



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:37 AM UTC

PDB ID : 1HTQ / pdb_00001htq
Title : Multicopy crystallographic structure of a relaxed glutamine synthetase from Mycobacterium tuberculosis
Authors : Gill, H.S.; Pfluegl, G.M.; Eisenberg, D.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2001-01-01
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

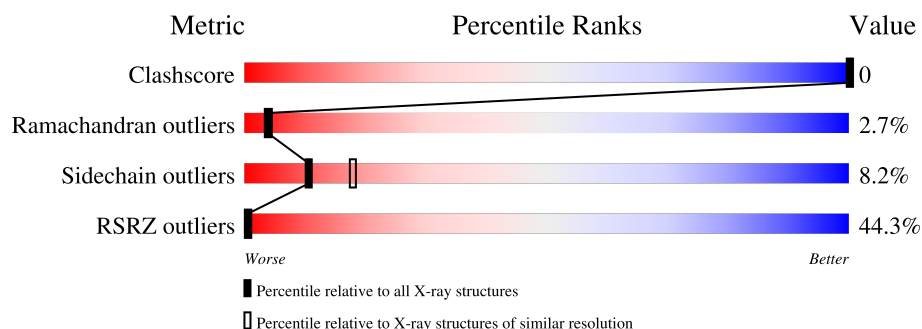
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	477	43% 89% 11%
1	1-B	477	42% 89% 11%
1	1-C	477	40% 89% 11%
1	1-D	477	45% 89% 11%
1	1-E	477	44% 89% 11%
1	1-F	477	48% 89% 11%

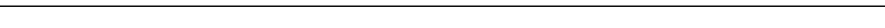
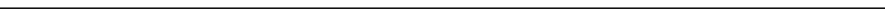
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	1-G	477	49% 89% 11%
1	1-H	477	43% 89% 11%
1	1-I	477	39% 89% 11%
1	1-J	477	41% 89% 11%
1	1-K	477	44% 89% 11%
1	1-L	477	53% 89% 11%
1	1-M	477	43% 89% 11%
1	1-N	477	44% 89% 11%
1	1-O	477	40% 89% 11%
1	1-P	477	48% 89% 11%
1	1-Q	477	45% 89% 11%
1	1-R	477	48% 89% 11%
1	1-S	477	48% 89% 11%
1	1-T	477	43% 89% 11%
1	1-U	477	43% 89% 11%
1	1-V	477	41% 89% 11%
1	1-W	477	43% 89% 11%
1	1-X	477	46% 89% 11%
1	10-A	477	89% 10%
1	10-B	477	89% 10%
1	10-C	477	89% 10%
1	10-D	477	89% 10%
1	10-E	477	89% 10%
1	10-F	477	89% 10%
1	10-G	477	89% 10%

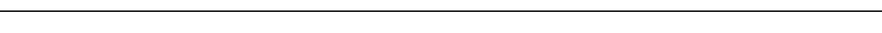
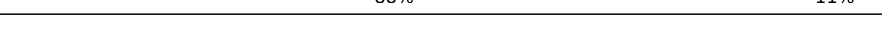
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	10-H	477	 89% 10%
1	10-I	477	 89% 10%
1	10-J	477	 89% 10%
1	10-K	477	 89% 10%
1	10-L	477	 89% 10%
1	10-M	477	 89% 10%
1	10-N	477	 89% 10%
1	10-O	477	 89% 10%
1	10-P	477	 89% 10%
1	10-Q	477	 89% 10%
1	10-R	477	 89% 10%
1	10-S	477	 89% 10%
1	10-T	477	 89% 10%
1	10-U	477	 89% 10%
1	10-V	477	 89% 10%
1	10-W	477	 89% 10%
1	10-X	477	 89% 10%
1	2-A	477	 88% 11%
1	2-B	477	 88% 11%
1	2-C	477	 88% 11%
1	2-D	477	 88% 11%
1	2-E	477	 88% 11%
1	2-F	477	 88% 11%
1	2-G	477	 88% 11%
1	2-H	477	 88% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	2-I	477	 88% 11%
1	2-J	477	 88% 11%
1	2-K	477	 88% 11%
1	2-L	477	 88% 11%
1	2-M	477	 88% 11%
1	2-N	477	 88% 11%
1	2-O	477	 88% 11%
1	2-P	477	 88% 11%
1	2-Q	477	 88% 11%
1	2-R	477	 88% 11%
1	2-S	477	 88% 11%
1	2-T	477	 88% 11%
1	2-U	477	 88% 11%
1	2-V	477	 88% 11%
1	2-W	477	 88% 11%
1	2-X	477	 88% 11%
1	3-A	477	 90% 10%
1	3-B	477	 90% 10%
1	3-C	477	 90% 10%
1	3-D	477	 90% 10%
1	3-E	477	 90% 10%
1	3-F	477	 90% 10%
1	3-G	477	 90% 10%
1	3-H	477	 90% 10%
1	3-I	477	 90% 10%

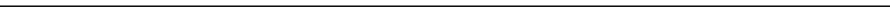
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	3-J	477		90% 10%
1	3-K	477		90% 10%
1	3-L	477		90% 10%
1	3-M	477		90% 10%
1	3-N	477		90% 10%
1	3-O	477		90% 10%
1	3-P	477		90% 10%
1	3-Q	477		90% 10%
1	3-R	477		90% 10%
1	3-S	477		90% 10%
1	3-T	477		90% 10%
1	3-U	477		90% 10%
1	3-V	477		90% 10%
1	3-W	477		90% 10%
1	3-X	477		90% 10%
1	4-A	477		89% 11%
1	4-B	477		89% 11%
1	4-C	477		89% 11%
1	4-D	477		89% 11%
1	4-E	477		89% 11%
1	4-F	477		89% 11%
1	4-G	477		89% 11%
1	4-H	477		89% 11%
1	4-I	477		89% 11%
1	4-J	477		89% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	4-K	477		89% 11%
1	4-L	477		89% 11%
1	4-M	477		89% 11%
1	4-N	477		89% 11%
1	4-O	477		89% 11%
1	4-P	477		89% 11%
1	4-Q	477		89% 11%
1	4-R	477		89% 11%
1	4-S	477		89% 11%
1	4-T	477		89% 11%
1	4-U	477		89% 11%
1	4-V	477		89% 11%
1	4-W	477		89% 11%
1	4-X	477		89% 11%
1	5-A	477		90% 10%
1	5-B	477		90% 10%
1	5-C	477		90% 10%
1	5-D	477		90% 10%
1	5-E	477		90% 10%
1	5-F	477		90% 10%
1	5-G	477		90% 10%
1	5-H	477		90% 10%
1	5-I	477		90% 10%
1	5-J	477		90% 10%
1	5-K	477		90% 10%

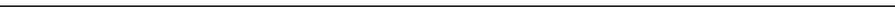
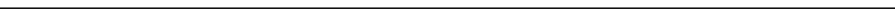
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	5-L	477		90% 10%
1	5-M	477		90% 10%
1	5-N	477		90% 10%
1	5-O	477		90% 10%
1	5-P	477		90% 10%
1	5-Q	477		90% 10%
1	5-R	477		90% 10%
1	5-S	477		90% 10%
1	5-T	477		90% 10%
1	5-U	477		90% 10%
1	5-V	477		90% 10%
1	5-W	477		90% 10%
1	5-X	477		90% 10%
1	6-A	477		89% 10%
1	6-B	477		90% 10%
1	6-C	477		89% 10%
1	6-D	477		90% 10%
1	6-E	477		90% 10%
1	6-F	477		89% 10%
1	6-G	477		89% 10%
1	6-H	477		90% 10%
1	6-I	477		89% 10%
1	6-J	477		89% 10%
1	6-K	477		89% 10%
1	6-L	477		89% 10%

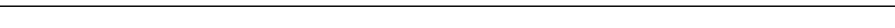
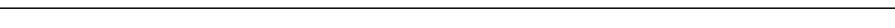
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	6-M	477	 90% 10%
1	6-N	477	 89% 10%
1	6-O	477	 89% 10%
1	6-P	477	 90% 10%
1	6-Q	477	 89% 10%
1	6-R	477	 89% 10%
1	6-S	477	 90% 10%
1	6-T	477	 90% 10%
1	6-U	477	 89% 10%
1	6-V	477	 89% 10%
1	6-W	477	 89% 10%
1	6-X	477	 90% 10%
1	7-A	477	 89% 10% .
1	7-B	477	 89% 10% .
1	7-C	477	 89% 10% .
1	7-D	477	 89% 10% .
1	7-E	477	 89% 10% .
1	7-F	477	 89% 10% .
1	7-G	477	 89% 10% .
1	7-H	477	 89% 10% .
1	7-I	477	 89% 10% .
1	7-J	477	 89% 10% .
1	7-K	477	 89% 10% .
1	7-L	477	 89% 10% .
1	7-M	477	 89% 10% .

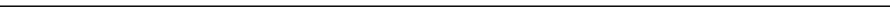
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	7-N	477	 89% 10% .
1	7-O	477	 89% 10% .
1	7-P	477	 89% 10% .
1	7-Q	477	 89% 10% .
1	7-R	477	 89% 10% .
1	7-S	477	 89% 10% .
1	7-T	477	 89% 10% .
1	7-U	477	 89% 10% .
1	7-V	477	 89% 10% .
1	7-W	477	 89% 10% .
1	7-X	477	 89% 10% .
1	8-A	477	 90% 10%
1	8-B	477	 90% 10%
1	8-C	477	 90% 10%
1	8-D	477	 90% 10%
1	8-E	477	 90% 10%
1	8-F	477	 90% 10%
1	8-G	477	 90% 10%
1	8-H	477	 90% 10%
1	8-I	477	 90% 10%
1	8-J	477	 90% 10%
1	8-K	477	 90% 10%
1	8-L	477	 90% 10%
1	8-M	477	 90% 10%
1	8-N	477	 90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	8-O	477		90% 10%
1	8-P	477		90% 10%
1	8-Q	477		90% 10%
1	8-R	477		90% 10%
1	8-S	477		90% 10%
1	8-T	477		90% 10%
1	8-U	477		90% 10%
1	8-V	477		90% 10%
1	8-W	477		90% 10%
1	8-X	477		90% 10%
1	9-A	477		90% 10%
1	9-B	477		90% 10%
1	9-C	477		90% 10%
1	9-D	477		90% 10%
1	9-E	477		90% 10%
1	9-F	477		90% 10%
1	9-G	477		90% 10%
1	9-H	477		90% 10%
1	9-I	477		90% 10%
1	9-J	477		90% 10%
1	9-K	477		90% 10%
1	9-L	477		90% 10%
1	9-M	477		90% 10%
1	9-N	477		90% 10%
1	9-O	477		90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	9-P	477	 90% 10%
1	9-Q	477	 90% 10%
1	9-R	477	 90% 10%
1	9-S	477	 90% 10%
1	9-T	477	 90% 10%
1	9-U	477	 90% 10%
1	9-V	477	 90% 10%
1	9-W	477	 90% 10%
1	9-X	477	 90% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	1-G	470	-	-	-	X
4	CIT	1-A	7476	-	X	-	-
4	CIT	1-B	7478	-	X	-	-
4	CIT	1-C	7480	-	X	-	-
4	CIT	1-D	7482	-	X	-	-
4	CIT	1-E	7484	-	X	-	-
4	CIT	1-F	7486	-	X	-	-
4	CIT	1-G	7488	-	X	-	-
4	CIT	1-H	7490	-	X	-	-
4	CIT	1-I	7492	-	X	-	-
4	CIT	1-J	7494	-	X	-	-
4	CIT	1-K	7496	-	X	-	-
4	CIT	1-L	7498	-	X	-	-
4	CIT	1-M	7500	-	X	-	-
4	CIT	1-N	7502	-	X	-	-
4	CIT	1-O	7504	-	X	-	-
4	CIT	1-P	7506	-	X	-	-
4	CIT	1-Q	7508	-	X	-	-
4	CIT	1-R	7510	-	X	-	-
4	CIT	1-S	7512	-	X	-	-
4	CIT	1-T	7514	-	X	-	-
4	CIT	1-U	7516	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	1-V	7518	-	X	-	-
4	CIT	1-W	7520	-	X	-	-
4	CIT	1-X	7522	-	X	-	-
4	CIT	10-A	7476	-	X	-	-
4	CIT	10-B	7478	-	X	-	-
4	CIT	10-C	7480	-	X	-	-
4	CIT	10-D	7482	-	X	-	-
4	CIT	10-E	7484	-	X	-	-
4	CIT	10-F	7486	-	X	-	-
4	CIT	10-G	7488	-	X	-	-
4	CIT	10-H	7490	-	X	-	-
4	CIT	10-I	7492	-	X	-	-
4	CIT	10-J	7494	-	X	-	-
4	CIT	10-K	7496	-	X	-	-
4	CIT	10-L	7498	-	X	-	-
4	CIT	10-M	7500	-	X	-	-
4	CIT	10-N	7502	-	X	-	-
4	CIT	10-O	7504	-	X	-	-
4	CIT	10-P	7506	-	X	-	-
4	CIT	10-Q	7508	-	X	-	-
4	CIT	10-R	7510	-	X	-	-
4	CIT	10-S	7512	-	X	-	-
4	CIT	10-T	7514	-	X	-	-
4	CIT	10-U	7516	-	X	-	-
4	CIT	10-V	7518	-	X	-	-
4	CIT	10-W	7520	-	X	-	-
4	CIT	10-X	7522	-	X	-	-
4	CIT	2-A	7476	-	X	-	-
4	CIT	2-B	7478	-	X	-	-
4	CIT	2-C	7480	-	X	-	-
4	CIT	2-D	7482	-	X	-	-
4	CIT	2-E	7484	-	X	-	-
4	CIT	2-F	7486	-	X	-	-
4	CIT	2-G	7488	-	X	-	-
4	CIT	2-H	7490	-	X	-	-
4	CIT	2-I	7492	-	X	-	-
4	CIT	2-J	7494	-	X	-	-
4	CIT	2-K	7496	-	X	-	-
4	CIT	2-L	7498	-	X	-	-
4	CIT	2-M	7500	-	X	-	-
4	CIT	2-N	7502	-	X	-	-
4	CIT	2-O	7504	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	2-P	7506	-	X	-	-
4	CIT	2-Q	7508	-	X	-	-
4	CIT	2-R	7510	-	X	-	-
4	CIT	2-S	7512	-	X	-	-
4	CIT	2-T	7514	-	X	-	-
4	CIT	2-U	7516	-	X	-	-
4	CIT	2-V	7518	-	X	-	-
4	CIT	2-W	7520	-	X	-	-
4	CIT	2-X	7522	-	X	-	-
4	CIT	3-A	7476	-	X	-	-
4	CIT	3-B	7478	-	X	-	-
4	CIT	3-C	7480	-	X	-	-
4	CIT	3-D	7482	-	X	-	-
4	CIT	3-E	7484	-	X	-	-
4	CIT	3-F	7486	-	X	-	-
4	CIT	3-G	7488	-	X	-	-
4	CIT	3-H	7490	-	X	-	-
4	CIT	3-I	7492	-	X	-	-
4	CIT	3-J	7494	-	X	-	-
4	CIT	3-K	7496	-	X	-	-
4	CIT	3-L	7498	-	X	-	-
4	CIT	3-M	7500	-	X	-	-
4	CIT	3-N	7502	-	X	-	-
4	CIT	3-O	7504	-	X	-	-
4	CIT	3-P	7506	-	X	-	-
4	CIT	3-Q	7508	-	X	-	-
4	CIT	3-R	7510	-	X	-	-
4	CIT	3-S	7512	-	X	-	-
4	CIT	3-T	7514	-	X	-	-
4	CIT	3-U	7516	-	X	-	-
4	CIT	3-V	7518	-	X	-	-
4	CIT	3-W	7520	-	X	-	-
4	CIT	3-X	7522	-	X	-	-
4	CIT	4-A	7476	-	X	-	-
4	CIT	4-B	7478	-	X	-	-
4	CIT	4-C	7480	-	X	-	-
4	CIT	4-D	7482	-	X	-	-
4	CIT	4-E	7484	-	X	-	-
4	CIT	4-F	7486	-	X	-	-
4	CIT	4-G	7488	-	X	-	-
4	CIT	4-H	7490	-	X	-	-
4	CIT	4-I	7492	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	4-J	7494	-	X	-	-
4	CIT	4-K	7496	-	X	-	-
4	CIT	4-L	7498	-	X	-	-
4	CIT	4-M	7500	-	X	-	-
4	CIT	4-N	7502	-	X	-	-
4	CIT	4-O	7504	-	X	-	-
4	CIT	4-P	7506	-	X	-	-
4	CIT	4-Q	7508	-	X	-	-
4	CIT	4-R	7510	-	X	-	-
4	CIT	4-S	7512	-	X	-	-
4	CIT	4-T	7514	-	X	-	-
4	CIT	4-U	7516	-	X	-	-
4	CIT	4-V	7518	-	X	-	-
4	CIT	4-W	7520	-	X	-	-
4	CIT	4-X	7522	-	X	-	-
4	CIT	5-A	7476	-	X	-	-
4	CIT	5-B	7478	-	X	-	-
4	CIT	5-C	7480	-	X	-	-
4	CIT	5-D	7482	-	X	-	-
4	CIT	5-E	7484	-	X	-	-
4	CIT	5-F	7486	-	X	-	-
4	CIT	5-G	7488	-	X	-	-
4	CIT	5-H	7490	-	X	-	-
4	CIT	5-I	7492	-	X	-	-
4	CIT	5-J	7494	-	X	-	-
4	CIT	5-K	7496	-	X	-	-
4	CIT	5-L	7498	-	X	-	-
4	CIT	5-M	7500	-	X	-	-
4	CIT	5-N	7502	-	X	-	-
4	CIT	5-O	7504	-	X	-	-
4	CIT	5-P	7506	-	X	-	-
4	CIT	5-Q	7508	-	X	-	-
4	CIT	5-R	7510	-	X	-	-
4	CIT	5-S	7512	-	X	-	-
4	CIT	5-T	7514	-	X	-	-
4	CIT	5-U	7516	-	X	-	-
4	CIT	5-V	7518	-	X	-	-
4	CIT	5-W	7520	-	X	-	-
4	CIT	5-X	7522	-	X	-	-
4	CIT	6-A	7476	-	X	-	-
4	CIT	6-B	7478	-	X	-	-
4	CIT	6-C	7480	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	6-D	7482	-	X	-	-
4	CIT	6-E	7484	-	X	-	-
4	CIT	6-F	7486	-	X	-	-
4	CIT	6-G	7488	-	X	-	-
4	CIT	6-H	7490	-	X	-	-
4	CIT	6-I	7492	-	X	-	-
4	CIT	6-J	7494	-	X	-	-
4	CIT	6-K	7496	-	X	-	-
4	CIT	6-L	7498	-	X	-	-
4	CIT	6-M	7500	-	X	-	-
4	CIT	6-N	7502	-	X	-	-
4	CIT	6-O	7504	-	X	-	-
4	CIT	6-P	7506	-	X	-	-
4	CIT	6-Q	7508	-	X	-	-
4	CIT	6-R	7510	-	X	-	-
4	CIT	6-S	7512	-	X	-	-
4	CIT	6-T	7514	-	X	-	-
4	CIT	6-U	7516	-	X	-	-
4	CIT	6-V	7518	-	X	-	-
4	CIT	6-W	7520	-	X	-	-
4	CIT	6-X	7522	-	X	-	-
4	CIT	7-A	7476	-	X	-	-
4	CIT	7-B	7478	-	X	-	-
4	CIT	7-C	7480	-	X	-	-
4	CIT	7-D	7482	-	X	-	-
4	CIT	7-E	7484	-	X	-	-
4	CIT	7-F	7486	-	X	-	-
4	CIT	7-G	7488	-	X	-	-
4	CIT	7-H	7490	-	X	-	-
4	CIT	7-I	7492	-	X	-	-
4	CIT	7-J	7494	-	X	-	-
4	CIT	7-K	7496	-	X	-	-
4	CIT	7-L	7498	-	X	-	-
4	CIT	7-M	7500	-	X	-	-
4	CIT	7-N	7502	-	X	-	-
4	CIT	7-O	7504	-	X	-	-
4	CIT	7-P	7506	-	X	-	-
4	CIT	7-Q	7508	-	X	-	-
4	CIT	7-R	7510	-	X	-	-
4	CIT	7-S	7512	-	X	-	-
4	CIT	7-T	7514	-	X	-	-
4	CIT	7-U	7516	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	7-V	7518	-	X	-	-
4	CIT	7-W	7520	-	X	-	-
4	CIT	7-X	7522	-	X	-	-
4	CIT	8-A	7476	-	X	-	-
4	CIT	8-B	7478	-	X	-	-
4	CIT	8-C	7480	-	X	-	-
4	CIT	8-D	7482	-	X	-	-
4	CIT	8-E	7484	-	X	-	-
4	CIT	8-F	7486	-	X	-	-
4	CIT	8-G	7488	-	X	-	-
4	CIT	8-H	7490	-	X	-	-
4	CIT	8-I	7492	-	X	-	-
4	CIT	8-J	7494	-	X	-	-
4	CIT	8-K	7496	-	X	-	-
4	CIT	8-L	7498	-	X	-	-
4	CIT	8-M	7500	-	X	-	-
4	CIT	8-N	7502	-	X	-	-
4	CIT	8-O	7504	-	X	-	-
4	CIT	8-P	7506	-	X	-	-
4	CIT	8-Q	7508	-	X	-	-
4	CIT	8-R	7510	-	X	-	-
4	CIT	8-S	7512	-	X	-	-
4	CIT	8-T	7514	-	X	-	-
4	CIT	8-U	7516	-	X	-	-
4	CIT	8-V	7518	-	X	-	-
4	CIT	8-W	7520	-	X	-	-
4	CIT	8-X	7522	-	X	-	-
4	CIT	9-A	7476	-	X	-	-
4	CIT	9-B	7478	-	X	-	-
4	CIT	9-C	7480	-	X	-	-
4	CIT	9-D	7482	-	X	-	-
4	CIT	9-E	7484	-	X	-	-
4	CIT	9-F	7486	-	X	-	-
4	CIT	9-G	7488	-	X	-	-
4	CIT	9-H	7490	-	X	-	-
4	CIT	9-I	7492	-	X	-	-
4	CIT	9-J	7494	-	X	-	-
4	CIT	9-K	7496	-	X	-	-
4	CIT	9-L	7498	-	X	-	-
4	CIT	9-M	7500	-	X	-	-
4	CIT	9-N	7502	-	X	-	-
4	CIT	9-O	7504	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	9-P	7506	-	X	-	-
4	CIT	9-Q	7508	-	X	-	-
4	CIT	9-R	7510	-	X	-	-
4	CIT	9-S	7512	-	X	-	-
4	CIT	9-T	7514	-	X	-	-
4	CIT	9-U	7516	-	X	-	-
4	CIT	9-V	7518	-	X	-	-
4	CIT	9-W	7520	-	X	-	-
4	CIT	9-X	7522	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 978720 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	7-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	8-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	9-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	10-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	3-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	4-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	5-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	6-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	7-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	1	Total	Mn	0	0
			1	1		
2	2-A	1	Total	Mn	0	0
			1	1		
2	3-A	1	Total	Mn	0	0
			1	1		
2	4-A	1	Total	Mn	0	0
			1	1		
2	5-A	1	Total	Mn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	6-A	1	Total 1	Mn 1	0	0
2	7-A	1	Total 1	Mn 1	0	0
2	8-A	1	Total 1	Mn 1	0	0
2	9-A	1	Total 1	Mn 1	0	0
2	10-A	1	Total 1	Mn 1	0	0
2	1-B	1	Total 1	Mn 1	0	0
2	2-B	1	Total 1	Mn 1	0	0
2	3-B	1	Total 1	Mn 1	0	0
2	4-B	1	Total 1	Mn 1	0	0
2	5-B	1	Total 1	Mn 1	0	0
2	6-B	1	Total 1	Mn 1	0	0
2	7-B	1	Total 1	Mn 1	0	0
2	8-B	1	Total 1	Mn 1	0	0
2	9-B	1	Total 1	Mn 1	0	0
2	10-B	1	Total 1	Mn 1	0	0
2	1-C	1	Total 1	Mn 1	0	0
2	2-C	1	Total 1	Mn 1	0	0
2	3-C	1	Total 1	Mn 1	0	0
2	4-C	1	Total 1	Mn 1	0	0
2	5-C	1	Total 1	Mn 1	0	0
2	6-C	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7-C	1	Total 1	Mn 1	0	0
2	8-C	1	Total 1	Mn 1	0	0
2	9-C	1	Total 1	Mn 1	0	0
2	10-C	1	Total 1	Mn 1	0	0
2	1-D	1	Total 1	Mn 1	0	0
2	2-D	1	Total 1	Mn 1	0	0
2	3-D	1	Total 1	Mn 1	0	0
2	4-D	1	Total 1	Mn 1	0	0
2	5-D	1	Total 1	Mn 1	0	0
2	6-D	1	Total 1	Mn 1	0	0
2	7-D	1	Total 1	Mn 1	0	0
2	8-D	1	Total 1	Mn 1	0	0
2	9-D	1	Total 1	Mn 1	0	0
2	10-D	1	Total 1	Mn 1	0	0
2	1-E	1	Total 1	Mn 1	0	0
2	2-E	1	Total 1	Mn 1	0	0
2	3-E	1	Total 1	Mn 1	0	0
2	4-E	1	Total 1	Mn 1	0	0
2	5-E	1	Total 1	Mn 1	0	0
2	6-E	1	Total 1	Mn 1	0	0
2	7-E	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	8-E	1	Total 1	Mn 1	0	0
2	9-E	1	Total 1	Mn 1	0	0
2	10-E	1	Total 1	Mn 1	0	0
2	1-F	1	Total 1	Mn 1	0	0
2	2-F	1	Total 1	Mn 1	0	0
2	3-F	1	Total 1	Mn 1	0	0
2	4-F	1	Total 1	Mn 1	0	0
2	5-F	1	Total 1	Mn 1	0	0
2	6-F	1	Total 1	Mn 1	0	0
2	7-F	1	Total 1	Mn 1	0	0
2	8-F	1	Total 1	Mn 1	0	0
2	9-F	1	Total 1	Mn 1	0	0
2	10-F	1	Total 1	Mn 1	0	0
2	1-G	1	Total 1	Mn 1	0	0
2	2-G	1	Total 1	Mn 1	0	0
2	3-G	1	Total 1	Mn 1	0	0
2	4-G	1	Total 1	Mn 1	0	0
2	5-G	1	Total 1	Mn 1	0	0
2	6-G	1	Total 1	Mn 1	0	0
2	7-G	1	Total 1	Mn 1	0	0
2	8-G	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	9-G	1	Total 1	Mn 1	0	0
2	10-G	1	Total 1	Mn 1	0	0
2	1-H	1	Total 1	Mn 1	0	0
2	2-H	1	Total 1	Mn 1	0	0
2	3-H	1	Total 1	Mn 1	0	0
2	4-H	1	Total 1	Mn 1	0	0
2	5-H	1	Total 1	Mn 1	0	0
2	6-H	1	Total 1	Mn 1	0	0
2	7-H	1	Total 1	Mn 1	0	0
2	8-H	1	Total 1	Mn 1	0	0
2	9-H	1	Total 1	Mn 1	0	0
2	10-H	1	Total 1	Mn 1	0	0
2	1-I	1	Total 1	Mn 1	0	0
2	2-I	1	Total 1	Mn 1	0	0
2	3-I	1	Total 1	Mn 1	0	0
2	4-I	1	Total 1	Mn 1	0	0
2	5-I	1	Total 1	Mn 1	0	0
2	6-I	1	Total 1	Mn 1	0	0
2	7-I	1	Total 1	Mn 1	0	0
2	8-I	1	Total 1	Mn 1	0	0
2	9-I	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	10-I	1	Total 1	Mn 1	0	0
2	1-J	1	Total 1	Mn 1	0	0
2	2-J	1	Total 1	Mn 1	0	0
2	3-J	1	Total 1	Mn 1	0	0
2	4-J	1	Total 1	Mn 1	0	0
2	5-J	1	Total 1	Mn 1	0	0
2	6-J	1	Total 1	Mn 1	0	0
2	7-J	1	Total 1	Mn 1	0	0
2	8-J	1	Total 1	Mn 1	0	0
2	9-J	1	Total 1	Mn 1	0	0
2	10-J	1	Total 1	Mn 1	0	0
2	1-K	1	Total 1	Mn 1	0	0
2	2-K	1	Total 1	Mn 1	0	0
2	3-K	1	Total 1	Mn 1	0	0
2	4-K	1	Total 1	Mn 1	0	0
2	5-K	1	Total 1	Mn 1	0	0
2	6-K	1	Total 1	Mn 1	0	0
2	7-K	1	Total 1	Mn 1	0	0
2	8-K	1	Total 1	Mn 1	0	0
2	9-K	1	Total 1	Mn 1	0	0
2	10-K	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-L	1	Total 1	Mn 1	0	0
2	2-L	1	Total 1	Mn 1	0	0
2	3-L	1	Total 1	Mn 1	0	0
2	4-L	1	Total 1	Mn 1	0	0
2	5-L	1	Total 1	Mn 1	0	0
2	6-L	1	Total 1	Mn 1	0	0
2	7-L	1	Total 1	Mn 1	0	0
2	8-L	1	Total 1	Mn 1	0	0
2	9-L	1	Total 1	Mn 1	0	0
2	10-L	1	Total 1	Mn 1	0	0
2	1-M	1	Total 1	Mn 1	0	0
2	2-M	1	Total 1	Mn 1	0	0
2	3-M	1	Total 1	Mn 1	0	0
2	4-M	1	Total 1	Mn 1	0	0
2	5-M	1	Total 1	Mn 1	0	0
2	6-M	1	Total 1	Mn 1	0	0
2	7-M	1	Total 1	Mn 1	0	0
2	8-M	1	Total 1	Mn 1	0	0
2	9-M	1	Total 1	Mn 1	0	0
2	10-M	1	Total 1	Mn 1	0	0
2	1-N	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	2-N	1	Total 1	Mn 1	0	0
2	3-N	1	Total 1	Mn 1	0	0
2	4-N	1	Total 1	Mn 1	0	0
2	5-N	1	Total 1	Mn 1	0	0
2	6-N	1	Total 1	Mn 1	0	0
2	7-N	1	Total 1	Mn 1	0	0
2	8-N	1	Total 1	Mn 1	0	0
2	9-N	1	Total 1	Mn 1	0	0
2	10-N	1	Total 1	Mn 1	0	0
2	1-O	1	Total 1	Mn 1	0	0
2	2-O	1	Total 1	Mn 1	0	0
2	3-O	1	Total 1	Mn 1	0	0
2	4-O	1	Total 1	Mn 1	0	0
2	5-O	1	Total 1	Mn 1	0	0
2	6-O	1	Total 1	Mn 1	0	0
2	7-O	1	Total 1	Mn 1	0	0
2	8-O	1	Total 1	Mn 1	0	0
2	9-O	1	Total 1	Mn 1	0	0
2	10-O	1	Total 1	Mn 1	0	0
2	1-P	1	Total 1	Mn 1	0	0
2	2-P	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-P	1	Total 1	Mn 1	0	0
2	4-P	1	Total 1	Mn 1	0	0
2	5-P	1	Total 1	Mn 1	0	0
2	6-P	1	Total 1	Mn 1	0	0
2	7-P	1	Total 1	Mn 1	0	0
2	8-P	1	Total 1	Mn 1	0	0
2	9-P	1	Total 1	Mn 1	0	0
2	10-P	1	Total 1	Mn 1	0	0
2	1-Q	1	Total 1	Mn 1	0	0
2	2-Q	1	Total 1	Mn 1	0	0
2	3-Q	1	Total 1	Mn 1	0	0
2	4-Q	1	Total 1	Mn 1	0	0
2	5-Q	1	Total 1	Mn 1	0	0
2	6-Q	1	Total 1	Mn 1	0	0
2	7-Q	1	Total 1	Mn 1	0	0
2	8-Q	1	Total 1	Mn 1	0	0
2	9-Q	1	Total 1	Mn 1	0	0
2	10-Q	1	Total 1	Mn 1	0	0
2	1-R	1	Total 1	Mn 1	0	0
2	2-R	1	Total 1	Mn 1	0	0
2	3-R	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	4-R	1	Total 1	Mn 1	0	0
2	5-R	1	Total 1	Mn 1	0	0
2	6-R	1	Total 1	Mn 1	0	0
2	7-R	1	Total 1	Mn 1	0	0
2	8-R	1	Total 1	Mn 1	0	0
2	9-R	1	Total 1	Mn 1	0	0
2	10-R	1	Total 1	Mn 1	0	0
2	1-S	1	Total 1	Mn 1	0	0
2	2-S	1	Total 1	Mn 1	0	0
2	3-S	1	Total 1	Mn 1	0	0
2	4-S	1	Total 1	Mn 1	0	0
2	5-S	1	Total 1	Mn 1	0	0
2	6-S	1	Total 1	Mn 1	0	0
2	7-S	1	Total 1	Mn 1	0	0
2	8-S	1	Total 1	Mn 1	0	0
2	9-S	1	Total 1	Mn 1	0	0
2	10-S	1	Total 1	Mn 1	0	0
2	1-T	1	Total 1	Mn 1	0	0
2	2-T	1	Total 1	Mn 1	0	0
2	3-T	1	Total 1	Mn 1	0	0
2	4-T	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	5-T	1	Total 1	Mn 1	0	0
2	6-T	1	Total 1	Mn 1	0	0
2	7-T	1	Total 1	Mn 1	0	0
2	8-T	1	Total 1	Mn 1	0	0
2	9-T	1	Total 1	Mn 1	0	0
2	10-T	1	Total 1	Mn 1	0	0
2	1-U	1	Total 1	Mn 1	0	0
2	2-U	1	Total 1	Mn 1	0	0
2	3-U	1	Total 1	Mn 1	0	0
2	4-U	1	Total 1	Mn 1	0	0
2	5-U	1	Total 1	Mn 1	0	0
2	6-U	1	Total 1	Mn 1	0	0
2	7-U	1	Total 1	Mn 1	0	0
2	8-U	1	Total 1	Mn 1	0	0
2	9-U	1	Total 1	Mn 1	0	0
2	10-U	1	Total 1	Mn 1	0	0
2	1-V	1	Total 1	Mn 1	0	0
2	2-V	1	Total 1	Mn 1	0	0
2	3-V	1	Total 1	Mn 1	0	0
2	4-V	1	Total 1	Mn 1	0	0
2	5-V	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

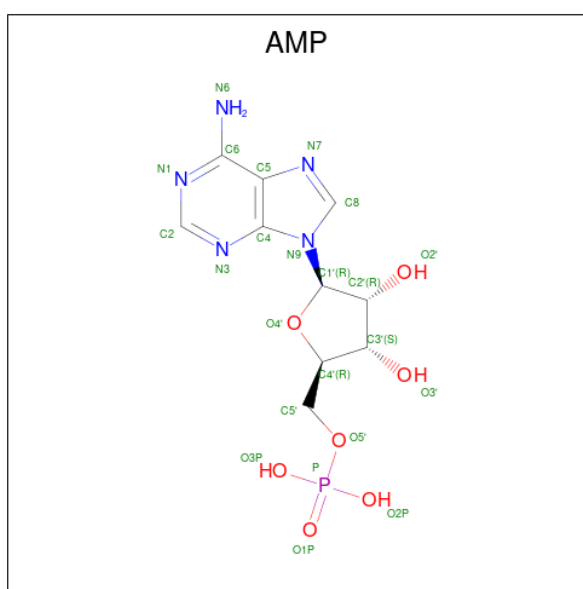
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	6-V	1	Total 1	Mn 1	0	0
2	7-V	1	Total 1	Mn 1	0	0
2	8-V	1	Total 1	Mn 1	0	0
2	9-V	1	Total 1	Mn 1	0	0
2	10-V	1	Total 1	Mn 1	0	0
2	1-W	1	Total 1	Mn 1	0	0
2	2-W	1	Total 1	Mn 1	0	0
2	3-W	1	Total 1	Mn 1	0	0
2	4-W	1	Total 1	Mn 1	0	0
2	5-W	1	Total 1	Mn 1	0	0
2	6-W	1	Total 1	Mn 1	0	0
2	7-W	1	Total 1	Mn 1	0	0
2	8-W	1	Total 1	Mn 1	0	0
2	9-W	1	Total 1	Mn 1	0	0
2	10-W	1	Total 1	Mn 1	0	0
2	1-X	1	Total 1	Mn 1	0	0
2	2-X	1	Total 1	Mn 1	0	0
2	3-X	1	Total 1	Mn 1	0	0
2	4-X	1	Total 1	Mn 1	0	0
2	5-X	1	Total 1	Mn 1	0	0
2	6-X	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7-X	1	Total	Mn	0	0
			1	1		
2	8-X	1	Total	Mn	0	0
			1	1		
2	9-X	1	Total	Mn	0	0
			1	1		
2	10-X	1	Total	Mn	0	0
			1	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	5-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	6-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	7-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	8-A	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-A	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-A	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-C	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	9-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-E	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	10-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-G	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-J	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	2-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-L	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	3-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-N	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	4-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-P	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	5-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-R	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	6-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-T	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	7-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-V	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

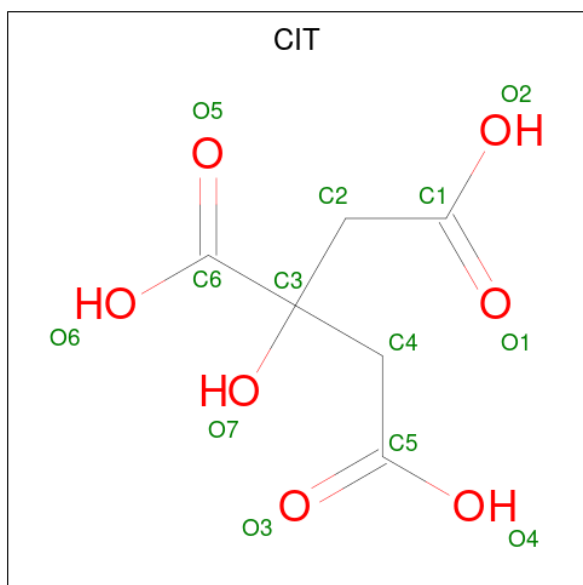
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	8-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-X	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	9-X	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	10-X	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-A	1	Total	C	O	0	0
			13	6	7		
4	2-A	1	Total	C	O	0	0
			13	6	7		
4	3-A	1	Total	C	O	0	0
			13	6	7		
4	4-A	1	Total	C	O	0	0
			13	6	7		
4	5-A	1	Total	C	O	0	0
			13	6	7		
4	6-A	1	Total	C	O	0	0
			13	6	7		
4	7-A	1	Total	C	O	0	0
			13	6	7		
4	8-A	1	Total	C	O	0	0
			13	6	7		
4	9-A	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	10-A	1	Total	C	O	0	0
			13	6	7		
4	1-B	1	Total	C	O	0	0
			13	6	7		
4	2-B	1	Total	C	O	0	0
			13	6	7		
4	3-B	1	Total	C	O	0	0
			13	6	7		
4	4-B	1	Total	C	O	0	0
			13	6	7		
4	5-B	1	Total	C	O	0	0
			13	6	7		
4	6-B	1	Total	C	O	0	0
			13	6	7		
4	7-B	1	Total	C	O	0	0
			13	6	7		
4	8-B	1	Total	C	O	0	0
			13	6	7		
4	9-B	1	Total	C	O	0	0
			13	6	7		
4	10-B	1	Total	C	O	0	0
			13	6	7		
4	1-C	1	Total	C	O	0	0
			13	6	7		
4	2-C	1	Total	C	O	0	0
			13	6	7		
4	3-C	1	Total	C	O	0	0
			13	6	7		
4	4-C	1	Total	C	O	0	0
			13	6	7		
4	5-C	1	Total	C	O	0	0
			13	6	7		
4	6-C	1	Total	C	O	0	0
			13	6	7		
4	7-C	1	Total	C	O	0	0
			13	6	7		
4	8-C	1	Total	C	O	0	0
			13	6	7		
4	9-C	1	Total	C	O	0	0
			13	6	7		
4	10-C	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-D	1	Total	C	O	0	0
			13	6	7		
4	2-D	1	Total	C	O	0	0
			13	6	7		
4	3-D	1	Total	C	O	0	0
			13	6	7		
4	4-D	1	Total	C	O	0	0
			13	6	7		
4	5-D	1	Total	C	O	0	0
			13	6	7		
4	6-D	1	Total	C	O	0	0
			13	6	7		
4	7-D	1	Total	C	O	0	0
			13	6	7		
4	8-D	1	Total	C	O	0	0
			13	6	7		
4	9-D	1	Total	C	O	0	0
			13	6	7		
4	10-D	1	Total	C	O	0	0
			13	6	7		
4	1-E	1	Total	C	O	0	0
			13	6	7		
4	2-E	1	Total	C	O	0	0
			13	6	7		
4	3-E	1	Total	C	O	0	0
			13	6	7		
4	4-E	1	Total	C	O	0	0
			13	6	7		
4	5-E	1	Total	C	O	0	0
			13	6	7		
4	6-E	1	Total	C	O	0	0
			13	6	7		
4	7-E	1	Total	C	O	0	0
			13	6	7		
4	8-E	1	Total	C	O	0	0
			13	6	7		
4	9-E	1	Total	C	O	0	0
			13	6	7		
4	10-E	1	Total	C	O	0	0
			13	6	7		
4	1-F	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	2-F	1	Total	C	O	0	0
			13	6	7		
4	3-F	1	Total	C	O	0	0
			13	6	7		
4	4-F	1	Total	C	O	0	0
			13	6	7		
4	5-F	1	Total	C	O	0	0
			13	6	7		
4	6-F	1	Total	C	O	0	0
			13	6	7		
4	7-F	1	Total	C	O	0	0
			13	6	7		
4	8-F	1	Total	C	O	0	0
			13	6	7		
4	9-F	1	Total	C	O	0	0
			13	6	7		
4	10-F	1	Total	C	O	0	0
			13	6	7		
4	1-G	1	Total	C	O	0	0
			13	6	7		
4	2-G	1	Total	C	O	0	0
			13	6	7		
4	3-G	1	Total	C	O	0	0
			13	6	7		
4	4-G	1	Total	C	O	0	0
			13	6	7		
4	5-G	1	Total	C	O	0	0
			13	6	7		
4	6-G	1	Total	C	O	0	0
			13	6	7		
4	7-G	1	Total	C	O	0	0
			13	6	7		
4	8-G	1	Total	C	O	0	0
			13	6	7		
4	9-G	1	Total	C	O	0	0
			13	6	7		
4	10-G	1	Total	C	O	0	0
			13	6	7		
4	1-H	1	Total	C	O	0	0
			13	6	7		
4	2-H	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	3-H	1	Total	C	O	0	0
			13	6	7		
4	4-H	1	Total	C	O	0	0
			13	6	7		
4	5-H	1	Total	C	O	0	0
			13	6	7		
4	6-H	1	Total	C	O	0	0
			13	6	7		
4	7-H	1	Total	C	O	0	0
			13	6	7		
4	8-H	1	Total	C	O	0	0
			13	6	7		
4	9-H	1	Total	C	O	0	0
			13	6	7		
4	10-H	1	Total	C	O	0	0
			13	6	7		
4	1-I	1	Total	C	O	0	0
			13	6	7		
4	2-I	1	Total	C	O	0	0
			13	6	7		
4	3-I	1	Total	C	O	0	0
			13	6	7		
4	4-I	1	Total	C	O	0	0
			13	6	7		
4	5-I	1	Total	C	O	0	0
			13	6	7		
4	6-I	1	Total	C	O	0	0
			13	6	7		
4	7-I	1	Total	C	O	0	0
			13	6	7		
4	8-I	1	Total	C	O	0	0
			13	6	7		
4	9-I	1	Total	C	O	0	0
			13	6	7		
4	10-I	1	Total	C	O	0	0
			13	6	7		
4	1-J	1	Total	C	O	0	0
			13	6	7		
4	2-J	1	Total	C	O	0	0
			13	6	7		
4	3-J	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	4-J	1	Total	C	O	0	0
			13	6	7		
4	5-J	1	Total	C	O	0	0
			13	6	7		
4	6-J	1	Total	C	O	0	0
			13	6	7		
4	7-J	1	Total	C	O	0	0
			13	6	7		
4	8-J	1	Total	C	O	0	0
			13	6	7		
4	9-J	1	Total	C	O	0	0
			13	6	7		
4	10-J	1	Total	C	O	0	0
			13	6	7		
4	1-K	1	Total	C	O	0	0
			13	6	7		
4	2-K	1	Total	C	O	0	0
			13	6	7		
4	3-K	1	Total	C	O	0	0
			13	6	7		
4	4-K	1	Total	C	O	0	0
			13	6	7		
4	5-K	1	Total	C	O	0	0
			13	6	7		
4	6-K	1	Total	C	O	0	0
			13	6	7		
4	7-K	1	Total	C	O	0	0
			13	6	7		
4	8-K	1	Total	C	O	0	0
			13	6	7		
4	9-K	1	Total	C	O	0	0
			13	6	7		
4	10-K	1	Total	C	O	0	0
			13	6	7		
4	1-L	1	Total	C	O	0	0
			13	6	7		
4	2-L	1	Total	C	O	0	0
			13	6	7		
4	3-L	1	Total	C	O	0	0
			13	6	7		
4	4-L	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	5-L	1	Total	C	O	0	0
			13	6	7		
4	6-L	1	Total	C	O	0	0
			13	6	7		
4	7-L	1	Total	C	O	0	0
			13	6	7		
4	8-L	1	Total	C	O	0	0
			13	6	7		
4	9-L	1	Total	C	O	0	0
			13	6	7		
4	10-L	1	Total	C	O	0	0
			13	6	7		
4	1-M	1	Total	C	O	0	0
			13	6	7		
4	2-M	1	Total	C	O	0	0
			13	6	7		
4	3-M	1	Total	C	O	0	0
			13	6	7		
4	4-M	1	Total	C	O	0	0
			13	6	7		
4	5-M	1	Total	C	O	0	0
			13	6	7		
4	6-M	1	Total	C	O	0	0
			13	6	7		
4	7-M	1	Total	C	O	0	0
			13	6	7		
4	8-M	1	Total	C	O	0	0
			13	6	7		
4	9-M	1	Total	C	O	0	0
			13	6	7		
4	10-M	1	Total	C	O	0	0
			13	6	7		
4	1-N	1	Total	C	O	0	0
			13	6	7		
4	2-N	1	Total	C	O	0	0
			13	6	7		
4	3-N	1	Total	C	O	0	0
			13	6	7		
4	4-N	1	Total	C	O	0	0
			13	6	7		
4	5-N	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	6-N	1	Total	C	O	0	0
			13	6	7		
4	7-N	1	Total	C	O	0	0
			13	6	7		
4	8-N	1	Total	C	O	0	0
			13	6	7		
4	9-N	1	Total	C	O	0	0
			13	6	7		
4	10-N	1	Total	C	O	0	0
			13	6	7		
4	1-O	1	Total	C	O	0	0
			13	6	7		
4	2-O	1	Total	C	O	0	0
			13	6	7		
4	3-O	1	Total	C	O	0	0
			13	6	7		
4	4-O	1	Total	C	O	0	0
			13	6	7		
4	5-O	1	Total	C	O	0	0
			13	6	7		
4	6-O	1	Total	C	O	0	0
			13	6	7		
4	7-O	1	Total	C	O	0	0
			13	6	7		
4	8-O	1	Total	C	O	0	0
			13	6	7		
4	9-O	1	Total	C	O	0	0
			13	6	7		
4	10-O	1	Total	C	O	0	0
			13	6	7		
4	1-P	1	Total	C	O	0	0
			13	6	7		
4	2-P	1	Total	C	O	0	0
			13	6	7		
4	3-P	1	Total	C	O	0	0
			13	6	7		
4	4-P	1	Total	C	O	0	0
			13	6	7		
4	5-P	1	Total	C	O	0	0
			13	6	7		
4	6-P	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	7-P	1	Total	C	O	0	0
			13	6	7		
4	8-P	1	Total	C	O	0	0
			13	6	7		
4	9-P	1	Total	C	O	0	0
			13	6	7		
4	10-P	1	Total	C	O	0	0
			13	6	7		
4	1-Q	1	Total	C	O	0	0
			13	6	7		
4	2-Q	1	Total	C	O	0	0
			13	6	7		
4	3-Q	1	Total	C	O	0	0
			13	6	7		
4	4-Q	1	Total	C	O	0	0
			13	6	7		
4	5-Q	1	Total	C	O	0	0
			13	6	7		
4	6-Q	1	Total	C	O	0	0
			13	6	7		
4	7-Q	1	Total	C	O	0	0
			13	6	7		
4	8-Q	1	Total	C	O	0	0
			13	6	7		
4	9-Q	1	Total	C	O	0	0
			13	6	7		
4	10-Q	1	Total	C	O	0	0
			13	6	7		
4	1-R	1	Total	C	O	0	0
			13	6	7		
4	2-R	1	Total	C	O	0	0
			13	6	7		
4	3-R	1	Total	C	O	0	0
			13	6	7		
4	4-R	1	Total	C	O	0	0
			13	6	7		
4	5-R	1	Total	C	O	0	0
			13	6	7		
4	6-R	1	Total	C	O	0	0
			13	6	7		
4	7-R	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	8-R	1	Total	C	O	0	0
			13	6	7		
4	9-R	1	Total	C	O	0	0
			13	6	7		
4	10-R	1	Total	C	O	0	0
			13	6	7		
4	1-S	1	Total	C	O	0	0
			13	6	7		
4	2-S	1	Total	C	O	0	0
			13	6	7		
4	3-S	1	Total	C	O	0	0
			13	6	7		
4	4-S	1	Total	C	O	0	0
			13	6	7		
4	5-S	1	Total	C	O	0	0
			13	6	7		
4	6-S	1	Total	C	O	0	0
			13	6	7		
4	7-S	1	Total	C	O	0	0
			13	6	7		
4	8-S	1	Total	C	O	0	0
			13	6	7		
4	9-S	1	Total	C	O	0	0
			13	6	7		
4	10-S	1	Total	C	O	0	0
			13	6	7		
4	1-T	1	Total	C	O	0	0
			13	6	7		
4	2-T	1	Total	C	O	0	0
			13	6	7		
4	3-T	1	Total	C	O	0	0
			13	6	7		
4	4-T	1	Total	C	O	0	0
			13	6	7		
4	5-T	1	Total	C	O	0	0
			13	6	7		
4	6-T	1	Total	C	O	0	0
			13	6	7		
4	7-T	1	Total	C	O	0	0
			13	6	7		
4	8-T	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	9-T	1	Total	C	O	0	0
			13	6	7		
4	10-T	1	Total	C	O	0	0
			13	6	7		
4	1-U	1	Total	C	O	0	0
			13	6	7		
4	2-U	1	Total	C	O	0	0
			13	6	7		
4	3-U	1	Total	C	O	0	0
			13	6	7		
4	4-U	1	Total	C	O	0	0
			13	6	7		
4	5-U	1	Total	C	O	0	0
			13	6	7		
4	6-U	1	Total	C	O	0	0
			13	6	7		
4	7-U	1	Total	C	O	0	0
			13	6	7		
4	8-U	1	Total	C	O	0	0
			13	6	7		
4	9-U	1	Total	C	O	0	0
			13	6	7		
4	10-U	1	Total	C	O	0	0
			13	6	7		
4	1-V	1	Total	C	O	0	0
			13	6	7		
4	2-V	1	Total	C	O	0	0
			13	6	7		
4	3-V	1	Total	C	O	0	0
			13	6	7		
4	4-V	1	Total	C	O	0	0
			13	6	7		
4	5-V	1	Total	C	O	0	0
			13	6	7		
4	6-V	1	Total	C	O	0	0
			13	6	7		
4	7-V	1	Total	C	O	0	0
			13	6	7		
4	8-V	1	Total	C	O	0	0
			13	6	7		
4	9-V	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	10-V	1	Total	C	O	0	0
			13	6	7		
4	1-W	1	Total	C	O	0	0
			13	6	7		
4	2-W	1	Total	C	O	0	0
			13	6	7		
4	3-W	1	Total	C	O	0	0
			13	6	7		
4	4-W	1	Total	C	O	0	0
			13	6	7		
4	5-W	1	Total	C	O	0	0
			13	6	7		
4	6-W	1	Total	C	O	0	0
			13	6	7		
4	7-W	1	Total	C	O	0	0
			13	6	7		
4	8-W	1	Total	C	O	0	0
			13	6	7		
4	9-W	1	Total	C	O	0	0
			13	6	7		
4	10-W	1	Total	C	O	0	0
			13	6	7		
4	1-X	1	Total	C	O	0	0
			13	6	7		
4	2-X	1	Total	C	O	0	0
			13	6	7		
4	3-X	1	Total	C	O	0	0
			13	6	7		
4	4-X	1	Total	C	O	0	0
			13	6	7		
4	5-X	1	Total	C	O	0	0
			13	6	7		
4	6-X	1	Total	C	O	0	0
			13	6	7		
4	7-X	1	Total	C	O	0	0
			13	6	7		
4	8-X	1	Total	C	O	0	0
			13	6	7		
4	9-X	1	Total	C	O	0	0
			13	6	7		
4	10-X	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	261	Total O 261 261	0	0
5	2-A	262	Total O 262 262	0	0
5	3-A	261	Total O 261 261	0	0
5	4-A	263	Total O 263 263	0	0
5	5-A	261	Total O 261 261	0	0
5	6-A	257	Total O 257 257	0	0
5	7-A	265	Total O 265 265	0	0
5	8-A	259	Total O 259 259	0	0
5	9-A	265	Total O 265 265	0	0
5	10-A	262	Total O 262 262	0	0
5	1-B	264	Total O 264 264	0	0
5	2-B	261	Total O 261 261	0	0
5	3-B	263	Total O 263 263	0	0
5	4-B	262	Total O 262 262	0	0
5	5-B	261	Total O 261 261	0	0
5	6-B	265	Total O 265 265	0	0
5	7-B	264	Total O 264 264	0	0
5	8-B	264	Total O 264 264	0	0
5	9-B	258	Total O 258 258	0	0
5	10-B	263	Total O 263 263	0	0
5	1-C	261	Total O 261 261	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-C	264	Total 264	O 264	0	0
5	3-C	265	Total 265	O 265	0	0
5	4-C	261	Total 261	O 261	0	0
5	5-C	263	Total 263	O 263	0	0
5	6-C	262	Total 262	O 262	0	0
5	7-C	262	Total 262	O 262	0	0
5	8-C	263	Total 263	O 263	0	0
5	9-C	261	Total 261	O 261	0	0
5	10-C	262	Total 262	O 262	0	0
5	1-D	260	Total 260	O 260	0	0
5	2-D	269	Total 269	O 269	0	0
5	3-D	260	Total 260	O 260	0	0
5	4-D	263	Total 263	O 263	0	0
5	5-D	262	Total 262	O 262	0	0
5	6-D	265	Total 265	O 265	0	0
5	7-D	261	Total 261	O 261	0	0
5	8-D	265	Total 265	O 265	0	0
5	9-D	266	Total 266	O 266	0	0
5	10-D	262	Total 262	O 262	0	0
5	1-E	261	Total 261	O 261	0	0
5	2-E	254	Total 254	O 254	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	3-E	257	Total 257	O 257	0	0
5	4-E	263	Total 263	O 263	0	0
5	5-E	259	Total 259	O 259	0	0
5	6-E	262	Total 262	O 262	0	0
5	7-E	265	Total 265	O 265	0	0
5	8-E	257	Total 257	O 257	0	0
5	9-E	262	Total 262	O 262	0	0
5	10-E	257	Total 257	O 257	0	0
5	1-F	262	Total 262	O 262	0	0
5	2-F	263	Total 263	O 263	0	0
5	3-F	272	Total 272	O 272	0	0
5	4-F	264	Total 264	O 264	0	0
5	5-F	266	Total 266	O 266	0	0
5	6-F	263	Total 263	O 263	0	0
5	7-F	262	Total 262	O 262	0	0
5	8-F	268	Total 268	O 268	0	0
5	9-F	262	Total 262	O 262	0	0
5	10-F	261	Total 261	O 261	0	0
5	1-G	265	Total 265	O 265	0	0
5	2-G	262	Total 262	O 262	0	0
5	3-G	257	Total 257	O 257	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	4-G	261	Total 261	O 261	0	0
5	5-G	263	Total 263	O 263	0	0
5	6-G	267	Total 267	O 267	0	0
5	7-G	259	Total 259	O 259	0	0
5	8-G	265	Total 265	O 265	0	0
5	9-G	263	Total 263	O 263	0	0
5	10-G	264	Total 264	O 264	0	0
5	1-H	262	Total 262	O 262	0	0
5	2-H	263	Total 263	O 263	0	0
5	3-H	261	Total 261	O 261	0	0
5	4-H	266	Total 266	O 266	0	0
5	5-H	270	Total 270	O 270	0	0
5	6-H	263	Total 263	O 263	0	0
5	7-H	262	Total 262	O 262	0	0
5	8-H	261	Total 261	O 261	0	0
5	9-H	268	Total 268	O 268	0	0
5	10-H	264	Total 264	O 264	0	0
5	1-I	265	Total 265	O 265	0	0
5	2-I	265	Total 265	O 265	0	0
5	3-I	266	Total 266	O 266	0	0
5	4-I	263	Total 263	O 263	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	5-I	260	Total 260	O 260	0	0
5	6-I	263	Total 263	O 263	0	0
5	7-I	261	Total 261	O 261	0	0
5	8-I	265	Total 265	O 265	0	0
5	9-I	262	Total 262	O 262	0	0
5	10-I	263	Total 263	O 263	0	0
5	1-J	262	Total 262	O 262	0	0
5	2-J	258	Total 258	O 258	0	0
5	3-J	260	Total 260	O 260	0	0
5	4-J	260	Total 260	O 260	0	0
5	5-J	263	Total 263	O 263	0	0
5	6-J	259	Total 259	O 259	0	0
5	7-J	266	Total 266	O 266	0	0
5	8-J	263	Total 263	O 263	0	0
5	9-J	260	Total 260	O 260	0	0
5	10-J	264	Total 264	O 264	0	0
5	1-K	272	Total 272	O 272	0	0
5	2-K	271	Total 271	O 271	0	0
5	3-K	268	Total 268	O 268	0	0
5	4-K	267	Total 267	O 267	0	0
5	5-K	268	Total 268	O 268	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	6-K	270	Total 270	O 270	0	0
5	7-K	263	Total 263	O 263	0	0
5	8-K	264	Total 264	O 264	0	0
5	9-K	269	Total 269	O 269	0	0
5	10-K	271	Total 271	O 271	0	0
5	1-L	261	Total 261	O 261	0	0
5	2-L	264	Total 264	O 264	0	0
5	3-L	266	Total 266	O 266	0	0
5	4-L	263	Total 263	O 263	0	0
5	5-L	260	Total 260	O 260	0	0
5	6-L	260	Total 260	O 260	0	0
5	7-L	266	Total 266	O 266	0	0
5	8-L	262	Total 262	O 262	0	0
5	9-L	260	Total 260	O 260	0	0
5	10-L	263	Total 263	O 263	0	0
5	1-M	261	Total 261	O 261	0	0
5	2-M	264	Total 264	O 264	0	0
5	3-M	259	Total 259	O 259	0	0
5	4-M	264	Total 264	O 264	0	0
5	5-M	264	Total 264	O 264	0	0
5	6-M	262	Total 262	O 262	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	7-M	260	Total 260	O 260	0	0
5	8-M	260	Total 260	O 260	0	0
5	9-M	265	Total 265	O 265	0	0
5	10-M	263	Total 263	O 263	0	0
5	1-N	263	Total 263	O 263	0	0
5	2-N	261	Total 261	O 261	0	0
5	3-N	263	Total 263	O 263	0	0
5	4-N	263	Total 263	O 263	0	0
5	5-N	265	Total 265	O 265	0	0
5	6-N	260	Total 260	O 260	0	0
5	7-N	266	Total 266	O 266	0	0
5	8-N	263	Total 263	O 263	0	0
5	9-N	261	Total 261	O 261	0	0
5	10-N	259	Total 259	O 259	0	0
5	1-O	263	Total 263	O 263	0	0
5	2-O	267	Total 267	O 267	0	0
5	3-O	265	Total 265	O 265	0	0
5	4-O	263	Total 263	O 263	0	0
5	5-O	267	Total 267	O 267	0	0
5	6-O	265	Total 265	O 265	0	0
5	7-O	262	Total 262	O 262	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	8-O	265	Total 265	O 265	0	0
5	9-O	263	Total 263	O 263	0	0
5	10-O	263	Total 263	O 263	0	0
5	1-P	261	Total 261	O 261	0	0
5	2-P	264	Total 264	O 264	0	0
5	3-P	260	Total 260	O 260	0	0
5	4-P	259	Total 259	O 259	0	0
5	5-P	262	Total 262	O 262	0	0
5	6-P	262	Total 262	O 262	0	0
5	7-P	261	Total 261	O 261	0	0
5	8-P	263	Total 263	O 263	0	0
5	9-P	265	Total 265	O 265	0	0
5	10-P	264	Total 264	O 264	0	0
5	1-Q	260	Total 260	O 260	0	0
5	2-Q	257	Total 257	O 257	0	0
5	3-Q	259	Total 259	O 259	0	0
5	4-Q	264	Total 264	O 264	0	0
5	5-Q	261	Total 261	O 261	0	0
5	6-Q	260	Total 260	O 260	0	0
5	7-Q	264	Total 264	O 264	0	0
5	8-Q	257	Total 257	O 257	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	9-Q	263	Total 263	O 263	0	0
5	10-Q	257	Total 257	O 257	0	0
5	1-R	261	Total 261	O 261	0	0
5	2-R	265	Total 265	O 265	0	0
5	3-R	268	Total 268	O 268	0	0
5	4-R	263	Total 263	O 263	0	0
5	5-R	265	Total 265	O 265	0	0
5	6-R	266	Total 266	O 266	0	0
5	7-R	264	Total 264	O 264	0	0
5	8-R	265	Total 265	O 265	0	0
5	9-R	264	Total 264	O 264	0	0
5	10-R	262	Total 262	O 262	0	0
5	1-S	265	Total 265	O 265	0	0
5	2-S	259	Total 259	O 259	0	0
5	3-S	264	Total 264	O 264	0	0
5	4-S	260	Total 260	O 260	0	0
5	5-S	263	Total 263	O 263	0	0
5	6-S	266	Total 266	O 266	0	0
5	7-S	263	Total 263	O 263	0	0
5	8-S	269	Total 269	O 269	0	0
5	9-S	259	Total 259	O 259	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	10-S	266	Total 266	O 266	0	0
5	1-T	261	Total 261	O 261	0	0
5	2-T	259	Total 259	O 259	0	0
5	3-T	262	Total 262	O 262	0	0
5	4-T	262	Total 262	O 262	0	0
5	5-T	258	Total 258	O 258	0	0
5	6-T	257	Total 257	O 257	0	0
5	7-T	263	Total 263	O 263	0	0
5	8-T	259	Total 259	O 259	0	0
5	9-T	265	Total 265	O 265	0	0
5	10-T	262	Total 262	O 262	0	0
5	1-U	263	Total 263	O 263	0	0
5	2-U	267	Total 267	O 267	0	0
5	3-U	267	Total 267	O 267	0	0
5	4-U	264	Total 264	O 264	0	0
5	5-U	263	Total 263	O 263	0	0
5	6-U	265	Total 265	O 265	0	0
5	7-U	262	Total 262	O 262	0	0
5	8-U	263	Total 263	O 263	0	0
5	9-U	265	Total 265	O 265	0	0
5	10-U	264	Total 264	O 264	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-V	265	Total 265	O 265	0	0
5	2-V	260	Total 260	O 260	0	0
5	3-V	258	Total 258	O 258	0	0
5	4-V	266	Total 266	O 266	0	0
5	5-V	261	Total 261	O 261	0	0
5	6-V	265	Total 265	O 265	0	0
5	7-V	265	Total 265	O 265	0	0
5	8-V	264	Total 264	O 264	0	0
5	9-V	259	Total 259	O 259	0	0
5	10-V	265	Total 265	O 265	0	0
5	1-W	269	Total 269	O 269	0	0
5	2-W	266	Total 266	O 266	0	0
5	3-W	266	Total 266	O 266	0	0
5	4-W	263	Total 263	O 263	0	0
5	5-W	262	Total 262	O 262	0	0
5	6-W	264	Total 264	O 264	0	0
5	7-W	265	Total 265	O 265	0	0
5	8-W	263	Total 263	O 263	0	0
5	9-W	261	Total 261	O 261	0	0
5	10-W	265	Total 265	O 265	0	0
5	1-X	264	Total 264	O 264	0	0

Continued on next page...

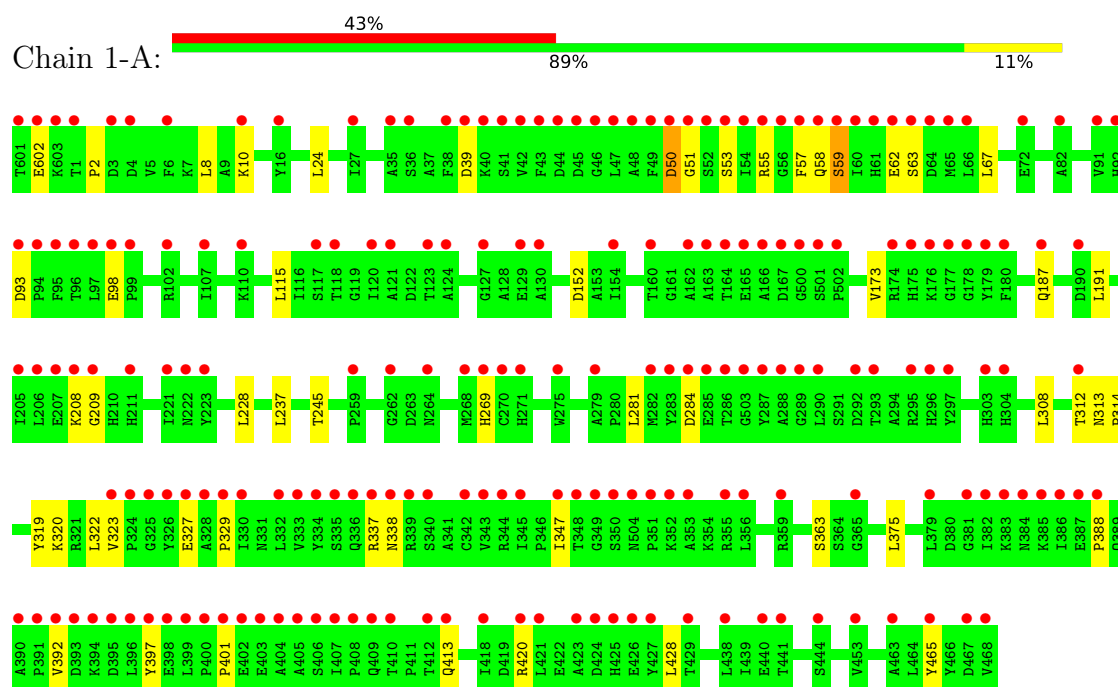
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-X	267	Total 267	O 267	0	0
5	3-X	265	Total 265	O 265	0	0
5	4-X	265	Total 265	O 265	0	0
5	5-X	265	Total 265	O 265	0	0
5	6-X	264	Total 264	O 264	0	0
5	7-X	261	Total 261	O 261	0	0
5	8-X	265	Total 265	O 265	0	0
5	9-X	266	Total 266	O 266	0	0
5	10-X	266	Total 266	O 266	0	0

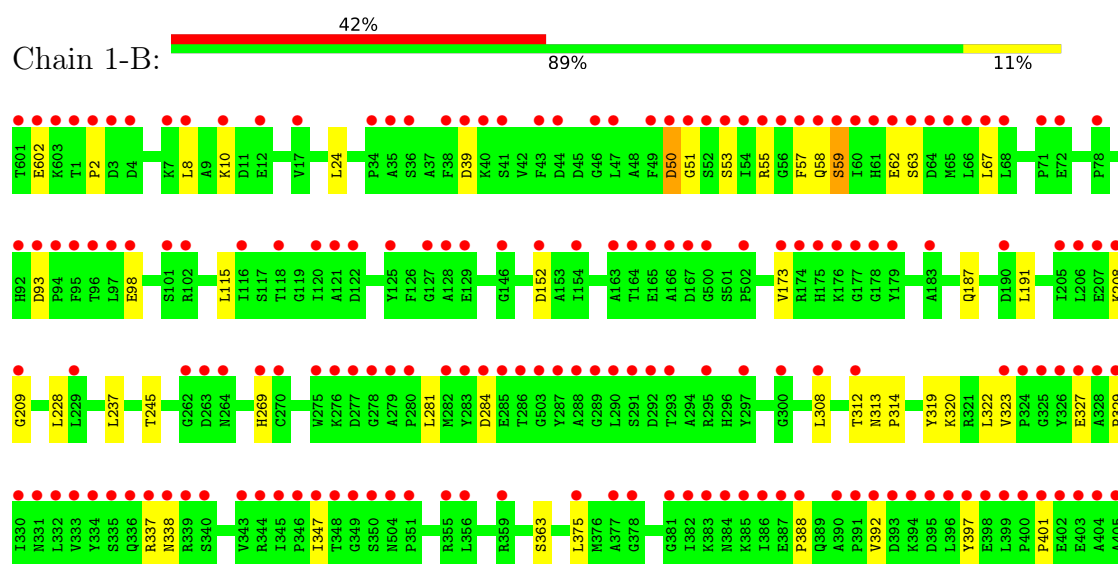
3 Residue-property plots [i](#)

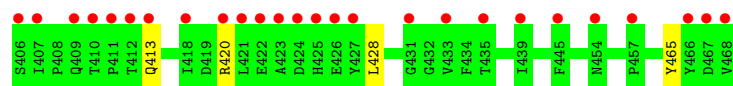
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: glutamine synthetase

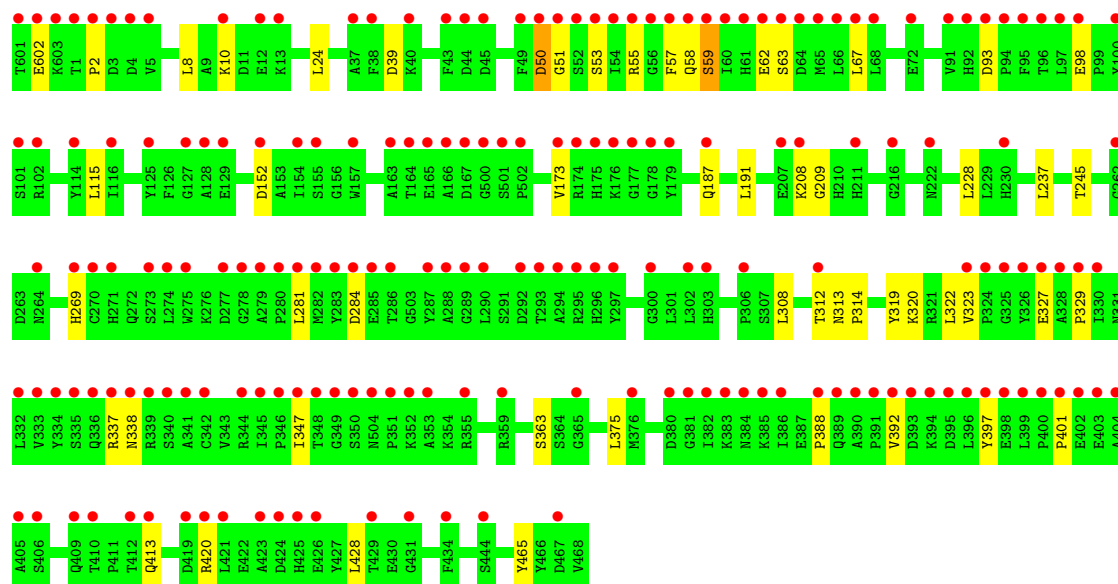
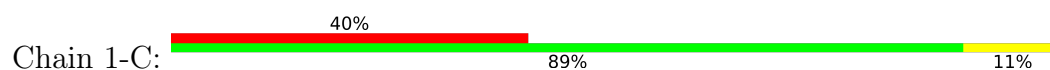


- Molecule 1: glutamine synthetase

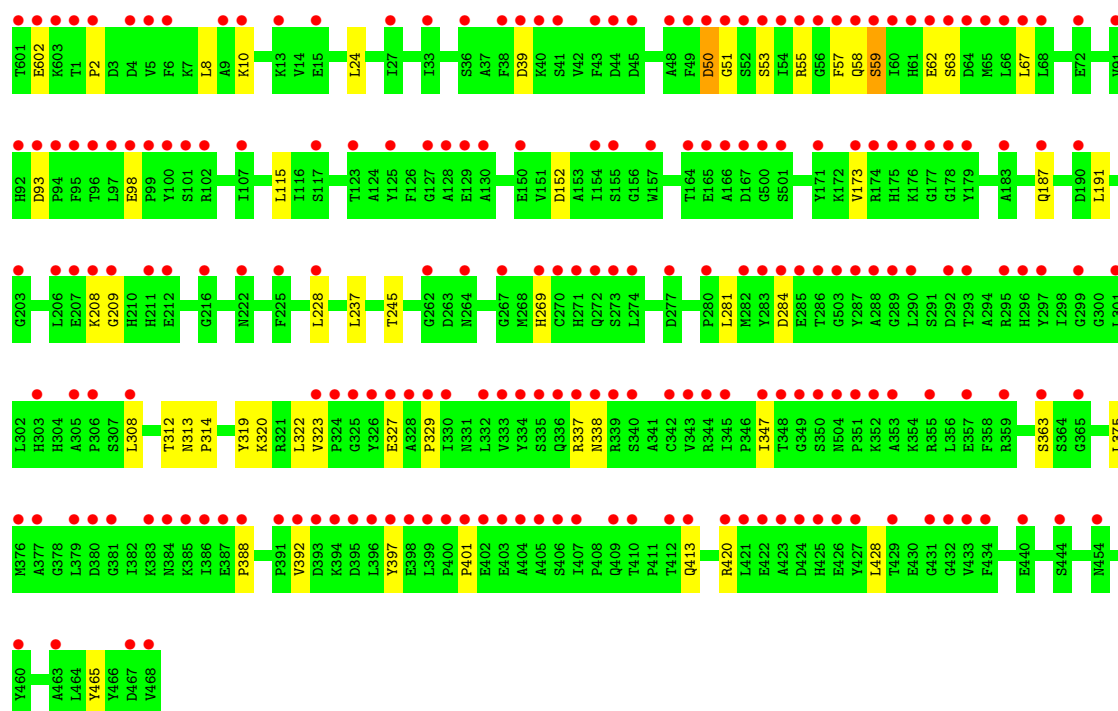




• Molecule 1: glutamine synthetase

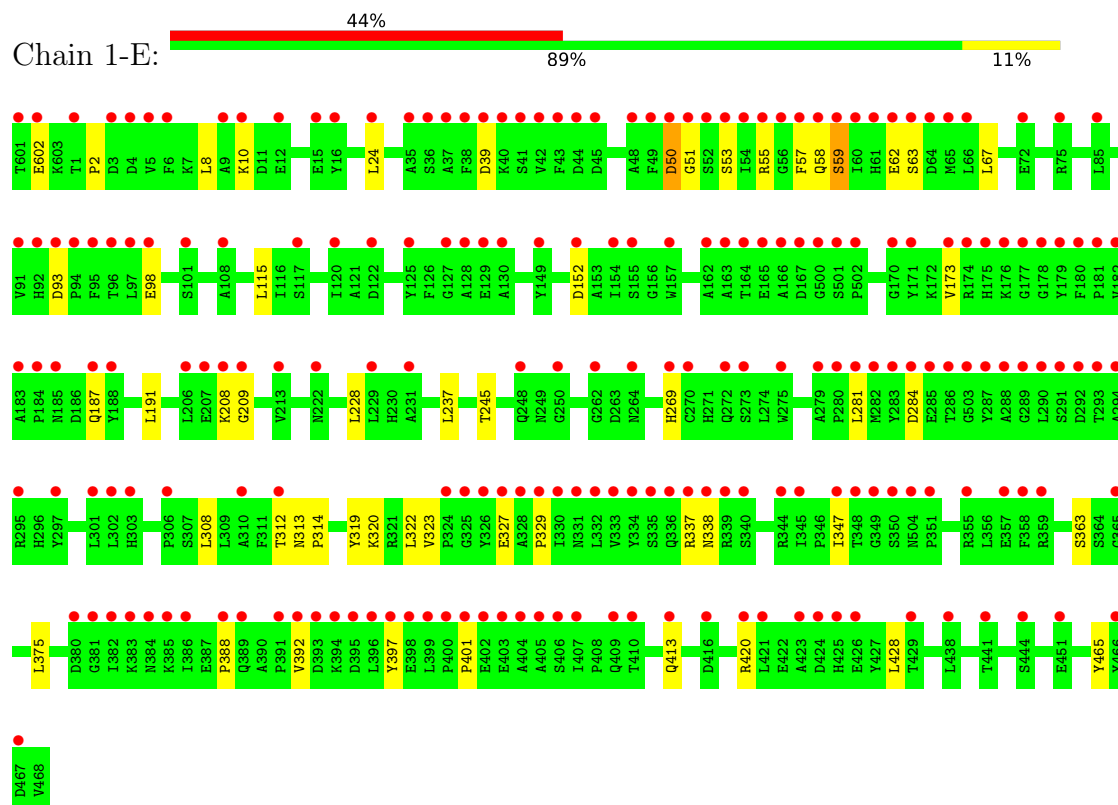


• Molecule 1: glutamine synthetase



- Molecule 1: glutamine synthetase

Chain 1-E:



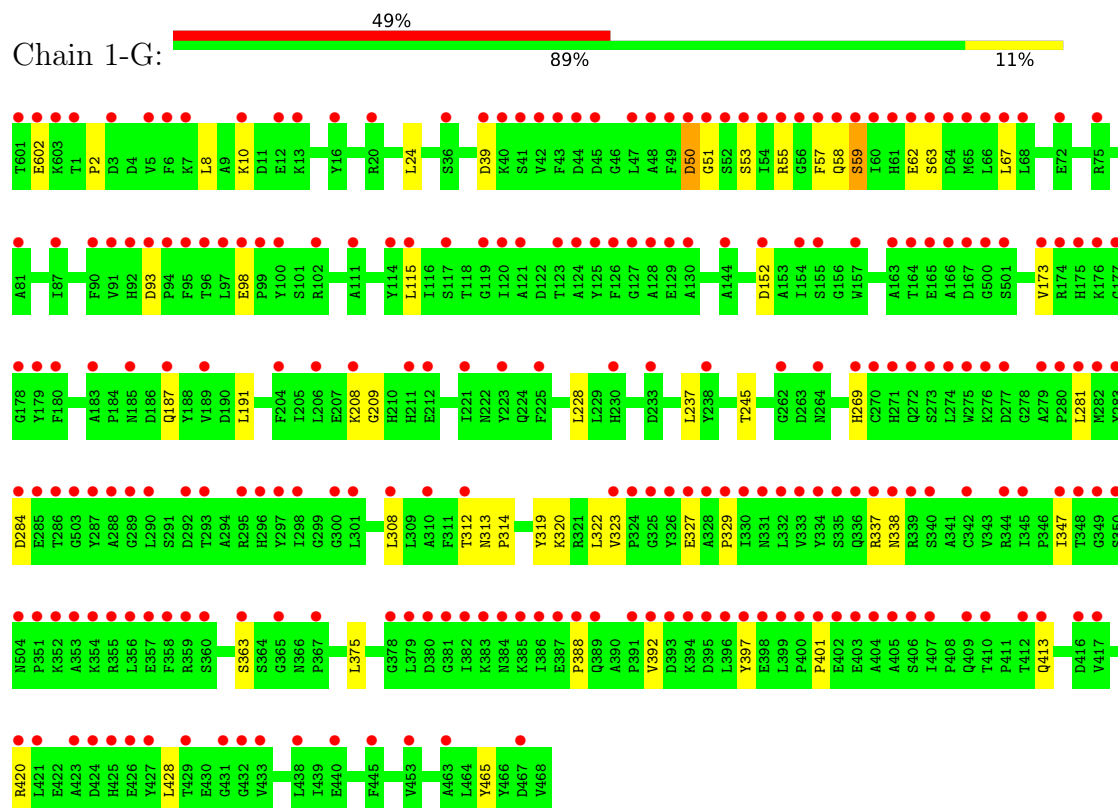
- Molecule 1: glutamine synthetase

Chain 1-F:



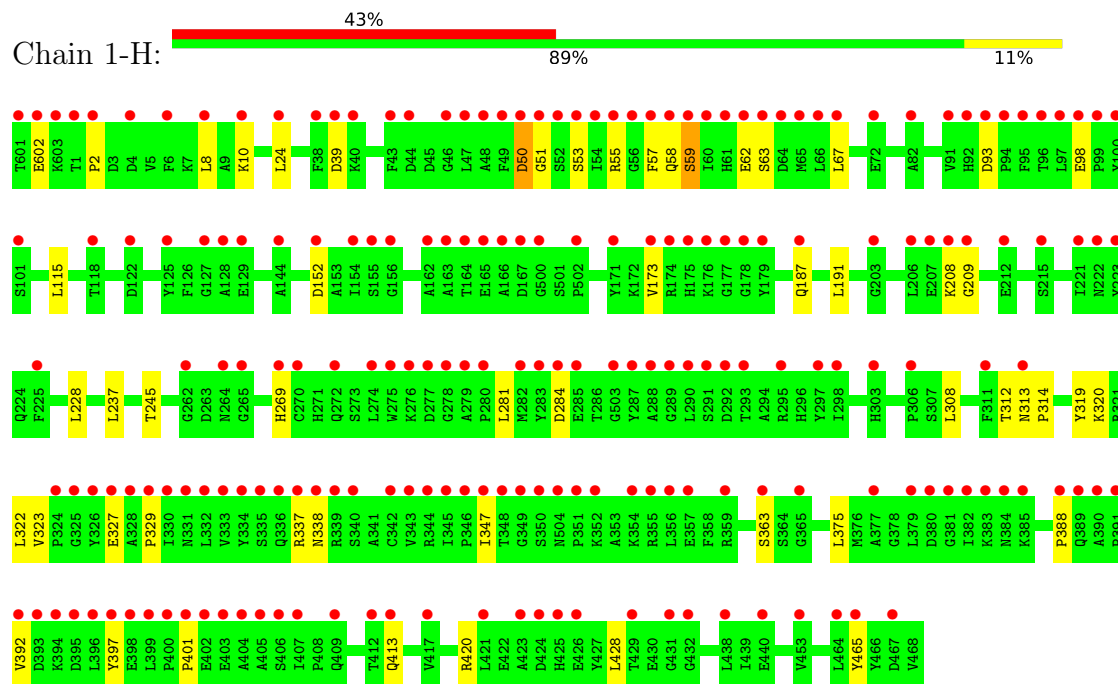
- Molecule 1: glutamine synthetase

Chain 1-G:



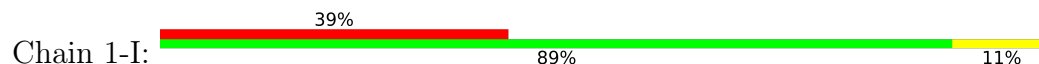
- Molecule 1: glutamine synthetase

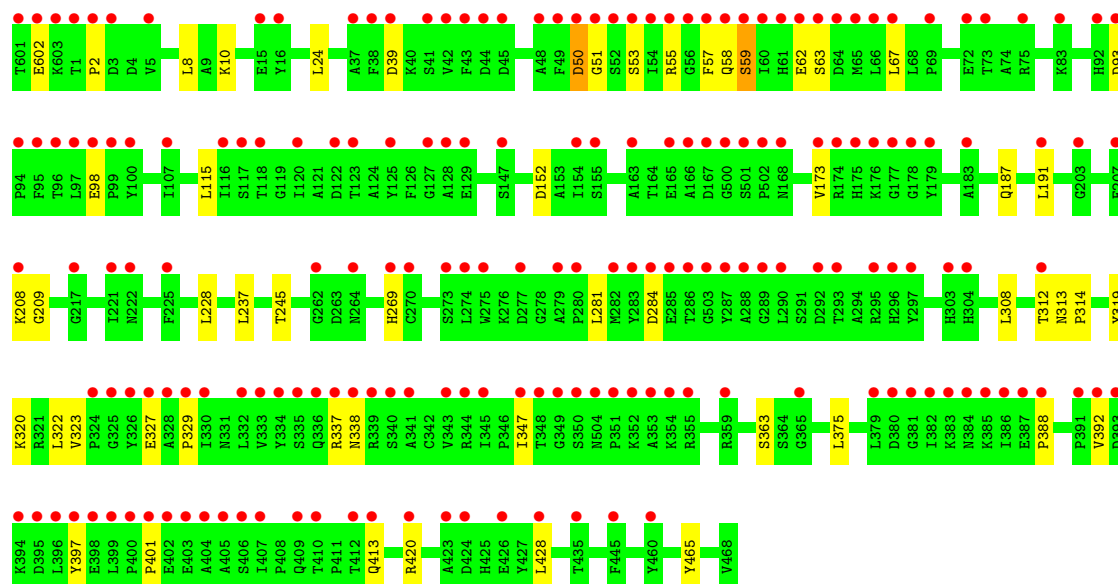
Chain 1-H:



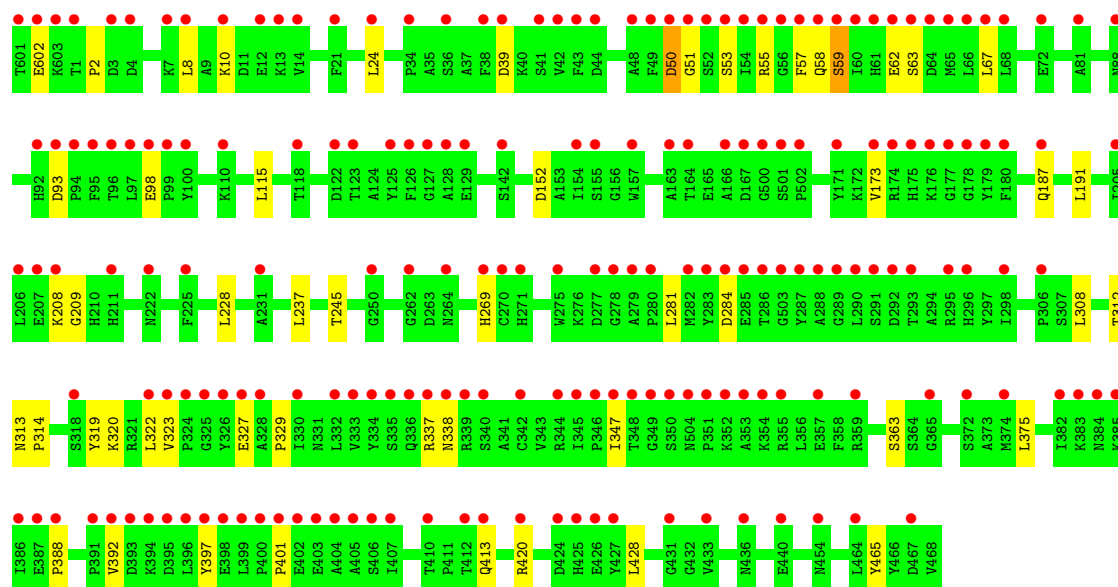
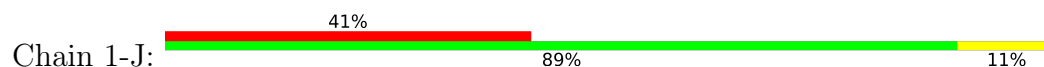
- Molecule 1: glutamine synthetase

Chain 1-I:

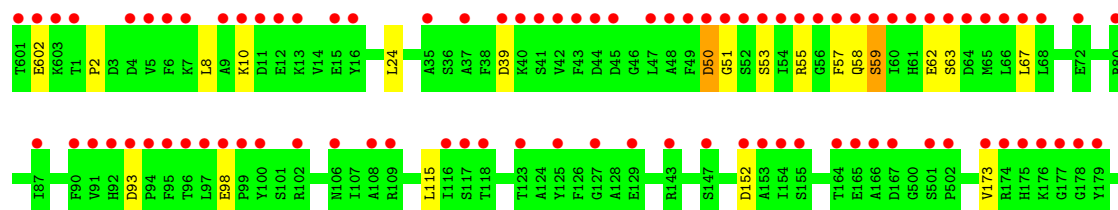
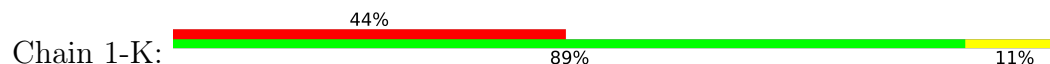


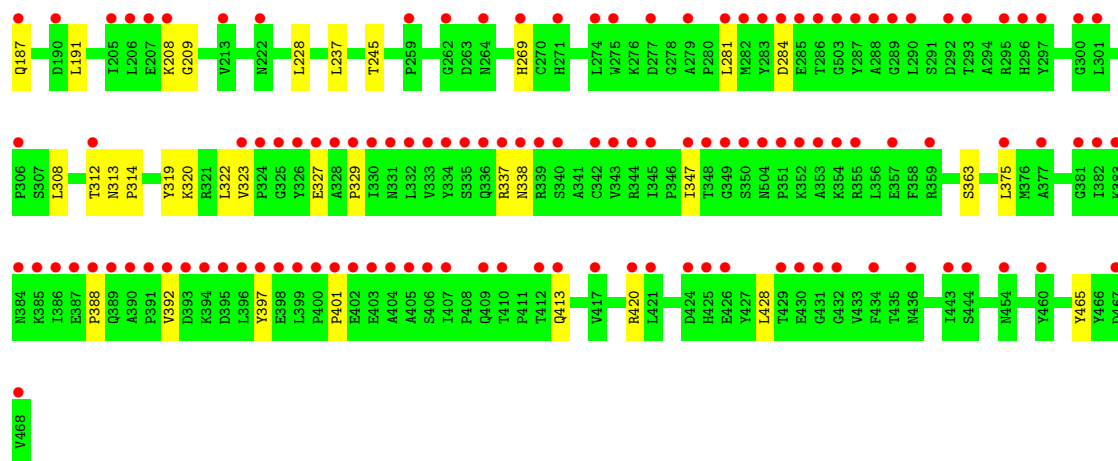


• Molecule 1: glutamine synthetase

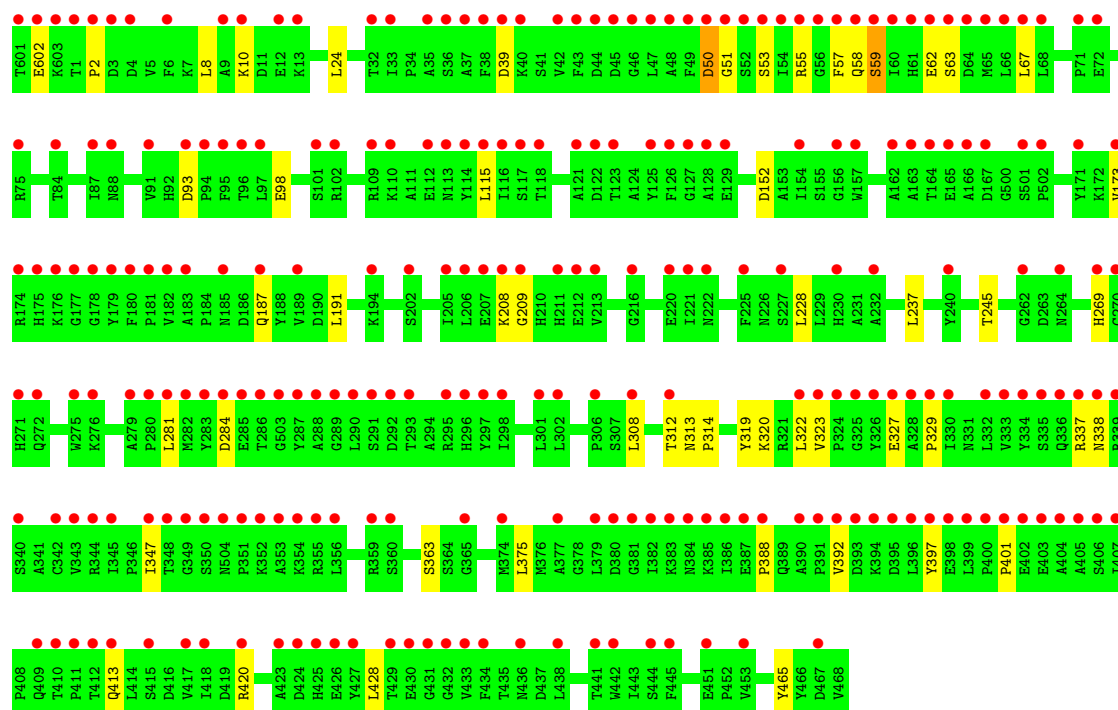
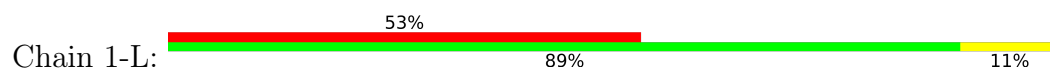


• Molecule 1: glutamine synthetase

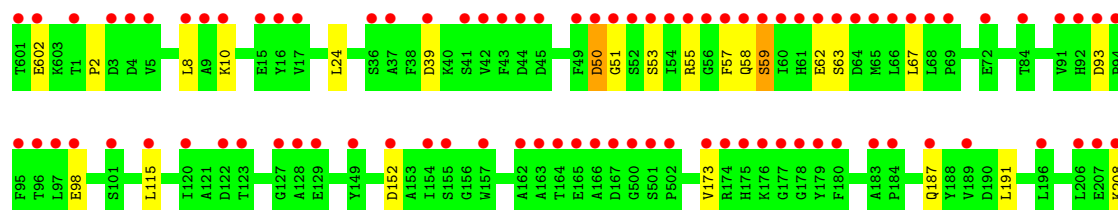


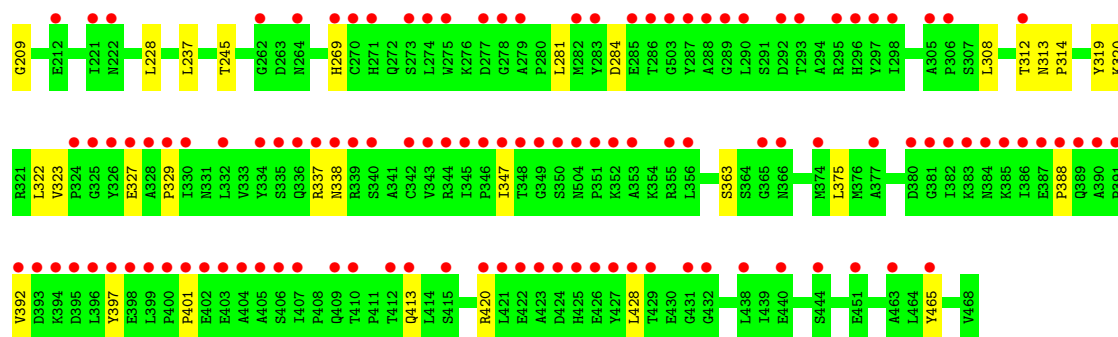


- Molecule 1: glutamine synthetase

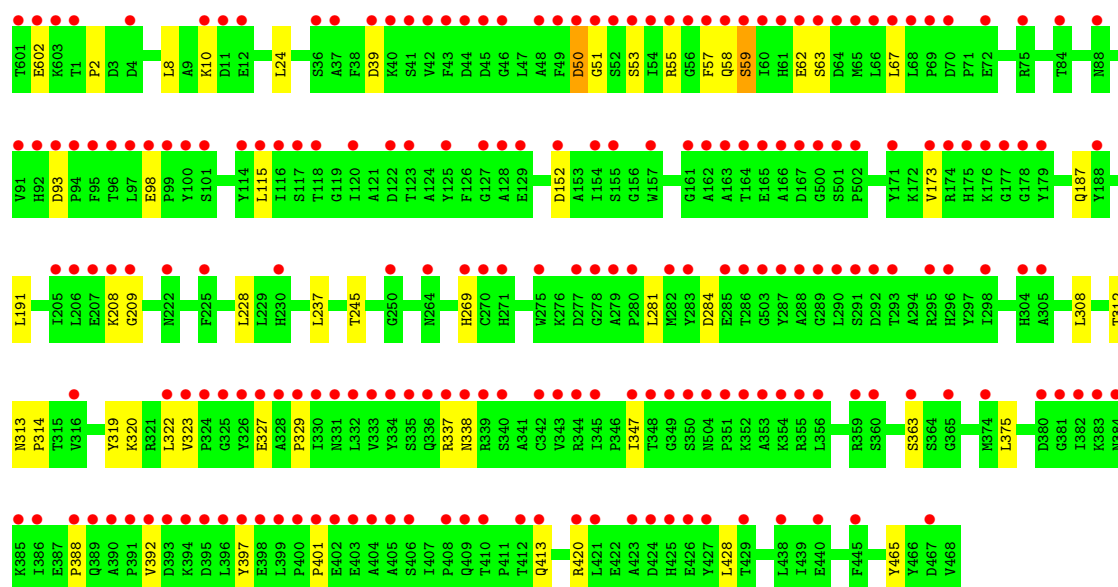


- Molecule 1: glutamine synthetase

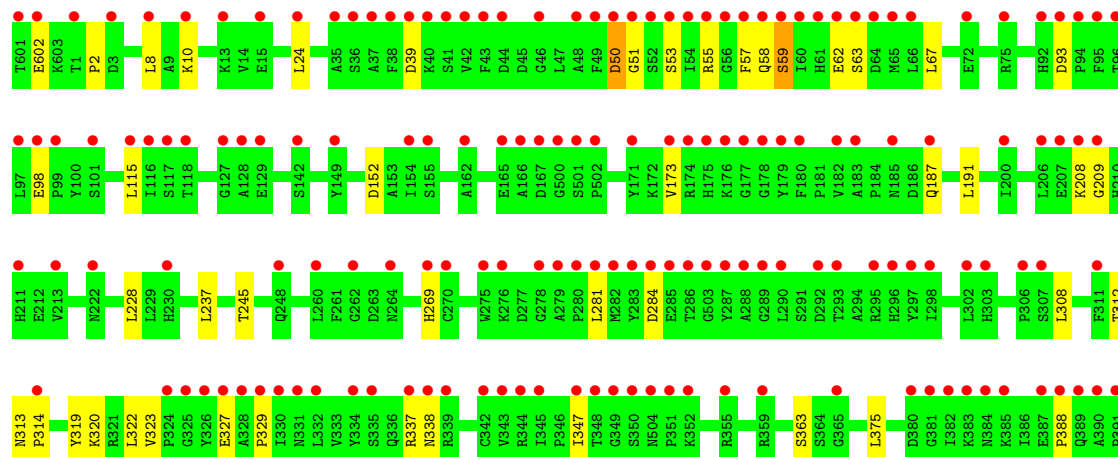
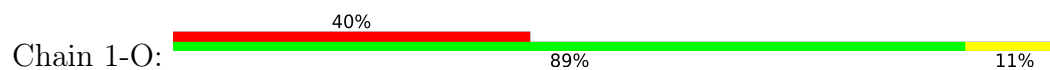




• Molecule 1: glutamine synthetase

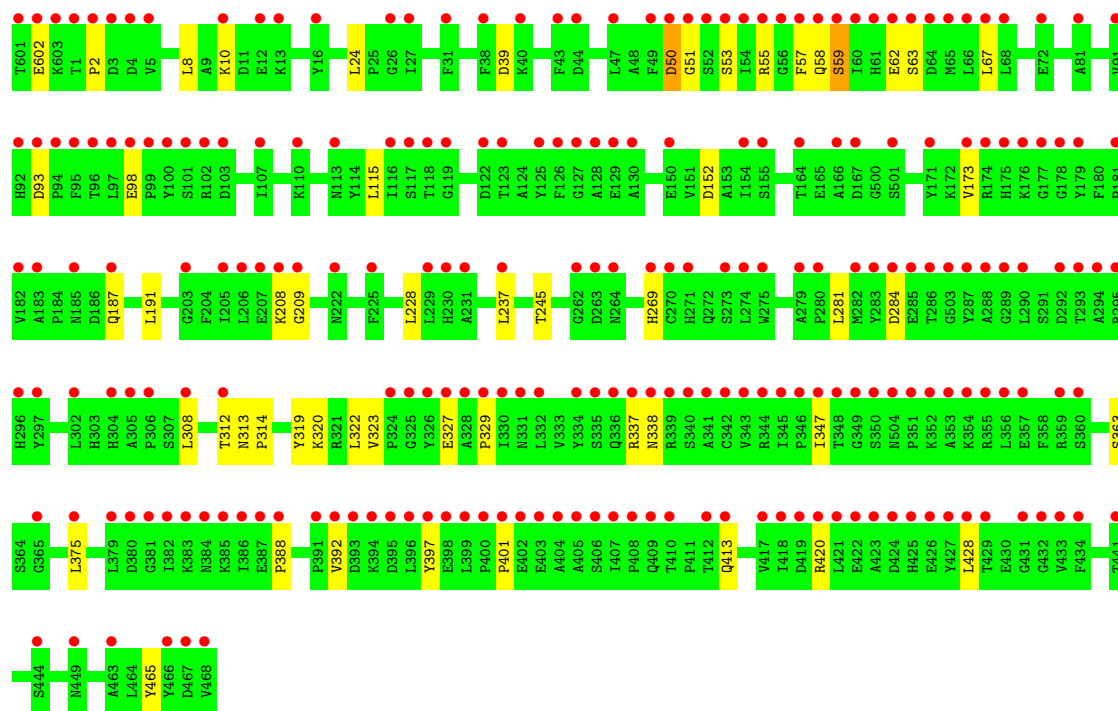
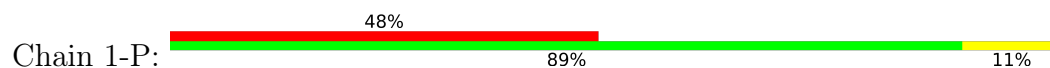


• Molecule 1: glutamine synthetase

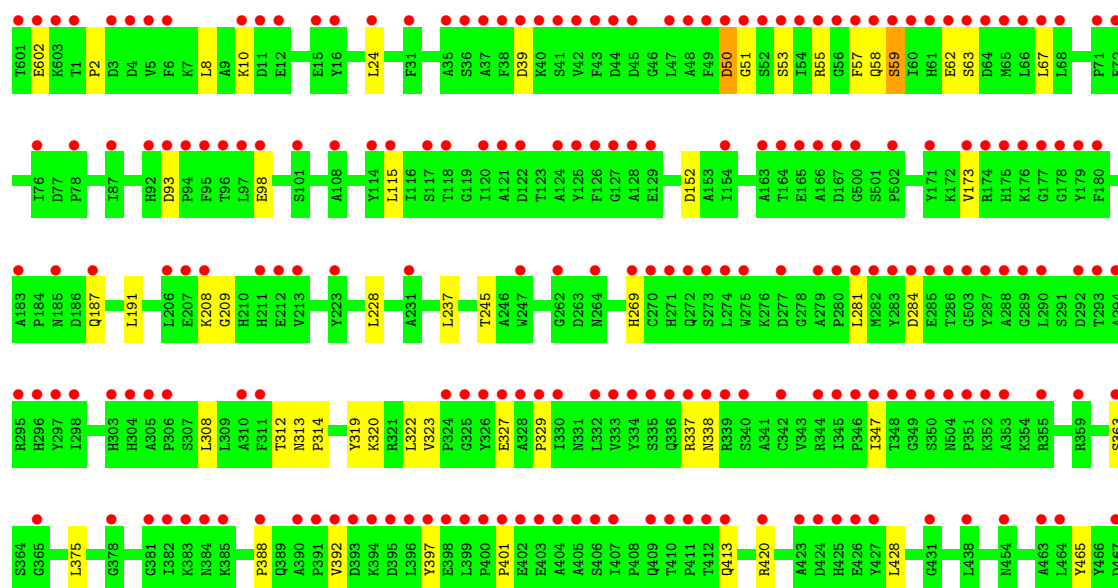
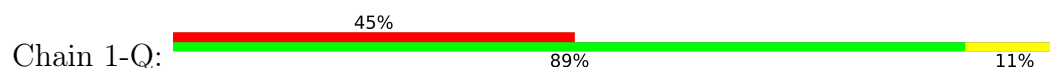




- Molecule 1: glutamine synthetase

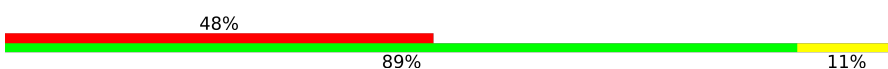


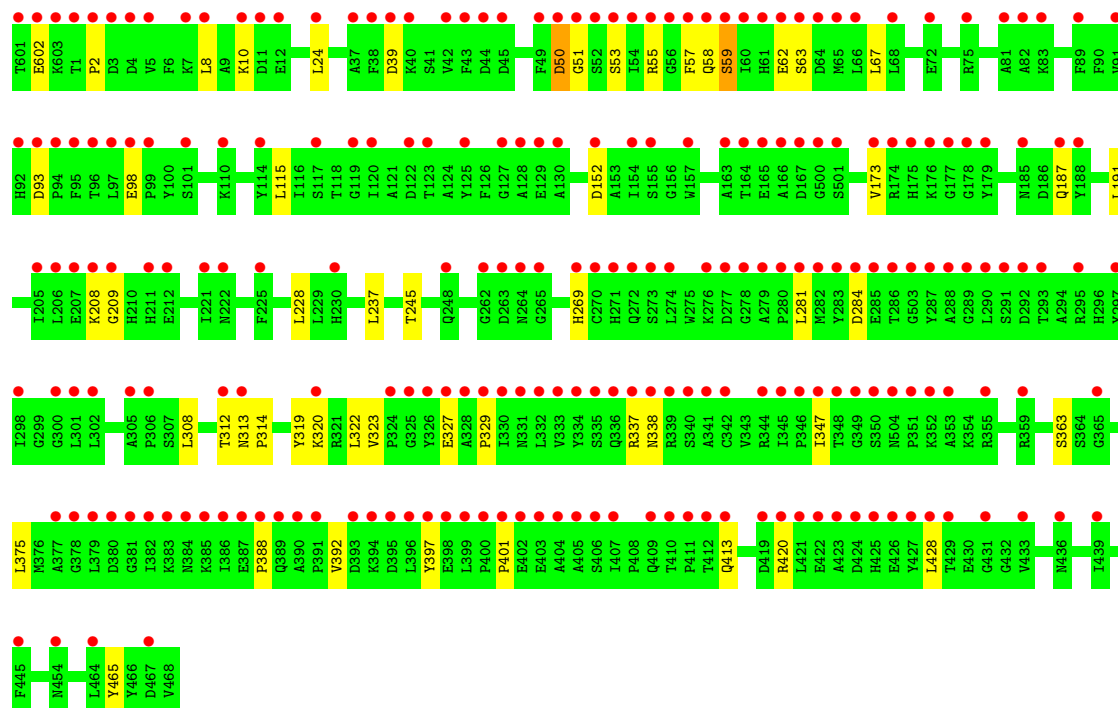
- Molecule 1: glutamine synthetase



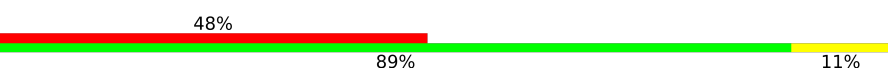
V468

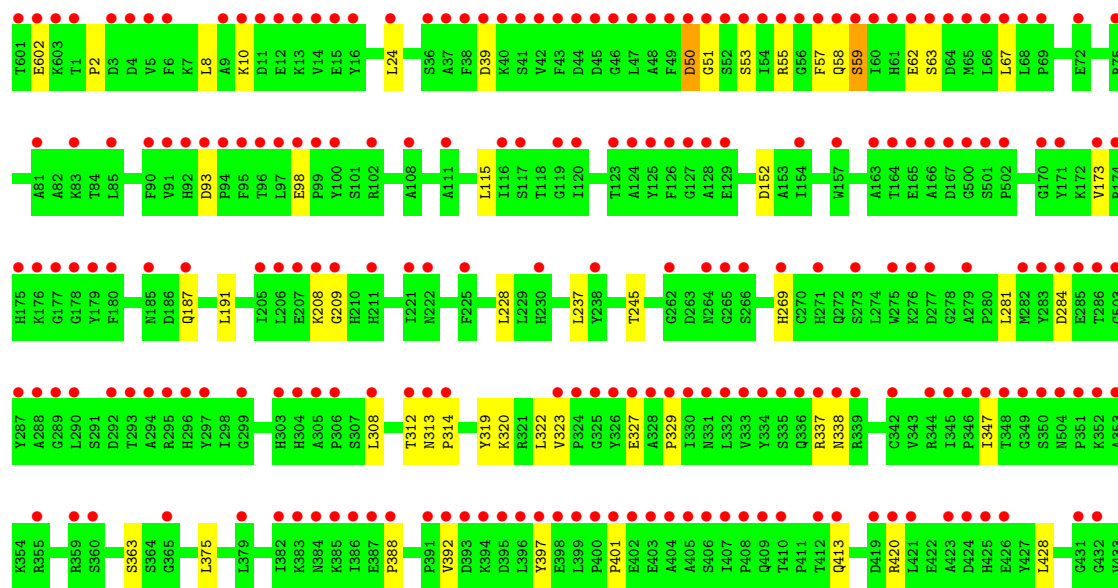
- Molecule 1: glutamine synthetase

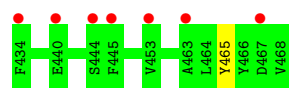
Chain 1-R: 



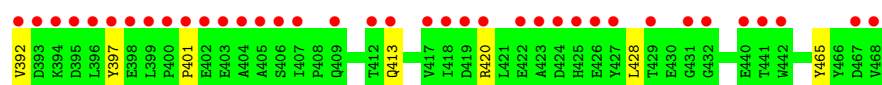
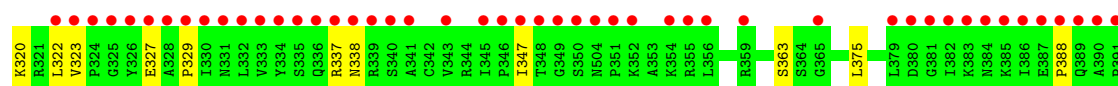
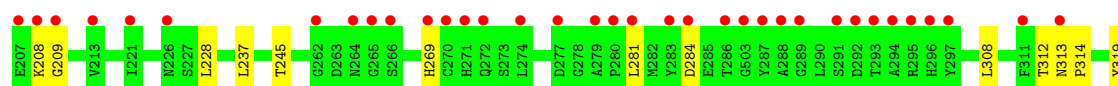
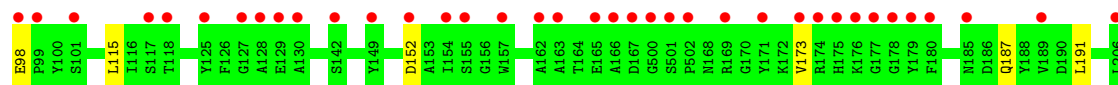
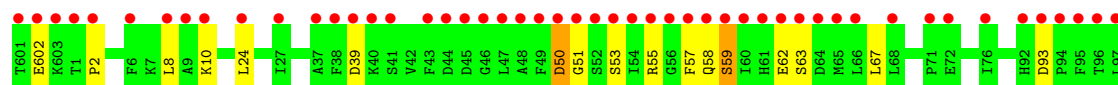
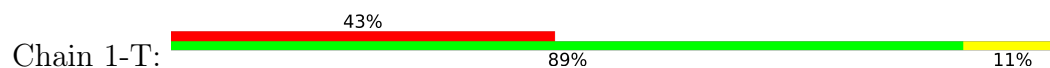
- Molecule 1: glutamine synthetase

Chain 1-S: 

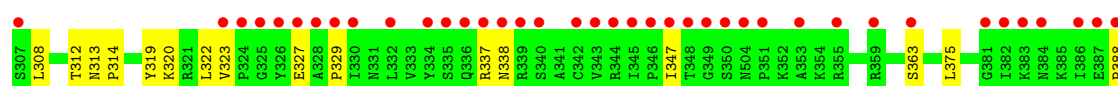
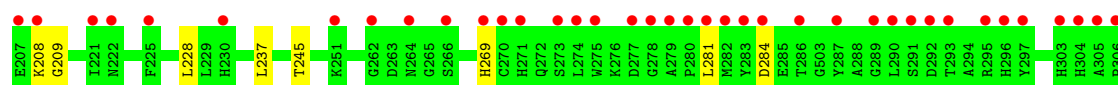
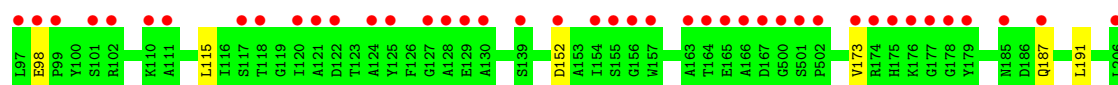
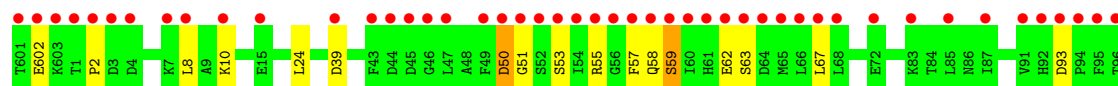




- Molecule 1: glutamine synthetase

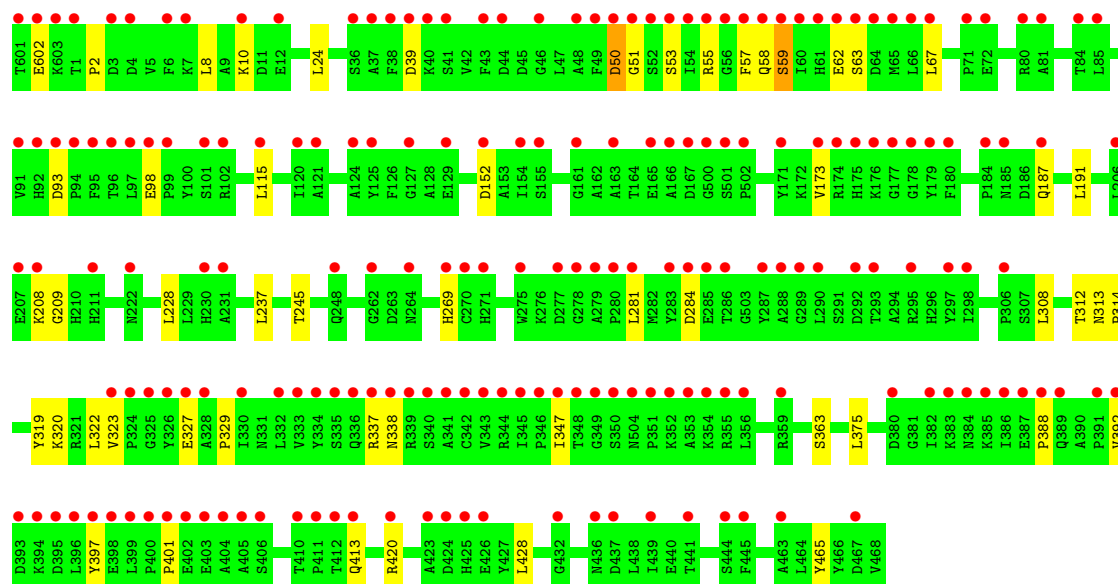


- Molecule 1: glutamine synthetase

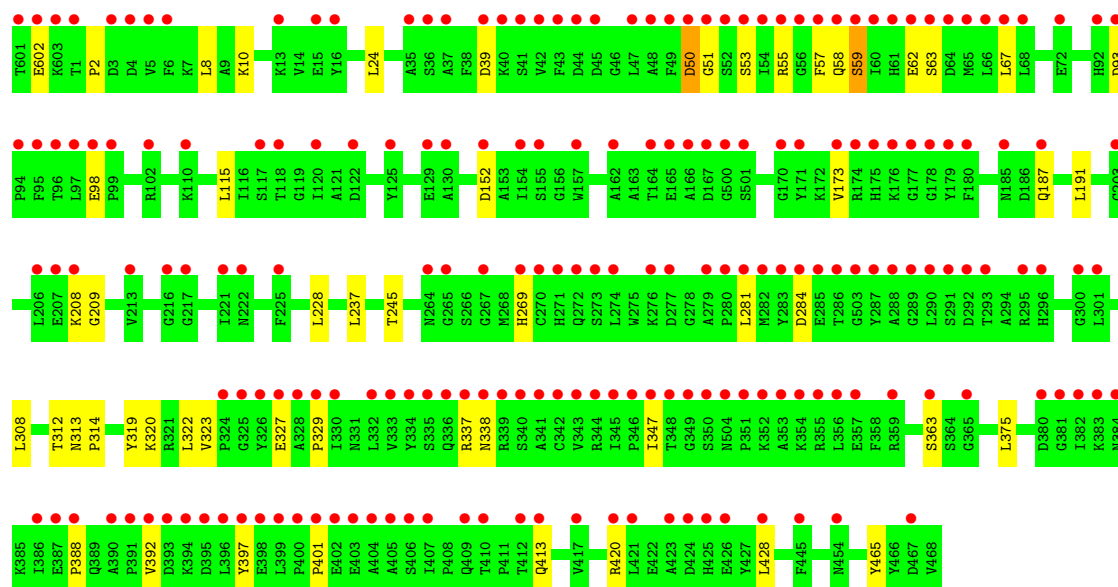
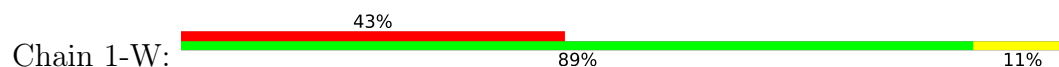


- Molecule 1: glutamine synthetase

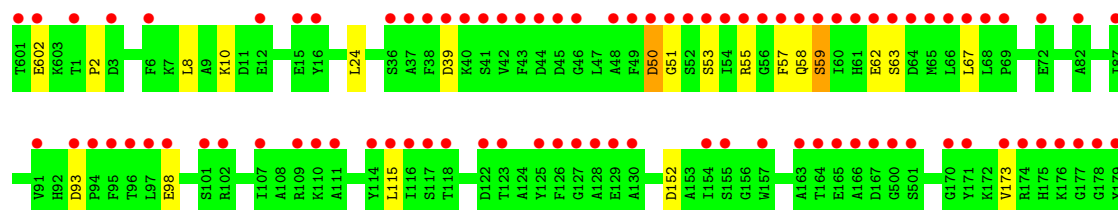
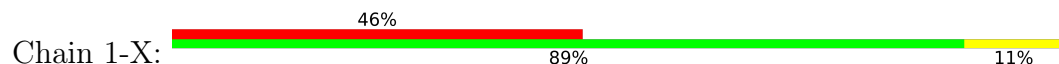


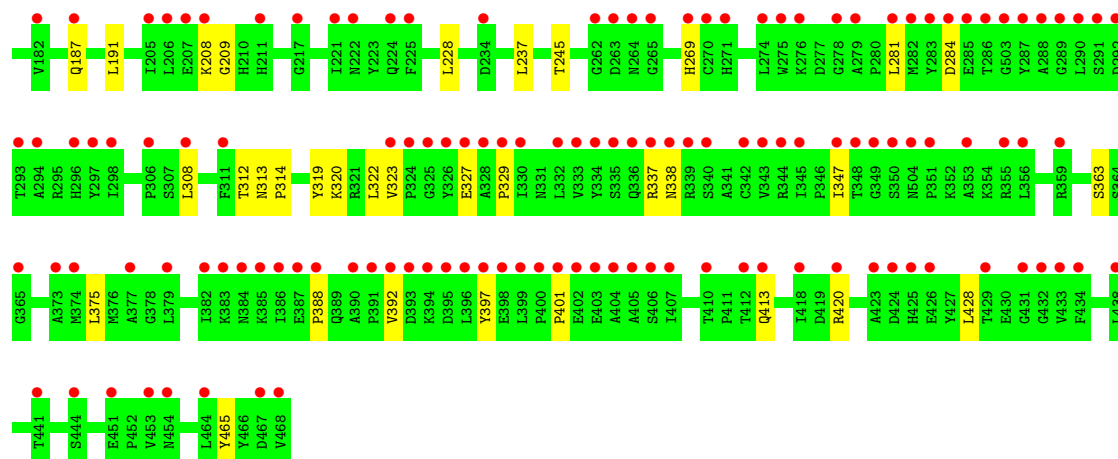


• Molecule 1: glutamine synthetase



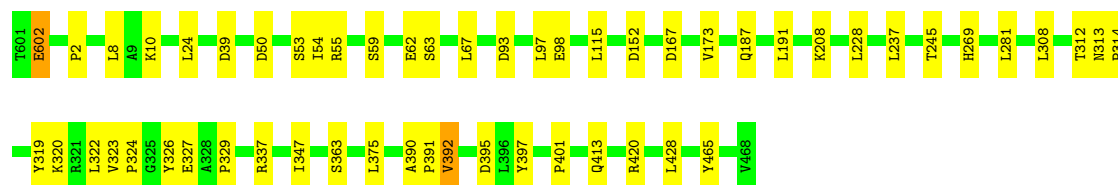
• Molecule 1: glutamine synthetase





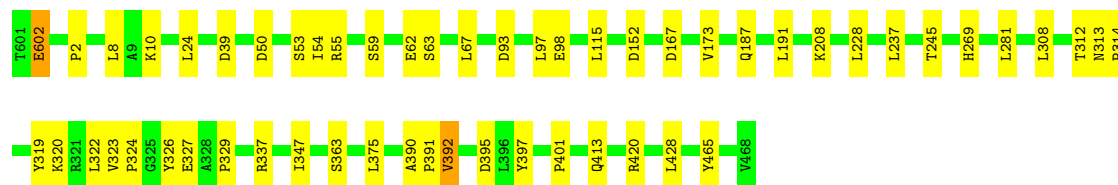
- Molecule 1: glutamine synthetase

Chain 2-A: 88% 11%



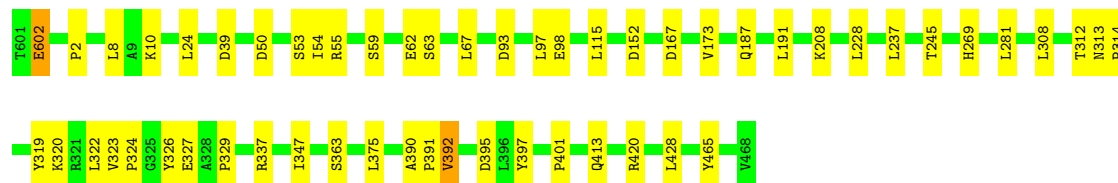
- Molecule 1: glutamine synthetase

Chain 2-B: 88% 11%



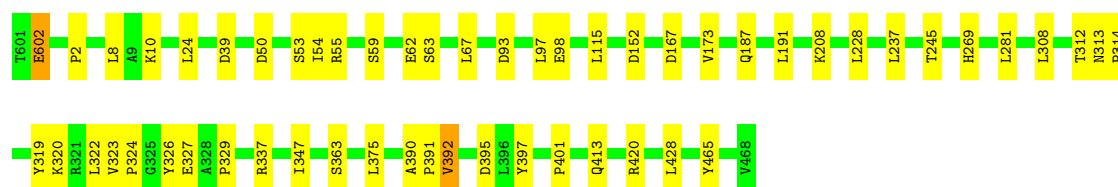
- Molecule 1: glutamine synthetase

Chain 2-C: 88% 11%



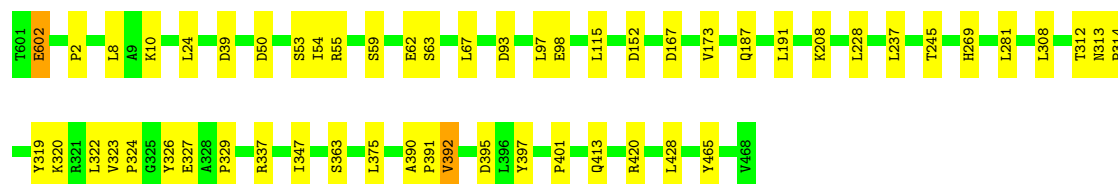
- Molecule 1: glutamine synthetase

Chain 2-D: 88% 11%



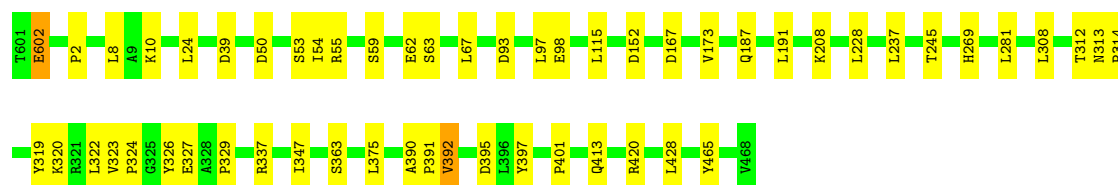
- Molecule 1: glutamine synthetase

Chain 2-E: 88% 11%



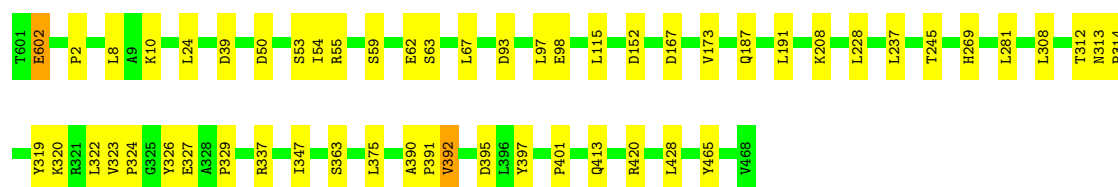
- Molecule 1: glutamine synthetase

Chain 2-F: 88% 11%



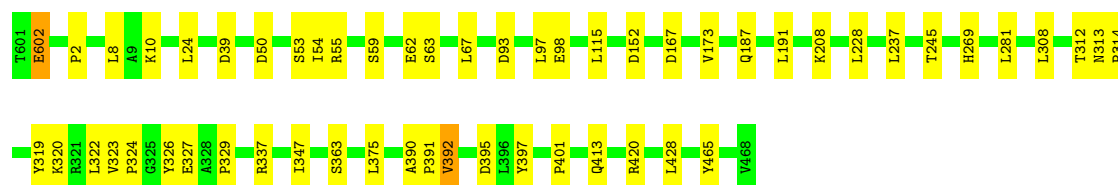
- Molecule 1: glutamine synthetase

Chain 2-G: 88% 11%



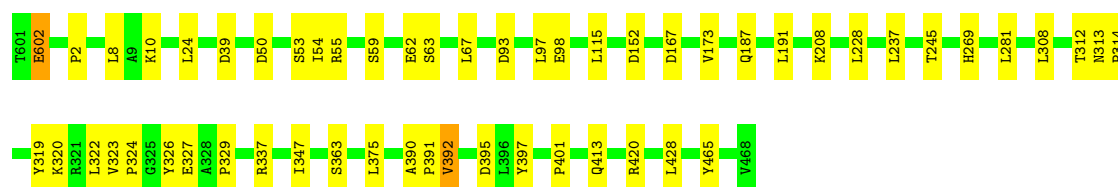
- Molecule 1: glutamine synthetase

Chain 2-H: 88% 11%



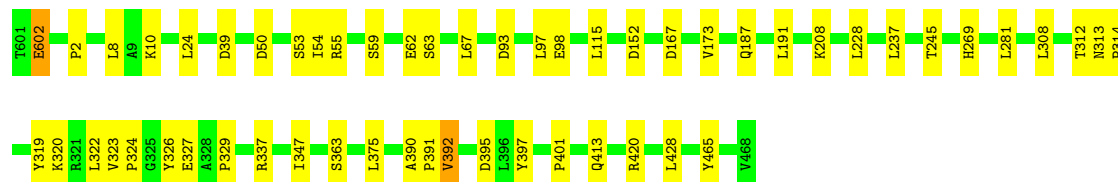
- Molecule 1: glutamine synthetase

Chain 2-I: 88% 11%



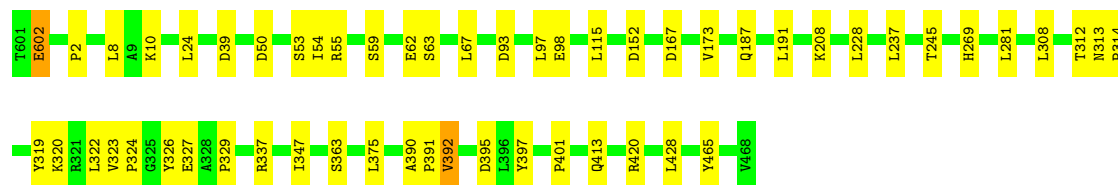
- Molecule 1: glutamine synthetase

Chain 2-J: 88% 11%



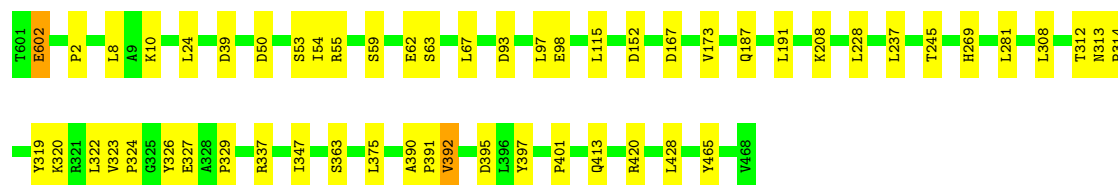
- Molecule 1: glutamine synthetase

Chain 2-K: 88% 11%



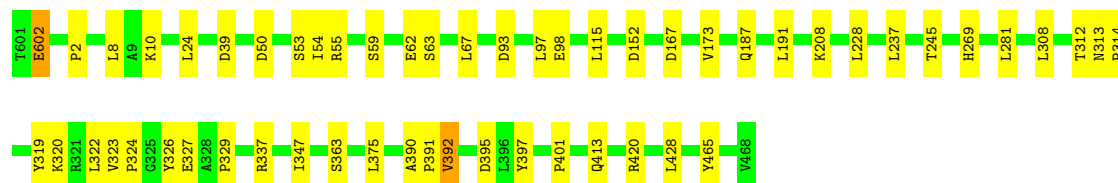
- Molecule 1: glutamine synthetase

Chain 2-L: 88% 11%



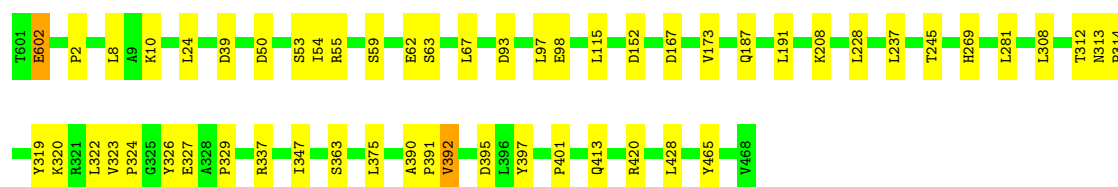
- Molecule 1: glutamine synthetase

Chain 2-M: 88% 11%



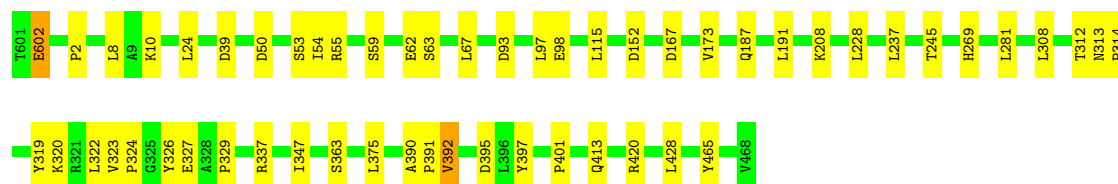
- Molecule 1: glutamine synthetase

Chain 2-N: 88% 11%



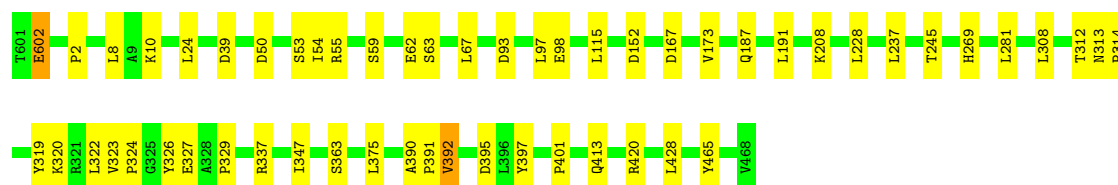
- Molecule 1: glutamine synthetase

Chain 2-O:
88% 11%



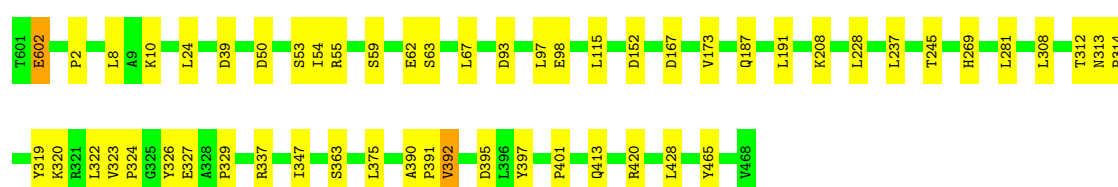
- Molecule 1: glutamine synthetase

Chain 2-P:
88% 11%



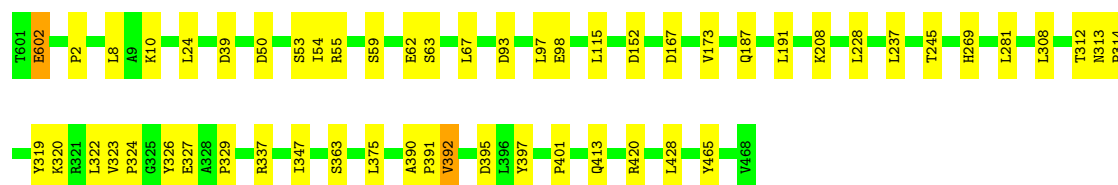
- Molecule 1: glutamine synthetase

Chain 2-Q:
88% 11%



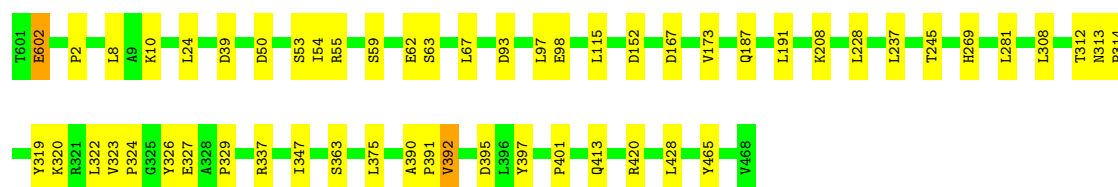
- Molecule 1: glutamine synthetase

Chain 2-R:
88% 11%



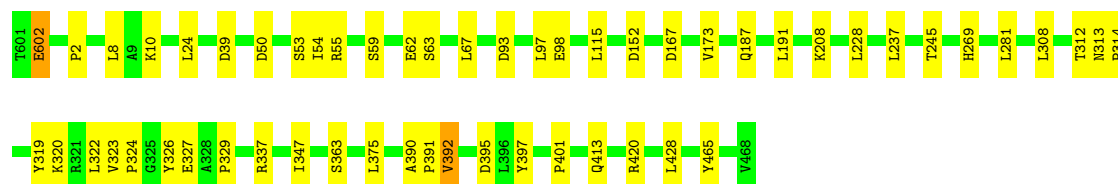
- Molecule 1: glutamine synthetase

Chain 2-S:
88% 11%



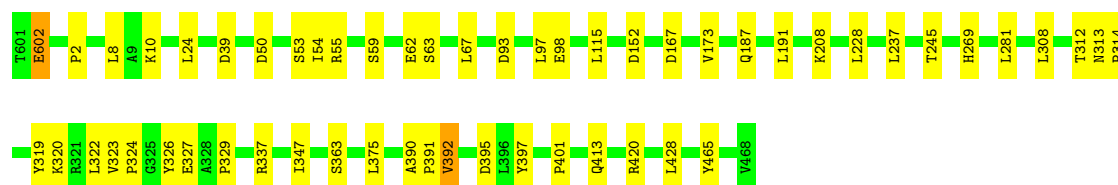
- Molecule 1: glutamine synthetase

Chain 2-T: 88% 11%



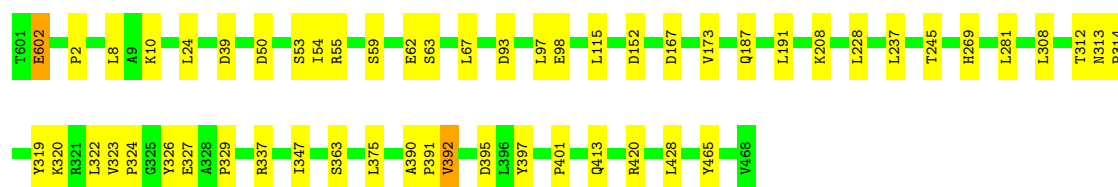
- Molecule 1: glutamine synthetase

Chain 2-U: 88% 11%



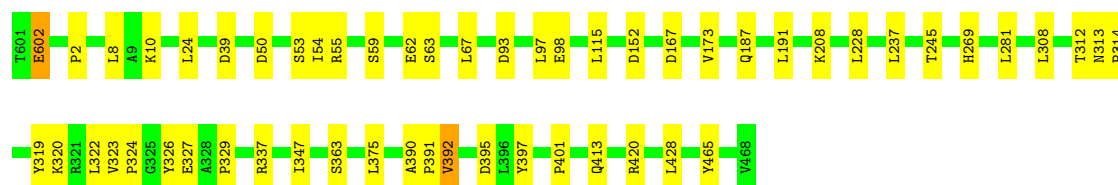
- Molecule 1: glutamine synthetase

Chain 2-V: 88% 11%



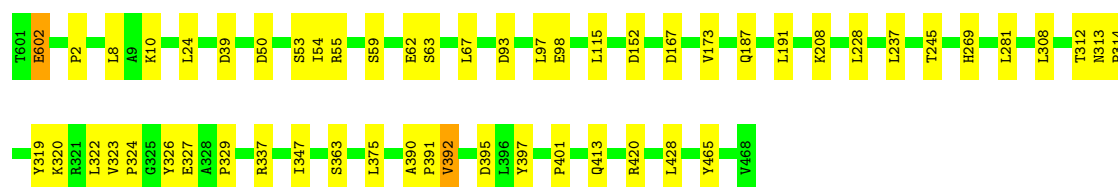
- Molecule 1: glutamine synthetase

Chain 2-W: 88% 11%



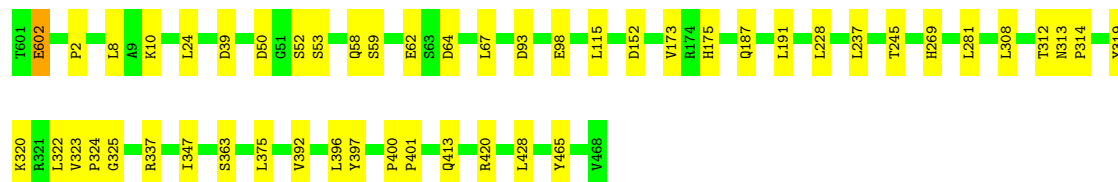
- Molecule 1: glutamine synthetase

Chain 2-X: 88% 11%



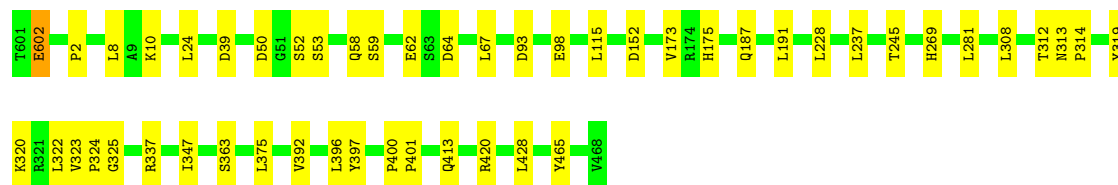
- Molecule 1: glutamine synthetase

Chain 3-A: 90% 10%



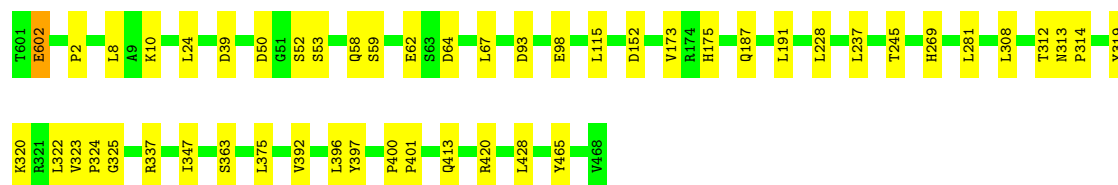
- Molecule 1: glutamine synthetase

Chain 3-B: 90% 10%



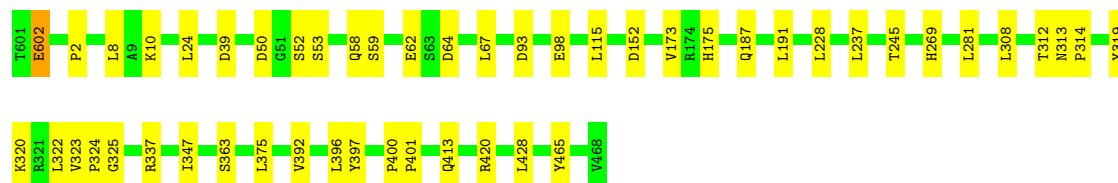
- Molecule 1: glutamine synthetase

Chain 3-C: 90% 10%



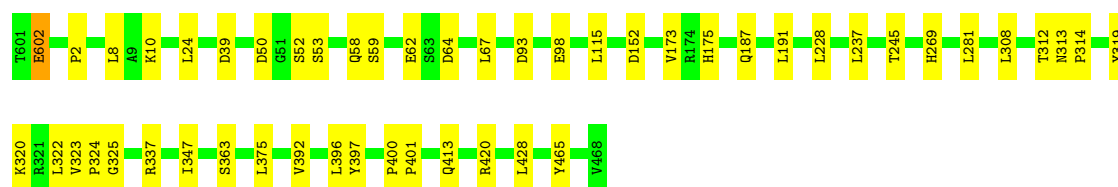
- Molecule 1: glutamine synthetase

Chain 3-D: 90% 10%



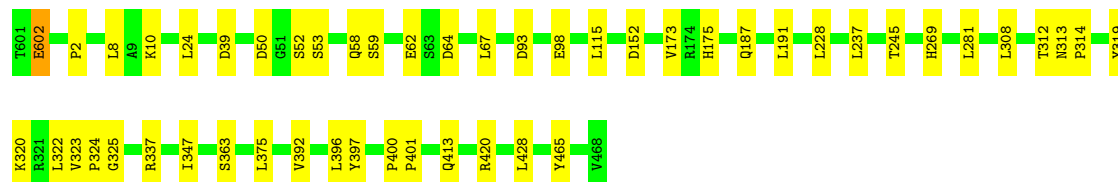
- Molecule 1: glutamine synthetase

Chain 3-E: 90% 10%



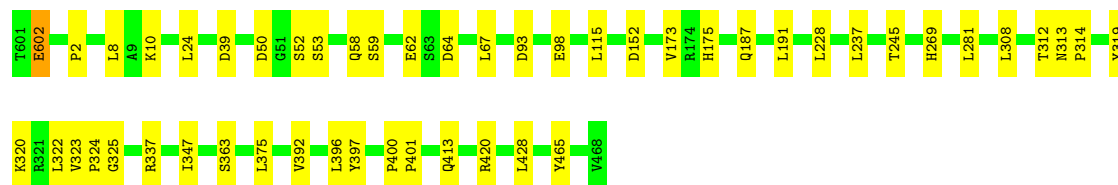
- Molecule 1: glutamine synthetase

Chain 3-F: 90% 10%



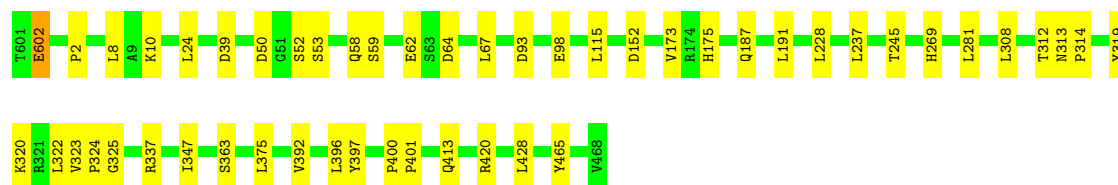
- Molecule 1: glutamine synthetase

Chain 3-G: 90% 10%



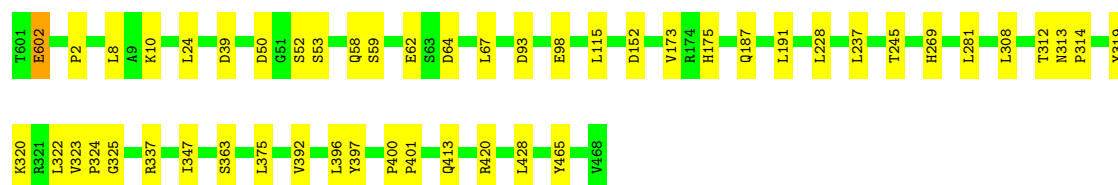
- Molecule 1: glutamine synthetase

Chain 3-H: 90% 10%



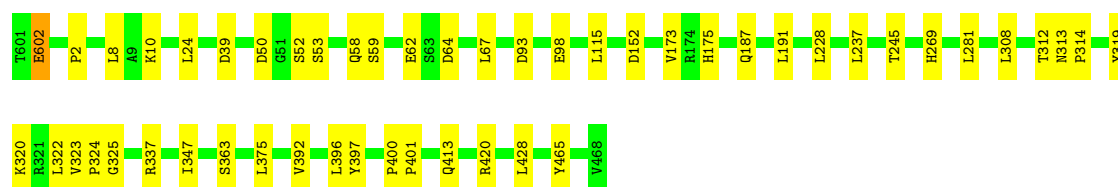
- Molecule 1: glutamine synthetase

Chain 3-I: 90% 10%



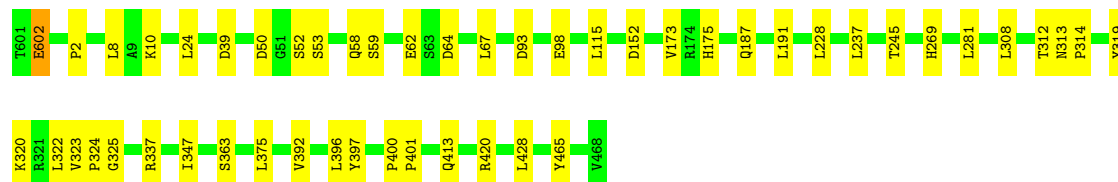
- Molecule 1: glutamine synthetase

Chain 3-J: 90% 10%



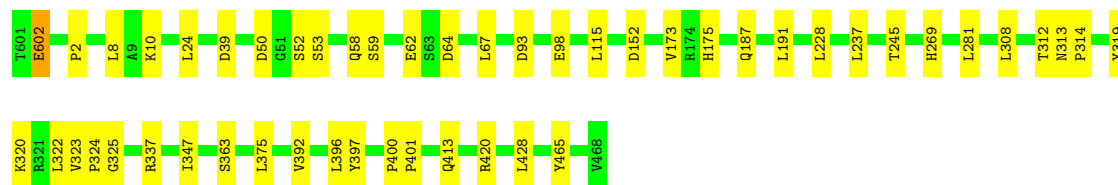
- Molecule 1: glutamine synthetase

Chain 3-K: 90% 10%



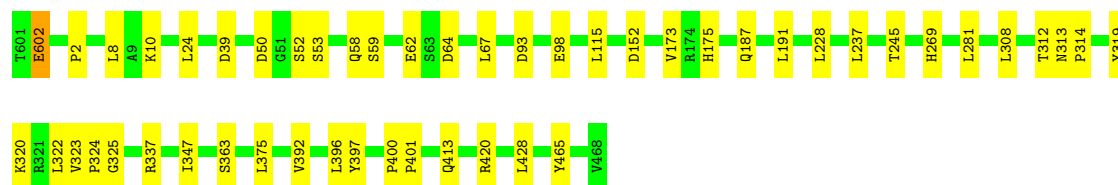
- Molecule 1: glutamine synthetase

Chain 3-L: 90% 10%



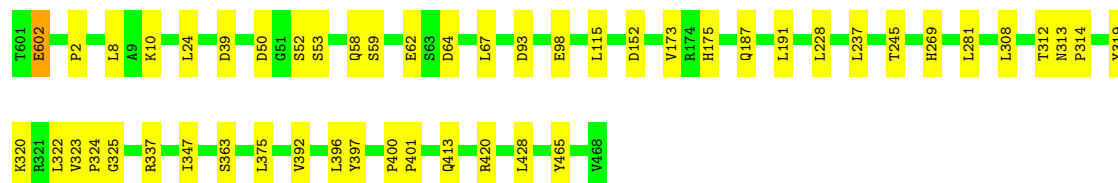
- Molecule 1: glutamine synthetase

Chain 3-M: 90% 10%



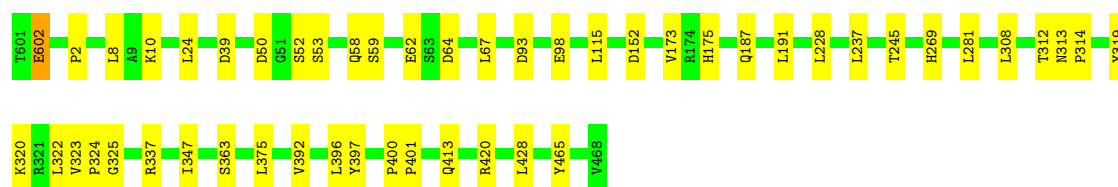
- Molecule 1: glutamine synthetase

Chain 3-N: 90% 10%



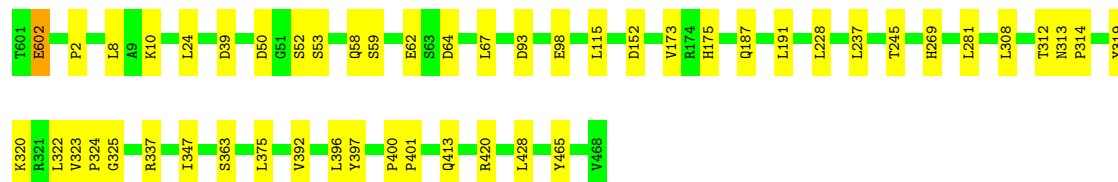
- Molecule 1: glutamine synthetase

Chain 3-O: 90% 10%



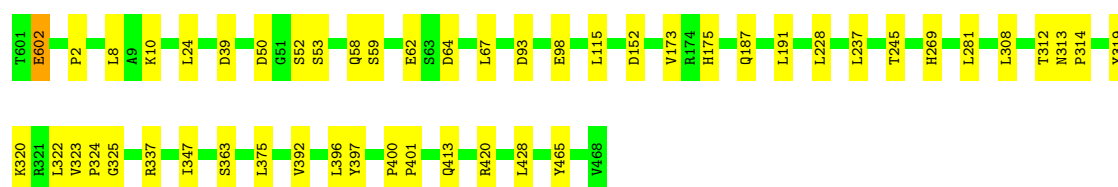
- Molecule 1: glutamine synthetase

Chain 3-P: 90% 10%



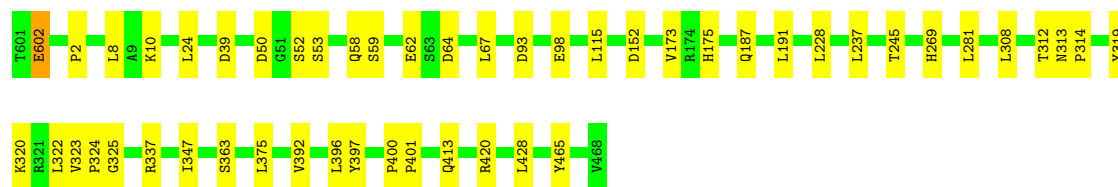
- Molecule 1: glutamine synthetase

Chain 3-Q: 90% 10%



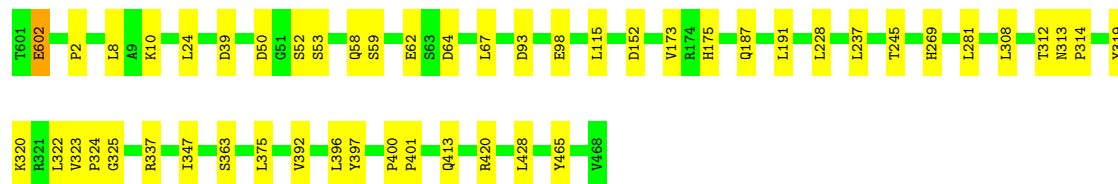
- Molecule 1: glutamine synthetase

Chain 3-R: 90% 10%



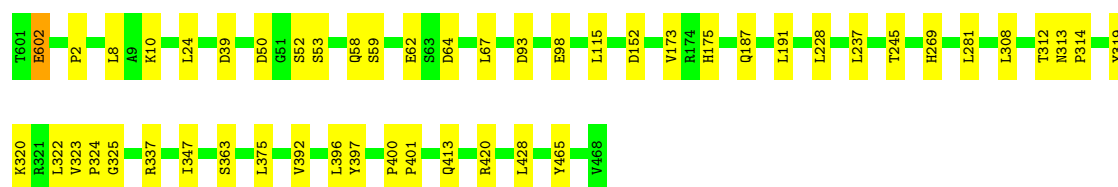
- Molecule 1: glutamine synthetase

Chain 3-S: 90% 10%



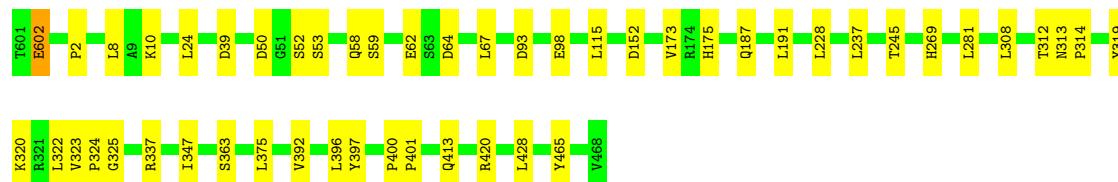
- Molecule 1: glutamine synthetase

Chain 3-T: 90% 10%



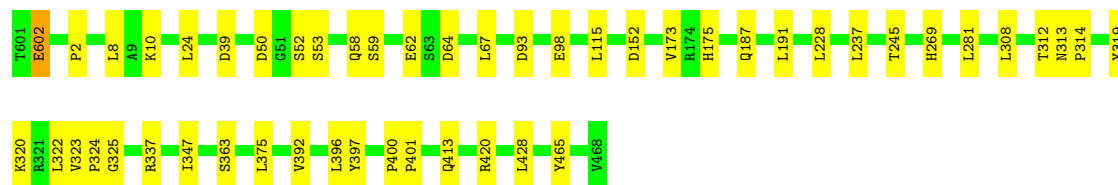
- Molecule 1: glutamine synthetase

Chain 3-U: 90% 10%



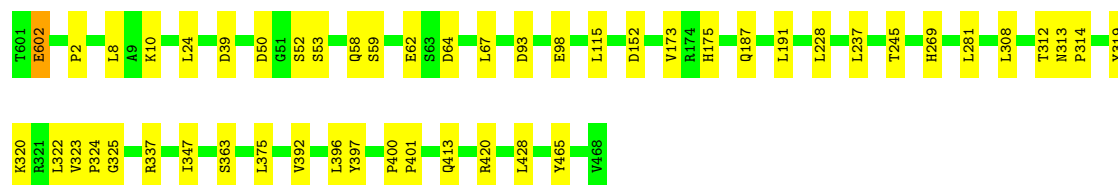
- Molecule 1: glutamine synthetase

Chain 3-V: 90% 10%



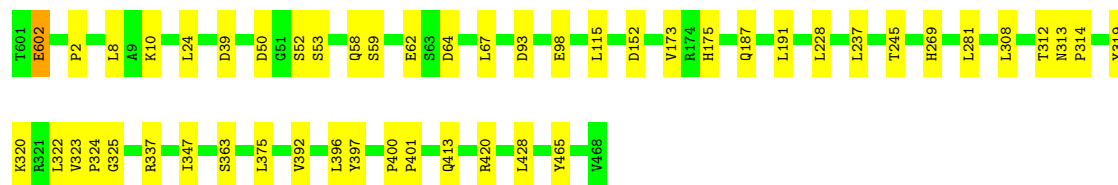
- Molecule 1: glutamine synthetase

Chain 3-W: 90% 10%



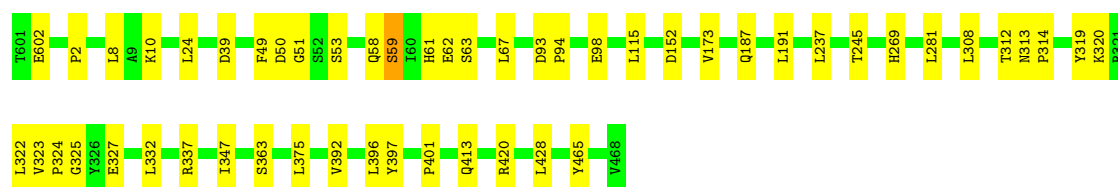
- Molecule 1: glutamine synthetase

Chain 3-X: 90% 10%

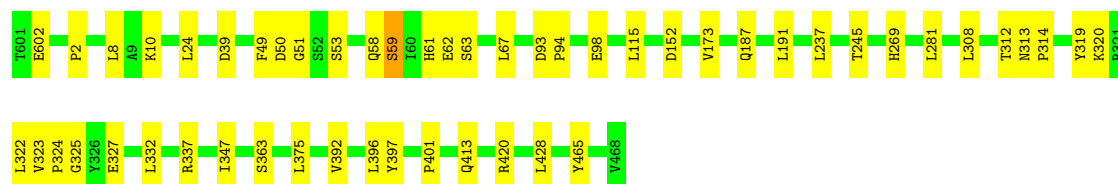


- Molecule 1: glutamine synthetase

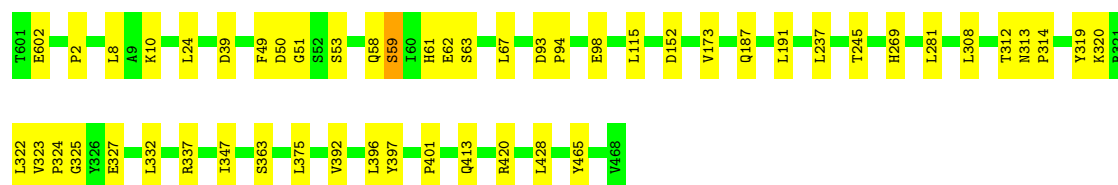
Chain 4-A: 89% 11%



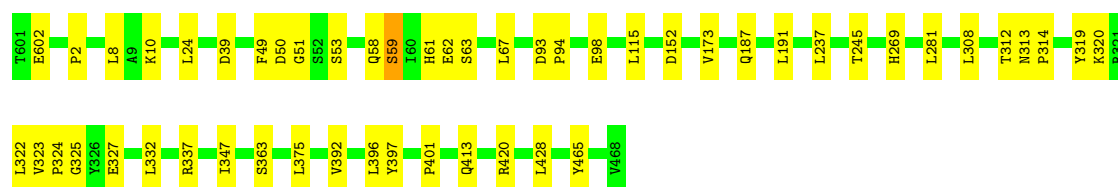
Chain 4-B: 89% 11%



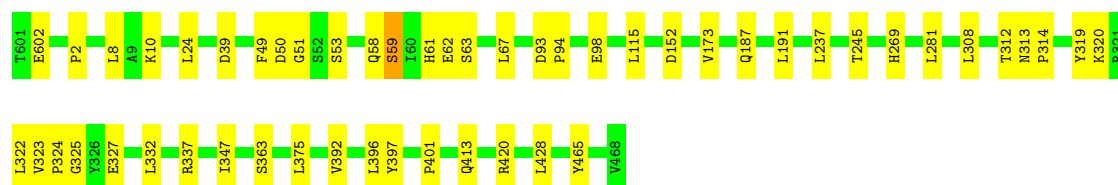
Chain 4-C: 89% 11%



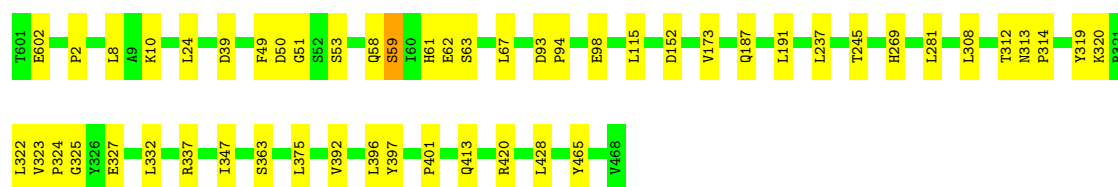
Chain 4-D: 89% 11%



Chain 4-E: 89% 11%

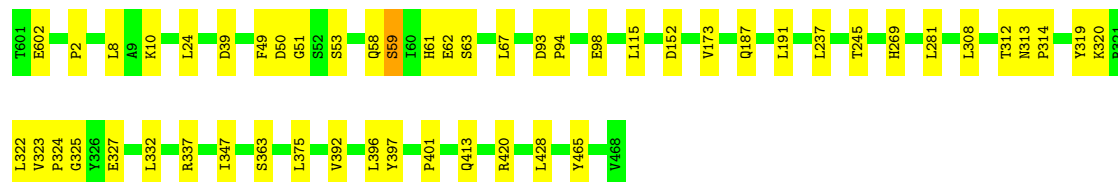


Chain 4-F: 89% 11%



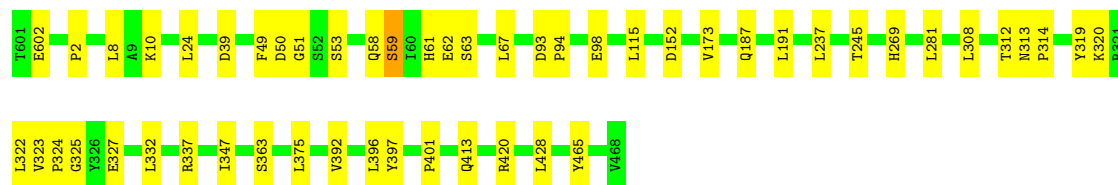
- Molecule 1: glutamine synthetase

Chain 4-G:  89% 11%



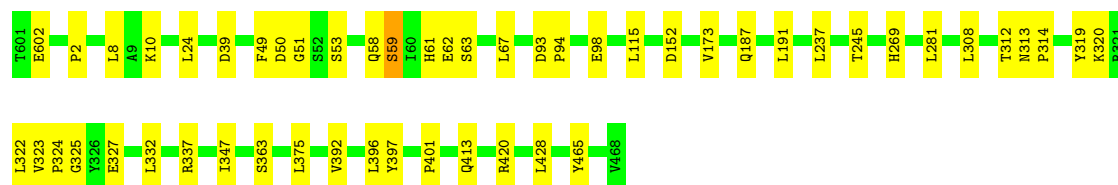
- Molecule 1: glutamine synthetase

Chain 4-H:  89% 11%



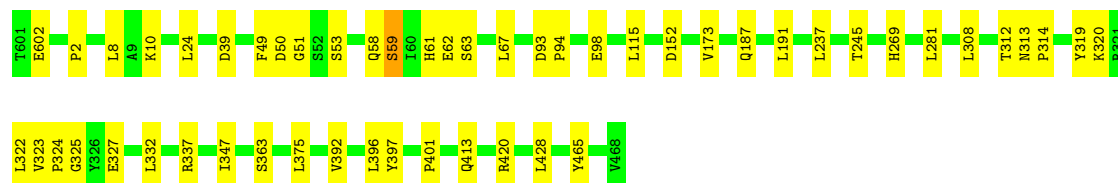
- Molecule 1: glutamine synthetase

Chain 4-I:  89% 11%



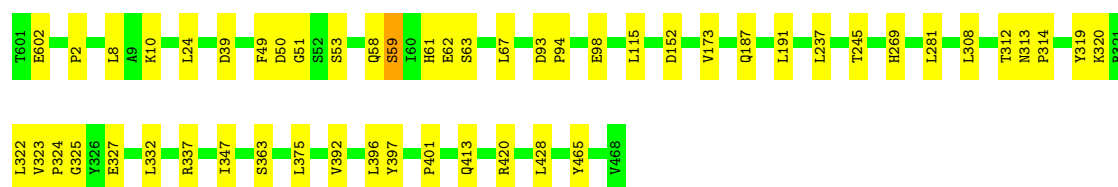
- Molecule 1: glutamine synthetase

Chain 4-J:  89% 11%



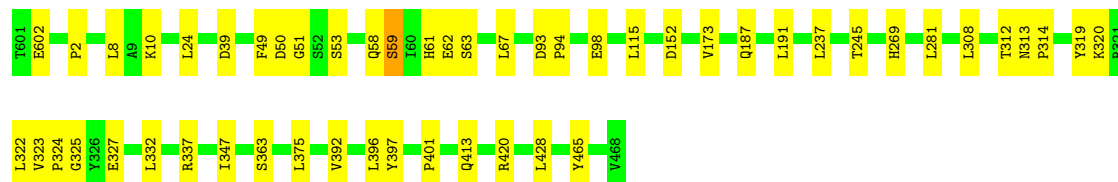
- Molecule 1: glutamine synthetase

Chain 4-K:  89% 11%



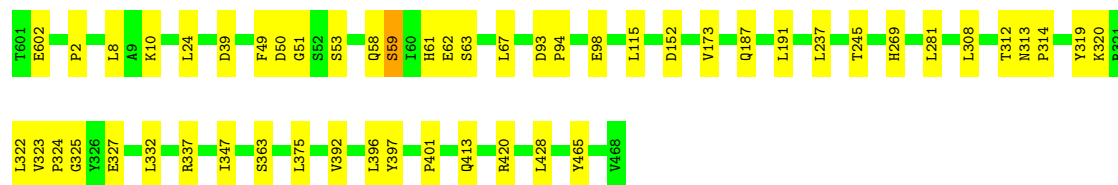
- Molecule 1: glutamine synthetase

Chain 4-L: 89% 11%



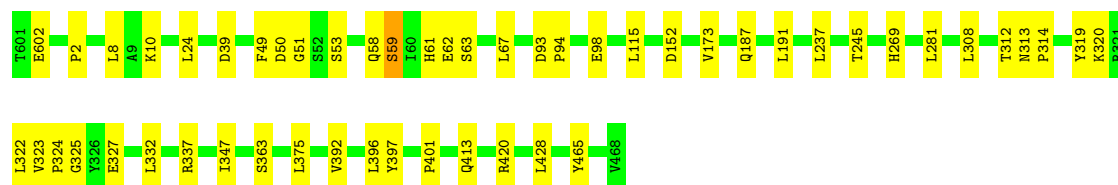
- Molecule 1: glutamine synthetase

Chain 4-M: 89% 11%



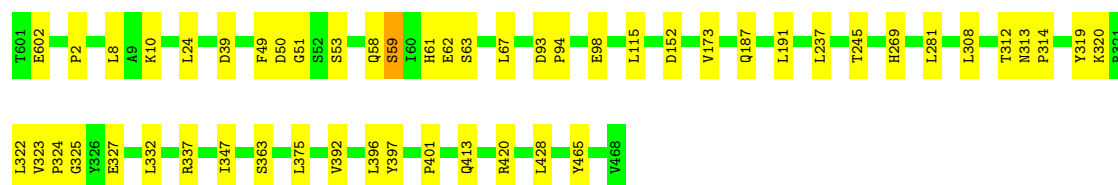
- Molecule 1: glutamine synthetase

Chain 4-N: 89% 11%



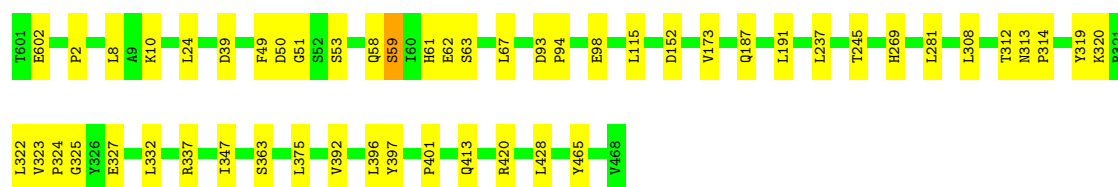
- Molecule 1: glutamine synthetase

Chain 4-O: 89% 11%



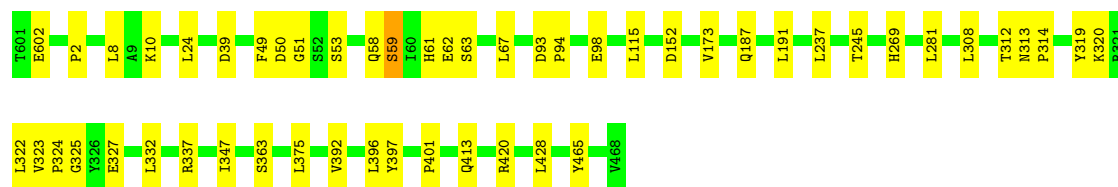
- Molecule 1: glutamine synthetase

Chain 4-P: 89% 11%



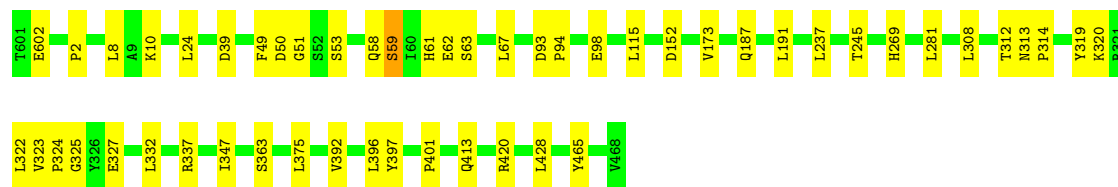
- Molecule 1: glutamine synthetase

Chain 4-Q: 89% 11%



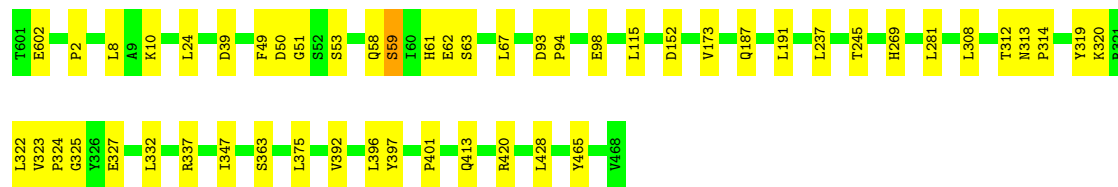
- Molecule 1: glutamine synthetase

Chain 4-R: 89% 11%



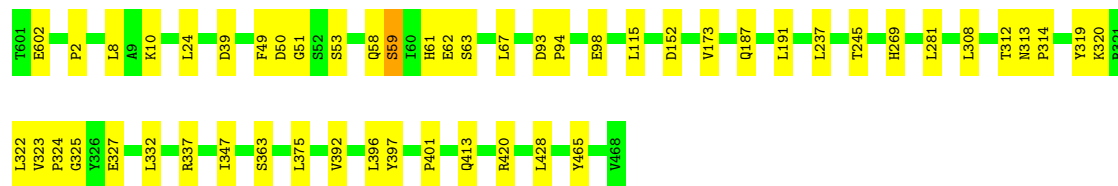
- Molecule 1: glutamine synthetase

Chain 4-S: 89% 11%



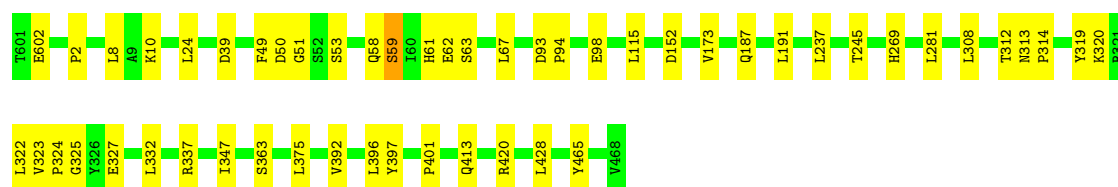
- Molecule 1: glutamine synthetase

Chain 4-T: 89% 11%



- Molecule 1: glutamine synthetase

Chain 4-U: 89% 11%



- Molecule 1: glutamine synthetase



- Molecule 1: glutamine synthetase



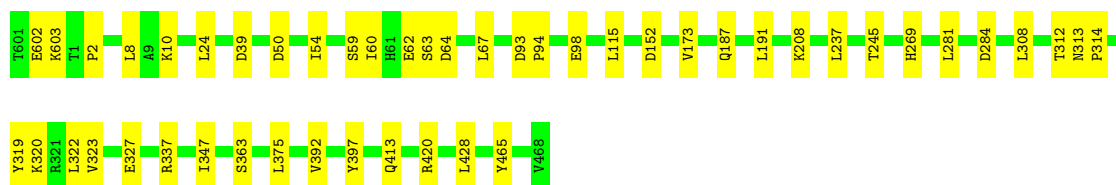
- Molecule 1: glutamine synthetase



- Molecule 1: glutamine synthetase

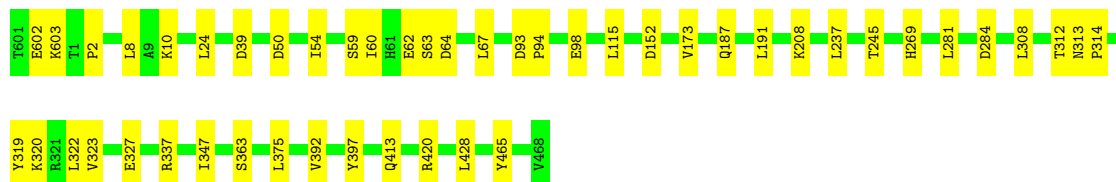


- Molecule 1: glutamine synthetase



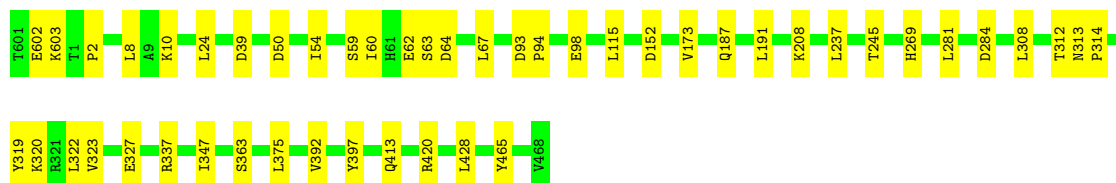
- Molecule 1: glutamine synthetase

Chain 5-C:  90% 10%



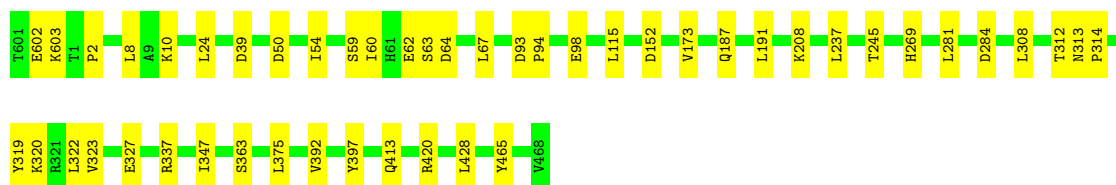
- Molecule 1: glutamine synthetase

Chain 5-D:  90% 10%



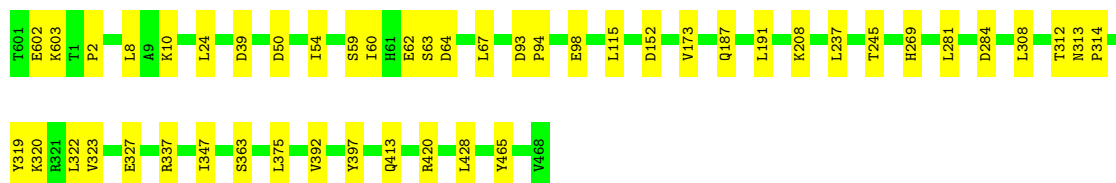
- Molecule 1: glutamine synthetase

Chain 5-E:  90% 10%



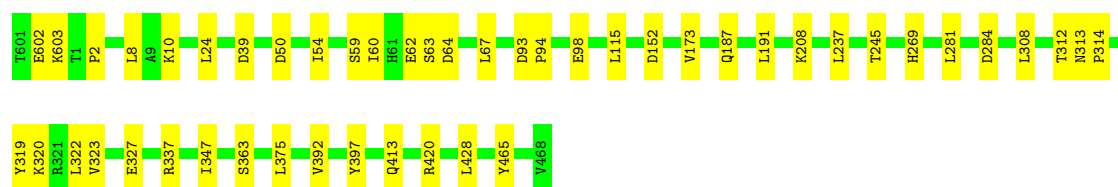
- Molecule 1: glutamine synthetase

Chain 5-F:  90% 10%



- Molecule 1: glutamine synthetase

Chain 5-G:  90% 10%



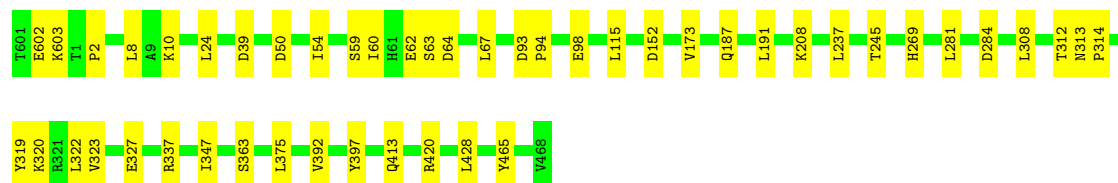
- Molecule 1: glutamine synthetase

Chain 5-H: 90% 10%



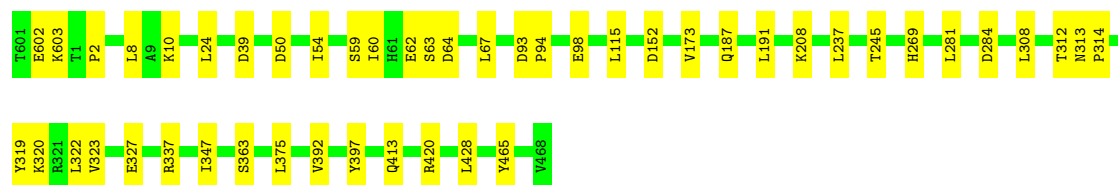
- Molecule 1: glutamine synthetase

Chain 5-I: 90% 10%



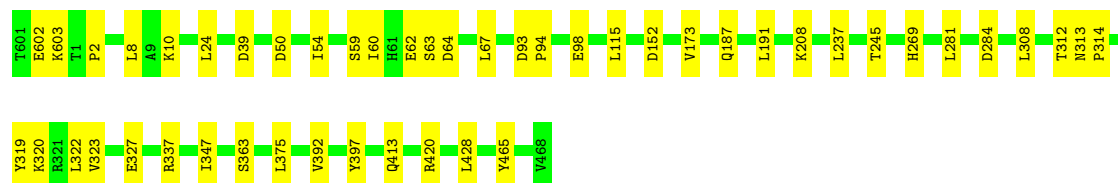
- Molecule 1: glutamine synthetase

Chain 5-J: 90% 10%



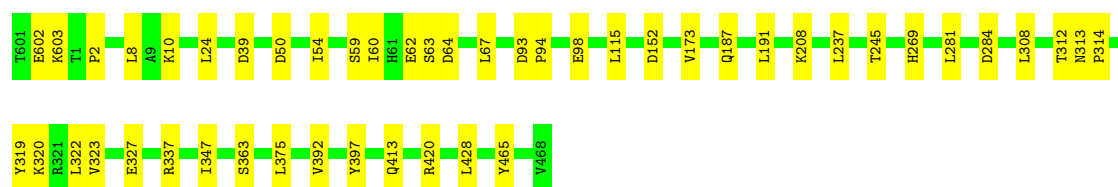
- Molecule 1: glutamine synthetase

Chain 5-K: 90% 10%



- Molecule 1: glutamine synthetase

Chain 5-L: 90% 10%



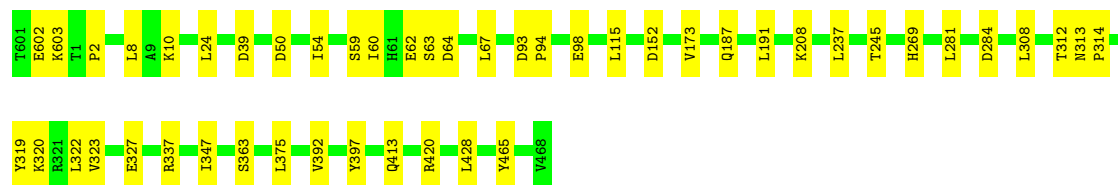
- Molecule 1: glutamine synthetase

Chain 5-M: 90% 10%



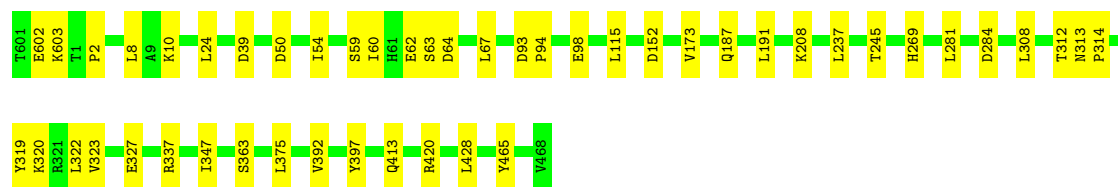
- Molecule 1: glutamine synthetase

Chain 5-N: 90% 10%



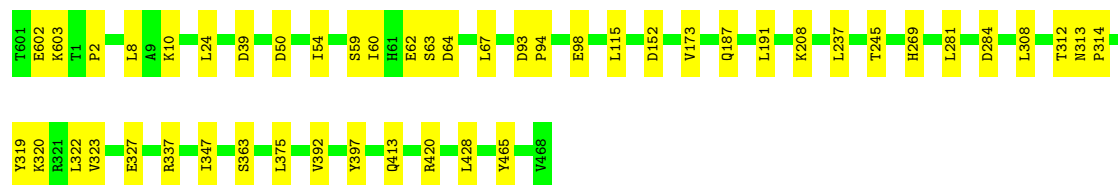
- Molecule 1: glutamine synthetase

Chain 5-O: 90% 10%



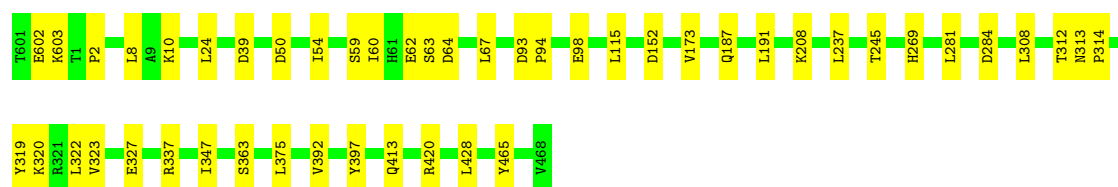
- Molecule 1: glutamine synthetase

Chain 5-P: 90% 10%



- Molecule 1: glutamine synthetase

Chain 5-Q: 90% 10%



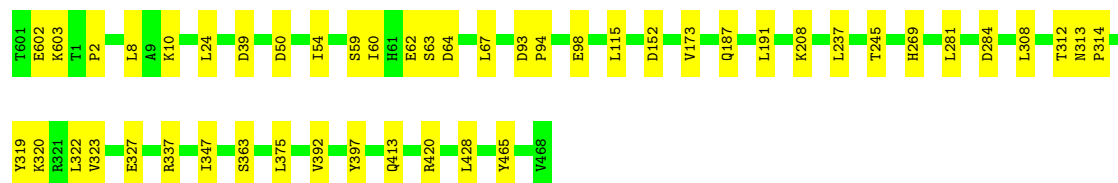
- Molecule 1: glutamine synthetase

Chain 5-R: 90% 10%



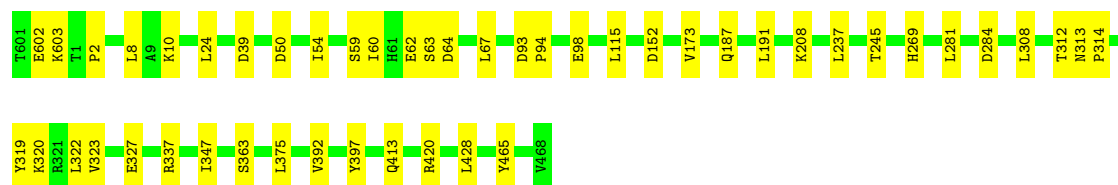
- Molecule 1: glutamine synthetase

Chain 5-S: 90% 10%



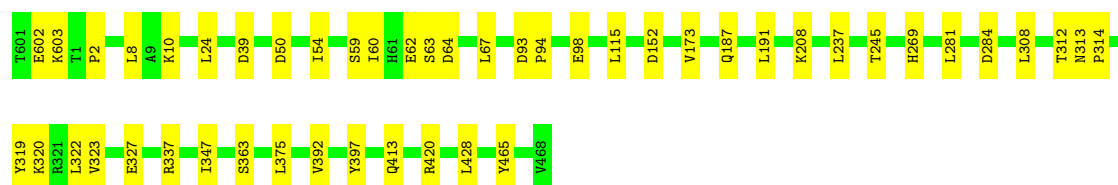
- Molecule 1: glutamine synthetase

Chain 5-T: 90% 10%



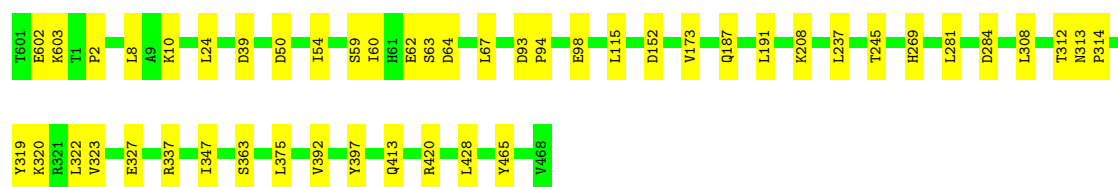
- Molecule 1: glutamine synthetase

Chain 5-U: 90% 10%



- Molecule 1: glutamine synthetase

Chain 5-V: 90% 10%



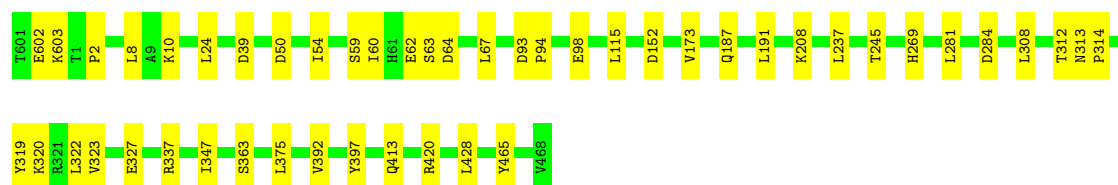
- Molecule 1: glutamine synthetase

Chain 5-W: 90% 10%



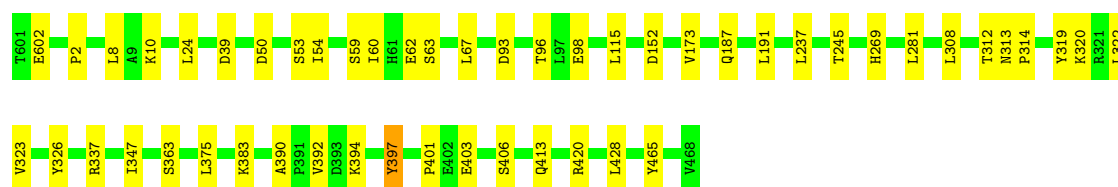
- Molecule 1: glutamine synthetase

Chain 5-X: 90% 10%



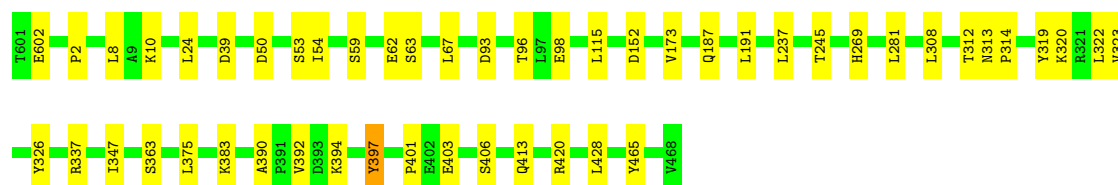
- Molecule 1: glutamine synthetase

Chain 6-A: 89% 10%



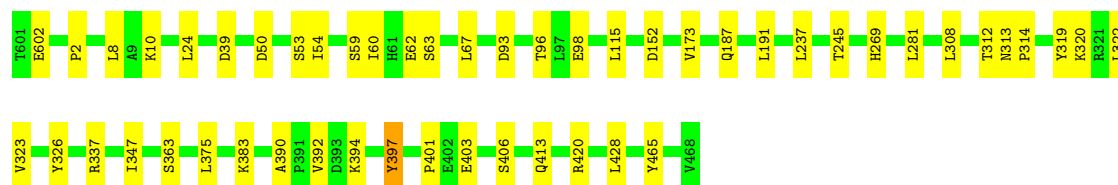
- Molecule 1: glutamine synthetase

Chain 6-B: 90% 10%



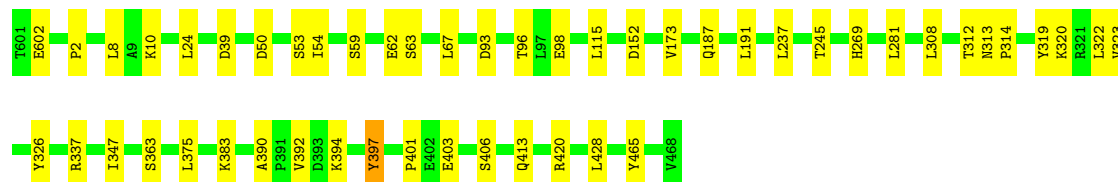
- Molecule 1: glutamine synthetase

Chain 6-C: 89% 10%



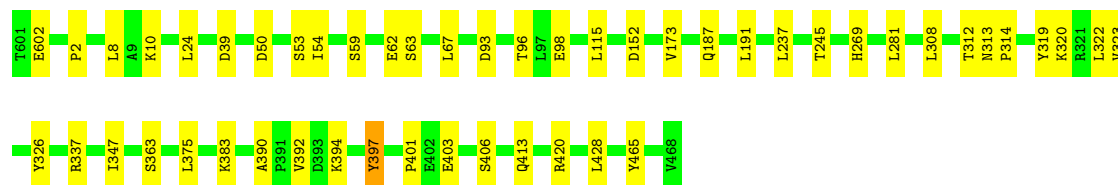
- Molecule 1: glutamine synthetase

Chain 6-D: 90% 10%



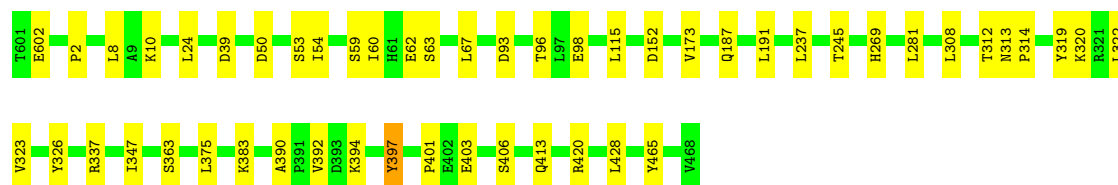
- Molecule 1: glutamine synthetase

Chain 6-E: 90% 10%



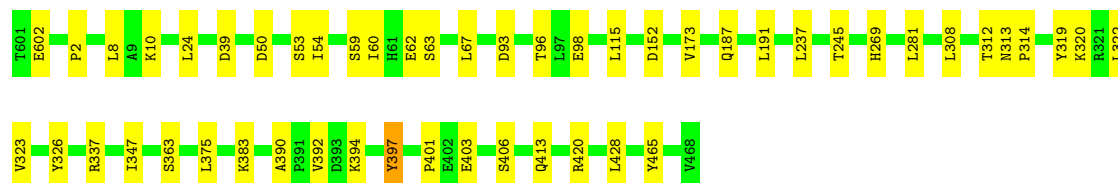
- Molecule 1: glutamine synthetase

Chain 6-F: 89% 10%



- Molecule 1: glutamine synthetase

Chain 6-G: 89% 10%



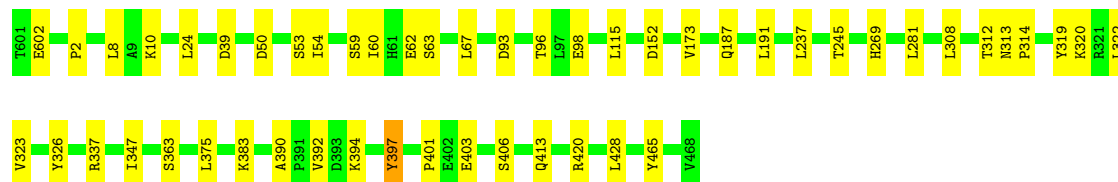
- Molecule 1: glutamine synthetase

Chain 6-H: 90% 10%



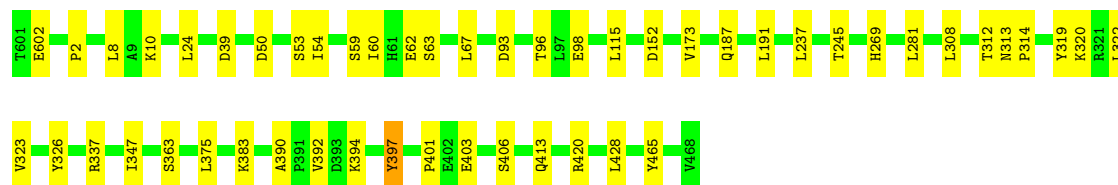
- Molecule 1: glutamine synthetase

Chain 6-I: 89% 10%



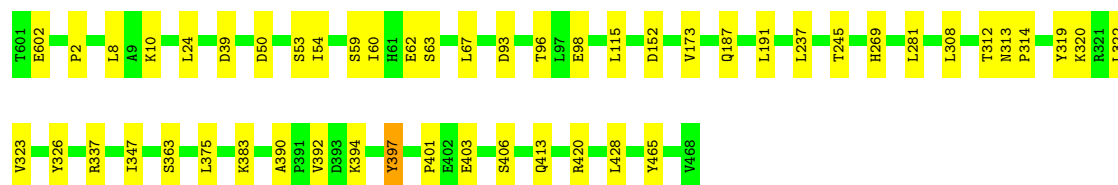
- Molecule 1: glutamine synthetase

Chain 6-J: 89% 10%



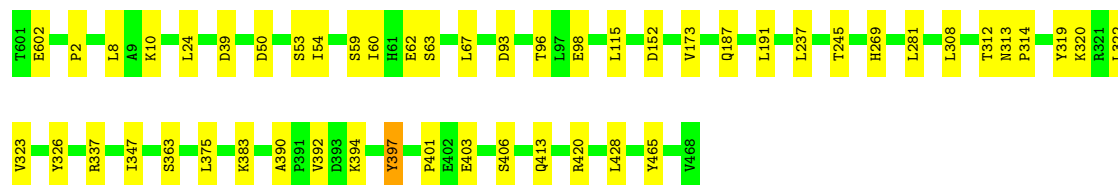
- Molecule 1: glutamine synthetase

Chain 6-K: 89% 10%



- Molecule 1: glutamine synthetase

Chain 6-L: 89% 10%



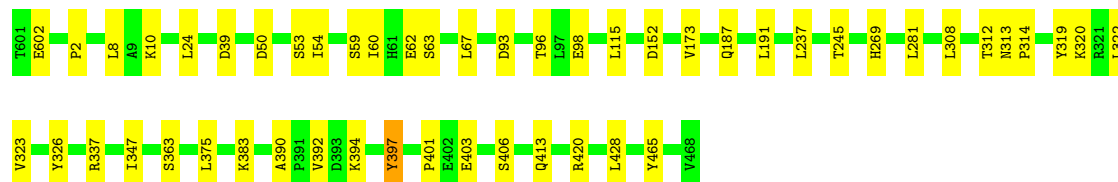
- Molecule 1: glutamine synthetase

Chain 6-M: 90% 10%



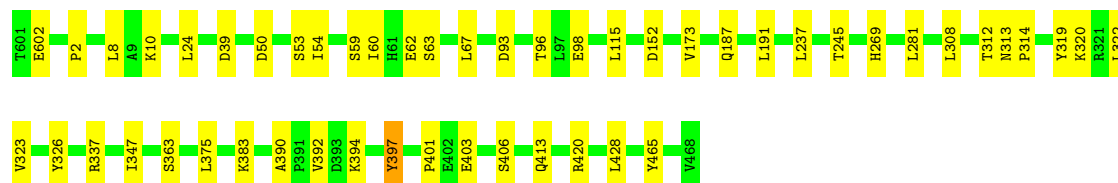
- Molecule 1: glutamine synthetase

Chain 6-N: 89% 10%



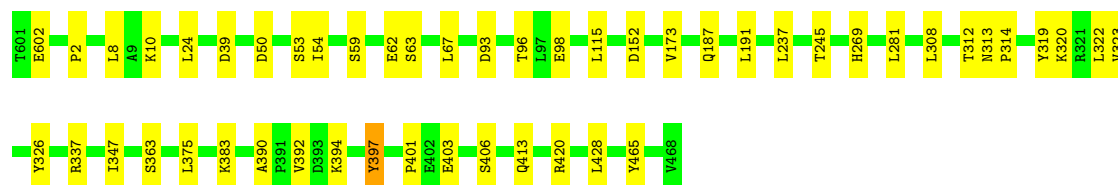
- Molecule 1: glutamine synthetase

Chain 6-O: 89% 10%



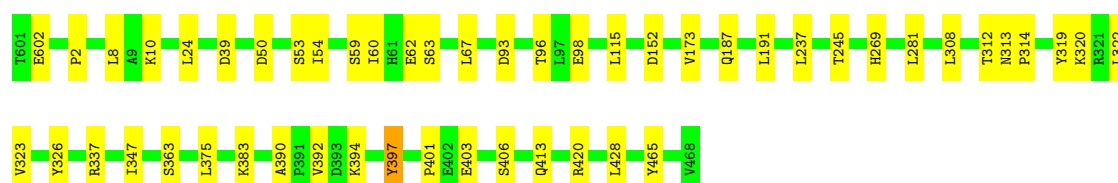
- Molecule 1: glutamine synthetase

Chain 6-P: 90% 10%



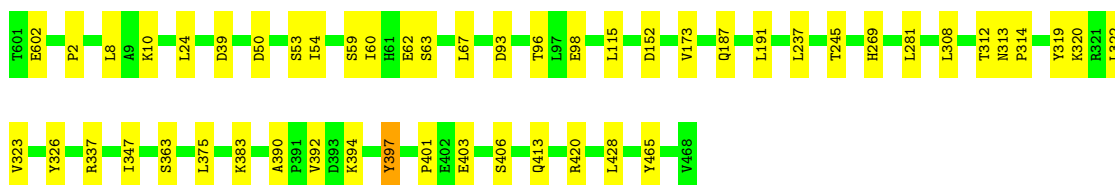
- Molecule 1: glutamine synthetase

Chain 6-Q: 89% 10%



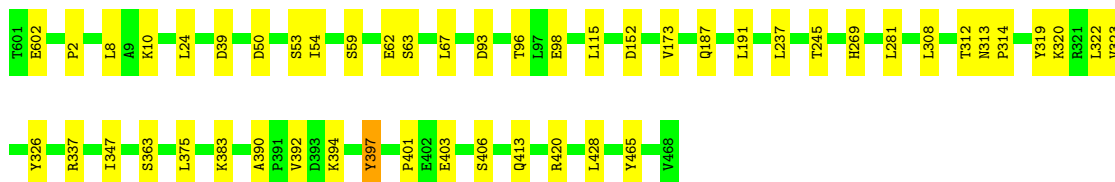
- Molecule 1: glutamine synthetase

Chain 6-R: 89% 10%



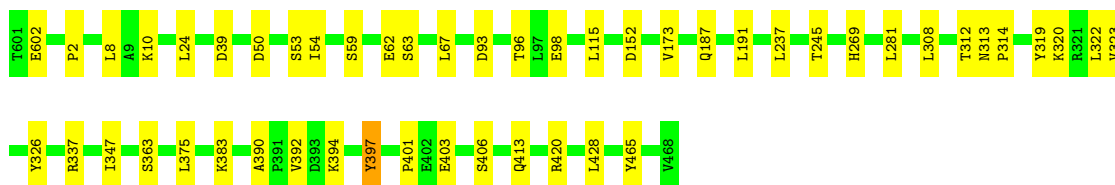
- Molecule 1: glutamine synthetase

Chain 6-S: 90% 10%



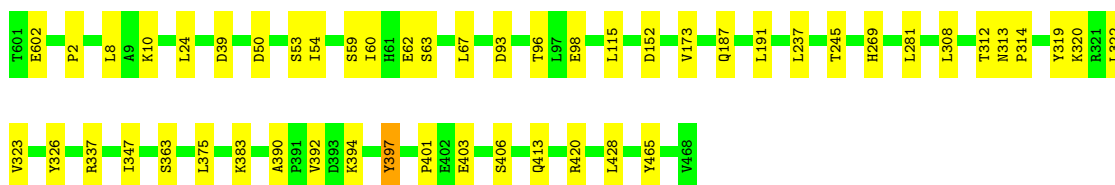
- Molecule 1: glutamine synthetase

Chain 6-T: 90% 10%



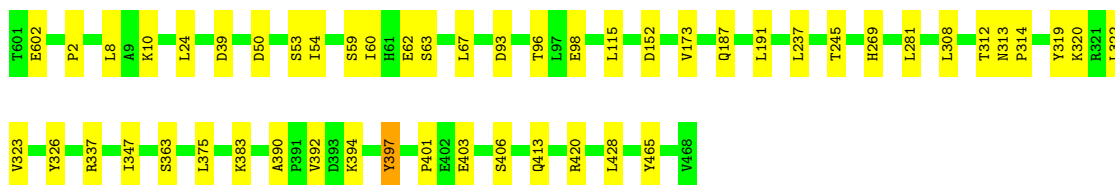
- Molecule 1: glutamine synthetase

Chain 6-U: 89% 10%



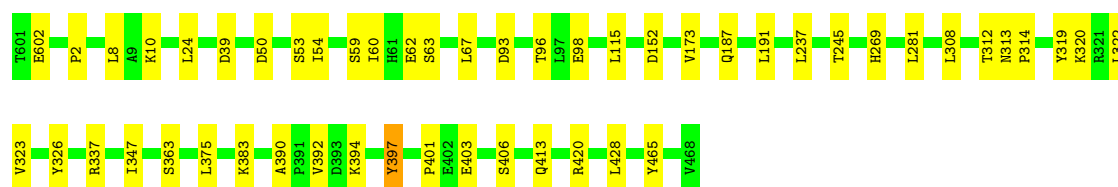
- Molecule 1: glutamine synthetase

Chain 6-V: 89% 10%



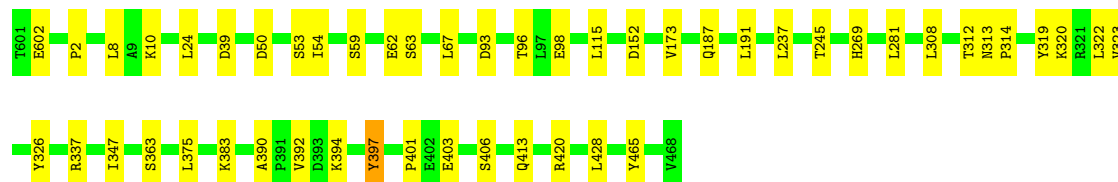
- Molecule 1: glutamine synthetase

Chain 6-W: 89% 10%



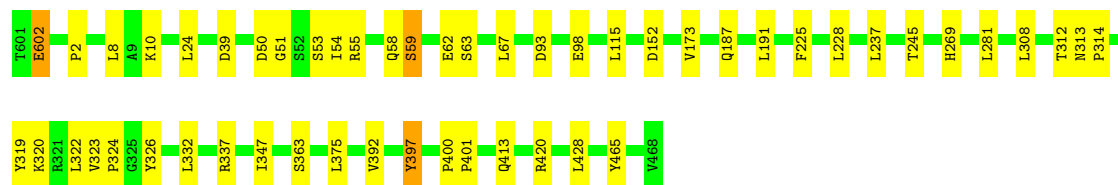
- Molecule 1: glutamine synthetase

Chain 6-X: 90% 10%



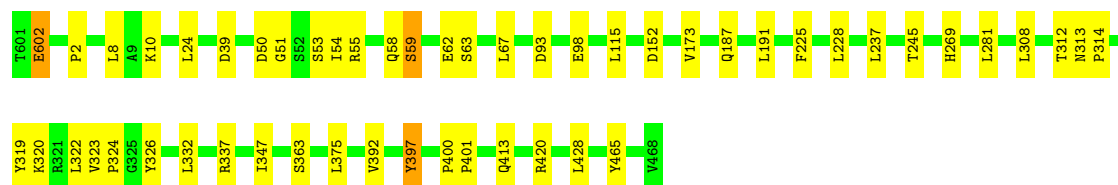
- Molecule 1: glutamine synthetase

Chain 7-A: 89% 10%



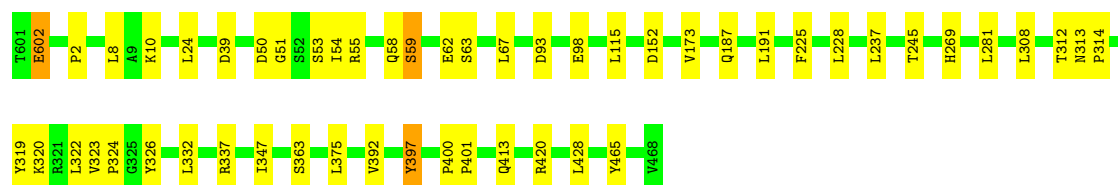
- Molecule 1: glutamine synthetase

Chain 7-B: 89% 10%



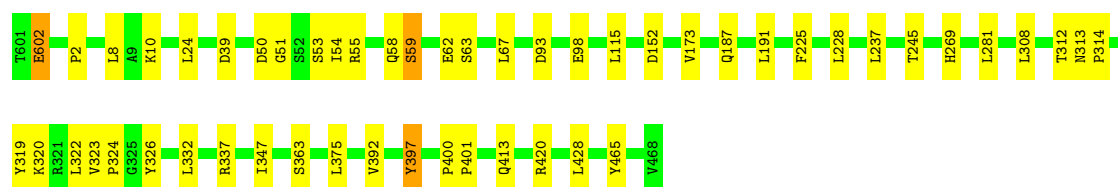
- Molecule 1: glutamine synthetase

Chain 7-C: 89% 10%



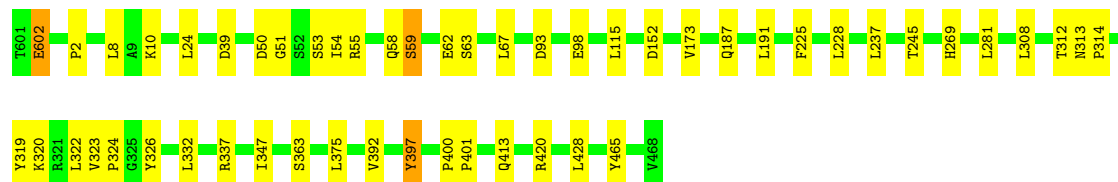
- Molecule 1: glutamine synthetase

Chain 7-D: 89% 10%



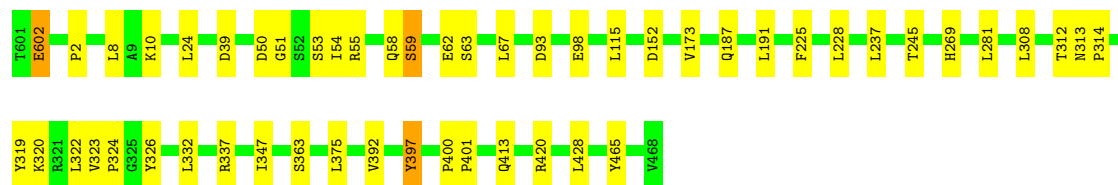
- Molecule 1: glutamine synthetase

Chain 7-E: 89% 10%



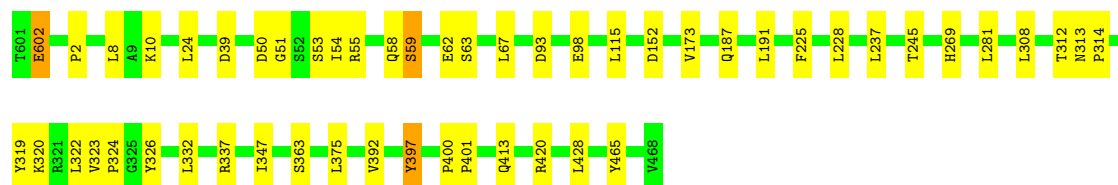
- Molecule 1: glutamine synthetase

Chain 7-F: 89% 10%



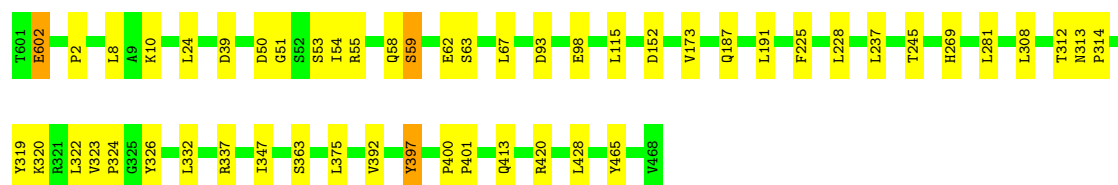
- Molecule 1: glutamine synthetase

Chain 7-G: 89% 10%



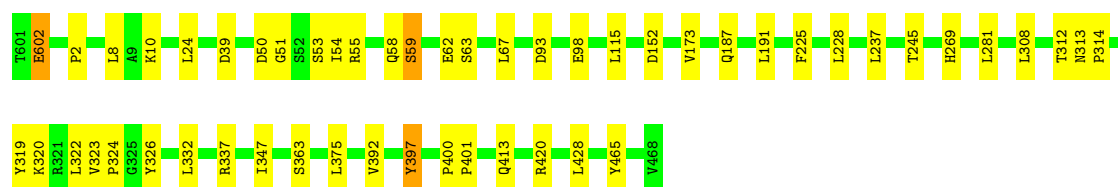
- Molecule 1: glutamine synthetase

Chain 7-H: 89% 10%



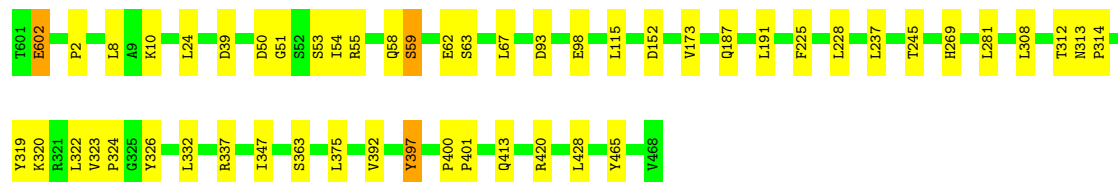
- Molecule 1: glutamine synthetase

Chain 7-I: 89% 10%



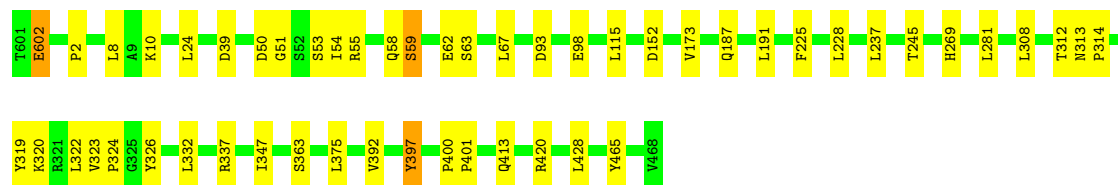
- Molecule 1: glutamine synthetase

Chain 7-J: 89% 10% .



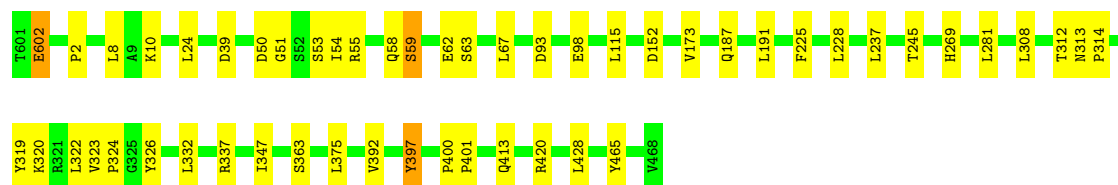
- Molecule 1: glutamine synthetase

Chain 7-K: 89% 10% .



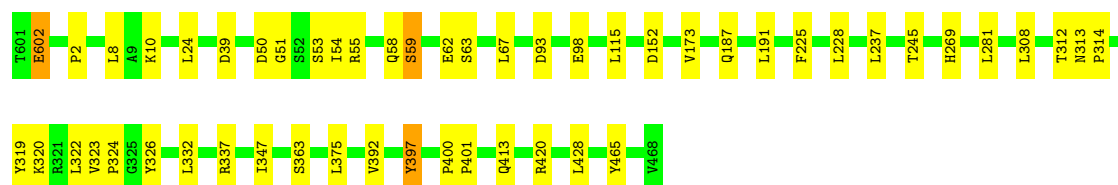
- Molecule 1: glutamine synthetase

Chain 7-L: 89% 10% .



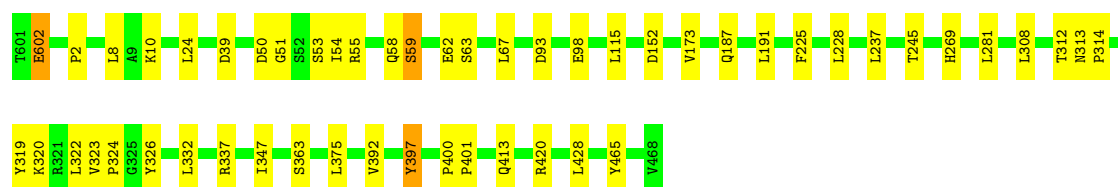
- Molecule 1: glutamine synthetase

Chain 7-M: 89% 10% .



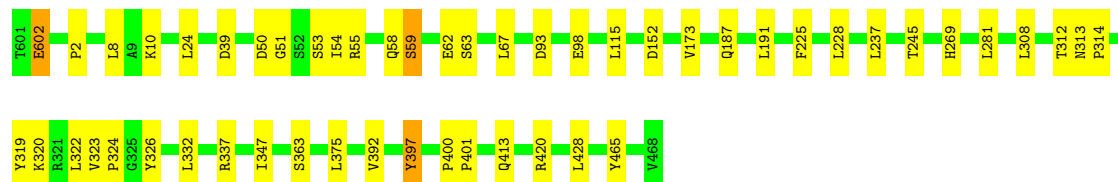
- Molecule 1: glutamine synthetase

Chain 7-N: 89% 10% .



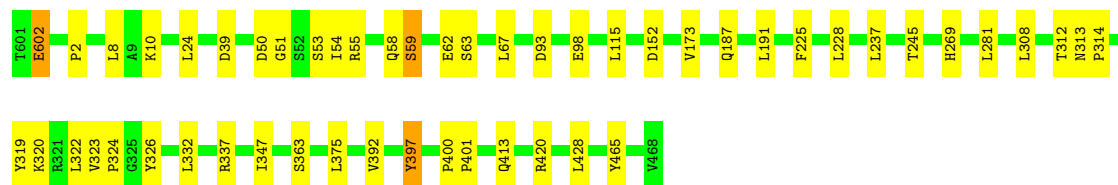
- Molecule 1: glutamine synthetase

Chain 7-O:
89% 10%



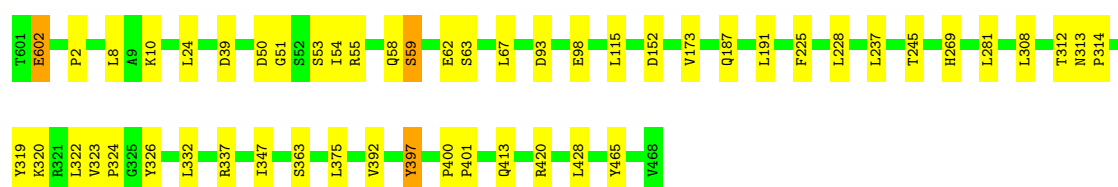
- Molecule 1: glutamine synthetase

Chain 7-P:
89% 10%



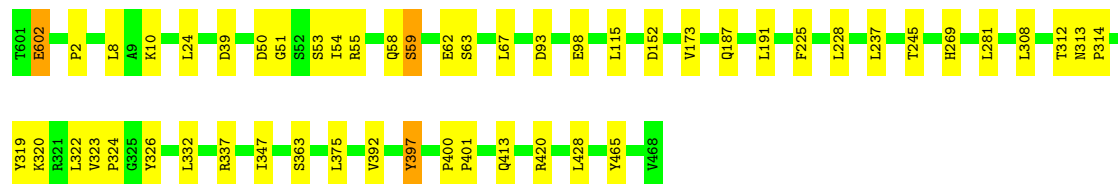
- Molecule 1: glutamine synthetase

Chain 7-Q:
89% 10%



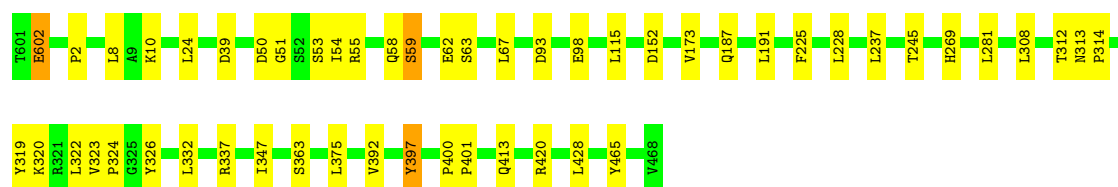
- Molecule 1: glutamine synthetase

Chain 7-R:
89% 10%



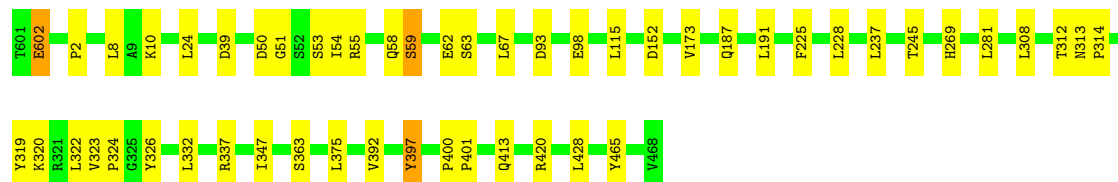
- Molecule 1: glutamine synthetase

Chain 7-S:
89% 10%



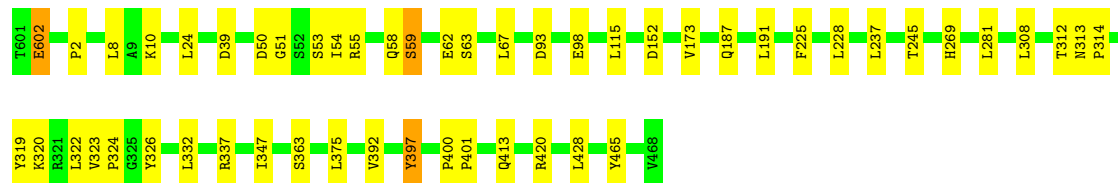
- Molecule 1: glutamine synthetase

Chain 7-T: 89% 10% .



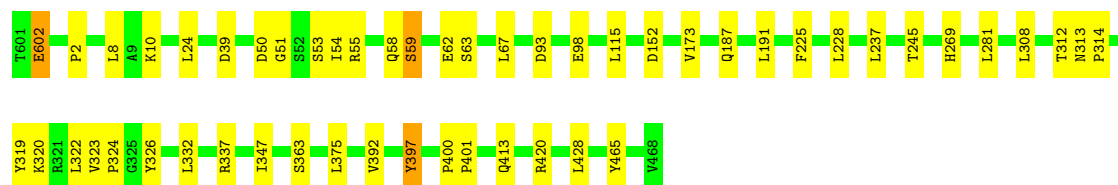
- Molecule 1: glutamine synthetase

Chain 7-U: 89% 10% .



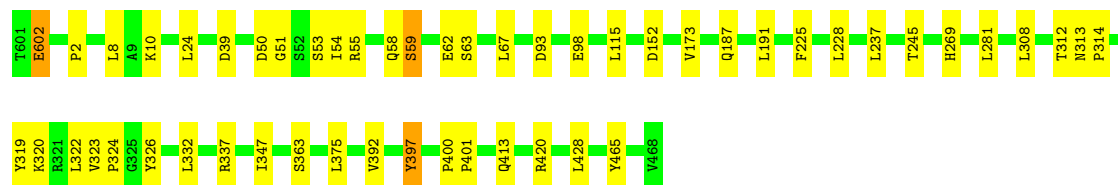
- Molecule 1: glutamine synthetase

Chain 7-V: 89% 10% .



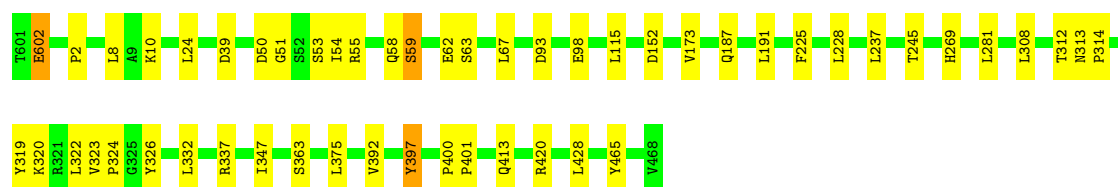
- Molecule 1: glutamine synthetase

Chain 7-W: 89% 10% .



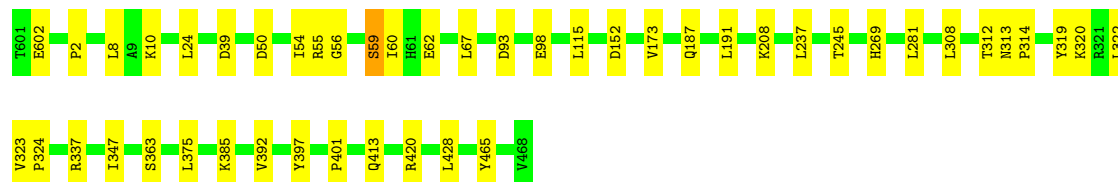
- Molecule 1: glutamine synthetase

Chain 7-X: 89% 10% .



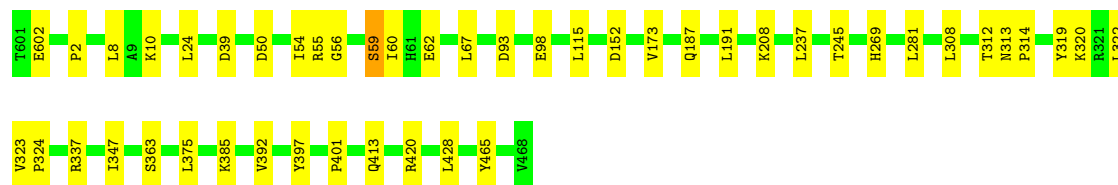
- Molecule 1: glutamine synthetase

Chain 8-A: 90% 10%



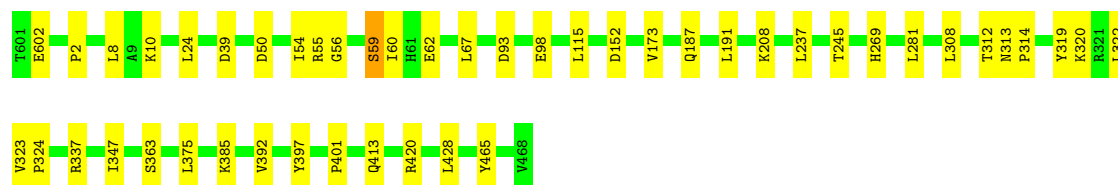
- Molecule 1: glutamine synthetase

Chain 8-B: 90% 10%



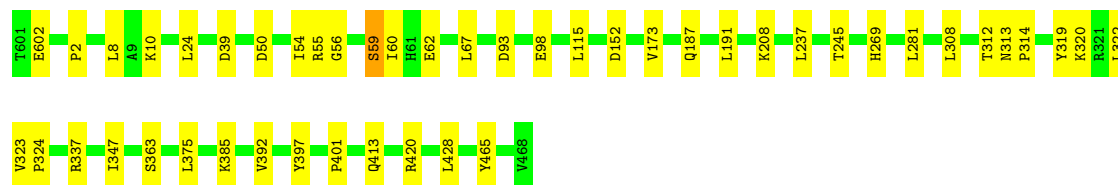
- Molecule 1: glutamine synthetase

Chain 8-C: 90% 10%



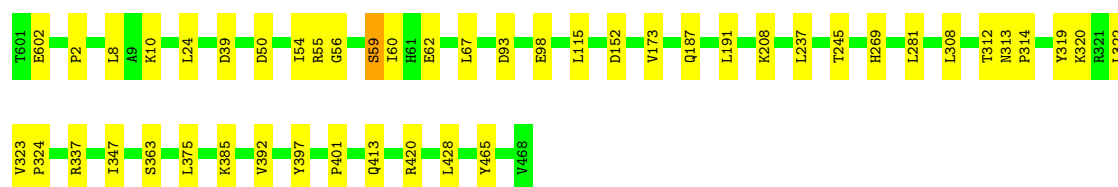
- Molecule 1: glutamine synthetase

Chain 8-D: 90% 10%



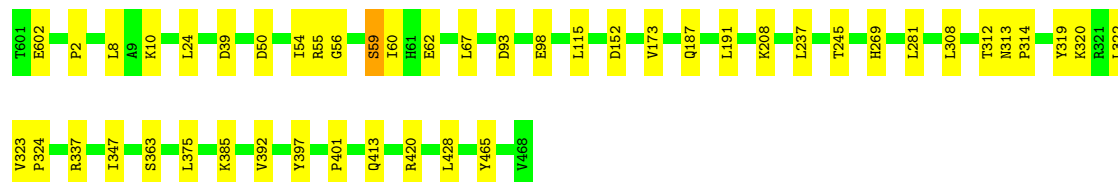
- Molecule 1: glutamine synthetase

Chain 8-E: 90% 10%



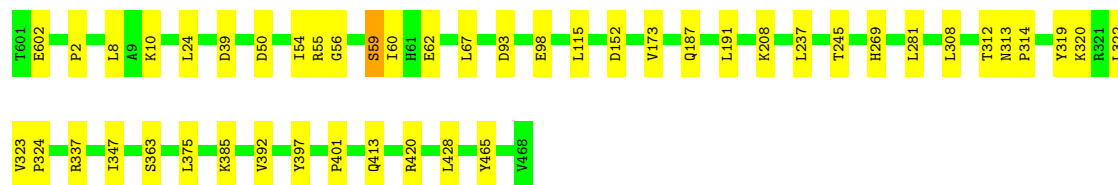
- Molecule 1: glutamine synthetase

Chain 8-F: 90% 10%



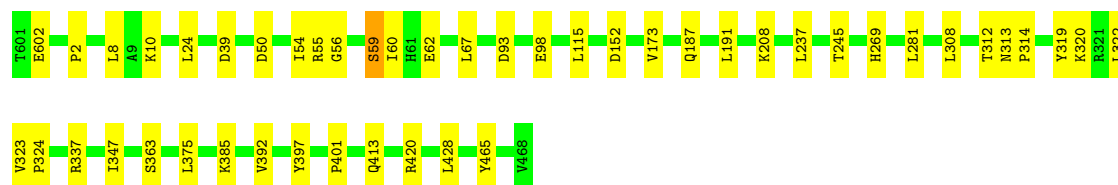
- Molecule 1: glutamine synthetase

Chain 8-G: 90% 10%



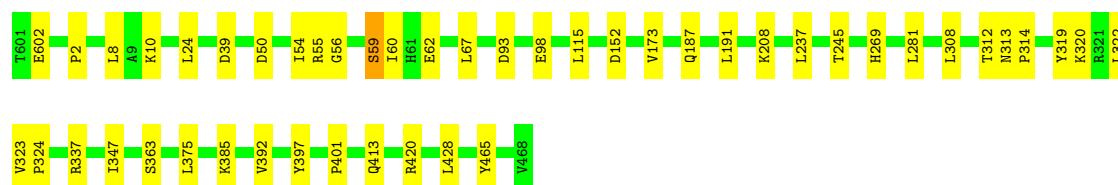
- Molecule 1: glutamine synthetase

Chain 8-H: 90% 10%



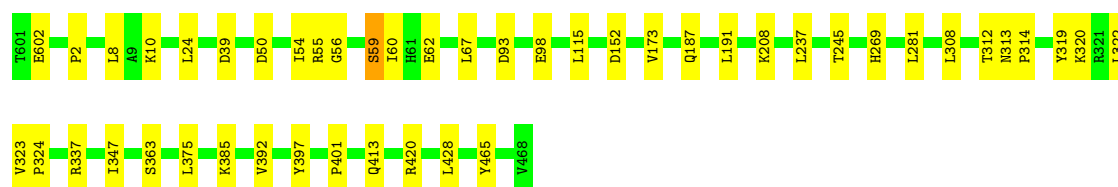
- Molecule 1: glutamine synthetase

Chain 8-I: 90% 10%



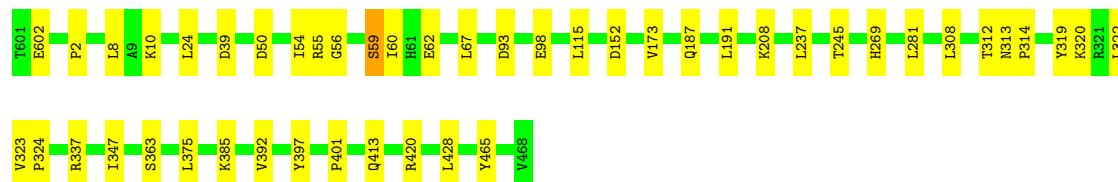
- Molecule 1: glutamine synthetase

Chain 8-J: 90% 10%



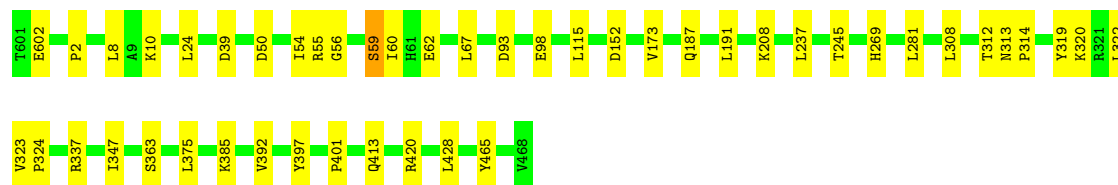
- Molecule 1: glutamine synthetase

Chain 8-K: 90% 10%



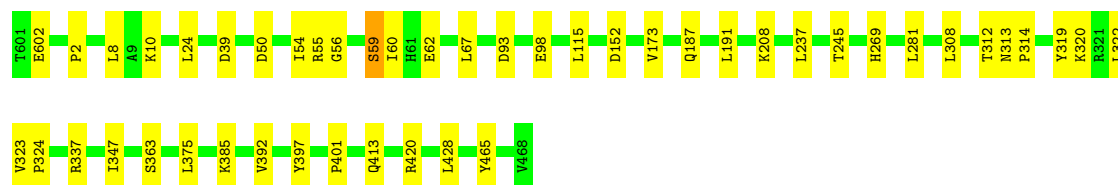
- Molecule 1: glutamine synthetase

Chain 8-L: 90% 10%



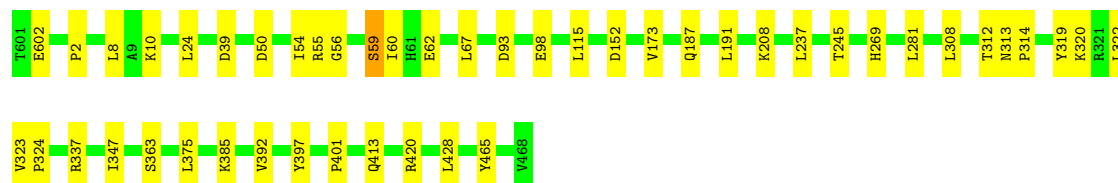
- Molecule 1: glutamine synthetase

Chain 8-M: 90% 10%



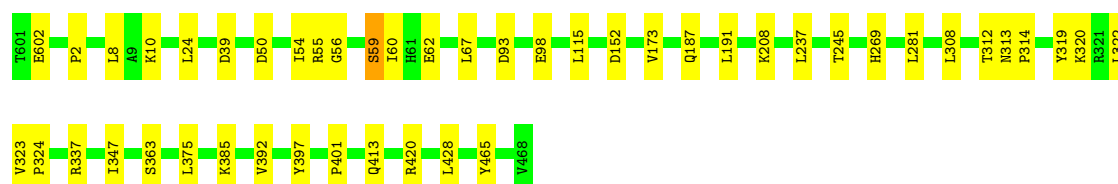
- Molecule 1: glutamine synthetase

Chain 8-N: 90% 10%



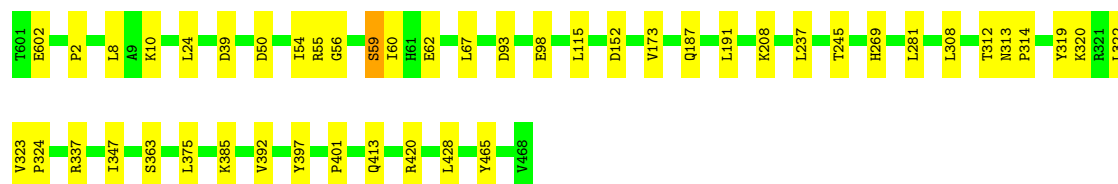
- Molecule 1: glutamine synthetase

Chain 8-O: 90% 10%



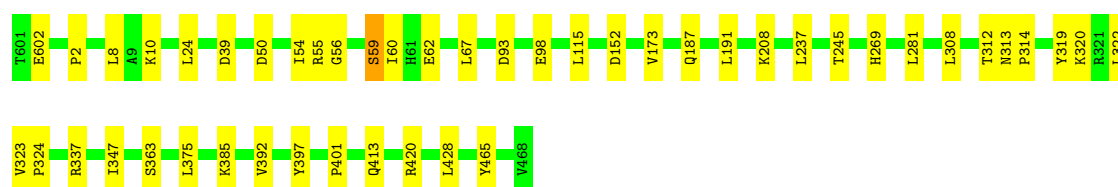
- Molecule 1: glutamine synthetase

Chain 8-P: 90% 10%



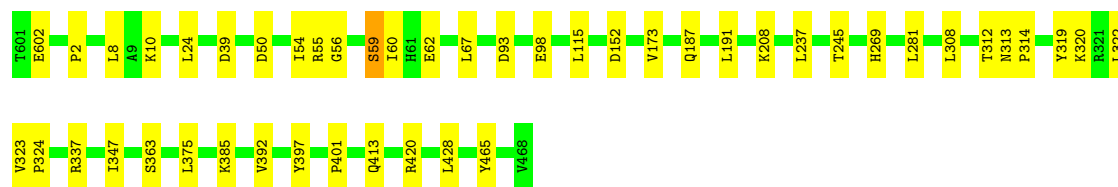
- Molecule 1: glutamine synthetase

Chain 8-Q: 90% 10%



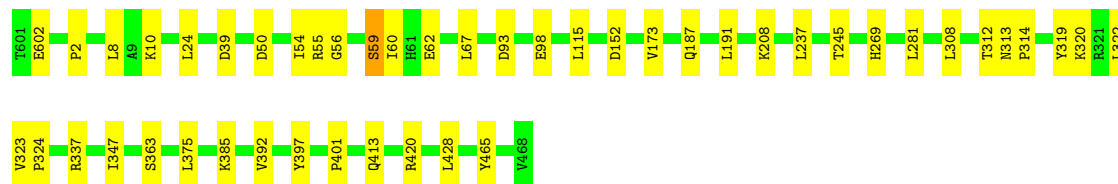
- Molecule 1: glutamine synthetase

Chain 8-R: 90% 10%



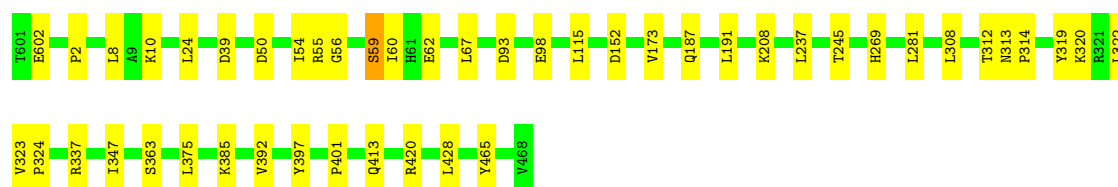
- Molecule 1: glutamine synthetase

Chain 8-S: 90% 10%



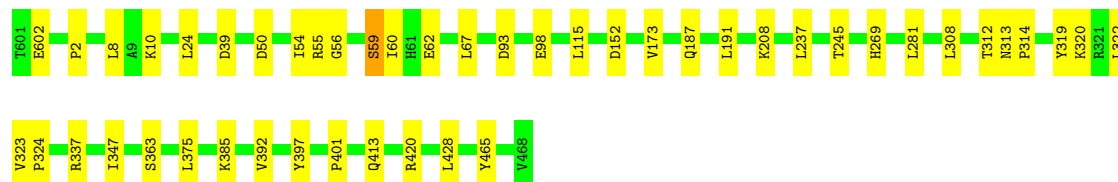
- Molecule 1: glutamine synthetase

Chain 8-T: 90% 10%



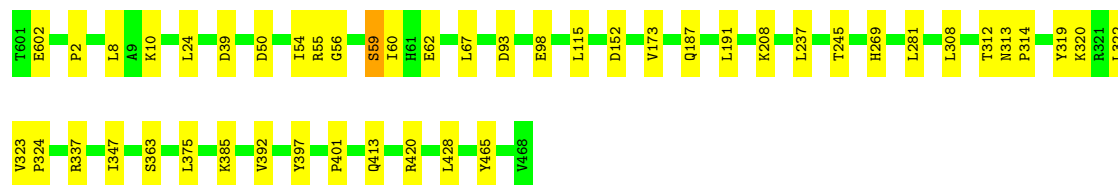
- Molecule 1: glutamine synthetase

Chain 8-U: 90% 10%



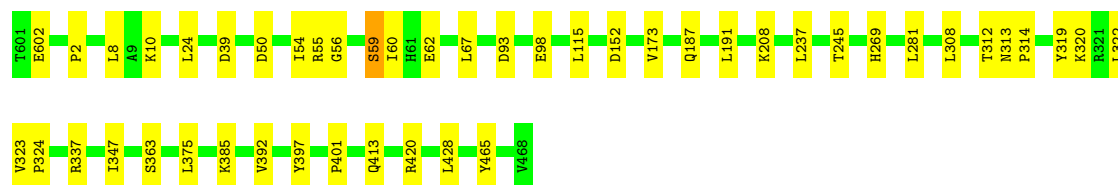
- Molecule 1: glutamine synthetase

Chain 8-V: 90% 10%



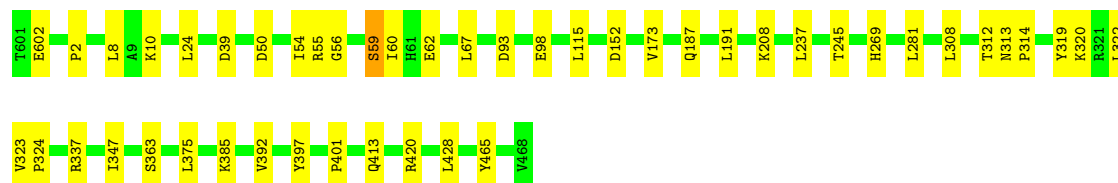
- Molecule 1: glutamine synthetase

Chain 8-W: 90% 10%



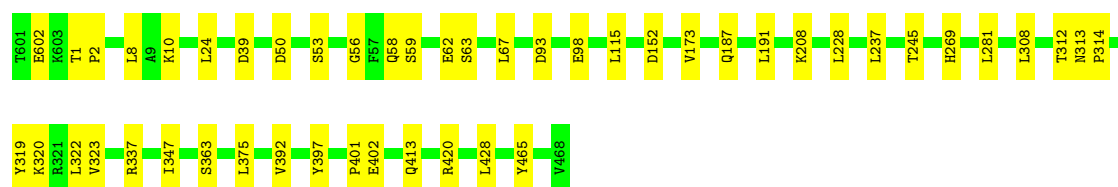
- Molecule 1: glutamine synthetase

Chain 8-X: 90% 10%



- Molecule 1: glutamine synthetase

Chain 9-A: 90% 10%



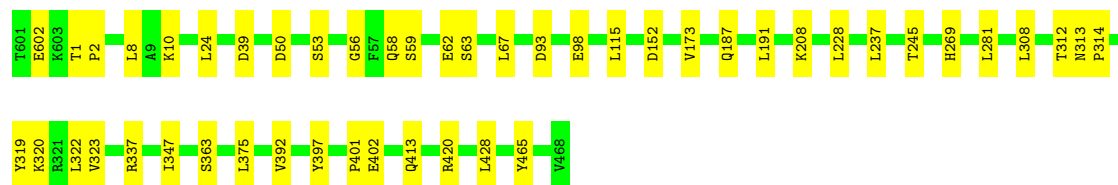
- Molecule 1: glutamine synthetase

Chain 9-B: 90% 10%



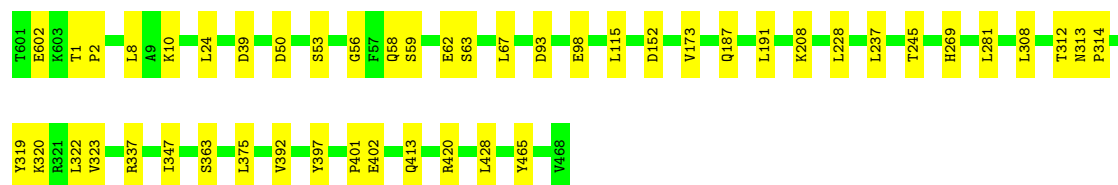
- Molecule 1: glutamine synthetase

Chain 9-C: 90% 10%



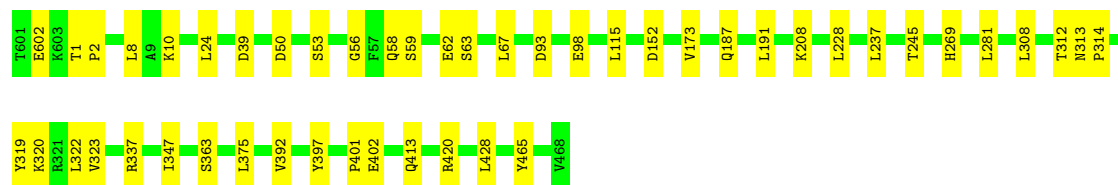
- Molecule 1: glutamine synthetase

Chain 9-D: 90% 10%



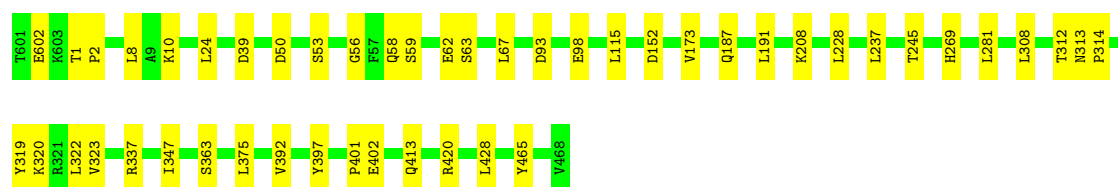
- Molecule 1: glutamine synthetase

Chain 9-E: 90% 10%



- Molecule 1: glutamine synthetase

Chain 9-F: 90% 10%



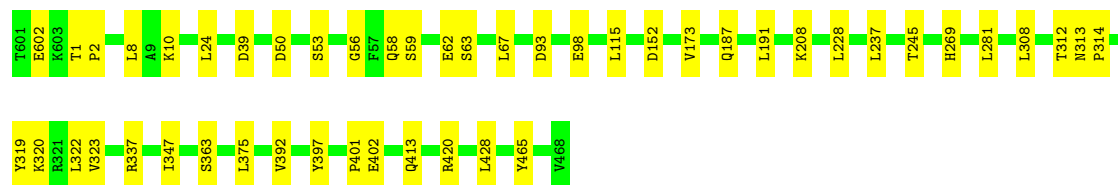
- Molecule 1: glutamine synthetase

Chain 9-G: 90% 10%



- Molecule 1: glutamine synthetase

Chain 9-H: 90% 10%



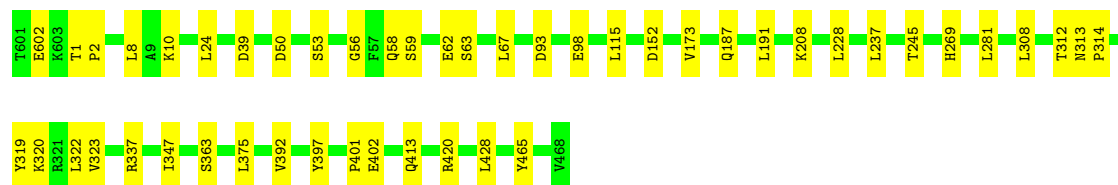
- Molecule 1: glutamine synthetase

Chain 9-I: 90% 10%



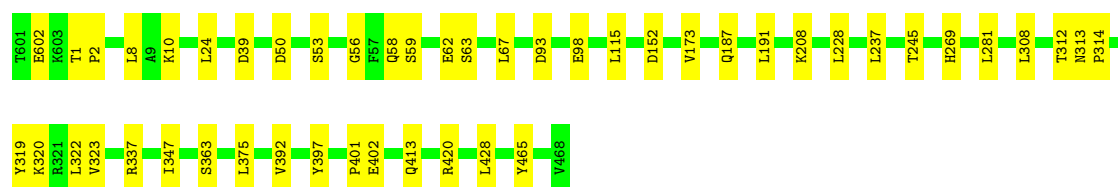
- Molecule 1: glutamine synthetase

Chain 9-J: 90% 10%



- Molecule 1: glutamine synthetase

Chain 9-K: 90% 10%



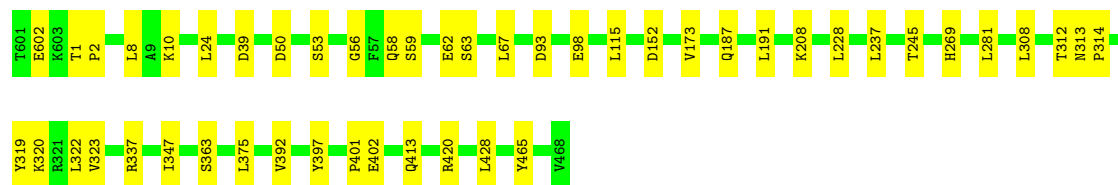
- Molecule 1: glutamine synthetase

Chain 9-L: 90% 10%



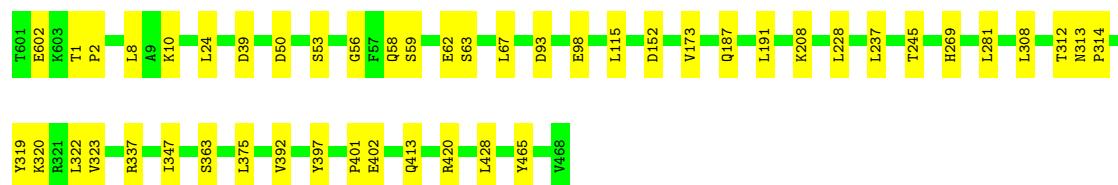
- Molecule 1: glutamine synthetase

Chain 9-M: 90% 10%



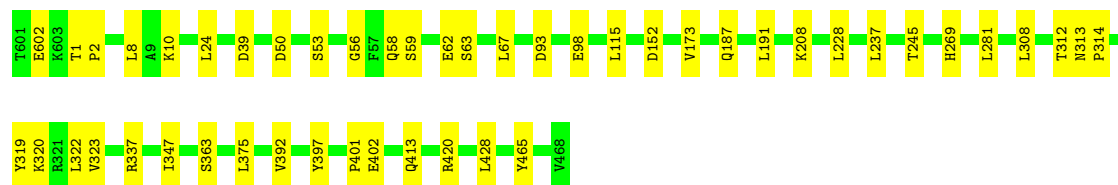
- Molecule 1: glutamine synthetase

Chain 9-N: 90% 10%



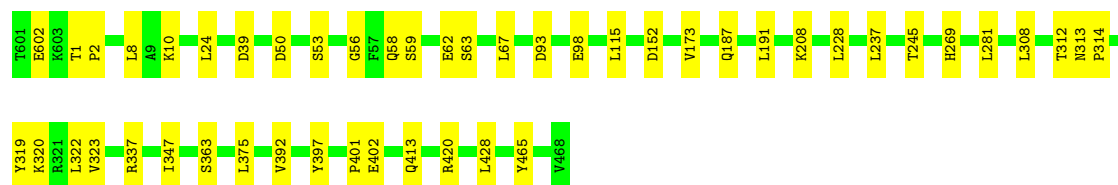
- Molecule 1: glutamine synthetase

Chain 9-O: 90% 10%



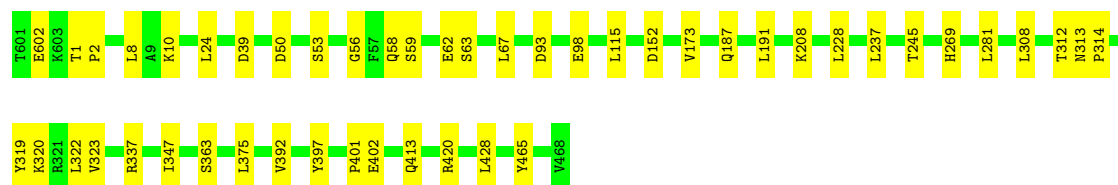
- Molecule 1: glutamine synthetase

Chain 9-P: 90% 10%



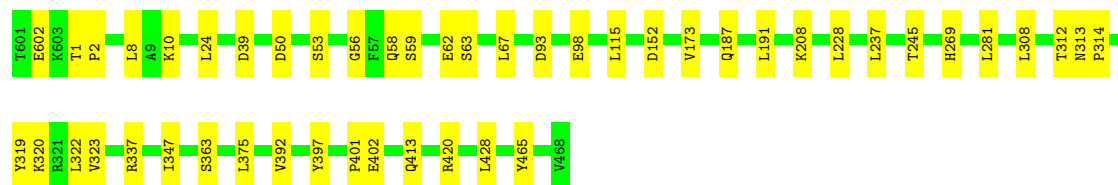
- Molecule 1: glutamine synthetase

Chain 9-Q: 90% 10%



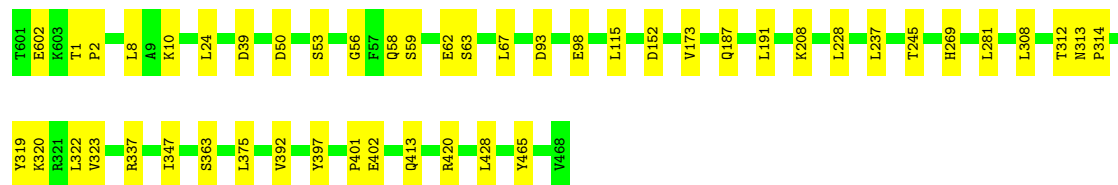
- Molecule 1: glutamine synthetase

Chain 9-R: 90% 10%



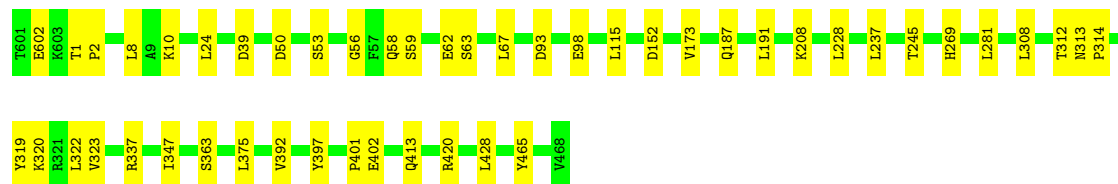
- Molecule 1: glutamine synthetase

Chain 9-S: 90% 10%



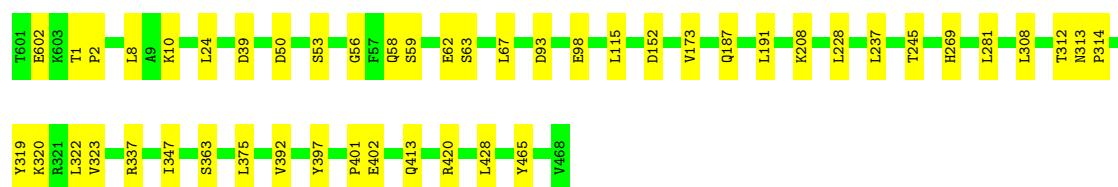
- Molecule 1: glutamine synthetase

Chain 9-T: 90% 10%



- Molecule 1: glutamine synthetase

Chain 9-U: 90% 10%



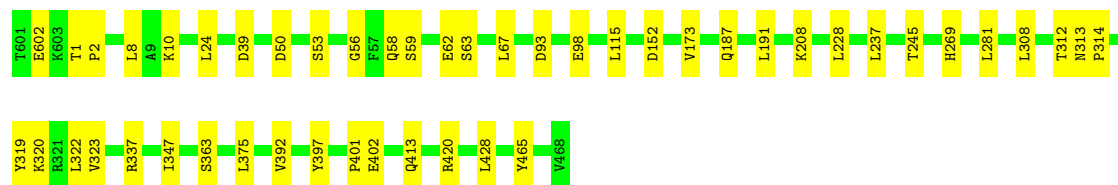
- Molecule 1: glutamine synthetase

Chain 9-V:
90% 10%



- Molecule 1: glutamine synthetase

Chain 9-W:
90% 10%



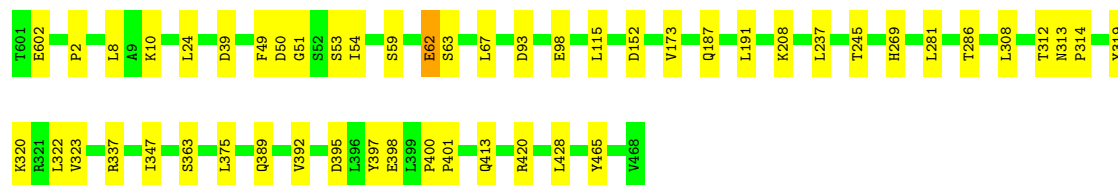
- Molecule 1: glutamine synthetase

Chain 9-X:
90% 10%



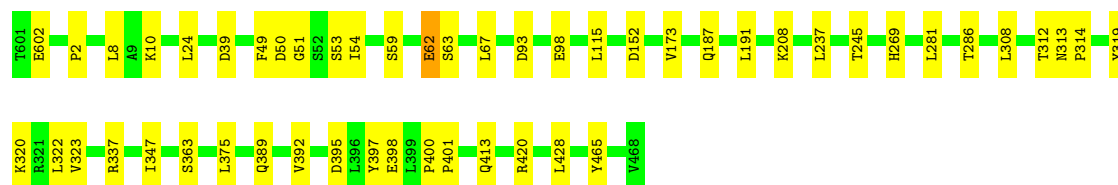
- Molecule 1: glutamine synthetase

Chain 10-A:
89% 10%



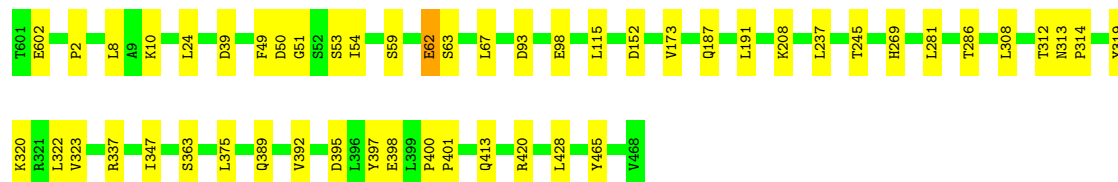
- Molecule 1: glutamine synthetase

Chain 10-B:
89% 10%



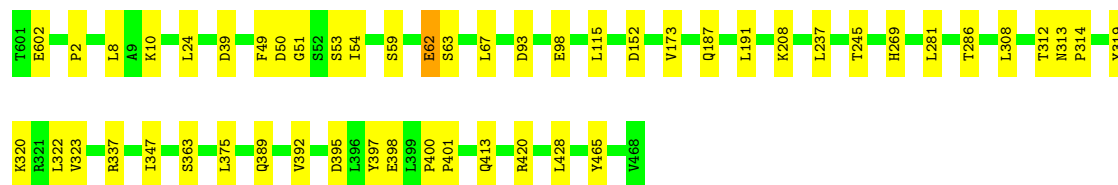
- Molecule 1: glutamine synthetase

Chain 10-C: 89% 10%



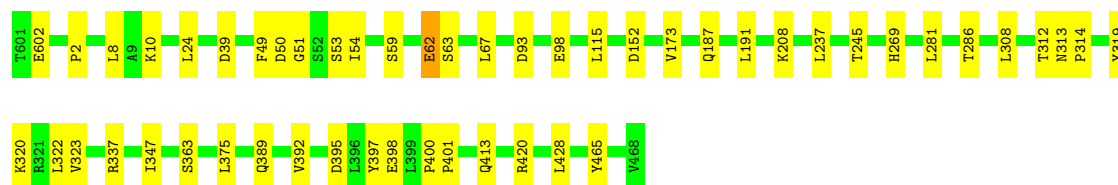
- Molecule 1: glutamine synthetase

Chain 10-D: 89% 10%



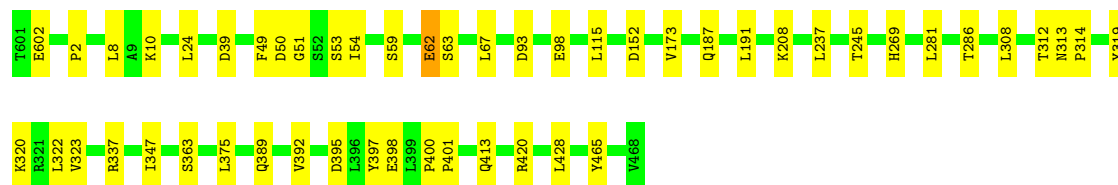
- Molecule 1: glutamine synthetase

Chain 10-E: 89% 10%



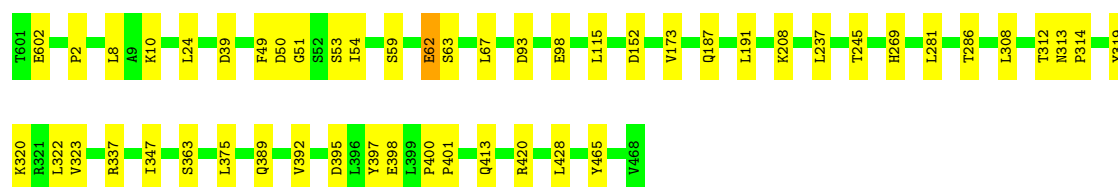
- Molecule 1: glutamine synthetase

Chain 10-F: 89% 10%



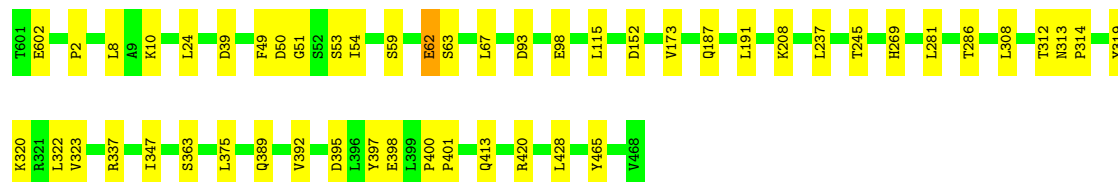
- Molecule 1: glutamine synthetase

Chain 10-G: 89% 10%



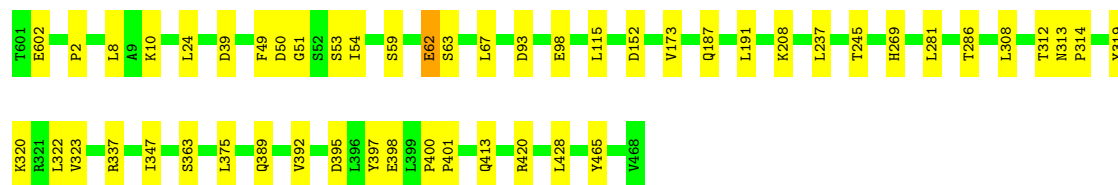
- Molecule 1: glutamine synthetase

Chain 10-H: 89% 10%



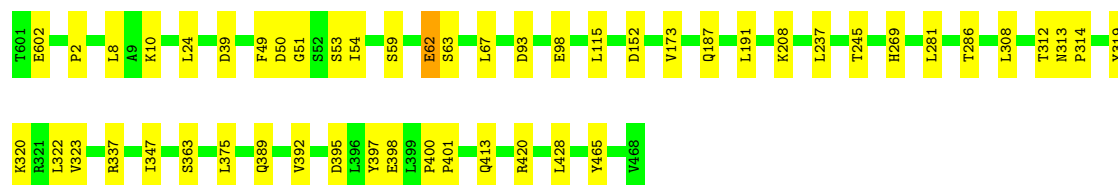
- Molecule 1: glutamine synthetase

Chain 10-I: 89% 10%



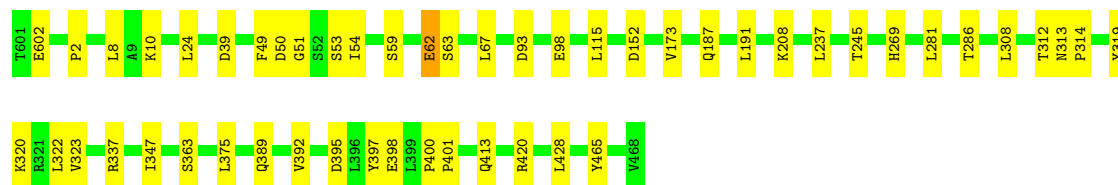
- Molecule 1: glutamine synthetase

Chain 10-J: 89% 10%



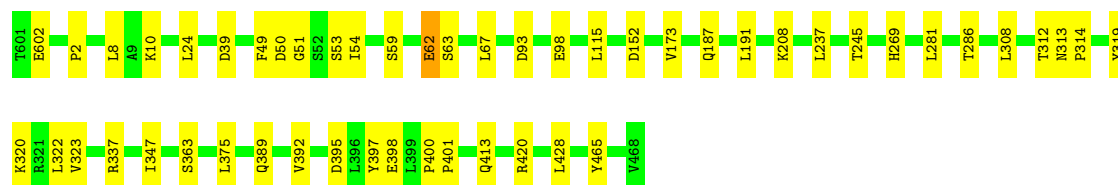
- Molecule 1: glutamine synthetase

Chain 10-K: 89% 10%



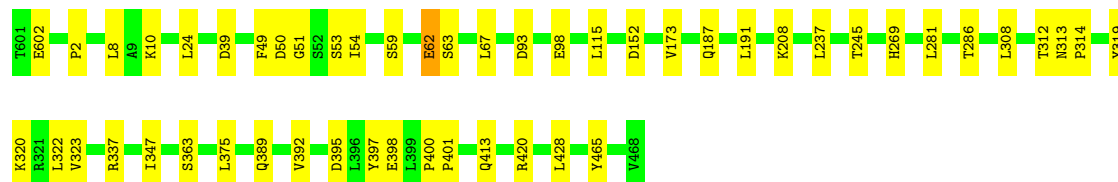
- Molecule 1: glutamine synthetase

Chain 10-L: 89% 10%



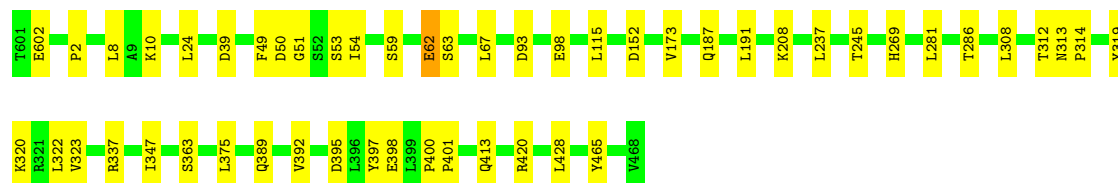
- Molecule 1: glutamine synthetase

Chain 10-M: 89% 10%



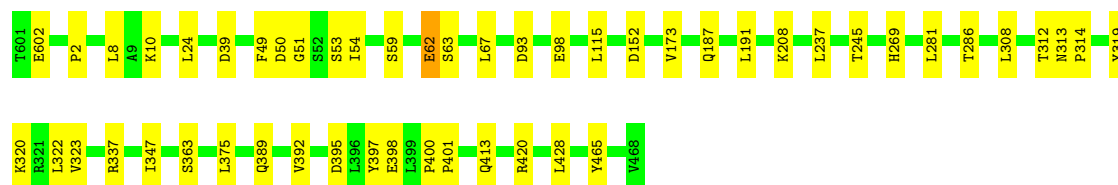
- Molecule 1: glutamine synthetase

Chain 10-N: 89% 10%



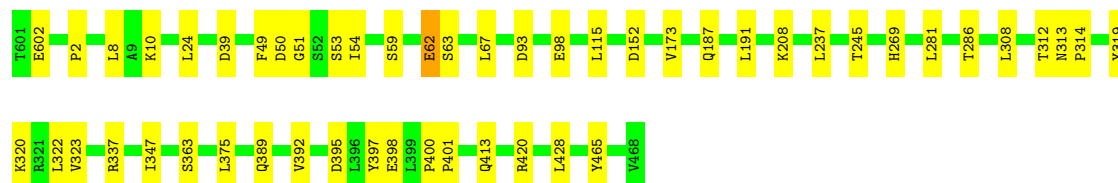
- Molecule 1: glutamine synthetase

Chain 10-O: 89% 10%



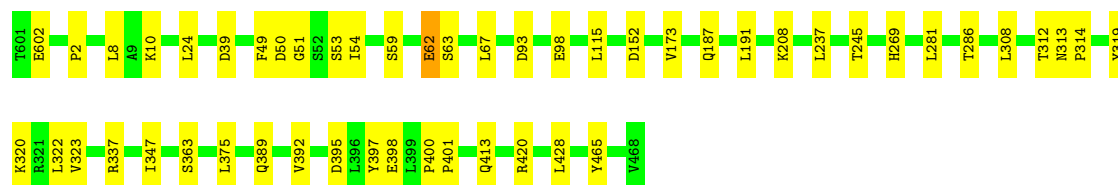
- Molecule 1: glutamine synthetase

Chain 10-P: 89% 10%



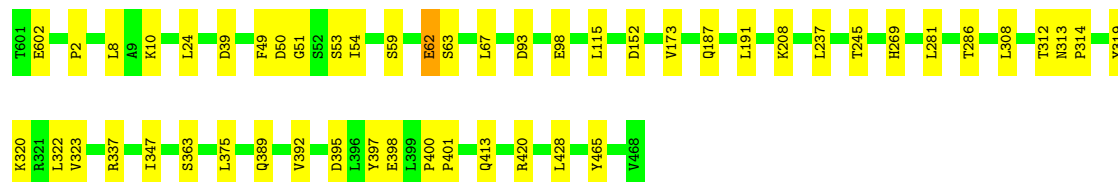
- Molecule 1: glutamine synthetase

Chain 10-Q: 89% 10%



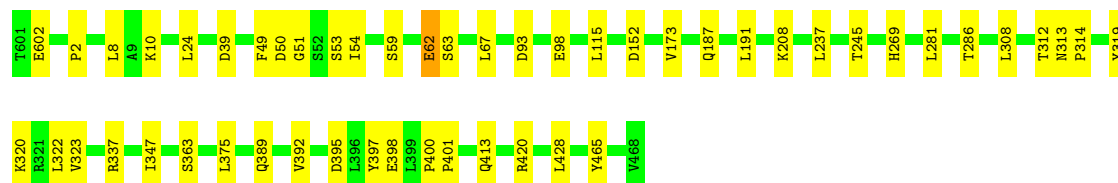
- Molecule 1: glutamine synthetase

Chain 10-R: 89% 10%



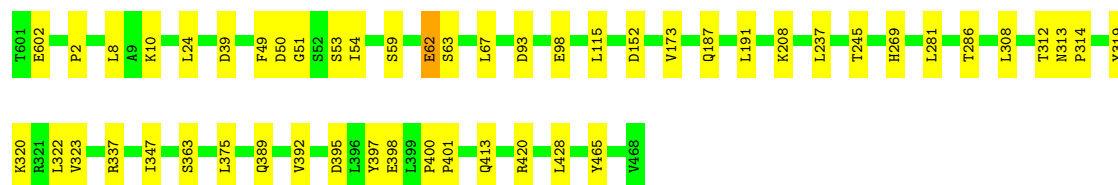
- Molecule 1: glutamine synthetase

Chain 10-S: 89% 10%



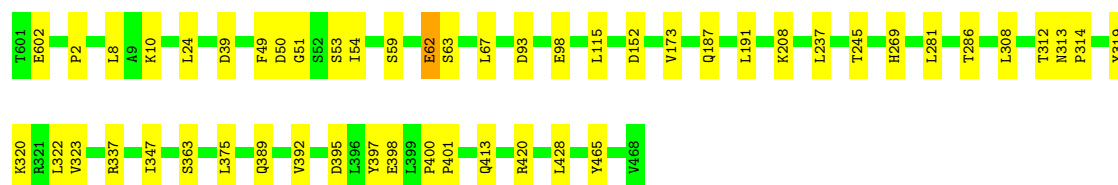
- Molecule 1: glutamine synthetase

Chain 10-T: 89% 10%



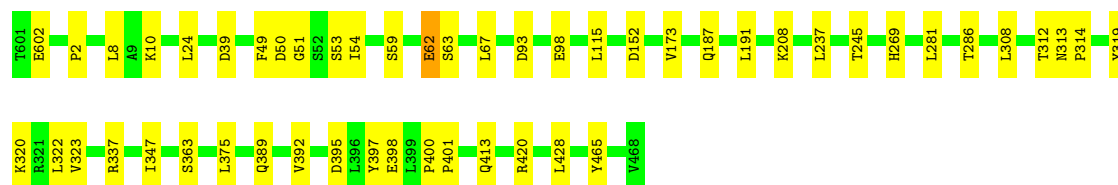
- Molecule 1: glutamine synthetase

Chain 10-U: 89% 10%



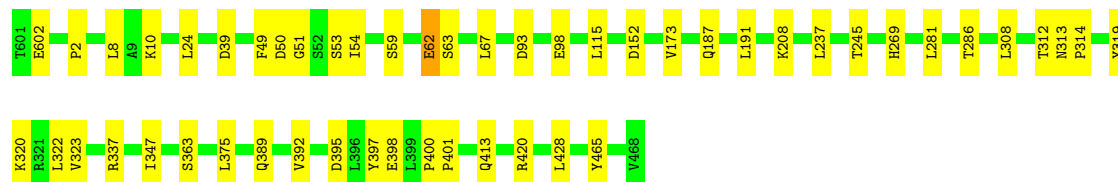
- Molecule 1: glutamine synthetase

Chain 10-V: 89% 10%



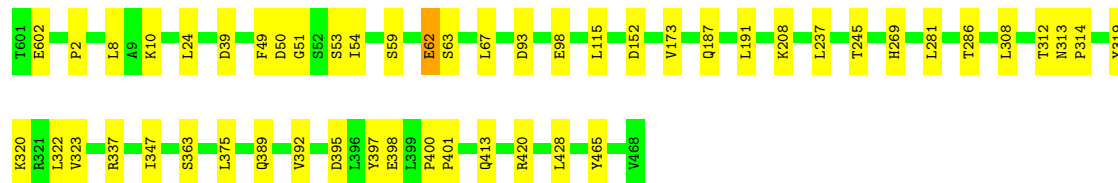
- Molecule 1: glutamine synthetase

Chain 10-W: 89% 10%



- Molecule 1: glutamine synthetase

Chain 10-X: 89% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.72Å 257.69Å 274.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.40) 99.5 (20.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.38 (at 2.41Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.204 , 0.223 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.03 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	978720	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0949e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, AMP, CIT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1-A	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-B	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-C	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-D	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-E	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-F	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-G	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-H	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-I	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-J	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-K	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-L	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-M	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-N	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-O	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-P	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-Q	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-R	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-S	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-T	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-U	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-V	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-W	0.28	0/3884	0.58	6/5279 (0.1%)
1	1-X	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-A	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-B	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-C	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-D	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-E	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-F	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-G	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-H	0.28	0/3884	0.58	6/5279 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2-I	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-J	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-K	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-L	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-M	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-N	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-O	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-P	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-Q	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-R	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-S	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-T	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-U	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-V	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-W	0.28	0/3884	0.58	6/5279 (0.1%)
1	2-X	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-A	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-B	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-C	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-D	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-E	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-F	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-G	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-H	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-I	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-J	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-K	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-L	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-M	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-N	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-O	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-P	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-Q	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-R	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-S	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-T	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-U	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-V	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-W	0.28	0/3884	0.58	6/5279 (0.1%)
1	3-X	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-A	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-B	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-C	0.28	0/3884	0.58	6/5279 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	4-D	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-E	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-F	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-G	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-H	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-I	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-J	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-K	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-L	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-M	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-N	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-O	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-P	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-Q	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-R	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-S	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-T	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-U	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-V	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-W	0.28	0/3884	0.58	6/5279 (0.1%)
1	4-X	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-A	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-B	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-C	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-D	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-E	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-F	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-G	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-H	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-I	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-J	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-K	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-L	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-M	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-N	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-O	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-P	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-Q	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-R	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-S	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-T	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-U	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-V	0.28	0/3884	0.58	6/5279 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	5-W	0.28	0/3884	0.58	6/5279 (0.1%)
1	5-X	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-A	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-B	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-C	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-D	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-E	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-F	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-G	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-H	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-I	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-J	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-K	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-L	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-M	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-N	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-O	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-P	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-Q	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-R	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-S	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-T	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-U	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-V	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-W	0.28	0/3884	0.58	6/5279 (0.1%)
1	6-X	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-A	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-B	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-C	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-D	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-E	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-F	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-G	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-H	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-I	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-J	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-K	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-L	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-M	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-N	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-O	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-P	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-Q	0.28	0/3884	0.58	6/5279 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	7-R	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-S	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-T	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-U	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-V	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-W	0.28	0/3884	0.58	6/5279 (0.1%)
1	7-X	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-A	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-B	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-C	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-D	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-E	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-F	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-G	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-H	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-I	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-J	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-K	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-L	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-M	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-N	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-O	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-P	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-Q	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-R	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-S	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-T	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-U	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-V	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-W	0.28	0/3884	0.58	6/5279 (0.1%)
1	8-X	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-A	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-B	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-C	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-D	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-E	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-F	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-G	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-H	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-I	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-J	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-K	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-L	0.28	0/3884	0.58	6/5279 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	9-M	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-N	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-O	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-P	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-Q	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-R	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-S	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-T	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-U	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-V	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-W	0.28	0/3884	0.58	6/5279 (0.1%)
1	9-X	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-A	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-B	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-C	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-D	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-E	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-F	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-G	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-H	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-I	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-J	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-K	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-L	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-M	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-N	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-O	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-P	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-Q	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-R	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-S	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-T	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-U	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-V	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-W	0.28	0/3884	0.58	6/5279 (0.1%)
1	10-X	0.28	0/3884	0.58	6/5279 (0.1%)
All	All	0.28	0/932160	0.58	1440/1266960 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	1-B	0	1
1	1-C	0	1
1	1-D	0	1
1	1-E	0	1
1	1-F	0	1
1	1-G	0	1
1	1-H	0	1
1	1-I	0	1
1	1-J	0	1
1	1-K	0	1
1	1-L	0	1
1	1-M	0	1
1	1-N	0	1
1	1-O	0	1
1	1-P	0	1
1	1-Q	0	1
1	1-R	0	1
1	1-S	0	1
1	1-T	0	1
1	1-U	0	1
1	1-V	0	1
1	1-W	0	1
1	1-X	0	1
1	2-A	0	1
1	2-B	0	1
1	2-C	0	1
1	2-D	0	1
1	2-E	0	1
1	2-F	0	1
1	2-G	0	1
1	2-H	0	1
1	2-I	0	1
1	2-J	0	1
1	2-K	0	1
1	2-L	0	1
1	2-M	0	1
1	2-N	0	1
1	2-O	0	1
1	2-P	0	1
1	2-Q	0	1
1	2-R	0	1
1	2-S	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-T	0	1
1	2-U	0	1
1	2-V	0	1
1	2-W	0	1
1	2-X	0	1
1	3-A	0	1
1	3-B	0	1
1	3-C	0	1
1	3-D	0	1
1	3-E	0	1
1	3-F	0	1
1	3-G	0	1
1	3-H	0	1
1	3-I	0	1
1	3-J	0	1
1	3-K	0	1
1	3-L	0	1
1	3-M	0	1
1	3-N	0	1
1	3-O	0	1
1	3-P	0	1
1	3-Q	0	1
1	3-R	0	1
1	3-S	0	1
1	3-T	0	1
1	3-U	0	1
1	3-V	0	1
1	3-W	0	1
1	3-X	0	1
1	4-A	0	1
1	4-B	0	1
1	4-C	0	1
1	4-D	0	1
1	4-E	0	1
1	4-F	0	1
1	4-G	0	1
1	4-H	0	1
1	4-I	0	1
1	4-J	0	1
1	4-K	0	1
1	4-L	0	1
1	4-M	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4-N	0	1
1	4-O	0	1
1	4-P	0	1
1	4-Q	0	1
1	4-R	0	1
1	4-S	0	1
1	4-T	0	1
1	4-U	0	1
1	4-V	0	1
1	4-W	0	1
1	4-X	0	1
1	5-A	0	1
1	5-B	0	1
1	5-C	0	1
1	5-D	0	1
1	5-E	0	1
1	5-F	0	1
1	5-G	0	1
1	5-H	0	1
1	5-I	0	1
1	5-J	0	1
1	5-K	0	1
1	5-L	0	1
1	5-M	0	1
1	5-N	0	1
1	5-O	0	1
1	5-P	0	1
1	5-Q	0	1
1	5-R	0	1
1	5-S	0	1
1	5-T	0	1
1	5-U	0	1
1	5-V	0	1
1	5-W	0	1
1	5-X	0	1
1	6-A	0	1
1	6-B	0	1
1	6-C	0	1
1	6-D	0	1
1	6-E	0	1
1	6-F	0	1
1	6-G	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	6-H	0	1
1	6-I	0	1
1	6-J	0	1
1	6-K	0	1
1	6-L	0	1
1	6-M	0	1
1	6-N	0	1
1	6-O	0	1
1	6-P	0	1
1	6-Q	0	1
1	6-R	0	1
1	6-S	0	1
1	6-T	0	1
1	6-U	0	1
1	6-V	0	1
1	6-W	0	1
1	6-X	0	1
1	7-A	0	1
1	7-B	0	1
1	7-C	0	1
1	7-D	0	1
1	7-E	0	1
1	7-F	0	1
1	7-G	0	1
1	7-H	0	1
1	7-I	0	1
1	7-J	0	1
1	7-K	0	1
1	7-L	0	1
1	7-M	0	1
1	7-N	0	1
1	7-O	0	1
1	7-P	0	1
1	7-Q	0	1
1	7-R	0	1
1	7-S	0	1
1	7-T	0	1
1	7-U	0	1
1	7-V	0	1
1	7-W	0	1
1	7-X	0	1
1	8-A	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	8-B	0	1
1	8-C	0	1
1	8-D	0	1
1	8-E	0	1
1	8-F	0	1
1	8-G	0	1
1	8-H	0	1
1	8-I	0	1
1	8-J	0	1
1	8-K	0	1
1	8-L	0	1
1	8-M	0	1
1	8-N	0	1
1	8-O	0	1
1	8-P	0	1
1	8-Q	0	1
1	8-R	0	1
1	8-S	0	1
1	8-T	0	1
1	8-U	0	1
1	8-V	0	1
1	8-W	0	1
1	8-X	0	1
1	9-A	0	1
1	9-B	0	1
1	9-C	0	1
1	9-D	0	1
1	9-E	0	1
1	9-F	0	1
1	9-G	0	1
1	9-H	0	1
1	9-I	0	1
1	9-J	0	1
1	9-K	0	1
1	9-L	0	1
1	9-M	0	1
1	9-N	0	1
1	9-O	0	1
1	9-P	0	1
1	9-Q	0	1
1	9-R	0	1
1	9-S	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	9-T	0	1
1	9-U	0	1
1	9-V	0	1
1	9-W	0	1
1	9-X	0	1
1	10-A	0	1
1	10-B	0	1
1	10-C	0	1
1	10-D	0	1
1	10-E	0	1
1	10-F	0	1
1	10-G	0	1
1	10-H	0	1
1	10-I	0	1
1	10-J	0	1
1	10-K	0	1
1	10-L	0	1
1	10-M	0	1
1	10-N	0	1
1	10-O	0	1
1	10-P	0	1
1	10-Q	0	1
1	10-R	0	1
1	10-S	0	1
1	10-T	0	1
1	10-U	0	1
1	10-V	0	1
1	10-W	0	1
1	10-X	0	1
All	All	0	240

There are no bond length outliers.

All (1440) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-U	320	LYS	N-CA-C	-7.00	104.56	113.23
1	2-U	320	LYS	N-CA-C	-7.00	104.56	113.23
1	3-U	320	LYS	N-CA-C	-7.00	104.56	113.23
1	4-U	320	LYS	N-CA-C	-7.00	104.56	113.23
1	5-U	320	LYS	N-CA-C	-7.00	104.56	113.23
1	6-U	320	LYS	N-CA-C	-7.00	104.56	113.23
1	7-U	320	LYS	N-CA-C	-7.00	104.56	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-U	320	LYS	N-CA-C	-7.00	104.56	113.23
1	9-U	320	LYS	N-CA-C	-7.00	104.56	113.23
1	10-U	320	LYS	N-CA-C	-7.00	104.56	113.23
1	1-G	320	LYS	N-CA-C	-6.99	104.56	113.23
1	2-G	320	LYS	N-CA-C	-6.99	104.56	113.23
1	3-G	320	LYS	N-CA-C	-6.99	104.56	113.23
1	4-G	320	LYS	N-CA-C	-6.99	104.56	113.23
1	5-G	320	LYS	N-CA-C	-6.99	104.56	113.23
1	6-G	320	LYS	N-CA-C	-6.99	104.56	113.23
1	7-G	320	LYS	N-CA-C	-6.99	104.56	113.23
1	8-G	320	LYS	N-CA-C	-6.99	104.56	113.23
1	9-G	320	LYS	N-CA-C	-6.99	104.56	113.23
1	10-G	320	LYS	N-CA-C	-6.99	104.56	113.23
1	1-J	320	LYS	N-CA-C	-6.99	104.56	113.23
1	2-J	320	LYS	N-CA-C	-6.99	104.56	113.23
1	3-J	320	LYS	N-CA-C	-6.99	104.56	113.23
1	4-J	320	LYS	N-CA-C	-6.99	104.56	113.23
1	5-J	320	LYS	N-CA-C	-6.99	104.56	113.23
1	6-J	320	LYS	N-CA-C	-6.99	104.56	113.23
1	7-J	320	LYS	N-CA-C	-6.99	104.56	113.23
1	8-J	320	LYS	N-CA-C	-6.99	104.56	113.23
1	9-J	320	LYS	N-CA-C	-6.99	104.56	113.23
1	10-J	320	LYS	N-CA-C	-6.99	104.56	113.23
1	1-S	320	LYS	N-CA-C	-6.99	104.57	113.23
1	2-S	320	LYS	N-CA-C	-6.99	104.57	113.23
1	3-S	320	LYS	N-CA-C	-6.99	104.57	113.23
1	4-S	320	LYS	N-CA-C	-6.99	104.57	113.23
1	5-S	320	LYS	N-CA-C	-6.99	104.57	113.23
1	6-S	320	LYS	N-CA-C	-6.99	104.57	113.23
1	7-S	320	LYS	N-CA-C	-6.99	104.57	113.23
1	8-S	320	LYS	N-CA-C	-6.99	104.57	113.23
1	9-S	320	LYS	N-CA-C	-6.99	104.57	113.23
1	10-S	320	LYS	N-CA-C	-6.99	104.57	113.23
1	1-F	320	LYS	N-CA-C	-6.98	104.57	113.23
1	2-F	320	LYS	N-CA-C	-6.98	104.57	113.23
1	3-F	320	LYS	N-CA-C	-6.98	104.57	113.23
1	4-F	320	LYS	N-CA-C	-6.98	104.57	113.23
1	5-F	320	LYS	N-CA-C	-6.98	104.57	113.23
1	6-F	320	LYS	N-CA-C	-6.98	104.57	113.23
1	7-F	320	LYS	N-CA-C	-6.98	104.57	113.23
1	8-F	320	LYS	N-CA-C	-6.98	104.57	113.23
1	9-F	320	LYS	N-CA-C	-6.98	104.57	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-F	320	LYS	N-CA-C	-6.98	104.57	113.23
1	1-B	320	LYS	N-CA-C	-6.98	104.58	113.23
1	2-B	320	LYS	N-CA-C	-6.98	104.58	113.23
1	3-B	320	LYS	N-CA-C	-6.98	104.58	113.23
1	4-B	320	LYS	N-CA-C	-6.98	104.58	113.23
1	5-B	320	LYS	N-CA-C	-6.98	104.58	113.23
1	6-B	320	LYS	N-CA-C	-6.98	104.58	113.23
1	7-B	320	LYS	N-CA-C	-6.98	104.58	113.23
1	8-B	320	LYS	N-CA-C	-6.98	104.58	113.23
1	9-B	320	LYS	N-CA-C	-6.98	104.58	113.23
1	10-B	320	LYS	N-CA-C	-6.98	104.58	113.23
1	1-C	320	LYS	N-CA-C	-6.97	104.58	113.23
1	2-C	320	LYS	N-CA-C	-6.97	104.58	113.23
1	3-C	320	LYS	N-CA-C	-6.97	104.58	113.23
1	4-C	320	LYS	N-CA-C	-6.97	104.58	113.23
1	5-C	320	LYS	N-CA-C	-6.97	104.58	113.23
1	6-C	320	LYS	N-CA-C	-6.97	104.58	113.23
1	7-C	320	LYS	N-CA-C	-6.97	104.58	113.23
1	8-C	320	LYS	N-CA-C	-6.97	104.58	113.23
1	9-C	320	LYS	N-CA-C	-6.97	104.58	113.23
1	10-C	320	LYS	N-CA-C	-6.97	104.58	113.23
1	1-K	320	LYS	N-CA-C	-6.97	104.58	113.23
1	2-K	320	LYS	N-CA-C	-6.97	104.58	113.23
1	3-K	320	LYS	N-CA-C	-6.97	104.58	113.23
1	4-K	320	LYS	N-CA-C	-6.97	104.58	113.23
1	5-K	320	LYS	N-CA-C	-6.97	104.58	113.23
1	6-K	320	LYS	N-CA-C	-6.97	104.58	113.23
1	7-K	320	LYS	N-CA-C	-6.97	104.58	113.23
1	8-K	320	LYS	N-CA-C	-6.97	104.58	113.23
1	9-K	320	LYS	N-CA-C	-6.97	104.58	113.23
1	10-K	320	LYS	N-CA-C	-6.97	104.58	113.23
1	1-I	320	LYS	N-CA-C	-6.96	104.59	113.23
1	2-I	320	LYS	N-CA-C	-6.96	104.59	113.23
1	3-I	320	LYS	N-CA-C	-6.96	104.59	113.23
1	4-I	320	LYS	N-CA-C	-6.96	104.59	113.23
1	5-I	320	LYS	N-CA-C	-6.96	104.59	113.23
1	6-I	320	LYS	N-CA-C	-6.96	104.59	113.23
1	7-I	320	LYS	N-CA-C	-6.96	104.59	113.23
1	8-I	320	LYS	N-CA-C	-6.96	104.59	113.23
1	9-I	320	LYS	N-CA-C	-6.96	104.59	113.23
1	10-I	320	LYS	N-CA-C	-6.96	104.59	113.23
1	1-A	320	LYS	N-CA-C	-6.96	104.60	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	320	LYS	N-CA-C	-6.96	104.60	113.23
1	3-A	320	LYS	N-CA-C	-6.96	104.60	113.23
1	4-A	320	LYS	N-CA-C	-6.96	104.60	113.23
1	5-A	320	LYS	N-CA-C	-6.96	104.60	113.23
1	6-A	320	LYS	N-CA-C	-6.96	104.60	113.23
1	7-A	320	LYS	N-CA-C	-6.96	104.60	113.23
1	8-A	320	LYS	N-CA-C	-6.96	104.60	113.23
1	9-A	320	LYS	N-CA-C	-6.96	104.60	113.23
1	10-A	320	LYS	N-CA-C	-6.96	104.60	113.23
1	1-H	320	LYS	N-CA-C	-6.96	104.60	113.23
1	1-T	320	LYS	N-CA-C	-6.96	104.60	113.23
1	1-W	320	LYS	N-CA-C	-6.96	104.60	113.23
1	1-X	320	LYS	N-CA-C	-6.96	104.60	113.23
1	2-H	320	LYS	N-CA-C	-6.96	104.60	113.23
1	2-T	320	LYS	N-CA-C	-6.96	104.60	113.23
1	2-W	320	LYS	N-CA-C	-6.96	104.60	113.23
1	2-X	320	LYS	N-CA-C	-6.96	104.60	113.23
1	3-H	320	LYS	N-CA-C	-6.96	104.60	113.23
1	3-T	320	LYS	N-CA-C	-6.96	104.60	113.23
1	3-W	320	LYS	N-CA-C	-6.96	104.60	113.23
1	3-X	320	LYS	N-CA-C	-6.96	104.60	113.23
1	4-H	320	LYS	N-CA-C	-6.96	104.60	113.23
1	4-T	320	LYS	N-CA-C	-6.96	104.60	113.23
1	4-W	320	LYS	N-CA-C	-6.96	104.60	113.23
1	4-X	320	LYS	N-CA-C	-6.96	104.60	113.23
1	5-H	320	LYS	N-CA-C	-6.96	104.60	113.23
1	5-T	320	LYS	N-CA-C	-6.96	104.60	113.23
1	5-W	320	LYS	N-CA-C	-6.96	104.60	113.23
1	5-X	320	LYS	N-CA-C	-6.96	104.60	113.23
1	6-H	320	LYS	N-CA-C	-6.96	104.60	113.23
1	6-T	320	LYS	N-CA-C	-6.96	104.60	113.23
1	6-W	320	LYS	N-CA-C	-6.96	104.60	113.23
1	6-X	320	LYS	N-CA-C	-6.96	104.60	113.23
1	7-H	320	LYS	N-CA-C	-6.96	104.60	113.23
1	7-T	320	LYS	N-CA-C	-6.96	104.60	113.23
1	7-W	320	LYS	N-CA-C	-6.96	104.60	113.23
1	7-X	320	LYS	N-CA-C	-6.96	104.60	113.23
1	8-H	320	LYS	N-CA-C	-6.96	104.60	113.23
1	8-T	320	LYS	N-CA-C	-6.96	104.60	113.23
1	8-W	320	LYS	N-CA-C	-6.96	104.60	113.23
1	8-X	320	LYS	N-CA-C	-6.96	104.60	113.23
1	9-H	320	LYS	N-CA-C	-6.96	104.60	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-T	320	LYS	N-CA-C	-6.96	104.60	113.23
1	9-W	320	LYS	N-CA-C	-6.96	104.60	113.23
1	9-X	320	LYS	N-CA-C	-6.96	104.60	113.23
1	10-H	320	LYS	N-CA-C	-6.96	104.60	113.23
1	10-T	320	LYS	N-CA-C	-6.96	104.60	113.23
1	10-W	320	LYS	N-CA-C	-6.96	104.60	113.23
1	10-X	320	LYS	N-CA-C	-6.96	104.60	113.23
1	1-P	320	LYS	N-CA-C	-6.96	104.60	113.23
1	2-P	320	LYS	N-CA-C	-6.96	104.60	113.23
1	3-P	320	LYS	N-CA-C	-6.96	104.60	113.23
1	4-P	320	LYS	N-CA-C	-6.96	104.60	113.23
1	5-P	320	LYS	N-CA-C	-6.96	104.60	113.23
1	6-P	320	LYS	N-CA-C	-6.96	104.60	113.23
1	7-P	320	LYS	N-CA-C	-6.96	104.60	113.23
1	8-P	320	LYS	N-CA-C	-6.96	104.60	113.23
1	9-P	320	LYS	N-CA-C	-6.96	104.60	113.23
1	10-P	320	LYS	N-CA-C	-6.96	104.60	113.23
1	1-L	320	LYS	N-CA-C	-6.96	104.61	113.23
1	2-L	320	LYS	N-CA-C	-6.96	104.61	113.23
1	3-L	320	LYS	N-CA-C	-6.96	104.61	113.23
1	4-L	320	LYS	N-CA-C	-6.96	104.61	113.23
1	5-L	320	LYS	N-CA-C	-6.96	104.61	113.23
1	6-L	320	LYS	N-CA-C	-6.96	104.61	113.23
1	7-L	320	LYS	N-CA-C	-6.96	104.61	113.23
1	8-L	320	LYS	N-CA-C	-6.96	104.61	113.23
1	9-L	320	LYS	N-CA-C	-6.96	104.61	113.23
1	10-L	320	LYS	N-CA-C	-6.96	104.61	113.23
1	1-Q	320	LYS	N-CA-C	-6.95	104.61	113.23
1	1-R	320	LYS	N-CA-C	-6.95	104.61	113.23
1	2-Q	320	LYS	N-CA-C	-6.95	104.61	113.23
1	2-R	320	LYS	N-CA-C	-6.95	104.61	113.23
1	3-Q	320	LYS	N-CA-C	-6.95	104.61	113.23
1	3-R	320	LYS	N-CA-C	-6.95	104.61	113.23
1	4-Q	320	LYS	N-CA-C	-6.95	104.61	113.23
1	4-R	320	LYS	N-CA-C	-6.95	104.61	113.23
1	5-Q	320	LYS	N-CA-C	-6.95	104.61	113.23
1	5-R	320	LYS	N-CA-C	-6.95	104.61	113.23
1	6-Q	320	LYS	N-CA-C	-6.95	104.61	113.23
1	6-R	320	LYS	N-CA-C	-6.95	104.61	113.23
1	7-Q	320	LYS	N-CA-C	-6.95	104.61	113.23
1	7-R	320	LYS	N-CA-C	-6.95	104.61	113.23
1	8-Q	320	LYS	N-CA-C	-6.95	104.61	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-R	320	LYS	N-CA-C	-6.95	104.61	113.23
1	9-Q	320	LYS	N-CA-C	-6.95	104.61	113.23
1	9-R	320	LYS	N-CA-C	-6.95	104.61	113.23
1	10-Q	320	LYS	N-CA-C	-6.95	104.61	113.23
1	10-R	320	LYS	N-CA-C	-6.95	104.61	113.23
1	1-D	320	LYS	N-CA-C	-6.95	104.61	113.23
1	1-M	320	LYS	N-CA-C	-6.95	104.61	113.23
1	2-D	320	LYS	N-CA-C	-6.95	104.61	113.23
1	2-M	320	LYS	N-CA-C	-6.95	104.61	113.23
1	3-D	320	LYS	N-CA-C	-6.95	104.61	113.23
1	3-M	320	LYS	N-CA-C	-6.95	104.61	113.23
1	4-D	320	LYS	N-CA-C	-6.95	104.61	113.23
1	4-M	320	LYS	N-CA-C	-6.95	104.61	113.23
1	5-D	320	LYS	N-CA-C	-6.95	104.61	113.23
1	5-M	320	LYS	N-CA-C	-6.95	104.61	113.23
1	6-D	320	LYS	N-CA-C	-6.95	104.61	113.23
1	6-M	320	LYS	N-CA-C	-6.95	104.61	113.23
1	7-D	320	LYS	N-CA-C	-6.95	104.61	113.23
1	7-M	320	LYS	N-CA-C	-6.95	104.61	113.23
1	8-D	320	LYS	N-CA-C	-6.95	104.61	113.23
1	8-M	320	LYS	N-CA-C	-6.95	104.61	113.23
1	9-D	320	LYS	N-CA-C	-6.95	104.61	113.23
1	9-M	320	LYS	N-CA-C	-6.95	104.61	113.23
1	10-D	320	LYS	N-CA-C	-6.95	104.61	113.23
1	10-M	320	LYS	N-CA-C	-6.95	104.61	113.23
1	1-O	320	LYS	N-CA-C	-6.94	104.62	113.23
1	2-O	320	LYS	N-CA-C	-6.94	104.62	113.23
1	3-O	320	LYS	N-CA-C	-6.94	104.62	113.23
1	4-O	320	LYS	N-CA-C	-6.94	104.62	113.23
1	5-O	320	LYS	N-CA-C	-6.94	104.62	113.23
1	6-O	320	LYS	N-CA-C	-6.94	104.62	113.23
1	7-O	320	LYS	N-CA-C	-6.94	104.62	113.23
1	8-O	320	LYS	N-CA-C	-6.94	104.62	113.23
1	9-O	320	LYS	N-CA-C	-6.94	104.62	113.23
1	10-O	320	LYS	N-CA-C	-6.94	104.62	113.23
1	1-E	320	LYS	N-CA-C	-6.94	104.62	113.23
1	2-E	320	LYS	N-CA-C	-6.94	104.62	113.23
1	3-E	320	LYS	N-CA-C	-6.94	104.62	113.23
1	4-E	320	LYS	N-CA-C	-6.94	104.62	113.23
1	5-E	320	LYS	N-CA-C	-6.94	104.62	113.23
1	6-E	320	LYS	N-CA-C	-6.94	104.62	113.23
1	7-E	320	LYS	N-CA-C	-6.94	104.62	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-E	320	LYS	N-CA-C	-6.94	104.62	113.23
1	9-E	320	LYS	N-CA-C	-6.94	104.62	113.23
1	10-E	320	LYS	N-CA-C	-6.94	104.62	113.23
1	1-N	320	LYS	N-CA-C	-6.94	104.63	113.23
1	2-N	320	LYS	N-CA-C	-6.94	104.63	113.23
1	3-N	320	LYS	N-CA-C	-6.94	104.63	113.23
1	4-N	320	LYS	N-CA-C	-6.94	104.63	113.23
1	5-N	320	LYS	N-CA-C	-6.94	104.63	113.23
1	6-N	320	LYS	N-CA-C	-6.94	104.63	113.23
1	7-N	320	LYS	N-CA-C	-6.94	104.63	113.23
1	8-N	320	LYS	N-CA-C	-6.94	104.63	113.23
1	9-N	320	LYS	N-CA-C	-6.94	104.63	113.23
1	10-N	320	LYS	N-CA-C	-6.94	104.63	113.23
1	1-V	320	LYS	N-CA-C	-6.93	104.63	113.23
1	2-V	320	LYS	N-CA-C	-6.93	104.63	113.23
1	3-V	320	LYS	N-CA-C	-6.93	104.63	113.23
1	4-V	320	LYS	N-CA-C	-6.93	104.63	113.23
1	5-V	320	LYS	N-CA-C	-6.93	104.63	113.23
1	6-V	320	LYS	N-CA-C	-6.93	104.63	113.23
1	7-V	320	LYS	N-CA-C	-6.93	104.63	113.23
1	8-V	320	LYS	N-CA-C	-6.93	104.63	113.23
1	9-V	320	LYS	N-CA-C	-6.93	104.63	113.23
1	10-V	320	LYS	N-CA-C	-6.93	104.63	113.23
1	1-P	465	TYR	N-CA-C	6.72	123.69	113.61
1	2-P	465	TYR	N-CA-C	6.72	123.69	113.61
1	3-P	465	TYR	N-CA-C	6.72	123.69	113.61
1	4-P	465	TYR	N-CA-C	6.72	123.69	113.61
1	5-P	465	TYR	N-CA-C	6.72	123.69	113.61
1	6-P	465	TYR	N-CA-C	6.72	123.69	113.61
1	7-P	465	TYR	N-CA-C	6.72	123.69	113.61
1	8-P	465	TYR	N-CA-C	6.72	123.69	113.61
1	9-P	465	TYR	N-CA-C	6.72	123.69	113.61
1	10-P	465	TYR	N-CA-C	6.72	123.69	113.61
1	1-E	465	TYR	N-CA-C	6.72	123.69	113.61
1	2-E	465	TYR	N-CA-C	6.72	123.69	113.61
1	3-E	465	TYR	N-CA-C	6.72	123.69	113.61
1	4-E	465	TYR	N-CA-C	6.72	123.69	113.61
1	5-E	465	TYR	N-CA-C	6.72	123.69	113.61
1	6-E	465	TYR	N-CA-C	6.72	123.69	113.61
1	7-E	465	TYR	N-CA-C	6.72	123.69	113.61
1	8-E	465	TYR	N-CA-C	6.72	123.69	113.61
1	9-E	465	TYR	N-CA-C	6.72	123.69	113.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-E	465	TYR	N-CA-C	6.72	123.69	113.61
1	1-R	465	TYR	N-CA-C	6.71	123.68	113.61
1	2-R	465	TYR	N-CA-C	6.71	123.68	113.61
1	3-R	465	TYR	N-CA-C	6.71	123.68	113.61
1	4-R	465	TYR	N-CA-C	6.71	123.68	113.61
1	5-R	465	TYR	N-CA-C	6.71	123.68	113.61
1	6-R	465	TYR	N-CA-C	6.71	123.68	113.61
1	7-R	465	TYR	N-CA-C	6.71	123.68	113.61
1	8-R	465	TYR	N-CA-C	6.71	123.68	113.61
1	9-R	465	TYR	N-CA-C	6.71	123.68	113.61
1	10-R	465	TYR	N-CA-C	6.71	123.68	113.61
1	1-Q	465	TYR	N-CA-C	6.71	123.68	113.61
1	2-Q	465	TYR	N-CA-C	6.71	123.68	113.61
1	3-Q	465	TYR	N-CA-C	6.71	123.68	113.61
1	4-Q	465	TYR	N-CA-C	6.71	123.68	113.61
1	5-Q	465	TYR	N-CA-C	6.71	123.68	113.61
1	6-Q	465	TYR	N-CA-C	6.71	123.68	113.61
1	7-Q	465	TYR	N-CA-C	6.71	123.68	113.61
1	8-Q	465	TYR	N-CA-C	6.71	123.68	113.61
1	9-Q	465	TYR	N-CA-C	6.71	123.68	113.61
1	10-Q	465	TYR	N-CA-C	6.71	123.68	113.61
1	1-N	465	TYR	N-CA-C	6.71	123.67	113.61
1	2-N	465	TYR	N-CA-C	6.71	123.67	113.61
1	3-N	465	TYR	N-CA-C	6.71	123.67	113.61
1	4-N	465	TYR	N-CA-C	6.71	123.67	113.61
1	5-N	465	TYR	N-CA-C	6.71	123.67	113.61
1	6-N	465	TYR	N-CA-C	6.71	123.67	113.61
1	7-N	465	TYR	N-CA-C	6.71	123.67	113.61
1	8-N	465	TYR	N-CA-C	6.71	123.67	113.61
1	9-N	465	TYR	N-CA-C	6.71	123.67	113.61
1	10-N	465	TYR	N-CA-C	6.71	123.67	113.61
1	1-U	465	TYR	N-CA-C	6.71	123.67	113.61
1	2-U	465	TYR	N-CA-C	6.71	123.67	113.61
1	3-U	465	TYR	N-CA-C	6.71	123.67	113.61
1	4-U	465	TYR	N-CA-C	6.71	123.67	113.61
1	5-U	465	TYR	N-CA-C	6.71	123.67	113.61
1	6-U	465	TYR	N-CA-C	6.71	123.67	113.61
1	7-U	465	TYR	N-CA-C	6.71	123.67	113.61
1	8-U	465	TYR	N-CA-C	6.71	123.67	113.61
1	9-U	465	TYR	N-CA-C	6.71	123.67	113.61
1	10-U	465	TYR	N-CA-C	6.71	123.67	113.61
1	1-B	465	TYR	N-CA-C	6.71	123.67	113.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-M	465	TYR	N-CA-C	6.71	123.67	113.61
1	2-B	465	TYR	N-CA-C	6.71	123.67	113.61
1	2-M	465	TYR	N-CA-C	6.71	123.67	113.61
1	3-B	465	TYR	N-CA-C	6.71	123.67	113.61
1	3-M	465	TYR	N-CA-C	6.71	123.67	113.61
1	4-B	465	TYR	N-CA-C	6.71	123.67	113.61
1	4-M	465	TYR	N-CA-C	6.71	123.67	113.61
1	5-B	465	TYR	N-CA-C	6.71	123.67	113.61
1	5-M	465	TYR	N-CA-C	6.71	123.67	113.61
1	6-B	465	TYR	N-CA-C	6.71	123.67	113.61
1	6-M	465	TYR	N-CA-C	6.71	123.67	113.61
1	7-B	465	TYR	N-CA-C	6.71	123.67	113.61
1	7-M	465	TYR	N-CA-C	6.71	123.67	113.61
1	8-B	465	TYR	N-CA-C	6.71	123.67	113.61
1	8-M	465	TYR	N-CA-C	6.71	123.67	113.61
1	9-B	465	TYR	N-CA-C	6.71	123.67	113.61
1	9-M	465	TYR	N-CA-C	6.71	123.67	113.61
1	10-B	465	TYR	N-CA-C	6.71	123.67	113.61
1	10-M	465	TYR	N-CA-C	6.71	123.67	113.61
1	1-H	465	TYR	N-CA-C	6.70	123.66	113.61
1	1-V	465	TYR	N-CA-C	6.70	123.66	113.61
1	2-H	465	TYR	N-CA-C	6.70	123.66	113.61
1	2-V	465	TYR	N-CA-C	6.70	123.66	113.61
1	3-H	465	TYR	N-CA-C	6.70	123.66	113.61
1	3-V	465	TYR	N-CA-C	6.70	123.66	113.61
1	4-H	465	TYR	N-CA-C	6.70	123.66	113.61
1	4-V	465	TYR	N-CA-C	6.70	123.66	113.61
1	5-H	465	TYR	N-CA-C	6.70	123.66	113.61
1	5-V	465	TYR	N-CA-C	6.70	123.66	113.61
1	6-H	465	TYR	N-CA-C	6.70	123.66	113.61
1	6-V	465	TYR	N-CA-C	6.70	123.66	113.61
1	7-H	465	TYR	N-CA-C	6.70	123.66	113.61
1	7-V	465	TYR	N-CA-C	6.70	123.66	113.61
1	8-H	465	TYR	N-CA-C	6.70	123.66	113.61
1	8-V	465	TYR	N-CA-C	6.70	123.66	113.61
1	9-H	465	TYR	N-CA-C	6.70	123.66	113.61
1	9-V	465	TYR	N-CA-C	6.70	123.66	113.61
1	10-H	465	TYR	N-CA-C	6.70	123.66	113.61
1	10-V	465	TYR	N-CA-C	6.70	123.66	113.61
1	1-A	465	TYR	N-CA-C	6.70	123.66	113.61
1	1-G	465	TYR	N-CA-C	6.70	123.66	113.61
1	2-A	465	TYR	N-CA-C	6.70	123.66	113.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-G	465	TYR	N-CA-C	6.70	123.66	113.61
1	3-A	465	TYR	N-CA-C	6.70	123.66	113.61
1	3-G	465	TYR	N-CA-C	6.70	123.66	113.61
1	4-A	465	TYR	N-CA-C	6.70	123.66	113.61
1	4-G	465	TYR	N-CA-C	6.70	123.66	113.61
1	5-A	465	TYR	N-CA-C	6.70	123.66	113.61
1	5-G	465	TYR	N-CA-C	6.70	123.66	113.61
1	6-A	465	TYR	N-CA-C	6.70	123.66	113.61
1	6-G	465	TYR	N-CA-C	6.70	123.66	113.61
1	7-A	465	TYR	N-CA-C	6.70	123.66	113.61
1	7-G	465	TYR	N-CA-C	6.70	123.66	113.61
1	8-A	465	TYR	N-CA-C	6.70	123.66	113.61
1	8-G	465	TYR	N-CA-C	6.70	123.66	113.61
1	9-A	465	TYR	N-CA-C	6.70	123.66	113.61
1	9-G	465	TYR	N-CA-C	6.70	123.66	113.61
1	10-A	465	TYR	N-CA-C	6.70	123.66	113.61
1	10-G	465	TYR	N-CA-C	6.70	123.66	113.61
1	1-L	465	TYR	N-CA-C	6.69	123.65	113.61
1	1-X	465	TYR	N-CA-C	6.69	123.65	113.61
1	2-L	465	TYR	N-CA-C	6.69	123.65	113.61
1	2-X	465	TYR	N-CA-C	6.69	123.65	113.61
1	3-L	465	TYR	N-CA-C	6.69	123.65	113.61
1	3-X	465	TYR	N-CA-C	6.69	123.65	113.61
1	4-L	465	TYR	N-CA-C	6.69	123.65	113.61
1	4-X	465	TYR	N-CA-C	6.69	123.65	113.61
1	5-L	465	TYR	N-CA-C	6.69	123.65	113.61
1	5-X	465	TYR	N-CA-C	6.69	123.65	113.61
1	6-L	465	TYR	N-CA-C	6.69	123.65	113.61
1	6-X	465	TYR	N-CA-C	6.69	123.65	113.61
1	7-L	465	TYR	N-CA-C	6.69	123.65	113.61
1	7-X	465	TYR	N-CA-C	6.69	123.65	113.61
1	8-L	465	TYR	N-CA-C	6.69	123.65	113.61
1	8-X	465	TYR	N-CA-C	6.69	123.65	113.61
1	9-L	465	TYR	N-CA-C	6.69	123.65	113.61
1	9-X	465	TYR	N-CA-C	6.69	123.65	113.61
1	10-L	465	TYR	N-CA-C	6.69	123.65	113.61
1	10-X	465	TYR	N-CA-C	6.69	123.65	113.61
1	1-W	465	TYR	N-CA-C	6.69	123.65	113.61
1	2-W	465	TYR	N-CA-C	6.69	123.65	113.61
1	3-W	465	TYR	N-CA-C	6.69	123.65	113.61
1	4-W	465	TYR	N-CA-C	6.69	123.65	113.61
1	5-W	465	TYR	N-CA-C	6.69	123.65	113.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-W	465	TYR	N-CA-C	6.69	123.65	113.61
1	7-W	465	TYR	N-CA-C	6.69	123.65	113.61
1	8-W	465	TYR	N-CA-C	6.69	123.65	113.61
1	9-W	465	TYR	N-CA-C	6.69	123.65	113.61
1	10-W	465	TYR	N-CA-C	6.69	123.65	113.61
1	1-I	465	TYR	N-CA-C	6.69	123.65	113.61
1	2-I	465	TYR	N-CA-C	6.69	123.65	113.61
1	3-I	465	TYR	N-CA-C	6.69	123.65	113.61
1	4-I	465	TYR	N-CA-C	6.69	123.65	113.61
1	5-I	465	TYR	N-CA-C	6.69	123.65	113.61
1	6-I	465	TYR	N-CA-C	6.69	123.65	113.61
1	7-I	465	TYR	N-CA-C	6.69	123.65	113.61
1	8-I	465	TYR	N-CA-C	6.69	123.65	113.61
1	9-I	465	TYR	N-CA-C	6.69	123.65	113.61
1	10-I	465	TYR	N-CA-C	6.69	123.65	113.61
1	1-T	465	TYR	N-CA-C	6.69	123.64	113.61
1	2-T	465	TYR	N-CA-C	6.69	123.64	113.61
1	3-T	465	TYR	N-CA-C	6.69	123.64	113.61
1	4-T	465	TYR	N-CA-C	6.69	123.64	113.61
1	5-T	465	TYR	N-CA-C	6.69	123.64	113.61
1	6-T	465	TYR	N-CA-C	6.69	123.64	113.61
1	7-T	465	TYR	N-CA-C	6.69	123.64	113.61
1	8-T	465	TYR	N-CA-C	6.69	123.64	113.61
1	9-T	465	TYR	N-CA-C	6.69	123.64	113.61
1	10-T	465	TYR	N-CA-C	6.69	123.64	113.61
1	1-J	465	TYR	N-CA-C	6.68	123.63	113.61
1	2-J	465	TYR	N-CA-C	6.68	123.63	113.61
1	3-J	465	TYR	N-CA-C	6.68	123.63	113.61
1	4-J	465	TYR	N-CA-C	6.68	123.63	113.61
1	5-J	465	TYR	N-CA-C	6.68	123.63	113.61
1	6-J	465	TYR	N-CA-C	6.68	123.63	113.61
1	7-J	465	TYR	N-CA-C	6.68	123.63	113.61
1	8-J	465	TYR	N-CA-C	6.68	123.63	113.61
1	9-J	465	TYR	N-CA-C	6.68	123.63	113.61
1	10-J	465	TYR	N-CA-C	6.68	123.63	113.61
1	1-F	465	TYR	N-CA-C	6.68	123.63	113.61
1	1-K	465	TYR	N-CA-C	6.68	123.63	113.61
1	2-F	465	TYR	N-CA-C	6.68	123.63	113.61
1	2-K	465	TYR	N-CA-C	6.68	123.63	113.61
1	3-F	465	TYR	N-CA-C	6.68	123.63	113.61
1	3-K	465	TYR	N-CA-C	6.68	123.63	113.61
1	4-F	465	TYR	N-CA-C	6.68	123.63	113.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-K	465	TYR	N-CA-C	6.68	123.63	113.61
1	5-F	465	TYR	N-CA-C	6.68	123.63	113.61
1	5-K	465	TYR	N-CA-C	6.68	123.63	113.61
1	6-F	465	TYR	N-CA-C	6.68	123.63	113.61
1	6-K	465	TYR	N-CA-C	6.68	123.63	113.61
1	7-F	465	TYR	N-CA-C	6.68	123.63	113.61
1	7-K	465	TYR	N-CA-C	6.68	123.63	113.61
1	8-F	465	TYR	N-CA-C	6.68	123.63	113.61
1	8-K	465	TYR	N-CA-C	6.68	123.63	113.61
1	9-F	465	TYR	N-CA-C	6.68	123.63	113.61
1	9-K	465	TYR	N-CA-C	6.68	123.63	113.61
1	10-F	465	TYR	N-CA-C	6.68	123.63	113.61
1	10-K	465	TYR	N-CA-C	6.68	123.63	113.61
1	1-D	465	TYR	N-CA-C	6.68	123.63	113.61
1	1-S	465	TYR	N-CA-C	6.68	123.62	113.61
1	2-D	465	TYR	N-CA-C	6.68	123.63	113.61
1	2-S	465	TYR	N-CA-C	6.68	123.62	113.61
1	3-D	465	TYR	N-CA-C	6.68	123.63	113.61
1	3-S	465	TYR	N-CA-C	6.68	123.62	113.61
1	4-D	465	TYR	N-CA-C	6.68	123.63	113.61
1	4-S	465	TYR	N-CA-C	6.68	123.62	113.61
1	5-D	465	TYR	N-CA-C	6.68	123.63	113.61
1	5-S	465	TYR	N-CA-C	6.68	123.62	113.61
1	6-D	465	TYR	N-CA-C	6.68	123.63	113.61
1	6-S	465	TYR	N-CA-C	6.68	123.62	113.61
1	7-D	465	TYR	N-CA-C	6.68	123.63	113.61
1	7-S	465	TYR	N-CA-C	6.68	123.62	113.61
1	8-D	465	TYR	N-CA-C	6.68	123.63	113.61
1	8-S	465	TYR	N-CA-C	6.68	123.62	113.61
1	9-D	465	TYR	N-CA-C	6.68	123.63	113.61
1	9-S	465	TYR	N-CA-C	6.68	123.62	113.61
1	10-D	465	TYR	N-CA-C	6.68	123.63	113.61
1	10-S	465	TYR	N-CA-C	6.68	123.62	113.61
1	1-O	465	TYR	N-CA-C	6.67	123.62	113.61
1	2-O	465	TYR	N-CA-C	6.67	123.62	113.61
1	3-O	465	TYR	N-CA-C	6.67	123.62	113.61
1	4-O	465	TYR	N-CA-C	6.67	123.62	113.61
1	5-O	465	TYR	N-CA-C	6.67	123.62	113.61
1	6-O	465	TYR	N-CA-C	6.67	123.62	113.61
1	7-O	465	TYR	N-CA-C	6.67	123.62	113.61
1	8-O	465	TYR	N-CA-C	6.67	123.62	113.61
1	9-O	465	TYR	N-CA-C	6.67	123.62	113.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-O	465	TYR	N-CA-C	6.67	123.62	113.61
1	1-C	465	TYR	N-CA-C	6.67	123.62	113.61
1	2-C	465	TYR	N-CA-C	6.67	123.62	113.61
1	3-C	465	TYR	N-CA-C	6.67	123.62	113.61
1	4-C	465	TYR	N-CA-C	6.67	123.62	113.61
1	5-C	465	TYR	N-CA-C	6.67	123.62	113.61
1	6-C	465	TYR	N-CA-C	6.67	123.62	113.61
1	7-C	465	TYR	N-CA-C	6.67	123.62	113.61
1	8-C	465	TYR	N-CA-C	6.67	123.62	113.61
1	9-C	465	TYR	N-CA-C	6.67	123.62	113.61
1	10-C	465	TYR	N-CA-C	6.67	123.62	113.61
1	1-S	314	PRO	N-CA-C	6.05	121.46	114.20
1	2-S	314	PRO	N-CA-C	6.05	121.46	114.20
1	3-S	314	PRO	N-CA-C	6.05	121.46	114.20
1	4-S	314	PRO	N-CA-C	6.05	121.46	114.20
1	5-S	314	PRO	N-CA-C	6.05	121.46	114.20
1	6-S	314	PRO	N-CA-C	6.05	121.46	114.20
1	7-S	314	PRO	N-CA-C	6.05	121.46	114.20
1	8-S	314	PRO	N-CA-C	6.05	121.46	114.20
1	9-S	314	PRO	N-CA-C	6.05	121.46	114.20
1	10-S	314	PRO	N-CA-C	6.05	121.46	114.20
1	1-F	314	PRO	N-CA-C	6.04	121.44	114.20
1	2-F	314	PRO	N-CA-C	6.04	121.44	114.20
1	3-F	314	PRO	N-CA-C	6.04	121.44	114.20
1	4-F	314	PRO	N-CA-C	6.04	121.44	114.20
1	5-F	314	PRO	N-CA-C	6.04	121.44	114.20
1	6-F	314	PRO	N-CA-C	6.04	121.44	114.20
1	7-F	314	PRO	N-CA-C	6.04	121.44	114.20
1	8-F	314	PRO	N-CA-C	6.04	121.44	114.20
1	9-F	314	PRO	N-CA-C	6.04	121.44	114.20
1	10-F	314	PRO	N-CA-C	6.04	121.44	114.20
1	1-G	314	PRO	N-CA-C	6.03	121.44	114.20
1	2-G	314	PRO	N-CA-C	6.03	121.44	114.20
1	3-G	314	PRO	N-CA-C	6.03	121.44	114.20
1	4-G	314	PRO	N-CA-C	6.03	121.44	114.20
1	5-G	314	PRO	N-CA-C	6.03	121.44	114.20
1	6-G	314	PRO	N-CA-C	6.03	121.44	114.20
1	7-G	314	PRO	N-CA-C	6.03	121.44	114.20
1	8-G	314	PRO	N-CA-C	6.03	121.44	114.20
1	9-G	314	PRO	N-CA-C	6.03	121.44	114.20
1	10-G	314	PRO	N-CA-C	6.03	121.44	114.20
1	1-E	314	PRO	N-CA-C	6.03	121.43	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-E	314	PRO	N-CA-C	6.03	121.43	114.20
1	3-E	314	PRO	N-CA-C	6.03	121.43	114.20
1	4-E	314	PRO	N-CA-C	6.03	121.43	114.20
1	5-E	314	PRO	N-CA-C	6.03	121.43	114.20
1	6-E	314	PRO	N-CA-C	6.03	121.43	114.20
1	7-E	314	PRO	N-CA-C	6.03	121.43	114.20
1	8-E	314	PRO	N-CA-C	6.03	121.43	114.20
1	9-E	314	PRO	N-CA-C	6.03	121.43	114.20
1	10-E	314	PRO	N-CA-C	6.03	121.43	114.20
1	1-H	314	PRO	N-CA-C	6.02	121.43	114.20
1	2-H	314	PRO	N-CA-C	6.02	121.43	114.20
1	3-H	314	PRO	N-CA-C	6.02	121.43	114.20
1	4-H	314	PRO	N-CA-C	6.02	121.43	114.20
1	5-H	314	PRO	N-CA-C	6.02	121.43	114.20
1	6-H	314	PRO	N-CA-C	6.02	121.43	114.20
1	7-H	314	PRO	N-CA-C	6.02	121.43	114.20
1	8-H	314	PRO	N-CA-C	6.02	121.43	114.20
1	9-H	314	PRO	N-CA-C	6.02	121.43	114.20
1	10-H	314	PRO	N-CA-C	6.02	121.43	114.20
1	1-C	314	PRO	N-CA-C	6.02	121.42	114.20
1	2-C	314	PRO	N-CA-C	6.02	121.42	114.20
1	3-C	314	PRO	N-CA-C	6.02	121.42	114.20
1	4-C	314	PRO	N-CA-C	6.02	121.42	114.20
1	5-C	314	PRO	N-CA-C	6.02	121.42	114.20
1	6-C	314	PRO	N-CA-C	6.02	121.42	114.20
1	7-C	314	PRO	N-CA-C	6.02	121.42	114.20
1	8-C	314	PRO	N-CA-C	6.02	121.42	114.20
1	9-C	314	PRO	N-CA-C	6.02	121.42	114.20
1	10-C	314	PRO	N-CA-C	6.02	121.42	114.20
1	1-K	314	PRO	N-CA-C	6.02	121.42	114.20
1	2-K	314	PRO	N-CA-C	6.02	121.42	114.20
1	3-K	314	PRO	N-CA-C	6.02	121.42	114.20
1	4-K	314	PRO	N-CA-C	6.02	121.42	114.20
1	5-K	314	PRO	N-CA-C	6.02	121.42	114.20
1	6-K	314	PRO	N-CA-C	6.02	121.42	114.20
1	7-K	314	PRO	N-CA-C	6.02	121.42	114.20
1	8-K	314	PRO	N-CA-C	6.02	121.42	114.20
1	9-K	314	PRO	N-CA-C	6.02	121.42	114.20
1	10-K	314	PRO	N-CA-C	6.02	121.42	114.20
1	1-X	314	PRO	N-CA-C	6.01	121.42	114.20
1	2-X	314	PRO	N-CA-C	6.01	121.42	114.20
1	3-X	314	PRO	N-CA-C	6.01	121.42	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-X	314	PRO	N-CA-C	6.01	121.42	114.20
1	5-X	314	PRO	N-CA-C	6.01	121.42	114.20
1	6-X	314	PRO	N-CA-C	6.01	121.42	114.20
1	7-X	314	PRO	N-CA-C	6.01	121.42	114.20
1	8-X	314	PRO	N-CA-C	6.01	121.42	114.20
1	9-X	314	PRO	N-CA-C	6.01	121.42	114.20
1	10-X	314	PRO	N-CA-C	6.01	121.42	114.20
1	1-A	314	PRO	N-CA-C	6.01	121.41	114.20
1	1-U	314	PRO	N-CA-C	6.01	121.41	114.20
1	2-A	314	PRO	N-CA-C	6.01	121.41	114.20
1	2-U	314	PRO	N-CA-C	6.01	121.41	114.20
1	3-A	314	PRO	N-CA-C	6.01	121.41	114.20
1	3-U	314	PRO	N-CA-C	6.01	121.41	114.20
1	4-A	314	PRO	N-CA-C	6.01	121.41	114.20
1	4-U	314	PRO	N-CA-C	6.01	121.41	114.20
1	5-A	314	PRO	N-CA-C	6.01	121.41	114.20
1	5-U	314	PRO	N-CA-C	6.01	121.41	114.20
1	6-A	314	PRO	N-CA-C	6.01	121.41	114.20
1	6-U	314	PRO	N-CA-C	6.01	121.41	114.20
1	7-A	314	PRO	N-CA-C	6.01	121.41	114.20
1	7-U	314	PRO	N-CA-C	6.01	121.41	114.20
1	8-A	314	PRO	N-CA-C	6.01	121.41	114.20
1	8-U	314	PRO	N-CA-C	6.01	121.41	114.20
1	9-A	314	PRO	N-CA-C	6.01	121.41	114.20
1	9-U	314	PRO	N-CA-C	6.01	121.41	114.20
1	10-A	314	PRO	N-CA-C	6.01	121.41	114.20
1	10-U	314	PRO	N-CA-C	6.01	121.41	114.20
1	1-L	314	PRO	N-CA-C	6.01	121.41	114.20
1	1-R	314	PRO	N-CA-C	6.01	121.41	114.20
1	2-L	314	PRO	N-CA-C	6.01	121.41	114.20
1	2-R	314	PRO	N-CA-C	6.01	121.41	114.20
1	3-L	314	PRO	N-CA-C	6.01	121.41	114.20
1	3-R	314	PRO	N-CA-C	6.01	121.41	114.20
1	4-L	314	PRO	N-CA-C	6.01	121.41	114.20
1	4-R	314	PRO	N-CA-C	6.01	121.41	114.20
1	5-L	314	PRO	N-CA-C	6.01	121.41	114.20
1	5-R	314	PRO	N-CA-C	6.01	121.41	114.20
1	6-L	314	PRO	N-CA-C	6.01	121.41	114.20
1	6-R	314	PRO	N-CA-C	6.01	121.41	114.20
1	7-L	314	PRO	N-CA-C	6.01	121.41	114.20
1	7-R	314	PRO	N-CA-C	6.01	121.41	114.20
1	8-L	314	PRO	N-CA-C	6.01	121.41	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-R	314	PRO	N-CA-C	6.01	121.41	114.20
1	9-L	314	PRO	N-CA-C	6.01	121.41	114.20
1	9-R	314	PRO	N-CA-C	6.01	121.41	114.20
1	10-L	314	PRO	N-CA-C	6.01	121.41	114.20
1	10-R	314	PRO	N-CA-C	6.01	121.41	114.20
1	1-W	314	PRO	N-CA-C	6.00	121.41	114.20
1	2-W	314	PRO	N-CA-C	6.00	121.41	114.20
1	3-W	314	PRO	N-CA-C	6.00	121.41	114.20
1	4-W	314	PRO	N-CA-C	6.00	121.41	114.20
1	5-W	314	PRO	N-CA-C	6.00	121.41	114.20
1	6-W	314	PRO	N-CA-C	6.00	121.41	114.20
1	7-W	314	PRO	N-CA-C	6.00	121.41	114.20
1	8-W	314	PRO	N-CA-C	6.00	121.41	114.20
1	9-W	314	PRO	N-CA-C	6.00	121.41	114.20
1	10-W	314	PRO	N-CA-C	6.00	121.41	114.20
1	1-V	314	PRO	N-CA-C	6.00	121.40	114.20
1	2-V	314	PRO	N-CA-C	6.00	121.40	114.20
1	3-V	314	PRO	N-CA-C	6.00	121.40	114.20
1	4-V	314	PRO	N-CA-C	6.00	121.40	114.20
1	5-V	314	PRO	N-CA-C	6.00	121.40	114.20
1	6-V	314	PRO	N-CA-C	6.00	121.40	114.20
1	7-V	314	PRO	N-CA-C	6.00	121.40	114.20
1	8-V	314	PRO	N-CA-C	6.00	121.40	114.20
1	9-V	314	PRO	N-CA-C	6.00	121.40	114.20
1	10-V	314	PRO	N-CA-C	6.00	121.40	114.20
1	1-D	314	PRO	N-CA-C	6.00	121.40	114.20
1	1-M	314	PRO	N-CA-C	6.00	121.40	114.20
1	2-D	314	PRO	N-CA-C	6.00	121.40	114.20
1	2-M	314	PRO	N-CA-C	6.00	121.40	114.20
1	3-D	314	PRO	N-CA-C	6.00	121.40	114.20
1	3-M	314	PRO	N-CA-C	6.00	121.40	114.20
1	4-D	314	PRO	N-CA-C	6.00	121.40	114.20
1	4-M	314	PRO	N-CA-C	6.00	121.40	114.20
1	5-D	314	PRO	N-CA-C	6.00	121.40	114.20
1	5-M	314	PRO	N-CA-C	6.00	121.40	114.20
1	6-D	314	PRO	N-CA-C	6.00	121.40	114.20
1	6-M	314	PRO	N-CA-C	6.00	121.40	114.20
1	7-D	314	PRO	N-CA-C	6.00	121.40	114.20
1	7-M	314	PRO	N-CA-C	6.00	121.40	114.20
1	8-D	314	PRO	N-CA-C	6.00	121.40	114.20
1	8-M	314	PRO	N-CA-C	6.00	121.40	114.20
1	9-D	314	PRO	N-CA-C	6.00	121.40	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-M	314	PRO	N-CA-C	6.00	121.40	114.20
1	10-D	314	PRO	N-CA-C	6.00	121.40	114.20
1	10-M	314	PRO	N-CA-C	6.00	121.40	114.20
1	1-T	314	PRO	N-CA-C	6.00	121.39	114.20
1	2-T	314	PRO	N-CA-C	6.00	121.39	114.20
1	3-T	314	PRO	N-CA-C	6.00	121.39	114.20
1	4-T	314	PRO	N-CA-C	6.00	121.39	114.20
1	5-T	314	PRO	N-CA-C	6.00	121.39	114.20
1	6-T	314	PRO	N-CA-C	6.00	121.39	114.20
1	7-T	314	PRO	N-CA-C	6.00	121.39	114.20
1	8-T	314	PRO	N-CA-C	6.00	121.39	114.20
1	9-T	314	PRO	N-CA-C	6.00	121.39	114.20
1	10-T	314	PRO	N-CA-C	6.00	121.39	114.20
1	1-N	314	PRO	N-CA-C	5.99	121.39	114.20
1	1-O	314	PRO	N-CA-C	5.99	121.39	114.20
1	2-N	314	PRO	N-CA-C	5.99	121.39	114.20
1	2-O	314	PRO	N-CA-C	5.99	121.39	114.20
1	3-N	314	PRO	N-CA-C	5.99	121.39	114.20
1	3-O	314	PRO	N-CA-C	5.99	121.39	114.20
1	4-N	314	PRO	N-CA-C	5.99	121.39	114.20
1	4-O	314	PRO	N-CA-C	5.99	121.39	114.20
1	5-N	314	PRO	N-CA-C	5.99	121.39	114.20
1	5-O	314	PRO	N-CA-C	5.99	121.39	114.20
1	6-N	314	PRO	N-CA-C	5.99	121.39	114.20
1	6-O	314	PRO	N-CA-C	5.99	121.39	114.20
1	7-N	314	PRO	N-CA-C	5.99	121.39	114.20
1	7-O	314	PRO	N-CA-C	5.99	121.39	114.20
1	8-N	314	PRO	N-CA-C	5.99	121.39	114.20
1	8-O	314	PRO	N-CA-C	5.99	121.39	114.20
1	9-N	314	PRO	N-CA-C	5.99	121.39	114.20
1	9-O	314	PRO	N-CA-C	5.99	121.39	114.20
1	10-N	314	PRO	N-CA-C	5.99	121.39	114.20
1	10-O	314	PRO	N-CA-C	5.99	121.39	114.20
1	1-B	314	PRO	N-CA-C	5.99	121.39	114.20
1	2-B	314	PRO	N-CA-C	5.99	121.39	114.20
1	3-B	314	PRO	N-CA-C	5.99	121.39	114.20
1	4-B	314	PRO	N-CA-C	5.99	121.39	114.20
1	5-B	314	PRO	N-CA-C	5.99	121.39	114.20
1	6-B	314	PRO	N-CA-C	5.99	121.39	114.20
1	7-B	314	PRO	N-CA-C	5.99	121.39	114.20
1	8-B	314	PRO	N-CA-C	5.99	121.39	114.20
1	9-B	314	PRO	N-CA-C	5.99	121.39	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-B	314	PRO	N-CA-C	5.99	121.39	114.20
1	1-I	314	PRO	N-CA-C	5.99	121.39	114.20
1	2-I	314	PRO	N-CA-C	5.99	121.39	114.20
1	3-I	314	PRO	N-CA-C	5.99	121.39	114.20
1	4-I	314	PRO	N-CA-C	5.99	121.39	114.20
1	5-I	314	PRO	N-CA-C	5.99	121.39	114.20
1	6-I	314	PRO	N-CA-C	5.99	121.39	114.20
1	7-I	314	PRO	N-CA-C	5.99	121.39	114.20
1	8-I	314	PRO	N-CA-C	5.99	121.39	114.20
1	9-I	314	PRO	N-CA-C	5.99	121.39	114.20
1	10-I	314	PRO	N-CA-C	5.99	121.39	114.20
1	1-Q	314	PRO	N-CA-C	5.99	121.38	114.20
1	2-Q	314	PRO	N-CA-C	5.99	121.38	114.20
1	3-Q	314	PRO	N-CA-C	5.99	121.38	114.20
1	4-Q	314	PRO	N-CA-C	5.99	121.38	114.20
1	5-Q	314	PRO	N-CA-C	5.99	121.38	114.20
1	6-Q	314	PRO	N-CA-C	5.99	121.38	114.20
1	7-Q	314	PRO	N-CA-C	5.99	121.38	114.20
1	8-Q	314	PRO	N-CA-C	5.99	121.38	114.20
1	9-Q	314	PRO	N-CA-C	5.99	121.38	114.20
1	10-Q	314	PRO	N-CA-C	5.99	121.38	114.20
1	1-P	314	PRO	N-CA-C	5.98	121.38	114.20
1	2-P	314	PRO	N-CA-C	5.98	121.38	114.20
1	3-P	314	PRO	N-CA-C	5.98	121.38	114.20
1	4-P	314	PRO	N-CA-C	5.98	121.38	114.20
1	5-P	314	PRO	N-CA-C	5.98	121.38	114.20
1	6-P	314	PRO	N-CA-C	5.98	121.38	114.20
1	7-P	314	PRO	N-CA-C	5.98	121.38	114.20
1	8-P	314	PRO	N-CA-C	5.98	121.38	114.20
1	9-P	314	PRO	N-CA-C	5.98	121.38	114.20
1	10-P	314	PRO	N-CA-C	5.98	121.38	114.20
1	1-J	314	PRO	N-CA-C	5.98	121.38	114.20
1	2-J	314	PRO	N-CA-C	5.98	121.38	114.20
1	3-J	314	PRO	N-CA-C	5.98	121.38	114.20
1	4-J	314	PRO	N-CA-C	5.98	121.38	114.20
1	5-J	314	PRO	N-CA-C	5.98	121.38	114.20
1	6-J	314	PRO	N-CA-C	5.98	121.38	114.20
1	7-J	314	PRO	N-CA-C	5.98	121.38	114.20
1	8-J	314	PRO	N-CA-C	5.98	121.38	114.20
1	9-J	314	PRO	N-CA-C	5.98	121.38	114.20
1	10-J	314	PRO	N-CA-C	5.98	121.38	114.20
1	1-I	313	ASN	CA-C-N	5.55	126.49	120.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-I	313	ASN	C-N-CA	5.55	126.49	120.83
1	2-I	313	ASN	CA-C-N	5.55	126.49	120.83
1	2-I	313	ASN	C-N-CA	5.55	126.49	120.83
1	3-I	313	ASN	CA-C-N	5.55	126.49	120.83
1	3-I	313	ASN	C-N-CA	5.55	126.49	120.83
1	4-I	313	ASN	CA-C-N	5.55	126.49	120.83
1	4-I	313	ASN	C-N-CA	5.55	126.49	120.83
1	5-I	313	ASN	CA-C-N	5.55	126.49	120.83
1	5-I	313	ASN	C-N-CA	5.55	126.49	120.83
1	6-I	313	ASN	CA-C-N	5.55	126.49	120.83
1	6-I	313	ASN	C-N-CA	5.55	126.49	120.83
1	7-I	313	ASN	CA-C-N	5.55	126.49	120.83
1	7-I	313	ASN	C-N-CA	5.55	126.49	120.83
1	8-I	313	ASN	CA-C-N	5.55	126.49	120.83
1	8-I	313	ASN	C-N-CA	5.55	126.49	120.83
1	9-I	313	ASN	CA-C-N	5.55	126.49	120.83
1	9-I	313	ASN	C-N-CA	5.55	126.49	120.83
1	10-I	313	ASN	CA-C-N	5.55	126.49	120.83
1	10-I	313	ASN	C-N-CA	5.55	126.49	120.83
1	1-K	313	ASN	CA-C-N	5.54	126.27	120.12
1	1-K	313	ASN	C-N-CA	5.54	126.27	120.12
1	1-X	313	ASN	CA-C-N	5.54	126.27	120.12
1	1-X	313	ASN	C-N-CA	5.54	126.27	120.12
1	2-K	313	ASN	CA-C-N	5.54	126.27	120.12
1	2-K	313	ASN	C-N-CA	5.54	126.27	120.12
1	2-X	313	ASN	CA-C-N	5.54	126.27	120.12
1	2-X	313	ASN	C-N-CA	5.54	126.27	120.12
1	3-K	313	ASN	CA-C-N	5.54	126.27	120.12
1	3-K	313	ASN	C-N-CA	5.54	126.27	120.12
1	3-X	313	ASN	CA-C-N	5.54	126.27	120.12
1	3-X	313	ASN	C-N-CA	5.54	126.27	120.12
1	4-K	313	ASN	CA-C-N	5.54	126.27	120.12
1	4-K	313	ASN	C-N-CA	5.54	126.27	120.12
1	4-X	313	ASN	CA-C-N	5.54	126.27	120.12
1	4-X	313	ASN	C-N-CA	5.54	126.27	120.12
1	5-K	313	ASN	CA-C-N	5.54	126.27	120.12
1	5-K	313	ASN	C-N-CA	5.54	126.27	120.12
1	5-X	313	ASN	CA-C-N	5.54	126.27	120.12
1	5-X	313	ASN	C-N-CA	5.54	126.27	120.12
1	6-K	313	ASN	CA-C-N	5.54	126.27	120.12
1	6-K	313	ASN	C-N-CA	5.54	126.27	120.12
1	6-X	313	ASN	CA-C-N	5.54	126.27	120.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-X	313	ASN	C-N-CA	5.54	126.27	120.12
1	7-K	313	ASN	CA-C-N	5.54	126.27	120.12
1	7-K	313	ASN	C-N-CA	5.54	126.27	120.12
1	7-X	313	ASN	CA-C-N	5.54	126.27	120.12
1	7-X	313	ASN	C-N-CA	5.54	126.27	120.12
1	8-K	313	ASN	CA-C-N	5.54	126.27	120.12
1	8-K	313	ASN	C-N-CA	5.54	126.27	120.12
1	8-X	313	ASN	CA-C-N	5.54	126.27	120.12
1	8-X	313	ASN	C-N-CA	5.54	126.27	120.12
1	9-K	313	ASN	CA-C-N	5.54	126.27	120.12
1	9-K	313	ASN	C-N-CA	5.54	126.27	120.12
1	9-X	313	ASN	CA-C-N	5.54	126.27	120.12
1	9-X	313	ASN	C-N-CA	5.54	126.27	120.12
1	10-K	313	ASN	CA-C-N	5.54	126.27	120.12
1	10-K	313	ASN	C-N-CA	5.54	126.27	120.12
1	10-X	313	ASN	CA-C-N	5.54	126.27	120.12
1	10-X	313	ASN	C-N-CA	5.54	126.27	120.12
1	1-Q	313	ASN	CA-C-N	5.53	126.26	120.12
1	1-Q	313	ASN	C-N-CA	5.53	126.26	120.12
1	2-Q	313	ASN	CA-C-N	5.53	126.26	120.12
1	2-Q	313	ASN	C-N-CA	5.53	126.26	120.12
1	3-Q	313	ASN	CA-C-N	5.53	126.26	120.12
1	3-Q	313	ASN	C-N-CA	5.53	126.26	120.12
1	4-Q	313	ASN	CA-C-N	5.53	126.26	120.12
1	4-Q	313	ASN	C-N-CA	5.53	126.26	120.12
1	5-Q	313	ASN	CA-C-N	5.53	126.26	120.12
1	5-Q	313	ASN	C-N-CA	5.53	126.26	120.12
1	6-Q	313	ASN	CA-C-N	5.53	126.26	120.12
1	6-Q	313	ASN	C-N-CA	5.53	126.26	120.12
1	7-Q	313	ASN	CA-C-N	5.53	126.26	120.12
1	7-Q	313	ASN	C-N-CA	5.53	126.26	120.12
1	8-Q	313	ASN	CA-C-N	5.53	126.26	120.12
1	8-Q	313	ASN	C-N-CA	5.53	126.26	120.12
1	9-Q	313	ASN	CA-C-N	5.53	126.26	120.12
1	9-Q	313	ASN	C-N-CA	5.53	126.26	120.12
1	10-Q	313	ASN	CA-C-N	5.53	126.26	120.12
1	10-Q	313	ASN	C-N-CA	5.53	126.26	120.12
1	1-P	313	ASN	CA-C-N	5.53	126.26	120.12
1	1-P	313	ASN	C-N-CA	5.53	126.26	120.12
1	2-P	313	ASN	CA-C-N	5.53	126.26	120.12
1	2-P	313	ASN	C-N-CA	5.53	126.26	120.12
1	3-P	313	ASN	CA-C-N	5.53	126.26	120.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-P	313	ASN	C-N-CA	5.53	126.26	120.12
1	4-P	313	ASN	CA-C-N	5.53	126.26	120.12
1	4-P	313	ASN	C-N-CA	5.53	126.26	120.12
1	5-P	313	ASN	CA-C-N	5.53	126.26	120.12
1	5-P	313	ASN	C-N-CA	5.53	126.26	120.12
1	6-P	313	ASN	CA-C-N	5.53	126.26	120.12
1	6-P	313	ASN	C-N-CA	5.53	126.26	120.12
1	7-P	313	ASN	CA-C-N	5.53	126.26	120.12
1	7-P	313	ASN	C-N-CA	5.53	126.26	120.12
1	8-P	313	ASN	CA-C-N	5.53	126.26	120.12
1	8-P	313	ASN	C-N-CA	5.53	126.26	120.12
1	9-P	313	ASN	CA-C-N	5.53	126.26	120.12
1	9-P	313	ASN	C-N-CA	5.53	126.26	120.12
1	10-P	313	ASN	CA-C-N	5.53	126.26	120.12
1	10-P	313	ASN	C-N-CA	5.53	126.26	120.12
1	1-O	313	ASN	CA-C-N	5.52	126.46	120.83
1	1-O	313	ASN	C-N-CA	5.52	126.46	120.83
1	2-O	313	ASN	CA-C-N	5.52	126.46	120.83
1	2-O	313	ASN	C-N-CA	5.52	126.46	120.83
1	3-O	313	ASN	CA-C-N	5.52	126.46	120.83
1	3-O	313	ASN	C-N-CA	5.52	126.46	120.83
1	4-O	313	ASN	CA-C-N	5.52	126.46	120.83
1	4-O	313	ASN	C-N-CA	5.52	126.46	120.83
1	5-O	313	ASN	CA-C-N	5.52	126.46	120.83
1	5-O	313	ASN	C-N-CA	5.52	126.46	120.83
1	6-O	313	ASN	CA-C-N	5.52	126.46	120.83
1	6-O	313	ASN	C-N-CA	5.52	126.46	120.83
1	7-O	313	ASN	CA-C-N	5.52	126.46	120.83
1	7-O	313	ASN	C-N-CA	5.52	126.46	120.83
1	8-O	313	ASN	CA-C-N	5.52	126.46	120.83
1	8-O	313	ASN	C-N-CA	5.52	126.46	120.83
1	9-O	313	ASN	CA-C-N	5.52	126.46	120.83
1	9-O	313	ASN	C-N-CA	5.52	126.46	120.83
1	10-O	313	ASN	CA-C-N	5.52	126.46	120.83
1	10-O	313	ASN	C-N-CA	5.52	126.46	120.83
1	1-A	313	ASN	CA-C-N	5.52	126.46	120.83
1	1-A	313	ASN	C-N-CA	5.52	126.46	120.83
1	2-A	313	ASN	CA-C-N	5.52	126.46	120.83
1	2-A	313	ASN	C-N-CA	5.52	126.46	120.83
1	3-A	313	ASN	CA-C-N	5.52	126.46	120.83
1	3-A	313	ASN	C-N-CA	5.52	126.46	120.83
1	4-A	313	ASN	CA-C-N	5.52	126.46	120.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	313	ASN	C-N-CA	5.52	126.46	120.83
1	5-A	313	ASN	CA-C-N	5.52	126.46	120.83
1	5-A	313	ASN	C-N-CA	5.52	126.46	120.83
1	6-A	313	ASN	CA-C-N	5.52	126.46	120.83
1	6-A	313	ASN	C-N-CA	5.52	126.46	120.83
1	7-A	313	ASN	CA-C-N	5.52	126.46	120.83
1	7-A	313	ASN	C-N-CA	5.52	126.46	120.83
1	8-A	313	ASN	CA-C-N	5.52	126.46	120.83
1	8-A	313	ASN	C-N-CA	5.52	126.46	120.83
1	9-A	313	ASN	CA-C-N	5.52	126.46	120.83
1	9-A	313	ASN	C-N-CA	5.52	126.46	120.83
1	10-A	313	ASN	CA-C-N	5.52	126.46	120.83
1	10-A	313	ASN	C-N-CA	5.52	126.46	120.83
1	1-F	313	ASN	CA-C-N	5.52	126.24	120.12
1	1-F	313	ASN	C-N-CA	5.52	126.24	120.12
1	1-S	313	ASN	CA-C-N	5.52	126.25	120.12
1	1-S	313	ASN	C-N-CA	5.52	126.25	120.12
1	2-F	313	ASN	CA-C-N	5.52	126.24	120.12
1	2-F	313	ASN	C-N-CA	5.52	126.24	120.12
1	2-S	313	ASN	CA-C-N	5.52	126.25	120.12
1	2-S	313	ASN	C-N-CA	5.52	126.25	120.12
1	3-F	313	ASN	CA-C-N	5.52	126.24	120.12
1	3-F	313	ASN	C-N-CA	5.52	126.24	120.12
1	3-S	313	ASN	CA-C-N	5.52	126.25	120.12
1	3-S	313	ASN	C-N-CA	5.52	126.25	120.12
1	4-F	313	ASN	CA-C-N	5.52	126.24	120.12
1	4-F	313	ASN	C-N-CA	5.52	126.24	120.12
1	4-S	313	ASN	CA-C-N	5.52	126.25	120.12
1	4-S	313	ASN	C-N-CA	5.52	126.25	120.12
1	5-F	313	ASN	CA-C-N	5.52	126.24	120.12
1	5-F	313	ASN	C-N-CA	5.52	126.24	120.12
1	5-S	313	ASN	CA-C-N	5.52	126.25	120.12
1	5-S	313	ASN	C-N-CA	5.52	126.25	120.12
1	6-F	313	ASN	CA-C-N	5.52	126.24	120.12
1	6-F	313	ASN	C-N-CA	5.52	126.24	120.12
1	6-S	313	ASN	CA-C-N	5.52	126.25	120.12
1	6-S	313	ASN	C-N-CA	5.52	126.25	120.12
1	7-F	313	ASN	CA-C-N	5.52	126.24	120.12
1	7-F	313	ASN	C-N-CA	5.52	126.24	120.12
1	7-S	313	ASN	CA-C-N	5.52	126.25	120.12
1	7-S	313	ASN	C-N-CA	5.52	126.25	120.12
1	8-F	313	ASN	CA-C-N	5.52	126.24	120.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-F	313	ASN	C-N-CA	5.52	126.24	120.12
1	8-S	313	ASN	CA-C-N	5.52	126.25	120.12
1	8-S	313	ASN	C-N-CA	5.52	126.25	120.12
1	9-F	313	ASN	CA-C-N	5.52	126.24	120.12
1	9-F	313	ASN	C-N-CA	5.52	126.24	120.12
1	9-S	313	ASN	CA-C-N	5.52	126.25	120.12
1	9-S	313	ASN	C-N-CA	5.52	126.25	120.12
1	10-F	313	ASN	CA-C-N	5.52	126.24	120.12
1	10-F	313	ASN	C-N-CA	5.52	126.24	120.12
1	10-S	313	ASN	CA-C-N	5.52	126.25	120.12
1	10-S	313	ASN	C-N-CA	5.52	126.25	120.12
1	1-G	313	ASN	CA-C-N	5.52	126.46	120.83
1	1-G	313	ASN	C-N-CA	5.52	126.46	120.83
1	2-G	313	ASN	CA-C-N	5.52	126.46	120.83
1	2-G	313	ASN	C-N-CA	5.52	126.46	120.83
1	3-G	313	ASN	CA-C-N	5.52	126.46	120.83
1	3-G	313	ASN	C-N-CA	5.52	126.46	120.83
1	4-G	313	ASN	CA-C-N	5.52	126.46	120.83
1	4-G	313	ASN	C-N-CA	5.52	126.46	120.83
1	5-G	313	ASN	CA-C-N	5.52	126.46	120.83
1	5-G	313	ASN	C-N-CA	5.52	126.46	120.83
1	6-G	313	ASN	CA-C-N	5.52	126.46	120.83
1	6-G	313	ASN	C-N-CA	5.52	126.46	120.83
1	7-G	313	ASN	CA-C-N	5.52	126.46	120.83
1	7-G	313	ASN	C-N-CA	5.52	126.46	120.83
1	8-G	313	ASN	CA-C-N	5.52	126.46	120.83
1	8-G	313	ASN	C-N-CA	5.52	126.46	120.83
1	9-G	313	ASN	CA-C-N	5.52	126.46	120.83
1	9-G	313	ASN	C-N-CA	5.52	126.46	120.83
1	10-G	313	ASN	CA-C-N	5.52	126.46	120.83
1	10-G	313	ASN	C-N-CA	5.52	126.46	120.83
1	1-R	313	ASN	CA-C-N	5.51	126.45	120.83
1	1-R	313	ASN	C-N-CA	5.51	126.45	120.83
1	2-R	313	ASN	CA-C-N	5.51	126.45	120.83
1	2-R	313	ASN	C-N-CA	5.51	126.45	120.83
1	3-R	313	ASN	CA-C-N	5.51	126.45	120.83
1	3-R	313	ASN	C-N-CA	5.51	126.45	120.83
1	4-R	313	ASN	CA-C-N	5.51	126.45	120.83
1	4-R	313	ASN	C-N-CA	5.51	126.45	120.83
1	5-R	313	ASN	CA-C-N	5.51	126.45	120.83
1	5-R	313	ASN	C-N-CA	5.51	126.45	120.83
1	6-R	313	ASN	CA-C-N	5.51	126.45	120.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-R	313	ASN	C-N-CA	5.51	126.45	120.83
1	7-R	313	ASN	CA-C-N	5.51	126.45	120.83
1	7-R	313	ASN	C-N-CA	5.51	126.45	120.83
1	8-R	313	ASN	CA-C-N	5.51	126.45	120.83
1	8-R	313	ASN	C-N-CA	5.51	126.45	120.83
1	9-R	313	ASN	CA-C-N	5.51	126.45	120.83
1	9-R	313	ASN	C-N-CA	5.51	126.45	120.83
1	10-R	313	ASN	CA-C-N	5.51	126.45	120.83
1	10-R	313	ASN	C-N-CA	5.51	126.45	120.83
1	1-T	313	ASN	CA-C-N	5.51	126.24	120.12
1	1-T	313	ASN	C-N-CA	5.51	126.24	120.12
1	2-T	313	ASN	CA-C-N	5.51	126.24	120.12
1	2-T	313	ASN	C-N-CA	5.51	126.24	120.12
1	3-T	313	ASN	CA-C-N	5.51	126.24	120.12
1	3-T	313	ASN	C-N-CA	5.51	126.24	120.12
1	4-T	313	ASN	CA-C-N	5.51	126.24	120.12
1	4-T	313	ASN	C-N-CA	5.51	126.24	120.12
1	5-T	313	ASN	CA-C-N	5.51	126.24	120.12
1	5-T	313	ASN	C-N-CA	5.51	126.24	120.12
1	6-T	313	ASN	CA-C-N	5.51	126.24	120.12
1	6-T	313	ASN	C-N-CA	5.51	126.24	120.12
1	7-T	313	ASN	CA-C-N	5.51	126.24	120.12
1	7-T	313	ASN	C-N-CA	5.51	126.24	120.12
1	8-T	313	ASN	CA-C-N	5.51	126.24	120.12
1	8-T	313	ASN	C-N-CA	5.51	126.24	120.12
1	9-T	313	ASN	CA-C-N	5.51	126.24	120.12
1	9-T	313	ASN	C-N-CA	5.51	126.24	120.12
1	10-T	313	ASN	CA-C-N	5.51	126.24	120.12
1	10-T	313	ASN	C-N-CA	5.51	126.24	120.12
1	1-L	313	ASN	CA-C-N	5.51	126.45	120.83
1	1-L	313	ASN	C-N-CA	5.51	126.45	120.83
1	1-V	313	ASN	CA-C-N	5.51	126.45	120.83
1	1-V	313	ASN	C-N-CA	5.51	126.45	120.83
1	2-L	313	ASN	CA-C-N	5.51	126.45	120.83
1	2-L	313	ASN	C-N-CA	5.51	126.45	120.83
1	2-V	313	ASN	CA-C-N	5.51	126.45	120.83
1	2-V	313	ASN	C-N-CA	5.51	126.45	120.83
1	3-L	313	ASN	CA-C-N	5.51	126.45	120.83
1	3-L	313	ASN	C-N-CA	5.51	126.45	120.83
1	3-V	313	ASN	CA-C-N	5.51	126.45	120.83
1	3-V	313	ASN	C-N-CA	5.51	126.45	120.83
1	4-L	313	ASN	CA-C-N	5.51	126.45	120.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-L	313	ASN	C-N-CA	5.51	126.45	120.83
1	4-V	313	ASN	CA-C-N	5.51	126.45	120.83
1	4-V	313	ASN	C-N-CA	5.51	126.45	120.83
1	5-L	313	ASN	CA-C-N	5.51	126.45	120.83
1	5-L	313	ASN	C-N-CA	5.51	126.45	120.83
1	5-V	313	ASN	CA-C-N	5.51	126.45	120.83
1	5-V	313	ASN	C-N-CA	5.51	126.45	120.83
1	6-L	313	ASN	CA-C-N	5.51	126.45	120.83
1	6-L	313	ASN	C-N-CA	5.51	126.45	120.83
1	6-V	313	ASN	CA-C-N	5.51	126.45	120.83
1	6-V	313	ASN	C-N-CA	5.51	126.45	120.83
1	7-L	313	ASN	CA-C-N	5.51	126.45	120.83
1	7-L	313	ASN	C-N-CA	5.51	126.45	120.83
1	7-V	313	ASN	CA-C-N	5.51	126.45	120.83
1	7-V	313	ASN	C-N-CA	5.51	126.45	120.83
1	8-L	313	ASN	CA-C-N	5.51	126.45	120.83
1	8-L	313	ASN	C-N-CA	5.51	126.45	120.83
1	8-V	313	ASN	CA-C-N	5.51	126.45	120.83
1	8-V	313	ASN	C-N-CA	5.51	126.45	120.83
1	9-L	313	ASN	CA-C-N	5.51	126.45	120.83
1	9-L	313	ASN	C-N-CA	5.51	126.45	120.83
1	9-V	313	ASN	CA-C-N	5.51	126.45	120.83
1	9-V	313	ASN	C-N-CA	5.51	126.45	120.83
1	10-L	313	ASN	CA-C-N	5.51	126.45	120.83
1	10-L	313	ASN	C-N-CA	5.51	126.45	120.83
1	10-V	313	ASN	CA-C-N	5.51	126.45	120.83
1	10-V	313	ASN	C-N-CA	5.51	126.45	120.83
1	1-N	313	ASN	CA-C-N	5.51	126.45	120.83
1	1-N	313	ASN	C-N-CA	5.51	126.45	120.83
1	2-N	313	ASN	CA-C-N	5.51	126.45	120.83
1	2-N	313	ASN	C-N-CA	5.51	126.45	120.83
1	3-N	313	ASN	CA-C-N	5.51	126.45	120.83
1	3-N	313	ASN	C-N-CA	5.51	126.45	120.83
1	4-N	313	ASN	CA-C-N	5.51	126.45	120.83
1	4-N	313	ASN	C-N-CA	5.51	126.45	120.83
1	5-N	313	ASN	CA-C-N	5.51	126.45	120.83
1	5-N	313	ASN	C-N-CA	5.51	126.45	120.83
1	6-N	313	ASN	CA-C-N	5.51	126.45	120.83
1	6-N	313	ASN	C-N-CA	5.51	126.45	120.83
1	7-N	313	ASN	CA-C-N	5.51	126.45	120.83
1	7-N	313	ASN	C-N-CA	5.51	126.45	120.83
1	8-N	313	ASN	CA-C-N	5.51	126.45	120.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-N	313	ASN	C-N-CA	5.51	126.45	120.83
1	9-N	313	ASN	CA-C-N	5.51	126.45	120.83
1	9-N	313	ASN	C-N-CA	5.51	126.45	120.83
1	10-N	313	ASN	CA-C-N	5.51	126.45	120.83
1	10-N	313	ASN	C-N-CA	5.51	126.45	120.83
1	1-U	313	ASN	CA-C-N	5.50	126.22	120.12
1	1-U	313	ASN	C-N-CA	5.50	126.22	120.12
1	1-W	313	ASN	CA-C-N	5.50	126.44	120.83
1	1-W	313	ASN	C-N-CA	5.50	126.44	120.83
1	2-U	313	ASN	CA-C-N	5.50	126.22	120.12
1	2-U	313	ASN	C-N-CA	5.50	126.22	120.12
1	2-W	313	ASN	CA-C-N	5.50	126.44	120.83
1	2-W	313	ASN	C-N-CA	5.50	126.44	120.83
1	3-U	313	ASN	CA-C-N	5.50	126.22	120.12
1	3-U	313	ASN	C-N-CA	5.50	126.22	120.12
1	3-W	313	ASN	CA-C-N	5.50	126.44	120.83
1	3-W	313	ASN	C-N-CA	5.50	126.44	120.83
1	4-U	313	ASN	CA-C-N	5.50	126.22	120.12
1	4-U	313	ASN	C-N-CA	5.50	126.22	120.12
1	4-W	313	ASN	CA-C-N	5.50	126.44	120.83
1	4-W	313	ASN	C-N-CA	5.50	126.44	120.83
1	5-U	313	ASN	CA-C-N	5.50	126.22	120.12
1	5-U	313	ASN	C-N-CA	5.50	126.22	120.12
1	5-W	313	ASN	CA-C-N	5.50	126.44	120.83
1	5-W	313	ASN	C-N-CA	5.50	126.44	120.83
1	6-U	313	ASN	CA-C-N	5.50	126.22	120.12
1	6-U	313	ASN	C-N-CA	5.50	126.22	120.12
1	6-W	313	ASN	CA-C-N	5.50	126.44	120.83
1	6-W	313	ASN	C-N-CA	5.50	126.44	120.83
1	7-U	313	ASN	CA-C-N	5.50	126.22	120.12
1	7-U	313	ASN	C-N-CA	5.50	126.22	120.12
1	7-W	313	ASN	CA-C-N	5.50	126.44	120.83
1	7-W	313	ASN	C-N-CA	5.50	126.44	120.83
1	8-U	313	ASN	CA-C-N	5.50	126.22	120.12
1	8-U	313	ASN	C-N-CA	5.50	126.22	120.12
1	8-W	313	ASN	CA-C-N	5.50	126.44	120.83
1	8-W	313	ASN	C-N-CA	5.50	126.44	120.83
1	9-U	313	ASN	CA-C-N	5.50	126.22	120.12
1	9-U	313	ASN	C-N-CA	5.50	126.22	120.12
1	9-W	313	ASN	CA-C-N	5.50	126.44	120.83
1	9-W	313	ASN	C-N-CA	5.50	126.44	120.83
1	10-U	313	ASN	CA-C-N	5.50	126.22	120.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-U	313	ASN	C-N-CA	5.50	126.22	120.12
1	10-W	313	ASN	CA-C-N	5.50	126.44	120.83
1	10-W	313	ASN	C-N-CA	5.50	126.44	120.83
1	1-J	313	ASN	CA-C-N	5.49	126.43	120.83
1	1-J	313	ASN	C-N-CA	5.49	126.43	120.83
1	2-J	313	ASN	CA-C-N	5.49	126.43	120.83
1	2-J	313	ASN	C-N-CA	5.49	126.43	120.83
1	3-J	313	ASN	CA-C-N	5.49	126.43	120.83
1	3-J	313	ASN	C-N-CA	5.49	126.43	120.83
1	4-J	313	ASN	CA-C-N	5.49	126.43	120.83
1	4-J	313	ASN	C-N-CA	5.49	126.43	120.83
1	5-J	313	ASN	CA-C-N	5.49	126.43	120.83
1	5-J	313	ASN	C-N-CA	5.49	126.43	120.83
1	6-J	313	ASN	CA-C-N	5.49	126.43	120.83
1	6-J	313	ASN	C-N-CA	5.49	126.43	120.83
1	7-J	313	ASN	CA-C-N	5.49	126.43	120.83
1	7-J	313	ASN	C-N-CA	5.49	126.43	120.83
1	8-J	313	ASN	CA-C-N	5.49	126.43	120.83
1	8-J	313	ASN	C-N-CA	5.49	126.43	120.83
1	9-J	313	ASN	CA-C-N	5.49	126.43	120.83
1	9-J	313	ASN	C-N-CA	5.49	126.43	120.83
1	10-J	313	ASN	CA-C-N	5.49	126.43	120.83
1	10-J	313	ASN	C-N-CA	5.49	126.43	120.83
1	1-H	313	ASN	CA-C-N	5.49	126.43	120.83
1	1-H	313	ASN	C-N-CA	5.49	126.43	120.83
1	2-H	313	ASN	CA-C-N	5.49	126.43	120.83
1	2-H	313	ASN	C-N-CA	5.49	126.43	120.83
1	3-H	313	ASN	CA-C-N	5.49	126.43	120.83
1	3-H	313	ASN	C-N-CA	5.49	126.43	120.83
1	4-H	313	ASN	CA-C-N	5.49	126.43	120.83
1	4-H	313	ASN	C-N-CA	5.49	126.43	120.83
1	5-H	313	ASN	CA-C-N	5.49	126.43	120.83
1	5-H	313	ASN	C-N-CA	5.49	126.43	120.83
1	6-H	313	ASN	CA-C-N	5.49	126.43	120.83
1	6-H	313	ASN	C-N-CA	5.49	126.43	120.83
1	7-H	313	ASN	CA-C-N	5.49	126.43	120.83
1	7-H	313	ASN	C-N-CA	5.49	126.43	120.83
1	8-H	313	ASN	CA-C-N	5.49	126.43	120.83
1	8-H	313	ASN	C-N-CA	5.49	126.43	120.83
1	9-H	313	ASN	CA-C-N	5.49	126.43	120.83
1	9-H	313	ASN	C-N-CA	5.49	126.43	120.83
1	10-H	313	ASN	CA-C-N	5.49	126.43	120.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-H	313	ASN	C-N-CA	5.49	126.43	120.83
1	1-M	313	ASN	CA-C-N	5.48	126.42	120.83
1	1-M	313	ASN	C-N-CA	5.48	126.42	120.83
1	2-M	313	ASN	CA-C-N	5.48	126.42	120.83
1	2-M	313	ASN	C-N-CA	5.48	126.42	120.83
1	3-M	313	ASN	CA-C-N	5.48	126.42	120.83
1	3-M	313	ASN	C-N-CA	5.48	126.42	120.83
1	4-M	313	ASN	CA-C-N	5.48	126.42	120.83
1	4-M	313	ASN	C-N-CA	5.48	126.42	120.83
1	5-M	313	ASN	CA-C-N	5.48	126.42	120.83
1	5-M	313	ASN	C-N-CA	5.48	126.42	120.83
1	6-M	313	ASN	CA-C-N	5.48	126.42	120.83
1	6-M	313	ASN	C-N-CA	5.48	126.42	120.83
1	7-M	313	ASN	CA-C-N	5.48	126.42	120.83
1	7-M	313	ASN	C-N-CA	5.48	126.42	120.83
1	8-M	313	ASN	CA-C-N	5.48	126.42	120.83
1	8-M	313	ASN	C-N-CA	5.48	126.42	120.83
1	9-M	313	ASN	CA-C-N	5.48	126.42	120.83
1	9-M	313	ASN	C-N-CA	5.48	126.42	120.83
1	10-M	313	ASN	CA-C-N	5.48	126.42	120.83
1	10-M	313	ASN	C-N-CA	5.48	126.42	120.83
1	1-B	313	ASN	CA-C-N	5.48	126.42	120.83
1	1-B	313	ASN	C-N-CA	5.48	126.42	120.83
1	1-D	313	ASN	CA-C-N	5.48	126.42	120.83
1	1-D	313	ASN	C-N-CA	5.48	126.42	120.83
1	2-B	313	ASN	CA-C-N	5.48	126.42	120.83
1	2-B	313	ASN	C-N-CA	5.48	126.42	120.83
1	2-D	313	ASN	CA-C-N	5.48	126.42	120.83
1	2-D	313	ASN	C-N-CA	5.48	126.42	120.83
1	3-B	313	ASN	CA-C-N	5.48	126.42	120.83
1	3-B	313	ASN	C-N-CA	5.48	126.42	120.83
1	3-D	313	ASN	CA-C-N	5.48	126.42	120.83
1	3-D	313	ASN	C-N-CA	5.48	126.42	120.83
1	4-B	313	ASN	CA-C-N	5.48	126.42	120.83
1	4-B	313	ASN	C-N-CA	5.48	126.42	120.83
1	4-D	313	ASN	CA-C-N	5.48	126.42	120.83
1	4-D	313	ASN	C-N-CA	5.48	126.42	120.83
1	5-B	313	ASN	CA-C-N	5.48	126.42	120.83
1	5-B	313	ASN	C-N-CA	5.48	126.42	120.83
1	5-D	313	ASN	CA-C-N	5.48	126.42	120.83
1	5-D	313	ASN	C-N-CA	5.48	126.42	120.83
1	6-B	313	ASN	CA-C-N	5.48	126.42	120.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-B	313	ASN	C-N-CA	5.48	126.42	120.83
1	6-D	313	ASN	CA-C-N	5.48	126.42	120.83
1	6-D	313	ASN	C-N-CA	5.48	126.42	120.83
1	7-B	313	ASN	CA-C-N	5.48	126.42	120.83
1	7-B	313	ASN	C-N-CA	5.48	126.42	120.83
1	7-D	313	ASN	CA-C-N	5.48	126.42	120.83
1	7-D	313	ASN	C-N-CA	5.48	126.42	120.83
1	8-B	313	ASN	CA-C-N	5.48	126.42	120.83
1	8-B	313	ASN	C-N-CA	5.48	126.42	120.83
1	8-D	313	ASN	CA-C-N	5.48	126.42	120.83
1	8-D	313	ASN	C-N-CA	5.48	126.42	120.83
1	9-B	313	ASN	CA-C-N	5.48	126.42	120.83
1	9-B	313	ASN	C-N-CA	5.48	126.42	120.83
1	9-D	313	ASN	CA-C-N	5.48	126.42	120.83
1	9-D	313	ASN	C-N-CA	5.48	126.42	120.83
1	10-B	313	ASN	CA-C-N	5.48	126.42	120.83
1	10-B	313	ASN	C-N-CA	5.48	126.42	120.83
1	10-D	313	ASN	CA-C-N	5.48	126.42	120.83
1	10-D	313	ASN	C-N-CA	5.48	126.42	120.83
1	1-C	313	ASN	CA-C-N	5.48	126.42	120.83
1	1-C	313	ASN	C-N-CA	5.48	126.42	120.83
1	1-E	313	ASN	CA-C-N	5.48	126.42	120.83
1	1-E	313	ASN	C-N-CA	5.48	126.42	120.83
1	2-C	313	ASN	CA-C-N	5.48	126.42	120.83
1	2-C	313	ASN	C-N-CA	5.48	126.42	120.83
1	2-E	313	ASN	CA-C-N	5.48	126.42	120.83
1	2-E	313	ASN	C-N-CA	5.48	126.42	120.83
1	3-C	313	ASN	CA-C-N	5.48	126.42	120.83
1	3-C	313	ASN	C-N-CA	5.48	126.42	120.83
1	3-E	313	ASN	CA-C-N	5.48	126.42	120.83
1	3-E	313	ASN	C-N-CA	5.48	126.42	120.83
1	4-C	313	ASN	CA-C-N	5.48	126.42	120.83
1	4-C	313	ASN	C-N-CA	5.48	126.42	120.83
1	4-E	313	ASN	CA-C-N	5.48	126.42	120.83
1	4-E	313	ASN	C-N-CA	5.48	126.42	120.83
1	5-C	313	ASN	CA-C-N	5.48	126.42	120.83
1	5-C	313	ASN	C-N-CA	5.48	126.42	120.83
1	5-E	313	ASN	CA-C-N	5.48	126.42	120.83
1	5-E	313	ASN	C-N-CA	5.48	126.42	120.83
1	6-C	313	ASN	CA-C-N	5.48	126.42	120.83
1	6-C	313	ASN	C-N-CA	5.48	126.42	120.83
1	6-E	313	ASN	CA-C-N	5.48	126.42	120.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-E	313	ASN	C-N-CA	5.48	126.42	120.83
1	7-C	313	ASN	CA-C-N	5.48	126.42	120.83
1	7-C	313	ASN	C-N-CA	5.48	126.42	120.83
1	7-E	313	ASN	CA-C-N	5.48	126.42	120.83
1	7-E	313	ASN	C-N-CA	5.48	126.42	120.83
1	8-C	313	ASN	CA-C-N	5.48	126.42	120.83
1	8-C	313	ASN	C-N-CA	5.48	126.42	120.83
1	8-E	313	ASN	CA-C-N	5.48	126.42	120.83
1	8-E	313	ASN	C-N-CA	5.48	126.42	120.83
1	9-C	313	ASN	CA-C-N	5.48	126.42	120.83
1	9-C	313	ASN	C-N-CA	5.48	126.42	120.83
1	9-E	313	ASN	CA-C-N	5.48	126.42	120.83
1	9-E	313	ASN	C-N-CA	5.48	126.42	120.83
1	10-C	313	ASN	CA-C-N	5.48	126.42	120.83
1	10-C	313	ASN	C-N-CA	5.48	126.42	120.83
1	10-E	313	ASN	CA-C-N	5.48	126.42	120.83
1	10-E	313	ASN	C-N-CA	5.48	126.42	120.83
1	1-W	245	THR	N-CA-C	-5.24	105.64	111.36
1	2-W	245	THR	N-CA-C	-5.24	105.64	111.36
1	3-W	245	THR	N-CA-C	-5.24	105.64	111.36
1	4-W	245	THR	N-CA-C	-5.24	105.64	111.36
1	5-W	245	THR	N-CA-C	-5.24	105.64	111.36
1	6-W	245	THR	N-CA-C	-5.24	105.64	111.36
1	7-W	245	THR	N-CA-C	-5.24	105.64	111.36
1	8-W	245	THR	N-CA-C	-5.24	105.64	111.36
1	9-W	245	THR	N-CA-C	-5.24	105.64	111.36
1	10-W	245	THR	N-CA-C	-5.24	105.64	111.36
1	1-K	245	THR	N-CA-C	-5.24	105.65	111.36
1	2-K	245	THR	N-CA-C	-5.24	105.65	111.36
1	3-K	245	THR	N-CA-C	-5.24	105.65	111.36
1	4-K	245	THR	N-CA-C	-5.24	105.65	111.36
1	5-K	245	THR	N-CA-C	-5.24	105.65	111.36
1	6-K	245	THR	N-CA-C	-5.24	105.65	111.36
1	7-K	245	THR	N-CA-C	-5.24	105.65	111.36
1	8-K	245	THR	N-CA-C	-5.24	105.65	111.36
1	9-K	245	THR	N-CA-C	-5.24	105.65	111.36
1	10-K	245	THR	N-CA-C	-5.24	105.65	111.36
1	1-G	245	THR	N-CA-C	-5.22	105.67	111.36
1	2-G	245	THR	N-CA-C	-5.22	105.67	111.36
1	3-G	245	THR	N-CA-C	-5.22	105.67	111.36
1	4-G	245	THR	N-CA-C	-5.22	105.67	111.36
1	5-G	245	THR	N-CA-C	-5.22	105.67	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-G	245	THR	N-CA-C	-5.22	105.67	111.36
1	7-G	245	THR	N-CA-C	-5.22	105.67	111.36
1	8-G	245	THR	N-CA-C	-5.22	105.67	111.36
1	9-G	245	THR	N-CA-C	-5.22	105.67	111.36
1	10-G	245	THR	N-CA-C	-5.22	105.67	111.36
1	1-E	245	THR	N-CA-C	-5.22	105.67	111.36
1	1-N	245	THR	N-CA-C	-5.22	105.67	111.36
1	2-E	245	THR	N-CA-C	-5.22	105.67	111.36
1	2-N	245	THR	N-CA-C	-5.22	105.67	111.36
1	3-E	245	THR	N-CA-C	-5.22	105.67	111.36
1	3-N	245	THR	N-CA-C	-5.22	105.67	111.36
1	4-E	245	THR	N-CA-C	-5.22	105.67	111.36
1	4-N	245	THR	N-CA-C	-5.22	105.67	111.36
1	5-E	245	THR	N-CA-C	-5.22	105.67	111.36
1	5-N	245	THR	N-CA-C	-5.22	105.67	111.36
1	6-E	245	THR	N-CA-C	-5.22	105.67	111.36
1	6-N	245	THR	N-CA-C	-5.22	105.67	111.36
1	7-E	245	THR	N-CA-C	-5.22	105.67	111.36
1	7-N	245	THR	N-CA-C	-5.22	105.67	111.36
1	8-E	245	THR	N-CA-C	-5.22	105.67	111.36
1	8-N	245	THR	N-CA-C	-5.22	105.67	111.36
1	9-E	245	THR	N-CA-C	-5.22	105.67	111.36
1	9-N	245	THR	N-CA-C	-5.22	105.67	111.36
1	10-E	245	THR	N-CA-C	-5.22	105.67	111.36
1	10-N	245	THR	N-CA-C	-5.22	105.67	111.36
1	1-I	245	THR	N-CA-C	-5.22	105.67	111.36
1	2-I	245	THR	N-CA-C	-5.22	105.67	111.36
1	3-I	245	THR	N-CA-C	-5.22	105.67	111.36
1	4-I	245	THR	N-CA-C	-5.22	105.67	111.36
1	5-I	245	THR	N-CA-C	-5.22	105.67	111.36
1	6-I	245	THR	N-CA-C	-5.22	105.67	111.36
1	7-I	245	THR	N-CA-C	-5.22	105.67	111.36
1	8-I	245	THR	N-CA-C	-5.22	105.67	111.36
1	9-I	245	THR	N-CA-C	-5.22	105.67	111.36
1	10-I	245	THR	N-CA-C	-5.22	105.67	111.36
1	1-C	245	THR	N-CA-C	-5.22	105.67	111.36
1	1-J	245	THR	N-CA-C	-5.22	105.67	111.36
1	2-C	245	THR	N-CA-C	-5.22	105.67	111.36
1	2-J	245	THR	N-CA-C	-5.22	105.67	111.36
1	3-C	245	THR	N-CA-C	-5.22	105.67	111.36
1	3-J	245	THR	N-CA-C	-5.22	105.67	111.36
1	4-C	245	THR	N-CA-C	-5.22	105.67	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-J	245	THR	N-CA-C	-5.22	105.67	111.36
1	5-C	245	THR	N-CA-C	-5.22	105.67	111.36
1	5-J	245	THR	N-CA-C	-5.22	105.67	111.36
1	6-C	245	THR	N-CA-C	-5.22	105.67	111.36
1	6-J	245	THR	N-CA-C	-5.22	105.67	111.36
1	7-C	245	THR	N-CA-C	-5.22	105.67	111.36
1	7-J	245	THR	N-CA-C	-5.22	105.67	111.36
1	8-C	245	THR	N-CA-C	-5.22	105.67	111.36
1	8-J	245	THR	N-CA-C	-5.22	105.67	111.36
1	9-C	245	THR	N-CA-C	-5.22	105.67	111.36
1	9-J	245	THR	N-CA-C	-5.22	105.67	111.36
1	10-C	245	THR	N-CA-C	-5.22	105.67	111.36
1	10-J	245	THR	N-CA-C	-5.22	105.67	111.36
1	1-T	245	THR	N-CA-C	-5.22	105.67	111.36
1	2-T	245	THR	N-CA-C	-5.22	105.67	111.36
1	3-T	245	THR	N-CA-C	-5.22	105.67	111.36
1	4-T	245	THR	N-CA-C	-5.22	105.67	111.36
1	5-T	245	THR	N-CA-C	-5.22	105.67	111.36
1	6-T	245	THR	N-CA-C	-5.22	105.67	111.36
1	7-T	245	THR	N-CA-C	-5.22	105.67	111.36
1	8-T	245	THR	N-CA-C	-5.22	105.67	111.36
1	9-T	245	THR	N-CA-C	-5.22	105.67	111.36
1	10-T	245	THR	N-CA-C	-5.22	105.67	111.36
1	1-O	245	THR	N-CA-C	-5.21	105.68	111.36
1	2-O	245	THR	N-CA-C	-5.21	105.68	111.36
1	3-O	245	THR	N-CA-C	-5.21	105.68	111.36
1	4-O	245	THR	N-CA-C	-5.21	105.68	111.36
1	5-O	245	THR	N-CA-C	-5.21	105.68	111.36
1	6-O	245	THR	N-CA-C	-5.21	105.68	111.36
1	7-O	245	THR	N-CA-C	-5.21	105.68	111.36
1	8-O	245	THR	N-CA-C	-5.21	105.68	111.36
1	9-O	245	THR	N-CA-C	-5.21	105.68	111.36
1	10-O	245	THR	N-CA-C	-5.21	105.68	111.36
1	1-F	245	THR	N-CA-C	-5.21	105.68	111.36
1	1-H	245	THR	N-CA-C	-5.21	105.68	111.36
1	2-F	245	THR	N-CA-C	-5.21	105.68	111.36
1	2-H	245	THR	N-CA-C	-5.21	105.68	111.36
1	3-F	245	THR	N-CA-C	-5.21	105.68	111.36
1	3-H	245	THR	N-CA-C	-5.21	105.68	111.36
1	4-F	245	THR	N-CA-C	-5.21	105.68	111.36
1	4-H	245	THR	N-CA-C	-5.21	105.68	111.36
1	5-F	245	THR	N-CA-C	-5.21	105.68	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-H	245	THR	N-CA-C	-5.21	105.68	111.36
1	6-F	245	THR	N-CA-C	-5.21	105.68	111.36
1	6-H	245	THR	N-CA-C	-5.21	105.68	111.36
1	7-F	245	THR	N-CA-C	-5.21	105.68	111.36
1	7-H	245	THR	N-CA-C	-5.21	105.68	111.36
1	8-F	245	THR	N-CA-C	-5.21	105.68	111.36
1	8-H	245	THR	N-CA-C	-5.21	105.68	111.36
1	9-F	245	THR	N-CA-C	-5.21	105.68	111.36
1	9-H	245	THR	N-CA-C	-5.21	105.68	111.36
1	10-F	245	THR	N-CA-C	-5.21	105.68	111.36
1	10-H	245	THR	N-CA-C	-5.21	105.68	111.36
1	1-A	245	THR	N-CA-C	-5.21	105.68	111.36
1	1-U	245	THR	N-CA-C	-5.21	105.68	111.36
1	2-A	245	THR	N-CA-C	-5.21	105.68	111.36
1	2-U	245	THR	N-CA-C	-5.21	105.68	111.36
1	3-A	245	THR	N-CA-C	-5.21	105.68	111.36
1	3-U	245	THR	N-CA-C	-5.21	105.68	111.36
1	4-A	245	THR	N-CA-C	-5.21	105.68	111.36
1	4-U	245	THR	N-CA-C	-5.21	105.68	111.36
1	5-A	245	THR	N-CA-C	-5.21	105.68	111.36
1	5-U	245	THR	N-CA-C	-5.21	105.68	111.36
1	6-A	245	THR	N-CA-C	-5.21	105.68	111.36
1	6-U	245	THR	N-CA-C	-5.21	105.68	111.36
1	7-A	245	THR	N-CA-C	-5.21	105.68	111.36
1	7-U	245	THR	N-CA-C	-5.21	105.68	111.36
1	8-A	245	THR	N-CA-C	-5.21	105.68	111.36
1	8-U	245	THR	N-CA-C	-5.21	105.68	111.36
1	9-A	245	THR	N-CA-C	-5.21	105.68	111.36
1	9-U	245	THR	N-CA-C	-5.21	105.68	111.36
1	10-A	245	THR	N-CA-C	-5.21	105.68	111.36
1	10-U	245	THR	N-CA-C	-5.21	105.68	111.36
1	1-B	245	THR	N-CA-C	-5.21	105.68	111.36
1	1-X	245	THR	N-CA-C	-5.21	105.68	111.36
1	2-B	245	THR	N-CA-C	-5.21	105.68	111.36
1	2-X	245	THR	N-CA-C	-5.21	105.68	111.36
1	3-B	245	THR	N-CA-C	-5.21	105.68	111.36
1	3-X	245	THR	N-CA-C	-5.21	105.68	111.36
1	4-B	245	THR	N-CA-C	-5.21	105.68	111.36
1	4-X	245	THR	N-CA-C	-5.21	105.68	111.36
1	5-B	245	THR	N-CA-C	-5.21	105.68	111.36
1	5-X	245	THR	N-CA-C	-5.21	105.68	111.36
1	6-B	245	THR	N-CA-C	-5.21	105.68	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-X	245	THR	N-CA-C	-5.21	105.68	111.36
1	7-B	245	THR	N-CA-C	-5.21	105.68	111.36
1	7-X	245	THR	N-CA-C	-5.21	105.68	111.36
1	8-B	245	THR	N-CA-C	-5.21	105.68	111.36
1	8-X	245	THR	N-CA-C	-5.21	105.68	111.36
1	9-B	245	THR	N-CA-C	-5.21	105.68	111.36
1	9-X	245	THR	N-CA-C	-5.21	105.68	111.36
1	10-B	245	THR	N-CA-C	-5.21	105.68	111.36
1	10-X	245	THR	N-CA-C	-5.21	105.68	111.36
1	1-Q	245	THR	N-CA-C	-5.20	105.69	111.36
1	1-S	245	THR	N-CA-C	-5.20	105.69	111.36
1	2-Q	245	THR	N-CA-C	-5.20	105.69	111.36
1	2-S	245	THR	N-CA-C	-5.20	105.69	111.36
1	3-Q	245	THR	N-CA-C	-5.20	105.69	111.36
1	3-S	245	THR	N-CA-C	-5.20	105.69	111.36
1	4-Q	245	THR	N-CA-C	-5.20	105.69	111.36
1	4-S	245	THR	N-CA-C	-5.20	105.69	111.36
1	5-Q	245	THR	N-CA-C	-5.20	105.69	111.36
1	5-S	245	THR	N-CA-C	-5.20	105.69	111.36
1	6-Q	245	THR	N-CA-C	-5.20	105.69	111.36
1	6-S	245	THR	N-CA-C	-5.20	105.69	111.36
1	7-Q	245	THR	N-CA-C	-5.20	105.69	111.36
1	7-S	245	THR	N-CA-C	-5.20	105.69	111.36
1	8-Q	245	THR	N-CA-C	-5.20	105.69	111.36
1	8-S	245	THR	N-CA-C	-5.20	105.69	111.36
1	9-Q	245	THR	N-CA-C	-5.20	105.69	111.36
1	9-S	245	THR	N-CA-C	-5.20	105.69	111.36
1	10-Q	245	THR	N-CA-C	-5.20	105.69	111.36
1	10-S	245	THR	N-CA-C	-5.20	105.69	111.36
1	1-L	245	THR	N-CA-C	-5.20	105.69	111.36
1	2-L	245	THR	N-CA-C	-5.20	105.69	111.36
1	3-L	245	THR	N-CA-C	-5.20	105.69	111.36
1	4-L	245	THR	N-CA-C	-5.20	105.69	111.36
1	5-L	245	THR	N-CA-C	-5.20	105.69	111.36
1	6-L	245	THR	N-CA-C	-5.20	105.69	111.36
1	7-L	245	THR	N-CA-C	-5.20	105.69	111.36
1	8-L	245	THR	N-CA-C	-5.20	105.69	111.36
1	9-L	245	THR	N-CA-C	-5.20	105.69	111.36
1	10-L	245	THR	N-CA-C	-5.20	105.69	111.36
1	1-M	245	THR	N-CA-C	-5.20	105.69	111.36
1	1-V	245	THR	N-CA-C	-5.20	105.69	111.36
1	2-M	245	THR	N-CA-C	-5.20	105.69	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-V	245	THR	N-CA-C	-5.20	105.69	111.36
1	3-M	245	THR	N-CA-C	-5.20	105.69	111.36
1	3-V	245	THR	N-CA-C	-5.20	105.69	111.36
1	4-M	245	THR	N-CA-C	-5.20	105.69	111.36
1	4-V	245	THR	N-CA-C	-5.20	105.69	111.36
1	5-M	245	THR	N-CA-C	-5.20	105.69	111.36
1	5-V	245	THR	N-CA-C	-5.20	105.69	111.36
1	6-M	245	THR	N-CA-C	-5.20	105.69	111.36
1	6-V	245	THR	N-CA-C	-5.20	105.69	111.36
1	7-M	245	THR	N-CA-C	-5.20	105.69	111.36
1	7-V	245	THR	N-CA-C	-5.20	105.69	111.36
1	8-M	245	THR	N-CA-C	-5.20	105.69	111.36
1	8-V	245	THR	N-CA-C	-5.20	105.69	111.36
1	9-M	245	THR	N-CA-C	-5.20	105.69	111.36
1	9-V	245	THR	N-CA-C	-5.20	105.69	111.36
1	10-M	245	THR	N-CA-C	-5.20	105.69	111.36
1	10-V	245	THR	N-CA-C	-5.20	105.69	111.36
1	1-D	245	THR	N-CA-C	-5.19	105.70	111.36
1	2-D	245	THR	N-CA-C	-5.19	105.70	111.36
1	3-D	245	THR	N-CA-C	-5.19	105.70	111.36
1	4-D	245	THR	N-CA-C	-5.19	105.70	111.36
1	5-D	245	THR	N-CA-C	-5.19	105.70	111.36
1	6-D	245	THR	N-CA-C	-5.19	105.70	111.36
1	7-D	245	THR	N-CA-C	-5.19	105.70	111.36
1	8-D	245	THR	N-CA-C	-5.19	105.70	111.36
1	9-D	245	THR	N-CA-C	-5.19	105.70	111.36
1	10-D	245	THR	N-CA-C	-5.19	105.70	111.36
1	1-R	245	THR	N-CA-C	-5.17	105.72	111.36
1	2-R	245	THR	N-CA-C	-5.17	105.72	111.36
1	3-R	245	THR	N-CA-C	-5.17	105.72	111.36
1	4-R	245	THR	N-CA-C	-5.17	105.72	111.36
1	5-R	245	THR	N-CA-C	-5.17	105.72	111.36
1	6-R	245	THR	N-CA-C	-5.17	105.72	111.36
1	7-R	245	THR	N-CA-C	-5.17	105.72	111.36
1	8-R	245	THR	N-CA-C	-5.17	105.72	111.36
1	9-R	245	THR	N-CA-C	-5.17	105.72	111.36
1	10-R	245	THR	N-CA-C	-5.17	105.72	111.36
1	1-P	245	THR	N-CA-C	-5.16	105.73	111.36
1	2-P	245	THR	N-CA-C	-5.16	105.73	111.36
1	3-P	245	THR	N-CA-C	-5.16	105.73	111.36
1	4-P	245	THR	N-CA-C	-5.16	105.73	111.36
1	5-P	245	THR	N-CA-C	-5.16	105.73	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-P	245	THR	N-CA-C	-5.16	105.73	111.36
1	7-P	245	THR	N-CA-C	-5.16	105.73	111.36
1	8-P	245	THR	N-CA-C	-5.16	105.73	111.36
1	9-P	245	THR	N-CA-C	-5.16	105.73	111.36
1	10-P	245	THR	N-CA-C	-5.16	105.73	111.36

There are no chirality outliers.

All (240) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	319	TYR	Sidechain
1	1-B	319	TYR	Sidechain
1	1-C	319	TYR	Sidechain
1	1-D	319	TYR	Sidechain
1	1-E	319	TYR	Sidechain
1	1-F	319	TYR	Sidechain
1	1-G	319	TYR	Sidechain
1	1-H	319	TYR	Sidechain
1	1-I	319	TYR	Sidechain
1	1-J	319	TYR	Sidechain
1	1-K	319	TYR	Sidechain
1	1-L	319	TYR	Sidechain
1	1-M	319	TYR	Sidechain
1	1-N	319	TYR	Sidechain
1	1-O	319	TYR	Sidechain
1	1-P	319	TYR	Sidechain
1	1-Q	319	TYR	Sidechain
1	1-R	319	TYR	Sidechain
1	1-S	319	TYR	Sidechain
1	1-T	319	TYR	Sidechain
1	1-U	319	TYR	Sidechain
1	1-V	319	TYR	Sidechain
1	1-W	319	TYR	Sidechain
1	1-X	319	TYR	Sidechain
1	10-A	319	TYR	Sidechain
1	10-B	319	TYR	Sidechain
1	10-C	319	TYR	Sidechain
1	10-D	319	TYR	Sidechain
1	10-E	319	TYR	Sidechain
1	10-F	319	TYR	Sidechain
1	10-G	319	TYR	Sidechain
1	10-H	319	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	10-I	319	TYR	Sidechain
1	10-J	319	TYR	Sidechain
1	10-K	319	TYR	Sidechain
1	10-L	319	TYR	Sidechain
1	10-M	319	TYR	Sidechain
1	10-N	319	TYR	Sidechain
1	10-O	319	TYR	Sidechain
1	10-P	319	TYR	Sidechain
1	10-Q	319	TYR	Sidechain
1	10-R	319	TYR	Sidechain
1	10-S	319	TYR	Sidechain
1	10-T	319	TYR	Sidechain
1	10-U	319	TYR	Sidechain
1	10-V	319	TYR	Sidechain
1	10-W	319	TYR	Sidechain
1	10-X	319	TYR	Sidechain
1	2-A	319	TYR	Sidechain
1	2-B	319	TYR	Sidechain
1	2-C	319	TYR	Sidechain
1	2-D	319	TYR	Sidechain
1	2-E	319	TYR	Sidechain
1	2-F	319	TYR	Sidechain
1	2-G	319	TYR	Sidechain
1	2-H	319	TYR	Sidechain
1	2-I	319	TYR	Sidechain
1	2-J	319	TYR	Sidechain
1	2-K	319	TYR	Sidechain
1	2-L	319	TYR	Sidechain
1	2-M	319	TYR	Sidechain
1	2-N	319	TYR	Sidechain
1	2-O	319	TYR	Sidechain
1	2-P	319	TYR	Sidechain
1	2-Q	319	TYR	Sidechain
1	2-R	319	TYR	Sidechain
1	2-S	319	TYR	Sidechain
1	2-T	319	TYR	Sidechain
1	2-U	319	TYR	Sidechain
1	2-V	319	TYR	Sidechain
1	2-W	319	TYR	Sidechain
1	2-X	319	TYR	Sidechain
1	3-A	319	TYR	Sidechain
1	3-B	319	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	3-C	319	TYR	Sidechain
1	3-D	319	TYR	Sidechain
1	3-E	319	TYR	Sidechain
1	3-F	319	TYR	Sidechain
1	3-G	319	TYR	Sidechain
1	3-H	319	TYR	Sidechain
1	3-I	319	TYR	Sidechain
1	3-J	319	TYR	Sidechain
1	3-K	319	TYR	Sidechain
1	3-L	319	TYR	Sidechain
1	3-M	319	TYR	Sidechain
1	3-N	319	TYR	Sidechain
1	3-O	319	TYR	Sidechain
1	3-P	319	TYR	Sidechain
1	3-Q	319	TYR	Sidechain
1	3-R	319	TYR	Sidechain
1	3-S	319	TYR	Sidechain
1	3-T	319	TYR	Sidechain
1	3-U	319	TYR	Sidechain
1	3-V	319	TYR	Sidechain
1	3-W	319	TYR	Sidechain
1	3-X	319	TYR	Sidechain
1	4-A	319	TYR	Sidechain
1	4-B	319	TYR	Sidechain
1	4-C	319	TYR	Sidechain
1	4-D	319	TYR	Sidechain
1	4-E	319	TYR	Sidechain
1	4-F	319	TYR	Sidechain
1	4-G	319	TYR	Sidechain
1	4-H	319	TYR	Sidechain
1	4-I	319	TYR	Sidechain
1	4-J	319	TYR	Sidechain
1	4-K	319	TYR	Sidechain
1	4-L	319	TYR	Sidechain
1	4-M	319	TYR	Sidechain
1	4-N	319	TYR	Sidechain
1	4-O	319	TYR	Sidechain
1	4-P	319	TYR	Sidechain
1	4-Q	319	TYR	Sidechain
1	4-R	319	TYR	Sidechain
1	4-S	319	TYR	Sidechain
1	4-T	319	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	4-U	319	TYR	Sidechain
1	4-V	319	TYR	Sidechain
1	4-W	319	TYR	Sidechain
1	4-X	319	TYR	Sidechain
1	5-A	319	TYR	Sidechain
1	5-B	319	TYR	Sidechain
1	5-C	319	TYR	Sidechain
1	5-D	319	TYR	Sidechain
1	5-E	319	TYR	Sidechain
1	5-F	319	TYR	Sidechain
1	5-G	319	TYR	Sidechain
1	5-H	319	TYR	Sidechain
1	5-I	319	TYR	Sidechain
1	5-J	319	TYR	Sidechain
1	5-K	319	TYR	Sidechain
1	5-L	319	TYR	Sidechain
1	5-M	319	TYR	Sidechain
1	5-N	319	TYR	Sidechain
1	5-O	319	TYR	Sidechain
1	5-P	319	TYR	Sidechain
1	5-Q	319	TYR	Sidechain
1	5-R	319	TYR	Sidechain
1	5-S	319	TYR	Sidechain
1	5-T	319	TYR	Sidechain
1	5-U	319	TYR	Sidechain
1	5-V	319	TYR	Sidechain
1	5-W	319	TYR	Sidechain
1	5-X	319	TYR	Sidechain
1	6-A	319	TYR	Sidechain
1	6-B	319	TYR	Sidechain
1	6-C	319	TYR	Sidechain
1	6-D	319	TYR	Sidechain
1	6-E	319	TYR	Sidechain
1	6-F	319	TYR	Sidechain
1	6-G	319	TYR	Sidechain
1	6-H	319	TYR	Sidechain
1	6-I	319	TYR	Sidechain
1	6-J	319	TYR	Sidechain
1	6-K	319	TYR	Sidechain
1	6-L	319	TYR	Sidechain
1	6-M	319	TYR	Sidechain
1	6-N	319	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	6-O	319	TYR	Sidechain
1	6-P	319	TYR	Sidechain
1	6-Q	319	TYR	Sidechain
1	6-R	319	TYR	Sidechain
1	6-S	319	TYR	Sidechain
1	6-T	319	TYR	Sidechain
1	6-U	319	TYR	Sidechain
1	6-V	319	TYR	Sidechain
1	6-W	319	TYR	Sidechain
1	6-X	319	TYR	Sidechain
1	7-A	319	TYR	Sidechain
1	7-B	319	TYR	Sidechain
1	7-C	319	TYR	Sidechain
1	7-D	319	TYR	Sidechain
1	7-E	319	TYR	Sidechain
1	7-F	319	TYR	Sidechain
1	7-G	319	TYR	Sidechain
1	7-H	319	TYR	Sidechain
1	7-I	319	TYR	Sidechain
1	7-J	319	TYR	Sidechain
1	7-K	319	TYR	Sidechain
1	7-L	319	TYR	Sidechain
1	7-M	319	TYR	Sidechain
1	7-N	319	TYR	Sidechain
1	7-O	319	TYR	Sidechain
1	7-P	319	TYR	Sidechain
1	7-Q	319	TYR	Sidechain
1	7-R	319	TYR	Sidechain
1	7-S	319	TYR	Sidechain
1	7-T	319	TYR	Sidechain
1	7-U	319	TYR	Sidechain
1	7-V	319	TYR	Sidechain
1	7-W	319	TYR	Sidechain
1	7-X	319	TYR	Sidechain
1	8-A	319	TYR	Sidechain
1	8-B	319	TYR	Sidechain
1	8-C	319	TYR	Sidechain
1	8-D	319	TYR	Sidechain
1	8-E	319	TYR	Sidechain
1	8-F	319	TYR	Sidechain
1	8-G	319	TYR	Sidechain
1	8-H	319	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	8-I	319	TYR	Sidechain
1	8-J	319	TYR	Sidechain
1	8-K	319	TYR	Sidechain
1	8-L	319	TYR	Sidechain
1	8-M	319	TYR	Sidechain
1	8-N	319	TYR	Sidechain
1	8-O	319	TYR	Sidechain
1	8-P	319	TYR	Sidechain
1	8-Q	319	TYR	Sidechain
1	8-R	319	TYR	Sidechain
1	8-S	319	TYR	Sidechain
1	8-T	319	TYR	Sidechain
1	8-U	319	TYR	Sidechain
1	8-V	319	TYR	Sidechain
1	8-W	319	TYR	Sidechain
1	8-X	319	TYR	Sidechain
1	9-A	319	TYR	Sidechain
1	9-B	319	TYR	Sidechain
1	9-C	319	TYR	Sidechain
1	9-D	319	TYR	Sidechain
1	9-E	319	TYR	Sidechain
1	9-F	319	TYR	Sidechain
1	9-G	319	TYR	Sidechain
1	9-H	319	TYR	Sidechain
1	9-I	319	TYR	Sidechain
1	9-J	319	TYR	Sidechain
1	9-K	319	TYR	Sidechain
1	9-L	319	TYR	Sidechain
1	9-M	319	TYR	Sidechain
1	9-N	319	TYR	Sidechain
1	9-O	319	TYR	Sidechain
1	9-P	319	TYR	Sidechain
1	9-Q	319	TYR	Sidechain
1	9-R	319	TYR	Sidechain
1	9-S	319	TYR	Sidechain
1	9-T	319	TYR	Sidechain
1	9-U	319	TYR	Sidechain
1	9-V	319	TYR	Sidechain
1	9-W	319	TYR	Sidechain
1	9-X	319	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	3778	0	3604	0	0
1	1-B	3778	0	3604	0	0
1	1-C	3778	0	3604	0	0
1	1-D	3778	0	3604	0	0
1	1-E	3778	0	3604	0	0
1	1-F	3778	0	3604	0	0
1	1-G	3778	0	3604	0	0
1	1-H	3778	0	3604	0	0
1	1-I	3778	0	3604	0	0
1	1-J	3778	0	3604	0	0
1	1-K	3778	0	3604	0	0
1	1-L	3778	0	3604	0	0
1	1-M	3778	0	3604	0	0
1	1-N	3778	0	3604	0	0
1	1-O	3778	0	3604	0	0
1	1-P	3778	0	3604	0	0
1	1-Q	3778	0	3604	0	0
1	1-R	3778	0	3604	0	0
1	1-S	3778	0	3604	0	0
1	1-T	3778	0	3604	0	0
1	1-U	3778	0	3604	0	0
1	1-V	3778	0	3604	0	0
1	1-W	3778	0	3604	0	0
1	1-X	3778	0	3604	0	0
1	2-A	3778	0	3604	0	0
1	2-B	3778	0	3604	0	0
1	2-C	3778	0	3604	0	0
1	2-D	3778	0	3604	0	0
1	2-E	3778	0	3604	0	0
1	2-F	3778	0	3604	0	0
1	2-G	3778	0	3604	0	0
1	2-H	3778	0	3604	0	0
1	2-I	3778	0	3604	0	0
1	2-J	3778	0	3604	0	0
1	2-K	3778	0	3604	0	0
1	2-L	3778	0	3604	0	0
1	2-M	3778	0	3604	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2-N	3778	0	3604	0	0
1	2-O	3778	0	3604	0	0
1	2-P	3778	0	3604	0	0
1	2-Q	3778	0	3604	0	0
1	2-R	3778	0	3604	0	0
1	2-S	3778	0	3604	0	0
1	2-T	3778	0	3604	0	0
1	2-U	3778	0	3604	0	0
1	2-V	3778	0	3604	0	0
1	2-W	3778	0	3604	0	0
1	2-X	3778	0	3604	0	0
1	3-A	3778	0	3604	0	0
1	3-B	3778	0	3604	0	0
1	3-C	3778	0	3604	0	0
1	3-D	3778	0	3604	0	0
1	3-E	3778	0	3604	0	0
1	3-F	3778	0	3604	0	0
1	3-G	3778	0	3604	0	0
1	3-H	3778	0	3604	0	0
1	3-I	3778	0	3604	0	0
1	3-J	3778	0	3604	0	0
1	3-K	3778	0	3604	0	0
1	3-L	3778	0	3604	0	0
1	3-M	3778	0	3604	0	0
1	3-N	3778	0	3604	0	0
1	3-O	3778	0	3604	0	0
1	3-P	3778	0	3604	0	0
1	3-Q	3778	0	3604	0	0
1	3-R	3778	0	3604	0	0
1	3-S	3778	0	3604	0	0
1	3-T	3778	0	3604	0	0
1	3-U	3778	0	3602	0	0
1	3-V	3778	0	3604	0	0
1	3-W	3778	0	3604	0	0
1	3-X	3778	0	3604	0	0
1	4-A	3778	0	3604	0	0
1	4-B	3778	0	3604	0	0
1	4-C	3778	0	3604	0	0
1	4-D	3778	0	3604	0	0
1	4-E	3778	0	3604	0	0
1	4-F	3778	0	3604	0	0
1	4-G	3778	0	3604	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4-H	3778	0	3604	0	0
1	4-I	3778	0	3604	0	0
1	4-J	3778	0	3604	0	0
1	4-K	3778	0	3604	0	0
1	4-L	3778	0	3604	0	0
1	4-M	3778	0	3604	0	0
1	4-N	3778	0	3604	0	0
1	4-O	3778	0	3604	0	0
1	4-P	3778	0	3604	0	0
1	4-Q	3778	0	3604	0	0
1	4-R	3778	0	3604	0	0
1	4-S	3778	0	3602	0	0
1	4-T	3778	0	3604	0	0
1	4-U	3778	0	3604	0	0
1	4-V	3778	0	3604	0	0
1	4-W	3778	0	3604	0	0
1	4-X	3778	0	3604	0	0
1	5-A	3778	0	3604	0	0
1	5-B	3778	0	3604	0	0
1	5-C	3778	0	3604	0	0
1	5-D	3778	0	3604	0	0
1	5-E	3778	0	3604	0	0
1	5-F	3778	0	3604	0	0
1	5-G	3778	0	3604	0	0
1	5-H	3778	0	3604	0	0
1	5-I	3778	0	3604	0	0
1	5-J	3778	0	3604	0	0
1	5-K	3778	0	3604	0	0
1	5-L	3778	0	3604	0	0
1	5-M	3778	0	3604	0	0
1	5-N	3778	0	3604	0	0
1	5-O	3778	0	3604	0	0
1	5-P	3778	0	3604	0	0
1	5-Q	3778	0	3604	0	0
1	5-R	3778	0	3604	0	0
1	5-S	3778	0	3604	0	0
1	5-T	3778	0	3604	0	0
1	5-U	3778	0	3604	0	0
1	5-V	3778	0	3604	0	0
1	5-W	3778	0	3604	0	0
1	5-X	3778	0	3604	0	0
1	6-A	3778	0	3604	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6-B	3778	0	3604	0	0
1	6-C	3778	0	3604	0	0
1	6-D	3778	0	3604	0	0
1	6-E	3778	0	3604	0	0
1	6-F	3778	0	3604	0	0
1	6-G	3778	0	3604	0	0
1	6-H	3778	0	3604	0	0
1	6-I	3778	0	3604	0	0
1	6-J	3778	0	3604	0	0
1	6-K	3778	0	3604	0	0
1	6-L	3778	0	3604	0	0
1	6-M	3778	0	3604	0	0
1	6-N	3778	0	3604	0	0
1	6-O	3778	0	3604	0	0
1	6-P	3778	0	3604	0	0
1	6-Q	3778	0	3604	0	0
1	6-R	3778	0	3604	0	0
1	6-S	3778	0	3604	0	0
1	6-T	3778	0	3604	0	0
1	6-U	3778	0	3604	0	0
1	6-V	3778	0	3604	0	0
1	6-W	3778	0	3604	0	0
1	6-X	3778	0	3604	0	0
1	7-A	3778	0	3604	0	0
1	7-B	3778	0	3604	0	0
1	7-C	3778	0	3604	0	0
1	7-D	3778	0	3604	0	0
1	7-E	3778	0	3604	0	0
1	7-F	3778	0	3604	0	0
1	7-G	3778	0	3604	0	0
1	7-H	3778	0	3604	0	0
1	7-I	3778	0	3604	0	0
1	7-J	3778	0	3604	0	0
1	7-K	3778	0	3604	0	0
1	7-L	3778	0	3604	0	0
1	7-M	3778	0	3604	0	0
1	7-N	3778	0	3604	0	0
1	7-O	3778	0	3604	0	0
1	7-P	3778	0	3604	0	0
1	7-Q	3778	0	3604	0	0
1	7-R	3778	0	3604	0	0
1	7-S	3778	0	3601	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7-T	3778	0	3604	0	0
1	7-U	3778	0	3604	0	0
1	7-V	3778	0	3604	0	0
1	7-W	3778	0	3604	0	0
1	7-X	3778	0	3604	0	0
1	8-A	3778	0	3604	0	0
1	8-B	3778	0	3604	0	0
1	8-C	3778	0	3604	0	0
1	8-D	3778	0	3604	0	0
1	8-E	3778	0	3604	0	0
1	8-F	3778	0	3604	0	0
1	8-G	3778	0	3604	0	0
1	8-H	3778	0	3604	0	0
1	8-I	3778	0	3604	0	0
1	8-J	3778	0	3604	0	0
1	8-K	3778	0	3604	0	0
1	8-L	3778	0	3604	0	0
1	8-M	3778	0	3604	0	0
1	8-N	3778	0	3604	0	0
1	8-O	3778	0	3604	0	0
1	8-P	3778	0	3604	0	0
1	8-Q	3778	0	3604	0	0
1	8-R	3778	0	3604	0	0
1	8-S	3778	0	3604	0	0
1	8-T	3778	0	3604	0	0
1	8-U	3778	0	3604	0	0
1	8-V	3778	0	3604	0	0
1	8-W	3778	0	3604	0	0
1	8-X	3778	0	3604	0	0
1	9-A	3778	0	3604	0	0
1	9-B	3778	0	3604	0	0
1	9-C	3778	0	3604	0	0
1	9-D	3778	0	3604	0	0
1	9-E	3778	0	3604	0	0
1	9-F	3778	0	3604	0	0
1	9-G	3778	0	3604	0	0
1	9-H	3778	0	3604	0	0
1	9-I	3778	0	3604	0	0
1	9-J	3778	0	3604	0	0
1	9-K	3778	0	3604	0	0
1	9-L	3778	0	3604	0	0
1	9-M	3778	0	3604	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9-N	3778	0	3604	0	0
1	9-O	3778	0	3604	0	0
1	9-P	3778	0	3604	0	0
1	9-Q	3778	0	3604	0	0
1	9-R	3778	0	3604	0	0
1	9-S	3778	0	3602	0	0
1	9-T	3778	0	3604	0	0
1	9-U	3778	0	3604	0	0
1	9-V	3778	0	3604	0	0
1	9-W	3778	0	3604	0	0
1	9-X	3778	0	3604	0	0
1	10-A	3778	0	3604	0	0
1	10-B	3778	0	3604	0	0
1	10-C	3778	0	3604	0	0
1	10-D	3778	0	3604	0	0
1	10-E	3778	0	3604	0	0
1	10-F	3778	0	3604	0	0
1	10-G	3778	0	3604	0	0
1	10-H	3778	0	3604	0	0
1	10-I	3778	0	3604	0	0
1	10-J	3778	0	3604	0	0
1	10-K	3778	0	3604	0	0
1	10-L	3778	0	3604	0	0
1	10-M	3778	0	3604	0	0
1	10-N	3778	0	3604	0	0
1	10-O	3778	0	3604	0	0
1	10-P	3778	0	3604	0	0
1	10-Q	3778	0	3604	0	0
1	10-R	3778	0	3604	0	0
1	10-S	3778	0	3604	0	0
1	10-T	3778	0	3604	0	0
1	10-U	3778	0	3604	0	0
1	10-V	3778	0	3604	0	0
1	10-W	3778	0	3604	0	0
1	10-X	3778	0	3604	0	0
2	1-A	1	0	0	0	0
2	1-B	1	0	0	0	0
2	1-C	1	0	0	0	0
2	1-D	1	0	0	0	0
2	1-E	1	0	0	0	0
2	1-F	1	0	0	0	0
2	1-G	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1-H	1	0	0	0	0
2	1-I	1	0	0	0	0
2	1-J	1	0	0	0	0
2	1-K	1	0	0	0	0
2	1-L	1	0	0	0	0
2	1-M	1	0	0	0	0
2	1-N	1	0	0	0	0
2	1-O	1	0	0	0	0
2	1-P	1	0	0	0	0
2	1-Q	1	0	0	0	0
2	1-R	1	0	0	0	0
2	1-S	1	0	0	0	0
2	1-T	1	0	0	0	0
2	1-U	1	0	0	0	0
2	1-V	1	0	0	0	0
2	1-W	1	0	0	0	0
2	1-X	1	0	0	0	0
2	2-A	1	0	0	0	0
2	2-B	1	0	0	0	0
2	2-C	1	0	0	0	0
2	2-D	1	0	0	0	0
2	2-E	1	0	0	0	0
2	2-F	1	0	0	0	0
2	2-G	1	0	0	0	0
2	2-H	1	0	0	0	0
2	2-I	1	0	0	0	0
2	2-J	1	0	0	0	0
2	2-K	1	0	0	0	0
2	2-L	1	0	0	0	0
2	2-M	1	0	0	0	0
2	2-N	1	0	0	0	0
2	2-O	1	0	0	0	0
2	2-P	1	0	0	0	0
2	2-Q	1	0	0	0	0
2	2-R	1	0	0	0	0
2	2-S	1	0	0	0	0
2	2-T	1	0	0	0	0
2	2-U	1	0	0	0	0
2	2-V	1	0	0	0	0
2	2-W	1	0	0	0	0
2	2-X	1	0	0	0	0
2	3-A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3-B	1	0	0	0	0
2	3-C	1	0	0	0	0
2	3-D	1	0	0	0	0
2	3-E	1	0	0	0	0
2	3-F	1	0	0	0	0
2	3-G	1	0	0	0	0
2	3-H	1	0	0	0	0
2	3-I	1	0	0	0	0
2	3-J	1	0	0	0	0
2	3-K	1	0	0	0	0
2	3-L	1	0	0	0	0
2	3-M	1	0	0	0	0
2	3-N	1	0	0	0	0
2	3-O	1	0	0	0	0
2	3-P	1	0	0	0	0
2	3-Q	1	0	0	0	0
2	3-R	1	0	0	0	0
2	3-S	1	0	0	0	0
2	3-T	1	0	0	0	0
2	3-U	1	0	0	0	0
2	3-V	1	0	0	0	0
2	3-W	1	0	0	0	0
2	3-X	1	0	0	0	0
2	4-A	1	0	0	0	0
2	4-B	1	0	0	0	0
2	4-C	1	0	0	0	0
2	4-D	1	0	0	0	0
2	4-E	1	0	0	0	0
2	4-F	1	0	0	0	0
2	4-G	1	0	0	0	0
2	4-H	1	0	0	0	0
2	4-I	1	0	0	0	0
2	4-J	1	0	0	0	0
2	4-K	1	0	0	0	0
2	4-L	1	0	0	0	0
2	4-M	1	0	0	0	0
2	4-N	1	0	0	0	0
2	4-O	1	0	0	0	0
2	4-P	1	0	0	0	0
2	4-Q	1	0	0	0	0
2	4-R	1	0	0	0	0
2	4-S	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4-T	1	0	0	0	0
2	4-U	1	0	0	0	0
2	4-V	1	0	0	0	0
2	4-W	1	0	0	0	0
2	4-X	1	0	0	0	0
2	5-A	1	0	0	0	0
2	5-B	1	0	0	0	0
2	5-C	1	0	0	0	0
2	5-D	1	0	0	0	0
2	5-E	1	0	0	0	0
2	5-F	1	0	0	0	0
2	5-G	1	0	0	0	0
2	5-H	1	0	0	0	0
2	5-I	1	0	0	0	0
2	5-J	1	0	0	0	0
2	5-K	1	0	0	0	0
2	5-L	1	0	0	0	0
2	5-M	1	0	0	0	0
2	5-N	1	0	0	0	0
2	5-O	1	0	0	0	0
2	5-P	1	0	0	0	0
2	5-Q	1	0	0	0	0
2	5-R	1	0	0	0	0
2	5-S	1	0	0	0	0
2	5-T	1	0	0	0	0
2	5-U	1	0	0	0	0
2	5-V	1	0	0	0	0
2	5-W	1	0	0	0	0
2	5-X	1	0	0	0	0
2	6-A	1	0	0	0	0
2	6-B	1	0	0	0	0
2	6-C	1	0	0	0	0
2	6-D	1	0	0	0	0
2	6-E	1	0	0	0	0
2	6-F	1	0	0	0	0
2	6-G	1	0	0	0	0
2	6-H	1	0	0	0	0
2	6-I	1	0	0	0	0
2	6-J	1	0	0	0	0
2	6-K	1	0	0	0	0
2	6-L	1	0	0	0	0
2	6-M	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-N	1	0	0	0	0
2	6-O	1	0	0	0	0
2	6-P	1	0	0	0	0
2	6-Q	1	0	0	0	0
2	6-R	1	0	0	0	0
2	6-S	1	0	0	0	0
2	6-T	1	0	0	0	0
2	6-U	1	0	0	0	0
2	6-V	1	0	0	0	0
2	6-W	1	0	0	0	0
2	6-X	1	0	0	0	0
2	7-A	1	0	0	0	0
2	7-B	1	0	0	0	0
2	7-C	1	0	0	0	0
2	7-D	1	0	0	0	0
2	7-E	1	0	0	0	0
2	7-F	1	0	0	0	0
2	7-G	1	0	0	0	0
2	7-H	1	0	0	0	0
2	7-I	1	0	0	0	0
2	7-J	1	0	0	0	0
2	7-K	1	0	0	0	0
2	7-L	1	0	0	0	0
2	7-M	1	0	0	0	0
2	7-N	1	0	0	0	0
2	7-O	1	0	0	0	0
2	7-P	1	0	0	0	0
2	7-Q	1	0	0	0	0
2	7-R	1	0	0	0	0
2	7-S	1	0	0	0	0
2	7-T	1	0	0	0	0
2	7-U	1	0	0	0	0
2	7-V	1	0	0	0	0
2	7-W	1	0	0	0	0
2	7-X	1	0	0	0	0
2	8-A	1	0	0	0	0
2	8-B	1	0	0	0	0
2	8-C	1	0	0	0	0
2	8-D	1	0	0	0	0
2	8-E	1	0	0	0	0
2	8-F	1	0	0	0	0
2	8-G	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	8-H	1	0	0	0	0
2	8-I	1	0	0	0	0
2	8-J	1	0	0	0	0
2	8-K	1	0	0	0	0
2	8-L	1	0	0	0	0
2	8-M	1	0	0	0	0
2	8-N	1	0	0	0	0
2	8-O	1	0	0	0	0
2	8-P	1	0	0	0	0
2	8-Q	1	0	0	0	0
2	8-R	1	0	0	0	0
2	8-S	1	0	0	0	0
2	8-T	1	0	0	0	0
2	8-U	1	0	0	0	0
2	8-V	1	0	0	0	0
2	8-W	1	0	0	0	0
2	8-X	1	0	0	0	0
2	9-A	1	0	0	0	0
2	9-B	1	0	0	0	0
2	9-C	1	0	0	0	0
2	9-D	1	0	0	0	0
2	9-E	1	0	0	0	0
2	9-F	1	0	0	0	0
2	9-G	1	0	0	0	0
2	9-H	1	0	0	0	0
2	9-I	1	0	0	0	0
2	9-J	1	0	0	0	0
2	9-K	1	0	0	0	0
2	9-L	1	0	0	0	0
2	9-M	1	0	0	0	0
2	9-N	1	0	0	0	0
2	9-O	1	0	0	0	0
2	9-P	1	0	0	0	0
2	9-Q	1	0	0	0	0
2	9-R	1	0	0	0	0
2	9-S	1	0	0	0	0
2	9-T	1	0	0	0	0
2	9-U	1	0	0	0	0
2	9-V	1	0	0	0	0
2	9-W	1	0	0	0	0
2	9-X	1	0	0	0	0
2	10-A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	10-B	1	0	0	0	0
2	10-C	1	0	0	0	0
2	10-D	1	0	0	0	0
2	10-E	1	0	0	0	0
2	10-F	1	0	0	0	0
2	10-G	1	0	0	0	0
2	10-H	1	0	0	0	0
2	10-I	1	0	0	0	0
2	10-J	1	0	0	0	0
2	10-K	1	0	0	0	0
2	10-L	1	0	0	0	0
2	10-M	1	0	0	0	0
2	10-N	1	0	0	0	0
2	10-O	1	0	0	0	0
2	10-P	1	0	0	0	0
2	10-Q	1	0	0	0	0
2	10-R	1	0	0	0	0
2	10-S	1	0	0	0	0
2	10-T	1	0	0	0	0
2	10-U	1	0	0	0	0
2	10-V	1	0	0	0	0
2	10-W	1	0	0	0	0
2	10-X	1	0	0	0	0
3	1-A	23	0	10	0	0
3	1-B	23	0	10	0	0
3	1-C	23	0	10	0	0
3	1-D	23	0	10	0	0
3	1-E	23	0	10	0	0
3	1-F	23	0	10	0	0
3	1-G	23	0	10	0	0
3	1-H	23	0	10	0	0
3	1-I	23	0	10	0	0
3	1-J	23	0	10	0	0
3	1-K	23	0	10	0	0
3	1-L	23	0	10	0	0
3	1-M	23	0	10	0	0
3	1-N	23	0	10	0	0
3	1-O	23	0	10	0	0
3	1-P	23	0	10	0	0
3	1-Q	23	0	10	0	0
3	1-R	23	0	10	0	0
3	1-S	23	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1-T	23	0	10	0	0
3	1-U	23	0	10	0	0
3	1-V	23	0	10	0	0
3	1-W	23	0	10	0	0
3	1-X	23	0	10	0	0
3	2-A	23	0	10	0	0
3	2-B	23	0	10	0	0
3	2-C	23	0	10	0	0
3	2-D	23	0	10	0	0
3	2-E	23	0	10	0	0
3	2-F	23	0	10	0	0
3	2-G	23	0	10	0	0
3	2-H	23	0	10	0	0
3	2-I	23	0	10	0	0
3	2-J	23	0	10	0	0
3	2-K	23	0	10	0	0
3	2-L	23	0	10	0	0
3	2-M	23	0	10	0	0
3	2-N	23	0	10	0	0
3	2-O	23	0	10	0	0
3	2-P	23	0	10	0	0
3	2-Q	23	0	10	0	0
3	2-R	23	0	10	0	0
3	2-S	23	0	10	0	0
3	2-T	23	0	10	0	0
3	2-U	23	0	10	0	0
3	2-V	23	0	10	0	0
3	2-W	23	0	10	0	0
3	2-X	23	0	10	0	0
3	3-A	23	0	10	0	0
3	3-B	23	0	10	0	0
3	3-C	23	0	10	0	0
3	3-D	23	0	10	0	0
3	3-E	23	0	10	0	0
3	3-F	23	0	10	0	0
3	3-G	23	0	10	0	0
3	3-H	23	0	10	0	0
3	3-I	23	0	10	0	0
3	3-J	23	0	10	0	0
3	3-K	23	0	10	0	0
3	3-L	23	0	10	0	0
3	3-M	23	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3-N	23	0	10	0	0
3	3-O	23	0	10	0	0
3	3-P	23	0	10	0	0
3	3-Q	23	0	10	0	0
3	3-R	23	0	10	0	0
3	3-S	23	0	10	0	0
3	3-T	23	0	10	0	0
3	3-U	23	0	10	0	0
3	3-V	23	0	10	0	0
3	3-W	23	0	10	0	0
3	3-X	23	0	10	0	0
3	4-A	23	0	10	0	0
3	4-B	23	0	10	0	0
3	4-C	23	0	10	0	0
3	4-D	23	0	10	0	0
3	4-E	23	0	10	0	0
3	4-F	23	0	10	0	0
3	4-G	23	0	10	0	0
3	4-H	23	0	10	0	0
3	4-I	23	0	10	0	0
3	4-J	23	0	10	0	0
3	4-K	23	0	10	0	0
3	4-L	23	0	10	0	0
3	4-M	23	0	10	0	0
3	4-N	23	0	10	0	0
3	4-O	23	0	10	0	0
3	4-P	23	0	10	0	0
3	4-Q	23	0	10	0	0
3	4-R	23	0	10	0	0
3	4-S	23	0	10	0	0
3	4-T	23	0	10	0	0
3	4-U	23	0	10	0	0
3	4-V	23	0	10	0	0
3	4-W	23	0	10	0	0
3	4-X	23	0	10	0	0
3	5-A	23	0	10	0	0
3	5-B	23	0	10	0	0
3	5-C	23	0	10	0	0
3	5-D	23	0	10	0	0
3	5-E	23	0	10	0	0
3	5-F	23	0	10	0	0
3	5-G	23	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	5-H	23	0	10	0	0
3	5-I	23	0	10	0	0
3	5-J	23	0	10	0	0
3	5-K	23	0	10	0	0
3	5-L	23	0	10	0	0
3	5-M	23	0	10	0	0
3	5-N	23	0	10	0	0
3	5-O	23	0	10	0	0
3	5-P	23	0	10	0	0
3	5-Q	23	0	10	0	0
3	5-R	23	0	10	0	0
3	5-S	23	0	10	0	0
3	5-T	23	0	10	0	0
3	5-U	23	0	10	0	0
3	5-V	23	0	10	0	0
3	5-W	23	0	10	0	0
3	5-X	23	0	10	0	0
3	6-A	23	0	10	0	0
3	6-B	23	0	10	0	0
3	6-C	23	0	10	0	0
3	6-D	23	0	10	0	0
3	6-E	23	0	10	0	0
3	6-F	23	0	10	0	0
3	6-G	23	0	10	0	0
3	6-H	23	0	10	0	0
3	6-I	23	0	10	0	0
3	6-J	23	0	10	0	0
3	6-K	23	0	10	0	0
3	6-L	23	0	10	0	0
3	6-M	23	0	10	0	0
3	6-N	23	0	10	0	0
3	6-O	23	0	10	0	0
3	6-P	23	0	10	0	0
3	6-Q	23	0	10	0	0
3	6-R	23	0	10	0	0
3	6-S	23	0	10	0	0
3	6-T	23	0	10	0	0
3	6-U	23	0	10	0	0
3	6-V	23	0	10	0	0
3	6-W	23	0	10	0	0
3	6-X	23	0	10	0	0
3	7-A	23	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7-B	23	0	10	0	0
3	7-C	23	0	10	0	0
3	7-D	23	0	10	0	0
3	7-E	23	0	10	0	0
3	7-F	23	0	10	0	0
3	7-G	23	0	10	0	0
3	7-H	23	0	10	0	0
3	7-I	23	0	10	0	0
3	7-J	23	0	10	0	0
3	7-K	23	0	10	0	0
3	7-L	23	0	10	0	0
3	7-M	23	0	10	0	0
3	7-N	23	0	10	0	0
3	7-O	23	0	10	0	0
3	7-P	23	0	10	0	0
3	7-Q	23	0	10	0	0
3	7-R	23	0	10	0	0
3	7-S	23	0	10	0	0
3	7-T	23	0	10	0	0
3	7-U	23	0	10	0	0
3	7-V	23	0	10	0	0
3	7-W	23	0	10	0	0
3	7-X	23	0	10	0	0
3	8-A	23	0	10	0	0
3	8-B	23	0	10	0	0
3	8-C	23	0	10	0	0
3	8-D	23	0	10	0	0
3	8-E	23	0	10	0	0
3	8-F	23	0	10	0	0
3	8-G	23	0	10	0	0
3	8-H	23	0	10	0	0
3	8-I	23	0	10	0	0
3	8-J	23	0	10	0	0
3	8-K	23	0	10	0	0
3	8-L	23	0	10	0	0
3	8-M	23	0	10	0	0
3	8-N	23	0	10	0	0
3	8-O	23	0	10	0	0
3	8-P	23	0	10	0	0
3	8-Q	23	0	10	0	0
3	8-R	23	0	10	0	0
3	8-S	23	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8-T	23	0	10	0	0
3	8-U	23	0	10	0	0
3	8-V	23	0	10	0	0
3	8-W	23	0	10	0	0
3	8-X	23	0	10	0	0
3	9-A	23	0	10	0	0
3	9-B	23	0	10	0	0
3	9-C	23	0	10	0	0
3	9-D	23	0	10	0	0
3	9-E	23	0	10	0	0
3	9-F	23	0	10	0	0
3	9-G	23	0	10	0	0
3	9-H	23	0	10	0	0
3	9-I	23	0	10	0	0
3	9-J	23	0	10	0	0
3	9-K	23	0	10	0	0
3	9-L	23	0	10	0	0
3	9-M	23	0	10	0	0
3	9-N	23	0	10	0	0
3	9-O	23	0	10	0	0
3	9-P	23	0	10	0	0
3	9-Q	23	0	10	0	0
3	9-R	23	0	10	0	0
3	9-S	23	0	10	0	0
3	9-T	23	0	10	0	0
3	9-U	23	0	10	0	0
3	9-V	23	0	10	0	0
3	9-W	23	0	10	0	0
3	9-X	23	0	10	0	0
3	10-A	23	0	10	0	0
3	10-B	23	0	10	0	0
3	10-C	23	0	10	0	0
3	10-D	23	0	10	0	0
3	10-E	23	0	10	0	0
3	10-F	23	0	10	0	0
3	10-G	23	0	10	0	0
3	10-H	23	0	10	0	0
3	10-I	23	0	10	0	0
3	10-J	23	0	10	0	0
3	10-K	23	0	10	0	0
3	10-L	23	0	10	0	0
3	10-M	23	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	10-N	23	0	10	0	0
3	10-O	23	0	10	0	0
3	10-P	23	0	10	0	0
3	10-Q	23	0	10	0	0
3	10-R	23	0	10	0	0
3	10-S	23	0	10	0	0
3	10-T	23	0	10	0	0
3	10-U	23	0	10	0	0
3	10-V	23	0	10	0	0
3	10-W	23	0	10	0	0
3	10-X	23	0	10	0	0
4	1-A	13	0	5	0	0
4	1-B	13	0	5	0	0
4	1-C	13	0	5	0	0
4	1-D	13	0	5	0	0
4	1-E	13	0	5	0	0
4	1-F	13	0	5	0	0
4	1-G	13	0	5	0	0
4	1-H	13	0	5	0	0
4	1-I	13	0	5	0	0
4	1-J	13	0	5	0	0
4	1-K	13	0	5	0	0
4	1-L	13	0	5	0	0
4	1-M	13	0	5	0	0
4	1-N	13	0	5	0	0
4	1-O	13	0	5	0	0
4	1-P	13	0	5	0	0
4	1-Q	13	0	5	0	0
4	1-R	13	0	5	0	0
4	1-S	13	0	5	0	0
4	1-T	13	0	5	0	0
4	1-U	13	0	5	0	0
4	1-V	13	0	5	0	0
4	1-W	13	0	5	0	0
4	1-X	13	0	5	0	0
4	2-A	13	0	5	0	0
4	2-B	13	0	5	0	0
4	2-C	13	0	5	0	0
4	2-D	13	0	5	0	0
4	2-E	13	0	5	0	0
4	2-F	13	0	5	0	0
4	2-G	13	0	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2-H	13	0	5	0	0
4	2-I	13	0	5	0	0
4	2-J	13	0	5	0	0
4	2-K	13	0	5	0	0
4	2-L	13	0	5	0	0
4	2-M	13	0	5	0	0
4	2-N	13	0	5	0	0
4	2-O	13	0	5	0	0
4	2-P	13	0	5	0	0
4	2-Q	13	0	5	0	0
4	2-R	13	0	5	0	0
4	2-S	13	0	5	0	0
4	2-T	13	0	5	0	0
4	2-U	13	0	5	0	0
4	2-V	13	0	5	0	0
4	2-W	13	0	5	0	0
4	2-X	13	0	5	0	0
4	3-A	13	0	5	0	0
4	3-B	13	0	5	0	0
4	3-C	13	0	5	0	0
4	3-D	13	0	5	0	0
4	3-E	13	0	5	0	0
4	3-F	13	0	5	0	0
4	3-G	13	0	5	0	0
4	3-H	13	0	5	0	0
4	3-I	13	0	5	0	0
4	3-J	13	0	5	0	0
4	3-K	13	0	5	0	0
4	3-L	13	0	5	0	0
4	3-M	13	0	5	0	0
4	3-N	13	0	5	0	0
4	3-O	13	0	5	0	0
4	3-P	13	0	5	0	0
4	3-Q	13	0	5	0	0
4	3-R	13	0	5	0	0
4	3-S	13	0	5	0	0
4	3-T	13	0	5	0	0
4	3-U	13	0	5	0	0
4	3-V	13	0	5	0	0
4	3-W	13	0	5	0	0
4	3-X	13	0	5	0	0
4	4-A	13	0	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4-B	13	0	5	0	0
4	4-C	13	0	5	0	0
4	4-D	13	0	5	0	0
4	4-E	13	0	5	0	0
4	4-F	13	0	5	0	0
4	4-G	13	0	5	0	0
4	4-H	13	0	5	0	0
4	4-I	13	0	5	0	0
4	4-J	13	0	5	0	0
4	4-K	13	0	5	0	0
4	4-L	13	0	5	0	0
4	4-M	13	0	5	0	0
4	4-N	13	0	5	0	0
4	4-O	13	0	5	0	0
4	4-P	13	0	5	0	0
4	4-Q	13	0	5	0	0
4	4-R	13	0	5	0	0
4	4-S	13	0	5	0	0
4	4-T	13	0	5	0	0
4	4-U	13	0	5	0	0
4	4-V	13	0	5	0	0
4	4-W	13	0	5	0	0
4	4-X	13	0	5	0	0
4	5-A	13	0	5	0	0
4	5-B	13	0	5	0	0
4	5-C	13	0	5	0	0
4	5-D	13	0	5	0	0
4	5-E	13	0	5	0	0
4	5-F	13	0	5	0	0
4	5-G	13	0	5	0	0
4	5-H	13	0	5	0	0
4	5-I	13	0	5	0	0
4	5-J	13	0	5	0	0
4	5-K	13	0	5	0	0
4	5-L	13	0	5	0	0
4	5-M	13	0	5	0	0
4	5-N	13	0	5	0	0
4	5-O	13	0	5	0	0
4	5-P	13	0	5	0	0
4	5-Q	13	0	5	0	0
4	5-R	13	0	5	0	0
4	5-S	13	0	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	5-T	13	0	5	0	0
4	5-U	13	0	5	0	0
4	5-V	13	0	5	0	0
4	5-W	13	0	5	0	0
4	5-X	13	0	5	0	0
4	6-A	13	0	5	0	0
4	6-B	13	0	5	0	0
4	6-C	13	0	5	0	0
4	6-D	13	0	5	0	0
4	6-E	13	0	5	0	0
4	6-F	13	0	5	0	0
4	6-G	13	0	5	0	0
4	6-H	13	0	5	0	0
4	6-I	13	0	5	0	0
4	6-J	13	0	5	0	0
4	6-K	13	0	5	0	0
4	6-L	13	0	5	0	0
4	6-M	13	0	5	0	0
4	6-N	13	0	5	0	0
4	6-O	13	0	5	0	0
4	6-P	13	0	5	0	0
4	6-Q	13	0	5	0	0
4	6-R	13	0	5	0	0
4	6-S	13	0	5	0	0
4	6-T	13	0	5	0	0
4	6-U	13	0	5	0	0
4	6-V	13	0	5	0	0
4	6-W	13	0	5	0	0
4	6-X	13	0	5	0	0
4	7-A	13	0	5	0	0
4	7-B	13	0	5	0	0
4	7-C	13	0	5	0	0
4	7-D	13	0	5	0	0
4	7-E	13	0	5	0	0
4	7-F	13	0	5	0	0
4	7-G	13	0	5	0	0
4	7-H	13	0	5	0	0
4	7-I	13	0	5	0	0
4	7-J	13	0	5	0	0
4	7-K	13	0	5	0	0
4	7-L	13	0	5	0	0
4	7-M	13	0	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	7-N	13	0	5	0	0
4	7-O	13	0	5	0	0
4	7-P	13	0	5	0	0
4	7-Q	13	0	5	0	0
4	7-R	13	0	5	0	0
4	7-S	13	0	5	0	0
4	7-T	13	0	5	0	0
4	7-U	13	0	5	0	0
4	7-V	13	0	5	0	0
4	7-W	13	0	5	0	0
4	7-X	13	0	5	0	0
4	8-A	13	0	5	0	0
4	8-B	13	0	5	0	0
4	8-C	13	0	5	0	0
4	8-D	13	0	5	0	0
4	8-E	13	0	5	0	0
4	8-F	13	0	5	0	0
4	8-G	13	0	5	0	0
4	8-H	13	0	5	0	0
4	8-I	13	0	5	0	0
4	8-J	13	0	5	0	0
4	8-K	13	0	5	0	0
4	8-L	13	0	5	0	0
4	8-M	13	0	5	0	0
4	8-N	13	0	5	0	0
4	8-O	13	0	5	0	0
4	8-P	13	0	5	0	0
4	8-Q	13	0	5	0	0
4	8-R	13	0	5	0	0
4	8-S	13	0	5	0	0
4	8-T	13	0	5	0	0
4	8-U	13	0	5	0	0
4	8-V	13	0	5	0	0
4	8-W	13	0	5	0	0
4	8-X	13	0	5	0	0
4	9-A	13	0	5	0	0
4	9-B	13	0	5	0	0
4	9-C	13	0	5	0	0
4	9-D	13	0	5	0	0
4	9-E	13	0	5	0	0
4	9-F	13	0	5	0	0
4	9-G	13	0	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	9-H	13	0	5	0	0
4	9-I	13	0	5	0	0
4	9-J	13	0	5	0	0
4	9-K	13	0	5	0	0
4	9-L	13	0	5	0	0
4	9-M	13	0	5	0	0
4	9-N	13	0	5	0	0
4	9-O	13	0	5	0	0
4	9-P	13	0	5	0	0
4	9-Q	13	0	5	0	0
4	9-R	13	0	5	0	0
4	9-S	13	0	5	0	0
4	9-T	13	0	5	0	0
4	9-U	13	0	5	0	0
4	9-V	13	0	5	0	0
4	9-W	13	0	5	0	0
4	9-X	13	0	5	0	0
4	10-A	13	0	5	0	0
4	10-B	13	0	5	0	0
4	10-C	13	0	5	0	0
4	10-D	13	0	5	0	0
4	10-E	13	0	5	0	0
4	10-F	13	0	5	0	0
4	10-G	13	0	5	0	0
4	10-H	13	0	5	0	0
4	10-I	13	0	5	0	0
4	10-J	13	0	5	0	0
4	10-K	13	0	5	0	0
4	10-L	13	0	5	0	0
4	10-M	13	0	5	0	0
4	10-N	13	0	5	0	0
4	10-O	13	0	5	0	0
4	10-P	13	0	5	0	0
4	10-Q	13	0	5	0	0
4	10-R	13	0	5	0	0
4	10-S	13	0	5	0	0
4	10-T	13	0	5	0	0
4	10-U	13	0	5	0	0
4	10-V	13	0	5	0	0
4	10-W	13	0	5	0	0
4	10-X	13	0	5	0	0
5	1-A	261	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1-B	264	0	0	0	0
5	1-C	261	0	0	0	0
5	1-D	260	0	0	0	0
5	1-E	261	0	0	0	0
5	1-F	262	0	0	0	0
5	1-G	265	0	0	0	0
5	1-H	262	0	0	0	0
5	1-I	265	0	0	0	0
5	1-J	262	0	0	0	0
5	1-K	272	0	0	0	0
5	1-L	261	0	0	0	0
5	1-M	261	0	0	0	0
5	1-N	263	0	0	0	0
5	1-O	263	0	0	0	0
5	1-P	261	0	0	0	0
5	1-Q	260	0	0	0	0
5	1-R	261	0	0	0	0
5	1-S	265	0	0	0	0
5	1-T	261	0	0	0	0
5	1-U	263	0	0	0	0
5	1-V	265	0	0	0	0
5	1-W	269	0	0	0	0
5	1-X	264	0	0	0	0
5	2-A	262	0	0	0	0
5	2-B	261	0	0	0	0
5	2-C	264	0	0	0	0
5	2-D	269	0	0	0	0
5	2-E	254	0	0	0	0
5	2-F	263	0	0	0	0
5	2-G	262	0	0	0	0
5	2-H	263	0	0	0	0
5	2-I	265	0	0	0	0
5	2-J	258	0	0	0	0
5	2-K	271	0	0	0	0
5	2-L	264	0	0	0	0
5	2-M	264	0	0	0	0
5	2-N	261	0	0	0	0
5	2-O	267	0	0	0	0
5	2-P	264	0	0	0	0
5	2-Q	257	0	0	0	0
5	2-R	265	0	0	0	0
5	2-S	259	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	2-T	259	0	0	0	0
5	2-U	267	0	0	0	0
5	2-V	260	0	0	0	0
5	2-W	266	0	0	0	0
5	2-X	267	0	0	0	0
5	3-A	261	0	0	0	0
5	3-B	263	0	0	0	0
5	3-C	265	0	0	0	0
5	3-D	260	0	0	0	0
5	3-E	257	0	0	0	0
5	3-F	272	0	0	0	0
5	3-G	257	0	0	0	0
5	3-H	261	0	0	0	0
5	3-I	266	0	0	0	0
5	3-J	260	0	0	0	0
5	3-K	268	0	0	0	0
5	3-L	266	0	0	0	0
5	3-M	259	0	0	0	0
5	3-N	263	0	0	0	0
5	3-O	265	0	0	0	0
5	3-P	260	0	0	0	0
5	3-Q	259	0	0	0	0
5	3-R	268	0	0	0	0
5	3-S	264	0	0	0	0
5	3-T	262	0	0	0	0
5	3-U	267	0	0	0	0
5	3-V	258	0	0	0	0
5	3-W	266	0	0	0	0
5	3-X	265	0	0	0	0
5	4-A	263	0	0	0	0
5	4-B	262	0	0	0	0
5	4-C	261	0	0	0	0
5	4-D	263	0	0	0	0
5	4-E	263	0	0	0	0
5	4-F	264	0	0	0	0
5	4-G	261	0	0	0	0
5	4-H	266	0	0	0	0
5	4-I	263	0	0	0	0
5	4-J	260	0	0	0	0
5	4-K	267	0	0	0	0
5	4-L	263	0	0	0	0
5	4-M	264	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4-N	263	0	0	0	0
5	4-O	263	0	0	0	0
5	4-P	259	0	0	0	0
5	4-Q	264	0	0	0	0
5	4-R	263	0	0	0	0
5	4-S	260	0	0	0	0
5	4-T	262	0	0	0	0
5	4-U	264	0	0	0	0
5	4-V	266	0	0	0	0
5	4-W	263	0	0	0	0
5	4-X	265	0	0	0	0
5	5-A	261	0	0	0	0
5	5-B	261	0	0	0	0
5	5-C	263	0	0	0	0
5	5-D	262	0	0	0	0
5	5-E	259	0	0	0	0
5	5-F	266	0	0	0	0
5	5-G	263	0	0	0	0
5	5-H	270	0	0	0	0
5	5-I	260	0	0	0	0
5	5-J	263	0	0	0	0
5	5-K	268	0	0	0	0
5	5-L	260	0	0	0	0
5	5-M	264	0	0	0	0
5	5-N	265	0	0	0	0
5	5-O	267	0	0	0	0
5	5-P	262	0	0	0	0
5	5-Q	261	0	0	0	0
5	5-R	265	0	0	0	0
5	5-S	263	0	0	0	0
5	5-T	258	0	0	0	0
5	5-U	263	0	0	0	0
5	5-V	261	0	0	0	0
5	5-W	262	0	0	0	0
5	5-X	265	0	0	0	0
5	6-A	257	0	0	0	0
5	6-B	265	0	0	0	0
5	6-C	262	0	0	0	0
5	6-D	265	0	0	0	0
5	6-E	262	0	0	0	0
5	6-F	263	0	0	0	0
5	6-G	267	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	6-H	263	0	0	0	0
5	6-I	263	0	0	0	0
5	6-J	259	0	0	0	0
5	6-K	270	0	0	0	0
5	6-L	260	0	0	0	0
5	6-M	262	0	0	0	0
5	6-N	260	0	0	0	0
5	6-O	265	0	0	0	0
5	6-P	262	0	0	0	0
5	6-Q	260	0	0	0	0
5	6-R	266	0	0	0	0
5	6-S	266	0	0	0	0
5	6-T	257	0	0	0	0
5	6-U	265	0	0	0	0
5	6-V	265	0	0	0	0
5	6-W	264	0	0	0	0
5	6-X	264	0	0	0	0
5	7-A	265	0	0	0	0
5	7-B	264	0	0	0	0
5	7-C	262	0	0	0	0
5	7-D	261	0	0	0	0
5	7-E	265	0	0	0	0
5	7-F	262	0	0	0	0
5	7-G	259	0	0	0	0
5	7-H	262	0	0	0	0
5	7-I	261	0	0	0	0
5	7-J	266	0	0	0	0
5	7-K	263	0	0	0	0
5	7-L	266	0	0	0	0
5	7-M	260	0	0	0	0
5	7-N	266	0	0	0	0
5	7-O	262	0	0	0	0
5	7-P	261	0	0	0	0
5	7-Q	264	0	0	0	0
5	7-R	264	0	0	0	0
5	7-S	263	0	0	0	0
5	7-T	263	0	0	0	0
5	7-U	262	0	0	0	0
5	7-V	265	0	0	0	0
5	7-W	265	0	0	0	0
5	7-X	261	0	0	0	0
5	8-A	259	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	8-B	264	0	0	0	0
5	8-C	263	0	0	0	0
5	8-D	265	0	0	0	0
5	8-E	257	0	0	0	0
5	8-F	268	0	0	0	0
5	8-G	265	0	0	0	0
5	8-H	261	0	0	0	0
5	8-I	265	0	0	0	0
5	8-J	263	0	0	0	0
5	8-K	264	0	0	0	0
5	8-L	262	0	0	0	0
5	8-M	260	0	0	0	0
5	8-N	263	0	0	0	0
5	8-O	265	0	0	0	0
5	8-P	263	0	0	0	0
5	8-Q	257	0	0	0	0
5	8-R	265	0	0	0	0
5	8-S	269	0	0	0	0
5	8-T	259	0	0	0	0
5	8-U	263	0	0	0	0
5	8-V	264	0	0	0	0
5	8-W	263	0	0	0	0
5	8-X	265	0	0	0	0
5	9-A	265	0	0	0	0
5	9-B	258	0	0	0	0
5	9-C	261	0	0	0	0
5	9-D	266	0	0	0	0
5	9-E	262	0	0	0	0
5	9-F	262	0	0	0	0
5	9-G	263	0	0	0	0
5	9-H	268	0	0	0	0
5	9-I	262	0	0	0	0
5	9-J	260	0	0	0	0
5	9-K	269	0	0	0	0
5	9-L	260	0	0	0	0
5	9-M	265	0	0	0	0
5	9-N	261	0	0	0	0
5	9-O	263	0	0	0	0
5	9-P	265	0	0	0	0
5	9-Q	263	0	0	0	0
5	9-R	264	0	0	0	0
5	9-S	259	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	9-T	265	0	0	0	0
5	9-U	265	0	0	0	0
5	9-V	259	0	0	0	0
5	9-W	261	0	0	0	0
5	9-X	266	0	0	0	0
5	10-A	262	0	0	0	0
5	10-B	263	0	0	0	0
5	10-C	262	0	0	0	0
5	10-D	262	0	0	0	0
5	10-E	257	0	0	0	0
5	10-F	261	0	0	0	0
5	10-G	264	0	0	0	0
5	10-H	264	0	0	0	0
5	10-I	263	0	0	0	0
5	10-J	264	0	0	0	0
5	10-K	271	0	0	0	0
5	10-L	263	0	0	0	0
5	10-M	263	0	0	0	0
5	10-N	259	0	0	0	0
5	10-O	263	0	0	0	0
5	10-P	264	0	0	0	0
5	10-Q	257	0	0	0	0
5	10-R	262	0	0	0	0
5	10-S	266	0	0	0	0
5	10-T	262	0	0	0	0
5	10-U	264	0	0	0	0
5	10-V	265	0	0	0	0
5	10-W	265	0	0	0	0
5	10-X	266	0	0	0	0
All	All	978720	0	868551	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-B	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-C	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	2	2
1	1-D	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-E	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-F	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-G	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	2	2
1	1-H	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	2	2
1	1-I	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-J	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-K	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-L	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-M	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	2	2
1	1-N	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-O	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-P	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-Q	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-R	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-S	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	2	2
1	1-T	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-U	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-V	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-W	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	2	2
1	1-X	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	2	2
1	2-A	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-B	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-C	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-D	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-E	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-F	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-G	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-H	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-I	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-J	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-K	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-L	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-M	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-N	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-O	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-P	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-Q	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-R	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-S	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-T	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-U	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-V	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-W	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	2-X	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	2	2
1	3-A	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5
1	3-B	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5
1	3-C	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	4	5
1	3-D	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5
1	3-E	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	4	5
1	3-F	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	4	5
1	3-G	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5
1	3-H	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	3-I	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5	
1	3-J	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	4	5	
1	3-K	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5	
1	3-L	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	4	5	
1	3-M	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5	
1	3-N	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5	
1	3-O	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	4	5	
1	3-P	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	4	5	
1	3-Q	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5	
1	3-R	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5	
1	3-S	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5	
1	3-T	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5	
1	3-U	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	4	5	
1	3-V	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	4	5	
1	3-W	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	4	5	
1	3-X	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	4	5	
1	4-A	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-B	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-C	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-D	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-E	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-F	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-G	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-H	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-I	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-J	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-K	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-L	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-M	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-N	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	
1	4-O	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4-P	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3
1	4-Q	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3
1	4-R	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3
1	4-S	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3
1	4-T	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3
1	4-U	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3
1	4-V	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3
1	4-W	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3
1	4-X	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	3	3
1	5-A	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-B	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-C	475/477 (100%)	423 (89%)	43 (9%)	9 (2%)	6	8
1	5-D	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-E	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-F	475/477 (100%)	423 (89%)	43 (9%)	9 (2%)	6	8
1	5-G	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-H	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-I	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-J	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-K	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-L	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-M	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-N	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-O	475/477 (100%)	423 (89%)	43 (9%)	9 (2%)	6	8
1	5-P	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-Q	475/477 (100%)	423 (89%)	43 (9%)	9 (2%)	6	8
1	5-R	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-S	475/477 (100%)	423 (89%)	43 (9%)	9 (2%)	6	8
1	5-T	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-U	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-V	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-W	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	5-X	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	6	8
1	6-A	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-B	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	4	5
1	6-C	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-D	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	4	5
1	6-E	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	4	5
1	6-F	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-G	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-H	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	4	5
1	6-I	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-J	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-K	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-L	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-M	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	4	5
1	6-N	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-O	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-P	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	4	5
1	6-Q	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-R	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-S	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	4	5
1	6-T	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	4	5
1	6-U	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-V	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-W	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	4	4
1	6-X	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	4	5
1	7-A	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-B	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-C	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-D	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-E	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7-F	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-G	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	2
1	7-H	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-I	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	2
1	7-J	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-K	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-L	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-M	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-N	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	2
1	7-O	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-P	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	2
1	7-Q	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-R	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-S	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-T	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-U	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-V	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	2
1	7-W	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	7-X	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	2
1	8-A	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-B	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-C	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-D	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-E	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-F	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-G	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-H	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-I	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-J	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-K	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-L	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-M	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-N	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-O	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-P	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-Q	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-R	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-S	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-T	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-U	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-V	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-W	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	8-X	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	6	8
1	9-A	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-B	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	6	8
1	9-C	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-D	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-E	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	6	8
1	9-F	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-G	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-H	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-I	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	6	8
1	9-J	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	6	8
1	9-K	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-L	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	6	8
1	9-M	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-N	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-O	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-P	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	6	8
1	9-Q	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-R	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-S	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-T	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	6	8
1	9-U	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-V	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	9-W	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	6	8
1	9-X	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	6	8
1	10-A	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-B	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-C	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-D	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-E	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-F	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-G	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-H	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-I	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-J	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-K	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-L	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-M	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-N	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-O	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-P	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-Q	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-R	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-S	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-T	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-U	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-V	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-W	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
1	10-X	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	4	4
All	All	114000/114480 (100%)	102469 (90%)	8420 (7%)	3111 (3%)	4	4

All (3111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	57	PHE
1	1-A	59	SER
1	1-A	63	SER
1	1-A	327	GLU
1	1-B	57	PHE
1	1-B	59	SER
1	1-B	63	SER
1	1-B	327	GLU
1	1-C	57	PHE
1	1-C	59	SER
1	1-C	63	SER
1	1-C	327	GLU
1	1-D	57	PHE
1	1-D	59	SER
1	1-D	63	SER
1	1-D	327	GLU
1	1-E	57	PHE
1	1-E	59	SER
1	1-E	63	SER
1	1-E	327	GLU
1	1-F	57	PHE
1	1-F	59	SER
1	1-F	63	SER
1	1-F	327	GLU
1	1-G	57	PHE
1	1-G	59	SER
1	1-G	63	SER
1	1-G	327	GLU
1	1-H	57	PHE
1	1-H	59	SER
1	1-H	63	SER
1	1-H	327	GLU
1	1-I	57	PHE
1	1-I	59	SER
1	1-I	63	SER
1	1-I	327	GLU
1	1-J	57	PHE
1	1-J	59	SER
1	1-J	63	SER
1	1-J	327	GLU
1	1-K	57	PHE
1	1-K	59	SER
1	1-K	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-K	327	GLU
1	1-L	57	PHE
1	1-L	59	SER
1	1-L	63	SER
1	1-L	327	GLU
1	1-M	57	PHE
1	1-M	59	SER
1	1-M	63	SER
1	1-M	327	GLU
1	1-N	57	PHE
1	1-N	59	SER
1	1-N	63	SER
1	1-N	327	GLU
1	1-O	57	PHE
1	1-O	59	SER
1	1-O	63	SER
1	1-O	327	GLU
1	1-P	57	PHE
1	1-P	59	SER
1	1-P	63	SER
1	1-P	327	GLU
1	1-Q	57	PHE
1	1-Q	59	SER
1	1-Q	63	SER
1	1-Q	327	GLU
1	1-R	57	PHE
1	1-R	59	SER
1	1-R	63	SER
1	1-R	327	GLU
1	1-S	57	PHE
1	1-S	59	SER
1	1-S	63	SER
1	1-S	327	GLU
1	1-T	57	PHE
1	1-T	59	SER
1	1-T	63	SER
1	1-T	327	GLU
1	1-U	57	PHE
1	1-U	59	SER
1	1-U	63	SER
1	1-U	327	GLU
1	1-V	57	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-V	59	SER
1	1-V	63	SER
1	1-V	327	GLU
1	1-W	57	PHE
1	1-W	59	SER
1	1-W	63	SER
1	1-W	327	GLU
1	1-X	57	PHE
1	1-X	59	SER
1	1-X	63	SER
1	1-X	327	GLU
1	2-A	602	GLU
1	2-A	54	ILE
1	2-A	63	SER
1	2-A	97	LEU
1	2-A	208	LYS
1	2-A	327	GLU
1	2-A	390	ALA
1	2-B	602	GLU
1	2-B	54	ILE
1	2-B	63	SER
1	2-B	97	LEU
1	2-B	208	LYS
1	2-B	327	GLU
1	2-B	390	ALA
1	2-C	602	GLU
1	2-C	54	ILE
1	2-C	63	SER
1	2-C	97	LEU
1	2-C	208	LYS
1	2-C	327	GLU
1	2-C	390	ALA
1	2-D	602	GLU
1	2-D	54	ILE
1	2-D	63	SER
1	2-D	97	LEU
1	2-D	208	LYS
1	2-D	327	GLU
1	2-D	390	ALA
1	2-E	602	GLU
1	2-E	54	ILE
1	2-E	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-E	97	LEU
1	2-E	208	LYS
1	2-E	327	GLU
1	2-E	390	ALA
1	2-F	602	GLU
1	2-F	54	ILE
1	2-F	63	SER
1	2-F	97	LEU
1	2-F	208	LYS
1	2-F	327	GLU
1	2-F	390	ALA
1	2-G	602	GLU
1	2-G	54	ILE
1	2-G	63	SER
1	2-G	97	LEU
1	2-G	208	LYS
1	2-G	327	GLU
1	2-G	390	ALA
1	2-H	602	GLU
1	2-H	54	ILE
1	2-H	63	SER
1	2-H	97	LEU
1	2-H	208	LYS
1	2-H	327	GLU
1	2-H	390	ALA
1	2-I	602	GLU
1	2-I	54	ILE
1	2-I	63	SER
1	2-I	97	LEU
1	2-I	208	LYS
1	2-I	327	GLU
1	2-I	390	ALA
1	2-J	602	GLU
1	2-J	54	ILE
1	2-J	63	SER
1	2-J	97	LEU
1	2-J	208	LYS
1	2-J	327	GLU
1	2-J	390	ALA
1	2-K	602	GLU
1	2-K	54	ILE
1	2-K	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-K	97	LEU
1	2-K	208	LYS
1	2-K	327	GLU
1	2-K	390	ALA
1	2-L	602	GLU
1	2-L	54	ILE
1	2-L	63	SER
1	2-L	97	LEU
1	2-L	208	LYS
1	2-L	327	GLU
1	2-L	390	ALA
1	2-M	602	GLU
1	2-M	54	ILE
1	2-M	63	SER
1	2-M	97	LEU
1	2-M	208	LYS
1	2-M	327	GLU
1	2-M	390	ALA
1	2-N	602	GLU
1	2-N	54	ILE
1	2-N	63	SER
1	2-N	97	LEU
1	2-N	208	LYS
1	2-N	327	GLU
1	2-N	390	ALA
1	2-O	602	GLU
1	2-O	54	ILE
1	2-O	63	SER
1	2-O	97	LEU
1	2-O	208	LYS
1	2-O	327	GLU
1	2-O	390	ALA
1	2-P	602	GLU
1	2-P	54	ILE
1	2-P	63	SER
1	2-P	97	LEU
1	2-P	208	LYS
1	2-P	327	GLU
1	2-P	390	ALA
1	2-Q	602	GLU
1	2-Q	54	ILE
1	2-Q	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-Q	97	LEU
1	2-Q	208	LYS
1	2-Q	327	GLU
1	2-Q	390	ALA
1	2-R	602	GLU
1	2-R	54	ILE
1	2-R	63	SER
1	2-R	97	LEU
1	2-R	208	LYS
1	2-R	327	GLU
1	2-R	390	ALA
1	2-S	602	GLU
1	2-S	54	ILE
1	2-S	63	SER
1	2-S	97	LEU
1	2-S	208	LYS
1	2-S	327	GLU
1	2-S	390	ALA
1	2-T	602	GLU
1	2-T	54	ILE
1	2-T	63	SER
1	2-T	97	LEU
1	2-T	208	LYS
1	2-T	327	GLU
1	2-T	390	ALA
1	2-U	602	GLU
1	2-U	54	ILE
1	2-U	63	SER
1	2-U	97	LEU
1	2-U	208	LYS
1	2-U	327	GLU
1	2-U	390	ALA
1	2-V	602	GLU
1	2-V	54	ILE
1	2-V	63	SER
1	2-V	97	LEU
1	2-V	208	LYS
1	2-V	327	GLU
1	2-V	390	ALA
1	2-W	602	GLU
1	2-W	54	ILE
1	2-W	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-W	97	LEU
1	2-W	208	LYS
1	2-W	327	GLU
1	2-W	390	ALA
1	2-X	602	GLU
1	2-X	54	ILE
1	2-X	63	SER
1	2-X	97	LEU
1	2-X	208	LYS
1	2-X	327	GLU
1	2-X	390	ALA
1	3-A	602	GLU
1	3-A	52	SER
1	3-A	53	SER
1	3-A	401	PRO
1	3-B	602	GLU
1	3-B	52	SER
1	3-B	53	SER
1	3-B	401	PRO
1	3-C	602	GLU
1	3-C	52	SER
1	3-C	53	SER
1	3-C	401	PRO
1	3-D	602	GLU
1	3-D	52	SER
1	3-D	53	SER
1	3-D	401	PRO
1	3-E	602	GLU
1	3-E	52	SER
1	3-E	53	SER
1	3-E	401	PRO
1	3-F	602	GLU
1	3-F	52	SER
1	3-F	53	SER
1	3-F	401	PRO
1	3-G	602	GLU
1	3-G	52	SER
1	3-G	53	SER
1	3-G	401	PRO
1	3-H	602	GLU
1	3-H	52	SER
1	3-H	53	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-H	401	PRO
1	3-I	602	GLU
1	3-I	52	SER
1	3-I	53	SER
1	3-I	401	PRO
1	3-J	602	GLU
1	3-J	52	SER
1	3-J	53	SER
1	3-J	401	PRO
1	3-K	602	GLU
1	3-K	52	SER
1	3-K	53	SER
1	3-K	401	PRO
1	3-L	602	GLU
1	3-L	52	SER
1	3-L	53	SER
1	3-L	401	PRO
1	3-M	602	GLU
1	3-M	52	SER
1	3-M	53	SER
1	3-M	401	PRO
1	3-N	602	GLU
1	3-N	52	SER
1	3-N	53	SER
1	3-N	401	PRO
1	3-O	602	GLU
1	3-O	52	SER
1	3-O	53	SER
1	3-O	401	PRO
1	3-P	602	GLU
1	3-P	52	SER
1	3-P	53	SER
1	3-P	401	PRO
1	3-Q	602	GLU
1	3-Q	52	SER
1	3-Q	53	SER
1	3-Q	401	PRO
1	3-R	602	GLU
1	3-R	52	SER
1	3-R	53	SER
1	3-R	401	PRO
1	3-S	602	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-S	52	SER
1	3-S	53	SER
1	3-S	401	PRO
1	3-T	602	GLU
1	3-T	52	SER
1	3-T	53	SER
1	3-T	401	PRO
1	3-U	602	GLU
1	3-U	52	SER
1	3-U	53	SER
1	3-U	401	PRO
1	3-V	602	GLU
1	3-V	52	SER
1	3-V	53	SER
1	3-V	401	PRO
1	3-W	602	GLU
1	3-W	52	SER
1	3-W	53	SER
1	3-W	401	PRO
1	3-X	602	GLU
1	3-X	52	SER
1	3-X	53	SER
1	3-X	401	PRO
1	4-A	49	PHE
1	4-A	53	SER
1	4-A	63	SER
1	4-A	324	PRO
1	4-B	49	PHE
1	4-B	53	SER
1	4-B	63	SER
1	4-B	324	PRO
1	4-C	49	PHE
1	4-C	53	SER
1	4-C	63	SER
1	4-C	324	PRO
1	4-D	49	PHE
1	4-D	53	SER
1	4-D	63	SER
1	4-D	324	PRO
1	4-E	49	PHE
1	4-E	53	SER
1	4-E	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-E	324	PRO
1	4-F	49	PHE
1	4-F	53	SER
1	4-F	63	SER
1	4-F	324	PRO
1	4-G	49	PHE
1	4-G	53	SER
1	4-G	63	SER
1	4-G	324	PRO
1	4-H	49	PHE
1	4-H	53	SER
1	4-H	63	SER
1	4-H	324	PRO
1	4-I	49	PHE
1	4-I	53	SER
1	4-I	63	SER
1	4-I	324	PRO
1	4-J	49	PHE
1	4-J	53	SER
1	4-J	63	SER
1	4-J	324	PRO
1	4-K	49	PHE
1	4-K	53	SER
1	4-K	63	SER
1	4-K	324	PRO
1	4-L	49	PHE
1	4-L	53	SER
1	4-L	63	SER
1	4-L	324	PRO
1	4-M	49	PHE
1	4-M	53	SER
1	4-M	63	SER
1	4-M	324	PRO
1	4-N	49	PHE
1	4-N	53	SER
1	4-N	63	SER
1	4-N	324	PRO
1	4-O	49	PHE
1	4-O	53	SER
1	4-O	63	SER
1	4-O	324	PRO
1	4-P	49	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-P	53	SER
1	4-P	63	SER
1	4-P	324	PRO
1	4-Q	49	PHE
1	4-Q	53	SER
1	4-Q	63	SER
1	4-Q	324	PRO
1	4-R	49	PHE
1	4-R	53	SER
1	4-R	63	SER
1	4-R	324	PRO
1	4-S	49	PHE
1	4-S	53	SER
1	4-S	63	SER
1	4-S	324	PRO
1	4-T	49	PHE
1	4-T	53	SER
1	4-T	63	SER
1	4-T	324	PRO
1	4-U	49	PHE
1	4-U	53	SER
1	4-U	63	SER
1	4-U	324	PRO
1	4-V	49	PHE
1	4-V	53	SER
1	4-V	63	SER
1	4-V	324	PRO
1	4-W	49	PHE
1	4-W	53	SER
1	4-W	63	SER
1	4-W	324	PRO
1	4-X	49	PHE
1	4-X	53	SER
1	4-X	63	SER
1	4-X	324	PRO
1	5-A	63	SER
1	5-A	64	ASP
1	5-A	208	LYS
1	5-B	63	SER
1	5-B	64	ASP
1	5-B	208	LYS
1	5-C	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-C	64	ASP
1	5-C	208	LYS
1	5-D	63	SER
1	5-D	64	ASP
1	5-D	208	LYS
1	5-E	63	SER
1	5-E	64	ASP
1	5-E	208	LYS
1	5-F	63	SER
1	5-F	64	ASP
1	5-F	208	LYS
1	5-G	63	SER
1	5-G	64	ASP
1	5-G	208	LYS
1	5-H	63	SER
1	5-H	64	ASP
1	5-H	208	LYS
1	5-I	63	SER
1	5-I	64	ASP
1	5-I	208	LYS
1	5-J	63	SER
1	5-J	64	ASP
1	5-J	208	LYS
1	5-K	63	SER
1	5-K	64	ASP
1	5-K	208	LYS
1	5-L	63	SER
1	5-L	64	ASP
1	5-L	208	LYS
1	5-M	63	SER
1	5-M	64	ASP
1	5-M	208	LYS
1	5-N	63	SER
1	5-N	64	ASP
1	5-N	208	LYS
1	5-O	63	SER
1	5-O	64	ASP
1	5-O	208	LYS
1	5-P	63	SER
1	5-P	64	ASP
1	5-P	208	LYS
1	5-Q	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-Q	64	ASP
1	5-Q	208	LYS
1	5-R	63	SER
1	5-R	64	ASP
1	5-R	208	LYS
1	5-S	63	SER
1	5-S	64	ASP
1	5-S	208	LYS
1	5-T	63	SER
1	5-T	64	ASP
1	5-T	208	LYS
1	5-U	63	SER
1	5-U	64	ASP
1	5-U	208	LYS
1	5-V	63	SER
1	5-V	64	ASP
1	5-V	208	LYS
1	5-W	63	SER
1	5-W	64	ASP
1	5-W	208	LYS
1	5-X	63	SER
1	5-X	64	ASP
1	5-X	208	LYS
1	6-A	53	SER
1	6-A	54	ILE
1	6-A	96	THR
1	6-A	326	TYR
1	6-A	394	LYS
1	6-B	53	SER
1	6-B	54	ILE
1	6-B	96	THR
1	6-B	326	TYR
1	6-B	394	LYS
1	6-C	53	SER
1	6-C	54	ILE
1	6-C	96	THR
1	6-C	326	TYR
1	6-C	394	LYS
1	6-D	53	SER
1	6-D	54	ILE
1	6-D	96	THR
1	6-D	326	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-D	394	LYS
1	6-E	53	SER
1	6-E	54	ILE
1	6-E	96	THR
1	6-E	326	TYR
1	6-E	394	LYS
1	6-F	53	SER
1	6-F	54	ILE
1	6-F	96	THR
1	6-F	326	TYR
1	6-F	394	LYS
1	6-G	53	SER
1	6-G	54	ILE
1	6-G	96	THR
1	6-G	326	TYR
1	6-G	394	LYS
1	6-H	53	SER
1	6-H	54	ILE
1	6-H	96	THR
1	6-H	326	TYR
1	6-H	394	LYS
1	6-I	53	SER
1	6-I	54	ILE
1	6-I	96	THR
1	6-I	326	TYR
1	6-I	394	LYS
1	6-J	53	SER
1	6-J	54	ILE
1	6-J	96	THR
1	6-J	326	TYR
1	6-J	394	LYS
1	6-K	53	SER
1	6-K	54	ILE
1	6-K	96	THR
1	6-K	326	TYR
1	6-K	394	LYS
1	6-L	53	SER
1	6-L	54	ILE
1	6-L	96	THR
1	6-L	326	TYR
1	6-L	394	LYS
1	6-M	53	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-M	54	ILE
1	6-M	96	THR
1	6-M	326	TYR
1	6-M	394	LYS
1	6-N	53	SER
1	6-N	54	ILE
1	6-N	96	THR
1	6-N	326	TYR
1	6-N	394	LYS
1	6-O	53	SER
1	6-O	54	ILE
1	6-O	96	THR
1	6-O	326	TYR
1	6-O	394	LYS
1	6-P	53	SER
1	6-P	54	ILE
1	6-P	96	THR
1	6-P	326	TYR
1	6-P	394	LYS
1	6-Q	53	SER
1	6-Q	54	ILE
1	6-Q	96	THR
1	6-Q	326	TYR
1	6-Q	394	LYS
1	6-R	53	SER
1	6-R	54	ILE
1	6-R	96	THR
1	6-R	326	TYR
1	6-R	394	LYS
1	6-S	53	SER
1	6-S	54	ILE
1	6-S	96	THR
1	6-S	326	TYR
1	6-S	394	LYS
1	6-T	53	SER
1	6-T	54	ILE
1	6-T	96	THR
1	6-T	326	TYR
1	6-T	394	LYS
1	6-U	53	SER
1	6-U	54	ILE
1	6-U	96	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-U	326	TYR
1	6-U	394	LYS
1	6-V	53	SER
1	6-V	54	ILE
1	6-V	96	THR
1	6-V	326	TYR
1	6-V	394	LYS
1	6-W	53	SER
1	6-W	54	ILE
1	6-W	96	THR
1	6-W	326	TYR
1	6-W	394	LYS
1	6-X	53	SER
1	6-X	54	ILE
1	6-X	96	THR
1	6-X	326	TYR
1	6-X	394	LYS
1	7-A	602	GLU
1	7-A	53	SER
1	7-A	55	ARG
1	7-A	58	GLN
1	7-A	59	SER
1	7-A	326	TYR
1	7-A	397	TYR
1	7-A	401	PRO
1	7-B	602	GLU
1	7-B	53	SER
1	7-B	55	ARG
1	7-B	58	GLN
1	7-B	59	SER
1	7-B	326	TYR
1	7-B	397	TYR
1	7-B	401	PRO
1	7-C	602	GLU
1	7-C	53	SER
1	7-C	55	ARG
1	7-C	58	GLN
1	7-C	59	SER
1	7-C	326	TYR
1	7-C	397	TYR
1	7-C	401	PRO
1	7-D	602	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-D	53	SER
1	7-D	55	ARG
1	7-D	58	GLN
1	7-D	59	SER
1	7-D	326	TYR
1	7-D	397	TYR
1	7-D	401	PRO
1	7-E	602	GLU
1	7-E	53	SER
1	7-E	55	ARG
1	7-E	58	GLN
1	7-E	59	SER
1	7-E	326	TYR
1	7-E	397	TYR
1	7-E	401	PRO
1	7-F	602	GLU
1	7-F	53	SER
1	7-F	55	ARG
1	7-F	58	GLN
1	7-F	59	SER
1	7-F	326	TYR
1	7-F	397	TYR
1	7-F	401	PRO
1	7-G	602	GLU
1	7-G	53	SER
1	7-G	55	ARG
1	7-G	58	GLN
1	7-G	59	SER
1	7-G	326	TYR
1	7-G	397	TYR
1	7-G	401	PRO
1	7-H	602	GLU
1	7-H	53	SER
1	7-H	55	ARG
1	7-H	58	GLN
1	7-H	59	SER
1	7-H	326	TYR
1	7-H	397	TYR
1	7-H	401	PRO
1	7-I	602	GLU
1	7-I	53	SER
1	7-I	55	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-I	58	GLN
1	7-I	59	SER
1	7-I	326	TYR
1	7-I	397	TYR
1	7-I	401	PRO
1	7-J	602	GLU
1	7-J	53	SER
1	7-J	55	ARG
1	7-J	58	GLN
1	7-J	59	SER
1	7-J	326	TYR
1	7-J	397	TYR
1	7-J	401	PRO
1	7-K	602	GLU
1	7-K	53	SER
1	7-K	55	ARG
1	7-K	58	GLN
1	7-K	59	SER
1	7-K	326	TYR
1	7-K	397	TYR
1	7-K	401	PRO
1	7-L	602	GLU
1	7-L	53	SER
1	7-L	55	ARG
1	7-L	58	GLN
1	7-L	59	SER
1	7-L	326	TYR
1	7-L	397	TYR
1	7-L	401	PRO
1	7-M	602	GLU
1	7-M	53	SER
1	7-M	55	ARG
1	7-M	58	GLN
1	7-M	59	SER
1	7-M	326	TYR
1	7-M	397	TYR
1	7-M	401	PRO
1	7-N	602	GLU
1	7-N	53	SER
1	7-N	55	ARG
1	7-N	58	GLN
1	7-N	59	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-N	326	TYR
1	7-N	397	TYR
1	7-N	401	PRO
1	7-O	602	GLU
1	7-O	53	SER
1	7-O	55	ARG
1	7-O	58	GLN
1	7-O	59	SER
1	7-O	326	TYR
1	7-O	397	TYR
1	7-O	401	PRO
1	7-P	602	GLU
1	7-P	53	SER
1	7-P	55	ARG
1	7-P	58	GLN
1	7-P	59	SER
1	7-P	326	TYR
1	7-P	397	TYR
1	7-P	401	PRO
1	7-Q	602	GLU
1	7-Q	53	SER
1	7-Q	55	ARG
1	7-Q	58	GLN
1	7-Q	59	SER
1	7-Q	326	TYR
1	7-Q	397	TYR
1	7-Q	401	PRO
1	7-R	602	GLU
1	7-R	53	SER
1	7-R	55	ARG
1	7-R	58	GLN
1	7-R	59	SER
1	7-R	326	TYR
1	7-R	397	TYR
1	7-R	401	PRO
1	7-S	602	GLU
1	7-S	53	SER
1	7-S	55	ARG
1	7-S	58	GLN
1	7-S	59	SER
1	7-S	326	TYR
1	7-S	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-S	401	PRO
1	7-T	602	GLU
1	7-T	53	SER
1	7-T	55	ARG
1	7-T	58	GLN
1	7-T	59	SER
1	7-T	326	TYR
1	7-T	397	TYR
1	7-T	401	PRO
1	7-U	602	GLU
1	7-U	53	SER
1	7-U	55	ARG
1	7-U	58	GLN
1	7-U	59	SER
1	7-U	326	TYR
1	7-U	397	TYR
1	7-U	401	PRO
1	7-V	602	GLU
1	7-V	53	SER
1	7-V	55	ARG
1	7-V	58	GLN
1	7-V	59	SER
1	7-V	326	TYR
1	7-V	397	TYR
1	7-V	401	PRO
1	7-W	602	GLU
1	7-W	53	SER
1	7-W	55	ARG
1	7-W	58	GLN
1	7-W	59	SER
1	7-W	326	TYR
1	7-W	397	TYR
1	7-W	401	PRO
1	7-X	602	GLU
1	7-X	53	SER
1	7-X	55	ARG
1	7-X	58	GLN
1	7-X	59	SER
1	7-X	326	TYR
1	7-X	397	TYR
1	7-X	401	PRO
1	8-A	54	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-A	208	LYS
1	8-B	54	ILE
1	8-B	208	LYS
1	8-C	54	ILE
1	8-C	208	LYS
1	8-D	54	ILE
1	8-D	208	LYS
1	8-E	54	ILE
1	8-E	208	LYS
1	8-F	54	ILE
1	8-F	208	LYS
1	8-G	54	ILE
1	8-G	208	LYS
1	8-H	54	ILE
1	8-H	208	LYS
1	8-I	54	ILE
1	8-I	208	LYS
1	8-J	54	ILE
1	8-J	208	LYS
1	8-K	54	ILE
1	8-K	208	LYS
1	8-L	54	ILE
1	8-L	208	LYS
1	8-M	54	ILE
1	8-M	208	LYS
1	8-N	54	ILE
1	8-N	208	LYS
1	8-O	54	ILE
1	8-O	208	LYS
1	8-P	54	ILE
1	8-P	208	LYS
1	8-Q	54	ILE
1	8-Q	208	LYS
1	8-R	54	ILE
1	8-R	208	LYS
1	8-S	54	ILE
1	8-S	208	LYS
1	8-T	54	ILE
1	8-T	208	LYS
1	8-U	54	ILE
1	8-U	208	LYS
1	8-V	54	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-V	208	LYS
1	8-W	54	ILE
1	8-W	208	LYS
1	8-X	54	ILE
1	8-X	208	LYS
1	9-A	208	LYS
1	9-A	401	PRO
1	9-A	402	GLU
1	9-B	208	LYS
1	9-B	401	PRO
1	9-B	402	GLU
1	9-C	208	LYS
1	9-C	401	PRO
1	9-C	402	GLU
1	9-D	208	LYS
1	9-D	401	PRO
1	9-D	402	GLU
1	9-E	208	LYS
1	9-E	401	PRO
1	9-E	402	GLU
1	9-F	208	LYS
1	9-F	401	PRO
1	9-F	402	GLU
1	9-G	208	LYS
1	9-G	401	PRO
1	9-G	402	GLU
1	9-H	208	LYS
1	9-H	401	PRO
1	9-H	402	GLU
1	9-I	208	LYS
1	9-I	401	PRO
1	9-I	402	GLU
1	9-J	208	LYS
1	9-J	401	PRO
1	9-J	402	GLU
1	9-K	208	LYS
1	9-K	401	PRO
1	9-K	402	GLU
1	9-L	208	LYS
1	9-L	401	PRO
1	9-L	402	GLU
1	9-M	208	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-M	401	PRO
1	9-M	402	GLU
1	9-N	208	LYS
1	9-N	401	PRO
1	9-N	402	GLU
1	9-O	208	LYS
1	9-O	401	PRO
1	9-O	402	GLU
1	9-P	208	LYS
1	9-P	401	PRO
1	9-P	402	GLU
1	9-Q	208	LYS
1	9-Q	401	PRO
1	9-Q	402	GLU
1	9-R	208	LYS
1	9-R	401	PRO
1	9-R	402	GLU
1	9-S	208	LYS
1	9-S	401	PRO
1	9-S	402	GLU
1	9-T	208	LYS
1	9-T	401	PRO
1	9-T	402	GLU
1	9-U	208	LYS
1	9-U	401	PRO
1	9-U	402	GLU
1	9-V	208	LYS
1	9-V	401	PRO
1	9-V	402	GLU
1	9-W	208	LYS
1	9-W	401	PRO
1	9-W	402	GLU
1	9-X	208	LYS
1	9-X	401	PRO
1	9-X	402	GLU
1	10-A	51	GLY
1	10-A	53	SER
1	10-A	54	ILE
1	10-A	63	SER
1	10-A	401	PRO
1	10-B	51	GLY
1	10-B	53	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-B	54	ILE
1	10-B	63	SER
1	10-B	401	PRO
1	10-C	51	GLY
1	10-C	53	SER
1	10-C	54	ILE
1	10-C	63	SER
1	10-C	401	PRO
1	10-D	51	GLY
1	10-D	53	SER
1	10-D	54	ILE
1	10-D	63	SER
1	10-D	401	PRO
1	10-E	51	GLY
1	10-E	53	SER
1	10-E	54	ILE
1	10-E	63	SER
1	10-E	401	PRO
1	10-F	51	GLY
1	10-F	53	SER
1	10-F	54	ILE
1	10-F	63	SER
1	10-F	401	PRO
1	10-G	51	GLY
1	10-G	53	SER
1	10-G	54	ILE
1	10-G	63	SER
1	10-G	401	PRO
1	10-H	51	GLY
1	10-H	53	SER
1	10-H	54	ILE
1	10-H	63	SER
1	10-H	401	PRO
1	10-I	51	GLY
1	10-I	53	SER
1	10-I	54	ILE
1	10-I	63	SER
1	10-I	401	PRO
1	10-J	51	GLY
1	10-J	53	SER
1	10-J	54	ILE
1	10-J	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-J	401	PRO
1	10-K	51	GLY
1	10-K	53	SER
1	10-K	54	ILE
1	10-K	63	SER
1	10-K	401	PRO
1	10-L	51	GLY
1	10-L	53	SER
1	10-L	54	ILE
1	10-L	63	SER
1	10-L	401	PRO
1	10-M	51	GLY
1	10-M	53	SER
1	10-M	54	ILE
1	10-M	63	SER
1	10-M	401	PRO
1	10-N	51	GLY
1	10-N	53	SER
1	10-N	54	ILE
1	10-N	63	SER
1	10-N	401	PRO
1	10-O	51	GLY
1	10-O	53	SER
1	10-O	54	ILE
1	10-O	63	SER
1	10-O	401	PRO
1	10-P	51	GLY
1	10-P	53	SER
1	10-P	54	ILE
1	10-P	63	SER
1	10-P	401	PRO
1	10-Q	51	GLY
1	10-Q	53	SER
1	10-Q	54	ILE
1	10-Q	63	SER
1	10-Q	401	PRO
1	10-R	51	GLY
1	10-R	53	SER
1	10-R	54	ILE
1	10-R	63	SER
1	10-R	401	PRO
1	10-S	51	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-S	53	SER
1	10-S	54	ILE
1	10-S	63	SER
1	10-S	401	PRO
1	10-T	51	GLY
1	10-T	53	SER
1	10-T	54	ILE
1	10-T	63	SER
1	10-T	401	PRO
1	10-U	51	GLY
1	10-U	53	SER
1	10-U	54	ILE
1	10-U	63	SER
1	10-U	401	PRO
1	10-V	51	GLY
1	10-V	53	SER
1	10-V	54	ILE
1	10-V	63	SER
1	10-V	401	PRO
1	10-W	51	GLY
1	10-W	53	SER
1	10-W	54	ILE
1	10-W	63	SER
1	10-W	401	PRO
1	10-X	51	GLY
1	10-X	53	SER
1	10-X	54	ILE
1	10-X	63	SER
1	10-X	401	PRO
1	1-A	51	GLY
1	1-A	58	GLN
1	1-A	208	LYS
1	1-B	51	GLY
1	1-B	58	GLN
1	1-B	208	LYS
1	1-C	51	GLY
1	1-C	58	GLN
1	1-C	208	LYS
1	1-D	51	GLY
1	1-D	58	GLN
1	1-D	208	LYS
1	1-E	51	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-E	58	GLN
1	1-E	208	LYS
1	1-F	51	GLY
1	1-F	58	GLN
1	1-F	208	LYS
1	1-G	51	GLY
1	1-G	58	GLN
1	1-G	208	LYS
1	1-H	51	GLY
1	1-H	58	GLN
1	1-H	208	LYS
1	1-I	51	GLY
1	1-I	58	GLN
1	1-I	208	LYS
1	1-J	51	GLY
1	1-J	58	GLN
1	1-J	208	LYS
1	1-K	51	GLY
1	1-K	58	GLN
1	1-K	208	LYS
1	1-L	51	GLY
1	1-L	58	GLN
1	1-L	208	LYS
1	1-M	51	GLY
1	1-M	58	GLN
1	1-M	208	LYS
1	1-N	51	GLY
1	1-N	58	GLN
1	1-N	208	LYS
1	1-O	51	GLY
1	1-O	58	GLN
1	1-O	208	LYS
1	1-P	51	GLY
1	1-P	58	GLN
1	1-P	208	LYS
1	1-Q	51	GLY
1	1-Q	58	GLN
1	1-Q	208	LYS
1	1-R	51	GLY
1	1-R	58	GLN
1	1-R	208	LYS
1	1-S	51	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-S	58	GLN
1	1-S	208	LYS
1	1-T	51	GLY
1	1-T	58	GLN
1	1-T	208	LYS
1	1-U	51	GLY
1	1-U	58	GLN
1	1-U	208	LYS
1	1-V	51	GLY
1	1-V	58	GLN
1	1-V	208	LYS
1	1-W	51	GLY
1	1-W	58	GLN
1	1-W	208	LYS
1	1-X	51	GLY
1	1-X	58	GLN
1	1-X	208	LYS
1	2-A	324	PRO
1	2-A	395	ASP
1	2-B	324	PRO
1	2-B	395	ASP
1	2-C	324	PRO
1	2-C	395	ASP
1	2-D	324	PRO
1	2-D	395	ASP
1	2-E	324	PRO
1	2-E	395	ASP
1	2-F	324	PRO
1	2-F	395	ASP
1	2-G	324	PRO
1	2-G	395	ASP
1	2-H	324	PRO
1	2-H	395	ASP
1	2-I	324	PRO
1	2-I	395	ASP
1	2-J	324	PRO
1	2-J	395	ASP
1	2-K	324	PRO
1	2-K	395	ASP
1	2-L	324	PRO
1	2-L	395	ASP
1	2-M	324	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-M	395	ASP
1	2-N	324	PRO
1	2-N	395	ASP
1	2-O	324	PRO
1	2-O	395	ASP
1	2-P	324	PRO
1	2-P	395	ASP
1	2-Q	324	PRO
1	2-Q	395	ASP
1	2-R	324	PRO
1	2-R	395	ASP
1	2-S	324	PRO
1	2-S	395	ASP
1	2-T	324	PRO
1	2-T	395	ASP
1	2-U	324	PRO
1	2-U	395	ASP
1	2-V	324	PRO
1	2-V	395	ASP
1	2-W	324	PRO
1	2-W	395	ASP
1	2-X	324	PRO
1	2-X	395	ASP
1	3-A	175	HIS
1	3-A	325	GLY
1	3-B	175	HIS
1	3-B	325	GLY
1	3-C	175	HIS
1	3-C	325	GLY
1	3-D	175	HIS
1	3-D	325	GLY
1	3-E	175	HIS
1	3-E	325	GLY
1	3-F	175	HIS
1	3-F	325	GLY
1	3-G	175	HIS
1	3-G	325	GLY
1	3-H	175	HIS
1	3-H	325	GLY
1	3-I	175	HIS
1	3-I	325	GLY
1	3-J	175	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-J	325	GLY
1	3-K	175	HIS
1	3-K	325	GLY
1	3-L	175	HIS
1	3-L	325	GLY
1	3-M	175	HIS
1	3-M	325	GLY
1	3-N	175	HIS
1	3-N	325	GLY
1	3-O	175	HIS
1	3-O	325	GLY
1	3-P	175	HIS
1	3-P	325	GLY
1	3-Q	175	HIS
1	3-Q	325	GLY
1	3-R	175	HIS
1	3-R	325	GLY
1	3-S	175	HIS
1	3-S	325	GLY
1	3-T	175	HIS
1	3-T	325	GLY
1	3-U	175	HIS
1	3-U	325	GLY
1	3-V	175	HIS
1	3-V	325	GLY
1	3-W	175	HIS
1	3-W	325	GLY
1	3-X	175	HIS
1	3-X	325	GLY
1	4-A	58	GLN
1	4-B	58	GLN
1	4-C	58	GLN
1	4-D	58	GLN
1	4-E	58	GLN
1	4-F	58	GLN
1	4-G	58	GLN
1	4-H	58	GLN
1	4-I	58	GLN
1	4-J	58	GLN
1	4-K	58	GLN
1	4-L	58	GLN
1	4-M	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-N	58	GLN
1	4-O	58	GLN
1	4-P	58	GLN
1	4-Q	58	GLN
1	4-R	58	GLN
1	4-S	58	GLN
1	4-T	58	GLN
1	4-U	58	GLN
1	4-V	58	GLN
1	4-W	58	GLN
1	4-X	58	GLN
1	5-A	327	GLU
1	5-B	327	GLU
1	5-C	327	GLU
1	5-D	327	GLU
1	5-E	327	GLU
1	5-F	327	GLU
1	5-G	327	GLU
1	5-H	327	GLU
1	5-I	327	GLU
1	5-J	327	GLU
1	5-K	327	GLU
1	5-L	327	GLU
1	5-M	327	GLU
1	5-N	327	GLU
1	5-O	327	GLU
1	5-P	327	GLU
1	5-Q	327	GLU
1	5-R	327	GLU
1	5-S	327	GLU
1	5-T	327	GLU
1	5-U	327	GLU
1	5-V	327	GLU
1	5-W	327	GLU
1	5-X	327	GLU
1	6-A	63	SER
1	6-A	397	TYR
1	6-A	403	GLU
1	6-B	63	SER
1	6-B	397	TYR
1	6-B	403	GLU
1	6-C	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-C	397	TYR
1	6-C	403	GLU
1	6-D	63	SER
1	6-D	397	TYR
1	6-D	403	GLU
1	6-E	63	SER
1	6-E	397	TYR
1	6-E	403	GLU
1	6-F	63	SER
1	6-F	397	TYR
1	6-F	403	GLU
1	6-G	63	SER
1	6-G	397	TYR
1	6-G	403	GLU
1	6-H	63	SER
1	6-H	397	TYR
1	6-H	403	GLU
1	6-I	63	SER
1	6-I	397	TYR
1	6-I	403	GLU
1	6-J	63	SER
1	6-J	397	TYR
1	6-J	403	GLU
1	6-K	63	SER
1	6-K	397	TYR
1	6-K	403	GLU
1	6-L	63	SER
1	6-L	397	TYR
1	6-L	403	GLU
1	6-M	63	SER
1	6-M	397	TYR
1	6-M	403	GLU
1	6-N	63	SER
1	6-N	397	TYR
1	6-N	403	GLU
1	6-O	63	SER
1	6-O	397	TYR
1	6-O	403	GLU
1	6-P	63	SER
1	6-P	397	TYR
1	6-P	403	GLU
1	6-Q	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-Q	397	TYR
1	6-Q	403	GLU
1	6-R	63	SER
1	6-R	397	TYR
1	6-R	403	GLU
1	6-S	63	SER
1	6-S	397	TYR
1	6-S	403	GLU
1	6-T	63	SER
1	6-T	397	TYR
1	6-T	403	GLU
1	6-U	63	SER
1	6-U	397	TYR
1	6-U	403	GLU
1	6-V	63	SER
1	6-V	397	TYR
1	6-V	403	GLU
1	6-W	63	SER
1	6-W	397	TYR
1	6-W	403	GLU
1	6-X	63	SER
1	6-X	397	TYR
1	6-X	403	GLU
1	7-A	51	GLY
1	7-A	63	SER
1	7-B	51	GLY
1	7-B	63	SER
1	7-C	51	GLY
1	7-C	63	SER
1	7-D	51	GLY
1	7-D	63	SER
1	7-E	51	GLY
1	7-E	63	SER
1	7-F	51	GLY
1	7-F	63	SER
1	7-G	51	GLY
1	7-G	63	SER
1	7-H	51	GLY
1	7-H	63	SER
1	7-I	51	GLY
1	7-I	63	SER
1	7-J	51	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-J	63	SER
1	7-K	51	GLY
1	7-K	63	SER
1	7-L	51	GLY
1	7-L	63	SER
1	7-M	51	GLY
1	7-M	63	SER
1	7-N	51	GLY
1	7-N	63	SER
1	7-O	51	GLY
1	7-O	63	SER
1	7-P	51	GLY
1	7-P	63	SER
1	7-Q	51	GLY
1	7-Q	63	SER
1	7-R	51	GLY
1	7-R	63	SER
1	7-S	51	GLY
1	7-S	63	SER
1	7-T	51	GLY
1	7-T	63	SER
1	7-U	51	GLY
1	7-U	63	SER
1	7-V	51	GLY
1	7-V	63	SER
1	7-W	51	GLY
1	7-W	63	SER
1	7-X	51	GLY
1	7-X	63	SER
1	8-A	55	ARG
1	8-B	55	ARG
1	8-C	55	ARG
1	8-D	55	ARG
1	8-E	55	ARG
1	8-F	55	ARG
1	8-G	55	ARG
1	8-H	55	ARG
1	8-I	55	ARG
1	8-J	55	ARG
1	8-K	55	ARG
1	8-L	55	ARG
1	8-M	55	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-N	55	ARG
1	8-O	55	ARG
1	8-P	55	ARG
1	8-Q	55	ARG
1	8-R	55	ARG
1	8-S	55	ARG
1	8-T	55	ARG
1	8-U	55	ARG
1	8-V	55	ARG
1	8-W	55	ARG
1	8-X	55	ARG
1	10-A	398	GLU
1	10-A	400	PRO
1	10-B	398	GLU
1	10-B	400	PRO
1	10-C	398	GLU
1	10-C	400	PRO
1	10-D	398	GLU
1	10-D	400	PRO
1	10-E	398	GLU
1	10-E	400	PRO
1	10-F	398	GLU
1	10-F	400	PRO
1	10-G	398	GLU
1	10-G	400	PRO
1	10-H	398	GLU
1	10-H	400	PRO
1	10-I	398	GLU
1	10-I	400	PRO
1	10-J	398	GLU
1	10-J	400	PRO
1	10-K	398	GLU
1	10-K	400	PRO
1	10-L	398	GLU
1	10-L	400	PRO
1	10-M	398	GLU
1	10-M	400	PRO
1	10-N	398	GLU
1	10-N	400	PRO
1	10-O	398	GLU
1	10-O	400	PRO
1	10-P	398	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-P	400	PRO
1	10-Q	398	GLU
1	10-Q	400	PRO
1	10-R	398	GLU
1	10-R	400	PRO
1	10-S	398	GLU
1	10-S	400	PRO
1	10-T	398	GLU
1	10-T	400	PRO
1	10-U	398	GLU
1	10-U	400	PRO
1	10-V	398	GLU
1	10-V	400	PRO
1	10-W	398	GLU
1	10-W	400	PRO
1	10-X	398	GLU
1	10-X	400	PRO
1	1-A	55	ARG
1	1-A	329	PRO
1	1-A	338	ASN
1	1-A	388	PRO
1	1-A	401	PRO
1	1-B	55	ARG
1	1-B	329	PRO
1	1-B	338	ASN
1	1-B	388	PRO
1	1-B	401	PRO
1	1-C	55	ARG
1	1-C	329	PRO
1	1-C	338	ASN
1	1-C	388	PRO
1	1-C	401	PRO
1	1-D	55	ARG
1	1-D	329	PRO
1	1-D	338	ASN
1	1-D	388	PRO
1	1-D	401	PRO
1	1-E	55	ARG
1	1-E	329	PRO
1	1-E	338	ASN
1	1-E	388	PRO
1	1-E	401	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-F	55	ARG
1	1-F	329	PRO
1	1-F	338	ASN
1	1-F	388	PRO
1	1-F	401	PRO
1	1-G	55	ARG
1	1-G	329	PRO
1	1-G	338	ASN
1	1-G	388	PRO
1	1-G	401	PRO
1	1-H	55	ARG
1	1-H	329	PRO
1	1-H	338	ASN
1	1-H	388	PRO
1	1-H	401	PRO
1	1-I	55	ARG
1	1-I	329	PRO
1	1-I	338	ASN
1	1-I	388	PRO
1	1-I	401	PRO
1	1-J	55	ARG
1	1-J	329	PRO
1	1-J	338	ASN
1	1-J	388	PRO
1	1-J	401	PRO
1	1-K	55	ARG
1	1-K	329	PRO
1	1-K	338	ASN
1	1-K	388	PRO
1	1-K	401	PRO
1	1-L	55	ARG
1	1-L	329	PRO
1	1-L	338	ASN
1	1-L	388	PRO
1	1-L	401	PRO
1	1-M	55	ARG
1	1-M	329	PRO
1	1-M	338	ASN
1	1-M	388	PRO
1	1-M	401	PRO
1	1-N	55	ARG
1	1-N	329	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-N	338	ASN
1	1-N	388	PRO
1	1-N	401	PRO
1	1-O	55	ARG
1	1-O	329	PRO
1	1-O	338	ASN
1	1-O	388	PRO
1	1-O	401	PRO
1	1-P	55	ARG
1	1-P	329	PRO
1	1-P	338	ASN
1	1-P	388	PRO
1	1-P	401	PRO
1	1-Q	55	ARG
1	1-Q	329	PRO
1	1-Q	338	ASN
1	1-Q	388	PRO
1	1-Q	401	PRO
1	1-R	55	ARG
1	1-R	329	PRO
1	1-R	338	ASN
1	1-R	388	PRO
1	1-R	401	PRO
1	1-S	55	ARG
1	1-S	329	PRO
1	1-S	338	ASN
1	1-S	388	PRO
1	1-S	401	PRO
1	1-T	55	ARG
1	1-T	329	PRO
1	1-T	338	ASN
1	1-T	388	PRO
1	1-T	401	PRO
1	1-U	55	ARG
1	1-U	329	PRO
1	1-U	338	ASN
1	1-U	388	PRO
1	1-U	401	PRO
1	1-V	55	ARG
1	1-V	329	PRO
1	1-V	338	ASN
1	1-V	388	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-V	401	PRO
1	1-W	55	ARG
1	1-W	329	PRO
1	1-W	338	ASN
1	1-W	388	PRO
1	1-W	401	PRO
1	1-X	55	ARG
1	1-X	329	PRO
1	1-X	338	ASN
1	1-X	388	PRO
1	1-X	401	PRO
1	2-A	53	SER
1	2-A	167	ASP
1	2-A	326	TYR
1	2-B	53	SER
1	2-B	167	ASP
1	2-B	326	TYR
1	2-C	53	SER
1	2-C	167	ASP
1	2-C	326	TYR
1	2-D	53	SER
1	2-D	167	ASP
1	2-D	326	TYR
1	2-E	53	SER
1	2-E	167	ASP
1	2-E	326	TYR
1	2-F	53	SER
1	2-F	167	ASP
1	2-F	326	TYR
1	2-G	53	SER
1	2-G	167	ASP
1	2-G	326	TYR
1	2-H	53	SER
1	2-H	167	ASP
1	2-H	326	TYR
1	2-I	53	SER
1	2-I	167	ASP
1	2-I	326	TYR
1	2-J	53	SER
1	2-J	167	ASP
1	2-J	326	TYR
1	2-K	53	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-K	167	ASP
1	2-K	326	TYR
1	2-L	53	SER
1	2-L	167	ASP
1	2-L	326	TYR
1	2-M	53	SER
1	2-M	167	ASP
1	2-M	326	TYR
1	2-N	53	SER
1	2-N	167	ASP
1	2-N	326	TYR
1	2-O	53	SER
1	2-O	167	ASP
1	2-O	326	TYR
1	2-P	53	SER
1	2-P	167	ASP
1	2-P	326	TYR
1	2-Q	53	SER
1	2-Q	167	ASP
1	2-Q	326	TYR
1	2-R	53	SER
1	2-R	167	ASP
1	2-R	326	TYR
1	2-S	53	SER
1	2-S	167	ASP
1	2-S	326	TYR
1	2-T	53	SER
1	2-T	167	ASP
1	2-T	326	TYR
1	2-U	53	SER
1	2-U	167	ASP
1	2-U	326	TYR
1	2-V	53	SER
1	2-V	167	ASP
1	2-V	326	TYR
1	2-W	53	SER
1	2-W	167	ASP
1	2-W	326	TYR
1	2-X	53	SER
1	2-X	167	ASP
1	2-X	326	TYR
1	3-A	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-A	396	LEU
1	3-B	58	GLN
1	3-B	396	LEU
1	3-C	58	GLN
1	3-C	396	LEU
1	3-D	58	GLN
1	3-D	396	LEU
1	3-E	58	GLN
1	3-E	396	LEU
1	3-F	58	GLN
1	3-F	396	LEU
1	3-G	58	GLN
1	3-G	396	LEU
1	3-H	58	GLN
1	3-H	396	LEU
1	3-I	58	GLN
1	3-I	396	LEU
1	3-J	58	GLN
1	3-J	396	LEU
1	3-K	58	GLN
1	3-K	396	LEU
1	3-L	58	GLN
1	3-L	396	LEU
1	3-M	58	GLN
1	3-M	396	LEU
1	3-N	58	GLN
1	3-N	396	LEU
1	3-O	58	GLN
1	3-O	396	LEU
1	3-P	58	GLN
1	3-P	396	LEU
1	3-Q	58	GLN
1	3-Q	396	LEU
1	3-R	58	GLN
1	3-R	396	LEU
1	3-S	58	GLN
1	3-S	396	LEU
1	3-T	58	GLN
1	3-T	396	LEU
1	3-U	58	GLN
1	3-U	396	LEU
1	3-V	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-V	396	LEU
1	3-W	58	GLN
1	3-W	396	LEU
1	3-X	58	GLN
1	3-X	396	LEU
1	4-A	59	SER
1	4-A	94	PRO
1	4-B	59	SER
1	4-B	94	PRO
1	4-C	59	SER
1	4-C	94	PRO
1	4-D	59	SER
1	4-D	94	PRO
1	4-E	59	SER
1	4-E	94	PRO
1	4-F	59	SER
1	4-F	94	PRO
1	4-G	59	SER
1	4-G	94	PRO
1	4-H	59	SER
1	4-H	94	PRO
1	4-I	59	SER
1	4-I	94	PRO
1	4-J	59	SER
1	4-J	94	PRO
1	4-K	59	SER
1	4-K	94	PRO
1	4-L	59	SER
1	4-L	94	PRO
1	4-M	59	SER
1	4-M	94	PRO
1	4-N	59	SER
1	4-N	94	PRO
1	4-O	59	SER
1	4-O	94	PRO
1	4-P	59	SER
1	4-P	94	PRO
1	4-Q	59	SER
1	4-Q	94	PRO
1	4-R	59	SER
1	4-R	94	PRO
1	4-S	59	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-S	94	PRO
1	4-T	59	SER
1	4-T	94	PRO
1	4-U	59	SER
1	4-U	94	PRO
1	4-V	59	SER
1	4-V	94	PRO
1	4-W	59	SER
1	4-W	94	PRO
1	4-X	59	SER
1	4-X	94	PRO
1	5-A	603	LYS
1	5-B	603	LYS
1	5-C	603	LYS
1	5-D	603	LYS
1	5-E	603	LYS
1	5-F	603	LYS
1	5-G	603	LYS
1	5-H	603	LYS
1	5-I	603	LYS
1	5-J	603	LYS
1	5-K	603	LYS
1	5-L	603	LYS
1	5-M	603	LYS
1	5-N	603	LYS
1	5-O	603	LYS
1	5-P	603	LYS
1	5-Q	603	LYS
1	5-R	603	LYS
1	5-S	603	LYS
1	5-T	603	LYS
1	5-U	603	LYS
1	5-V	603	LYS
1	5-W	603	LYS
1	5-X	603	LYS
1	6-A	401	PRO
1	6-B	401	PRO
1	6-C	401	PRO
1	6-D	401	PRO
1	6-E	401	PRO
1	6-F	401	PRO
1	6-G	401	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-H	401	PRO
1	6-I	401	PRO
1	6-J	401	PRO
1	6-K	401	PRO
1	6-L	401	PRO
1	6-M	401	PRO
1	6-N	401	PRO
1	6-O	401	PRO
1	6-P	401	PRO
1	6-Q	401	PRO
1	6-R	401	PRO
1	6-S	401	PRO
1	6-T	401	PRO
1	6-U	401	PRO
1	6-V	401	PRO
1	6-W	401	PRO
1	6-X	401	PRO
1	7-A	332	LEU
1	7-A	400	PRO
1	7-B	332	LEU
1	7-B	400	PRO
1	7-C	332	LEU
1	7-C	400	PRO
1	7-D	332	LEU
1	7-D	400	PRO
1	7-E	332	LEU
1	7-E	400	PRO
1	7-F	332	LEU
1	7-F	400	PRO
1	7-G	332	LEU
1	7-G	400	PRO
1	7-H	332	LEU
1	7-H	400	PRO
1	7-I	332	LEU
1	7-I	400	PRO
1	7-J	332	LEU
1	7-J	400	PRO
1	7-K	332	LEU
1	7-K	400	PRO
1	7-L	332	LEU
1	7-L	400	PRO
1	7-M	332	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-M	400	PRO
1	7-N	332	LEU
1	7-N	400	PRO
1	7-O	332	LEU
1	7-O	400	PRO
1	7-P	332	LEU
1	7-P	400	PRO
1	7-Q	332	LEU
1	7-Q	400	PRO
1	7-R	332	LEU
1	7-R	400	PRO
1	7-S	332	LEU
1	7-S	400	PRO
1	7-T	332	LEU
1	7-T	400	PRO
1	7-U	332	LEU
1	7-U	400	PRO
1	7-V	332	LEU
1	7-V	400	PRO
1	7-W	332	LEU
1	7-W	400	PRO
1	7-X	332	LEU
1	7-X	400	PRO
1	8-A	385	LYS
1	8-A	401	PRO
1	8-B	385	LYS
1	8-B	401	PRO
1	8-C	385	LYS
1	8-C	401	PRO
1	8-D	385	LYS
1	8-D	401	PRO
1	8-E	385	LYS
1	8-E	401	PRO
1	8-F	385	LYS
1	8-F	401	PRO
1	8-G	385	LYS
1	8-G	401	PRO
1	8-H	385	LYS
1	8-H	401	PRO
1	8-I	385	LYS
1	8-I	401	PRO
1	8-J	385	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-J	401	PRO
1	8-K	385	LYS
1	8-K	401	PRO
1	8-L	385	LYS
1	8-L	401	PRO
1	8-M	385	LYS
1	8-M	401	PRO
1	8-N	385	LYS
1	8-N	401	PRO
1	8-O	385	LYS
1	8-O	401	PRO
1	8-P	385	LYS
1	8-P	401	PRO
1	8-Q	385	LYS
1	8-Q	401	PRO
1	8-R	385	LYS
1	8-R	401	PRO
1	8-S	385	LYS
1	8-S	401	PRO
1	8-T	385	LYS
1	8-T	401	PRO
1	8-U	385	LYS
1	8-U	401	PRO
1	8-V	385	LYS
1	8-V	401	PRO
1	8-W	385	LYS
1	8-W	401	PRO
1	8-X	385	LYS
1	8-X	401	PRO
1	9-A	63	SER
1	9-B	63	SER
1	9-C	63	SER
1	9-D	63	SER
1	9-E	63	SER
1	9-F	63	SER
1	9-G	63	SER
1	9-H	63	SER
1	9-I	63	SER
1	9-J	63	SER
1	9-K	63	SER
1	9-L	63	SER
1	9-M	63	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-N	63	SER
1	9-O	63	SER
1	9-P	63	SER
1	9-Q	63	SER
1	9-R	63	SER
1	9-S	63	SER
1	9-T	63	SER
1	9-U	63	SER
1	9-V	63	SER
1	9-W	63	SER
1	9-X	63	SER
1	10-A	286	THR
1	10-A	395	ASP
1	10-B	286	THR
1	10-B	395	ASP
1	10-C	286	THR
1	10-C	395	ASP
1	10-D	286	THR
1	10-D	395	ASP
1	10-E	286	THR
1	10-E	395	ASP
1	10-F	286	THR
1	10-F	395	ASP
1	10-G	286	THR
1	10-G	395	ASP
1	10-H	286	THR
1	10-H	395	ASP
1	10-I	286	THR
1	10-I	395	ASP
1	10-J	286	THR
1	10-J	395	ASP
1	10-K	286	THR
1	10-K	395	ASP
1	10-L	286	THR
1	10-L	395	ASP
1	10-M	286	THR
1	10-M	395	ASP
1	10-N	286	THR
1	10-N	395	ASP
1	10-O	286	THR
1	10-O	395	ASP
1	10-P	286	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-P	395	ASP
1	10-Q	286	THR
1	10-Q	395	ASP
1	10-R	286	THR
1	10-R	395	ASP
1	10-S	286	THR
1	10-S	395	ASP
1	10-T	286	THR
1	10-T	395	ASP
1	10-U	286	THR
1	10-U	395	ASP
1	10-V	286	THR
1	10-V	395	ASP
1	10-W	286	THR
1	10-W	395	ASP
1	10-X	286	THR
1	10-X	395	ASP
1	1-A	50	ASP
1	1-A	53	SER
1	1-A	209	GLY
1	1-A	228	LEU
1	1-A	284	ASP
1	1-B	50	ASP
1	1-B	53	SER
1	1-B	209	GLY
1	1-B	228	LEU
1	1-B	284	ASP
1	1-C	50	ASP
1	1-C	53	SER
1	1-C	209	GLY
1	1-C	228	LEU
1	1-C	284	ASP
1	1-D	50	ASP
1	1-D	53	SER
1	1-D	209	GLY
1	1-D	228	LEU
1	1-D	284	ASP
1	1-E	50	ASP
1	1-E	53	SER
1	1-E	209	GLY
1	1-E	228	LEU
1	1-E	284	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-F	50	ASP
1	1-F	53	SER
1	1-F	209	GLY
1	1-F	228	LEU
1	1-F	284	ASP
1	1-G	50	ASP
1	1-G	53	SER
1	1-G	209	GLY
1	1-G	228	LEU
1	1-G	284	ASP
1	1-H	50	ASP
1	1-H	53	SER
1	1-H	209	GLY
1	1-H	228	LEU
1	1-H	284	ASP
1	1-I	50	ASP
1	1-I	53	SER
1	1-I	209	GLY
1	1-I	228	LEU
1	1-I	284	ASP
1	1-J	50	ASP
1	1-J	53	SER
1	1-J	209	GLY
1	1-J	228	LEU
1	1-J	284	ASP
1	1-K	50	ASP
1	1-K	53	SER
1	1-K	209	GLY
1	1-K	228	LEU
1	1-K	284	ASP
1	1-L	50	ASP
1	1-L	53	SER
1	1-L	209	GLY
1	1-L	228	LEU
1	1-L	284	ASP
1	1-M	50	ASP
1	1-M	53	SER
1	1-M	209	GLY
1	1-M	228	LEU
1	1-M	284	ASP
1	1-N	50	ASP
1	1-N	53	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-N	209	GLY
1	1-N	228	LEU
1	1-N	284	ASP
1	1-O	50	ASP
1	1-O	53	SER
1	1-O	209	GLY
1	1-O	228	LEU
1	1-O	284	ASP
1	1-P	50	ASP
1	1-P	53	SER
1	1-P	209	GLY
1	1-P	228	LEU
1	1-P	284	ASP
1	1-Q	50	ASP
1	1-Q	53	SER
1	1-Q	209	GLY
1	1-Q	228	LEU
1	1-Q	284	ASP
1	1-R	50	ASP
1	1-R	53	SER
1	1-R	209	GLY
1	1-R	228	LEU
1	1-R	284	ASP
1	1-S	50	ASP
1	1-S	53	SER
1	1-S	209	GLY
1	1-S	228	LEU
1	1-S	284	ASP
1	1-T	50	ASP
1	1-T	53	SER
1	1-T	209	GLY
1	1-T	228	LEU
1	1-T	284	ASP
1	1-U	50	ASP
1	1-U	53	SER
1	1-U	209	GLY
1	1-U	228	LEU
1	1-U	284	ASP
1	1-V	50	ASP
1	1-V	53	SER
1	1-V	209	GLY
1	1-V	228	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-V	284	ASP
1	1-W	50	ASP
1	1-W	53	SER
1	1-W	209	GLY
1	1-W	228	LEU
1	1-W	284	ASP
1	1-X	50	ASP
1	1-X	53	SER
1	1-X	209	GLY
1	1-X	228	LEU
1	1-X	284	ASP
1	2-A	391	PRO
1	2-A	392	VAL
1	2-B	391	PRO
1	2-B	392	VAL
1	2-C	391	PRO
1	2-C	392	VAL
1	2-D	391	PRO
1	2-D	392	VAL
1	2-E	391	PRO
1	2-E	392	VAL
1	2-F	391	PRO
1	2-F	392	VAL
1	2-G	391	PRO
1	2-G	392	VAL
1	2-H	391	PRO
1	2-H	392	VAL
1	2-I	391	PRO
1	2-I	392	VAL
1	2-J	391	PRO
1	2-J	392	VAL
1	2-K	391	PRO
1	2-K	392	VAL
1	2-L	391	PRO
1	2-L	392	VAL
1	2-M	391	PRO
1	2-M	392	VAL
1	2-N	391	PRO
1	2-N	392	VAL
1	2-O	391	PRO
1	2-O	392	VAL
1	2-P	391	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-P	392	VAL
1	2-Q	391	PRO
1	2-Q	392	VAL
1	2-R	391	PRO
1	2-R	392	VAL
1	2-S	391	PRO
1	2-S	392	VAL
1	2-T	391	PRO
1	2-T	392	VAL
1	2-U	391	PRO
1	2-U	392	VAL
1	2-V	391	PRO
1	2-V	392	VAL
1	2-W	391	PRO
1	2-W	392	VAL
1	2-X	391	PRO
1	2-X	392	VAL
1	3-A	64	ASP
1	3-A	228	LEU
1	3-B	64	ASP
1	3-B	228	LEU
1	3-C	64	ASP
1	3-C	228	LEU
1	3-D	64	ASP
1	3-D	228	LEU
1	3-E	64	ASP
1	3-E	228	LEU
1	3-F	64	ASP
1	3-F	228	LEU
1	3-G	64	ASP
1	3-G	228	LEU
1	3-H	64	ASP
1	3-H	228	LEU
1	3-I	64	ASP
1	3-I	228	LEU
1	3-J	64	ASP
1	3-J	228	LEU
1	3-K	64	ASP
1	3-K	228	LEU
1	3-L	64	ASP
1	3-L	228	LEU
1	3-M	64	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-M	228	LEU
1	3-N	64	ASP
1	3-N	228	LEU
1	3-O	64	ASP
1	3-O	228	LEU
1	3-P	64	ASP
1	3-P	228	LEU
1	3-Q	64	ASP
1	3-Q	228	LEU
1	3-R	64	ASP
1	3-R	228	LEU
1	3-S	64	ASP
1	3-S	228	LEU
1	3-T	64	ASP
1	3-T	228	LEU
1	3-U	64	ASP
1	3-U	228	LEU
1	3-V	64	ASP
1	3-V	228	LEU
1	3-W	64	ASP
1	3-W	228	LEU
1	3-X	64	ASP
1	3-X	228	LEU
1	4-A	61	HIS
1	4-B	61	HIS
1	4-C	61	HIS
1	4-D	61	HIS
1	4-E	61	HIS
1	4-F	61	HIS
1	4-G	61	HIS
1	4-H	61	HIS
1	4-I	61	HIS
1	4-J	61	HIS
1	4-K	61	HIS
1	4-L	61	HIS
1	4-M	61	HIS
1	4-N	61	HIS
1	4-O	61	HIS
1	4-P	61	HIS
1	4-Q	61	HIS
1	4-R	61	HIS
1	4-S	61	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-T	61	HIS
1	4-U	61	HIS
1	4-V	61	HIS
1	4-W	61	HIS
1	4-X	61	HIS
1	5-A	94	PRO
1	5-B	94	PRO
1	5-C	94	PRO
1	5-D	94	PRO
1	5-E	94	PRO
1	5-F	94	PRO
1	5-G	94	PRO
1	5-H	94	PRO
1	5-I	94	PRO
1	5-J	94	PRO
1	5-K	94	PRO
1	5-L	94	PRO
1	5-M	94	PRO
1	5-N	94	PRO
1	5-O	94	PRO
1	5-P	94	PRO
1	5-Q	94	PRO
1	5-R	94	PRO
1	5-S	94	PRO
1	5-T	94	PRO
1	5-U	94	PRO
1	5-V	94	PRO
1	5-W	94	PRO
1	5-X	94	PRO
1	6-A	383	LYS
1	6-B	383	LYS
1	6-C	383	LYS
1	6-D	383	LYS
1	6-E	383	LYS
1	6-F	383	LYS
1	6-G	383	LYS
1	6-H	383	LYS
1	6-I	383	LYS
1	6-J	383	LYS
1	6-K	383	LYS
1	6-L	383	LYS
1	6-M	383	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-N	383	LYS
1	6-O	383	LYS
1	6-P	383	LYS
1	6-Q	383	LYS
1	6-R	383	LYS
1	6-S	383	LYS
1	6-T	383	LYS
1	6-U	383	LYS
1	6-V	383	LYS
1	6-W	383	LYS
1	6-X	383	LYS
1	9-A	58	GLN
1	9-B	58	GLN
1	9-C	58	GLN
1	9-D	58	GLN
1	9-E	58	GLN
1	9-F	58	GLN
1	9-G	58	GLN
1	9-H	58	GLN
1	9-I	58	GLN
1	9-J	58	GLN
1	9-K	58	GLN
1	9-L	58	GLN
1	9-M	58	GLN
1	9-N	58	GLN
1	9-O	58	GLN
1	9-P	58	GLN
1	9-Q	58	GLN
1	9-R	58	GLN
1	9-S	58	GLN
1	9-T	58	GLN
1	9-U	58	GLN
1	9-V	58	GLN
1	9-W	58	GLN
1	9-X	58	GLN
1	10-A	208	LYS
1	10-B	208	LYS
1	10-C	208	LYS
1	10-D	208	LYS
1	10-E	208	LYS
1	10-F	208	LYS
1	10-G	208	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-H	208	LYS
1	10-I	208	LYS
1	10-J	208	LYS
1	10-K	208	LYS
1	10-L	208	LYS
1	10-M	208	LYS
1	10-N	208	LYS
1	10-O	208	LYS
1	10-P	208	LYS
1	10-Q	208	LYS
1	10-R	208	LYS
1	10-S	208	LYS
1	10-T	208	LYS
1	10-U	208	LYS
1	10-V	208	LYS
1	10-W	208	LYS
1	10-X	208	LYS
1	2-A	55	ARG
1	2-A	228	LEU
1	2-B	55	ARG
1	2-B	228	LEU
1	2-C	55	ARG
1	2-C	228	LEU
1	2-D	55	ARG
1	2-D	228	LEU
1	2-E	55	ARG
1	2-E	228	LEU
1	2-F	55	ARG
1	2-F	228	LEU
1	2-G	55	ARG
1	2-G	228	LEU
1	2-H	55	ARG
1	2-H	228	LEU
1	2-I	55	ARG
1	2-I	228	LEU
1	2-J	55	ARG
1	2-J	228	LEU
1	2-K	55	ARG
1	2-K	228	LEU
1	2-L	55	ARG
1	2-L	228	LEU
1	2-M	55	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-M	228	LEU
1	2-N	55	ARG
1	2-N	228	LEU
1	2-O	55	ARG
1	2-O	228	LEU
1	2-P	55	ARG
1	2-P	228	LEU
1	2-Q	55	ARG
1	2-Q	228	LEU
1	2-R	55	ARG
1	2-R	228	LEU
1	2-S	55	ARG
1	2-S	228	LEU
1	2-T	55	ARG
1	2-T	228	LEU
1	2-U	55	ARG
1	2-U	228	LEU
1	2-V	55	ARG
1	2-V	228	LEU
1	2-W	55	ARG
1	2-W	228	LEU
1	2-X	55	ARG
1	2-X	228	LEU
1	3-A	324	PRO
1	3-B	324	PRO
1	3-C	324	PRO
1	3-D	324	PRO
1	3-E	324	PRO
1	3-F	324	PRO
1	3-G	324	PRO
1	3-H	324	PRO
1	3-I	324	PRO
1	3-J	324	PRO
1	3-K	324	PRO
1	3-L	324	PRO
1	3-M	324	PRO
1	3-N	324	PRO
1	3-O	324	PRO
1	3-P	324	PRO
1	3-Q	324	PRO
1	3-R	324	PRO
1	3-S	324	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-T	324	PRO
1	3-U	324	PRO
1	3-V	324	PRO
1	3-W	324	PRO
1	3-X	324	PRO
1	4-A	332	LEU
1	4-A	396	LEU
1	4-B	332	LEU
1	4-B	396	LEU
1	4-C	332	LEU
1	4-C	396	LEU
1	4-D	332	LEU
1	4-D	396	LEU
1	4-E	332	LEU
1	4-E	396	LEU
1	4-F	332	LEU
1	4-F	396	LEU
1	4-G	332	LEU
1	4-G	396	LEU
1	4-H	332	LEU
1	4-H	396	LEU
1	4-I	332	LEU
1	4-I	396	LEU
1	4-J	332	LEU
1	4-J	396	LEU
1	4-K	332	LEU
1	4-K	396	LEU
1	4-L	332	LEU
1	4-L	396	LEU
1	4-M	332	LEU
1	4-M	396	LEU
1	4-N	332	LEU
1	4-N	396	LEU
1	4-O	332	LEU
1	4-O	396	LEU
1	4-P	332	LEU
1	4-P	396	LEU
1	4-Q	332	LEU
1	4-Q	396	LEU
1	4-R	332	LEU
1	4-R	396	LEU
1	4-S	332	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-S	396	LEU
1	4-T	332	LEU
1	4-T	396	LEU
1	4-U	332	LEU
1	4-U	396	LEU
1	4-V	332	LEU
1	4-V	396	LEU
1	4-W	332	LEU
1	4-W	396	LEU
1	4-X	332	LEU
1	4-X	396	LEU
1	5-A	54	ILE
1	5-A	60	ILE
1	5-A	284	ASP
1	5-B	54	ILE
1	5-B	60	ILE
1	5-B	284	ASP
1	5-C	54	ILE
1	5-C	60	ILE
1	5-C	284	ASP
1	5-D	54	ILE
1	5-D	60	ILE
1	5-D	284	ASP
1	5-E	54	ILE
1	5-E	60	ILE
1	5-E	284	ASP
1	5-F	54	ILE
1	5-F	60	ILE
1	5-F	284	ASP
1	5-G	54	ILE
1	5-G	60	ILE
1	5-G	284	ASP
1	5-H	54	ILE
1	5-H	60	ILE
1	5-H	284	ASP
1	5-I	54	ILE
1	5-I	60	ILE
1	5-I	284	ASP
1	5-J	54	ILE
1	5-J	60	ILE
1	5-J	284	ASP
1	5-K	54	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-K	60	ILE
1	5-K	284	ASP
1	5-L	54	ILE
1	5-L	60	ILE
1	5-L	284	ASP
1	5-M	54	ILE
1	5-M	60	ILE
1	5-M	284	ASP
1	5-N	54	ILE
1	5-N	60	ILE
1	5-N	284	ASP
1	5-O	54	ILE
1	5-O	60	ILE
1	5-O	284	ASP
1	5-P	54	ILE
1	5-P	60	ILE
1	5-P	284	ASP
1	5-Q	54	ILE
1	5-Q	60	ILE
1	5-Q	284	ASP
1	5-R	54	ILE
1	5-R	60	ILE
1	5-R	284	ASP
1	5-S	54	ILE
1	5-S	60	ILE
1	5-S	284	ASP
1	5-T	54	ILE
1	5-T	60	ILE
1	5-T	284	ASP
1	5-U	54	ILE
1	5-U	60	ILE
1	5-U	284	ASP
1	5-V	54	ILE
1	5-V	60	ILE
1	5-V	284	ASP
1	5-W	54	ILE
1	5-W	60	ILE
1	5-W	284	ASP
1	5-X	54	ILE
1	5-X	60	ILE
1	5-X	284	ASP
1	6-A	390	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-A	406	SER
1	6-B	390	ALA
1	6-B	406	SER
1	6-C	390	ALA
1	6-C	406	SER
1	6-D	390	ALA
1	6-D	406	SER
1	6-E	390	ALA
1	6-E	406	SER
1	6-F	390	ALA
1	6-F	406	SER
1	6-G	390	ALA
1	6-G	406	SER
1	6-H	390	ALA
1	6-H	406	SER
1	6-I	390	ALA
1	6-I	406	SER
1	6-J	390	ALA
1	6-J	406	SER
1	6-K	390	ALA
1	6-K	406	SER
1	6-L	390	ALA
1	6-L	406	SER
1	6-M	390	ALA
1	6-M	406	SER
1	6-N	390	ALA
1	6-N	406	SER
1	6-O	390	ALA
1	6-O	406	SER
1	6-P	390	ALA
1	6-P	406	SER
1	6-Q	390	ALA
1	6-Q	406	SER
1	6-R	390	ALA
1	6-R	406	SER
1	6-S	390	ALA
1	6-S	406	SER
1	6-T	390	ALA
1	6-T	406	SER
1	6-U	390	ALA
1	6-U	406	SER
1	6-V	390	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-V	406	SER
1	6-W	390	ALA
1	6-W	406	SER
1	6-X	390	ALA
1	6-X	406	SER
1	7-A	225	PHE
1	7-A	228	LEU
1	7-A	324	PRO
1	7-B	225	PHE
1	7-B	228	LEU
1	7-B	324	PRO
1	7-C	225	PHE
1	7-C	228	LEU
1	7-C	324	PRO
1	7-D	225	PHE
1	7-D	228	LEU
1	7-D	324	PRO
1	7-E	225	PHE
1	7-E	228	LEU
1	7-E	324	PRO
1	7-F	225	PHE
1	7-F	228	LEU
1	7-F	324	PRO
1	7-G	225	PHE
1	7-G	228	LEU
1	7-G	324	PRO
1	7-H	225	PHE
1	7-H	228	LEU
1	7-H	324	PRO
1	7-I	225	PHE
1	7-I	228	LEU
1	7-I	324	PRO
1	7-J	225	PHE
1	7-J	228	LEU
1	7-J	324	PRO
1	7-K	225	PHE
1	7-K	228	LEU
1	7-K	324	PRO
1	7-L	225	PHE
1	7-L	228	LEU
1	7-L	324	PRO
1	7-M	225	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-M	228	LEU
1	7-M	324	PRO
1	7-N	225	PHE
1	7-N	228	LEU
1	7-N	324	PRO
1	7-O	225	PHE
1	7-O	228	LEU
1	7-O	324	PRO
1	7-P	225	PHE
1	7-P	228	LEU
1	7-P	324	PRO
1	7-Q	225	PHE
1	7-Q	228	LEU
1	7-Q	324	PRO
1	7-R	225	PHE
1	7-R	228	LEU
1	7-R	324	PRO
1	7-S	225	PHE
1	7-S	228	LEU
1	7-S	324	PRO
1	7-T	225	PHE
1	7-T	228	LEU
1	7-T	324	PRO
1	7-U	225	PHE
1	7-U	228	LEU
1	7-U	324	PRO
1	7-V	225	PHE
1	7-V	228	LEU
1	7-V	324	PRO
1	7-W	225	PHE
1	7-W	228	LEU
1	7-W	324	PRO
1	7-X	225	PHE
1	7-X	228	LEU
1	7-X	324	PRO
1	8-A	59	SER
1	8-B	59	SER
1	8-C	59	SER
1	8-D	59	SER
1	8-E	59	SER
1	8-F	59	SER
1	8-G	59	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-H	59	SER
1	8-I	59	SER
1	8-J	59	SER
1	8-K	59	SER
1	8-L	59	SER
1	8-M	59	SER
1	8-N	59	SER
1	8-O	59	SER
1	8-P	59	SER
1	8-Q	59	SER
1	8-R	59	SER
1	8-S	59	SER
1	8-T	59	SER
1	8-U	59	SER
1	8-V	59	SER
1	8-W	59	SER
1	8-X	59	SER
1	9-A	53	SER
1	9-A	228	LEU
1	9-B	53	SER
1	9-B	228	LEU
1	9-C	53	SER
1	9-C	228	LEU
1	9-D	53	SER
1	9-D	228	LEU
1	9-E	53	SER
1	9-E	228	LEU
1	9-F	53	SER
1	9-F	228	LEU
1	9-G	53	SER
1	9-G	228	LEU
1	9-H	53	SER
1	9-H	228	LEU
1	9-I	53	SER
1	9-I	228	LEU
1	9-J	53	SER
1	9-J	228	LEU
1	9-K	53	SER
1	9-K	228	LEU
1	9-L	53	SER
1	9-L	228	LEU
1	9-M	53	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-M	228	LEU
1	9-N	53	SER
1	9-N	228	LEU
1	9-O	53	SER
1	9-O	228	LEU
1	9-P	53	SER
1	9-P	228	LEU
1	9-Q	53	SER
1	9-Q	228	LEU
1	9-R	53	SER
1	9-R	228	LEU
1	9-S	53	SER
1	9-S	228	LEU
1	9-T	53	SER
1	9-T	228	LEU
1	9-U	53	SER
1	9-U	228	LEU
1	9-V	53	SER
1	9-V	228	LEU
1	9-W	53	SER
1	9-W	228	LEU
1	9-X	53	SER
1	9-X	228	LEU
1	10-A	389	GLN
1	10-B	389	GLN
1	10-C	389	GLN
1	10-D	389	GLN
1	10-E	389	GLN
1	10-F	389	GLN
1	10-G	389	GLN
1	10-H	389	GLN
1	10-I	389	GLN
1	10-J	389	GLN
1	10-K	389	GLN
1	10-L	389	GLN
1	10-M	389	GLN
1	10-N	389	GLN
1	10-O	389	GLN
1	10-P	389	GLN
1	10-Q	389	GLN
1	10-R	389	GLN
1	10-S	389	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-T	389	GLN
1	10-U	389	GLN
1	10-V	389	GLN
1	10-W	389	GLN
1	10-X	389	GLN
1	4-A	325	GLY
1	4-A	327	GLU
1	4-B	325	GLY
1	4-B	327	GLU
1	4-C	325	GLY
1	4-C	327	GLU
1	4-D	325	GLY
1	4-D	327	GLU
1	4-E	325	GLY
1	4-E	327	GLU
1	4-F	325	GLY
1	4-F	327	GLU
1	4-G	325	GLY
1	4-G	327	GLU
1	4-H	325	GLY
1	4-H	327	GLU
1	4-I	325	GLY
1	4-I	327	GLU
1	4-J	325	GLY
1	4-J	327	GLU
1	4-K	325	GLY
1	4-K	327	GLU
1	4-L	325	GLY
1	4-L	327	GLU
1	4-M	325	GLY
1	4-M	327	GLU
1	4-N	325	GLY
1	4-N	327	GLU
1	4-O	325	GLY
1	4-O	327	GLU
1	4-P	325	GLY
1	4-P	327	GLU
1	4-Q	325	GLY
1	4-Q	327	GLU
1	4-R	325	GLY
1	4-R	327	GLU
1	4-S	325	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-S	327	GLU
1	4-T	325	GLY
1	4-T	327	GLU
1	4-U	325	GLY
1	4-U	327	GLU
1	4-V	325	GLY
1	4-V	327	GLU
1	4-W	325	GLY
1	4-W	327	GLU
1	4-X	325	GLY
1	4-X	327	GLU
1	10-A	49	PHE
1	10-A	62	GLU
1	10-B	49	PHE
1	10-B	62	GLU
1	10-C	49	PHE
1	10-C	62	GLU
1	10-D	49	PHE
1	10-D	62	GLU
1	10-E	49	PHE
1	10-E	62	GLU
1	10-F	49	PHE
1	10-F	62	GLU
1	10-G	49	PHE
1	10-G	62	GLU
1	10-H	49	PHE
1	10-H	62	GLU
1	10-I	49	PHE
1	10-I	62	GLU
1	10-J	49	PHE
1	10-J	62	GLU
1	10-K	49	PHE
1	10-K	62	GLU
1	10-L	49	PHE
1	10-L	62	GLU
1	10-M	49	PHE
1	10-M	62	GLU
1	10-N	49	PHE
1	10-N	62	GLU
1	10-O	49	PHE
1	10-O	62	GLU
1	10-P	49	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-P	62	GLU
1	10-Q	49	PHE
1	10-Q	62	GLU
1	10-R	49	PHE
1	10-R	62	GLU
1	10-S	49	PHE
1	10-S	62	GLU
1	10-T	49	PHE
1	10-T	62	GLU
1	10-U	49	PHE
1	10-U	62	GLU
1	10-V	49	PHE
1	10-V	62	GLU
1	10-W	49	PHE
1	10-W	62	GLU
1	10-X	49	PHE
1	10-X	62	GLU
1	2-E	401	PRO
1	2-J	401	PRO
1	2-R	401	PRO
1	2-S	401	PRO
1	2-T	401	PRO
1	2-W	401	PRO
1	4-A	51	GLY
1	4-B	51	GLY
1	4-C	51	GLY
1	4-D	51	GLY
1	4-E	51	GLY
1	4-F	51	GLY
1	4-G	51	GLY
1	4-H	51	GLY
1	4-I	51	GLY
1	4-J	51	GLY
1	4-K	51	GLY
1	4-L	51	GLY
1	4-M	51	GLY
1	4-N	51	GLY
1	4-O	51	GLY
1	4-P	51	GLY
1	4-Q	51	GLY
1	4-R	51	GLY
1	4-S	51	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-T	51	GLY
1	4-U	51	GLY
1	4-V	51	GLY
1	4-W	51	GLY
1	4-X	51	GLY
1	8-A	56	GLY
1	8-A	324	PRO
1	8-B	56	GLY
1	8-B	324	PRO
1	8-C	56	GLY
1	8-C	324	PRO
1	8-D	56	GLY
1	8-D	324	PRO
1	8-E	56	GLY
1	8-E	324	PRO
1	8-F	56	GLY
1	8-F	324	PRO
1	8-G	56	GLY
1	8-G	324	PRO
1	8-H	56	GLY
1	8-H	324	PRO
1	8-I	56	GLY
1	8-I	324	PRO
1	8-J	56	GLY
1	8-J	324	PRO
1	8-K	56	GLY
1	8-K	324	PRO
1	8-L	56	GLY
1	8-L	324	PRO
1	8-M	56	GLY
1	8-M	324	PRO
1	8-N	56	GLY
1	8-N	324	PRO
1	8-O	56	GLY
1	8-O	324	PRO
1	8-P	56	GLY
1	8-P	324	PRO
1	8-Q	56	GLY
1	8-Q	324	PRO
1	8-R	56	GLY
1	8-R	324	PRO
1	8-S	56	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-S	324	PRO
1	8-T	56	GLY
1	8-T	324	PRO
1	8-U	56	GLY
1	8-U	324	PRO
1	8-V	56	GLY
1	8-V	324	PRO
1	8-W	56	GLY
1	8-W	324	PRO
1	8-X	56	GLY
1	8-X	324	PRO
1	2-A	401	PRO
1	2-B	401	PRO
1	2-C	401	PRO
1	2-D	401	PRO
1	2-F	401	PRO
1	2-G	401	PRO
1	2-H	401	PRO
1	2-I	401	PRO
1	2-K	401	PRO
1	2-L	401	PRO
1	2-M	401	PRO
1	2-N	401	PRO
1	2-O	401	PRO
1	2-P	401	PRO
1	2-Q	401	PRO
1	2-U	401	PRO
1	2-V	401	PRO
1	2-X	401	PRO
1	4-A	401	PRO
1	4-B	401	PRO
1	4-C	401	PRO
1	4-E	401	PRO
1	4-F	401	PRO
1	4-G	401	PRO
1	4-H	401	PRO
1	4-I	401	PRO
1	4-J	401	PRO
1	4-K	401	PRO
1	4-L	401	PRO
1	4-M	401	PRO
1	4-N	401	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-O	401	PRO
1	4-P	401	PRO
1	4-Q	401	PRO
1	4-R	401	PRO
1	4-T	401	PRO
1	4-U	401	PRO
1	4-W	401	PRO
1	4-X	401	PRO
1	9-A	56	GLY
1	9-B	56	GLY
1	9-C	56	GLY
1	9-D	56	GLY
1	9-E	56	GLY
1	9-F	56	GLY
1	9-G	56	GLY
1	9-H	56	GLY
1	9-I	56	GLY
1	9-J	56	GLY
1	9-K	56	GLY
1	9-L	56	GLY
1	9-M	56	GLY
1	9-N	56	GLY
1	9-O	56	GLY
1	9-P	56	GLY
1	9-Q	56	GLY
1	9-R	56	GLY
1	9-S	56	GLY
1	9-T	56	GLY
1	9-U	56	GLY
1	9-V	56	GLY
1	9-W	56	GLY
1	9-X	56	GLY
1	2-A	329	PRO
1	2-B	329	PRO
1	2-C	329	PRO
1	2-D	329	PRO
1	2-E	329	PRO
1	2-F	329	PRO
1	2-G	329	PRO
1	2-H	329	PRO
1	2-I	329	PRO
1	2-J	329	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-K	329	PRO
1	2-L	329	PRO
1	2-M	329	PRO
1	2-N	329	PRO
1	2-O	329	PRO
1	2-P	329	PRO
1	2-Q	329	PRO
1	2-R	329	PRO
1	2-S	329	PRO
1	2-T	329	PRO
1	2-U	329	PRO
1	2-V	329	PRO
1	2-W	329	PRO
1	2-X	329	PRO
1	3-A	400	PRO
1	3-B	400	PRO
1	3-C	400	PRO
1	3-D	400	PRO
1	3-E	400	PRO
1	3-F	400	PRO
1	3-G	400	PRO
1	3-H	400	PRO
1	3-I	400	PRO
1	3-J	400	PRO
1	3-K	400	PRO
1	3-L	400	PRO
1	3-M	400	PRO
1	3-N	400	PRO
1	3-O	400	PRO
1	3-P	400	PRO
1	3-Q	400	PRO
1	3-R	400	PRO
1	3-S	400	PRO
1	3-T	400	PRO
1	3-U	400	PRO
1	3-V	400	PRO
1	3-W	400	PRO
1	3-X	400	PRO
1	4-D	401	PRO
1	4-S	401	PRO
1	4-V	401	PRO
1	7-A	54	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-B	54	ILE
1	7-C	54	ILE
1	7-D	54	ILE
1	7-E	54	ILE
1	7-F	54	ILE
1	7-G	54	ILE
1	7-H	54	ILE
1	7-I	54	ILE
1	7-J	54	ILE
1	7-K	54	ILE
1	7-L	54	ILE
1	7-M	54	ILE
1	7-N	54	ILE
1	7-O	54	ILE
1	7-P	54	ILE
1	7-Q	54	ILE
1	7-R	54	ILE
1	7-S	54	ILE
1	7-T	54	ILE
1	7-U	54	ILE
1	7-V	54	ILE
1	7-W	54	ILE
1	7-X	54	ILE
1	8-A	60	ILE
1	8-B	60	ILE
1	8-C	60	ILE
1	8-D	60	ILE
1	8-E	60	ILE
1	8-F	60	ILE
1	8-G	60	ILE
1	8-H	60	ILE
1	8-I	60	ILE
1	8-J	60	ILE
1	8-K	60	ILE
1	8-L	60	ILE
1	8-M	60	ILE
1	8-N	60	ILE
1	8-O	60	ILE
1	8-P	60	ILE
1	8-Q	60	ILE
1	8-R	60	ILE
1	8-S	60	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-T	60	ILE
1	8-U	60	ILE
1	8-V	60	ILE
1	8-W	60	ILE
1	8-X	60	ILE
1	9-A	1	THR
1	9-B	1	THR
1	9-C	1	THR
1	9-D	1	THR
1	9-E	1	THR
1	9-F	1	THR
1	9-G	1	THR
1	9-H	1	THR
1	9-I	1	THR
1	9-J	1	THR
1	9-K	1	THR
1	9-L	1	THR
1	9-M	1	THR
1	9-N	1	THR
1	9-O	1	THR
1	9-P	1	THR
1	9-Q	1	THR
1	9-R	1	THR
1	9-S	1	THR
1	9-T	1	THR
1	9-U	1	THR
1	9-V	1	THR
1	9-W	1	THR
1	9-X	1	THR
1	6-A	60	ILE
1	6-C	60	ILE
1	6-F	60	ILE
1	6-G	60	ILE
1	6-I	60	ILE
1	6-J	60	ILE
1	6-K	60	ILE
1	6-L	60	ILE
1	6-N	60	ILE
1	6-O	60	ILE
1	6-Q	60	ILE
1	6-R	60	ILE
1	6-U	60	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-V	60	ILE
1	6-W	60	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-B	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-C	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-D	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-E	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-F	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-G	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-H	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-I	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-J	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-K	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-L	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-M	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-N	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-O	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-P	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-Q	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-R	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-S	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-T	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-U	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-V	404/404 (100%)	371 (92%)	33 (8%)	10	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-W	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	1-X	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-A	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-B	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-C	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-D	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-E	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-F	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-G	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-H	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-I	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-J	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-K	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-L	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-M	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-N	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-O	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-P	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-Q	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-R	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-S	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-T	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-U	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-V	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-W	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	2-X	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-A	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-B	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-C	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-D	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-E	404/404 (100%)	371 (92%)	33 (8%)	10	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3-F	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-G	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-H	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-I	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-J	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-K	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-L	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-M	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-N	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-O	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-P	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-Q	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-R	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-S	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-T	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-U	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-V	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-W	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	3-X	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-A	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-B	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-C	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-D	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-E	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-F	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-G	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-H	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-I	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-J	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-K	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-L	404/404 (100%)	371 (92%)	33 (8%)	10	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4-M	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-N	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-O	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-P	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-Q	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-R	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-S	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-T	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-U	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-V	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-W	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	4-X	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-A	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-B	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-C	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-D	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-E	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-F	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-G	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-H	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-I	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-J	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-K	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-L	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-M	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-N	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-O	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-P	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-Q	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-R	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-S	404/404 (100%)	371 (92%)	33 (8%)	10	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5-T	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-U	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-V	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-W	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	5-X	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-A	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-B	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-C	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-D	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-E	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-F	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-G	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-H	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-I	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-J	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-K	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-L	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-M	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-N	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-O	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-P	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-Q	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-R	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-S	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-T	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-U	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-V	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-W	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	6-X	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-A	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-B	404/404 (100%)	371 (92%)	33 (8%)	10	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7-C	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-D	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-E	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-F	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-G	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-H	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-I	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-J	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-K	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-L	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-M	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-N	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-O	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-P	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-Q	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-R	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-S	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-T	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-U	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-V	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-W	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	7-X	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-A	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-B	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-C	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-D	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-E	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-F	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-G	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-H	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-I	404/404 (100%)	371 (92%)	33 (8%)	10	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-J	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-K	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-L	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-M	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-N	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-O	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-P	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-Q	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-R	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-S	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-T	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-U	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-V	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-W	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	8-X	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-A	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-B	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-C	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-D	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-E	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-F	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-G	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-H	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-I	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-J	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-K	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-L	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-M	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-N	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-O	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-P	404/404 (100%)	371 (92%)	33 (8%)	10	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9-Q	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-R	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-S	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-T	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-U	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-V	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-W	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	9-X	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-A	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-B	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-C	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-D	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-E	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-F	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-G	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-H	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-I	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-J	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-K	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-L	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-M	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-N	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-O	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-P	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-Q	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-R	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-S	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-T	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-U	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-V	404/404 (100%)	371 (92%)	33 (8%)	10	18
1	10-W	404/404 (100%)	371 (92%)	33 (8%)	10	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	10-X	404/404 (100%)	371 (92%)	33 (8%)	10	18
All	All	96960/96960 (100%)	89040 (92%)	7920 (8%)	10	18

All (7920) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	602	GLU
1	1-A	2	PRO
1	1-A	8	LEU
1	1-A	10	LYS
1	1-A	24	LEU
1	1-A	39	ASP
1	1-A	50	ASP
1	1-A	59	SER
1	1-A	62	GLU
1	1-A	67	LEU
1	1-A	93	ASP
1	1-A	98	GLU
1	1-A	115	LEU
1	1-A	152	ASP
1	1-A	173	VAL
1	1-A	187	GLN
1	1-A	191	LEU
1	1-A	237	LEU
1	1-A	269	HIS
1	1-A	281	LEU
1	1-A	308	LEU
1	1-A	312	THR
1	1-A	322	LEU
1	1-A	323	VAL
1	1-A	337	ARG
1	1-A	347	ILE
1	1-A	363	SER
1	1-A	375	LEU
1	1-A	392	VAL
1	1-A	397	TYR
1	1-A	413	GLN
1	1-A	420	ARG
1	1-A	428	LEU
1	1-B	602	GLU
1	1-B	2	PRO
1	1-B	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-B	10	LYS
1	1-B	24	LEU
1	1-B	39	ASP
1	1-B	50	ASP
1	1-B	59	SER
1	1-B	62	GLU
1	1-B	67	LEU
1	1-B	93	ASP
1	1-B	98	GLU
1	1-B	115	LEU
1	1-B	152	ASP
1	1-B	173	VAL
1	1-B	187	GLN
1	1-B	191	LEU
1	1-B	237	LEU
1	1-B	269	HIS
1	1-B	281	LEU
1	1-B	308	LEU
1	1-B	312	THR
1	1-B	322	LEU
1	1-B	323	VAL
1	1-B	337	ARG
1	1-B	347	ILE
1	1-B	363	SER
1	1-B	375	LEU
1	1-B	392	VAL
1	1-B	397	TYR
1	1-B	413	GLN
1	1-B	420	ARG
1	1-B	428	LEU
1	1-C	602	GLU
1	1-C	2	PRO
1	1-C	8	LEU
1	1-C	10	LYS
1	1-C	24	LEU
1	1-C	39	ASP
1	1-C	50	ASP
1	1-C	59	SER
1	1-C	62	GLU
1	1-C	67	LEU
1	1-C	93	ASP
1	1-C	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-C	115	LEU
1	1-C	152	ASP
1	1-C	173	VAL
1	1-C	187	GLN
1	1-C	191	LEU
1	1-C	237	LEU
1	1-C	269	HIS
1	1-C	281	LEU
1	1-C	308	LEU
1	1-C	312	THR
1	1-C	322	LEU
1	1-C	323	VAL
1	1-C	337	ARG
1	1-C	347	ILE
1	1-C	363	SER
1	1-C	375	LEU
1	1-C	392	VAL
1	1-C	397	TYR
1	1-C	413	GLN
1	1-C	420	ARG
1	1-C	428	LEU
1	1-D	602	GLU
1	1-D	2	PRO
1	1-D	8	LEU
1	1-D	10	LYS
1	1-D	24	LEU
1	1-D	39	ASP
1	1-D	50	ASP
1	1-D	59	SER
1	1-D	62	GLU
1	1-D	67	LEU
1	1-D	93	ASP
1	1-D	98	GLU
1	1-D	115	LEU
1	1-D	152	ASP
1	1-D	173	VAL
1	1-D	187	GLN
1	1-D	191	LEU
1	1-D	237	LEU
1	1-D	269	HIS
1	1-D	281	LEU
1	1-D	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-D	312	THR
1	1-D	322	LEU
1	1-D	323	VAL
1	1-D	337	ARG
1	1-D	347	ILE
1	1-D	363	SER
1	1-D	375	LEU
1	1-D	392	VAL
1	1-D	397	TYR
1	1-D	413	GLN
1	1-D	420	ARG
1	1-D	428	LEU
1	1-E	602	GLU
1	1-E	2	PRO
1	1-E	8	LEU
1	1-E	10	LYS
1	1-E	24	LEU
1	1-E	39	ASP
1	1-E	50	ASP
1	1-E	59	SER
1	1-E	62	GLU
1	1-E	67	LEU
1	1-E	93	ASP
1	1-E	98	GLU
1	1-E	115	LEU
1	1-E	152	ASP
1	1-E	173	VAL
1	1-E	187	GLN
1	1-E	191	LEU
1	1-E	237	LEU
1	1-E	269	HIS
1	1-E	281	LEU
1	1-E	308	LEU
1	1-E	312	THR
1	1-E	322	LEU
1	1-E	323	VAL
1	1-E	337	ARG
1	1-E	347	ILE
1	1-E	363	SER
1	1-E	375	LEU
1	1-E	392	VAL
1	1-E	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-E	413	GLN
1	1-E	420	ARG
1	1-E	428	LEU
1	1-F	602	GLU
1	1-F	2	PRO
1	1-F	8	LEU
1	1-F	10	LYS
1	1-F	24	LEU
1	1-F	39	ASP
1	1-F	50	ASP
1	1-F	59	SER
1	1-F	62	GLU
1	1-F	67	LEU
1	1-F	93	ASP
1	1-F	98	GLU
1	1-F	115	LEU
1	1-F	152	ASP
1	1-F	173	VAL
1	1-F	187	GLN
1	1-F	191	LEU
1	1-F	237	LEU
1	1-F	269	HIS
1	1-F	281	LEU
1	1-F	308	LEU
1	1-F	312	THR
1	1-F	322	LEU
1	1-F	323	VAL
1	1-F	337	ARG
1	1-F	347	ILE
1	1-F	363	SER
1	1-F	375	LEU
1	1-F	392	VAL
1	1-F	397	TYR
1	1-F	413	GLN
1	1-F	420	ARG
1	1-F	428	LEU
1	1-G	602	GLU
1	1-G	2	PRO
1	1-G	8	LEU
1	1-G	10	LYS
1	1-G	24	LEU
1	1-G	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-G	50	ASP
1	1-G	59	SER
1	1-G	62	GLU
1	1-G	67	LEU
1	1-G	93	ASP
1	1-G	98	GLU
1	1-G	115	LEU
1	1-G	152	ASP
1	1-G	173	VAL
1	1-G	187	GLN
1	1-G	191	LEU
1	1-G	237	LEU
1	1-G	269	HIS
1	1-G	281	LEU
1	1-G	308	LEU
1	1-G	312	THR
1	1-G	322	LEU
1	1-G	323	VAL
1	1-G	337	ARG
1	1-G	347	ILE
1	1-G	363	SER
1	1-G	375	LEU
1	1-G	392	VAL
1	1-G	397	TYR
1	1-G	413	GLN
1	1-G	420	ARG
1	1-G	428	LEU
1	1-H	602	GLU
1	1-H	2	PRO
1	1-H	8	LEU
1	1-H	10	LYS
1	1-H	24	LEU
1	1-H	39	ASP
1	1-H	50	ASP
1	1-H	59	SER
1	1-H	62	GLU
1	1-H	67	LEU
1	1-H	93	ASP
1	1-H	98	GLU
1	1-H	115	LEU
1	1-H	152	ASP
1	1-H	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-H	187	GLN
1	1-H	191	LEU
1	1-H	237	LEU
1	1-H	269	HIS
1	1-H	281	LEU
1	1-H	308	LEU
1	1-H	312	THR
1	1-H	322	LEU
1	1-H	323	VAL
1	1-H	337	ARG
1	1-H	347	ILE
1	1-H	363	SER
1	1-H	375	LEU
1	1-H	392	VAL
1	1-H	397	TYR
1	1-H	413	GLN
1	1-H	420	ARG
1	1-H	428	LEU
1	1-I	602	GLU
1	1-I	2	PRO
1	1-I	8	LEU
1	1-I	10	LYS
1	1-I	24	LEU
1	1-I	39	ASP
1	1-I	50	ASP
1	1-I	59	SER
1	1-I	62	GLU
1	1-I	67	LEU
1	1-I	93	ASP
1	1-I	98	GLU
1	1-I	115	LEU
1	1-I	152	ASP
1	1-I	173	VAL
1	1-I	187	GLN
1	1-I	191	LEU
1	1-I	237	LEU
1	1-I	269	HIS
1	1-I	281	LEU
1	1-I	308	LEU
1	1-I	312	THR
1	1-I	322	LEU
1	1-I	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-I	337	ARG
1	1-I	347	ILE
1	1-I	363	SER
1	1-I	375	LEU
1	1-I	392	VAL
1	1-I	397	TYR
1	1-I	413	GLN
1	1-I	420	ARG
1	1-I	428	LEU
1	1-J	602	GLU
1	1-J	2	PRO
1	1-J	8	LEU
1	1-J	10	LYS
1	1-J	24	LEU
1	1-J	39	ASP
1	1-J	50	ASP
1	1-J	59	SER
1	1-J	62	GLU
1	1-J	67	LEU
1	1-J	93	ASP
1	1-J	98	GLU
1	1-J	115	LEU
1	1-J	152	ASP
1	1-J	173	VAL
1	1-J	187	GLN
1	1-J	191	LEU
1	1-J	237	LEU
1	1-J	269	HIS
1	1-J	281	LEU
1	1-J	308	LEU
1	1-J	312	THR
1	1-J	322	LEU
1	1-J	323	VAL
1	1-J	337	ARG
1	1-J	347	ILE
1	1-J	363	SER
1	1-J	375	LEU
1	1-J	392	VAL
1	1-J	397	TYR
1	1-J	413	GLN
1	1-J	420	ARG
1	1-J	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-K	602	GLU
1	1-K	2	PRO
1	1-K	8	LEU
1	1-K	10	LYS
1	1-K	24	LEU
1	1-K	39	ASP
1	1-K	50	ASP
1	1-K	59	SER
1	1-K	62	GLU
1	1-K	67	LEU
1	1-K	93	ASP
1	1-K	98	GLU
1	1-K	115	LEU
1	1-K	152	ASP
1	1-K	173	VAL
1	1-K	187	GLN
1	1-K	191	LEU
1	1-K	237	LEU
1	1-K	269	HIS
1	1-K	281	LEU
1	1-K	308	LEU
1	1-K	312	THR
1	1-K	322	LEU
1	1-K	323	VAL
1	1-K	337	ARG
1	1-K	347	ILE
1	1-K	363	SER
1	1-K	375	LEU
1	1-K	392	VAL
1	1-K	397	TYR
1	1-K	413	GLN
1	1-K	420	ARG
1	1-K	428	LEU
1	1-L	602	GLU
1	1-L	2	PRO
1	1-L	8	LEU
1	1-L	10	LYS
1	1-L	24	LEU
1	1-L	39	ASP
1	1-L	50	ASP
1	1-L	59	SER
1	1-L	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-L	67	LEU
1	1-L	93	ASP
1	1-L	98	GLU
1	1-L	115	LEU
1	1-L	152	ASP
1	1-L	173	VAL
1	1-L	187	GLN
1	1-L	191	LEU
1	1-L	237	LEU
1	1-L	269	HIS
1	1-L	281	LEU
1	1-L	308	LEU
1	1-L	312	THR
1	1-L	322	LEU
1	1-L	323	VAL
1	1-L	337	ARG
1	1-L	347	ILE
1	1-L	363	SER
1	1-L	375	LEU
1	1-L	392	VAL
1	1-L	397	TYR
1	1-L	413	GLN
1	1-L	420	ARG
1	1-L	428	LEU
1	1-M	602	GLU
1	1-M	2	PRO
1	1-M	8	LEU
1	1-M	10	LYS
1	1-M	24	LEU
1	1-M	39	ASP
1	1-M	50	ASP
1	1-M	59	SER
1	1-M	62	GLU
1	1-M	67	LEU
1	1-M	93	ASP
1	1-M	98	GLU
1	1-M	115	LEU
1	1-M	152	ASP
1	1-M	173	VAL
1	1-M	187	GLN
1	1-M	191	LEU
1	1-M	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-M	269	HIS
1	1-M	281	LEU
1	1-M	308	LEU
1	1-M	312	THR
1	1-M	322	LEU
1	1-M	323	VAL
1	1-M	337	ARG
1	1-M	347	ILE
1	1-M	363	SER
1	1-M	375	LEU
1	1-M	392	VAL
1	1-M	397	TYR
1	1-M	413	GLN
1	1-M	420	ARG
1	1-M	428	LEU
1	1-N	602	GLU
1	1-N	2	PRO
1	1-N	8	LEU
1	1-N	10	LYS
1	1-N	24	LEU
1	1-N	39	ASP
1	1-N	50	ASP
1	1-N	59	SER
1	1-N	62	GLU
1	1-N	67	LEU
1	1-N	93	ASP
1	1-N	98	GLU
1	1-N	115	LEU
1	1-N	152	ASP
1	1-N	173	VAL
1	1-N	187	GLN
1	1-N	191	LEU
1	1-N	237	LEU
1	1-N	269	HIS
1	1-N	281	LEU
1	1-N	308	LEU
1	1-N	312	THR
1	1-N	322	LEU
1	1-N	323	VAL
1	1-N	337	ARG
1	1-N	347	ILE
1	1-N	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-N	375	LEU
1	1-N	392	VAL
1	1-N	397	TYR
1	1-N	413	GLN
1	1-N	420	ARG
1	1-N	428	LEU
1	1-O	602	GLU
1	1-O	2	PRO
1	1-O	8	LEU
1	1-O	10	LYS
1	1-O	24	LEU
1	1-O	39	ASP
1	1-O	50	ASP
1	1-O	59	SER
1	1-O	62	GLU
1	1-O	67	LEU
1	1-O	93	ASP
1	1-O	98	GLU
1	1-O	115	LEU
1	1-O	152	ASP
1	1-O	173	VAL
1	1-O	187	GLN
1	1-O	191	LEU
1	1-O	237	LEU
1	1-O	269	HIS
1	1-O	281	LEU
1	1-O	308	LEU
1	1-O	312	THR
1	1-O	322	LEU
1	1-O	323	VAL
1	1-O	337	ARG
1	1-O	347	ILE
1	1-O	363	SER
1	1-O	375	LEU
1	1-O	392	VAL
1	1-O	397	TYR
1	1-O	413	GLN
1	1-O	420	ARG
1	1-O	428	LEU
1	1-P	602	GLU
1	1-P	2	PRO
1	1-P	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-P	10	LYS
1	1-P	24	LEU
1	1-P	39	ASP
1	1-P	50	ASP
1	1-P	59	SER
1	1-P	62	GLU
1	1-P	67	LEU
1	1-P	93	ASP
1	1-P	98	GLU
1	1-P	115	LEU
1	1-P	152	ASP
1	1-P	173	VAL
1	1-P	187	GLN
1	1-P	191	LEU
1	1-P	237	LEU
1	1-P	269	HIS
1	1-P	281	LEU
1	1-P	308	LEU
1	1-P	312	THR
1	1-P	322	LEU
1	1-P	323	VAL
1	1-P	337	ARG
1	1-P	347	ILE
1	1-P	363	SER
1	1-P	375	LEU
1	1-P	392	VAL
1	1-P	397	TYR
1	1-P	413	GLN
1	1-P	420	ARG
1	1-P	428	LEU
1	1-Q	602	GLU
1	1-Q	2	PRO
1	1-Q	8	LEU
1	1-Q	10	LYS
1	1-Q	24	LEU
1	1-Q	39	ASP
1	1-Q	50	ASP
1	1-Q	59	SER
1	1-Q	62	GLU
1	1-Q	67	LEU
1	1-Q	93	ASP
1	1-Q	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-Q	115	LEU
1	1-Q	152	ASP
1	1-Q	173	VAL
1	1-Q	187	GLN
1	1-Q	191	LEU
1	1-Q	237	LEU
1	1-Q	269	HIS
1	1-Q	281	LEU
1	1-Q	308	LEU
1	1-Q	312	THR
1	1-Q	322	LEU
1	1-Q	323	VAL
1	1-Q	337	ARG
1	1-Q	347	ILE
1	1-Q	363	SER
1	1-Q	375	LEU
1	1-Q	392	VAL
1	1-Q	397	TYR
1	1-Q	413	GLN
1	1-Q	420	ARG
1	1-Q	428	LEU
1	1-R	602	GLU
1	1-R	2	PRO
1	1-R	8	LEU
1	1-R	10	LYS
1	1-R	24	LEU
1	1-R	39	ASP
1	1-R	50	ASP
1	1-R	59	SER
1	1-R	62	GLU
1	1-R	67	LEU
1	1-R	93	ASP
1	1-R	98	GLU
1	1-R	115	LEU
1	1-R	152	ASP
1	1-R	173	VAL
1	1-R	187	GLN
1	1-R	191	LEU
1	1-R	237	LEU
1	1-R	269	HIS
1	1-R	281	LEU
1	1-R	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-R	312	THR
1	1-R	322	LEU
1	1-R	323	VAL
1	1-R	337	ARG
1	1-R	347	ILE
1	1-R	363	SER
1	1-R	375	LEU
1	1-R	392	VAL
1	1-R	397	TYR
1	1-R	413	GLN
1	1-R	420	ARG
1	1-R	428	LEU
1	1-S	602	GLU
1	1-S	2	PRO
1	1-S	8	LEU
1	1-S	10	LYS
1	1-S	24	LEU
1	1-S	39	ASP
1	1-S	50	ASP
1	1-S	59	SER
1	1-S	62	GLU
1	1-S	67	LEU
1	1-S	93	ASP
1	1-S	98	GLU
1	1-S	115	LEU
1	1-S	152	ASP
1	1-S	173	VAL
1	1-S	187	GLN
1	1-S	191	LEU
1	1-S	237	LEU
1	1-S	269	HIS
1	1-S	281	LEU
1	1-S	308	LEU
1	1-S	312	THR
1	1-S	322	LEU
1	1-S	323	VAL
1	1-S	337	ARG
1	1-S	347	ILE
1	1-S	363	SER
1	1-S	375	LEU
1	1-S	392	VAL
1	1-S	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-S	413	GLN
1	1-S	420	ARG
1	1-S	428	LEU
1	1-T	602	GLU
1	1-T	2	PRO
1	1-T	8	LEU
1	1-T	10	LYS
1	1-T	24	LEU
1	1-T	39	ASP
1	1-T	50	ASP
1	1-T	59	SER
1	1-T	62	GLU
1	1-T	67	LEU
1	1-T	93	ASP
1	1-T	98	GLU
1	1-T	115	LEU
1	1-T	152	ASP
1	1-T	173	VAL
1	1-T	187	GLN
1	1-T	191	LEU
1	1-T	237	LEU
1	1-T	269	HIS
1	1-T	281	LEU
1	1-T	308	LEU
1	1-T	312	THR
1	1-T	322	LEU
1	1-T	323	VAL
1	1-T	337	ARG
1	1-T	347	ILE
1	1-T	363	SER
1	1-T	375	LEU
1	1-T	392	VAL
1	1-T	397	TYR
1	1-T	413	GLN
1	1-T	420	ARG
1	1-T	428	LEU
1	1-U	602	GLU
1	1-U	2	PRO
1	1-U	8	LEU
1	1-U	10	LYS
1	1-U	24	LEU
1	1-U	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-U	50	ASP
1	1-U	59	SER
1	1-U	62	GLU
1	1-U	67	LEU
1	1-U	93	ASP
1	1-U	98	GLU
1	1-U	115	LEU
1	1-U	152	ASP
1	1-U	173	VAL
1	1-U	187	GLN
1	1-U	191	LEU
1	1-U	237	LEU
1	1-U	269	HIS
1	1-U	281	LEU
1	1-U	308	LEU
1	1-U	312	THR
1	1-U	322	LEU
1	1-U	323	VAL
1	1-U	337	ARG
1	1-U	347	ILE
1	1-U	363	SER
1	1-U	375	LEU
1	1-U	392	VAL
1	1-U	397	TYR
1	1-U	413	GLN
1	1-U	420	ARG
1	1-U	428	LEU
1	1-V	602	GLU
1	1-V	2	PRO
1	1-V	8	LEU
1	1-V	10	LYS
1	1-V	24	LEU
1	1-V	39	ASP
1	1-V	50	ASP
1	1-V	59	SER
1	1-V	62	GLU
1	1-V	67	LEU
1	1-V	93	ASP
1	1-V	98	GLU
1	1-V	115	LEU
1	1-V	152	ASP
1	1-V	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-V	187	GLN
1	1-V	191	LEU
1	1-V	237	LEU
1	1-V	269	HIS
1	1-V	281	LEU
1	1-V	308	LEU
1	1-V	312	THR
1	1-V	322	LEU
1	1-V	323	VAL
1	1-V	337	ARG
1	1-V	347	ILE
1	1-V	363	SER
1	1-V	375	LEU
1	1-V	392	VAL
1	1-V	397	TYR
1	1-V	413	GLN
1	1-V	420	ARG
1	1-V	428	LEU
1	1-W	602	GLU
1	1-W	2	PRO
1	1-W	8	LEU
1	1-W	10	LYS
1	1-W	24	LEU
1	1-W	39	ASP
1	1-W	50	ASP
1	1-W	59	SER
1	1-W	62	GLU
1	1-W	67	LEU
1	1-W	93	ASP
1	1-W	98	GLU
1	1-W	115	LEU
1	1-W	152	ASP
1	1-W	173	VAL
1	1-W	187	GLN
1	1-W	191	LEU
1	1-W	237	LEU
1	1-W	269	HIS
1	1-W	281	LEU
1	1-W	308	LEU
1	1-W	312	THR
1	1-W	322	LEU
1	1-W	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-W	337	ARG
1	1-W	347	ILE
1	1-W	363	SER
1	1-W	375	LEU
1	1-W	392	VAL
1	1-W	397	TYR
1	1-W	413	GLN
1	1-W	420	ARG
1	1-W	428	LEU
1	1-X	602	GLU
1	1-X	2	PRO
1	1-X	8	LEU
1	1-X	10	LYS
1	1-X	24	LEU
1	1-X	39	ASP
1	1-X	50	ASP
1	1-X	59	SER
1	1-X	62	GLU
1	1-X	67	LEU
1	1-X	93	ASP
1	1-X	98	GLU
1	1-X	115	LEU
1	1-X	152	ASP
1	1-X	173	VAL
1	1-X	187	GLN
1	1-X	191	LEU
1	1-X	237	LEU
1	1-X	269	HIS
1	1-X	281	LEU
1	1-X	308	LEU
1	1-X	312	THR
1	1-X	322	LEU
1	1-X	323	VAL
1	1-X	337	ARG
1	1-X	347	ILE
1	1-X	363	SER
1	1-X	375	LEU
1	1-X	392	VAL
1	1-X	397	TYR
1	1-X	413	GLN
1	1-X	420	ARG
1	1-X	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-A	602	GLU
1	2-A	2	PRO
1	2-A	8	LEU
1	2-A	10	LYS
1	2-A	24	LEU
1	2-A	39	ASP
1	2-A	50	ASP
1	2-A	59	SER
1	2-A	62	GLU
1	2-A	67	LEU
1	2-A	93	ASP
1	2-A	98	GLU
1	2-A	115	LEU
1	2-A	152	ASP
1	2-A	173	VAL
1	2-A	187	GLN
1	2-A	191	LEU
1	2-A	237	LEU
1	2-A	269	HIS
1	2-A	281	LEU
1	2-A	308	LEU
1	2-A	312	THR
1	2-A	322	LEU
1	2-A	323	VAL
1	2-A	337	ARG
1	2-A	347	ILE
1	2-A	363	SER
1	2-A	375	LEU
1	2-A	392	VAL
1	2-A	397	TYR
1	2-A	413	GLN
1	2-A	420	ARG
1	2-A	428	LEU
1	2-B	602	GLU
1	2-B	2	PRO
1	2-B	8	LEU
1	2-B	10	LYS
1	2-B	24	LEU
1	2-B	39	ASP
1	2-B	50	ASP
1	2-B	59	SER
1	2-B	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-B	67	LEU
1	2-B	93	ASP
1	2-B	98	GLU
1	2-B	115	LEU
1	2-B	152	ASP
1	2-B	173	VAL
1	2-B	187	GLN
1	2-B	191	LEU
1	2-B	237	LEU
1	2-B	269	HIS
1	2-B	281	LEU
1	2-B	308	LEU
1	2-B	312	THR
1	2-B	322	LEU
1	2-B	323	VAL
1	2-B	337	ARG
1	2-B	347	ILE
1	2-B	363	SER
1	2-B	375	LEU
1	2-B	392	VAL
1	2-B	397	TYR
1	2-B	413	GLN
1	2-B	420	ARG
1	2-B	428	LEU
1	2-C	602	GLU
1	2-C	2	PRO
1	2-C	8	LEU
1	2-C	10	LYS
1	2-C	24	LEU
1	2-C	39	ASP
1	2-C	50	ASP
1	2-C	59	SER
1	2-C	62	GLU
1	2-C	67	LEU
1	2-C	93	ASP
1	2-C	98	GLU
1	2-C	115	LEU
1	2-C	152	ASP
1	2-C	173	VAL
1	2-C	187	GLN
1	2-C	191	LEU
1	2-C	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-C	269	HIS
1	2-C	281	LEU
1	2-C	308	LEU
1	2-C	312	THR
1	2-C	322	LEU
1	2-C	323	VAL
1	2-C	337	ARG
1	2-C	347	ILE
1	2-C	363	SER
1	2-C	375	LEU
1	2-C	392	VAL
1	2-C	397	TYR
1	2-C	413	GLN
1	2-C	420	ARG
1	2-C	428	LEU
1	2-D	602	GLU
1	2-D	2	PRO
1	2-D	8	LEU
1	2-D	10	LYS
1	2-D	24	LEU
1	2-D	39	ASP
1	2-D	50	ASP
1	2-D	59	SER
1	2-D	62	GLU
1	2-D	67	LEU
1	2-D	93	ASP
1	2-D	98	GLU
1	2-D	115	LEU
1	2-D	152	ASP
1	2-D	173	VAL
1	2-D	187	GLN
1	2-D	191	LEU
1	2-D	237	LEU
1	2-D	269	HIS
1	2-D	281	LEU
1	2-D	308	LEU
1	2-D	312	THR
1	2-D	322	LEU
1	2-D	323	VAL
1	2-D	337	ARG
1	2-D	347	ILE
1	2-D	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-D	375	LEU
1	2-D	392	VAL
1	2-D	397	TYR
1	2-D	413	GLN
1	2-D	420	ARG
1	2-D	428	LEU
1	2-E	602	GLU
1	2-E	2	PRO
1	2-E	8	LEU
1	2-E	10	LYS
1	2-E	24	LEU
1	2-E	39	ASP
1	2-E	50	ASP
1	2-E	59	SER
1	2-E	62	GLU
1	2-E	67	LEU
1	2-E	93	ASP
1	2-E	98	GLU
1	2-E	115	LEU
1	2-E	152	ASP
1	2-E	173	VAL
1	2-E	187	GLN
1	2-E	191	LEU
1	2-E	237	LEU
1	2-E	269	HIS
1	2-E	281	LEU
1	2-E	308	LEU
1	2-E	312	THR
1	2-E	322	LEU
1	2-E	323	VAL
1	2-E	337	ARG
1	2-E	347	ILE
1	2-E	363	SER
1	2-E	375	LEU
1	2-E	392	VAL
1	2-E	397	TYR
1	2-E	413	GLN
1	2-E	420	ARG
1	2-E	428	LEU
1	2-F	602	GLU
1	2-F	2	PRO
1	2-F	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-F	10	LYS
1	2-F	24	LEU
1	2-F	39	ASP
1	2-F	50	ASP
1	2-F	59	SER
1	2-F	62	GLU
1	2-F	67	LEU
1	2-F	93	ASP
1	2-F	98	GLU
1	2-F	115	LEU
1	2-F	152	ASP
1	2-F	173	VAL
1	2-F	187	GLN
1	2-F	191	LEU
1	2-F	237	LEU
1	2-F	269	HIS
1	2-F	281	LEU
1	2-F	308	LEU
1	2-F	312	THR
1	2-F	322	LEU
1	2-F	323	VAL
1	2-F	337	ARG
1	2-F	347	ILE
1	2-F	363	SER
1	2-F	375	LEU
1	2-F	392	VAL
1	2-F	397	TYR
1	2-F	413	GLN
1	2-F	420	ARG
1	2-F	428	LEU
1	2-G	602	GLU
1	2-G	2	PRO
1	2-G	8	LEU
1	2-G	10	LYS
1	2-G	24	LEU
1	2-G	39	ASP
1	2-G	50	ASP
1	2-G	59	SER
1	2-G	62	GLU
1	2-G	67	LEU
1	2-G	93	ASP
1	2-G	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-G	115	LEU
1	2-G	152	ASP
1	2-G	173	VAL
1	2-G	187	GLN
1	2-G	191	LEU
1	2-G	237	LEU
1	2-G	269	HIS
1	2-G	281	LEU
1	2-G	308	LEU
1	2-G	312	THR
1	2-G	322	LEU
1	2-G	323	VAL
1	2-G	337	ARG
1	2-G	347	ILE
1	2-G	363	SER
1	2-G	375	LEU
1	2-G	392	VAL
1	2-G	397	TYR
1	2-G	413	GLN
1	2-G	420	ARG
1	2-G	428	LEU
1	2-H	602	GLU
1	2-H	2	PRO
1	2-H	8	LEU
1	2-H	10	LYS
1	2-H	24	LEU
1	2-H	39	ASP
1	2-H	50	ASP
1	2-H	59	SER
1	2-H	62	GLU
1	2-H	67	LEU
1	2-H	93	ASP
1	2-H	98	GLU
1	2-H	115	LEU
1	2-H	152	ASP
1	2-H	173	VAL
1	2-H	187	GLN
1	2-H	191	LEU
1	2-H	237	LEU
1	2-H	269	HIS
1	2-H	281	LEU
1	2-H	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-H	312	THR
1	2-H	322	LEU
1	2-H	323	VAL
1	2-H	337	ARG
1	2-H	347	ILE
1	2-H	363	SER
1	2-H	375	LEU
1	2-H	392	VAL
1	2-H	397	TYR
1	2-H	413	GLN
1	2-H	420	ARG
1	2-H	428	LEU
1	2-I	602	GLU
1	2-I	2	PRO
1	2-I	8	LEU
1	2-I	10	LYS
1	2-I	24	LEU
1	2-I	39	ASP
1	2-I	50	ASP
1	2-I	59	SER
1	2-I	62	GLU
1	2-I	67	LEU
1	2-I	93	ASP
1	2-I	98	GLU
1	2-I	115	LEU
1	2-I	152	ASP
1	2-I	173	VAL
1	2-I	187	GLN
1	2-I	191	LEU
1	2-I	237	LEU
1	2-I	269	HIS
1	2-I	281	LEU
1	2-I	308	LEU
1	2-I	312	THR
1	2-I	322	LEU
1	2-I	323	VAL
1	2-I	337	ARG
1	2-I	347	ILE
1	2-I	363	SER
1	2-I	375	LEU
1	2-I	392	VAL
1	2-I	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-I	413	GLN
1	2-I	420	ARG
1	2-I	428	LEU
1	2-J	602	GLU
1	2-J	2	PRO
1	2-J	8	LEU
1	2-J	10	LYS
1	2-J	24	LEU
1	2-J	39	ASP
1	2-J	50	ASP
1	2-J	59	SER
1	2-J	62	GLU
1	2-J	67	LEU
1	2-J	93	ASP
1	2-J	98	GLU
1	2-J	115	LEU
1	2-J	152	ASP
1	2-J	173	VAL
1	2-J	187	GLN
1	2-J	191	LEU
1	2-J	237	LEU
1	2-J	269	HIS
1	2-J	281	LEU
1	2-J	308	LEU
1	2-J	312	THR
1	2-J	322	LEU
1	2-J	323	VAL
1	2-J	337	ARG
1	2-J	347	ILE
1	2-J	363	SER
1	2-J	375	LEU
1	2-J	392	VAL
1	2-J	397	TYR
1	2-J	413	GLN
1	2-J	420	ARG
1	2-J	428	LEU
1	2-K	602	GLU
1	2-K	2	PRO
1	2-K	8	LEU
1	2-K	10	LYS
1	2-K	24	LEU
1	2-K	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-K	50	ASP
1	2-K	59	SER
1	2-K	62	GLU
1	2-K	67	LEU
1	2-K	93	ASP
1	2-K	98	GLU
1	2-K	115	LEU
1	2-K	152	ASP
1	2-K	173	VAL
1	2-K	187	GLN
1	2-K	191	LEU
1	2-K	237	LEU
1	2-K	269	HIS
1	2-K	281	LEU
1	2-K	308	LEU
1	2-K	312	THR
1	2-K	322	LEU
1	2-K	323	VAL
1	2-K	337	ARG
1	2-K	347	ILE
1	2-K	363	SER
1	2-K	375	LEU
1	2-K	392	VAL
1	2-K	397	TYR
1	2-K	413	GLN
1	2-K	420	ARG
1	2-K	428	LEU
1	2-L	602	GLU
1	2-L	2	PRO
1	2-L	8	LEU
1	2-L	10	LYS
1	2-L	24	LEU
1	2-L	39	ASP
1	2-L	50	ASP
1	2-L	59	SER
1	2-L	62	GLU
1	2-L	67	LEU
1	2-L	93	ASP
1	2-L	98	GLU
1	2-L	115	LEU
1	2-L	152	ASP
1	2-L	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-L	187	GLN
1	2-L	191	LEU
1	2-L	237	LEU
1	2-L	269	HIS
1	2-L	281	LEU
1	2-L	308	LEU
1	2-L	312	THR
1	2-L	322	LEU
1	2-L	323	VAL
1	2-L	337	ARG
1	2-L	347	ILE
1	2-L	363	SER
1	2-L	375	LEU
1	2-L	392	VAL
1	2-L	397	TYR
1	2-L	413	GLN
1	2-L	420	ARG
1	2-L	428	LEU
1	2-M	602	GLU
1	2-M	2	PRO
1	2-M	8	LEU
1	2-M	10	LYS
1	2-M	24	LEU
1	2-M	39	ASP
1	2-M	50	ASP
1	2-M	59	SER
1	2-M	62	GLU
1	2-M	67	LEU
1	2-M	93	ASP
1	2-M	98	GLU
1	2-M	115	LEU
1	2-M	152	ASP
1	2-M	173	VAL
1	2-M	187	GLN
1	2-M	191	LEU
1	2-M	237	LEU
1	2-M	269	HIS
1	2-M	281	LEU
1	2-M	308	LEU
1	2-M	312	THR
1	2-M	322	LEU
1	2-M	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-M	337	ARG
1	2-M	347	ILE
1	2-M	363	SER
1	2-M	375	LEU
1	2-M	392	VAL
1	2-M	397	TYR
1	2-M	413	GLN
1	2-M	420	ARG
1	2-M	428	LEU
1	2-N	602	GLU
1	2-N	2	PRO
1	2-N	8	LEU
1	2-N	10	LYS
1	2-N	24	LEU
1	2-N	39	ASP
1	2-N	50	ASP
1	2-N	59	SER
1	2-N	62	GLU
1	2-N	67	LEU
1	2-N	93	ASP
1	2-N	98	GLU
1	2-N	115	LEU
1	2-N	152	ASP
1	2-N	173	VAL
1	2-N	187	GLN
1	2-N	191	LEU
1	2-N	237	LEU
1	2-N	269	HIS
1	2-N	281	LEU
1	2-N	308	LEU
1	2-N	312	THR
1	2-N	322	LEU
1	2-N	323	VAL
1	2-N	337	ARG
1	2-N	347	ILE
1	2-N	363	SER
1	2-N	375	LEU
1	2-N	392	VAL
1	2-N	397	TYR
1	2-N	413	GLN
1	2-N	420	ARG
1	2-N	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-O	602	GLU
1	2-O	2	PRO
1	2-O	8	LEU
1	2-O	10	LYS
1	2-O	24	LEU
1	2-O	39	ASP
1	2-O	50	ASP
1	2-O	59	SER
1	2-O	62	GLU
1	2-O	67	LEU
1	2-O	93	ASP
1	2-O	98	GLU
1	2-O	115	LEU
1	2-O	152	ASP
1	2-O	173	VAL
1	2-O	187	GLN
1	2-O	191	LEU
1	2-O	237	LEU
1	2-O	269	HIS
1	2-O	281	LEU
1	2-O	308	LEU
1	2-O	312	THR
1	2-O	322	LEU
1	2-O	323	VAL
1	2-O	337	ARG
1	2-O	347	ILE
1	2-O	363	SER
1	2-O	375	LEU
1	2-O	392	VAL
1	2-O	397	TYR
1	2-O	413	GLN
1	2-O	420	ARG
1	2-O	428	LEU
1	2-P	602	GLU
1	2-P	2	PRO
1	2-P	8	LEU
1	2-P	10	LYS
1	2-P	24	LEU
1	2-P	39	ASP
1	2-P	50	ASP
1	2-P	59	SER
1	2-P	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-P	67	LEU
1	2-P	93	ASP
1	2-P	98	GLU
1	2-P	115	LEU
1	2-P	152	ASP
1	2-P	173	VAL
1	2-P	187	GLN
1	2-P	191	LEU
1	2-P	237	LEU
1	2-P	269	HIS
1	2-P	281	LEU
1	2-P	308	LEU
1	2-P	312	THR
1	2-P	322	LEU
1	2-P	323	VAL
1	2-P	337	ARG
1	2-P	347	ILE
1	2-P	363	SER
1	2-P	375	LEU
1	2-P	392	VAL
1	2-P	397	TYR
1	2-P	413	GLN
1	2-P	420	ARG
1	2-P	428	LEU
1	2-Q	602	GLU
1	2-Q	2	PRO
1	2-Q	8	LEU
1	2-Q	10	LYS
1	2-Q	24	LEU
1	2-Q	39	ASP
1	2-Q	50	ASP
1	2-Q	59	SER
1	2-Q	62	GLU
1	2-Q	67	LEU
1	2-Q	93	ASP
1	2-Q	98	GLU
1	2-Q	115	LEU
1	2-Q	152	ASP
1	2-Q	173	VAL
1	2-Q	187	GLN
1	2-Q	191	LEU
1	2-Q	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-Q	269	HIS
1	2-Q	281	LEU
1	2-Q	308	LEU
1	2-Q	312	THR
1	2-Q	322	LEU
1	2-Q	323	VAL
1	2-Q	337	ARG
1	2-Q	347	ILE
1	2-Q	363	SER
1	2-Q	375	LEU
1	2-Q	392	VAL
1	2-Q	397	TYR
1	2-Q	413	GLN
1	2-Q	420	ARG
1	2-Q	428	LEU
1	2-R	602	GLU
1	2-R	2	PRO
1	2-R	8	LEU
1	2-R	10	LYS
1	2-R	24	LEU
1	2-R	39	ASP
1	2-R	50	ASP
1	2-R	59	SER
1	2-R	62	GLU
1	2-R	67	LEU
1	2-R	93	ASP
1	2-R	98	GLU
1	2-R	115	LEU
1	2-R	152	ASP
1	2-R	173	VAL
1	2-R	187	GLN
1	2-R	191	LEU
1	2-R	237	LEU
1	2-R	269	HIS
1	2-R	281	LEU
1	2-R	308	LEU
1	2-R	312	THR
1	2-R	322	LEU
1	2-R	323	VAL
1	2-R	337	ARG
1	2-R	347	ILE
1	2-R	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-R	375	LEU
1	2-R	392	VAL
1	2-R	397	TYR
1	2-R	413	GLN
1	2-R	420	ARG
1	2-R	428	LEU
1	2-S	602	GLU
1	2-S	2	PRO
1	2-S	8	LEU
1	2-S	10	LYS
1	2-S	24	LEU
1	2-S	39	ASP
1	2-S	50	ASP
1	2-S	59	SER
1	2-S	62	GLU
1	2-S	67	LEU
1	2-S	93	ASP
1	2-S	98	GLU
1	2-S	115	LEU
1	2-S	152	ASP
1	2-S	173	VAL
1	2-S	187	GLN
1	2-S	191	LEU
1	2-S	237	LEU
1	2-S	269	HIS
1	2-S	281	LEU
1	2-S	308	LEU
1	2-S	312	THR
1	2-S	322	LEU
1	2-S	323	VAL
1	2-S	337	ARG
1	2-S	347	ILE
1	2-S	363	SER
1	2-S	375	LEU
1	2-S	392	VAL
1	2-S	397	TYR
1	2-S	413	GLN
1	2-S	420	ARG
1	2-S	428	LEU
1	2-T	602	GLU
1	2-T	2	PRO
1	2-T	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-T	10	LYS
1	2-T	24	LEU
1	2-T	39	ASP
1	2-T	50	ASP
1	2-T	59	SER
1	2-T	62	GLU
1	2-T	67	LEU
1	2-T	93	ASP
1	2-T	98	GLU
1	2-T	115	LEU
1	2-T	152	ASP
1	2-T	173	VAL
1	2-T	187	GLN
1	2-T	191	LEU
1	2-T	237	LEU
1	2-T	269	HIS
1	2-T	281	LEU
1	2-T	308	LEU
1	2-T	312	THR
1	2-T	322	LEU
1	2-T	323	VAL
1	2-T	337	ARG
1	2-T	347	ILE
1	2-T	363	SER
1	2-T	375	LEU
1	2-T	392	VAL
1	2-T	397	TYR
1	2-T	413	GLN
1	2-T	420	ARG
1	2-T	428	LEU
1	2-U	602	GLU
1	2-U	2	PRO
1	2-U	8	LEU
1	2-U	10	LYS
1	2-U	24	LEU
1	2-U	39	ASP
1	2-U	50	ASP
1	2-U	59	SER
1	2-U	62	GLU
1	2-U	67	LEU
1	2-U	93	ASP
1	2-U	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-U	115	LEU
1	2-U	152	ASP
1	2-U	173	VAL
1	2-U	187	GLN
1	2-U	191	LEU
1	2-U	237	LEU
1	2-U	269	HIS
1	2-U	281	LEU
1	2-U	308	LEU
1	2-U	312	THR
1	2-U	322	LEU
1	2-U	323	VAL
1	2-U	337	ARG
1	2-U	347	ILE
1	2-U	363	SER
1	2-U	375	LEU
1	2-U	392	VAL
1	2-U	397	TYR
1	2-U	413	GLN
1	2-U	420	ARG
1	2-U	428	LEU
1	2-V	602	GLU
1	2-V	2	PRO
1	2-V	8	LEU
1	2-V	10	LYS
1	2-V	24	LEU
1	2-V	39	ASP
1	2-V	50	ASP
1	2-V	59	SER
1	2-V	62	GLU
1	2-V	67	LEU
1	2-V	93	ASP
1	2-V	98	GLU
1	2-V	115	LEU
1	2-V	152	ASP
1	2-V	173	VAL
1	2-V	187	GLN
1	2-V	191	LEU
1	2-V	237	LEU
1	2-V	269	HIS
1	2-V	281	LEU
1	2-V	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-V	312	THR
1	2-V	322	LEU
1	2-V	323	VAL
1	2-V	337	ARG
1	2-V	347	ILE
1	2-V	363	SER
1	2-V	375	LEU
1	2-V	392	VAL
1	2-V	397	TYR
1	2-V	413	GLN
1	2-V	420	ARG
1	2-V	428	LEU
1	2-W	602	GLU
1	2-W	2	PRO
1	2-W	8	LEU
1	2-W	10	LYS
1	2-W	24	LEU
1	2-W	39	ASP
1	2-W	50	ASP
1	2-W	59	SER
1	2-W	62	GLU
1	2-W	67	LEU
1	2-W	93	ASP
1	2-W	98	GLU
1	2-W	115	LEU
1	2-W	152	ASP
1	2-W	173	VAL
1	2-W	187	GLN
1	2-W	191	LEU
1	2-W	237	LEU
1	2-W	269	HIS
1	2-W	281	LEU
1	2-W	308	LEU
1	2-W	312	THR
1	2-W	322	LEU
1	2-W	323	VAL
1	2-W	337	ARG
1	2-W	347	ILE
1	2-W	363	SER
1	2-W	375	LEU
1	2-W	392	VAL
1	2-W	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-W	413	GLN
1	2-W	420	ARG
1	2-W	428	LEU
1	2-X	602	GLU
1	2-X	2	PRO
1	2-X	8	LEU
1	2-X	10	LYS
1	2-X	24	LEU
1	2-X	39	ASP
1	2-X	50	ASP
1	2-X	59	SER
1	2-X	62	GLU
1	2-X	67	LEU
1	2-X	93	ASP
1	2-X	98	GLU
1	2-X	115	LEU
1	2-X	152	ASP
1	2-X	173	VAL
1	2-X	187	GLN
1	2-X	191	LEU
1	2-X	237	LEU
1	2-X	269	HIS
1	2-X	281	LEU
1	2-X	308	LEU
1	2-X	312	THR
1	2-X	322	LEU
1	2-X	323	VAL
1	2-X	337	ARG
1	2-X	347	ILE
1	2-X	363	SER
1	2-X	375	LEU
1	2-X	392	VAL
1	2-X	397	TYR
1	2-X	413	GLN
1	2-X	420	ARG
1	2-X	428	LEU
1	3-A	602	GLU
1	3-A	2	PRO
1	3-A	8	LEU
1	3-A	10	LYS
1	3-A	24	LEU
1	3-A	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-A	50	ASP
1	3-A	59	SER
1	3-A	62	GLU
1	3-A	67	LEU
1	3-A	93	ASP
1	3-A	98	GLU
1	3-A	115	LEU
1	3-A	152	ASP
1	3-A	173	VAL
1	3-A	187	GLN
1	3-A	191	LEU
1	3-A	237	LEU
1	3-A	269	HIS
1	3-A	281	LEU
1	3-A	308	LEU
1	3-A	312	THR
1	3-A	322	LEU
1	3-A	323	VAL
1	3-A	337	ARG
1	3-A	347	ILE
1	3-A	363	SER
1	3-A	375	LEU
1	3-A	392	VAL
1	3-A	397	TYR
1	3-A	413	GLN
1	3-A	420	ARG
1	3-A	428	LEU
1	3-B	602	GLU
1	3-B	2	PRO
1	3-B	8	LEU
1	3-B	10	LYS
1	3-B	24	LEU
1	3-B	39	ASP
1	3-B	50	ASP
1	3-B	59	SER
1	3-B	62	GLU
1	3-B	67	LEU
1	3-B	93	ASP
1	3-B	98	GLU
1	3-B	115	LEU
1	3-B	152	ASP
1	3-B	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-B	187	GLN
1	3-B	191	LEU
1	3-B	237	LEU
1	3-B	269	HIS
1	3-B	281	LEU
1	3-B	308	LEU
1	3-B	312	THR
1	3-B	322	LEU
1	3-B	323	VAL
1	3-B	337	ARG
1	3-B	347	ILE
1	3-B	363	SER
1	3-B	375	LEU
1	3-B	392	VAL
1	3-B	397	TYR
1	3-B	413	GLN
1	3-B	420	ARG
1	3-B	428	LEU
1	3-C	602	GLU
1	3-C	2	PRO
1	3-C	8	LEU
1	3-C	10	LYS
1	3-C	24	LEU
1	3-C	39	ASP
1	3-C	50	ASP
1	3-C	59	SER
1	3-C	62	GLU
1	3-C	67	LEU
1	3-C	93	ASP
1	3-C	98	GLU
1	3-C	115	LEU
1	3-C	152	ASP
1	3-C	173	VAL
1	3-C	187	GLN
1	3-C	191	LEU
1	3-C	237	LEU
1	3-C	269	HIS
1	3-C	281	LEU
1	3-C	308	LEU
1	3-C	312	THR
1	3-C	322	LEU
1	3-C	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-C	337	ARG
1	3-C	347	ILE
1	3-C	363	SER
1	3-C	375	LEU
1	3-C	392	VAL
1	3-C	397	TYR
1	3-C	413	GLN
1	3-C	420	ARG
1	3-C	428	LEU
1	3-D	602	GLU
1	3-D	2	PRO
1	3-D	8	LEU
1	3-D	10	LYS
1	3-D	24	LEU
1	3-D	39	ASP
1	3-D	50	ASP
1	3-D	59	SER
1	3-D	62	GLU
1	3-D	67	LEU
1	3-D	93	ASP
1	3-D	98	GLU
1	3-D	115	LEU
1	3-D	152	ASP
1	3-D	173	VAL
1	3-D	187	GLN
1	3-D	191	LEU
1	3-D	237	LEU
1	3-D	269	HIS
1	3-D	281	LEU
1	3-D	308	LEU
1	3-D	312	THR
1	3-D	322	LEU
1	3-D	323	VAL
1	3-D	337	ARG
1	3-D	347	ILE
1	3-D	363	SER
1	3-D	375	LEU
1	3-D	392	VAL
1	3-D	397	TYR
1	3-D	413	GLN
1	3-D	420	ARG
1	3-D	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-E	602	GLU
1	3-E	2	PRO
1	3-E	8	LEU
1	3-E	10	LYS
1	3-E	24	LEU
1	3-E	39	ASP
1	3-E	50	ASP
1	3-E	59	SER
1	3-E	62	GLU
1	3-E	67	LEU
1	3-E	93	ASP
1	3-E	98	GLU
1	3-E	115	LEU
1	3-E	152	ASP
1	3-E	173	VAL
1	3-E	187	GLN
1	3-E	191	LEU
1	3-E	237	LEU
1	3-E	269	HIS
1	3-E	281	LEU
1	3-E	308	LEU
1	3-E	312	THR
1	3-E	322	LEU
1	3-E	323	VAL
1	3-E	337	ARG
1	3-E	347	ILE
1	3-E	363	SER
1	3-E	375	LEU
1	3-E	392	VAL
1	3-E	397	TYR
1	3-E	413	GLN
1	3-E	420	ARG
1	3-E	428	LEU
1	3-F	602	GLU
1	3-F	2	PRO
1	3-F	8	LEU
1	3-F	10	LYS
1	3-F	24	LEU
1	3-F	39	ASP
1	3-F	50	ASP
1	3-F	59	SER
1	3-F	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-F	67	LEU
1	3-F	93	ASP
1	3-F	98	GLU
1	3-F	115	LEU
1	3-F	152	ASP
1	3-F	173	VAL
1	3-F	187	GLN
1	3-F	191	LEU
1	3-F	237	LEU
1	3-F	269	HIS
1	3-F	281	LEU
1	3-F	308	LEU
1	3-F	312	THR
1	3-F	322	LEU
1	3-F	323	VAL
1	3-F	337	ARG
1	3-F	347	ILE
1	3-F	363	SER
1	3-F	375	LEU
1	3-F	392	VAL
1	3-F	397	TYR
1	3-F	413	GLN
1	3-F	420	ARG
1	3-F	428	LEU
1	3-G	602	GLU
1	3-G	2	PRO
1	3-G	8	LEU
1	3-G	10	LYS
1	3-G	24	LEU
1	3-G	39	ASP
1	3-G	50	ASP
1	3-G	59	SER
1	3-G	62	GLU
1	3-G	67	LEU
1	3-G	93	ASP
1	3-G	98	GLU
1	3-G	115	LEU
1	3-G	152	ASP
1	3-G	173	VAL
1	3-G	187	GLN
1	3-G	191	LEU
1	3-G	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-G	269	HIS
1	3-G	281	LEU
1	3-G	308	LEU
1	3-G	312	THR
1	3-G	322	LEU
1	3-G	323	VAL
1	3-G	337	ARG
1	3-G	347	ILE
1	3-G	363	SER
1	3-G	375	LEU
1	3-G	392	VAL
1	3-G	397	TYR
1	3-G	413	GLN
1	3-G	420	ARG
1	3-G	428	LEU
1	3-H	602	GLU
1	3-H	2	PRO
1	3-H	8	LEU
1	3-H	10	LYS
1	3-H	24	LEU
1	3-H	39	ASP
1	3-H	50	ASP
1	3-H	59	SER
1	3-H	62	GLU
1	3-H	67	LEU
1	3-H	93	ASP
1	3-H	98	GLU
1	3-H	115	LEU
1	3-H	152	ASP
1	3-H	173	VAL
1	3-H	187	GLN
1	3-H	191	LEU
1	3-H	237	LEU
1	3-H	269	HIS
1	3-H	281	LEU
1	3-H	308	LEU
1	3-H	312	THR
1	3-H	322	LEU
1	3-H	323	VAL
1	3-H	337	ARG
1	3-H	347	ILE
1	3-H	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-H	375	LEU
1	3-H	392	VAL
1	3-H	397	TYR
1	3-H	413	GLN
1	3-H	420	ARG
1	3-H	428	LEU
1	3-I	602	GLU
1	3-I	2	PRO
1	3-I	8	LEU
1	3-I	10	LYS
1	3-I	24	LEU
1	3-I	39	ASP
1	3-I	50	ASP
1	3-I	59	SER
1	3-I	62	GLU
1	3-I	67	LEU
1	3-I	93	ASP
1	3-I	98	GLU
1	3-I	115	LEU
1	3-I	152	ASP
1	3-I	173	VAL
1	3-I	187	GLN
1	3-I	191	LEU
1	3-I	237	LEU
1	3-I	269	HIS
1	3-I	281	LEU
1	3-I	308	LEU
1	3-I	312	THR
1	3-I	322	LEU
1	3-I	323	VAL
1	3-I	337	ARG
1	3-I	347	ILE
1	3-I	363	SER
1	3-I	375	LEU
1	3-I	392	VAL
1	3-I	397	TYR
1	3-I	413	GLN
1	3-I	420	ARG
1	3-I	428	LEU
1	3-J	602	GLU
1	3-J	2	PRO
1	3-J	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-J	10	LYS
1	3-J	24	LEU
1	3-J	39	ASP
1	3-J	50	ASP
1	3-J	59	SER
1	3-J	62	GLU
1	3-J	67	LEU
1	3-J	93	ASP
1	3-J	98	GLU
1	3-J	115	LEU
1	3-J	152	ASP
1	3-J	173	VAL
1	3-J	187	GLN
1	3-J	191	LEU
1	3-J	237	LEU
1	3-J	269	HIS
1	3-J	281	LEU
1	3-J	308	LEU
1	3-J	312	THR
1	3-J	322	LEU
1	3-J	323	VAL
1	3-J	337	ARG
1	3-J	347	ILE
1	3-J	363	SER
1	3-J	375	LEU
1	3-J	392	VAL
1	3-J	397	TYR
1	3-J	413	GLN
1	3-J	420	ARG
1	3-J	428	LEU
1	3-K	602	GLU
1	3-K	2	PRO
1	3-K	8	LEU
1	3-K	10	LYS
1	3-K	24	LEU
1	3-K	39	ASP
1	3-K	50	ASP
1	3-K	59	SER
1	3-K	62	GLU
1	3-K	67	LEU
1	3-K	93	ASP
1	3-K	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-K	115	LEU
1	3-K	152	ASP
1	3-K	173	VAL
1	3-K	187	GLN
1	3-K	191	LEU
1	3-K	237	LEU
1	3-K	269	HIS
1	3-K	281	LEU
1	3-K	308	LEU
1	3-K	312	THR
1	3-K	322	LEU
1	3-K	323	VAL
1	3-K	337	ARG
1	3-K	347	ILE
1	3-K	363	SER
1	3-K	375	LEU
1	3-K	392	VAL
1	3-K	397	TYR
1	3-K	413	GLN
1	3-K	420	ARG
1	3-K	428	LEU
1	3-L	602	GLU
1	3-L	2	PRO
1	3-L	8	LEU
1	3-L	10	LYS
1	3-L	24	LEU
1	3-L	39	ASP
1	3-L	50	ASP
1	3-L	59	SER
1	3-L	62	GLU
1	3-L	67	LEU
1	3-L	93	ASP
1	3-L	98	GLU
1	3-L	115	LEU
1	3-L	152	ASP
1	3-L	173	VAL
1	3-L	187	GLN
1	3-L	191	LEU
1	3-L	237	LEU
1	3-L	269	HIS
1	3-L	281	LEU
1	3-L	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-L	312	THR
1	3-L	322	LEU
1	3-L	323	VAL
1	3-L	337	ARG
1	3-L	347	ILE
1	3-L	363	SER
1	3-L	375	LEU
1	3-L	392	VAL
1	3-L	397	TYR
1	3-L	413	GLN
1	3-L	420	ARG
1	3-L	428	LEU
1	3-M	602	GLU
1	3-M	2	PRO
1	3-M	8	LEU
1	3-M	10	LYS
1	3-M	24	LEU
1	3-M	39	ASP
1	3-M	50	ASP
1	3-M	59	SER
1	3-M	62	GLU
1	3-M	67	LEU
1	3-M	93	ASP
1	3-M	98	GLU
1	3-M	115	LEU
1	3-M	152	ASP
1	3-M	173	VAL
1	3-M	187	GLN
1	3-M	191	LEU
1	3-M	237	LEU
1	3-M	269	HIS
1	3-M	281	LEU
1	3-M	308	LEU
1	3-M	312	THR
1	3-M	322	LEU
1	3-M	323	VAL
1	3-M	337	ARG
1	3-M	347	ILE
1	3-M	363	SER
1	3-M	375	LEU
1	3-M	392	VAL
1	3-M	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-M	413	GLN
1	3-M	420	ARG
1	3-M	428	LEU
1	3-N	602	GLU
1	3-N	2	PRO
1	3-N	8	LEU
1	3-N	10	LYS
1	3-N	24	LEU
1	3-N	39	ASP
1	3-N	50	ASP
1	3-N	59	SER
1	3-N	62	GLU
1	3-N	67	LEU
1	3-N	93	ASP
1	3-N	98	GLU
1	3-N	115	LEU
1	3-N	152	ASP
1	3-N	173	VAL
1	3-N	187	GLN
1	3-N	191	LEU
1	3-N	237	LEU
1	3-N	269	HIS
1	3-N	281	LEU
1	3-N	308	LEU
1	3-N	312	THR
1	3-N	322	LEU
1	3-N	323	VAL
1	3-N	337	ARG
1	3-N	347	ILE
1	3-N	363	SER
1	3-N	375	LEU
1	3-N	392	VAL
1	3-N	397	TYR
1	3-N	413	GLN
1	3-N	420	ARG
1	3-N	428	LEU
1	3-O	602	GLU
1	3-O	2	PRO
1	3-O	8	LEU
1	3-O	10	LYS
1	3-O	24	LEU
1	3-O	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-O	50	ASP
1	3-O	59	SER
1	3-O	62	GLU
1	3-O	67	LEU
1	3-O	93	ASP
1	3-O	98	GLU
1	3-O	115	LEU
1	3-O	152	ASP
1	3-O	173	VAL
1	3-O	187	GLN
1	3-O	191	LEU
1	3-O	237	LEU
1	3-O	269	HIS
1	3-O	281	LEU
1	3-O	308	LEU
1	3-O	312	THR
1	3-O	322	LEU
1	3-O	323	VAL
1	3-O	337	ARG
1	3-O	347	ILE
1	3-O	363	SER
1	3-O	375	LEU
1	3-O	392	VAL
1	3-O	397	TYR
1	3-O	413	GLN
1	3-O	420	ARG
1	3-O	428	LEU
1	3-P	602	GLU
1	3-P	2	PRO
1	3-P	8	LEU
1	3-P	10	LYS
1	3-P	24	LEU
1	3-P	39	ASP
1	3-P	50	ASP
1	3-P	59	SER
1	3-P	62	GLU
1	3-P	67	LEU
1	3-P	93	ASP
1	3-P	98	GLU
1	3-P	115	LEU
1	3-P	152	ASP
1	3-P	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-P	187	GLN
1	3-P	191	LEU
1	3-P	237	LEU
1	3-P	269	HIS
1	3-P	281	LEU
1	3-P	308	LEU
1	3-P	312	THR
1	3-P	322	LEU
1	3-P	323	VAL
1	3-P	337	ARG
1	3-P	347	ILE
1	3-P	363	SER
1	3-P	375	LEU
1	3-P	392	VAL
1	3-P	397	TYR
1	3-P	413	GLN
1	3-P	420	ARG
1	3-P	428	LEU
1	3-Q	602	GLU
1	3-Q	2	PRO
1	3-Q	8	LEU
1	3-Q	10	LYS
1	3-Q	24	LEU
1	3-Q	39	ASP
1	3-Q	50	ASP
1	3-Q	59	SER
1	3-Q	62	GLU
1	3-Q	67	LEU
1	3-Q	93	ASP
1	3-Q	98	GLU
1	3-Q	115	LEU
1	3-Q	152	ASP
1	3-Q	173	VAL
1	3-Q	187	GLN
1	3-Q	191	LEU
1	3-Q	237	LEU
1	3-Q	269	HIS
1	3-Q	281	LEU
1	3-Q	308	LEU
1	3-Q	312	THR
1	3-Q	322	LEU
1	3-Q	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-Q	337	ARG
1	3-Q	347	ILE
1	3-Q	363	SER
1	3-Q	375	LEU
1	3-Q	392	VAL
1	3-Q	397	TYR
1	3-Q	413	GLN
1	3-Q	420	ARG
1	3-Q	428	LEU
1	3-R	602	GLU
1	3-R	2	PRO
1	3-R	8	LEU
1	3-R	10	LYS
1	3-R	24	LEU
1	3-R	39	ASP
1	3-R	50	ASP
1	3-R	59	SER
1	3-R	62	GLU
1	3-R	67	LEU
1	3-R	93	ASP
1	3-R	98	GLU
1	3-R	115	LEU
1	3-R	152	ASP
1	3-R	173	VAL
1	3-R	187	GLN
1	3-R	191	LEU
1	3-R	237	LEU
1	3-R	269	HIS
1	3-R	281	LEU
1	3-R	308	LEU
1	3-R	312	THR
1	3-R	322	LEU
1	3-R	323	VAL
1	3-R	337	ARG
1	3-R	347	ILE
1	3-R	363	SER
1	3-R	375	LEU
1	3-R	392	VAL
1	3-R	397	TYR
1	3-R	413	GLN
1	3-R	420	ARG
1	3-R	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-S	602	GLU
1	3-S	2	PRO
1	3-S	8	LEU
1	3-S	10	LYS
1	3-S	24	LEU
1	3-S	39	ASP
1	3-S	50	ASP
1	3-S	59	SER
1	3-S	62	GLU
1	3-S	67	LEU
1	3-S	93	ASP
1	3-S	98	GLU
1	3-S	115	LEU
1	3-S	152	ASP
1	3-S	173	VAL
1	3-S	187	GLN
1	3-S	191	LEU
1	3-S	237	LEU
1	3-S	269	HIS
1	3-S	281	LEU
1	3-S	308	LEU
1	3-S	312	THR
1	3-S	322	LEU
1	3-S	323	VAL
1	3-S	337	ARG
1	3-S	347	ILE
1	3-S	363	SER
1	3-S	375	LEU
1	3-S	392	VAL
1	3-S	397	TYR
1	3-S	413	GLN
1	3-S	420	ARG
1	3-S	428	LEU
1	3-T	602	GLU
1	3-T	2	PRO
1	3-T	8	LEU
1	3-T	10	LYS
1	3-T	24	LEU
1	3-T	39	ASP
1	3-T	50	ASP
1	3-T	59	SER
1	3-T	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-T	67	LEU
1	3-T	93	ASP
1	3-T	98	GLU
1	3-T	115	LEU
1	3-T	152	ASP
1	3-T	173	VAL
1	3-T	187	GLN
1	3-T	191	LEU
1	3-T	237	LEU
1	3-T	269	HIS
1	3-T	281	LEU
1	3-T	308	LEU
1	3-T	312	THR
1	3-T	322	LEU
1	3-T	323	VAL
1	3-T	337	ARG
1	3-T	347	ILE
1	3-T	363	SER
1	3-T	375	LEU
1	3-T	392	VAL
1	3-T	397	TYR
1	3-T	413	GLN
1	3-T	420	ARG
1	3-T	428	LEU
1	3-U	602	GLU
1	3-U	2	PRO
1	3-U	8	LEU
1	3-U	10	LYS
1	3-U	24	LEU
1	3-U	39	ASP
1	3-U	50	ASP
1	3-U	59	SER
1	3-U	62	GLU
1	3-U	67	LEU
1	3-U	93	ASP
1	3-U	98	GLU
1	3-U	115	LEU
1	3-U	152	ASP
1	3-U	173	VAL
1	3-U	187	GLN
1	3-U	191	LEU
1	3-U	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-U	269	HIS
1	3-U	281	LEU
1	3-U	308	LEU
1	3-U	312	THR
1	3-U	322	LEU
1	3-U	323	VAL
1	3-U	337	ARG
1	3-U	347	ILE
1	3-U	363	SER
1	3-U	375	LEU
1	3-U	392	VAL
1	3-U	397	TYR
1	3-U	413	GLN
1	3-U	420	ARG
1	3-U	428	LEU
1	3-V	602	GLU
1	3-V	2	PRO
1	3-V	8	LEU
1	3-V	10	LYS
1	3-V	24	LEU
1	3-V	39	ASP
1	3-V	50	ASP
1	3-V	59	SER
1	3-V	62	GLU
1	3-V	67	LEU
1	3-V	93	ASP
1	3-V	98	GLU
1	3-V	115	LEU
1	3-V	152	ASP
1	3-V	173	VAL
1	3-V	187	GLN
1	3-V	191	LEU
1	3-V	237	LEU
1	3-V	269	HIS
1	3-V	281	LEU
1	3-V	308	LEU
1	3-V	312	THR
1	3-V	322	LEU
1	3-V	323	VAL
1	3-V	337	ARG
1	3-V	347	ILE
1	3-V	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-V	375	LEU
1	3-V	392	VAL
1	3-V	397	TYR
1	3-V	413	GLN
1	3-V	420	ARG
1	3-V	428	LEU
1	3-W	602	GLU
1	3-W	2	PRO
1	3-W	8	LEU
1	3-W	10	LYS
1	3-W	24	LEU
1	3-W	39	ASP
1	3-W	50	ASP
1	3-W	59	SER
1	3-W	62	GLU
1	3-W	67	LEU
1	3-W	93	ASP
1	3-W	98	GLU
1	3-W	115	LEU
1	3-W	152	ASP
1	3-W	173	VAL
1	3-W	187	GLN
1	3-W	191	LEU
1	3-W	237	LEU
1	3-W	269	HIS
1	3-W	281	LEU
1	3-W	308	LEU
1	3-W	312	THR
1	3-W	322	LEU
1	3-W	323	VAL
1	3-W	337	ARG
1	3-W	347	ILE
1	3-W	363	SER
1	3-W	375	LEU
1	3-W	392	VAL
1	3-W	397	TYR
1	3-W	413	GLN
1	3-W	420	ARG
1	3-W	428	LEU
1	3-X	602	GLU
1	3-X	2	PRO
1	3-X	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-X	10	LYS
1	3-X	24	LEU
1	3-X	39	ASP
1	3-X	50	ASP
1	3-X	59	SER
1	3-X	62	GLU
1	3-X	67	LEU
1	3-X	93	ASP
1	3-X	98	GLU
1	3-X	115	LEU
1	3-X	152	ASP
1	3-X	173	VAL
1	3-X	187	GLN
1	3-X	191	LEU
1	3-X	237	LEU
1	3-X	269	HIS
1	3-X	281	LEU
1	3-X	308	LEU
1	3-X	312	THR
1	3-X	322	LEU
1	3-X	323	VAL
1	3-X	337	ARG
1	3-X	347	ILE
1	3-X	363	SER
1	3-X	375	LEU
1	3-X	392	VAL
1	3-X	397	TYR
1	3-X	413	GLN
1	3-X	420	ARG
1	3-X	428	LEU
1	4-A	602	GLU
1	4-A	2	PRO
1	4-A	8	LEU
1	4-A	10	LYS
1	4-A	24	LEU
1	4-A	39	ASP
1	4-A	50	ASP
1	4-A	59	SER
1	4-A	62	GLU
1	4-A	67	LEU
1	4-A	93	ASP
1	4-A	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-A	115	LEU
1	4-A	152	ASP
1	4-A	173	VAL
1	4-A	187	GLN
1	4-A	191	LEU
1	4-A	237	LEU
1	4-A	269	HIS
1	4-A	281	LEU
1	4-A	308	LEU
1	4-A	312	THR
1	4-A	322	LEU
1	4-A	323	VAL
1	4-A	337	ARG
1	4-A	347	ILE
1	4-A	363	SER
1	4-A	375	LEU
1	4-A	392	VAL
1	4-A	397	TYR
1	4-A	413	GLN
1	4-A	420	ARG
1	4-A	428	LEU
1	4-B	602	GLU
1	4-B	2	PRO
1	4-B	8	LEU
1	4-B	10	LYS
1	4-B	24	LEU
1	4-B	39	ASP
1	4-B	50	ASP
1	4-B	59	SER
1	4-B	62	GLU
1	4-B	67	LEU
1	4-B	93	ASP
1	4-B	98	GLU
1	4-B	115	LEU
1	4-B	152	ASP
1	4-B	173	VAL
1	4-B	187	GLN
1	4-B	191	LEU
1	4-B	237	LEU
1	4-B	269	HIS
1	4-B	281	LEU
1	4-B	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-B	312	THR
1	4-B	322	LEU
1	4-B	323	VAL
1	4-B	337	ARG
1	4-B	347	ILE
1	4-B	363	SER
1	4-B	375	LEU
1	4-B	392	VAL
1	4-B	397	TYR
1	4-B	413	GLN
1	4-B	420	ARG
1	4-B	428	LEU
1	4-C	602	GLU
1	4-C	2	PRO
1	4-C	8	LEU
1	4-C	10	LYS
1	4-C	24	LEU
1	4-C	39	ASP
1	4-C	50	ASP
1	4-C	59	SER
1	4-C	62	GLU
1	4-C	67	LEU
1	4-C	93	ASP
1	4-C	98	GLU
1	4-C	115	LEU
1	4-C	152	ASP
1	4-C	173	VAL
1	4-C	187	GLN
1	4-C	191	LEU
1	4-C	237	LEU
1	4-C	269	HIS
1	4-C	281	LEU
1	4-C	308	LEU
1	4-C	312	THR
1	4-C	322	LEU
1	4-C	323	VAL
1	4-C	337	ARG
1	4-C	347	ILE
1	4-C	363	SER
1	4-C	375	LEU
1	4-C	392	VAL
1	4-C	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-C	413	GLN
1	4-C	420	ARG
1	4-C	428	LEU
1	4-D	602	GLU
1	4-D	2	PRO
1	4-D	8	LEU
1	4-D	10	LYS
1	4-D	24	LEU
1	4-D	39	ASP
1	4-D	50	ASP
1	4-D	59	SER
1	4-D	62	GLU
1	4-D	67	LEU
1	4-D	93	ASP
1	4-D	98	GLU
1	4-D	115	LEU
1	4-D	152	ASP
1	4-D	173	VAL
1	4-D	187	GLN
1	4-D	191	LEU
1	4-D	237	LEU
1	4-D	269	HIS
1	4-D	281	LEU
1	4-D	308	LEU
1	4-D	312	THR
1	4-D	322	LEU
1	4-D	323	VAL
1	4-D	337	ARG
1	4-D	347	ILE
1	4-D	363	SER
1	4-D	375	LEU
1	4-D	392	VAL
1	4-D	397	TYR
1	4-D	413	GLN
1	4-D	420	ARG
1	4-D	428	LEU
1	4-E	602	GLU
1	4-E	2	PRO
1	4-E	8	LEU
1	4-E	10	LYS
1	4-E	24	LEU
1	4-E	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-E	50	ASP
1	4-E	59	SER
1	4-E	62	GLU
1	4-E	67	LEU
1	4-E	93	ASP
1	4-E	98	GLU
1	4-E	115	LEU
1	4-E	152	ASP
1	4-E	173	VAL
1	4-E	187	GLN
1	4-E	191	LEU
1	4-E	237	LEU
1	4-E	269	HIS
1	4-E	281	LEU
1	4-E	308	LEU
1	4-E	312	THR
1	4-E	322	LEU
1	4-E	323	VAL
1	4-E	337	ARG
1	4-E	347	ILE
1	4-E	363	SER
1	4-E	375	LEU
1	4-E	392	VAL
1	4-E	397	TYR
1	4-E	413	GLN
1	4-E	420	ARG
1	4-E	428	LEU
1	4-F	602	GLU
1	4-F	2	PRO
1	4-F	8	LEU
1	4-F	10	LYS
1	4-F	24	LEU
1	4-F	39	ASP
1	4-F	50	ASP
1	4-F	59	SER
1	4-F	62	GLU
1	4-F	67	LEU
1	4-F	93	ASP
1	4-F	98	GLU
1	4-F	115	LEU
1	4-F	152	ASP
1	4-F	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-F	187	GLN
1	4-F	191	LEU
1	4-F	237	LEU
1	4-F	269	HIS
1	4-F	281	LEU
1	4-F	308	LEU
1	4-F	312	THR
1	4-F	322	LEU
1	4-F	323	VAL
1	4-F	337	ARG
1	4-F	347	ILE
1	4-F	363	SER
1	4-F	375	LEU
1	4-F	392	VAL
1	4-F	397	TYR
1	4-F	413	GLN
1	4-F	420	ARG
1	4-F	428	LEU
1	4-G	602	GLU
1	4-G	2	PRO
1	4-G	8	LEU
1	4-G	10	LYS
1	4-G	24	LEU
1	4-G	39	ASP
1	4-G	50	ASP
1	4-G	59	SER
1	4-G	62	GLU
1	4-G	67	LEU
1	4-G	93	ASP
1	4-G	98	GLU
1	4-G	115	LEU
1	4-G	152	ASP
1	4-G	173	VAL
1	4-G	187	GLN
1	4-G	191	LEU
1	4-G	237	LEU
1	4-G	269	HIS
1	4-G	281	LEU
1	4-G	308	LEU
1	4-G	312	THR
1	4-G	322	LEU
1	4-G	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-G	337	ARG
1	4-G	347	ILE
1	4-G	363	SER
1	4-G	375	LEU
1	4-G	392	VAL
1	4-G	397	TYR
1	4-G	413	GLN
1	4-G	420	ARG
1	4-G	428	LEU
1	4-H	602	GLU
1	4-H	2	PRO
1	4-H	8	LEU
1	4-H	10	LYS
1	4-H	24	LEU
1	4-H	39	ASP
1	4-H	50	ASP
1	4-H	59	SER
1	4-H	62	GLU
1	4-H	67	LEU
1	4-H	93	ASP
1	4-H	98	GLU
1	4-H	115	LEU
1	4-H	152	ASP
1	4-H	173	VAL
1	4-H	187	GLN
1	4-H	191	LEU
1	4-H	237	LEU
1	4-H	269	HIS
1	4-H	281	LEU
1	4-H	308	LEU
1	4-H	312	THR
1	4-H	322	LEU
1	4-H	323	VAL
1	4-H	337	ARG
1	4-H	347	ILE
1	4-H	363	SER
1	4-H	375	LEU
1	4-H	392	VAL
1	4-H	397	TYR
1	4-H	413	GLN
1	4-H	420	ARG
1	4-H	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-I	602	GLU
1	4-I	2	PRO
1	4-I	8	LEU
1	4-I	10	LYS
1	4-I	24	LEU
1	4-I	39	ASP
1	4-I	50	ASP
1	4-I	59	SER
1	4-I	62	GLU
1	4-I	67	LEU
1	4-I	93	ASP
1	4-I	98	GLU
1	4-I	115	LEU
1	4-I	152	ASP
1	4-I	173	VAL
1	4-I	187	GLN
1	4-I	191	LEU
1	4-I	237	LEU
1	4-I	269	HIS
1	4-I	281	LEU
1	4-I	308	LEU
1	4-I	312	THR
1	4-I	322	LEU
1	4-I	323	VAL
1	4-I	337	ARG
1	4-I	347	ILE
1	4-I	363	SER
1	4-I	375	LEU
1	4-I	392	VAL
1	4-I	397	TYR
1	4-I	413	GLN
1	4-I	420	ARG
1	4-I	428	LEU
1	4-J	602	GLU
1	4-J	2	PRO
1	4-J	8	LEU
1	4-J	10	LYS
1	4-J	24	LEU
1	4-J	39	ASP
1	4-J	50	ASP
1	4-J	59	SER
1	4-J	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-J	67	LEU
1	4-J	93	ASP
1	4-J	98	GLU
1	4-J	115	LEU
1	4-J	152	ASP
1	4-J	173	VAL
1	4-J	187	GLN
1	4-J	191	LEU
1	4-J	237	LEU
1	4-J	269	HIS
1	4-J	281	LEU
1	4-J	308	LEU
1	4-J	312	THR
1	4-J	322	LEU
1	4-J	323	VAL
1	4-J	337	ARG
1	4-J	347	ILE
1	4-J	363	SER
1	4-J	375	LEU
1	4-J	392	VAL
1	4-J	397	TYR
1	4-J	413	GLN
1	4-J	420	ARG
1	4-J	428	LEU
1	4-K	602	GLU
1	4-K	2	PRO
1	4-K	8	LEU
1	4-K	10	LYS
1	4-K	24	LEU
1	4-K	39	ASP
1	4-K	50	ASP
1	4-K	59	SER
1	4-K	62	GLU
1	4-K	67	LEU
1	4-K	93	ASP
1	4-K	98	GLU
1	4-K	115	LEU
1	4-K	152	ASP
1	4-K	173	VAL
1	4-K	187	GLN
1	4-K	191	LEU
1	4-K	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-K	269	HIS
1	4-K	281	LEU
1	4-K	308	LEU
1	4-K	312	THR
1	4-K	322	LEU
1	4-K	323	VAL
1	4-K	337	ARG
1	4-K	347	ILE
1	4-K	363	SER
1	4-K	375	LEU
1	4-K	392	VAL
1	4-K	397	TYR
1	4-K	413	GLN
1	4-K	420	ARG
1	4-K	428	LEU
1	4-L	602	GLU
1	4-L	2	PRO
1	4-L	8	LEU
1	4-L	10	LYS
1	4-L	24	LEU
1	4-L	39	ASP
1	4-L	50	ASP
1	4-L	59	SER
1	4-L	62	GLU
1	4-L	67	LEU
1	4-L	93	ASP
1	4-L	98	GLU
1	4-L	115	LEU
1	4-L	152	ASP
1	4-L	173	VAL
1	4-L	187	GLN
1	4-L	191	LEU
1	4-L	237	LEU
1	4-L	269	HIS
1	4-L	281	LEU
1	4-L	308	LEU
1	4-L	312	THR
1	4-L	322	LEU
1	4-L	323	VAL
1	4-L	337	ARG
1	4-L	347	ILE
1	4-L	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-L	375	LEU
1	4-L	392	VAL
1	4-L	397	TYR
1	4-L	413	GLN
1	4-L	420	ARG
1	4-L	428	LEU
1	4-M	602	GLU
1	4-M	2	PRO
1	4-M	8	LEU
1	4-M	10	LYS
1	4-M	24	LEU
1	4-M	39	ASP
1	4-M	50	ASP
1	4-M	59	SER
1	4-M	62	GLU
1	4-M	67	LEU
1	4-M	93	ASP
1	4-M	98	GLU
1	4-M	115	LEU
1	4-M	152	ASP
1	4-M	173	VAL
1	4-M	187	GLN
1	4-M	191	LEU
1	4-M	237	LEU
1	4-M	269	HIS
1	4-M	281	LEU
1	4-M	308	LEU
1	4-M	312	THR
1	4-M	322	LEU
1	4-M	323	VAL
1	4-M	337	ARG
1	4-M	347	ILE
1	4-M	363	SER
1	4-M	375	LEU
1	4-M	392	VAL
1	4-M	397	TYR
1	4-M	413	GLN
1	4-M	420	ARG
1	4-M	428	LEU
1	4-N	602	GLU
1	4-N	2	PRO
1	4-N	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-N	10	LYS
1	4-N	24	LEU
1	4-N	39	ASP
1	4-N	50	ASP
1	4-N	59	SER
1	4-N	62	GLU
1	4-N	67	LEU
1	4-N	93	ASP
1	4-N	98	GLU
1	4-N	115	LEU
1	4-N	152	ASP
1	4-N	173	VAL
1	4-N	187	GLN
1	4-N	191	LEU
1	4-N	237	LEU
1	4-N	269	HIS
1	4-N	281	LEU
1	4-N	308	LEU
1	4-N	312	THR
1	4-N	322	LEU
1	4-N	323	VAL
1	4-N	337	ARG
1	4-N	347	ILE
1	4-N	363	SER
1	4-N	375	LEU
1	4-N	392	VAL
1	4-N	397	TYR
1	4-N	413	GLN
1	4-N	420	ARG
1	4-N	428	LEU
1	4-O	602	GLU
1	4-O	2	PRO
1	4-O	8	LEU
1	4-O	10	LYS
1	4-O	24	LEU
1	4-O	39	ASP
1	4-O	50	ASP
1	4-O	59	SER
1	4-O	62	GLU
1	4-O	67	LEU
1	4-O	93	ASP
1	4-O	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-O	115	LEU
1	4-O	152	ASP
1	4-O	173	VAL
1	4-O	187	GLN
1	4-O	191	LEU
1	4-O	237	LEU
1	4-O	269	HIS
1	4-O	281	LEU
1	4-O	308	LEU
1	4-O	312	THR
1	4-O	322	LEU
1	4-O	323	VAL
1	4-O	337	ARG
1	4-O	347	ILE
1	4-O	363	SER
1	4-O	375	LEU
1	4-O	392	VAL
1	4-O	397	TYR
1	4-O	413	GLN
1	4-O	420	ARG
1	4-O	428	LEU
1	4-P	602	GLU
1	4-P	2	PRO
1	4-P	8	LEU
1	4-P	10	LYS
1	4-P	24	LEU
1	4-P	39	ASP
1	4-P	50	ASP
1	4-P	59	SER
1	4-P	62	GLU
1	4-P	67	LEU
1	4-P	93	ASP
1	4-P	98	GLU
1	4-P	115	LEU
1	4-P	152	ASP
1	4-P	173	VAL
1	4-P	187	GLN
1	4-P	191	LEU
1	4-P	237	LEU
1	4-P	269	HIS
1	4-P	281	LEU
1	4-P	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-P	312	THR
1	4-P	322	LEU
1	4-P	323	VAL
1	4-P	337	ARG
1	4-P	347	ILE
1	4-P	363	SER
1	4-P	375	LEU
1	4-P	392	VAL
1	4-P	397	TYR
1	4-P	413	GLN
1	4-P	420	ARG
1	4-P	428	LEU
1	4-Q	602	GLU
1	4-Q	2	PRO
1	4-Q	8	LEU
1	4-Q	10	LYS
1	4-Q	24	LEU
1	4-Q	39	ASP
1	4-Q	50	ASP
1	4-Q	59	SER
1	4-Q	62	GLU
1	4-Q	67	LEU
1	4-Q	93	ASP
1	4-Q	98	GLU
1	4-Q	115	LEU
1	4-Q	152	ASP
1	4-Q	173	VAL
1	4-Q	187	GLN
1	4-Q	191	LEU
1	4-Q	237	LEU
1	4-Q	269	HIS
1	4-Q	281	LEU
1	4-Q	308	LEU
1	4-Q	312	THR
1	4-Q	322	LEU
1	4-Q	323	VAL
1	4-Q	337	ARG
1	4-Q	347	ILE
1	4-Q	363	SER
1	4-Q	375	LEU
1	4-Q	392	VAL
1	4-Q	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-Q	413	GLN
1	4-Q	420	ARG
1	4-Q	428	LEU
1	4-R	602	GLU
1	4-R	2	PRO
1	4-R	8	LEU
1	4-R	10	LYS
1	4-R	24	LEU
1	4-R	39	ASP
1	4-R	50	ASP
1	4-R	59	SER
1	4-R	62	GLU
1	4-R	67	LEU
1	4-R	93	ASP
1	4-R	98	GLU
1	4-R	115	LEU
1	4-R	152	ASP
1	4-R	173	VAL
1	4-R	187	GLN
1	4-R	191	LEU
1	4-R	237	LEU
1	4-R	269	HIS
1	4-R	281	LEU
1	4-R	308	LEU
1	4-R	312	THR
1	4-R	322	LEU
1	4-R	323	VAL
1	4-R	337	ARG
1	4-R	347	ILE
1	4-R	363	SER
1	4-R	375	LEU
1	4-R	392	VAL
1	4-R	397	TYR
1	4-R	413	GLN
1	4-R	420	ARG
1	4-R	428	LEU
1	4-S	602	GLU
1	4-S	2	PRO
1	4-S	8	LEU
1	4-S	10	LYS
1	4-S	24	LEU
1	4-S	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-S	50	ASP
1	4-S	59	SER
1	4-S	62	GLU
1	4-S	67	LEU
1	4-S	93	ASP
1	4-S	98	GLU
1	4-S	115	LEU
1	4-S	152	ASP
1	4-S	173	VAL
1	4-S	187	GLN
1	4-S	191	LEU
1	4-S	237	LEU
1	4-S	269	HIS
1	4-S	281	LEU
1	4-S	308	LEU
1	4-S	312	THR
1	4-S	322	LEU
1	4-S	323	VAL
1	4-S	337	ARG
1	4-S	347	ILE
1	4-S	363	SER
1	4-S	375	LEU
1	4-S	392	VAL
1	4-S	397	TYR
1	4-S	413	GLN
1	4-S	420	ARG
1	4-S	428	LEU
1	4-T	602	GLU
1	4-T	2	PRO
1	4-T	8	LEU
1	4-T	10	LYS
1	4-T	24	LEU
1	4-T	39	ASP
1	4-T	50	ASP
1	4-T	59	SER
1	4-T	62	GLU
1	4-T	67	LEU
1	4-T	93	ASP
1	4-T	98	GLU
1	4-T	115	LEU
1	4-T	152	ASP
1	4-T	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-T	187	GLN
1	4-T	191	LEU
1	4-T	237	LEU
1	4-T	269	HIS
1	4-T	281	LEU
1	4-T	308	LEU
1	4-T	312	THR
1	4-T	322	LEU
1	4-T	323	VAL
1	4-T	337	ARG
1	4-T	347	ILE
1	4-T	363	SER
1	4-T	375	LEU
1	4-T	392	VAL
1	4-T	397	TYR
1	4-T	413	GLN
1	4-T	420	ARG
1	4-T	428	LEU
1	4-U	602	GLU
1	4-U	2	PRO
1	4-U	8	LEU
1	4-U	10	LYS
1	4-U	24	LEU
1	4-U	39	ASP
1	4-U	50	ASP
1	4-U	59	SER
1	4-U	62	GLU
1	4-U	67	LEU
1	4-U	93	ASP
1	4-U	98	GLU
1	4-U	115	LEU
1	4-U	152	ASP
1	4-U	173	VAL
1	4-U	187	GLN
1	4-U	191	LEU
1	4-U	237	LEU
1	4-U	269	HIS
1	4-U	281	LEU
1	4-U	308	LEU
1	4-U	312	THR
1	4-U	322	LEU
1	4-U	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-U	337	ARG
1	4-U	347	ILE
1	4-U	363	SER
1	4-U	375	LEU
1	4-U	392	VAL
1	4-U	397	TYR
1	4-U	413	GLN
1	4-U	420	ARG
1	4-U	428	LEU
1	4-V	602	GLU
1	4-V	2	PRO
1	4-V	8	LEU
1	4-V	10	LYS
1	4-V	24	LEU
1	4-V	39	ASP
1	4-V	50	ASP
1	4-V	59	SER
1	4-V	62	GLU
1	4-V	67	LEU
1	4-V	93	ASP
1	4-V	98	GLU
1	4-V	115	LEU
1	4-V	152	ASP
1	4-V	173	VAL
1	4-V	187	GLN
1	4-V	191	LEU
1	4-V	237	LEU
1	4-V	269	HIS
1	4-V	281	LEU
1	4-V	308	LEU
1	4-V	312	THR
1	4-V	322	LEU
1	4-V	323	VAL
1	4-V	337	ARG
1	4-V	347	ILE
1	4-V	363	SER
1	4-V	375	LEU
1	4-V	392	VAL
1	4-V	397	TYR
1	4-V	413	GLN
1	4-V	420	ARG
1	4-V	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-W	602	GLU
1	4-W	2	PRO
1	4-W	8	LEU
1	4-W	10	LYS
1	4-W	24	LEU
1	4-W	39	ASP
1	4-W	50	ASP
1	4-W	59	SER
1	4-W	62	GLU
1	4-W	67	LEU
1	4-W	93	ASP
1	4-W	98	GLU
1	4-W	115	LEU
1	4-W	152	ASP
1	4-W	173	VAL
1	4-W	187	GLN
1	4-W	191	LEU
1	4-W	237	LEU
1	4-W	269	HIS
1	4-W	281	LEU
1	4-W	308	LEU
1	4-W	312	THR
1	4-W	322	LEU
1	4-W	323	VAL
1	4-W	337	ARG
1	4-W	347	ILE
1	4-W	363	SER
1	4-W	375	LEU
1	4-W	392	VAL
1	4-W	397	TYR
1	4-W	413	GLN
1	4-W	420	ARG
1	4-W	428	LEU
1	4-X	602	GLU
1	4-X	2	PRO
1	4-X	8	LEU
1	4-X	10	LYS
1	4-X	24	LEU
1	4-X	39	ASP
1	4-X	50	ASP
1	4-X	59	SER
1	4-X	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-X	67	LEU
1	4-X	93	ASP
1	4-X	98	GLU
1	4-X	115	LEU
1	4-X	152	ASP
1	4-X	173	VAL
1	4-X	187	GLN
1	4-X	191	LEU
1	4-X	237	LEU
1	4-X	269	HIS
1	4-X	281	LEU
1	4-X	308	LEU
1	4-X	312	THR
1	4-X	322	LEU
1	4-X	323	VAL
1	4-X	337	ARG
1	4-X	347	ILE
1	4-X	363	SER
1	4-X	375	LEU
1	4-X	392	VAL
1	4-X	397	TYR
1	4-X	413	GLN
1	4-X	420	ARG
1	4-X	428	LEU
1	5-A	602	GLU
1	5-A	2	PRO
1	5-A	8	LEU
1	5-A	10	LYS
1	5-A	24	LEU
1	5-A	39	ASP
1	5-A	50	ASP
1	5-A	59	SER
1	5-A	62	GLU
1	5-A	67	LEU
1	5-A	93	ASP
1	5-A	98	GLU
1	5-A	115	LEU
1	5-A	152	ASP
1	5-A	173	VAL
1	5-A	187	GLN
1	5-A	191	LEU
1	5-A	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-A	269	HIS
1	5-A	281	LEU
1	5-A	308	LEU
1	5-A	312	THR
1	5-A	322	LEU
1	5-A	323	VAL
1	5-A	337	ARG
1	5-A	347	ILE
1	5-A	363	SER
1	5-A	375	LEU
1	5-A	392	VAL
1	5-A	397	TYR
1	5-A	413	GLN
1	5-A	420	ARG
1	5-A	428	LEU
1	5-B	602	GLU
1	5-B	2	PRO
1	5-B	8	LEU
1	5-B	10	LYS
1	5-B	24	LEU
1	5-B	39	ASP
1	5-B	50	ASP
1	5-B	59	SER
1	5-B	62	GLU
1	5-B	67	LEU
1	5-B	93	ASP
1	5-B	98	GLU
1	5-B	115	LEU
1	5-B	152	ASP
1	5-B	173	VAL
1	5-B	187	GLN
1	5-B	191	LEU
1	5-B	237	LEU
1	5-B	269	HIS
1	5-B	281	LEU
1	5-B	308	LEU
1	5-B	312	THR
1	5-B	322	LEU
1	5-B	323	VAL
1	5-B	337	ARG
1	5-B	347	ILE
1	5-B	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-B	375	LEU
1	5-B	392	VAL
1	5-B	397	TYR
1	5-B	413	GLN
1	5-B	420	ARG
1	5-B	428	LEU
1	5-C	602	GLU
1	5-C	2	PRO
1	5-C	8	LEU
1	5-C	10	LYS
1	5-C	24	LEU
1	5-C	39	ASP
1	5-C	50	ASP
1	5-C	59	SER
1	5-C	62	GLU
1	5-C	67	LEU
1	5-C	93	ASP
1	5-C	98	GLU
1	5-C	115	LEU
1	5-C	152	ASP
1	5-C	173	VAL
1	5-C	187	GLN
1	5-C	191	LEU
1	5-C	237	LEU
1	5-C	269	HIS
1	5-C	281	LEU
1	5-C	308	LEU
1	5-C	312	THR
1	5-C	322	LEU
1	5-C	323	VAL
1	5-C	337	ARG
1	5-C	347	ILE
1	5-C	363	SER
1	5-C	375	LEU
1	5-C	392	VAL
1	5-C	397	TYR
1	5-C	413	GLN
1	5-C	420	ARG
1	5-C	428	LEU
1	5-D	602	GLU
1	5-D	2	PRO
1	5-D	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-D	10	LYS
1	5-D	24	LEU
1	5-D	39	ASP
1	5-D	50	ASP
1	5-D	59	SER
1	5-D	62	GLU
1	5-D	67	LEU
1	5-D	93	ASP
1	5-D	98	GLU
1	5-D	115	LEU
1	5-D	152	ASP
1	5-D	173	VAL
1	5-D	187	GLN
1	5-D	191	LEU
1	5-D	237	LEU
1	5-D	269	HIS
1	5-D	281	LEU
1	5-D	308	LEU
1	5-D	312	THR
1	5-D	322	LEU
1	5-D	323	VAL
1	5-D	337	ARG
1	5-D	347	ILE
1	5-D	363	SER
1	5-D	375	LEU
1	5-D	392	VAL
1	5-D	397	TYR
1	5-D	413	GLN
1	5-D	420	ARG
1	5-D	428	LEU
1	5-E	602	GLU
1	5-E	2	PRO
1	5-E	8	LEU
1	5-E	10	LYS
1	5-E	24	LEU
1	5-E	39	ASP
1	5-E	50	ASP
1	5-E	59	SER
1	5-E	62	GLU
1	5-E	67	LEU
1	5-E	93	ASP
1	5-E	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-E	115	LEU
1	5-E	152	ASP
1	5-E	173	VAL
1	5-E	187	GLN
1	5-E	191	LEU
1	5-E	237	LEU
1	5-E	269	HIS
1	5-E	281	LEU
1	5-E	308	LEU
1	5-E	312	THR
1	5-E	322	LEU
1	5-E	323	VAL
1	5-E	337	ARG
1	5-E	347	ILE
1	5-E	363	SER
1	5-E	375	LEU
1	5-E	392	VAL
1	5-E	397	TYR
1	5-E	413	GLN
1	5-E	420	ARG
1	5-E	428	LEU
1	5-F	602	GLU
1	5-F	2	PRO
1	5-F	8	LEU
1	5-F	10	LYS
1	5-F	24	LEU
1	5-F	39	ASP
1	5-F	50	ASP
1	5-F	59	SER
1	5-F	62	GLU
1	5-F	67	LEU
1	5-F	93	ASP
1	5-F	98	GLU
1	5-F	115	LEU
1	5-F	152	ASP
1	5-F	173	VAL
1	5-F	187	GLN
1	5-F	191	LEU
1	5-F	237	LEU
1	5-F	269	HIS
1	5-F	281	LEU
1	5-F	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-F	312	THR
1	5-F	322	LEU
1	5-F	323	VAL
1	5-F	337	ARG
1	5-F	347	ILE
1	5-F	363	SER
1	5-F	375	LEU
1	5-F	392	VAL
1	5-F	397	TYR
1	5-F	413	GLN
1	5-F	420	ARG
1	5-F	428	LEU
1	5-G	602	GLU
1	5-G	2	PRO
1	5-G	8	LEU
1	5-G	10	LYS
1	5-G	24	LEU
1	5-G	39	ASP
1	5-G	50	ASP
1	5-G	59	SER
1	5-G	62	GLU
1	5-G	67	LEU
1	5-G	93	ASP
1	5-G	98	GLU
1	5-G	115	LEU
1	5-G	152	ASP
1	5-G	173	VAL
1	5-G	187	GLN
1	5-G	191	LEU
1	5-G	237	LEU
1	5-G	269	HIS
1	5-G	281	LEU
1	5-G	308	LEU
1	5-G	312	THR
1	5-G	322	LEU
1	5-G	323	VAL
1	5-G	337	ARG
1	5-G	347	ILE
1	5-G	363	SER
1	5-G	375	LEU
1	5-G	392	VAL
1	5-G	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-G	413	GLN
1	5-G	420	ARG
1	5-G	428	LEU
1	5-H	602	GLU
1	5-H	2	PRO
1	5-H	8	LEU
1	5-H	10	LYS
1	5-H	24	LEU
1	5-H	39	ASP
1	5-H	50	ASP
1	5-H	59	SER
1	5-H	62	GLU
1	5-H	67	LEU
1	5-H	93	ASP
1	5-H	98	GLU
1	5-H	115	LEU
1	5-H	152	ASP
1	5-H	173	VAL
1	5-H	187	GLN
1	5-H	191	LEU
1	5-H	237	LEU
1	5-H	269	HIS
1	5-H	281	LEU
1	5-H	308	LEU
1	5-H	312	THR
1	5-H	322	LEU
1	5-H	323	VAL
1	5-H	337	ARG
1	5-H	347	ILE
1	5-H	363	SER
1	5-H	375	LEU
1	5-H	392	VAL
1	5-H	397	TYR
1	5-H	413	GLN
1	5-H	420	ARG
1	5-H	428	LEU
1	5-I	602	GLU
1	5-I	2	PRO
1	5-I	8	LEU
1	5-I	10	LYS
1	5-I	24	LEU
1	5-I	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-I	50	ASP
1	5-I	59	SER
1	5-I	62	GLU
1	5-I	67	LEU
1	5-I	93	ASP
1	5-I	98	GLU
1	5-I	115	LEU
1	5-I	152	ASP
1	5-I	173	VAL
1	5-I	187	GLN
1	5-I	191	LEU
1	5-I	237	LEU
1	5-I	269	HIS
1	5-I	281	LEU
1	5-I	308	LEU
1	5-I	312	THR
1	5-I	322	LEU
1	5-I	323	VAL
1	5-I	337	ARG
1	5-I	347	ILE
1	5-I	363	SER
1	5-I	375	LEU
1	5-I	392	VAL
1	5-I	397	TYR
1	5-I	413	GLN
1	5-I	420	ARG
1	5-I	428	LEU
1	5-J	602	GLU
1	5-J	2	PRO
1	5-J	8	LEU
1	5-J	10	LYS
1	5-J	24	LEU
1	5-J	39	ASP
1	5-J	50	ASP
1	5-J	59	SER
1	5-J	62	GLU
1	5-J	67	LEU
1	5-J	93	ASP
1	5-J	98	GLU
1	5-J	115	LEU
1	5-J	152	ASP
1	5-J	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-J	187	GLN
1	5-J	191	LEU
1	5-J	237	LEU
1	5-J	269	HIS
1	5-J	281	LEU
1	5-J	308	LEU
1	5-J	312	THR
1	5-J	322	LEU
1	5-J	323	VAL
1	5-J	337	ARG
1	5-J	347	ILE
1	5-J	363	SER
1	5-J	375	LEU
1	5-J	392	VAL
1	5-J	397	TYR
1	5-J	413	GLN
1	5-J	420	ARG
1	5-J	428	LEU
1	5-K	602	GLU
1	5-K	2	PRO
1	5-K	8	LEU
1	5-K	10	LYS
1	5-K	24	LEU
1	5-K	39	ASP
1	5-K	50	ASP
1	5-K	59	SER
1	5-K	62	GLU
1	5-K	67	LEU
1	5-K	93	ASP
1	5-K	98	GLU
1	5-K	115	LEU
1	5-K	152	ASP
1	5-K	173	VAL
1	5-K	187	GLN
1	5-K	191	LEU
1	5-K	237	LEU
1	5-K	269	HIS
1	5-K	281	LEU
1	5-K	308	LEU
1	5-K	312	THR
1	5-K	322	LEU
1	5-K	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-K	337	ARG
1	5-K	347	ILE
1	5-K	363	SER
1	5-K	375	LEU
1	5-K	392	VAL
1	5-K	397	TYR
1	5-K	413	GLN
1	5-K	420	ARG
1	5-K	428	LEU
1	5-L	602	GLU
1	5-L	2	PRO
1	5-L	8	LEU
1	5-L	10	LYS
1	5-L	24	LEU
1	5-L	39	ASP
1	5-L	50	ASP
1	5-L	59	SER
1	5-L	62	GLU
1	5-L	67	LEU
1	5-L	93	ASP
1	5-L	98	GLU
1	5-L	115	LEU
1	5-L	152	ASP
1	5-L	173	VAL
1	5-L	187	GLN
1	5-L	191	LEU
1	5-L	237	LEU
1	5-L	269	HIS
1	5-L	281	LEU
1	5-L	308	LEU
1	5-L	312	THR
1	5-L	322	LEU
1	5-L	323	VAL
1	5-L	337	ARG
1	5-L	347	ILE
1	5-L	363	SER
1	5-L	375	LEU
1	5-L	392	VAL
1	5-L	397	TYR
1	5-L	413	GLN
1	5-L	420	ARG
1	5-L	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-M	602	GLU
1	5-M	2	PRO
1	5-M	8	LEU
1	5-M	10	LYS
1	5-M	24	LEU
1	5-M	39	ASP
1	5-M	50	ASP
1	5-M	59	SER
1	5-M	62	GLU
1	5-M	67	LEU
1	5-M	93	ASP
1	5-M	98	GLU
1	5-M	115	LEU
1	5-M	152	ASP
1	5-M	173	VAL
1	5-M	187	GLN
1	5-M	191	LEU
1	5-M	237	LEU
1	5-M	269	HIS
1	5-M	281	LEU
1	5-M	308	LEU
1	5-M	312	THR
1	5-M	322	LEU
1	5-M	323	VAL
1	5-M	337	ARG
1	5-M	347	ILE
1	5-M	363	SER
1	5-M	375	LEU
1	5-M	392	VAL
1	5-M	397	TYR
1	5-M	413	GLN
1	5-M	420	ARG
1	5-M	428	LEU
1	5-N	602	GLU
1	5-N	2	PRO
1	5-N	8	LEU
1	5-N	10	LYS
1	5-N	24	LEU
1	5-N	39	ASP
1	5-N	50	ASP
1	5-N	59	SER
1	5-N	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-N	67	LEU
1	5-N	93	ASP
1	5-N	98	GLU
1	5-N	115	LEU
1	5-N	152	ASP
1	5-N	173	VAL
1	5-N	187	GLN
1	5-N	191	LEU
1	5-N	237	LEU
1	5-N	269	HIS
1	5-N	281	LEU
1	5-N	308	LEU
1	5-N	312	THR
1	5-N	322	LEU
1	5-N	323	VAL
1	5-N	337	ARG
1	5-N	347	ILE
1	5-N	363	SER
1	5-N	375	LEU
1	5-N	392	VAL
1	5-N	397	TYR
1	5-N	413	GLN
1	5-N	420	ARG
1	5-N	428	LEU
1	5-O	602	GLU
1	5-O	2	PRO
1	5-O	8	LEU
1	5-O	10	LYS
1	5-O	24	LEU
1	5-O	39	ASP
1	5-O	50	ASP
1	5-O	59	SER
1	5-O	62	GLU
1	5-O	67	LEU
1	5-O	93	ASP
1	5-O	98	GLU
1	5-O	115	LEU
1	5-O	152	ASP
1	5-O	173	VAL
1	5-O	187	GLN
1	5-O	191	LEU
1	5-O	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-O	269	HIS
1	5-O	281	LEU
1	5-O	308	LEU
1	5-O	312	THR
1	5-O	322	LEU
1	5-O	323	VAL
1	5-O	337	ARG
1	5-O	347	ILE
1	5-O	363	SER
1	5-O	375	LEU
1	5-O	392	VAL
1	5-O	397	TYR
1	5-O	413	GLN
1	5-O	420	ARG
1	5-O	428	LEU
1	5-P	602	GLU
1	5-P	2	PRO
1	5-P	8	LEU
1	5-P	10	LYS
1	5-P	24	LEU
1	5-P	39	ASP
1	5-P	50	ASP
1	5-P	59	SER
1	5-P	62	GLU
1	5-P	67	LEU
1	5-P	93	ASP
1	5-P	98	GLU
1	5-P	115	LEU
1	5-P	152	ASP
1	5-P	173	VAL
1	5-P	187	GLN
1	5-P	191	LEU
1	5-P	237	LEU
1	5-P	269	HIS
1	5-P	281	LEU
1	5-P	308	LEU
1	5-P	312	THR
1	5-P	322	LEU
1	5-P	323	VAL
1	5-P	337	ARG
1	5-P	347	ILE
1	5-P	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-P	375	LEU
1	5-P	392	VAL
1	5-P	397	TYR
1	5-P	413	GLN
1	5-P	420	ARG
1	5-P	428	LEU
1	5-Q	602	GLU
1	5-Q	2	PRO
1	5-Q	8	LEU
1	5-Q	10	LYS
1	5-Q	24	LEU
1	5-Q	39	ASP
1	5-Q	50	ASP
1	5-Q	59	SER
1	5-Q	62	GLU
1	5-Q	67	LEU
1	5-Q	93	ASP
1	5-Q	98	GLU
1	5-Q	115	LEU
1	5-Q	152	ASP
1	5-Q	173	VAL
1	5-Q	187	GLN
1	5-Q	191	LEU
1	5-Q	237	LEU
1	5-Q	269	HIS
1	5-Q	281	LEU
1	5-Q	308	LEU
1	5-Q	312	THR
1	5-Q	322	LEU
1	5-Q	323	VAL
1	5-Q	337	ARG
1	5-Q	347	ILE
1	5-Q	363	SER
1	5-Q	375	LEU
1	5-Q	392	VAL
1	5-Q	397	TYR
1	5-Q	413	GLN
1	5-Q	420	ARG
1	5-Q	428	LEU
1	5-R	602	GLU
1	5-R	2	PRO
1	5-R	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-R	10	LYS
1	5-R	24	LEU
1	5-R	39	ASP
1	5-R	50	ASP
1	5-R	59	SER
1	5-R	62	GLU
1	5-R	67	LEU
1	5-R	93	ASP
1	5-R	98	GLU
1	5-R	115	LEU
1	5-R	152	ASP
1	5-R	173	VAL
1	5-R	187	GLN
1	5-R	191	LEU
1	5-R	237	LEU
1	5-R	269	HIS
1	5-R	281	LEU
1	5-R	308	LEU
1	5-R	312	THR
1	5-R	322	LEU
1	5-R	323	VAL
1	5-R	337	ARG
1	5-R	347	ILE
1	5-R	363	SER
1	5-R	375	LEU
1	5-R	392	VAL
1	5-R	397	TYR
1	5-R	413	GLN
1	5-R	420	ARG
1	5-R	428	LEU
1	5-S	602	GLU
1	5-S	2	PRO
1	5-S	8	LEU
1	5-S	10	LYS
1	5-S	24	LEU
1	5-S	39	ASP
1	5-S	50	ASP
1	5-S	59	SER
1	5-S	62	GLU
1	5-S	67	LEU
1	5-S	93	ASP
1	5-S	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-S	115	LEU
1	5-S	152	ASP
1	5-S	173	VAL
1	5-S	187	GLN
1	5-S	191	LEU
1	5-S	237	LEU
1	5-S	269	HIS
1	5-S	281	LEU
1	5-S	308	LEU
1	5-S	312	THR
1	5-S	322	LEU
1	5-S	323	VAL
1	5-S	337	ARG
1	5-S	347	ILE
1	5-S	363	SER
1	5-S	375	LEU
1	5-S	392	VAL
1	5-S	397	TYR
1	5-S	413	GLN
1	5-S	420	ARG
1	5-S	428	LEU
1	5-T	602	GLU
1	5-T	2	PRO
1	5-T	8	LEU
1	5-T	10	LYS
1	5-T	24	LEU
1	5-T	39	ASP
1	5-T	50	ASP
1	5-T	59	SER
1	5-T	62	GLU
1	5-T	67	LEU
1	5-T	93	ASP
1	5-T	98	GLU
1	5-T	115	LEU
1	5-T	152	ASP
1	5-T	173	VAL
1	5-T	187	GLN
1	5-T	191	LEU
1	5-T	237	LEU
1	5-T	269	HIS
1	5-T	281	LEU
1	5-T	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-T	312	THR
1	5-T	322	LEU
1	5-T	323	VAL
1	5-T	337	ARG
1	5-T	347	ILE
1	5-T	363	SER
1	5-T	375	LEU
1	5-T	392	VAL
1	5-T	397	TYR
1	5-T	413	GLN
1	5-T	420	ARG
1	5-T	428	LEU
1	5-U	602	GLU
1	5-U	2	PRO
1	5-U	8	LEU
1	5-U	10	LYS
1	5-U	24	LEU
1	5-U	39	ASP
1	5-U	50	ASP
1	5-U	59	SER
1	5-U	62	GLU
1	5-U	67	LEU
1	5-U	93	ASP
1	5-U	98	GLU
1	5-U	115	LEU
1	5-U	152	ASP
1	5-U	173	VAL
1	5-U	187	GLN
1	5-U	191	LEU
1	5-U	237	LEU
1	5-U	269	HIS
1	5-U	281	LEU
1	5-U	308	LEU
1	5-U	312	THR
1	5-U	322	LEU
1	5-U	323	VAL
1	5-U	337	ARG
1	5-U	347	ILE
1	5-U	363	SER
1	5-U	375	LEU
1	5-U	392	VAL
1	5-U	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-U	413	GLN
1	5-U	420	ARG
1	5-U	428	LEU
1	5-V	602	GLU
1	5-V	2	PRO
1	5-V	8	LEU
1	5-V	10	LYS
1	5-V	24	LEU
1	5-V	39	ASP
1	5-V	50	ASP
1	5-V	59	SER
1	5-V	62	GLU
1	5-V	67	LEU
1	5-V	93	ASP
1	5-V	98	GLU
1	5-V	115	LEU
1	5-V	152	ASP
1	5-V	173	VAL
1	5-V	187	GLN
1	5-V	191	LEU
1	5-V	237	LEU
1	5-V	269	HIS
1	5-V	281	LEU
1	5-V	308	LEU
1	5-V	312	THR
1	5-V	322	LEU
1	5-V	323	VAL
1	5-V	337	ARG
1	5-V	347	ILE
1	5-V	363	SER
1	5-V	375	LEU
1	5-V	392	VAL
1	5-V	397	TYR
1	5-V	413	GLN
1	5-V	420	ARG
1	5-V	428	LEU
1	5-W	602	GLU
1	5-W	2	PRO
1	5-W	8	LEU
1	5-W	10	LYS
1	5-W	24	LEU
1	5-W	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-W	50	ASP
1	5-W	59	SER
1	5-W	62	GLU
1	5-W	67	LEU
1	5-W	93	ASP
1	5-W	98	GLU
1	5-W	115	LEU
1	5-W	152	ASP
1	5-W	173	VAL
1	5-W	187	GLN
1	5-W	191	LEU
1	5-W	237	LEU
1	5-W	269	HIS
1	5-W	281	LEU
1	5-W	308	LEU
1	5-W	312	THR
1	5-W	322	LEU
1	5-W	323	VAL
1	5-W	337	ARG
1	5-W	347	ILE
1	5-W	363	SER
1	5-W	375	LEU
1	5-W	392	VAL
1	5-W	397	TYR
1	5-W	413	GLN
1	5-W	420	ARG
1	5-W	428	LEU
1	5-X	602	GLU
1	5-X	2	PRO
1	5-X	8	LEU
1	5-X	10	LYS
1	5-X	24	LEU
1	5-X	39	ASP
1	5-X	50	ASP
1	5-X	59	SER
1	5-X	62	GLU
1	5-X	67	LEU
1	5-X	93	ASP
1	5-X	98	GLU
1	5-X	115	LEU
1	5-X	152	ASP
1	5-X	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-X	187	GLN
1	5-X	191	LEU
1	5-X	237	LEU
1	5-X	269	HIS
1	5-X	281	LEU
1	5-X	308	LEU
1	5-X	312	THR
1	5-X	322	LEU
1	5-X	323	VAL
1	5-X	337	ARG
1	5-X	347	ILE
1	5-X	363	SER
1	5-X	375	LEU
1	5-X	392	VAL
1	5-X	397	TYR
1	5-X	413	GLN
1	5-X	420	ARG
1	5-X	428	LEU
1	6-A	602	GLU
1	6-A	2	PRO
1	6-A	8	LEU
1	6-A	10	LYS
1	6-A	24	LEU
1	6-A	39	ASP
1	6-A	50	ASP
1	6-A	59	SER
1	6-A	62	GLU
1	6-A	67	LEU
1	6-A	93	ASP
1	6-A	98	GLU
1	6-A	115	LEU
1	6-A	152	ASP
1	6-A	173	VAL
1	6-A	187	GLN
1	6-A	191	LEU
1	6-A	237	LEU
1	6-A	269	HIS
1	6-A	281	LEU
1	6-A	308	LEU
1	6-A	312	THR
1	6-A	322	LEU
1	6-A	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-A	337	ARG
1	6-A	347	ILE
1	6-A	363	SER
1	6-A	375	LEU
1	6-A	392	VAL
1	6-A	397	TYR
1	6-A	413	GLN
1	6-A	420	ARG
1	6-A	428	LEU
1	6-B	602	GLU
1	6-B	2	PRO
1	6-B	8	LEU
1	6-B	10	LYS
1	6-B	24	LEU
1	6-B	39	ASP
1	6-B	50	ASP
1	6-B	59	SER
1	6-B	62	GLU
1	6-B	67	LEU
1	6-B	93	ASP
1	6-B	98	GLU
1	6-B	115	LEU
1	6-B	152	ASP
1	6-B	173	VAL
1	6-B	187	GLN
1	6-B	191	LEU
1	6-B	237	LEU
1	6-B	269	HIS
1	6-B	281	LEU
1	6-B	308	LEU
1	6-B	312	THR
1	6-B	322	LEU
1	6-B	323	VAL
1	6-B	337	ARG
1	6-B	347	ILE
1	6-B	363	SER
1	6-B	375	LEU
1	6-B	392	VAL
1	6-B	397	TYR
1	6-B	413	GLN
1	6-B	420	ARG
1	6-B	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-C	602	GLU
1	6-C	2	PRO
1	6-C	8	LEU
1	6-C	10	LYS
1	6-C	24	LEU
1	6-C	39	ASP
1	6-C	50	ASP
1	6-C	59	SER
1	6-C	62	GLU
1	6-C	67	LEU
1	6-C	93	ASP
1	6-C	98	GLU
1	6-C	115	LEU
1	6-C	152	ASP
1	6-C	173	VAL
1	6-C	187	GLN
1	6-C	191	LEU
1	6-C	237	LEU
1	6-C	269	HIS
1	6-C	281	LEU
1	6-C	308	LEU
1	6-C	312	THR
1	6-C	322	LEU
1	6-C	323	VAL
1	6-C	337	ARG
1	6-C	347	ILE
1	6-C	363	SER
1	6-C	375	LEU
1	6-C	392	VAL
1	6-C	397	TYR
1	6-C	413	GLN
1	6-C	420	ARG
1	6-C	428	LEU
1	6-D	602	GLU
1	6-D	2	PRO
1	6-D	8	LEU
1	6-D	10	LYS
1	6-D	24	LEU
1	6-D	39	ASP
1	6-D	50	ASP
1	6-D	59	SER
1	6-D	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-D	67	LEU
1	6-D	93	ASP
1	6-D	98	GLU
1	6-D	115	LEU
1	6-D	152	ASP
1	6-D	173	VAL
1	6-D	187	GLN
1	6-D	191	LEU
1	6-D	237	LEU
1	6-D	269	HIS
1	6-D	281	LEU
1	6-D	308	LEU
1	6-D	312	THR
1	6-D	322	LEU
1	6-D	323	VAL
1	6-D	337	ARG
1	6-D	347	ILE
1	6-D	363	SER
1	6-D	375	LEU
1	6-D	392	VAL
1	6-D	397	TYR
1	6-D	413	GLN
1	6-D	420	ARG
1	6-D	428	LEU
1	6-E	602	GLU
1	6-E	2	PRO
1	6-E	8	LEU
1	6-E	10	LYS
1	6-E	24	LEU
1	6-E	39	ASP
1	6-E	50	ASP
1	6-E	59	SER
1	6-E	62	GLU
1	6-E	67	LEU
1	6-E	93	ASP
1	6-E	98	GLU
1	6-E	115	LEU
1	6-E	152	ASP
1	6-E	173	VAL
1	6-E	187	GLN
1	6-E	191	LEU
1	6-E	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-E	269	HIS
1	6-E	281	LEU
1	6-E	308	LEU
1	6-E	312	THR
1	6-E	322	LEU
1	6-E	323	VAL
1	6-E	337	ARG
1	6-E	347	ILE
1	6-E	363	SER
1	6-E	375	LEU
1	6-E	392	VAL
1	6-E	397	TYR
1	6-E	413	GLN
1	6-E	420	ARG
1	6-E	428	LEU
1	6-F	602	GLU
1	6-F	2	PRO
1	6-F	8	LEU
1	6-F	10	LYS
1	6-F	24	LEU
1	6-F	39	ASP
1	6-F	50	ASP
1	6-F	59	SER
1	6-F	62	GLU
1	6-F	67	LEU
1	6-F	93	ASP
1	6-F	98	GLU
1	6-F	115	LEU
1	6-F	152	ASP
1	6-F	173	VAL
1	6-F	187	GLN
1	6-F	191	LEU
1	6-F	237	LEU
1	6-F	269	HIS
1	6-F	281	LEU
1	6-F	308	LEU
1	6-F	312	THR
1	6-F	322	LEU
1	6-F	323	VAL
1	6-F	337	ARG
1	6-F	347	ILE
1	6-F	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-F	375	LEU
1	6-F	392	VAL
1	6-F	397	TYR
1	6-F	413	GLN
1	6-F	420	ARG
1	6-F	428	LEU
1	6-G	602	GLU
1	6-G	2	PRO
1	6-G	8	LEU
1	6-G	10	LYS
1	6-G	24	LEU
1	6-G	39	ASP
1	6-G	50	ASP
1	6-G	59	SER
1	6-G	62	GLU
1	6-G	67	LEU
1	6-G	93	ASP
1	6-G	98	GLU
1	6-G	115	LEU
1	6-G	152	ASP
1	6-G	173	VAL
1	6-G	187	GLN
1	6-G	191	LEU
1	6-G	237	LEU
1	6-G	269	HIS
1	6-G	281	LEU
1	6-G	308	LEU
1	6-G	312	THR
1	6-G	322	LEU
1	6-G	323	VAL
1	6-G	337	ARG
1	6-G	347	ILE
1	6-G	363	SER
1	6-G	375	LEU
1	6-G	392	VAL
1	6-G	397	TYR
1	6-G	413	GLN
1	6-G	420	ARG
1	6-G	428	LEU
1	6-H	602	GLU
1	6-H	2	PRO
1	6-H	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-H	10	LYS
1	6-H	24	LEU
1	6-H	39	ASP
1	6-H	50	ASP
1	6-H	59	SER
1	6-H	62	GLU
1	6-H	67	LEU
1	6-H	93	ASP
1	6-H	98	GLU
1	6-H	115	LEU
1	6-H	152	ASP
1	6-H	173	VAL
1	6-H	187	GLN
1	6-H	191	LEU
1	6-H	237	LEU
1	6-H	269	HIS
1	6-H	281	LEU
1	6-H	308	LEU
1	6-H	312	THR
1	6-H	322	LEU
1	6-H	323	VAL
1	6-H	337	ARG
1	6-H	347	ILE
1	6-H	363	SER
1	6-H	375	LEU
1	6-H	392	VAL
1	6-H	397	TYR
1	6-H	413	GLN
1	6-H	420	ARG
1	6-H	428	LEU
1	6-I	602	GLU
1	6-I	2	PRO
1	6-I	8	LEU
1	6-I	10	LYS
1	6-I	24	LEU
1	6-I	39	ASP
1	6-I	50	ASP
1	6-I	59	SER
1	6-I	62	GLU
1	6-I	67	LEU
1	6-I	93	ASP
1	6-I	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-I	115	LEU
1	6-I	152	ASP
1	6-I	173	VAL
1	6-I	187	GLN
1	6-I	191	LEU
1	6-I	237	LEU
1	6-I	269	HIS
1	6-I	281	LEU
1	6-I	308	LEU
1	6-I	312	THR
1	6-I	322	LEU
1	6-I	323	VAL
1	6-I	337	ARG
1	6-I	347	ILE
1	6-I	363	SER
1	6-I	375	LEU
1	6-I	392	VAL
1	6-I	397	TYR
1	6-I	413	GLN
1	6-I	420	ARG
1	6-I	428	LEU
1	6-J	602	GLU
1	6-J	2	PRO
1	6-J	8	LEU
1	6-J	10	LYS
1	6-J	24	LEU
1	6-J	39	ASP
1	6-J	50	ASP
1	6-J	59	SER
1	6-J	62	GLU
1	6-J	67	LEU
1	6-J	93	ASP
1	6-J	98	GLU
1	6-J	115	LEU
1	6-J	152	ASP
1	6-J	173	VAL
1	6-J	187	GLN
1	6-J	191	LEU
1	6-J	237	LEU
1	6-J	269	HIS
1	6-J	281	LEU
1	6-J	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-J	312	THR
1	6-J	322	LEU
1	6-J	323	VAL
1	6-J	337	ARG
1	6-J	347	ILE
1	6-J	363	SER
1	6-J	375	LEU
1	6-J	392	VAL
1	6-J	397	TYR
1	6-J	413	GLN
1	6-J	420	ARG
1	6-J	428	LEU
1	6-K	602	GLU
1	6-K	2	PRO
1	6-K	8	LEU
1	6-K	10	LYS
1	6-K	24	LEU
1	6-K	39	ASP
1	6-K	50	ASP
1	6-K	59	SER
1	6-K	62	GLU
1	6-K	67	LEU
1	6-K	93	ASP
1	6-K	98	GLU
1	6-K	115	LEU
1	6-K	152	ASP
1	6-K	173	VAL
1	6-K	187	GLN
1	6-K	191	LEU
1	6-K	237	LEU
1	6-K	269	HIS
1	6-K	281	LEU
1	6-K	308	LEU
1	6-K	312	THR
1	6-K	322	LEU
1	6-K	323	VAL
1	6-K	337	ARG
1	6-K	347	ILE
1	6-K	363	SER
1	6-K	375	LEU
1	6-K	392	VAL
1	6-K	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-K	413	GLN
1	6-K	420	ARG
1	6-K	428	LEU
1	6-L	602	GLU
1	6-L	2	PRO
1	6-L	8	LEU
1	6-L	10	LYS
1	6-L	24	LEU
1	6-L	39	ASP
1	6-L	50	ASP
1	6-L	59	SER
1	6-L	62	GLU
1	6-L	67	LEU
1	6-L	93	ASP
1	6-L	98	GLU
1	6-L	115	LEU
1	6-L	152	ASP
1	6-L	173	VAL
1	6-L	187	GLN
1	6-L	191	LEU
1	6-L	237	LEU
1	6-L	269	HIS
1	6-L	281	LEU
1	6-L	308	LEU
1	6-L	312	THR
1	6-L	322	LEU
1	6-L	323	VAL
1	6-L	337	ARG
1	6-L	347	ILE
1	6-L	363	SER
1	6-L	375	LEU
1	6-L	392	VAL
1	6-L	397	TYR
1	6-L	413	GLN
1	6-L	420	ARG
1	6-L	428	LEU
1	6-M	602	GLU
1	6-M	2	PRO
1	6-M	8	LEU
1	6-M	10	LYS
1	6-M	24	LEU
1	6-M	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-M	50	ASP
1	6-M	59	SER
1	6-M	62	GLU
1	6-M	67	LEU
1	6-M	93	ASP
1	6-M	98	GLU
1	6-M	115	LEU
1	6-M	152	ASP
1	6-M	173	VAL
1	6-M	187	GLN
1	6-M	191	LEU
1	6-M	237	LEU
1	6-M	269	HIS
1	6-M	281	LEU
1	6-M	308	LEU
1	6-M	312	THR
1	6-M	322	LEU
1	6-M	323	VAL
1	6-M	337	ARG
1	6-M	347	ILE
1	6-M	363	SER
1	6-M	375	LEU
1	6-M	392	VAL
1	6-M	397	TYR
1	6-M	413	GLN
1	6-M	420	ARG
1	6-M	428	LEU
1	6-N	602	GLU
1	6-N	2	PRO
1	6-N	8	LEU
1	6-N	10	LYS
1	6-N	24	LEU
1	6-N	39	ASP
1	6-N	50	ASP
1	6-N	59	SER
1	6-N	62	GLU
1	6-N	67	LEU
1	6-N	93	ASP
1	6-N	98	GLU
1	6-N	115	LEU
1	6-N	152	ASP
1	6-N	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-N	187	GLN
1	6-N	191	LEU
1	6-N	237	LEU
1	6-N	269	HIS
1	6-N	281	LEU
1	6-N	308	LEU
1	6-N	312	THR
1	6-N	322	LEU
1	6-N	323	VAL
1	6-N	337	ARG
1	6-N	347	ILE
1	6-N	363	SER
1	6-N	375	LEU
1	6-N	392	VAL
1	6-N	397	TYR
1	6-N	413	GLN
1	6-N	420	ARG
1	6-N	428	LEU
1	6-O	602	GLU
1	6-O	2	PRO
1	6-O	8	LEU
1	6-O	10	LYS
1	6-O	24	LEU
1	6-O	39	ASP
1	6-O	50	ASP
1	6-O	59	SER
1	6-O	62	GLU
1	6-O	67	LEU
1	6-O	93	ASP
1	6-O	98	GLU
1	6-O	115	LEU
1	6-O	152	ASP
1	6-O	173	VAL
1	6-O	187	GLN
1	6-O	191	LEU
1	6-O	237	LEU
1	6-O	269	HIS
1	6-O	281	LEU
1	6-O	308	LEU
1	6-O	312	THR
1	6-O	322	LEU
1	6-O	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-O	337	ARG
1	6-O	347	ILE
1	6-O	363	SER
1	6-O	375	LEU
1	6-O	392	VAL
1	6-O	397	TYR
1	6-O	413	GLN
1	6-O	420	ARG
1	6-O	428	LEU
1	6-P	602	GLU
1	6-P	2	PRO
1	6-P	8	LEU
1	6-P	10	LYS
1	6-P	24	LEU
1	6-P	39	ASP
1	6-P	50	ASP
1	6-P	59	SER
1	6-P	62	GLU
1	6-P	67	LEU
1	6-P	93	ASP
1	6-P	98	GLU
1	6-P	115	LEU
1	6-P	152	ASP
1	6-P	173	VAL
1	6-P	187	GLN
1	6-P	191	LEU
1	6-P	237	LEU
1	6-P	269	HIS
1	6-P	281	LEU
1	6-P	308	LEU
1	6-P	312	THR
1	6-P	322	LEU
1	6-P	323	VAL
1	6-P	337	ARG
1	6-P	347	ILE
1	6-P	363	SER
1	6-P	375	LEU
1	6-P	392	VAL
1	6-P	397	TYR
1	6-P	413	GLN
1	6-P	420	ARG
1	6-P	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-Q	602	GLU
1	6-Q	2	PRO
1	6-Q	8	LEU
1	6-Q	10	LYS
1	6-Q	24	LEU
1	6-Q	39	ASP
1	6-Q	50	ASP
1	6-Q	59	SER
1	6-Q	62	GLU
1	6-Q	67	LEU
1	6-Q	93	ASP
1	6-Q	98	GLU
1	6-Q	115	LEU
1	6-Q	152	ASP
1	6-Q	173	VAL
1	6-Q	187	GLN
1	6-Q	191	LEU
1	6-Q	237	LEU
1	6-Q	269	HIS
1	6-Q	281	LEU
1	6-Q	308	LEU
1	6-Q	312	THR
1	6-Q	322	LEU
1	6-Q	323	VAL
1	6-Q	337	ARG
1	6-Q	347	ILE
1	6-Q	363	SER
1	6-Q	375	LEU
1	6-Q	392	VAL
1	6-Q	397	TYR
1	6-Q	413	GLN
1	6-Q	420	ARG
1	6-Q	428	LEU
1	6-R	602	GLU
1	6-R	2	PRO
1	6-R	8	LEU
1	6-R	10	LYS
1	6-R	24	LEU
1	6-R	39	ASP
1	6-R	50	ASP
1	6-R	59	SER
1	6-R	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-R	67	LEU
1	6-R	93	ASP
1	6-R	98	GLU
1	6-R	115	LEU
1	6-R	152	ASP
1	6-R	173	VAL
1	6-R	187	GLN
1	6-R	191	LEU
1	6-R	237	LEU
1	6-R	269	HIS
1	6-R	281	LEU
1	6-R	308	LEU
1	6-R	312	THR
1	6-R	322	LEU
1	6-R	323	VAL
1	6-R	337	ARG
1	6-R	347	ILE
1	6-R	363	SER
1	6-R	375	LEU
1	6-R	392	VAL
1	6-R	397	TYR
1	6-R	413	GLN
1	6-R	420	ARG
1	6-R	428	LEU
1	6-S	602	GLU
1	6-S	2	PRO
1	6-S	8	LEU
1	6-S	10	LYS
1	6-S	24	LEU
1	6-S	39	ASP
1	6-S	50	ASP
1	6-S	59	SER
1	6-S	62	GLU
1	6-S	67	LEU
1	6-S	93	ASP
1	6-S	98	GLU
1	6-S	115	LEU
1	6-S	152	ASP
1	6-S	173	VAL
1	6-S	187	GLN
1	6-S	191	LEU
1	6-S	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-S	269	HIS
1	6-S	281	LEU
1	6-S	308	LEU
1	6-S	312	THR
1	6-S	322	LEU
1	6-S	323	VAL
1	6-S	337	ARG
1	6-S	347	ILE
1	6-S	363	SER
1	6-S	375	LEU
1	6-S	392	VAL
1	6-S	397	TYR
1	6-S	413	GLN
1	6-S	420	ARG
1	6-S	428	LEU
1	6-T	602	GLU
1	6-T	2	PRO
1	6-T	8	LEU
1	6-T	10	LYS
1	6-T	24	LEU
1	6-T	39	ASP
1	6-T	50	ASP
1	6-T	59	SER
1	6-T	62	GLU
1	6-T	67	LEU
1	6-T	93	ASP
1	6-T	98	GLU
1	6-T	115	LEU
1	6-T	152	ASP
1	6-T	173	VAL
1	6-T	187	GLN
1	6-T	191	LEU
1	6-T	237	LEU
1	6-T	269	HIS
1	6-T	281	LEU
1	6-T	308	LEU
1	6-T	312	THR
1	6-T	322	LEU
1	6-T	323	VAL
1	6-T	337	ARG
1	6-T	347	ILE
1	6-T	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-T	375	LEU
1	6-T	392	VAL
1	6-T	397	TYR
1	6-T	413	GLN
1	6-T	420	ARG
1	6-T	428	LEU
1	6-U	602	GLU
1	6-U	2	PRO
1	6-U	8	LEU
1	6-U	10	LYS
1	6-U	24	LEU
1	6-U	39	ASP
1	6-U	50	ASP
1	6-U	59	SER
1	6-U	62	GLU
1	6-U	67	LEU
1	6-U	93	ASP
1	6-U	98	GLU
1	6-U	115	LEU
1	6-U	152	ASP
1	6-U	173	VAL
1	6-U	187	GLN
1	6-U	191	LEU
1	6-U	237	LEU
1	6-U	269	HIS
1	6-U	281	LEU
1	6-U	308	LEU
1	6-U	312	THR
1	6-U	322	LEU
1	6-U	323	VAL
1	6-U	337	ARG
1	6-U	347	ILE
1	6-U	363	SER
1	6-U	375	LEU
1	6-U	392	VAL
1	6-U	397	TYR
1	6-U	413	GLN
1	6-U	420	ARG
1	6-U	428	LEU
1	6-V	602	GLU
1	6-V	2	PRO
1	6-V	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-V	10	LYS
1	6-V	24	LEU
1	6-V	39	ASP
1	6-V	50	ASP
1	6-V	59	SER
1	6-V	62	GLU
1	6-V	67	LEU
1	6-V	93	ASP
1	6-V	98	GLU
1	6-V	115	LEU
1	6-V	152	ASP
1	6-V	173	VAL
1	6-V	187	GLN
1	6-V	191	LEU
1	6-V	237	LEU
1	6-V	269	HIS
1	6-V	281	LEU
1	6-V	308	LEU
1	6-V	312	THR
1	6-V	322	LEU
1	6-V	323	VAL
1	6-V	337	ARG
1	6-V	347	ILE
1	6-V	363	SER
1	6-V	375	LEU
1	6-V	392	VAL
1	6-V	397	TYR
1	6-V	413	GLN
1	6-V	420	ARG
1	6-V	428	LEU
1	6-W	602	GLU
1	6-W	2	PRO
1	6-W	8	LEU
1	6-W	10	LYS
1	6-W	24	LEU
1	6-W	39	ASP
1	6-W	50	ASP
1	6-W	59	SER
1	6-W	62	GLU
1	6-W	67	LEU
1	6-W	93	ASP
1	6-W	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-W	115	LEU
1	6-W	152	ASP
1	6-W	173	VAL
1	6-W	187	GLN
1	6-W	191	LEU
1	6-W	237	LEU
1	6-W	269	HIS
1	6-W	281	LEU
1	6-W	308	LEU
1	6-W	312	THR
1	6-W	322	LEU
1	6-W	323	VAL
1	6-W	337	ARG
1	6-W	347	ILE
1	6-W	363	SER
1	6-W	375	LEU
1	6-W	392	VAL
1	6-W	397	TYR
1	6-W	413	GLN
1	6-W	420	ARG
1	6-W	428	LEU
1	6-X	602	GLU
1	6-X	2	PRO
1	6-X	8	LEU
1	6-X	10	LYS
1	6-X	24	LEU
1	6-X	39	ASP
1	6-X	50	ASP
1	6-X	59	SER
1	6-X	62	GLU
1	6-X	67	LEU
1	6-X	93	ASP
1	6-X	98	GLU
1	6-X	115	LEU
1	6-X	152	ASP
1	6-X	173	VAL
1	6-X	187	GLN
1	6-X	191	LEU
1	6-X	237	LEU
1	6-X	269	HIS
1	6-X	281	LEU
1	6-X	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-X	312	THR
1	6-X	322	LEU
1	6-X	323	VAL
1	6-X	337	ARG
1	6-X	347	ILE
1	6-X	363	SER
1	6-X	375	LEU
1	6-X	392	VAL
1	6-X	397	TYR
1	6-X	413	GLN
1	6-X	420	ARG
1	6-X	428	LEU
1	7-A	602	GLU
1	7-A	2	PRO
1	7-A	8	LEU
1	7-A	10	LYS
1	7-A	24	LEU
1	7-A	39	ASP
1	7-A	50	ASP
1	7-A	59	SER
1	7-A	62	GLU
1	7-A	67	LEU
1	7-A	93	ASP
1	7-A	98	GLU
1	7-A	115	LEU
1	7-A	152	ASP
1	7-A	173	VAL
1	7-A	187	GLN
1	7-A	191	LEU
1	7-A	237	LEU
1	7-A	269	HIS
1	7-A	281	LEU
1	7-A	308	LEU
1	7-A	312	THR
1	7-A	322	LEU
1	7-A	323	VAL
1	7-A	337	ARG
1	7-A	347	ILE
1	7-A	363	SER
1	7-A	375	LEU
1	7-A	392	VAL
1	7-A	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-A	413	GLN
1	7-A	420	ARG
1	7-A	428	LEU
1	7-B	602	GLU
1	7-B	2	PRO
1	7-B	8	LEU
1	7-B	10	LYS
1	7-B	24	LEU
1	7-B	39	ASP
1	7-B	50	ASP
1	7-B	59	SER
1	7-B	62	GLU
1	7-B	67	LEU
1	7-B	93	ASP
1	7-B	98	GLU
1	7-B	115	LEU
1	7-B	152	ASP
1	7-B	173	VAL
1	7-B	187	GLN
1	7-B	191	LEU
1	7-B	237	LEU
1	7-B	269	HIS
1	7-B	281	LEU
1	7-B	308	LEU
1	7-B	312	THR
1	7-B	322	LEU
1	7-B	323	VAL
1	7-B	337	ARG
1	7-B	347	ILE
1	7-B	363	SER
1	7-B	375	LEU
1	7-B	392	VAL
1	7-B	397	TYR
1	7-B	413	GLN
1	7-B	420	ARG
1	7-B	428	LEU
1	7-C	602	GLU
1	7-C	2	PRO
1	7-C	8	LEU
1	7-C	10	LYS
1	7-C	24	LEU
1	7-C	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-C	50	ASP
1	7-C	59	SER
1	7-C	62	GLU
1	7-C	67	LEU
1	7-C	93	ASP
1	7-C	98	GLU
1	7-C	115	LEU
1	7-C	152	ASP
1	7-C	173	VAL
1	7-C	187	GLN
1	7-C	191	LEU
1	7-C	237	LEU
1	7-C	269	HIS
1	7-C	281	LEU
1	7-C	308	LEU
1	7-C	312	THR
1	7-C	322	LEU
1	7-C	323	VAL
1	7-C	337	ARG
1	7-C	347	ILE
1	7-C	363	SER
1	7-C	375	LEU
1	7-C	392	VAL
1	7-C	397	TYR
1	7-C	413	GLN
1	7-C	420	ARG
1	7-C	428	LEU
1	7-D	602	GLU
1	7-D	2	PRO
1	7-D	8	LEU
1	7-D	10	LYS
1	7-D	24	LEU
1	7-D	39	ASP
1	7-D	50	ASP
1	7-D	59	SER
1	7-D	62	GLU
1	7-D	67	LEU
1	7-D	93	ASP
1	7-D	98	GLU
1	7-D	115	LEU
1	7-D	152	ASP
1	7-D	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-D	187	GLN
1	7-D	191	LEU
1	7-D	237	LEU
1	7-D	269	HIS
1	7-D	281	LEU
1	7-D	308	LEU
1	7-D	312	THR
1	7-D	322	LEU
1	7-D	323	VAL
1	7-D	337	ARG
1	7-D	347	ILE
1	7-D	363	SER
1	7-D	375	LEU
1	7-D	392	VAL
1	7-D	397	TYR
1	7-D	413	GLN
1	7-D	420	ARG
1	7-D	428	LEU
1	7-E	602	GLU
1	7-E	2	PRO
1	7-E	8	LEU
1	7-E	10	LYS
1	7-E	24	LEU
1	7-E	39	ASP
1	7-E	50	ASP
1	7-E	59	SER
1	7-E	62	GLU
1	7-E	67	LEU
1	7-E	93	ASP
1	7-E	98	GLU
1	7-E	115	LEU
1	7-E	152	ASP
1	7-E	173	VAL
1	7-E	187	GLN
1	7-E	191	LEU
1	7-E	237	LEU
1	7-E	269	HIS
1	7-E	281	LEU
1	7-E	308	LEU
1	7-E	312	THR
1	7-E	322	LEU
1	7-E	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-E	337	ARG
1	7-E	347	ILE
1	7-E	363	SER
1	7-E	375	LEU
1	7-E	392	VAL
1	7-E	397	TYR
1	7-E	413	GLN
1	7-E	420	ARG
1	7-E	428	LEU
1	7-F	602	GLU
1	7-F	2	PRO
1	7-F	8	LEU
1	7-F	10	LYS
1	7-F	24	LEU
1	7-F	39	ASP
1	7-F	50	ASP
1	7-F	59	SER
1	7-F	62	GLU
1	7-F	67	LEU
1	7-F	93	ASP
1	7-F	98	GLU
1	7-F	115	LEU
1	7-F	152	ASP
1	7-F	173	VAL
1	7-F	187	GLN
1	7-F	191	LEU
1	7-F	237	LEU
1	7-F	269	HIS
1	7-F	281	LEU
1	7-F	308	LEU
1	7-F	312	THR
1	7-F	322	LEU
1	7-F	323	VAL
1	7-F	337	ARG
1	7-F	347	ILE
1	7-F	363	SER
1	7-F	375	LEU
1	7-F	392	VAL
1	7-F	397	TYR
1	7-F	413	GLN
1	7-F	420	ARG
1	7-F	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-G	602	GLU
1	7-G	2	PRO
1	7-G	8	LEU
1	7-G	10	LYS
1	7-G	24	LEU
1	7-G	39	ASP
1	7-G	50	ASP
1	7-G	59	SER
1	7-G	62	GLU
1	7-G	67	LEU
1	7-G	93	ASP
1	7-G	98	GLU
1	7-G	115	LEU
1	7-G	152	ASP
1	7-G	173	VAL
1	7-G	187	GLN
1	7-G	191	LEU
1	7-G	237	LEU
1	7-G	269	HIS
1	7-G	281	LEU
1	7-G	308	LEU
1	7-G	312	THR
1	7-G	322	LEU
1	7-G	323	VAL
1	7-G	337	ARG
1	7-G	347	ILE
1	7-G	363	SER
1	7-G	375	LEU
1	7-G	392	VAL
1	7-G	397	TYR
1	7-G	413	GLN
1	7-G	420	ARG
1	7-G	428	LEU
1	7-H	602	GLU
1	7-H	2	PRO
1	7-H	8	LEU
1	7-H	10	LYS
1	7-H	24	LEU
1	7-H	39	ASP
1	7-H	50	ASP
1	7-H	59	SER
1	7-H	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-H	67	LEU
1	7-H	93	ASP
1	7-H	98	GLU
1	7-H	115	LEU
1	7-H	152	ASP
1	7-H	173	VAL
1	7-H	187	GLN
1	7-H	191	LEU
1	7-H	237	LEU
1	7-H	269	HIS
1	7-H	281	LEU
1	7-H	308	LEU
1	7-H	312	THR
1	7-H	322	LEU
1	7-H	323	VAL
1	7-H	337	ARG
1	7-H	347	ILE
1	7-H	363	SER
1	7-H	375	LEU
1	7-H	392	VAL
1	7-H	397	TYR
1	7-H	413	GLN
1	7-H	420	ARG
1	7-H	428	LEU
1	7-I	602	GLU
1	7-I	2	PRO
1	7-I	8	LEU
1	7-I	10	LYS
1	7-I	24	LEU
1	7-I	39	ASP
1	7-I	50	ASP
1	7-I	59	SER
1	7-I	62	GLU
1	7-I	67	LEU
1	7-I	93	ASP
1	7-I	98	GLU
1	7-I	115	LEU
1	7-I	152	ASP
1	7-I	173	VAL
1	7-I	187	GLN
1	7-I	191	LEU
1	7-I	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-I	269	HIS
1	7-I	281	LEU
1	7-I	308	LEU
1	7-I	312	THR
1	7-I	322	LEU
1	7-I	323	VAL
1	7-I	337	ARG
1	7-I	347	ILE
1	7-I	363	SER
1	7-I	375	LEU
1	7-I	392	VAL
1	7-I	397	TYR
1	7-I	413	GLN
1	7-I	420	ARG
1	7-I	428	LEU
1	7-J	602	GLU
1	7-J	2	PRO
1	7-J	8	LEU
1	7-J	10	LYS
1	7-J	24	LEU
1	7-J	39	ASP
1	7-J	50	ASP
1	7-J	59	SER
1	7-J	62	GLU
1	7-J	67	LEU
1	7-J	93	ASP
1	7-J	98	GLU
1	7-J	115	LEU
1	7-J	152	ASP
1	7-J	173	VAL
1	7-J	187	GLN
1	7-J	191	LEU
1	7-J	237	LEU
1	7-J	269	HIS
1	7-J	281	LEU
1	7-J	308	LEU
1	7-J	312	THR
1	7-J	322	LEU
1	7-J	323	VAL
1	7-J	337	ARG
1	7-J	347	ILE
1	7-J	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-J	375	LEU
1	7-J	392	VAL
1	7-J	397	TYR
1	7-J	413	GLN
1	7-J	420	ARG
1	7-J	428	LEU
1	7-K	602	GLU
1	7-K	2	PRO
1	7-K	8	LEU
1	7-K	10	LYS
1	7-K	24	LEU
1	7-K	39	ASP
1	7-K	50	ASP
1	7-K	59	SER
1	7-K	62	GLU
1	7-K	67	LEU
1	7-K	93	ASP
1	7-K	98	GLU
1	7-K	115	LEU
1	7-K	152	ASP
1	7-K	173	VAL
1	7-K	187	GLN
1	7-K	191	LEU
1	7-K	237	LEU
1	7-K	269	HIS
1	7-K	281	LEU
1	7-K	308	LEU
1	7-K	312	THR
1	7-K	322	LEU
1	7-K	323	VAL
1	7-K	337	ARG
1	7-K	347	ILE
1	7-K	363	SER
1	7-K	375	LEU
1	7-K	392	VAL
1	7-K	397	TYR
1	7-K	413	GLN
1	7-K	420	ARG
1	7-K	428	LEU
1	7-L	602	GLU
1	7-L	2	PRO
1	7-L	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-L	10	LYS
1	7-L	24	LEU
1	7-L	39	ASP
1	7-L	50	ASP
1	7-L	59	SER
1	7-L	62	GLU
1	7-L	67	LEU
1	7-L	93	ASP
1	7-L	98	GLU
1	7-L	115	LEU
1	7-L	152	ASP
1	7-L	173	VAL
1	7-L	187	GLN
1	7-L	191	LEU
1	7-L	237	LEU
1	7-L	269	HIS
1	7-L	281	LEU
1	7-L	308	LEU
1	7-L	312	THR
1	7-L	322	LEU
1	7-L	323	VAL
1	7-L	337	ARG
1	7-L	347	ILE
1	7-L	363	SER
1	7-L	375	LEU
1	7-L	392	VAL
1	7-L	397	TYR
1	7-L	413	GLN
1	7-L	420	ARG
1	7-L	428	LEU
1	7-M	602	GLU
1	7-M	2	PRO
1	7-M	8	LEU
1	7-M	10	LYS
1	7-M	24	LEU
1	7-M	39	ASP
1	7-M	50	ASP
1	7-M	59	SER
1	7-M	62	GLU
1	7-M	67	LEU
1	7-M	93	ASP
1	7-M	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-M	115	LEU
1	7-M	152	ASP
1	7-M	173	VAL
1	7-M	187	GLN
1	7-M	191	LEU
1	7-M	237	LEU
1	7-M	269	HIS
1	7-M	281	LEU
1	7-M	308	LEU
1	7-M	312	THR
1	7-M	322	LEU
1	7-M	323	VAL
1	7-M	337	ARG
1	7-M	347	ILE
1	7-M	363	SER
1	7-M	375	LEU
1	7-M	392	VAL
1	7-M	397	TYR
1	7-M	413	GLN
1	7-M	420	ARG
1	7-M	428	LEU
1	7-N	602	GLU
1	7-N	2	PRO
1	7-N	8	LEU
1	7-N	10	LYS
1	7-N	24	LEU
1	7-N	39	ASP
1	7-N	50	ASP
1	7-N	59	SER
1	7-N	62	GLU
1	7-N	67	LEU
1	7-N	93	ASP
1	7-N	98	GLU
1	7-N	115	LEU
1	7-N	152	ASP
1	7-N	173	VAL
1	7-N	187	GLN
1	7-N	191	LEU
1	7-N	237	LEU
1	7-N	269	HIS
1	7-N	281	LEU
1	7-N	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-N	312	THR
1	7-N	322	LEU
1	7-N	323	VAL
1	7-N	337	ARG
1	7-N	347	ILE
1	7-N	363	SER
1	7-N	375	LEU
1	7-N	392	VAL
1	7-N	397	TYR
1	7-N	413	GLN
1	7-N	420	ARG
1	7-N	428	LEU
1	7-O	602	GLU
1	7-O	2	PRO
1	7-O	8	LEU
1	7-O	10	LYS
1	7-O	24	LEU
1	7-O	39	ASP
1	7-O	50	ASP
1	7-O	59	SER
1	7-O	62	GLU
1	7-O	67	LEU
1	7-O	93	ASP
1	7-O	98	GLU
1	7-O	115	LEU
1	7-O	152	ASP
1	7-O	173	VAL
1	7-O	187	GLN
1	7-O	191	LEU
1	7-O	237	LEU
1	7-O	269	HIS
1	7-O	281	LEU
1	7-O	308	LEU
1	7-O	312	THR
1	7-O	322	LEU
1	7-O	323	VAL
1	7-O	337	ARG
1	7-O	347	ILE
1	7-O	363	SER
1	7-O	375	LEU
1	7-O	392	VAL
1	7-O	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-O	413	GLN
1	7-O	420	ARG
1	7-O	428	LEU
1	7-P	602	GLU
1	7-P	2	PRO
1	7-P	8	LEU
1	7-P	10	LYS
1	7-P	24	LEU
1	7-P	39	ASP
1	7-P	50	ASP
1	7-P	59	SER
1	7-P	62	GLU
1	7-P	67	LEU
1	7-P	93	ASP
1	7-P	98	GLU
1	7-P	115	LEU
1	7-P	152	ASP
1	7-P	173	VAL
1	7-P	187	GLN
1	7-P	191	LEU
1	7-P	237	LEU
1	7-P	269	HIS
1	7-P	281	LEU
1	7-P	308	LEU
1	7-P	312	THR
1	7-P	322	LEU
1	7-P	323	VAL
1	7-P	337	ARG
1	7-P	347	ILE
1	7-P	363	SER
1	7-P	375	LEU
1	7-P	392	VAL
1	7-P	397	TYR
1	7-P	413	GLN
1	7-P	420	ARG
1	7-P	428	LEU
1	7-Q	602	GLU
1	7-Q	2	PRO
1	7-Q	8	LEU
1	7-Q	10	LYS
1	7-Q	24	LEU
1	7-Q	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-Q	50	ASP
1	7-Q	59	SER
1	7-Q	62	GLU
1	7-Q	67	LEU
1	7-Q	93	ASP
1	7-Q	98	GLU
1	7-Q	115	LEU
1	7-Q	152	ASP
1	7-Q	173	VAL
1	7-Q	187	GLN
1	7-Q	191	LEU
1	7-Q	237	LEU
1	7-Q	269	HIS
1	7-Q	281	LEU
1	7-Q	308	LEU
1	7-Q	312	THR
1	7-Q	322	LEU
1	7-Q	323	VAL
1	7-Q	337	ARG
1	7-Q	347	ILE
1	7-Q	363	SER
1	7-Q	375	LEU
1	7-Q	392	VAL
1	7-Q	397	TYR
1	7-Q	413	GLN
1	7-Q	420	ARG
1	7-Q	428	LEU
1	7-R	602	GLU
1	7-R	2	PRO
1	7-R	8	LEU
1	7-R	10	LYS
1	7-R	24	LEU
1	7-R	39	ASP
1	7-R	50	ASP
1	7-R	59	SER
1	7-R	62	GLU
1	7-R	67	LEU
1	7-R	93	ASP
1	7-R	98	GLU
1	7-R	115	LEU
1	7-R	152	ASP
1	7-R	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-R	187	GLN
1	7-R	191	LEU
1	7-R	237	LEU
1	7-R	269	HIS
1	7-R	281	LEU
1	7-R	308	LEU
1	7-R	312	THR
1	7-R	322	LEU
1	7-R	323	VAL
1	7-R	337	ARG
1	7-R	347	ILE
1	7-R	363	SER
1	7-R	375	LEU
1	7-R	392	VAL
1	7-R	397	TYR
1	7-R	413	GLN
1	7-R	420	ARG
1	7-R	428	LEU
1	7-S	602	GLU
1	7-S	2	PRO
1	7-S	8	LEU
1	7-S	10	LYS
1	7-S	24	LEU
1	7-S	39	ASP
1	7-S	50	ASP
1	7-S	59	SER
1	7-S	62	GLU
1	7-S	67	LEU
1	7-S	93	ASP
1	7-S	98	GLU
1	7-S	115	LEU
1	7-S	152	ASP
1	7-S	173	VAL
1	7-S	187	GLN
1	7-S	191	LEU
1	7-S	237	LEU
1	7-S	269	HIS
1	7-S	281	LEU
1	7-S	308	LEU
1	7-S	312	THR
1	7-S	322	LEU
1	7-S	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-S	337	ARG
1	7-S	347	ILE
1	7-S	363	SER
1	7-S	375	LEU
1	7-S	392	VAL
1	7-S	397	TYR
1	7-S	413	GLN
1	7-S	420	ARG
1	7-S	428	LEU
1	7-T	602	GLU
1	7-T	2	PRO
1	7-T	8	LEU
1	7-T	10	LYS
1	7-T	24	LEU
1	7-T	39	ASP
1	7-T	50	ASP
1	7-T	59	SER
1	7-T	62	GLU
1	7-T	67	LEU
1	7-T	93	ASP
1	7-T	98	GLU
1	7-T	115	LEU
1	7-T	152	ASP
1	7-T	173	VAL
1	7-T	187	GLN
1	7-T	191	LEU
1	7-T	237	LEU
1	7-T	269	HIS
1	7-T	281	LEU
1	7-T	308	LEU
1	7-T	312	THR
1	7-T	322	LEU
1	7-T	323	VAL
1	7-T	337	ARG
1	7-T	347	ILE
1	7-T	363	SER
1	7-T	375	LEU
1	7-T	392	VAL
1	7-T	397	TYR
1	7-T	413	GLN
1	7-T	420	ARG
1	7-T	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-U	602	GLU
1	7-U	2	PRO
1	7-U	8	LEU
1	7-U	10	LYS
1	7-U	24	LEU
1	7-U	39	ASP
1	7-U	50	ASP
1	7-U	59	SER
1	7-U	62	GLU
1	7-U	67	LEU
1	7-U	93	ASP
1	7-U	98	GLU
1	7-U	115	LEU
1	7-U	152	ASP
1	7-U	173	VAL
1	7-U	187	GLN
1	7-U	191	LEU
1	7-U	237	LEU
1	7-U	269	HIS
1	7-U	281	LEU
1	7-U	308	LEU
1	7-U	312	THR
1	7-U	322	LEU
1	7-U	323	VAL
1	7-U	337	ARG
1	7-U	347	ILE
1	7-U	363	SER
1	7-U	375	LEU
1	7-U	392	VAL
1	7-U	397	TYR
1	7-U	413	GLN
1	7-U	420	ARG
1	7-U	428	LEU
1	7-V	602	GLU
1	7-V	2	PRO
1	7-V	8	LEU
1	7-V	10	LYS
1	7-V	24	LEU
1	7-V	39	ASP
1	7-V	50	ASP
1	7-V	59	SER
1	7-V	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-V	67	LEU
1	7-V	93	ASP
1	7-V	98	GLU
1	7-V	115	LEU
1	7-V	152	ASP
1	7-V	173	VAL
1	7-V	187	GLN
1	7-V	191	LEU
1	7-V	237	LEU
1	7-V	269	HIS
1	7-V	281	LEU
1	7-V	308	LEU
1	7-V	312	THR
1	7-V	322	LEU
1	7-V	323	VAL
1	7-V	337	ARG
1	7-V	347	ILE
1	7-V	363	SER
1	7-V	375	LEU
1	7-V	392	VAL
1	7-V	397	TYR
1	7-V	413	GLN
1	7-V	420	ARG
1	7-V	428	LEU
1	7-W	602	GLU
1	7-W	2	PRO
1	7-W	8	LEU
1	7-W	10	LYS
1	7-W	24	LEU
1	7-W	39	ASP
1	7-W	50	ASP
1	7-W	59	SER
1	7-W	62	GLU
1	7-W	67	LEU
1	7-W	93	ASP
1	7-W	98	GLU
1	7-W	115	LEU
1	7-W	152	ASP
1	7-W	173	VAL
1	7-W	187	GLN
1	7-W	191	LEU
1	7-W	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-W	269	HIS
1	7-W	281	LEU
1	7-W	308	LEU
1	7-W	312	THR
1	7-W	322	LEU
1	7-W	323	VAL
1	7-W	337	ARG
1	7-W	347	ILE
1	7-W	363	SER
1	7-W	375	LEU
1	7-W	392	VAL
1	7-W	397	TYR
1	7-W	413	GLN
1	7-W	420	ARG
1	7-W	428	LEU
1	7-X	602	GLU
1	7-X	2	PRO
1	7-X	8	LEU
1	7-X	10	LYS
1	7-X	24	LEU
1	7-X	39	ASP
1	7-X	50	ASP
1	7-X	59	SER
1	7-X	62	GLU
1	7-X	67	LEU
1	7-X	93	ASP
1	7-X	98	GLU
1	7-X	115	LEU
1	7-X	152	ASP
1	7-X	173	VAL
1	7-X	187	GLN
1	7-X	191	LEU
1	7-X	237	LEU
1	7-X	269	HIS
1	7-X	281	LEU
1	7-X	308	LEU
1	7-X	312	THR
1	7-X	322	LEU
1	7-X	323	VAL
1	7-X	337	ARG
1	7-X	347	ILE
1	7-X	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-X	375	LEU
1	7-X	392	VAL
1	7-X	397	TYR
1	7-X	413	GLN
1	7-X	420	ARG
1	7-X	428	LEU
1	8-A	602	GLU
1	8-A	2	PRO
1	8-A	8	LEU
1	8-A	10	LYS
1	8-A	24	LEU
1	8-A	39	ASP
1	8-A	50	ASP
1	8-A	59	SER
1	8-A	62	GLU
1	8-A	67	LEU
1	8-A	93	ASP
1	8-A	98	GLU
1	8-A	115	LEU
1	8-A	152	ASP
1	8-A	173	VAL
1	8-A	187	GLN
1	8-A	191	LEU
1	8-A	237	LEU
1	8-A	269	HIS
1	8-A	281	LEU
1	8-A	308	LEU
1	8-A	312	THR
1	8-A	322	LEU
1	8-A	323	VAL
1	8-A	337	ARG
1	8-A	347	ILE
1	8-A	363	SER
1	8-A	375	LEU
1	8-A	392	VAL
1	8-A	397	TYR
1	8-A	413	GLN
1	8-A	420	ARG
1	8-A	428	LEU
1	8-B	602	GLU
1	8-B	2	PRO
1	8-B	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-B	10	LYS
1	8-B	24	LEU
1	8-B	39	ASP
1	8-B	50	ASP
1	8-B	59	SER
1	8-B	62	GLU
1	8-B	67	LEU
1	8-B	93	ASP
1	8-B	98	GLU
1	8-B	115	LEU
1	8-B	152	ASP
1	8-B	173	VAL
1	8-B	187	GLN
1	8-B	191	LEU
1	8-B	237	LEU
1	8-B	269	HIS
1	8-B	281	LEU
1	8-B	308	LEU
1	8-B	312	THR
1	8-B	322	LEU
1	8-B	323	VAL
1	8-B	337	ARG
1	8-B	347	ILE
1	8-B	363	SER
1	8-B	375	LEU
1	8-B	392	VAL
1	8-B	397	TYR
1	8-B	413	GLN
1	8-B	420	ARG
1	8-B	428	LEU
1	8-C	602	GLU
1	8-C	2	PRO
1	8-C	8	LEU
1	8-C	10	LYS
1	8-C	24	LEU
1	8-C	39	ASP
1	8-C	50	ASP
1	8-C	59	SER
1	8-C	62	GLU
1	8-C	67	LEU
1	8-C	93	ASP
1	8-C	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-C	115	LEU
1	8-C	152	ASP
1	8-C	173	VAL
1	8-C	187	GLN
1	8-C	191	LEU
1	8-C	237	LEU
1	8-C	269	HIS
1	8-C	281	LEU
1	8-C	308	LEU
1	8-C	312	THR
1	8-C	322	LEU
1	8-C	323	VAL
1	8-C	337	ARG
1	8-C	347	ILE
1	8-C	363	SER
1	8-C	375	LEU
1	8-C	392	VAL
1	8-C	397	TYR
1	8-C	413	GLN
1	8-C	420	ARG
1	8-C	428	LEU
1	8-D	602	GLU
1	8-D	2	PRO
1	8-D	8	LEU
1	8-D	10	LYS
1	8-D	24	LEU
1	8-D	39	ASP
1	8-D	50	ASP
1	8-D	59	SER
1	8-D	62	GLU
1	8-D	67	LEU
1	8-D	93	ASP
1	8-D	98	GLU
1	8-D	115	LEU
1	8-D	152	ASP
1	8-D	173	VAL
1	8-D	187	GLN
1	8-D	191	LEU
1	8-D	237	LEU
1	8-D	269	HIS
1	8-D	281	LEU
1	8-D	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-D	312	THR
1	8-D	322	LEU
1	8-D	323	VAL
1	8-D	337	ARG
1	8-D	347	ILE
1	8-D	363	SER
1	8-D	375	LEU
1	8-D	392	VAL
1	8-D	397	TYR
1	8-D	413	GLN
1	8-D	420	ARG
1	8-D	428	LEU
1	8-E	602	GLU
1	8-E	2	PRO
1	8-E	8	LEU
1	8-E	10	LYS
1	8-E	24	LEU
1	8-E	39	ASP
1	8-E	50	ASP
1	8-E	59	SER
1	8-E	62	GLU
1	8-E	67	LEU
1	8-E	93	ASP
1	8-E	98	GLU
1	8-E	115	LEU
1	8-E	152	ASP
1	8-E	173	VAL
1	8-E	187	GLN
1	8-E	191	LEU
1	8-E	237	LEU
1	8-E	269	HIS
1	8-E	281	LEU
1	8-E	308	LEU
1	8-E	312	THR
1	8-E	322	LEU
1	8-E	323	VAL
1	8-E	337	ARG
1	8-E	347	ILE
1	8-E	363	SER
1	8-E	375	LEU
1	8-E	392	VAL
1	8-E	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-E	413	GLN
1	8-E	420	ARG
1	8-E	428	LEU
1	8-F	602	GLU
1	8-F	2	PRO
1	8-F	8	LEU
1	8-F	10	LYS
1	8-F	24	LEU
1	8-F	39	ASP
1	8-F	50	ASP
1	8-F	59	SER
1	8-F	62	GLU
1	8-F	67	LEU
1	8-F	93	ASP
1	8-F	98	GLU
1	8-F	115	LEU
1	8-F	152	ASP
1	8-F	173	VAL
1	8-F	187	GLN
1	8-F	191	LEU
1	8-F	237	LEU
1	8-F	269	HIS
1	8-F	281	LEU
1	8-F	308	LEU
1	8-F	312	THR
1	8-F	322	LEU
1	8-F	323	VAL
1	8-F	337	ARG
1	8-F	347	ILE
1	8-F	363	SER
1	8-F	375	LEU
1	8-F	392	VAL
1	8-F	397	TYR
1	8-F	413	GLN
1	8-F	420	ARG
1	8-F	428	LEU
1	8-G	602	GLU
1	8-G	2	PRO
1	8-G	8	LEU
1	8-G	10	LYS
1	8-G	24	LEU
1	8-G	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-G	50	ASP
1	8-G	59	SER
1	8-G	62	GLU
1	8-G	67	LEU
1	8-G	93	ASP
1	8-G	98	GLU
1	8-G	115	LEU
1	8-G	152	ASP
1	8-G	173	VAL
1	8-G	187	GLN
1	8-G	191	LEU
1	8-G	237	LEU
1	8-G	269	HIS
1	8-G	281	LEU
1	8-G	308	LEU
1	8-G	312	THR
1	8-G	322	LEU
1	8-G	323	VAL
1	8-G	337	ARG
1	8-G	347	ILE
1	8-G	363	SER
1	8-G	375	LEU
1	8-G	392	VAL
1	8-G	397	TYR
1	8-G	413	GLN
1	8-G	420	ARG
1	8-G	428	LEU
1	8-H	602	GLU
1	8-H	2	PRO
1	8-H	8	LEU
1	8-H	10	LYS
1	8-H	24	LEU
1	8-H	39	ASP
1	8-H	50	ASP
1	8-H	59	SER
1	8-H	62	GLU
1	8-H	67	LEU
1	8-H	93	ASP
1	8-H	98	GLU
1	8-H	115	LEU
1	8-H	152	ASP
1	8-H	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-H	187	GLN
1	8-H	191	LEU
1	8-H	237	LEU
1	8-H	269	HIS
1	8-H	281	LEU
1	8-H	308	LEU
1	8-H	312	THR
1	8-H	322	LEU
1	8-H	323	VAL
1	8-H	337	ARG
1	8-H	347	ILE
1	8-H	363	SER
1	8-H	375	LEU
1	8-H	392	VAL
1	8-H	397	TYR
1	8-H	413	GLN
1	8-H	420	ARG
1	8-H	428	LEU
1	8-I	602	GLU
1	8-I	2	PRO
1	8-I	8	LEU
1	8-I	10	LYS
1	8-I	24	LEU
1	8-I	39	ASP
1	8-I	50	ASP
1	8-I	59	SER
1	8-I	62	GLU
1	8-I	67	LEU
1	8-I	93	ASP
1	8-I	98	GLU
1	8-I	115	LEU
1	8-I	152	ASP
1	8-I	173	VAL
1	8-I	187	GLN
1	8-I	191	LEU
1	8-I	237	LEU
1	8-I	269	HIS
1	8-I	281	LEU
1	8-I	308	LEU
1	8-I	312	THR
1	8-I	322	LEU
1	8-I	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-I	337	ARG
1	8-I	347	ILE
1	8-I	363	SER
1	8-I	375	LEU
1	8-I	392	VAL
1	8-I	397	TYR
1	8-I	413	GLN
1	8-I	420	ARG
1	8-I	428	LEU
1	8-J	602	GLU
1	8-J	2	PRO
1	8-J	8	LEU
1	8-J	10	LYS
1	8-J	24	LEU
1	8-J	39	ASP
1	8-J	50	ASP
1	8-J	59	SER
1	8-J	62	GLU
1	8-J	67	LEU
1	8-J	93	ASP
1	8-J	98	GLU
1	8-J	115	LEU
1	8-J	152	ASP
1	8-J	173	VAL
1	8-J	187	GLN
1	8-J	191	LEU
1	8-J	237	LEU
1	8-J	269	HIS
1	8-J	281	LEU
1	8-J	308	LEU
1	8-J	312	THR
1	8-J	322	LEU
1	8-J	323	VAL
1	8-J	337	ARG
1	8-J	347	ILE
1	8-J	363	SER
1	8-J	375	LEU
1	8-J	392	VAL
1	8-J	397	TYR
1	8-J	413	GLN
1	8-J	420	ARG
1	8-J	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-K	602	GLU
1	8-K	2	PRO
1	8-K	8	LEU
1	8-K	10	LYS
1	8-K	24	LEU
1	8-K	39	ASP
1	8-K	50	ASP
1	8-K	59	SER
1	8-K	62	GLU
1	8-K	67	LEU
1	8-K	93	ASP
1	8-K	98	GLU
1	8-K	115	LEU
1	8-K	152	ASP
1	8-K	173	VAL
1	8-K	187	GLN
1	8-K	191	LEU
1	8-K	237	LEU
1	8-K	269	HIS
1	8-K	281	LEU
1	8-K	308	LEU
1	8-K	312	THR
1	8-K	322	LEU
1	8-K	323	VAL
1	8-K	337	ARG
1	8-K	347	ILE
1	8-K	363	SER
1	8-K	375	LEU
1	8-K	392	VAL
1	8-K	397	TYR
1	8-K	413	GLN
1	8-K	420	ARG
1	8-K	428	LEU
1	8-L	602	GLU
1	8-L	2	PRO
1	8-L	8	LEU
1	8-L	10	LYS
1	8-L	24	LEU
1	8-L	39	ASP
1	8-L	50	ASP
1	8-L	59	SER
1	8-L	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-L	67	LEU
1	8-L	93	ASP
1	8-L	98	GLU
1	8-L	115	LEU
1	8-L	152	ASP
1	8-L	173	VAL
1	8-L	187	GLN
1	8-L	191	LEU
1	8-L	237	LEU
1	8-L	269	HIS
1	8-L	281	LEU
1	8-L	308	LEU
1	8-L	312	THR
1	8-L	322	LEU
1	8-L	323	VAL
1	8-L	337	ARG
1	8-L	347	ILE
1	8-L	363	SER
1	8-L	375	LEU
1	8-L	392	VAL
1	8-L	397	TYR
1	8-L	413	GLN
1	8-L	420	ARG
1	8-L	428	LEU
1	8-M	602	GLU
1	8-M	2	PRO
1	8-M	8	LEU
1	8-M	10	LYS
1	8-M	24	LEU
1	8-M	39	ASP
1	8-M	50	ASP
1	8-M	59	SER
1	8-M	62	GLU
1	8-M	67	LEU
1	8-M	93	ASP
1	8-M	98	GLU
1	8-M	115	LEU
1	8-M	152	ASP
1	8-M	173	VAL
1	8-M	187	GLN
1	8-M	191	LEU
1	8-M	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-M	269	HIS
1	8-M	281	LEU
1	8-M	308	LEU
1	8-M	312	THR
1	8-M	322	LEU
1	8-M	323	VAL
1	8-M	337	ARG
1	8-M	347	ILE
1	8-M	363	SER
1	8-M	375	LEU
1	8-M	392	VAL
1	8-M	397	TYR
1	8-M	413	GLN
1	8-M	420	ARG
1	8-M	428	LEU
1	8-N	602	GLU
1	8-N	2	PRO
1	8-N	8	LEU
1	8-N	10	LYS
1	8-N	24	LEU
1	8-N	39	ASP
1	8-N	50	ASP
1	8-N	59	SER
1	8-N	62	GLU
1	8-N	67	LEU
1	8-N	93	ASP
1	8-N	98	GLU
1	8-N	115	LEU
1	8-N	152	ASP
1	8-N	173	VAL
1	8-N	187	GLN
1	8-N	191	LEU
1	8-N	237	LEU
1	8-N	269	HIS
1	8-N	281	LEU
1	8-N	308	LEU
1	8-N	312	THR
1	8-N	322	LEU
1	8-N	323	VAL
1	8-N	337	ARG
1	8-N	347	ILE
1	8-N	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-N	375	LEU
1	8-N	392	VAL
1	8-N	397	TYR
1	8-N	413	GLN
1	8-N	420	ARG
1	8-N	428	LEU
1	8-O	602	GLU
1	8-O	2	PRO
1	8-O	8	LEU
1	8-O	10	LYS
1	8-O	24	LEU
1	8-O	39	ASP
1	8-O	50	ASP
1	8-O	59	SER
1	8-O	62	GLU
1	8-O	67	LEU
1	8-O	93	ASP
1	8-O	98	GLU
1	8-O	115	LEU
1	8-O	152	ASP
1	8-O	173	VAL
1	8-O	187	GLN
1	8-O	191	LEU
1	8-O	237	LEU
1	8-O	269	HIS
1	8-O	281	LEU
1	8-O	308	LEU
1	8-O	312	THR
1	8-O	322	LEU
1	8-O	323	VAL
1	8-O	337	ARG
1	8-O	347	ILE
1	8-O	363	SER
1	8-O	375	LEU
1	8-O	392	VAL
1	8-O	397	TYR
1	8-O	413	GLN
1	8-O	420	ARG
1	8-O	428	LEU
1	8-P	602	GLU
1	8-P	2	PRO
1	8-P	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-P	10	LYS
1	8-P	24	LEU
1	8-P	39	ASP
1	8-P	50	ASP
1	8-P	59	SER
1	8-P	62	GLU
1	8-P	67	LEU
1	8-P	93	ASP
1	8-P	98	GLU
1	8-P	115	LEU
1	8-P	152	ASP
1	8-P	173	VAL
1	8-P	187	GLN
1	8-P	191	LEU
1	8-P	237	LEU
1	8-P	269	HIS
1	8-P	281	LEU
1	8-P	308	LEU
1	8-P	312	THR
1	8-P	322	LEU
1	8-P	323	VAL
1	8-P	337	ARG
1	8-P	347	ILE
1	8-P	363	SER
1	8-P	375	LEU
1	8-P	392	VAL
1	8-P	397	TYR
1	8-P	413	GLN
1	8-P	420	ARG
1	8-P	428	LEU
1	8-Q	602	GLU
1	8-Q	2	PRO
1	8-Q	8	LEU
1	8-Q	10	LYS
1	8-Q	24	LEU
1	8-Q	39	ASP
1	8-Q	50	ASP
1	8-Q	59	SER
1	8-Q	62	GLU
1	8-Q	67	LEU
1	8-Q	93	ASP
1	8-Q	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-Q	115	LEU
1	8-Q	152	ASP
1	8-Q	173	VAL
1	8-Q	187	GLN
1	8-Q	191	LEU
1	8-Q	237	LEU
1	8-Q	269	HIS
1	8-Q	281	LEU
1	8-Q	308	LEU
1	8-Q	312	THR
1	8-Q	322	LEU
1	8-Q	323	VAL
1	8-Q	337	ARG
1	8-Q	347	ILE
1	8-Q	363	SER
1	8-Q	375	LEU
1	8-Q	392	VAL
1	8-Q	397	TYR
1	8-Q	413	GLN
1	8-Q	420	ARG
1	8-Q	428	LEU
1	8-R	602	GLU
1	8-R	2	PRO
1	8-R	8	LEU
1	8-R	10	LYS
1	8-R	24	LEU
1	8-R	39	ASP
1	8-R	50	ASP
1	8-R	59	SER
1	8-R	62	GLU
1	8-R	67	LEU
1	8-R	93	ASP
1	8-R	98	GLU
1	8-R	115	LEU
1	8-R	152	ASP
1	8-R	173	VAL
1	8-R	187	GLN
1	8-R	191	LEU
1	8-R	237	LEU
1	8-R	269	HIS
1	8-R	281	LEU
1	8-R	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-R	312	THR
1	8-R	322	LEU
1	8-R	323	VAL
1	8-R	337	ARG
1	8-R	347	ILE
1	8-R	363	SER
1	8-R	375	LEU
1	8-R	392	VAL
1	8-R	397	TYR
1	8-R	413	GLN
1	8-R	420	ARG
1	8-R	428	LEU
1	8-S	602	GLU
1	8-S	2	PRO
1	8-S	8	LEU
1	8-S	10	LYS
1	8-S	24	LEU
1	8-S	39	ASP
1	8-S	50	ASP
1	8-S	59	SER
1	8-S	62	GLU
1	8-S	67	LEU
1	8-S	93	ASP
1	8-S	98	GLU
1	8-S	115	LEU
1	8-S	152	ASP
1	8-S	173	VAL
1	8-S	187	GLN
1	8-S	191	LEU
1	8-S	237	LEU
1	8-S	269	HIS
1	8-S	281	LEU
1	8-S	308	LEU
1	8-S	312	THR
1	8-S	322	LEU
1	8-S	323	VAL
1	8-S	337	ARG
1	8-S	347	ILE
1	8-S	363	SER
1	8-S	375	LEU
1	8-S	392	VAL
1	8-S	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-S	413	GLN
1	8-S	420	ARG
1	8-S	428	LEU
1	8-T	602	GLU
1	8-T	2	PRO
1	8-T	8	LEU
1	8-T	10	LYS
1	8-T	24	LEU
1	8-T	39	ASP
1	8-T	50	ASP
1	8-T	59	SER
1	8-T	62	GLU
1	8-T	67	LEU
1	8-T	93	ASP
1	8-T	98	GLU
1	8-T	115	LEU
1	8-T	152	ASP
1	8-T	173	VAL
1	8-T	187	GLN
1	8-T	191	LEU
1	8-T	237	LEU
1	8-T	269	HIS
1	8-T	281	LEU
1	8-T	308	LEU
1	8-T	312	THR
1	8-T	322	LEU
1	8-T	323	VAL
1	8-T	337	ARG
1	8-T	347	ILE
1	8-T	363	SER
1	8-T	375	LEU
1	8-T	392	VAL
1	8-T	397	TYR
1	8-T	413	GLN
1	8-T	420	ARG
1	8-T	428	LEU
1	8-U	602	GLU
1	8-U	2	PRO
1	8-U	8	LEU
1	8-U	10	LYS
1	8-U	24	LEU
1	8-U	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-U	50	ASP
1	8-U	59	SER
1	8-U	62	GLU
1	8-U	67	LEU
1	8-U	93	ASP
1	8-U	98	GLU
1	8-U	115	LEU
1	8-U	152	ASP
1	8-U	173	VAL
1	8-U	187	GLN
1	8-U	191	LEU
1	8-U	237	LEU
1	8-U	269	HIS
1	8-U	281	LEU
1	8-U	308	LEU
1	8-U	312	THR
1	8-U	322	LEU
1	8-U	323	VAL
1	8-U	337	ARG
1	8-U	347	ILE
1	8-U	363	SER
1	8-U	375	LEU
1	8-U	392	VAL
1	8-U	397	TYR
1	8-U	413	GLN
1	8-U	420	ARG
1	8-U	428	LEU
1	8-V	602	GLU
1	8-V	2	PRO
1	8-V	8	LEU
1	8-V	10	LYS
1	8-V	24	LEU
1	8-V	39	ASP
1	8-V	50	ASP
1	8-V	59	SER
1	8-V	62	GLU
1	8-V	67	LEU
1	8-V	93	ASP
1	8-V	98	GLU
1	8-V	115	LEU
1	8-V	152	ASP
1	8-V	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-V	187	GLN
1	8-V	191	LEU
1	8-V	237	LEU
1	8-V	269	HIS
1	8-V	281	LEU
1	8-V	308	LEU
1	8-V	312	THR
1	8-V	322	LEU
1	8-V	323	VAL
1	8-V	337	ARG
1	8-V	347	ILE
1	8-V	363	SER
1	8-V	375	LEU
1	8-V	392	VAL
1	8-V	397	TYR
1	8-V	413	GLN
1	8-V	420	ARG
1	8-V	428	LEU
1	8-W	602	GLU
1	8-W	2	PRO
1	8-W	8	LEU
1	8-W	10	LYS
1	8-W	24	LEU
1	8-W	39	ASP
1	8-W	50	ASP
1	8-W	59	SER
1	8-W	62	GLU
1	8-W	67	LEU
1	8-W	93	ASP
1	8-W	98	GLU
1	8-W	115	LEU
1	8-W	152	ASP
1	8-W	173	VAL
1	8-W	187	GLN
1	8-W	191	LEU
1	8-W	237	LEU
1	8-W	269	HIS
1	8-W	281	LEU
1	8-W	308	LEU
1	8-W	312	THR
1	8-W	322	LEU
1	8-W	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-W	337	ARG
1	8-W	347	ILE
1	8-W	363	SER
1	8-W	375	LEU
1	8-W	392	VAL
1	8-W	397	TYR
1	8-W	413	GLN
1	8-W	420	ARG
1	8-W	428	LEU
1	8-X	602	GLU
1	8-X	2	PRO
1	8-X	8	LEU
1	8-X	10	LYS
1	8-X	24	LEU
1	8-X	39	ASP
1	8-X	50	ASP
1	8-X	59	SER
1	8-X	62	GLU
1	8-X	67	LEU
1	8-X	93	ASP
1	8-X	98	GLU
1	8-X	115	LEU
1	8-X	152	ASP
1	8-X	173	VAL
1	8-X	187	GLN
1	8-X	191	LEU
1	8-X	237	LEU
1	8-X	269	HIS
1	8-X	281	LEU
1	8-X	308	LEU
1	8-X	312	THR
1	8-X	322	LEU
1	8-X	323	VAL
1	8-X	337	ARG
1	8-X	347	ILE
1	8-X	363	SER
1	8-X	375	LEU
1	8-X	392	VAL
1	8-X	397	TYR
1	8-X	413	GLN
1	8-X	420	ARG
1	8-X	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-A	602	GLU
1	9-A	2	PRO
1	9-A	8	LEU
1	9-A	10	LYS
1	9-A	24	LEU
1	9-A	39	ASP
1	9-A	50	ASP
1	9-A	59	SER
1	9-A	62	GLU
1	9-A	67	LEU
1	9-A	93	ASP
1	9-A	98	GLU
1	9-A	115	LEU
1	9-A	152	ASP
1	9-A	173	VAL
1	9-A	187	GLN
1	9-A	191	LEU
1	9-A	237	LEU
1	9-A	269	HIS
1	9-A	281	LEU
1	9-A	308	LEU
1	9-A	312	THR
1	9-A	322	LEU
1	9-A	323	VAL
1	9-A	337	ARG
1	9-A	347	ILE
1	9-A	363	SER
1	9-A	375	LEU
1	9-A	392	VAL
1	9-A	397	TYR
1	9-A	413	GLN
1	9-A	420	ARG
1	9-A	428	LEU
1	9-B	602	GLU
1	9-B	2	PRO
1	9-B	8	LEU
1	9-B	10	LYS
1	9-B	24	LEU
1	9-B	39	ASP
1	9-B	50	ASP
1	9-B	59	SER
1	9-B	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-B	67	LEU
1	9-B	93	ASP
1	9-B	98	GLU
1	9-B	115	LEU
1	9-B	152	ASP
1	9-B	173	VAL
1	9-B	187	GLN
1	9-B	191	LEU
1	9-B	237	LEU
1	9-B	269	HIS
1	9-B	281	LEU
1	9-B	308	LEU
1	9-B	312	THR
1	9-B	322	LEU
1	9-B	323	VAL
1	9-B	337	ARG
1	9-B	347	ILE
1	9-B	363	SER
1	9-B	375	LEU
1	9-B	392	VAL
1	9-B	397	TYR
1	9-B	413	GLN
1	9-B	420	ARG
1	9-B	428	LEU
1	9-C	602	GLU
1	9-C	2	PRO
1	9-C	8	LEU
1	9-C	10	LYS
1	9-C	24	LEU
1	9-C	39	ASP
1	9-C	50	ASP
1	9-C	59	SER
1	9-C	62	GLU
1	9-C	67	LEU
1	9-C	93	ASP
1	9-C	98	GLU
1	9-C	115	LEU
1	9-C	152	ASP
1	9-C	173	VAL
1	9-C	187	GLN
1	9-C	191	LEU
1	9-C	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-C	269	HIS
1	9-C	281	LEU
1	9-C	308	LEU
1	9-C	312	THR
1	9-C	322	LEU
1	9-C	323	VAL
1	9-C	337	ARG
1	9-C	347	ILE
1	9-C	363	SER
1	9-C	375	LEU
1	9-C	392	VAL
1	9-C	397	TYR
1	9-C	413	GLN
1	9-C	420	ARG
1	9-C	428	LEU
1	9-D	602	GLU
1	9-D	2	PRO
1	9-D	8	LEU
1	9-D	10	LYS
1	9-D	24	LEU
1	9-D	39	ASP
1	9-D	50	ASP
1	9-D	59	SER
1	9-D	62	GLU
1	9-D	67	LEU
1	9-D	93	ASP
1	9-D	98	GLU
1	9-D	115	LEU
1	9-D	152	ASP
1	9-D	173	VAL
1	9-D	187	GLN
1	9-D	191	LEU
1	9-D	237	LEU
1	9-D	269	HIS
1	9-D	281	LEU
1	9-D	308	LEU
1	9-D	312	THR
1	9-D	322	LEU
1	9-D	323	VAL
1	9-D	337	ARG
1	9-D	347	ILE
1	9-D	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-D	375	LEU
1	9-D	392	VAL
1	9-D	397	TYR
1	9-D	413	GLN
1	9-D	420	ARG
1	9-D	428	LEU
1	9-E	602	GLU
1	9-E	2	PRO
1	9-E	8	LEU
1	9-E	10	LYS
1	9-E	24	LEU
1	9-E	39	ASP
1	9-E	50	ASP
1	9-E	59	SER
1	9-E	62	GLU
1	9-E	67	LEU
1	9-E	93	ASP
1	9-E	98	GLU
1	9-E	115	LEU
1	9-E	152	ASP
1	9-E	173	VAL
1	9-E	187	GLN
1	9-E	191	LEU
1	9-E	237	LEU
1	9-E	269	HIS
1	9-E	281	LEU
1	9-E	308	LEU
1	9-E	312	THR
1	9-E	322	LEU
1	9-E	323	VAL
1	9-E	337	ARG
1	9-E	347	ILE
1	9-E	363	SER
1	9-E	375	LEU
1	9-E	392	VAL
1	9-E	397	TYR
1	9-E	413	GLN
1	9-E	420	ARG
1	9-E	428	LEU
1	9-F	602	GLU
1	9-F	2	PRO
1	9-F	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-F	10	LYS
1	9-F	24	LEU
1	9-F	39	ASP
1	9-F	50	ASP
1	9-F	59	SER
1	9-F	62	GLU
1	9-F	67	LEU
1	9-F	93	ASP
1	9-F	98	GLU
1	9-F	115	LEU
1	9-F	152	ASP
1	9-F	173	VAL
1	9-F	187	GLN
1	9-F	191	LEU
1	9-F	237	LEU
1	9-F	269	HIS
1	9-F	281	LEU
1	9-F	308	LEU
1	9-F	312	THR
1	9-F	322	LEU
1	9-F	323	VAL
1	9-F	337	ARG
1	9-F	347	ILE
1	9-F	363	SER
1	9-F	375	LEU
1	9-F	392	VAL
1	9-F	397	TYR
1	9-F	413	GLN
1	9-F	420	ARG
1	9-F	428	LEU
1	9-G	602	GLU
1	9-G	2	PRO
1	9-G	8	LEU
1	9-G	10	LYS
1	9-G	24	LEU
1	9-G	39	ASP
1	9-G	50	ASP
1	9-G	59	SER
1	9-G	62	GLU
1	9-G	67	LEU
1	9-G	93	ASP
1	9-G	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-G	115	LEU
1	9-G	152	ASP
1	9-G	173	VAL
1	9-G	187	GLN
1	9-G	191	LEU
1	9-G	237	LEU
1	9-G	269	HIS
1	9-G	281	LEU
1	9-G	308	LEU
1	9-G	312	THR
1	9-G	322	LEU
1	9-G	323	VAL
1	9-G	337	ARG
1	9-G	347	ILE
1	9-G	363	SER
1	9-G	375	LEU
1	9-G	392	VAL
1	9-G	397	TYR
1	9-G	413	GLN
1	9-G	420	ARG
1	9-G	428	LEU
1	9-H	602	GLU
1	9-H	2	PRO
1	9-H	8	LEU
1	9-H	10	LYS
1	9-H	24	LEU
1	9-H	39	ASP
1	9-H	50	ASP
1	9-H	59	SER
1	9-H	62	GLU
1	9-H	67	LEU
1	9-H	93	ASP
1	9-H	98	GLU
1	9-H	115	LEU
1	9-H	152	ASP
1	9-H	173	VAL
1	9-H	187	GLN
1	9-H	191	LEU
1	9-H	237	LEU
1	9-H	269	HIS
1	9-H	281	LEU
1	9-H	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-H	312	THR
1	9-H	322	LEU
1	9-H	323	VAL
1	9-H	337	ARG
1	9-H	347	ILE
1	9-H	363	SER
1	9-H	375	LEU
1	9-H	392	VAL
1	9-H	397	TYR
1	9-H	413	GLN
1	9-H	420	ARG
1	9-H	428	LEU
1	9-I	602	GLU
1	9-I	2	PRO
1	9-I	8	LEU
1	9-I	10	LYS
1	9-I	24	LEU
1	9-I	39	ASP
1	9-I	50	ASP
1	9-I	59	SER
1	9-I	62	GLU
1	9-I	67	LEU
1	9-I	93	ASP
1	9-I	98	GLU
1	9-I	115	LEU
1	9-I	152	ASP
1	9-I	173	VAL
1	9-I	187	GLN
1	9-I	191	LEU
1	9-I	237	LEU
1	9-I	269	HIS
1	9-I	281	LEU
1	9-I	308	LEU
1	9-I	312	THR
1	9-I	322	LEU
1	9-I	323	VAL
1	9-I	337	ARG
1	9-I	347	ILE
1	9-I	363	SER
1	9-I	375	LEU
1	9-I	392	VAL
1	9-I	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-I	413	GLN
1	9-I	420	ARG
1	9-I	428	LEU
1	9-J	602	GLU
1	9-J	2	PRO
1	9-J	8	LEU
1	9-J	10	LYS
1	9-J	24	LEU
1	9-J	39	ASP
1	9-J	50	ASP
1	9-J	59	SER
1	9-J	62	GLU
1	9-J	67	LEU
1	9-J	93	ASP
1	9-J	98	GLU
1	9-J	115	LEU
1	9-J	152	ASP
1	9-J	173	VAL
1	9-J	187	GLN
1	9-J	191	LEU
1	9-J	237	LEU
1	9-J	269	HIS
1	9-J	281	LEU
1	9-J	308	LEU
1	9-J	312	THR
1	9-J	322	LEU
1	9-J	323	VAL
1	9-J	337	ARG
1	9-J	347	ILE
1	9-J	363	SER
1	9-J	375	LEU
1	9-J	392	VAL
1	9-J	397	TYR
1	9-J	413	GLN
1	9-J	420	ARG
1	9-J	428	LEU
1	9-K	602	GLU
1	9-K	2	PRO
1	9-K	8	LEU
1	9-K	10	LYS
1	9-K	24	LEU
1	9-K	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-K	50	ASP
1	9-K	59	SER
1	9-K	62	GLU
1	9-K	67	LEU
1	9-K	93	ASP
1	9-K	98	GLU
1	9-K	115	LEU
1	9-K	152	ASP
1	9-K	173	VAL
1	9-K	187	GLN
1	9-K	191	LEU
1	9-K	237	LEU
1	9-K	269	HIS
1	9-K	281	LEU
1	9-K	308	LEU
1	9-K	312	THR
1	9-K	322	LEU
1	9-K	323	VAL
1	9-K	337	ARG
1	9-K	347	ILE
1	9-K	363	SER
1	9-K	375	LEU
1	9-K	392	VAL
1	9-K	397	TYR
1	9-K	413	GLN
1	9-K	420	ARG
1	9-K	428	LEU
1	9-L	602	GLU
1	9-L	2	PRO
1	9-L	8	LEU
1	9-L	10	LYS
1	9-L	24	LEU
1	9-L	39	ASP
1	9-L	50	ASP
1	9-L	59	SER
1	9-L	62	GLU
1	9-L	67	LEU
1	9-L	93	ASP
1	9-L	98	GLU
1	9-L	115	LEU
1	9-L	152	ASP
1	9-L	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-L	187	GLN
1	9-L	191	LEU
1	9-L	237	LEU
1	9-L	269	HIS
1	9-L	281	LEU
1	9-L	308	LEU
1	9-L	312	THR
1	9-L	322	LEU
1	9-L	323	VAL
1	9-L	337	ARG
1	9-L	347	ILE
1	9-L	363	SER
1	9-L	375	LEU
1	9-L	392	VAL
1	9-L	397	TYR
1	9-L	413	GLN
1	9-L	420	ARG
1	9-L	428	LEU
1	9-M	602	GLU
1	9-M	2	PRO
1	9-M	8	LEU
1	9-M	10	LYS
1	9-M	24	LEU
1	9-M	39	ASP
1	9-M	50	ASP
1	9-M	59	SER
1	9-M	62	GLU
1	9-M	67	LEU
1	9-M	93	ASP
1	9-M	98	GLU
1	9-M	115	LEU
1	9-M	152	ASP
1	9-M	173	VAL
1	9-M	187	GLN
1	9-M	191	LEU
1	9-M	237	LEU
1	9-M	269	HIS
1	9-M	281	LEU
1	9-M	308	LEU
1	9-M	312	THR
1	9-M	322	LEU
1	9-M	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-M	337	ARG
1	9-M	347	ILE
1	9-M	363	SER
1	9-M	375	LEU
1	9-M	392	VAL
1	9-M	397	TYR
1	9-M	413	GLN
1	9-M	420	ARG
1	9-M	428	LEU
1	9-N	602	GLU
1	9-N	2	PRO
1	9-N	8	LEU
1	9-N	10	LYS
1	9-N	24	LEU
1	9-N	39	ASP
1	9-N	50	ASP
1	9-N	59	SER
1	9-N	62	GLU
1	9-N	67	LEU
1	9-N	93	ASP
1	9-N	98	GLU
1	9-N	115	LEU
1	9-N	152	ASP
1	9-N	173	VAL
1	9-N	187	GLN
1	9-N	191	LEU
1	9-N	237	LEU
1	9-N	269	HIS
1	9-N	281	LEU
1	9-N	308	LEU
1	9-N	312	THR
1	9-N	322	LEU
1	9-N	323	VAL
1	9-N	337	ARG
1	9-N	347	ILE
1	9-N	363	SER
1	9-N	375	LEU
1	9-N	392	VAL
1	9-N	397	TYR
1	9-N	413	GLN
1	9-N	420	ARG
1	9-N	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-O	602	GLU
1	9-O	2	PRO
1	9-O	8	LEU
1	9-O	10	LYS
1	9-O	24	LEU
1	9-O	39	ASP
1	9-O	50	ASP
1	9-O	59	SER
1	9-O	62	GLU
1	9-O	67	LEU
1	9-O	93	ASP
1	9-O	98	GLU
1	9-O	115	LEU
1	9-O	152	ASP
1	9-O	173	VAL
1	9-O	187	GLN
1	9-O	191	LEU
1	9-O	237	LEU
1	9-O	269	HIS
1	9-O	281	LEU
1	9-O	308	LEU
1	9-O	312	THR
1	9-O	322	LEU
1	9-O	323	VAL
1	9-O	337	ARG
1	9-O	347	ILE
1	9-O	363	SER
1	9-O	375	LEU
1	9-O	392	VAL
1	9-O	397	TYR
1	9-O	413	GLN
1	9-O	420	ARG
1	9-O	428	LEU
1	9-P	602	GLU
1	9-P	2	PRO
1	9-P	8	LEU
1	9-P	10	LYS
1	9-P	24	LEU
1	9-P	39	ASP
1	9-P	50	ASP
1	9-P	59	SER
1	9-P	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-P	67	LEU
1	9-P	93	ASP
1	9-P	98	GLU
1	9-P	115	LEU
1	9-P	152	ASP
1	9-P	173	VAL
1	9-P	187	GLN
1	9-P	191	LEU
1	9-P	237	LEU
1	9-P	269	HIS
1	9-P	281	LEU
1	9-P	308	LEU
1	9-P	312	THR
1	9-P	322	LEU
1	9-P	323	VAL
1	9-P	337	ARG
1	9-P	347	ILE
1	9-P	363	SER
1	9-P	375	LEU
1	9-P	392	VAL
1	9-P	397	TYR
1	9-P	413	GLN
1	9-P	420	ARG
1	9-P	428	LEU
1	9-Q	602	GLU
1	9-Q	2	PRO
1	9-Q	8	LEU
1	9-Q	10	LYS
1	9-Q	24	LEU
1	9-Q	39	ASP
1	9-Q	50	ASP
1	9-Q	59	SER
1	9-Q	62	GLU
1	9-Q	67	LEU
1	9-Q	93	ASP
1	9-Q	98	GLU
1	9-Q	115	LEU
1	9-Q	152	ASP
1	9-Q	173	VAL
1	9-Q	187	GLN
1	9-Q	191	LEU
1	9-Q	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-Q	269	HIS
1	9-Q	281	LEU
1	9-Q	308	LEU
1	9-Q	312	THR
1	9-Q	322	LEU
1	9-Q	323	VAL
1	9-Q	337	ARG
1	9-Q	347	ILE
1	9-Q	363	SER
1	9-Q	375	LEU
1	9-Q	392	VAL
1	9-Q	397	TYR
1	9-Q	413	GLN
1	9-Q	420	ARG
1	9-Q	428	LEU
1	9-R	602	GLU
1	9-R	2	PRO
1	9-R	8	LEU
1	9-R	10	LYS
1	9-R	24	LEU
1	9-R	39	ASP
1	9-R	50	ASP
1	9-R	59	SER
1	9-R	62	GLU
1	9-R	67	LEU
1	9-R	93	ASP
1	9-R	98	GLU
1	9-R	115	LEU
1	9-R	152	ASP
1	9-R	173	VAL
1	9-R	187	GLN
1	9-R	191	LEU
1	9-R	237	LEU
1	9-R	269	HIS
1	9-R	281	LEU
1	9-R	308	LEU
1	9-R	312	THR
1	9-R	322	LEU
1	9-R	323	VAL
1	9-R	337	ARG
1	9-R	347	ILE
1	9-R	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-R	375	LEU
1	9-R	392	VAL
1	9-R	397	TYR
1	9-R	413	GLN
1	9-R	420	ARG
1	9-R	428	LEU
1	9-S	602	GLU
1	9-S	2	PRO
1	9-S	8	LEU
1	9-S	10	LYS
1	9-S	24	LEU
1	9-S	39	ASP
1	9-S	50	ASP
1	9-S	59	SER
1	9-S	62	GLU
1	9-S	67	LEU
1	9-S	93	ASP
1	9-S	98	GLU
1	9-S	115	LEU
1	9-S	152	ASP
1	9-S	173	VAL
1	9-S	187	GLN
1	9-S	191	LEU
1	9-S	237	LEU
1	9-S	269	HIS
1	9-S	281	LEU
1	9-S	308	LEU
1	9-S	312	THR
1	9-S	322	LEU
1	9-S	323	VAL
1	9-S	337	ARG
1	9-S	347	ILE
1	9-S	363	SER
1	9-S	375	LEU
1	9-S	392	VAL
1	9-S	397	TYR
1	9-S	413	GLN
1	9-S	420	ARG
1	9-S	428	LEU
1	9-T	602	GLU
1	9-T	2	PRO
1	9-T	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-T	10	LYS
1	9-T	24	LEU
1	9-T	39	ASP
1	9-T	50	ASP
1	9-T	59	SER
1	9-T	62	GLU
1	9-T	67	LEU
1	9-T	93	ASP
1	9-T	98	GLU
1	9-T	115	LEU
1	9-T	152	ASP
1	9-T	173	VAL
1	9-T	187	GLN
1	9-T	191	LEU
1	9-T	237	LEU
1	9-T	269	HIS
1	9-T	281	LEU
1	9-T	308	LEU
1	9-T	312	THR
1	9-T	322	LEU
1	9-T	323	VAL
1	9-T	337	ARG
1	9-T	347	ILE
1	9-T	363	SER
1	9-T	375	LEU
1	9-T	392	VAL
1	9-T	397	TYR
1	9-T	413	GLN
1	9-T	420	ARG
1	9-T	428	LEU
1	9-U	602	GLU
1	9-U	2	PRO
1	9-U	8	LEU
1	9-U	10	LYS
1	9-U	24	LEU
1	9-U	39	ASP
1	9-U	50	ASP
1	9-U	59	SER
1	9-U	62	GLU
1	9-U	67	LEU
1	9-U	93	ASP
1	9-U	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-U	115	LEU
1	9-U	152	ASP
1	9-U	173	VAL
1	9-U	187	GLN
1	9-U	191	LEU
1	9-U	237	LEU
1	9-U	269	HIS
1	9-U	281	LEU
1	9-U	308	LEU
1	9-U	312	THR
1	9-U	322	LEU
1	9-U	323	VAL
1	9-U	337	ARG
1	9-U	347	ILE
1	9-U	363	SER
1	9-U	375	LEU
1	9-U	392	VAL
1	9-U	397	TYR
1	9-U	413	GLN
1	9-U	420	ARG
1	9-U	428	LEU
1	9-V	602	GLU
1	9-V	2	PRO
1	9-V	8	LEU
1	9-V	10	LYS
1	9-V	24	LEU
1	9-V	39	ASP
1	9-V	50	ASP
1	9-V	59	SER
1	9-V	62	GLU
1	9-V	67	LEU
1	9-V	93	ASP
1	9-V	98	GLU
1	9-V	115	LEU
1	9-V	152	ASP
1	9-V	173	VAL
1	9-V	187	GLN
1	9-V	191	LEU
1	9-V	237	LEU
1	9-V	269	HIS
1	9-V	281	LEU
1	9-V	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-V	312	THR
1	9-V	322	LEU
1	9-V	323	VAL
1	9-V	337	ARG
1	9-V	347	ILE
1	9-V	363	SER
1	9-V	375	LEU
1	9-V	392	VAL
1	9-V	397	TYR
1	9-V	413	GLN
1	9-V	420	ARG
1	9-V	428	LEU
1	9-W	602	GLU
1	9-W	2	PRO
1	9-W	8	LEU
1	9-W	10	LYS
1	9-W	24	LEU
1	9-W	39	ASP
1	9-W	50	ASP
1	9-W	59	SER
1	9-W	62	GLU
1	9-W	67	LEU
1	9-W	93	ASP
1	9-W	98	GLU
1	9-W	115	LEU
1	9-W	152	ASP
1	9-W	173	VAL
1	9-W	187	GLN
1	9-W	191	LEU
1	9-W	237	LEU
1	9-W	269	HIS
1	9-W	281	LEU
1	9-W	308	LEU
1	9-W	312	THR
1	9-W	322	LEU
1	9-W	323	VAL
1	9-W	337	ARG
1	9-W	347	ILE
1	9-W	363	SER
1	9-W	375	LEU
1	9-W	392	VAL
1	9-W	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-W	413	GLN
1	9-W	420	ARG
1	9-W	428	LEU
1	9-X	602	GLU
1	9-X	2	PRO
1	9-X	8	LEU
1	9-X	10	LYS
1	9-X	24	LEU
1	9-X	39	ASP
1	9-X	50	ASP
1	9-X	59	SER
1	9-X	62	GLU
1	9-X	67	LEU
1	9-X	93	ASP
1	9-X	98	GLU
1	9-X	115	LEU
1	9-X	152	ASP
1	9-X	173	VAL
1	9-X	187	GLN
1	9-X	191	LEU
1	9-X	237	LEU
1	9-X	269	HIS
1	9-X	281	LEU
1	9-X	308	LEU
1	9-X	312	THR
1	9-X	322	LEU
1	9-X	323	VAL
1	9-X	337	ARG
1	9-X	347	ILE
1	9-X	363	SER
1	9-X	375	LEU
1	9-X	392	VAL
1	9-X	397	TYR
1	9-X	413	GLN
1	9-X	420	ARG
1	9-X	428	LEU
1	10-A	602	GLU
1	10-A	2	PRO
1	10-A	8	LEU
1	10-A	10	LYS
1	10-A	24	LEU
1	10-A	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-A	50	ASP
1	10-A	59	SER
1	10-A	62	GLU
1	10-A	67	LEU
1	10-A	93	ASP
1	10-A	98	GLU
1	10-A	115	LEU
1	10-A	152	ASP
1	10-A	173	VAL
1	10-A	187	GLN
1	10-A	191	LEU
1	10-A	237	LEU
1	10-A	269	HIS
1	10-A	281	LEU
1	10-A	308	LEU
1	10-A	312	THR
1	10-A	322	LEU
1	10-A	323	VAL
1	10-A	337	ARG
1	10-A	347	ILE
1	10-A	363	SER
1	10-A	375	LEU
1	10-A	392	VAL
1	10-A	397	TYR
1	10-A	413	GLN
1	10-A	420	ARG
1	10-A	428	LEU
1	10-B	602	GLU
1	10-B	2	PRO
1	10-B	8	LEU
1	10-B	10	LYS
1	10-B	24	LEU
1	10-B	39	ASP
1	10-B	50	ASP
1	10-B	59	SER
1	10-B	62	GLU
1	10-B	67	LEU
1	10-B	93	ASP
1	10-B	98	GLU
1	10-B	115	LEU
1	10-B	152	ASP
1	10-B	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-B	187	GLN
1	10-B	191	LEU
1	10-B	237	LEU
1	10-B	269	HIS
1	10-B	281	LEU
1	10-B	308	LEU
1	10-B	312	THR
1	10-B	322	LEU
1	10-B	323	VAL
1	10-B	337	ARG
1	10-B	347	ILE
1	10-B	363	SER
1	10-B	375	LEU
1	10-B	392	VAL
1	10-B	397	TYR
1	10-B	413	GLN
1	10-B	420	ARG
1	10-B	428	LEU
1	10-C	602	GLU
1	10-C	2	PRO
1	10-C	8	LEU
1	10-C	10	LYS
1	10-C	24	LEU
1	10-C	39	ASP
1	10-C	50	ASP
1	10-C	59	SER
1	10-C	62	GLU
1	10-C	67	LEU
1	10-C	93	ASP
1	10-C	98	GLU
1	10-C	115	LEU
1	10-C	152	ASP
1	10-C	173	VAL
1	10-C	187	GLN
1	10-C	191	LEU
1	10-C	237	LEU
1	10-C	269	HIS
1	10-C	281	LEU
1	10-C	308	LEU
1	10-C	312	THR
1	10-C	322	LEU
1	10-C	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-C	337	ARG
1	10-C	347	ILE
1	10-C	363	SER
1	10-C	375	LEU
1	10-C	392	VAL
1	10-C	397	TYR
1	10-C	413	GLN
1	10-C	420	ARG
1	10-C	428	LEU
1	10-D	602	GLU
1	10-D	2	PRO
1	10-D	8	LEU
1	10-D	10	LYS
1	10-D	24	LEU
1	10-D	39	ASP
1	10-D	50	ASP
1	10-D	59	SER
1	10-D	62	GLU
1	10-D	67	LEU
1	10-D	93	ASP
1	10-D	98	GLU
1	10-D	115	LEU
1	10-D	152	ASP
1	10-D	173	VAL
1	10-D	187	GLN
1	10-D	191	LEU
1	10-D	237	LEU
1	10-D	269	HIS
1	10-D	281	LEU
1	10-D	308	LEU
1	10-D	312	THR
1	10-D	322	LEU
1	10-D	323	VAL
1	10-D	337	ARG
1	10-D	347	ILE
1	10-D	363	SER
1	10-D	375	LEU
1	10-D	392	VAL
1	10-D	397	TYR
1	10-D	413	GLN
1	10-D	420	ARG
1	10-D	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-E	602	GLU
1	10-E	2	PRO
1	10-E	8	LEU
1	10-E	10	LYS
1	10-E	24	LEU
1	10-E	39	ASP
1	10-E	50	ASP
1	10-E	59	SER
1	10-E	62	GLU
1	10-E	67	LEU
1	10-E	93	ASP
1	10-E	98	GLU
1	10-E	115	LEU
1	10-E	152	ASP
1	10-E	173	VAL
1	10-E	187	GLN
1	10-E	191	LEU
1	10-E	237	LEU
1	10-E	269	HIS
1	10-E	281	LEU
1	10-E	308	LEU
1	10-E	312	THR
1	10-E	322	LEU
1	10-E	323	VAL
1	10-E	337	ARG
1	10-E	347	ILE
1	10-E	363	SER
1	10-E	375	LEU
1	10-E	392	VAL
1	10-E	397	TYR
1	10-E	413	GLN
1	10-E	420	ARG
1	10-E	428	LEU
1	10-F	602	GLU
1	10-F	2	PRO
1	10-F	8	LEU
1	10-F	10	LYS
1	10-F	24	LEU
1	10-F	39	ASP
1	10-F	50	ASP
1	10-F	59	SER
1	10-F	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-F	67	LEU
1	10-F	93	ASP
1	10-F	98	GLU
1	10-F	115	LEU
1	10-F	152	ASP
1	10-F	173	VAL
1	10-F	187	GLN
1	10-F	191	LEU
1	10-F	237	LEU
1	10-F	269	HIS
1	10-F	281	LEU
1	10-F	308	LEU
1	10-F	312	THR
1	10-F	322	LEU
1	10-F	323	VAL
1	10-F	337	ARG
1	10-F	347	ILE
1	10-F	363	SER
1	10-F	375	LEU
1	10-F	392	VAL
1	10-F	397	TYR
1	10-F	413	GLN
1	10-F	420	ARG
1	10-F	428	LEU
1	10-G	602	GLU
1	10-G	2	PRO
1	10-G	8	LEU
1	10-G	10	LYS
1	10-G	24	LEU
1	10-G	39	ASP
1	10-G	50	ASP
1	10-G	59	SER
1	10-G	62	GLU
1	10-G	67	LEU
1	10-G	93	ASP
1	10-G	98	GLU
1	10-G	115	LEU
1	10-G	152	ASP
1	10-G	173	VAL
1	10-G	187	GLN
1	10-G	191	LEU
1	10-G	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-G	269	HIS
1	10-G	281	LEU
1	10-G	308	LEU
1	10-G	312	THR
1	10-G	322	LEU
1	10-G	323	VAL
1	10-G	337	ARG
1	10-G	347	ILE
1	10-G	363	SER
1	10-G	375	LEU
1	10-G	392	VAL
1	10-G	397	TYR
1	10-G	413	GLN
1	10-G	420	ARG
1	10-G	428	LEU
1	10-H	602	GLU
1	10-H	2	PRO
1	10-H	8	LEU
1	10-H	10	LYS
1	10-H	24	LEU
1	10-H	39	ASP
1	10-H	50	ASP
1	10-H	59	SER
1	10-H	62	GLU
1	10-H	67	LEU
1	10-H	93	ASP
1	10-H	98	GLU
1	10-H	115	LEU
1	10-H	152	ASP
1	10-H	173	VAL
1	10-H	187	GLN
1	10-H	191	LEU
1	10-H	237	LEU
1	10-H	269	HIS
1	10-H	281	LEU
1	10-H	308	LEU
1	10-H	312	THR
1	10-H	322	LEU
1	10-H	323	VAL
1	10-H	337	ARG
1	10-H	347	ILE
1	10-H	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-H	375	LEU
1	10-H	392	VAL
1	10-H	397	TYR
1	10-H	413	GLN
1	10-H	420	ARG
1	10-H	428	LEU
1	10-I	602	GLU
1	10-I	2	PRO
1	10-I	8	LEU
1	10-I	10	LYS
1	10-I	24	LEU
1	10-I	39	ASP
1	10-I	50	ASP
1	10-I	59	SER
1	10-I	62	GLU
1	10-I	67	LEU
1	10-I	93	ASP
1	10-I	98	GLU
1	10-I	115	LEU
1	10-I	152	ASP
1	10-I	173	VAL
1	10-I	187	GLN
1	10-I	191	LEU
1	10-I	237	LEU
1	10-I	269	HIS
1	10-I	281	LEU
1	10-I	308	LEU
1	10-I	312	THR
1	10-I	322	LEU
1	10-I	323	VAL
1	10-I	337	ARG
1	10-I	347	ILE
1	10-I	363	SER
1	10-I	375	LEU
1	10-I	392	VAL
1	10-I	397	TYR
1	10-I	413	GLN
1	10-I	420	ARG
1	10-I	428	LEU
1	10-J	602	GLU
1	10-J	2	PRO
1	10-J	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-J	10	LYS
1	10-J	24	LEU
1	10-J	39	ASP
1	10-J	50	ASP
1	10-J	59	SER
1	10-J	62	GLU
1	10-J	67	LEU
1	10-J	93	ASP
1	10-J	98	GLU
1	10-J	115	LEU
1	10-J	152	ASP
1	10-J	173	VAL
1	10-J	187	GLN
1	10-J	191	LEU
1	10-J	237	LEU
1	10-J	269	HIS
1	10-J	281	LEU
1	10-J	308	LEU
1	10-J	312	THR
1	10-J	322	LEU
1	10-J	323	VAL
1	10-J	337	ARG
1	10-J	347	ILE
1	10-J	363	SER
1	10-J	375	LEU
1	10-J	392	VAL
1	10-J	397	TYR
1	10-J	413	GLN
1	10-J	420	ARG
1	10-J	428	LEU
1	10-K	602	GLU
1	10-K	2	PRO
1	10-K	8	LEU
1	10-K	10	LYS
1	10-K	24	LEU
1	10-K	39	ASP
1	10-K	50	ASP
1	10-K	59	SER
1	10-K	62	GLU
1	10-K	67	LEU
1	10-K	93	ASP
1	10-K	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-K	115	LEU
1	10-K	152	ASP
1	10-K	173	VAL
1	10-K	187	GLN
1	10-K	191	LEU
1	10-K	237	LEU
1	10-K	269	HIS
1	10-K	281	LEU
1	10-K	308	LEU
1	10-K	312	THR
1	10-K	322	LEU
1	10-K	323	VAL
1	10-K	337	ARG
1	10-K	347	ILE
1	10-K	363	SER
1	10-K	375	LEU
1	10-K	392	VAL
1	10-K	397	TYR
1	10-K	413	GLN
1	10-K	420	ARG
1	10-K	428	LEU
1	10-L	602	GLU
1	10-L	2	PRO
1	10-L	8	LEU
1	10-L	10	LYS
1	10-L	24	LEU
1	10-L	39	ASP
1	10-L	50	ASP
1	10-L	59	SER
1	10-L	62	GLU
1	10-L	67	LEU
1	10-L	93	ASP
1	10-L	98	GLU
1	10-L	115	LEU
1	10-L	152	ASP
1	10-L	173	VAL
1	10-L	187	GLN
1	10-L	191	LEU
1	10-L	237	LEU
1	10-L	269	HIS
1	10-L	281	LEU
1	10-L	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-L	312	THR
1	10-L	322	LEU
1	10-L	323	VAL
1	10-L	337	ARG
1	10-L	347	ILE
1	10-L	363	SER
1	10-L	375	LEU
1	10-L	392	VAL
1	10-L	397	TYR
1	10-L	413	GLN
1	10-L	420	ARG
1	10-L	428	LEU
1	10-M	602	GLU
1	10-M	2	PRO
1	10-M	8	LEU
1	10-M	10	LYS
1	10-M	24	LEU
1	10-M	39	ASP
1	10-M	50	ASP
1	10-M	59	SER
1	10-M	62	GLU
1	10-M	67	LEU
1	10-M	93	ASP
1	10-M	98	GLU
1	10-M	115	LEU
1	10-M	152	ASP
1	10-M	173	VAL
1	10-M	187	GLN
1	10-M	191	LEU
1	10-M	237	LEU
1	10-M	269	HIS
1	10-M	281	LEU
1	10-M	308	LEU
1	10-M	312	THR
1	10-M	322	LEU
1	10-M	323	VAL
1	10-M	337	ARG
1	10-M	347	ILE
1	10-M	363	SER
1	10-M	375	LEU
1	10-M	392	VAL
1	10-M	397	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-M	413	GLN
1	10-M	420	ARG
1	10-M	428	LEU
1	10-N	602	GLU
1	10-N	2	PRO
1	10-N	8	LEU
1	10-N	10	LYS
1	10-N	24	LEU
1	10-N	39	ASP
1	10-N	50	ASP
1	10-N	59	SER
1	10-N	62	GLU
1	10-N	67	LEU
1	10-N	93	ASP
1	10-N	98	GLU
1	10-N	115	LEU
1	10-N	152	ASP
1	10-N	173	VAL
1	10-N	187	GLN
1	10-N	191	LEU
1	10-N	237	LEU
1	10-N	269	HIS
1	10-N	281	LEU
1	10-N	308	LEU
1	10-N	312	THR
1	10-N	322	LEU
1	10-N	323	VAL
1	10-N	337	ARG
1	10-N	347	ILE
1	10-N	363	SER
1	10-N	375	LEU
1	10-N	392	VAL
1	10-N	397	TYR
1	10-N	413	GLN
1	10-N	420	ARG
1	10-N	428	LEU
1	10-O	602	GLU
1	10-O	2	PRO
1	10-O	8	LEU
1	10-O	10	LYS
1	10-O	24	LEU
1	10-O	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-O	50	ASP
1	10-O	59	SER
1	10-O	62	GLU
1	10-O	67	LEU
1	10-O	93	ASP
1	10-O	98	GLU
1	10-O	115	LEU
1	10-O	152	ASP
1	10-O	173	VAL
1	10-O	187	GLN
1	10-O	191	LEU
1	10-O	237	LEU
1	10-O	269	HIS
1	10-O	281	LEU
1	10-O	308	LEU
1	10-O	312	THR
1	10-O	322	LEU
1	10-O	323	VAL
1	10-O	337	ARG
1	10-O	347	ILE
1	10-O	363	SER
1	10-O	375	LEU
1	10-O	392	VAL
1	10-O	397	TYR
1	10-O	413	GLN
1	10-O	420	ARG
1	10-O	428	LEU
1	10-P	602	GLU
1	10-P	2	PRO
1	10-P	8	LEU
1	10-P	10	LYS
1	10-P	24	LEU
1	10-P	39	ASP
1	10-P	50	ASP
1	10-P	59	SER
1	10-P	62	GLU
1	10-P	67	LEU
1	10-P	93	ASP
1	10-P	98	GLU
1	10-P	115	LEU
1	10-P	152	ASP
1	10-P	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-P	187	GLN
1	10-P	191	LEU
1	10-P	237	LEU
1	10-P	269	HIS
1	10-P	281	LEU
1	10-P	308	LEU
1	10-P	312	THR
1	10-P	322	LEU
1	10-P	323	VAL
1	10-P	337	ARG
1	10-P	347	ILE
1	10-P	363	SER
1	10-P	375	LEU
1	10-P	392	VAL
1	10-P	397	TYR
1	10-P	413	GLN
1	10-P	420	ARG
1	10-P	428	LEU
1	10-Q	602	GLU
1	10-Q	2	PRO
1	10-Q	8	LEU
1	10-Q	10	LYS
1	10-Q	24	LEU
1	10-Q	39	ASP
1	10-Q	50	ASP
1	10-Q	59	SER
1	10-Q	62	GLU
1	10-Q	67	LEU
1	10-Q	93	ASP
1	10-Q	98	GLU
1	10-Q	115	LEU
1	10-Q	152	ASP
1	10-Q	173	VAL
1	10-Q	187	GLN
1	10-Q	191	LEU
1	10-Q	237	LEU
1	10-Q	269	HIS
1	10-Q	281	LEU
1	10-Q	308	LEU
1	10-Q	312	THR
1	10-Q	322	LEU
1	10-Q	323	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-Q	337	ARG
1	10-Q	347	ILE
1	10-Q	363	SER
1	10-Q	375	LEU
1	10-Q	392	VAL
1	10-Q	397	TYR
1	10-Q	413	GLN
1	10-Q	420	ARG
1	10-Q	428	LEU
1	10-R	602	GLU
1	10-R	2	PRO
1	10-R	8	LEU
1	10-R	10	LYS
1	10-R	24	LEU
1	10-R	39	ASP
1	10-R	50	ASP
1	10-R	59	SER
1	10-R	62	GLU
1	10-R	67	LEU
1	10-R	93	ASP
1	10-R	98	GLU
1	10-R	115	LEU
1	10-R	152	ASP
1	10-R	173	VAL
1	10-R	187	GLN
1	10-R	191	LEU
1	10-R	237	LEU
1	10-R	269	HIS
1	10-R	281	LEU
1	10-R	308	LEU
1	10-R	312	THR
1	10-R	322	LEU
1	10-R	323	VAL
1	10-R	337	ARG
1	10-R	347	ILE
1	10-R	363	SER
1	10-R	375	LEU
1	10-R	392	VAL
1	10-R	397	TYR
1	10-R	413	GLN
1	10-R	420	ARG
1	10-R	428	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-S	602	GLU
1	10-S	2	PRO
1	10-S	8	LEU
1	10-S	10	LYS
1	10-S	24	LEU
1	10-S	39	ASP
1	10-S	50	ASP
1	10-S	59	SER
1	10-S	62	GLU
1	10-S	67	LEU
1	10-S	93	ASP
1	10-S	98	GLU
1	10-S	115	LEU
1	10-S	152	ASP
1	10-S	173	VAL
1	10-S	187	GLN
1	10-S	191	LEU
1	10-S	237	LEU
1	10-S	269	HIS
1	10-S	281	LEU
1	10-S	308	LEU
1	10-S	312	THR
1	10-S	322	LEU
1	10-S	323	VAL
1	10-S	337	ARG
1	10-S	347	ILE
1	10-S	363	SER
1	10-S	375	LEU
1	10-S	392	VAL
1	10-S	397	TYR
1	10-S	413	GLN
1	10-S	420	ARG
1	10-S	428	LEU
1	10-T	602	GLU
1	10-T	2	PRO
1	10-T	8	LEU
1	10-T	10	LYS
1	10-T	24	LEU
1	10-T	39	ASP
1	10-T	50	ASP
1	10-T	59	SER
1	10-T	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-T	67	LEU
1	10-T	93	ASP
1	10-T	98	GLU
1	10-T	115	LEU
1	10-T	152	ASP
1	10-T	173	VAL
1	10-T	187	GLN
1	10-T	191	LEU
1	10-T	237	LEU
1	10-T	269	HIS
1	10-T	281	LEU
1	10-T	308	LEU
1	10-T	312	THR
1	10-T	322	LEU
1	10-T	323	VAL
1	10-T	337	ARG
1	10-T	347	ILE
1	10-T	363	SER
1	10-T	375	LEU
1	10-T	392	VAL
1	10-T	397	TYR
1	10-T	413	GLN
1	10-T	420	ARG
1	10-T	428	LEU
1	10-U	602	GLU
1	10-U	2	PRO
1	10-U	8	LEU
1	10-U	10	LYS
1	10-U	24	LEU
1	10-U	39	ASP
1	10-U	50	ASP
1	10-U	59	SER
1	10-U	62	GLU
1	10-U	67	LEU
1	10-U	93	ASP
1	10-U	98	GLU
1	10-U	115	LEU
1	10-U	152	ASP
1	10-U	173	VAL
1	10-U	187	GLN
1	10-U	191	LEU
1	10-U	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-U	269	HIS
1	10-U	281	LEU
1	10-U	308	LEU
1	10-U	312	THR
1	10-U	322	LEU
1	10-U	323	VAL
1	10-U	337	ARG
1	10-U	347	ILE
1	10-U	363	SER
1	10-U	375	LEU
1	10-U	392	VAL
1	10-U	397	TYR
1	10-U	413	GLN
1	10-U	420	ARG
1	10-U	428	LEU
1	10-V	602	GLU
1	10-V	2	PRO
1	10-V	8	LEU
1	10-V	10	LYS
1	10-V	24	LEU
1	10-V	39	ASP
1	10-V	50	ASP
1	10-V	59	SER
1	10-V	62	GLU
1	10-V	67	LEU
1	10-V	93	ASP
1	10-V	98	GLU
1	10-V	115	LEU
1	10-V	152	ASP
1	10-V	173	VAL
1	10-V	187	GLN
1	10-V	191	LEU
1	10-V	237	LEU
1	10-V	269	HIS
1	10-V	281	LEU
1	10-V	308	LEU
1	10-V	312	THR
1	10-V	322	LEU
1	10-V	323	VAL
1	10-V	337	ARG
1	10-V	347	ILE
1	10-V	363	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-V	375	LEU
1	10-V	392	VAL
1	10-V	397	TYR
1	10-V	413	GLN
1	10-V	420	ARG
1	10-V	428	LEU
1	10-W	602	GLU
1	10-W	2	PRO
1	10-W	8	LEU
1	10-W	10	LYS
1	10-W	24	LEU
1	10-W	39	ASP
1	10-W	50	ASP
1	10-W	59	SER
1	10-W	62	GLU
1	10-W	67	LEU
1	10-W	93	ASP
1	10-W	98	GLU
1	10-W	115	LEU
1	10-W	152	ASP
1	10-W	173	VAL
1	10-W	187	GLN
1	10-W	191	LEU
1	10-W	237	LEU
1	10-W	269	HIS
1	10-W	281	LEU
1	10-W	308	LEU
1	10-W	312	THR
1	10-W	322	LEU
1	10-W	323	VAL
1	10-W	337	ARG
1	10-W	347	ILE
1	10-W	363	SER
1	10-W	375	LEU
1	10-W	392	VAL
1	10-W	397	TYR
1	10-W	413	GLN
1	10-W	420	ARG
1	10-W	428	LEU
1	10-X	602	GLU
1	10-X	2	PRO
1	10-X	8	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-X	10	LYS
1	10-X	24	LEU
1	10-X	39	ASP
1	10-X	50	ASP
1	10-X	59	SER
1	10-X	62	GLU
1	10-X	67	LEU
1	10-X	93	ASP
1	10-X	98	GLU
1	10-X	115	LEU
1	10-X	152	ASP
1	10-X	173	VAL
1	10-X	187	GLN
1	10-X	191	LEU
1	10-X	237	LEU
1	10-X	269	HIS
1	10-X	281	LEU
1	10-X	308	LEU
1	10-X	312	THR
1	10-X	322	LEU
1	10-X	323	VAL
1	10-X	337	ARG
1	10-X	347	ILE
1	10-X	363	SER
1	10-X	375	LEU
1	10-X	392	VAL
1	10-X	397	TYR
1	10-X	413	GLN
1	10-X	420	ARG
1	10-X	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4099) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	30	HIS
1	1-A	58	GLN
1	1-A	86	ASN
1	1-A	106	ASN
1	1-A	113	ASN
1	1-A	187	GLN
1	1-A	210	HIS
1	1-A	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-A	230	HIS
1	1-A	244	ASN
1	1-A	264	ASN
1	1-A	272	GLN
1	1-A	303	HIS
1	1-A	313	ASN
1	1-A	454	ASN
1	1-A	458	HIS
1	1-B	30	HIS
1	1-B	58	GLN
1	1-B	86	ASN
1	1-B	106	ASN
1	1-B	113	ASN
1	1-B	187	GLN
1	1-B	210	HIS
1	1-B	218	GLN
1	1-B	230	HIS
1	1-B	244	ASN
1	1-B	264	ASN
1	1-B	272	GLN
1	1-B	313	ASN
1	1-B	458	HIS
1	1-C	30	HIS
1	1-C	58	GLN
1	1-C	86	ASN
1	1-C	106	ASN
1	1-C	113	ASN
1	1-C	187	GLN
1	1-C	210	HIS
1	1-C	218	GLN
1	1-C	230	HIS
1	1-C	244	ASN
1	1-C	264	ASN
1	1-C	272	GLN
1	1-C	303	HIS
1	1-C	313	ASN
1	1-C	458	HIS
1	1-D	30	HIS
1	1-D	58	GLN
1	1-D	61	HIS
1	1-D	86	ASN
1	1-D	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-D	113	ASN
1	1-D	187	GLN
1	1-D	210	HIS
1	1-D	211	HIS
1	1-D	218	GLN
1	1-D	230	HIS
1	1-D	244	ASN
1	1-D	264	ASN
1	1-D	272	GLN
1	1-D	303	HIS
1	1-D	313	ASN
1	1-D	458	HIS
1	1-E	58	GLN
1	1-E	86	ASN
1	1-E	106	ASN
1	1-E	113	ASN
1	1-E	187	GLN
1	1-E	210	HIS
1	1-E	218	GLN
1	1-E	230	HIS
1	1-E	244	ASN
1	1-E	264	ASN
1	1-E	272	GLN
1	1-E	303	HIS
1	1-E	313	ASN
1	1-E	458	HIS
1	1-F	30	HIS
1	1-F	58	GLN
1	1-F	86	ASN
1	1-F	106	ASN
1	1-F	113	ASN
1	1-F	187	GLN
1	1-F	210	HIS
1	1-F	211	HIS
1	1-F	218	GLN
1	1-F	230	HIS
1	1-F	244	ASN
1	1-F	264	ASN
1	1-F	272	GLN
1	1-F	303	HIS
1	1-F	313	ASN
1	1-F	458	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-G	30	HIS
1	1-G	58	GLN
1	1-G	86	ASN
1	1-G	106	ASN
1	1-G	113	ASN
1	1-G	187	GLN
1	1-G	210	HIS
1	1-G	211	HIS
1	1-G	218	GLN
1	1-G	230	HIS
1	1-G	244	ASN
1	1-G	264	ASN
1	1-G	272	GLN
1	1-G	313	ASN
1	1-G	413	GLN
1	1-G	458	HIS
1	1-H	30	HIS
1	1-H	58	GLN
1	1-H	86	ASN
1	1-H	106	ASN
1	1-H	113	ASN
1	1-H	187	GLN
1	1-H	210	HIS
1	1-H	218	GLN
1	1-H	230	HIS
1	1-H	244	ASN
1	1-H	264	ASN
1	1-H	272	GLN
1	1-H	303	HIS
1	1-H	313	ASN
1	1-H	458	HIS
1	1-I	30	HIS
1	1-I	58	GLN
1	1-I	86	ASN
1	1-I	106	ASN
1	1-I	113	ASN
1	1-I	187	GLN
1	1-I	210	HIS
1	1-I	218	GLN
1	1-I	230	HIS
1	1-I	244	ASN
1	1-I	264	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-I	272	GLN
1	1-I	303	HIS
1	1-I	313	ASN
1	1-I	458	HIS
1	1-J	58	GLN
1	1-J	86	ASN
1	1-J	106	ASN
1	1-J	113	ASN
1	1-J	187	GLN
1	1-J	210	HIS
1	1-J	218	GLN
1	1-J	230	HIS
1	1-J	244	ASN
1	1-J	264	ASN
1	1-J	272	GLN
1	1-J	303	HIS
1	1-J	313	ASN
1	1-J	458	HIS
1	1-K	30	HIS
1	1-K	58	GLN
1	1-K	86	ASN
1	1-K	106	ASN
1	1-K	113	ASN
1	1-K	187	GLN
1	1-K	210	HIS
1	1-K	211	HIS
1	1-K	218	GLN
1	1-K	230	HIS
1	1-K	244	ASN
1	1-K	264	ASN
1	1-K	272	GLN
1	1-K	303	HIS
1	1-K	313	ASN
1	1-K	458	HIS
1	1-L	58	GLN
1	1-L	86	ASN
1	1-L	106	ASN
1	1-L	113	ASN
1	1-L	187	GLN
1	1-L	210	HIS
1	1-L	218	GLN
1	1-L	230	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-L	244	ASN
1	1-L	264	ASN
1	1-L	272	GLN
1	1-L	303	HIS
1	1-L	313	ASN
1	1-L	458	HIS
1	1-M	30	HIS
1	1-M	58	GLN
1	1-M	86	ASN
1	1-M	106	ASN
1	1-M	113	ASN
1	1-M	187	GLN
1	1-M	210	HIS
1	1-M	218	GLN
1	1-M	230	HIS
1	1-M	244	ASN
1	1-M	264	ASN
1	1-M	272	GLN
1	1-M	303	HIS
1	1-M	313	ASN
1	1-M	454	ASN
1	1-M	458	HIS
1	1-N	30	HIS
1	1-N	58	GLN
1	1-N	86	ASN
1	1-N	106	ASN
1	1-N	113	ASN
1	1-N	187	GLN
1	1-N	210	HIS
1	1-N	218	GLN
1	1-N	230	HIS
1	1-N	244	ASN
1	1-N	264	ASN
1	1-N	272	GLN
1	1-N	303	HIS
1	1-N	313	ASN
1	1-N	458	HIS
1	1-O	30	HIS
1	1-O	58	GLN
1	1-O	86	ASN
1	1-O	106	ASN
1	1-O	113	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-O	187	GLN
1	1-O	210	HIS
1	1-O	218	GLN
1	1-O	230	HIS
1	1-O	244	ASN
1	1-O	264	ASN
1	1-O	272	GLN
1	1-O	303	HIS
1	1-O	313	ASN
1	1-O	458	HIS
1	1-P	30	HIS
1	1-P	58	GLN
1	1-P	86	ASN
1	1-P	106	ASN
1	1-P	113	ASN
1	1-P	187	GLN
1	1-P	210	HIS
1	1-P	211	HIS
1	1-P	218	GLN
1	1-P	230	HIS
1	1-P	244	ASN
1	1-P	264	ASN
1	1-P	272	GLN
1	1-P	303	HIS
1	1-P	313	ASN
1	1-P	458	HIS
1	1-Q	58	GLN
1	1-Q	86	ASN
1	1-Q	106	ASN
1	1-Q	113	ASN
1	1-Q	187	GLN
1	1-Q	210	HIS
1	1-Q	218	GLN
1	1-Q	230	HIS
1	1-Q	244	ASN
1	1-Q	264	ASN
1	1-Q	272	GLN
1	1-Q	303	HIS
1	1-Q	313	ASN
1	1-Q	458	HIS
1	1-R	30	HIS
1	1-R	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-R	86	ASN
1	1-R	106	ASN
1	1-R	113	ASN
1	1-R	187	GLN
1	1-R	210	HIS
1	1-R	218	GLN
1	1-R	230	HIS
1	1-R	244	ASN
1	1-R	264	ASN
1	1-R	272	GLN
1	1-R	303	HIS
1	1-R	313	ASN
1	1-R	458	HIS
1	1-S	30	HIS
1	1-S	58	GLN
1	1-S	86	ASN
1	1-S	106	ASN
1	1-S	113	ASN
1	1-S	187	GLN
1	1-S	210	HIS
1	1-S	211	HIS
1	1-S	218	GLN
1	1-S	244	ASN
1	1-S	264	ASN
1	1-S	272	GLN
1	1-S	313	ASN
1	1-S	413	GLN
1	1-S	458	HIS
1	1-T	30	HIS
1	1-T	58	GLN
1	1-T	86	ASN
1	1-T	106	ASN
1	1-T	113	ASN
1	1-T	187	GLN
1	1-T	210	HIS
1	1-T	218	GLN
1	1-T	244	ASN
1	1-T	264	ASN
1	1-T	272	GLN
1	1-T	303	HIS
1	1-T	313	ASN
1	1-T	458	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-U	30	HIS
1	1-U	58	GLN
1	1-U	86	ASN
1	1-U	106	ASN
1	1-U	113	ASN
1	1-U	187	GLN
1	1-U	210	HIS
1	1-U	211	HIS
1	1-U	218	GLN
1	1-U	230	HIS
1	1-U	244	ASN
1	1-U	264	ASN
1	1-U	272	GLN
1	1-U	303	HIS
1	1-U	313	ASN
1	1-U	458	HIS
1	1-V	30	HIS
1	1-V	58	GLN
1	1-V	86	ASN
1	1-V	106	ASN
1	1-V	113	ASN
1	1-V	187	GLN
1	1-V	210	HIS
1	1-V	218	GLN
1	1-V	230	HIS
1	1-V	244	ASN
1	1-V	264	ASN
1	1-V	272	GLN
1	1-V	303	HIS
1	1-V	313	ASN
1	1-V	458	HIS
1	1-W	30	HIS
1	1-W	58	GLN
1	1-W	86	ASN
1	1-W	106	ASN
1	1-W	113	ASN
1	1-W	187	GLN
1	1-W	210	HIS
1	1-W	211	HIS
1	1-W	218	GLN
1	1-W	230	HIS
1	1-W	244	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-W	264	ASN
1	1-W	272	GLN
1	1-W	303	HIS
1	1-W	313	ASN
1	1-W	458	HIS
1	1-X	30	HIS
1	1-X	58	GLN
1	1-X	86	ASN
1	1-X	106	ASN
1	1-X	113	ASN
1	1-X	187	GLN
1	1-X	210	HIS
1	1-X	218	GLN
1	1-X	230	HIS
1	1-X	244	ASN
1	1-X	264	ASN
1	1-X	272	GLN
1	1-X	303	HIS
1	1-X	313	ASN
1	1-X	458	HIS
1	2-A	58	GLN
1	2-A	86	ASN
1	2-A	106	ASN
1	2-A	113	ASN
1	2-A	187	GLN
1	2-A	210	HIS
1	2-A	218	GLN
1	2-A	224	GLN
1	2-A	244	ASN
1	2-A	264	ASN
1	2-A	272	GLN
1	2-A	303	HIS
1	2-A	313	ASN
1	2-A	336	GLN
1	2-A	338	ASN
1	2-A	449	ASN
1	2-A	458	HIS
1	2-B	30	HIS
1	2-B	58	GLN
1	2-B	86	ASN
1	2-B	106	ASN
1	2-B	113	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-B	187	GLN
1	2-B	210	HIS
1	2-B	218	GLN
1	2-B	224	GLN
1	2-B	244	ASN
1	2-B	264	ASN
1	2-B	272	GLN
1	2-B	303	HIS
1	2-B	313	ASN
1	2-B	336	GLN
1	2-B	338	ASN
1	2-B	458	HIS
1	2-C	30	HIS
1	2-C	58	GLN
1	2-C	86	ASN
1	2-C	106	ASN
1	2-C	113	ASN
1	2-C	187	GLN
1	2-C	210	HIS
1	2-C	218	GLN
1	2-C	244	ASN
1	2-C	264	ASN
1	2-C	272	GLN
1	2-C	303	HIS
1	2-C	313	ASN
1	2-C	336	GLN
1	2-C	338	ASN
1	2-C	449	ASN
1	2-C	458	HIS
1	2-D	30	HIS
1	2-D	58	GLN
1	2-D	86	ASN
1	2-D	106	ASN
1	2-D	113	ASN
1	2-D	175	HIS
1	2-D	185	ASN
1	2-D	187	GLN
1	2-D	210	HIS
1	2-D	218	GLN
1	2-D	244	ASN
1	2-D	264	ASN
1	2-D	272	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-D	303	HIS
1	2-D	313	ASN
1	2-D	336	GLN
1	2-D	338	ASN
1	2-D	449	ASN
1	2-D	454	ASN
1	2-D	458	HIS
1	2-E	58	GLN
1	2-E	86	ASN
1	2-E	106	ASN
1	2-E	113	ASN
1	2-E	187	GLN
1	2-E	210	HIS
1	2-E	218	GLN
1	2-E	244	ASN
1	2-E	264	ASN
1	2-E	272	GLN
1	2-E	303	HIS
1	2-E	313	ASN
1	2-E	336	GLN
1	2-E	338	ASN
1	2-E	413	GLN
1	2-E	449	ASN
1	2-E	458	HIS
1	2-F	30	HIS
1	2-F	58	GLN
1	2-F	86	ASN
1	2-F	106	ASN
1	2-F	113	ASN
1	2-F	187	GLN
1	2-F	210	HIS
1	2-F	218	GLN
1	2-F	224	GLN
1	2-F	244	ASN
1	2-F	264	ASN
1	2-F	272	GLN
1	2-F	303	HIS
1	2-F	313	ASN
1	2-F	336	GLN
1	2-F	338	ASN
1	2-F	413	GLN
1	2-F	449	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-F	458	HIS
1	2-G	30	HIS
1	2-G	58	GLN
1	2-G	86	ASN
1	2-G	106	ASN
1	2-G	113	ASN
1	2-G	187	GLN
1	2-G	210	HIS
1	2-G	218	GLN
1	2-G	244	ASN
1	2-G	264	ASN
1	2-G	272	GLN
1	2-G	303	HIS
1	2-G	313	ASN
1	2-G	336	GLN
1	2-G	338	ASN
1	2-G	449	ASN
1	2-G	458	HIS
1	2-H	30	HIS
1	2-H	58	GLN
1	2-H	86	ASN
1	2-H	106	ASN
1	2-H	113	ASN
1	2-H	187	GLN
1	2-H	210	HIS
1	2-H	218	GLN
1	2-H	224	GLN
1	2-H	244	ASN
1	2-H	264	ASN
1	2-H	272	GLN
1	2-H	303	HIS
1	2-H	313	ASN
1	2-H	336	GLN
1	2-H	338	ASN
1	2-H	449	ASN
1	2-H	458	HIS
1	2-I	30	HIS
1	2-I	58	GLN
1	2-I	86	ASN
1	2-I	106	ASN
1	2-I	113	ASN
1	2-I	187	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-I	210	HIS
1	2-I	218	GLN
1	2-I	244	ASN
1	2-I	264	ASN
1	2-I	272	GLN
1	2-I	303	HIS
1	2-I	313	ASN
1	2-I	336	GLN
1	2-I	338	ASN
1	2-I	449	ASN
1	2-I	458	HIS
1	2-J	58	GLN
1	2-J	86	ASN
1	2-J	106	ASN
1	2-J	113	ASN
1	2-J	187	GLN
1	2-J	210	HIS
1	2-J	218	GLN
1	2-J	224	GLN
1	2-J	244	ASN
1	2-J	264	ASN
1	2-J	272	GLN
1	2-J	303	HIS
1	2-J	313	ASN
1	2-J	336	GLN
1	2-J	338	ASN
1	2-J	413	GLN
1	2-J	449	ASN
1	2-J	458	HIS
1	2-K	30	HIS
1	2-K	58	GLN
1	2-K	86	ASN
1	2-K	106	ASN
1	2-K	113	ASN
1	2-K	175	HIS
1	2-K	187	GLN
1	2-K	210	HIS
1	2-K	218	GLN
1	2-K	244	ASN
1	2-K	264	ASN
1	2-K	272	GLN
1	2-K	303	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-K	313	ASN
1	2-K	336	GLN
1	2-K	338	ASN
1	2-K	449	ASN
1	2-K	454	ASN
1	2-K	458	HIS
1	2-L	58	GLN
1	2-L	86	ASN
1	2-L	106	ASN
1	2-L	113	ASN
1	2-L	187	GLN
1	2-L	210	HIS
1	2-L	218	GLN
1	2-L	244	ASN
1	2-L	264	ASN
1	2-L	272	GLN
1	2-L	303	HIS
1	2-L	313	ASN
1	2-L	336	GLN
1	2-L	338	ASN
1	2-L	413	GLN
1	2-L	449	ASN
1	2-L	458	HIS
1	2-M	30	HIS
1	2-M	58	GLN
1	2-M	86	ASN
1	2-M	106	ASN
1	2-M	113	ASN
1	2-M	187	GLN
1	2-M	210	HIS
1	2-M	218	GLN
1	2-M	224	GLN
1	2-M	264	ASN
1	2-M	272	GLN
1	2-M	303	HIS
1	2-M	313	ASN
1	2-M	336	GLN
1	2-M	338	ASN
1	2-M	449	ASN
1	2-M	458	HIS
1	2-N	30	HIS
1	2-N	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-N	86	ASN
1	2-N	106	ASN
1	2-N	113	ASN
1	2-N	187	GLN
1	2-N	210	HIS
1	2-N	218	GLN
1	2-N	224	GLN
1	2-N	244	ASN
1	2-N	264	ASN
1	2-N	272	GLN
1	2-N	303	HIS
1	2-N	313	ASN
1	2-N	336	GLN
1	2-N	338	ASN
1	2-N	449	ASN
1	2-N	458	HIS
1	2-O	30	HIS
1	2-O	58	GLN
1	2-O	86	ASN
1	2-O	106	ASN
1	2-O	113	ASN
1	2-O	187	GLN
1	2-O	210	HIS
1	2-O	218	GLN
1	2-O	244	ASN
1	2-O	264	ASN
1	2-O	272	GLN
1	2-O	303	HIS
1	2-O	313	ASN
1	2-O	336	GLN
1	2-O	338	ASN
1	2-O	413	GLN
1	2-O	449	ASN
1	2-O	458	HIS
1	2-P	30	HIS
1	2-P	58	GLN
1	2-P	86	ASN
1	2-P	106	ASN
1	2-P	113	ASN
1	2-P	187	GLN
1	2-P	210	HIS
1	2-P	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-P	224	GLN
1	2-P	244	ASN
1	2-P	264	ASN
1	2-P	272	GLN
1	2-P	303	HIS
1	2-P	313	ASN
1	2-P	336	GLN
1	2-P	338	ASN
1	2-P	449	ASN
1	2-P	454	ASN
1	2-P	458	HIS
1	2-Q	58	GLN
1	2-Q	86	ASN
1	2-Q	106	ASN
1	2-Q	113	ASN
1	2-Q	187	GLN
1	2-Q	210	HIS
1	2-Q	218	GLN
1	2-Q	244	ASN
1	2-Q	264	ASN
1	2-Q	272	GLN
1	2-Q	303	HIS
1	2-Q	313	ASN
1	2-Q	336	GLN
1	2-Q	338	ASN
1	2-Q	449	ASN
1	2-Q	458	HIS
1	2-R	30	HIS
1	2-R	58	GLN
1	2-R	86	ASN
1	2-R	106	ASN
1	2-R	113	ASN
1	2-R	187	GLN
1	2-R	210	HIS
1	2-R	218	GLN
1	2-R	224	GLN
1	2-R	244	ASN
1	2-R	264	ASN
1	2-R	272	GLN
1	2-R	303	HIS
1	2-R	313	ASN
1	2-R	336	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-R	338	ASN
1	2-R	413	GLN
1	2-R	449	ASN
1	2-R	458	HIS
1	2-S	30	HIS
1	2-S	58	GLN
1	2-S	86	ASN
1	2-S	106	ASN
1	2-S	113	ASN
1	2-S	187	GLN
1	2-S	210	HIS
1	2-S	218	GLN
1	2-S	244	ASN
1	2-S	264	ASN
1	2-S	272	GLN
1	2-S	303	HIS
1	2-S	313	ASN
1	2-S	336	GLN
1	2-S	338	ASN
1	2-S	449	ASN
1	2-S	458	HIS
1	2-T	30	HIS
1	2-T	58	GLN
1	2-T	86	ASN
1	2-T	106	ASN
1	2-T	113	ASN
1	2-T	187	GLN
1	2-T	210	HIS
1	2-T	218	GLN
1	2-T	224	GLN
1	2-T	264	ASN
1	2-T	272	GLN
1	2-T	303	HIS
1	2-T	313	ASN
1	2-T	336	GLN
1	2-T	338	ASN
1	2-T	449	ASN
1	2-T	458	HIS
1	2-U	30	HIS
1	2-U	58	GLN
1	2-U	86	ASN
1	2-U	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-U	113	ASN
1	2-U	187	GLN
1	2-U	210	HIS
1	2-U	218	GLN
1	2-U	244	ASN
1	2-U	264	ASN
1	2-U	272	GLN
1	2-U	303	HIS
1	2-U	313	ASN
1	2-U	336	GLN
1	2-U	338	ASN
1	2-U	413	GLN
1	2-U	449	ASN
1	2-U	458	HIS
1	2-V	30	HIS
1	2-V	58	GLN
1	2-V	86	ASN
1	2-V	106	ASN
1	2-V	113	ASN
1	2-V	187	GLN
1	2-V	210	HIS
1	2-V	218	GLN
1	2-V	244	ASN
1	2-V	264	ASN
1	2-V	272	GLN
1	2-V	303	HIS
1	2-V	313	ASN
1	2-V	336	GLN
1	2-V	338	ASN
1	2-V	413	GLN
1	2-V	449	ASN
1	2-V	458	HIS
1	2-W	30	HIS
1	2-W	58	GLN
1	2-W	86	ASN
1	2-W	106	ASN
1	2-W	113	ASN
1	2-W	187	GLN
1	2-W	210	HIS
1	2-W	218	GLN
1	2-W	224	GLN
1	2-W	264	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-W	272	GLN
1	2-W	303	HIS
1	2-W	313	ASN
1	2-W	336	GLN
1	2-W	338	ASN
1	2-W	449	ASN
1	2-W	458	HIS
1	2-X	30	HIS
1	2-X	58	GLN
1	2-X	86	ASN
1	2-X	106	ASN
1	2-X	113	ASN
1	2-X	187	GLN
1	2-X	210	HIS
1	2-X	218	GLN
1	2-X	244	ASN
1	2-X	264	ASN
1	2-X	272	GLN
1	2-X	303	HIS
1	2-X	313	ASN
1	2-X	336	GLN
1	2-X	338	ASN
1	2-X	413	GLN
1	2-X	449	ASN
1	2-X	458	HIS
1	3-A	86	ASN
1	3-A	106	ASN
1	3-A	113	ASN
1	3-A	175	HIS
1	3-A	187	GLN
1	3-A	210	HIS
1	3-A	218	GLN
1	3-A	230	HIS
1	3-A	244	ASN
1	3-A	248	GLN
1	3-A	264	ASN
1	3-A	272	GLN
1	3-A	313	ASN
1	3-A	338	ASN
1	3-A	409	GLN
1	3-A	413	GLN
1	3-A	436	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-A	458	HIS
1	3-B	30	HIS
1	3-B	86	ASN
1	3-B	106	ASN
1	3-B	113	ASN
1	3-B	175	HIS
1	3-B	185	ASN
1	3-B	187	GLN
1	3-B	210	HIS
1	3-B	211	HIS
1	3-B	218	GLN
1	3-B	230	HIS
1	3-B	244	ASN
1	3-B	248	GLN
1	3-B	264	ASN
1	3-B	272	GLN
1	3-B	313	ASN
1	3-B	338	ASN
1	3-B	409	GLN
1	3-B	436	ASN
1	3-B	458	HIS
1	3-C	30	HIS
1	3-C	86	ASN
1	3-C	106	ASN
1	3-C	113	ASN
1	3-C	175	HIS
1	3-C	187	GLN
1	3-C	210	HIS
1	3-C	211	HIS
1	3-C	218	GLN
1	3-C	230	HIS
1	3-C	244	ASN
1	3-C	248	GLN
1	3-C	264	ASN
1	3-C	272	GLN
1	3-C	313	ASN
1	3-C	338	ASN
1	3-C	409	GLN
1	3-C	436	ASN
1	3-C	458	HIS
1	3-D	30	HIS
1	3-D	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-D	106	ASN
1	3-D	113	ASN
1	3-D	175	HIS
1	3-D	187	GLN
1	3-D	210	HIS
1	3-D	218	GLN
1	3-D	230	HIS
1	3-D	244	ASN
1	3-D	248	GLN
1	3-D	264	ASN
1	3-D	272	GLN
1	3-D	313	ASN
1	3-D	338	ASN
1	3-D	409	GLN
1	3-D	413	GLN
1	3-D	436	ASN
1	3-D	458	HIS
1	3-E	86	ASN
1	3-E	106	ASN
1	3-E	113	ASN
1	3-E	187	GLN
1	3-E	210	HIS
1	3-E	211	HIS
1	3-E	218	GLN
1	3-E	230	HIS
1	3-E	244	ASN
1	3-E	248	GLN
1	3-E	264	ASN
1	3-E	272	GLN
1	3-E	313	ASN
1	3-E	338	ASN
1	3-E	409	GLN
1	3-E	413	GLN
1	3-E	436	ASN
1	3-E	458	HIS
1	3-F	30	HIS
1	3-F	86	ASN
1	3-F	106	ASN
1	3-F	113	ASN
1	3-F	175	HIS
1	3-F	187	GLN
1	3-F	210	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-F	218	GLN
1	3-F	230	HIS
1	3-F	244	ASN
1	3-F	248	GLN
1	3-F	264	ASN
1	3-F	272	GLN
1	3-F	313	ASN
1	3-F	338	ASN
1	3-F	409	GLN
1	3-F	436	ASN
1	3-F	458	HIS
1	3-G	30	HIS
1	3-G	86	ASN
1	3-G	106	ASN
1	3-G	113	ASN
1	3-G	175	HIS
1	3-G	187	GLN
1	3-G	210	HIS
1	3-G	218	GLN
1	3-G	230	HIS
1	3-G	244	ASN
1	3-G	248	GLN
1	3-G	264	ASN
1	3-G	272	GLN
1	3-G	313	ASN
1	3-G	338	ASN
1	3-G	409	GLN
1	3-G	413	GLN
1	3-G	436	ASN
1	3-G	458	HIS
1	3-H	30	HIS
1	3-H	86	ASN
1	3-H	106	ASN
1	3-H	113	ASN
1	3-H	175	HIS
1	3-H	187	GLN
1	3-H	210	HIS
1	3-H	218	GLN
1	3-H	230	HIS
1	3-H	244	ASN
1	3-H	248	GLN
1	3-H	264	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-H	272	GLN
1	3-H	313	ASN
1	3-H	338	ASN
1	3-H	389	GLN
1	3-H	409	GLN
1	3-H	436	ASN
1	3-H	458	HIS
1	3-I	30	HIS
1	3-I	86	ASN
1	3-I	106	ASN
1	3-I	113	ASN
1	3-I	175	HIS
1	3-I	185	ASN
1	3-I	187	GLN
1	3-I	210	HIS
1	3-I	211	HIS
1	3-I	218	GLN
1	3-I	230	HIS
1	3-I	244	ASN
1	3-I	248	GLN
1	3-I	264	ASN
1	3-I	272	GLN
1	3-I	313	ASN
1	3-I	338	ASN
1	3-I	409	GLN
1	3-I	436	ASN
1	3-I	458	HIS
1	3-J	30	HIS
1	3-J	86	ASN
1	3-J	106	ASN
1	3-J	113	ASN
1	3-J	175	HIS
1	3-J	185	ASN
1	3-J	187	GLN
1	3-J	210	HIS
1	3-J	218	GLN
1	3-J	230	HIS
1	3-J	248	GLN
1	3-J	264	ASN
1	3-J	272	GLN
1	3-J	313	ASN
1	3-J	338	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-J	409	GLN
1	3-J	413	GLN
1	3-J	436	ASN
1	3-J	458	HIS
1	3-K	30	HIS
1	3-K	86	ASN
1	3-K	106	ASN
1	3-K	113	ASN
1	3-K	175	HIS
1	3-K	187	GLN
1	3-K	210	HIS
1	3-K	218	GLN
1	3-K	230	HIS
1	3-K	244	ASN
1	3-K	248	GLN
1	3-K	264	ASN
1	3-K	272	GLN
1	3-K	313	ASN
1	3-K	338	ASN
1	3-K	409	GLN
1	3-K	413	GLN
1	3-K	436	ASN
1	3-K	458	HIS
1	3-L	86	ASN
1	3-L	106	ASN
1	3-L	113	ASN
1	3-L	175	HIS
1	3-L	187	GLN
1	3-L	210	HIS
1	3-L	218	GLN
1	3-L	230	HIS
1	3-L	244	ASN
1	3-L	264	ASN
1	3-L	272	GLN
1	3-L	313	ASN
1	3-L	338	ASN
1	3-L	389	GLN
1	3-L	409	GLN
1	3-L	436	ASN
1	3-L	458	HIS
1	3-M	30	HIS
1	3-M	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-M	106	ASN
1	3-M	113	ASN
1	3-M	175	HIS
1	3-M	187	GLN
1	3-M	210	HIS
1	3-M	218	GLN
1	3-M	230	HIS
1	3-M	248	GLN
1	3-M	264	ASN
1	3-M	272	GLN
1	3-M	313	ASN
1	3-M	338	ASN
1	3-M	409	GLN
1	3-M	436	ASN
1	3-M	458	HIS
1	3-N	30	HIS
1	3-N	86	ASN
1	3-N	106	ASN
1	3-N	113	ASN
1	3-N	175	HIS
1	3-N	187	GLN
1	3-N	210	HIS
1	3-N	218	GLN
1	3-N	230	HIS
1	3-N	248	GLN
1	3-N	264	ASN
1	3-N	272	GLN
1	3-N	313	ASN
1	3-N	338	ASN
1	3-N	389	GLN
1	3-N	409	GLN
1	3-N	436	ASN
1	3-N	458	HIS
1	3-O	30	HIS
1	3-O	86	ASN
1	3-O	106	ASN
1	3-O	113	ASN
1	3-O	175	HIS
1	3-O	185	ASN
1	3-O	187	GLN
1	3-O	210	HIS
1	3-O	211	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-O	218	GLN
1	3-O	230	HIS
1	3-O	244	ASN
1	3-O	248	GLN
1	3-O	264	ASN
1	3-O	272	GLN
1	3-O	313	ASN
1	3-O	338	ASN
1	3-O	409	GLN
1	3-O	436	ASN
1	3-O	458	HIS
1	3-P	30	HIS
1	3-P	86	ASN
1	3-P	106	ASN
1	3-P	113	ASN
1	3-P	175	HIS
1	3-P	187	GLN
1	3-P	210	HIS
1	3-P	218	GLN
1	3-P	230	HIS
1	3-P	244	ASN
1	3-P	248	GLN
1	3-P	264	ASN
1	3-P	272	GLN
1	3-P	313	ASN
1	3-P	338	ASN
1	3-P	409	GLN
1	3-P	413	GLN
1	3-P	436	ASN
1	3-P	458	HIS
1	3-Q	86	ASN
1	3-Q	106	ASN
1	3-Q	113	ASN
1	3-Q	187	GLN
1	3-Q	210	HIS
1	3-Q	218	GLN
1	3-Q	230	HIS
1	3-Q	244	ASN
1	3-Q	248	GLN
1	3-Q	264	ASN
1	3-Q	272	GLN
1	3-Q	313	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-Q	338	ASN
1	3-Q	409	GLN
1	3-Q	436	ASN
1	3-Q	458	HIS
1	3-R	30	HIS
1	3-R	86	ASN
1	3-R	106	ASN
1	3-R	113	ASN
1	3-R	175	HIS
1	3-R	185	ASN
1	3-R	187	GLN
1	3-R	210	HIS
1	3-R	211	HIS
1	3-R	218	GLN
1	3-R	230	HIS
1	3-R	244	ASN
1	3-R	248	GLN
1	3-R	264	ASN
1	3-R	272	GLN
1	3-R	313	ASN
1	3-R	338	ASN
1	3-R	389	GLN
1	3-R	409	GLN
1	3-R	436	ASN
1	3-R	458	HIS
1	3-S	30	HIS
1	3-S	86	ASN
1	3-S	106	ASN
1	3-S	113	ASN
1	3-S	175	HIS
1	3-S	187	GLN
1	3-S	210	HIS
1	3-S	218	GLN
1	3-S	230	HIS
1	3-S	244	ASN
1	3-S	248	GLN
1	3-S	264	ASN
1	3-S	272	GLN
1	3-S	313	ASN
1	3-S	338	ASN
1	3-S	389	GLN
1	3-S	409	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-S	436	ASN
1	3-S	458	HIS
1	3-T	30	HIS
1	3-T	86	ASN
1	3-T	106	ASN
1	3-T	113	ASN
1	3-T	175	HIS
1	3-T	187	GLN
1	3-T	210	HIS
1	3-T	218	GLN
1	3-T	230	HIS
1	3-T	248	GLN
1	3-T	264	ASN
1	3-T	272	GLN
1	3-T	313	ASN
1	3-T	338	ASN
1	3-T	409	GLN
1	3-T	436	ASN
1	3-T	458	HIS
1	3-U	30	HIS
1	3-U	86	ASN
1	3-U	106	ASN
1	3-U	113	ASN
1	3-U	175	HIS
1	3-U	185	ASN
1	3-U	187	GLN
1	3-U	210	HIS
1	3-U	218	GLN
1	3-U	230	HIS
1	3-U	244	ASN
1	3-U	248	GLN
1	3-U	264	ASN
1	3-U	272	GLN
1	3-U	313	ASN
1	3-U	338	ASN
1	3-U	409	GLN
1	3-U	436	ASN
1	3-U	458	HIS
1	3-V	30	HIS
1	3-V	86	ASN
1	3-V	106	ASN
1	3-V	113	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-V	185	ASN
1	3-V	187	GLN
1	3-V	210	HIS
1	3-V	211	HIS
1	3-V	218	GLN
1	3-V	230	HIS
1	3-V	248	GLN
1	3-V	264	ASN
1	3-V	272	GLN
1	3-V	313	ASN
1	3-V	338	ASN
1	3-V	409	GLN
1	3-V	413	GLN
1	3-V	436	ASN
1	3-V	458	HIS
1	3-W	30	HIS
1	3-W	86	ASN
1	3-W	106	ASN
1	3-W	113	ASN
1	3-W	175	HIS
1	3-W	187	GLN
1	3-W	210	HIS
1	3-W	218	GLN
1	3-W	230	HIS
1	3-W	248	GLN
1	3-W	264	ASN
1	3-W	272	GLN
1	3-W	313	ASN
1	3-W	338	ASN
1	3-W	409	GLN
1	3-W	436	ASN
1	3-W	458	HIS
1	3-X	30	HIS
1	3-X	86	ASN
1	3-X	106	ASN
1	3-X	113	ASN
1	3-X	175	HIS
1	3-X	187	GLN
1	3-X	210	HIS
1	3-X	218	GLN
1	3-X	230	HIS
1	3-X	244	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-X	264	ASN
1	3-X	272	GLN
1	3-X	313	ASN
1	3-X	338	ASN
1	3-X	409	GLN
1	3-X	436	ASN
1	3-X	458	HIS
1	4-A	86	ASN
1	4-A	106	ASN
1	4-A	113	ASN
1	4-A	175	HIS
1	4-A	218	GLN
1	4-A	244	ASN
1	4-A	264	ASN
1	4-A	272	GLN
1	4-A	296	HIS
1	4-A	313	ASN
1	4-A	331	ASN
1	4-A	389	GLN
1	4-A	413	GLN
1	4-A	458	HIS
1	4-B	30	HIS
1	4-B	86	ASN
1	4-B	106	ASN
1	4-B	113	ASN
1	4-B	175	HIS
1	4-B	218	GLN
1	4-B	244	ASN
1	4-B	264	ASN
1	4-B	272	GLN
1	4-B	296	HIS
1	4-B	313	ASN
1	4-B	331	ASN
1	4-B	389	GLN
1	4-B	413	GLN
1	4-B	458	HIS
1	4-C	30	HIS
1	4-C	86	ASN
1	4-C	106	ASN
1	4-C	113	ASN
1	4-C	175	HIS
1	4-C	185	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-C	218	GLN
1	4-C	244	ASN
1	4-C	264	ASN
1	4-C	272	GLN
1	4-C	296	HIS
1	4-C	313	ASN
1	4-C	331	ASN
1	4-C	389	GLN
1	4-C	413	GLN
1	4-C	458	HIS
1	4-D	30	HIS
1	4-D	86	ASN
1	4-D	106	ASN
1	4-D	113	ASN
1	4-D	175	HIS
1	4-D	211	HIS
1	4-D	218	GLN
1	4-D	244	ASN
1	4-D	264	ASN
1	4-D	272	GLN
1	4-D	296	HIS
1	4-D	313	ASN
1	4-D	331	ASN
1	4-D	389	GLN
1	4-D	413	GLN
1	4-D	458	HIS
1	4-E	86	ASN
1	4-E	106	ASN
1	4-E	113	ASN
1	4-E	175	HIS
1	4-E	218	GLN
1	4-E	244	ASN
1	4-E	264	ASN
1	4-E	272	GLN
1	4-E	296	HIS
1	4-E	313	ASN
1	4-E	331	ASN
1	4-E	458	HIS
1	4-F	30	HIS
1	4-F	86	ASN
1	4-F	106	ASN
1	4-F	113	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-F	175	HIS
1	4-F	211	HIS
1	4-F	218	GLN
1	4-F	244	ASN
1	4-F	264	ASN
1	4-F	272	GLN
1	4-F	296	HIS
1	4-F	313	ASN
1	4-F	331	ASN
1	4-F	338	ASN
1	4-F	389	GLN
1	4-F	413	GLN
1	4-F	458	HIS
1	4-G	30	HIS
1	4-G	86	ASN
1	4-G	106	ASN
1	4-G	113	ASN
1	4-G	175	HIS
1	4-G	211	HIS
1	4-G	218	GLN
1	4-G	244	ASN
1	4-G	264	ASN
1	4-G	272	GLN
1	4-G	296	HIS
1	4-G	313	ASN
1	4-G	389	GLN
1	4-G	413	GLN
1	4-G	458	HIS
1	4-H	30	HIS
1	4-H	86	ASN
1	4-H	106	ASN
1	4-H	113	ASN
1	4-H	175	HIS
1	4-H	218	GLN
1	4-H	244	ASN
1	4-H	264	ASN
1	4-H	272	GLN
1	4-H	296	HIS
1	4-H	313	ASN
1	4-H	389	GLN
1	4-H	413	GLN
1	4-H	458	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-I	30	HIS
1	4-I	86	ASN
1	4-I	106	ASN
1	4-I	113	ASN
1	4-I	175	HIS
1	4-I	211	HIS
1	4-I	218	GLN
1	4-I	244	ASN
1	4-I	264	ASN
1	4-I	272	GLN
1	4-I	296	HIS
1	4-I	313	ASN
1	4-I	331	ASN
1	4-I	389	GLN
1	4-I	413	GLN
1	4-I	458	HIS
1	4-J	86	ASN
1	4-J	106	ASN
1	4-J	113	ASN
1	4-J	175	HIS
1	4-J	211	HIS
1	4-J	218	GLN
1	4-J	264	ASN
1	4-J	272	GLN
1	4-J	296	HIS
1	4-J	313	ASN
1	4-J	331	ASN
1	4-J	389	GLN
1	4-J	413	GLN
1	4-J	458	HIS
1	4-K	30	HIS
1	4-K	86	ASN
1	4-K	106	ASN
1	4-K	113	ASN
1	4-K	175	HIS
1	4-K	211	HIS
1	4-K	218	GLN
1	4-K	244	ASN
1	4-K	264	ASN
1	4-K	272	GLN
1	4-K	296	HIS
1	4-K	313	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-K	331	ASN
1	4-K	389	GLN
1	4-K	413	GLN
1	4-K	454	ASN
1	4-K	458	HIS
1	4-L	86	ASN
1	4-L	106	ASN
1	4-L	113	ASN
1	4-L	175	HIS
1	4-L	218	GLN
1	4-L	244	ASN
1	4-L	264	ASN
1	4-L	272	GLN
1	4-L	296	HIS
1	4-L	313	ASN
1	4-L	413	GLN
1	4-L	458	HIS
1	4-M	30	HIS
1	4-M	86	ASN
1	4-M	106	ASN
1	4-M	113	ASN
1	4-M	175	HIS
1	4-M	211	HIS
1	4-M	218	GLN
1	4-M	264	ASN
1	4-M	272	GLN
1	4-M	296	HIS
1	4-M	313	ASN
1	4-M	331	ASN
1	4-M	389	GLN
1	4-M	413	GLN
1	4-M	458	HIS
1	4-N	30	HIS
1	4-N	86	ASN
1	4-N	106	ASN
1	4-N	113	ASN
1	4-N	175	HIS
1	4-N	211	HIS
1	4-N	218	GLN
1	4-N	244	ASN
1	4-N	264	ASN
1	4-N	272	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-N	296	HIS
1	4-N	313	ASN
1	4-N	331	ASN
1	4-N	389	GLN
1	4-N	413	GLN
1	4-N	458	HIS
1	4-O	30	HIS
1	4-O	86	ASN
1	4-O	106	ASN
1	4-O	113	ASN
1	4-O	175	HIS
1	4-O	218	GLN
1	4-O	244	ASN
1	4-O	264	ASN
1	4-O	272	GLN
1	4-O	296	HIS
1	4-O	313	ASN
1	4-O	331	ASN
1	4-O	389	GLN
1	4-O	413	GLN
1	4-O	458	HIS
1	4-P	30	HIS
1	4-P	86	ASN
1	4-P	106	ASN
1	4-P	113	ASN
1	4-P	175	HIS
1	4-P	211	HIS
1	4-P	218	GLN
1	4-P	244	ASN
1	4-P	264	ASN
1	4-P	272	GLN
1	4-P	296	HIS
1	4-P	313	ASN
1	4-P	331	ASN
1	4-P	389	GLN
1	4-P	413	GLN
1	4-P	454	ASN
1	4-P	458	HIS
1	4-Q	86	ASN
1	4-Q	106	ASN
1	4-Q	113	ASN
1	4-Q	175	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-Q	218	GLN
1	4-Q	244	ASN
1	4-Q	264	ASN
1	4-Q	272	GLN
1	4-Q	296	HIS
1	4-Q	313	ASN
1	4-Q	389	GLN
1	4-Q	413	GLN
1	4-Q	458	HIS
1	4-R	30	HIS
1	4-R	86	ASN
1	4-R	106	ASN
1	4-R	113	ASN
1	4-R	175	HIS
1	4-R	211	HIS
1	4-R	218	GLN
1	4-R	244	ASN
1	4-R	264	ASN
1	4-R	272	GLN
1	4-R	296	HIS
1	4-R	313	ASN
1	4-R	331	ASN
1	4-R	338	ASN
1	4-R	389	GLN
1	4-R	458	HIS
1	4-S	30	HIS
1	4-S	86	ASN
1	4-S	106	ASN
1	4-S	113	ASN
1	4-S	175	HIS
1	4-S	211	HIS
1	4-S	218	GLN
1	4-S	244	ASN
1	4-S	264	ASN
1	4-S	272	GLN
1	4-S	296	HIS
1	4-S	313	ASN
1	4-S	338	ASN
1	4-S	389	GLN
1	4-S	413	GLN
1	4-S	458	HIS
1	4-T	30	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-T	86	ASN
1	4-T	106	ASN
1	4-T	113	ASN
1	4-T	175	HIS
1	4-T	218	GLN
1	4-T	264	ASN
1	4-T	272	GLN
1	4-T	296	HIS
1	4-T	313	ASN
1	4-T	389	GLN
1	4-T	413	GLN
1	4-T	458	HIS
1	4-U	30	HIS
1	4-U	86	ASN
1	4-U	106	ASN
1	4-U	113	ASN
1	4-U	175	HIS
1	4-U	211	HIS
1	4-U	218	GLN
1	4-U	244	ASN
1	4-U	264	ASN
1	4-U	272	GLN
1	4-U	296	HIS
1	4-U	313	ASN
1	4-U	331	ASN
1	4-U	389	GLN
1	4-U	413	GLN
1	4-U	458	HIS
1	4-V	30	HIS
1	4-V	86	ASN
1	4-V	106	ASN
1	4-V	113	ASN
1	4-V	175	HIS
1	4-V	218	GLN
1	4-V	264	ASN
1	4-V	272	GLN
1	4-V	296	HIS
1	4-V	313	ASN
1	4-V	331	ASN
1	4-V	389	GLN
1	4-V	458	HIS
1	4-W	30	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-W	86	ASN
1	4-W	106	ASN
1	4-W	113	ASN
1	4-W	175	HIS
1	4-W	211	HIS
1	4-W	218	GLN
1	4-W	264	ASN
1	4-W	272	GLN
1	4-W	296	HIS
1	4-W	313	ASN
1	4-W	331	ASN
1	4-W	389	GLN
1	4-W	413	GLN
1	4-W	458	HIS
1	4-X	30	HIS
1	4-X	86	ASN
1	4-X	106	ASN
1	4-X	113	ASN
1	4-X	175	HIS
1	4-X	211	HIS
1	4-X	218	GLN
1	4-X	244	ASN
1	4-X	264	ASN
1	4-X	272	GLN
1	4-X	296	HIS
1	4-X	313	ASN
1	4-X	389	GLN
1	4-X	413	GLN
1	4-X	454	ASN
1	4-X	458	HIS
1	5-A	58	GLN
1	5-A	86	ASN
1	5-A	92	HIS
1	5-A	106	ASN
1	5-A	113	ASN
1	5-A	187	GLN
1	5-A	210	HIS
1	5-A	211	HIS
1	5-A	218	GLN
1	5-A	244	ASN
1	5-A	272	GLN
1	5-A	296	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-A	313	ASN
1	5-A	338	ASN
1	5-A	449	ASN
1	5-A	458	HIS
1	5-B	30	HIS
1	5-B	58	GLN
1	5-B	86	ASN
1	5-B	92	HIS
1	5-B	106	ASN
1	5-B	113	ASN
1	5-B	187	GLN
1	5-B	210	HIS
1	5-B	211	HIS
1	5-B	218	GLN
1	5-B	244	ASN
1	5-B	272	GLN
1	5-B	296	HIS
1	5-B	313	ASN
1	5-B	338	ASN
1	5-B	449	ASN
1	5-B	458	HIS
1	5-C	30	HIS
1	5-C	58	GLN
1	5-C	86	ASN
1	5-C	92	HIS
1	5-C	106	ASN
1	5-C	113	ASN
1	5-C	187	GLN
1	5-C	210	HIS
1	5-C	211	HIS
1	5-C	218	GLN
1	5-C	272	GLN
1	5-C	296	HIS
1	5-C	313	ASN
1	5-C	338	ASN
1	5-C	449	ASN
1	5-C	458	HIS
1	5-D	30	HIS
1	5-D	58	GLN
1	5-D	86	ASN
1	5-D	92	HIS
1	5-D	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-D	113	ASN
1	5-D	187	GLN
1	5-D	210	HIS
1	5-D	211	HIS
1	5-D	218	GLN
1	5-D	272	GLN
1	5-D	296	HIS
1	5-D	313	ASN
1	5-D	338	ASN
1	5-D	449	ASN
1	5-D	458	HIS
1	5-E	58	GLN
1	5-E	86	ASN
1	5-E	92	HIS
1	5-E	106	ASN
1	5-E	113	ASN
1	5-E	187	GLN
1	5-E	210	HIS
1	5-E	218	GLN
1	5-E	244	ASN
1	5-E	272	GLN
1	5-E	296	HIS
1	5-E	313	ASN
1	5-E	338	ASN
1	5-E	449	ASN
1	5-E	458	HIS
1	5-F	30	HIS
1	5-F	58	GLN
1	5-F	86	ASN
1	5-F	92	HIS
1	5-F	106	ASN
1	5-F	113	ASN
1	5-F	187	GLN
1	5-F	210	HIS
1	5-F	211	HIS
1	5-F	218	GLN
1	5-F	244	ASN
1	5-F	272	GLN
1	5-F	296	HIS
1	5-F	313	ASN
1	5-F	338	ASN
1	5-F	449	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-F	458	HIS
1	5-G	30	HIS
1	5-G	58	GLN
1	5-G	86	ASN
1	5-G	92	HIS
1	5-G	106	ASN
1	5-G	113	ASN
1	5-G	185	ASN
1	5-G	187	GLN
1	5-G	210	HIS
1	5-G	211	HIS
1	5-G	218	GLN
1	5-G	272	GLN
1	5-G	296	HIS
1	5-G	313	ASN
1	5-G	338	ASN
1	5-G	449	ASN
1	5-G	458	HIS
1	5-H	30	HIS
1	5-H	58	GLN
1	5-H	86	ASN
1	5-H	92	HIS
1	5-H	106	ASN
1	5-H	113	ASN
1	5-H	187	GLN
1	5-H	210	HIS
1	5-H	211	HIS
1	5-H	218	GLN
1	5-H	272	GLN
1	5-H	296	HIS
1	5-H	313	ASN
1	5-H	338	ASN
1	5-H	449	ASN
1	5-H	458	HIS
1	5-I	30	HIS
1	5-I	58	GLN
1	5-I	86	ASN
1	5-I	92	HIS
1	5-I	106	ASN
1	5-I	113	ASN
1	5-I	187	GLN
1	5-I	210	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-I	211	HIS
1	5-I	218	GLN
1	5-I	272	GLN
1	5-I	296	HIS
1	5-I	313	ASN
1	5-I	338	ASN
1	5-I	449	ASN
1	5-I	458	HIS
1	5-J	58	GLN
1	5-J	86	ASN
1	5-J	92	HIS
1	5-J	106	ASN
1	5-J	113	ASN
1	5-J	187	GLN
1	5-J	210	HIS
1	5-J	211	HIS
1	5-J	218	GLN
1	5-J	272	GLN
1	5-J	296	HIS
1	5-J	313	ASN
1	5-J	338	ASN
1	5-J	449	ASN
1	5-J	458	HIS
1	5-K	30	HIS
1	5-K	58	GLN
1	5-K	86	ASN
1	5-K	92	HIS
1	5-K	106	ASN
1	5-K	113	ASN
1	5-K	187	GLN
1	5-K	210	HIS
1	5-K	211	HIS
1	5-K	244	ASN
1	5-K	272	GLN
1	5-K	296	HIS
1	5-K	313	ASN
1	5-K	338	ASN
1	5-K	449	ASN
1	5-K	458	HIS
1	5-L	58	GLN
1	5-L	86	ASN
1	5-L	92	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-L	106	ASN
1	5-L	113	ASN
1	5-L	187	GLN
1	5-L	210	HIS
1	5-L	211	HIS
1	5-L	218	GLN
1	5-L	244	ASN
1	5-L	272	GLN
1	5-L	296	HIS
1	5-L	313	ASN
1	5-L	338	ASN
1	5-L	449	ASN
1	5-L	458	HIS
1	5-M	30	HIS
1	5-M	58	GLN
1	5-M	86	ASN
1	5-M	92	HIS
1	5-M	106	ASN
1	5-M	113	ASN
1	5-M	187	GLN
1	5-M	210	HIS
1	5-M	211	HIS
1	5-M	218	GLN
1	5-M	272	GLN
1	5-M	296	HIS
1	5-M	313	ASN
1	5-M	338	ASN
1	5-M	449	ASN
1	5-M	458	HIS
1	5-N	30	HIS
1	5-N	58	GLN
1	5-N	86	ASN
1	5-N	92	HIS
1	5-N	106	ASN
1	5-N	113	ASN
1	5-N	187	GLN
1	5-N	210	HIS
1	5-N	211	HIS
1	5-N	272	GLN
1	5-N	296	HIS
1	5-N	313	ASN
1	5-N	338	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-N	449	ASN
1	5-N	458	HIS
1	5-O	30	HIS
1	5-O	58	GLN
1	5-O	86	ASN
1	5-O	92	HIS
1	5-O	106	ASN
1	5-O	113	ASN
1	5-O	187	GLN
1	5-O	210	HIS
1	5-O	218	GLN
1	5-O	244	ASN
1	5-O	272	GLN
1	5-O	296	HIS
1	5-O	313	ASN
1	5-O	338	ASN
1	5-O	413	GLN
1	5-O	449	ASN
1	5-O	458	HIS
1	5-P	30	HIS
1	5-P	58	GLN
1	5-P	86	ASN
1	5-P	92	HIS
1	5-P	106	ASN
1	5-P	113	ASN
1	5-P	187	GLN
1	5-P	210	HIS
1	5-P	211	HIS
1	5-P	218	GLN
1	5-P	244	ASN
1	5-P	272	GLN
1	5-P	296	HIS
1	5-P	313	ASN
1	5-P	338	ASN
1	5-P	413	GLN
1	5-P	449	ASN
1	5-P	458	HIS
1	5-Q	58	GLN
1	5-Q	86	ASN
1	5-Q	92	HIS
1	5-Q	106	ASN
1	5-Q	113	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-Q	185	ASN
1	5-Q	187	GLN
1	5-Q	210	HIS
1	5-Q	211	HIS
1	5-Q	218	GLN
1	5-Q	244	ASN
1	5-Q	272	GLN
1	5-Q	296	HIS
1	5-Q	313	ASN
1	5-Q	338	ASN
1	5-Q	449	ASN
1	5-Q	458	HIS
1	5-R	30	HIS
1	5-R	58	GLN
1	5-R	86	ASN
1	5-R	92	HIS
1	5-R	106	ASN
1	5-R	113	ASN
1	5-R	187	GLN
1	5-R	210	HIS
1	5-R	211	HIS
1	5-R	218	GLN
1	5-R	244	ASN
1	5-R	272	GLN
1	5-R	296	HIS
1	5-R	313	ASN
1	5-R	338	ASN
1	5-R	449	ASN
1	5-R	458	HIS
1	5-S	30	HIS
1	5-S	58	GLN
1	5-S	86	ASN
1	5-S	92	HIS
1	5-S	106	ASN
1	5-S	113	ASN
1	5-S	185	ASN
1	5-S	187	GLN
1	5-S	210	HIS
1	5-S	211	HIS
1	5-S	218	GLN
1	5-S	244	ASN
1	5-S	272	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-S	296	HIS
1	5-S	313	ASN
1	5-S	338	ASN
1	5-S	449	ASN
1	5-S	458	HIS
1	5-T	58	GLN
1	5-T	86	ASN
1	5-T	92	HIS
1	5-T	106	ASN
1	5-T	113	ASN
1	5-T	187	GLN
1	5-T	210	HIS
1	5-T	211	HIS
1	5-T	218	GLN
1	5-T	272	GLN
1	5-T	296	HIS
1	5-T	313	ASN
1	5-T	338	ASN
1	5-T	449	ASN
1	5-T	458	HIS
1	5-U	30	HIS
1	5-U	58	GLN
1	5-U	86	ASN
1	5-U	92	HIS
1	5-U	106	ASN
1	5-U	113	ASN
1	5-U	187	GLN
1	5-U	210	HIS
1	5-U	211	HIS
1	5-U	218	GLN
1	5-U	244	ASN
1	5-U	272	GLN
1	5-U	296	HIS
1	5-U	313	ASN
1	5-U	338	ASN
1	5-U	449	ASN
1	5-U	458	HIS
1	5-V	30	HIS
1	5-V	58	GLN
1	5-V	86	ASN
1	5-V	92	HIS
1	5-V	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-V	113	ASN
1	5-V	187	GLN
1	5-V	210	HIS
1	5-V	211	HIS
1	5-V	218	GLN
1	5-V	272	GLN
1	5-V	296	HIS
1	5-V	313	ASN
1	5-V	338	ASN
1	5-V	449	ASN
1	5-V	458	HIS
1	5-W	30	HIS
1	5-W	58	GLN
1	5-W	86	ASN
1	5-W	92	HIS
1	5-W	106	ASN
1	5-W	113	ASN
1	5-W	187	GLN
1	5-W	210	HIS
1	5-W	211	HIS
1	5-W	272	GLN
1	5-W	296	HIS
1	5-W	313	ASN
1	5-W	338	ASN
1	5-W	449	ASN
1	5-W	458	HIS
1	5-X	58	GLN
1	5-X	86	ASN
1	5-X	92	HIS
1	5-X	106	ASN
1	5-X	113	ASN
1	5-X	187	GLN
1	5-X	210	HIS
1	5-X	211	HIS
1	5-X	218	GLN
1	5-X	272	GLN
1	5-X	296	HIS
1	5-X	313	ASN
1	5-X	338	ASN
1	5-X	413	GLN
1	5-X	449	ASN
1	5-X	458	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-A	30	HIS
1	6-A	86	ASN
1	6-A	92	HIS
1	6-A	106	ASN
1	6-A	113	ASN
1	6-A	175	HIS
1	6-A	210	HIS
1	6-A	218	GLN
1	6-A	244	ASN
1	6-A	272	GLN
1	6-A	296	HIS
1	6-A	304	HIS
1	6-A	313	ASN
1	6-A	331	ASN
1	6-A	409	GLN
1	6-A	458	HIS
1	6-B	30	HIS
1	6-B	86	ASN
1	6-B	92	HIS
1	6-B	106	ASN
1	6-B	113	ASN
1	6-B	175	HIS
1	6-B	210	HIS
1	6-B	211	HIS
1	6-B	218	GLN
1	6-B	244	ASN
1	6-B	272	GLN
1	6-B	296	HIS
1	6-B	304	HIS
1	6-B	313	ASN
1	6-B	331	ASN
1	6-B	409	GLN
1	6-B	458	HIS
1	6-C	29	GLN
1	6-C	30	HIS
1	6-C	86	ASN
1	6-C	92	HIS
1	6-C	106	ASN
1	6-C	113	ASN
1	6-C	175	HIS
1	6-C	210	HIS
1	6-C	211	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-C	218	GLN
1	6-C	244	ASN
1	6-C	272	GLN
1	6-C	296	HIS
1	6-C	304	HIS
1	6-C	313	ASN
1	6-C	331	ASN
1	6-C	409	GLN
1	6-C	413	GLN
1	6-C	458	HIS
1	6-D	29	GLN
1	6-D	30	HIS
1	6-D	86	ASN
1	6-D	92	HIS
1	6-D	106	ASN
1	6-D	113	ASN
1	6-D	175	HIS
1	6-D	210	HIS
1	6-D	218	GLN
1	6-D	244	ASN
1	6-D	272	GLN
1	6-D	296	HIS
1	6-D	304	HIS
1	6-D	313	ASN
1	6-D	331	ASN
1	6-D	409	GLN
1	6-D	458	HIS
1	6-E	30	HIS
1	6-E	86	ASN
1	6-E	92	HIS
1	6-E	106	ASN
1	6-E	113	ASN
1	6-E	175	HIS
1	6-E	210	HIS
1	6-E	211	HIS
1	6-E	218	GLN
1	6-E	244	ASN
1	6-E	248	GLN
1	6-E	272	GLN
1	6-E	296	HIS
1	6-E	304	HIS
1	6-E	313	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-E	331	ASN
1	6-E	409	GLN
1	6-E	458	HIS
1	6-F	29	GLN
1	6-F	30	HIS
1	6-F	86	ASN
1	6-F	92	HIS
1	6-F	106	ASN
1	6-F	113	ASN
1	6-F	175	HIS
1	6-F	210	HIS
1	6-F	211	HIS
1	6-F	218	GLN
1	6-F	244	ASN
1	6-F	248	GLN
1	6-F	272	GLN
1	6-F	296	HIS
1	6-F	304	HIS
1	6-F	313	ASN
1	6-F	331	ASN
1	6-F	409	GLN
1	6-F	413	GLN
1	6-F	458	HIS
1	6-G	30	HIS
1	6-G	86	ASN
1	6-G	92	HIS
1	6-G	106	ASN
1	6-G	113	ASN
1	6-G	175	HIS
1	6-G	210	HIS
1	6-G	218	GLN
1	6-G	244	ASN
1	6-G	248	GLN
1	6-G	272	GLN
1	6-G	296	HIS
1	6-G	304	HIS
1	6-G	313	ASN
1	6-G	331	ASN
1	6-G	409	GLN
1	6-G	458	HIS
1	6-H	30	HIS
1	6-H	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-H	92	HIS
1	6-H	106	ASN
1	6-H	113	ASN
1	6-H	175	HIS
1	6-H	210	HIS
1	6-H	211	HIS
1	6-H	218	GLN
1	6-H	248	GLN
1	6-H	272	GLN
1	6-H	296	HIS
1	6-H	304	HIS
1	6-H	313	ASN
1	6-H	331	ASN
1	6-H	409	GLN
1	6-H	458	HIS
1	6-I	30	HIS
1	6-I	86	ASN
1	6-I	92	HIS
1	6-I	106	ASN
1	6-I	113	ASN
1	6-I	175	HIS
1	6-I	210	HIS
1	6-I	211	HIS
1	6-I	218	GLN
1	6-I	244	ASN
1	6-I	272	GLN
1	6-I	296	HIS
1	6-I	304	HIS
1	6-I	313	ASN
1	6-I	331	ASN
1	6-I	409	GLN
1	6-I	413	GLN
1	6-I	458	HIS
1	6-J	30	HIS
1	6-J	86	ASN
1	6-J	92	HIS
1	6-J	106	ASN
1	6-J	113	ASN
1	6-J	175	HIS
1	6-J	210	HIS
1	6-J	218	GLN
1	6-J	272	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-J	296	HIS
1	6-J	304	HIS
1	6-J	313	ASN
1	6-J	331	ASN
1	6-J	409	GLN
1	6-J	413	GLN
1	6-J	458	HIS
1	6-K	30	HIS
1	6-K	86	ASN
1	6-K	92	HIS
1	6-K	106	ASN
1	6-K	113	ASN
1	6-K	175	HIS
1	6-K	210	HIS
1	6-K	218	GLN
1	6-K	244	ASN
1	6-K	272	GLN
1	6-K	296	HIS
1	6-K	304	HIS
1	6-K	313	ASN
1	6-K	331	ASN
1	6-K	409	GLN
1	6-K	458	HIS
1	6-L	30	HIS
1	6-L	86	ASN
1	6-L	92	HIS
1	6-L	106	ASN
1	6-L	113	ASN
1	6-L	175	HIS
1	6-L	210	HIS
1	6-L	211	HIS
1	6-L	218	GLN
1	6-L	244	ASN
1	6-L	272	GLN
1	6-L	296	HIS
1	6-L	304	HIS
1	6-L	313	ASN
1	6-L	331	ASN
1	6-L	409	GLN
1	6-L	458	HIS
1	6-M	30	HIS
1	6-M	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-M	92	HIS
1	6-M	106	ASN
1	6-M	113	ASN
1	6-M	175	HIS
1	6-M	210	HIS
1	6-M	211	HIS
1	6-M	218	GLN
1	6-M	272	GLN
1	6-M	296	HIS
1	6-M	304	HIS
1	6-M	313	ASN
1	6-M	331	ASN
1	6-M	409	GLN
1	6-M	413	GLN
1	6-M	458	HIS
1	6-N	30	HIS
1	6-N	86	ASN
1	6-N	92	HIS
1	6-N	106	ASN
1	6-N	113	ASN
1	6-N	175	HIS
1	6-N	210	HIS
1	6-N	218	GLN
1	6-N	272	GLN
1	6-N	296	HIS
1	6-N	304	HIS
1	6-N	313	ASN
1	6-N	331	ASN
1	6-N	409	GLN
1	6-N	458	HIS
1	6-O	30	HIS
1	6-O	86	ASN
1	6-O	92	HIS
1	6-O	106	ASN
1	6-O	113	ASN
1	6-O	175	HIS
1	6-O	210	HIS
1	6-O	211	HIS
1	6-O	218	GLN
1	6-O	244	ASN
1	6-O	272	GLN
1	6-O	296	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-O	304	HIS
1	6-O	313	ASN
1	6-O	331	ASN
1	6-O	409	GLN
1	6-O	458	HIS
1	6-P	30	HIS
1	6-P	86	ASN
1	6-P	92	HIS
1	6-P	106	ASN
1	6-P	113	ASN
1	6-P	175	HIS
1	6-P	210	HIS
1	6-P	218	GLN
1	6-P	244	ASN
1	6-P	272	GLN
1	6-P	296	HIS
1	6-P	304	HIS
1	6-P	313	ASN
1	6-P	331	ASN
1	6-P	409	GLN
1	6-P	454	ASN
1	6-P	458	HIS
1	6-Q	30	HIS
1	6-Q	86	ASN
1	6-Q	92	HIS
1	6-Q	106	ASN
1	6-Q	113	ASN
1	6-Q	175	HIS
1	6-Q	210	HIS
1	6-Q	218	GLN
1	6-Q	244	ASN
1	6-Q	248	GLN
1	6-Q	272	GLN
1	6-Q	296	HIS
1	6-Q	304	HIS
1	6-Q	313	ASN
1	6-Q	331	ASN
1	6-Q	409	GLN
1	6-Q	458	HIS
1	6-R	29	GLN
1	6-R	30	HIS
1	6-R	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-R	92	HIS
1	6-R	106	ASN
1	6-R	113	ASN
1	6-R	175	HIS
1	6-R	210	HIS
1	6-R	211	HIS
1	6-R	218	GLN
1	6-R	244	ASN
1	6-R	248	GLN
1	6-R	272	GLN
1	6-R	296	HIS
1	6-R	304	HIS
1	6-R	313	ASN
1	6-R	331	ASN
1	6-R	409	GLN
1	6-R	458	HIS
1	6-S	30	HIS
1	6-S	86	ASN
1	6-S	92	HIS
1	6-S	106	ASN
1	6-S	113	ASN
1	6-S	175	HIS
1	6-S	210	HIS
1	6-S	211	HIS
1	6-S	218	GLN
1	6-S	244	ASN
1	6-S	248	GLN
1	6-S	272	GLN
1	6-S	296	HIS
1	6-S	304	HIS
1	6-S	313	ASN
1	6-S	331	ASN
1	6-S	409	GLN
1	6-S	458	HIS
1	6-T	30	HIS
1	6-T	86	ASN
1	6-T	92	HIS
1	6-T	106	ASN
1	6-T	113	ASN
1	6-T	175	HIS
1	6-T	210	HIS
1	6-T	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-T	272	GLN
1	6-T	296	HIS
1	6-T	304	HIS
1	6-T	313	ASN
1	6-T	331	ASN
1	6-T	409	GLN
1	6-T	458	HIS
1	6-U	29	GLN
1	6-U	30	HIS
1	6-U	86	ASN
1	6-U	92	HIS
1	6-U	106	ASN
1	6-U	113	ASN
1	6-U	175	HIS
1	6-U	210	HIS
1	6-U	211	HIS
1	6-U	218	GLN
1	6-U	244	ASN
1	6-U	272	GLN
1	6-U	296	HIS
1	6-U	304	HIS
1	6-U	313	ASN
1	6-U	331	ASN
1	6-U	409	GLN
1	6-U	458	HIS
1	6-V	30	HIS
1	6-V	86	ASN
1	6-V	92	HIS
1	6-V	106	ASN
1	6-V	113	ASN
1	6-V	175	HIS
1	6-V	210	HIS
1	6-V	211	HIS
1	6-V	218	GLN
1	6-V	272	GLN
1	6-V	296	HIS
1	6-V	304	HIS
1	6-V	313	ASN
1	6-V	331	ASN
1	6-V	409	GLN
1	6-V	413	GLN
1	6-V	458	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-W	30	HIS
1	6-W	86	ASN
1	6-W	92	HIS
1	6-W	106	ASN
1	6-W	113	ASN
1	6-W	175	HIS
1	6-W	210	HIS
1	6-W	218	GLN
1	6-W	272	GLN
1	6-W	296	HIS
1	6-W	304	HIS
1	6-W	313	ASN
1	6-W	331	ASN
1	6-W	409	GLN
1	6-W	458	HIS
1	6-X	30	HIS
1	6-X	86	ASN
1	6-X	92	HIS
1	6-X	106	ASN
1	6-X	113	ASN
1	6-X	175	HIS
1	6-X	210	HIS
1	6-X	211	HIS
1	6-X	218	GLN
1	6-X	272	GLN
1	6-X	296	HIS
1	6-X	304	HIS
1	6-X	313	ASN
1	6-X	331	ASN
1	6-X	409	GLN
1	6-X	458	HIS
1	7-A	30	HIS
1	7-A	61	HIS
1	7-A	86	ASN
1	7-A	92	HIS
1	7-A	106	ASN
1	7-A	113	ASN
1	7-A	187	GLN
1	7-A	210	HIS
1	7-A	211	HIS
1	7-A	218	GLN
1	7-A	230	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-A	244	ASN
1	7-A	248	GLN
1	7-A	264	ASN
1	7-A	313	ASN
1	7-A	338	ASN
1	7-A	413	GLN
1	7-A	454	ASN
1	7-A	458	HIS
1	7-B	30	HIS
1	7-B	61	HIS
1	7-B	86	ASN
1	7-B	92	HIS
1	7-B	106	ASN
1	7-B	113	ASN
1	7-B	187	GLN
1	7-B	210	HIS
1	7-B	211	HIS
1	7-B	218	GLN
1	7-B	230	HIS
1	7-B	244	ASN
1	7-B	248	GLN
1	7-B	264	ASN
1	7-B	271	HIS
1	7-B	272	GLN
1	7-B	313	ASN
1	7-B	338	ASN
1	7-B	413	GLN
1	7-B	454	ASN
1	7-B	458	HIS
1	7-C	30	HIS
1	7-C	61	HIS
1	7-C	86	ASN
1	7-C	92	HIS
1	7-C	106	ASN
1	7-C	113	ASN
1	7-C	187	GLN
1	7-C	210	HIS
1	7-C	211	HIS
1	7-C	218	GLN
1	7-C	230	HIS
1	7-C	244	ASN
1	7-C	248	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-C	264	ASN
1	7-C	313	ASN
1	7-C	338	ASN
1	7-C	413	GLN
1	7-C	454	ASN
1	7-C	458	HIS
1	7-D	30	HIS
1	7-D	61	HIS
1	7-D	86	ASN
1	7-D	92	HIS
1	7-D	106	ASN
1	7-D	113	ASN
1	7-D	187	GLN
1	7-D	210	HIS
1	7-D	218	GLN
1	7-D	230	HIS
1	7-D	244	ASN
1	7-D	248	GLN
1	7-D	264	ASN
1	7-D	272	GLN
1	7-D	313	ASN
1	7-D	338	ASN
1	7-D	413	GLN
1	7-D	454	ASN
1	7-D	458	HIS
1	7-E	61	HIS
1	7-E	86	ASN
1	7-E	92	HIS
1	7-E	106	ASN
1	7-E	113	ASN
1	7-E	187	GLN
1	7-E	210	HIS
1	7-E	211	HIS
1	7-E	218	GLN
1	7-E	230	HIS
1	7-E	244	ASN
1	7-E	248	GLN
1	7-E	264	ASN
1	7-E	313	ASN
1	7-E	338	ASN
1	7-E	413	GLN
1	7-E	454	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-E	458	HIS
1	7-F	30	HIS
1	7-F	86	ASN
1	7-F	92	HIS
1	7-F	106	ASN
1	7-F	113	ASN
1	7-F	187	GLN
1	7-F	210	HIS
1	7-F	211	HIS
1	7-F	218	GLN
1	7-F	230	HIS
1	7-F	244	ASN
1	7-F	248	GLN
1	7-F	264	ASN
1	7-F	313	ASN
1	7-F	338	ASN
1	7-F	413	GLN
1	7-F	454	ASN
1	7-F	458	HIS
1	7-G	30	HIS
1	7-G	61	HIS
1	7-G	86	ASN
1	7-G	92	HIS
1	7-G	106	ASN
1	7-G	113	ASN
1	7-G	185	ASN
1	7-G	187	GLN
1	7-G	210	HIS
1	7-G	218	GLN
1	7-G	230	HIS
1	7-G	244	ASN
1	7-G	248	GLN
1	7-G	264	ASN
1	7-G	313	ASN
1	7-G	338	ASN
1	7-G	413	GLN
1	7-G	454	ASN
1	7-G	458	HIS
1	7-H	30	HIS
1	7-H	61	HIS
1	7-H	86	ASN
1	7-H	92	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-H	106	ASN
1	7-H	113	ASN
1	7-H	187	GLN
1	7-H	210	HIS
1	7-H	211	HIS
1	7-H	218	GLN
1	7-H	230	HIS
1	7-H	244	ASN
1	7-H	248	GLN
1	7-H	264	ASN
1	7-H	313	ASN
1	7-H	338	ASN
1	7-H	413	GLN
1	7-H	454	ASN
1	7-H	458	HIS
1	7-I	30	HIS
1	7-I	61	HIS
1	7-I	86	ASN
1	7-I	92	HIS
1	7-I	106	ASN
1	7-I	113	ASN
1	7-I	187	GLN
1	7-I	210	HIS
1	7-I	211	HIS
1	7-I	218	GLN
1	7-I	230	HIS
1	7-I	244	ASN
1	7-I	248	GLN
1	7-I	264	ASN
1	7-I	272	GLN
1	7-I	313	ASN
1	7-I	338	ASN
1	7-I	413	GLN
1	7-I	454	ASN
1	7-I	458	HIS
1	7-J	30	HIS
1	7-J	61	HIS
1	7-J	86	ASN
1	7-J	92	HIS
1	7-J	106	ASN
1	7-J	113	ASN
1	7-J	187	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-J	210	HIS
1	7-J	211	HIS
1	7-J	218	GLN
1	7-J	230	HIS
1	7-J	244	ASN
1	7-J	248	GLN
1	7-J	264	ASN
1	7-J	271	HIS
1	7-J	313	ASN
1	7-J	338	ASN
1	7-J	413	GLN
1	7-J	454	ASN
1	7-J	458	HIS
1	7-K	30	HIS
1	7-K	61	HIS
1	7-K	86	ASN
1	7-K	92	HIS
1	7-K	106	ASN
1	7-K	113	ASN
1	7-K	185	ASN
1	7-K	187	GLN
1	7-K	210	HIS
1	7-K	218	GLN
1	7-K	230	HIS
1	7-K	244	ASN
1	7-K	248	GLN
1	7-K	264	ASN
1	7-K	313	ASN
1	7-K	338	ASN
1	7-K	413	GLN
1	7-K	454	ASN
1	7-K	458	HIS
1	7-L	61	HIS
1	7-L	86	ASN
1	7-L	92	HIS
1	7-L	106	ASN
1	7-L	113	ASN
1	7-L	187	GLN
1	7-L	210	HIS
1	7-L	211	HIS
1	7-L	218	GLN
1	7-L	230	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-L	244	ASN
1	7-L	248	GLN
1	7-L	264	ASN
1	7-L	271	HIS
1	7-L	313	ASN
1	7-L	338	ASN
1	7-L	413	GLN
1	7-L	454	ASN
1	7-L	458	HIS
1	7-M	30	HIS
1	7-M	61	HIS
1	7-M	86	ASN
1	7-M	92	HIS
1	7-M	106	ASN
1	7-M	113	ASN
1	7-M	187	GLN
1	7-M	210	HIS
1	7-M	211	HIS
1	7-M	218	GLN
1	7-M	230	HIS
1	7-M	248	GLN
1	7-M	264	ASN
1	7-M	313	ASN
1	7-M	338	ASN
1	7-M	413	GLN
1	7-M	454	ASN
1	7-M	458	HIS
1	7-N	30	HIS
1	7-N	61	HIS
1	7-N	86	ASN
1	7-N	92	HIS
1	7-N	106	ASN
1	7-N	113	ASN
1	7-N	187	GLN
1	7-N	210	HIS
1	7-N	211	HIS
1	7-N	218	GLN
1	7-N	230	HIS
1	7-N	248	GLN
1	7-N	264	ASN
1	7-N	271	HIS
1	7-N	313	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-N	338	ASN
1	7-N	413	GLN
1	7-N	454	ASN
1	7-N	458	HIS
1	7-O	30	HIS
1	7-O	61	HIS
1	7-O	86	ASN
1	7-O	92	HIS
1	7-O	106	ASN
1	7-O	113	ASN
1	7-O	187	GLN
1	7-O	210	HIS
1	7-O	211	HIS
1	7-O	218	GLN
1	7-O	230	HIS
1	7-O	244	ASN
1	7-O	248	GLN
1	7-O	264	ASN
1	7-O	313	ASN
1	7-O	338	ASN
1	7-O	413	GLN
1	7-O	454	ASN
1	7-O	458	HIS
1	7-P	30	HIS
1	7-P	61	HIS
1	7-P	86	ASN
1	7-P	92	HIS
1	7-P	106	ASN
1	7-P	113	ASN
1	7-P	187	GLN
1	7-P	210	HIS
1	7-P	218	GLN
1	7-P	230	HIS
1	7-P	244	ASN
1	7-P	248	GLN
1	7-P	264	ASN
1	7-P	313	ASN
1	7-P	338	ASN
1	7-P	413	GLN
1	7-P	454	ASN
1	7-P	458	HIS
1	7-Q	61	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-Q	86	ASN
1	7-Q	92	HIS
1	7-Q	106	ASN
1	7-Q	113	ASN
1	7-Q	187	GLN
1	7-Q	210	HIS
1	7-Q	211	HIS
1	7-Q	218	GLN
1	7-Q	230	HIS
1	7-Q	244	ASN
1	7-Q	248	GLN
1	7-Q	264	ASN
1	7-Q	313	ASN
1	7-Q	338	ASN
1	7-Q	413	GLN
1	7-Q	454	ASN
1	7-Q	458	HIS
1	7-R	30	HIS
1	7-R	86	ASN
1	7-R	92	HIS
1	7-R	106	ASN
1	7-R	113	ASN
1	7-R	187	GLN
1	7-R	210	HIS
1	7-R	211	HIS
1	7-R	218	GLN
1	7-R	230	HIS
1	7-R	244	ASN
1	7-R	248	GLN
1	7-R	264	ASN
1	7-R	313	ASN
1	7-R	338	ASN
1	7-R	413	GLN
1	7-R	454	ASN
1	7-R	458	HIS
1	7-S	30	HIS
1	7-S	61	HIS
1	7-S	86	ASN
1	7-S	92	HIS
1	7-S	106	ASN
1	7-S	113	ASN
1	7-S	185	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-S	187	GLN
1	7-S	210	HIS
1	7-S	211	HIS
1	7-S	218	GLN
1	7-S	230	HIS
1	7-S	244	ASN
1	7-S	248	GLN
1	7-S	264	ASN
1	7-S	313	ASN
1	7-S	338	ASN
1	7-S	413	GLN
1	7-S	454	ASN
1	7-S	458	HIS
1	7-T	30	HIS
1	7-T	61	HIS
1	7-T	86	ASN
1	7-T	92	HIS
1	7-T	106	ASN
1	7-T	113	ASN
1	7-T	187	GLN
1	7-T	210	HIS
1	7-T	211	HIS
1	7-T	218	GLN
1	7-T	230	HIS
1	7-T	244	ASN
1	7-T	248	GLN
1	7-T	264	ASN
1	7-T	313	ASN
1	7-T	338	ASN
1	7-T	413	GLN
1	7-T	454	ASN
1	7-T	458	HIS
1	7-U	30	HIS
1	7-U	61	HIS
1	7-U	86	ASN
1	7-U	92	HIS
1	7-U	106	ASN
1	7-U	113	ASN
1	7-U	187	GLN
1	7-U	210	HIS
1	7-U	211	HIS
1	7-U	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-U	230	HIS
1	7-U	244	ASN
1	7-U	248	GLN
1	7-U	264	ASN
1	7-U	313	ASN
1	7-U	338	ASN
1	7-U	413	GLN
1	7-U	454	ASN
1	7-U	458	HIS
1	7-V	30	HIS
1	7-V	61	HIS
1	7-V	86	ASN
1	7-V	92	HIS
1	7-V	106	ASN
1	7-V	113	ASN
1	7-V	187	GLN
1	7-V	210	HIS
1	7-V	211	HIS
1	7-V	218	GLN
1	7-V	230	HIS
1	7-V	248	GLN
1	7-V	264	ASN
1	7-V	271	HIS
1	7-V	313	ASN
1	7-V	338	ASN
1	7-V	413	GLN
1	7-V	454	ASN
1	7-V	458	HIS
1	7-W	30	HIS
1	7-W	61	HIS
1	7-W	86	ASN
1	7-W	92	HIS
1	7-W	106	ASN
1	7-W	113	ASN
1	7-W	187	GLN
1	7-W	210	HIS
1	7-W	211	HIS
1	7-W	218	GLN
1	7-W	230	HIS
1	7-W	248	GLN
1	7-W	264	ASN
1	7-W	313	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-W	338	ASN
1	7-W	413	GLN
1	7-W	454	ASN
1	7-W	458	HIS
1	7-X	30	HIS
1	7-X	61	HIS
1	7-X	86	ASN
1	7-X	92	HIS
1	7-X	106	ASN
1	7-X	113	ASN
1	7-X	187	GLN
1	7-X	210	HIS
1	7-X	211	HIS
1	7-X	218	GLN
1	7-X	230	HIS
1	7-X	244	ASN
1	7-X	248	GLN
1	7-X	264	ASN
1	7-X	271	HIS
1	7-X	313	ASN
1	7-X	338	ASN
1	7-X	413	GLN
1	7-X	454	ASN
1	7-X	458	HIS
1	8-A	58	GLN
1	8-A	61	HIS
1	8-A	86	ASN
1	8-A	92	HIS
1	8-A	106	ASN
1	8-A	113	ASN
1	8-A	187	GLN
1	8-A	210	HIS
1	8-A	218	GLN
1	8-A	222	ASN
1	8-A	244	ASN
1	8-A	248	GLN
1	8-A	296	HIS
1	8-A	303	HIS
1	8-A	313	ASN
1	8-A	409	GLN
1	8-A	458	HIS
1	8-B	30	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-B	58	GLN
1	8-B	61	HIS
1	8-B	86	ASN
1	8-B	92	HIS
1	8-B	106	ASN
1	8-B	113	ASN
1	8-B	187	GLN
1	8-B	210	HIS
1	8-B	218	GLN
1	8-B	222	ASN
1	8-B	244	ASN
1	8-B	296	HIS
1	8-B	303	HIS
1	8-B	313	ASN
1	8-B	409	GLN
1	8-B	458	HIS
1	8-C	30	HIS
1	8-C	58	GLN
1	8-C	61	HIS
1	8-C	86	ASN
1	8-C	92	HIS
1	8-C	106	ASN
1	8-C	113	ASN
1	8-C	175	HIS
1	8-C	187	GLN
1	8-C	210	HIS
1	8-C	218	GLN
1	8-C	222	ASN
1	8-C	244	ASN
1	8-C	296	HIS
1	8-C	303	HIS
1	8-C	313	ASN
1	8-C	336	GLN
1	8-C	409	GLN
1	8-C	458	HIS
1	8-D	30	HIS
1	8-D	58	GLN
1	8-D	61	HIS
1	8-D	86	ASN
1	8-D	92	HIS
1	8-D	106	ASN
1	8-D	113	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-D	175	HIS
1	8-D	185	ASN
1	8-D	187	GLN
1	8-D	210	HIS
1	8-D	218	GLN
1	8-D	222	ASN
1	8-D	224	GLN
1	8-D	244	ASN
1	8-D	248	GLN
1	8-D	296	HIS
1	8-D	303	HIS
1	8-D	313	ASN
1	8-D	409	GLN
1	8-D	458	HIS
1	8-E	58	GLN
1	8-E	61	HIS
1	8-E	86	ASN
1	8-E	92	HIS
1	8-E	106	ASN
1	8-E	113	ASN
1	8-E	187	GLN
1	8-E	210	HIS
1	8-E	218	GLN
1	8-E	222	ASN
1	8-E	244	ASN
1	8-E	296	HIS
1	8-E	303	HIS
1	8-E	313	ASN
1	8-E	409	GLN
1	8-E	458	HIS
1	8-F	30	HIS
1	8-F	58	GLN
1	8-F	61	HIS
1	8-F	86	ASN
1	8-F	92	HIS
1	8-F	106	ASN
1	8-F	113	ASN
1	8-F	175	HIS
1	8-F	187	GLN
1	8-F	210	HIS
1	8-F	218	GLN
1	8-F	222	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-F	224	GLN
1	8-F	244	ASN
1	8-F	296	HIS
1	8-F	303	HIS
1	8-F	313	ASN
1	8-F	409	GLN
1	8-F	458	HIS
1	8-G	30	HIS
1	8-G	58	GLN
1	8-G	61	HIS
1	8-G	86	ASN
1	8-G	92	HIS
1	8-G	106	ASN
1	8-G	113	ASN
1	8-G	175	HIS
1	8-G	185	ASN
1	8-G	187	GLN
1	8-G	210	HIS
1	8-G	218	GLN
1	8-G	222	ASN
1	8-G	244	ASN
1	8-G	248	GLN
1	8-G	296	HIS
1	8-G	303	HIS
1	8-G	313	ASN
1	8-G	409	GLN
1	8-G	458	HIS
1	8-H	30	HIS
1	8-H	58	GLN
1	8-H	61	HIS
1	8-H	86	ASN
1	8-H	92	HIS
1	8-H	106	ASN
1	8-H	113	ASN
1	8-H	187	GLN
1	8-H	210	HIS
1	8-H	218	GLN
1	8-H	222	ASN
1	8-H	224	GLN
1	8-H	244	ASN
1	8-H	296	HIS
1	8-H	303	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-H	313	ASN
1	8-H	336	GLN
1	8-H	409	GLN
1	8-H	458	HIS
1	8-I	30	HIS
1	8-I	58	GLN
1	8-I	61	HIS
1	8-I	86	ASN
1	8-I	92	HIS
1	8-I	106	ASN
1	8-I	113	ASN
1	8-I	187	GLN
1	8-I	210	HIS
1	8-I	218	GLN
1	8-I	222	ASN
1	8-I	224	GLN
1	8-I	244	ASN
1	8-I	248	GLN
1	8-I	296	HIS
1	8-I	303	HIS
1	8-I	313	ASN
1	8-I	409	GLN
1	8-I	458	HIS
1	8-J	58	GLN
1	8-J	61	HIS
1	8-J	86	ASN
1	8-J	92	HIS
1	8-J	106	ASN
1	8-J	113	ASN
1	8-J	187	GLN
1	8-J	210	HIS
1	8-J	218	GLN
1	8-J	222	ASN
1	8-J	296	HIS
1	8-J	303	HIS
1	8-J	313	ASN
1	8-J	336	GLN
1	8-J	409	GLN
1	8-J	458	HIS
1	8-K	30	HIS
1	8-K	58	GLN
1	8-K	61	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-K	86	ASN
1	8-K	92	HIS
1	8-K	106	ASN
1	8-K	113	ASN
1	8-K	175	HIS
1	8-K	187	GLN
1	8-K	210	HIS
1	8-K	218	GLN
1	8-K	222	ASN
1	8-K	224	GLN
1	8-K	244	ASN
1	8-K	296	HIS
1	8-K	303	HIS
1	8-K	313	ASN
1	8-K	409	GLN
1	8-K	458	HIS
1	8-L	58	GLN
1	8-L	61	HIS
1	8-L	86	ASN
1	8-L	92	HIS
1	8-L	106	ASN
1	8-L	113	ASN
1	8-L	187	GLN
1	8-L	210	HIS
1	8-L	218	GLN
1	8-L	222	ASN
1	8-L	244	ASN
1	8-L	296	HIS
1	8-L	303	HIS
1	8-L	313	ASN
1	8-L	409	GLN
1	8-L	458	HIS
1	8-M	30	HIS
1	8-M	58	GLN
1	8-M	61	HIS
1	8-M	86	ASN
1	8-M	92	HIS
1	8-M	106	ASN
1	8-M	113	ASN
1	8-M	187	GLN
1	8-M	210	HIS
1	8-M	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-M	222	ASN
1	8-M	248	GLN
1	8-M	296	HIS
1	8-M	303	HIS
1	8-M	313	ASN
1	8-M	336	GLN
1	8-M	409	GLN
1	8-M	458	HIS
1	8-N	30	HIS
1	8-N	58	GLN
1	8-N	61	HIS
1	8-N	86	ASN
1	8-N	92	HIS
1	8-N	106	ASN
1	8-N	113	ASN
1	8-N	187	GLN
1	8-N	210	HIS
1	8-N	218	GLN
1	8-N	222	ASN
1	8-N	224	GLN
1	8-N	244	ASN
1	8-N	296	HIS
1	8-N	303	HIS
1	8-N	313	ASN
1	8-N	409	GLN
1	8-N	458	HIS
1	8-O	30	HIS
1	8-O	58	GLN
1	8-O	61	HIS
1	8-O	86	ASN
1	8-O	92	HIS
1	8-O	106	ASN
1	8-O	113	ASN
1	8-O	187	GLN
1	8-O	210	HIS
1	8-O	218	GLN
1	8-O	222	ASN
1	8-O	224	GLN
1	8-O	244	ASN
1	8-O	296	HIS
1	8-O	303	HIS
1	8-O	313	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-O	336	GLN
1	8-O	409	GLN
1	8-O	458	HIS
1	8-P	30	HIS
1	8-P	58	GLN
1	8-P	61	HIS
1	8-P	86	ASN
1	8-P	92	HIS
1	8-P	106	ASN
1	8-P	113	ASN
1	8-P	175	HIS
1	8-P	187	GLN
1	8-P	210	HIS
1	8-P	218	GLN
1	8-P	222	ASN
1	8-P	224	GLN
1	8-P	244	ASN
1	8-P	296	HIS
1	8-P	303	HIS
1	8-P	313	ASN
1	8-P	409	GLN
1	8-P	458	HIS
1	8-Q	58	GLN
1	8-Q	61	HIS
1	8-Q	86	ASN
1	8-Q	92	HIS
1	8-Q	106	ASN
1	8-Q	113	ASN
1	8-Q	187	GLN
1	8-Q	210	HIS
1	8-Q	218	GLN
1	8-Q	222	ASN
1	8-Q	244	ASN
1	8-Q	296	HIS
1	8-Q	303	HIS
1	8-Q	313	ASN
1	8-Q	409	GLN
1	8-Q	458	HIS
1	8-R	30	HIS
1	8-R	58	GLN
1	8-R	61	HIS
1	8-R	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-R	92	HIS
1	8-R	106	ASN
1	8-R	113	ASN
1	8-R	175	HIS
1	8-R	187	GLN
1	8-R	210	HIS
1	8-R	218	GLN
1	8-R	222	ASN
1	8-R	224	GLN
1	8-R	244	ASN
1	8-R	296	HIS
1	8-R	303	HIS
1	8-R	313	ASN
1	8-R	409	GLN
1	8-R	458	HIS
1	8-S	30	HIS
1	8-S	58	GLN
1	8-S	61	HIS
1	8-S	86	ASN
1	8-S	92	HIS
1	8-S	106	ASN
1	8-S	113	ASN
1	8-S	187	GLN
1	8-S	210	HIS
1	8-S	218	GLN
1	8-S	222	ASN
1	8-S	244	ASN
1	8-S	248	GLN
1	8-S	296	HIS
1	8-S	303	HIS
1	8-S	313	ASN
1	8-S	409	GLN
1	8-S	458	HIS
1	8-T	58	GLN
1	8-T	61	HIS
1	8-T	86	ASN
1	8-T	92	HIS
1	8-T	106	ASN
1	8-T	113	ASN
1	8-T	187	GLN
1	8-T	210	HIS
1	8-T	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-T	222	ASN
1	8-T	224	GLN
1	8-T	244	ASN
1	8-T	296	HIS
1	8-T	303	HIS
1	8-T	313	ASN
1	8-T	336	GLN
1	8-T	409	GLN
1	8-T	458	HIS
1	8-U	30	HIS
1	8-U	58	GLN
1	8-U	61	HIS
1	8-U	86	ASN
1	8-U	92	HIS
1	8-U	106	ASN
1	8-U	113	ASN
1	8-U	175	HIS
1	8-U	187	GLN
1	8-U	210	HIS
1	8-U	218	GLN
1	8-U	222	ASN
1	8-U	224	GLN
1	8-U	244	ASN
1	8-U	248	GLN
1	8-U	296	HIS
1	8-U	303	HIS
1	8-U	313	ASN
1	8-U	409	GLN
1	8-U	458	HIS
1	8-V	30	HIS
1	8-V	58	GLN
1	8-V	61	HIS
1	8-V	86	ASN
1	8-V	92	HIS
1	8-V	106	ASN
1	8-V	113	ASN
1	8-V	187	GLN
1	8-V	210	HIS
1	8-V	218	GLN
1	8-V	222	ASN
1	8-V	224	GLN
1	8-V	244	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-V	296	HIS
1	8-V	303	HIS
1	8-V	313	ASN
1	8-V	336	GLN
1	8-V	409	GLN
1	8-V	458	HIS
1	8-W	30	HIS
1	8-W	58	GLN
1	8-W	61	HIS
1	8-W	86	ASN
1	8-W	92	HIS
1	8-W	106	ASN
1	8-W	113	ASN
1	8-W	175	HIS
1	8-W	187	GLN
1	8-W	210	HIS
1	8-W	218	GLN
1	8-W	222	ASN
1	8-W	224	GLN
1	8-W	296	HIS
1	8-W	303	HIS
1	8-W	313	ASN
1	8-W	409	GLN
1	8-W	458	HIS
1	8-X	30	HIS
1	8-X	58	GLN
1	8-X	61	HIS
1	8-X	86	ASN
1	8-X	92	HIS
1	8-X	106	ASN
1	8-X	113	ASN
1	8-X	187	GLN
1	8-X	210	HIS
1	8-X	218	GLN
1	8-X	222	ASN
1	8-X	224	GLN
1	8-X	244	ASN
1	8-X	296	HIS
1	8-X	303	HIS
1	8-X	313	ASN
1	8-X	409	GLN
1	8-X	458	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-A	61	HIS
1	9-A	86	ASN
1	9-A	106	ASN
1	9-A	113	ASN
1	9-A	187	GLN
1	9-A	210	HIS
1	9-A	211	HIS
1	9-A	218	GLN
1	9-A	244	ASN
1	9-A	248	GLN
1	9-A	264	ASN
1	9-A	272	GLN
1	9-A	313	ASN
1	9-A	338	ASN
1	9-A	504	ASN
1	9-A	389	GLN
1	9-A	458	HIS
1	9-B	30	HIS
1	9-B	61	HIS
1	9-B	86	ASN
1	9-B	106	ASN
1	9-B	113	ASN
1	9-B	187	GLN
1	9-B	210	HIS
1	9-B	211	HIS
1	9-B	218	GLN
1	9-B	244	ASN
1	9-B	248	GLN
1	9-B	264	ASN
1	9-B	272	GLN
1	9-B	313	ASN
1	9-B	338	ASN
1	9-B	504	ASN
1	9-B	389	GLN
1	9-B	458	HIS
1	9-C	30	HIS
1	9-C	61	HIS
1	9-C	86	ASN
1	9-C	106	ASN
1	9-C	113	ASN
1	9-C	175	HIS
1	9-C	187	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-C	210	HIS
1	9-C	211	HIS
1	9-C	218	GLN
1	9-C	244	ASN
1	9-C	248	GLN
1	9-C	264	ASN
1	9-C	272	GLN
1	9-C	313	ASN
1	9-C	338	ASN
1	9-C	504	ASN
1	9-C	389	GLN
1	9-C	458	HIS
1	9-D	30	HIS
1	9-D	61	HIS
1	9-D	86	ASN
1	9-D	106	ASN
1	9-D	113	ASN
1	9-D	175	HIS
1	9-D	187	GLN
1	9-D	210	HIS
1	9-D	211	HIS
1	9-D	218	GLN
1	9-D	244	ASN
1	9-D	248	GLN
1	9-D	264	ASN
1	9-D	272	GLN
1	9-D	313	ASN
1	9-D	338	ASN
1	9-D	504	ASN
1	9-D	389	GLN
1	9-D	458	HIS
1	9-E	61	HIS
1	9-E	86	ASN
1	9-E	106	ASN
1	9-E	113	ASN
1	9-E	187	GLN
1	9-E	210	HIS
1	9-E	218	GLN
1	9-E	244	ASN
1	9-E	248	GLN
1	9-E	264	ASN
1	9-E	272	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-E	313	ASN
1	9-E	338	ASN
1	9-E	504	ASN
1	9-E	389	GLN
1	9-E	458	HIS
1	9-F	30	HIS
1	9-F	61	HIS
1	9-F	86	ASN
1	9-F	106	ASN
1	9-F	113	ASN
1	9-F	175	HIS
1	9-F	187	GLN
1	9-F	210	HIS
1	9-F	211	HIS
1	9-F	218	GLN
1	9-F	248	GLN
1	9-F	264	ASN
1	9-F	272	GLN
1	9-F	313	ASN
1	9-F	338	ASN
1	9-F	504	ASN
1	9-F	389	GLN
1	9-F	458	HIS
1	9-G	30	HIS
1	9-G	61	HIS
1	9-G	86	ASN
1	9-G	106	ASN
1	9-G	113	ASN
1	9-G	175	HIS
1	9-G	187	GLN
1	9-G	210	HIS
1	9-G	211	HIS
1	9-G	218	GLN
1	9-G	244	ASN
1	9-G	248	GLN
1	9-G	264	ASN
1	9-G	272	GLN
1	9-G	313	ASN
1	9-G	338	ASN
1	9-G	504	ASN
1	9-G	389	GLN
1	9-G	458	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-H	30	HIS
1	9-H	61	HIS
1	9-H	86	ASN
1	9-H	106	ASN
1	9-H	113	ASN
1	9-H	175	HIS
1	9-H	187	GLN
1	9-H	210	HIS
1	9-H	218	GLN
1	9-H	244	ASN
1	9-H	248	GLN
1	9-H	264	ASN
1	9-H	272	GLN
1	9-H	313	ASN
1	9-H	338	ASN
1	9-H	504	ASN
1	9-H	389	GLN
1	9-H	458	HIS
1	9-I	30	HIS
1	9-I	61	HIS
1	9-I	86	ASN
1	9-I	106	ASN
1	9-I	113	ASN
1	9-I	187	GLN
1	9-I	210	HIS
1	9-I	211	HIS
1	9-I	218	GLN
1	9-I	244	ASN
1	9-I	248	GLN
1	9-I	264	ASN
1	9-I	272	GLN
1	9-I	313	ASN
1	9-I	338	ASN
1	9-I	504	ASN
1	9-I	389	GLN
1	9-I	458	HIS
1	9-J	61	HIS
1	9-J	86	ASN
1	9-J	106	ASN
1	9-J	113	ASN
1	9-J	175	HIS
1	9-J	187	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-J	210	HIS
1	9-J	211	HIS
1	9-J	218	GLN
1	9-J	244	ASN
1	9-J	248	GLN
1	9-J	264	ASN
1	9-J	272	GLN
1	9-J	313	ASN
1	9-J	338	ASN
1	9-J	504	ASN
1	9-J	389	GLN
1	9-J	458	HIS
1	9-K	30	HIS
1	9-K	61	HIS
1	9-K	86	ASN
1	9-K	106	ASN
1	9-K	113	ASN
1	9-K	175	HIS
1	9-K	187	GLN
1	9-K	210	HIS
1	9-K	211	HIS
1	9-K	218	GLN
1	9-K	244	ASN
1	9-K	248	GLN
1	9-K	264	ASN
1	9-K	272	GLN
1	9-K	313	ASN
1	9-K	338	ASN
1	9-K	504	ASN
1	9-K	389	GLN
1	9-K	458	HIS
1	9-L	61	HIS
1	9-L	86	ASN
1	9-L	106	ASN
1	9-L	113	ASN
1	9-L	187	GLN
1	9-L	210	HIS
1	9-L	211	HIS
1	9-L	218	GLN
1	9-L	244	ASN
1	9-L	248	GLN
1	9-L	264	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-L	272	GLN
1	9-L	313	ASN
1	9-L	338	ASN
1	9-L	504	ASN
1	9-L	389	GLN
1	9-L	458	HIS
1	9-M	30	HIS
1	9-M	61	HIS
1	9-M	86	ASN
1	9-M	106	ASN
1	9-M	113	ASN
1	9-M	187	GLN
1	9-M	210	HIS
1	9-M	211	HIS
1	9-M	218	GLN
1	9-M	244	ASN
1	9-M	248	GLN
1	9-M	264	ASN
1	9-M	272	GLN
1	9-M	313	ASN
1	9-M	338	ASN
1	9-M	504	ASN
1	9-M	389	GLN
1	9-M	458	HIS
1	9-N	30	HIS
1	9-N	61	HIS
1	9-N	86	ASN
1	9-N	106	ASN
1	9-N	113	ASN
1	9-N	187	GLN
1	9-N	210	HIS
1	9-N	211	HIS
1	9-N	218	GLN
1	9-N	244	ASN
1	9-N	248	GLN
1	9-N	264	ASN
1	9-N	272	GLN
1	9-N	313	ASN
1	9-N	338	ASN
1	9-N	504	ASN
1	9-N	389	GLN
1	9-N	458	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-O	30	HIS
1	9-O	61	HIS
1	9-O	86	ASN
1	9-O	106	ASN
1	9-O	113	ASN
1	9-O	175	HIS
1	9-O	187	GLN
1	9-O	210	HIS
1	9-O	218	GLN
1	9-O	244	ASN
1	9-O	248	GLN
1	9-O	264	ASN
1	9-O	272	GLN
1	9-O	313	ASN
1	9-O	338	ASN
1	9-O	504	ASN
1	9-O	389	GLN
1	9-O	458	HIS
1	9-P	30	HIS
1	9-P	61	HIS
1	9-P	86	ASN
1	9-P	106	ASN
1	9-P	113	ASN
1	9-P	175	HIS
1	9-P	187	GLN
1	9-P	210	HIS
1	9-P	211	HIS
1	9-P	218	GLN
1	9-P	244	ASN
1	9-P	248	GLN
1	9-P	264	ASN
1	9-P	272	GLN
1	9-P	313	ASN
1	9-P	338	ASN
1	9-P	504	ASN
1	9-P	389	GLN
1	9-P	458	HIS
1	9-Q	61	HIS
1	9-Q	86	ASN
1	9-Q	106	ASN
1	9-Q	113	ASN
1	9-Q	175	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-Q	210	HIS
1	9-Q	211	HIS
1	9-Q	218	GLN
1	9-Q	244	ASN
1	9-Q	248	GLN
1	9-Q	264	ASN
1	9-Q	272	GLN
1	9-Q	313	ASN
1	9-Q	338	ASN
1	9-Q	504	ASN
1	9-Q	389	GLN
1	9-Q	458	HIS
1	9-R	30	HIS
1	9-R	61	HIS
1	9-R	86	ASN
1	9-R	106	ASN
1	9-R	113	ASN
1	9-R	175	HIS
1	9-R	187	GLN
1	9-R	210	HIS
1	9-R	211	HIS
1	9-R	218	GLN
1	9-R	244	ASN
1	9-R	248	GLN
1	9-R	264	ASN
1	9-R	272	GLN
1	9-R	313	ASN
1	9-R	338	ASN
1	9-R	504	ASN
1	9-R	389	GLN
1	9-R	458	HIS
1	9-S	30	HIS
1	9-S	61	HIS
1	9-S	86	ASN
1	9-S	106	ASN
1	9-S	113	ASN
1	9-S	175	HIS
1	9-S	187	GLN
1	9-S	210	HIS
1	9-S	211	HIS
1	9-S	218	GLN
1	9-S	244	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-S	248	GLN
1	9-S	264	ASN
1	9-S	272	GLN
1	9-S	313	ASN
1	9-S	338	ASN
1	9-S	504	ASN
1	9-S	389	GLN
1	9-S	458	HIS
1	9-T	30	HIS
1	9-T	61	HIS
1	9-T	86	ASN
1	9-T	106	ASN
1	9-T	113	ASN
1	9-T	187	GLN
1	9-T	210	HIS
1	9-T	211	HIS
1	9-T	218	GLN
1	9-T	248	GLN
1	9-T	264	ASN
1	9-T	272	GLN
1	9-T	313	ASN
1	9-T	338	ASN
1	9-T	504	ASN
1	9-T	389	GLN
1	9-T	458	HIS
1	9-U	30	HIS
1	9-U	61	HIS
1	9-U	86	ASN
1	9-U	106	ASN
1	9-U	113	ASN
1	9-U	175	HIS
1	9-U	187	GLN
1	9-U	210	HIS
1	9-U	211	HIS
1	9-U	218	GLN
1	9-U	244	ASN
1	9-U	248	GLN
1	9-U	264	ASN
1	9-U	272	GLN
1	9-U	313	ASN
1	9-U	338	ASN
1	9-U	504	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-U	389	GLN
1	9-U	458	HIS
1	9-V	30	HIS
1	9-V	61	HIS
1	9-V	86	ASN
1	9-V	106	ASN
1	9-V	113	ASN
1	9-V	187	GLN
1	9-V	210	HIS
1	9-V	211	HIS
1	9-V	218	GLN
1	9-V	244	ASN
1	9-V	248	GLN
1	9-V	264	ASN
1	9-V	272	GLN
1	9-V	313	ASN
1	9-V	338	ASN
1	9-V	504	ASN
1	9-V	389	GLN
1	9-V	458	HIS
1	9-W	30	HIS
1	9-W	61	HIS
1	9-W	86	ASN
1	9-W	106	ASN
1	9-W	113	ASN
1	9-W	175	HIS
1	9-W	187	GLN
1	9-W	210	HIS
1	9-W	211	HIS
1	9-W	218	GLN
1	9-W	248	GLN
1	9-W	264	ASN
1	9-W	272	GLN
1	9-W	313	ASN
1	9-W	338	ASN
1	9-W	504	ASN
1	9-W	389	GLN
1	9-W	458	HIS
1	9-X	61	HIS
1	9-X	86	ASN
1	9-X	106	ASN
1	9-X	113	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-X	187	GLN
1	9-X	210	HIS
1	9-X	211	HIS
1	9-X	218	GLN
1	9-X	244	ASN
1	9-X	248	GLN
1	9-X	264	ASN
1	9-X	272	GLN
1	9-X	313	ASN
1	9-X	338	ASN
1	9-X	504	ASN
1	9-X	389	GLN
1	9-X	458	HIS
1	10-A	30	HIS
1	10-A	86	ASN
1	10-A	92	HIS
1	10-A	106	ASN
1	10-A	113	ASN
1	10-A	175	HIS
1	10-A	187	GLN
1	10-A	210	HIS
1	10-A	211	HIS
1	10-A	218	GLN
1	10-A	264	ASN
1	10-A	304	HIS
1	10-A	313	ASN
1	10-A	458	HIS
1	10-B	30	HIS
1	10-B	86	ASN
1	10-B	92	HIS
1	10-B	106	ASN
1	10-B	113	ASN
1	10-B	175	HIS
1	10-B	185	ASN
1	10-B	187	GLN
1	10-B	210	HIS
1	10-B	211	HIS
1	10-B	218	GLN
1	10-B	224	GLN
1	10-B	244	ASN
1	10-B	264	ASN
1	10-B	304	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-B	313	ASN
1	10-B	336	GLN
1	10-B	413	GLN
1	10-B	458	HIS
1	10-C	30	HIS
1	10-C	86	ASN
1	10-C	92	HIS
1	10-C	106	ASN
1	10-C	113	ASN
1	10-C	175	HIS
1	10-C	185	ASN
1	10-C	187	GLN
1	10-C	210	HIS
1	10-C	211	HIS
1	10-C	218	GLN
1	10-C	224	GLN
1	10-C	244	ASN
1	10-C	264	ASN
1	10-C	304	HIS
1	10-C	313	ASN
1	10-C	413	GLN
1	10-C	458	HIS
1	10-D	30	HIS
1	10-D	86	ASN
1	10-D	92	HIS
1	10-D	106	ASN
1	10-D	113	ASN
1	10-D	175	HIS
1	10-D	187	GLN
1	10-D	210	HIS
1	10-D	211	HIS
1	10-D	218	GLN
1	10-D	244	ASN
1	10-D	264	ASN
1	10-D	304	HIS
1	10-D	313	ASN
1	10-D	454	ASN
1	10-D	458	HIS
1	10-E	30	HIS
1	10-E	86	ASN
1	10-E	92	HIS
1	10-E	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-E	113	ASN
1	10-E	175	HIS
1	10-E	187	GLN
1	10-E	210	HIS
1	10-E	211	HIS
1	10-E	218	GLN
1	10-E	244	ASN
1	10-E	264	ASN
1	10-E	304	HIS
1	10-E	313	ASN
1	10-E	458	HIS
1	10-F	30	HIS
1	10-F	86	ASN
1	10-F	92	HIS
1	10-F	106	ASN
1	10-F	113	ASN
1	10-F	175	HIS
1	10-F	187	GLN
1	10-F	210	HIS
1	10-F	211	HIS
1	10-F	218	GLN
1	10-F	264	ASN
1	10-F	304	HIS
1	10-F	313	ASN
1	10-F	336	GLN
1	10-F	413	GLN
1	10-F	458	HIS
1	10-G	30	HIS
1	10-G	86	ASN
1	10-G	92	HIS
1	10-G	106	ASN
1	10-G	113	ASN
1	10-G	175	HIS
1	10-G	187	GLN
1	10-G	210	HIS
1	10-G	211	HIS
1	10-G	218	GLN
1	10-G	244	ASN
1	10-G	264	ASN
1	10-G	304	HIS
1	10-G	313	ASN
1	10-G	458	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-H	30	HIS
1	10-H	86	ASN
1	10-H	92	HIS
1	10-H	106	ASN
1	10-H	113	ASN
1	10-H	175	HIS
1	10-H	187	GLN
1	10-H	210	HIS
1	10-H	211	HIS
1	10-H	218	GLN
1	10-H	224	GLN
1	10-H	264	ASN
1	10-H	304	HIS
1	10-H	313	ASN
1	10-H	458	HIS
1	10-I	30	HIS
1	10-I	86	ASN
1	10-I	92	HIS
1	10-I	106	ASN
1	10-I	113	ASN
1	10-I	175	HIS
1	10-I	185	ASN
1	10-I	187	GLN
1	10-I	210	HIS
1	10-I	211	HIS
1	10-I	218	GLN
1	10-I	264	ASN
1	10-I	304	HIS
1	10-I	313	ASN
1	10-I	413	GLN
1	10-I	458	HIS
1	10-J	30	HIS
1	10-J	86	ASN
1	10-J	92	HIS
1	10-J	106	ASN
1	10-J	113	ASN
1	10-J	175	HIS
1	10-J	185	ASN
1	10-J	187	GLN
1	10-J	210	HIS
1	10-J	211	HIS
1	10-J	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-J	224	GLN
1	10-J	264	ASN
1	10-J	304	HIS
1	10-J	313	ASN
1	10-J	454	ASN
1	10-J	458	HIS
1	10-K	30	HIS
1	10-K	86	ASN
1	10-K	92	HIS
1	10-K	106	ASN
1	10-K	113	ASN
1	10-K	175	HIS
1	10-K	187	GLN
1	10-K	210	HIS
1	10-K	218	GLN
1	10-K	244	ASN
1	10-K	264	ASN
1	10-K	304	HIS
1	10-K	313	ASN
1	10-K	454	ASN
1	10-K	458	HIS
1	10-L	86	ASN
1	10-L	92	HIS
1	10-L	106	ASN
1	10-L	113	ASN
1	10-L	175	HIS
1	10-L	187	GLN
1	10-L	210	HIS
1	10-L	211	HIS
1	10-L	218	GLN
1	10-L	244	ASN
1	10-L	264	ASN
1	10-L	304	HIS
1	10-L	313	ASN
1	10-L	413	GLN
1	10-L	458	HIS
1	10-M	30	HIS
1	10-M	86	ASN
1	10-M	92	HIS
1	10-M	106	ASN
1	10-M	113	ASN
1	10-M	175	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-M	187	GLN
1	10-M	210	HIS
1	10-M	211	HIS
1	10-M	218	GLN
1	10-M	264	ASN
1	10-M	304	HIS
1	10-M	313	ASN
1	10-M	336	GLN
1	10-M	413	GLN
1	10-M	458	HIS
1	10-N	30	HIS
1	10-N	86	ASN
1	10-N	92	HIS
1	10-N	106	ASN
1	10-N	113	ASN
1	10-N	175	HIS
1	10-N	185	ASN
1	10-N	187	GLN
1	10-N	210	HIS
1	10-N	211	HIS
1	10-N	218	GLN
1	10-N	244	ASN
1	10-N	264	ASN
1	10-N	304	HIS
1	10-N	313	ASN
1	10-N	336	GLN
1	10-N	458	HIS
1	10-O	30	HIS
1	10-O	86	ASN
1	10-O	92	HIS
1	10-O	106	ASN
1	10-O	113	ASN
1	10-O	175	HIS
1	10-O	185	ASN
1	10-O	187	GLN
1	10-O	210	HIS
1	10-O	211	HIS
1	10-O	218	GLN
1	10-O	224	GLN
1	10-O	244	ASN
1	10-O	264	ASN
1	10-O	304	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-O	313	ASN
1	10-O	413	GLN
1	10-O	454	ASN
1	10-O	458	HIS
1	10-P	30	HIS
1	10-P	86	ASN
1	10-P	92	HIS
1	10-P	106	ASN
1	10-P	113	ASN
1	10-P	175	HIS
1	10-P	187	GLN
1	10-P	210	HIS
1	10-P	211	HIS
1	10-P	218	GLN
1	10-P	264	ASN
1	10-P	304	HIS
1	10-P	313	ASN
1	10-P	454	ASN
1	10-P	458	HIS
1	10-Q	30	HIS
1	10-Q	86	ASN
1	10-Q	92	HIS
1	10-Q	106	ASN
1	10-Q	113	ASN
1	10-Q	175	HIS
1	10-Q	187	GLN
1	10-Q	210	HIS
1	10-Q	211	HIS
1	10-Q	218	GLN
1	10-Q	264	ASN
1	10-Q	304	HIS
1	10-Q	313	ASN
1	10-Q	413	GLN
1	10-Q	458	HIS
1	10-R	30	HIS
1	10-R	86	ASN
1	10-R	92	HIS
1	10-R	106	ASN
1	10-R	113	ASN
1	10-R	175	HIS
1	10-R	187	GLN
1	10-R	210	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-R	211	HIS
1	10-R	218	GLN
1	10-R	244	ASN
1	10-R	264	ASN
1	10-R	304	HIS
1	10-R	313	ASN
1	10-R	336	GLN
1	10-R	413	GLN
1	10-R	458	HIS
1	10-S	30	HIS
1	10-S	86	ASN
1	10-S	92	HIS
1	10-S	106	ASN
1	10-S	113	ASN
1	10-S	175	HIS
1	10-S	187	GLN
1	10-S	210	HIS
1	10-S	211	HIS
1	10-S	218	GLN
1	10-S	244	ASN
1	10-S	264	ASN
1	10-S	304	HIS
1	10-S	313	ASN
1	10-S	336	GLN
1	10-S	413	GLN
1	10-S	458	HIS
1	10-T	30	HIS
1	10-T	86	ASN
1	10-T	92	HIS
1	10-T	106	ASN
1	10-T	113	ASN
1	10-T	175	HIS
1	10-T	187	GLN
1	10-T	210	HIS
1	10-T	211	HIS
1	10-T	218	GLN
1	10-T	224	GLN
1	10-T	264	ASN
1	10-T	304	HIS
1	10-T	313	ASN
1	10-T	458	HIS
1	10-U	30	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-U	86	ASN
1	10-U	92	HIS
1	10-U	106	ASN
1	10-U	113	ASN
1	10-U	175	HIS
1	10-U	185	ASN
1	10-U	187	GLN
1	10-U	210	HIS
1	10-U	211	HIS
1	10-U	218	GLN
1	10-U	264	ASN
1	10-U	304	HIS
1	10-U	313	ASN
1	10-U	458	HIS
1	10-V	30	HIS
1	10-V	86	ASN
1	10-V	92	HIS
1	10-V	106	ASN
1	10-V	113	ASN
1	10-V	175	HIS
1	10-V	185	ASN
1	10-V	187	GLN
1	10-V	210	HIS
1	10-V	211	HIS
1	10-V	218	GLN
1	10-V	224	GLN
1	10-V	264	ASN
1	10-V	304	HIS
1	10-V	313	ASN
1	10-V	454	ASN
1	10-V	458	HIS
1	10-W	30	HIS
1	10-W	86	ASN
1	10-W	92	HIS
1	10-W	106	ASN
1	10-W	113	ASN
1	10-W	175	HIS
1	10-W	187	GLN
1	10-W	210	HIS
1	10-W	218	GLN
1	10-W	264	ASN
1	10-W	304	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-W	313	ASN
1	10-W	458	HIS
1	10-X	30	HIS
1	10-X	86	ASN
1	10-X	92	HIS
1	10-X	106	ASN
1	10-X	113	ASN
1	10-X	175	HIS
1	10-X	187	GLN
1	10-X	210	HIS
1	10-X	211	HIS
1	10-X	218	GLN
1	10-X	264	ASN
1	10-X	304	HIS
1	10-X	313	ASN
1	10-X	413	GLN
1	10-X	458	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 720 ligands modelled in this entry, 240 are monoatomic - leaving 480 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	9-I	7491	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	2-G	7487	-	25,25,25	4.09	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	10-G	7487	-	25,25,25	4.09	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	2-P	7506	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	9-R	7510	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-A	7475	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	9-N	7502	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	9-A	7475	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	8-K	7496	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	5-L	7498	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	9-S	7511	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	1-U	7515	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	7-V	7518	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	7-H	7489	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	2-K	7496	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	7-E	7484	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	9-Q	7508	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	1-J	7493	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	5-A	7475	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	2-P	7505	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	6-C	7480	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	1-M	7500	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	7-F	7485	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	4-J	7493	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-N	7502	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	6-O	7503	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	8-U	7515	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	5-B	7477	-	25,25,25	4.11	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	4-D	7481	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	3-S	7511	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	8-R	7509	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	4-R	7509	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	5-C	7480	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	3-H	7490	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	7-R	7509	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	8-R	7510	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	7-Q	7508	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	6-R	7510	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	2-A	7476	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	7-W	7520	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	3-I	7491	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	1-P	7506	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	5-S	7511	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	10-S	7511	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	4-J	7494	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	5-D	7481	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	10-H	7490	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	10-M	7499	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	9-J	7493	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	8-T	7514	-	12,12,12	3.40	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	2-L	7497	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	8-U	7516	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	9-M	7500	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	1-D	7482	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	1-Q	7507	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	5-I	7491	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	10-P	7506	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	3-K	7496	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	5-N	7501	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	1-P	7505	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	7-T	7513	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	4-C	7479	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	9-T	7513	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	7-I	7491	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	6-A	7476	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	4-M	7499	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	8-J	7493	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	3-P	7505	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	4-H	7490	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	3-F	7485	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	2-K	7495	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	2-R	7509	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	3-T	7513	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	5-P	7505	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	9-K	7496	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	9-R	7509	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	8-G	7487	-	25,25,25	4.09	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	6-I	7492	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	6-D	7482	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	1-W	7519	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	7-G	7487	-	25,25,25	4.09	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-C	7480	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	5-W	7519	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	1-U	7516	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	8-H	7490	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	6-C	7479	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	5-G	7488	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	6-E	7484	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	10-K	7495	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	10-B	7478	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	1-F	7486	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	1-N	7502	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	4-L	7497	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	2-I	7492	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	1-D	7481	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	10-U	7516	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	4-X	7522	-	12,12,12	3.39	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	4-A	7475	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	8-Q	7508	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	1-V	7518	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	10-J	7493	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	7-N	7501	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	10-N	7501	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	2-T	7513	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	10-X	7521	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	9-N	7501	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	4-Q	7508	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	9-W	7519	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	5-H	7490	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	10-C	7479	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	5-O	7504	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	9-X	7521	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	7-V	7517	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	8-L	7498	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	7-C	7479	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	9-K	7495	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	10-P	7505	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	9-F	7486	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	2-B	7477	-	25,25,25	4.11	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-X	7522	-	12,12,12	3.39	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	1-T	7514	-	12,12,12	3.40	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	3-R	7510	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-X	7521	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	2-H	7490	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	8-A	7475	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	6-M	7499	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	2-L	7498	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	2-V	7517	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	10-F	7486	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	1-L	7497	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	7-O	7503	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	8-V	7518	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	10-C	7480	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	4-P	7505	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	4-L	7498	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	8-C	7479	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	1-W	7520	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	10-I	7492	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	5-W	7520	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	3-U	7516	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	6-R	7509	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	8-D	7481	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	2-C	7480	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	3-B	7478	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	3-U	7515	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	10-M	7500	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	3-X	7521	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	8-K	7495	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	1-Q	7508	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	2-V	7518	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	6-H	7490	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	9-X	7522	-	12,12,12	3.39	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	8-J	7494	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	1-A	7475	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	9-G	7488	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	4-B	7477	-	25,25,25	4.11	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	6-Q	7508	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	9-L	7497	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-E	7484	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	5-B	7478	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	1-I	7492	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	4-V	7518	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	1-S	7512	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	7-U	7515	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	2-W	7520	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	3-D	7481	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	5-V	7517	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	9-W	7520	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	4-V	7517	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	3-S	7512	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	1-L	7498	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	3-E	7483	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	2-B	7478	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	1-T	7513	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	6-L	7497	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	8-P	7505	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	10-D	7481	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	6-K	7495	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	10-Q	7507	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	8-S	7511	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	3-M	7499	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	10-E	7484	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	6-H	7489	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	7-S	7512	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	6-J	7493	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	10-T	7513	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	5-V	7518	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	1-B	7477	-	25,25,25	4.11	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	8-T	7513	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	3-G	7487	-	25,25,25	4.09	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	9-S	7512	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	8-I	7491	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	4-N	7501	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	2-X	7522	-	12,12,12	3.39	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	6-B	7478	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	3-L	7497	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	8-A	7476	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	5-D	7482	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	9-L	7498	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	4-K	7495	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	10-E	7483	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	5-N	7502	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	5-S	7512	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	1-S	7511	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	10-A	7476	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	5-K	7495	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	4-S	7511	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	9-C	7480	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	8-I	7492	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	4-U	7516	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	6-G	7487	-	25,25,25	4.09	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-W	7520	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	2-U	7516	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	7-C	7480	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	1-K	7496	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	10-L	7497	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	9-B	7478	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	10-S	7512	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	4-C	7480	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	9-B	7477	-	25,25,25	4.11	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	6-K	7496	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	3-C	7479	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	8-M	7499	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	4-F	7485	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	1-N	7501	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	4-R	7510	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	8-W	7519	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	10-W	7520	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	8-E	7484	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	9-P	7506	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	7-L	7497	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	8-G	7488	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	8-F	7485	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	3-R	7509	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	4-T	7513	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	6-L	7498	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	5-F	7486	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	5-G	7487	-	25,25,25	4.09	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	7-H	7490	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	9-O	7503	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	1-X	7522	-	12,12,12	3.39	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	8-X	7521	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	8-L	7497	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	5-K	7496	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-I	7491	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	8-C	7480	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	10-X	7522	-	12,12,12	3.39	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	10-A	7475	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	1-G	7488	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	4-G	7488	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	6-N	7501	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	8-X	7522	-	12,12,12	3.39	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	1-K	7495	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	3-V	7517	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	5-F	7485	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-O	7504	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	5-T	7513	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	2-F	7486	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	3-A	7476	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-N	7501	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	2-H	7489	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	5-A	7476	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	5-U	7515	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	4-A	7476	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	8-E	7483	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	6-M	7500	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	6-D	7481	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	10-F	7485	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	4-S	7512	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	9-V	7517	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	3-D	7482	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	4-H	7489	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	1-X	7521	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	3-N	7501	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	5-X	7521	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	2-E	7484	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	4-X	7521	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-V	7518	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	8-H	7489	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	7-B	7478	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	7-D	7482	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	1-E	7484	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	7-N	7502	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	10-B	7477	-	25,25,25	4.11	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	8-W	7520	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	2-Q	7507	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	3-Q	7507	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	1-A	7476	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	4-D	7482	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	2-G	7488	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	10-O	7504	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	4-Q	7507	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	2-O	7503	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	4-F	7486	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	2-C	7479	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	10-N	7502	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	6-U	7516	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	8-D	7482	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	8-F	7486	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	8-N	7502	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	7-R	7510	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	10-D	7482	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-E	7483	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	3-K	7495	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	8-B	7477	-	25,25,25	4.11	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	5-E	7483	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	3-O	7503	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	6-X	7521	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	5-O	7503	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	2-N	7502	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	1-I	7491	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	9-H	7489	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	1-H	7489	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	5-H	7489	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	4-I	7491	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	9-H	7490	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	5-R	7510	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	9-U	7516	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	6-W	7519	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	2-J	7494	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	8-N	7501	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	7-E	7483	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	7-O	7504	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	7-A	7476	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	6-B	7477	-	25,25,25	4.11	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	10-K	7496	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	2-D	7482	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	4-W	7519	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-Q	7508	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	5-P	7506	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	9-D	7482	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	3-J	7493	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	10-O	7503	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	6-P	7506	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	6-X	7522	-	12,12,12	3.39	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	4-N	7502	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	7-L	7498	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	9-F	7485	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	7-M	7499	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	3-A	7475	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	1-C	7479	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	4-I	7492	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	5-C	7479	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	5-J	7493	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	6-Q	7507	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	1-V	7517	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	5-J	7494	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	5-M	7500	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	7-I	7492	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	1-H	7490	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	7-J	7493	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	7-X	7522	-	12,12,12	3.39	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	3-B	7477	-	25,25,25	4.11	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	4-U	7515	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-J	7494	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	4-B	7478	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	9-D	7481	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	9-U	7515	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-P	7506	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	4-E	7483	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	6-W	7520	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	1-C	7480	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	4-O	7503	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	7-U	7516	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	7-K	7496	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-F	7485	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	9-J	7494	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	5-R	7509	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	6-J	7494	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-W	7519	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	6-I	7491	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	4-E	7484	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	10-R	7510	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-M	7499	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	3-H	7489	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-L	7498	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	1-F	7485	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	2-T	7514	-	12,12,12	3.40	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	6-A	7475	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	6-V	7518	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	4-W	7520	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	10-H	7489	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	9-G	7487	-	25,25,25	4.09	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	6-F	7486	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	2-O	7504	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	10-G	7488	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	6-V	7517	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	4-O	7504	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	5-U	7516	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	8-O	7503	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	1-B	7478	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	4-T	7514	-	12,12,12	3.40	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	9-P	7505	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	1-O	7504	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	1-R	7509	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	5-E	7484	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	7-T	7514	-	12,12,12	3.40	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	10-U	7515	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	6-O	7504	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	3-F	7486	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	3-M	7500	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	9-C	7479	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	9-E	7483	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	9-O	7504	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	9-A	7476	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	5-Q	7508	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	1-M	7499	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	7-A	7475	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	5-M	7499	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	8-S	7512	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	7-B	7477	-	25,25,25	4.11	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	8-V	7517	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	10-I	7491	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	7-M	7500	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	9-I	7492	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	1-J	7494	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	1-E	7483	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	5-Q	7507	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	7-S	7511	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	10-J	7494	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	10-V	7517	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	10-L	7498	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
3	AMP	7-D	7481	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	6-N	7502	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	6 (35%)
4	CIT	3-T	7514	-	12,12,12	3.40	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	1-O	7503	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	6-S	7511	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	9-E	7484	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	6-G	7488	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	5-T	7514	-	12,12,12	3.40	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	7-K	7495	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	4-K	7496	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	4-P	7506	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	9-V	7518	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	7-J	7494	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	4-G	7487	-	25,25,25	4.09	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	6-T	7513	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	3-I	7492	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	10-T	7514	-	12,12,12	3.40	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	8-O	7504	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	2-Q	7508	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	1-G	7487	-	25,25,25	4.09	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	8-P	7506	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	7-W	7519	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	5-I	7492	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	7-P	7506	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	5-L	7497	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	9-M	7499	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	10-V	7518	-	12,12,12	3.43	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	8-B	7478	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	7-F	7486	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
4	CIT	10-Q	7508	-	12,12,12	3.41	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	9-Q	7507	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	3-G	7488	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	2-R	7510	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	8-Q	7507	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	3-W	7519	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	7-Q	7507	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	9-T	7514	-	12,12,12	3.40	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	2-U	7515	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	7-P	7505	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	1-R	7510	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	6-P	7505	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	6-S	7512	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	2-S	7512	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-J	7493	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	10-W	7519	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	7-G	7488	-	12,12,12	3.41	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-S	7511	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	2-M	7500	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	2-D	7481	-	25,25,25	4.10	16 (64%)	37,38,38	3.18	14 (37%)
4	CIT	4-M	7500	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)
4	CIT	6-T	7514	-	12,12,12	3.40	9 (75%)	17,17,17	1.83	7 (41%)
3	AMP	6-F	7485	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	5-X	7522	-	12,12,12	3.39	9 (75%)	17,17,17	1.84	7 (41%)
3	AMP	7-X	7521	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	6-E	7483	-	25,25,25	4.09	16 (64%)	37,38,38	3.18	14 (37%)
3	AMP	10-R	7509	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
3	AMP	6-U	7515	-	25,25,25	4.10	16 (64%)	37,38,38	3.17	14 (37%)
4	CIT	8-M	7500	-	12,12,12	3.40	9 (75%)	17,17,17	1.84	7 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	9-I	7491	-	-	6/10/26/26	0/3/3/3
3	AMP	2-G	7487	-	-	6/10/26/26	0/3/3/3
3	AMP	10-G	7487	-	-	6/10/26/26	0/3/3/3
4	CIT	2-P	7506	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	9-R	7510	-	-	3/16/16/16	-
3	AMP	2-A	7475	-	-	6/10/26/26	0/3/3/3
4	CIT	9-N	7502	-	-	3/16/16/16	-
3	AMP	9-A	7475	-	-	6/10/26/26	0/3/3/3
4	CIT	8-K	7496	-	-	3/16/16/16	-
4	CIT	5-L	7498	-	-	3/16/16/16	-
3	AMP	9-S	7511	-	-	6/10/26/26	0/3/3/3
3	AMP	1-U	7515	-	-	6/10/26/26	0/3/3/3
4	CIT	7-V	7518	-	-	3/16/16/16	-
3	AMP	7-H	7489	-	-	6/10/26/26	0/3/3/3
4	CIT	2-K	7496	-	-	3/16/16/16	-
4	CIT	7-E	7484	-	-	3/16/16/16	-
4	CIT	9-Q	7508	-	-	3/16/16/16	-
3	AMP	1-J	7493	-	-	6/10/26/26	0/3/3/3
3	AMP	5-A	7475	-	-	6/10/26/26	0/3/3/3
3	AMP	2-P	7505	-	-	6/10/26/26	0/3/3/3
4	CIT	6-C	7480	-	-	3/16/16/16	-
4	CIT	1-M	7500	-	-	3/16/16/16	-
3	AMP	7-F	7485	-	-	6/10/26/26	0/3/3/3
3	AMP	4-J	7493	-	-	6/10/26/26	0/3/3/3
4	CIT	3-N	7502	-	-	3/16/16/16	-
3	AMP	6-O	7503	-	-	6/10/26/26	0/3/3/3
3	AMP	8-U	7515	-	-	6/10/26/26	0/3/3/3
3	AMP	5-B	7477	-	-	6/10/26/26	0/3/3/3
3	AMP	4-D	7481	-	-	6/10/26/26	0/3/3/3
3	AMP	3-S	7511	-	-	6/10/26/26	0/3/3/3
3	AMP	8-R	7509	-	-	6/10/26/26	0/3/3/3
3	AMP	4-R	7509	-	-	6/10/26/26	0/3/3/3
4	CIT	5-C	7480	-	-	3/16/16/16	-
4	CIT	3-H	7490	-	-	3/16/16/16	-
3	AMP	7-R	7509	-	-	6/10/26/26	0/3/3/3
4	CIT	8-R	7510	-	-	3/16/16/16	-
4	CIT	7-Q	7508	-	-	3/16/16/16	-
4	CIT	6-R	7510	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	2-A	7476	-	-	3/16/16/16	-
4	CIT	7-W	7520	-	-	3/16/16/16	-
3	AMP	3-I	7491	-	-	6/10/26/26	0/3/3/3
4	CIT	1-P	7506	-	-	3/16/16/16	-
3	AMP	5-S	7511	-	-	6/10/26/26	0/3/3/3
3	AMP	10-S	7511	-	-	6/10/26/26	0/3/3/3
4	CIT	4-J	7494	-	-	3/16/16/16	-
3	AMP	5-D	7481	-	-	6/10/26/26	0/3/3/3
4	CIT	10-H	7490	-	-	3/16/16/16	-
3	AMP	10-M	7499	-	-	6/10/26/26	0/3/3/3
3	AMP	9-J	7493	-	-	6/10/26/26	0/3/3/3
4	CIT	8-T	7514	-	-	3/16/16/16	-
3	AMP	2-L	7497	-	-	6/10/26/26	0/3/3/3
4	CIT	8-U	7516	-	-	3/16/16/16	-
4	CIT	9-M	7500	-	-	3/16/16/16	-
4	CIT	1-D	7482	-	-	3/16/16/16	-
3	AMP	1-Q	7507	-	-	6/10/26/26	0/3/3/3
3	AMP	5-I	7491	-	-	6/10/26/26	0/3/3/3
4	CIT	10-P	7506	-	-	3/16/16/16	-
4	CIT	3-K	7496	-	-	3/16/16/16	-
3	AMP	5-N	7501	-	-	6/10/26/26	0/3/3/3
3	AMP	1-P	7505	-	-	6/10/26/26	0/3/3/3
3	AMP	7-T	7513	-	-	6/10/26/26	0/3/3/3
3	AMP	4-C	7479	-	-	6/10/26/26	0/3/3/3
3	AMP	9-T	7513	-	-	6/10/26/26	0/3/3/3
3	AMP	7-I	7491	-	-	6/10/26/26	0/3/3/3
4	CIT	6-A	7476	-	-	3/16/16/16	-
3	AMP	4-M	7499	-	-	6/10/26/26	0/3/3/3
3	AMP	8-J	7493	-	-	6/10/26/26	0/3/3/3
3	AMP	3-P	7505	-	-	6/10/26/26	0/3/3/3
4	CIT	4-H	7490	-	-	3/16/16/16	-
3	AMP	3-F	7485	-	-	6/10/26/26	0/3/3/3
3	AMP	2-K	7495	-	-	6/10/26/26	0/3/3/3
3	AMP	2-R	7509	-	-	6/10/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	3-T	7513	-	-	6/10/26/26	0/3/3/3
3	AMP	5-P	7505	-	-	6/10/26/26	0/3/3/3
4	CIT	9-K	7496	-	-	3/16/16/16	-
3	AMP	9-R	7509	-	-	6/10/26/26	0/3/3/3
3	AMP	8-G	7487	-	-	6/10/26/26	0/3/3/3
4	CIT	6-I	7492	-	-	3/16/16/16	-
4	CIT	6-D	7482	-	-	3/16/16/16	-
3	AMP	1-W	7519	-	-	6/10/26/26	0/3/3/3
3	AMP	7-G	7487	-	-	6/10/26/26	0/3/3/3
4	CIT	3-C	7480	-	-	3/16/16/16	-
3	AMP	5-W	7519	-	-	6/10/26/26	0/3/3/3
4	CIT	1-U	7516	-	-	3/16/16/16	-
4	CIT	8-H	7490	-	-	3/16/16/16	-
3	AMP	6-C	7479	-	-	6/10/26/26	0/3/3/3
4	CIT	5-G	7488	-	-	3/16/16/16	-
4	CIT	6-E	7484	-	-	3/16/16/16	-
3	AMP	10-K	7495	-	-	6/10/26/26	0/3/3/3
4	CIT	10-B	7478	-	-	3/16/16/16	-
4	CIT	1-F	7486	-	-	3/16/16/16	-
4	CIT	1-N	7502	-	-	3/16/16/16	-
3	AMP	4-L	7497	-	-	6/10/26/26	0/3/3/3
4	CIT	2-I	7492	-	-	3/16/16/16	-
3	AMP	1-D	7481	-	-	6/10/26/26	0/3/3/3
4	CIT	10-U	7516	-	-	3/16/16/16	-
4	CIT	4-X	7522	-	-	3/16/16/16	-
3	AMP	4-A	7475	-	-	6/10/26/26	0/3/3/3
4	CIT	8-Q	7508	-	-	3/16/16/16	-
4	CIT	1-V	7518	-	-	3/16/16/16	-
3	AMP	10-J	7493	-	-	6/10/26/26	0/3/3/3
3	AMP	7-N	7501	-	-	6/10/26/26	0/3/3/3
3	AMP	10-N	7501	-	-	6/10/26/26	0/3/3/3
3	AMP	2-T	7513	-	-	6/10/26/26	0/3/3/3
3	AMP	10-X	7521	-	-	6/10/26/26	0/3/3/3
3	AMP	9-N	7501	-	-	6/10/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	4-Q	7508	-	-	3/16/16/16	-
3	AMP	9-W	7519	-	-	6/10/26/26	0/3/3/3
4	CIT	5-H	7490	-	-	3/16/16/16	-
3	AMP	10-C	7479	-	-	6/10/26/26	0/3/3/3
4	CIT	5-O	7504	-	-	3/16/16/16	-
3	AMP	9-X	7521	-	-	6/10/26/26	0/3/3/3
3	AMP	7-V	7517	-	-	6/10/26/26	0/3/3/3
4	CIT	8-L	7498	-	-	3/16/16/16	-
3	AMP	7-C	7479	-	-	6/10/26/26	0/3/3/3
3	AMP	9-K	7495	-	-	6/10/26/26	0/3/3/3
3	AMP	10-P	7505	-	-	6/10/26/26	0/3/3/3
4	CIT	9-F	7486	-	-	3/16/16/16	-
3	AMP	2-B	7477	-	-	6/10/26/26	0/3/3/3
4	CIT	3-X	7522	-	-	3/16/16/16	-
4	CIT	1-T	7514	-	-	3/16/16/16	-
4	CIT	3-R	7510	-	-	3/16/16/16	-
3	AMP	2-X	7521	-	-	6/10/26/26	0/3/3/3
4	CIT	2-H	7490	-	-	3/16/16/16	-
3	AMP	8-A	7475	-	-	6/10/26/26	0/3/3/3
3	AMP	6-M	7499	-	-	6/10/26/26	0/3/3/3
4	CIT	2-L	7498	-	-	3/16/16/16	-
3	AMP	2-V	7517	-	-	6/10/26/26	0/3/3/3
4	CIT	10-F	7486	-	-	3/16/16/16	-
3	AMP	1-L	7497	-	-	6/10/26/26	0/3/3/3
3	AMP	7-O	7503	-	-	6/10/26/26	0/3/3/3
4	CIT	8-V	7518	-	-	3/16/16/16	-
4	CIT	10-C	7480	-	-	3/16/16/16	-
3	AMP	4-P	7505	-	-	6/10/26/26	0/3/3/3
4	CIT	4-L	7498	-	-	3/16/16/16	-
3	AMP	8-C	7479	-	-	6/10/26/26	0/3/3/3
4	CIT	1-W	7520	-	-	3/16/16/16	-
4	CIT	10-I	7492	-	-	3/16/16/16	-
4	CIT	5-W	7520	-	-	3/16/16/16	-
4	CIT	3-U	7516	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	6-R	7509	-	-	6/10/26/26	0/3/3/3
3	AMP	8-D	7481	-	-	6/10/26/26	0/3/3/3
4	CIT	2-C	7480	-	-	3/16/16/16	-
4	CIT	3-B	7478	-	-	3/16/16/16	-
3	AMP	3-U	7515	-	-	6/10/26/26	0/3/3/3
4	CIT	10-M	7500	-	-	3/16/16/16	-
3	AMP	3-X	7521	-	-	6/10/26/26	0/3/3/3
3	AMP	8-K	7495	-	-	6/10/26/26	0/3/3/3
4	CIT	1-Q	7508	-	-	3/16/16/16	-
4	CIT	2-V	7518	-	-	3/16/16/16	-
4	CIT	6-H	7490	-	-	3/16/16/16	-
4	CIT	9-X	7522	-	-	3/16/16/16	-
4	CIT	8-J	7494	-	-	3/16/16/16	-
3	AMP	1-A	7475	-	-	6/10/26/26	0/3/3/3
4	CIT	9-G	7488	-	-	3/16/16/16	-
3	AMP	4-B	7477	-	-	6/10/26/26	0/3/3/3
4	CIT	6-Q	7508	-	-	3/16/16/16	-
3	AMP	9-L	7497	-	-	6/10/26/26	0/3/3/3
4	CIT	3-E	7484	-	-	3/16/16/16	-
4	CIT	5-B	7478	-	-	3/16/16/16	-
4	CIT	1-I	7492	-	-	3/16/16/16	-
4	CIT	4-V	7518	-	-	3/16/16/16	-
4	CIT	1-S	7512	-	-	3/16/16/16	-
3	AMP	7-U	7515	-	-	6/10/26/26	0/3/3/3
4	CIT	2-W	7520	-	-	3/16/16/16	-
3	AMP	3-D	7481	-	-	6/10/26/26	0/3/3/3
3	AMP	5-V	7517	-	-	6/10/26/26	0/3/3/3
4	CIT	9-W	7520	-	-	3/16/16/16	-
3	AMP	4-V	7517	-	-	6/10/26/26	0/3/3/3
4	CIT	3-S	7512	-	-	3/16/16/16	-
4	CIT	1-L	7498	-	-	3/16/16/16	-
3	AMP	3-E	7483	-	-	6/10/26/26	0/3/3/3
4	CIT	2-B	7478	-	-	3/16/16/16	-
3	AMP	1-T	7513	-	-	6/10/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	6-L	7497	-	-	6/10/26/26	0/3/3/3
3	AMP	8-P	7505	-	-	6/10/26/26	0/3/3/3
3	AMP	10-D	7481	-	-	6/10/26/26	0/3/3/3
3	AMP	6-K	7495	-	-	6/10/26/26	0/3/3/3
3	AMP	10-Q	7507	-	-	6/10/26/26	0/3/3/3
3	AMP	8-S	7511	-	-	6/10/26/26	0/3/3/3
3	AMP	3-M	7499	-	-	6/10/26/26	0/3/3/3
4	CIT	10-E	7484	-	-	3/16/16/16	-
3	AMP	6-H	7489	-	-	6/10/26/26	0/3/3/3
4	CIT	7-S	7512	-	-	3/16/16/16	-
3	AMP	6-J	7493	-	-	6/10/26/26	0/3/3/3
3	AMP	10-T	7513	-	-	6/10/26/26	0/3/3/3
4	CIT	5-V	7518	-	-	3/16/16/16	-
3	AMP	1-B	7477	-	-	6/10/26/26	0/3/3/3
3	AMP	8-T	7513	-	-	6/10/26/26	0/3/3/3
3	AMP	3-G	7487	-	-	6/10/26/26	0/3/3/3
4	CIT	9-S	7512	-	-	3/16/16/16	-
3	AMP	8-I	7491	-	-	6/10/26/26	0/3/3/3
3	AMP	4-N	7501	-	-	6/10/26/26	0/3/3/3
4	CIT	2-X	7522	-	-	3/16/16/16	-
4	CIT	6-B	7478	-	-	3/16/16/16	-
3	AMP	3-L	7497	-	-	6/10/26/26	0/3/3/3
4	CIT	8-A	7476	-	-	3/16/16/16	-
4	CIT	5-D	7482	-	-	3/16/16/16	-
4	CIT	9-L	7498	-	-	3/16/16/16	-
3	AMP	4-K	7495	-	-	6/10/26/26	0/3/3/3
3	AMP	10-E	7483	-	-	6/10/26/26	0/3/3/3
4	CIT	5-N	7502	-	-	3/16/16/16	-
4	CIT	5-S	7512	-	-	3/16/16/16	-
3	AMP	1-S	7511	-	-	6/10/26/26	0/3/3/3
4	CIT	10-A	7476	-	-	3/16/16/16	-
3	AMP	5-K	7495	-	-	6/10/26/26	0/3/3/3
3	AMP	4-S	7511	-	-	6/10/26/26	0/3/3/3
4	CIT	9-C	7480	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	8-I	7492	-	-	3/16/16/16	-
4	CIT	4-U	7516	-	-	3/16/16/16	-
3	AMP	6-G	7487	-	-	6/10/26/26	0/3/3/3
4	CIT	3-W	7520	-	-	3/16/16/16	-
4	CIT	2-U	7516	-	-	3/16/16/16	-
4	CIT	7-C	7480	-	-	3/16/16/16	-
4	CIT	1-K	7496	-	-	3/16/16/16	-
3	AMP	10-L	7497	-	-	6/10/26/26	0/3/3/3
4	CIT	9-B	7478	-	-	3/16/16/16	-
4	CIT	10-S	7512	-	-	3/16/16/16	-
4	CIT	4-C	7480	-	-	3/16/16/16	-
3	AMP	9-B	7477	-	-	6/10/26/26	0/3/3/3
4	CIT	6-K	7496	-	-	3/16/16/16	-
3	AMP	3-C	7479	-	-	6/10/26/26	0/3/3/3
3	AMP	8-M	7499	-	-	6/10/26/26	0/3/3/3
3	AMP	4-F	7485	-	-	6/10/26/26	0/3/3/3
3	AMP	1-N	7501	-	-	6/10/26/26	0/3/3/3
4	CIT	4-R	7510	-	-	3/16/16/16	-
3	AMP	8-W	7519	-	-	6/10/26/26	0/3/3/3
4	CIT	10-W	7520	-	-	3/16/16/16	-
4	CIT	8-E	7484	-	-	3/16/16/16	-
4	CIT	9-P	7506	-	-	3/16/16/16	-
3	AMP	7-L	7497	-	-	6/10/26/26	0/3/3/3
4	CIT	8-G	7488	-	-	3/16/16/16	-
3	AMP	8-F	7485	-	-	6/10/26/26	0/3/3/3
3	AMP	3-R	7509	-	-	6/10/26/26	0/3/3/3
3	AMP	4-T	7513	-	-	6/10/26/26	0/3/3/3
4	CIT	6-L	7498	-	-	3/16/16/16	-
4	CIT	5-F	7486	-	-	3/16/16/16	-
3	AMP	5-G	7487	-	-	6/10/26/26	0/3/3/3
4	CIT	7-H	7490	-	-	3/16/16/16	-
3	AMP	9-O	7503	-	-	6/10/26/26	0/3/3/3
4	CIT	1-X	7522	-	-	3/16/16/16	-
3	AMP	8-X	7521	-	-	6/10/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	8-L	7497	-	-	6/10/26/26	0/3/3/3
4	CIT	5-K	7496	-	-	3/16/16/16	-
3	AMP	2-I	7491	-	-	6/10/26/26	0/3/3/3
4	CIT	8-C	7480	-	-	3/16/16/16	-
4	CIT	10-X	7522	-	-	3/16/16/16	-
3	AMP	10-A	7475	-	-	6/10/26/26	0/3/3/3
4	CIT	1-G	7488	-	-	3/16/16/16	-
4	CIT	4-G	7488	-	-	3/16/16/16	-
3	AMP	6-N	7501	-	-	6/10/26/26	0/3/3/3
4	CIT	8-X	7522	-	-	3/16/16/16	-
3	AMP	1-K	7495	-	-	6/10/26/26	0/3/3/3
3	AMP	3-V	7517	-	-	6/10/26/26	0/3/3/3
3	AMP	5-F	7485	-	-	6/10/26/26	0/3/3/3
4	CIT	3-O	7504	-	-	3/16/16/16	-
3	AMP	5-T	7513	-	-	6/10/26/26	0/3/3/3
4	CIT	2-F	7486	-	-	3/16/16/16	-
4	CIT	3-A	7476	-	-	3/16/16/16	-
3	AMP	2-N	7501	-	-	6/10/26/26	0/3/3/3
3	AMP	2-H	7489	-	-	6/10/26/26	0/3/3/3
4	CIT	5-A	7476	-	-	3/16/16/16	-
3	AMP	5-U	7515	-	-	6/10/26/26	0/3/3/3
4	CIT	4-A	7476	-	-	3/16/16/16	-
3	AMP	8-E	7483	-	-	6/10/26/26	0/3/3/3
4	CIT	6-M	7500	-	-	3/16/16/16	-
3	AMP	6-D	7481	-	-	6/10/26/26	0/3/3/3
3	AMP	10-F	7485	-	-	6/10/26/26	0/3/3/3
4	CIT	4-S	7512	-	-	3/16/16/16	-
3	AMP	9-V	7517	-	-	6/10/26/26	0/3/3/3
4	CIT	3-D	7482	-	-	3/16/16/16	-
3	AMP	4-H	7489	-	-	6/10/26/26	0/3/3/3
3	AMP	1-X	7521	-	-	6/10/26/26	0/3/3/3
3	AMP	3-N	7501	-	-	6/10/26/26	0/3/3/3
3	AMP	5-X	7521	-	-	6/10/26/26	0/3/3/3
4	CIT	2-E	7484	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	4-X	7521	-	-	6/10/26/26	0/3/3/3
4	CIT	3-V	7518	-	-	3/16/16/16	-
3	AMP	8-H	7489	-	-	6/10/26/26	0/3/3/3
4	CIT	7-B	7478	-	-	3/16/16/16	-
4	CIT	7-D	7482	-	-	3/16/16/16	-
4	CIT	1-E	7484	-	-	3/16/16/16	-
4	CIT	7-N	7502	-	-	3/16/16/16	-
3	AMP	10-B	7477	-	-	6/10/26/26	0/3/3/3
4	CIT	8-W	7520	-	-	3/16/16/16	-
3	AMP	2-Q	7507	-	-	6/10/26/26	0/3/3/3
3	AMP	3-Q	7507	-	-	6/10/26/26	0/3/3/3
4	CIT	1-A	7476	-	-	3/16/16/16	-
4	CIT	4-D	7482	-	-	3/16/16/16	-
4	CIT	2-G	7488	-	-	3/16/16/16	-
4	CIT	10-O	7504	-	-	3/16/16/16	-
3	AMP	4-Q	7507	-	-	6/10/26/26	0/3/3/3
3	AMP	2-O	7503	-	-	6/10/26/26	0/3/3/3
4	CIT	4-F	7486	-	-	3/16/16/16	-
3	AMP	2-C	7479	-	-	6/10/26/26	0/3/3/3
4	CIT	10-N	7502	-	-	3/16/16/16	-
4	CIT	6-U	7516	-	-	3/16/16/16	-
4	CIT	8-D	7482	-	-	3/16/16/16	-
4	CIT	8-F	7486	-	-	3/16/16/16	-
4	CIT	8-N	7502	-	-	3/16/16/16	-
4	CIT	7-R	7510	-	-	3/16/16/16	-
4	CIT	10-D	7482	-	-	3/16/16/16	-
3	AMP	2-E	7483	-	-	6/10/26/26	0/3/3/3
3	AMP	3-K	7495	-	-	6/10/26/26	0/3/3/3
3	AMP	8-B	7477	-	-	6/10/26/26	0/3/3/3
3	AMP	5-E	7483	-	-	6/10/26/26	0/3/3/3
3	AMP	3-O	7503	-	-	6/10/26/26	0/3/3/3
3	AMP	6-X	7521	-	-	6/10/26/26	0/3/3/3
3	AMP	5-O	7503	-	-	6/10/26/26	0/3/3/3
4	CIT	2-N	7502	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	1-I	7491	-	-	6/10/26/26	0/3/3/3
3	AMP	9-H	7489	-	-	6/10/26/26	0/3/3/3
3	AMP	1-H	7489	-	-	6/10/26/26	0/3/3/3
3	AMP	5-H	7489	-	-	6/10/26/26	0/3/3/3
3	AMP	4-I	7491	-	-	6/10/26/26	0/3/3/3
4	CIT	9-H	7490	-	-	3/16/16/16	-
4	CIT	5-R	7510	-	-	3/16/16/16	-
4	CIT	9-U	7516	-	-	3/16/16/16	-
3	AMP	6-W	7519	-	-	6/10/26/26	0/3/3/3
4	CIT	2-J	7494	-	-	3/16/16/16	-
3	AMP	8-N	7501	-	-	6/10/26/26	0/3/3/3
3	AMP	7-E	7483	-	-	6/10/26/26	0/3/3/3
4	CIT	7-O	7504	-	-	3/16/16/16	-
4	CIT	7-A	7476	-	-	3/16/16/16	-
3	AMP	6-B	7477	-	-	6/10/26/26	0/3/3/3
4	CIT	10-K	7496	-	-	3/16/16/16	-
4	CIT	2-D	7482	-	-	3/16/16/16	-
3	AMP	4-W	7519	-	-	6/10/26/26	0/3/3/3
4	CIT	3-Q	7508	-	-	3/16/16/16	-
4	CIT	5-P	7506	-	-	3/16/16/16	-
4	CIT	9-D	7482	-	-	3/16/16/16	-
3	AMP	3-J	7493	-	-	6/10/26/26	0/3/3/3
3	AMP	10-O	7503	-	-	6/10/26/26	0/3/3/3
4	CIT	6-P	7506	-	-	3/16/16/16	-
4	CIT	6-X	7522	-	-	3/16/16/16	-
4	CIT	4-N	7502	-	-	3/16/16/16	-
4	CIT	7-L	7498	-	-	3/16/16/16	-
3	AMP	9-F	7485	-	-	6/10/26/26	0/3/3/3
3	AMP	7-M	7499	-	-	6/10/26/26	0/3/3/3
3	AMP	3-A	7475	-	-	6/10/26/26	0/3/3/3
3	AMP	1-C	7479	-	-	6/10/26/26	0/3/3/3
4	CIT	4-I	7492	-	-	3/16/16/16	-
3	AMP	5-C	7479	-	-	6/10/26/26	0/3/3/3
3	AMP	5-J	7493	-	-	6/10/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	6-Q	7507	-	-	6/10/26/26	0/3/3/3
3	AMP	1-V	7517	-	-	6/10/26/26	0/3/3/3
4	CIT	5-J	7494	-	-	3/16/16/16	-
4	CIT	5-M	7500	-	-	3/16/16/16	-
4	CIT	7-I	7492	-	-	3/16/16/16	-
4	CIT	1-H	7490	-	-	3/16/16/16	-
3	AMP	7-J	7493	-	-	6/10/26/26	0/3/3/3
4	CIT	7-X	7522	-	-	3/16/16/16	-
3	AMP	3-B	7477	-	-	6/10/26/26	0/3/3/3
3	AMP	4-U	7515	-	-	6/10/26/26	0/3/3/3
4	CIT	3-J	7494	-	-	3/16/16/16	-
4	CIT	4-B	7478	-	-	3/16/16/16	-
3	AMP	9-D	7481	-	-	6/10/26/26	0/3/3/3
3	AMP	9-U	7515	-	-	6/10/26/26	0/3/3/3
4	CIT	3-P	7506	-	-	3/16/16/16	-
3	AMP	4-E	7483	-	-	6/10/26/26	0/3/3/3
4	CIT	6-W	7520	-	-	3/16/16/16	-
4	CIT	1-C	7480	-	-	3/16/16/16	-
3	AMP	4-O	7503	-	-	6/10/26/26	0/3/3/3
4	CIT	7-U	7516	-	-	3/16/16/16	-
4	CIT	7-K	7496	-	-	3/16/16/16	-
3	AMP	2-F	7485	-	-	6/10/26/26	0/3/3/3
4	CIT	9-J	7494	-	-	3/16/16/16	-
3	AMP	5-R	7509	-	-	6/10/26/26	0/3/3/3
4	CIT	6-J	7494	-	-	3/16/16/16	-
3	AMP	2-W	7519	-	-	6/10/26/26	0/3/3/3
3	AMP	6-I	7491	-	-	6/10/26/26	0/3/3/3
4	CIT	4-E	7484	-	-	3/16/16/16	-
4	CIT	10-R	7510	-	-	3/16/16/16	-
3	AMP	2-M	7499	-	-	6/10/26/26	0/3/3/3
3	AMP	3-H	7489	-	-	6/10/26/26	0/3/3/3
4	CIT	3-L	7498	-	-	3/16/16/16	-
3	AMP	1-F	7485	-	-	6/10/26/26	0/3/3/3
4	CIT	2-T	7514	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	6-A	7475	-	-	6/10/26/26	0/3/3/3
4	CIT	6-V	7518	-	-	3/16/16/16	-
4	CIT	4-W	7520	-	-	3/16/16/16	-
3	AMP	10-H	7489	-	-	6/10/26/26	0/3/3/3
3	AMP	9-G	7487	-	-	6/10/26/26	0/3/3/3
4	CIT	6-F	7486	-	-	3/16/16/16	-
4	CIT	2-O	7504	-	-	3/16/16/16	-
4	CIT	10-G	7488	-	-	3/16/16/16	-
3	AMP	6-V	7517	-	-	6/10/26/26	0/3/3/3
4	CIT	4-O	7504	-	-	3/16/16/16	-
4	CIT	5-U	7516	-	-	3/16/16/16	-
3	AMP	8-O	7503	-	-	6/10/26/26	0/3/3/3
4	CIT	1-B	7478	-	-	3/16/16/16	-
4	CIT	4-T	7514	-	-	3/16/16/16	-
3	AMP	9-P	7505	-	-	6/10/26/26	0/3/3/3
4	CIT	1-O	7504	-	-	3/16/16/16	-
3	AMP	1-R	7509	-	-	6/10/26/26	0/3/3/3
4	CIT	5-E	7484	-	-	3/16/16/16	-
4	CIT	7-T	7514	-	-	3/16/16/16	-
3	AMP	10-U	7515	-	-	6/10/26/26	0/3/3/3
4	CIT	6-O	7504	-	-	3/16/16/16	-
4	CIT	3-F	7486	-	-	3/16/16/16	-
4	CIT	3-M	7500	-	-	3/16/16/16	-
3	AMP	9-C	7479	-	-	6/10/26/26	0/3/3/3
3	AMP	9-E	7483	-	-	6/10/26/26	0/3/3/3
4	CIT	9-O	7504	-	-	3/16/16/16	-
4	CIT	9-A	7476	-	-	3/16/16/16	-
4	CIT	5-Q	7508	-	-	3/16/16/16	-
3	AMP	1-M	7499	-	-	6/10/26/26	0/3/3/3
3	AMP	7-A	7475	-	-	6/10/26/26	0/3/3/3
3	AMP	5-M	7499	-	-	6/10/26/26	0/3/3/3
4	CIT	8-S	7512	-	-	3/16/16/16	-
3	AMP	7-B	7477	-	-	6/10/26/26	0/3/3/3
3	AMP	8-V	7517	-	-	6/10/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	10-I	7491	-	-	6/10/26/26	0/3/3/3
4	CIT	7-M	7500	-	-	3/16/16/16	-
4	CIT	9-I	7492	-	-	3/16/16/16	-
4	CIT	1-J	7494	-	-	3/16/16/16	-
3	AMP	1-E	7483	-	-	6/10/26/26	0/3/3/3
3	AMP	5-Q	7507	-	-	6/10/26/26	0/3/3/3
3	AMP	7-S	7511	-	-	6/10/26/26	0/3/3/3
4	CIT	10-J	7494	-	-	3/16/16/16	-
3	AMP	10-V	7517	-	-	6/10/26/26	0/3/3/3
4	CIT	10-L	7498	-	-	3/16/16/16	-
3	AMP	7-D	7481	-	-	6/10/26/26	0/3/3/3
4	CIT	6-N	7502	-	-	3/16/16/16	-
4	CIT	3-T	7514	-	-	3/16/16/16	-
3	AMP	1-O	7503	-	-	6/10/26/26	0/3/3/3
3	AMP	6-S	7511	-	-	6/10/26/26	0/3/3/3
4	CIT	9-E	7484	-	-	3/16/16/16	-
4	CIT	6-G	7488	-	-	3/16/16/16	-
4	CIT	5-T	7514	-	-	3/16/16/16	-
3	AMP	7-K	7495	-	-	6/10/26/26	0/3/3/3
4	CIT	4-K	7496	-	-	3/16/16/16	-
4	CIT	4-P	7506	-	-	3/16/16/16	-
4	CIT	9-V	7518	-	-	3/16/16/16	-
4	CIT	7-J	7494	-	-	3/16/16/16	-
3	AMP	4-G	7487	-	-	6/10/26/26	0/3/3/3
3	AMP	6-T	7513	-	-	6/10/26/26	0/3/3/3
4	CIT	3-I	7492	-	-	3/16/16/16	-
4	CIT	10-T	7514	-	-	3/16/16/16	-
4	CIT	8-O	7504	-	-	3/16/16/16	-
4	CIT	2-Q	7508	-	-	3/16/16/16	-
3	AMP	1-G	7487	-	-	6/10/26/26	0/3/3/3
4	CIT	8-P	7506	-	-	3/16/16/16	-
3	AMP	7-W	7519	-	-	6/10/26/26	0/3/3/3
4	CIT	5-I	7492	-	-	3/16/16/16	-
4	CIT	7-P	7506	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	5-L	7497	-	-	6/10/26/26	0/3/3/3
3	AMP	9-M	7499	-	-	6/10/26/26	0/3/3/3
4	CIT	10-V	7518	-	-	3/16/16/16	-
4	CIT	8-B	7478	-	-	3/16/16/16	-
4	CIT	7-F	7486	-	-	3/16/16/16	-
4	CIT	10-Q	7508	-	-	3/16/16/16	-
3	AMP	9-Q	7507	-	-	6/10/26/26	0/3/3/3
4	CIT	3-G	7488	-	-	3/16/16/16	-
4	CIT	2-R	7510	-	-	3/16/16/16	-
3	AMP	8-Q	7507	-	-	6/10/26/26	0/3/3/3
3	AMP	3-W	7519	-	-	6/10/26/26	0/3/3/3
3	AMP	7-Q	7507	-	-	6/10/26/26	0/3/3/3
4	CIT	9-T	7514	-	-	3/16/16/16	-
3	AMP	2-U	7515	-	-	6/10/26/26	0/3/3/3
3	AMP	7-P	7505	-	-	6/10/26/26	0/3/3/3
4	CIT	1-R	7510	-	-	3/16/16/16	-
3	AMP	6-P	7505	-	-	6/10/26/26	0/3/3/3
4	CIT	6-S	7512	-	-	3/16/16/16	-
4	CIT	2-S	7512	-	-	3/16/16/16	-
3	AMP	2-J	7493	-	-	6/10/26/26	0/3/3/3
3	AMP	10-W	7519	-	-	6/10/26/26	0/3/3/3
4	CIT	7-G	7488	-	-	3/16/16/16	-
3	AMP	2-S	7511	-	-	6/10/26/26	0/3/3/3
4	CIT	2-M	7500	-	-	3/16/16/16	-
3	AMP	2-D	7481	-	-	6/10/26/26	0/3/3/3
4	CIT	4-M	7500	-	-	3/16/16/16	-
4	CIT	6-T	7514	-	-	3/16/16/16	-
3	AMP	6-F	7485	-	-	6/10/26/26	0/3/3/3
4	CIT	5-X	7522	-	-	3/16/16/16	-
3	AMP	7-X	7521	-	-	6/10/26/26	0/3/3/3
3	AMP	6-E	7483	-	-	6/10/26/26	0/3/3/3
3	AMP	10-R	7509	-	-	6/10/26/26	0/3/3/3
3	AMP	6-U	7515	-	-	6/10/26/26	0/3/3/3
4	CIT	8-M	7500	-	-	3/16/16/16	-

All (6000) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-R	7509	AMP	C1'-N9	10.96	1.76	1.46
3	2-R	7509	AMP	C1'-N9	10.96	1.76	1.46
3	3-R	7509	AMP	C1'-N9	10.96	1.76	1.46
3	4-R	7509	AMP	C1'-N9	10.96	1.76	1.46
3	5-R	7509	AMP	C1'-N9	10.96	1.76	1.46
3	6-R	7509	AMP	C1'-N9	10.96	1.76	1.46
3	7-R	7509	AMP	C1'-N9	10.96	1.76	1.46
3	8-R	7509	AMP	C1'-N9	10.96	1.76	1.46
3	9-R	7509	AMP	C1'-N9	10.96	1.76	1.46
3	10-R	7509	AMP	C1'-N9	10.96	1.76	1.46
3	1-Q	7507	AMP	C1'-N9	10.96	1.76	1.46
3	2-Q	7507	AMP	C1'-N9	10.96	1.76	1.46
3	3-Q	7507	AMP	C1'-N9	10.96	1.76	1.46
3	4-Q	7507	AMP	C1'-N9	10.96	1.76	1.46
3	5-Q	7507	AMP	C1'-N9	10.96	1.76	1.46
3	6-Q	7507	AMP	C1'-N9	10.96	1.76	1.46
3	7-Q	7507	AMP	C1'-N9	10.96	1.76	1.46
3	8-Q	7507	AMP	C1'-N9	10.96	1.76	1.46
3	9-Q	7507	AMP	C1'-N9	10.96	1.76	1.46
3	10-Q	7507	AMP	C1'-N9	10.96	1.76	1.46
3	1-H	7489	AMP	C1'-N9	10.96	1.76	1.46
3	2-H	7489	AMP	C1'-N9	10.96	1.76	1.46
3	3-H	7489	AMP	C1'-N9	10.96	1.76	1.46
3	4-H	7489	AMP	C1'-N9	10.96	1.76	1.46
3	5-H	7489	AMP	C1'-N9	10.96	1.76	1.46
3	6-H	7489	AMP	C1'-N9	10.96	1.76	1.46
3	7-H	7489	AMP	C1'-N9	10.96	1.76	1.46
3	8-H	7489	AMP	C1'-N9	10.96	1.76	1.46
3	9-H	7489	AMP	C1'-N9	10.96	1.76	1.46
3	10-H	7489	AMP	C1'-N9	10.96	1.76	1.46
3	1-I	7491	AMP	C1'-N9	10.95	1.76	1.46
3	2-I	7491	AMP	C1'-N9	10.95	1.76	1.46
3	3-I	7491	AMP	C1'-N9	10.95	1.76	1.46
3	4-I	7491	AMP	C1'-N9	10.95	1.76	1.46
3	5-I	7491	AMP	C1'-N9	10.95	1.76	1.46
3	6-I	7491	AMP	C1'-N9	10.95	1.76	1.46
3	7-I	7491	AMP	C1'-N9	10.95	1.76	1.46
3	8-I	7491	AMP	C1'-N9	10.95	1.76	1.46
3	9-I	7491	AMP	C1'-N9	10.95	1.76	1.46
3	10-I	7491	AMP	C1'-N9	10.95	1.76	1.46
3	1-B	7477	AMP	C1'-N9	10.95	1.76	1.46
3	2-B	7477	AMP	C1'-N9	10.95	1.76	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	7477	AMP	C1'-N9	10.95	1.76	1.46
3	4-B	7477	AMP	C1'-N9	10.95	1.76	1.46
3	5-B	7477	AMP	C1'-N9	10.95	1.76	1.46
3	6-B	7477	AMP	C1'-N9	10.95	1.76	1.46
3	7-B	7477	AMP	C1'-N9	10.95	1.76	1.46
3	8-B	7477	AMP	C1'-N9	10.95	1.76	1.46
3	9-B	7477	AMP	C1'-N9	10.95	1.76	1.46
3	10-B	7477	AMP	C1'-N9	10.95	1.76	1.46
3	1-L	7497	AMP	C1'-N9	10.94	1.76	1.46
3	2-L	7497	AMP	C1'-N9	10.94	1.76	1.46
3	3-L	7497	AMP	C1'-N9	10.94	1.76	1.46
3	4-L	7497	AMP	C1'-N9	10.94	1.76	1.46
3	5-L	7497	AMP	C1'-N9	10.94	1.76	1.46
3	6-L	7497	AMP	C1'-N9	10.94	1.76	1.46
3	7-L	7497	AMP	C1'-N9	10.94	1.76	1.46
3	8-L	7497	AMP	C1'-N9	10.94	1.76	1.46
3	9-L	7497	AMP	C1'-N9	10.94	1.76	1.46
3	10-L	7497	AMP	C1'-N9	10.94	1.76	1.46
3	1-U	7515	AMP	C1'-N9	10.94	1.76	1.46
3	2-U	7515	AMP	C1'-N9	10.94	1.76	1.46
3	3-U	7515	AMP	C1'-N9	10.94	1.76	1.46
3	4-U	7515	AMP	C1'-N9	10.94	1.76	1.46
3	5-U	7515	AMP	C1'-N9	10.94	1.76	1.46
3	6-U	7515	AMP	C1'-N9	10.94	1.76	1.46
3	7-U	7515	AMP	C1'-N9	10.94	1.76	1.46
3	8-U	7515	AMP	C1'-N9	10.94	1.76	1.46
3	9-U	7515	AMP	C1'-N9	10.94	1.76	1.46
3	10-U	7515	AMP	C1'-N9	10.94	1.76	1.46
3	1-S	7511	AMP	C1'-N9	10.94	1.76	1.46
3	2-S	7511	AMP	C1'-N9	10.94	1.76	1.46
3	3-S	7511	AMP	C1'-N9	10.94	1.76	1.46
3	4-S	7511	AMP	C1'-N9	10.94	1.76	1.46
3	5-S	7511	AMP	C1'-N9	10.94	1.76	1.46
3	6-S	7511	AMP	C1'-N9	10.94	1.76	1.46
3	7-S	7511	AMP	C1'-N9	10.94	1.76	1.46
3	8-S	7511	AMP	C1'-N9	10.94	1.76	1.46
3	9-S	7511	AMP	C1'-N9	10.94	1.76	1.46
3	10-S	7511	AMP	C1'-N9	10.94	1.76	1.46
3	1-X	7521	AMP	C1'-N9	10.94	1.76	1.46
3	2-X	7521	AMP	C1'-N9	10.94	1.76	1.46
3	3-X	7521	AMP	C1'-N9	10.94	1.76	1.46
3	4-X	7521	AMP	C1'-N9	10.94	1.76	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-X	7521	AMP	C1'-N9	10.94	1.76	1.46
3	6-X	7521	AMP	C1'-N9	10.94	1.76	1.46
3	7-X	7521	AMP	C1'-N9	10.94	1.76	1.46
3	8-X	7521	AMP	C1'-N9	10.94	1.76	1.46
3	9-X	7521	AMP	C1'-N9	10.94	1.76	1.46
3	10-X	7521	AMP	C1'-N9	10.94	1.76	1.46
3	1-C	7479	AMP	C1'-N9	10.94	1.76	1.46
3	2-C	7479	AMP	C1'-N9	10.94	1.76	1.46
3	3-C	7479	AMP	C1'-N9	10.94	1.76	1.46
3	4-C	7479	AMP	C1'-N9	10.94	1.76	1.46
3	5-C	7479	AMP	C1'-N9	10.94	1.76	1.46
3	6-C	7479	AMP	C1'-N9	10.94	1.76	1.46
3	7-C	7479	AMP	C1'-N9	10.94	1.76	1.46
3	8-C	7479	AMP	C1'-N9	10.94	1.76	1.46
3	9-C	7479	AMP	C1'-N9	10.94	1.76	1.46
3	10-C	7479	AMP	C1'-N9	10.94	1.76	1.46
3	1-W	7519	AMP	C1'-N9	10.94	1.76	1.46
3	2-W	7519	AMP	C1'-N9	10.94	1.76	1.46
3	3-W	7519	AMP	C1'-N9	10.94	1.76	1.46
3	4-W	7519	AMP	C1'-N9	10.94	1.76	1.46
3	5-W	7519	AMP	C1'-N9	10.94	1.76	1.46
3	6-W	7519	AMP	C1'-N9	10.94	1.76	1.46
3	7-W	7519	AMP	C1'-N9	10.94	1.76	1.46
3	8-W	7519	AMP	C1'-N9	10.94	1.76	1.46
3	9-W	7519	AMP	C1'-N9	10.94	1.76	1.46
3	10-W	7519	AMP	C1'-N9	10.94	1.76	1.46
3	1-P	7505	AMP	C1'-N9	10.94	1.76	1.46
3	2-P	7505	AMP	C1'-N9	10.94	1.76	1.46
3	3-P	7505	AMP	C1'-N9	10.94	1.76	1.46
3	4-P	7505	AMP	C1'-N9	10.94	1.76	1.46
3	5-P	7505	AMP	C1'-N9	10.94	1.76	1.46
3	6-P	7505	AMP	C1'-N9	10.94	1.76	1.46
3	7-P	7505	AMP	C1'-N9	10.94	1.76	1.46
3	8-P	7505	AMP	C1'-N9	10.94	1.76	1.46
3	9-P	7505	AMP	C1'-N9	10.94	1.76	1.46
3	10-P	7505	AMP	C1'-N9	10.94	1.76	1.46
3	1-A	7475	AMP	C1'-N9	10.93	1.76	1.46
3	2-A	7475	AMP	C1'-N9	10.93	1.76	1.46
3	3-A	7475	AMP	C1'-N9	10.93	1.76	1.46
3	4-A	7475	AMP	C1'-N9	10.93	1.76	1.46
3	5-A	7475	AMP	C1'-N9	10.93	1.76	1.46
3	6-A	7475	AMP	C1'-N9	10.93	1.76	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-A	7475	AMP	C1'-N9	10.93	1.76	1.46
3	8-A	7475	AMP	C1'-N9	10.93	1.76	1.46
3	9-A	7475	AMP	C1'-N9	10.93	1.76	1.46
3	10-A	7475	AMP	C1'-N9	10.93	1.76	1.46
3	1-D	7481	AMP	C1'-N9	10.93	1.76	1.46
3	2-D	7481	AMP	C1'-N9	10.93	1.76	1.46
3	3-D	7481	AMP	C1'-N9	10.93	1.76	1.46
3	4-D	7481	AMP	C1'-N9	10.93	1.76	1.46
3	5-D	7481	AMP	C1'-N9	10.93	1.76	1.46
3	6-D	7481	AMP	C1'-N9	10.93	1.76	1.46
3	7-D	7481	AMP	C1'-N9	10.93	1.76	1.46
3	8-D	7481	AMP	C1'-N9	10.93	1.76	1.46
3	9-D	7481	AMP	C1'-N9	10.93	1.76	1.46
3	10-D	7481	AMP	C1'-N9	10.93	1.76	1.46
3	1-F	7485	AMP	C1'-N9	10.93	1.76	1.46
3	2-F	7485	AMP	C1'-N9	10.93	1.76	1.46
3	3-F	7485	AMP	C1'-N9	10.93	1.76	1.46
3	4-F	7485	AMP	C1'-N9	10.93	1.76	1.46
3	5-F	7485	AMP	C1'-N9	10.93	1.76	1.46
3	6-F	7485	AMP	C1'-N9	10.93	1.76	1.46
3	7-F	7485	AMP	C1'-N9	10.93	1.76	1.46
3	8-F	7485	AMP	C1'-N9	10.93	1.76	1.46
3	9-F	7485	AMP	C1'-N9	10.93	1.76	1.46
3	10-F	7485	AMP	C1'-N9	10.93	1.76	1.46
3	1-E	7483	AMP	C1'-N9	10.93	1.76	1.46
3	2-E	7483	AMP	C1'-N9	10.93	1.76	1.46
3	3-E	7483	AMP	C1'-N9	10.93	1.76	1.46
3	4-E	7483	AMP	C1'-N9	10.93	1.76	1.46
3	5-E	7483	AMP	C1'-N9	10.93	1.76	1.46
3	6-E	7483	AMP	C1'-N9	10.93	1.76	1.46
3	7-E	7483	AMP	C1'-N9	10.93	1.76	1.46
3	8-E	7483	AMP	C1'-N9	10.93	1.76	1.46
3	9-E	7483	AMP	C1'-N9	10.93	1.76	1.46
3	10-E	7483	AMP	C1'-N9	10.93	1.76	1.46
3	1-G	7487	AMP	C1'-N9	10.93	1.76	1.46
3	2-G	7487	AMP	C1'-N9	10.93	1.76	1.46
3	3-G	7487	AMP	C1'-N9	10.93	1.76	1.46
3	4-G	7487	AMP	C1'-N9	10.93	1.76	1.46
3	5-G	7487	AMP	C1'-N9	10.93	1.76	1.46
3	6-G	7487	AMP	C1'-N9	10.93	1.76	1.46
3	7-G	7487	AMP	C1'-N9	10.93	1.76	1.46
3	8-G	7487	AMP	C1'-N9	10.93	1.76	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-G	7487	AMP	C1'-N9	10.93	1.76	1.46
3	10-G	7487	AMP	C1'-N9	10.93	1.76	1.46
3	1-J	7493	AMP	C1'-N9	10.93	1.76	1.46
3	2-J	7493	AMP	C1'-N9	10.93	1.76	1.46
3	3-J	7493	AMP	C1'-N9	10.93	1.76	1.46
3	4-J	7493	AMP	C1'-N9	10.93	1.76	1.46
3	5-J	7493	AMP	C1'-N9	10.93	1.76	1.46
3	6-J	7493	AMP	C1'-N9	10.93	1.76	1.46
3	7-J	7493	AMP	C1'-N9	10.93	1.76	1.46
3	8-J	7493	AMP	C1'-N9	10.93	1.76	1.46
3	9-J	7493	AMP	C1'-N9	10.93	1.76	1.46
3	10-J	7493	AMP	C1'-N9	10.93	1.76	1.46
3	1-V	7517	AMP	C1'-N9	10.93	1.76	1.46
3	2-V	7517	AMP	C1'-N9	10.93	1.76	1.46
3	3-V	7517	AMP	C1'-N9	10.93	1.76	1.46
3	4-V	7517	AMP	C1'-N9	10.93	1.76	1.46
3	5-V	7517	AMP	C1'-N9	10.93	1.76	1.46
3	6-V	7517	AMP	C1'-N9	10.93	1.76	1.46
3	7-V	7517	AMP	C1'-N9	10.93	1.76	1.46
3	8-V	7517	AMP	C1'-N9	10.93	1.76	1.46
3	9-V	7517	AMP	C1'-N9	10.93	1.76	1.46
3	10-V	7517	AMP	C1'-N9	10.93	1.76	1.46
3	1-M	7499	AMP	C1'-N9	10.93	1.76	1.46
3	2-M	7499	AMP	C1'-N9	10.93	1.76	1.46
3	3-M	7499	AMP	C1'-N9	10.93	1.76	1.46
3	4-M	7499	AMP	C1'-N9	10.93	1.76	1.46
3	5-M	7499	AMP	C1'-N9	10.93	1.76	1.46
3	6-M	7499	AMP	C1'-N9	10.93	1.76	1.46
3	7-M	7499	AMP	C1'-N9	10.93	1.76	1.46
3	8-M	7499	AMP	C1'-N9	10.93	1.76	1.46
3	9-M	7499	AMP	C1'-N9	10.93	1.76	1.46
3	10-M	7499	AMP	C1'-N9	10.93	1.76	1.46
3	1-O	7503	AMP	C1'-N9	10.92	1.76	1.46
3	2-O	7503	AMP	C1'-N9	10.92	1.76	1.46
3	3-O	7503	AMP	C1'-N9	10.92	1.76	1.46
3	4-O	7503	AMP	C1'-N9	10.92	1.76	1.46
3	5-O	7503	AMP	C1'-N9	10.92	1.76	1.46
3	6-O	7503	AMP	C1'-N9	10.92	1.76	1.46
3	7-O	7503	AMP	C1'-N9	10.92	1.76	1.46
3	8-O	7503	AMP	C1'-N9	10.92	1.76	1.46
3	9-O	7503	AMP	C1'-N9	10.92	1.76	1.46
3	10-O	7503	AMP	C1'-N9	10.92	1.76	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-K	7495	AMP	C1'-N9	10.91	1.76	1.46
3	2-K	7495	AMP	C1'-N9	10.91	1.76	1.46
3	3-K	7495	AMP	C1'-N9	10.91	1.76	1.46
3	4-K	7495	AMP	C1'-N9	10.91	1.76	1.46
3	5-K	7495	AMP	C1'-N9	10.91	1.76	1.46
3	6-K	7495	AMP	C1'-N9	10.91	1.76	1.46
3	7-K	7495	AMP	C1'-N9	10.91	1.76	1.46
3	8-K	7495	AMP	C1'-N9	10.91	1.76	1.46
3	9-K	7495	AMP	C1'-N9	10.91	1.76	1.46
3	10-K	7495	AMP	C1'-N9	10.91	1.76	1.46
3	1-T	7513	AMP	C1'-N9	10.91	1.76	1.46
3	2-T	7513	AMP	C1'-N9	10.91	1.76	1.46
3	3-T	7513	AMP	C1'-N9	10.91	1.76	1.46
3	4-T	7513	AMP	C1'-N9	10.91	1.76	1.46
3	5-T	7513	AMP	C1'-N9	10.91	1.76	1.46
3	6-T	7513	AMP	C1'-N9	10.91	1.76	1.46
3	7-T	7513	AMP	C1'-N9	10.91	1.76	1.46
3	8-T	7513	AMP	C1'-N9	10.91	1.76	1.46
3	9-T	7513	AMP	C1'-N9	10.91	1.76	1.46
3	10-T	7513	AMP	C1'-N9	10.91	1.76	1.46
3	1-N	7501	AMP	C1'-N9	10.91	1.76	1.46
3	2-N	7501	AMP	C1'-N9	10.91	1.76	1.46
3	3-N	7501	AMP	C1'-N9	10.91	1.76	1.46
3	4-N	7501	AMP	C1'-N9	10.91	1.76	1.46
3	5-N	7501	AMP	C1'-N9	10.91	1.76	1.46
3	6-N	7501	AMP	C1'-N9	10.91	1.76	1.46
3	7-N	7501	AMP	C1'-N9	10.91	1.76	1.46
3	8-N	7501	AMP	C1'-N9	10.91	1.76	1.46
3	9-N	7501	AMP	C1'-N9	10.91	1.76	1.46
3	10-N	7501	AMP	C1'-N9	10.91	1.76	1.46
3	1-W	7519	AMP	C8-N9	7.92	1.51	1.37
3	2-W	7519	AMP	C8-N9	7.92	1.51	1.37
3	3-W	7519	AMP	C8-N9	7.92	1.51	1.37
3	4-W	7519	AMP	C8-N9	7.92	1.51	1.37
3	5-W	7519	AMP	C8-N9	7.92	1.51	1.37
3	6-W	7519	AMP	C8-N9	7.92	1.51	1.37
3	7-W	7519	AMP	C8-N9	7.92	1.51	1.37
3	8-W	7519	AMP	C8-N9	7.92	1.51	1.37
3	9-W	7519	AMP	C8-N9	7.92	1.51	1.37
3	10-W	7519	AMP	C8-N9	7.92	1.51	1.37
3	1-D	7481	AMP	C8-N9	7.91	1.51	1.37
3	2-D	7481	AMP	C8-N9	7.91	1.51	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-D	7481	AMP	C8-N9	7.91	1.51	1.37
3	4-D	7481	AMP	C8-N9	7.91	1.51	1.37
3	5-D	7481	AMP	C8-N9	7.91	1.51	1.37
3	6-D	7481	AMP	C8-N9	7.91	1.51	1.37
3	7-D	7481	AMP	C8-N9	7.91	1.51	1.37
3	8-D	7481	AMP	C8-N9	7.91	1.51	1.37
3	9-D	7481	AMP	C8-N9	7.91	1.51	1.37
3	10-D	7481	AMP	C8-N9	7.91	1.51	1.37
3	1-K	7495	AMP	C8-N9	7.91	1.51	1.37
3	2-K	7495	AMP	C8-N9	7.91	1.51	1.37
3	3-K	7495	AMP	C8-N9	7.91	1.51	1.37
3	4-K	7495	AMP	C8-N9	7.91	1.51	1.37
3	5-K	7495	AMP	C8-N9	7.91	1.51	1.37
3	6-K	7495	AMP	C8-N9	7.91	1.51	1.37
3	7-K	7495	AMP	C8-N9	7.91	1.51	1.37
3	8-K	7495	AMP	C8-N9	7.91	1.51	1.37
3	9-K	7495	AMP	C8-N9	7.91	1.51	1.37
3	10-K	7495	AMP	C8-N9	7.91	1.51	1.37
3	1-B	7477	AMP	C8-N9	7.91	1.51	1.37
3	2-B	7477	AMP	C8-N9	7.91	1.51	1.37
3	3-B	7477	AMP	C8-N9	7.91	1.51	1.37
3	4-B	7477	AMP	C8-N9	7.91	1.51	1.37
3	5-B	7477	AMP	C8-N9	7.91	1.51	1.37
3	6-B	7477	AMP	C8-N9	7.91	1.51	1.37
3	7-B	7477	AMP	C8-N9	7.91	1.51	1.37
3	8-B	7477	AMP	C8-N9	7.91	1.51	1.37
3	9-B	7477	AMP	C8-N9	7.91	1.51	1.37
3	10-B	7477	AMP	C8-N9	7.91	1.51	1.37
3	1-L	7497	AMP	C8-N9	7.90	1.51	1.37
3	2-L	7497	AMP	C8-N9	7.90	1.51	1.37
3	3-L	7497	AMP	C8-N9	7.90	1.51	1.37
3	4-L	7497	AMP	C8-N9	7.90	1.51	1.37
3	5-L	7497	AMP	C8-N9	7.90	1.51	1.37
3	6-L	7497	AMP	C8-N9	7.90	1.51	1.37
3	7-L	7497	AMP	C8-N9	7.90	1.51	1.37
3	8-L	7497	AMP	C8-N9	7.90	1.51	1.37
3	9-L	7497	AMP	C8-N9	7.90	1.51	1.37
3	10-L	7497	AMP	C8-N9	7.90	1.51	1.37
3	1-U	7515	AMP	C8-N9	7.90	1.51	1.37
3	2-U	7515	AMP	C8-N9	7.90	1.51	1.37
3	3-U	7515	AMP	C8-N9	7.90	1.51	1.37
3	4-U	7515	AMP	C8-N9	7.90	1.51	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-U	7515	AMP	C8-N9	7.90	1.51	1.37
3	6-U	7515	AMP	C8-N9	7.90	1.51	1.37
3	7-U	7515	AMP	C8-N9	7.90	1.51	1.37
3	8-U	7515	AMP	C8-N9	7.90	1.51	1.37
3	9-U	7515	AMP	C8-N9	7.90	1.51	1.37
3	10-U	7515	AMP	C8-N9	7.90	1.51	1.37
3	1-F	7485	AMP	C8-N9	7.89	1.51	1.37
3	2-F	7485	AMP	C8-N9	7.89	1.51	1.37
3	3-F	7485	AMP	C8-N9	7.89	1.51	1.37
3	4-F	7485	AMP	C8-N9	7.89	1.51	1.37
3	5-F	7485	AMP	C8-N9	7.89	1.51	1.37
3	6-F	7485	AMP	C8-N9	7.89	1.51	1.37
3	7-F	7485	AMP	C8-N9	7.89	1.51	1.37
3	8-F	7485	AMP	C8-N9	7.89	1.51	1.37
3	9-F	7485	AMP	C8-N9	7.89	1.51	1.37
3	10-F	7485	AMP	C8-N9	7.89	1.51	1.37
3	1-P	7505	AMP	C8-N9	7.89	1.51	1.37
3	2-P	7505	AMP	C8-N9	7.89	1.51	1.37
3	3-P	7505	AMP	C8-N9	7.89	1.51	1.37
3	4-P	7505	AMP	C8-N9	7.89	1.51	1.37
3	5-P	7505	AMP	C8-N9	7.89	1.51	1.37
3	6-P	7505	AMP	C8-N9	7.89	1.51	1.37
3	7-P	7505	AMP	C8-N9	7.89	1.51	1.37
3	8-P	7505	AMP	C8-N9	7.89	1.51	1.37
3	9-P	7505	AMP	C8-N9	7.89	1.51	1.37
3	10-P	7505	AMP	C8-N9	7.89	1.51	1.37
3	1-H	7489	AMP	C8-N9	7.89	1.51	1.37
3	2-H	7489	AMP	C8-N9	7.89	1.51	1.37
3	3-H	7489	AMP	C8-N9	7.89	1.51	1.37
3	4-H	7489	AMP	C8-N9	7.89	1.51	1.37
3	5-H	7489	AMP	C8-N9	7.89	1.51	1.37
3	6-H	7489	AMP	C8-N9	7.89	1.51	1.37
3	7-H	7489	AMP	C8-N9	7.89	1.51	1.37
3	8-H	7489	AMP	C8-N9	7.89	1.51	1.37
3	9-H	7489	AMP	C8-N9	7.89	1.51	1.37
3	10-H	7489	AMP	C8-N9	7.89	1.51	1.37
3	1-N	7501	AMP	C8-N9	7.89	1.51	1.37
3	2-N	7501	AMP	C8-N9	7.89	1.51	1.37
3	3-N	7501	AMP	C8-N9	7.89	1.51	1.37
3	4-N	7501	AMP	C8-N9	7.89	1.51	1.37
3	5-N	7501	AMP	C8-N9	7.89	1.51	1.37
3	6-N	7501	AMP	C8-N9	7.89	1.51	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-N	7501	AMP	C8-N9	7.89	1.51	1.37
3	8-N	7501	AMP	C8-N9	7.89	1.51	1.37
3	9-N	7501	AMP	C8-N9	7.89	1.51	1.37
3	10-N	7501	AMP	C8-N9	7.89	1.51	1.37
3	1-J	7493	AMP	C8-N9	7.89	1.51	1.37
3	2-J	7493	AMP	C8-N9	7.89	1.51	1.37
3	3-J	7493	AMP	C8-N9	7.89	1.51	1.37
3	4-J	7493	AMP	C8-N9	7.89	1.51	1.37
3	5-J	7493	AMP	C8-N9	7.89	1.51	1.37
3	6-J	7493	AMP	C8-N9	7.89	1.51	1.37
3	7-J	7493	AMP	C8-N9	7.89	1.51	1.37
3	8-J	7493	AMP	C8-N9	7.89	1.51	1.37
3	9-J	7493	AMP	C8-N9	7.89	1.51	1.37
3	10-J	7493	AMP	C8-N9	7.89	1.51	1.37
3	1-A	7475	AMP	C8-N9	7.88	1.50	1.37
3	2-A	7475	AMP	C8-N9	7.88	1.50	1.37
3	3-A	7475	AMP	C8-N9	7.88	1.50	1.37
3	4-A	7475	AMP	C8-N9	7.88	1.50	1.37
3	5-A	7475	AMP	C8-N9	7.88	1.50	1.37
3	6-A	7475	AMP	C8-N9	7.88	1.50	1.37
3	7-A	7475	AMP	C8-N9	7.88	1.50	1.37
3	8-A	7475	AMP	C8-N9	7.88	1.50	1.37
3	9-A	7475	AMP	C8-N9	7.88	1.50	1.37
3	10-A	7475	AMP	C8-N9	7.88	1.50	1.37
3	1-Q	7507	AMP	C8-N9	7.88	1.50	1.37
3	2-Q	7507	AMP	C8-N9	7.88	1.50	1.37
3	3-Q	7507	AMP	C8-N9	7.88	1.50	1.37
3	4-Q	7507	AMP	C8-N9	7.88	1.50	1.37
3	5-Q	7507	AMP	C8-N9	7.88	1.50	1.37
3	6-Q	7507	AMP	C8-N9	7.88	1.50	1.37
3	7-Q	7507	AMP	C8-N9	7.88	1.50	1.37
3	8-Q	7507	AMP	C8-N9	7.88	1.50	1.37
3	9-Q	7507	AMP	C8-N9	7.88	1.50	1.37
3	10-Q	7507	AMP	C8-N9	7.88	1.50	1.37
3	1-M	7499	AMP	C8-N9	7.88	1.50	1.37
3	2-M	7499	AMP	C8-N9	7.88	1.50	1.37
3	3-M	7499	AMP	C8-N9	7.88	1.50	1.37
3	4-M	7499	AMP	C8-N9	7.88	1.50	1.37
3	5-M	7499	AMP	C8-N9	7.88	1.50	1.37
3	6-M	7499	AMP	C8-N9	7.88	1.50	1.37
3	7-M	7499	AMP	C8-N9	7.88	1.50	1.37
3	8-M	7499	AMP	C8-N9	7.88	1.50	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-M	7499	AMP	C8-N9	7.88	1.50	1.37
3	10-M	7499	AMP	C8-N9	7.88	1.50	1.37
3	1-O	7503	AMP	C8-N9	7.87	1.50	1.37
3	2-O	7503	AMP	C8-N9	7.87	1.50	1.37
3	3-O	7503	AMP	C8-N9	7.87	1.50	1.37
3	4-O	7503	AMP	C8-N9	7.87	1.50	1.37
3	5-O	7503	AMP	C8-N9	7.87	1.50	1.37
3	6-O	7503	AMP	C8-N9	7.87	1.50	1.37
3	7-O	7503	AMP	C8-N9	7.87	1.50	1.37
3	8-O	7503	AMP	C8-N9	7.87	1.50	1.37
3	9-O	7503	AMP	C8-N9	7.87	1.50	1.37
3	10-O	7503	AMP	C8-N9	7.87	1.50	1.37
3	1-V	7517	AMP	C8-N9	7.87	1.50	1.37
3	2-V	7517	AMP	C8-N9	7.87	1.50	1.37
3	3-V	7517	AMP	C8-N9	7.87	1.50	1.37
3	4-V	7517	AMP	C8-N9	7.87	1.50	1.37
3	5-V	7517	AMP	C8-N9	7.87	1.50	1.37
3	6-V	7517	AMP	C8-N9	7.87	1.50	1.37
3	7-V	7517	AMP	C8-N9	7.87	1.50	1.37
3	8-V	7517	AMP	C8-N9	7.87	1.50	1.37
3	9-V	7517	AMP	C8-N9	7.87	1.50	1.37
3	10-V	7517	AMP	C8-N9	7.87	1.50	1.37
3	1-S	7511	AMP	C8-N9	7.86	1.50	1.37
3	2-S	7511	AMP	C8-N9	7.86	1.50	1.37
3	3-S	7511	AMP	C8-N9	7.86	1.50	1.37
3	4-S	7511	AMP	C8-N9	7.86	1.50	1.37
3	5-S	7511	AMP	C8-N9	7.86	1.50	1.37
3	6-S	7511	AMP	C8-N9	7.86	1.50	1.37
3	7-S	7511	AMP	C8-N9	7.86	1.50	1.37
3	8-S	7511	AMP	C8-N9	7.86	1.50	1.37
3	9-S	7511	AMP	C8-N9	7.86	1.50	1.37
3	10-S	7511	AMP	C8-N9	7.86	1.50	1.37
3	1-R	7509	AMP	C8-N9	7.86	1.50	1.37
3	2-R	7509	AMP	C8-N9	7.86	1.50	1.37
3	3-R	7509	AMP	C8-N9	7.86	1.50	1.37
3	4-R	7509	AMP	C8-N9	7.86	1.50	1.37
3	5-R	7509	AMP	C8-N9	7.86	1.50	1.37
3	6-R	7509	AMP	C8-N9	7.86	1.50	1.37
3	7-R	7509	AMP	C8-N9	7.86	1.50	1.37
3	8-R	7509	AMP	C8-N9	7.86	1.50	1.37
3	9-R	7509	AMP	C8-N9	7.86	1.50	1.37
3	10-R	7509	AMP	C8-N9	7.86	1.50	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-X	7521	AMP	C8-N9	7.86	1.50	1.37
3	2-X	7521	AMP	C8-N9	7.86	1.50	1.37
3	3-X	7521	AMP	C8-N9	7.86	1.50	1.37
3	4-X	7521	AMP	C8-N9	7.86	1.50	1.37
3	5-X	7521	AMP	C8-N9	7.86	1.50	1.37
3	6-X	7521	AMP	C8-N9	7.86	1.50	1.37
3	7-X	7521	AMP	C8-N9	7.86	1.50	1.37
3	8-X	7521	AMP	C8-N9	7.86	1.50	1.37
3	9-X	7521	AMP	C8-N9	7.86	1.50	1.37
3	10-X	7521	AMP	C8-N9	7.86	1.50	1.37
3	1-C	7479	AMP	C8-N9	7.84	1.50	1.37
3	2-C	7479	AMP	C8-N9	7.84	1.50	1.37
3	3-C	7479	AMP	C8-N9	7.84	1.50	1.37
3	4-C	7479	AMP	C8-N9	7.84	1.50	1.37
3	5-C	7479	AMP	C8-N9	7.84	1.50	1.37
3	6-C	7479	AMP	C8-N9	7.84	1.50	1.37
3	7-C	7479	AMP	C8-N9	7.84	1.50	1.37
3	8-C	7479	AMP	C8-N9	7.84	1.50	1.37
3	9-C	7479	AMP	C8-N9	7.84	1.50	1.37
3	10-C	7479	AMP	C8-N9	7.84	1.50	1.37
3	1-T	7513	AMP	C8-N9	7.84	1.50	1.37
3	2-T	7513	AMP	C8-N9	7.84	1.50	1.37
3	3-T	7513	AMP	C8-N9	7.84	1.50	1.37
3	4-T	7513	AMP	C8-N9	7.84	1.50	1.37
3	5-T	7513	AMP	C8-N9	7.84	1.50	1.37
3	6-T	7513	AMP	C8-N9	7.84	1.50	1.37
3	7-T	7513	AMP	C8-N9	7.84	1.50	1.37
3	8-T	7513	AMP	C8-N9	7.84	1.50	1.37
3	9-T	7513	AMP	C8-N9	7.84	1.50	1.37
3	10-T	7513	AMP	C8-N9	7.84	1.50	1.37
3	1-G	7487	AMP	C8-N9	7.84	1.50	1.37
3	2-G	7487	AMP	C8-N9	7.84	1.50	1.37
3	3-G	7487	AMP	C8-N9	7.84	1.50	1.37
3	4-G	7487	AMP	C8-N9	7.84	1.50	1.37
3	5-G	7487	AMP	C8-N9	7.84	1.50	1.37
3	6-G	7487	AMP	C8-N9	7.84	1.50	1.37
3	7-G	7487	AMP	C8-N9	7.84	1.50	1.37
3	8-G	7487	AMP	C8-N9	7.84	1.50	1.37
3	9-G	7487	AMP	C8-N9	7.84	1.50	1.37
3	10-G	7487	AMP	C8-N9	7.84	1.50	1.37
3	1-I	7491	AMP	C8-N9	7.84	1.50	1.37
3	2-I	7491	AMP	C8-N9	7.84	1.50	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-I	7491	AMP	C8-N9	7.84	1.50	1.37
3	4-I	7491	AMP	C8-N9	7.84	1.50	1.37
3	5-I	7491	AMP	C8-N9	7.84	1.50	1.37
3	6-I	7491	AMP	C8-N9	7.84	1.50	1.37
3	7-I	7491	AMP	C8-N9	7.84	1.50	1.37
3	8-I	7491	AMP	C8-N9	7.84	1.50	1.37
3	9-I	7491	AMP	C8-N9	7.84	1.50	1.37
3	10-I	7491	AMP	C8-N9	7.84	1.50	1.37
3	1-E	7483	AMP	C8-N9	7.83	1.50	1.37
3	2-E	7483	AMP	C8-N9	7.83	1.50	1.37
3	3-E	7483	AMP	C8-N9	7.83	1.50	1.37
3	4-E	7483	AMP	C8-N9	7.83	1.50	1.37
3	5-E	7483	AMP	C8-N9	7.83	1.50	1.37
3	6-E	7483	AMP	C8-N9	7.83	1.50	1.37
3	7-E	7483	AMP	C8-N9	7.83	1.50	1.37
3	8-E	7483	AMP	C8-N9	7.83	1.50	1.37
3	9-E	7483	AMP	C8-N9	7.83	1.50	1.37
3	10-E	7483	AMP	C8-N9	7.83	1.50	1.37
4	1-C	7480	CIT	C3-C6	-6.97	1.46	1.53
4	2-C	7480	CIT	C3-C6	-6.97	1.46	1.53
4	3-C	7480	CIT	C3-C6	-6.97	1.46	1.53
4	4-C	7480	CIT	C3-C6	-6.97	1.46	1.53
4	5-C	7480	CIT	C3-C6	-6.97	1.46	1.53
4	6-C	7480	CIT	C3-C6	-6.97	1.46	1.53
4	7-C	7480	CIT	C3-C6	-6.97	1.46	1.53
4	8-C	7480	CIT	C3-C6	-6.97	1.46	1.53
4	9-C	7480	CIT	C3-C6	-6.97	1.46	1.53
4	10-C	7480	CIT	C3-C6	-6.97	1.46	1.53
4	1-V	7518	CIT	C3-C6	-6.96	1.46	1.53
4	2-V	7518	CIT	C3-C6	-6.96	1.46	1.53
4	3-V	7518	CIT	C3-C6	-6.96	1.46	1.53
4	4-V	7518	CIT	C3-C6	-6.96	1.46	1.53
4	5-V	7518	CIT	C3-C6	-6.96	1.46	1.53
4	6-V	7518	CIT	C3-C6	-6.96	1.46	1.53
4	7-V	7518	CIT	C3-C6	-6.96	1.46	1.53
4	8-V	7518	CIT	C3-C6	-6.96	1.46	1.53
4	9-V	7518	CIT	C3-C6	-6.96	1.46	1.53
4	10-V	7518	CIT	C3-C6	-6.96	1.46	1.53
4	1-O	7504	CIT	C3-C6	-6.95	1.46	1.53
4	2-O	7504	CIT	C3-C6	-6.95	1.46	1.53
4	3-O	7504	CIT	C3-C6	-6.95	1.46	1.53
4	4-O	7504	CIT	C3-C6	-6.95	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5-O	7504	CIT	C3-C6	-6.95	1.46	1.53
4	6-O	7504	CIT	C3-C6	-6.95	1.46	1.53
4	7-O	7504	CIT	C3-C6	-6.95	1.46	1.53
4	8-O	7504	CIT	C3-C6	-6.95	1.46	1.53
4	9-O	7504	CIT	C3-C6	-6.95	1.46	1.53
4	10-O	7504	CIT	C3-C6	-6.95	1.46	1.53
4	1-R	7510	CIT	C3-C6	-6.94	1.46	1.53
4	2-R	7510	CIT	C3-C6	-6.94	1.46	1.53
4	3-R	7510	CIT	C3-C6	-6.94	1.46	1.53
4	4-R	7510	CIT	C3-C6	-6.94	1.46	1.53
4	5-R	7510	CIT	C3-C6	-6.94	1.46	1.53
4	6-R	7510	CIT	C3-C6	-6.94	1.46	1.53
4	7-R	7510	CIT	C3-C6	-6.94	1.46	1.53
4	8-R	7510	CIT	C3-C6	-6.94	1.46	1.53
4	9-R	7510	CIT	C3-C6	-6.94	1.46	1.53
4	10-R	7510	CIT	C3-C6	-6.94	1.46	1.53
4	1-P	7506	CIT	C3-C6	-6.93	1.46	1.53
4	2-P	7506	CIT	C3-C6	-6.93	1.46	1.53
4	3-P	7506	CIT	C3-C6	-6.93	1.46	1.53
4	4-P	7506	CIT	C3-C6	-6.93	1.46	1.53
4	5-P	7506	CIT	C3-C6	-6.93	1.46	1.53
4	6-P	7506	CIT	C3-C6	-6.93	1.46	1.53
4	7-P	7506	CIT	C3-C6	-6.93	1.46	1.53
4	8-P	7506	CIT	C3-C6	-6.93	1.46	1.53
4	9-P	7506	CIT	C3-C6	-6.93	1.46	1.53
4	10-P	7506	CIT	C3-C6	-6.93	1.46	1.53
4	1-S	7512	CIT	C3-C6	-6.92	1.46	1.53
4	2-S	7512	CIT	C3-C6	-6.92	1.46	1.53
4	3-S	7512	CIT	C3-C6	-6.92	1.46	1.53
4	4-S	7512	CIT	C3-C6	-6.92	1.46	1.53
4	5-S	7512	CIT	C3-C6	-6.92	1.46	1.53
4	6-S	7512	CIT	C3-C6	-6.92	1.46	1.53
4	7-S	7512	CIT	C3-C6	-6.92	1.46	1.53
4	8-S	7512	CIT	C3-C6	-6.92	1.46	1.53
4	9-S	7512	CIT	C3-C6	-6.92	1.46	1.53
4	10-S	7512	CIT	C3-C6	-6.92	1.46	1.53
4	1-G	7488	CIT	C3-C6	-6.91	1.46	1.53
4	2-G	7488	CIT	C3-C6	-6.91	1.46	1.53
4	3-G	7488	CIT	C3-C6	-6.91	1.46	1.53
4	4-G	7488	CIT	C3-C6	-6.91	1.46	1.53
4	5-G	7488	CIT	C3-C6	-6.91	1.46	1.53
4	6-G	7488	CIT	C3-C6	-6.91	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-G	7488	CIT	C3-C6	-6.91	1.46	1.53
4	8-G	7488	CIT	C3-C6	-6.91	1.46	1.53
4	9-G	7488	CIT	C3-C6	-6.91	1.46	1.53
4	10-G	7488	CIT	C3-C6	-6.91	1.46	1.53
4	1-K	7496	CIT	C3-C6	-6.91	1.46	1.53
4	2-K	7496	CIT	C3-C6	-6.91	1.46	1.53
4	3-K	7496	CIT	C3-C6	-6.91	1.46	1.53
4	4-K	7496	CIT	C3-C6	-6.91	1.46	1.53
4	5-K	7496	CIT	C3-C6	-6.91	1.46	1.53
4	6-K	7496	CIT	C3-C6	-6.91	1.46	1.53
4	7-K	7496	CIT	C3-C6	-6.91	1.46	1.53
4	8-K	7496	CIT	C3-C6	-6.91	1.46	1.53
4	9-K	7496	CIT	C3-C6	-6.91	1.46	1.53
4	10-K	7496	CIT	C3-C6	-6.91	1.46	1.53
4	1-N	7502	CIT	C3-C6	-6.90	1.46	1.53
4	2-N	7502	CIT	C3-C6	-6.90	1.46	1.53
4	3-N	7502	CIT	C3-C6	-6.90	1.46	1.53
4	4-N	7502	CIT	C3-C6	-6.90	1.46	1.53
4	5-N	7502	CIT	C3-C6	-6.90	1.46	1.53
4	6-N	7502	CIT	C3-C6	-6.90	1.46	1.53
4	7-N	7502	CIT	C3-C6	-6.90	1.46	1.53
4	8-N	7502	CIT	C3-C6	-6.90	1.46	1.53
4	9-N	7502	CIT	C3-C6	-6.90	1.46	1.53
4	10-N	7502	CIT	C3-C6	-6.90	1.46	1.53
4	1-E	7484	CIT	C3-C6	-6.90	1.46	1.53
4	2-E	7484	CIT	C3-C6	-6.90	1.46	1.53
4	3-E	7484	CIT	C3-C6	-6.90	1.46	1.53
4	4-E	7484	CIT	C3-C6	-6.90	1.46	1.53
4	5-E	7484	CIT	C3-C6	-6.90	1.46	1.53
4	6-E	7484	CIT	C3-C6	-6.90	1.46	1.53
4	7-E	7484	CIT	C3-C6	-6.90	1.46	1.53
4	8-E	7484	CIT	C3-C6	-6.90	1.46	1.53
4	9-E	7484	CIT	C3-C6	-6.90	1.46	1.53
4	10-E	7484	CIT	C3-C6	-6.90	1.46	1.53
4	1-I	7492	CIT	C3-C6	-6.90	1.46	1.53
4	2-I	7492	CIT	C3-C6	-6.90	1.46	1.53
4	3-I	7492	CIT	C3-C6	-6.90	1.46	1.53
4	4-I	7492	CIT	C3-C6	-6.90	1.46	1.53
4	5-I	7492	CIT	C3-C6	-6.90	1.46	1.53
4	6-I	7492	CIT	C3-C6	-6.90	1.46	1.53
4	7-I	7492	CIT	C3-C6	-6.90	1.46	1.53
4	8-I	7492	CIT	C3-C6	-6.90	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9-I	7492	CIT	C3-C6	-6.90	1.46	1.53
4	10-I	7492	CIT	C3-C6	-6.90	1.46	1.53
4	1-Q	7508	CIT	C3-C6	-6.90	1.46	1.53
4	2-Q	7508	CIT	C3-C6	-6.90	1.46	1.53
4	3-Q	7508	CIT	C3-C6	-6.90	1.46	1.53
4	4-Q	7508	CIT	C3-C6	-6.90	1.46	1.53
4	5-Q	7508	CIT	C3-C6	-6.90	1.46	1.53
4	6-Q	7508	CIT	C3-C6	-6.90	1.46	1.53
4	7-Q	7508	CIT	C3-C6	-6.90	1.46	1.53
4	8-Q	7508	CIT	C3-C6	-6.90	1.46	1.53
4	9-Q	7508	CIT	C3-C6	-6.90	1.46	1.53
4	10-Q	7508	CIT	C3-C6	-6.90	1.46	1.53
4	1-J	7494	CIT	C3-C6	-6.89	1.46	1.53
4	2-J	7494	CIT	C3-C6	-6.89	1.46	1.53
4	3-J	7494	CIT	C3-C6	-6.89	1.46	1.53
4	4-J	7494	CIT	C3-C6	-6.89	1.46	1.53
4	5-J	7494	CIT	C3-C6	-6.89	1.46	1.53
4	6-J	7494	CIT	C3-C6	-6.89	1.46	1.53
4	7-J	7494	CIT	C3-C6	-6.89	1.46	1.53
4	8-J	7494	CIT	C3-C6	-6.89	1.46	1.53
4	9-J	7494	CIT	C3-C6	-6.89	1.46	1.53
4	10-J	7494	CIT	C3-C6	-6.89	1.46	1.53
4	1-F	7486	CIT	C3-C6	-6.89	1.46	1.53
4	2-F	7486	CIT	C3-C6	-6.89	1.46	1.53
4	3-F	7486	CIT	C3-C6	-6.89	1.46	1.53
4	4-F	7486	CIT	C3-C6	-6.89	1.46	1.53
4	5-F	7486	CIT	C3-C6	-6.89	1.46	1.53
4	6-F	7486	CIT	C3-C6	-6.89	1.46	1.53
4	7-F	7486	CIT	C3-C6	-6.89	1.46	1.53
4	8-F	7486	CIT	C3-C6	-6.89	1.46	1.53
4	9-F	7486	CIT	C3-C6	-6.89	1.46	1.53
4	10-F	7486	CIT	C3-C6	-6.89	1.46	1.53
4	1-A	7476	CIT	C3-C6	-6.88	1.46	1.53
4	2-A	7476	CIT	C3-C6	-6.88	1.46	1.53
4	3-A	7476	CIT	C3-C6	-6.88	1.46	1.53
4	4-A	7476	CIT	C3-C6	-6.88	1.46	1.53
4	5-A	7476	CIT	C3-C6	-6.88	1.46	1.53
4	6-A	7476	CIT	C3-C6	-6.88	1.46	1.53
4	7-A	7476	CIT	C3-C6	-6.88	1.46	1.53
4	8-A	7476	CIT	C3-C6	-6.88	1.46	1.53
4	9-A	7476	CIT	C3-C6	-6.88	1.46	1.53
4	10-A	7476	CIT	C3-C6	-6.88	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-T	7514	CIT	C3-C6	-6.88	1.46	1.53
4	2-T	7514	CIT	C3-C6	-6.88	1.46	1.53
4	3-T	7514	CIT	C3-C6	-6.88	1.46	1.53
4	4-T	7514	CIT	C3-C6	-6.88	1.46	1.53
4	5-T	7514	CIT	C3-C6	-6.88	1.46	1.53
4	6-T	7514	CIT	C3-C6	-6.88	1.46	1.53
4	7-T	7514	CIT	C3-C6	-6.88	1.46	1.53
4	8-T	7514	CIT	C3-C6	-6.88	1.46	1.53
4	9-T	7514	CIT	C3-C6	-6.88	1.46	1.53
4	10-T	7514	CIT	C3-C6	-6.88	1.46	1.53
4	1-W	7520	CIT	C3-C6	-6.88	1.46	1.53
4	2-W	7520	CIT	C3-C6	-6.88	1.46	1.53
4	3-W	7520	CIT	C3-C6	-6.88	1.46	1.53
4	4-W	7520	CIT	C3-C6	-6.88	1.46	1.53
4	5-W	7520	CIT	C3-C6	-6.88	1.46	1.53
4	6-W	7520	CIT	C3-C6	-6.88	1.46	1.53
4	7-W	7520	CIT	C3-C6	-6.88	1.46	1.53
4	8-W	7520	CIT	C3-C6	-6.88	1.46	1.53
4	9-W	7520	CIT	C3-C6	-6.88	1.46	1.53
4	10-W	7520	CIT	C3-C6	-6.88	1.46	1.53
4	1-D	7482	CIT	C3-C6	-6.87	1.46	1.53
4	2-D	7482	CIT	C3-C6	-6.87	1.46	1.53
4	3-D	7482	CIT	C3-C6	-6.87	1.46	1.53
4	4-D	7482	CIT	C3-C6	-6.87	1.46	1.53
4	5-D	7482	CIT	C3-C6	-6.87	1.46	1.53
4	6-D	7482	CIT	C3-C6	-6.87	1.46	1.53
4	7-D	7482	CIT	C3-C6	-6.87	1.46	1.53
4	8-D	7482	CIT	C3-C6	-6.87	1.46	1.53
4	9-D	7482	CIT	C3-C6	-6.87	1.46	1.53
4	10-D	7482	CIT	C3-C6	-6.87	1.46	1.53
4	1-B	7478	CIT	C3-C6	-6.86	1.46	1.53
4	2-B	7478	CIT	C3-C6	-6.86	1.46	1.53
4	3-B	7478	CIT	C3-C6	-6.86	1.46	1.53
4	4-B	7478	CIT	C3-C6	-6.86	1.46	1.53
4	5-B	7478	CIT	C3-C6	-6.86	1.46	1.53
4	6-B	7478	CIT	C3-C6	-6.86	1.46	1.53
4	7-B	7478	CIT	C3-C6	-6.86	1.46	1.53
4	8-B	7478	CIT	C3-C6	-6.86	1.46	1.53
4	9-B	7478	CIT	C3-C6	-6.86	1.46	1.53
4	10-B	7478	CIT	C3-C6	-6.86	1.46	1.53
4	1-M	7500	CIT	C3-C6	-6.86	1.46	1.53
4	2-M	7500	CIT	C3-C6	-6.86	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-M	7500	CIT	C3-C6	-6.86	1.46	1.53
4	4-M	7500	CIT	C3-C6	-6.86	1.46	1.53
4	5-M	7500	CIT	C3-C6	-6.86	1.46	1.53
4	6-M	7500	CIT	C3-C6	-6.86	1.46	1.53
4	7-M	7500	CIT	C3-C6	-6.86	1.46	1.53
4	8-M	7500	CIT	C3-C6	-6.86	1.46	1.53
4	9-M	7500	CIT	C3-C6	-6.86	1.46	1.53
4	10-M	7500	CIT	C3-C6	-6.86	1.46	1.53
4	1-L	7498	CIT	C3-C6	-6.86	1.46	1.53
4	2-L	7498	CIT	C3-C6	-6.86	1.46	1.53
4	3-L	7498	CIT	C3-C6	-6.86	1.46	1.53
4	4-L	7498	CIT	C3-C6	-6.86	1.46	1.53
4	5-L	7498	CIT	C3-C6	-6.86	1.46	1.53
4	6-L	7498	CIT	C3-C6	-6.86	1.46	1.53
4	7-L	7498	CIT	C3-C6	-6.86	1.46	1.53
4	8-L	7498	CIT	C3-C6	-6.86	1.46	1.53
4	9-L	7498	CIT	C3-C6	-6.86	1.46	1.53
4	10-L	7498	CIT	C3-C6	-6.86	1.46	1.53
4	1-H	7490	CIT	C3-C6	-6.86	1.46	1.53
4	2-H	7490	CIT	C3-C6	-6.86	1.46	1.53
4	3-H	7490	CIT	C3-C6	-6.86	1.46	1.53
4	4-H	7490	CIT	C3-C6	-6.86	1.46	1.53
4	5-H	7490	CIT	C3-C6	-6.86	1.46	1.53
4	6-H	7490	CIT	C3-C6	-6.86	1.46	1.53
4	7-H	7490	CIT	C3-C6	-6.86	1.46	1.53
4	8-H	7490	CIT	C3-C6	-6.86	1.46	1.53
4	9-H	7490	CIT	C3-C6	-6.86	1.46	1.53
4	10-H	7490	CIT	C3-C6	-6.86	1.46	1.53
4	1-U	7516	CIT	C3-C6	-6.85	1.46	1.53
4	2-U	7516	CIT	C3-C6	-6.85	1.46	1.53
4	3-U	7516	CIT	C3-C6	-6.85	1.46	1.53
4	4-U	7516	CIT	C3-C6	-6.85	1.46	1.53
4	5-U	7516	CIT	C3-C6	-6.85	1.46	1.53
4	6-U	7516	CIT	C3-C6	-6.85	1.46	1.53
4	7-U	7516	CIT	C3-C6	-6.85	1.46	1.53
4	8-U	7516	CIT	C3-C6	-6.85	1.46	1.53
4	9-U	7516	CIT	C3-C6	-6.85	1.46	1.53
4	10-U	7516	CIT	C3-C6	-6.85	1.46	1.53
4	1-X	7522	CIT	C3-C6	-6.82	1.46	1.53
4	2-X	7522	CIT	C3-C6	-6.82	1.46	1.53
4	3-X	7522	CIT	C3-C6	-6.82	1.46	1.53
4	4-X	7522	CIT	C3-C6	-6.82	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5-X	7522	CIT	C3-C6	-6.82	1.46	1.53
4	6-X	7522	CIT	C3-C6	-6.82	1.46	1.53
4	7-X	7522	CIT	C3-C6	-6.82	1.46	1.53
4	8-X	7522	CIT	C3-C6	-6.82	1.46	1.53
4	9-X	7522	CIT	C3-C6	-6.82	1.46	1.53
4	10-X	7522	CIT	C3-C6	-6.82	1.46	1.53
4	1-L	7498	CIT	C2-C3	5.60	1.60	1.54
4	2-L	7498	CIT	C2-C3	5.60	1.60	1.54
4	3-L	7498	CIT	C2-C3	5.60	1.60	1.54
4	4-L	7498	CIT	C2-C3	5.60	1.60	1.54
4	5-L	7498	CIT	C2-C3	5.60	1.60	1.54
4	6-L	7498	CIT	C2-C3	5.60	1.60	1.54
4	7-L	7498	CIT	C2-C3	5.60	1.60	1.54
4	8-L	7498	CIT	C2-C3	5.60	1.60	1.54
4	9-L	7498	CIT	C2-C3	5.60	1.60	1.54
4	10-L	7498	CIT	C2-C3	5.60	1.60	1.54
4	1-C	7480	CIT	C2-C3	5.57	1.60	1.54
4	2-C	7480	CIT	C2-C3	5.57	1.60	1.54
4	3-C	7480	CIT	C2-C3	5.57	1.60	1.54
4	4-C	7480	CIT	C2-C3	5.57	1.60	1.54
4	5-C	7480	CIT	C2-C3	5.57	1.60	1.54
4	6-C	7480	CIT	C2-C3	5.57	1.60	1.54
4	7-C	7480	CIT	C2-C3	5.57	1.60	1.54
4	8-C	7480	CIT	C2-C3	5.57	1.60	1.54
4	9-C	7480	CIT	C2-C3	5.57	1.60	1.54
4	10-C	7480	CIT	C2-C3	5.57	1.60	1.54
4	1-V	7518	CIT	C2-C3	5.56	1.60	1.54
4	2-V	7518	CIT	C2-C3	5.56	1.60	1.54
4	3-V	7518	CIT	C2-C3	5.56	1.60	1.54
4	4-V	7518	CIT	C2-C3	5.56	1.60	1.54
4	5-V	7518	CIT	C2-C3	5.56	1.60	1.54
4	6-V	7518	CIT	C2-C3	5.56	1.60	1.54
4	7-V	7518	CIT	C2-C3	5.56	1.60	1.54
4	8-V	7518	CIT	C2-C3	5.56	1.60	1.54
4	9-V	7518	CIT	C2-C3	5.56	1.60	1.54
4	10-V	7518	CIT	C2-C3	5.56	1.60	1.54
4	1-I	7492	CIT	C2-C3	5.53	1.60	1.54
4	2-I	7492	CIT	C2-C3	5.53	1.60	1.54
4	3-I	7492	CIT	C2-C3	5.53	1.60	1.54
4	4-I	7492	CIT	C2-C3	5.53	1.60	1.54
4	5-I	7492	CIT	C2-C3	5.53	1.60	1.54
4	6-I	7492	CIT	C2-C3	5.53	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-I	7492	CIT	C2-C3	5.53	1.60	1.54
4	8-I	7492	CIT	C2-C3	5.53	1.60	1.54
4	9-I	7492	CIT	C2-C3	5.53	1.60	1.54
4	10-I	7492	CIT	C2-C3	5.53	1.60	1.54
4	1-N	7502	CIT	C2-C3	5.53	1.60	1.54
4	2-N	7502	CIT	C2-C3	5.53	1.60	1.54
4	3-N	7502	CIT	C2-C3	5.53	1.60	1.54
4	4-N	7502	CIT	C2-C3	5.53	1.60	1.54
4	5-N	7502	CIT	C2-C3	5.53	1.60	1.54
4	6-N	7502	CIT	C2-C3	5.53	1.60	1.54
4	7-N	7502	CIT	C2-C3	5.53	1.60	1.54
4	8-N	7502	CIT	C2-C3	5.53	1.60	1.54
4	9-N	7502	CIT	C2-C3	5.53	1.60	1.54
4	10-N	7502	CIT	C2-C3	5.53	1.60	1.54
4	1-F	7486	CIT	C2-C3	5.53	1.60	1.54
4	2-F	7486	CIT	C2-C3	5.53	1.60	1.54
4	3-F	7486	CIT	C2-C3	5.53	1.60	1.54
4	4-F	7486	CIT	C2-C3	5.53	1.60	1.54
4	5-F	7486	CIT	C2-C3	5.53	1.60	1.54
4	6-F	7486	CIT	C2-C3	5.53	1.60	1.54
4	7-F	7486	CIT	C2-C3	5.53	1.60	1.54
4	8-F	7486	CIT	C2-C3	5.53	1.60	1.54
4	9-F	7486	CIT	C2-C3	5.53	1.60	1.54
4	10-F	7486	CIT	C2-C3	5.53	1.60	1.54
4	1-D	7482	CIT	C2-C3	5.52	1.60	1.54
4	2-D	7482	CIT	C2-C3	5.52	1.60	1.54
4	3-D	7482	CIT	C2-C3	5.52	1.60	1.54
4	4-D	7482	CIT	C2-C3	5.52	1.60	1.54
4	5-D	7482	CIT	C2-C3	5.52	1.60	1.54
4	6-D	7482	CIT	C2-C3	5.52	1.60	1.54
4	7-D	7482	CIT	C2-C3	5.52	1.60	1.54
4	8-D	7482	CIT	C2-C3	5.52	1.60	1.54
4	9-D	7482	CIT	C2-C3	5.52	1.60	1.54
4	10-D	7482	CIT	C2-C3	5.52	1.60	1.54
4	1-W	7520	CIT	C2-C3	5.51	1.60	1.54
4	2-W	7520	CIT	C2-C3	5.51	1.60	1.54
4	3-W	7520	CIT	C2-C3	5.51	1.60	1.54
4	4-W	7520	CIT	C2-C3	5.51	1.60	1.54
4	5-W	7520	CIT	C2-C3	5.51	1.60	1.54
4	6-W	7520	CIT	C2-C3	5.51	1.60	1.54
4	7-W	7520	CIT	C2-C3	5.51	1.60	1.54
4	8-W	7520	CIT	C2-C3	5.51	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9-W	7520	CIT	C2-C3	5.51	1.60	1.54
4	10-W	7520	CIT	C2-C3	5.51	1.60	1.54
4	1-E	7484	CIT	C2-C3	5.51	1.60	1.54
4	2-E	7484	CIT	C2-C3	5.51	1.60	1.54
4	3-E	7484	CIT	C2-C3	5.51	1.60	1.54
4	4-E	7484	CIT	C2-C3	5.51	1.60	1.54
4	5-E	7484	CIT	C2-C3	5.51	1.60	1.54
4	6-E	7484	CIT	C2-C3	5.51	1.60	1.54
4	7-E	7484	CIT	C2-C3	5.51	1.60	1.54
4	8-E	7484	CIT	C2-C3	5.51	1.60	1.54
4	9-E	7484	CIT	C2-C3	5.51	1.60	1.54
4	10-E	7484	CIT	C2-C3	5.51	1.60	1.54
4	1-S	7512	CIT	C2-C3	5.51	1.60	1.54
4	2-S	7512	CIT	C2-C3	5.51	1.60	1.54
4	3-S	7512	CIT	C2-C3	5.51	1.60	1.54
4	4-S	7512	CIT	C2-C3	5.51	1.60	1.54
4	5-S	7512	CIT	C2-C3	5.51	1.60	1.54
4	6-S	7512	CIT	C2-C3	5.51	1.60	1.54
4	7-S	7512	CIT	C2-C3	5.51	1.60	1.54
4	8-S	7512	CIT	C2-C3	5.51	1.60	1.54
4	9-S	7512	CIT	C2-C3	5.51	1.60	1.54
4	10-S	7512	CIT	C2-C3	5.51	1.60	1.54
4	1-A	7476	CIT	C2-C3	5.50	1.60	1.54
4	2-A	7476	CIT	C2-C3	5.50	1.60	1.54
4	3-A	7476	CIT	C2-C3	5.50	1.60	1.54
4	4-A	7476	CIT	C2-C3	5.50	1.60	1.54
4	5-A	7476	CIT	C2-C3	5.50	1.60	1.54
4	6-A	7476	CIT	C2-C3	5.50	1.60	1.54
4	7-A	7476	CIT	C2-C3	5.50	1.60	1.54
4	8-A	7476	CIT	C2-C3	5.50	1.60	1.54
4	9-A	7476	CIT	C2-C3	5.50	1.60	1.54
4	10-A	7476	CIT	C2-C3	5.50	1.60	1.54
4	1-B	7478	CIT	C2-C3	5.50	1.60	1.54
4	2-B	7478	CIT	C2-C3	5.50	1.60	1.54
4	3-B	7478	CIT	C2-C3	5.50	1.60	1.54
4	4-B	7478	CIT	C2-C3	5.50	1.60	1.54
4	5-B	7478	CIT	C2-C3	5.50	1.60	1.54
4	6-B	7478	CIT	C2-C3	5.50	1.60	1.54
4	7-B	7478	CIT	C2-C3	5.50	1.60	1.54
4	8-B	7478	CIT	C2-C3	5.50	1.60	1.54
4	9-B	7478	CIT	C2-C3	5.50	1.60	1.54
4	10-B	7478	CIT	C2-C3	5.50	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-Q	7508	CIT	C2-C3	5.50	1.60	1.54
4	2-Q	7508	CIT	C2-C3	5.50	1.60	1.54
4	3-Q	7508	CIT	C2-C3	5.50	1.60	1.54
4	4-Q	7508	CIT	C2-C3	5.50	1.60	1.54
4	5-Q	7508	CIT	C2-C3	5.50	1.60	1.54
4	6-Q	7508	CIT	C2-C3	5.50	1.60	1.54
4	7-Q	7508	CIT	C2-C3	5.50	1.60	1.54
4	8-Q	7508	CIT	C2-C3	5.50	1.60	1.54
4	9-Q	7508	CIT	C2-C3	5.50	1.60	1.54
4	10-Q	7508	CIT	C2-C3	5.50	1.60	1.54
4	1-G	7488	CIT	C2-C3	5.50	1.60	1.54
4	2-G	7488	CIT	C2-C3	5.50	1.60	1.54
4	3-G	7488	CIT	C2-C3	5.50	1.60	1.54
4	4-G	7488	CIT	C2-C3	5.50	1.60	1.54
4	5-G	7488	CIT	C2-C3	5.50	1.60	1.54
4	6-G	7488	CIT	C2-C3	5.50	1.60	1.54
4	7-G	7488	CIT	C2-C3	5.50	1.60	1.54
4	8-G	7488	CIT	C2-C3	5.50	1.60	1.54
4	9-G	7488	CIT	C2-C3	5.50	1.60	1.54
4	10-G	7488	CIT	C2-C3	5.50	1.60	1.54
4	1-O	7504	CIT	C2-C3	5.49	1.60	1.54
4	2-O	7504	CIT	C2-C3	5.49	1.60	1.54
4	3-O	7504	CIT	C2-C3	5.49	1.60	1.54
4	4-O	7504	CIT	C2-C3	5.49	1.60	1.54
4	5-O	7504	CIT	C2-C3	5.49	1.60	1.54
4	6-O	7504	CIT	C2-C3	5.49	1.60	1.54
4	7-O	7504	CIT	C2-C3	5.49	1.60	1.54
4	8-O	7504	CIT	C2-C3	5.49	1.60	1.54
4	9-O	7504	CIT	C2-C3	5.49	1.60	1.54
4	10-O	7504	CIT	C2-C3	5.49	1.60	1.54
4	1-J	7494	CIT	C2-C3	5.49	1.60	1.54
4	2-J	7494	CIT	C2-C3	5.49	1.60	1.54
4	3-J	7494	CIT	C2-C3	5.49	1.60	1.54
4	4-J	7494	CIT	C2-C3	5.49	1.60	1.54
4	5-J	7494	CIT	C2-C3	5.49	1.60	1.54
4	6-J	7494	CIT	C2-C3	5.49	1.60	1.54
4	7-J	7494	CIT	C2-C3	5.49	1.60	1.54
4	8-J	7494	CIT	C2-C3	5.49	1.60	1.54
4	9-J	7494	CIT	C2-C3	5.49	1.60	1.54
4	10-J	7494	CIT	C2-C3	5.49	1.60	1.54
3	1-L	7497	AMP	C4-N3	5.48	1.44	1.34
3	2-L	7497	AMP	C4-N3	5.48	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-L	7497	AMP	C4-N3	5.48	1.44	1.34
3	4-L	7497	AMP	C4-N3	5.48	1.44	1.34
3	5-L	7497	AMP	C4-N3	5.48	1.44	1.34
3	6-L	7497	AMP	C4-N3	5.48	1.44	1.34
3	7-L	7497	AMP	C4-N3	5.48	1.44	1.34
3	8-L	7497	AMP	C4-N3	5.48	1.44	1.34
3	9-L	7497	AMP	C4-N3	5.48	1.44	1.34
3	10-L	7497	AMP	C4-N3	5.48	1.44	1.34
4	1-P	7506	CIT	C2-C3	5.48	1.60	1.54
4	2-P	7506	CIT	C2-C3	5.48	1.60	1.54
4	3-P	7506	CIT	C2-C3	5.48	1.60	1.54
4	4-P	7506	CIT	C2-C3	5.48	1.60	1.54
4	5-P	7506	CIT	C2-C3	5.48	1.60	1.54
4	6-P	7506	CIT	C2-C3	5.48	1.60	1.54
4	7-P	7506	CIT	C2-C3	5.48	1.60	1.54
4	8-P	7506	CIT	C2-C3	5.48	1.60	1.54
4	9-P	7506	CIT	C2-C3	5.48	1.60	1.54
4	10-P	7506	CIT	C2-C3	5.48	1.60	1.54
3	1-H	7489	AMP	C4-N3	5.48	1.44	1.34
3	2-H	7489	AMP	C4-N3	5.48	1.44	1.34
3	3-H	7489	AMP	C4-N3	5.48	1.44	1.34
3	4-H	7489	AMP	C4-N3	5.48	1.44	1.34
3	5-H	7489	AMP	C4-N3	5.48	1.44	1.34
3	6-H	7489	AMP	C4-N3	5.48	1.44	1.34
3	7-H	7489	AMP	C4-N3	5.48	1.44	1.34
3	8-H	7489	AMP	C4-N3	5.48	1.44	1.34
3	9-H	7489	AMP	C4-N3	5.48	1.44	1.34
3	10-H	7489	AMP	C4-N3	5.48	1.44	1.34
4	1-U	7516	CIT	C2-C3	5.48	1.60	1.54
4	2-U	7516	CIT	C2-C3	5.48	1.60	1.54
4	3-U	7516	CIT	C2-C3	5.48	1.60	1.54
4	4-U	7516	CIT	C2-C3	5.48	1.60	1.54
4	5-U	7516	CIT	C2-C3	5.48	1.60	1.54
4	6-U	7516	CIT	C2-C3	5.48	1.60	1.54
4	7-U	7516	CIT	C2-C3	5.48	1.60	1.54
4	8-U	7516	CIT	C2-C3	5.48	1.60	1.54
4	9-U	7516	CIT	C2-C3	5.48	1.60	1.54
4	10-U	7516	CIT	C2-C3	5.48	1.60	1.54
4	1-K	7496	CIT	C2-C3	5.47	1.60	1.54
4	2-K	7496	CIT	C2-C3	5.47	1.60	1.54
4	3-K	7496	CIT	C2-C3	5.47	1.60	1.54
4	4-K	7496	CIT	C2-C3	5.47	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5-K	7496	CIT	C2-C3	5.47	1.60	1.54
4	6-K	7496	CIT	C2-C3	5.47	1.60	1.54
4	7-K	7496	CIT	C2-C3	5.47	1.60	1.54
4	8-K	7496	CIT	C2-C3	5.47	1.60	1.54
4	9-K	7496	CIT	C2-C3	5.47	1.60	1.54
4	10-K	7496	CIT	C2-C3	5.47	1.60	1.54
3	1-B	7477	AMP	C4-N3	5.47	1.44	1.34
3	2-B	7477	AMP	C4-N3	5.47	1.44	1.34
3	3-B	7477	AMP	C4-N3	5.47	1.44	1.34
3	4-B	7477	AMP	C4-N3	5.47	1.44	1.34
3	5-B	7477	AMP	C4-N3	5.47	1.44	1.34
3	6-B	7477	AMP	C4-N3	5.47	1.44	1.34
3	7-B	7477	AMP	C4-N3	5.47	1.44	1.34
3	8-B	7477	AMP	C4-N3	5.47	1.44	1.34
3	9-B	7477	AMP	C4-N3	5.47	1.44	1.34
3	10-B	7477	AMP	C4-N3	5.47	1.44	1.34
3	1-U	7515	AMP	C4-N3	5.47	1.44	1.34
3	2-U	7515	AMP	C4-N3	5.47	1.44	1.34
3	3-U	7515	AMP	C4-N3	5.47	1.44	1.34
3	4-U	7515	AMP	C4-N3	5.47	1.44	1.34
3	5-U	7515	AMP	C4-N3	5.47	1.44	1.34
3	6-U	7515	AMP	C4-N3	5.47	1.44	1.34
3	7-U	7515	AMP	C4-N3	5.47	1.44	1.34
3	8-U	7515	AMP	C4-N3	5.47	1.44	1.34
3	9-U	7515	AMP	C4-N3	5.47	1.44	1.34
3	10-U	7515	AMP	C4-N3	5.47	1.44	1.34
4	1-H	7490	CIT	C2-C3	5.47	1.60	1.54
4	2-H	7490	CIT	C2-C3	5.47	1.60	1.54
4	3-H	7490	CIT	C2-C3	5.47	1.60	1.54
4	4-H	7490	CIT	C2-C3	5.47	1.60	1.54
4	5-H	7490	CIT	C2-C3	5.47	1.60	1.54
4	6-H	7490	CIT	C2-C3	5.47	1.60	1.54
4	7-H	7490	CIT	C2-C3	5.47	1.60	1.54
4	8-H	7490	CIT	C2-C3	5.47	1.60	1.54
4	9-H	7490	CIT	C2-C3	5.47	1.60	1.54
4	10-H	7490	CIT	C2-C3	5.47	1.60	1.54
4	1-R	7510	CIT	C2-C3	5.46	1.60	1.54
4	2-R	7510	CIT	C2-C3	5.46	1.60	1.54
4	3-R	7510	CIT	C2-C3	5.46	1.60	1.54
4	4-R	7510	CIT	C2-C3	5.46	1.60	1.54
4	5-R	7510	CIT	C2-C3	5.46	1.60	1.54
4	6-R	7510	CIT	C2-C3	5.46	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-R	7510	CIT	C2-C3	5.46	1.60	1.54
4	8-R	7510	CIT	C2-C3	5.46	1.60	1.54
4	9-R	7510	CIT	C2-C3	5.46	1.60	1.54
4	10-R	7510	CIT	C2-C3	5.46	1.60	1.54
4	1-X	7522	CIT	C2-C3	5.46	1.60	1.54
4	2-X	7522	CIT	C2-C3	5.46	1.60	1.54
4	3-X	7522	CIT	C2-C3	5.46	1.60	1.54
4	4-X	7522	CIT	C2-C3	5.46	1.60	1.54
4	5-X	7522	CIT	C2-C3	5.46	1.60	1.54
4	6-X	7522	CIT	C2-C3	5.46	1.60	1.54
4	7-X	7522	CIT	C2-C3	5.46	1.60	1.54
4	8-X	7522	CIT	C2-C3	5.46	1.60	1.54
4	9-X	7522	CIT	C2-C3	5.46	1.60	1.54
4	10-X	7522	CIT	C2-C3	5.46	1.60	1.54
3	1-D	7481	AMP	C4-N3	5.46	1.44	1.34
3	2-D	7481	AMP	C4-N3	5.46	1.44	1.34
3	3-D	7481	AMP	C4-N3	5.46	1.44	1.34
3	4-D	7481	AMP	C4-N3	5.46	1.44	1.34
3	5-D	7481	AMP	C4-N3	5.46	1.44	1.34
3	6-D	7481	AMP	C4-N3	5.46	1.44	1.34
3	7-D	7481	AMP	C4-N3	5.46	1.44	1.34
3	8-D	7481	AMP	C4-N3	5.46	1.44	1.34
3	9-D	7481	AMP	C4-N3	5.46	1.44	1.34
3	10-D	7481	AMP	C4-N3	5.46	1.44	1.34
3	1-J	7493	AMP	C4-N3	5.46	1.44	1.34
3	2-J	7493	AMP	C4-N3	5.46	1.44	1.34
3	3-J	7493	AMP	C4-N3	5.46	1.44	1.34
3	4-J	7493	AMP	C4-N3	5.46	1.44	1.34
3	5-J	7493	AMP	C4-N3	5.46	1.44	1.34
3	6-J	7493	AMP	C4-N3	5.46	1.44	1.34
3	7-J	7493	AMP	C4-N3	5.46	1.44	1.34
3	8-J	7493	AMP	C4-N3	5.46	1.44	1.34
3	9-J	7493	AMP	C4-N3	5.46	1.44	1.34
3	10-J	7493	AMP	C4-N3	5.46	1.44	1.34
3	1-W	7519	AMP	C4-N3	5.46	1.44	1.34
3	2-W	7519	AMP	C4-N3	5.46	1.44	1.34
3	3-W	7519	AMP	C4-N3	5.46	1.44	1.34
3	4-W	7519	AMP	C4-N3	5.46	1.44	1.34
3	5-W	7519	AMP	C4-N3	5.46	1.44	1.34
3	6-W	7519	AMP	C4-N3	5.46	1.44	1.34
3	7-W	7519	AMP	C4-N3	5.46	1.44	1.34
3	8-W	7519	AMP	C4-N3	5.46	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-W	7519	AMP	C4-N3	5.46	1.44	1.34
3	10-W	7519	AMP	C4-N3	5.46	1.44	1.34
3	1-I	7491	AMP	C4-N3	5.45	1.44	1.34
3	2-I	7491	AMP	C4-N3	5.45	1.44	1.34
3	3-I	7491	AMP	C4-N3	5.45	1.44	1.34
3	4-I	7491	AMP	C4-N3	5.45	1.44	1.34
3	5-I	7491	AMP	C4-N3	5.45	1.44	1.34
3	6-I	7491	AMP	C4-N3	5.45	1.44	1.34
3	7-I	7491	AMP	C4-N3	5.45	1.44	1.34
3	8-I	7491	AMP	C4-N3	5.45	1.44	1.34
3	9-I	7491	AMP	C4-N3	5.45	1.44	1.34
3	10-I	7491	AMP	C4-N3	5.45	1.44	1.34
3	1-F	7485	AMP	C4-N3	5.45	1.44	1.34
3	2-F	7485	AMP	C4-N3	5.45	1.44	1.34
3	3-F	7485	AMP	C4-N3	5.45	1.44	1.34
3	4-F	7485	AMP	C4-N3	5.45	1.44	1.34
3	5-F	7485	AMP	C4-N3	5.45	1.44	1.34
3	6-F	7485	AMP	C4-N3	5.45	1.44	1.34
3	7-F	7485	AMP	C4-N3	5.45	1.44	1.34
3	8-F	7485	AMP	C4-N3	5.45	1.44	1.34
3	9-F	7485	AMP	C4-N3	5.45	1.44	1.34
3	10-F	7485	AMP	C4-N3	5.45	1.44	1.34
3	1-M	7499	AMP	C4-N3	5.45	1.44	1.34
3	2-M	7499	AMP	C4-N3	5.45	1.44	1.34
3	3-M	7499	AMP	C4-N3	5.45	1.44	1.34
3	4-M	7499	AMP	C4-N3	5.45	1.44	1.34
3	5-M	7499	AMP	C4-N3	5.45	1.44	1.34
3	6-M	7499	AMP	C4-N3	5.45	1.44	1.34
3	7-M	7499	AMP	C4-N3	5.45	1.44	1.34
3	8-M	7499	AMP	C4-N3	5.45	1.44	1.34
3	9-M	7499	AMP	C4-N3	5.45	1.44	1.34
3	10-M	7499	AMP	C4-N3	5.45	1.44	1.34
4	1-M	7500	CIT	C2-C3	5.45	1.60	1.54
4	2-M	7500	CIT	C2-C3	5.45	1.60	1.54
4	3-M	7500	CIT	C2-C3	5.45	1.60	1.54
4	4-M	7500	CIT	C2-C3	5.45	1.60	1.54
4	5-M	7500	CIT	C2-C3	5.45	1.60	1.54
4	6-M	7500	CIT	C2-C3	5.45	1.60	1.54
4	7-M	7500	CIT	C2-C3	5.45	1.60	1.54
4	8-M	7500	CIT	C2-C3	5.45	1.60	1.54
4	9-M	7500	CIT	C2-C3	5.45	1.60	1.54
4	10-M	7500	CIT	C2-C3	5.45	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-A	7475	AMP	C4-N3	5.44	1.44	1.34
3	2-A	7475	AMP	C4-N3	5.44	1.44	1.34
3	3-A	7475	AMP	C4-N3	5.44	1.44	1.34
3	4-A	7475	AMP	C4-N3	5.44	1.44	1.34
3	5-A	7475	AMP	C4-N3	5.44	1.44	1.34
3	6-A	7475	AMP	C4-N3	5.44	1.44	1.34
3	7-A	7475	AMP	C4-N3	5.44	1.44	1.34
3	8-A	7475	AMP	C4-N3	5.44	1.44	1.34
3	9-A	7475	AMP	C4-N3	5.44	1.44	1.34
3	10-A	7475	AMP	C4-N3	5.44	1.44	1.34
3	1-N	7501	AMP	C4-N3	5.44	1.44	1.34
3	2-N	7501	AMP	C4-N3	5.44	1.44	1.34
3	3-N	7501	AMP	C4-N3	5.44	1.44	1.34
3	4-N	7501	AMP	C4-N3	5.44	1.44	1.34
3	5-N	7501	AMP	C4-N3	5.44	1.44	1.34
3	6-N	7501	AMP	C4-N3	5.44	1.44	1.34
3	7-N	7501	AMP	C4-N3	5.44	1.44	1.34
3	8-N	7501	AMP	C4-N3	5.44	1.44	1.34
3	9-N	7501	AMP	C4-N3	5.44	1.44	1.34
3	10-N	7501	AMP	C4-N3	5.44	1.44	1.34
3	1-V	7517	AMP	C4-N3	5.44	1.44	1.34
3	2-V	7517	AMP	C4-N3	5.44	1.44	1.34
3	3-V	7517	AMP	C4-N3	5.44	1.44	1.34
3	4-V	7517	AMP	C4-N3	5.44	1.44	1.34
3	5-V	7517	AMP	C4-N3	5.44	1.44	1.34
3	6-V	7517	AMP	C4-N3	5.44	1.44	1.34
3	7-V	7517	AMP	C4-N3	5.44	1.44	1.34
3	8-V	7517	AMP	C4-N3	5.44	1.44	1.34
3	9-V	7517	AMP	C4-N3	5.44	1.44	1.34
3	10-V	7517	AMP	C4-N3	5.44	1.44	1.34
3	1-G	7487	AMP	C4-N3	5.44	1.44	1.34
3	2-G	7487	AMP	C4-N3	5.44	1.44	1.34
3	3-G	7487	AMP	C4-N3	5.44	1.44	1.34
3	4-G	7487	AMP	C4-N3	5.44	1.44	1.34
3	5-G	7487	AMP	C4-N3	5.44	1.44	1.34
3	6-G	7487	AMP	C4-N3	5.44	1.44	1.34
3	7-G	7487	AMP	C4-N3	5.44	1.44	1.34
3	8-G	7487	AMP	C4-N3	5.44	1.44	1.34
3	9-G	7487	AMP	C4-N3	5.44	1.44	1.34
3	10-G	7487	AMP	C4-N3	5.44	1.44	1.34
3	1-P	7505	AMP	C4-N3	5.44	1.44	1.34
3	2-P	7505	AMP	C4-N3	5.44	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-P	7505	AMP	C4-N3	5.44	1.44	1.34
3	4-P	7505	AMP	C4-N3	5.44	1.44	1.34
3	5-P	7505	AMP	C4-N3	5.44	1.44	1.34
3	6-P	7505	AMP	C4-N3	5.44	1.44	1.34
3	7-P	7505	AMP	C4-N3	5.44	1.44	1.34
3	8-P	7505	AMP	C4-N3	5.44	1.44	1.34
3	9-P	7505	AMP	C4-N3	5.44	1.44	1.34
3	10-P	7505	AMP	C4-N3	5.44	1.44	1.34
3	1-T	7513	AMP	C4-N3	5.44	1.44	1.34
3	2-T	7513	AMP	C4-N3	5.44	1.44	1.34
3	3-T	7513	AMP	C4-N3	5.44	1.44	1.34
3	4-T	7513	AMP	C4-N3	5.44	1.44	1.34
3	5-T	7513	AMP	C4-N3	5.44	1.44	1.34
3	6-T	7513	AMP	C4-N3	5.44	1.44	1.34
3	7-T	7513	AMP	C4-N3	5.44	1.44	1.34
3	8-T	7513	AMP	C4-N3	5.44	1.44	1.34
3	9-T	7513	AMP	C4-N3	5.44	1.44	1.34
3	10-T	7513	AMP	C4-N3	5.44	1.44	1.34
4	1-T	7514	CIT	C2-C3	5.44	1.60	1.54
4	2-T	7514	CIT	C2-C3	5.44	1.60	1.54
4	3-T	7514	CIT	C2-C3	5.44	1.60	1.54
4	4-T	7514	CIT	C2-C3	5.44	1.60	1.54
4	5-T	7514	CIT	C2-C3	5.44	1.60	1.54
4	6-T	7514	CIT	C2-C3	5.44	1.60	1.54
4	7-T	7514	CIT	C2-C3	5.44	1.60	1.54
4	8-T	7514	CIT	C2-C3	5.44	1.60	1.54
4	9-T	7514	CIT	C2-C3	5.44	1.60	1.54
4	10-T	7514	CIT	C2-C3	5.44	1.60	1.54
3	1-R	7509	AMP	C4-N3	5.43	1.44	1.34
3	2-R	7509	AMP	C4-N3	5.43	1.44	1.34
3	3-R	7509	AMP	C4-N3	5.43	1.44	1.34
3	4-R	7509	AMP	C4-N3	5.43	1.44	1.34
3	5-R	7509	AMP	C4-N3	5.43	1.44	1.34
3	6-R	7509	AMP	C4-N3	5.43	1.44	1.34
3	7-R	7509	AMP	C4-N3	5.43	1.44	1.34
3	8-R	7509	AMP	C4-N3	5.43	1.44	1.34
3	9-R	7509	AMP	C4-N3	5.43	1.44	1.34
3	10-R	7509	AMP	C4-N3	5.43	1.44	1.34
3	1-X	7521	AMP	C4-N3	5.43	1.44	1.34
3	2-X	7521	AMP	C4-N3	5.43	1.44	1.34
3	3-X	7521	AMP	C4-N3	5.43	1.44	1.34
3	4-X	7521	AMP	C4-N3	5.43	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-X	7521	AMP	C4-N3	5.43	1.44	1.34
3	6-X	7521	AMP	C4-N3	5.43	1.44	1.34
3	7-X	7521	AMP	C4-N3	5.43	1.44	1.34
3	8-X	7521	AMP	C4-N3	5.43	1.44	1.34
3	9-X	7521	AMP	C4-N3	5.43	1.44	1.34
3	10-X	7521	AMP	C4-N3	5.43	1.44	1.34
3	1-O	7503	AMP	C4-N3	5.43	1.44	1.34
3	2-O	7503	AMP	C4-N3	5.43	1.44	1.34
3	3-O	7503	AMP	C4-N3	5.43	1.44	1.34
3	4-O	7503	AMP	C4-N3	5.43	1.44	1.34
3	5-O	7503	AMP	C4-N3	5.43	1.44	1.34
3	6-O	7503	AMP	C4-N3	5.43	1.44	1.34
3	7-O	7503	AMP	C4-N3	5.43	1.44	1.34
3	8-O	7503	AMP	C4-N3	5.43	1.44	1.34
3	9-O	7503	AMP	C4-N3	5.43	1.44	1.34
3	10-O	7503	AMP	C4-N3	5.43	1.44	1.34
3	1-E	7483	AMP	C4-N3	5.43	1.44	1.34
3	2-E	7483	AMP	C4-N3	5.43	1.44	1.34
3	3-E	7483	AMP	C4-N3	5.43	1.44	1.34
3	4-E	7483	AMP	C4-N3	5.43	1.44	1.34
3	5-E	7483	AMP	C4-N3	5.43	1.44	1.34
3	6-E	7483	AMP	C4-N3	5.43	1.44	1.34
3	7-E	7483	AMP	C4-N3	5.43	1.44	1.34
3	8-E	7483	AMP	C4-N3	5.43	1.44	1.34
3	9-E	7483	AMP	C4-N3	5.43	1.44	1.34
3	10-E	7483	AMP	C4-N3	5.43	1.44	1.34
3	1-S	7511	AMP	C4-N3	5.43	1.44	1.34
3	2-S	7511	AMP	C4-N3	5.43	1.44	1.34
3	3-S	7511	AMP	C4-N3	5.43	1.44	1.34
3	4-S	7511	AMP	C4-N3	5.43	1.44	1.34
3	5-S	7511	AMP	C4-N3	5.43	1.44	1.34
3	6-S	7511	AMP	C4-N3	5.43	1.44	1.34
3	7-S	7511	AMP	C4-N3	5.43	1.44	1.34
3	8-S	7511	AMP	C4-N3	5.43	1.44	1.34
3	9-S	7511	AMP	C4-N3	5.43	1.44	1.34
3	10-S	7511	AMP	C4-N3	5.43	1.44	1.34
3	1-Q	7507	AMP	C4-N3	5.42	1.44	1.34
3	2-Q	7507	AMP	C4-N3	5.42	1.44	1.34
3	3-Q	7507	AMP	C4-N3	5.42	1.44	1.34
3	4-Q	7507	AMP	C4-N3	5.42	1.44	1.34
3	5-Q	7507	AMP	C4-N3	5.42	1.44	1.34
3	6-Q	7507	AMP	C4-N3	5.42	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-Q	7507	AMP	C4-N3	5.42	1.44	1.34
3	8-Q	7507	AMP	C4-N3	5.42	1.44	1.34
3	9-Q	7507	AMP	C4-N3	5.42	1.44	1.34
3	10-Q	7507	AMP	C4-N3	5.42	1.44	1.34
3	1-C	7479	AMP	C4-N3	5.42	1.44	1.34
3	2-C	7479	AMP	C4-N3	5.42	1.44	1.34
3	3-C	7479	AMP	C4-N3	5.42	1.44	1.34
3	4-C	7479	AMP	C4-N3	5.42	1.44	1.34
3	5-C	7479	AMP	C4-N3	5.42	1.44	1.34
3	6-C	7479	AMP	C4-N3	5.42	1.44	1.34
3	7-C	7479	AMP	C4-N3	5.42	1.44	1.34
3	8-C	7479	AMP	C4-N3	5.42	1.44	1.34
3	9-C	7479	AMP	C4-N3	5.42	1.44	1.34
3	10-C	7479	AMP	C4-N3	5.42	1.44	1.34
3	1-K	7495	AMP	C4-N3	5.40	1.44	1.34
3	2-K	7495	AMP	C4-N3	5.40	1.44	1.34
3	3-K	7495	AMP	C4-N3	5.40	1.44	1.34
3	4-K	7495	AMP	C4-N3	5.40	1.44	1.34
3	5-K	7495	AMP	C4-N3	5.40	1.44	1.34
3	6-K	7495	AMP	C4-N3	5.40	1.44	1.34
3	7-K	7495	AMP	C4-N3	5.40	1.44	1.34
3	8-K	7495	AMP	C4-N3	5.40	1.44	1.34
3	9-K	7495	AMP	C4-N3	5.40	1.44	1.34
3	10-K	7495	AMP	C4-N3	5.40	1.44	1.34
3	1-N	7501	AMP	P-O3P	5.05	1.73	1.54
3	2-N	7501	AMP	P-O3P	5.05	1.73	1.54
3	3-N	7501	AMP	P-O3P	5.05	1.73	1.54
3	4-N	7501	AMP	P-O3P	5.05	1.73	1.54
3	5-N	7501	AMP	P-O3P	5.05	1.73	1.54
3	6-N	7501	AMP	P-O3P	5.05	1.73	1.54
3	7-N	7501	AMP	P-O3P	5.05	1.73	1.54
3	8-N	7501	AMP	P-O3P	5.05	1.73	1.54
3	9-N	7501	AMP	P-O3P	5.05	1.73	1.54
3	10-N	7501	AMP	P-O3P	5.05	1.73	1.54
3	1-W	7519	AMP	P-O3P	5.05	1.73	1.54
3	2-W	7519	AMP	P-O3P	5.05	1.73	1.54
3	3-W	7519	AMP	P-O3P	5.05	1.73	1.54
3	4-W	7519	AMP	P-O3P	5.05	1.73	1.54
3	5-W	7519	AMP	P-O3P	5.05	1.73	1.54
3	6-W	7519	AMP	P-O3P	5.05	1.73	1.54
3	7-W	7519	AMP	P-O3P	5.05	1.73	1.54
3	8-W	7519	AMP	P-O3P	5.05	1.73	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-W	7519	AMP	P-O3P	5.05	1.73	1.54
3	10-W	7519	AMP	P-O3P	5.05	1.73	1.54
3	1-B	7477	AMP	P-O3P	5.05	1.73	1.54
3	2-B	7477	AMP	P-O3P	5.05	1.73	1.54
3	3-B	7477	AMP	P-O3P	5.05	1.73	1.54
3	4-B	7477	AMP	P-O3P	5.05	1.73	1.54
3	5-B	7477	AMP	P-O3P	5.05	1.73	1.54
3	6-B	7477	AMP	P-O3P	5.05	1.73	1.54
3	7-B	7477	AMP	P-O3P	5.05	1.73	1.54
3	8-B	7477	AMP	P-O3P	5.05	1.73	1.54
3	9-B	7477	AMP	P-O3P	5.05	1.73	1.54
3	10-B	7477	AMP	P-O3P	5.05	1.73	1.54
3	1-X	7521	AMP	P-O3P	5.04	1.73	1.54
3	2-X	7521	AMP	P-O3P	5.04	1.73	1.54
3	3-X	7521	AMP	P-O3P	5.04	1.73	1.54
3	4-X	7521	AMP	P-O3P	5.04	1.73	1.54
3	5-X	7521	AMP	P-O3P	5.04	1.73	1.54
3	6-X	7521	AMP	P-O3P	5.04	1.73	1.54
3	7-X	7521	AMP	P-O3P	5.04	1.73	1.54
3	8-X	7521	AMP	P-O3P	5.04	1.73	1.54
3	9-X	7521	AMP	P-O3P	5.04	1.73	1.54
3	10-X	7521	AMP	P-O3P	5.04	1.73	1.54
3	1-J	7493	AMP	P-O3P	5.04	1.73	1.54
3	2-J	7493	AMP	P-O3P	5.04	1.73	1.54
3	3-J	7493	AMP	P-O3P	5.04	1.73	1.54
3	4-J	7493	AMP	P-O3P	5.04	1.73	1.54
3	5-J	7493	AMP	P-O3P	5.04	1.73	1.54
3	6-J	7493	AMP	P-O3P	5.04	1.73	1.54
3	7-J	7493	AMP	P-O3P	5.04	1.73	1.54
3	8-J	7493	AMP	P-O3P	5.04	1.73	1.54
3	9-J	7493	AMP	P-O3P	5.04	1.73	1.54
3	10-J	7493	AMP	P-O3P	5.04	1.73	1.54
3	1-M	7499	AMP	P-O3P	5.04	1.73	1.54
3	2-M	7499	AMP	P-O3P	5.04	1.73	1.54
3	3-M	7499	AMP	P-O3P	5.04	1.73	1.54
3	4-M	7499	AMP	P-O3P	5.04	1.73	1.54
3	5-M	7499	AMP	P-O3P	5.04	1.73	1.54
3	6-M	7499	AMP	P-O3P	5.04	1.73	1.54
3	7-M	7499	AMP	P-O3P	5.04	1.73	1.54
3	8-M	7499	AMP	P-O3P	5.04	1.73	1.54
3	9-M	7499	AMP	P-O3P	5.04	1.73	1.54
3	10-M	7499	AMP	P-O3P	5.04	1.73	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-Q	7507	AMP	P-O3P	5.03	1.73	1.54
3	2-Q	7507	AMP	P-O3P	5.03	1.73	1.54
3	3-Q	7507	AMP	P-O3P	5.03	1.73	1.54
3	4-Q	7507	AMP	P-O3P	5.03	1.73	1.54
3	5-Q	7507	AMP	P-O3P	5.03	1.73	1.54
3	6-Q	7507	AMP	P-O3P	5.03	1.73	1.54
3	7-Q	7507	AMP	P-O3P	5.03	1.73	1.54
3	8-Q	7507	AMP	P-O3P	5.03	1.73	1.54
3	9-Q	7507	AMP	P-O3P	5.03	1.73	1.54
3	10-Q	7507	AMP	P-O3P	5.03	1.73	1.54
3	1-R	7509	AMP	P-O3P	5.03	1.73	1.54
3	2-R	7509	AMP	P-O3P	5.03	1.73	1.54
3	3-R	7509	AMP	P-O3P	5.03	1.73	1.54
3	4-R	7509	AMP	P-O3P	5.03	1.73	1.54
3	5-R	7509	AMP	P-O3P	5.03	1.73	1.54
3	6-R	7509	AMP	P-O3P	5.03	1.73	1.54
3	7-R	7509	AMP	P-O3P	5.03	1.73	1.54
3	8-R	7509	AMP	P-O3P	5.03	1.73	1.54
3	9-R	7509	AMP	P-O3P	5.03	1.73	1.54
3	10-R	7509	AMP	P-O3P	5.03	1.73	1.54
3	1-C	7479	AMP	P-O3P	5.03	1.73	1.54
3	2-C	7479	AMP	P-O3P	5.03	1.73	1.54
3	3-C	7479	AMP	P-O3P	5.03	1.73	1.54
3	4-C	7479	AMP	P-O3P	5.03	1.73	1.54
3	5-C	7479	AMP	P-O3P	5.03	1.73	1.54
3	6-C	7479	AMP	P-O3P	5.03	1.73	1.54
3	7-C	7479	AMP	P-O3P	5.03	1.73	1.54
3	8-C	7479	AMP	P-O3P	5.03	1.73	1.54
3	9-C	7479	AMP	P-O3P	5.03	1.73	1.54
3	10-C	7479	AMP	P-O3P	5.03	1.73	1.54
3	1-L	7497	AMP	P-O3P	5.03	1.73	1.54
3	2-L	7497	AMP	P-O3P	5.03	1.73	1.54
3	3-L	7497	AMP	P-O3P	5.03	1.73	1.54
3	4-L	7497	AMP	P-O3P	5.03	1.73	1.54
3	5-L	7497	AMP	P-O3P	5.03	1.73	1.54
3	6-L	7497	AMP	P-O3P	5.03	1.73	1.54
3	7-L	7497	AMP	P-O3P	5.03	1.73	1.54
3	8-L	7497	AMP	P-O3P	5.03	1.73	1.54
3	9-L	7497	AMP	P-O3P	5.03	1.73	1.54
3	10-L	7497	AMP	P-O3P	5.03	1.73	1.54
3	1-F	7485	AMP	P-O3P	5.03	1.73	1.54
3	2-F	7485	AMP	P-O3P	5.03	1.73	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-F	7485	AMP	P-O3P	5.03	1.73	1.54
3	4-F	7485	AMP	P-O3P	5.03	1.73	1.54
3	5-F	7485	AMP	P-O3P	5.03	1.73	1.54
3	6-F	7485	AMP	P-O3P	5.03	1.73	1.54
3	7-F	7485	AMP	P-O3P	5.03	1.73	1.54
3	8-F	7485	AMP	P-O3P	5.03	1.73	1.54
3	9-F	7485	AMP	P-O3P	5.03	1.73	1.54
3	10-F	7485	AMP	P-O3P	5.03	1.73	1.54
3	1-A	7475	AMP	P-O3P	5.03	1.73	1.54
3	2-A	7475	AMP	P-O3P	5.03	1.73	1.54
3	3-A	7475	AMP	P-O3P	5.03	1.73	1.54
3	4-A	7475	AMP	P-O3P	5.03	1.73	1.54
3	5-A	7475	AMP	P-O3P	5.03	1.73	1.54
3	6-A	7475	AMP	P-O3P	5.03	1.73	1.54
3	7-A	7475	AMP	P-O3P	5.03	1.73	1.54
3	8-A	7475	AMP	P-O3P	5.03	1.73	1.54
3	9-A	7475	AMP	P-O3P	5.03	1.73	1.54
3	10-A	7475	AMP	P-O3P	5.03	1.73	1.54
3	1-E	7483	AMP	P-O3P	5.03	1.73	1.54
3	2-E	7483	AMP	P-O3P	5.03	1.73	1.54
3	3-E	7483	AMP	P-O3P	5.03	1.73	1.54
3	4-E	7483	AMP	P-O3P	5.03	1.73	1.54
3	5-E	7483	AMP	P-O3P	5.03	1.73	1.54
3	6-E	7483	AMP	P-O3P	5.03	1.73	1.54
3	7-E	7483	AMP	P-O3P	5.03	1.73	1.54
3	8-E	7483	AMP	P-O3P	5.03	1.73	1.54
3	9-E	7483	AMP	P-O3P	5.03	1.73	1.54
3	10-E	7483	AMP	P-O3P	5.03	1.73	1.54
3	1-O	7503	AMP	P-O3P	5.03	1.73	1.54
3	2-O	7503	AMP	P-O3P	5.03	1.73	1.54
3	3-O	7503	AMP	P-O3P	5.03	1.73	1.54
3	4-O	7503	AMP	P-O3P	5.03	1.73	1.54
3	5-O	7503	AMP	P-O3P	5.03	1.73	1.54
3	6-O	7503	AMP	P-O3P	5.03	1.73	1.54
3	7-O	7503	AMP	P-O3P	5.03	1.73	1.54
3	8-O	7503	AMP	P-O3P	5.03	1.73	1.54
3	9-O	7503	AMP	P-O3P	5.03	1.73	1.54
3	10-O	7503	AMP	P-O3P	5.03	1.73	1.54
3	1-P	7505	AMP	P-O3P	5.02	1.73	1.54
3	2-P	7505	AMP	P-O3P	5.02	1.73	1.54
3	3-P	7505	AMP	P-O3P	5.02	1.73	1.54
3	4-P	7505	AMP	P-O3P	5.02	1.73	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-P	7505	AMP	P-O3P	5.02	1.73	1.54
3	6-P	7505	AMP	P-O3P	5.02	1.73	1.54
3	7-P	7505	AMP	P-O3P	5.02	1.73	1.54
3	8-P	7505	AMP	P-O3P	5.02	1.73	1.54
3	9-P	7505	AMP	P-O3P	5.02	1.73	1.54
3	10-P	7505	AMP	P-O3P	5.02	1.73	1.54
3	1-K	7495	AMP	P-O3P	5.02	1.73	1.54
3	2-K	7495	AMP	P-O3P	5.02	1.73	1.54
3	3-K	7495	AMP	P-O3P	5.02	1.73	1.54
3	4-K	7495	AMP	P-O3P	5.02	1.73	1.54
3	5-K	7495	AMP	P-O3P	5.02	1.73	1.54
3	6-K	7495	AMP	P-O3P	5.02	1.73	1.54
3	7-K	7495	AMP	P-O3P	5.02	1.73	1.54
3	8-K	7495	AMP	P-O3P	5.02	1.73	1.54
3	9-K	7495	AMP	P-O3P	5.02	1.73	1.54
3	10-K	7495	AMP	P-O3P	5.02	1.73	1.54
3	1-I	7491	AMP	P-O3P	5.02	1.73	1.54
3	2-I	7491	AMP	P-O3P	5.02	1.73	1.54
3	3-I	7491	AMP	P-O3P	5.02	1.73	1.54
3	4-I	7491	AMP	P-O3P	5.02	1.73	1.54
3	5-I	7491	AMP	P-O3P	5.02	1.73	1.54
3	6-I	7491	AMP	P-O3P	5.02	1.73	1.54
3	7-I	7491	AMP	P-O3P	5.02	1.73	1.54
3	8-I	7491	AMP	P-O3P	5.02	1.73	1.54
3	9-I	7491	AMP	P-O3P	5.02	1.73	1.54
3	10-I	7491	AMP	P-O3P	5.02	1.73	1.54
3	1-V	7517	AMP	P-O3P	5.02	1.73	1.54
3	2-V	7517	AMP	P-O3P	5.02	1.73	1.54
3	3-V	7517	AMP	P-O3P	5.02	1.73	1.54
3	4-V	7517	AMP	P-O3P	5.02	1.73	1.54
3	5-V	7517	AMP	P-O3P	5.02	1.73	1.54
3	6-V	7517	AMP	P-O3P	5.02	1.73	1.54
3	7-V	7517	AMP	P-O3P	5.02	1.73	1.54
3	8-V	7517	AMP	P-O3P	5.02	1.73	1.54
3	9-V	7517	AMP	P-O3P	5.02	1.73	1.54
3	10-V	7517	AMP	P-O3P	5.02	1.73	1.54
3	1-D	7481	AMP	P-O3P	5.02	1.73	1.54
3	2-D	7481	AMP	P-O3P	5.02	1.73	1.54
3	3-D	7481	AMP	P-O3P	5.02	1.73	1.54
3	4-D	7481	AMP	P-O3P	5.02	1.73	1.54
3	5-D	7481	AMP	P-O3P	5.02	1.73	1.54
3	6-D	7481	AMP	P-O3P	5.02	1.73	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-D	7481	AMP	P-O3P	5.02	1.73	1.54
3	8-D	7481	AMP	P-O3P	5.02	1.73	1.54
3	9-D	7481	AMP	P-O3P	5.02	1.73	1.54
3	10-D	7481	AMP	P-O3P	5.02	1.73	1.54
3	1-G	7487	AMP	P-O3P	5.02	1.73	1.54
3	2-G	7487	AMP	P-O3P	5.02	1.73	1.54
3	3-G	7487	AMP	P-O3P	5.02	1.73	1.54
3	4-G	7487	AMP	P-O3P	5.02	1.73	1.54
3	5-G	7487	AMP	P-O3P	5.02	1.73	1.54
3	6-G	7487	AMP	P-O3P	5.02	1.73	1.54
3	7-G	7487	AMP	P-O3P	5.02	1.73	1.54
3	8-G	7487	AMP	P-O3P	5.02	1.73	1.54
3	9-G	7487	AMP	P-O3P	5.02	1.73	1.54
3	10-G	7487	AMP	P-O3P	5.02	1.73	1.54
3	1-U	7515	AMP	P-O3P	5.02	1.73	1.54
3	2-U	7515	AMP	P-O3P	5.02	1.73	1.54
3	3-U	7515	AMP	P-O3P	5.02	1.73	1.54
3	4-U	7515	AMP	P-O3P	5.02	1.73	1.54
3	5-U	7515	AMP	P-O3P	5.02	1.73	1.54
3	6-U	7515	AMP	P-O3P	5.02	1.73	1.54
3	7-U	7515	AMP	P-O3P	5.02	1.73	1.54
3	8-U	7515	AMP	P-O3P	5.02	1.73	1.54
3	9-U	7515	AMP	P-O3P	5.02	1.73	1.54
3	10-U	7515	AMP	P-O3P	5.02	1.73	1.54
3	1-T	7513	AMP	P-O3P	5.01	1.73	1.54
3	2-T	7513	AMP	P-O3P	5.01	1.73	1.54
3	3-T	7513	AMP	P-O3P	5.01	1.73	1.54
3	4-T	7513	AMP	P-O3P	5.01	1.73	1.54
3	5-T	7513	AMP	P-O3P	5.01	1.73	1.54
3	6-T	7513	AMP	P-O3P	5.01	1.73	1.54
3	7-T	7513	AMP	P-O3P	5.01	1.73	1.54
3	8-T	7513	AMP	P-O3P	5.01	1.73	1.54
3	9-T	7513	AMP	P-O3P	5.01	1.73	1.54
3	10-T	7513	AMP	P-O3P	5.01	1.73	1.54
3	1-H	7489	AMP	P-O3P	5.01	1.73	1.54
3	2-H	7489	AMP	P-O3P	5.01	1.73	1.54
3	3-H	7489	AMP	P-O3P	5.01	1.73	1.54
3	4-H	7489	AMP	P-O3P	5.01	1.73	1.54
3	5-H	7489	AMP	P-O3P	5.01	1.73	1.54
3	6-H	7489	AMP	P-O3P	5.01	1.73	1.54
3	7-H	7489	AMP	P-O3P	5.01	1.73	1.54
3	8-H	7489	AMP	P-O3P	5.01	1.73	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-H	7489	AMP	P-O3P	5.01	1.73	1.54
3	10-H	7489	AMP	P-O3P	5.01	1.73	1.54
3	1-S	7511	AMP	P-O3P	5.00	1.73	1.54
3	2-S	7511	AMP	P-O3P	5.00	1.73	1.54
3	3-S	7511	AMP	P-O3P	5.00	1.73	1.54
3	4-S	7511	AMP	P-O3P	5.00	1.73	1.54
3	5-S	7511	AMP	P-O3P	5.00	1.73	1.54
3	6-S	7511	AMP	P-O3P	5.00	1.73	1.54
3	7-S	7511	AMP	P-O3P	5.00	1.73	1.54
3	8-S	7511	AMP	P-O3P	5.00	1.73	1.54
3	9-S	7511	AMP	P-O3P	5.00	1.73	1.54
3	10-S	7511	AMP	P-O3P	5.00	1.73	1.54
3	1-X	7521	AMP	O4'-C1'	4.82	1.53	1.42
3	2-X	7521	AMP	O4'-C1'	4.82	1.53	1.42
3	3-X	7521	AMP	O4'-C1'	4.82	1.53	1.42
3	4-X	7521	AMP	O4'-C1'	4.82	1.53	1.42
3	5-X	7521	AMP	O4'-C1'	4.82	1.53	1.42
3	6-X	7521	AMP	O4'-C1'	4.82	1.53	1.42
3	7-X	7521	AMP	O4'-C1'	4.82	1.53	1.42
3	8-X	7521	AMP	O4'-C1'	4.82	1.53	1.42
3	9-X	7521	AMP	O4'-C1'	4.82	1.53	1.42
3	10-X	7521	AMP	O4'-C1'	4.82	1.53	1.42
3	1-S	7511	AMP	C5-C4	4.81	1.47	1.39
3	2-S	7511	AMP	C5-C4	4.81	1.47	1.39
3	3-S	7511	AMP	C5-C4	4.81	1.47	1.39
3	4-S	7511	AMP	C5-C4	4.81	1.47	1.39
3	5-S	7511	AMP	C5-C4	4.81	1.47	1.39
3	6-S	7511	AMP	C5-C4	4.81	1.47	1.39
3	7-S	7511	AMP	C5-C4	4.81	1.47	1.39
3	8-S	7511	AMP	C5-C4	4.81	1.47	1.39
3	9-S	7511	AMP	C5-C4	4.81	1.47	1.39
3	10-S	7511	AMP	C5-C4	4.81	1.47	1.39
3	1-N	7501	AMP	O4'-C1'	4.81	1.53	1.42
3	2-N	7501	AMP	O4'-C1'	4.81	1.53	1.42
3	3-N	7501	AMP	O4'-C1'	4.81	1.53	1.42
3	4-N	7501	AMP	O4'-C1'	4.81	1.53	1.42
3	5-N	7501	AMP	O4'-C1'	4.81	1.53	1.42
3	6-N	7501	AMP	O4'-C1'	4.81	1.53	1.42
3	7-N	7501	AMP	O4'-C1'	4.81	1.53	1.42
3	8-N	7501	AMP	O4'-C1'	4.81	1.53	1.42
3	9-N	7501	AMP	O4'-C1'	4.81	1.53	1.42
3	10-N	7501	AMP	O4'-C1'	4.81	1.53	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	7477	AMP	C5-C4	4.81	1.47	1.39
3	2-B	7477	AMP	C5-C4	4.81	1.47	1.39
3	3-B	7477	AMP	C5-C4	4.81	1.47	1.39
3	4-B	7477	AMP	C5-C4	4.81	1.47	1.39
3	5-B	7477	AMP	C5-C4	4.81	1.47	1.39
3	6-B	7477	AMP	C5-C4	4.81	1.47	1.39
3	7-B	7477	AMP	C5-C4	4.81	1.47	1.39
3	8-B	7477	AMP	C5-C4	4.81	1.47	1.39
3	9-B	7477	AMP	C5-C4	4.81	1.47	1.39
3	10-B	7477	AMP	C5-C4	4.81	1.47	1.39
3	1-X	7521	AMP	C5-C4	4.81	1.47	1.39
3	2-X	7521	AMP	C5-C4	4.81	1.47	1.39
3	3-X	7521	AMP	C5-C4	4.81	1.47	1.39
3	4-X	7521	AMP	C5-C4	4.81	1.47	1.39
3	5-X	7521	AMP	C5-C4	4.81	1.47	1.39
3	6-X	7521	AMP	C5-C4	4.81	1.47	1.39
3	7-X	7521	AMP	C5-C4	4.81	1.47	1.39
3	8-X	7521	AMP	C5-C4	4.81	1.47	1.39
3	9-X	7521	AMP	C5-C4	4.81	1.47	1.39
3	10-X	7521	AMP	C5-C4	4.81	1.47	1.39
3	1-B	7477	AMP	O4'-C1'	4.81	1.53	1.42
3	2-B	7477	AMP	O4'-C1'	4.81	1.53	1.42
3	3-B	7477	AMP	O4'-C1'	4.81	1.53	1.42
3	4-B	7477	AMP	O4'-C1'	4.81	1.53	1.42
3	5-B	7477	AMP	O4'-C1'	4.81	1.53	1.42
3	6-B	7477	AMP	O4'-C1'	4.81	1.53	1.42
3	7-B	7477	AMP	O4'-C1'	4.81	1.53	1.42
3	8-B	7477	AMP	O4'-C1'	4.81	1.53	1.42
3	9-B	7477	AMP	O4'-C1'	4.81	1.53	1.42
3	10-B	7477	AMP	O4'-C1'	4.81	1.53	1.42
3	1-K	7495	AMP	O4'-C1'	4.81	1.53	1.42
3	2-K	7495	AMP	O4'-C1'	4.81	1.53	1.42
3	3-K	7495	AMP	O4'-C1'	4.81	1.53	1.42
3	4-K	7495	AMP	O4'-C1'	4.81	1.53	1.42
3	5-K	7495	AMP	O4'-C1'	4.81	1.53	1.42
3	6-K	7495	AMP	O4'-C1'	4.81	1.53	1.42
3	7-K	7495	AMP	O4'-C1'	4.81	1.53	1.42
3	8-K	7495	AMP	O4'-C1'	4.81	1.53	1.42
3	9-K	7495	AMP	O4'-C1'	4.81	1.53	1.42
3	10-K	7495	AMP	O4'-C1'	4.81	1.53	1.42
3	1-T	7513	AMP	C5-C4	4.80	1.47	1.39
3	2-T	7513	AMP	C5-C4	4.80	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-T	7513	AMP	C5-C4	4.80	1.47	1.39
3	4-T	7513	AMP	C5-C4	4.80	1.47	1.39
3	5-T	7513	AMP	C5-C4	4.80	1.47	1.39
3	6-T	7513	AMP	C5-C4	4.80	1.47	1.39
3	7-T	7513	AMP	C5-C4	4.80	1.47	1.39
3	8-T	7513	AMP	C5-C4	4.80	1.47	1.39
3	9-T	7513	AMP	C5-C4	4.80	1.47	1.39
3	10-T	7513	AMP	C5-C4	4.80	1.47	1.39
3	1-W	7519	AMP	O4'-C1'	4.80	1.53	1.42
3	2-W	7519	AMP	O4'-C1'	4.80	1.53	1.42
3	3-W	7519	AMP	O4'-C1'	4.80	1.53	1.42
3	4-W	7519	AMP	O4'-C1'	4.80	1.53	1.42
3	5-W	7519	AMP	O4'-C1'	4.80	1.53	1.42
3	6-W	7519	AMP	O4'-C1'	4.80	1.53	1.42
3	7-W	7519	AMP	O4'-C1'	4.80	1.53	1.42
3	8-W	7519	AMP	O4'-C1'	4.80	1.53	1.42
3	9-W	7519	AMP	O4'-C1'	4.80	1.53	1.42
3	10-W	7519	AMP	O4'-C1'	4.80	1.53	1.42
3	1-C	7479	AMP	O4'-C1'	4.80	1.53	1.42
3	2-C	7479	AMP	O4'-C1'	4.80	1.53	1.42
3	3-C	7479	AMP	O4'-C1'	4.80	1.53	1.42
3	4-C	7479	AMP	O4'-C1'	4.80	1.53	1.42
3	5-C	7479	AMP	O4'-C1'	4.80	1.53	1.42
3	6-C	7479	AMP	O4'-C1'	4.80	1.53	1.42
3	7-C	7479	AMP	O4'-C1'	4.80	1.53	1.42
3	8-C	7479	AMP	O4'-C1'	4.80	1.53	1.42
3	9-C	7479	AMP	O4'-C1'	4.80	1.53	1.42
3	10-C	7479	AMP	O4'-C1'	4.80	1.53	1.42
3	1-P	7505	AMP	C5-C4	4.80	1.47	1.39
3	2-P	7505	AMP	C5-C4	4.80	1.47	1.39
3	3-P	7505	AMP	C5-C4	4.80	1.47	1.39
3	4-P	7505	AMP	C5-C4	4.80	1.47	1.39
3	5-P	7505	AMP	C5-C4	4.80	1.47	1.39
3	6-P	7505	AMP	C5-C4	4.80	1.47	1.39
3	7-P	7505	AMP	C5-C4	4.80	1.47	1.39
3	8-P	7505	AMP	C5-C4	4.80	1.47	1.39
3	9-P	7505	AMP	C5-C4	4.80	1.47	1.39
3	10-P	7505	AMP	C5-C4	4.80	1.47	1.39
3	1-G	7487	AMP	O4'-C1'	4.80	1.53	1.42
3	2-G	7487	AMP	O4'-C1'	4.80	1.53	1.42
3	3-G	7487	AMP	O4'-C1'	4.80	1.53	1.42
3	4-G	7487	AMP	O4'-C1'	4.80	1.53	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-G	7487	AMP	O4'-C1'	4.80	1.53	1.42
3	6-G	7487	AMP	O4'-C1'	4.80	1.53	1.42
3	7-G	7487	AMP	O4'-C1'	4.80	1.53	1.42
3	8-G	7487	AMP	O4'-C1'	4.80	1.53	1.42
3	9-G	7487	AMP	O4'-C1'	4.80	1.53	1.42
3	10-G	7487	AMP	O4'-C1'	4.80	1.53	1.42
3	1-R	7509	AMP	C5-C4	4.79	1.47	1.39
3	2-R	7509	AMP	C5-C4	4.79	1.47	1.39
3	3-R	7509	AMP	C5-C4	4.79	1.47	1.39
3	4-R	7509	AMP	C5-C4	4.79	1.47	1.39
3	5-R	7509	AMP	C5-C4	4.79	1.47	1.39
3	6-R	7509	AMP	C5-C4	4.79	1.47	1.39
3	7-R	7509	AMP	C5-C4	4.79	1.47	1.39
3	8-R	7509	AMP	C5-C4	4.79	1.47	1.39
3	9-R	7509	AMP	C5-C4	4.79	1.47	1.39
3	10-R	7509	AMP	C5-C4	4.79	1.47	1.39
3	1-P	7505	AMP	O4'-C1'	4.79	1.53	1.42
3	2-P	7505	AMP	O4'-C1'	4.79	1.53	1.42
3	3-P	7505	AMP	O4'-C1'	4.79	1.53	1.42
3	4-P	7505	AMP	O4'-C1'	4.79	1.53	1.42
3	5-P	7505	AMP	O4'-C1'	4.79	1.53	1.42
3	6-P	7505	AMP	O4'-C1'	4.79	1.53	1.42
3	7-P	7505	AMP	O4'-C1'	4.79	1.53	1.42
3	8-P	7505	AMP	O4'-C1'	4.79	1.53	1.42
3	9-P	7505	AMP	O4'-C1'	4.79	1.53	1.42
3	10-P	7505	AMP	O4'-C1'	4.79	1.53	1.42
3	1-U	7515	AMP	C5-C4	4.79	1.47	1.39
3	2-U	7515	AMP	C5-C4	4.79	1.47	1.39
3	3-U	7515	AMP	C5-C4	4.79	1.47	1.39
3	4-U	7515	AMP	C5-C4	4.79	1.47	1.39
3	5-U	7515	AMP	C5-C4	4.79	1.47	1.39
3	6-U	7515	AMP	C5-C4	4.79	1.47	1.39
3	7-U	7515	AMP	C5-C4	4.79	1.47	1.39
3	8-U	7515	AMP	C5-C4	4.79	1.47	1.39
3	9-U	7515	AMP	C5-C4	4.79	1.47	1.39
3	10-U	7515	AMP	C5-C4	4.79	1.47	1.39
3	1-E	7483	AMP	O4'-C1'	4.79	1.53	1.42
3	2-E	7483	AMP	O4'-C1'	4.79	1.53	1.42
3	3-E	7483	AMP	O4'-C1'	4.79	1.53	1.42
3	4-E	7483	AMP	O4'-C1'	4.79	1.53	1.42
3	5-E	7483	AMP	O4'-C1'	4.79	1.53	1.42
3	6-E	7483	AMP	O4'-C1'	4.79	1.53	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-E	7483	AMP	O4'-C1'	4.79	1.53	1.42
3	8-E	7483	AMP	O4'-C1'	4.79	1.53	1.42
3	9-E	7483	AMP	O4'-C1'	4.79	1.53	1.42
3	10-E	7483	AMP	O4'-C1'	4.79	1.53	1.42
3	1-J	7493	AMP	O4'-C1'	4.79	1.53	1.42
3	2-J	7493	AMP	O4'-C1'	4.79	1.53	1.42
3	3-J	7493	AMP	O4'-C1'	4.79	1.53	1.42
3	4-J	7493	AMP	O4'-C1'	4.79	1.53	1.42
3	5-J	7493	AMP	O4'-C1'	4.79	1.53	1.42
3	6-J	7493	AMP	O4'-C1'	4.79	1.53	1.42
3	7-J	7493	AMP	O4'-C1'	4.79	1.53	1.42
3	8-J	7493	AMP	O4'-C1'	4.79	1.53	1.42
3	9-J	7493	AMP	O4'-C1'	4.79	1.53	1.42
3	10-J	7493	AMP	O4'-C1'	4.79	1.53	1.42
3	1-M	7499	AMP	O4'-C1'	4.79	1.53	1.42
3	2-M	7499	AMP	O4'-C1'	4.79	1.53	1.42
3	3-M	7499	AMP	O4'-C1'	4.79	1.53	1.42
3	4-M	7499	AMP	O4'-C1'	4.79	1.53	1.42
3	5-M	7499	AMP	O4'-C1'	4.79	1.53	1.42
3	6-M	7499	AMP	O4'-C1'	4.79	1.53	1.42
3	7-M	7499	AMP	O4'-C1'	4.79	1.53	1.42
3	8-M	7499	AMP	O4'-C1'	4.79	1.53	1.42
3	9-M	7499	AMP	O4'-C1'	4.79	1.53	1.42
3	10-M	7499	AMP	O4'-C1'	4.79	1.53	1.42
3	1-D	7481	AMP	C5-C4	4.79	1.47	1.39
3	2-D	7481	AMP	C5-C4	4.79	1.47	1.39
3	3-D	7481	AMP	C5-C4	4.79	1.47	1.39
3	4-D	7481	AMP	C5-C4	4.79	1.47	1.39
3	5-D	7481	AMP	C5-C4	4.79	1.47	1.39
3	6-D	7481	AMP	C5-C4	4.79	1.47	1.39
3	7-D	7481	AMP	C5-C4	4.79	1.47	1.39
3	8-D	7481	AMP	C5-C4	4.79	1.47	1.39
3	9-D	7481	AMP	C5-C4	4.79	1.47	1.39
3	10-D	7481	AMP	C5-C4	4.79	1.47	1.39
3	1-T	7513	AMP	O4'-C1'	4.79	1.53	1.42
3	2-T	7513	AMP	O4'-C1'	4.79	1.53	1.42
3	3-T	7513	AMP	O4'-C1'	4.79	1.53	1.42
3	4-T	7513	AMP	O4'-C1'	4.79	1.53	1.42
3	5-T	7513	AMP	O4'-C1'	4.79	1.53	1.42
3	6-T	7513	AMP	O4'-C1'	4.79	1.53	1.42
3	7-T	7513	AMP	O4'-C1'	4.79	1.53	1.42
3	8-T	7513	AMP	O4'-C1'	4.79	1.53	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-T	7513	AMP	O4'-C1'	4.79	1.53	1.42
3	10-T	7513	AMP	O4'-C1'	4.79	1.53	1.42
3	1-C	7479	AMP	C5-C4	4.78	1.47	1.39
3	2-C	7479	AMP	C5-C4	4.78	1.47	1.39
3	3-C	7479	AMP	C5-C4	4.78	1.47	1.39
3	4-C	7479	AMP	C5-C4	4.78	1.47	1.39
3	5-C	7479	AMP	C5-C4	4.78	1.47	1.39
3	6-C	7479	AMP	C5-C4	4.78	1.47	1.39
3	7-C	7479	AMP	C5-C4	4.78	1.47	1.39
3	8-C	7479	AMP	C5-C4	4.78	1.47	1.39
3	9-C	7479	AMP	C5-C4	4.78	1.47	1.39
3	10-C	7479	AMP	C5-C4	4.78	1.47	1.39
3	1-A	7475	AMP	O4'-C1'	4.78	1.53	1.42
3	2-A	7475	AMP	O4'-C1'	4.78	1.53	1.42
3	3-A	7475	AMP	O4'-C1'	4.78	1.53	1.42
3	4-A	7475	AMP	O4'-C1'	4.78	1.53	1.42
3	5-A	7475	AMP	O4'-C1'	4.78	1.53	1.42
3	6-A	7475	AMP	O4'-C1'	4.78	1.53	1.42
3	7-A	7475	AMP	O4'-C1'	4.78	1.53	1.42
3	8-A	7475	AMP	O4'-C1'	4.78	1.53	1.42
3	9-A	7475	AMP	O4'-C1'	4.78	1.53	1.42
3	10-A	7475	AMP	O4'-C1'	4.78	1.53	1.42
3	1-F	7485	AMP	O4'-C1'	4.78	1.53	1.42
3	2-F	7485	AMP	O4'-C1'	4.78	1.53	1.42
3	3-F	7485	AMP	O4'-C1'	4.78	1.53	1.42
3	4-F	7485	AMP	O4'-C1'	4.78	1.53	1.42
3	5-F	7485	AMP	O4'-C1'	4.78	1.53	1.42
3	6-F	7485	AMP	O4'-C1'	4.78	1.53	1.42
3	7-F	7485	AMP	O4'-C1'	4.78	1.53	1.42
3	8-F	7485	AMP	O4'-C1'	4.78	1.53	1.42
3	9-F	7485	AMP	O4'-C1'	4.78	1.53	1.42
3	10-F	7485	AMP	O4'-C1'	4.78	1.53	1.42
3	1-D	7481	AMP	O4'-C1'	4.78	1.53	1.42
3	2-D	7481	AMP	O4'-C1'	4.78	1.53	1.42
3	3-D	7481	AMP	O4'-C1'	4.78	1.53	1.42
3	4-D	7481	AMP	O4'-C1'	4.78	1.53	1.42
3	5-D	7481	AMP	O4'-C1'	4.78	1.53	1.42
3	6-D	7481	AMP	O4'-C1'	4.78	1.53	1.42
3	7-D	7481	AMP	O4'-C1'	4.78	1.53	1.42
3	8-D	7481	AMP	O4'-C1'	4.78	1.53	1.42
3	9-D	7481	AMP	O4'-C1'	4.78	1.53	1.42
3	10-D	7481	AMP	O4'-C1'	4.78	1.53	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-S	7511	AMP	O4'-C1'	4.78	1.53	1.42
3	2-S	7511	AMP	O4'-C1'	4.78	1.53	1.42
3	3-S	7511	AMP	O4'-C1'	4.78	1.53	1.42
3	4-S	7511	AMP	O4'-C1'	4.78	1.53	1.42
3	5-S	7511	AMP	O4'-C1'	4.78	1.53	1.42
3	6-S	7511	AMP	O4'-C1'	4.78	1.53	1.42
3	7-S	7511	AMP	O4'-C1'	4.78	1.53	1.42
3	8-S	7511	AMP	O4'-C1'	4.78	1.53	1.42
3	9-S	7511	AMP	O4'-C1'	4.78	1.53	1.42
3	10-S	7511	AMP	O4'-C1'	4.78	1.53	1.42
3	1-M	7499	AMP	C5-C4	4.78	1.47	1.39
3	2-M	7499	AMP	C5-C4	4.78	1.47	1.39
3	3-M	7499	AMP	C5-C4	4.78	1.47	1.39
3	4-M	7499	AMP	C5-C4	4.78	1.47	1.39
3	5-M	7499	AMP	C5-C4	4.78	1.47	1.39
3	6-M	7499	AMP	C5-C4	4.78	1.47	1.39
3	7-M	7499	AMP	C5-C4	4.78	1.47	1.39
3	8-M	7499	AMP	C5-C4	4.78	1.47	1.39
3	9-M	7499	AMP	C5-C4	4.78	1.47	1.39
3	10-M	7499	AMP	C5-C4	4.78	1.47	1.39
3	1-O	7503	AMP	O4'-C1'	4.78	1.53	1.42
3	2-O	7503	AMP	O4'-C1'	4.78	1.53	1.42
3	3-O	7503	AMP	O4'-C1'	4.78	1.53	1.42
3	4-O	7503	AMP	O4'-C1'	4.78	1.53	1.42
3	5-O	7503	AMP	O4'-C1'	4.78	1.53	1.42
3	6-O	7503	AMP	O4'-C1'	4.78	1.53	1.42
3	7-O	7503	AMP	O4'-C1'	4.78	1.53	1.42
3	8-O	7503	AMP	O4'-C1'	4.78	1.53	1.42
3	9-O	7503	AMP	O4'-C1'	4.78	1.53	1.42
3	10-O	7503	AMP	O4'-C1'	4.78	1.53	1.42
3	1-R	7509	AMP	O4'-C1'	4.78	1.53	1.42
3	2-R	7509	AMP	O4'-C1'	4.78	1.53	1.42
3	3-R	7509	AMP	O4'-C1'	4.78	1.53	1.42
3	4-R	7509	AMP	O4'-C1'	4.78	1.53	1.42
3	5-R	7509	AMP	O4'-C1'	4.78	1.53	1.42
3	6-R	7509	AMP	O4'-C1'	4.78	1.53	1.42
3	7-R	7509	AMP	O4'-C1'	4.78	1.53	1.42
3	8-R	7509	AMP	O4'-C1'	4.78	1.53	1.42
3	9-R	7509	AMP	O4'-C1'	4.78	1.53	1.42
3	10-R	7509	AMP	O4'-C1'	4.78	1.53	1.42
3	1-F	7485	AMP	C5-C4	4.78	1.47	1.39
3	2-F	7485	AMP	C5-C4	4.78	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-F	7485	AMP	C5-C4	4.78	1.47	1.39
3	4-F	7485	AMP	C5-C4	4.78	1.47	1.39
3	5-F	7485	AMP	C5-C4	4.78	1.47	1.39
3	6-F	7485	AMP	C5-C4	4.78	1.47	1.39
3	7-F	7485	AMP	C5-C4	4.78	1.47	1.39
3	8-F	7485	AMP	C5-C4	4.78	1.47	1.39
3	9-F	7485	AMP	C5-C4	4.78	1.47	1.39
3	10-F	7485	AMP	C5-C4	4.78	1.47	1.39
3	1-K	7495	AMP	C5-C4	4.78	1.47	1.39
3	2-K	7495	AMP	C5-C4	4.78	1.47	1.39
3	3-K	7495	AMP	C5-C4	4.78	1.47	1.39
3	4-K	7495	AMP	C5-C4	4.78	1.47	1.39
3	5-K	7495	AMP	C5-C4	4.78	1.47	1.39
3	6-K	7495	AMP	C5-C4	4.78	1.47	1.39
3	7-K	7495	AMP	C5-C4	4.78	1.47	1.39
3	8-K	7495	AMP	C5-C4	4.78	1.47	1.39
3	9-K	7495	AMP	C5-C4	4.78	1.47	1.39
3	10-K	7495	AMP	C5-C4	4.78	1.47	1.39
3	1-L	7497	AMP	O4'-C1'	4.78	1.53	1.42
3	2-L	7497	AMP	O4'-C1'	4.78	1.53	1.42
3	3-L	7497	AMP	O4'-C1'	4.78	1.53	1.42
3	4-L	7497	AMP	O4'-C1'	4.78	1.53	1.42
3	5-L	7497	AMP	O4'-C1'	4.78	1.53	1.42
3	6-L	7497	AMP	O4'-C1'	4.78	1.53	1.42
3	7-L	7497	AMP	O4'-C1'	4.78	1.53	1.42
3	8-L	7497	AMP	O4'-C1'	4.78	1.53	1.42
3	9-L	7497	AMP	O4'-C1'	4.78	1.53	1.42
3	10-L	7497	AMP	O4'-C1'	4.78	1.53	1.42
3	1-I	7491	AMP	C5-C4	4.77	1.47	1.39
3	2-I	7491	AMP	C5-C4	4.77	1.47	1.39
3	3-I	7491	AMP	C5-C4	4.77	1.47	1.39
3	4-I	7491	AMP	C5-C4	4.77	1.47	1.39
3	5-I	7491	AMP	C5-C4	4.77	1.47	1.39
3	6-I	7491	AMP	C5-C4	4.77	1.47	1.39
3	7-I	7491	AMP	C5-C4	4.77	1.47	1.39
3	8-I	7491	AMP	C5-C4	4.77	1.47	1.39
3	9-I	7491	AMP	C5-C4	4.77	1.47	1.39
3	10-I	7491	AMP	C5-C4	4.77	1.47	1.39
3	1-A	7475	AMP	C5-C4	4.77	1.47	1.39
3	2-A	7475	AMP	C5-C4	4.77	1.47	1.39
3	3-A	7475	AMP	C5-C4	4.77	1.47	1.39
3	4-A	7475	AMP	C5-C4	4.77	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-A	7475	AMP	C5-C4	4.77	1.47	1.39
3	6-A	7475	AMP	C5-C4	4.77	1.47	1.39
3	7-A	7475	AMP	C5-C4	4.77	1.47	1.39
3	8-A	7475	AMP	C5-C4	4.77	1.47	1.39
3	9-A	7475	AMP	C5-C4	4.77	1.47	1.39
3	10-A	7475	AMP	C5-C4	4.77	1.47	1.39
3	1-W	7519	AMP	C5-C4	4.77	1.47	1.39
3	2-W	7519	AMP	C5-C4	4.77	1.47	1.39
3	3-W	7519	AMP	C5-C4	4.77	1.47	1.39
3	4-W	7519	AMP	C5-C4	4.77	1.47	1.39
3	5-W	7519	AMP	C5-C4	4.77	1.47	1.39
3	6-W	7519	AMP	C5-C4	4.77	1.47	1.39
3	7-W	7519	AMP	C5-C4	4.77	1.47	1.39
3	8-W	7519	AMP	C5-C4	4.77	1.47	1.39
3	9-W	7519	AMP	C5-C4	4.77	1.47	1.39
3	10-W	7519	AMP	C5-C4	4.77	1.47	1.39
3	1-U	7515	AMP	O4'-C1'	4.77	1.53	1.42
3	2-U	7515	AMP	O4'-C1'	4.77	1.53	1.42
3	3-U	7515	AMP	O4'-C1'	4.77	1.53	1.42
3	4-U	7515	AMP	O4'-C1'	4.77	1.53	1.42
3	5-U	7515	AMP	O4'-C1'	4.77	1.53	1.42
3	6-U	7515	AMP	O4'-C1'	4.77	1.53	1.42
3	7-U	7515	AMP	O4'-C1'	4.77	1.53	1.42
3	8-U	7515	AMP	O4'-C1'	4.77	1.53	1.42
3	9-U	7515	AMP	O4'-C1'	4.77	1.53	1.42
3	10-U	7515	AMP	O4'-C1'	4.77	1.53	1.42
3	1-H	7489	AMP	O4'-C1'	4.77	1.53	1.42
3	2-H	7489	AMP	O4'-C1'	4.77	1.53	1.42
3	3-H	7489	AMP	O4'-C1'	4.77	1.53	1.42
3	4-H	7489	AMP	O4'-C1'	4.77	1.53	1.42
3	5-H	7489	AMP	O4'-C1'	4.77	1.53	1.42
3	6-H	7489	AMP	O4'-C1'	4.77	1.53	1.42
3	7-H	7489	AMP	O4'-C1'	4.77	1.53	1.42
3	8-H	7489	AMP	O4'-C1'	4.77	1.53	1.42
3	9-H	7489	AMP	O4'-C1'	4.77	1.53	1.42
3	10-H	7489	AMP	O4'-C1'	4.77	1.53	1.42
3	1-G	7487	AMP	C5-C4	4.77	1.47	1.39
3	2-G	7487	AMP	C5-C4	4.77	1.47	1.39
3	3-G	7487	AMP	C5-C4	4.77	1.47	1.39
3	4-G	7487	AMP	C5-C4	4.77	1.47	1.39
3	5-G	7487	AMP	C5-C4	4.77	1.47	1.39
3	6-G	7487	AMP	C5-C4	4.77	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-G	7487	AMP	C5-C4	4.77	1.47	1.39
3	8-G	7487	AMP	C5-C4	4.77	1.47	1.39
3	9-G	7487	AMP	C5-C4	4.77	1.47	1.39
3	10-G	7487	AMP	C5-C4	4.77	1.47	1.39
3	1-Q	7507	AMP	C5-C4	4.77	1.47	1.39
3	2-Q	7507	AMP	C5-C4	4.77	1.47	1.39
3	3-Q	7507	AMP	C5-C4	4.77	1.47	1.39
3	4-Q	7507	AMP	C5-C4	4.77	1.47	1.39
3	5-Q	7507	AMP	C5-C4	4.77	1.47	1.39
3	6-Q	7507	AMP	C5-C4	4.77	1.47	1.39
3	7-Q	7507	AMP	C5-C4	4.77	1.47	1.39
3	8-Q	7507	AMP	C5-C4	4.77	1.47	1.39
3	9-Q	7507	AMP	C5-C4	4.77	1.47	1.39
3	10-Q	7507	AMP	C5-C4	4.77	1.47	1.39
3	1-Q	7507	AMP	O4'-C1'	4.76	1.53	1.42
3	2-Q	7507	AMP	O4'-C1'	4.76	1.53	1.42
3	3-Q	7507	AMP	O4'-C1'	4.76	1.53	1.42
3	4-Q	7507	AMP	O4'-C1'	4.76	1.53	1.42
3	5-Q	7507	AMP	O4'-C1'	4.76	1.53	1.42
3	6-Q	7507	AMP	O4'-C1'	4.76	1.53	1.42
3	7-Q	7507	AMP	O4'-C1'	4.76	1.53	1.42
3	8-Q	7507	AMP	O4'-C1'	4.76	1.53	1.42
3	9-Q	7507	AMP	O4'-C1'	4.76	1.53	1.42
3	10-Q	7507	AMP	O4'-C1'	4.76	1.53	1.42
3	1-N	7501	AMP	C5-C4	4.76	1.47	1.39
3	2-N	7501	AMP	C5-C4	4.76	1.47	1.39
3	3-N	7501	AMP	C5-C4	4.76	1.47	1.39
3	4-N	7501	AMP	C5-C4	4.76	1.47	1.39
3	5-N	7501	AMP	C5-C4	4.76	1.47	1.39
3	6-N	7501	AMP	C5-C4	4.76	1.47	1.39
3	7-N	7501	AMP	C5-C4	4.76	1.47	1.39
3	8-N	7501	AMP	C5-C4	4.76	1.47	1.39
3	9-N	7501	AMP	C5-C4	4.76	1.47	1.39
3	10-N	7501	AMP	C5-C4	4.76	1.47	1.39
3	1-I	7491	AMP	O4'-C1'	4.75	1.53	1.42
3	2-I	7491	AMP	O4'-C1'	4.75	1.53	1.42
3	3-I	7491	AMP	O4'-C1'	4.75	1.53	1.42
3	4-I	7491	AMP	O4'-C1'	4.75	1.53	1.42
3	5-I	7491	AMP	O4'-C1'	4.75	1.53	1.42
3	6-I	7491	AMP	O4'-C1'	4.75	1.53	1.42
3	7-I	7491	AMP	O4'-C1'	4.75	1.53	1.42
3	8-I	7491	AMP	O4'-C1'	4.75	1.53	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-I	7491	AMP	O4'-C1'	4.75	1.53	1.42
3	10-I	7491	AMP	O4'-C1'	4.75	1.53	1.42
3	1-H	7489	AMP	C5-C4	4.75	1.47	1.39
3	2-H	7489	AMP	C5-C4	4.75	1.47	1.39
3	3-H	7489	AMP	C5-C4	4.75	1.47	1.39
3	4-H	7489	AMP	C5-C4	4.75	1.47	1.39
3	5-H	7489	AMP	C5-C4	4.75	1.47	1.39
3	6-H	7489	AMP	C5-C4	4.75	1.47	1.39
3	7-H	7489	AMP	C5-C4	4.75	1.47	1.39
3	8-H	7489	AMP	C5-C4	4.75	1.47	1.39
3	9-H	7489	AMP	C5-C4	4.75	1.47	1.39
3	10-H	7489	AMP	C5-C4	4.75	1.47	1.39
3	1-O	7503	AMP	C5-C4	4.75	1.47	1.39
3	2-O	7503	AMP	C5-C4	4.75	1.47	1.39
3	3-O	7503	AMP	C5-C4	4.75	1.47	1.39
3	4-O	7503	AMP	C5-C4	4.75	1.47	1.39
3	5-O	7503	AMP	C5-C4	4.75	1.47	1.39
3	6-O	7503	AMP	C5-C4	4.75	1.47	1.39
3	7-O	7503	AMP	C5-C4	4.75	1.47	1.39
3	8-O	7503	AMP	C5-C4	4.75	1.47	1.39
3	9-O	7503	AMP	C5-C4	4.75	1.47	1.39
3	10-O	7503	AMP	C5-C4	4.75	1.47	1.39
3	1-V	7517	AMP	C5-C4	4.75	1.47	1.39
3	2-V	7517	AMP	C5-C4	4.75	1.47	1.39
3	3-V	7517	AMP	C5-C4	4.75	1.47	1.39
3	4-V	7517	AMP	C5-C4	4.75	1.47	1.39
3	5-V	7517	AMP	C5-C4	4.75	1.47	1.39
3	6-V	7517	AMP	C5-C4	4.75	1.47	1.39
3	7-V	7517	AMP	C5-C4	4.75	1.47	1.39
3	8-V	7517	AMP	C5-C4	4.75	1.47	1.39
3	9-V	7517	AMP	C5-C4	4.75	1.47	1.39
3	10-V	7517	AMP	C5-C4	4.75	1.47	1.39
3	1-V	7517	AMP	O4'-C1'	4.75	1.53	1.42
3	2-V	7517	AMP	O4'-C1'	4.75	1.53	1.42
3	3-V	7517	AMP	O4'-C1'	4.75	1.53	1.42
3	4-V	7517	AMP	O4'-C1'	4.75	1.53	1.42
3	5-V	7517	AMP	O4'-C1'	4.75	1.53	1.42
3	6-V	7517	AMP	O4'-C1'	4.75	1.53	1.42
3	7-V	7517	AMP	O4'-C1'	4.75	1.53	1.42
3	8-V	7517	AMP	O4'-C1'	4.75	1.53	1.42
3	9-V	7517	AMP	O4'-C1'	4.75	1.53	1.42
3	10-V	7517	AMP	O4'-C1'	4.75	1.53	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-J	7493	AMP	C5-C4	4.74	1.47	1.39
3	2-J	7493	AMP	C5-C4	4.74	1.47	1.39
3	3-J	7493	AMP	C5-C4	4.74	1.47	1.39
3	4-J	7493	AMP	C5-C4	4.74	1.47	1.39
3	5-J	7493	AMP	C5-C4	4.74	1.47	1.39
3	6-J	7493	AMP	C5-C4	4.74	1.47	1.39
3	7-J	7493	AMP	C5-C4	4.74	1.47	1.39
3	8-J	7493	AMP	C5-C4	4.74	1.47	1.39
3	9-J	7493	AMP	C5-C4	4.74	1.47	1.39
3	10-J	7493	AMP	C5-C4	4.74	1.47	1.39
3	1-E	7483	AMP	C5-C4	4.72	1.47	1.39
3	2-E	7483	AMP	C5-C4	4.72	1.47	1.39
3	3-E	7483	AMP	C5-C4	4.72	1.47	1.39
3	4-E	7483	AMP	C5-C4	4.72	1.47	1.39
3	5-E	7483	AMP	C5-C4	4.72	1.47	1.39
3	6-E	7483	AMP	C5-C4	4.72	1.47	1.39
3	7-E	7483	AMP	C5-C4	4.72	1.47	1.39
3	8-E	7483	AMP	C5-C4	4.72	1.47	1.39
3	9-E	7483	AMP	C5-C4	4.72	1.47	1.39
3	10-E	7483	AMP	C5-C4	4.72	1.47	1.39
3	1-L	7497	AMP	C5-C4	4.72	1.47	1.39
3	2-L	7497	AMP	C5-C4	4.72	1.47	1.39
3	3-L	7497	AMP	C5-C4	4.72	1.47	1.39
3	4-L	7497	AMP	C5-C4	4.72	1.47	1.39
3	5-L	7497	AMP	C5-C4	4.72	1.47	1.39
3	6-L	7497	AMP	C5-C4	4.72	1.47	1.39
3	7-L	7497	AMP	C5-C4	4.72	1.47	1.39
3	8-L	7497	AMP	C5-C4	4.72	1.47	1.39
3	9-L	7497	AMP	C5-C4	4.72	1.47	1.39
3	10-L	7497	AMP	C5-C4	4.72	1.47	1.39
3	1-K	7495	AMP	C4-N9	4.65	1.47	1.37
3	2-K	7495	AMP	C4-N9	4.65	1.47	1.37
3	3-K	7495	AMP	C4-N9	4.65	1.47	1.37
3	4-K	7495	AMP	C4-N9	4.65	1.47	1.37
3	5-K	7495	AMP	C4-N9	4.65	1.47	1.37
3	6-K	7495	AMP	C4-N9	4.65	1.47	1.37
3	7-K	7495	AMP	C4-N9	4.65	1.47	1.37
3	8-K	7495	AMP	C4-N9	4.65	1.47	1.37
3	9-K	7495	AMP	C4-N9	4.65	1.47	1.37
3	10-K	7495	AMP	C4-N9	4.65	1.47	1.37
3	1-I	7491	AMP	C4-N9	4.64	1.47	1.37
3	2-I	7491	AMP	C4-N9	4.64	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-I	7491	AMP	C4-N9	4.64	1.47	1.37
3	4-I	7491	AMP	C4-N9	4.64	1.47	1.37
3	5-I	7491	AMP	C4-N9	4.64	1.47	1.37
3	6-I	7491	AMP	C4-N9	4.64	1.47	1.37
3	7-I	7491	AMP	C4-N9	4.64	1.47	1.37
3	8-I	7491	AMP	C4-N9	4.64	1.47	1.37
3	9-I	7491	AMP	C4-N9	4.64	1.47	1.37
3	10-I	7491	AMP	C4-N9	4.64	1.47	1.37
3	1-X	7521	AMP	C4-N9	4.64	1.47	1.37
3	2-X	7521	AMP	C4-N9	4.64	1.47	1.37
3	3-X	7521	AMP	C4-N9	4.64	1.47	1.37
3	4-X	7521	AMP	C4-N9	4.64	1.47	1.37
3	5-X	7521	AMP	C4-N9	4.64	1.47	1.37
3	6-X	7521	AMP	C4-N9	4.64	1.47	1.37
3	7-X	7521	AMP	C4-N9	4.64	1.47	1.37
3	8-X	7521	AMP	C4-N9	4.64	1.47	1.37
3	9-X	7521	AMP	C4-N9	4.64	1.47	1.37
3	10-X	7521	AMP	C4-N9	4.64	1.47	1.37
3	1-T	7513	AMP	C4-N9	4.63	1.47	1.37
3	2-T	7513	AMP	C4-N9	4.63	1.47	1.37
3	3-T	7513	AMP	C4-N9	4.63	1.47	1.37
3	4-T	7513	AMP	C4-N9	4.63	1.47	1.37
3	5-T	7513	AMP	C4-N9	4.63	1.47	1.37
3	6-T	7513	AMP	C4-N9	4.63	1.47	1.37
3	7-T	7513	AMP	C4-N9	4.63	1.47	1.37
3	8-T	7513	AMP	C4-N9	4.63	1.47	1.37
3	9-T	7513	AMP	C4-N9	4.63	1.47	1.37
3	10-T	7513	AMP	C4-N9	4.63	1.47	1.37
3	1-M	7499	AMP	C4-N9	4.63	1.47	1.37
3	2-M	7499	AMP	C4-N9	4.63	1.47	1.37
3	3-M	7499	AMP	C4-N9	4.63	1.47	1.37
3	4-M	7499	AMP	C4-N9	4.63	1.47	1.37
3	5-M	7499	AMP	C4-N9	4.63	1.47	1.37
3	6-M	7499	AMP	C4-N9	4.63	1.47	1.37
3	7-M	7499	AMP	C4-N9	4.63	1.47	1.37
3	8-M	7499	AMP	C4-N9	4.63	1.47	1.37
3	9-M	7499	AMP	C4-N9	4.63	1.47	1.37
3	10-M	7499	AMP	C4-N9	4.63	1.47	1.37
3	1-J	7493	AMP	C4-N9	4.63	1.47	1.37
3	2-J	7493	AMP	C4-N9	4.63	1.47	1.37
3	3-J	7493	AMP	C4-N9	4.63	1.47	1.37
3	4-J	7493	AMP	C4-N9	4.63	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-J	7493	AMP	C4-N9	4.63	1.47	1.37
3	6-J	7493	AMP	C4-N9	4.63	1.47	1.37
3	7-J	7493	AMP	C4-N9	4.63	1.47	1.37
3	8-J	7493	AMP	C4-N9	4.63	1.47	1.37
3	9-J	7493	AMP	C4-N9	4.63	1.47	1.37
3	10-J	7493	AMP	C4-N9	4.63	1.47	1.37
3	1-L	7497	AMP	C6-N6	-4.62	1.22	1.34
3	2-L	7497	AMP	C6-N6	-4.62	1.22	1.34
3	3-L	7497	AMP	C6-N6	-4.62	1.22	1.34
3	4-L	7497	AMP	C6-N6	-4.62	1.22	1.34
3	5-L	7497	AMP	C6-N6	-4.62	1.22	1.34
3	6-L	7497	AMP	C6-N6	-4.62	1.22	1.34
3	7-L	7497	AMP	C6-N6	-4.62	1.22	1.34
3	8-L	7497	AMP	C6-N6	-4.62	1.22	1.34
3	9-L	7497	AMP	C6-N6	-4.62	1.22	1.34
3	10-L	7497	AMP	C6-N6	-4.62	1.22	1.34
3	1-S	7511	AMP	C6-N6	-4.62	1.22	1.34
3	2-S	7511	AMP	C6-N6	-4.62	1.22	1.34
3	3-S	7511	AMP	C6-N6	-4.62	1.22	1.34
3	4-S	7511	AMP	C6-N6	-4.62	1.22	1.34
3	5-S	7511	AMP	C6-N6	-4.62	1.22	1.34
3	6-S	7511	AMP	C6-N6	-4.62	1.22	1.34
3	7-S	7511	AMP	C6-N6	-4.62	1.22	1.34
3	8-S	7511	AMP	C6-N6	-4.62	1.22	1.34
3	9-S	7511	AMP	C6-N6	-4.62	1.22	1.34
3	10-S	7511	AMP	C6-N6	-4.62	1.22	1.34
3	1-A	7475	AMP	C4-N9	4.62	1.47	1.37
3	2-A	7475	AMP	C4-N9	4.62	1.47	1.37
3	3-A	7475	AMP	C4-N9	4.62	1.47	1.37
3	4-A	7475	AMP	C4-N9	4.62	1.47	1.37
3	5-A	7475	AMP	C4-N9	4.62	1.47	1.37
3	6-A	7475	AMP	C4-N9	4.62	1.47	1.37
3	7-A	7475	AMP	C4-N9	4.62	1.47	1.37
3	8-A	7475	AMP	C4-N9	4.62	1.47	1.37
3	9-A	7475	AMP	C4-N9	4.62	1.47	1.37
3	10-A	7475	AMP	C4-N9	4.62	1.47	1.37
3	1-O	7503	AMP	C4-N9	4.62	1.47	1.37
3	2-O	7503	AMP	C4-N9	4.62	1.47	1.37
3	3-O	7503	AMP	C4-N9	4.62	1.47	1.37
3	4-O	7503	AMP	C4-N9	4.62	1.47	1.37
3	5-O	7503	AMP	C4-N9	4.62	1.47	1.37
3	6-O	7503	AMP	C4-N9	4.62	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-O	7503	AMP	C4-N9	4.62	1.47	1.37
3	8-O	7503	AMP	C4-N9	4.62	1.47	1.37
3	9-O	7503	AMP	C4-N9	4.62	1.47	1.37
3	10-O	7503	AMP	C4-N9	4.62	1.47	1.37
3	1-E	7483	AMP	C4-N9	4.62	1.47	1.37
3	2-E	7483	AMP	C4-N9	4.62	1.47	1.37
3	3-E	7483	AMP	C4-N9	4.62	1.47	1.37
3	4-E	7483	AMP	C4-N9	4.62	1.47	1.37
3	5-E	7483	AMP	C4-N9	4.62	1.47	1.37
3	6-E	7483	AMP	C4-N9	4.62	1.47	1.37
3	7-E	7483	AMP	C4-N9	4.62	1.47	1.37
3	8-E	7483	AMP	C4-N9	4.62	1.47	1.37
3	9-E	7483	AMP	C4-N9	4.62	1.47	1.37
3	10-E	7483	AMP	C4-N9	4.62	1.47	1.37
3	1-D	7481	AMP	C6-N6	-4.62	1.22	1.34
3	2-D	7481	AMP	C6-N6	-4.62	1.22	1.34
3	3-D	7481	AMP	C6-N6	-4.62	1.22	1.34
3	4-D	7481	AMP	C6-N6	-4.62	1.22	1.34
3	5-D	7481	AMP	C6-N6	-4.62	1.22	1.34
3	6-D	7481	AMP	C6-N6	-4.62	1.22	1.34
3	7-D	7481	AMP	C6-N6	-4.62	1.22	1.34
3	8-D	7481	AMP	C6-N6	-4.62	1.22	1.34
3	9-D	7481	AMP	C6-N6	-4.62	1.22	1.34
3	10-D	7481	AMP	C6-N6	-4.62	1.22	1.34
3	1-N	7501	AMP	C4-N9	4.62	1.47	1.37
3	2-N	7501	AMP	C4-N9	4.62	1.47	1.37
3	3-N	7501	AMP	C4-N9	4.62	1.47	1.37
3	4-N	7501	AMP	C4-N9	4.62	1.47	1.37
3	5-N	7501	AMP	C4-N9	4.62	1.47	1.37
3	6-N	7501	AMP	C4-N9	4.62	1.47	1.37
3	7-N	7501	AMP	C4-N9	4.62	1.47	1.37
3	8-N	7501	AMP	C4-N9	4.62	1.47	1.37
3	9-N	7501	AMP	C4-N9	4.62	1.47	1.37
3	10-N	7501	AMP	C4-N9	4.62	1.47	1.37
3	1-W	7519	AMP	C4-N9	4.62	1.47	1.37
3	2-W	7519	AMP	C4-N9	4.62	1.47	1.37
3	3-W	7519	AMP	C4-N9	4.62	1.47	1.37
3	4-W	7519	AMP	C4-N9	4.62	1.47	1.37
3	5-W	7519	AMP	C4-N9	4.62	1.47	1.37
3	6-W	7519	AMP	C4-N9	4.62	1.47	1.37
3	7-W	7519	AMP	C4-N9	4.62	1.47	1.37
3	8-W	7519	AMP	C4-N9	4.62	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-W	7519	AMP	C4-N9	4.62	1.47	1.37
3	10-W	7519	AMP	C4-N9	4.62	1.47	1.37
3	1-V	7517	AMP	C4-N9	4.62	1.47	1.37
3	2-V	7517	AMP	C4-N9	4.62	1.47	1.37
3	3-V	7517	AMP	C4-N9	4.62	1.47	1.37
3	4-V	7517	AMP	C4-N9	4.62	1.47	1.37
3	5-V	7517	AMP	C4-N9	4.62	1.47	1.37
3	6-V	7517	AMP	C4-N9	4.62	1.47	1.37
3	7-V	7517	AMP	C4-N9	4.62	1.47	1.37
3	8-V	7517	AMP	C4-N9	4.62	1.47	1.37
3	9-V	7517	AMP	C4-N9	4.62	1.47	1.37
3	10-V	7517	AMP	C4-N9	4.62	1.47	1.37
3	1-K	7495	AMP	C6-N6	-4.62	1.22	1.34
3	2-K	7495	AMP	C6-N6	-4.62	1.22	1.34
3	3-K	7495	AMP	C6-N6	-4.62	1.22	1.34
3	4-K	7495	AMP	C6-N6	-4.62	1.22	1.34
3	5-K	7495	AMP	C6-N6	-4.62	1.22	1.34
3	6-K	7495	AMP	C6-N6	-4.62	1.22	1.34
3	7-K	7495	AMP	C6-N6	-4.62	1.22	1.34
3	8-K	7495	AMP	C6-N6	-4.62	1.22	1.34
3	9-K	7495	AMP	C6-N6	-4.62	1.22	1.34
3	10-K	7495	AMP	C6-N6	-4.62	1.22	1.34
3	1-R	7509	AMP	C4-N9	4.62	1.47	1.37
3	2-R	7509	AMP	C4-N9	4.62	1.47	1.37
3	3-R	7509	AMP	C4-N9	4.62	1.47	1.37
3	4-R	7509	AMP	C4-N9	4.62	1.47	1.37
3	5-R	7509	AMP	C4-N9	4.62	1.47	1.37
3	6-R	7509	AMP	C4-N9	4.62	1.47	1.37
3	7-R	7509	AMP	C4-N9	4.62	1.47	1.37
3	8-R	7509	AMP	C4-N9	4.62	1.47	1.37
3	9-R	7509	AMP	C4-N9	4.62	1.47	1.37
3	10-R	7509	AMP	C4-N9	4.62	1.47	1.37
3	1-G	7487	AMP	C4-N9	4.61	1.47	1.37
3	2-G	7487	AMP	C4-N9	4.61	1.47	1.37
3	3-G	7487	AMP	C4-N9	4.61	1.47	1.37
3	4-G	7487	AMP	C4-N9	4.61	1.47	1.37
3	5-G	7487	AMP	C4-N9	4.61	1.47	1.37
3	6-G	7487	AMP	C4-N9	4.61	1.47	1.37
3	7-G	7487	AMP	C4-N9	4.61	1.47	1.37
3	8-G	7487	AMP	C4-N9	4.61	1.47	1.37
3	9-G	7487	AMP	C4-N9	4.61	1.47	1.37
3	10-G	7487	AMP	C4-N9	4.61	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-Q	7507	AMP	C4-N9	4.61	1.47	1.37
3	2-Q	7507	AMP	C4-N9	4.61	1.47	1.37
3	3-Q	7507	AMP	C4-N9	4.61	1.47	1.37
3	4-Q	7507	AMP	C4-N9	4.61	1.47	1.37
3	5-Q	7507	AMP	C4-N9	4.61	1.47	1.37
3	6-Q	7507	AMP	C4-N9	4.61	1.47	1.37
3	7-Q	7507	AMP	C4-N9	4.61	1.47	1.37
3	8-Q	7507	AMP	C4-N9	4.61	1.47	1.37
3	9-Q	7507	AMP	C4-N9	4.61	1.47	1.37
3	10-Q	7507	AMP	C4-N9	4.61	1.47	1.37
3	1-S	7511	AMP	C4-N9	4.61	1.47	1.37
3	2-S	7511	AMP	C4-N9	4.61	1.47	1.37
3	3-S	7511	AMP	C4-N9	4.61	1.47	1.37
3	4-S	7511	AMP	C4-N9	4.61	1.47	1.37
3	5-S	7511	AMP	C4-N9	4.61	1.47	1.37
3	6-S	7511	AMP	C4-N9	4.61	1.47	1.37
3	7-S	7511	AMP	C4-N9	4.61	1.47	1.37
3	8-S	7511	AMP	C4-N9	4.61	1.47	1.37
3	9-S	7511	AMP	C4-N9	4.61	1.47	1.37
3	10-S	7511	AMP	C4-N9	4.61	1.47	1.37
3	1-U	7515	AMP	C6-N6	-4.61	1.22	1.34
3	2-U	7515	AMP	C6-N6	-4.61	1.22	1.34
3	3-U	7515	AMP	C6-N6	-4.61	1.22	1.34
3	4-U	7515	AMP	C6-N6	-4.61	1.22	1.34
3	5-U	7515	AMP	C6-N6	-4.61	1.22	1.34
3	6-U	7515	AMP	C6-N6	-4.61	1.22	1.34
3	7-U	7515	AMP	C6-N6	-4.61	1.22	1.34
3	8-U	7515	AMP	C6-N6	-4.61	1.22	1.34
3	9-U	7515	AMP	C6-N6	-4.61	1.22	1.34
3	10-U	7515	AMP	C6-N6	-4.61	1.22	1.34
3	1-Q	7507	AMP	C6-N6	-4.61	1.22	1.34
3	2-Q	7507	AMP	C6-N6	-4.61	1.22	1.34
3	3-Q	7507	AMP	C6-N6	-4.61	1.22	1.34
3	4-Q	7507	AMP	C6-N6	-4.61	1.22	1.34
3	5-Q	7507	AMP	C6-N6	-4.61	1.22	1.34
3	6-Q	7507	AMP	C6-N6	-4.61	1.22	1.34
3	7-Q	7507	AMP	C6-N6	-4.61	1.22	1.34
3	8-Q	7507	AMP	C6-N6	-4.61	1.22	1.34
3	9-Q	7507	AMP	C6-N6	-4.61	1.22	1.34
3	10-Q	7507	AMP	C6-N6	-4.61	1.22	1.34
3	1-U	7515	AMP	C4-N9	4.61	1.47	1.37
3	2-U	7515	AMP	C4-N9	4.61	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-U	7515	AMP	C4-N9	4.61	1.47	1.37
3	4-U	7515	AMP	C4-N9	4.61	1.47	1.37
3	5-U	7515	AMP	C4-N9	4.61	1.47	1.37
3	6-U	7515	AMP	C4-N9	4.61	1.47	1.37
3	7-U	7515	AMP	C4-N9	4.61	1.47	1.37
3	8-U	7515	AMP	C4-N9	4.61	1.47	1.37
3	9-U	7515	AMP	C4-N9	4.61	1.47	1.37
3	10-U	7515	AMP	C4-N9	4.61	1.47	1.37
3	1-R	7509	AMP	C6-N6	-4.60	1.22	1.34
3	2-R	7509	AMP	C6-N6	-4.60	1.22	1.34
3	3-R	7509	AMP	C6-N6	-4.60	1.22	1.34
3	4-R	7509	AMP	C6-N6	-4.60	1.22	1.34
3	5-R	7509	AMP	C6-N6	-4.60	1.22	1.34
3	6-R	7509	AMP	C6-N6	-4.60	1.22	1.34
3	7-R	7509	AMP	C6-N6	-4.60	1.22	1.34
3	8-R	7509	AMP	C6-N6	-4.60	1.22	1.34
3	9-R	7509	AMP	C6-N6	-4.60	1.22	1.34
3	10-R	7509	AMP	C6-N6	-4.60	1.22	1.34
3	1-J	7493	AMP	C6-N6	-4.60	1.22	1.34
3	2-J	7493	AMP	C6-N6	-4.60	1.22	1.34
3	3-J	7493	AMP	C6-N6	-4.60	1.22	1.34
3	4-J	7493	AMP	C6-N6	-4.60	1.22	1.34
3	5-J	7493	AMP	C6-N6	-4.60	1.22	1.34
3	6-J	7493	AMP	C6-N6	-4.60	1.22	1.34
3	7-J	7493	AMP	C6-N6	-4.60	1.22	1.34
3	8-J	7493	AMP	C6-N6	-4.60	1.22	1.34
3	9-J	7493	AMP	C6-N6	-4.60	1.22	1.34
3	10-J	7493	AMP	C6-N6	-4.60	1.22	1.34
3	1-I	7491	AMP	C6-N6	-4.60	1.22	1.34
3	2-I	7491	AMP	C6-N6	-4.60	1.22	1.34
3	3-I	7491	AMP	C6-N6	-4.60	1.22	1.34
3	4-I	7491	AMP	C6-N6	-4.60	1.22	1.34
3	5-I	7491	AMP	C6-N6	-4.60	1.22	1.34
3	6-I	7491	AMP	C6-N6	-4.60	1.22	1.34
3	7-I	7491	AMP	C6-N6	-4.60	1.22	1.34
3	8-I	7491	AMP	C6-N6	-4.60	1.22	1.34
3	9-I	7491	AMP	C6-N6	-4.60	1.22	1.34
3	10-I	7491	AMP	C6-N6	-4.60	1.22	1.34
3	1-B	7477	AMP	C4-N9	4.60	1.47	1.37
3	2-B	7477	AMP	C4-N9	4.60	1.47	1.37
3	3-B	7477	AMP	C4-N9	4.60	1.47	1.37
3	4-B	7477	AMP	C4-N9	4.60	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-B	7477	AMP	C4-N9	4.60	1.47	1.37
3	6-B	7477	AMP	C4-N9	4.60	1.47	1.37
3	7-B	7477	AMP	C4-N9	4.60	1.47	1.37
3	8-B	7477	AMP	C4-N9	4.60	1.47	1.37
3	9-B	7477	AMP	C4-N9	4.60	1.47	1.37
3	10-B	7477	AMP	C4-N9	4.60	1.47	1.37
3	1-H	7489	AMP	C4-N9	4.60	1.47	1.37
3	2-H	7489	AMP	C4-N9	4.60	1.47	1.37
3	3-H	7489	AMP	C4-N9	4.60	1.47	1.37
3	4-H	7489	AMP	C4-N9	4.60	1.47	1.37
3	5-H	7489	AMP	C4-N9	4.60	1.47	1.37
3	6-H	7489	AMP	C4-N9	4.60	1.47	1.37
3	7-H	7489	AMP	C4-N9	4.60	1.47	1.37
3	8-H	7489	AMP	C4-N9	4.60	1.47	1.37
3	9-H	7489	AMP	C4-N9	4.60	1.47	1.37
3	10-H	7489	AMP	C4-N9	4.60	1.47	1.37
3	1-W	7519	AMP	C6-N6	-4.59	1.22	1.34
3	2-W	7519	AMP	C6-N6	-4.59	1.22	1.34
3	3-W	7519	AMP	C6-N6	-4.59	1.22	1.34
3	4-W	7519	AMP	C6-N6	-4.59	1.22	1.34
3	5-W	7519	AMP	C6-N6	-4.59	1.22	1.34
3	6-W	7519	AMP	C6-N6	-4.59	1.22	1.34
3	7-W	7519	AMP	C6-N6	-4.59	1.22	1.34
3	8-W	7519	AMP	C6-N6	-4.59	1.22	1.34
3	9-W	7519	AMP	C6-N6	-4.59	1.22	1.34
3	10-W	7519	AMP	C6-N6	-4.59	1.22	1.34
3	1-E	7483	AMP	C6-N6	-4.59	1.22	1.34
3	2-E	7483	AMP	C6-N6	-4.59	1.22	1.34
3	3-E	7483	AMP	C6-N6	-4.59	1.22	1.34
3	4-E	7483	AMP	C6-N6	-4.59	1.22	1.34
3	5-E	7483	AMP	C6-N6	-4.59	1.22	1.34
3	6-E	7483	AMP	C6-N6	-4.59	1.22	1.34
3	7-E	7483	AMP	C6-N6	-4.59	1.22	1.34
3	8-E	7483	AMP	C6-N6	-4.59	1.22	1.34
3	9-E	7483	AMP	C6-N6	-4.59	1.22	1.34
3	10-E	7483	AMP	C6-N6	-4.59	1.22	1.34
3	1-X	7521	AMP	C6-N6	-4.59	1.22	1.34
3	2-X	7521	AMP	C6-N6	-4.59	1.22	1.34
3	3-X	7521	AMP	C6-N6	-4.59	1.22	1.34
3	4-X	7521	AMP	C6-N6	-4.59	1.22	1.34
3	5-X	7521	AMP	C6-N6	-4.59	1.22	1.34
3	6-X	7521	AMP	C6-N6	-4.59	1.22	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-X	7521	AMP	C6-N6	-4.59	1.22	1.34
3	8-X	7521	AMP	C6-N6	-4.59	1.22	1.34
3	9-X	7521	AMP	C6-N6	-4.59	1.22	1.34
3	10-X	7521	AMP	C6-N6	-4.59	1.22	1.34
3	1-C	7479	AMP	C6-N6	-4.59	1.22	1.34
3	2-C	7479	AMP	C6-N6	-4.59	1.22	1.34
3	3-C	7479	AMP	C6-N6	-4.59	1.22	1.34
3	4-C	7479	AMP	C6-N6	-4.59	1.22	1.34
3	5-C	7479	AMP	C6-N6	-4.59	1.22	1.34
3	6-C	7479	AMP	C6-N6	-4.59	1.22	1.34
3	7-C	7479	AMP	C6-N6	-4.59	1.22	1.34
3	8-C	7479	AMP	C6-N6	-4.59	1.22	1.34
3	9-C	7479	AMP	C6-N6	-4.59	1.22	1.34
3	10-C	7479	AMP	C6-N6	-4.59	1.22	1.34
3	1-A	7475	AMP	C6-N6	-4.59	1.22	1.34
3	2-A	7475	AMP	C6-N6	-4.59	1.22	1.34
3	3-A	7475	AMP	C6-N6	-4.59	1.22	1.34
3	4-A	7475	AMP	C6-N6	-4.59	1.22	1.34
3	5-A	7475	AMP	C6-N6	-4.59	1.22	1.34
3	6-A	7475	AMP	C6-N6	-4.59	1.22	1.34
3	7-A	7475	AMP	C6-N6	-4.59	1.22	1.34
3	8-A	7475	AMP	C6-N6	-4.59	1.22	1.34
3	9-A	7475	AMP	C6-N6	-4.59	1.22	1.34
3	10-A	7475	AMP	C6-N6	-4.59	1.22	1.34
3	1-T	7513	AMP	C6-N6	-4.59	1.22	1.34
3	2-T	7513	AMP	C6-N6	-4.59	1.22	1.34
3	3-T	7513	AMP	C6-N6	-4.59	1.22	1.34
3	4-T	7513	AMP	C6-N6	-4.59	1.22	1.34
3	5-T	7513	AMP	C6-N6	-4.59	1.22	1.34
3	6-T	7513	AMP	C6-N6	-4.59	1.22	1.34
3	7-T	7513	AMP	C6-N6	-4.59	1.22	1.34
3	8-T	7513	AMP	C6-N6	-4.59	1.22	1.34
3	9-T	7513	AMP	C6-N6	-4.59	1.22	1.34
3	10-T	7513	AMP	C6-N6	-4.59	1.22	1.34
3	1-C	7479	AMP	C4-N9	4.59	1.47	1.37
3	2-C	7479	AMP	C4-N9	4.59	1.47	1.37
3	3-C	7479	AMP	C4-N9	4.59	1.47	1.37
3	4-C	7479	AMP	C4-N9	4.59	1.47	1.37
3	5-C	7479	AMP	C4-N9	4.59	1.47	1.37
3	6-C	7479	AMP	C4-N9	4.59	1.47	1.37
3	7-C	7479	AMP	C4-N9	4.59	1.47	1.37
3	8-C	7479	AMP	C4-N9	4.59	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-C	7479	AMP	C4-N9	4.59	1.47	1.37
3	10-C	7479	AMP	C4-N9	4.59	1.47	1.37
3	1-D	7481	AMP	C4-N9	4.58	1.47	1.37
3	2-D	7481	AMP	C4-N9	4.58	1.47	1.37
3	3-D	7481	AMP	C4-N9	4.58	1.47	1.37
3	4-D	7481	AMP	C4-N9	4.58	1.47	1.37
3	5-D	7481	AMP	C4-N9	4.58	1.47	1.37
3	6-D	7481	AMP	C4-N9	4.58	1.47	1.37
3	7-D	7481	AMP	C4-N9	4.58	1.47	1.37
3	8-D	7481	AMP	C4-N9	4.58	1.47	1.37
3	9-D	7481	AMP	C4-N9	4.58	1.47	1.37
3	10-D	7481	AMP	C4-N9	4.58	1.47	1.37
3	1-L	7497	AMP	C4-N9	4.58	1.47	1.37
3	2-L	7497	AMP	C4-N9	4.58	1.47	1.37
3	3-L	7497	AMP	C4-N9	4.58	1.47	1.37
3	4-L	7497	AMP	C4-N9	4.58	1.47	1.37
3	5-L	7497	AMP	C4-N9	4.58	1.47	1.37
3	6-L	7497	AMP	C4-N9	4.58	1.47	1.37
3	7-L	7497	AMP	C4-N9	4.58	1.47	1.37
3	8-L	7497	AMP	C4-N9	4.58	1.47	1.37
3	9-L	7497	AMP	C4-N9	4.58	1.47	1.37
3	10-L	7497	AMP	C4-N9	4.58	1.47	1.37
3	1-P	7505	AMP	C4-N9	4.58	1.47	1.37
3	2-P	7505	AMP	C4-N9	4.58	1.47	1.37
3	3-P	7505	AMP	C4-N9	4.58	1.47	1.37
3	4-P	7505	AMP	C4-N9	4.58	1.47	1.37
3	5-P	7505	AMP	C4-N9	4.58	1.47	1.37
3	6-P	7505	AMP	C4-N9	4.58	1.47	1.37
3	7-P	7505	AMP	C4-N9	4.58	1.47	1.37
3	8-P	7505	AMP	C4-N9	4.58	1.47	1.37
3	9-P	7505	AMP	C4-N9	4.58	1.47	1.37
3	10-P	7505	AMP	C4-N9	4.58	1.47	1.37
3	1-G	7487	AMP	C6-N6	-4.58	1.22	1.34
3	2-G	7487	AMP	C6-N6	-4.58	1.22	1.34
3	3-G	7487	AMP	C6-N6	-4.58	1.22	1.34
3	4-G	7487	AMP	C6-N6	-4.58	1.22	1.34
3	5-G	7487	AMP	C6-N6	-4.58	1.22	1.34
3	6-G	7487	AMP	C6-N6	-4.58	1.22	1.34
3	7-G	7487	AMP	C6-N6	-4.58	1.22	1.34
3	8-G	7487	AMP	C6-N6	-4.58	1.22	1.34
3	9-G	7487	AMP	C6-N6	-4.58	1.22	1.34
3	10-G	7487	AMP	C6-N6	-4.58	1.22	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-N	7501	AMP	C6-N6	-4.58	1.22	1.34
3	2-N	7501	AMP	C6-N6	-4.58	1.22	1.34
3	3-N	7501	AMP	C6-N6	-4.58	1.22	1.34
3	4-N	7501	AMP	C6-N6	-4.58	1.22	1.34
3	5-N	7501	AMP	C6-N6	-4.58	1.22	1.34
3	6-N	7501	AMP	C6-N6	-4.58	1.22	1.34
3	7-N	7501	AMP	C6-N6	-4.58	1.22	1.34
3	8-N	7501	AMP	C6-N6	-4.58	1.22	1.34
3	9-N	7501	AMP	C6-N6	-4.58	1.22	1.34
3	10-N	7501	AMP	C6-N6	-4.58	1.22	1.34
3	1-F	7485	AMP	C4-N9	4.58	1.47	1.37
3	2-F	7485	AMP	C4-N9	4.58	1.47	1.37
3	3-F	7485	AMP	C4-N9	4.58	1.47	1.37
3	4-F	7485	AMP	C4-N9	4.58	1.47	1.37
3	5-F	7485	AMP	C4-N9	4.58	1.47	1.37
3	6-F	7485	AMP	C4-N9	4.58	1.47	1.37
3	7-F	7485	AMP	C4-N9	4.58	1.47	1.37
3	8-F	7485	AMP	C4-N9	4.58	1.47	1.37
3	9-F	7485	AMP	C4-N9	4.58	1.47	1.37
3	10-F	7485	AMP	C4-N9	4.58	1.47	1.37
3	1-M	7499	AMP	C6-N6	-4.57	1.22	1.34
3	2-M	7499	AMP	C6-N6	-4.57	1.22	1.34
3	3-M	7499	AMP	C6-N6	-4.57	1.22	1.34
3	4-M	7499	AMP	C6-N6	-4.57	1.22	1.34
3	5-M	7499	AMP	C6-N6	-4.57	1.22	1.34
3	6-M	7499	AMP	C6-N6	-4.57	1.22	1.34
3	7-M	7499	AMP	C6-N6	-4.57	1.22	1.34
3	8-M	7499	AMP	C6-N6	-4.57	1.22	1.34
3	9-M	7499	AMP	C6-N6	-4.57	1.22	1.34
3	10-M	7499	AMP	C6-N6	-4.57	1.22	1.34
3	1-F	7485	AMP	C6-N6	-4.57	1.22	1.34
3	2-F	7485	AMP	C6-N6	-4.57	1.22	1.34
3	3-F	7485	AMP	C6-N6	-4.57	1.22	1.34
3	4-F	7485	AMP	C6-N6	-4.57	1.22	1.34
3	5-F	7485	AMP	C6-N6	-4.57	1.22	1.34
3	6-F	7485	AMP	C6-N6	-4.57	1.22	1.34
3	7-F	7485	AMP	C6-N6	-4.57	1.22	1.34
3	8-F	7485	AMP	C6-N6	-4.57	1.22	1.34
3	9-F	7485	AMP	C6-N6	-4.57	1.22	1.34
3	10-F	7485	AMP	C6-N6	-4.57	1.22	1.34
3	1-P	7505	AMP	C6-N6	-4.57	1.22	1.34
3	2-P	7505	AMP	C6-N6	-4.57	1.22	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-P	7505	AMP	C6-N6	-4.57	1.22	1.34
3	4-P	7505	AMP	C6-N6	-4.57	1.22	1.34
3	5-P	7505	AMP	C6-N6	-4.57	1.22	1.34
3	6-P	7505	AMP	C6-N6	-4.57	1.22	1.34
3	7-P	7505	AMP	C6-N6	-4.57	1.22	1.34
3	8-P	7505	AMP	C6-N6	-4.57	1.22	1.34
3	9-P	7505	AMP	C6-N6	-4.57	1.22	1.34
3	10-P	7505	AMP	C6-N6	-4.57	1.22	1.34
3	1-H	7489	AMP	C6-N6	-4.57	1.22	1.34
3	2-H	7489	AMP	C6-N6	-4.57	1.22	1.34
3	3-H	7489	AMP	C6-N6	-4.57	1.22	1.34
3	4-H	7489	AMP	C6-N6	-4.57	1.22	1.34
3	5-H	7489	AMP	C6-N6	-4.57	1.22	1.34
3	6-H	7489	AMP	C6-N6	-4.57	1.22	1.34
3	7-H	7489	AMP	C6-N6	-4.57	1.22	1.34
3	8-H	7489	AMP	C6-N6	-4.57	1.22	1.34
3	9-H	7489	AMP	C6-N6	-4.57	1.22	1.34
3	10-H	7489	AMP	C6-N6	-4.57	1.22	1.34
3	1-B	7477	AMP	C6-N6	-4.57	1.22	1.34
3	2-B	7477	AMP	C6-N6	-4.57	1.22	1.34
3	3-B	7477	AMP	C6-N6	-4.57	1.22	1.34
3	4-B	7477	AMP	C6-N6	-4.57	1.22	1.34
3	5-B	7477	AMP	C6-N6	-4.57	1.22	1.34
3	6-B	7477	AMP	C6-N6	-4.57	1.22	1.34
3	7-B	7477	AMP	C6-N6	-4.57	1.22	1.34
3	8-B	7477	AMP	C6-N6	-4.57	1.22	1.34
3	9-B	7477	AMP	C6-N6	-4.57	1.22	1.34
3	10-B	7477	AMP	C6-N6	-4.57	1.22	1.34
3	1-V	7517	AMP	C6-N6	-4.57	1.22	1.34
3	2-V	7517	AMP	C6-N6	-4.57	1.22	1.34
3	3-V	7517	AMP	C6-N6	-4.57	1.22	1.34
3	4-V	7517	AMP	C6-N6	-4.57	1.22	1.34
3	5-V	7517	AMP	C6-N6	-4.57	1.22	1.34
3	6-V	7517	AMP	C6-N6	-4.57	1.22	1.34
3	7-V	7517	AMP	C6-N6	-4.57	1.22	1.34
3	8-V	7517	AMP	C6-N6	-4.57	1.22	1.34
3	9-V	7517	AMP	C6-N6	-4.57	1.22	1.34
3	10-V	7517	AMP	C6-N6	-4.57	1.22	1.34
3	1-O	7503	AMP	C6-N6	-4.56	1.22	1.34
3	2-O	7503	AMP	C6-N6	-4.56	1.22	1.34
3	3-O	7503	AMP	C6-N6	-4.56	1.22	1.34
3	4-O	7503	AMP	C6-N6	-4.56	1.22	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-O	7503	AMP	C6-N6	-4.56	1.22	1.34
3	6-O	7503	AMP	C6-N6	-4.56	1.22	1.34
3	7-O	7503	AMP	C6-N6	-4.56	1.22	1.34
3	8-O	7503	AMP	C6-N6	-4.56	1.22	1.34
3	9-O	7503	AMP	C6-N6	-4.56	1.22	1.34
3	10-O	7503	AMP	C6-N6	-4.56	1.22	1.34
3	1-Q	7507	AMP	O4'-C4'	4.33	1.54	1.45
3	2-Q	7507	AMP	O4'-C4'	4.33	1.54	1.45
3	3-Q	7507	AMP	O4'-C4'	4.33	1.54	1.45
3	4-Q	7507	AMP	O4'-C4'	4.33	1.54	1.45
3	5-Q	7507	AMP	O4'-C4'	4.33	1.54	1.45
3	6-Q	7507	AMP	O4'-C4'	4.33	1.54	1.45
3	7-Q	7507	AMP	O4'-C4'	4.33	1.54	1.45
3	8-Q	7507	AMP	O4'-C4'	4.33	1.54	1.45
3	9-Q	7507	AMP	O4'-C4'	4.33	1.54	1.45
3	10-Q	7507	AMP	O4'-C4'	4.33	1.54	1.45
3	1-S	7511	AMP	O4'-C4'	4.33	1.54	1.45
3	2-S	7511	AMP	O4'-C4'	4.33	1.54	1.45
3	3-S	7511	AMP	O4'-C4'	4.33	1.54	1.45
3	4-S	7511	AMP	O4'-C4'	4.33	1.54	1.45
3	5-S	7511	AMP	O4'-C4'	4.33	1.54	1.45
3	6-S	7511	AMP	O4'-C4'	4.33	1.54	1.45
3	7-S	7511	AMP	O4'-C4'	4.33	1.54	1.45
3	8-S	7511	AMP	O4'-C4'	4.33	1.54	1.45
3	9-S	7511	AMP	O4'-C4'	4.33	1.54	1.45
3	10-S	7511	AMP	O4'-C4'	4.33	1.54	1.45
3	1-M	7499	AMP	O4'-C4'	4.33	1.54	1.45
3	2-M	7499	AMP	O4'-C4'	4.33	1.54	1.45
3	3-M	7499	AMP	O4'-C4'	4.33	1.54	1.45
3	4-M	7499	AMP	O4'-C4'	4.33	1.54	1.45
3	5-M	7499	AMP	O4'-C4'	4.33	1.54	1.45
3	6-M	7499	AMP	O4'-C4'	4.33	1.54	1.45
3	7-M	7499	AMP	O4'-C4'	4.33	1.54	1.45
3	8-M	7499	AMP	O4'-C4'	4.33	1.54	1.45
3	9-M	7499	AMP	O4'-C4'	4.33	1.54	1.45
3	10-M	7499	AMP	O4'-C4'	4.33	1.54	1.45
3	1-H	7489	AMP	O4'-C4'	4.33	1.54	1.45
3	2-H	7489	AMP	O4'-C4'	4.33	1.54	1.45
3	3-H	7489	AMP	O4'-C4'	4.33	1.54	1.45
3	4-H	7489	AMP	O4'-C4'	4.33	1.54	1.45
3	5-H	7489	AMP	O4'-C4'	4.33	1.54	1.45
3	6-H	7489	AMP	O4'-C4'	4.33	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-H	7489	AMP	O4'-C4'	4.33	1.54	1.45
3	8-H	7489	AMP	O4'-C4'	4.33	1.54	1.45
3	9-H	7489	AMP	O4'-C4'	4.33	1.54	1.45
3	10-H	7489	AMP	O4'-C4'	4.33	1.54	1.45
3	1-V	7517	AMP	O4'-C4'	4.33	1.54	1.45
3	2-V	7517	AMP	O4'-C4'	4.33	1.54	1.45
3	3-V	7517	AMP	O4'-C4'	4.33	1.54	1.45
3	4-V	7517	AMP	O4'-C4'	4.33	1.54	1.45
3	5-V	7517	AMP	O4'-C4'	4.33	1.54	1.45
3	6-V	7517	AMP	O4'-C4'	4.33	1.54	1.45
3	7-V	7517	AMP	O4'-C4'	4.33	1.54	1.45
3	8-V	7517	AMP	O4'-C4'	4.33	1.54	1.45
3	9-V	7517	AMP	O4'-C4'	4.33	1.54	1.45
3	10-V	7517	AMP	O4'-C4'	4.33	1.54	1.45
3	1-F	7485	AMP	O4'-C4'	4.33	1.54	1.45
3	2-F	7485	AMP	O4'-C4'	4.33	1.54	1.45
3	3-F	7485	AMP	O4'-C4'	4.33	1.54	1.45
3	4-F	7485	AMP	O4'-C4'	4.33	1.54	1.45
3	5-F	7485	AMP	O4'-C4'	4.33	1.54	1.45
3	6-F	7485	AMP	O4'-C4'	4.33	1.54	1.45
3	7-F	7485	AMP	O4'-C4'	4.33	1.54	1.45
3	8-F	7485	AMP	O4'-C4'	4.33	1.54	1.45
3	9-F	7485	AMP	O4'-C4'	4.33	1.54	1.45
3	10-F	7485	AMP	O4'-C4'	4.33	1.54	1.45
3	1-X	7521	AMP	O4'-C4'	4.32	1.54	1.45
3	2-X	7521	AMP	O4'-C4'	4.32	1.54	1.45
3	3-X	7521	AMP	O4'-C4'	4.32	1.54	1.45
3	4-X	7521	AMP	O4'-C4'	4.32	1.54	1.45
3	5-X	7521	AMP	O4'-C4'	4.32	1.54	1.45
3	6-X	7521	AMP	O4'-C4'	4.32	1.54	1.45
3	7-X	7521	AMP	O4'-C4'	4.32	1.54	1.45
3	8-X	7521	AMP	O4'-C4'	4.32	1.54	1.45
3	9-X	7521	AMP	O4'-C4'	4.32	1.54	1.45
3	10-X	7521	AMP	O4'-C4'	4.32	1.54	1.45
3	1-I	7491	AMP	O4'-C4'	4.32	1.54	1.45
3	2-I	7491	AMP	O4'-C4'	4.32	1.54	1.45
3	3-I	7491	AMP	O4'-C4'	4.32	1.54	1.45
3	4-I	7491	AMP	O4'-C4'	4.32	1.54	1.45
3	5-I	7491	AMP	O4'-C4'	4.32	1.54	1.45
3	6-I	7491	AMP	O4'-C4'	4.32	1.54	1.45
3	7-I	7491	AMP	O4'-C4'	4.32	1.54	1.45
3	8-I	7491	AMP	O4'-C4'	4.32	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-I	7491	AMP	O4'-C4'	4.32	1.54	1.45
3	10-I	7491	AMP	O4'-C4'	4.32	1.54	1.45
3	1-J	7493	AMP	O4'-C4'	4.31	1.54	1.45
3	2-J	7493	AMP	O4'-C4'	4.31	1.54	1.45
3	3-J	7493	AMP	O4'-C4'	4.31	1.54	1.45
3	4-J	7493	AMP	O4'-C4'	4.31	1.54	1.45
3	5-J	7493	AMP	O4'-C4'	4.31	1.54	1.45
3	6-J	7493	AMP	O4'-C4'	4.31	1.54	1.45
3	7-J	7493	AMP	O4'-C4'	4.31	1.54	1.45
3	8-J	7493	AMP	O4'-C4'	4.31	1.54	1.45
3	9-J	7493	AMP	O4'-C4'	4.31	1.54	1.45
3	10-J	7493	AMP	O4'-C4'	4.31	1.54	1.45
3	1-B	7477	AMP	O4'-C4'	4.31	1.54	1.45
3	2-B	7477	AMP	O4'-C4'	4.31	1.54	1.45
3	3-B	7477	AMP	O4'-C4'	4.31	1.54	1.45
3	4-B	7477	AMP	O4'-C4'	4.31	1.54	1.45
3	5-B	7477	AMP	O4'-C4'	4.31	1.54	1.45
3	6-B	7477	AMP	O4'-C4'	4.31	1.54	1.45
3	7-B	7477	AMP	O4'-C4'	4.31	1.54	1.45
3	8-B	7477	AMP	O4'-C4'	4.31	1.54	1.45
3	9-B	7477	AMP	O4'-C4'	4.31	1.54	1.45
3	10-B	7477	AMP	O4'-C4'	4.31	1.54	1.45
3	1-A	7475	AMP	O4'-C4'	4.31	1.54	1.45
3	2-A	7475	AMP	O4'-C4'	4.31	1.54	1.45
3	3-A	7475	AMP	O4'-C4'	4.31	1.54	1.45
3	4-A	7475	AMP	O4'-C4'	4.31	1.54	1.45
3	5-A	7475	AMP	O4'-C4'	4.31	1.54	1.45
3	6-A	7475	AMP	O4'-C4'	4.31	1.54	1.45
3	7-A	7475	AMP	O4'-C4'	4.31	1.54	1.45
3	8-A	7475	AMP	O4'-C4'	4.31	1.54	1.45
3	9-A	7475	AMP	O4'-C4'	4.31	1.54	1.45
3	10-A	7475	AMP	O4'-C4'	4.31	1.54	1.45
3	1-O	7503	AMP	O4'-C4'	4.31	1.54	1.45
3	2-O	7503	AMP	O4'-C4'	4.31	1.54	1.45
3	3-O	7503	AMP	O4'-C4'	4.31	1.54	1.45
3	4-O	7503	AMP	O4'-C4'	4.31	1.54	1.45
3	5-O	7503	AMP	O4'-C4'	4.31	1.54	1.45
3	6-O	7503	AMP	O4'-C4'	4.31	1.54	1.45
3	7-O	7503	AMP	O4'-C4'	4.31	1.54	1.45
3	8-O	7503	AMP	O4'-C4'	4.31	1.54	1.45
3	9-O	7503	AMP	O4'-C4'	4.31	1.54	1.45
3	10-O	7503	AMP	O4'-C4'	4.31	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-L	7497	AMP	O4'-C4'	4.31	1.54	1.45
3	2-L	7497	AMP	O4'-C4'	4.31	1.54	1.45
3	3-L	7497	AMP	O4'-C4'	4.31	1.54	1.45
3	4-L	7497	AMP	O4'-C4'	4.31	1.54	1.45
3	5-L	7497	AMP	O4'-C4'	4.31	1.54	1.45
3	6-L	7497	AMP	O4'-C4'	4.31	1.54	1.45
3	7-L	7497	AMP	O4'-C4'	4.31	1.54	1.45
3	8-L	7497	AMP	O4'-C4'	4.31	1.54	1.45
3	9-L	7497	AMP	O4'-C4'	4.31	1.54	1.45
3	10-L	7497	AMP	O4'-C4'	4.31	1.54	1.45
3	1-G	7487	AMP	O4'-C4'	4.30	1.54	1.45
3	2-G	7487	AMP	O4'-C4'	4.30	1.54	1.45
3	3-G	7487	AMP	O4'-C4'	4.30	1.54	1.45
3	4-G	7487	AMP	O4'-C4'	4.30	1.54	1.45
3	5-G	7487	AMP	O4'-C4'	4.30	1.54	1.45
3	6-G	7487	AMP	O4'-C4'	4.30	1.54	1.45
3	7-G	7487	AMP	O4'-C4'	4.30	1.54	1.45
3	8-G	7487	AMP	O4'-C4'	4.30	1.54	1.45
3	9-G	7487	AMP	O4'-C4'	4.30	1.54	1.45
3	10-G	7487	AMP	O4'-C4'	4.30	1.54	1.45
3	1-K	7495	AMP	O4'-C4'	4.30	1.54	1.45
3	2-K	7495	AMP	O4'-C4'	4.30	1.54	1.45
3	3-K	7495	AMP	O4'-C4'	4.30	1.54	1.45
3	4-K	7495	AMP	O4'-C4'	4.30	1.54	1.45
3	5-K	7495	AMP	O4'-C4'	4.30	1.54	1.45
3	6-K	7495	AMP	O4'-C4'	4.30	1.54	1.45
3	7-K	7495	AMP	O4'-C4'	4.30	1.54	1.45
3	8-K	7495	AMP	O4'-C4'	4.30	1.54	1.45
3	9-K	7495	AMP	O4'-C4'	4.30	1.54	1.45
3	10-K	7495	AMP	O4'-C4'	4.30	1.54	1.45
3	1-D	7481	AMP	O4'-C4'	4.30	1.54	1.45
3	2-D	7481	AMP	O4'-C4'	4.30	1.54	1.45
3	3-D	7481	AMP	O4'-C4'	4.30	1.54	1.45
3	4-D	7481	AMP	O4'-C4'	4.30	1.54	1.45
3	5-D	7481	AMP	O4'-C4'	4.30	1.54	1.45
3	6-D	7481	AMP	O4'-C4'	4.30	1.54	1.45
3	7-D	7481	AMP	O4'-C4'	4.30	1.54	1.45
3	8-D	7481	AMP	O4'-C4'	4.30	1.54	1.45
3	9-D	7481	AMP	O4'-C4'	4.30	1.54	1.45
3	10-D	7481	AMP	O4'-C4'	4.30	1.54	1.45
3	1-U	7515	AMP	O4'-C4'	4.30	1.54	1.45
3	2-U	7515	AMP	O4'-C4'	4.30	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-U	7515	AMP	O4'-C4'	4.30	1.54	1.45
3	4-U	7515	AMP	O4'-C4'	4.30	1.54	1.45
3	5-U	7515	AMP	O4'-C4'	4.30	1.54	1.45
3	6-U	7515	AMP	O4'-C4'	4.30	1.54	1.45
3	7-U	7515	AMP	O4'-C4'	4.30	1.54	1.45
3	8-U	7515	AMP	O4'-C4'	4.30	1.54	1.45
3	9-U	7515	AMP	O4'-C4'	4.30	1.54	1.45
3	10-U	7515	AMP	O4'-C4'	4.30	1.54	1.45
3	1-E	7483	AMP	O4'-C4'	4.29	1.54	1.45
3	2-E	7483	AMP	O4'-C4'	4.29	1.54	1.45
3	3-E	7483	AMP	O4'-C4'	4.29	1.54	1.45
3	4-E	7483	AMP	O4'-C4'	4.29	1.54	1.45
3	5-E	7483	AMP	O4'-C4'	4.29	1.54	1.45
3	6-E	7483	AMP	O4'-C4'	4.29	1.54	1.45
3	7-E	7483	AMP	O4'-C4'	4.29	1.54	1.45
3	8-E	7483	AMP	O4'-C4'	4.29	1.54	1.45
3	9-E	7483	AMP	O4'-C4'	4.29	1.54	1.45
3	10-E	7483	AMP	O4'-C4'	4.29	1.54	1.45
3	1-R	7509	AMP	O4'-C4'	4.29	1.54	1.45
3	2-R	7509	AMP	O4'-C4'	4.29	1.54	1.45
3	3-R	7509	AMP	O4'-C4'	4.29	1.54	1.45
3	4-R	7509	AMP	O4'-C4'	4.29	1.54	1.45
3	5-R	7509	AMP	O4'-C4'	4.29	1.54	1.45
3	6-R	7509	AMP	O4'-C4'	4.29	1.54	1.45
3	7-R	7509	AMP	O4'-C4'	4.29	1.54	1.45
3	8-R	7509	AMP	O4'-C4'	4.29	1.54	1.45
3	9-R	7509	AMP	O4'-C4'	4.29	1.54	1.45
3	10-R	7509	AMP	O4'-C4'	4.29	1.54	1.45
3	1-W	7519	AMP	O4'-C4'	4.29	1.54	1.45
3	2-W	7519	AMP	O4'-C4'	4.29	1.54	1.45
3	3-W	7519	AMP	O4'-C4'	4.29	1.54	1.45
3	4-W	7519	AMP	O4'-C4'	4.29	1.54	1.45
3	5-W	7519	AMP	O4'-C4'	4.29	1.54	1.45
3	6-W	7519	AMP	O4'-C4'	4.29	1.54	1.45
3	7-W	7519	AMP	O4'-C4'	4.29	1.54	1.45
3	8-W	7519	AMP	O4'-C4'	4.29	1.54	1.45
3	9-W	7519	AMP	O4'-C4'	4.29	1.54	1.45
3	10-W	7519	AMP	O4'-C4'	4.29	1.54	1.45
3	1-N	7501	AMP	O4'-C4'	4.29	1.54	1.45
3	2-N	7501	AMP	O4'-C4'	4.29	1.54	1.45
3	3-N	7501	AMP	O4'-C4'	4.29	1.54	1.45
3	4-N	7501	AMP	O4'-C4'	4.29	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-N	7501	AMP	O4'-C4'	4.29	1.54	1.45
3	6-N	7501	AMP	O4'-C4'	4.29	1.54	1.45
3	7-N	7501	AMP	O4'-C4'	4.29	1.54	1.45
3	8-N	7501	AMP	O4'-C4'	4.29	1.54	1.45
3	9-N	7501	AMP	O4'-C4'	4.29	1.54	1.45
3	10-N	7501	AMP	O4'-C4'	4.29	1.54	1.45
3	1-T	7513	AMP	O4'-C4'	4.29	1.54	1.45
3	2-T	7513	AMP	O4'-C4'	4.29	1.54	1.45
3	3-T	7513	AMP	O4'-C4'	4.29	1.54	1.45
3	4-T	7513	AMP	O4'-C4'	4.29	1.54	1.45
3	5-T	7513	AMP	O4'-C4'	4.29	1.54	1.45
3	6-T	7513	AMP	O4'-C4'	4.29	1.54	1.45
3	7-T	7513	AMP	O4'-C4'	4.29	1.54	1.45
3	8-T	7513	AMP	O4'-C4'	4.29	1.54	1.45
3	9-T	7513	AMP	O4'-C4'	4.29	1.54	1.45
3	10-T	7513	AMP	O4'-C4'	4.29	1.54	1.45
3	1-P	7505	AMP	O4'-C4'	4.28	1.54	1.45
3	2-P	7505	AMP	O4'-C4'	4.28	1.54	1.45
3	3-P	7505	AMP	O4'-C4'	4.28	1.54	1.45
3	4-P	7505	AMP	O4'-C4'	4.28	1.54	1.45
3	5-P	7505	AMP	O4'-C4'	4.28	1.54	1.45
3	6-P	7505	AMP	O4'-C4'	4.28	1.54	1.45
3	7-P	7505	AMP	O4'-C4'	4.28	1.54	1.45
3	8-P	7505	AMP	O4'-C4'	4.28	1.54	1.45
3	9-P	7505	AMP	O4'-C4'	4.28	1.54	1.45
3	10-P	7505	AMP	O4'-C4'	4.28	1.54	1.45
3	1-C	7479	AMP	O4'-C4'	4.28	1.54	1.45
3	2-C	7479	AMP	O4'-C4'	4.28	1.54	1.45
3	3-C	7479	AMP	O4'-C4'	4.28	1.54	1.45
3	4-C	7479	AMP	O4'-C4'	4.28	1.54	1.45
3	5-C	7479	AMP	O4'-C4'	4.28	1.54	1.45
3	6-C	7479	AMP	O4'-C4'	4.28	1.54	1.45
3	7-C	7479	AMP	O4'-C4'	4.28	1.54	1.45
3	8-C	7479	AMP	O4'-C4'	4.28	1.54	1.45
3	9-C	7479	AMP	O4'-C4'	4.28	1.54	1.45
3	10-C	7479	AMP	O4'-C4'	4.28	1.54	1.45
4	1-D	7482	CIT	O3-C5	4.18	1.35	1.22
4	2-D	7482	CIT	O3-C5	4.18	1.35	1.22
4	3-D	7482	CIT	O3-C5	4.18	1.35	1.22
4	4-D	7482	CIT	O3-C5	4.18	1.35	1.22
4	5-D	7482	CIT	O3-C5	4.18	1.35	1.22
4	6-D	7482	CIT	O3-C5	4.18	1.35	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-D	7482	CIT	O3-C5	4.18	1.35	1.22
4	8-D	7482	CIT	O3-C5	4.18	1.35	1.22
4	9-D	7482	CIT	O3-C5	4.18	1.35	1.22
4	10-D	7482	CIT	O3-C5	4.18	1.35	1.22
4	1-M	7500	CIT	O3-C5	4.17	1.35	1.22
4	2-M	7500	CIT	O3-C5	4.17	1.35	1.22
4	3-M	7500	CIT	O3-C5	4.17	1.35	1.22
4	4-M	7500	CIT	O3-C5	4.17	1.35	1.22
4	5-M	7500	CIT	O3-C5	4.17	1.35	1.22
4	6-M	7500	CIT	O3-C5	4.17	1.35	1.22
4	7-M	7500	CIT	O3-C5	4.17	1.35	1.22
4	8-M	7500	CIT	O3-C5	4.17	1.35	1.22
4	9-M	7500	CIT	O3-C5	4.17	1.35	1.22
4	10-M	7500	CIT	O3-C5	4.17	1.35	1.22
4	1-X	7522	CIT	O3-C5	4.17	1.35	1.22
4	2-X	7522	CIT	O3-C5	4.17	1.35	1.22
4	3-X	7522	CIT	O3-C5	4.17	1.35	1.22
4	4-X	7522	CIT	O3-C5	4.17	1.35	1.22
4	5-X	7522	CIT	O3-C5	4.17	1.35	1.22
4	6-X	7522	CIT	O3-C5	4.17	1.35	1.22
4	7-X	7522	CIT	O3-C5	4.17	1.35	1.22
4	8-X	7522	CIT	O3-C5	4.17	1.35	1.22
4	9-X	7522	CIT	O3-C5	4.17	1.35	1.22
4	10-X	7522	CIT	O3-C5	4.17	1.35	1.22
4	1-O	7504	CIT	O3-C5	4.16	1.35	1.22
4	2-O	7504	CIT	O3-C5	4.16	1.35	1.22
4	3-O	7504	CIT	O3-C5	4.16	1.35	1.22
4	4-O	7504	CIT	O3-C5	4.16	1.35	1.22
4	5-O	7504	CIT	O3-C5	4.16	1.35	1.22
4	6-O	7504	CIT	O3-C5	4.16	1.35	1.22
4	7-O	7504	CIT	O3-C5	4.16	1.35	1.22
4	8-O	7504	CIT	O3-C5	4.16	1.35	1.22
4	9-O	7504	CIT	O3-C5	4.16	1.35	1.22
4	10-O	7504	CIT	O3-C5	4.16	1.35	1.22
4	1-K	7496	CIT	O3-C5	4.16	1.35	1.22
4	2-K	7496	CIT	O3-C5	4.16	1.35	1.22
4	3-K	7496	CIT	O3-C5	4.16	1.35	1.22
4	4-K	7496	CIT	O3-C5	4.16	1.35	1.22
4	5-K	7496	CIT	O3-C5	4.16	1.35	1.22
4	6-K	7496	CIT	O3-C5	4.16	1.35	1.22
4	7-K	7496	CIT	O3-C5	4.16	1.35	1.22
4	8-K	7496	CIT	O3-C5	4.16	1.35	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9-K	7496	CIT	O3-C5	4.16	1.35	1.22
4	10-K	7496	CIT	O3-C5	4.16	1.35	1.22
4	1-U	7516	CIT	O3-C5	4.16	1.35	1.22
4	2-U	7516	CIT	O3-C5	4.16	1.35	1.22
4	3-U	7516	CIT	O3-C5	4.16	1.35	1.22
4	4-U	7516	CIT	O3-C5	4.16	1.35	1.22
4	5-U	7516	CIT	O3-C5	4.16	1.35	1.22
4	6-U	7516	CIT	O3-C5	4.16	1.35	1.22
4	7-U	7516	CIT	O3-C5	4.16	1.35	1.22
4	8-U	7516	CIT	O3-C5	4.16	1.35	1.22
4	9-U	7516	CIT	O3-C5	4.16	1.35	1.22
4	10-U	7516	CIT	O3-C5	4.16	1.35	1.22
4	1-F	7486	CIT	O3-C5	4.16	1.35	1.22
4	2-F	7486	CIT	O3-C5	4.16	1.35	1.22
4	3-F	7486	CIT	O3-C5	4.16	1.35	1.22
4	4-F	7486	CIT	O3-C5	4.16	1.35	1.22
4	5-F	7486	CIT	O3-C5	4.16	1.35	1.22
4	6-F	7486	CIT	O3-C5	4.16	1.35	1.22
4	7-F	7486	CIT	O3-C5	4.16	1.35	1.22
4	8-F	7486	CIT	O3-C5	4.16	1.35	1.22
4	9-F	7486	CIT	O3-C5	4.16	1.35	1.22
4	10-F	7486	CIT	O3-C5	4.16	1.35	1.22
4	1-N	7502	CIT	O3-C5	4.16	1.35	1.22
4	2-N	7502	CIT	O3-C5	4.16	1.35	1.22
4	3-N	7502	CIT	O3-C5	4.16	1.35	1.22
4	4-N	7502	CIT	O3-C5	4.16	1.35	1.22
4	5-N	7502	CIT	O3-C5	4.16	1.35	1.22
4	6-N	7502	CIT	O3-C5	4.16	1.35	1.22
4	7-N	7502	CIT	O3-C5	4.16	1.35	1.22
4	8-N	7502	CIT	O3-C5	4.16	1.35	1.22
4	9-N	7502	CIT	O3-C5	4.16	1.35	1.22
4	10-N	7502	CIT	O3-C5	4.16	1.35	1.22
4	1-W	7520	CIT	O3-C5	4.16	1.35	1.22
4	2-W	7520	CIT	O3-C5	4.16	1.35	1.22
4	3-W	7520	CIT	O3-C5	4.16	1.35	1.22
4	4-W	7520	CIT	O3-C5	4.16	1.35	1.22
4	5-W	7520	CIT	O3-C5	4.16	1.35	1.22
4	6-W	7520	CIT	O3-C5	4.16	1.35	1.22
4	7-W	7520	CIT	O3-C5	4.16	1.35	1.22
4	8-W	7520	CIT	O3-C5	4.16	1.35	1.22
4	9-W	7520	CIT	O3-C5	4.16	1.35	1.22
4	10-W	7520	CIT	O3-C5	4.16	1.35	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-A	7476	CIT	O3-C5	4.15	1.35	1.22
4	2-A	7476	CIT	O3-C5	4.15	1.35	1.22
4	3-A	7476	CIT	O3-C5	4.15	1.35	1.22
4	4-A	7476	CIT	O3-C5	4.15	1.35	1.22
4	5-A	7476	CIT	O3-C5	4.15	1.35	1.22
4	6-A	7476	CIT	O3-C5	4.15	1.35	1.22
4	7-A	7476	CIT	O3-C5	4.15	1.35	1.22
4	8-A	7476	CIT	O3-C5	4.15	1.35	1.22
4	9-A	7476	CIT	O3-C5	4.15	1.35	1.22
4	10-A	7476	CIT	O3-C5	4.15	1.35	1.22
4	1-B	7478	CIT	O3-C5	4.15	1.35	1.22
4	2-B	7478	CIT	O3-C5	4.15	1.35	1.22
4	3-B	7478	CIT	O3-C5	4.15	1.35	1.22
4	4-B	7478	CIT	O3-C5	4.15	1.35	1.22
4	5-B	7478	CIT	O3-C5	4.15	1.35	1.22
4	6-B	7478	CIT	O3-C5	4.15	1.35	1.22
4	7-B	7478	CIT	O3-C5	4.15	1.35	1.22
4	8-B	7478	CIT	O3-C5	4.15	1.35	1.22
4	9-B	7478	CIT	O3-C5	4.15	1.35	1.22
4	10-B	7478	CIT	O3-C5	4.15	1.35	1.22
4	1-G	7488	CIT	O3-C5	4.15	1.35	1.22
4	2-G	7488	CIT	O3-C5	4.15	1.35	1.22
4	3-G	7488	CIT	O3-C5	4.15	1.35	1.22
4	4-G	7488	CIT	O3-C5	4.15	1.35	1.22
4	5-G	7488	CIT	O3-C5	4.15	1.35	1.22
4	6-G	7488	CIT	O3-C5	4.15	1.35	1.22
4	7-G	7488	CIT	O3-C5	4.15	1.35	1.22
4	8-G	7488	CIT	O3-C5	4.15	1.35	1.22
4	9-G	7488	CIT	O3-C5	4.15	1.35	1.22
4	10-G	7488	CIT	O3-C5	4.15	1.35	1.22
4	1-T	7514	CIT	O3-C5	4.15	1.35	1.22
4	2-T	7514	CIT	O3-C5	4.15	1.35	1.22
4	3-T	7514	CIT	O3-C5	4.15	1.35	1.22
4	4-T	7514	CIT	O3-C5	4.15	1.35	1.22
4	5-T	7514	CIT	O3-C5	4.15	1.35	1.22
4	6-T	7514	CIT	O3-C5	4.15	1.35	1.22
4	7-T	7514	CIT	O3-C5	4.15	1.35	1.22
4	8-T	7514	CIT	O3-C5	4.15	1.35	1.22
4	9-T	7514	CIT	O3-C5	4.15	1.35	1.22
4	10-T	7514	CIT	O3-C5	4.15	1.35	1.22
4	1-I	7492	CIT	O3-C5	4.15	1.35	1.22
4	2-I	7492	CIT	O3-C5	4.15	1.35	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-I	7492	CIT	O3-C5	4.15	1.35	1.22
4	4-I	7492	CIT	O3-C5	4.15	1.35	1.22
4	5-I	7492	CIT	O3-C5	4.15	1.35	1.22
4	6-I	7492	CIT	O3-C5	4.15	1.35	1.22
4	7-I	7492	CIT	O3-C5	4.15	1.35	1.22
4	8-I	7492	CIT	O3-C5	4.15	1.35	1.22
4	9-I	7492	CIT	O3-C5	4.15	1.35	1.22
4	10-I	7492	CIT	O3-C5	4.15	1.35	1.22
4	1-E	7484	CIT	O3-C5	4.15	1.35	1.22
4	2-E	7484	CIT	O3-C5	4.15	1.35	1.22
4	3-E	7484	CIT	O3-C5	4.15	1.35	1.22
4	4-E	7484	CIT	O3-C5	4.15	1.35	1.22
4	5-E	7484	CIT	O3-C5	4.15	1.35	1.22
4	6-E	7484	CIT	O3-C5	4.15	1.35	1.22
4	7-E	7484	CIT	O3-C5	4.15	1.35	1.22
4	8-E	7484	CIT	O3-C5	4.15	1.35	1.22
4	9-E	7484	CIT	O3-C5	4.15	1.35	1.22
4	10-E	7484	CIT	O3-C5	4.15	1.35	1.22
4	1-H	7490	CIT	O3-C5	4.15	1.35	1.22
4	2-H	7490	CIT	O3-C5	4.15	1.35	1.22
4	3-H	7490	CIT	O3-C5	4.15	1.35	1.22
4	4-H	7490	CIT	O3-C5	4.15	1.35	1.22
4	5-H	7490	CIT	O3-C5	4.15	1.35	1.22
4	6-H	7490	CIT	O3-C5	4.15	1.35	1.22
4	7-H	7490	CIT	O3-C5	4.15	1.35	1.22
4	8-H	7490	CIT	O3-C5	4.15	1.35	1.22
4	9-H	7490	CIT	O3-C5	4.15	1.35	1.22
4	10-H	7490	CIT	O3-C5	4.15	1.35	1.22
4	1-V	7518	CIT	O3-C5	4.15	1.35	1.22
4	2-V	7518	CIT	O3-C5	4.15	1.35	1.22
4	3-V	7518	CIT	O3-C5	4.15	1.35	1.22
4	4-V	7518	CIT	O3-C5	4.15	1.35	1.22
4	5-V	7518	CIT	O3-C5	4.15	1.35	1.22
4	6-V	7518	CIT	O3-C5	4.15	1.35	1.22
4	7-V	7518	CIT	O3-C5	4.15	1.35	1.22
4	8-V	7518	CIT	O3-C5	4.15	1.35	1.22
4	9-V	7518	CIT	O3-C5	4.15	1.35	1.22
4	10-V	7518	CIT	O3-C5	4.15	1.35	1.22
4	1-P	7506	CIT	O3-C5	4.15	1.35	1.22
4	2-P	7506	CIT	O3-C5	4.15	1.35	1.22
4	3-P	7506	CIT	O3-C5	4.15	1.35	1.22
4	4-P	7506	CIT	O3-C5	4.15	1.35	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5-P	7506	CIT	O3-C5	4.15	1.35	1.22
4	6-P	7506	CIT	O3-C5	4.15	1.35	1.22
4	7-P	7506	CIT	O3-C5	4.15	1.35	1.22
4	8-P	7506	CIT	O3-C5	4.15	1.35	1.22
4	9-P	7506	CIT	O3-C5	4.15	1.35	1.22
4	10-P	7506	CIT	O3-C5	4.15	1.35	1.22
4	1-S	7512	CIT	O3-C5	4.14	1.35	1.22
4	2-S	7512	CIT	O3-C5	4.14	1.35	1.22
4	3-S	7512	CIT	O3-C5	4.14	1.35	1.22
4	4-S	7512	CIT	O3-C5	4.14	1.35	1.22
4	5-S	7512	CIT	O3-C5	4.14	1.35	1.22
4	6-S	7512	CIT	O3-C5	4.14	1.35	1.22
4	7-S	7512	CIT	O3-C5	4.14	1.35	1.22
4	8-S	7512	CIT	O3-C5	4.14	1.35	1.22
4	9-S	7512	CIT	O3-C5	4.14	1.35	1.22
4	10-S	7512	CIT	O3-C5	4.14	1.35	1.22
4	1-J	7494	CIT	O3-C5	4.14	1.35	1.22
4	2-J	7494	CIT	O3-C5	4.14	1.35	1.22
4	3-J	7494	CIT	O3-C5	4.14	1.35	1.22
4	4-J	7494	CIT	O3-C5	4.14	1.35	1.22
4	5-J	7494	CIT	O3-C5	4.14	1.35	1.22
4	6-J	7494	CIT	O3-C5	4.14	1.35	1.22
4	7-J	7494	CIT	O3-C5	4.14	1.35	1.22
4	8-J	7494	CIT	O3-C5	4.14	1.35	1.22
4	9-J	7494	CIT	O3-C5	4.14	1.35	1.22
4	10-J	7494	CIT	O3-C5	4.14	1.35	1.22
4	1-R	7510	CIT	O3-C5	4.14	1.35	1.22
4	2-R	7510	CIT	O3-C5	4.14	1.35	1.22
4	3-R	7510	CIT	O3-C5	4.14	1.35	1.22
4	4-R	7510	CIT	O3-C5	4.14	1.35	1.22
4	5-R	7510	CIT	O3-C5	4.14	1.35	1.22
4	6-R	7510	CIT	O3-C5	4.14	1.35	1.22
4	7-R	7510	CIT	O3-C5	4.14	1.35	1.22
4	8-R	7510	CIT	O3-C5	4.14	1.35	1.22
4	9-R	7510	CIT	O3-C5	4.14	1.35	1.22
4	10-R	7510	CIT	O3-C5	4.14	1.35	1.22
4	1-L	7498	CIT	O3-C5	4.14	1.35	1.22
4	2-L	7498	CIT	O3-C5	4.14	1.35	1.22
4	3-L	7498	CIT	O3-C5	4.14	1.35	1.22
4	4-L	7498	CIT	O3-C5	4.14	1.35	1.22
4	5-L	7498	CIT	O3-C5	4.14	1.35	1.22
4	6-L	7498	CIT	O3-C5	4.14	1.35	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-L	7498	CIT	O3-C5	4.14	1.35	1.22
4	8-L	7498	CIT	O3-C5	4.14	1.35	1.22
4	9-L	7498	CIT	O3-C5	4.14	1.35	1.22
4	10-L	7498	CIT	O3-C5	4.14	1.35	1.22
4	1-Q	7508	CIT	O3-C5	4.14	1.35	1.22
4	2-Q	7508	CIT	O3-C5	4.14	1.35	1.22
4	3-Q	7508	CIT	O3-C5	4.14	1.35	1.22
4	4-Q	7508	CIT	O3-C5	4.14	1.35	1.22
4	5-Q	7508	CIT	O3-C5	4.14	1.35	1.22
4	6-Q	7508	CIT	O3-C5	4.14	1.35	1.22
4	7-Q	7508	CIT	O3-C5	4.14	1.35	1.22
4	8-Q	7508	CIT	O3-C5	4.14	1.35	1.22
4	9-Q	7508	CIT	O3-C5	4.14	1.35	1.22
4	10-Q	7508	CIT	O3-C5	4.14	1.35	1.22
3	1-R	7509	AMP	C3'-C4'	-4.13	1.42	1.53
3	2-R	7509	AMP	C3'-C4'	-4.13	1.42	1.53
3	3-R	7509	AMP	C3'-C4'	-4.13	1.42	1.53
3	4-R	7509	AMP	C3'-C4'	-4.13	1.42	1.53
3	5-R	7509	AMP	C3'-C4'	-4.13	1.42	1.53
3	6-R	7509	AMP	C3'-C4'	-4.13	1.42	1.53
3	7-R	7509	AMP	C3'-C4'	-4.13	1.42	1.53
3	8-R	7509	AMP	C3'-C4'	-4.13	1.42	1.53
3	9-R	7509	AMP	C3'-C4'	-4.13	1.42	1.53
3	10-R	7509	AMP	C3'-C4'	-4.13	1.42	1.53
4	1-C	7480	CIT	O3-C5	4.12	1.35	1.22
4	2-C	7480	CIT	O3-C5	4.12	1.35	1.22
4	3-C	7480	CIT	O3-C5	4.12	1.35	1.22
4	4-C	7480	CIT	O3-C5	4.12	1.35	1.22
4	5-C	7480	CIT	O3-C5	4.12	1.35	1.22
4	6-C	7480	CIT	O3-C5	4.12	1.35	1.22
4	7-C	7480	CIT	O3-C5	4.12	1.35	1.22
4	8-C	7480	CIT	O3-C5	4.12	1.35	1.22
4	9-C	7480	CIT	O3-C5	4.12	1.35	1.22
4	10-C	7480	CIT	O3-C5	4.12	1.35	1.22
3	1-M	7499	AMP	C3'-C4'	-4.12	1.42	1.53
3	2-M	7499	AMP	C3'-C4'	-4.12	1.42	1.53
3	3-M	7499	AMP	C3'-C4'	-4.12	1.42	1.53
3	4-M	7499	AMP	C3'-C4'	-4.12	1.42	1.53
3	5-M	7499	AMP	C3'-C4'	-4.12	1.42	1.53
3	6-M	7499	AMP	C3'-C4'	-4.12	1.42	1.53
3	7-M	7499	AMP	C3'-C4'	-4.12	1.42	1.53
3	8-M	7499	AMP	C3'-C4'	-4.12	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-M	7499	AMP	C3'-C4'	-4.12	1.42	1.53
3	10-M	7499	AMP	C3'-C4'	-4.12	1.42	1.53
3	1-H	7489	AMP	C3'-C4'	-4.11	1.42	1.53
3	2-H	7489	AMP	C3'-C4'	-4.11	1.42	1.53
3	3-H	7489	AMP	C3'-C4'	-4.11	1.42	1.53
3	4-H	7489	AMP	C3'-C4'	-4.11	1.42	1.53
3	5-H	7489	AMP	C3'-C4'	-4.11	1.42	1.53
3	6-H	7489	AMP	C3'-C4'	-4.11	1.42	1.53
3	7-H	7489	AMP	C3'-C4'	-4.11	1.42	1.53
3	8-H	7489	AMP	C3'-C4'	-4.11	1.42	1.53
3	9-H	7489	AMP	C3'-C4'	-4.11	1.42	1.53
3	10-H	7489	AMP	C3'-C4'	-4.11	1.42	1.53
3	1-K	7495	AMP	C3'-C4'	-4.11	1.42	1.53
3	2-K	7495	AMP	C3'-C4'	-4.11	1.42	1.53
3	3-K	7495	AMP	C3'-C4'	-4.11	1.42	1.53
3	4-K	7495	AMP	C3'-C4'	-4.11	1.42	1.53
3	5-K	7495	AMP	C3'-C4'	-4.11	1.42	1.53
3	6-K	7495	AMP	C3'-C4'	-4.11	1.42	1.53
3	7-K	7495	AMP	C3'-C4'	-4.11	1.42	1.53
3	8-K	7495	AMP	C3'-C4'	-4.11	1.42	1.53
3	9-K	7495	AMP	C3'-C4'	-4.11	1.42	1.53
3	10-K	7495	AMP	C3'-C4'	-4.11	1.42	1.53
3	1-U	7515	AMP	C3'-C4'	-4.11	1.42	1.53
3	2-U	7515	AMP	C3'-C4'	-4.11	1.42	1.53
3	3-U	7515	AMP	C3'-C4'	-4.11	1.42	1.53
3	4-U	7515	AMP	C3'-C4'	-4.11	1.42	1.53
3	5-U	7515	AMP	C3'-C4'	-4.11	1.42	1.53
3	6-U	7515	AMP	C3'-C4'	-4.11	1.42	1.53
3	7-U	7515	AMP	C3'-C4'	-4.11	1.42	1.53
3	8-U	7515	AMP	C3'-C4'	-4.11	1.42	1.53
3	9-U	7515	AMP	C3'-C4'	-4.11	1.42	1.53
3	10-U	7515	AMP	C3'-C4'	-4.11	1.42	1.53
3	1-W	7519	AMP	C3'-C4'	-4.11	1.42	1.53
3	2-W	7519	AMP	C3'-C4'	-4.11	1.42	1.53
3	3-W	7519	AMP	C3'-C4'	-4.11	1.42	1.53
3	4-W	7519	AMP	C3'-C4'	-4.11	1.42	1.53
3	5-W	7519	AMP	C3'-C4'	-4.11	1.42	1.53
3	6-W	7519	AMP	C3'-C4'	-4.11	1.42	1.53
3	7-W	7519	AMP	C3'-C4'	-4.11	1.42	1.53
3	8-W	7519	AMP	C3'-C4'	-4.11	1.42	1.53
3	9-W	7519	AMP	C3'-C4'	-4.11	1.42	1.53
3	10-W	7519	AMP	C3'-C4'	-4.11	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-F	7485	AMP	C2-N3	4.10	1.41	1.33
3	2-F	7485	AMP	C2-N3	4.10	1.41	1.33
3	3-F	7485	AMP	C2-N3	4.10	1.41	1.33
3	4-F	7485	AMP	C2-N3	4.10	1.41	1.33
3	5-F	7485	AMP	C2-N3	4.10	1.41	1.33
3	6-F	7485	AMP	C2-N3	4.10	1.41	1.33
3	7-F	7485	AMP	C2-N3	4.10	1.41	1.33
3	8-F	7485	AMP	C2-N3	4.10	1.41	1.33
3	9-F	7485	AMP	C2-N3	4.10	1.41	1.33
3	10-F	7485	AMP	C2-N3	4.10	1.41	1.33
3	1-R	7509	AMP	C2-N3	4.09	1.41	1.33
3	2-R	7509	AMP	C2-N3	4.09	1.41	1.33
3	3-R	7509	AMP	C2-N3	4.09	1.41	1.33
3	4-R	7509	AMP	C2-N3	4.09	1.41	1.33
3	5-R	7509	AMP	C2-N3	4.09	1.41	1.33
3	6-R	7509	AMP	C2-N3	4.09	1.41	1.33
3	7-R	7509	AMP	C2-N3	4.09	1.41	1.33
3	8-R	7509	AMP	C2-N3	4.09	1.41	1.33
3	9-R	7509	AMP	C2-N3	4.09	1.41	1.33
3	10-R	7509	AMP	C2-N3	4.09	1.41	1.33
3	1-N	7501	AMP	C3'-C4'	-4.09	1.42	1.53
3	2-N	7501	AMP	C3'-C4'	-4.09	1.42	1.53
3	3-N	7501	AMP	C3'-C4'	-4.09	1.42	1.53
3	4-N	7501	AMP	C3'-C4'	-4.09	1.42	1.53
3	5-N	7501	AMP	C3'-C4'	-4.09	1.42	1.53
3	6-N	7501	AMP	C3'-C4'	-4.09	1.42	1.53
3	7-N	7501	AMP	C3'-C4'	-4.09	1.42	1.53
3	8-N	7501	AMP	C3'-C4'	-4.09	1.42	1.53
3	9-N	7501	AMP	C3'-C4'	-4.09	1.42	1.53
3	10-N	7501	AMP	C3'-C4'	-4.09	1.42	1.53
3	1-C	7479	AMP	C2-N3	4.09	1.41	1.33
3	2-C	7479	AMP	C2-N3	4.09	1.41	1.33
3	3-C	7479	AMP	C2-N3	4.09	1.41	1.33
3	4-C	7479	AMP	C2-N3	4.09	1.41	1.33
3	5-C	7479	AMP	C2-N3	4.09	1.41	1.33
3	6-C	7479	AMP	C2-N3	4.09	1.41	1.33
3	7-C	7479	AMP	C2-N3	4.09	1.41	1.33
3	8-C	7479	AMP	C2-N3	4.09	1.41	1.33
3	9-C	7479	AMP	C2-N3	4.09	1.41	1.33
3	10-C	7479	AMP	C2-N3	4.09	1.41	1.33
3	1-I	7491	AMP	C3'-C4'	-4.09	1.42	1.53
3	2-I	7491	AMP	C3'-C4'	-4.09	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-I	7491	AMP	C3'-C4'	-4.09	1.42	1.53
3	4-I	7491	AMP	C3'-C4'	-4.09	1.42	1.53
3	5-I	7491	AMP	C3'-C4'	-4.09	1.42	1.53
3	6-I	7491	AMP	C3'-C4'	-4.09	1.42	1.53
3	7-I	7491	AMP	C3'-C4'	-4.09	1.42	1.53
3	8-I	7491	AMP	C3'-C4'	-4.09	1.42	1.53
3	9-I	7491	AMP	C3'-C4'	-4.09	1.42	1.53
3	10-I	7491	AMP	C3'-C4'	-4.09	1.42	1.53
3	1-O	7503	AMP	C3'-C4'	-4.09	1.42	1.53
3	2-O	7503	AMP	C3'-C4'	-4.09	1.42	1.53
3	3-O	7503	AMP	C3'-C4'	-4.09	1.42	1.53
3	4-O	7503	AMP	C3'-C4'	-4.09	1.42	1.53
3	5-O	7503	AMP	C3'-C4'	-4.09	1.42	1.53
3	6-O	7503	AMP	C3'-C4'	-4.09	1.42	1.53
3	7-O	7503	AMP	C3'-C4'	-4.09	1.42	1.53
3	8-O	7503	AMP	C3'-C4'	-4.09	1.42	1.53
3	9-O	7503	AMP	C3'-C4'	-4.09	1.42	1.53
3	10-O	7503	AMP	C3'-C4'	-4.09	1.42	1.53
3	1-P	7505	AMP	C3'-C4'	-4.09	1.42	1.53
3	2-P	7505	AMP	C3'-C4'	-4.09	1.42	1.53
3	3-P	7505	AMP	C3'-C4'	-4.09	1.42	1.53
3	4-P	7505	AMP	C3'-C4'	-4.09	1.42	1.53
3	5-P	7505	AMP	C3'-C4'	-4.09	1.42	1.53
3	6-P	7505	AMP	C3'-C4'	-4.09	1.42	1.53
3	7-P	7505	AMP	C3'-C4'	-4.09	1.42	1.53
3	8-P	7505	AMP	C3'-C4'	-4.09	1.42	1.53
3	9-P	7505	AMP	C3'-C4'	-4.09	1.42	1.53
3	10-P	7505	AMP	C3'-C4'	-4.09	1.42	1.53
3	1-E	7483	AMP	C3'-C4'	-4.09	1.42	1.53
3	2-E	7483	AMP	C3'-C4'	-4.09	1.42	1.53
3	3-E	7483	AMP	C3'-C4'	-4.09	1.42	1.53
3	4-E	7483	AMP	C3'-C4'	-4.09	1.42	1.53
3	5-E	7483	AMP	C3'-C4'	-4.09	1.42	1.53
3	6-E	7483	AMP	C3'-C4'	-4.09	1.42	1.53
3	7-E	7483	AMP	C3'-C4'	-4.09	1.42	1.53
3	8-E	7483	AMP	C3'-C4'	-4.09	1.42	1.53
3	9-E	7483	AMP	C3'-C4'	-4.09	1.42	1.53
3	10-E	7483	AMP	C3'-C4'	-4.09	1.42	1.53
3	1-D	7481	AMP	C3'-C4'	-4.09	1.42	1.53
3	2-D	7481	AMP	C3'-C4'	-4.09	1.42	1.53
3	3-D	7481	AMP	C3'-C4'	-4.09	1.42	1.53
3	4-D	7481	AMP	C3'-C4'	-4.09	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-D	7481	AMP	C3'-C4'	-4.09	1.42	1.53
3	6-D	7481	AMP	C3'-C4'	-4.09	1.42	1.53
3	7-D	7481	AMP	C3'-C4'	-4.09	1.42	1.53
3	8-D	7481	AMP	C3'-C4'	-4.09	1.42	1.53
3	9-D	7481	AMP	C3'-C4'	-4.09	1.42	1.53
3	10-D	7481	AMP	C3'-C4'	-4.09	1.42	1.53
3	1-A	7475	AMP	C3'-C4'	-4.09	1.42	1.53
3	2-A	7475	AMP	C3'-C4'	-4.09	1.42	1.53
3	3-A	7475	AMP	C3'-C4'	-4.09	1.42	1.53
3	4-A	7475	AMP	C3'-C4'	-4.09	1.42	1.53
3	5-A	7475	AMP	C3'-C4'	-4.09	1.42	1.53
3	6-A	7475	AMP	C3'-C4'	-4.09	1.42	1.53
3	7-A	7475	AMP	C3'-C4'	-4.09	1.42	1.53
3	8-A	7475	AMP	C3'-C4'	-4.09	1.42	1.53
3	9-A	7475	AMP	C3'-C4'	-4.09	1.42	1.53
3	10-A	7475	AMP	C3'-C4'	-4.09	1.42	1.53
3	1-S	7511	AMP	C3'-C4'	-4.08	1.42	1.53
3	2-S	7511	AMP	C3'-C4'	-4.08	1.42	1.53
3	3-S	7511	AMP	C3'-C4'	-4.08	1.42	1.53
3	4-S	7511	AMP	C3'-C4'	-4.08	1.42	1.53
3	5-S	7511	AMP	C3'-C4'	-4.08	1.42	1.53
3	6-S	7511	AMP	C3'-C4'	-4.08	1.42	1.53
3	7-S	7511	AMP	C3'-C4'	-4.08	1.42	1.53
3	8-S	7511	AMP	C3'-C4'	-4.08	1.42	1.53
3	9-S	7511	AMP	C3'-C4'	-4.08	1.42	1.53
3	10-S	7511	AMP	C3'-C4'	-4.08	1.42	1.53
3	1-F	7485	AMP	C3'-C4'	-4.08	1.42	1.53
3	2-F	7485	AMP	C3'-C4'	-4.08	1.42	1.53
3	3-F	7485	AMP	C3'-C4'	-4.08	1.42	1.53
3	4-F	7485	AMP	C3'-C4'	-4.08	1.42	1.53
3	5-F	7485	AMP	C3'-C4'	-4.08	1.42	1.53
3	6-F	7485	AMP	C3'-C4'	-4.08	1.42	1.53
3	7-F	7485	AMP	C3'-C4'	-4.08	1.42	1.53
3	8-F	7485	AMP	C3'-C4'	-4.08	1.42	1.53
3	9-F	7485	AMP	C3'-C4'	-4.08	1.42	1.53
3	10-F	7485	AMP	C3'-C4'	-4.08	1.42	1.53
3	1-Q	7507	AMP	C3'-C4'	-4.08	1.42	1.53
3	2-Q	7507	AMP	C3'-C4'	-4.08	1.42	1.53
3	3-Q	7507	AMP	C3'-C4'	-4.08	1.42	1.53
3	4-Q	7507	AMP	C3'-C4'	-4.08	1.42	1.53
3	5-Q	7507	AMP	C3'-C4'	-4.08	1.42	1.53
3	6-Q	7507	AMP	C3'-C4'	-4.08	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-Q	7507	AMP	C3'-C4'	-4.08	1.42	1.53
3	8-Q	7507	AMP	C3'-C4'	-4.08	1.42	1.53
3	9-Q	7507	AMP	C3'-C4'	-4.08	1.42	1.53
3	10-Q	7507	AMP	C3'-C4'	-4.08	1.42	1.53
3	1-U	7515	AMP	C2-N3	4.08	1.41	1.33
3	2-U	7515	AMP	C2-N3	4.08	1.41	1.33
3	3-U	7515	AMP	C2-N3	4.08	1.41	1.33
3	4-U	7515	AMP	C2-N3	4.08	1.41	1.33
3	5-U	7515	AMP	C2-N3	4.08	1.41	1.33
3	6-U	7515	AMP	C2-N3	4.08	1.41	1.33
3	7-U	7515	AMP	C2-N3	4.08	1.41	1.33
3	8-U	7515	AMP	C2-N3	4.08	1.41	1.33
3	9-U	7515	AMP	C2-N3	4.08	1.41	1.33
3	10-U	7515	AMP	C2-N3	4.08	1.41	1.33
3	1-T	7513	AMP	C3'-C4'	-4.08	1.42	1.53
3	2-T	7513	AMP	C3'-C4'	-4.08	1.42	1.53
3	3-T	7513	AMP	C3'-C4'	-4.08	1.42	1.53
3	4-T	7513	AMP	C3'-C4'	-4.08	1.42	1.53
3	5-T	7513	AMP	C3'-C4'	-4.08	1.42	1.53
3	6-T	7513	AMP	C3'-C4'	-4.08	1.42	1.53
3	7-T	7513	AMP	C3'-C4'	-4.08	1.42	1.53
3	8-T	7513	AMP	C3'-C4'	-4.08	1.42	1.53
3	9-T	7513	AMP	C3'-C4'	-4.08	1.42	1.53
3	10-T	7513	AMP	C3'-C4'	-4.08	1.42	1.53
3	1-D	7481	AMP	C2-N3	4.08	1.41	1.33
3	2-D	7481	AMP	C2-N3	4.08	1.41	1.33
3	3-D	7481	AMP	C2-N3	4.08	1.41	1.33
3	4-D	7481	AMP	C2-N3	4.08	1.41	1.33
3	5-D	7481	AMP	C2-N3	4.08	1.41	1.33
3	6-D	7481	AMP	C2-N3	4.08	1.41	1.33
3	7-D	7481	AMP	C2-N3	4.08	1.41	1.33
3	8-D	7481	AMP	C2-N3	4.08	1.41	1.33
3	9-D	7481	AMP	C2-N3	4.08	1.41	1.33
3	10-D	7481	AMP	C2-N3	4.08	1.41	1.33
3	1-C	7479	AMP	C3'-C4'	-4.08	1.42	1.53
3	2-C	7479	AMP	C3'-C4'	-4.08	1.42	1.53
3	3-C	7479	AMP	C3'-C4'	-4.08	1.42	1.53
3	4-C	7479	AMP	C3'-C4'	-4.08	1.42	1.53
3	5-C	7479	AMP	C3'-C4'	-4.08	1.42	1.53
3	6-C	7479	AMP	C3'-C4'	-4.08	1.42	1.53
3	7-C	7479	AMP	C3'-C4'	-4.08	1.42	1.53
3	8-C	7479	AMP	C3'-C4'	-4.08	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-C	7479	AMP	C3'-C4'	-4.08	1.42	1.53
3	10-C	7479	AMP	C3'-C4'	-4.08	1.42	1.53
3	1-X	7521	AMP	C2-N3	4.08	1.41	1.33
3	2-X	7521	AMP	C2-N3	4.08	1.41	1.33
3	3-X	7521	AMP	C2-N3	4.08	1.41	1.33
3	4-X	7521	AMP	C2-N3	4.08	1.41	1.33
3	5-X	7521	AMP	C2-N3	4.08	1.41	1.33
3	6-X	7521	AMP	C2-N3	4.08	1.41	1.33
3	7-X	7521	AMP	C2-N3	4.08	1.41	1.33
3	8-X	7521	AMP	C2-N3	4.08	1.41	1.33
3	9-X	7521	AMP	C2-N3	4.08	1.41	1.33
3	10-X	7521	AMP	C2-N3	4.08	1.41	1.33
3	1-T	7513	AMP	C2-N3	4.08	1.41	1.33
3	2-T	7513	AMP	C2-N3	4.08	1.41	1.33
3	3-T	7513	AMP	C2-N3	4.08	1.41	1.33
3	4-T	7513	AMP	C2-N3	4.08	1.41	1.33
3	5-T	7513	AMP	C2-N3	4.08	1.41	1.33
3	6-T	7513	AMP	C2-N3	4.08	1.41	1.33
3	7-T	7513	AMP	C2-N3	4.08	1.41	1.33
3	8-T	7513	AMP	C2-N3	4.08	1.41	1.33
3	9-T	7513	AMP	C2-N3	4.08	1.41	1.33
3	10-T	7513	AMP	C2-N3	4.08	1.41	1.33
3	1-L	7497	AMP	C3'-C4'	-4.08	1.42	1.53
3	2-L	7497	AMP	C3'-C4'	-4.08	1.42	1.53
3	3-L	7497	AMP	C3'-C4'	-4.08	1.42	1.53
3	4-L	7497	AMP	C3'-C4'	-4.08	1.42	1.53
3	5-L	7497	AMP	C3'-C4'	-4.08	1.42	1.53
3	6-L	7497	AMP	C3'-C4'	-4.08	1.42	1.53
3	7-L	7497	AMP	C3'-C4'	-4.08	1.42	1.53
3	8-L	7497	AMP	C3'-C4'	-4.08	1.42	1.53
3	9-L	7497	AMP	C3'-C4'	-4.08	1.42	1.53
3	10-L	7497	AMP	C3'-C4'	-4.08	1.42	1.53
3	1-K	7495	AMP	C2-N3	4.08	1.41	1.33
3	2-K	7495	AMP	C2-N3	4.08	1.41	1.33
3	3-K	7495	AMP	C2-N3	4.08	1.41	1.33
3	4-K	7495	AMP	C2-N3	4.08	1.41	1.33
3	5-K	7495	AMP	C2-N3	4.08	1.41	1.33
3	6-K	7495	AMP	C2-N3	4.08	1.41	1.33
3	7-K	7495	AMP	C2-N3	4.08	1.41	1.33
3	8-K	7495	AMP	C2-N3	4.08	1.41	1.33
3	9-K	7495	AMP	C2-N3	4.08	1.41	1.33
3	10-K	7495	AMP	C2-N3	4.08	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-X	7521	AMP	C3'-C4'	-4.08	1.42	1.53
3	2-X	7521	AMP	C3'-C4'	-4.08	1.42	1.53
3	3-X	7521	AMP	C3'-C4'	-4.08	1.42	1.53
3	4-X	7521	AMP	C3'-C4'	-4.08	1.42	1.53
3	5-X	7521	AMP	C3'-C4'	-4.08	1.42	1.53
3	6-X	7521	AMP	C3'-C4'	-4.08	1.42	1.53
3	7-X	7521	AMP	C3'-C4'	-4.08	1.42	1.53
3	8-X	7521	AMP	C3'-C4'	-4.08	1.42	1.53
3	9-X	7521	AMP	C3'-C4'	-4.08	1.42	1.53
3	10-X	7521	AMP	C3'-C4'	-4.08	1.42	1.53
3	1-V	7517	AMP	C3'-C4'	-4.08	1.42	1.53
3	2-V	7517	AMP	C3'-C4'	-4.08	1.42	1.53
3	3-V	7517	AMP	C3'-C4'	-4.08	1.42	1.53
3	4-V	7517	AMP	C3'-C4'	-4.08	1.42	1.53
3	5-V	7517	AMP	C3'-C4'	-4.08	1.42	1.53
3	6-V	7517	AMP	C3'-C4'	-4.08	1.42	1.53
3	7-V	7517	AMP	C3'-C4'	-4.08	1.42	1.53
3	8-V	7517	AMP	C3'-C4'	-4.08	1.42	1.53
3	9-V	7517	AMP	C3'-C4'	-4.08	1.42	1.53
3	10-V	7517	AMP	C3'-C4'	-4.08	1.42	1.53
3	1-J	7493	AMP	C3'-C4'	-4.07	1.42	1.53
3	2-J	7493	AMP	C3'-C4'	-4.07	1.42	1.53
3	3-J	7493	AMP	C3'-C4'	-4.07	1.42	1.53
3	4-J	7493	AMP	C3'-C4'	-4.07	1.42	1.53
3	5-J	7493	AMP	C3'-C4'	-4.07	1.42	1.53
3	6-J	7493	AMP	C3'-C4'	-4.07	1.42	1.53
3	7-J	7493	AMP	C3'-C4'	-4.07	1.42	1.53
3	8-J	7493	AMP	C3'-C4'	-4.07	1.42	1.53
3	9-J	7493	AMP	C3'-C4'	-4.07	1.42	1.53
3	10-J	7493	AMP	C3'-C4'	-4.07	1.42	1.53
3	1-I	7491	AMP	C2-N3	4.07	1.41	1.33
3	2-I	7491	AMP	C2-N3	4.07	1.41	1.33
3	3-I	7491	AMP	C2-N3	4.07	1.41	1.33
3	4-I	7491	AMP	C2-N3	4.07	1.41	1.33
3	5-I	7491	AMP	C2-N3	4.07	1.41	1.33
3	6-I	7491	AMP	C2-N3	4.07	1.41	1.33
3	7-I	7491	AMP	C2-N3	4.07	1.41	1.33
3	8-I	7491	AMP	C2-N3	4.07	1.41	1.33
3	9-I	7491	AMP	C2-N3	4.07	1.41	1.33
3	10-I	7491	AMP	C2-N3	4.07	1.41	1.33
3	1-J	7493	AMP	C2-N3	4.07	1.41	1.33
3	2-J	7493	AMP	C2-N3	4.07	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-J	7493	AMP	C2-N3	4.07	1.41	1.33
3	4-J	7493	AMP	C2-N3	4.07	1.41	1.33
3	5-J	7493	AMP	C2-N3	4.07	1.41	1.33
3	6-J	7493	AMP	C2-N3	4.07	1.41	1.33
3	7-J	7493	AMP	C2-N3	4.07	1.41	1.33
3	8-J	7493	AMP	C2-N3	4.07	1.41	1.33
3	9-J	7493	AMP	C2-N3	4.07	1.41	1.33
3	10-J	7493	AMP	C2-N3	4.07	1.41	1.33
3	1-W	7519	AMP	C2-N3	4.07	1.41	1.33
3	2-W	7519	AMP	C2-N3	4.07	1.41	1.33
3	3-W	7519	AMP	C2-N3	4.07	1.41	1.33
3	4-W	7519	AMP	C2-N3	4.07	1.41	1.33
3	5-W	7519	AMP	C2-N3	4.07	1.41	1.33
3	6-W	7519	AMP	C2-N3	4.07	1.41	1.33
3	7-W	7519	AMP	C2-N3	4.07	1.41	1.33
3	8-W	7519	AMP	C2-N3	4.07	1.41	1.33
3	9-W	7519	AMP	C2-N3	4.07	1.41	1.33
3	10-W	7519	AMP	C2-N3	4.07	1.41	1.33
3	1-B	7477	AMP	C3'-C4'	-4.07	1.42	1.53
3	2-B	7477	AMP	C3'-C4'	-4.07	1.42	1.53
3	3-B	7477	AMP	C3'-C4'	-4.07	1.42	1.53
3	4-B	7477	AMP	C3'-C4'	-4.07	1.42	1.53
3	5-B	7477	AMP	C3'-C4'	-4.07	1.42	1.53
3	6-B	7477	AMP	C3'-C4'	-4.07	1.42	1.53
3	7-B	7477	AMP	C3'-C4'	-4.07	1.42	1.53
3	8-B	7477	AMP	C3'-C4'	-4.07	1.42	1.53
3	9-B	7477	AMP	C3'-C4'	-4.07	1.42	1.53
3	10-B	7477	AMP	C3'-C4'	-4.07	1.42	1.53
3	1-G	7487	AMP	C3'-C4'	-4.07	1.42	1.53
3	2-G	7487	AMP	C3'-C4'	-4.07	1.42	1.53
3	3-G	7487	AMP	C3'-C4'	-4.07	1.42	1.53
3	4-G	7487	AMP	C3'-C4'	-4.07	1.42	1.53
3	5-G	7487	AMP	C3'-C4'	-4.07	1.42	1.53
3	6-G	7487	AMP	C3'-C4'	-4.07	1.42	1.53
3	7-G	7487	AMP	C3'-C4'	-4.07	1.42	1.53
3	8-G	7487	AMP	C3'-C4'	-4.07	1.42	1.53
3	9-G	7487	AMP	C3'-C4'	-4.07	1.42	1.53
3	10-G	7487	AMP	C3'-C4'	-4.07	1.42	1.53
3	1-L	7497	AMP	C2-N3	4.07	1.41	1.33
3	2-L	7497	AMP	C2-N3	4.07	1.41	1.33
3	3-L	7497	AMP	C2-N3	4.07	1.41	1.33
3	4-L	7497	AMP	C2-N3	4.07	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-L	7497	AMP	C2-N3	4.07	1.41	1.33
3	6-L	7497	AMP	C2-N3	4.07	1.41	1.33
3	7-L	7497	AMP	C2-N3	4.07	1.41	1.33
3	8-L	7497	AMP	C2-N3	4.07	1.41	1.33
3	9-L	7497	AMP	C2-N3	4.07	1.41	1.33
3	10-L	7497	AMP	C2-N3	4.07	1.41	1.33
3	1-O	7503	AMP	C2-N3	4.07	1.41	1.33
3	2-O	7503	AMP	C2-N3	4.07	1.41	1.33
3	3-O	7503	AMP	C2-N3	4.07	1.41	1.33
3	4-O	7503	AMP	C2-N3	4.07	1.41	1.33
3	5-O	7503	AMP	C2-N3	4.07	1.41	1.33
3	6-O	7503	AMP	C2-N3	4.07	1.41	1.33
3	7-O	7503	AMP	C2-N3	4.07	1.41	1.33
3	8-O	7503	AMP	C2-N3	4.07	1.41	1.33
3	9-O	7503	AMP	C2-N3	4.07	1.41	1.33
3	10-O	7503	AMP	C2-N3	4.07	1.41	1.33
3	1-A	7475	AMP	C2-N3	4.06	1.41	1.33
3	2-A	7475	AMP	C2-N3	4.06	1.41	1.33
3	3-A	7475	AMP	C2-N3	4.06	1.41	1.33
3	4-A	7475	AMP	C2-N3	4.06	1.41	1.33
3	5-A	7475	AMP	C2-N3	4.06	1.41	1.33
3	6-A	7475	AMP	C2-N3	4.06	1.41	1.33
3	7-A	7475	AMP	C2-N3	4.06	1.41	1.33
3	8-A	7475	AMP	C2-N3	4.06	1.41	1.33
3	9-A	7475	AMP	C2-N3	4.06	1.41	1.33
3	10-A	7475	AMP	C2-N3	4.06	1.41	1.33
3	1-B	7477	AMP	C2-N3	4.06	1.41	1.33
3	2-B	7477	AMP	C2-N3	4.06	1.41	1.33
3	3-B	7477	AMP	C2-N3	4.06	1.41	1.33
3	4-B	7477	AMP	C2-N3	4.06	1.41	1.33
3	5-B	7477	AMP	C2-N3	4.06	1.41	1.33
3	6-B	7477	AMP	C2-N3	4.06	1.41	1.33
3	7-B	7477	AMP	C2-N3	4.06	1.41	1.33
3	8-B	7477	AMP	C2-N3	4.06	1.41	1.33
3	9-B	7477	AMP	C2-N3	4.06	1.41	1.33
3	10-B	7477	AMP	C2-N3	4.06	1.41	1.33
3	1-G	7487	AMP	C2-N3	4.06	1.41	1.33
3	2-G	7487	AMP	C2-N3	4.06	1.41	1.33
3	3-G	7487	AMP	C2-N3	4.06	1.41	1.33
3	4-G	7487	AMP	C2-N3	4.06	1.41	1.33
3	5-G	7487	AMP	C2-N3	4.06	1.41	1.33
3	6-G	7487	AMP	C2-N3	4.06	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-G	7487	AMP	C2-N3	4.06	1.41	1.33
3	8-G	7487	AMP	C2-N3	4.06	1.41	1.33
3	9-G	7487	AMP	C2-N3	4.06	1.41	1.33
3	10-G	7487	AMP	C2-N3	4.06	1.41	1.33
3	1-H	7489	AMP	C2-N3	4.06	1.41	1.33
3	2-H	7489	AMP	C2-N3	4.06	1.41	1.33
3	3-H	7489	AMP	C2-N3	4.06	1.41	1.33
3	4-H	7489	AMP	C2-N3	4.06	1.41	1.33
3	5-H	7489	AMP	C2-N3	4.06	1.41	1.33
3	6-H	7489	AMP	C2-N3	4.06	1.41	1.33
3	7-H	7489	AMP	C2-N3	4.06	1.41	1.33
3	8-H	7489	AMP	C2-N3	4.06	1.41	1.33
3	9-H	7489	AMP	C2-N3	4.06	1.41	1.33
3	10-H	7489	AMP	C2-N3	4.06	1.41	1.33
3	1-Q	7507	AMP	C2-N3	4.06	1.41	1.33
3	2-Q	7507	AMP	C2-N3	4.06	1.41	1.33
3	3-Q	7507	AMP	C2-N3	4.06	1.41	1.33
3	4-Q	7507	AMP	C2-N3	4.06	1.41	1.33
3	5-Q	7507	AMP	C2-N3	4.06	1.41	1.33
3	6-Q	7507	AMP	C2-N3	4.06	1.41	1.33
3	7-Q	7507	AMP	C2-N3	4.06	1.41	1.33
3	8-Q	7507	AMP	C2-N3	4.06	1.41	1.33
3	9-Q	7507	AMP	C2-N3	4.06	1.41	1.33
3	10-Q	7507	AMP	C2-N3	4.06	1.41	1.33
3	1-N	7501	AMP	C2-N3	4.06	1.41	1.33
3	2-N	7501	AMP	C2-N3	4.06	1.41	1.33
3	3-N	7501	AMP	C2-N3	4.06	1.41	1.33
3	4-N	7501	AMP	C2-N3	4.06	1.41	1.33
3	5-N	7501	AMP	C2-N3	4.06	1.41	1.33
3	6-N	7501	AMP	C2-N3	4.06	1.41	1.33
3	7-N	7501	AMP	C2-N3	4.06	1.41	1.33
3	8-N	7501	AMP	C2-N3	4.06	1.41	1.33
3	9-N	7501	AMP	C2-N3	4.06	1.41	1.33
3	10-N	7501	AMP	C2-N3	4.06	1.41	1.33
3	1-E	7483	AMP	C2-N3	4.06	1.41	1.33
3	2-E	7483	AMP	C2-N3	4.06	1.41	1.33
3	3-E	7483	AMP	C2-N3	4.06	1.41	1.33
3	4-E	7483	AMP	C2-N3	4.06	1.41	1.33
3	5-E	7483	AMP	C2-N3	4.06	1.41	1.33
3	6-E	7483	AMP	C2-N3	4.06	1.41	1.33
3	7-E	7483	AMP	C2-N3	4.06	1.41	1.33
3	8-E	7483	AMP	C2-N3	4.06	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-E	7483	AMP	C2-N3	4.06	1.41	1.33
3	10-E	7483	AMP	C2-N3	4.06	1.41	1.33
3	1-P	7505	AMP	C2-N3	4.05	1.41	1.33
3	2-P	7505	AMP	C2-N3	4.05	1.41	1.33
3	3-P	7505	AMP	C2-N3	4.05	1.41	1.33
3	4-P	7505	AMP	C2-N3	4.05	1.41	1.33
3	5-P	7505	AMP	C2-N3	4.05	1.41	1.33
3	6-P	7505	AMP	C2-N3	4.05	1.41	1.33
3	7-P	7505	AMP	C2-N3	4.05	1.41	1.33
3	8-P	7505	AMP	C2-N3	4.05	1.41	1.33
3	9-P	7505	AMP	C2-N3	4.05	1.41	1.33
3	10-P	7505	AMP	C2-N3	4.05	1.41	1.33
3	1-V	7517	AMP	C2-N3	4.05	1.41	1.33
3	2-V	7517	AMP	C2-N3	4.05	1.41	1.33
3	3-V	7517	AMP	C2-N3	4.05	1.41	1.33
3	4-V	7517	AMP	C2-N3	4.05	1.41	1.33
3	5-V	7517	AMP	C2-N3	4.05	1.41	1.33
3	6-V	7517	AMP	C2-N3	4.05	1.41	1.33
3	7-V	7517	AMP	C2-N3	4.05	1.41	1.33
3	8-V	7517	AMP	C2-N3	4.05	1.41	1.33
3	9-V	7517	AMP	C2-N3	4.05	1.41	1.33
3	10-V	7517	AMP	C2-N3	4.05	1.41	1.33
3	1-M	7499	AMP	C2-N3	4.03	1.41	1.33
3	2-M	7499	AMP	C2-N3	4.03	1.41	1.33
3	3-M	7499	AMP	C2-N3	4.03	1.41	1.33
3	4-M	7499	AMP	C2-N3	4.03	1.41	1.33
3	5-M	7499	AMP	C2-N3	4.03	1.41	1.33
3	6-M	7499	AMP	C2-N3	4.03	1.41	1.33
3	7-M	7499	AMP	C2-N3	4.03	1.41	1.33
3	8-M	7499	AMP	C2-N3	4.03	1.41	1.33
3	9-M	7499	AMP	C2-N3	4.03	1.41	1.33
3	10-M	7499	AMP	C2-N3	4.03	1.41	1.33
3	1-S	7511	AMP	C2-N3	4.02	1.41	1.33
3	2-S	7511	AMP	C2-N3	4.02	1.41	1.33
3	3-S	7511	AMP	C2-N3	4.02	1.41	1.33
3	4-S	7511	AMP	C2-N3	4.02	1.41	1.33
3	5-S	7511	AMP	C2-N3	4.02	1.41	1.33
3	6-S	7511	AMP	C2-N3	4.02	1.41	1.33
3	7-S	7511	AMP	C2-N3	4.02	1.41	1.33
3	8-S	7511	AMP	C2-N3	4.02	1.41	1.33
3	9-S	7511	AMP	C2-N3	4.02	1.41	1.33
3	10-S	7511	AMP	C2-N3	4.02	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-T	7514	CIT	C4-C3	3.77	1.58	1.54
4	2-T	7514	CIT	C4-C3	3.77	1.58	1.54
4	3-T	7514	CIT	C4-C3	3.77	1.58	1.54
4	4-T	7514	CIT	C4-C3	3.77	1.58	1.54
4	5-T	7514	CIT	C4-C3	3.77	1.58	1.54
4	6-T	7514	CIT	C4-C3	3.77	1.58	1.54
4	7-T	7514	CIT	C4-C3	3.77	1.58	1.54
4	8-T	7514	CIT	C4-C3	3.77	1.58	1.54
4	9-T	7514	CIT	C4-C3	3.77	1.58	1.54
4	10-T	7514	CIT	C4-C3	3.77	1.58	1.54
4	1-Q	7508	CIT	C4-C3	3.76	1.58	1.54
4	2-Q	7508	CIT	C4-C3	3.76	1.58	1.54
4	3-Q	7508	CIT	C4-C3	3.76	1.58	1.54
4	4-Q	7508	CIT	C4-C3	3.76	1.58	1.54
4	5-Q	7508	CIT	C4-C3	3.76	1.58	1.54
4	6-Q	7508	CIT	C4-C3	3.76	1.58	1.54
4	7-Q	7508	CIT	C4-C3	3.76	1.58	1.54
4	8-Q	7508	CIT	C4-C3	3.76	1.58	1.54
4	9-Q	7508	CIT	C4-C3	3.76	1.58	1.54
4	10-Q	7508	CIT	C4-C3	3.76	1.58	1.54
4	1-V	7518	CIT	C4-C3	3.76	1.58	1.54
4	2-V	7518	CIT	C4-C3	3.76	1.58	1.54
4	3-V	7518	CIT	C4-C3	3.76	1.58	1.54
4	4-V	7518	CIT	C4-C3	3.76	1.58	1.54
4	5-V	7518	CIT	C4-C3	3.76	1.58	1.54
4	6-V	7518	CIT	C4-C3	3.76	1.58	1.54
4	7-V	7518	CIT	C4-C3	3.76	1.58	1.54
4	8-V	7518	CIT	C4-C3	3.76	1.58	1.54
4	9-V	7518	CIT	C4-C3	3.76	1.58	1.54
4	10-V	7518	CIT	C4-C3	3.76	1.58	1.54
4	1-R	7510	CIT	C4-C3	3.75	1.58	1.54
4	2-R	7510	CIT	C4-C3	3.75	1.58	1.54
4	3-R	7510	CIT	C4-C3	3.75	1.58	1.54
4	4-R	7510	CIT	C4-C3	3.75	1.58	1.54
4	5-R	7510	CIT	C4-C3	3.75	1.58	1.54
4	6-R	7510	CIT	C4-C3	3.75	1.58	1.54
4	7-R	7510	CIT	C4-C3	3.75	1.58	1.54
4	8-R	7510	CIT	C4-C3	3.75	1.58	1.54
4	9-R	7510	CIT	C4-C3	3.75	1.58	1.54
4	10-R	7510	CIT	C4-C3	3.75	1.58	1.54
4	1-B	7478	CIT	C4-C3	3.75	1.58	1.54
4	2-B	7478	CIT	C4-C3	3.75	1.58	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-B	7478	CIT	C4-C3	3.75	1.58	1.54
4	4-B	7478	CIT	C4-C3	3.75	1.58	1.54
4	5-B	7478	CIT	C4-C3	3.75	1.58	1.54
4	6-B	7478	CIT	C4-C3	3.75	1.58	1.54
4	7-B	7478	CIT	C4-C3	3.75	1.58	1.54
4	8-B	7478	CIT	C4-C3	3.75	1.58	1.54
4	9-B	7478	CIT	C4-C3	3.75	1.58	1.54
4	10-B	7478	CIT	C4-C3	3.75	1.58	1.54
4	1-W	7520	CIT	C4-C3	3.75	1.58	1.54
4	2-W	7520	CIT	C4-C3	3.75	1.58	1.54
4	3-W	7520	CIT	C4-C3	3.75	1.58	1.54
4	4-W	7520	CIT	C4-C3	3.75	1.58	1.54
4	5-W	7520	CIT	C4-C3	3.75	1.58	1.54
4	6-W	7520	CIT	C4-C3	3.75	1.58	1.54
4	7-W	7520	CIT	C4-C3	3.75	1.58	1.54
4	8-W	7520	CIT	C4-C3	3.75	1.58	1.54
4	9-W	7520	CIT	C4-C3	3.75	1.58	1.54
4	10-W	7520	CIT	C4-C3	3.75	1.58	1.54
4	1-H	7490	CIT	C4-C3	3.74	1.58	1.54
4	2-H	7490	CIT	C4-C3	3.74	1.58	1.54
4	3-H	7490	CIT	C4-C3	3.74	1.58	1.54
4	4-H	7490	CIT	C4-C3	3.74	1.58	1.54
4	5-H	7490	CIT	C4-C3	3.74	1.58	1.54
4	6-H	7490	CIT	C4-C3	3.74	1.58	1.54
4	7-H	7490	CIT	C4-C3	3.74	1.58	1.54
4	8-H	7490	CIT	C4-C3	3.74	1.58	1.54
4	9-H	7490	CIT	C4-C3	3.74	1.58	1.54
4	10-H	7490	CIT	C4-C3	3.74	1.58	1.54
4	1-E	7484	CIT	C4-C3	3.73	1.58	1.54
4	2-E	7484	CIT	C4-C3	3.73	1.58	1.54
4	3-E	7484	CIT	C4-C3	3.73	1.58	1.54
4	4-E	7484	CIT	C4-C3	3.73	1.58	1.54
4	5-E	7484	CIT	C4-C3	3.73	1.58	1.54
4	6-E	7484	CIT	C4-C3	3.73	1.58	1.54
4	7-E	7484	CIT	C4-C3	3.73	1.58	1.54
4	8-E	7484	CIT	C4-C3	3.73	1.58	1.54
4	9-E	7484	CIT	C4-C3	3.73	1.58	1.54
4	10-E	7484	CIT	C4-C3	3.73	1.58	1.54
4	1-P	7506	CIT	C4-C3	3.73	1.58	1.54
4	2-P	7506	CIT	C4-C3	3.73	1.58	1.54
4	3-P	7506	CIT	C4-C3	3.73	1.58	1.54
4	4-P	7506	CIT	C4-C3	3.73	1.58	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5-P	7506	CIT	C4-C3	3.73	1.58	1.54
4	6-P	7506	CIT	C4-C3	3.73	1.58	1.54
4	7-P	7506	CIT	C4-C3	3.73	1.58	1.54
4	8-P	7506	CIT	C4-C3	3.73	1.58	1.54
4	9-P	7506	CIT	C4-C3	3.73	1.58	1.54
4	10-P	7506	CIT	C4-C3	3.73	1.58	1.54
4	1-J	7494	CIT	C4-C3	3.73	1.58	1.54
4	2-J	7494	CIT	C4-C3	3.73	1.58	1.54
4	3-J	7494	CIT	C4-C3	3.73	1.58	1.54
4	4-J	7494	CIT	C4-C3	3.73	1.58	1.54
4	5-J	7494	CIT	C4-C3	3.73	1.58	1.54
4	6-J	7494	CIT	C4-C3	3.73	1.58	1.54
4	7-J	7494	CIT	C4-C3	3.73	1.58	1.54
4	8-J	7494	CIT	C4-C3	3.73	1.58	1.54
4	9-J	7494	CIT	C4-C3	3.73	1.58	1.54
4	10-J	7494	CIT	C4-C3	3.73	1.58	1.54
4	1-D	7482	CIT	C4-C3	3.73	1.58	1.54
4	2-D	7482	CIT	C4-C3	3.73	1.58	1.54
4	3-D	7482	CIT	C4-C3	3.73	1.58	1.54
4	4-D	7482	CIT	C4-C3	3.73	1.58	1.54
4	5-D	7482	CIT	C4-C3	3.73	1.58	1.54
4	6-D	7482	CIT	C4-C3	3.73	1.58	1.54
4	7-D	7482	CIT	C4-C3	3.73	1.58	1.54
4	8-D	7482	CIT	C4-C3	3.73	1.58	1.54
4	9-D	7482	CIT	C4-C3	3.73	1.58	1.54
4	10-D	7482	CIT	C4-C3	3.73	1.58	1.54
4	1-M	7500	CIT	C4-C3	3.73	1.58	1.54
4	2-M	7500	CIT	C4-C3	3.73	1.58	1.54
4	3-M	7500	CIT	C4-C3	3.73	1.58	1.54
4	4-M	7500	CIT	C4-C3	3.73	1.58	1.54
4	5-M	7500	CIT	C4-C3	3.73	1.58	1.54
4	6-M	7500	CIT	C4-C3	3.73	1.58	1.54
4	7-M	7500	CIT	C4-C3	3.73	1.58	1.54
4	8-M	7500	CIT	C4-C3	3.73	1.58	1.54
4	9-M	7500	CIT	C4-C3	3.73	1.58	1.54
4	10-M	7500	CIT	C4-C3	3.73	1.58	1.54
4	1-S	7512	CIT	C4-C3	3.73	1.58	1.54
4	2-S	7512	CIT	C4-C3	3.73	1.58	1.54
4	3-S	7512	CIT	C4-C3	3.73	1.58	1.54
4	4-S	7512	CIT	C4-C3	3.73	1.58	1.54
4	5-S	7512	CIT	C4-C3	3.73	1.58	1.54
4	6-S	7512	CIT	C4-C3	3.73	1.58	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-S	7512	CIT	C4-C3	3.73	1.58	1.54
4	8-S	7512	CIT	C4-C3	3.73	1.58	1.54
4	9-S	7512	CIT	C4-C3	3.73	1.58	1.54
4	10-S	7512	CIT	C4-C3	3.73	1.58	1.54
4	1-C	7480	CIT	C4-C3	3.72	1.58	1.54
4	2-C	7480	CIT	C4-C3	3.72	1.58	1.54
4	3-C	7480	CIT	C4-C3	3.72	1.58	1.54
4	4-C	7480	CIT	C4-C3	3.72	1.58	1.54
4	5-C	7480	CIT	C4-C3	3.72	1.58	1.54
4	6-C	7480	CIT	C4-C3	3.72	1.58	1.54
4	7-C	7480	CIT	C4-C3	3.72	1.58	1.54
4	8-C	7480	CIT	C4-C3	3.72	1.58	1.54
4	9-C	7480	CIT	C4-C3	3.72	1.58	1.54
4	10-C	7480	CIT	C4-C3	3.72	1.58	1.54
4	1-F	7486	CIT	C4-C3	3.72	1.58	1.54
4	2-F	7486	CIT	C4-C3	3.72	1.58	1.54
4	3-F	7486	CIT	C4-C3	3.72	1.58	1.54
4	4-F	7486	CIT	C4-C3	3.72	1.58	1.54
4	5-F	7486	CIT	C4-C3	3.72	1.58	1.54
4	6-F	7486	CIT	C4-C3	3.72	1.58	1.54
4	7-F	7486	CIT	C4-C3	3.72	1.58	1.54
4	8-F	7486	CIT	C4-C3	3.72	1.58	1.54
4	9-F	7486	CIT	C4-C3	3.72	1.58	1.54
4	10-F	7486	CIT	C4-C3	3.72	1.58	1.54
4	1-A	7476	CIT	C4-C3	3.71	1.58	1.54
4	2-A	7476	CIT	C4-C3	3.71	1.58	1.54
4	3-A	7476	CIT	C4-C3	3.71	1.58	1.54
4	4-A	7476	CIT	C4-C3	3.71	1.58	1.54
4	5-A	7476	CIT	C4-C3	3.71	1.58	1.54
4	6-A	7476	CIT	C4-C3	3.71	1.58	1.54
4	7-A	7476	CIT	C4-C3	3.71	1.58	1.54
4	8-A	7476	CIT	C4-C3	3.71	1.58	1.54
4	9-A	7476	CIT	C4-C3	3.71	1.58	1.54
4	10-A	7476	CIT	C4-C3	3.71	1.58	1.54
4	1-N	7502	CIT	C4-C3	3.71	1.58	1.54
4	2-N	7502	CIT	C4-C3	3.71	1.58	1.54
4	3-N	7502	CIT	C4-C3	3.71	1.58	1.54
4	4-N	7502	CIT	C4-C3	3.71	1.58	1.54
4	5-N	7502	CIT	C4-C3	3.71	1.58	1.54
4	6-N	7502	CIT	C4-C3	3.71	1.58	1.54
4	7-N	7502	CIT	C4-C3	3.71	1.58	1.54
4	8-N	7502	CIT	C4-C3	3.71	1.58	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9-N	7502	CIT	C4-C3	3.71	1.58	1.54
4	10-N	7502	CIT	C4-C3	3.71	1.58	1.54
4	1-G	7488	CIT	C4-C3	3.70	1.58	1.54
4	2-G	7488	CIT	C4-C3	3.70	1.58	1.54
4	3-G	7488	CIT	C4-C3	3.70	1.58	1.54
4	4-G	7488	CIT	C4-C3	3.70	1.58	1.54
4	5-G	7488	CIT	C4-C3	3.70	1.58	1.54
4	6-G	7488	CIT	C4-C3	3.70	1.58	1.54
4	7-G	7488	CIT	C4-C3	3.70	1.58	1.54
4	8-G	7488	CIT	C4-C3	3.70	1.58	1.54
4	9-G	7488	CIT	C4-C3	3.70	1.58	1.54
4	10-G	7488	CIT	C4-C3	3.70	1.58	1.54
4	1-U	7516	CIT	C4-C3	3.70	1.58	1.54
4	2-U	7516	CIT	C4-C3	3.70	1.58	1.54
4	3-U	7516	CIT	C4-C3	3.70	1.58	1.54
4	4-U	7516	CIT	C4-C3	3.70	1.58	1.54
4	5-U	7516	CIT	C4-C3	3.70	1.58	1.54
4	6-U	7516	CIT	C4-C3	3.70	1.58	1.54
4	7-U	7516	CIT	C4-C3	3.70	1.58	1.54
4	8-U	7516	CIT	C4-C3	3.70	1.58	1.54
4	9-U	7516	CIT	C4-C3	3.70	1.58	1.54
4	10-U	7516	CIT	C4-C3	3.70	1.58	1.54
4	1-K	7496	CIT	C4-C3	3.69	1.58	1.54
4	2-K	7496	CIT	C4-C3	3.69	1.58	1.54
4	3-K	7496	CIT	C4-C3	3.69	1.58	1.54
4	4-K	7496	CIT	C4-C3	3.69	1.58	1.54
4	5-K	7496	CIT	C4-C3	3.69	1.58	1.54
4	6-K	7496	CIT	C4-C3	3.69	1.58	1.54
4	7-K	7496	CIT	C4-C3	3.69	1.58	1.54
4	8-K	7496	CIT	C4-C3	3.69	1.58	1.54
4	9-K	7496	CIT	C4-C3	3.69	1.58	1.54
4	10-K	7496	CIT	C4-C3	3.69	1.58	1.54
4	1-X	7522	CIT	C4-C3	3.69	1.58	1.54
4	2-X	7522	CIT	C4-C3	3.69	1.58	1.54
4	3-X	7522	CIT	C4-C3	3.69	1.58	1.54
4	4-X	7522	CIT	C4-C3	3.69	1.58	1.54
4	5-X	7522	CIT	C4-C3	3.69	1.58	1.54
4	6-X	7522	CIT	C4-C3	3.69	1.58	1.54
4	7-X	7522	CIT	C4-C3	3.69	1.58	1.54
4	8-X	7522	CIT	C4-C3	3.69	1.58	1.54
4	9-X	7522	CIT	C4-C3	3.69	1.58	1.54
4	10-X	7522	CIT	C4-C3	3.69	1.58	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-O	7504	CIT	C4-C3	3.68	1.58	1.54
4	2-O	7504	CIT	C4-C3	3.68	1.58	1.54
4	3-O	7504	CIT	C4-C3	3.68	1.58	1.54
4	4-O	7504	CIT	C4-C3	3.68	1.58	1.54
4	5-O	7504	CIT	C4-C3	3.68	1.58	1.54
4	6-O	7504	CIT	C4-C3	3.68	1.58	1.54
4	7-O	7504	CIT	C4-C3	3.68	1.58	1.54
4	8-O	7504	CIT	C4-C3	3.68	1.58	1.54
4	9-O	7504	CIT	C4-C3	3.68	1.58	1.54
4	10-O	7504	CIT	C4-C3	3.68	1.58	1.54
4	1-L	7498	CIT	C4-C3	3.67	1.58	1.54
4	2-L	7498	CIT	C4-C3	3.67	1.58	1.54
4	3-L	7498	CIT	C4-C3	3.67	1.58	1.54
4	4-L	7498	CIT	C4-C3	3.67	1.58	1.54
4	5-L	7498	CIT	C4-C3	3.67	1.58	1.54
4	6-L	7498	CIT	C4-C3	3.67	1.58	1.54
4	7-L	7498	CIT	C4-C3	3.67	1.58	1.54
4	8-L	7498	CIT	C4-C3	3.67	1.58	1.54
4	9-L	7498	CIT	C4-C3	3.67	1.58	1.54
4	10-L	7498	CIT	C4-C3	3.67	1.58	1.54
4	1-I	7492	CIT	C4-C3	3.66	1.58	1.54
4	2-I	7492	CIT	C4-C3	3.66	1.58	1.54
4	3-I	7492	CIT	C4-C3	3.66	1.58	1.54
4	4-I	7492	CIT	C4-C3	3.66	1.58	1.54
4	5-I	7492	CIT	C4-C3	3.66	1.58	1.54
4	6-I	7492	CIT	C4-C3	3.66	1.58	1.54
4	7-I	7492	CIT	C4-C3	3.66	1.58	1.54
4	8-I	7492	CIT	C4-C3	3.66	1.58	1.54
4	9-I	7492	CIT	C4-C3	3.66	1.58	1.54
4	10-I	7492	CIT	C4-C3	3.66	1.58	1.54
3	1-B	7477	AMP	P-O1P	3.26	1.60	1.50
3	2-B	7477	AMP	P-O1P	3.26	1.60	1.50
3	3-B	7477	AMP	P-O1P	3.26	1.60	1.50
3	4-B	7477	AMP	P-O1P	3.26	1.60	1.50
3	5-B	7477	AMP	P-O1P	3.26	1.60	1.50
3	6-B	7477	AMP	P-O1P	3.26	1.60	1.50
3	7-B	7477	AMP	P-O1P	3.26	1.60	1.50
3	8-B	7477	AMP	P-O1P	3.26	1.60	1.50
3	9-B	7477	AMP	P-O1P	3.26	1.60	1.50
3	10-B	7477	AMP	P-O1P	3.26	1.60	1.50
3	1-I	7491	AMP	P-O1P	3.24	1.60	1.50
3	2-I	7491	AMP	P-O1P	3.24	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-I	7491	AMP	P-O1P	3.24	1.60	1.50
3	4-I	7491	AMP	P-O1P	3.24	1.60	1.50
3	5-I	7491	AMP	P-O1P	3.24	1.60	1.50
3	6-I	7491	AMP	P-O1P	3.24	1.60	1.50
3	7-I	7491	AMP	P-O1P	3.24	1.60	1.50
3	8-I	7491	AMP	P-O1P	3.24	1.60	1.50
3	9-I	7491	AMP	P-O1P	3.24	1.60	1.50
3	10-I	7491	AMP	P-O1P	3.24	1.60	1.50
3	1-E	7483	AMP	P-O1P	3.24	1.60	1.50
3	2-E	7483	AMP	P-O1P	3.24	1.60	1.50
3	3-E	7483	AMP	P-O1P	3.24	1.60	1.50
3	4-E	7483	AMP	P-O1P	3.24	1.60	1.50
3	5-E	7483	AMP	P-O1P	3.24	1.60	1.50
3	6-E	7483	AMP	P-O1P	3.24	1.60	1.50
3	7-E	7483	AMP	P-O1P	3.24	1.60	1.50
3	8-E	7483	AMP	P-O1P	3.24	1.60	1.50
3	9-E	7483	AMP	P-O1P	3.24	1.60	1.50
3	10-E	7483	AMP	P-O1P	3.24	1.60	1.50
3	1-O	7503	AMP	P-O1P	3.24	1.60	1.50
3	2-O	7503	AMP	P-O1P	3.24	1.60	1.50
3	3-O	7503	AMP	P-O1P	3.24	1.60	1.50
3	4-O	7503	AMP	P-O1P	3.24	1.60	1.50
3	5-O	7503	AMP	P-O1P	3.24	1.60	1.50
3	6-O	7503	AMP	P-O1P	3.24	1.60	1.50
3	7-O	7503	AMP	P-O1P	3.24	1.60	1.50
3	8-O	7503	AMP	P-O1P	3.24	1.60	1.50
3	9-O	7503	AMP	P-O1P	3.24	1.60	1.50
3	10-O	7503	AMP	P-O1P	3.24	1.60	1.50
3	1-U	7515	AMP	P-O1P	3.24	1.60	1.50
3	2-U	7515	AMP	P-O1P	3.24	1.60	1.50
3	3-U	7515	AMP	P-O1P	3.24	1.60	1.50
3	4-U	7515	AMP	P-O1P	3.24	1.60	1.50
3	5-U	7515	AMP	P-O1P	3.24	1.60	1.50
3	6-U	7515	AMP	P-O1P	3.24	1.60	1.50
3	7-U	7515	AMP	P-O1P	3.24	1.60	1.50
3	8-U	7515	AMP	P-O1P	3.24	1.60	1.50
3	9-U	7515	AMP	P-O1P	3.24	1.60	1.50
3	10-U	7515	AMP	P-O1P	3.24	1.60	1.50
3	1-Q	7507	AMP	P-O1P	3.23	1.60	1.50
3	2-Q	7507	AMP	P-O1P	3.23	1.60	1.50
3	3-Q	7507	AMP	P-O1P	3.23	1.60	1.50
3	4-Q	7507	AMP	P-O1P	3.23	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-Q	7507	AMP	P-O1P	3.23	1.60	1.50
3	6-Q	7507	AMP	P-O1P	3.23	1.60	1.50
3	7-Q	7507	AMP	P-O1P	3.23	1.60	1.50
3	8-Q	7507	AMP	P-O1P	3.23	1.60	1.50
3	9-Q	7507	AMP	P-O1P	3.23	1.60	1.50
3	10-Q	7507	AMP	P-O1P	3.23	1.60	1.50
3	1-D	7481	AMP	P-O1P	3.23	1.60	1.50
3	2-D	7481	AMP	P-O1P	3.23	1.60	1.50
3	3-D	7481	AMP	P-O1P	3.23	1.60	1.50
3	4-D	7481	AMP	P-O1P	3.23	1.60	1.50
3	5-D	7481	AMP	P-O1P	3.23	1.60	1.50
3	6-D	7481	AMP	P-O1P	3.23	1.60	1.50
3	7-D	7481	AMP	P-O1P	3.23	1.60	1.50
3	8-D	7481	AMP	P-O1P	3.23	1.60	1.50
3	9-D	7481	AMP	P-O1P	3.23	1.60	1.50
3	10-D	7481	AMP	P-O1P	3.23	1.60	1.50
3	1-G	7487	AMP	P-O1P	3.23	1.60	1.50
3	2-G	7487	AMP	P-O1P	3.23	1.60	1.50
3	3-G	7487	AMP	P-O1P	3.23	1.60	1.50
3	4-G	7487	AMP	P-O1P	3.23	1.60	1.50
3	5-G	7487	AMP	P-O1P	3.23	1.60	1.50
3	6-G	7487	AMP	P-O1P	3.23	1.60	1.50
3	7-G	7487	AMP	P-O1P	3.23	1.60	1.50
3	8-G	7487	AMP	P-O1P	3.23	1.60	1.50
3	9-G	7487	AMP	P-O1P	3.23	1.60	1.50
3	10-G	7487	AMP	P-O1P	3.23	1.60	1.50
3	1-L	7497	AMP	P-O1P	3.23	1.60	1.50
3	2-L	7497	AMP	P-O1P	3.23	1.60	1.50
3	3-L	7497	AMP	P-O1P	3.23	1.60	1.50
3	4-L	7497	AMP	P-O1P	3.23	1.60	1.50
3	5-L	7497	AMP	P-O1P	3.23	1.60	1.50
3	6-L	7497	AMP	P-O1P	3.23	1.60	1.50
3	7-L	7497	AMP	P-O1P	3.23	1.60	1.50
3	8-L	7497	AMP	P-O1P	3.23	1.60	1.50
3	9-L	7497	AMP	P-O1P	3.23	1.60	1.50
3	10-L	7497	AMP	P-O1P	3.23	1.60	1.50
3	1-H	7489	AMP	P-O1P	3.23	1.60	1.50
3	2-H	7489	AMP	P-O1P	3.23	1.60	1.50
3	3-H	7489	AMP	P-O1P	3.23	1.60	1.50
3	4-H	7489	AMP	P-O1P	3.23	1.60	1.50
3	5-H	7489	AMP	P-O1P	3.23	1.60	1.50
3	6-H	7489	AMP	P-O1P	3.23	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-H	7489	AMP	P-O1P	3.23	1.60	1.50
3	8-H	7489	AMP	P-O1P	3.23	1.60	1.50
3	9-H	7489	AMP	P-O1P	3.23	1.60	1.50
3	10-H	7489	AMP	P-O1P	3.23	1.60	1.50
3	1-J	7493	AMP	P-O1P	3.23	1.60	1.50
3	2-J	7493	AMP	P-O1P	3.23	1.60	1.50
3	3-J	7493	AMP	P-O1P	3.23	1.60	1.50
3	4-J	7493	AMP	P-O1P	3.23	1.60	1.50
3	5-J	7493	AMP	P-O1P	3.23	1.60	1.50
3	6-J	7493	AMP	P-O1P	3.23	1.60	1.50
3	7-J	7493	AMP	P-O1P	3.23	1.60	1.50
3	8-J	7493	AMP	P-O1P	3.23	1.60	1.50
3	9-J	7493	AMP	P-O1P	3.23	1.60	1.50
3	10-J	7493	AMP	P-O1P	3.23	1.60	1.50
3	1-T	7513	AMP	P-O1P	3.23	1.60	1.50
3	2-T	7513	AMP	P-O1P	3.23	1.60	1.50
3	3-T	7513	AMP	P-O1P	3.23	1.60	1.50
3	4-T	7513	AMP	P-O1P	3.23	1.60	1.50
3	5-T	7513	AMP	P-O1P	3.23	1.60	1.50
3	6-T	7513	AMP	P-O1P	3.23	1.60	1.50
3	7-T	7513	AMP	P-O1P	3.23	1.60	1.50
3	8-T	7513	AMP	P-O1P	3.23	1.60	1.50
3	9-T	7513	AMP	P-O1P	3.23	1.60	1.50
3	10-T	7513	AMP	P-O1P	3.23	1.60	1.50
3	1-A	7475	AMP	P-O1P	3.23	1.60	1.50
3	2-A	7475	AMP	P-O1P	3.23	1.60	1.50
3	3-A	7475	AMP	P-O1P	3.23	1.60	1.50
3	4-A	7475	AMP	P-O1P	3.23	1.60	1.50
3	5-A	7475	AMP	P-O1P	3.23	1.60	1.50
3	6-A	7475	AMP	P-O1P	3.23	1.60	1.50
3	7-A	7475	AMP	P-O1P	3.23	1.60	1.50
3	8-A	7475	AMP	P-O1P	3.23	1.60	1.50
3	9-A	7475	AMP	P-O1P	3.23	1.60	1.50
3	10-A	7475	AMP	P-O1P	3.23	1.60	1.50
3	1-P	7505	AMP	P-O1P	3.23	1.60	1.50
3	2-P	7505	AMP	P-O1P	3.23	1.60	1.50
3	3-P	7505	AMP	P-O1P	3.23	1.60	1.50
3	4-P	7505	AMP	P-O1P	3.23	1.60	1.50
3	5-P	7505	AMP	P-O1P	3.23	1.60	1.50
3	6-P	7505	AMP	P-O1P	3.23	1.60	1.50
3	7-P	7505	AMP	P-O1P	3.23	1.60	1.50
3	8-P	7505	AMP	P-O1P	3.23	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-P	7505	AMP	P-O1P	3.23	1.60	1.50
3	10-P	7505	AMP	P-O1P	3.23	1.60	1.50
3	1-K	7495	AMP	P-O1P	3.23	1.60	1.50
3	2-K	7495	AMP	P-O1P	3.23	1.60	1.50
3	3-K	7495	AMP	P-O1P	3.23	1.60	1.50
3	4-K	7495	AMP	P-O1P	3.23	1.60	1.50
3	5-K	7495	AMP	P-O1P	3.23	1.60	1.50
3	6-K	7495	AMP	P-O1P	3.23	1.60	1.50
3	7-K	7495	AMP	P-O1P	3.23	1.60	1.50
3	8-K	7495	AMP	P-O1P	3.23	1.60	1.50
3	9-K	7495	AMP	P-O1P	3.23	1.60	1.50
3	10-K	7495	AMP	P-O1P	3.23	1.60	1.50
3	1-X	7521	AMP	P-O1P	3.22	1.60	1.50
3	2-X	7521	AMP	P-O1P	3.22	1.60	1.50
3	3-X	7521	AMP	P-O1P	3.22	1.60	1.50
3	4-X	7521	AMP	P-O1P	3.22	1.60	1.50
3	5-X	7521	AMP	P-O1P	3.22	1.60	1.50
3	6-X	7521	AMP	P-O1P	3.22	1.60	1.50
3	7-X	7521	AMP	P-O1P	3.22	1.60	1.50
3	8-X	7521	AMP	P-O1P	3.22	1.60	1.50
3	9-X	7521	AMP	P-O1P	3.22	1.60	1.50
3	10-X	7521	AMP	P-O1P	3.22	1.60	1.50
3	1-M	7499	AMP	P-O1P	3.22	1.60	1.50
3	2-M	7499	AMP	P-O1P	3.22	1.60	1.50
3	3-M	7499	AMP	P-O1P	3.22	1.60	1.50
3	4-M	7499	AMP	P-O1P	3.22	1.60	1.50
3	5-M	7499	AMP	P-O1P	3.22	1.60	1.50
3	6-M	7499	AMP	P-O1P	3.22	1.60	1.50
3	7-M	7499	AMP	P-O1P	3.22	1.60	1.50
3	8-M	7499	AMP	P-O1P	3.22	1.60	1.50
3	9-M	7499	AMP	P-O1P	3.22	1.60	1.50
3	10-M	7499	AMP	P-O1P	3.22	1.60	1.50
3	1-W	7519	AMP	P-O1P	3.22	1.60	1.50
3	2-W	7519	AMP	P-O1P	3.22	1.60	1.50
3	3-W	7519	AMP	P-O1P	3.22	1.60	1.50
3	4-W	7519	AMP	P-O1P	3.22	1.60	1.50
3	5-W	7519	AMP	P-O1P	3.22	1.60	1.50
3	6-W	7519	AMP	P-O1P	3.22	1.60	1.50
3	7-W	7519	AMP	P-O1P	3.22	1.60	1.50
3	8-W	7519	AMP	P-O1P	3.22	1.60	1.50
3	9-W	7519	AMP	P-O1P	3.22	1.60	1.50
3	10-W	7519	AMP	P-O1P	3.22	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-R	7509	AMP	P-O1P	3.22	1.60	1.50
3	2-R	7509	AMP	P-O1P	3.22	1.60	1.50
3	3-R	7509	AMP	P-O1P	3.22	1.60	1.50
3	4-R	7509	AMP	P-O1P	3.22	1.60	1.50
3	5-R	7509	AMP	P-O1P	3.22	1.60	1.50
3	6-R	7509	AMP	P-O1P	3.22	1.60	1.50
3	7-R	7509	AMP	P-O1P	3.22	1.60	1.50
3	8-R	7509	AMP	P-O1P	3.22	1.60	1.50
3	9-R	7509	AMP	P-O1P	3.22	1.60	1.50
3	10-R	7509	AMP	P-O1P	3.22	1.60	1.50
3	1-N	7501	AMP	P-O1P	3.22	1.60	1.50
3	2-N	7501	AMP	P-O1P	3.22	1.60	1.50
3	3-N	7501	AMP	P-O1P	3.22	1.60	1.50
3	4-N	7501	AMP	P-O1P	3.22	1.60	1.50
3	5-N	7501	AMP	P-O1P	3.22	1.60	1.50
3	6-N	7501	AMP	P-O1P	3.22	1.60	1.50
3	7-N	7501	AMP	P-O1P	3.22	1.60	1.50
3	8-N	7501	AMP	P-O1P	3.22	1.60	1.50
3	9-N	7501	AMP	P-O1P	3.22	1.60	1.50
3	10-N	7501	AMP	P-O1P	3.22	1.60	1.50
3	1-S	7511	AMP	P-O1P	3.22	1.60	1.50
3	2-S	7511	AMP	P-O1P	3.22	1.60	1.50
3	3-S	7511	AMP	P-O1P	3.22	1.60	1.50
3	4-S	7511	AMP	P-O1P	3.22	1.60	1.50
3	5-S	7511	AMP	P-O1P	3.22	1.60	1.50
3	6-S	7511	AMP	P-O1P	3.22	1.60	1.50
3	7-S	7511	AMP	P-O1P	3.22	1.60	1.50
3	8-S	7511	AMP	P-O1P	3.22	1.60	1.50
3	9-S	7511	AMP	P-O1P	3.22	1.60	1.50
3	10-S	7511	AMP	P-O1P	3.22	1.60	1.50
3	1-V	7517	AMP	P-O1P	3.21	1.60	1.50
3	2-V	7517	AMP	P-O1P	3.21	1.60	1.50
3	3-V	7517	AMP	P-O1P	3.21	1.60	1.50
3	4-V	7517	AMP	P-O1P	3.21	1.60	1.50
3	5-V	7517	AMP	P-O1P	3.21	1.60	1.50
3	6-V	7517	AMP	P-O1P	3.21	1.60	1.50
3	7-V	7517	AMP	P-O1P	3.21	1.60	1.50
3	8-V	7517	AMP	P-O1P	3.21	1.60	1.50
3	9-V	7517	AMP	P-O1P	3.21	1.60	1.50
3	10-V	7517	AMP	P-O1P	3.21	1.60	1.50
3	1-F	7485	AMP	P-O1P	3.21	1.60	1.50
3	2-F	7485	AMP	P-O1P	3.21	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-F	7485	AMP	P-O1P	3.21	1.60	1.50
3	4-F	7485	AMP	P-O1P	3.21	1.60	1.50
3	5-F	7485	AMP	P-O1P	3.21	1.60	1.50
3	6-F	7485	AMP	P-O1P	3.21	1.60	1.50
3	7-F	7485	AMP	P-O1P	3.21	1.60	1.50
3	8-F	7485	AMP	P-O1P	3.21	1.60	1.50
3	9-F	7485	AMP	P-O1P	3.21	1.60	1.50
3	10-F	7485	AMP	P-O1P	3.21	1.60	1.50
3	1-C	7479	AMP	P-O1P	3.20	1.60	1.50
3	2-C	7479	AMP	P-O1P	3.20	1.60	1.50
3	3-C	7479	AMP	P-O1P	3.20	1.60	1.50
3	4-C	7479	AMP	P-O1P	3.20	1.60	1.50
3	5-C	7479	AMP	P-O1P	3.20	1.60	1.50
3	6-C	7479	AMP	P-O1P	3.20	1.60	1.50
3	7-C	7479	AMP	P-O1P	3.20	1.60	1.50
3	8-C	7479	AMP	P-O1P	3.20	1.60	1.50
3	9-C	7479	AMP	P-O1P	3.20	1.60	1.50
3	10-C	7479	AMP	P-O1P	3.20	1.60	1.50
3	1-T	7513	AMP	P-O5'	2.58	1.68	1.60
3	2-T	7513	AMP	P-O5'	2.58	1.68	1.60
3	3-T	7513	AMP	P-O5'	2.58	1.68	1.60
3	4-T	7513	AMP	P-O5'	2.58	1.68	1.60
3	5-T	7513	AMP	P-O5'	2.58	1.68	1.60
3	6-T	7513	AMP	P-O5'	2.58	1.68	1.60
3	7-T	7513	AMP	P-O5'	2.58	1.68	1.60
3	8-T	7513	AMP	P-O5'	2.58	1.68	1.60
3	9-T	7513	AMP	P-O5'	2.58	1.68	1.60
3	10-T	7513	AMP	P-O5'	2.58	1.68	1.60
3	1-O	7503	AMP	P-O5'	2.57	1.68	1.60
3	2-O	7503	AMP	P-O5'	2.57	1.68	1.60
3	3-O	7503	AMP	P-O5'	2.57	1.68	1.60
3	4-O	7503	AMP	P-O5'	2.57	1.68	1.60
3	5-O	7503	AMP	P-O5'	2.57	1.68	1.60
3	6-O	7503	AMP	P-O5'	2.57	1.68	1.60
3	7-O	7503	AMP	P-O5'	2.57	1.68	1.60
3	8-O	7503	AMP	P-O5'	2.57	1.68	1.60
3	9-O	7503	AMP	P-O5'	2.57	1.68	1.60
3	10-O	7503	AMP	P-O5'	2.57	1.68	1.60
3	1-Q	7507	AMP	P-O5'	2.57	1.68	1.60
3	2-Q	7507	AMP	P-O5'	2.57	1.68	1.60
3	3-Q	7507	AMP	P-O5'	2.57	1.68	1.60
3	4-Q	7507	AMP	P-O5'	2.57	1.68	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-Q	7507	AMP	P-O5'	2.57	1.68	1.60
3	6-Q	7507	AMP	P-O5'	2.57	1.68	1.60
3	7-Q	7507	AMP	P-O5'	2.57	1.68	1.60
3	8-Q	7507	AMP	P-O5'	2.57	1.68	1.60
3	9-Q	7507	AMP	P-O5'	2.57	1.68	1.60
3	10-Q	7507	AMP	P-O5'	2.57	1.68	1.60
3	1-S	7511	AMP	P-O5'	2.57	1.68	1.60
3	2-S	7511	AMP	P-O5'	2.57	1.68	1.60
3	3-S	7511	AMP	P-O5'	2.57	1.68	1.60
3	4-S	7511	AMP	P-O5'	2.57	1.68	1.60
3	5-S	7511	AMP	P-O5'	2.57	1.68	1.60
3	6-S	7511	AMP	P-O5'	2.57	1.68	1.60
3	7-S	7511	AMP	P-O5'	2.57	1.68	1.60
3	8-S	7511	AMP	P-O5'	2.57	1.68	1.60
3	9-S	7511	AMP	P-O5'	2.57	1.68	1.60
3	10-S	7511	AMP	P-O5'	2.57	1.68	1.60
3	1-U	7515	AMP	P-O5'	2.57	1.68	1.60
3	2-U	7515	AMP	P-O5'	2.57	1.68	1.60
3	3-U	7515	AMP	P-O5'	2.57	1.68	1.60
3	4-U	7515	AMP	P-O5'	2.57	1.68	1.60
3	5-U	7515	AMP	P-O5'	2.57	1.68	1.60
3	6-U	7515	AMP	P-O5'	2.57	1.68	1.60
3	7-U	7515	AMP	P-O5'	2.57	1.68	1.60
3	8-U	7515	AMP	P-O5'	2.57	1.68	1.60
3	9-U	7515	AMP	P-O5'	2.57	1.68	1.60
3	10-U	7515	AMP	P-O5'	2.57	1.68	1.60
3	1-L	7497	AMP	P-O5'	2.56	1.68	1.60
3	2-L	7497	AMP	P-O5'	2.56	1.68	1.60
3	3-L	7497	AMP	P-O5'	2.56	1.68	1.60
3	4-L	7497	AMP	P-O5'	2.56	1.68	1.60
3	5-L	7497	AMP	P-O5'	2.56	1.68	1.60
3	6-L	7497	AMP	P-O5'	2.56	1.68	1.60
3	7-L	7497	AMP	P-O5'	2.56	1.68	1.60
3	8-L	7497	AMP	P-O5'	2.56	1.68	1.60
3	9-L	7497	AMP	P-O5'	2.56	1.68	1.60
3	10-L	7497	AMP	P-O5'	2.56	1.68	1.60
3	1-W	7519	AMP	P-O5'	2.56	1.68	1.60
3	2-W	7519	AMP	P-O5'	2.56	1.68	1.60
3	3-W	7519	AMP	P-O5'	2.56	1.68	1.60
3	4-W	7519	AMP	P-O5'	2.56	1.68	1.60
3	5-W	7519	AMP	P-O5'	2.56	1.68	1.60
3	6-W	7519	AMP	P-O5'	2.56	1.68	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-W	7519	AMP	P-O5'	2.56	1.68	1.60
3	8-W	7519	AMP	P-O5'	2.56	1.68	1.60
3	9-W	7519	AMP	P-O5'	2.56	1.68	1.60
3	10-W	7519	AMP	P-O5'	2.56	1.68	1.60
3	1-F	7485	AMP	P-O5'	2.56	1.68	1.60
3	2-F	7485	AMP	P-O5'	2.56	1.68	1.60
3	3-F	7485	AMP	P-O5'	2.56	1.68	1.60
3	4-F	7485	AMP	P-O5'	2.56	1.68	1.60
3	5-F	7485	AMP	P-O5'	2.56	1.68	1.60
3	6-F	7485	AMP	P-O5'	2.56	1.68	1.60
3	7-F	7485	AMP	P-O5'	2.56	1.68	1.60
3	8-F	7485	AMP	P-O5'	2.56	1.68	1.60
3	9-F	7485	AMP	P-O5'	2.56	1.68	1.60
3	10-F	7485	AMP	P-O5'	2.56	1.68	1.60
3	1-D	7481	AMP	P-O5'	2.56	1.68	1.60
3	2-D	7481	AMP	P-O5'	2.56	1.68	1.60
3	3-D	7481	AMP	P-O5'	2.56	1.68	1.60
3	4-D	7481	AMP	P-O5'	2.56	1.68	1.60
3	5-D	7481	AMP	P-O5'	2.56	1.68	1.60
3	6-D	7481	AMP	P-O5'	2.56	1.68	1.60
3	7-D	7481	AMP	P-O5'	2.56	1.68	1.60
3	8-D	7481	AMP	P-O5'	2.56	1.68	1.60
3	9-D	7481	AMP	P-O5'	2.56	1.68	1.60
3	10-D	7481	AMP	P-O5'	2.56	1.68	1.60
3	1-I	7491	AMP	P-O5'	2.56	1.68	1.60
3	2-I	7491	AMP	P-O5'	2.56	1.68	1.60
3	3-I	7491	AMP	P-O5'	2.56	1.68	1.60
3	4-I	7491	AMP	P-O5'	2.56	1.68	1.60
3	5-I	7491	AMP	P-O5'	2.56	1.68	1.60
3	6-I	7491	AMP	P-O5'	2.56	1.68	1.60
3	7-I	7491	AMP	P-O5'	2.56	1.68	1.60
3	8-I	7491	AMP	P-O5'	2.56	1.68	1.60
3	9-I	7491	AMP	P-O5'	2.56	1.68	1.60
3	10-I	7491	AMP	P-O5'	2.56	1.68	1.60
3	1-A	7475	AMP	P-O5'	2.56	1.68	1.60
3	2-A	7475	AMP	P-O5'	2.56	1.68	1.60
3	3-A	7475	AMP	P-O5'	2.56	1.68	1.60
3	4-A	7475	AMP	P-O5'	2.56	1.68	1.60
3	5-A	7475	AMP	P-O5'	2.56	1.68	1.60
3	6-A	7475	AMP	P-O5'	2.56	1.68	1.60
3	7-A	7475	AMP	P-O5'	2.56	1.68	1.60
3	8-A	7475	AMP	P-O5'	2.56	1.68	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-A	7475	AMP	P-O5'	2.56	1.68	1.60
3	10-A	7475	AMP	P-O5'	2.56	1.68	1.60
3	1-R	7509	AMP	P-O5'	2.56	1.68	1.60
3	2-R	7509	AMP	P-O5'	2.56	1.68	1.60
3	3-R	7509	AMP	P-O5'	2.56	1.68	1.60
3	4-R	7509	AMP	P-O5'	2.56	1.68	1.60
3	5-R	7509	AMP	P-O5'	2.56	1.68	1.60
3	6-R	7509	AMP	P-O5'	2.56	1.68	1.60
3	7-R	7509	AMP	P-O5'	2.56	1.68	1.60
3	8-R	7509	AMP	P-O5'	2.56	1.68	1.60
3	9-R	7509	AMP	P-O5'	2.56	1.68	1.60
3	10-R	7509	AMP	P-O5'	2.56	1.68	1.60
3	1-X	7521	AMP	P-O5'	2.55	1.68	1.60
3	2-X	7521	AMP	P-O5'	2.55	1.68	1.60
3	3-X	7521	AMP	P-O5'	2.55	1.68	1.60
3	4-X	7521	AMP	P-O5'	2.55	1.68	1.60
3	5-X	7521	AMP	P-O5'	2.55	1.68	1.60
3	6-X	7521	AMP	P-O5'	2.55	1.68	1.60
3	7-X	7521	AMP	P-O5'	2.55	1.68	1.60
3	8-X	7521	AMP	P-O5'	2.55	1.68	1.60
3	9-X	7521	AMP	P-O5'	2.55	1.68	1.60
3	10-X	7521	AMP	P-O5'	2.55	1.68	1.60
3	1-K	7495	AMP	P-O5'	2.55	1.68	1.60
3	2-K	7495	AMP	P-O5'	2.55	1.68	1.60
3	3-K	7495	AMP	P-O5'	2.55	1.68	1.60
3	4-K	7495	AMP	P-O5'	2.55	1.68	1.60
3	5-K	7495	AMP	P-O5'	2.55	1.68	1.60
3	6-K	7495	AMP	P-O5'	2.55	1.68	1.60
3	7-K	7495	AMP	P-O5'	2.55	1.68	1.60
3	8-K	7495	AMP	P-O5'	2.55	1.68	1.60
3	9-K	7495	AMP	P-O5'	2.55	1.68	1.60
3	10-K	7495	AMP	P-O5'	2.55	1.68	1.60
3	1-M	7499	AMP	P-O5'	2.55	1.68	1.60
3	2-M	7499	AMP	P-O5'	2.55	1.68	1.60
3	3-M	7499	AMP	P-O5'	2.55	1.68	1.60
3	4-M	7499	AMP	P-O5'	2.55	1.68	1.60
3	5-M	7499	AMP	P-O5'	2.55	1.68	1.60
3	6-M	7499	AMP	P-O5'	2.55	1.68	1.60
3	7-M	7499	AMP	P-O5'	2.55	1.68	1.60
3	8-M	7499	AMP	P-O5'	2.55	1.68	1.60
3	9-M	7499	AMP	P-O5'	2.55	1.68	1.60
3	10-M	7499	AMP	P-O5'	2.55	1.68	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-N	7501	AMP	P-O5'	2.55	1.68	1.60
3	2-N	7501	AMP	P-O5'	2.55	1.68	1.60
3	3-N	7501	AMP	P-O5'	2.55	1.68	1.60
3	4-N	7501	AMP	P-O5'	2.55	1.68	1.60
3	5-N	7501	AMP	P-O5'	2.55	1.68	1.60
3	6-N	7501	AMP	P-O5'	2.55	1.68	1.60
3	7-N	7501	AMP	P-O5'	2.55	1.68	1.60
3	8-N	7501	AMP	P-O5'	2.55	1.68	1.60
3	9-N	7501	AMP	P-O5'	2.55	1.68	1.60
3	10-N	7501	AMP	P-O5'	2.55	1.68	1.60
3	1-J	7493	AMP	P-O5'	2.55	1.68	1.60
3	2-J	7493	AMP	P-O5'	2.55	1.68	1.60
3	3-J	7493	AMP	P-O5'	2.55	1.68	1.60
3	4-J	7493	AMP	P-O5'	2.55	1.68	1.60
3	5-J	7493	AMP	P-O5'	2.55	1.68	1.60
3	6-J	7493	AMP	P-O5'	2.55	1.68	1.60
3	7-J	7493	AMP	P-O5'	2.55	1.68	1.60
3	8-J	7493	AMP	P-O5'	2.55	1.68	1.60
3	9-J	7493	AMP	P-O5'	2.55	1.68	1.60
3	10-J	7493	AMP	P-O5'	2.55	1.68	1.60
3	1-B	7477	AMP	P-O5'	2.55	1.68	1.60
3	2-B	7477	AMP	P-O5'	2.55	1.68	1.60
3	3-B	7477	AMP	P-O5'	2.55	1.68	1.60
3	4-B	7477	AMP	P-O5'	2.55	1.68	1.60
3	5-B	7477	AMP	P-O5'	2.55	1.68	1.60
3	6-B	7477	AMP	P-O5'	2.55	1.68	1.60
3	7-B	7477	AMP	P-O5'	2.55	1.68	1.60
3	8-B	7477	AMP	P-O5'	2.55	1.68	1.60
3	9-B	7477	AMP	P-O5'	2.55	1.68	1.60
3	10-B	7477	AMP	P-O5'	2.55	1.68	1.60
3	1-C	7479	AMP	P-O5'	2.55	1.68	1.60
3	2-C	7479	AMP	P-O5'	2.55	1.68	1.60
3	3-C	7479	AMP	P-O5'	2.55	1.68	1.60
3	4-C	7479	AMP	P-O5'	2.55	1.68	1.60
3	5-C	7479	AMP	P-O5'	2.55	1.68	1.60
3	6-C	7479	AMP	P-O5'	2.55	1.68	1.60
3	7-C	7479	AMP	P-O5'	2.55	1.68	1.60
3	8-C	7479	AMP	P-O5'	2.55	1.68	1.60
3	9-C	7479	AMP	P-O5'	2.55	1.68	1.60
3	10-C	7479	AMP	P-O5'	2.55	1.68	1.60
3	1-H	7489	AMP	P-O5'	2.55	1.68	1.60
3	2-H	7489	AMP	P-O5'	2.55	1.68	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-H	7489	AMP	P-O5'	2.55	1.68	1.60
3	4-H	7489	AMP	P-O5'	2.55	1.68	1.60
3	5-H	7489	AMP	P-O5'	2.55	1.68	1.60
3	6-H	7489	AMP	P-O5'	2.55	1.68	1.60
3	7-H	7489	AMP	P-O5'	2.55	1.68	1.60
3	8-H	7489	AMP	P-O5'	2.55	1.68	1.60
3	9-H	7489	AMP	P-O5'	2.55	1.68	1.60
3	10-H	7489	AMP	P-O5'	2.55	1.68	1.60
3	1-V	7517	AMP	P-O5'	2.54	1.68	1.60
3	2-V	7517	AMP	P-O5'	2.54	1.68	1.60
3	3-V	7517	AMP	P-O5'	2.54	1.68	1.60
3	4-V	7517	AMP	P-O5'	2.54	1.68	1.60
3	5-V	7517	AMP	P-O5'	2.54	1.68	1.60
3	6-V	7517	AMP	P-O5'	2.54	1.68	1.60
3	7-V	7517	AMP	P-O5'	2.54	1.68	1.60
3	8-V	7517	AMP	P-O5'	2.54	1.68	1.60
3	9-V	7517	AMP	P-O5'	2.54	1.68	1.60
3	10-V	7517	AMP	P-O5'	2.54	1.68	1.60
3	1-G	7487	AMP	P-O5'	2.54	1.68	1.60
3	2-G	7487	AMP	P-O5'	2.54	1.68	1.60
3	3-G	7487	AMP	P-O5'	2.54	1.68	1.60
3	4-G	7487	AMP	P-O5'	2.54	1.68	1.60
3	5-G	7487	AMP	P-O5'	2.54	1.68	1.60
3	6-G	7487	AMP	P-O5'	2.54	1.68	1.60
3	7-G	7487	AMP	P-O5'	2.54	1.68	1.60
3	8-G	7487	AMP	P-O5'	2.54	1.68	1.60
3	9-G	7487	AMP	P-O5'	2.54	1.68	1.60
3	10-G	7487	AMP	P-O5'	2.54	1.68	1.60
3	1-P	7505	AMP	P-O5'	2.54	1.68	1.60
3	2-P	7505	AMP	P-O5'	2.54	1.68	1.60
3	3-P	7505	AMP	P-O5'	2.54	1.68	1.60
3	4-P	7505	AMP	P-O5'	2.54	1.68	1.60
3	5-P	7505	AMP	P-O5'	2.54	1.68	1.60
3	6-P	7505	AMP	P-O5'	2.54	1.68	1.60
3	7-P	7505	AMP	P-O5'	2.54	1.68	1.60
3	8-P	7505	AMP	P-O5'	2.54	1.68	1.60
3	9-P	7505	AMP	P-O5'	2.54	1.68	1.60
3	10-P	7505	AMP	P-O5'	2.54	1.68	1.60
3	1-E	7483	AMP	P-O5'	2.54	1.68	1.60
3	2-E	7483	AMP	P-O5'	2.54	1.68	1.60
3	3-E	7483	AMP	P-O5'	2.54	1.68	1.60
3	4-E	7483	AMP	P-O5'	2.54	1.68	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-E	7483	AMP	P-O5'	2.54	1.68	1.60
3	6-E	7483	AMP	P-O5'	2.54	1.68	1.60
3	7-E	7483	AMP	P-O5'	2.54	1.68	1.60
3	8-E	7483	AMP	P-O5'	2.54	1.68	1.60
3	9-E	7483	AMP	P-O5'	2.54	1.68	1.60
3	10-E	7483	AMP	P-O5'	2.54	1.68	1.60
3	1-V	7517	AMP	C8-N7	2.49	1.36	1.31
3	2-V	7517	AMP	C8-N7	2.49	1.36	1.31
3	3-V	7517	AMP	C8-N7	2.49	1.36	1.31
3	4-V	7517	AMP	C8-N7	2.49	1.36	1.31
3	5-V	7517	AMP	C8-N7	2.49	1.36	1.31
3	6-V	7517	AMP	C8-N7	2.49	1.36	1.31
3	7-V	7517	AMP	C8-N7	2.49	1.36	1.31
3	8-V	7517	AMP	C8-N7	2.49	1.36	1.31
3	9-V	7517	AMP	C8-N7	2.49	1.36	1.31
3	10-V	7517	AMP	C8-N7	2.49	1.36	1.31
3	1-G	7487	AMP	P-O2P	2.49	1.64	1.54
3	2-G	7487	AMP	P-O2P	2.49	1.64	1.54
3	3-G	7487	AMP	P-O2P	2.49	1.64	1.54
3	4-G	7487	AMP	P-O2P	2.49	1.64	1.54
3	5-G	7487	AMP	P-O2P	2.49	1.64	1.54
3	6-G	7487	AMP	P-O2P	2.49	1.64	1.54
3	7-G	7487	AMP	P-O2P	2.49	1.64	1.54
3	8-G	7487	AMP	P-O2P	2.49	1.64	1.54
3	9-G	7487	AMP	P-O2P	2.49	1.64	1.54
3	10-G	7487	AMP	P-O2P	2.49	1.64	1.54
3	1-V	7517	AMP	P-O2P	2.49	1.64	1.54
3	2-V	7517	AMP	P-O2P	2.49	1.64	1.54
3	3-V	7517	AMP	P-O2P	2.49	1.64	1.54
3	4-V	7517	AMP	P-O2P	2.49	1.64	1.54
3	5-V	7517	AMP	P-O2P	2.49	1.64	1.54
3	6-V	7517	AMP	P-O2P	2.49	1.64	1.54
3	7-V	7517	AMP	P-O2P	2.49	1.64	1.54
3	8-V	7517	AMP	P-O2P	2.49	1.64	1.54
3	9-V	7517	AMP	P-O2P	2.49	1.64	1.54
3	10-V	7517	AMP	P-O2P	2.49	1.64	1.54
3	1-S	7511	AMP	P-O2P	2.49	1.64	1.54
3	2-S	7511	AMP	P-O2P	2.49	1.64	1.54
3	3-S	7511	AMP	P-O2P	2.49	1.64	1.54
3	4-S	7511	AMP	P-O2P	2.49	1.64	1.54
3	5-S	7511	AMP	P-O2P	2.49	1.64	1.54
3	6-S	7511	AMP	P-O2P	2.49	1.64	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-S	7511	AMP	P-O2P	2.49	1.64	1.54
3	8-S	7511	AMP	P-O2P	2.49	1.64	1.54
3	9-S	7511	AMP	P-O2P	2.49	1.64	1.54
3	10-S	7511	AMP	P-O2P	2.49	1.64	1.54
3	1-O	7503	AMP	P-O2P	2.49	1.64	1.54
3	2-O	7503	AMP	P-O2P	2.49	1.64	1.54
3	3-O	7503	AMP	P-O2P	2.49	1.64	1.54
3	4-O	7503	AMP	P-O2P	2.49	1.64	1.54
3	5-O	7503	AMP	P-O2P	2.49	1.64	1.54
3	6-O	7503	AMP	P-O2P	2.49	1.64	1.54
3	7-O	7503	AMP	P-O2P	2.49	1.64	1.54
3	8-O	7503	AMP	P-O2P	2.49	1.64	1.54
3	9-O	7503	AMP	P-O2P	2.49	1.64	1.54
3	10-O	7503	AMP	P-O2P	2.49	1.64	1.54
3	1-Q	7507	AMP	C8-N7	2.48	1.36	1.31
3	2-Q	7507	AMP	C8-N7	2.48	1.36	1.31
3	3-Q	7507	AMP	C8-N7	2.48	1.36	1.31
3	4-Q	7507	AMP	C8-N7	2.48	1.36	1.31
3	5-Q	7507	AMP	C8-N7	2.48	1.36	1.31
3	6-Q	7507	AMP	C8-N7	2.48	1.36	1.31
3	7-Q	7507	AMP	C8-N7	2.48	1.36	1.31
3	8-Q	7507	AMP	C8-N7	2.48	1.36	1.31
3	9-Q	7507	AMP	C8-N7	2.48	1.36	1.31
3	10-Q	7507	AMP	C8-N7	2.48	1.36	1.31
3	1-T	7513	AMP	C8-N7	2.48	1.36	1.31
3	2-T	7513	AMP	C8-N7	2.48	1.36	1.31
3	3-T	7513	AMP	C8-N7	2.48	1.36	1.31
3	4-T	7513	AMP	C8-N7	2.48	1.36	1.31
3	5-T	7513	AMP	C8-N7	2.48	1.36	1.31
3	6-T	7513	AMP	C8-N7	2.48	1.36	1.31
3	7-T	7513	AMP	C8-N7	2.48	1.36	1.31
3	8-T	7513	AMP	C8-N7	2.48	1.36	1.31
3	9-T	7513	AMP	C8-N7	2.48	1.36	1.31
3	10-T	7513	AMP	C8-N7	2.48	1.36	1.31
3	1-T	7513	AMP	P-O2P	2.48	1.64	1.54
3	2-T	7513	AMP	P-O2P	2.48	1.64	1.54
3	3-T	7513	AMP	P-O2P	2.48	1.64	1.54
3	4-T	7513	AMP	P-O2P	2.48	1.64	1.54
3	5-T	7513	AMP	P-O2P	2.48	1.64	1.54
3	6-T	7513	AMP	P-O2P	2.48	1.64	1.54
3	7-T	7513	AMP	P-O2P	2.48	1.64	1.54
3	8-T	7513	AMP	P-O2P	2.48	1.64	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-T	7513	AMP	P-O2P	2.48	1.64	1.54
3	10-T	7513	AMP	P-O2P	2.48	1.64	1.54
3	1-N	7501	AMP	C8-N7	2.48	1.36	1.31
3	2-N	7501	AMP	C8-N7	2.48	1.36	1.31
3	3-N	7501	AMP	C8-N7	2.48	1.36	1.31
3	4-N	7501	AMP	C8-N7	2.48	1.36	1.31
3	5-N	7501	AMP	C8-N7	2.48	1.36	1.31
3	6-N	7501	AMP	C8-N7	2.48	1.36	1.31
3	7-N	7501	AMP	C8-N7	2.48	1.36	1.31
3	8-N	7501	AMP	C8-N7	2.48	1.36	1.31
3	9-N	7501	AMP	C8-N7	2.48	1.36	1.31
3	10-N	7501	AMP	C8-N7	2.48	1.36	1.31
3	1-C	7479	AMP	P-O2P	2.48	1.64	1.54
3	2-C	7479	AMP	P-O2P	2.48	1.64	1.54
3	3-C	7479	AMP	P-O2P	2.48	1.64	1.54
3	4-C	7479	AMP	P-O2P	2.48	1.64	1.54
3	5-C	7479	AMP	P-O2P	2.48	1.64	1.54
3	6-C	7479	AMP	P-O2P	2.48	1.64	1.54
3	7-C	7479	AMP	P-O2P	2.48	1.64	1.54
3	8-C	7479	AMP	P-O2P	2.48	1.64	1.54
3	9-C	7479	AMP	P-O2P	2.48	1.64	1.54
3	10-C	7479	AMP	P-O2P	2.48	1.64	1.54
3	1-J	7493	AMP	P-O2P	2.48	1.64	1.54
3	2-J	7493	AMP	P-O2P	2.48	1.64	1.54
3	3-J	7493	AMP	P-O2P	2.48	1.64	1.54
3	4-J	7493	AMP	P-O2P	2.48	1.64	1.54
3	5-J	7493	AMP	P-O2P	2.48	1.64	1.54
3	6-J	7493	AMP	P-O2P	2.48	1.64	1.54
3	7-J	7493	AMP	P-O2P	2.48	1.64	1.54
3	8-J	7493	AMP	P-O2P	2.48	1.64	1.54
3	9-J	7493	AMP	P-O2P	2.48	1.64	1.54
3	10-J	7493	AMP	P-O2P	2.48	1.64	1.54
3	1-M	7499	AMP	C8-N7	2.48	1.36	1.31
3	2-M	7499	AMP	C8-N7	2.48	1.36	1.31
3	3-M	7499	AMP	C8-N7	2.48	1.36	1.31
3	4-M	7499	AMP	C8-N7	2.48	1.36	1.31
3	5-M	7499	AMP	C8-N7	2.48	1.36	1.31
3	6-M	7499	AMP	C8-N7	2.48	1.36	1.31
3	7-M	7499	AMP	C8-N7	2.48	1.36	1.31
3	8-M	7499	AMP	C8-N7	2.48	1.36	1.31
3	9-M	7499	AMP	C8-N7	2.48	1.36	1.31
3	10-M	7499	AMP	C8-N7	2.48	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	7477	AMP	P-O2P	2.48	1.64	1.54
3	2-B	7477	AMP	P-O2P	2.48	1.64	1.54
3	3-B	7477	AMP	P-O2P	2.48	1.64	1.54
3	4-B	7477	AMP	P-O2P	2.48	1.64	1.54
3	5-B	7477	AMP	P-O2P	2.48	1.64	1.54
3	6-B	7477	AMP	P-O2P	2.48	1.64	1.54
3	7-B	7477	AMP	P-O2P	2.48	1.64	1.54
3	8-B	7477	AMP	P-O2P	2.48	1.64	1.54
3	9-B	7477	AMP	P-O2P	2.48	1.64	1.54
3	10-B	7477	AMP	P-O2P	2.48	1.64	1.54
3	1-D	7481	AMP	P-O2P	2.48	1.64	1.54
3	2-D	7481	AMP	P-O2P	2.48	1.64	1.54
3	3-D	7481	AMP	P-O2P	2.48	1.64	1.54
3	4-D	7481	AMP	P-O2P	2.48	1.64	1.54
3	5-D	7481	AMP	P-O2P	2.48	1.64	1.54
3	6-D	7481	AMP	P-O2P	2.48	1.64	1.54
3	7-D	7481	AMP	P-O2P	2.48	1.64	1.54
3	8-D	7481	AMP	P-O2P	2.48	1.64	1.54
3	9-D	7481	AMP	P-O2P	2.48	1.64	1.54
3	10-D	7481	AMP	P-O2P	2.48	1.64	1.54
3	1-H	7489	AMP	C8-N7	2.48	1.36	1.31
3	2-H	7489	AMP	C8-N7	2.48	1.36	1.31
3	3-H	7489	AMP	C8-N7	2.48	1.36	1.31
3	4-H	7489	AMP	C8-N7	2.48	1.36	1.31
3	5-H	7489	AMP	C8-N7	2.48	1.36	1.31
3	6-H	7489	AMP	C8-N7	2.48	1.36	1.31
3	7-H	7489	AMP	C8-N7	2.48	1.36	1.31
3	8-H	7489	AMP	C8-N7	2.48	1.36	1.31
3	9-H	7489	AMP	C8-N7	2.48	1.36	1.31
3	10-H	7489	AMP	C8-N7	2.48	1.36	1.31
3	1-A	7475	AMP	P-O2P	2.48	1.64	1.54
3	2-A	7475	AMP	P-O2P	2.48	1.64	1.54
3	3-A	7475	AMP	P-O2P	2.48	1.64	1.54
3	4-A	7475	AMP	P-O2P	2.48	1.64	1.54
3	5-A	7475	AMP	P-O2P	2.48	1.64	1.54
3	6-A	7475	AMP	P-O2P	2.48	1.64	1.54
3	7-A	7475	AMP	P-O2P	2.48	1.64	1.54
3	8-A	7475	AMP	P-O2P	2.48	1.64	1.54
3	9-A	7475	AMP	P-O2P	2.48	1.64	1.54
3	10-A	7475	AMP	P-O2P	2.48	1.64	1.54
3	1-Q	7507	AMP	P-O2P	2.48	1.64	1.54
3	2-Q	7507	AMP	P-O2P	2.48	1.64	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-Q	7507	AMP	P-O2P	2.48	1.64	1.54
3	4-Q	7507	AMP	P-O2P	2.48	1.64	1.54
3	5-Q	7507	AMP	P-O2P	2.48	1.64	1.54
3	6-Q	7507	AMP	P-O2P	2.48	1.64	1.54
3	7-Q	7507	AMP	P-O2P	2.48	1.64	1.54
3	8-Q	7507	AMP	P-O2P	2.48	1.64	1.54
3	9-Q	7507	AMP	P-O2P	2.48	1.64	1.54
3	10-Q	7507	AMP	P-O2P	2.48	1.64	1.54
3	1-R	7509	AMP	P-O2P	2.48	1.64	1.54
3	2-R	7509	AMP	P-O2P	2.48	1.64	1.54
3	3-R	7509	AMP	P-O2P	2.48	1.64	1.54
3	4-R	7509	AMP	P-O2P	2.48	1.64	1.54
3	5-R	7509	AMP	P-O2P	2.48	1.64	1.54
3	6-R	7509	AMP	P-O2P	2.48	1.64	1.54
3	7-R	7509	AMP	P-O2P	2.48	1.64	1.54
3	8-R	7509	AMP	P-O2P	2.48	1.64	1.54
3	9-R	7509	AMP	P-O2P	2.48	1.64	1.54
3	10-R	7509	AMP	P-O2P	2.48	1.64	1.54
4	1-V	7518	CIT	O5-C6	2.48	1.29	1.22
4	2-V	7518	CIT	O5-C6	2.48	1.29	1.22
4	3-V	7518	CIT	O5-C6	2.48	1.29	1.22
4	4-V	7518	CIT	O5-C6	2.48	1.29	1.22
4	5-V	7518	CIT	O5-C6	2.48	1.29	1.22
4	6-V	7518	CIT	O5-C6	2.48	1.29	1.22
4	7-V	7518	CIT	O5-C6	2.48	1.29	1.22
4	8-V	7518	CIT	O5-C6	2.48	1.29	1.22
4	9-V	7518	CIT	O5-C6	2.48	1.29	1.22
4	10-V	7518	CIT	O5-C6	2.48	1.29	1.22
3	1-O	7503	AMP	C8-N7	2.48	1.36	1.31
3	2-O	7503	AMP	C8-N7	2.48	1.36	1.31
3	3-O	7503	AMP	C8-N7	2.48	1.36	1.31
3	4-O	7503	AMP	C8-N7	2.48	1.36	1.31
3	5-O	7503	AMP	C8-N7	2.48	1.36	1.31
3	6-O	7503	AMP	C8-N7	2.48	1.36	1.31
3	7-O	7503	AMP	C8-N7	2.48	1.36	1.31
3	8-O	7503	AMP	C8-N7	2.48	1.36	1.31
3	9-O	7503	AMP	C8-N7	2.48	1.36	1.31
3	10-O	7503	AMP	C8-N7	2.48	1.36	1.31
3	1-P	7505	AMP	P-O2P	2.47	1.64	1.54
3	2-P	7505	AMP	P-O2P	2.47	1.64	1.54
3	3-P	7505	AMP	P-O2P	2.47	1.64	1.54
3	4-P	7505	AMP	P-O2P	2.47	1.64	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-P	7505	AMP	P-O2P	2.47	1.64	1.54
3	6-P	7505	AMP	P-O2P	2.47	1.64	1.54
3	7-P	7505	AMP	P-O2P	2.47	1.64	1.54
3	8-P	7505	AMP	P-O2P	2.47	1.64	1.54
3	9-P	7505	AMP	P-O2P	2.47	1.64	1.54
3	10-P	7505	AMP	P-O2P	2.47	1.64	1.54
3	1-F	7485	AMP	P-O2P	2.47	1.64	1.54
3	2-F	7485	AMP	P-O2P	2.47	1.64	1.54
3	3-F	7485	AMP	P-O2P	2.47	1.64	1.54
3	4-F	7485	AMP	P-O2P	2.47	1.64	1.54
3	5-F	7485	AMP	P-O2P	2.47	1.64	1.54
3	6-F	7485	AMP	P-O2P	2.47	1.64	1.54
3	7-F	7485	AMP	P-O2P	2.47	1.64	1.54
3	8-F	7485	AMP	P-O2P	2.47	1.64	1.54
3	9-F	7485	AMP	P-O2P	2.47	1.64	1.54
3	10-F	7485	AMP	P-O2P	2.47	1.64	1.54
4	1-D	7482	CIT	O5-C6	2.47	1.29	1.22
4	2-D	7482	CIT	O5-C6	2.47	1.29	1.22
4	3-D	7482	CIT	O5-C6	2.47	1.29	1.22
4	4-D	7482	CIT	O5-C6	2.47	1.29	1.22
4	5-D	7482	CIT	O5-C6	2.47	1.29	1.22
4	6-D	7482	CIT	O5-C6	2.47	1.29	1.22
4	7-D	7482	CIT	O5-C6	2.47	1.29	1.22
4	8-D	7482	CIT	O5-C6	2.47	1.29	1.22
4	9-D	7482	CIT	O5-C6	2.47	1.29	1.22
4	10-D	7482	CIT	O5-C6	2.47	1.29	1.22
3	1-H	7489	AMP	P-O2P	2.47	1.64	1.54
3	2-H	7489	AMP	P-O2P	2.47	1.64	1.54
3	3-H	7489	AMP	P-O2P	2.47	1.64	1.54
3	4-H	7489	AMP	P-O2P	2.47	1.64	1.54
3	5-H	7489	AMP	P-O2P	2.47	1.64	1.54
3	6-H	7489	AMP	P-O2P	2.47	1.64	1.54
3	7-H	7489	AMP	P-O2P	2.47	1.64	1.54
3	8-H	7489	AMP	P-O2P	2.47	1.64	1.54
3	9-H	7489	AMP	P-O2P	2.47	1.64	1.54
3	10-H	7489	AMP	P-O2P	2.47	1.64	1.54
3	1-W	7519	AMP	P-O2P	2.47	1.64	1.54
3	2-W	7519	AMP	P-O2P	2.47	1.64	1.54
3	3-W	7519	AMP	P-O2P	2.47	1.64	1.54
3	4-W	7519	AMP	P-O2P	2.47	1.64	1.54
3	5-W	7519	AMP	P-O2P	2.47	1.64	1.54
3	6-W	7519	AMP	P-O2P	2.47	1.64	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-W	7519	AMP	P-O2P	2.47	1.64	1.54
3	8-W	7519	AMP	P-O2P	2.47	1.64	1.54
3	9-W	7519	AMP	P-O2P	2.47	1.64	1.54
3	10-W	7519	AMP	P-O2P	2.47	1.64	1.54
4	1-G	7488	CIT	O5-C6	2.47	1.29	1.22
4	2-G	7488	CIT	O5-C6	2.47	1.29	1.22
4	3-G	7488	CIT	O5-C6	2.47	1.29	1.22
4	4-G	7488	CIT	O5-C6	2.47	1.29	1.22
4	5-G	7488	CIT	O5-C6	2.47	1.29	1.22
4	6-G	7488	CIT	O5-C6	2.47	1.29	1.22
4	7-G	7488	CIT	O5-C6	2.47	1.29	1.22
4	8-G	7488	CIT	O5-C6	2.47	1.29	1.22
4	9-G	7488	CIT	O5-C6	2.47	1.29	1.22
4	10-G	7488	CIT	O5-C6	2.47	1.29	1.22
4	1-F	7486	CIT	O5-C6	2.47	1.29	1.22
4	2-F	7486	CIT	O5-C6	2.47	1.29	1.22
4	3-F	7486	CIT	O5-C6	2.47	1.29	1.22
4	4-F	7486	CIT	O5-C6	2.47	1.29	1.22
4	5-F	7486	CIT	O5-C6	2.47	1.29	1.22
4	6-F	7486	CIT	O5-C6	2.47	1.29	1.22
4	7-F	7486	CIT	O5-C6	2.47	1.29	1.22
4	8-F	7486	CIT	O5-C6	2.47	1.29	1.22
4	9-F	7486	CIT	O5-C6	2.47	1.29	1.22
4	10-F	7486	CIT	O5-C6	2.47	1.29	1.22
4	1-S	7512	CIT	O5-C6	2.47	1.29	1.22
4	2-S	7512	CIT	O5-C6	2.47	1.29	1.22
4	3-S	7512	CIT	O5-C6	2.47	1.29	1.22
4	4-S	7512	CIT	O5-C6	2.47	1.29	1.22
4	5-S	7512	CIT	O5-C6	2.47	1.29	1.22
4	6-S	7512	CIT	O5-C6	2.47	1.29	1.22
4	7-S	7512	CIT	O5-C6	2.47	1.29	1.22
4	8-S	7512	CIT	O5-C6	2.47	1.29	1.22
4	9-S	7512	CIT	O5-C6	2.47	1.29	1.22
4	10-S	7512	CIT	O5-C6	2.47	1.29	1.22
3	1-J	7493	AMP	C8-N7	2.47	1.36	1.31
3	2-J	7493	AMP	C8-N7	2.47	1.36	1.31
3	3-J	7493	AMP	C8-N7	2.47	1.36	1.31
3	4-J	7493	AMP	C8-N7	2.47	1.36	1.31
3	5-J	7493	AMP	C8-N7	2.47	1.36	1.31
3	6-J	7493	AMP	C8-N7	2.47	1.36	1.31
3	7-J	7493	AMP	C8-N7	2.47	1.36	1.31
3	8-J	7493	AMP	C8-N7	2.47	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-J	7493	AMP	C8-N7	2.47	1.36	1.31
3	10-J	7493	AMP	C8-N7	2.47	1.36	1.31
3	1-K	7495	AMP	P-O2P	2.47	1.64	1.54
3	2-K	7495	AMP	P-O2P	2.47	1.64	1.54
3	3-K	7495	AMP	P-O2P	2.47	1.64	1.54
3	4-K	7495	AMP	P-O2P	2.47	1.64	1.54
3	5-K	7495	AMP	P-O2P	2.47	1.64	1.54
3	6-K	7495	AMP	P-O2P	2.47	1.64	1.54
3	7-K	7495	AMP	P-O2P	2.47	1.64	1.54
3	8-K	7495	AMP	P-O2P	2.47	1.64	1.54
3	9-K	7495	AMP	P-O2P	2.47	1.64	1.54
3	10-K	7495	AMP	P-O2P	2.47	1.64	1.54
3	1-I	7491	AMP	P-O2P	2.47	1.64	1.54
3	2-I	7491	AMP	P-O2P	2.47	1.64	1.54
3	3-I	7491	AMP	P-O2P	2.47	1.64	1.54
3	4-I	7491	AMP	P-O2P	2.47	1.64	1.54
3	5-I	7491	AMP	P-O2P	2.47	1.64	1.54
3	6-I	7491	AMP	P-O2P	2.47	1.64	1.54
3	7-I	7491	AMP	P-O2P	2.47	1.64	1.54
3	8-I	7491	AMP	P-O2P	2.47	1.64	1.54
3	9-I	7491	AMP	P-O2P	2.47	1.64	1.54
3	10-I	7491	AMP	P-O2P	2.47	1.64	1.54
3	1-N	7501	AMP	P-O2P	2.47	1.64	1.54
3	2-N	7501	AMP	P-O2P	2.47	1.64	1.54
3	3-N	7501	AMP	P-O2P	2.47	1.64	1.54
3	4-N	7501	AMP	P-O2P	2.47	1.64	1.54
3	5-N	7501	AMP	P-O2P	2.47	1.64	1.54
3	6-N	7501	AMP	P-O2P	2.47	1.64	1.54
3	7-N	7501	AMP	P-O2P	2.47	1.64	1.54
3	8-N	7501	AMP	P-O2P	2.47	1.64	1.54
3	9-N	7501	AMP	P-O2P	2.47	1.64	1.54
3	10-N	7501	AMP	P-O2P	2.47	1.64	1.54
4	1-U	7516	CIT	O5-C6	2.47	1.29	1.22
4	2-U	7516	CIT	O5-C6	2.47	1.29	1.22
4	3-U	7516	CIT	O5-C6	2.47	1.29	1.22
4	4-U	7516	CIT	O5-C6	2.47	1.29	1.22
4	5-U	7516	CIT	O5-C6	2.47	1.29	1.22
4	6-U	7516	CIT	O5-C6	2.47	1.29	1.22
4	7-U	7516	CIT	O5-C6	2.47	1.29	1.22
4	8-U	7516	CIT	O5-C6	2.47	1.29	1.22
4	9-U	7516	CIT	O5-C6	2.47	1.29	1.22
4	10-U	7516	CIT	O5-C6	2.47	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-J	7494	CIT	O5-C6	2.47	1.29	1.22
4	2-J	7494	CIT	O5-C6	2.47	1.29	1.22
4	3-J	7494	CIT	O5-C6	2.47	1.29	1.22
4	4-J	7494	CIT	O5-C6	2.47	1.29	1.22
4	5-J	7494	CIT	O5-C6	2.47	1.29	1.22
4	6-J	7494	CIT	O5-C6	2.47	1.29	1.22
4	7-J	7494	CIT	O5-C6	2.47	1.29	1.22
4	8-J	7494	CIT	O5-C6	2.47	1.29	1.22
4	9-J	7494	CIT	O5-C6	2.47	1.29	1.22
4	10-J	7494	CIT	O5-C6	2.47	1.29	1.22
3	1-U	7515	AMP	P-O2P	2.47	1.64	1.54
3	2-U	7515	AMP	P-O2P	2.47	1.64	1.54
3	3-U	7515	AMP	P-O2P	2.47	1.64	1.54
3	4-U	7515	AMP	P-O2P	2.47	1.64	1.54
3	5-U	7515	AMP	P-O2P	2.47	1.64	1.54
3	6-U	7515	AMP	P-O2P	2.47	1.64	1.54
3	7-U	7515	AMP	P-O2P	2.47	1.64	1.54
3	8-U	7515	AMP	P-O2P	2.47	1.64	1.54
3	9-U	7515	AMP	P-O2P	2.47	1.64	1.54
3	10-U	7515	AMP	P-O2P	2.47	1.64	1.54
4	1-T	7514	CIT	O5-C6	2.47	1.29	1.22
4	2-T	7514	CIT	O5-C6	2.47	1.29	1.22
4	3-T	7514	CIT	O5-C6	2.47	1.29	1.22
4	4-T	7514	CIT	O5-C6	2.47	1.29	1.22
4	5-T	7514	CIT	O5-C6	2.47	1.29	1.22
4	6-T	7514	CIT	O5-C6	2.47	1.29	1.22
4	7-T	7514	CIT	O5-C6	2.47	1.29	1.22
4	8-T	7514	CIT	O5-C6	2.47	1.29	1.22
4	9-T	7514	CIT	O5-C6	2.47	1.29	1.22
4	10-T	7514	CIT	O5-C6	2.47	1.29	1.22
4	1-Q	7508	CIT	O5-C6	2.47	1.29	1.22
4	2-Q	7508	CIT	O5-C6	2.47	1.29	1.22
4	3-Q	7508	CIT	O5-C6	2.47	1.29	1.22
4	4-Q	7508	CIT	O5-C6	2.47	1.29	1.22
4	5-Q	7508	CIT	O5-C6	2.47	1.29	1.22
4	6-Q	7508	CIT	O5-C6	2.47	1.29	1.22
4	7-Q	7508	CIT	O5-C6	2.47	1.29	1.22
4	8-Q	7508	CIT	O5-C6	2.47	1.29	1.22
4	9-Q	7508	CIT	O5-C6	2.47	1.29	1.22
4	10-Q	7508	CIT	O5-C6	2.47	1.29	1.22
3	1-X	7521	AMP	P-O2P	2.47	1.64	1.54
3	2-X	7521	AMP	P-O2P	2.47	1.64	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-X	7521	AMP	P-O2P	2.47	1.64	1.54
3	4-X	7521	AMP	P-O2P	2.47	1.64	1.54
3	5-X	7521	AMP	P-O2P	2.47	1.64	1.54
3	6-X	7521	AMP	P-O2P	2.47	1.64	1.54
3	7-X	7521	AMP	P-O2P	2.47	1.64	1.54
3	8-X	7521	AMP	P-O2P	2.47	1.64	1.54
3	9-X	7521	AMP	P-O2P	2.47	1.64	1.54
3	10-X	7521	AMP	P-O2P	2.47	1.64	1.54
3	1-P	7505	AMP	C8-N7	2.46	1.36	1.31
3	2-P	7505	AMP	C8-N7	2.46	1.36	1.31
3	3-P	7505	AMP	C8-N7	2.46	1.36	1.31
3	4-P	7505	AMP	C8-N7	2.46	1.36	1.31
3	5-P	7505	AMP	C8-N7	2.46	1.36	1.31
3	6-P	7505	AMP	C8-N7	2.46	1.36	1.31
3	7-P	7505	AMP	C8-N7	2.46	1.36	1.31
3	8-P	7505	AMP	C8-N7	2.46	1.36	1.31
3	9-P	7505	AMP	C8-N7	2.46	1.36	1.31
3	10-P	7505	AMP	C8-N7	2.46	1.36	1.31
3	1-E	7483	AMP	P-O2P	2.46	1.63	1.54
3	2-E	7483	AMP	P-O2P	2.46	1.63	1.54
3	3-E	7483	AMP	P-O2P	2.46	1.63	1.54
3	4-E	7483	AMP	P-O2P	2.46	1.63	1.54
3	5-E	7483	AMP	P-O2P	2.46	1.63	1.54
3	6-E	7483	AMP	P-O2P	2.46	1.63	1.54
3	7-E	7483	AMP	P-O2P	2.46	1.63	1.54
3	8-E	7483	AMP	P-O2P	2.46	1.63	1.54
3	9-E	7483	AMP	P-O2P	2.46	1.63	1.54
3	10-E	7483	AMP	P-O2P	2.46	1.63	1.54
3	1-M	7499	AMP	P-O2P	2.46	1.63	1.54
3	2-M	7499	AMP	P-O2P	2.46	1.63	1.54
3	3-M	7499	AMP	P-O2P	2.46	1.63	1.54
3	4-M	7499	AMP	P-O2P	2.46	1.63	1.54
3	5-M	7499	AMP	P-O2P	2.46	1.63	1.54
3	6-M	7499	AMP	P-O2P	2.46	1.63	1.54
3	7-M	7499	AMP	P-O2P	2.46	1.63	1.54
3	8-M	7499	AMP	P-O2P	2.46	1.63	1.54
3	9-M	7499	AMP	P-O2P	2.46	1.63	1.54
3	10-M	7499	AMP	P-O2P	2.46	1.63	1.54
3	1-L	7497	AMP	P-O2P	2.46	1.63	1.54
3	2-L	7497	AMP	P-O2P	2.46	1.63	1.54
3	3-L	7497	AMP	P-O2P	2.46	1.63	1.54
3	4-L	7497	AMP	P-O2P	2.46	1.63	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-L	7497	AMP	P-O2P	2.46	1.63	1.54
3	6-L	7497	AMP	P-O2P	2.46	1.63	1.54
3	7-L	7497	AMP	P-O2P	2.46	1.63	1.54
3	8-L	7497	AMP	P-O2P	2.46	1.63	1.54
3	9-L	7497	AMP	P-O2P	2.46	1.63	1.54
3	10-L	7497	AMP	P-O2P	2.46	1.63	1.54
4	1-C	7480	CIT	O5-C6	2.46	1.29	1.22
4	2-C	7480	CIT	O5-C6	2.46	1.29	1.22
4	3-C	7480	CIT	O5-C6	2.46	1.29	1.22
4	4-C	7480	CIT	O5-C6	2.46	1.29	1.22
4	5-C	7480	CIT	O5-C6	2.46	1.29	1.22
4	6-C	7480	CIT	O5-C6	2.46	1.29	1.22
4	7-C	7480	CIT	O5-C6	2.46	1.29	1.22
4	8-C	7480	CIT	O5-C6	2.46	1.29	1.22
4	9-C	7480	CIT	O5-C6	2.46	1.29	1.22
4	10-C	7480	CIT	O5-C6	2.46	1.29	1.22
4	1-H	7490	CIT	O5-C6	2.46	1.29	1.22
4	2-H	7490	CIT	O5-C6	2.46	1.29	1.22
4	3-H	7490	CIT	O5-C6	2.46	1.29	1.22
4	4-H	7490	CIT	O5-C6	2.46	1.29	1.22
4	5-H	7490	CIT	O5-C6	2.46	1.29	1.22
4	6-H	7490	CIT	O5-C6	2.46	1.29	1.22
4	7-H	7490	CIT	O5-C6	2.46	1.29	1.22
4	8-H	7490	CIT	O5-C6	2.46	1.29	1.22
4	9-H	7490	CIT	O5-C6	2.46	1.29	1.22
4	10-H	7490	CIT	O5-C6	2.46	1.29	1.22
4	1-M	7500	CIT	O5-C6	2.46	1.29	1.22
4	2-M	7500	CIT	O5-C6	2.46	1.29	1.22
4	3-M	7500	CIT	O5-C6	2.46	1.29	1.22
4	4-M	7500	CIT	O5-C6	2.46	1.29	1.22
4	5-M	7500	CIT	O5-C6	2.46	1.29	1.22
4	6-M	7500	CIT	O5-C6	2.46	1.29	1.22
4	7-M	7500	CIT	O5-C6	2.46	1.29	1.22
4	8-M	7500	CIT	O5-C6	2.46	1.29	1.22
4	9-M	7500	CIT	O5-C6	2.46	1.29	1.22
4	10-M	7500	CIT	O5-C6	2.46	1.29	1.22
4	1-E	7484	CIT	O5-C6	2.46	1.29	1.22
4	2-E	7484	CIT	O5-C6	2.46	1.29	1.22
4	3-E	7484	CIT	O5-C6	2.46	1.29	1.22
4	4-E	7484	CIT	O5-C6	2.46	1.29	1.22
4	5-E	7484	CIT	O5-C6	2.46	1.29	1.22
4	6-E	7484	CIT	O5-C6	2.46	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-E	7484	CIT	O5-C6	2.46	1.29	1.22
4	8-E	7484	CIT	O5-C6	2.46	1.29	1.22
4	9-E	7484	CIT	O5-C6	2.46	1.29	1.22
4	10-E	7484	CIT	O5-C6	2.46	1.29	1.22
4	1-R	7510	CIT	O5-C6	2.46	1.29	1.22
4	2-R	7510	CIT	O5-C6	2.46	1.29	1.22
4	3-R	7510	CIT	O5-C6	2.46	1.29	1.22
4	4-R	7510	CIT	O5-C6	2.46	1.29	1.22
4	5-R	7510	CIT	O5-C6	2.46	1.29	1.22
4	6-R	7510	CIT	O5-C6	2.46	1.29	1.22
4	7-R	7510	CIT	O5-C6	2.46	1.29	1.22
4	8-R	7510	CIT	O5-C6	2.46	1.29	1.22
4	9-R	7510	CIT	O5-C6	2.46	1.29	1.22
4	10-R	7510	CIT	O5-C6	2.46	1.29	1.22
3	1-X	7521	AMP	C8-N7	2.45	1.36	1.31
3	2-X	7521	AMP	C8-N7	2.45	1.36	1.31
3	3-X	7521	AMP	C8-N7	2.45	1.36	1.31
3	4-X	7521	AMP	C8-N7	2.45	1.36	1.31
3	5-X	7521	AMP	C8-N7	2.45	1.36	1.31
3	6-X	7521	AMP	C8-N7	2.45	1.36	1.31
3	7-X	7521	AMP	C8-N7	2.45	1.36	1.31
3	8-X	7521	AMP	C8-N7	2.45	1.36	1.31
3	9-X	7521	AMP	C8-N7	2.45	1.36	1.31
3	10-X	7521	AMP	C8-N7	2.45	1.36	1.31
4	1-K	7496	CIT	O5-C6	2.45	1.29	1.22
4	2-K	7496	CIT	O5-C6	2.45	1.29	1.22
4	3-K	7496	CIT	O5-C6	2.45	1.29	1.22
4	4-K	7496	CIT	O5-C6	2.45	1.29	1.22
4	5-K	7496	CIT	O5-C6	2.45	1.29	1.22
4	6-K	7496	CIT	O5-C6	2.45	1.29	1.22
4	7-K	7496	CIT	O5-C6	2.45	1.29	1.22
4	8-K	7496	CIT	O5-C6	2.45	1.29	1.22
4	9-K	7496	CIT	O5-C6	2.45	1.29	1.22
4	10-K	7496	CIT	O5-C6	2.45	1.29	1.22
3	1-R	7509	AMP	C8-N7	2.45	1.36	1.31
3	2-R	7509	AMP	C8-N7	2.45	1.36	1.31
3	3-R	7509	AMP	C8-N7	2.45	1.36	1.31
3	4-R	7509	AMP	C8-N7	2.45	1.36	1.31
3	5-R	7509	AMP	C8-N7	2.45	1.36	1.31
3	6-R	7509	AMP	C8-N7	2.45	1.36	1.31
3	7-R	7509	AMP	C8-N7	2.45	1.36	1.31
3	8-R	7509	AMP	C8-N7	2.45	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-R	7509	AMP	C8-N7	2.45	1.36	1.31
3	10-R	7509	AMP	C8-N7	2.45	1.36	1.31
3	1-I	7491	AMP	C8-N7	2.45	1.36	1.31
3	2-I	7491	AMP	C8-N7	2.45	1.36	1.31
3	3-I	7491	AMP	C8-N7	2.45	1.36	1.31
3	4-I	7491	AMP	C8-N7	2.45	1.36	1.31
3	5-I	7491	AMP	C8-N7	2.45	1.36	1.31
3	6-I	7491	AMP	C8-N7	2.45	1.36	1.31
3	7-I	7491	AMP	C8-N7	2.45	1.36	1.31
3	8-I	7491	AMP	C8-N7	2.45	1.36	1.31
3	9-I	7491	AMP	C8-N7	2.45	1.36	1.31
3	10-I	7491	AMP	C8-N7	2.45	1.36	1.31
4	1-N	7502	CIT	O5-C6	2.45	1.29	1.22
4	2-N	7502	CIT	O5-C6	2.45	1.29	1.22
4	3-N	7502	CIT	O5-C6	2.45	1.29	1.22
4	4-N	7502	CIT	O5-C6	2.45	1.29	1.22
4	5-N	7502	CIT	O5-C6	2.45	1.29	1.22
4	6-N	7502	CIT	O5-C6	2.45	1.29	1.22
4	7-N	7502	CIT	O5-C6	2.45	1.29	1.22
4	8-N	7502	CIT	O5-C6	2.45	1.29	1.22
4	9-N	7502	CIT	O5-C6	2.45	1.29	1.22
4	10-N	7502	CIT	O5-C6	2.45	1.29	1.22
3	1-A	7475	AMP	C8-N7	2.45	1.36	1.31
3	2-A	7475	AMP	C8-N7	2.45	1.36	1.31
3	3-A	7475	AMP	C8-N7	2.45	1.36	1.31
3	4-A	7475	AMP	C8-N7	2.45	1.36	1.31
3	5-A	7475	AMP	C8-N7	2.45	1.36	1.31
3	6-A	7475	AMP	C8-N7	2.45	1.36	1.31
3	7-A	7475	AMP	C8-N7	2.45	1.36	1.31
3	8-A	7475	AMP	C8-N7	2.45	1.36	1.31
3	9-A	7475	AMP	C8-N7	2.45	1.36	1.31
3	10-A	7475	AMP	C8-N7	2.45	1.36	1.31
3	1-B	7477	AMP	C8-N7	2.45	1.36	1.31
3	2-B	7477	AMP	C8-N7	2.45	1.36	1.31
3	3-B	7477	AMP	C8-N7	2.45	1.36	1.31
3	4-B	7477	AMP	C8-N7	2.45	1.36	1.31
3	5-B	7477	AMP	C8-N7	2.45	1.36	1.31
3	6-B	7477	AMP	C8-N7	2.45	1.36	1.31
3	7-B	7477	AMP	C8-N7	2.45	1.36	1.31
3	8-B	7477	AMP	C8-N7	2.45	1.36	1.31
3	9-B	7477	AMP	C8-N7	2.45	1.36	1.31
3	10-B	7477	AMP	C8-N7	2.45	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-G	7487	AMP	C8-N7	2.45	1.36	1.31
3	2-G	7487	AMP	C8-N7	2.45	1.36	1.31
3	3-G	7487	AMP	C8-N7	2.45	1.36	1.31
3	4-G	7487	AMP	C8-N7	2.45	1.36	1.31
3	5-G	7487	AMP	C8-N7	2.45	1.36	1.31
3	6-G	7487	AMP	C8-N7	2.45	1.36	1.31
3	7-G	7487	AMP	C8-N7	2.45	1.36	1.31
3	8-G	7487	AMP	C8-N7	2.45	1.36	1.31
3	9-G	7487	AMP	C8-N7	2.45	1.36	1.31
3	10-G	7487	AMP	C8-N7	2.45	1.36	1.31
4	1-A	7476	CIT	O5-C6	2.45	1.29	1.22
4	2-A	7476	CIT	O5-C6	2.45	1.29	1.22
4	3-A	7476	CIT	O5-C6	2.45	1.29	1.22
4	4-A	7476	CIT	O5-C6	2.45	1.29	1.22
4	5-A	7476	CIT	O5-C6	2.45	1.29	1.22
4	6-A	7476	CIT	O5-C6	2.45	1.29	1.22
4	7-A	7476	CIT	O5-C6	2.45	1.29	1.22
4	8-A	7476	CIT	O5-C6	2.45	1.29	1.22
4	9-A	7476	CIT	O5-C6	2.45	1.29	1.22
4	10-A	7476	CIT	O5-C6	2.45	1.29	1.22
3	1-C	7479	AMP	C8-N7	2.45	1.36	1.31
3	2-C	7479	AMP	C8-N7	2.45	1.36	1.31
3	3-C	7479	AMP	C8-N7	2.45	1.36	1.31
3	4-C	7479	AMP	C8-N7	2.45	1.36	1.31
3	5-C	7479	AMP	C8-N7	2.45	1.36	1.31
3	6-C	7479	AMP	C8-N7	2.45	1.36	1.31
3	7-C	7479	AMP	C8-N7	2.45	1.36	1.31
3	8-C	7479	AMP	C8-N7	2.45	1.36	1.31
3	9-C	7479	AMP	C8-N7	2.45	1.36	1.31
3	10-C	7479	AMP	C8-N7	2.45	1.36	1.31
4	1-I	7492	CIT	O5-C6	2.45	1.29	1.22
4	2-I	7492	CIT	O5-C6	2.45	1.29	1.22
4	3-I	7492	CIT	O5-C6	2.45	1.29	1.22
4	4-I	7492	CIT	O5-C6	2.45	1.29	1.22
4	5-I	7492	CIT	O5-C6	2.45	1.29	1.22
4	6-I	7492	CIT	O5-C6	2.45	1.29	1.22
4	7-I	7492	CIT	O5-C6	2.45	1.29	1.22
4	8-I	7492	CIT	O5-C6	2.45	1.29	1.22
4	9-I	7492	CIT	O5-C6	2.45	1.29	1.22
4	10-I	7492	CIT	O5-C6	2.45	1.29	1.22
4	1-B	7478	CIT	O5-C6	2.45	1.29	1.22
4	2-B	7478	CIT	O5-C6	2.45	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-B	7478	CIT	O5-C6	2.45	1.29	1.22
4	4-B	7478	CIT	O5-C6	2.45	1.29	1.22
4	5-B	7478	CIT	O5-C6	2.45	1.29	1.22
4	6-B	7478	CIT	O5-C6	2.45	1.29	1.22
4	7-B	7478	CIT	O5-C6	2.45	1.29	1.22
4	8-B	7478	CIT	O5-C6	2.45	1.29	1.22
4	9-B	7478	CIT	O5-C6	2.45	1.29	1.22
4	10-B	7478	CIT	O5-C6	2.45	1.29	1.22
3	1-F	7485	AMP	C8-N7	2.44	1.36	1.31
3	2-F	7485	AMP	C8-N7	2.44	1.36	1.31
3	3-F	7485	AMP	C8-N7	2.44	1.36	1.31
3	4-F	7485	AMP	C8-N7	2.44	1.36	1.31
3	5-F	7485	AMP	C8-N7	2.44	1.36	1.31
3	6-F	7485	AMP	C8-N7	2.44	1.36	1.31
3	7-F	7485	AMP	C8-N7	2.44	1.36	1.31
3	8-F	7485	AMP	C8-N7	2.44	1.36	1.31
3	9-F	7485	AMP	C8-N7	2.44	1.36	1.31
3	10-F	7485	AMP	C8-N7	2.44	1.36	1.31
4	1-L	7498	CIT	O5-C6	2.44	1.29	1.22
4	2-L	7498	CIT	O5-C6	2.44	1.29	1.22
4	3-L	7498	CIT	O5-C6	2.44	1.29	1.22
4	4-L	7498	CIT	O5-C6	2.44	1.29	1.22
4	5-L	7498	CIT	O5-C6	2.44	1.29	1.22
4	6-L	7498	CIT	O5-C6	2.44	1.29	1.22
4	7-L	7498	CIT	O5-C6	2.44	1.29	1.22
4	8-L	7498	CIT	O5-C6	2.44	1.29	1.22
4	9-L	7498	CIT	O5-C6	2.44	1.29	1.22
4	10-L	7498	CIT	O5-C6	2.44	1.29	1.22
3	1-L	7497	AMP	C8-N7	2.44	1.36	1.31
3	2-L	7497	AMP	C8-N7	2.44	1.36	1.31
3	3-L	7497	AMP	C8-N7	2.44	1.36	1.31
3	4-L	7497	AMP	C8-N7	2.44	1.36	1.31
3	5-L	7497	AMP	C8-N7	2.44	1.36	1.31
3	6-L	7497	AMP	C8-N7	2.44	1.36	1.31
3	7-L	7497	AMP	C8-N7	2.44	1.36	1.31
3	8-L	7497	AMP	C8-N7	2.44	1.36	1.31
3	9-L	7497	AMP	C8-N7	2.44	1.36	1.31
3	10-L	7497	AMP	C8-N7	2.44	1.36	1.31
3	1-W	7519	AMP	C8-N7	2.44	1.36	1.31
3	2-W	7519	AMP	C8-N7	2.44	1.36	1.31
3	3-W	7519	AMP	C8-N7	2.44	1.36	1.31
3	4-W	7519	AMP	C8-N7	2.44	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-W	7519	AMP	C8-N7	2.44	1.36	1.31
3	6-W	7519	AMP	C8-N7	2.44	1.36	1.31
3	7-W	7519	AMP	C8-N7	2.44	1.36	1.31
3	8-W	7519	AMP	C8-N7	2.44	1.36	1.31
3	9-W	7519	AMP	C8-N7	2.44	1.36	1.31
3	10-W	7519	AMP	C8-N7	2.44	1.36	1.31
3	1-E	7483	AMP	C8-N7	2.44	1.36	1.31
3	2-E	7483	AMP	C8-N7	2.44	1.36	1.31
3	3-E	7483	AMP	C8-N7	2.44	1.36	1.31
3	4-E	7483	AMP	C8-N7	2.44	1.36	1.31
3	5-E	7483	AMP	C8-N7	2.44	1.36	1.31
3	6-E	7483	AMP	C8-N7	2.44	1.36	1.31
3	7-E	7483	AMP	C8-N7	2.44	1.36	1.31
3	8-E	7483	AMP	C8-N7	2.44	1.36	1.31
3	9-E	7483	AMP	C8-N7	2.44	1.36	1.31
3	10-E	7483	AMP	C8-N7	2.44	1.36	1.31
3	1-D	7481	AMP	C8-N7	2.44	1.36	1.31
3	2-D	7481	AMP	C8-N7	2.44	1.36	1.31
3	3-D	7481	AMP	C8-N7	2.44	1.36	1.31
3	4-D	7481	AMP	C8-N7	2.44	1.36	1.31
3	5-D	7481	AMP	C8-N7	2.44	1.36	1.31
3	6-D	7481	AMP	C8-N7	2.44	1.36	1.31
3	7-D	7481	AMP	C8-N7	2.44	1.36	1.31
3	8-D	7481	AMP	C8-N7	2.44	1.36	1.31
3	9-D	7481	AMP	C8-N7	2.44	1.36	1.31
3	10-D	7481	AMP	C8-N7	2.44	1.36	1.31
4	1-P	7506	CIT	O5-C6	2.44	1.29	1.22
4	2-P	7506	CIT	O5-C6	2.44	1.29	1.22
4	3-P	7506	CIT	O5-C6	2.44	1.29	1.22
4	4-P	7506	CIT	O5-C6	2.44	1.29	1.22
4	5-P	7506	CIT	O5-C6	2.44	1.29	1.22
4	6-P	7506	CIT	O5-C6	2.44	1.29	1.22
4	7-P	7506	CIT	O5-C6	2.44	1.29	1.22
4	8-P	7506	CIT	O5-C6	2.44	1.29	1.22
4	9-P	7506	CIT	O5-C6	2.44	1.29	1.22
4	10-P	7506	CIT	O5-C6	2.44	1.29	1.22
3	1-U	7515	AMP	C8-N7	2.44	1.36	1.31
3	2-U	7515	AMP	C8-N7	2.44	1.36	1.31
3	3-U	7515	AMP	C8-N7	2.44	1.36	1.31
3	4-U	7515	AMP	C8-N7	2.44	1.36	1.31
3	5-U	7515	AMP	C8-N7	2.44	1.36	1.31
3	6-U	7515	AMP	C8-N7	2.44	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-U	7515	AMP	C8-N7	2.44	1.36	1.31
3	8-U	7515	AMP	C8-N7	2.44	1.36	1.31
3	9-U	7515	AMP	C8-N7	2.44	1.36	1.31
3	10-U	7515	AMP	C8-N7	2.44	1.36	1.31
4	1-O	7504	CIT	O5-C6	2.44	1.29	1.22
4	2-O	7504	CIT	O5-C6	2.44	1.29	1.22
4	3-O	7504	CIT	O5-C6	2.44	1.29	1.22
4	4-O	7504	CIT	O5-C6	2.44	1.29	1.22
4	5-O	7504	CIT	O5-C6	2.44	1.29	1.22
4	6-O	7504	CIT	O5-C6	2.44	1.29	1.22
4	7-O	7504	CIT	O5-C6	2.44	1.29	1.22
4	8-O	7504	CIT	O5-C6	2.44	1.29	1.22
4	9-O	7504	CIT	O5-C6	2.44	1.29	1.22
4	10-O	7504	CIT	O5-C6	2.44	1.29	1.22
3	1-S	7511	AMP	C8-N7	2.43	1.36	1.31
3	2-S	7511	AMP	C8-N7	2.43	1.36	1.31
3	3-S	7511	AMP	C8-N7	2.43	1.36	1.31
3	4-S	7511	AMP	C8-N7	2.43	1.36	1.31
3	5-S	7511	AMP	C8-N7	2.43	1.36	1.31
3	6-S	7511	AMP	C8-N7	2.43	1.36	1.31
3	7-S	7511	AMP	C8-N7	2.43	1.36	1.31
3	8-S	7511	AMP	C8-N7	2.43	1.36	1.31
3	9-S	7511	AMP	C8-N7	2.43	1.36	1.31
3	10-S	7511	AMP	C8-N7	2.43	1.36	1.31
4	1-X	7522	CIT	O5-C6	2.43	1.29	1.22
4	2-X	7522	CIT	O5-C6	2.43	1.29	1.22
4	3-X	7522	CIT	O5-C6	2.43	1.29	1.22
4	4-X	7522	CIT	O5-C6	2.43	1.29	1.22
4	5-X	7522	CIT	O5-C6	2.43	1.29	1.22
4	6-X	7522	CIT	O5-C6	2.43	1.29	1.22
4	7-X	7522	CIT	O5-C6	2.43	1.29	1.22
4	8-X	7522	CIT	O5-C6	2.43	1.29	1.22
4	9-X	7522	CIT	O5-C6	2.43	1.29	1.22
4	10-X	7522	CIT	O5-C6	2.43	1.29	1.22
3	1-K	7495	AMP	C8-N7	2.43	1.36	1.31
3	2-K	7495	AMP	C8-N7	2.43	1.36	1.31
3	3-K	7495	AMP	C8-N7	2.43	1.36	1.31
3	4-K	7495	AMP	C8-N7	2.43	1.36	1.31
3	5-K	7495	AMP	C8-N7	2.43	1.36	1.31
3	6-K	7495	AMP	C8-N7	2.43	1.36	1.31
3	7-K	7495	AMP	C8-N7	2.43	1.36	1.31
3	8-K	7495	AMP	C8-N7	2.43	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-K	7495	AMP	C8-N7	2.43	1.36	1.31
3	10-K	7495	AMP	C8-N7	2.43	1.36	1.31
4	1-W	7520	CIT	O5-C6	2.42	1.29	1.22
4	2-W	7520	CIT	O5-C6	2.42	1.29	1.22
4	3-W	7520	CIT	O5-C6	2.42	1.29	1.22
4	4-W	7520	CIT	O5-C6	2.42	1.29	1.22
4	5-W	7520	CIT	O5-C6	2.42	1.29	1.22
4	6-W	7520	CIT	O5-C6	2.42	1.29	1.22
4	7-W	7520	CIT	O5-C6	2.42	1.29	1.22
4	8-W	7520	CIT	O5-C6	2.42	1.29	1.22
4	9-W	7520	CIT	O5-C6	2.42	1.29	1.22
4	10-W	7520	CIT	O5-C6	2.42	1.29	1.22
3	1-K	7495	AMP	C2'-C3'	2.34	1.59	1.53
3	2-K	7495	AMP	C2'-C3'	2.34	1.59	1.53
3	3-K	7495	AMP	C2'-C3'	2.34	1.59	1.53
3	4-K	7495	AMP	C2'-C3'	2.34	1.59	1.53
3	5-K	7495	AMP	C2'-C3'	2.34	1.59	1.53
3	6-K	7495	AMP	C2'-C3'	2.34	1.59	1.53
3	7-K	7495	AMP	C2'-C3'	2.34	1.59	1.53
3	8-K	7495	AMP	C2'-C3'	2.34	1.59	1.53
3	9-K	7495	AMP	C2'-C3'	2.34	1.59	1.53
3	10-K	7495	AMP	C2'-C3'	2.34	1.59	1.53
3	1-U	7515	AMP	C2'-C3'	2.34	1.59	1.53
3	2-U	7515	AMP	C2'-C3'	2.34	1.59	1.53
3	3-U	7515	AMP	C2'-C3'	2.34	1.59	1.53
3	4-U	7515	AMP	C2'-C3'	2.34	1.59	1.53
3	5-U	7515	AMP	C2'-C3'	2.34	1.59	1.53
3	6-U	7515	AMP	C2'-C3'	2.34	1.59	1.53
3	7-U	7515	AMP	C2'-C3'	2.34	1.59	1.53
3	8-U	7515	AMP	C2'-C3'	2.34	1.59	1.53
3	9-U	7515	AMP	C2'-C3'	2.34	1.59	1.53
3	10-U	7515	AMP	C2'-C3'	2.34	1.59	1.53
3	1-N	7501	AMP	C2'-C3'	2.33	1.59	1.53
3	2-N	7501	AMP	C2'-C3'	2.33	1.59	1.53
3	3-N	7501	AMP	C2'-C3'	2.33	1.59	1.53
3	4-N	7501	AMP	C2'-C3'	2.33	1.59	1.53
3	5-N	7501	AMP	C2'-C3'	2.33	1.59	1.53
3	6-N	7501	AMP	C2'-C3'	2.33	1.59	1.53
3	7-N	7501	AMP	C2'-C3'	2.33	1.59	1.53
3	8-N	7501	AMP	C2'-C3'	2.33	1.59	1.53
3	9-N	7501	AMP	C2'-C3'	2.33	1.59	1.53
3	10-N	7501	AMP	C2'-C3'	2.33	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	7477	AMP	C2'-C3'	2.33	1.59	1.53
3	2-B	7477	AMP	C2'-C3'	2.33	1.59	1.53
3	3-B	7477	AMP	C2'-C3'	2.33	1.59	1.53
3	4-B	7477	AMP	C2'-C3'	2.33	1.59	1.53
3	5-B	7477	AMP	C2'-C3'	2.33	1.59	1.53
3	6-B	7477	AMP	C2'-C3'	2.33	1.59	1.53
3	7-B	7477	AMP	C2'-C3'	2.33	1.59	1.53
3	8-B	7477	AMP	C2'-C3'	2.33	1.59	1.53
3	9-B	7477	AMP	C2'-C3'	2.33	1.59	1.53
3	10-B	7477	AMP	C2'-C3'	2.33	1.59	1.53
3	1-F	7485	AMP	C2'-C3'	2.33	1.59	1.53
3	2-F	7485	AMP	C2'-C3'	2.33	1.59	1.53
3	3-F	7485	AMP	C2'-C3'	2.33	1.59	1.53
3	4-F	7485	AMP	C2'-C3'	2.33	1.59	1.53
3	5-F	7485	AMP	C2'-C3'	2.33	1.59	1.53
3	6-F	7485	AMP	C2'-C3'	2.33	1.59	1.53
3	7-F	7485	AMP	C2'-C3'	2.33	1.59	1.53
3	8-F	7485	AMP	C2'-C3'	2.33	1.59	1.53
3	9-F	7485	AMP	C2'-C3'	2.33	1.59	1.53
3	10-F	7485	AMP	C2'-C3'	2.33	1.59	1.53
3	1-O	7503	AMP	C2'-C3'	2.33	1.59	1.53
3	2-O	7503	AMP	C2'-C3'	2.33	1.59	1.53
3	3-O	7503	AMP	C2'-C3'	2.33	1.59	1.53
3	4-O	7503	AMP	C2'-C3'	2.33	1.59	1.53
3	5-O	7503	AMP	C2'-C3'	2.33	1.59	1.53
3	6-O	7503	AMP	C2'-C3'	2.33	1.59	1.53
3	7-O	7503	AMP	C2'-C3'	2.33	1.59	1.53
3	8-O	7503	AMP	C2'-C3'	2.33	1.59	1.53
3	9-O	7503	AMP	C2'-C3'	2.33	1.59	1.53
3	10-O	7503	AMP	C2'-C3'	2.33	1.59	1.53
4	1-D	7482	CIT	O2-C1	-2.33	1.23	1.30
4	2-D	7482	CIT	O2-C1	-2.33	1.23	1.30
4	3-D	7482	CIT	O2-C1	-2.33	1.23	1.30
4	4-D	7482	CIT	O2-C1	-2.33	1.23	1.30
4	5-D	7482	CIT	O2-C1	-2.33	1.23	1.30
4	6-D	7482	CIT	O2-C1	-2.33	1.23	1.30
4	7-D	7482	CIT	O2-C1	-2.33	1.23	1.30
4	8-D	7482	CIT	O2-C1	-2.33	1.23	1.30
4	9-D	7482	CIT	O2-C1	-2.33	1.23	1.30
4	10-D	7482	CIT	O2-C1	-2.33	1.23	1.30
4	1-G	7488	CIT	O2-C1	-2.33	1.23	1.30
4	2-G	7488	CIT	O2-C1	-2.33	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-G	7488	CIT	O2-C1	-2.33	1.23	1.30
4	4-G	7488	CIT	O2-C1	-2.33	1.23	1.30
4	5-G	7488	CIT	O2-C1	-2.33	1.23	1.30
4	6-G	7488	CIT	O2-C1	-2.33	1.23	1.30
4	7-G	7488	CIT	O2-C1	-2.33	1.23	1.30
4	8-G	7488	CIT	O2-C1	-2.33	1.23	1.30
4	9-G	7488	CIT	O2-C1	-2.33	1.23	1.30
4	10-G	7488	CIT	O2-C1	-2.33	1.23	1.30
3	1-H	7489	AMP	C2'-C3'	2.33	1.59	1.53
3	2-H	7489	AMP	C2'-C3'	2.33	1.59	1.53
3	3-H	7489	AMP	C2'-C3'	2.33	1.59	1.53
3	4-H	7489	AMP	C2'-C3'	2.33	1.59	1.53
3	5-H	7489	AMP	C2'-C3'	2.33	1.59	1.53
3	6-H	7489	AMP	C2'-C3'	2.33	1.59	1.53
3	7-H	7489	AMP	C2'-C3'	2.33	1.59	1.53
3	8-H	7489	AMP	C2'-C3'	2.33	1.59	1.53
3	9-H	7489	AMP	C2'-C3'	2.33	1.59	1.53
3	10-H	7489	AMP	C2'-C3'	2.33	1.59	1.53
4	1-S	7512	CIT	O2-C1	-2.33	1.23	1.30
4	2-S	7512	CIT	O2-C1	-2.33	1.23	1.30
4	3-S	7512	CIT	O2-C1	-2.33	1.23	1.30
4	4-S	7512	CIT	O2-C1	-2.33	1.23	1.30
4	5-S	7512	CIT	O2-C1	-2.33	1.23	1.30
4	6-S	7512	CIT	O2-C1	-2.33	1.23	1.30
4	7-S	7512	CIT	O2-C1	-2.33	1.23	1.30
4	8-S	7512	CIT	O2-C1	-2.33	1.23	1.30
4	9-S	7512	CIT	O2-C1	-2.33	1.23	1.30
4	10-S	7512	CIT	O2-C1	-2.33	1.23	1.30
4	1-Q	7508	CIT	O2-C1	-2.32	1.23	1.30
4	2-Q	7508	CIT	O2-C1	-2.32	1.23	1.30
4	3-Q	7508	CIT	O2-C1	-2.32	1.23	1.30
4	4-Q	7508	CIT	O2-C1	-2.32	1.23	1.30
4	5-Q	7508	CIT	O2-C1	-2.32	1.23	1.30
4	6-Q	7508	CIT	O2-C1	-2.32	1.23	1.30
4	7-Q	7508	CIT	O2-C1	-2.32	1.23	1.30
4	8-Q	7508	CIT	O2-C1	-2.32	1.23	1.30
4	9-Q	7508	CIT	O2-C1	-2.32	1.23	1.30
4	10-Q	7508	CIT	O2-C1	-2.32	1.23	1.30
3	1-V	7517	AMP	C2'-C3'	2.32	1.59	1.53
3	2-V	7517	AMP	C2'-C3'	2.32	1.59	1.53
3	3-V	7517	AMP	C2'-C3'	2.32	1.59	1.53
3	4-V	7517	AMP	C2'-C3'	2.32	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-V	7517	AMP	C2'-C3'	2.32	1.59	1.53
3	6-V	7517	AMP	C2'-C3'	2.32	1.59	1.53
3	7-V	7517	AMP	C2'-C3'	2.32	1.59	1.53
3	8-V	7517	AMP	C2'-C3'	2.32	1.59	1.53
3	9-V	7517	AMP	C2'-C3'	2.32	1.59	1.53
3	10-V	7517	AMP	C2'-C3'	2.32	1.59	1.53
3	1-I	7491	AMP	C2'-C3'	2.32	1.59	1.53
3	2-I	7491	AMP	C2'-C3'	2.32	1.59	1.53
3	3-I	7491	AMP	C2'-C3'	2.32	1.59	1.53
3	4-I	7491	AMP	C2'-C3'	2.32	1.59	1.53
3	5-I	7491	AMP	C2'-C3'	2.32	1.59	1.53
3	6-I	7491	AMP	C2'-C3'	2.32	1.59	1.53
3	7-I	7491	AMP	C2'-C3'	2.32	1.59	1.53
3	8-I	7491	AMP	C2'-C3'	2.32	1.59	1.53
3	9-I	7491	AMP	C2'-C3'	2.32	1.59	1.53
3	10-I	7491	AMP	C2'-C3'	2.32	1.59	1.53
3	1-X	7521	AMP	C2'-C3'	2.32	1.59	1.53
3	2-X	7521	AMP	C2'-C3'	2.32	1.59	1.53
3	3-X	7521	AMP	C2'-C3'	2.32	1.59	1.53
3	4-X	7521	AMP	C2'-C3'	2.32	1.59	1.53
3	5-X	7521	AMP	C2'-C3'	2.32	1.59	1.53
3	6-X	7521	AMP	C2'-C3'	2.32	1.59	1.53
3	7-X	7521	AMP	C2'-C3'	2.32	1.59	1.53
3	8-X	7521	AMP	C2'-C3'	2.32	1.59	1.53
3	9-X	7521	AMP	C2'-C3'	2.32	1.59	1.53
3	10-X	7521	AMP	C2'-C3'	2.32	1.59	1.53
4	1-T	7514	CIT	O2-C1	-2.32	1.23	1.30
4	2-T	7514	CIT	O2-C1	-2.32	1.23	1.30
4	3-T	7514	CIT	O2-C1	-2.32	1.23	1.30
4	4-T	7514	CIT	O2-C1	-2.32	1.23	1.30
4	5-T	7514	CIT	O2-C1	-2.32	1.23	1.30
4	6-T	7514	CIT	O2-C1	-2.32	1.23	1.30
4	7-T	7514	CIT	O2-C1	-2.32	1.23	1.30
4	8-T	7514	CIT	O2-C1	-2.32	1.23	1.30
4	9-T	7514	CIT	O2-C1	-2.32	1.23	1.30
4	10-T	7514	CIT	O2-C1	-2.32	1.23	1.30
4	1-P	7506	CIT	O2-C1	-2.32	1.23	1.30
4	2-P	7506	CIT	O2-C1	-2.32	1.23	1.30
4	3-P	7506	CIT	O2-C1	-2.32	1.23	1.30
4	4-P	7506	CIT	O2-C1	-2.32	1.23	1.30
4	5-P	7506	CIT	O2-C1	-2.32	1.23	1.30
4	6-P	7506	CIT	O2-C1	-2.32	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-P	7506	CIT	O2-C1	-2.32	1.23	1.30
4	8-P	7506	CIT	O2-C1	-2.32	1.23	1.30
4	9-P	7506	CIT	O2-C1	-2.32	1.23	1.30
4	10-P	7506	CIT	O2-C1	-2.32	1.23	1.30
3	1-R	7509	AMP	C2'-C3'	2.32	1.59	1.53
3	2-R	7509	AMP	C2'-C3'	2.32	1.59	1.53
3	3-R	7509	AMP	C2'-C3'	2.32	1.59	1.53
3	4-R	7509	AMP	C2'-C3'	2.32	1.59	1.53
3	5-R	7509	AMP	C2'-C3'	2.32	1.59	1.53
3	6-R	7509	AMP	C2'-C3'	2.32	1.59	1.53
3	7-R	7509	AMP	C2'-C3'	2.32	1.59	1.53
3	8-R	7509	AMP	C2'-C3'	2.32	1.59	1.53
3	9-R	7509	AMP	C2'-C3'	2.32	1.59	1.53
3	10-R	7509	AMP	C2'-C3'	2.32	1.59	1.53
4	1-F	7486	CIT	O2-C1	-2.31	1.23	1.30
4	2-F	7486	CIT	O2-C1	-2.31	1.23	1.30
4	3-F	7486	CIT	O2-C1	-2.31	1.23	1.30
4	4-F	7486	CIT	O2-C1	-2.31	1.23	1.30
4	5-F	7486	CIT	O2-C1	-2.31	1.23	1.30
4	6-F	7486	CIT	O2-C1	-2.31	1.23	1.30
4	7-F	7486	CIT	O2-C1	-2.31	1.23	1.30
4	8-F	7486	CIT	O2-C1	-2.31	1.23	1.30
4	9-F	7486	CIT	O2-C1	-2.31	1.23	1.30
4	10-F	7486	CIT	O2-C1	-2.31	1.23	1.30
4	1-X	7522	CIT	O2-C1	-2.31	1.23	1.30
4	2-X	7522	CIT	O2-C1	-2.31	1.23	1.30
4	3-X	7522	CIT	O2-C1	-2.31	1.23	1.30
4	4-X	7522	CIT	O2-C1	-2.31	1.23	1.30
4	5-X	7522	CIT	O2-C1	-2.31	1.23	1.30
4	6-X	7522	CIT	O2-C1	-2.31	1.23	1.30
4	7-X	7522	CIT	O2-C1	-2.31	1.23	1.30
4	8-X	7522	CIT	O2-C1	-2.31	1.23	1.30
4	9-X	7522	CIT	O2-C1	-2.31	1.23	1.30
4	10-X	7522	CIT	O2-C1	-2.31	1.23	1.30
3	1-A	7475	AMP	C2'-C3'	2.31	1.59	1.53
3	2-A	7475	AMP	C2'-C3'	2.31	1.59	1.53
3	3-A	7475	AMP	C2'-C3'	2.31	1.59	1.53
3	4-A	7475	AMP	C2'-C3'	2.31	1.59	1.53
3	5-A	7475	AMP	C2'-C3'	2.31	1.59	1.53
3	6-A	7475	AMP	C2'-C3'	2.31	1.59	1.53
3	7-A	7475	AMP	C2'-C3'	2.31	1.59	1.53
3	8-A	7475	AMP	C2'-C3'	2.31	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-A	7475	AMP	C2'-C3'	2.31	1.59	1.53
3	10-A	7475	AMP	C2'-C3'	2.31	1.59	1.53
3	1-Q	7507	AMP	C2'-C3'	2.31	1.59	1.53
3	2-Q	7507	AMP	C2'-C3'	2.31	1.59	1.53
3	3-Q	7507	AMP	C2'-C3'	2.31	1.59	1.53
3	4-Q	7507	AMP	C2'-C3'	2.31	1.59	1.53
3	5-Q	7507	AMP	C2'-C3'	2.31	1.59	1.53
3	6-Q	7507	AMP	C2'-C3'	2.31	1.59	1.53
3	7-Q	7507	AMP	C2'-C3'	2.31	1.59	1.53
3	8-Q	7507	AMP	C2'-C3'	2.31	1.59	1.53
3	9-Q	7507	AMP	C2'-C3'	2.31	1.59	1.53
3	10-Q	7507	AMP	C2'-C3'	2.31	1.59	1.53
3	1-W	7519	AMP	C2'-C3'	2.31	1.59	1.53
3	2-W	7519	AMP	C2'-C3'	2.31	1.59	1.53
3	3-W	7519	AMP	C2'-C3'	2.31	1.59	1.53
3	4-W	7519	AMP	C2'-C3'	2.31	1.59	1.53
3	5-W	7519	AMP	C2'-C3'	2.31	1.59	1.53
3	6-W	7519	AMP	C2'-C3'	2.31	1.59	1.53
3	7-W	7519	AMP	C2'-C3'	2.31	1.59	1.53
3	8-W	7519	AMP	C2'-C3'	2.31	1.59	1.53
3	9-W	7519	AMP	C2'-C3'	2.31	1.59	1.53
3	10-W	7519	AMP	C2'-C3'	2.31	1.59	1.53
4	1-V	7518	CIT	O2-C1	-2.31	1.23	1.30
4	2-V	7518	CIT	O2-C1	-2.31	1.23	1.30
4	3-V	7518	CIT	O2-C1	-2.31	1.23	1.30
4	4-V	7518	CIT	O2-C1	-2.31	1.23	1.30
4	5-V	7518	CIT	O2-C1	-2.31	1.23	1.30
4	6-V	7518	CIT	O2-C1	-2.31	1.23	1.30
4	7-V	7518	CIT	O2-C1	-2.31	1.23	1.30
4	8-V	7518	CIT	O2-C1	-2.31	1.23	1.30
4	9-V	7518	CIT	O2-C1	-2.31	1.23	1.30
4	10-V	7518	CIT	O2-C1	-2.31	1.23	1.30
3	1-D	7481	AMP	C2'-C3'	2.31	1.59	1.53
3	2-D	7481	AMP	C2'-C3'	2.31	1.59	1.53
3	3-D	7481	AMP	C2'-C3'	2.31	1.59	1.53
3	4-D	7481	AMP	C2'-C3'	2.31	1.59	1.53
3	5-D	7481	AMP	C2'-C3'	2.31	1.59	1.53
3	6-D	7481	AMP	C2'-C3'	2.31	1.59	1.53
3	7-D	7481	AMP	C2'-C3'	2.31	1.59	1.53
3	8-D	7481	AMP	C2'-C3'	2.31	1.59	1.53
3	9-D	7481	AMP	C2'-C3'	2.31	1.59	1.53
3	10-D	7481	AMP	C2'-C3'	2.31	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-P	7505	AMP	C2'-C3'	2.31	1.59	1.53
3	2-P	7505	AMP	C2'-C3'	2.31	1.59	1.53
3	3-P	7505	AMP	C2'-C3'	2.31	1.59	1.53
3	4-P	7505	AMP	C2'-C3'	2.31	1.59	1.53
3	5-P	7505	AMP	C2'-C3'	2.31	1.59	1.53
3	6-P	7505	AMP	C2'-C3'	2.31	1.59	1.53
3	7-P	7505	AMP	C2'-C3'	2.31	1.59	1.53
3	8-P	7505	AMP	C2'-C3'	2.31	1.59	1.53
3	9-P	7505	AMP	C2'-C3'	2.31	1.59	1.53
3	10-P	7505	AMP	C2'-C3'	2.31	1.59	1.53
4	1-A	7476	CIT	O2-C1	-2.31	1.23	1.30
4	2-A	7476	CIT	O2-C1	-2.31	1.23	1.30
4	3-A	7476	CIT	O2-C1	-2.31	1.23	1.30
4	4-A	7476	CIT	O2-C1	-2.31	1.23	1.30
4	5-A	7476	CIT	O2-C1	-2.31	1.23	1.30
4	6-A	7476	CIT	O2-C1	-2.31	1.23	1.30
4	7-A	7476	CIT	O2-C1	-2.31	1.23	1.30
4	8-A	7476	CIT	O2-C1	-2.31	1.23	1.30
4	9-A	7476	CIT	O2-C1	-2.31	1.23	1.30
4	10-A	7476	CIT	O2-C1	-2.31	1.23	1.30
4	1-C	7480	CIT	O2-C1	-2.31	1.23	1.30
4	2-C	7480	CIT	O2-C1	-2.31	1.23	1.30
4	3-C	7480	CIT	O2-C1	-2.31	1.23	1.30
4	4-C	7480	CIT	O2-C1	-2.31	1.23	1.30
4	5-C	7480	CIT	O2-C1	-2.31	1.23	1.30
4	6-C	7480	CIT	O2-C1	-2.31	1.23	1.30
4	7-C	7480	CIT	O2-C1	-2.31	1.23	1.30
4	8-C	7480	CIT	O2-C1	-2.31	1.23	1.30
4	9-C	7480	CIT	O2-C1	-2.31	1.23	1.30
4	10-C	7480	CIT	O2-C1	-2.31	1.23	1.30
4	1-U	7516	CIT	O2-C1	-2.31	1.23	1.30
4	2-U	7516	CIT	O2-C1	-2.31	1.23	1.30
4	3-U	7516	CIT	O2-C1	-2.31	1.23	1.30
4	4-U	7516	CIT	O2-C1	-2.31	1.23	1.30
4	5-U	7516	CIT	O2-C1	-2.31	1.23	1.30
4	6-U	7516	CIT	O2-C1	-2.31	1.23	1.30
4	7-U	7516	CIT	O2-C1	-2.31	1.23	1.30
4	8-U	7516	CIT	O2-C1	-2.31	1.23	1.30
4	9-U	7516	CIT	O2-C1	-2.31	1.23	1.30
4	10-U	7516	CIT	O2-C1	-2.31	1.23	1.30
3	1-C	7479	AMP	C2'-C3'	2.31	1.59	1.53
3	2-C	7479	AMP	C2'-C3'	2.31	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-C	7479	AMP	C2'-C3'	2.31	1.59	1.53
3	4-C	7479	AMP	C2'-C3'	2.31	1.59	1.53
3	5-C	7479	AMP	C2'-C3'	2.31	1.59	1.53
3	6-C	7479	AMP	C2'-C3'	2.31	1.59	1.53
3	7-C	7479	AMP	C2'-C3'	2.31	1.59	1.53
3	8-C	7479	AMP	C2'-C3'	2.31	1.59	1.53
3	9-C	7479	AMP	C2'-C3'	2.31	1.59	1.53
3	10-C	7479	AMP	C2'-C3'	2.31	1.59	1.53
4	1-E	7484	CIT	O2-C1	-2.31	1.23	1.30
4	2-E	7484	CIT	O2-C1	-2.31	1.23	1.30
4	3-E	7484	CIT	O2-C1	-2.31	1.23	1.30
4	4-E	7484	CIT	O2-C1	-2.31	1.23	1.30
4	5-E	7484	CIT	O2-C1	-2.31	1.23	1.30
4	6-E	7484	CIT	O2-C1	-2.31	1.23	1.30
4	7-E	7484	CIT	O2-C1	-2.31	1.23	1.30
4	8-E	7484	CIT	O2-C1	-2.31	1.23	1.30
4	9-E	7484	CIT	O2-C1	-2.31	1.23	1.30
4	10-E	7484	CIT	O2-C1	-2.31	1.23	1.30
3	1-G	7487	AMP	C2'-C3'	2.31	1.59	1.53
3	2-G	7487	AMP	C2'-C3'	2.31	1.59	1.53
3	3-G	7487	AMP	C2'-C3'	2.31	1.59	1.53
3	4-G	7487	AMP	C2'-C3'	2.31	1.59	1.53
3	5-G	7487	AMP	C2'-C3'	2.31	1.59	1.53
3	6-G	7487	AMP	C2'-C3'	2.31	1.59	1.53
3	7-G	7487	AMP	C2'-C3'	2.31	1.59	1.53
3	8-G	7487	AMP	C2'-C3'	2.31	1.59	1.53
3	9-G	7487	AMP	C2'-C3'	2.31	1.59	1.53
3	10-G	7487	AMP	C2'-C3'	2.31	1.59	1.53
4	1-H	7490	CIT	O2-C1	-2.31	1.23	1.30
4	2-H	7490	CIT	O2-C1	-2.31	1.23	1.30
4	3-H	7490	CIT	O2-C1	-2.31	1.23	1.30
4	4-H	7490	CIT	O2-C1	-2.31	1.23	1.30
4	5-H	7490	CIT	O2-C1	-2.31	1.23	1.30
4	6-H	7490	CIT	O2-C1	-2.31	1.23	1.30
4	7-H	7490	CIT	O2-C1	-2.31	1.23	1.30
4	8-H	7490	CIT	O2-C1	-2.31	1.23	1.30
4	9-H	7490	CIT	O2-C1	-2.31	1.23	1.30
4	10-H	7490	CIT	O2-C1	-2.31	1.23	1.30
4	1-N	7502	CIT	O2-C1	-2.31	1.23	1.30
4	2-N	7502	CIT	O2-C1	-2.31	1.23	1.30
4	3-N	7502	CIT	O2-C1	-2.31	1.23	1.30
4	4-N	7502	CIT	O2-C1	-2.31	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5-N	7502	CIT	O2-C1	-2.31	1.23	1.30
4	6-N	7502	CIT	O2-C1	-2.31	1.23	1.30
4	7-N	7502	CIT	O2-C1	-2.31	1.23	1.30
4	8-N	7502	CIT	O2-C1	-2.31	1.23	1.30
4	9-N	7502	CIT	O2-C1	-2.31	1.23	1.30
4	10-N	7502	CIT	O2-C1	-2.31	1.23	1.30
4	1-K	7496	CIT	O2-C1	-2.31	1.23	1.30
4	2-K	7496	CIT	O2-C1	-2.31	1.23	1.30
4	3-K	7496	CIT	O2-C1	-2.31	1.23	1.30
4	4-K	7496	CIT	O2-C1	-2.31	1.23	1.30
4	5-K	7496	CIT	O2-C1	-2.31	1.23	1.30
4	6-K	7496	CIT	O2-C1	-2.31	1.23	1.30
4	7-K	7496	CIT	O2-C1	-2.31	1.23	1.30
4	8-K	7496	CIT	O2-C1	-2.31	1.23	1.30
4	9-K	7496	CIT	O2-C1	-2.31	1.23	1.30
4	10-K	7496	CIT	O2-C1	-2.31	1.23	1.30
3	1-T	7513	AMP	C2'-C3'	2.31	1.59	1.53
3	2-T	7513	AMP	C2'-C3'	2.31	1.59	1.53
3	3-T	7513	AMP	C2'-C3'	2.31	1.59	1.53
3	4-T	7513	AMP	C2'-C3'	2.31	1.59	1.53
3	5-T	7513	AMP	C2'-C3'	2.31	1.59	1.53
3	6-T	7513	AMP	C2'-C3'	2.31	1.59	1.53
3	7-T	7513	AMP	C2'-C3'	2.31	1.59	1.53
3	8-T	7513	AMP	C2'-C3'	2.31	1.59	1.53
3	9-T	7513	AMP	C2'-C3'	2.31	1.59	1.53
3	10-T	7513	AMP	C2'-C3'	2.31	1.59	1.53
4	1-W	7520	CIT	O2-C1	-2.31	1.23	1.30
4	2-W	7520	CIT	O2-C1	-2.31	1.23	1.30
4	3-W	7520	CIT	O2-C1	-2.31	1.23	1.30
4	4-W	7520	CIT	O2-C1	-2.31	1.23	1.30
4	5-W	7520	CIT	O2-C1	-2.31	1.23	1.30
4	6-W	7520	CIT	O2-C1	-2.31	1.23	1.30
4	7-W	7520	CIT	O2-C1	-2.31	1.23	1.30
4	8-W	7520	CIT	O2-C1	-2.31	1.23	1.30
4	9-W	7520	CIT	O2-C1	-2.31	1.23	1.30
4	10-W	7520	CIT	O2-C1	-2.31	1.23	1.30
3	1-J	7493	AMP	C2'-C3'	2.31	1.59	1.53
3	2-J	7493	AMP	C2'-C3'	2.31	1.59	1.53
3	3-J	7493	AMP	C2'-C3'	2.31	1.59	1.53
3	4-J	7493	AMP	C2'-C3'	2.31	1.59	1.53
3	5-J	7493	AMP	C2'-C3'	2.31	1.59	1.53
3	6-J	7493	AMP	C2'-C3'	2.31	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-J	7493	AMP	C2'-C3'	2.31	1.59	1.53
3	8-J	7493	AMP	C2'-C3'	2.31	1.59	1.53
3	9-J	7493	AMP	C2'-C3'	2.31	1.59	1.53
3	10-J	7493	AMP	C2'-C3'	2.31	1.59	1.53
3	1-E	7483	AMP	C2'-C3'	2.31	1.59	1.53
3	2-E	7483	AMP	C2'-C3'	2.31	1.59	1.53
3	3-E	7483	AMP	C2'-C3'	2.31	1.59	1.53
3	4-E	7483	AMP	C2'-C3'	2.31	1.59	1.53
3	5-E	7483	AMP	C2'-C3'	2.31	1.59	1.53
3	6-E	7483	AMP	C2'-C3'	2.31	1.59	1.53
3	7-E	7483	AMP	C2'-C3'	2.31	1.59	1.53
3	8-E	7483	AMP	C2'-C3'	2.31	1.59	1.53
3	9-E	7483	AMP	C2'-C3'	2.31	1.59	1.53
3	10-E	7483	AMP	C2'-C3'	2.31	1.59	1.53
4	1-O	7504	CIT	O2-C1	-2.31	1.23	1.30
4	2-O	7504	CIT	O2-C1	-2.31	1.23	1.30
4	3-O	7504	CIT	O2-C1	-2.31	1.23	1.30
4	4-O	7504	CIT	O2-C1	-2.31	1.23	1.30
4	5-O	7504	CIT	O2-C1	-2.31	1.23	1.30
4	6-O	7504	CIT	O2-C1	-2.31	1.23	1.30
4	7-O	7504	CIT	O2-C1	-2.31	1.23	1.30
4	8-O	7504	CIT	O2-C1	-2.31	1.23	1.30
4	9-O	7504	CIT	O2-C1	-2.31	1.23	1.30
4	10-O	7504	CIT	O2-C1	-2.31	1.23	1.30
3	1-M	7499	AMP	C2'-C3'	2.31	1.59	1.53
3	2-M	7499	AMP	C2'-C3'	2.31	1.59	1.53
3	3-M	7499	AMP	C2'-C3'	2.31	1.59	1.53
3	4-M	7499	AMP	C2'-C3'	2.31	1.59	1.53
3	5-M	7499	AMP	C2'-C3'	2.31	1.59	1.53
3	6-M	7499	AMP	C2'-C3'	2.31	1.59	1.53
3	7-M	7499	AMP	C2'-C3'	2.31	1.59	1.53
3	8-M	7499	AMP	C2'-C3'	2.31	1.59	1.53
3	9-M	7499	AMP	C2'-C3'	2.31	1.59	1.53
3	10-M	7499	AMP	C2'-C3'	2.31	1.59	1.53
4	1-I	7492	CIT	O2-C1	-2.30	1.23	1.30
4	2-I	7492	CIT	O2-C1	-2.30	1.23	1.30
4	3-I	7492	CIT	O2-C1	-2.30	1.23	1.30
4	4-I	7492	CIT	O2-C1	-2.30	1.23	1.30
4	5-I	7492	CIT	O2-C1	-2.30	1.23	1.30
4	6-I	7492	CIT	O2-C1	-2.30	1.23	1.30
4	7-I	7492	CIT	O2-C1	-2.30	1.23	1.30
4	8-I	7492	CIT	O2-C1	-2.30	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9-I	7492	CIT	O2-C1	-2.30	1.23	1.30
4	10-I	7492	CIT	O2-C1	-2.30	1.23	1.30
4	1-M	7500	CIT	O2-C1	-2.30	1.23	1.30
4	2-M	7500	CIT	O2-C1	-2.30	1.23	1.30
4	3-M	7500	CIT	O2-C1	-2.30	1.23	1.30
4	4-M	7500	CIT	O2-C1	-2.30	1.23	1.30
4	5-M	7500	CIT	O2-C1	-2.30	1.23	1.30
4	6-M	7500	CIT	O2-C1	-2.30	1.23	1.30
4	7-M	7500	CIT	O2-C1	-2.30	1.23	1.30
4	8-M	7500	CIT	O2-C1	-2.30	1.23	1.30
4	9-M	7500	CIT	O2-C1	-2.30	1.23	1.30
4	10-M	7500	CIT	O2-C1	-2.30	1.23	1.30
4	1-L	7498	CIT	O2-C1	-2.30	1.23	1.30
4	2-L	7498	CIT	O2-C1	-2.30	1.23	1.30
4	3-L	7498	CIT	O2-C1	-2.30	1.23	1.30
4	4-L	7498	CIT	O2-C1	-2.30	1.23	1.30
4	5-L	7498	CIT	O2-C1	-2.30	1.23	1.30
4	6-L	7498	CIT	O2-C1	-2.30	1.23	1.30
4	7-L	7498	CIT	O2-C1	-2.30	1.23	1.30
4	8-L	7498	CIT	O2-C1	-2.30	1.23	1.30
4	9-L	7498	CIT	O2-C1	-2.30	1.23	1.30
4	10-L	7498	CIT	O2-C1	-2.30	1.23	1.30
4	1-B	7478	CIT	O2-C1	-2.30	1.23	1.30
4	2-B	7478	CIT	O2-C1	-2.30	1.23	1.30
4	3-B	7478	CIT	O2-C1	-2.30	1.23	1.30
4	4-B	7478	CIT	O2-C1	-2.30	1.23	1.30
4	5-B	7478	CIT	O2-C1	-2.30	1.23	1.30
4	6-B	7478	CIT	O2-C1	-2.30	1.23	1.30
4	7-B	7478	CIT	O2-C1	-2.30	1.23	1.30
4	8-B	7478	CIT	O2-C1	-2.30	1.23	1.30
4	9-B	7478	CIT	O2-C1	-2.30	1.23	1.30
4	10-B	7478	CIT	O2-C1	-2.30	1.23	1.30
3	1-S	7511	AMP	C2'-C3'	2.30	1.59	1.53
3	2-S	7511	AMP	C2'-C3'	2.30	1.59	1.53
3	3-S	7511	AMP	C2'-C3'	2.30	1.59	1.53
3	4-S	7511	AMP	C2'-C3'	2.30	1.59	1.53
3	5-S	7511	AMP	C2'-C3'	2.30	1.59	1.53
3	6-S	7511	AMP	C2'-C3'	2.30	1.59	1.53
3	7-S	7511	AMP	C2'-C3'	2.30	1.59	1.53
3	8-S	7511	AMP	C2'-C3'	2.30	1.59	1.53
3	9-S	7511	AMP	C2'-C3'	2.30	1.59	1.53
3	10-S	7511	AMP	C2'-C3'	2.30	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-L	7497	AMP	C2'-C3'	2.30	1.59	1.53
3	2-L	7497	AMP	C2'-C3'	2.30	1.59	1.53
3	3-L	7497	AMP	C2'-C3'	2.30	1.59	1.53
3	4-L	7497	AMP	C2'-C3'	2.30	1.59	1.53
3	5-L	7497	AMP	C2'-C3'	2.30	1.59	1.53
3	6-L	7497	AMP	C2'-C3'	2.30	1.59	1.53
3	7-L	7497	AMP	C2'-C3'	2.30	1.59	1.53
3	8-L	7497	AMP	C2'-C3'	2.30	1.59	1.53
3	9-L	7497	AMP	C2'-C3'	2.30	1.59	1.53
3	10-L	7497	AMP	C2'-C3'	2.30	1.59	1.53
4	1-R	7510	CIT	O2-C1	-2.29	1.23	1.30
4	2-R	7510	CIT	O2-C1	-2.29	1.23	1.30
4	3-R	7510	CIT	O2-C1	-2.29	1.23	1.30
4	4-R	7510	CIT	O2-C1	-2.29	1.23	1.30
4	5-R	7510	CIT	O2-C1	-2.29	1.23	1.30
4	6-R	7510	CIT	O2-C1	-2.29	1.23	1.30
4	7-R	7510	CIT	O2-C1	-2.29	1.23	1.30
4	8-R	7510	CIT	O2-C1	-2.29	1.23	1.30
4	9-R	7510	CIT	O2-C1	-2.29	1.23	1.30
4	10-R	7510	CIT	O2-C1	-2.29	1.23	1.30
4	1-J	7494	CIT	O2-C1	-2.28	1.23	1.30
4	2-J	7494	CIT	O2-C1	-2.28	1.23	1.30
4	3-J	7494	CIT	O2-C1	-2.28	1.23	1.30
4	4-J	7494	CIT	O2-C1	-2.28	1.23	1.30
4	5-J	7494	CIT	O2-C1	-2.28	1.23	1.30
4	6-J	7494	CIT	O2-C1	-2.28	1.23	1.30
4	7-J	7494	CIT	O2-C1	-2.28	1.23	1.30
4	8-J	7494	CIT	O2-C1	-2.28	1.23	1.30
4	9-J	7494	CIT	O2-C1	-2.28	1.23	1.30
4	10-J	7494	CIT	O2-C1	-2.28	1.23	1.30
4	1-H	7490	CIT	C2-C1	2.27	1.57	1.50
4	2-H	7490	CIT	C2-C1	2.27	1.57	1.50
4	3-H	7490	CIT	C2-C1	2.27	1.57	1.50
4	4-H	7490	CIT	C2-C1	2.27	1.57	1.50
4	5-H	7490	CIT	C2-C1	2.27	1.57	1.50
4	6-H	7490	CIT	C2-C1	2.27	1.57	1.50
4	7-H	7490	CIT	C2-C1	2.27	1.57	1.50
4	8-H	7490	CIT	C2-C1	2.27	1.57	1.50
4	9-H	7490	CIT	C2-C1	2.27	1.57	1.50
4	10-H	7490	CIT	C2-C1	2.27	1.57	1.50
4	1-D	7482	CIT	C2-C1	2.27	1.57	1.50
4	2-D	7482	CIT	C2-C1	2.27	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-D	7482	CIT	C2-C1	2.27	1.57	1.50
4	4-D	7482	CIT	C2-C1	2.27	1.57	1.50
4	5-D	7482	CIT	C2-C1	2.27	1.57	1.50
4	6-D	7482	CIT	C2-C1	2.27	1.57	1.50
4	7-D	7482	CIT	C2-C1	2.27	1.57	1.50
4	8-D	7482	CIT	C2-C1	2.27	1.57	1.50
4	9-D	7482	CIT	C2-C1	2.27	1.57	1.50
4	10-D	7482	CIT	C2-C1	2.27	1.57	1.50
4	1-U	7516	CIT	C2-C1	2.27	1.57	1.50
4	2-U	7516	CIT	C2-C1	2.27	1.57	1.50
4	3-U	7516	CIT	C2-C1	2.27	1.57	1.50
4	4-U	7516	CIT	C2-C1	2.27	1.57	1.50
4	5-U	7516	CIT	C2-C1	2.27	1.57	1.50
4	6-U	7516	CIT	C2-C1	2.27	1.57	1.50
4	7-U	7516	CIT	C2-C1	2.27	1.57	1.50
4	8-U	7516	CIT	C2-C1	2.27	1.57	1.50
4	9-U	7516	CIT	C2-C1	2.27	1.57	1.50
4	10-U	7516	CIT	C2-C1	2.27	1.57	1.50
4	1-F	7486	CIT	C2-C1	2.26	1.57	1.50
4	2-F	7486	CIT	C2-C1	2.26	1.57	1.50
4	3-F	7486	CIT	C2-C1	2.26	1.57	1.50
4	4-F	7486	CIT	C2-C1	2.26	1.57	1.50
4	5-F	7486	CIT	C2-C1	2.26	1.57	1.50
4	6-F	7486	CIT	C2-C1	2.26	1.57	1.50
4	7-F	7486	CIT	C2-C1	2.26	1.57	1.50
4	8-F	7486	CIT	C2-C1	2.26	1.57	1.50
4	9-F	7486	CIT	C2-C1	2.26	1.57	1.50
4	10-F	7486	CIT	C2-C1	2.26	1.57	1.50
4	1-W	7520	CIT	C2-C1	2.26	1.57	1.50
4	2-W	7520	CIT	C2-C1	2.26	1.57	1.50
4	3-W	7520	CIT	C2-C1	2.26	1.57	1.50
4	4-W	7520	CIT	C2-C1	2.26	1.57	1.50
4	5-W	7520	CIT	C2-C1	2.26	1.57	1.50
4	6-W	7520	CIT	C2-C1	2.26	1.57	1.50
4	7-W	7520	CIT	C2-C1	2.26	1.57	1.50
4	8-W	7520	CIT	C2-C1	2.26	1.57	1.50
4	9-W	7520	CIT	C2-C1	2.26	1.57	1.50
4	10-W	7520	CIT	C2-C1	2.26	1.57	1.50
4	1-B	7478	CIT	C2-C1	2.26	1.57	1.50
4	2-B	7478	CIT	C2-C1	2.26	1.57	1.50
4	3-B	7478	CIT	C2-C1	2.26	1.57	1.50
4	4-B	7478	CIT	C2-C1	2.26	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5-B	7478	CIT	C2-C1	2.26	1.57	1.50
4	6-B	7478	CIT	C2-C1	2.26	1.57	1.50
4	7-B	7478	CIT	C2-C1	2.26	1.57	1.50
4	8-B	7478	CIT	C2-C1	2.26	1.57	1.50
4	9-B	7478	CIT	C2-C1	2.26	1.57	1.50
4	10-B	7478	CIT	C2-C1	2.26	1.57	1.50
4	1-M	7500	CIT	C2-C1	2.26	1.57	1.50
4	2-M	7500	CIT	C2-C1	2.26	1.57	1.50
4	3-M	7500	CIT	C2-C1	2.26	1.57	1.50
4	4-M	7500	CIT	C2-C1	2.26	1.57	1.50
4	5-M	7500	CIT	C2-C1	2.26	1.57	1.50
4	6-M	7500	CIT	C2-C1	2.26	1.57	1.50
4	7-M	7500	CIT	C2-C1	2.26	1.57	1.50
4	8-M	7500	CIT	C2-C1	2.26	1.57	1.50
4	9-M	7500	CIT	C2-C1	2.26	1.57	1.50
4	10-M	7500	CIT	C2-C1	2.26	1.57	1.50
4	1-O	7504	CIT	C2-C1	2.26	1.57	1.50
4	2-O	7504	CIT	C2-C1	2.26	1.57	1.50
4	3-O	7504	CIT	C2-C1	2.26	1.57	1.50
4	4-O	7504	CIT	C2-C1	2.26	1.57	1.50
4	5-O	7504	CIT	C2-C1	2.26	1.57	1.50
4	6-O	7504	CIT	C2-C1	2.26	1.57	1.50
4	7-O	7504	CIT	C2-C1	2.26	1.57	1.50
4	8-O	7504	CIT	C2-C1	2.26	1.57	1.50
4	9-O	7504	CIT	C2-C1	2.26	1.57	1.50
4	10-O	7504	CIT	C2-C1	2.26	1.57	1.50
4	1-I	7492	CIT	C2-C1	2.25	1.57	1.50
4	2-I	7492	CIT	C2-C1	2.25	1.57	1.50
4	3-I	7492	CIT	C2-C1	2.25	1.57	1.50
4	4-I	7492	CIT	C2-C1	2.25	1.57	1.50
4	5-I	7492	CIT	C2-C1	2.25	1.57	1.50
4	6-I	7492	CIT	C2-C1	2.25	1.57	1.50
4	7-I	7492	CIT	C2-C1	2.25	1.57	1.50
4	8-I	7492	CIT	C2-C1	2.25	1.57	1.50
4	9-I	7492	CIT	C2-C1	2.25	1.57	1.50
4	10-I	7492	CIT	C2-C1	2.25	1.57	1.50
4	1-Q	7508	CIT	C2-C1	2.25	1.57	1.50
4	2-Q	7508	CIT	C2-C1	2.25	1.57	1.50
4	3-Q	7508	CIT	C2-C1	2.25	1.57	1.50
4	4-Q	7508	CIT	C2-C1	2.25	1.57	1.50
4	5-Q	7508	CIT	C2-C1	2.25	1.57	1.50
4	6-Q	7508	CIT	C2-C1	2.25	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-Q	7508	CIT	C2-C1	2.25	1.57	1.50
4	8-Q	7508	CIT	C2-C1	2.25	1.57	1.50
4	9-Q	7508	CIT	C2-C1	2.25	1.57	1.50
4	10-Q	7508	CIT	C2-C1	2.25	1.57	1.50
4	1-P	7506	CIT	C2-C1	2.25	1.57	1.50
4	2-P	7506	CIT	C2-C1	2.25	1.57	1.50
4	3-P	7506	CIT	C2-C1	2.25	1.57	1.50
4	4-P	7506	CIT	C2-C1	2.25	1.57	1.50
4	5-P	7506	CIT	C2-C1	2.25	1.57	1.50
4	6-P	7506	CIT	C2-C1	2.25	1.57	1.50
4	7-P	7506	CIT	C2-C1	2.25	1.57	1.50
4	8-P	7506	CIT	C2-C1	2.25	1.57	1.50
4	9-P	7506	CIT	C2-C1	2.25	1.57	1.50
4	10-P	7506	CIT	C2-C1	2.25	1.57	1.50
4	1-R	7510	CIT	C2-C1	2.25	1.57	1.50
4	2-R	7510	CIT	C2-C1	2.25	1.57	1.50
4	3-R	7510	CIT	C2-C1	2.25	1.57	1.50
4	4-R	7510	CIT	C2-C1	2.25	1.57	1.50
4	5-R	7510	CIT	C2-C1	2.25	1.57	1.50
4	6-R	7510	CIT	C2-C1	2.25	1.57	1.50
4	7-R	7510	CIT	C2-C1	2.25	1.57	1.50
4	8-R	7510	CIT	C2-C1	2.25	1.57	1.50
4	9-R	7510	CIT	C2-C1	2.25	1.57	1.50
4	10-R	7510	CIT	C2-C1	2.25	1.57	1.50
4	1-E	7484	CIT	C2-C1	2.24	1.57	1.50
4	2-E	7484	CIT	C2-C1	2.24	1.57	1.50
4	3-E	7484	CIT	C2-C1	2.24	1.57	1.50
4	4-E	7484	CIT	C2-C1	2.24	1.57	1.50
4	5-E	7484	CIT	C2-C1	2.24	1.57	1.50
4	6-E	7484	CIT	C2-C1	2.24	1.57	1.50
4	7-E	7484	CIT	C2-C1	2.24	1.57	1.50
4	8-E	7484	CIT	C2-C1	2.24	1.57	1.50
4	9-E	7484	CIT	C2-C1	2.24	1.57	1.50
4	10-E	7484	CIT	C2-C1	2.24	1.57	1.50
4	1-G	7488	CIT	C2-C1	2.24	1.57	1.50
4	2-G	7488	CIT	C2-C1	2.24	1.57	1.50
4	3-G	7488	CIT	C2-C1	2.24	1.57	1.50
4	4-G	7488	CIT	C2-C1	2.24	1.57	1.50
4	5-G	7488	CIT	C2-C1	2.24	1.57	1.50
4	6-G	7488	CIT	C2-C1	2.24	1.57	1.50
4	7-G	7488	CIT	C2-C1	2.24	1.57	1.50
4	8-G	7488	CIT	C2-C1	2.24	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9-G	7488	CIT	C2-C1	2.24	1.57	1.50
4	10-G	7488	CIT	C2-C1	2.24	1.57	1.50
4	1-A	7476	CIT	C2-C1	2.24	1.57	1.50
4	2-A	7476	CIT	C2-C1	2.24	1.57	1.50
4	3-A	7476	CIT	C2-C1	2.24	1.57	1.50
4	4-A	7476	CIT	C2-C1	2.24	1.57	1.50
4	5-A	7476	CIT	C2-C1	2.24	1.57	1.50
4	6-A	7476	CIT	C2-C1	2.24	1.57	1.50
4	7-A	7476	CIT	C2-C1	2.24	1.57	1.50
4	8-A	7476	CIT	C2-C1	2.24	1.57	1.50
4	9-A	7476	CIT	C2-C1	2.24	1.57	1.50
4	10-A	7476	CIT	C2-C1	2.24	1.57	1.50
4	1-T	7514	CIT	C2-C1	2.24	1.57	1.50
4	2-T	7514	CIT	C2-C1	2.24	1.57	1.50
4	3-T	7514	CIT	C2-C1	2.24	1.57	1.50
4	4-T	7514	CIT	C2-C1	2.24	1.57	1.50
4	5-T	7514	CIT	C2-C1	2.24	1.57	1.50
4	6-T	7514	CIT	C2-C1	2.24	1.57	1.50
4	7-T	7514	CIT	C2-C1	2.24	1.57	1.50
4	8-T	7514	CIT	C2-C1	2.24	1.57	1.50
4	9-T	7514	CIT	C2-C1	2.24	1.57	1.50
4	10-T	7514	CIT	C2-C1	2.24	1.57	1.50
4	1-S	7512	CIT	C2-C1	2.24	1.57	1.50
4	2-S	7512	CIT	C2-C1	2.24	1.57	1.50
4	3-S	7512	CIT	C2-C1	2.24	1.57	1.50
4	4-S	7512	CIT	C2-C1	2.24	1.57	1.50
4	5-S	7512	CIT	C2-C1	2.24	1.57	1.50
4	6-S	7512	CIT	C2-C1	2.24	1.57	1.50
4	7-S	7512	CIT	C2-C1	2.24	1.57	1.50
4	8-S	7512	CIT	C2-C1	2.24	1.57	1.50
4	9-S	7512	CIT	C2-C1	2.24	1.57	1.50
4	10-S	7512	CIT	C2-C1	2.24	1.57	1.50
4	1-K	7496	CIT	C2-C1	2.24	1.57	1.50
4	2-K	7496	CIT	C2-C1	2.24	1.57	1.50
4	3-K	7496	CIT	C2-C1	2.24	1.57	1.50
4	4-K	7496	CIT	C2-C1	2.24	1.57	1.50
4	5-K	7496	CIT	C2-C1	2.24	1.57	1.50
4	6-K	7496	CIT	C2-C1	2.24	1.57	1.50
4	7-K	7496	CIT	C2-C1	2.24	1.57	1.50
4	8-K	7496	CIT	C2-C1	2.24	1.57	1.50
4	9-K	7496	CIT	C2-C1	2.24	1.57	1.50
4	10-K	7496	CIT	C2-C1	2.24	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-N	7502	CIT	C2-C1	2.23	1.57	1.50
4	2-N	7502	CIT	C2-C1	2.23	1.57	1.50
4	3-N	7502	CIT	C2-C1	2.23	1.57	1.50
4	4-N	7502	CIT	C2-C1	2.23	1.57	1.50
4	5-N	7502	CIT	C2-C1	2.23	1.57	1.50
4	6-N	7502	CIT	C2-C1	2.23	1.57	1.50
4	7-N	7502	CIT	C2-C1	2.23	1.57	1.50
4	8-N	7502	CIT	C2-C1	2.23	1.57	1.50
4	9-N	7502	CIT	C2-C1	2.23	1.57	1.50
4	10-N	7502	CIT	C2-C1	2.23	1.57	1.50
4	1-J	7494	CIT	C2-C1	2.23	1.57	1.50
4	2-J	7494	CIT	C2-C1	2.23	1.57	1.50
4	3-J	7494	CIT	C2-C1	2.23	1.57	1.50
4	4-J	7494	CIT	C2-C1	2.23	1.57	1.50
4	5-J	7494	CIT	C2-C1	2.23	1.57	1.50
4	6-J	7494	CIT	C2-C1	2.23	1.57	1.50
4	7-J	7494	CIT	C2-C1	2.23	1.57	1.50
4	8-J	7494	CIT	C2-C1	2.23	1.57	1.50
4	9-J	7494	CIT	C2-C1	2.23	1.57	1.50
4	10-J	7494	CIT	C2-C1	2.23	1.57	1.50
4	1-L	7498	CIT	C2-C1	2.23	1.57	1.50
4	2-L	7498	CIT	C2-C1	2.23	1.57	1.50
4	3-L	7498	CIT	C2-C1	2.23	1.57	1.50
4	4-L	7498	CIT	C2-C1	2.23	1.57	1.50
4	5-L	7498	CIT	C2-C1	2.23	1.57	1.50
4	6-L	7498	CIT	C2-C1	2.23	1.57	1.50
4	7-L	7498	CIT	C2-C1	2.23	1.57	1.50
4	8-L	7498	CIT	C2-C1	2.23	1.57	1.50
4	9-L	7498	CIT	C2-C1	2.23	1.57	1.50
4	10-L	7498	CIT	C2-C1	2.23	1.57	1.50
4	1-X	7522	CIT	C2-C1	2.23	1.57	1.50
4	2-X	7522	CIT	C2-C1	2.23	1.57	1.50
4	3-X	7522	CIT	C2-C1	2.23	1.57	1.50
4	4-X	7522	CIT	C2-C1	2.23	1.57	1.50
4	5-X	7522	CIT	C2-C1	2.23	1.57	1.50
4	6-X	7522	CIT	C2-C1	2.23	1.57	1.50
4	7-X	7522	CIT	C2-C1	2.23	1.57	1.50
4	8-X	7522	CIT	C2-C1	2.23	1.57	1.50
4	9-X	7522	CIT	C2-C1	2.23	1.57	1.50
4	10-X	7522	CIT	C2-C1	2.23	1.57	1.50
4	1-V	7518	CIT	C2-C1	2.22	1.57	1.50
4	2-V	7518	CIT	C2-C1	2.22	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-V	7518	CIT	C2-C1	2.22	1.57	1.50
4	4-V	7518	CIT	C2-C1	2.22	1.57	1.50
4	5-V	7518	CIT	C2-C1	2.22	1.57	1.50
4	6-V	7518	CIT	C2-C1	2.22	1.57	1.50
4	7-V	7518	CIT	C2-C1	2.22	1.57	1.50
4	8-V	7518	CIT	C2-C1	2.22	1.57	1.50
4	9-V	7518	CIT	C2-C1	2.22	1.57	1.50
4	10-V	7518	CIT	C2-C1	2.22	1.57	1.50
4	1-C	7480	CIT	C2-C1	2.21	1.57	1.50
4	2-C	7480	CIT	C2-C1	2.21	1.57	1.50
4	3-C	7480	CIT	C2-C1	2.21	1.57	1.50
4	4-C	7480	CIT	C2-C1	2.21	1.57	1.50
4	5-C	7480	CIT	C2-C1	2.21	1.57	1.50
4	6-C	7480	CIT	C2-C1	2.21	1.57	1.50
4	7-C	7480	CIT	C2-C1	2.21	1.57	1.50
4	8-C	7480	CIT	C2-C1	2.21	1.57	1.50
4	9-C	7480	CIT	C2-C1	2.21	1.57	1.50
4	10-C	7480	CIT	C2-C1	2.21	1.57	1.50
4	1-B	7478	CIT	O1-C1	-2.13	1.15	1.22
4	2-B	7478	CIT	O1-C1	-2.13	1.15	1.22
4	3-B	7478	CIT	O1-C1	-2.13	1.15	1.22
4	4-B	7478	CIT	O1-C1	-2.13	1.15	1.22
4	5-B	7478	CIT	O1-C1	-2.13	1.15	1.22
4	6-B	7478	CIT	O1-C1	-2.13	1.15	1.22
4	7-B	7478	CIT	O1-C1	-2.13	1.15	1.22
4	8-B	7478	CIT	O1-C1	-2.13	1.15	1.22
4	9-B	7478	CIT	O1-C1	-2.13	1.15	1.22
4	10-B	7478	CIT	O1-C1	-2.13	1.15	1.22
4	1-P	7506	CIT	O1-C1	-2.13	1.15	1.22
4	2-P	7506	CIT	O1-C1	-2.13	1.15	1.22
4	3-P	7506	CIT	O1-C1	-2.13	1.15	1.22
4	4-P	7506	CIT	O1-C1	-2.13	1.15	1.22
4	5-P	7506	CIT	O1-C1	-2.13	1.15	1.22
4	6-P	7506	CIT	O1-C1	-2.13	1.15	1.22
4	7-P	7506	CIT	O1-C1	-2.13	1.15	1.22
4	8-P	7506	CIT	O1-C1	-2.13	1.15	1.22
4	9-P	7506	CIT	O1-C1	-2.13	1.15	1.22
4	10-P	7506	CIT	O1-C1	-2.13	1.15	1.22
4	1-H	7490	CIT	O1-C1	-2.13	1.15	1.22
4	2-H	7490	CIT	O1-C1	-2.13	1.15	1.22
4	3-H	7490	CIT	O1-C1	-2.13	1.15	1.22
4	4-H	7490	CIT	O1-C1	-2.13	1.15	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5-H	7490	CIT	O1-C1	-2.13	1.15	1.22
4	6-H	7490	CIT	O1-C1	-2.13	1.15	1.22
4	7-H	7490	CIT	O1-C1	-2.13	1.15	1.22
4	8-H	7490	CIT	O1-C1	-2.13	1.15	1.22
4	9-H	7490	CIT	O1-C1	-2.13	1.15	1.22
4	10-H	7490	CIT	O1-C1	-2.13	1.15	1.22
4	1-Q	7508	CIT	O1-C1	-2.13	1.15	1.22
4	2-Q	7508	CIT	O1-C1	-2.13	1.15	1.22
4	3-Q	7508	CIT	O1-C1	-2.13	1.15	1.22
4	4-Q	7508	CIT	O1-C1	-2.13	1.15	1.22
4	5-Q	7508	CIT	O1-C1	-2.13	1.15	1.22
4	6-Q	7508	CIT	O1-C1	-2.13	1.15	1.22
4	7-Q	7508	CIT	O1-C1	-2.13	1.15	1.22
4	8-Q	7508	CIT	O1-C1	-2.13	1.15	1.22
4	9-Q	7508	CIT	O1-C1	-2.13	1.15	1.22
4	10-Q	7508	CIT	O1-C1	-2.13	1.15	1.22
4	1-E	7484	CIT	O1-C1	-2.13	1.15	1.22
4	2-E	7484	CIT	O1-C1	-2.13	1.15	1.22
4	3-E	7484	CIT	O1-C1	-2.13	1.15	1.22
4	4-E	7484	CIT	O1-C1	-2.13	1.15	1.22
4	5-E	7484	CIT	O1-C1	-2.13	1.15	1.22
4	6-E	7484	CIT	O1-C1	-2.13	1.15	1.22
4	7-E	7484	CIT	O1-C1	-2.13	1.15	1.22
4	8-E	7484	CIT	O1-C1	-2.13	1.15	1.22
4	9-E	7484	CIT	O1-C1	-2.13	1.15	1.22
4	10-E	7484	CIT	O1-C1	-2.13	1.15	1.22
4	1-V	7518	CIT	O1-C1	-2.13	1.15	1.22
4	2-V	7518	CIT	O1-C1	-2.13	1.15	1.22
4	3-V	7518	CIT	O1-C1	-2.13	1.15	1.22
4	4-V	7518	CIT	O1-C1	-2.13	1.15	1.22
4	5-V	7518	CIT	O1-C1	-2.13	1.15	1.22
4	6-V	7518	CIT	O1-C1	-2.13	1.15	1.22
4	7-V	7518	CIT	O1-C1	-2.13	1.15	1.22
4	8-V	7518	CIT	O1-C1	-2.13	1.15	1.22
4	9-V	7518	CIT	O1-C1	-2.13	1.15	1.22
4	10-V	7518	CIT	O1-C1	-2.13	1.15	1.22
4	1-K	7496	CIT	O1-C1	-2.12	1.15	1.22
4	2-K	7496	CIT	O1-C1	-2.12	1.15	1.22
4	3-K	7496	CIT	O1-C1	-2.12	1.15	1.22
4	4-K	7496	CIT	O1-C1	-2.12	1.15	1.22
4	5-K	7496	CIT	O1-C1	-2.12	1.15	1.22
4	6-K	7496	CIT	O1-C1	-2.12	1.15	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-K	7496	CIT	O1-C1	-2.12	1.15	1.22
4	8-K	7496	CIT	O1-C1	-2.12	1.15	1.22
4	9-K	7496	CIT	O1-C1	-2.12	1.15	1.22
4	10-K	7496	CIT	O1-C1	-2.12	1.15	1.22
4	1-W	7520	CIT	O1-C1	-2.12	1.15	1.22
4	2-W	7520	CIT	O1-C1	-2.12	1.15	1.22
4	3-W	7520	CIT	O1-C1	-2.12	1.15	1.22
4	4-W	7520	CIT	O1-C1	-2.12	1.15	1.22
4	5-W	7520	CIT	O1-C1	-2.12	1.15	1.22
4	6-W	7520	CIT	O1-C1	-2.12	1.15	1.22
4	7-W	7520	CIT	O1-C1	-2.12	1.15	1.22
4	8-W	7520	CIT	O1-C1	-2.12	1.15	1.22
4	9-W	7520	CIT	O1-C1	-2.12	1.15	1.22
4	10-W	7520	CIT	O1-C1	-2.12	1.15	1.22
4	1-F	7486	CIT	O1-C1	-2.12	1.15	1.22
4	2-F	7486	CIT	O1-C1	-2.12	1.15	1.22
4	3-F	7486	CIT	O1-C1	-2.12	1.15	1.22
4	4-F	7486	CIT	O1-C1	-2.12	1.15	1.22
4	5-F	7486	CIT	O1-C1	-2.12	1.15	1.22
4	6-F	7486	CIT	O1-C1	-2.12	1.15	1.22
4	7-F	7486	CIT	O1-C1	-2.12	1.15	1.22
4	8-F	7486	CIT	O1-C1	-2.12	1.15	1.22
4	9-F	7486	CIT	O1-C1	-2.12	1.15	1.22
4	10-F	7486	CIT	O1-C1	-2.12	1.15	1.22
4	1-U	7516	CIT	O1-C1	-2.12	1.15	1.22
4	2-U	7516	CIT	O1-C1	-2.12	1.15	1.22
4	3-U	7516	CIT	O1-C1	-2.12	1.15	1.22
4	4-U	7516	CIT	O1-C1	-2.12	1.15	1.22
4	5-U	7516	CIT	O1-C1	-2.12	1.15	1.22
4	6-U	7516	CIT	O1-C1	-2.12	1.15	1.22
4	7-U	7516	CIT	O1-C1	-2.12	1.15	1.22
4	8-U	7516	CIT	O1-C1	-2.12	1.15	1.22
4	9-U	7516	CIT	O1-C1	-2.12	1.15	1.22
4	10-U	7516	CIT	O1-C1	-2.12	1.15	1.22
4	1-M	7500	CIT	O1-C1	-2.12	1.15	1.22
4	2-M	7500	CIT	O1-C1	-2.12	1.15	1.22
4	3-M	7500	CIT	O1-C1	-2.12	1.15	1.22
4	4-M	7500	CIT	O1-C1	-2.12	1.15	1.22
4	5-M	7500	CIT	O1-C1	-2.12	1.15	1.22
4	6-M	7500	CIT	O1-C1	-2.12	1.15	1.22
4	7-M	7500	CIT	O1-C1	-2.12	1.15	1.22
4	8-M	7500	CIT	O1-C1	-2.12	1.15	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9-M	7500	CIT	O1-C1	-2.12	1.15	1.22
4	10-M	7500	CIT	O1-C1	-2.12	1.15	1.22
4	1-I	7492	CIT	O1-C1	-2.12	1.15	1.22
4	2-I	7492	CIT	O1-C1	-2.12	1.15	1.22
4	3-I	7492	CIT	O1-C1	-2.12	1.15	1.22
4	4-I	7492	CIT	O1-C1	-2.12	1.15	1.22
4	5-I	7492	CIT	O1-C1	-2.12	1.15	1.22
4	6-I	7492	CIT	O1-C1	-2.12	1.15	1.22
4	7-I	7492	CIT	O1-C1	-2.12	1.15	1.22
4	8-I	7492	CIT	O1-C1	-2.12	1.15	1.22
4	9-I	7492	CIT	O1-C1	-2.12	1.15	1.22
4	10-I	7492	CIT	O1-C1	-2.12	1.15	1.22
4	1-T	7514	CIT	O1-C1	-2.12	1.15	1.22
4	2-T	7514	CIT	O1-C1	-2.12	1.15	1.22
4	3-T	7514	CIT	O1-C1	-2.12	1.15	1.22
4	4-T	7514	CIT	O1-C1	-2.12	1.15	1.22
4	5-T	7514	CIT	O1-C1	-2.12	1.15	1.22
4	6-T	7514	CIT	O1-C1	-2.12	1.15	1.22
4	7-T	7514	CIT	O1-C1	-2.12	1.15	1.22
4	8-T	7514	CIT	O1-C1	-2.12	1.15	1.22
4	9-T	7514	CIT	O1-C1	-2.12	1.15	1.22
4	10-T	7514	CIT	O1-C1	-2.12	1.15	1.22
4	1-A	7476	CIT	O1-C1	-2.11	1.15	1.22
4	2-A	7476	CIT	O1-C1	-2.11	1.15	1.22
4	3-A	7476	CIT	O1-C1	-2.11	1.15	1.22
4	4-A	7476	CIT	O1-C1	-2.11	1.15	1.22
4	5-A	7476	CIT	O1-C1	-2.11	1.15	1.22
4	6-A	7476	CIT	O1-C1	-2.11	1.15	1.22
4	7-A	7476	CIT	O1-C1	-2.11	1.15	1.22
4	8-A	7476	CIT	O1-C1	-2.11	1.15	1.22
4	9-A	7476	CIT	O1-C1	-2.11	1.15	1.22
4	10-A	7476	CIT	O1-C1	-2.11	1.15	1.22
4	1-D	7482	CIT	O1-C1	-2.11	1.15	1.22
4	2-D	7482	CIT	O1-C1	-2.11	1.15	1.22
4	3-D	7482	CIT	O1-C1	-2.11	1.15	1.22
4	4-D	7482	CIT	O1-C1	-2.11	1.15	1.22
4	5-D	7482	CIT	O1-C1	-2.11	1.15	1.22
4	6-D	7482	CIT	O1-C1	-2.11	1.15	1.22
4	7-D	7482	CIT	O1-C1	-2.11	1.15	1.22
4	8-D	7482	CIT	O1-C1	-2.11	1.15	1.22
4	9-D	7482	CIT	O1-C1	-2.11	1.15	1.22
4	10-D	7482	CIT	O1-C1	-2.11	1.15	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-R	7510	CIT	O1-C1	-2.11	1.15	1.22
4	2-R	7510	CIT	O1-C1	-2.11	1.15	1.22
4	3-R	7510	CIT	O1-C1	-2.11	1.15	1.22
4	4-R	7510	CIT	O1-C1	-2.11	1.15	1.22
4	5-R	7510	CIT	O1-C1	-2.11	1.15	1.22
4	6-R	7510	CIT	O1-C1	-2.11	1.15	1.22
4	7-R	7510	CIT	O1-C1	-2.11	1.15	1.22
4	8-R	7510	CIT	O1-C1	-2.11	1.15	1.22
4	9-R	7510	CIT	O1-C1	-2.11	1.15	1.22
4	10-R	7510	CIT	O1-C1	-2.11	1.15	1.22
4	1-O	7504	CIT	O1-C1	-2.11	1.15	1.22
4	2-O	7504	CIT	O1-C1	-2.11	1.15	1.22
4	3-O	7504	CIT	O1-C1	-2.11	1.15	1.22
4	4-O	7504	CIT	O1-C1	-2.11	1.15	1.22
4	5-O	7504	CIT	O1-C1	-2.11	1.15	1.22
4	6-O	7504	CIT	O1-C1	-2.11	1.15	1.22
4	7-O	7504	CIT	O1-C1	-2.11	1.15	1.22
4	8-O	7504	CIT	O1-C1	-2.11	1.15	1.22
4	9-O	7504	CIT	O1-C1	-2.11	1.15	1.22
4	10-O	7504	CIT	O1-C1	-2.11	1.15	1.22
4	1-J	7494	CIT	O1-C1	-2.11	1.15	1.22
4	2-J	7494	CIT	O1-C1	-2.11	1.15	1.22
4	3-J	7494	CIT	O1-C1	-2.11	1.15	1.22
4	4-J	7494	CIT	O1-C1	-2.11	1.15	1.22
4	5-J	7494	CIT	O1-C1	-2.11	1.15	1.22
4	6-J	7494	CIT	O1-C1	-2.11	1.15	1.22
4	7-J	7494	CIT	O1-C1	-2.11	1.15	1.22
4	8-J	7494	CIT	O1-C1	-2.11	1.15	1.22
4	9-J	7494	CIT	O1-C1	-2.11	1.15	1.22
4	10-J	7494	CIT	O1-C1	-2.11	1.15	1.22
4	1-G	7488	CIT	O1-C1	-2.10	1.15	1.22
4	2-G	7488	CIT	O1-C1	-2.10	1.15	1.22
4	3-G	7488	CIT	O1-C1	-2.10	1.15	1.22
4	4-G	7488	CIT	O1-C1	-2.10	1.15	1.22
4	5-G	7488	CIT	O1-C1	-2.10	1.15	1.22
4	6-G	7488	CIT	O1-C1	-2.10	1.15	1.22
4	7-G	7488	CIT	O1-C1	-2.10	1.15	1.22
4	8-G	7488	CIT	O1-C1	-2.10	1.15	1.22
4	9-G	7488	CIT	O1-C1	-2.10	1.15	1.22
4	10-G	7488	CIT	O1-C1	-2.10	1.15	1.22
4	1-L	7498	CIT	O1-C1	-2.10	1.15	1.22
4	2-L	7498	CIT	O1-C1	-2.10	1.15	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-L	7498	CIT	O1-C1	-2.10	1.15	1.22
4	4-L	7498	CIT	O1-C1	-2.10	1.15	1.22
4	5-L	7498	CIT	O1-C1	-2.10	1.15	1.22
4	6-L	7498	CIT	O1-C1	-2.10	1.15	1.22
4	7-L	7498	CIT	O1-C1	-2.10	1.15	1.22
4	8-L	7498	CIT	O1-C1	-2.10	1.15	1.22
4	9-L	7498	CIT	O1-C1	-2.10	1.15	1.22
4	10-L	7498	CIT	O1-C1	-2.10	1.15	1.22
4	1-C	7480	CIT	O1-C1	-2.10	1.15	1.22
4	2-C	7480	CIT	O1-C1	-2.10	1.15	1.22
4	3-C	7480	CIT	O1-C1	-2.10	1.15	1.22
4	4-C	7480	CIT	O1-C1	-2.10	1.15	1.22
4	5-C	7480	CIT	O1-C1	-2.10	1.15	1.22
4	6-C	7480	CIT	O1-C1	-2.10	1.15	1.22
4	7-C	7480	CIT	O1-C1	-2.10	1.15	1.22
4	8-C	7480	CIT	O1-C1	-2.10	1.15	1.22
4	9-C	7480	CIT	O1-C1	-2.10	1.15	1.22
4	10-C	7480	CIT	O1-C1	-2.10	1.15	1.22
4	1-X	7522	CIT	O1-C1	-2.10	1.15	1.22
4	2-X	7522	CIT	O1-C1	-2.10	1.15	1.22
4	3-X	7522	CIT	O1-C1	-2.10	1.15	1.22
4	4-X	7522	CIT	O1-C1	-2.10	1.15	1.22
4	5-X	7522	CIT	O1-C1	-2.10	1.15	1.22
4	6-X	7522	CIT	O1-C1	-2.10	1.15	1.22
4	7-X	7522	CIT	O1-C1	-2.10	1.15	1.22
4	8-X	7522	CIT	O1-C1	-2.10	1.15	1.22
4	9-X	7522	CIT	O1-C1	-2.10	1.15	1.22
4	10-X	7522	CIT	O1-C1	-2.10	1.15	1.22
4	1-N	7502	CIT	O1-C1	-2.09	1.15	1.22
4	2-N	7502	CIT	O1-C1	-2.09	1.15	1.22
4	3-N	7502	CIT	O1-C1	-2.09	1.15	1.22
4	4-N	7502	CIT	O1-C1	-2.09	1.15	1.22
4	5-N	7502	CIT	O1-C1	-2.09	1.15	1.22
4	6-N	7502	CIT	O1-C1	-2.09	1.15	1.22
4	7-N	7502	CIT	O1-C1	-2.09	1.15	1.22
4	8-N	7502	CIT	O1-C1	-2.09	1.15	1.22
4	9-N	7502	CIT	O1-C1	-2.09	1.15	1.22
4	10-N	7502	CIT	O1-C1	-2.09	1.15	1.22
4	1-S	7512	CIT	O1-C1	-2.09	1.15	1.22
4	2-S	7512	CIT	O1-C1	-2.09	1.15	1.22
4	3-S	7512	CIT	O1-C1	-2.09	1.15	1.22
4	4-S	7512	CIT	O1-C1	-2.09	1.15	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5-S	7512	CIT	O1-C1	-2.09	1.15	1.22
4	6-S	7512	CIT	O1-C1	-2.09	1.15	1.22
4	7-S	7512	CIT	O1-C1	-2.09	1.15	1.22
4	8-S	7512	CIT	O1-C1	-2.09	1.15	1.22
4	9-S	7512	CIT	O1-C1	-2.09	1.15	1.22
4	10-S	7512	CIT	O1-C1	-2.09	1.15	1.22
4	1-G	7488	CIT	C4-C5	2.08	1.57	1.50
4	2-G	7488	CIT	C4-C5	2.08	1.57	1.50
4	3-G	7488	CIT	C4-C5	2.08	1.57	1.50
4	4-G	7488	CIT	C4-C5	2.08	1.57	1.50
4	5-G	7488	CIT	C4-C5	2.08	1.57	1.50
4	6-G	7488	CIT	C4-C5	2.08	1.57	1.50
4	7-G	7488	CIT	C4-C5	2.08	1.57	1.50
4	8-G	7488	CIT	C4-C5	2.08	1.57	1.50
4	9-G	7488	CIT	C4-C5	2.08	1.57	1.50
4	10-G	7488	CIT	C4-C5	2.08	1.57	1.50
4	1-N	7502	CIT	C4-C5	2.07	1.57	1.50
4	2-N	7502	CIT	C4-C5	2.07	1.57	1.50
4	3-N	7502	CIT	C4-C5	2.07	1.57	1.50
4	4-N	7502	CIT	C4-C5	2.07	1.57	1.50
4	5-N	7502	CIT	C4-C5	2.07	1.57	1.50
4	6-N	7502	CIT	C4-C5	2.07	1.57	1.50
4	7-N	7502	CIT	C4-C5	2.07	1.57	1.50
4	8-N	7502	CIT	C4-C5	2.07	1.57	1.50
4	9-N	7502	CIT	C4-C5	2.07	1.57	1.50
4	10-N	7502	CIT	C4-C5	2.07	1.57	1.50
4	1-C	7480	CIT	C4-C5	2.07	1.57	1.50
4	2-C	7480	CIT	C4-C5	2.07	1.57	1.50
4	3-C	7480	CIT	C4-C5	2.07	1.57	1.50
4	4-C	7480	CIT	C4-C5	2.07	1.57	1.50
4	5-C	7480	CIT	C4-C5	2.07	1.57	1.50
4	6-C	7480	CIT	C4-C5	2.07	1.57	1.50
4	7-C	7480	CIT	C4-C5	2.07	1.57	1.50
4	8-C	7480	CIT	C4-C5	2.07	1.57	1.50
4	9-C	7480	CIT	C4-C5	2.07	1.57	1.50
4	10-C	7480	CIT	C4-C5	2.07	1.57	1.50
4	1-R	7510	CIT	C4-C5	2.07	1.57	1.50
4	2-R	7510	CIT	C4-C5	2.07	1.57	1.50
4	3-R	7510	CIT	C4-C5	2.07	1.57	1.50
4	4-R	7510	CIT	C4-C5	2.07	1.57	1.50
4	5-R	7510	CIT	C4-C5	2.07	1.57	1.50
4	6-R	7510	CIT	C4-C5	2.07	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7-R	7510	CIT	C4-C5	2.07	1.57	1.50
4	8-R	7510	CIT	C4-C5	2.07	1.57	1.50
4	9-R	7510	CIT	C4-C5	2.07	1.57	1.50
4	10-R	7510	CIT	C4-C5	2.07	1.57	1.50
4	1-O	7504	CIT	C4-C5	2.07	1.57	1.50
4	2-O	7504	CIT	C4-C5	2.07	1.57	1.50
4	3-O	7504	CIT	C4-C5	2.07	1.57	1.50
4	4-O	7504	CIT	C4-C5	2.07	1.57	1.50
4	5-O	7504	CIT	C4-C5	2.07	1.57	1.50
4	6-O	7504	CIT	C4-C5	2.07	1.57	1.50
4	7-O	7504	CIT	C4-C5	2.07	1.57	1.50
4	8-O	7504	CIT	C4-C5	2.07	1.57	1.50
4	9-O	7504	CIT	C4-C5	2.07	1.57	1.50
4	10-O	7504	CIT	C4-C5	2.07	1.57	1.50
4	1-J	7494	CIT	C4-C5	2.07	1.57	1.50
4	2-J	7494	CIT	C4-C5	2.07	1.57	1.50
4	3-J	7494	CIT	C4-C5	2.07	1.57	1.50
4	4-J	7494	CIT	C4-C5	2.07	1.57	1.50
4	5-J	7494	CIT	C4-C5	2.07	1.57	1.50
4	6-J	7494	CIT	C4-C5	2.07	1.57	1.50
4	7-J	7494	CIT	C4-C5	2.07	1.57	1.50
4	8-J	7494	CIT	C4-C5	2.07	1.57	1.50
4	9-J	7494	CIT	C4-C5	2.07	1.57	1.50
4	10-J	7494	CIT	C4-C5	2.07	1.57	1.50
4	1-U	7516	CIT	C4-C5	2.06	1.57	1.50
4	2-U	7516	CIT	C4-C5	2.06	1.57	1.50
4	3-U	7516	CIT	C4-C5	2.06	1.57	1.50
4	4-U	7516	CIT	C4-C5	2.06	1.57	1.50
4	5-U	7516	CIT	C4-C5	2.06	1.57	1.50
4	6-U	7516	CIT	C4-C5	2.06	1.57	1.50
4	7-U	7516	CIT	C4-C5	2.06	1.57	1.50
4	8-U	7516	CIT	C4-C5	2.06	1.57	1.50
4	9-U	7516	CIT	C4-C5	2.06	1.57	1.50
4	10-U	7516	CIT	C4-C5	2.06	1.57	1.50
4	1-P	7506	CIT	C4-C5	2.06	1.57	1.50
4	2-P	7506	CIT	C4-C5	2.06	1.57	1.50
4	3-P	7506	CIT	C4-C5	2.06	1.57	1.50
4	4-P	7506	CIT	C4-C5	2.06	1.57	1.50
4	5-P	7506	CIT	C4-C5	2.06	1.57	1.50
4	6-P	7506	CIT	C4-C5	2.06	1.57	1.50
4	7-P	7506	CIT	C4-C5	2.06	1.57	1.50
4	8-P	7506	CIT	C4-C5	2.06	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9-P	7506	CIT	C4-C5	2.06	1.57	1.50
4	10-P	7506	CIT	C4-C5	2.06	1.57	1.50
4	1-L	7498	CIT	C4-C5	2.06	1.57	1.50
4	2-L	7498	CIT	C4-C5	2.06	1.57	1.50
4	3-L	7498	CIT	C4-C5	2.06	1.57	1.50
4	4-L	7498	CIT	C4-C5	2.06	1.57	1.50
4	5-L	7498	CIT	C4-C5	2.06	1.57	1.50
4	6-L	7498	CIT	C4-C5	2.06	1.57	1.50
4	7-L	7498	CIT	C4-C5	2.06	1.57	1.50
4	8-L	7498	CIT	C4-C5	2.06	1.57	1.50
4	9-L	7498	CIT	C4-C5	2.06	1.57	1.50
4	10-L	7498	CIT	C4-C5	2.06	1.57	1.50
4	1-X	7522	CIT	C4-C5	2.06	1.57	1.50
4	2-X	7522	CIT	C4-C5	2.06	1.57	1.50
4	3-X	7522	CIT	C4-C5	2.06	1.57	1.50
4	4-X	7522	CIT	C4-C5	2.06	1.57	1.50
4	5-X	7522	CIT	C4-C5	2.06	1.57	1.50
4	6-X	7522	CIT	C4-C5	2.06	1.57	1.50
4	7-X	7522	CIT	C4-C5	2.06	1.57	1.50
4	8-X	7522	CIT	C4-C5	2.06	1.57	1.50
4	9-X	7522	CIT	C4-C5	2.06	1.57	1.50
4	10-X	7522	CIT	C4-C5	2.06	1.57	1.50
4	1-F	7486	CIT	C4-C5	2.06	1.57	1.50
4	2-F	7486	CIT	C4-C5	2.06	1.57	1.50
4	3-F	7486	CIT	C4-C5	2.06	1.57	1.50
4	4-F	7486	CIT	C4-C5	2.06	1.57	1.50
4	5-F	7486	CIT	C4-C5	2.06	1.57	1.50
4	6-F	7486	CIT	C4-C5	2.06	1.57	1.50
4	7-F	7486	CIT	C4-C5	2.06	1.57	1.50
4	8-F	7486	CIT	C4-C5	2.06	1.57	1.50
4	9-F	7486	CIT	C4-C5	2.06	1.57	1.50
4	10-F	7486	CIT	C4-C5	2.06	1.57	1.50
4	1-Q	7508	CIT	C4-C5	2.06	1.57	1.50
4	2-Q	7508	CIT	C4-C5	2.06	1.57	1.50
4	3-Q	7508	CIT	C4-C5	2.06	1.57	1.50
4	4-Q	7508	CIT	C4-C5	2.06	1.57	1.50
4	5-Q	7508	CIT	C4-C5	2.06	1.57	1.50
4	6-Q	7508	CIT	C4-C5	2.06	1.57	1.50
4	7-Q	7508	CIT	C4-C5	2.06	1.57	1.50
4	8-Q	7508	CIT	C4-C5	2.06	1.57	1.50
4	9-Q	7508	CIT	C4-C5	2.06	1.57	1.50
4	10-Q	7508	CIT	C4-C5	2.06	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-I	7492	CIT	C4-C5	2.06	1.57	1.50
4	2-I	7492	CIT	C4-C5	2.06	1.57	1.50
4	3-I	7492	CIT	C4-C5	2.06	1.57	1.50
4	4-I	7492	CIT	C4-C5	2.06	1.57	1.50
4	5-I	7492	CIT	C4-C5	2.06	1.57	1.50
4	6-I	7492	CIT	C4-C5	2.06	1.57	1.50
4	7-I	7492	CIT	C4-C5	2.06	1.57	1.50
4	8-I	7492	CIT	C4-C5	2.06	1.57	1.50
4	9-I	7492	CIT	C4-C5	2.06	1.57	1.50
4	10-I	7492	CIT	C4-C5	2.06	1.57	1.50
4	1-M	7500	CIT	C4-C5	2.06	1.57	1.50
4	2-M	7500	CIT	C4-C5	2.06	1.57	1.50
4	3-M	7500	CIT	C4-C5	2.06	1.57	1.50
4	4-M	7500	CIT	C4-C5	2.06	1.57	1.50
4	5-M	7500	CIT	C4-C5	2.06	1.57	1.50
4	6-M	7500	CIT	C4-C5	2.06	1.57	1.50
4	7-M	7500	CIT	C4-C5	2.06	1.57	1.50
4	8-M	7500	CIT	C4-C5	2.06	1.57	1.50
4	9-M	7500	CIT	C4-C5	2.06	1.57	1.50
4	10-M	7500	CIT	C4-C5	2.06	1.57	1.50
4	1-A	7476	CIT	C4-C5	2.06	1.57	1.50
4	2-A	7476	CIT	C4-C5	2.06	1.57	1.50
4	3-A	7476	CIT	C4-C5	2.06	1.57	1.50
4	4-A	7476	CIT	C4-C5	2.06	1.57	1.50
4	5-A	7476	CIT	C4-C5	2.06	1.57	1.50
4	6-A	7476	CIT	C4-C5	2.06	1.57	1.50
4	7-A	7476	CIT	C4-C5	2.06	1.57	1.50
4	8-A	7476	CIT	C4-C5	2.06	1.57	1.50
4	9-A	7476	CIT	C4-C5	2.06	1.57	1.50
4	10-A	7476	CIT	C4-C5	2.06	1.57	1.50
4	1-B	7478	CIT	C4-C5	2.06	1.57	1.50
4	2-B	7478	CIT	C4-C5	2.06	1.57	1.50
4	3-B	7478	CIT	C4-C5	2.06	1.57	1.50
4	4-B	7478	CIT	C4-C5	2.06	1.57	1.50
4	5-B	7478	CIT	C4-C5	2.06	1.57	1.50
4	6-B	7478	CIT	C4-C5	2.06	1.57	1.50
4	7-B	7478	CIT	C4-C5	2.06	1.57	1.50
4	8-B	7478	CIT	C4-C5	2.06	1.57	1.50
4	9-B	7478	CIT	C4-C5	2.06	1.57	1.50
4	10-B	7478	CIT	C4-C5	2.06	1.57	1.50
4	1-W	7520	CIT	C4-C5	2.05	1.57	1.50
4	2-W	7520	CIT	C4-C5	2.05	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-W	7520	CIT	C4-C5	2.05	1.57	1.50
4	4-W	7520	CIT	C4-C5	2.05	1.57	1.50
4	5-W	7520	CIT	C4-C5	2.05	1.57	1.50
4	6-W	7520	CIT	C4-C5	2.05	1.57	1.50
4	7-W	7520	CIT	C4-C5	2.05	1.57	1.50
4	8-W	7520	CIT	C4-C5	2.05	1.57	1.50
4	9-W	7520	CIT	C4-C5	2.05	1.57	1.50
4	10-W	7520	CIT	C4-C5	2.05	1.57	1.50
4	1-K	7496	CIT	C4-C5	2.05	1.56	1.50
4	2-K	7496	CIT	C4-C5	2.05	1.56	1.50
4	3-K	7496	CIT	C4-C5	2.05	1.56	1.50
4	4-K	7496	CIT	C4-C5	2.05	1.56	1.50
4	5-K	7496	CIT	C4-C5	2.05	1.56	1.50
4	6-K	7496	CIT	C4-C5	2.05	1.56	1.50
4	7-K	7496	CIT	C4-C5	2.05	1.56	1.50
4	8-K	7496	CIT	C4-C5	2.05	1.56	1.50
4	9-K	7496	CIT	C4-C5	2.05	1.56	1.50
4	10-K	7496	CIT	C4-C5	2.05	1.56	1.50
4	1-E	7484	CIT	C4-C5	2.04	1.56	1.50
4	2-E	7484	CIT	C4-C5	2.04	1.56	1.50
4	3-E	7484	CIT	C4-C5	2.04	1.56	1.50
4	4-E	7484	CIT	C4-C5	2.04	1.56	1.50
4	5-E	7484	CIT	C4-C5	2.04	1.56	1.50
4	6-E	7484	CIT	C4-C5	2.04	1.56	1.50
4	7-E	7484	CIT	C4-C5	2.04	1.56	1.50
4	8-E	7484	CIT	C4-C5	2.04	1.56	1.50
4	9-E	7484	CIT	C4-C5	2.04	1.56	1.50
4	10-E	7484	CIT	C4-C5	2.04	1.56	1.50
4	1-V	7518	CIT	C4-C5	2.04	1.56	1.50
4	2-V	7518	CIT	C4-C5	2.04	1.56	1.50
4	3-V	7518	CIT	C4-C5	2.04	1.56	1.50
4	4-V	7518	CIT	C4-C5	2.04	1.56	1.50
4	5-V	7518	CIT	C4-C5	2.04	1.56	1.50
4	6-V	7518	CIT	C4-C5	2.04	1.56	1.50
4	7-V	7518	CIT	C4-C5	2.04	1.56	1.50
4	8-V	7518	CIT	C4-C5	2.04	1.56	1.50
4	9-V	7518	CIT	C4-C5	2.04	1.56	1.50
4	10-V	7518	CIT	C4-C5	2.04	1.56	1.50
4	1-D	7482	CIT	C4-C5	2.04	1.56	1.50
4	2-D	7482	CIT	C4-C5	2.04	1.56	1.50
4	3-D	7482	CIT	C4-C5	2.04	1.56	1.50
4	4-D	7482	CIT	C4-C5	2.04	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5-D	7482	CIT	C4-C5	2.04	1.56	1.50
4	6-D	7482	CIT	C4-C5	2.04	1.56	1.50
4	7-D	7482	CIT	C4-C5	2.04	1.56	1.50
4	8-D	7482	CIT	C4-C5	2.04	1.56	1.50
4	9-D	7482	CIT	C4-C5	2.04	1.56	1.50
4	10-D	7482	CIT	C4-C5	2.04	1.56	1.50
4	1-T	7514	CIT	C4-C5	2.04	1.56	1.50
4	2-T	7514	CIT	C4-C5	2.04	1.56	1.50
4	3-T	7514	CIT	C4-C5	2.04	1.56	1.50
4	4-T	7514	CIT	C4-C5	2.04	1.56	1.50
4	5-T	7514	CIT	C4-C5	2.04	1.56	1.50
4	6-T	7514	CIT	C4-C5	2.04	1.56	1.50
4	7-T	7514	CIT	C4-C5	2.04	1.56	1.50
4	8-T	7514	CIT	C4-C5	2.04	1.56	1.50
4	9-T	7514	CIT	C4-C5	2.04	1.56	1.50
4	10-T	7514	CIT	C4-C5	2.04	1.56	1.50
4	1-H	7490	CIT	C4-C5	2.04	1.56	1.50
4	2-H	7490	CIT	C4-C5	2.04	1.56	1.50
4	3-H	7490	CIT	C4-C5	2.04	1.56	1.50
4	4-H	7490	CIT	C4-C5	2.04	1.56	1.50
4	5-H	7490	CIT	C4-C5	2.04	1.56	1.50
4	6-H	7490	CIT	C4-C5	2.04	1.56	1.50
4	7-H	7490	CIT	C4-C5	2.04	1.56	1.50
4	8-H	7490	CIT	C4-C5	2.04	1.56	1.50
4	9-H	7490	CIT	C4-C5	2.04	1.56	1.50
4	10-H	7490	CIT	C4-C5	2.04	1.56	1.50
4	1-S	7512	CIT	C4-C5	2.03	1.56	1.50
4	2-S	7512	CIT	C4-C5	2.03	1.56	1.50
4	3-S	7512	CIT	C4-C5	2.03	1.56	1.50
4	4-S	7512	CIT	C4-C5	2.03	1.56	1.50
4	5-S	7512	CIT	C4-C5	2.03	1.56	1.50
4	6-S	7512	CIT	C4-C5	2.03	1.56	1.50
4	7-S	7512	CIT	C4-C5	2.03	1.56	1.50
4	8-S	7512	CIT	C4-C5	2.03	1.56	1.50
4	9-S	7512	CIT	C4-C5	2.03	1.56	1.50
4	10-S	7512	CIT	C4-C5	2.03	1.56	1.50

All (5010) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-P	7505	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	2-P	7505	AMP	O4'-C1'-C2'	-9.17	87.00	106.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-P	7505	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	4-P	7505	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	5-P	7505	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	6-P	7505	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	7-P	7505	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	8-P	7505	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	9-P	7505	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	10-P	7505	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	1-J	7493	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	2-J	7493	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	3-J	7493	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	4-J	7493	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	5-J	7493	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	6-J	7493	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	7-J	7493	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	8-J	7493	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	9-J	7493	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	10-J	7493	AMP	O4'-C1'-C2'	-9.17	87.00	106.62
3	1-E	7483	AMP	O4'-C1'-C2'	-9.16	87.00	106.62
3	2-E	7483	AMP	O4'-C1'-C2'	-9.16	87.00	106.62
3	3-E	7483	AMP	O4'-C1'-C2'	-9.16	87.00	106.62
3	4-E	7483	AMP	O4'-C1'-C2'	-9.16	87.00	106.62
3	5-E	7483	AMP	O4'-C1'-C2'	-9.16	87.00	106.62
3	6-E	7483	AMP	O4'-C1'-C2'	-9.16	87.00	106.62
3	7-E	7483	AMP	O4'-C1'-C2'	-9.16	87.00	106.62
3	8-E	7483	AMP	O4'-C1'-C2'	-9.16	87.00	106.62
3	9-E	7483	AMP	O4'-C1'-C2'	-9.16	87.00	106.62
3	10-E	7483	AMP	O4'-C1'-C2'	-9.16	87.00	106.62
3	1-N	7501	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	2-N	7501	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	3-N	7501	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	4-N	7501	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	5-N	7501	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	6-N	7501	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	7-N	7501	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	8-N	7501	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	9-N	7501	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	10-N	7501	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	1-G	7487	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	2-G	7487	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	3-G	7487	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	4-G	7487	AMP	O4'-C1'-C2'	-9.16	87.01	106.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-G	7487	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	6-G	7487	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	7-G	7487	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	8-G	7487	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	9-G	7487	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	10-G	7487	AMP	O4'-C1'-C2'	-9.16	87.01	106.62
3	1-O	7503	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	2-O	7503	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	3-O	7503	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	4-O	7503	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	5-O	7503	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	6-O	7503	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	7-O	7503	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	8-O	7503	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	9-O	7503	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	10-O	7503	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	1-M	7499	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	2-M	7499	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	3-M	7499	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	4-M	7499	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	5-M	7499	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	6-M	7499	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	7-M	7499	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	8-M	7499	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	9-M	7499	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	10-M	7499	AMP	O4'-C1'-C2'	-9.16	87.02	106.62
3	1-C	7479	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	2-C	7479	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	3-C	7479	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	4-C	7479	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	5-C	7479	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	6-C	7479	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	7-C	7479	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	8-C	7479	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	9-C	7479	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	10-C	7479	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	1-F	7485	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	2-F	7485	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	3-F	7485	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	4-F	7485	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	5-F	7485	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	6-F	7485	AMP	O4'-C1'-C2'	-9.15	87.03	106.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-F	7485	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	8-F	7485	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	9-F	7485	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	10-F	7485	AMP	O4'-C1'-C2'	-9.15	87.03	106.62
3	1-W	7519	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	2-W	7519	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	3-W	7519	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	4-W	7519	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	5-W	7519	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	6-W	7519	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	7-W	7519	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	8-W	7519	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	9-W	7519	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	10-W	7519	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	1-K	7495	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	2-K	7495	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	3-K	7495	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	4-K	7495	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	5-K	7495	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	6-K	7495	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	7-K	7495	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	8-K	7495	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	9-K	7495	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	10-K	7495	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	1-H	7489	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	2-H	7489	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	3-H	7489	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	4-H	7489	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	5-H	7489	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	6-H	7489	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	7-H	7489	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	8-H	7489	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	9-H	7489	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	10-H	7489	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	1-X	7521	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	2-X	7521	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	3-X	7521	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	4-X	7521	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	5-X	7521	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	6-X	7521	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	7-X	7521	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	8-X	7521	AMP	O4'-C1'-C2'	-9.15	87.04	106.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-X	7521	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	10-X	7521	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	1-A	7475	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	2-A	7475	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	3-A	7475	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	4-A	7475	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	5-A	7475	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	6-A	7475	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	7-A	7475	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	8-A	7475	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	9-A	7475	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	10-A	7475	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	1-D	7481	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	2-D	7481	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	3-D	7481	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	4-D	7481	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	5-D	7481	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	6-D	7481	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	7-D	7481	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	8-D	7481	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	9-D	7481	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	10-D	7481	AMP	O4'-C1'-C2'	-9.15	87.04	106.62
3	1-U	7515	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	2-U	7515	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	3-U	7515	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	4-U	7515	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	5-U	7515	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	6-U	7515	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	7-U	7515	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	8-U	7515	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	9-U	7515	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	10-U	7515	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	1-T	7513	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	2-T	7513	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	3-T	7513	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	4-T	7513	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	5-T	7513	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	6-T	7513	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	7-T	7513	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	8-T	7513	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	9-T	7513	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	10-T	7513	AMP	O4'-C1'-C2'	-9.14	87.05	106.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-L	7497	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	2-L	7497	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	3-L	7497	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	4-L	7497	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	5-L	7497	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	6-L	7497	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	7-L	7497	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	8-L	7497	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	9-L	7497	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	10-L	7497	AMP	O4'-C1'-C2'	-9.14	87.05	106.62
3	1-Q	7507	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	2-Q	7507	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	3-Q	7507	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	4-Q	7507	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	5-Q	7507	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	6-Q	7507	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	7-Q	7507	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	8-Q	7507	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	9-Q	7507	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	10-Q	7507	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	1-I	7491	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	2-I	7491	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	3-I	7491	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	4-I	7491	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	5-I	7491	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	6-I	7491	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	7-I	7491	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	8-I	7491	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	9-I	7491	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	10-I	7491	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	1-B	7477	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	2-B	7477	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	3-B	7477	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	4-B	7477	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	5-B	7477	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	6-B	7477	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	7-B	7477	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	8-B	7477	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	9-B	7477	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	10-B	7477	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	1-V	7517	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	2-V	7517	AMP	O4'-C1'-C2'	-9.14	87.06	106.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-V	7517	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	4-V	7517	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	5-V	7517	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	6-V	7517	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	7-V	7517	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	8-V	7517	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	9-V	7517	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	10-V	7517	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	1-R	7509	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	2-R	7509	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	3-R	7509	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	4-R	7509	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	5-R	7509	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	6-R	7509	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	7-R	7509	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	8-R	7509	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	9-R	7509	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	10-R	7509	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	1-S	7511	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	2-S	7511	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	3-S	7511	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	4-S	7511	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	5-S	7511	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	6-S	7511	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	7-S	7511	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	8-S	7511	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	9-S	7511	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	10-S	7511	AMP	O4'-C1'-C2'	-9.14	87.06	106.62
3	1-X	7521	AMP	O5'-C5'-C4'	8.49	137.89	108.99
3	2-X	7521	AMP	O5'-C5'-C4'	8.49	137.89	108.99
3	3-X	7521	AMP	O5'-C5'-C4'	8.49	137.89	108.99
3	4-X	7521	AMP	O5'-C5'-C4'	8.49	137.89	108.99
3	5-X	7521	AMP	O5'-C5'-C4'	8.49	137.89	108.99
3	6-X	7521	AMP	O5'-C5'-C4'	8.49	137.89	108.99
3	7-X	7521	AMP	O5'-C5'-C4'	8.49	137.89	108.99
3	8-X	7521	AMP	O5'-C5'-C4'	8.49	137.89	108.99
3	9-X	7521	AMP	O5'-C5'-C4'	8.49	137.89	108.99
3	10-X	7521	AMP	O5'-C5'-C4'	8.49	137.89	108.99
3	1-P	7505	AMP	O5'-C5'-C4'	8.49	137.88	108.99
3	2-P	7505	AMP	O5'-C5'-C4'	8.49	137.88	108.99
3	3-P	7505	AMP	O5'-C5'-C4'	8.49	137.88	108.99
3	4-P	7505	AMP	O5'-C5'-C4'	8.49	137.88	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-P	7505	AMP	O5'-C5'-C4'	8.49	137.88	108.99
3	6-P	7505	AMP	O5'-C5'-C4'	8.49	137.88	108.99
3	7-P	7505	AMP	O5'-C5'-C4'	8.49	137.88	108.99
3	8-P	7505	AMP	O5'-C5'-C4'	8.49	137.88	108.99
3	9-P	7505	AMP	O5'-C5'-C4'	8.49	137.88	108.99
3	10-P	7505	AMP	O5'-C5'-C4'	8.49	137.88	108.99
3	1-I	7491	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	2-I	7491	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	3-I	7491	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	4-I	7491	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	5-I	7491	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	6-I	7491	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	7-I	7491	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	8-I	7491	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	9-I	7491	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	10-I	7491	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	1-C	7479	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	2-C	7479	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	3-C	7479	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	4-C	7479	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	5-C	7479	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	6-C	7479	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	7-C	7479	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	8-C	7479	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	9-C	7479	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	10-C	7479	AMP	O5'-C5'-C4'	8.48	137.87	108.99
3	1-T	7513	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	2-T	7513	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	3-T	7513	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	4-T	7513	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	5-T	7513	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	6-T	7513	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	7-T	7513	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	8-T	7513	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	9-T	7513	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	10-T	7513	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	1-V	7517	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	2-V	7517	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	3-V	7517	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	4-V	7517	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	5-V	7517	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	6-V	7517	AMP	O5'-C5'-C4'	8.48	137.86	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-V	7517	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	8-V	7517	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	9-V	7517	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	10-V	7517	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	1-M	7499	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	2-M	7499	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	3-M	7499	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	4-M	7499	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	5-M	7499	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	6-M	7499	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	7-M	7499	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	8-M	7499	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	9-M	7499	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	10-M	7499	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	1-U	7515	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	2-U	7515	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	3-U	7515	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	4-U	7515	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	5-U	7515	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	6-U	7515	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	7-U	7515	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	8-U	7515	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	9-U	7515	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	10-U	7515	AMP	O5'-C5'-C4'	8.48	137.86	108.99
3	1-S	7511	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	2-S	7511	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	3-S	7511	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	4-S	7511	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	5-S	7511	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	6-S	7511	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	7-S	7511	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	8-S	7511	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	9-S	7511	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	10-S	7511	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	1-W	7519	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	2-W	7519	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	3-W	7519	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	4-W	7519	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	5-W	7519	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	6-W	7519	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	7-W	7519	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	8-W	7519	AMP	O5'-C5'-C4'	8.48	137.85	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-W	7519	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	10-W	7519	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	1-Q	7507	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	2-Q	7507	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	3-Q	7507	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	4-Q	7507	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	5-Q	7507	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	6-Q	7507	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	7-Q	7507	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	8-Q	7507	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	9-Q	7507	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	10-Q	7507	AMP	O5'-C5'-C4'	8.48	137.85	108.99
3	1-K	7495	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	2-K	7495	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	3-K	7495	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	4-K	7495	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	5-K	7495	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	6-K	7495	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	7-K	7495	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	8-K	7495	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	9-K	7495	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	10-K	7495	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	1-E	7483	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	2-E	7483	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	3-E	7483	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	4-E	7483	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	5-E	7483	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	6-E	7483	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	7-E	7483	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	8-E	7483	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	9-E	7483	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	10-E	7483	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	1-G	7487	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	2-G	7487	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	3-G	7487	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	4-G	7487	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	5-G	7487	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	6-G	7487	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	7-G	7487	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	8-G	7487	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	9-G	7487	AMP	O5'-C5'-C4'	8.47	137.85	108.99
3	10-G	7487	AMP	O5'-C5'-C4'	8.47	137.85	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-A	7475	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	2-A	7475	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	3-A	7475	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	4-A	7475	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	5-A	7475	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	6-A	7475	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	7-A	7475	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	8-A	7475	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	9-A	7475	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	10-A	7475	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	1-O	7503	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	2-O	7503	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	3-O	7503	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	4-O	7503	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	5-O	7503	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	6-O	7503	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	7-O	7503	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	8-O	7503	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	9-O	7503	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	10-O	7503	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	1-N	7501	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	2-N	7501	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	3-N	7501	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	4-N	7501	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	5-N	7501	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	6-N	7501	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	7-N	7501	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	8-N	7501	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	9-N	7501	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	10-N	7501	AMP	O5'-C5'-C4'	8.47	137.84	108.99
3	1-H	7489	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	2-H	7489	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	3-H	7489	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	4-H	7489	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	5-H	7489	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	6-H	7489	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	7-H	7489	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	8-H	7489	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	9-H	7489	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	10-H	7489	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	1-R	7509	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	2-R	7509	AMP	O5'-C5'-C4'	8.47	137.83	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-R	7509	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	4-R	7509	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	5-R	7509	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	6-R	7509	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	7-R	7509	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	8-R	7509	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	9-R	7509	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	10-R	7509	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	1-J	7493	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	2-J	7493	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	3-J	7493	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	4-J	7493	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	5-J	7493	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	6-J	7493	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	7-J	7493	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	8-J	7493	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	9-J	7493	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	10-J	7493	AMP	O5'-C5'-C4'	8.47	137.83	108.99
3	1-D	7481	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	2-D	7481	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	3-D	7481	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	4-D	7481	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	5-D	7481	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	6-D	7481	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	7-D	7481	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	8-D	7481	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	9-D	7481	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	10-D	7481	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	1-B	7477	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	2-B	7477	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	3-B	7477	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	4-B	7477	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	5-B	7477	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	6-B	7477	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	7-B	7477	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	8-B	7477	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	9-B	7477	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	10-B	7477	AMP	O5'-C5'-C4'	8.47	137.82	108.99
3	1-L	7497	AMP	O5'-C5'-C4'	8.46	137.80	108.99
3	2-L	7497	AMP	O5'-C5'-C4'	8.46	137.80	108.99
3	3-L	7497	AMP	O5'-C5'-C4'	8.46	137.80	108.99
3	4-L	7497	AMP	O5'-C5'-C4'	8.46	137.80	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-L	7497	AMP	O5'-C5'-C4'	8.46	137.80	108.99
3	6-L	7497	AMP	O5'-C5'-C4'	8.46	137.80	108.99
3	7-L	7497	AMP	O5'-C5'-C4'	8.46	137.80	108.99
3	8-L	7497	AMP	O5'-C5'-C4'	8.46	137.80	108.99
3	9-L	7497	AMP	O5'-C5'-C4'	8.46	137.80	108.99
3	10-L	7497	AMP	O5'-C5'-C4'	8.46	137.80	108.99
3	1-F	7485	AMP	O5'-C5'-C4'	8.46	137.79	108.99
3	2-F	7485	AMP	O5'-C5'-C4'	8.46	137.79	108.99
3	3-F	7485	AMP	O5'-C5'-C4'	8.46	137.79	108.99
3	4-F	7485	AMP	O5'-C5'-C4'	8.46	137.79	108.99
3	5-F	7485	AMP	O5'-C5'-C4'	8.46	137.79	108.99
3	6-F	7485	AMP	O5'-C5'-C4'	8.46	137.79	108.99
3	7-F	7485	AMP	O5'-C5'-C4'	8.46	137.79	108.99
3	8-F	7485	AMP	O5'-C5'-C4'	8.46	137.79	108.99
3	9-F	7485	AMP	O5'-C5'-C4'	8.46	137.79	108.99
3	10-F	7485	AMP	O5'-C5'-C4'	8.46	137.79	108.99
3	1-K	7495	AMP	C4-N9-C8	-6.53	98.88	105.74
3	2-K	7495	AMP	C4-N9-C8	-6.53	98.88	105.74
3	3-K	7495	AMP	C4-N9-C8	-6.53	98.88	105.74
3	4-K	7495	AMP	C4-N9-C8	-6.53	98.88	105.74
3	5-K	7495	AMP	C4-N9-C8	-6.53	98.88	105.74
3	6-K	7495	AMP	C4-N9-C8	-6.53	98.88	105.74
3	7-K	7495	AMP	C4-N9-C8	-6.53	98.88	105.74
3	8-K	7495	AMP	C4-N9-C8	-6.53	98.88	105.74
3	9-K	7495	AMP	C4-N9-C8	-6.53	98.88	105.74
3	10-K	7495	AMP	C4-N9-C8	-6.53	98.88	105.74
3	1-L	7497	AMP	C4-N9-C8	-6.53	98.89	105.74
3	2-L	7497	AMP	C4-N9-C8	-6.53	98.89	105.74
3	3-L	7497	AMP	C4-N9-C8	-6.53	98.89	105.74
3	4-L	7497	AMP	C4-N9-C8	-6.53	98.89	105.74
3	5-L	7497	AMP	C4-N9-C8	-6.53	98.89	105.74
3	6-L	7497	AMP	C4-N9-C8	-6.53	98.89	105.74
3	7-L	7497	AMP	C4-N9-C8	-6.53	98.89	105.74
3	8-L	7497	AMP	C4-N9-C8	-6.53	98.89	105.74
3	9-L	7497	AMP	C4-N9-C8	-6.53	98.89	105.74
3	10-L	7497	AMP	C4-N9-C8	-6.53	98.89	105.74
3	1-O	7503	AMP	C4-N9-C8	-6.52	98.89	105.74
3	2-O	7503	AMP	C4-N9-C8	-6.52	98.89	105.74
3	3-O	7503	AMP	C4-N9-C8	-6.52	98.89	105.74
3	4-O	7503	AMP	C4-N9-C8	-6.52	98.89	105.74
3	5-O	7503	AMP	C4-N9-C8	-6.52	98.89	105.74
3	6-O	7503	AMP	C4-N9-C8	-6.52	98.89	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-O	7503	AMP	C4-N9-C8	-6.52	98.89	105.74
3	8-O	7503	AMP	C4-N9-C8	-6.52	98.89	105.74
3	9-O	7503	AMP	C4-N9-C8	-6.52	98.89	105.74
3	10-O	7503	AMP	C4-N9-C8	-6.52	98.89	105.74
3	1-P	7505	AMP	C4-N9-C8	-6.52	98.90	105.74
3	2-P	7505	AMP	C4-N9-C8	-6.52	98.90	105.74
3	3-P	7505	AMP	C4-N9-C8	-6.52	98.90	105.74
3	4-P	7505	AMP	C4-N9-C8	-6.52	98.90	105.74
3	5-P	7505	AMP	C4-N9-C8	-6.52	98.90	105.74
3	6-P	7505	AMP	C4-N9-C8	-6.52	98.90	105.74
3	7-P	7505	AMP	C4-N9-C8	-6.52	98.90	105.74
3	8-P	7505	AMP	C4-N9-C8	-6.52	98.90	105.74
3	9-P	7505	AMP	C4-N9-C8	-6.52	98.90	105.74
3	10-P	7505	AMP	C4-N9-C8	-6.52	98.90	105.74
3	1-U	7515	AMP	C4-N9-C8	-6.52	98.90	105.74
3	2-U	7515	AMP	C4-N9-C8	-6.52	98.90	105.74
3	3-U	7515	AMP	C4-N9-C8	-6.52	98.90	105.74
3	4-U	7515	AMP	C4-N9-C8	-6.52	98.90	105.74
3	5-U	7515	AMP	C4-N9-C8	-6.52	98.90	105.74
3	6-U	7515	AMP	C4-N9-C8	-6.52	98.90	105.74
3	7-U	7515	AMP	C4-N9-C8	-6.52	98.90	105.74
3	8-U	7515	AMP	C4-N9-C8	-6.52	98.90	105.74
3	9-U	7515	AMP	C4-N9-C8	-6.52	98.90	105.74
3	10-U	7515	AMP	C4-N9-C8	-6.52	98.90	105.74
3	1-T	7513	AMP	C4-N9-C8	-6.51	98.90	105.74
3	2-T	7513	AMP	C4-N9-C8	-6.51	98.90	105.74
3	3-T	7513	AMP	C4-N9-C8	-6.51	98.90	105.74
3	4-T	7513	AMP	C4-N9-C8	-6.51	98.90	105.74
3	5-T	7513	AMP	C4-N9-C8	-6.51	98.90	105.74
3	6-T	7513	AMP	C4-N9-C8	-6.51	98.90	105.74
3	7-T	7513	AMP	C4-N9-C8	-6.51	98.90	105.74
3	8-T	7513	AMP	C4-N9-C8	-6.51	98.90	105.74
3	9-T	7513	AMP	C4-N9-C8	-6.51	98.90	105.74
3	10-T	7513	AMP	C4-N9-C8	-6.51	98.90	105.74
3	1-V	7517	AMP	C4-N9-C8	-6.51	98.90	105.74
3	2-V	7517	AMP	C4-N9-C8	-6.51	98.90	105.74
3	3-V	7517	AMP	C4-N9-C8	-6.51	98.90	105.74
3	4-V	7517	AMP	C4-N9-C8	-6.51	98.90	105.74
3	5-V	7517	AMP	C4-N9-C8	-6.51	98.90	105.74
3	6-V	7517	AMP	C4-N9-C8	-6.51	98.90	105.74
3	7-V	7517	AMP	C4-N9-C8	-6.51	98.90	105.74
3	8-V	7517	AMP	C4-N9-C8	-6.51	98.90	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-V	7517	AMP	C4-N9-C8	-6.51	98.90	105.74
3	10-V	7517	AMP	C4-N9-C8	-6.51	98.90	105.74
3	1-I	7491	AMP	C4-N9-C8	-6.51	98.90	105.74
3	2-I	7491	AMP	C4-N9-C8	-6.51	98.90	105.74
3	3-I	7491	AMP	C4-N9-C8	-6.51	98.90	105.74
3	4-I	7491	AMP	C4-N9-C8	-6.51	98.90	105.74
3	5-I	7491	AMP	C4-N9-C8	-6.51	98.90	105.74
3	6-I	7491	AMP	C4-N9-C8	-6.51	98.90	105.74
3	7-I	7491	AMP	C4-N9-C8	-6.51	98.90	105.74
3	8-I	7491	AMP	C4-N9-C8	-6.51	98.90	105.74
3	9-I	7491	AMP	C4-N9-C8	-6.51	98.90	105.74
3	10-I	7491	AMP	C4-N9-C8	-6.51	98.90	105.74
3	1-D	7481	AMP	C4-N9-C8	-6.51	98.90	105.74
3	2-D	7481	AMP	C4-N9-C8	-6.51	98.90	105.74
3	3-D	7481	AMP	C4-N9-C8	-6.51	98.90	105.74
3	4-D	7481	AMP	C4-N9-C8	-6.51	98.90	105.74
3	5-D	7481	AMP	C4-N9-C8	-6.51	98.90	105.74
3	6-D	7481	AMP	C4-N9-C8	-6.51	98.90	105.74
3	7-D	7481	AMP	C4-N9-C8	-6.51	98.90	105.74
3	8-D	7481	AMP	C4-N9-C8	-6.51	98.90	105.74
3	9-D	7481	AMP	C4-N9-C8	-6.51	98.90	105.74
3	10-D	7481	AMP	C4-N9-C8	-6.51	98.90	105.74
3	1-W	7519	AMP	C4-N9-C8	-6.50	98.91	105.74
3	2-W	7519	AMP	C4-N9-C8	-6.50	98.91	105.74
3	3-W	7519	AMP	C4-N9-C8	-6.50	98.91	105.74
3	4-W	7519	AMP	C4-N9-C8	-6.50	98.91	105.74
3	5-W	7519	AMP	C4-N9-C8	-6.50	98.91	105.74
3	6-W	7519	AMP	C4-N9-C8	-6.50	98.91	105.74
3	7-W	7519	AMP	C4-N9-C8	-6.50	98.91	105.74
3	8-W	7519	AMP	C4-N9-C8	-6.50	98.91	105.74
3	9-W	7519	AMP	C4-N9-C8	-6.50	98.91	105.74
3	10-W	7519	AMP	C4-N9-C8	-6.50	98.91	105.74
3	1-A	7475	AMP	C4-N9-C8	-6.50	98.91	105.74
3	2-A	7475	AMP	C4-N9-C8	-6.50	98.91	105.74
3	3-A	7475	AMP	C4-N9-C8	-6.50	98.91	105.74
3	4-A	7475	AMP	C4-N9-C8	-6.50	98.91	105.74
3	5-A	7475	AMP	C4-N9-C8	-6.50	98.91	105.74
3	6-A	7475	AMP	C4-N9-C8	-6.50	98.91	105.74
3	7-A	7475	AMP	C4-N9-C8	-6.50	98.91	105.74
3	8-A	7475	AMP	C4-N9-C8	-6.50	98.91	105.74
3	9-A	7475	AMP	C4-N9-C8	-6.50	98.91	105.74
3	10-A	7475	AMP	C4-N9-C8	-6.50	98.91	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-N	7501	AMP	C4-N9-C8	-6.50	98.91	105.74
3	2-N	7501	AMP	C4-N9-C8	-6.50	98.91	105.74
3	3-N	7501	AMP	C4-N9-C8	-6.50	98.91	105.74
3	4-N	7501	AMP	C4-N9-C8	-6.50	98.91	105.74
3	5-N	7501	AMP	C4-N9-C8	-6.50	98.91	105.74
3	6-N	7501	AMP	C4-N9-C8	-6.50	98.91	105.74
3	7-N	7501	AMP	C4-N9-C8	-6.50	98.91	105.74
3	8-N	7501	AMP	C4-N9-C8	-6.50	98.91	105.74
3	9-N	7501	AMP	C4-N9-C8	-6.50	98.91	105.74
3	10-N	7501	AMP	C4-N9-C8	-6.50	98.91	105.74
3	1-M	7499	AMP	C4-N9-C8	-6.50	98.91	105.74
3	2-M	7499	AMP	C4-N9-C8	-6.50	98.91	105.74
3	3-M	7499	AMP	C4-N9-C8	-6.50	98.91	105.74
3	4-M	7499	AMP	C4-N9-C8	-6.50	98.91	105.74
3	5-M	7499	AMP	C4-N9-C8	-6.50	98.91	105.74
3	6-M	7499	AMP	C4-N9-C8	-6.50	98.91	105.74
3	7-M	7499	AMP	C4-N9-C8	-6.50	98.91	105.74
3	8-M	7499	AMP	C4-N9-C8	-6.50	98.91	105.74
3	9-M	7499	AMP	C4-N9-C8	-6.50	98.91	105.74
3	10-M	7499	AMP	C4-N9-C8	-6.50	98.91	105.74
3	1-E	7483	AMP	C4-N9-C8	-6.50	98.92	105.74
3	2-E	7483	AMP	C4-N9-C8	-6.50	98.92	105.74
3	3-E	7483	AMP	C4-N9-C8	-6.50	98.92	105.74
3	4-E	7483	AMP	C4-N9-C8	-6.50	98.92	105.74
3	5-E	7483	AMP	C4-N9-C8	-6.50	98.92	105.74
3	6-E	7483	AMP	C4-N9-C8	-6.50	98.92	105.74
3	7-E	7483	AMP	C4-N9-C8	-6.50	98.92	105.74
3	8-E	7483	AMP	C4-N9-C8	-6.50	98.92	105.74
3	9-E	7483	AMP	C4-N9-C8	-6.50	98.92	105.74
3	10-E	7483	AMP	C4-N9-C8	-6.50	98.92	105.74
3	1-B	7477	AMP	C4-N9-C8	-6.50	98.92	105.74
3	2-B	7477	AMP	C4-N9-C8	-6.50	98.92	105.74
3	3-B	7477	AMP	C4-N9-C8	-6.50	98.92	105.74
3	4-B	7477	AMP	C4-N9-C8	-6.50	98.92	105.74
3	5-B	7477	AMP	C4-N9-C8	-6.50	98.92	105.74
3	6-B	7477	AMP	C4-N9-C8	-6.50	98.92	105.74
3	7-B	7477	AMP	C4-N9-C8	-6.50	98.92	105.74
3	8-B	7477	AMP	C4-N9-C8	-6.50	98.92	105.74
3	9-B	7477	AMP	C4-N9-C8	-6.50	98.92	105.74
3	10-B	7477	AMP	C4-N9-C8	-6.50	98.92	105.74
3	1-J	7493	AMP	C4-N9-C8	-6.49	98.92	105.74
3	2-J	7493	AMP	C4-N9-C8	-6.49	98.92	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-J	7493	AMP	C4-N9-C8	-6.49	98.92	105.74
3	4-J	7493	AMP	C4-N9-C8	-6.49	98.92	105.74
3	5-J	7493	AMP	C4-N9-C8	-6.49	98.92	105.74
3	6-J	7493	AMP	C4-N9-C8	-6.49	98.92	105.74
3	7-J	7493	AMP	C4-N9-C8	-6.49	98.92	105.74
3	8-J	7493	AMP	C4-N9-C8	-6.49	98.92	105.74
3	9-J	7493	AMP	C4-N9-C8	-6.49	98.92	105.74
3	10-J	7493	AMP	C4-N9-C8	-6.49	98.92	105.74
3	1-S	7511	AMP	C4-N9-C8	-6.49	98.93	105.74
3	2-S	7511	AMP	C4-N9-C8	-6.49	98.93	105.74
3	3-S	7511	AMP	C4-N9-C8	-6.49	98.93	105.74
3	4-S	7511	AMP	C4-N9-C8	-6.49	98.93	105.74
3	5-S	7511	AMP	C4-N9-C8	-6.49	98.93	105.74
3	6-S	7511	AMP	C4-N9-C8	-6.49	98.93	105.74
3	7-S	7511	AMP	C4-N9-C8	-6.49	98.93	105.74
3	8-S	7511	AMP	C4-N9-C8	-6.49	98.93	105.74
3	9-S	7511	AMP	C4-N9-C8	-6.49	98.93	105.74
3	10-S	7511	AMP	C4-N9-C8	-6.49	98.93	105.74
3	1-F	7485	AMP	C4-N9-C8	-6.49	98.93	105.74
3	2-F	7485	AMP	C4-N9-C8	-6.49	98.93	105.74
3	3-F	7485	AMP	C4-N9-C8	-6.49	98.93	105.74
3	4-F	7485	AMP	C4-N9-C8	-6.49	98.93	105.74
3	5-F	7485	AMP	C4-N9-C8	-6.49	98.93	105.74
3	6-F	7485	AMP	C4-N9-C8	-6.49	98.93	105.74
3	7-F	7485	AMP	C4-N9-C8	-6.49	98.93	105.74
3	8-F	7485	AMP	C4-N9-C8	-6.49	98.93	105.74
3	9-F	7485	AMP	C4-N9-C8	-6.49	98.93	105.74
3	10-F	7485	AMP	C4-N9-C8	-6.49	98.93	105.74
3	1-R	7509	AMP	C4-N9-C8	-6.49	98.93	105.74
3	2-R	7509	AMP	C4-N9-C8	-6.49	98.93	105.74
3	3-R	7509	AMP	C4-N9-C8	-6.49	98.93	105.74
3	4-R	7509	AMP	C4-N9-C8	-6.49	98.93	105.74
3	5-R	7509	AMP	C4-N9-C8	-6.49	98.93	105.74
3	6-R	7509	AMP	C4-N9-C8	-6.49	98.93	105.74
3	7-R	7509	AMP	C4-N9-C8	-6.49	98.93	105.74
3	8-R	7509	AMP	C4-N9-C8	-6.49	98.93	105.74
3	9-R	7509	AMP	C4-N9-C8	-6.49	98.93	105.74
3	10-R	7509	AMP	C4-N9-C8	-6.49	98.93	105.74
3	1-G	7487	AMP	C4-N9-C8	-6.48	98.93	105.74
3	2-G	7487	AMP	C4-N9-C8	-6.48	98.93	105.74
3	3-G	7487	AMP	C4-N9-C8	-6.48	98.93	105.74
3	4-G	7487	AMP	C4-N9-C8	-6.48	98.93	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-G	7487	AMP	C4-N9-C8	-6.48	98.93	105.74
3	6-G	7487	AMP	C4-N9-C8	-6.48	98.93	105.74
3	7-G	7487	AMP	C4-N9-C8	-6.48	98.93	105.74
3	8-G	7487	AMP	C4-N9-C8	-6.48	98.93	105.74
3	9-G	7487	AMP	C4-N9-C8	-6.48	98.93	105.74
3	10-G	7487	AMP	C4-N9-C8	-6.48	98.93	105.74
3	1-C	7479	AMP	C4-N9-C8	-6.48	98.93	105.74
3	2-C	7479	AMP	C4-N9-C8	-6.48	98.93	105.74
3	3-C	7479	AMP	C4-N9-C8	-6.48	98.93	105.74
3	4-C	7479	AMP	C4-N9-C8	-6.48	98.93	105.74
3	5-C	7479	AMP	C4-N9-C8	-6.48	98.93	105.74
3	6-C	7479	AMP	C4-N9-C8	-6.48	98.93	105.74
3	7-C	7479	AMP	C4-N9-C8	-6.48	98.93	105.74
3	8-C	7479	AMP	C4-N9-C8	-6.48	98.93	105.74
3	9-C	7479	AMP	C4-N9-C8	-6.48	98.93	105.74
3	10-C	7479	AMP	C4-N9-C8	-6.48	98.93	105.74
3	1-H	7489	AMP	C4-N9-C8	-6.47	98.94	105.74
3	2-H	7489	AMP	C4-N9-C8	-6.47	98.94	105.74
3	3-H	7489	AMP	C4-N9-C8	-6.47	98.94	105.74
3	4-H	7489	AMP	C4-N9-C8	-6.47	98.94	105.74
3	5-H	7489	AMP	C4-N9-C8	-6.47	98.94	105.74
3	6-H	7489	AMP	C4-N9-C8	-6.47	98.94	105.74
3	7-H	7489	AMP	C4-N9-C8	-6.47	98.94	105.74
3	8-H	7489	AMP	C4-N9-C8	-6.47	98.94	105.74
3	9-H	7489	AMP	C4-N9-C8	-6.47	98.94	105.74
3	10-H	7489	AMP	C4-N9-C8	-6.47	98.94	105.74
3	1-Q	7507	AMP	C4-N9-C8	-6.47	98.94	105.74
3	2-Q	7507	AMP	C4-N9-C8	-6.47	98.94	105.74
3	3-Q	7507	AMP	C4-N9-C8	-6.47	98.94	105.74
3	4-Q	7507	AMP	C4-N9-C8	-6.47	98.94	105.74
3	5-Q	7507	AMP	C4-N9-C8	-6.47	98.94	105.74
3	6-Q	7507	AMP	C4-N9-C8	-6.47	98.94	105.74
3	7-Q	7507	AMP	C4-N9-C8	-6.47	98.94	105.74
3	8-Q	7507	AMP	C4-N9-C8	-6.47	98.94	105.74
3	9-Q	7507	AMP	C4-N9-C8	-6.47	98.94	105.74
3	10-Q	7507	AMP	C4-N9-C8	-6.47	98.94	105.74
3	1-X	7521	AMP	C4-N9-C8	-6.45	98.96	105.74
3	2-X	7521	AMP	C4-N9-C8	-6.45	98.96	105.74
3	3-X	7521	AMP	C4-N9-C8	-6.45	98.96	105.74
3	4-X	7521	AMP	C4-N9-C8	-6.45	98.96	105.74
3	5-X	7521	AMP	C4-N9-C8	-6.45	98.96	105.74
3	6-X	7521	AMP	C4-N9-C8	-6.45	98.96	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-X	7521	AMP	C4-N9-C8	-6.45	98.96	105.74
3	8-X	7521	AMP	C4-N9-C8	-6.45	98.96	105.74
3	9-X	7521	AMP	C4-N9-C8	-6.45	98.96	105.74
3	10-X	7521	AMP	C4-N9-C8	-6.45	98.96	105.74
3	1-I	7491	AMP	O4'-C4'-C5'	4.82	124.79	109.33
3	2-I	7491	AMP	O4'-C4'-C5'	4.82	124.79	109.33
3	3-I	7491	AMP	O4'-C4'-C5'	4.82	124.79	109.33
3	4-I	7491	AMP	O4'-C4'-C5'	4.82	124.79	109.33
3	5-I	7491	AMP	O4'-C4'-C5'	4.82	124.79	109.33
3	6-I	7491	AMP	O4'-C4'-C5'	4.82	124.79	109.33
3	7-I	7491	AMP	O4'-C4'-C5'	4.82	124.79	109.33
3	8-I	7491	AMP	O4'-C4'-C5'	4.82	124.79	109.33
3	9-I	7491	AMP	O4'-C4'-C5'	4.82	124.79	109.33
3	10-I	7491	AMP	O4'-C4'-C5'	4.82	124.79	109.33
3	1-E	7483	AMP	O4'-C4'-C5'	4.82	124.78	109.33
3	2-E	7483	AMP	O4'-C4'-C5'	4.82	124.78	109.33
3	3-E	7483	AMP	O4'-C4'-C5'	4.82	124.78	109.33
3	4-E	7483	AMP	O4'-C4'-C5'	4.82	124.78	109.33
3	5-E	7483	AMP	O4'-C4'-C5'	4.82	124.78	109.33
3	6-E	7483	AMP	O4'-C4'-C5'	4.82	124.78	109.33
3	7-E	7483	AMP	O4'-C4'-C5'	4.82	124.78	109.33
3	8-E	7483	AMP	O4'-C4'-C5'	4.82	124.78	109.33
3	9-E	7483	AMP	O4'-C4'-C5'	4.82	124.78	109.33
3	10-E	7483	AMP	O4'-C4'-C5'	4.82	124.78	109.33
3	1-V	7517	AMP	O2'-C2'-C1'	4.82	126.70	110.10
3	2-V	7517	AMP	O2'-C2'-C1'	4.82	126.70	110.10
3	3-V	7517	AMP	O2'-C2'-C1'	4.82	126.70	110.10
3	4-V	7517	AMP	O2'-C2'-C1'	4.82	126.70	110.10
3	5-V	7517	AMP	O2'-C2'-C1'	4.82	126.70	110.10
3	6-V	7517	AMP	O2'-C2'-C1'	4.82	126.70	110.10
3	7-V	7517	AMP	O2'-C2'-C1'	4.82	126.70	110.10
3	8-V	7517	AMP	O2'-C2'-C1'	4.82	126.70	110.10
3	9-V	7517	AMP	O2'-C2'-C1'	4.82	126.70	110.10
3	10-V	7517	AMP	O2'-C2'-C1'	4.82	126.70	110.10
3	1-T	7513	AMP	O4'-C4'-C5'	4.82	124.77	109.33
3	2-T	7513	AMP	O4'-C4'-C5'	4.82	124.77	109.33
3	3-T	7513	AMP	O4'-C4'-C5'	4.82	124.77	109.33
3	4-T	7513	AMP	O4'-C4'-C5'	4.82	124.77	109.33
3	5-T	7513	AMP	O4'-C4'-C5'	4.82	124.77	109.33
3	6-T	7513	AMP	O4'-C4'-C5'	4.82	124.77	109.33
3	7-T	7513	AMP	O4'-C4'-C5'	4.82	124.77	109.33
3	8-T	7513	AMP	O4'-C4'-C5'	4.82	124.77	109.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-T	7513	AMP	O4'-C4'-C5'	4.82	124.77	109.33
3	10-T	7513	AMP	O4'-C4'-C5'	4.82	124.77	109.33
3	1-V	7517	AMP	O4'-C4'-C5'	4.82	124.76	109.33
3	2-V	7517	AMP	O4'-C4'-C5'	4.82	124.76	109.33
3	3-V	7517	AMP	O4'-C4'-C5'	4.82	124.76	109.33
3	4-V	7517	AMP	O4'-C4'-C5'	4.82	124.76	109.33
3	5-V	7517	AMP	O4'-C4'-C5'	4.82	124.76	109.33
3	6-V	7517	AMP	O4'-C4'-C5'	4.82	124.76	109.33
3	7-V	7517	AMP	O4'-C4'-C5'	4.82	124.76	109.33
3	8-V	7517	AMP	O4'-C4'-C5'	4.82	124.76	109.33
3	9-V	7517	AMP	O4'-C4'-C5'	4.82	124.76	109.33
3	10-V	7517	AMP	O4'-C4'-C5'	4.82	124.76	109.33
3	1-P	7505	AMP	O4'-C4'-C5'	4.81	124.76	109.33
3	2-P	7505	AMP	O4'-C4'-C5'	4.81	124.76	109.33
3	3-P	7505	AMP	O4'-C4'-C5'	4.81	124.76	109.33
3	4-P	7505	AMP	O4'-C4'-C5'	4.81	124.76	109.33
3	5-P	7505	AMP	O4'-C4'-C5'	4.81	124.76	109.33
3	6-P	7505	AMP	O4'-C4'-C5'	4.81	124.76	109.33
3	7-P	7505	AMP	O4'-C4'-C5'	4.81	124.76	109.33
3	8-P	7505	AMP	O4'-C4'-C5'	4.81	124.76	109.33
3	9-P	7505	AMP	O4'-C4'-C5'	4.81	124.76	109.33
3	10-P	7505	AMP	O4'-C4'-C5'	4.81	124.76	109.33
3	1-R	7509	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	2-R	7509	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	3-R	7509	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	4-R	7509	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	5-R	7509	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	6-R	7509	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	7-R	7509	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	8-R	7509	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	9-R	7509	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	10-R	7509	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	1-B	7477	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	2-B	7477	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	3-B	7477	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	4-B	7477	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	5-B	7477	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	6-B	7477	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	7-B	7477	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	8-B	7477	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	9-B	7477	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	10-B	7477	AMP	O2'-C2'-C1'	4.81	126.67	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-F	7485	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	2-F	7485	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	3-F	7485	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	4-F	7485	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	5-F	7485	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	6-F	7485	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	7-F	7485	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	8-F	7485	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	9-F	7485	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	10-F	7485	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	1-U	7515	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	2-U	7515	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	3-U	7515	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	4-U	7515	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	5-U	7515	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	6-U	7515	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	7-U	7515	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	8-U	7515	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	9-U	7515	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	10-U	7515	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	1-S	7511	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	2-S	7511	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	3-S	7511	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	4-S	7511	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	5-S	7511	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	6-S	7511	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	7-S	7511	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	8-S	7511	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	9-S	7511	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	10-S	7511	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	1-A	7475	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	2-A	7475	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	3-A	7475	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	4-A	7475	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	5-A	7475	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	6-A	7475	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	7-A	7475	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	8-A	7475	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	9-A	7475	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	10-A	7475	AMP	O4'-C4'-C5'	4.81	124.75	109.33
3	1-U	7515	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	2-U	7515	AMP	O2'-C2'-C1'	4.81	126.67	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-U	7515	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	4-U	7515	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	5-U	7515	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	6-U	7515	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	7-U	7515	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	8-U	7515	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	9-U	7515	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	10-U	7515	AMP	O2'-C2'-C1'	4.81	126.67	110.10
3	1-J	7493	AMP	O4'-C4'-C5'	4.81	124.74	109.33
3	2-J	7493	AMP	O4'-C4'-C5'	4.81	124.74	109.33
3	3-J	7493	AMP	O4'-C4'-C5'	4.81	124.74	109.33
3	4-J	7493	AMP	O4'-C4'-C5'	4.81	124.74	109.33
3	5-J	7493	AMP	O4'-C4'-C5'	4.81	124.74	109.33
3	6-J	7493	AMP	O4'-C4'-C5'	4.81	124.74	109.33
3	7-J	7493	AMP	O4'-C4'-C5'	4.81	124.74	109.33
3	8-J	7493	AMP	O4'-C4'-C5'	4.81	124.74	109.33
3	9-J	7493	AMP	O4'-C4'-C5'	4.81	124.74	109.33
3	10-J	7493	AMP	O4'-C4'-C5'	4.81	124.74	109.33
3	1-W	7519	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	2-W	7519	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	3-W	7519	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	4-W	7519	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	5-W	7519	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	6-W	7519	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	7-W	7519	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	8-W	7519	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	9-W	7519	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	10-W	7519	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	1-L	7497	AMP	O2'-C2'-C1'	4.81	126.66	110.10
3	2-L	7497	AMP	O2'-C2'-C1'	4.81	126.66	110.10
3	3-L	7497	AMP	O2'-C2'-C1'	4.81	126.66	110.10
3	4-L	7497	AMP	O2'-C2'-C1'	4.81	126.66	110.10
3	5-L	7497	AMP	O2'-C2'-C1'	4.81	126.66	110.10
3	6-L	7497	AMP	O2'-C2'-C1'	4.81	126.66	110.10
3	7-L	7497	AMP	O2'-C2'-C1'	4.81	126.66	110.10
3	8-L	7497	AMP	O2'-C2'-C1'	4.81	126.66	110.10
3	9-L	7497	AMP	O2'-C2'-C1'	4.81	126.66	110.10
3	10-L	7497	AMP	O2'-C2'-C1'	4.81	126.66	110.10
3	1-D	7481	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	2-D	7481	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	3-D	7481	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	4-D	7481	AMP	O4'-C4'-C5'	4.81	124.73	109.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-D	7481	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	6-D	7481	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	7-D	7481	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	8-D	7481	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	9-D	7481	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	10-D	7481	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	1-D	7481	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	2-D	7481	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	3-D	7481	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	4-D	7481	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	5-D	7481	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	6-D	7481	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	7-D	7481	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	8-D	7481	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	9-D	7481	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	10-D	7481	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	1-I	7491	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	2-I	7491	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	3-I	7491	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	4-I	7491	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	5-I	7491	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	6-I	7491	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	7-I	7491	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	8-I	7491	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	9-I	7491	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	10-I	7491	AMP	O2'-C2'-C1'	4.81	126.65	110.10
3	1-H	7489	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	2-H	7489	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	3-H	7489	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	4-H	7489	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	5-H	7489	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	6-H	7489	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	7-H	7489	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	8-H	7489	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	9-H	7489	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	10-H	7489	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	1-L	7497	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	2-L	7497	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	3-L	7497	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	4-L	7497	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	5-L	7497	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	6-L	7497	AMP	O4'-C4'-C5'	4.81	124.73	109.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-L	7497	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	8-L	7497	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	9-L	7497	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	10-L	7497	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	1-O	7503	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	2-O	7503	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	3-O	7503	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	4-O	7503	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	5-O	7503	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	6-O	7503	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	7-O	7503	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	8-O	7503	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	9-O	7503	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	10-O	7503	AMP	O4'-C4'-C5'	4.81	124.73	109.33
3	1-N	7501	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	2-N	7501	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	3-N	7501	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	4-N	7501	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	5-N	7501	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	6-N	7501	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	7-N	7501	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	8-N	7501	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	9-N	7501	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	10-N	7501	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	1-Q	7507	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	2-Q	7507	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	3-Q	7507	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	4-Q	7507	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	5-Q	7507	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	6-Q	7507	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	7-Q	7507	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	8-Q	7507	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	9-Q	7507	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	10-Q	7507	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	1-T	7513	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	2-T	7513	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	3-T	7513	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	4-T	7513	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	5-T	7513	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	6-T	7513	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	7-T	7513	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	8-T	7513	AMP	O2'-C2'-C1'	4.80	126.64	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-T	7513	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	10-T	7513	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	1-M	7499	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	2-M	7499	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	3-M	7499	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	4-M	7499	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	5-M	7499	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	6-M	7499	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	7-M	7499	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	8-M	7499	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	9-M	7499	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	10-M	7499	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	1-P	7505	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	2-P	7505	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	3-P	7505	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	4-P	7505	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	5-P	7505	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	6-P	7505	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	7-P	7505	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	8-P	7505	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	9-P	7505	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	10-P	7505	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	1-B	7477	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	2-B	7477	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	3-B	7477	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	4-B	7477	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	5-B	7477	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	6-B	7477	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	7-B	7477	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	8-B	7477	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	9-B	7477	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	10-B	7477	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	1-C	7479	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	2-C	7479	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	3-C	7479	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	4-C	7479	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	5-C	7479	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	6-C	7479	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	7-C	7479	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	8-C	7479	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	9-C	7479	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	10-C	7479	AMP	O4'-C4'-C5'	4.80	124.72	109.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-X	7521	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	2-X	7521	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	3-X	7521	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	4-X	7521	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	5-X	7521	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	6-X	7521	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	7-X	7521	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	8-X	7521	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	9-X	7521	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	10-X	7521	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	1-R	7509	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	2-R	7509	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	3-R	7509	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	4-R	7509	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	5-R	7509	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	6-R	7509	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	7-R	7509	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	8-R	7509	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	9-R	7509	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	10-R	7509	AMP	O4'-C4'-C5'	4.80	124.72	109.33
3	1-A	7475	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	2-A	7475	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	3-A	7475	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	4-A	7475	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	5-A	7475	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	6-A	7475	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	7-A	7475	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	8-A	7475	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	9-A	7475	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	10-A	7475	AMP	O2'-C2'-C1'	4.80	126.64	110.10
3	1-Q	7507	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	2-Q	7507	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	3-Q	7507	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	4-Q	7507	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	5-Q	7507	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	6-Q	7507	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	7-Q	7507	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	8-Q	7507	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	9-Q	7507	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	10-Q	7507	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	1-K	7495	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	2-K	7495	AMP	O4'-C4'-C5'	4.80	124.71	109.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-K	7495	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	4-K	7495	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	5-K	7495	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	6-K	7495	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	7-K	7495	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	8-K	7495	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	9-K	7495	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	10-K	7495	AMP	O4'-C4'-C5'	4.80	124.71	109.33
3	1-K	7495	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	2-K	7495	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	3-K	7495	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	4-K	7495	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	5-K	7495	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	6-K	7495	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	7-K	7495	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	8-K	7495	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	9-K	7495	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	10-K	7495	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	1-G	7487	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	2-G	7487	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	3-G	7487	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	4-G	7487	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	5-G	7487	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	6-G	7487	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	7-G	7487	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	8-G	7487	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	9-G	7487	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	10-G	7487	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	1-W	7519	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	2-W	7519	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	3-W	7519	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	4-W	7519	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	5-W	7519	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	6-W	7519	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	7-W	7519	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	8-W	7519	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	9-W	7519	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	10-W	7519	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	1-X	7521	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	2-X	7521	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	3-X	7521	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	4-X	7521	AMP	O2'-C2'-C1'	4.80	126.63	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-X	7521	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	6-X	7521	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	7-X	7521	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	8-X	7521	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	9-X	7521	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	10-X	7521	AMP	O2'-C2'-C1'	4.80	126.63	110.10
3	1-E	7483	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	2-E	7483	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	3-E	7483	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	4-E	7483	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	5-E	7483	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	6-E	7483	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	7-E	7483	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	8-E	7483	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	9-E	7483	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	10-E	7483	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	1-G	7487	AMP	O4'-C4'-C5'	4.80	124.70	109.33
3	2-G	7487	AMP	O4'-C4'-C5'	4.80	124.70	109.33
3	3-G	7487	AMP	O4'-C4'-C5'	4.80	124.70	109.33
3	4-G	7487	AMP	O4'-C4'-C5'	4.80	124.70	109.33
3	5-G	7487	AMP	O4'-C4'-C5'	4.80	124.70	109.33
3	6-G	7487	AMP	O4'-C4'-C5'	4.80	124.70	109.33
3	7-G	7487	AMP	O4'-C4'-C5'	4.80	124.70	109.33
3	8-G	7487	AMP	O4'-C4'-C5'	4.80	124.70	109.33
3	9-G	7487	AMP	O4'-C4'-C5'	4.80	124.70	109.33
3	10-G	7487	AMP	O4'-C4'-C5'	4.80	124.70	109.33
3	1-N	7501	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	2-N	7501	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	3-N	7501	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	4-N	7501	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	5-N	7501	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	6-N	7501	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	7-N	7501	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	8-N	7501	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	9-N	7501	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	10-N	7501	AMP	O2'-C2'-C1'	4.80	126.62	110.10
3	1-C	7479	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	2-C	7479	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	3-C	7479	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	4-C	7479	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	5-C	7479	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	6-C	7479	AMP	O2'-C2'-C1'	4.79	126.61	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-C	7479	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	8-C	7479	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	9-C	7479	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	10-C	7479	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	1-F	7485	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	2-F	7485	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	3-F	7485	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	4-F	7485	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	5-F	7485	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	6-F	7485	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	7-F	7485	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	8-F	7485	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	9-F	7485	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	10-F	7485	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	1-S	7511	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	2-S	7511	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	3-S	7511	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	4-S	7511	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	5-S	7511	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	6-S	7511	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	7-S	7511	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	8-S	7511	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	9-S	7511	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	10-S	7511	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	1-H	7489	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	2-H	7489	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	3-H	7489	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	4-H	7489	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	5-H	7489	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	6-H	7489	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	7-H	7489	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	8-H	7489	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	9-H	7489	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	10-H	7489	AMP	O2'-C2'-C1'	4.79	126.61	110.10
3	1-J	7493	AMP	O2'-C2'-C1'	4.79	126.60	110.10
3	2-J	7493	AMP	O2'-C2'-C1'	4.79	126.60	110.10
3	3-J	7493	AMP	O2'-C2'-C1'	4.79	126.60	110.10
3	4-J	7493	AMP	O2'-C2'-C1'	4.79	126.60	110.10
3	5-J	7493	AMP	O2'-C2'-C1'	4.79	126.60	110.10
3	6-J	7493	AMP	O2'-C2'-C1'	4.79	126.60	110.10
3	7-J	7493	AMP	O2'-C2'-C1'	4.79	126.60	110.10
3	8-J	7493	AMP	O2'-C2'-C1'	4.79	126.60	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-J	7493	AMP	O2'-C2'-C1'	4.79	126.60	110.10
3	10-J	7493	AMP	O2'-C2'-C1'	4.79	126.60	110.10
3	1-M	7499	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	2-M	7499	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	3-M	7499	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	4-M	7499	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	5-M	7499	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	6-M	7499	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	7-M	7499	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	8-M	7499	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	9-M	7499	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	10-M	7499	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	1-O	7503	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	2-O	7503	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	3-O	7503	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	4-O	7503	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	5-O	7503	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	6-O	7503	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	7-O	7503	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	8-O	7503	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	9-O	7503	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	10-O	7503	AMP	O2'-C2'-C1'	4.79	126.59	110.10
3	1-C	7479	AMP	O4'-C1'-N9	4.25	116.24	108.09
3	2-C	7479	AMP	O4'-C1'-N9	4.25	116.24	108.09
3	3-C	7479	AMP	O4'-C1'-N9	4.25	116.24	108.09
3	4-C	7479	AMP	O4'-C1'-N9	4.25	116.24	108.09
3	5-C	7479	AMP	O4'-C1'-N9	4.25	116.24	108.09
3	6-C	7479	AMP	O4'-C1'-N9	4.25	116.24	108.09
3	7-C	7479	AMP	O4'-C1'-N9	4.25	116.24	108.09
3	8-C	7479	AMP	O4'-C1'-N9	4.25	116.24	108.09
3	9-C	7479	AMP	O4'-C1'-N9	4.25	116.24	108.09
3	10-C	7479	AMP	O4'-C1'-N9	4.25	116.24	108.09
3	1-V	7517	AMP	O4'-C1'-N9	4.24	116.24	108.09
3	2-V	7517	AMP	O4'-C1'-N9	4.24	116.24	108.09
3	3-V	7517	AMP	O4'-C1'-N9	4.24	116.24	108.09
3	4-V	7517	AMP	O4'-C1'-N9	4.24	116.24	108.09
3	5-V	7517	AMP	O4'-C1'-N9	4.24	116.24	108.09
3	6-V	7517	AMP	O4'-C1'-N9	4.24	116.24	108.09
3	7-V	7517	AMP	O4'-C1'-N9	4.24	116.24	108.09
3	8-V	7517	AMP	O4'-C1'-N9	4.24	116.24	108.09
3	9-V	7517	AMP	O4'-C1'-N9	4.24	116.24	108.09
3	10-V	7517	AMP	O4'-C1'-N9	4.24	116.24	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-L	7497	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	2-L	7497	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	3-L	7497	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	4-L	7497	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	5-L	7497	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	6-L	7497	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	7-L	7497	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	8-L	7497	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	9-L	7497	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	10-L	7497	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	1-E	7483	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	2-E	7483	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	3-E	7483	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	4-E	7483	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	5-E	7483	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	6-E	7483	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	7-E	7483	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	8-E	7483	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	9-E	7483	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	10-E	7483	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	1-O	7503	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	2-O	7503	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	3-O	7503	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	4-O	7503	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	5-O	7503	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	6-O	7503	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	7-O	7503	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	8-O	7503	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	9-O	7503	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	10-O	7503	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	1-T	7513	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	2-T	7513	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	3-T	7513	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	4-T	7513	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	5-T	7513	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	6-T	7513	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	7-T	7513	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	8-T	7513	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	9-T	7513	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	10-T	7513	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	1-M	7499	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	2-M	7499	AMP	O4'-C1'-N9	4.23	116.22	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-M	7499	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	4-M	7499	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	5-M	7499	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	6-M	7499	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	7-M	7499	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	8-M	7499	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	9-M	7499	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	10-M	7499	AMP	O4'-C1'-N9	4.23	116.22	108.09
3	1-G	7487	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	2-G	7487	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	3-G	7487	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	4-G	7487	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	5-G	7487	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	6-G	7487	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	7-G	7487	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	8-G	7487	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	9-G	7487	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	10-G	7487	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	1-K	7495	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	2-K	7495	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	3-K	7495	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	4-K	7495	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	5-K	7495	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	6-K	7495	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	7-K	7495	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	8-K	7495	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	9-K	7495	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	10-K	7495	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	1-F	7485	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	2-F	7485	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	3-F	7485	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	4-F	7485	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	5-F	7485	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	6-F	7485	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	7-F	7485	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	8-F	7485	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	9-F	7485	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	10-F	7485	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	1-N	7501	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	2-N	7501	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	3-N	7501	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	4-N	7501	AMP	O4'-C1'-N9	4.23	116.21	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-N	7501	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	6-N	7501	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	7-N	7501	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	8-N	7501	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	9-N	7501	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	10-N	7501	AMP	O4'-C1'-N9	4.23	116.21	108.09
3	1-R	7509	AMP	O4'-C1'-N9	4.23	116.20	108.09
3	2-R	7509	AMP	O4'-C1'-N9	4.23	116.20	108.09
3	3-R	7509	AMP	O4'-C1'-N9	4.23	116.20	108.09
3	4-R	7509	AMP	O4'-C1'-N9	4.23	116.20	108.09
3	5-R	7509	AMP	O4'-C1'-N9	4.23	116.20	108.09
3	6-R	7509	AMP	O4'-C1'-N9	4.23	116.20	108.09
3	7-R	7509	AMP	O4'-C1'-N9	4.23	116.20	108.09
3	8-R	7509	AMP	O4'-C1'-N9	4.23	116.20	108.09
3	9-R	7509	AMP	O4'-C1'-N9	4.23	116.20	108.09
3	10-R	7509	AMP	O4'-C1'-N9	4.23	116.20	108.09
3	1-A	7475	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	2-A	7475	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	3-A	7475	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	4-A	7475	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	5-A	7475	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	6-A	7475	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	7-A	7475	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	8-A	7475	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	9-A	7475	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	10-A	7475	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	1-W	7519	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	2-W	7519	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	3-W	7519	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	4-W	7519	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	5-W	7519	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	6-W	7519	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	7-W	7519	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	8-W	7519	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	9-W	7519	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	10-W	7519	AMP	O4'-C1'-N9	4.22	116.20	108.09
3	1-I	7491	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	2-I	7491	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	3-I	7491	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	4-I	7491	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	5-I	7491	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	6-I	7491	AMP	O4'-C1'-N9	4.22	116.19	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-I	7491	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	8-I	7491	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	9-I	7491	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	10-I	7491	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	1-D	7481	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	2-D	7481	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	3-D	7481	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	4-D	7481	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	5-D	7481	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	6-D	7481	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	7-D	7481	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	8-D	7481	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	9-D	7481	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	10-D	7481	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	1-J	7493	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	2-J	7493	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	3-J	7493	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	4-J	7493	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	5-J	7493	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	6-J	7493	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	7-J	7493	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	8-J	7493	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	9-J	7493	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	10-J	7493	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	1-Q	7507	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	2-Q	7507	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	3-Q	7507	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	4-Q	7507	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	5-Q	7507	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	6-Q	7507	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	7-Q	7507	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	8-Q	7507	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	9-Q	7507	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	10-Q	7507	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	1-P	7505	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	2-P	7505	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	3-P	7505	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	4-P	7505	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	5-P	7505	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	6-P	7505	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	7-P	7505	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	8-P	7505	AMP	O4'-C1'-N9	4.22	116.19	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-P	7505	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	10-P	7505	AMP	O4'-C1'-N9	4.22	116.19	108.09
3	1-H	7489	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	2-H	7489	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	3-H	7489	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	4-H	7489	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	5-H	7489	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	6-H	7489	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	7-H	7489	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	8-H	7489	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	9-H	7489	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	10-H	7489	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	1-X	7521	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	2-X	7521	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	3-X	7521	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	4-X	7521	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	5-X	7521	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	6-X	7521	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	7-X	7521	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	8-X	7521	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	9-X	7521	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	10-X	7521	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	1-S	7511	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	2-S	7511	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	3-S	7511	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	4-S	7511	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	5-S	7511	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	6-S	7511	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	7-S	7511	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	8-S	7511	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	9-S	7511	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	10-S	7511	AMP	O4'-C1'-N9	4.21	116.18	108.09
3	1-U	7515	AMP	O4'-C1'-N9	4.21	116.17	108.09
3	2-U	7515	AMP	O4'-C1'-N9	4.21	116.17	108.09
3	3-U	7515	AMP	O4'-C1'-N9	4.21	116.17	108.09
3	4-U	7515	AMP	O4'-C1'-N9	4.21	116.17	108.09
3	5-U	7515	AMP	O4'-C1'-N9	4.21	116.17	108.09
3	6-U	7515	AMP	O4'-C1'-N9	4.21	116.17	108.09
3	7-U	7515	AMP	O4'-C1'-N9	4.21	116.17	108.09
3	8-U	7515	AMP	O4'-C1'-N9	4.21	116.17	108.09
3	9-U	7515	AMP	O4'-C1'-N9	4.21	116.17	108.09
3	10-U	7515	AMP	O4'-C1'-N9	4.21	116.17	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-B	7477	AMP	O4'-C1'-N9	4.20	116.15	108.09
3	2-B	7477	AMP	O4'-C1'-N9	4.20	116.15	108.09
3	3-B	7477	AMP	O4'-C1'-N9	4.20	116.15	108.09
3	4-B	7477	AMP	O4'-C1'-N9	4.20	116.15	108.09
3	5-B	7477	AMP	O4'-C1'-N9	4.20	116.15	108.09
3	6-B	7477	AMP	O4'-C1'-N9	4.20	116.15	108.09
3	7-B	7477	AMP	O4'-C1'-N9	4.20	116.15	108.09
3	8-B	7477	AMP	O4'-C1'-N9	4.20	116.15	108.09
3	9-B	7477	AMP	O4'-C1'-N9	4.20	116.15	108.09
3	10-B	7477	AMP	O4'-C1'-N9	4.20	116.15	108.09
3	1-E	7483	AMP	O3'-C3'-C2'	4.07	124.87	111.82
3	2-E	7483	AMP	O3'-C3'-C2'	4.07	124.87	111.82
3	3-E	7483	AMP	O3'-C3'-C2'	4.07	124.87	111.82
3	4-E	7483	AMP	O3'-C3'-C2'	4.07	124.87	111.82
3	5-E	7483	AMP	O3'-C3'-C2'	4.07	124.87	111.82
3	6-E	7483	AMP	O3'-C3'-C2'	4.07	124.87	111.82
3	7-E	7483	AMP	O3'-C3'-C2'	4.07	124.87	111.82
3	8-E	7483	AMP	O3'-C3'-C2'	4.07	124.87	111.82
3	9-E	7483	AMP	O3'-C3'-C2'	4.07	124.87	111.82
3	10-E	7483	AMP	O3'-C3'-C2'	4.07	124.87	111.82
3	1-C	7479	AMP	O3'-C3'-C2'	4.07	124.86	111.82
3	2-C	7479	AMP	O3'-C3'-C2'	4.07	124.86	111.82
3	3-C	7479	AMP	O3'-C3'-C2'	4.07	124.86	111.82
3	4-C	7479	AMP	O3'-C3'-C2'	4.07	124.86	111.82
3	5-C	7479	AMP	O3'-C3'-C2'	4.07	124.86	111.82
3	6-C	7479	AMP	O3'-C3'-C2'	4.07	124.86	111.82
3	7-C	7479	AMP	O3'-C3'-C2'	4.07	124.86	111.82
3	8-C	7479	AMP	O3'-C3'-C2'	4.07	124.86	111.82
3	9-C	7479	AMP	O3'-C3'-C2'	4.07	124.86	111.82
3	10-C	7479	AMP	O3'-C3'-C2'	4.07	124.86	111.82
3	1-O	7503	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	2-O	7503	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	3-O	7503	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	4-O	7503	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	5-O	7503	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	6-O	7503	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	7-O	7503	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	8-O	7503	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	9-O	7503	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	10-O	7503	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	1-T	7513	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	2-T	7513	AMP	O3'-C3'-C2'	4.06	124.84	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-T	7513	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	4-T	7513	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	5-T	7513	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	6-T	7513	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	7-T	7513	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	8-T	7513	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	9-T	7513	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	10-T	7513	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	1-V	7517	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	2-V	7517	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	3-V	7517	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	4-V	7517	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	5-V	7517	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	6-V	7517	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	7-V	7517	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	8-V	7517	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	9-V	7517	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	10-V	7517	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	1-M	7499	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	2-M	7499	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	3-M	7499	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	4-M	7499	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	5-M	7499	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	6-M	7499	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	7-M	7499	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	8-M	7499	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	9-M	7499	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	10-M	7499	AMP	O3'-C3'-C2'	4.06	124.84	111.82
3	1-K	7495	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	2-K	7495	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	3-K	7495	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	4-K	7495	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	5-K	7495	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	6-K	7495	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	7-K	7495	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	8-K	7495	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	9-K	7495	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	10-K	7495	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	1-S	7511	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	2-S	7511	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	3-S	7511	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	4-S	7511	AMP	O3'-C3'-C2'	4.06	124.83	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-S	7511	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	6-S	7511	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	7-S	7511	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	8-S	7511	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	9-S	7511	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	10-S	7511	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	1-G	7487	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	2-G	7487	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	3-G	7487	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	4-G	7487	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	5-G	7487	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	6-G	7487	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	7-G	7487	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	8-G	7487	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	9-G	7487	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	10-G	7487	AMP	O3'-C3'-C2'	4.06	124.83	111.82
3	1-B	7477	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	2-B	7477	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	3-B	7477	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	4-B	7477	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	5-B	7477	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	6-B	7477	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	7-B	7477	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	8-B	7477	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	9-B	7477	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	10-B	7477	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	1-R	7509	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	2-R	7509	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	3-R	7509	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	4-R	7509	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	5-R	7509	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	6-R	7509	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	7-R	7509	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	8-R	7509	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	9-R	7509	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	10-R	7509	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	1-X	7521	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	2-X	7521	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	3-X	7521	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	4-X	7521	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	5-X	7521	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	6-X	7521	AMP	O3'-C3'-C2'	4.06	124.82	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-X	7521	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	8-X	7521	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	9-X	7521	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	10-X	7521	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	1-F	7485	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	2-F	7485	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	3-F	7485	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	4-F	7485	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	5-F	7485	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	6-F	7485	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	7-F	7485	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	8-F	7485	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	9-F	7485	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	10-F	7485	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	1-J	7493	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	2-J	7493	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	3-J	7493	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	4-J	7493	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	5-J	7493	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	6-J	7493	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	7-J	7493	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	8-J	7493	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	9-J	7493	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	10-J	7493	AMP	O3'-C3'-C2'	4.06	124.82	111.82
3	1-A	7475	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	2-A	7475	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	3-A	7475	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	4-A	7475	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	5-A	7475	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	6-A	7475	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	7-A	7475	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	8-A	7475	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	9-A	7475	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	10-A	7475	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	1-H	7489	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	2-H	7489	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	3-H	7489	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	4-H	7489	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	5-H	7489	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	6-H	7489	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	7-H	7489	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	8-H	7489	AMP	O3'-C3'-C2'	4.05	124.81	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-H	7489	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	10-H	7489	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	1-W	7519	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	2-W	7519	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	3-W	7519	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	4-W	7519	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	5-W	7519	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	6-W	7519	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	7-W	7519	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	8-W	7519	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	9-W	7519	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	10-W	7519	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	1-L	7497	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	2-L	7497	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	3-L	7497	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	4-L	7497	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	5-L	7497	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	6-L	7497	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	7-L	7497	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	8-L	7497	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	9-L	7497	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	10-L	7497	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	1-P	7505	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	2-P	7505	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	3-P	7505	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	4-P	7505	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	5-P	7505	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	6-P	7505	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	7-P	7505	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	8-P	7505	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	9-P	7505	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	10-P	7505	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	1-I	7491	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	2-I	7491	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	3-I	7491	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	4-I	7491	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	5-I	7491	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	6-I	7491	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	7-I	7491	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	8-I	7491	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	9-I	7491	AMP	O3'-C3'-C2'	4.05	124.81	111.82
3	10-I	7491	AMP	O3'-C3'-C2'	4.05	124.81	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-Q	7507	AMP	O3'-C3'-C2'	4.05	124.80	111.82
3	2-Q	7507	AMP	O3'-C3'-C2'	4.05	124.80	111.82
3	3-Q	7507	AMP	O3'-C3'-C2'	4.05	124.80	111.82
3	4-Q	7507	AMP	O3'-C3'-C2'	4.05	124.80	111.82
3	5-Q	7507	AMP	O3'-C3'-C2'	4.05	124.80	111.82
3	6-Q	7507	AMP	O3'-C3'-C2'	4.05	124.80	111.82
3	7-Q	7507	AMP	O3'-C3'-C2'	4.05	124.80	111.82
3	8-Q	7507	AMP	O3'-C3'-C2'	4.05	124.80	111.82
3	9-Q	7507	AMP	O3'-C3'-C2'	4.05	124.80	111.82
3	10-Q	7507	AMP	O3'-C3'-C2'	4.05	124.80	111.82
3	1-D	7481	AMP	O3'-C3'-C2'	4.05	124.79	111.82
3	2-D	7481	AMP	O3'-C3'-C2'	4.05	124.79	111.82
3	3-D	7481	AMP	O3'-C3'-C2'	4.05	124.79	111.82
3	4-D	7481	AMP	O3'-C3'-C2'	4.05	124.79	111.82
3	5-D	7481	AMP	O3'-C3'-C2'	4.05	124.79	111.82
3	6-D	7481	AMP	O3'-C3'-C2'	4.05	124.79	111.82
3	7-D	7481	AMP	O3'-C3'-C2'	4.05	124.79	111.82
3	8-D	7481	AMP	O3'-C3'-C2'	4.05	124.79	111.82
3	9-D	7481	AMP	O3'-C3'-C2'	4.05	124.79	111.82
3	10-D	7481	AMP	O3'-C3'-C2'	4.05	124.79	111.82
3	1-U	7515	AMP	O3'-C3'-C2'	4.04	124.78	111.82
3	2-U	7515	AMP	O3'-C3'-C2'	4.04	124.78	111.82
3	3-U	7515	AMP	O3'-C3'-C2'	4.04	124.78	111.82
3	4-U	7515	AMP	O3'-C3'-C2'	4.04	124.78	111.82
3	5-U	7515	AMP	O3'-C3'-C2'	4.04	124.78	111.82
3	6-U	7515	AMP	O3'-C3'-C2'	4.04	124.78	111.82
3	7-U	7515	AMP	O3'-C3'-C2'	4.04	124.78	111.82
3	8-U	7515	AMP	O3'-C3'-C2'	4.04	124.78	111.82
3	9-U	7515	AMP	O3'-C3'-C2'	4.04	124.78	111.82
3	10-U	7515	AMP	O3'-C3'-C2'	4.04	124.78	111.82
3	1-N	7501	AMP	O3'-C3'-C2'	4.04	124.77	111.82
3	2-N	7501	AMP	O3'-C3'-C2'	4.04	124.77	111.82
3	3-N	7501	AMP	O3'-C3'-C2'	4.04	124.77	111.82
3	4-N	7501	AMP	O3'-C3'-C2'	4.04	124.77	111.82
3	5-N	7501	AMP	O3'-C3'-C2'	4.04	124.77	111.82
3	6-N	7501	AMP	O3'-C3'-C2'	4.04	124.77	111.82
3	7-N	7501	AMP	O3'-C3'-C2'	4.04	124.77	111.82
3	8-N	7501	AMP	O3'-C3'-C2'	4.04	124.77	111.82
3	9-N	7501	AMP	O3'-C3'-C2'	4.04	124.77	111.82
3	10-N	7501	AMP	O3'-C3'-C2'	4.04	124.77	111.82
4	1-X	7522	CIT	O4-C5-C4	3.99	126.97	114.35
4	2-X	7522	CIT	O4-C5-C4	3.99	126.97	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-X	7522	CIT	O4-C5-C4	3.99	126.97	114.35
4	4-X	7522	CIT	O4-C5-C4	3.99	126.97	114.35
4	5-X	7522	CIT	O4-C5-C4	3.99	126.97	114.35
4	6-X	7522	CIT	O4-C5-C4	3.99	126.97	114.35
4	7-X	7522	CIT	O4-C5-C4	3.99	126.97	114.35
4	8-X	7522	CIT	O4-C5-C4	3.99	126.97	114.35
4	9-X	7522	CIT	O4-C5-C4	3.99	126.97	114.35
4	10-X	7522	CIT	O4-C5-C4	3.99	126.97	114.35
4	1-M	7500	CIT	O4-C5-C4	3.98	126.97	114.35
4	2-M	7500	CIT	O4-C5-C4	3.98	126.97	114.35
4	3-M	7500	CIT	O4-C5-C4	3.98	126.97	114.35
4	4-M	7500	CIT	O4-C5-C4	3.98	126.97	114.35
4	5-M	7500	CIT	O4-C5-C4	3.98	126.97	114.35
4	6-M	7500	CIT	O4-C5-C4	3.98	126.97	114.35
4	7-M	7500	CIT	O4-C5-C4	3.98	126.97	114.35
4	8-M	7500	CIT	O4-C5-C4	3.98	126.97	114.35
4	9-M	7500	CIT	O4-C5-C4	3.98	126.97	114.35
4	10-M	7500	CIT	O4-C5-C4	3.98	126.97	114.35
4	1-K	7496	CIT	O4-C5-C4	3.98	126.97	114.35
4	2-K	7496	CIT	O4-C5-C4	3.98	126.97	114.35
4	3-K	7496	CIT	O4-C5-C4	3.98	126.97	114.35
4	4-K	7496	CIT	O4-C5-C4	3.98	126.97	114.35
4	5-K	7496	CIT	O4-C5-C4	3.98	126.97	114.35
4	6-K	7496	CIT	O4-C5-C4	3.98	126.97	114.35
4	7-K	7496	CIT	O4-C5-C4	3.98	126.97	114.35
4	8-K	7496	CIT	O4-C5-C4	3.98	126.97	114.35
4	9-K	7496	CIT	O4-C5-C4	3.98	126.97	114.35
4	10-K	7496	CIT	O4-C5-C4	3.98	126.97	114.35
4	1-E	7484	CIT	O4-C5-C4	3.98	126.96	114.35
4	2-E	7484	CIT	O4-C5-C4	3.98	126.96	114.35
4	3-E	7484	CIT	O4-C5-C4	3.98	126.96	114.35
4	4-E	7484	CIT	O4-C5-C4	3.98	126.96	114.35
4	5-E	7484	CIT	O4-C5-C4	3.98	126.96	114.35
4	6-E	7484	CIT	O4-C5-C4	3.98	126.96	114.35
4	7-E	7484	CIT	O4-C5-C4	3.98	126.96	114.35
4	8-E	7484	CIT	O4-C5-C4	3.98	126.96	114.35
4	9-E	7484	CIT	O4-C5-C4	3.98	126.96	114.35
4	10-E	7484	CIT	O4-C5-C4	3.98	126.96	114.35
4	1-O	7504	CIT	O4-C5-C4	3.98	126.96	114.35
4	2-O	7504	CIT	O4-C5-C4	3.98	126.96	114.35
4	3-O	7504	CIT	O4-C5-C4	3.98	126.96	114.35
4	4-O	7504	CIT	O4-C5-C4	3.98	126.96	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5-O	7504	CIT	O4-C5-C4	3.98	126.96	114.35
4	6-O	7504	CIT	O4-C5-C4	3.98	126.96	114.35
4	7-O	7504	CIT	O4-C5-C4	3.98	126.96	114.35
4	8-O	7504	CIT	O4-C5-C4	3.98	126.96	114.35
4	9-O	7504	CIT	O4-C5-C4	3.98	126.96	114.35
4	10-O	7504	CIT	O4-C5-C4	3.98	126.96	114.35
4	1-D	7482	CIT	O4-C5-C4	3.98	126.95	114.35
4	2-D	7482	CIT	O4-C5-C4	3.98	126.95	114.35
4	3-D	7482	CIT	O4-C5-C4	3.98	126.95	114.35
4	4-D	7482	CIT	O4-C5-C4	3.98	126.95	114.35
4	5-D	7482	CIT	O4-C5-C4	3.98	126.95	114.35
4	6-D	7482	CIT	O4-C5-C4	3.98	126.95	114.35
4	7-D	7482	CIT	O4-C5-C4	3.98	126.95	114.35
4	8-D	7482	CIT	O4-C5-C4	3.98	126.95	114.35
4	9-D	7482	CIT	O4-C5-C4	3.98	126.95	114.35
4	10-D	7482	CIT	O4-C5-C4	3.98	126.95	114.35
4	1-B	7478	CIT	O4-C5-C4	3.98	126.95	114.35
4	2-B	7478	CIT	O4-C5-C4	3.98	126.95	114.35
4	3-B	7478	CIT	O4-C5-C4	3.98	126.95	114.35
4	4-B	7478	CIT	O4-C5-C4	3.98	126.95	114.35
4	5-B	7478	CIT	O4-C5-C4	3.98	126.95	114.35
4	6-B	7478	CIT	O4-C5-C4	3.98	126.95	114.35
4	7-B	7478	CIT	O4-C5-C4	3.98	126.95	114.35
4	8-B	7478	CIT	O4-C5-C4	3.98	126.95	114.35
4	9-B	7478	CIT	O4-C5-C4	3.98	126.95	114.35
4	10-B	7478	CIT	O4-C5-C4	3.98	126.95	114.35
4	1-G	7488	CIT	O4-C5-C4	3.97	126.93	114.35
4	2-G	7488	CIT	O4-C5-C4	3.97	126.93	114.35
4	3-G	7488	CIT	O4-C5-C4	3.97	126.93	114.35
4	4-G	7488	CIT	O4-C5-C4	3.97	126.93	114.35
4	5-G	7488	CIT	O4-C5-C4	3.97	126.93	114.35
4	6-G	7488	CIT	O4-C5-C4	3.97	126.93	114.35
4	7-G	7488	CIT	O4-C5-C4	3.97	126.93	114.35
4	8-G	7488	CIT	O4-C5-C4	3.97	126.93	114.35
4	9-G	7488	CIT	O4-C5-C4	3.97	126.93	114.35
4	10-G	7488	CIT	O4-C5-C4	3.97	126.93	114.35
4	1-S	7512	CIT	O4-C5-C4	3.97	126.93	114.35
4	2-S	7512	CIT	O4-C5-C4	3.97	126.93	114.35
4	3-S	7512	CIT	O4-C5-C4	3.97	126.93	114.35
4	4-S	7512	CIT	O4-C5-C4	3.97	126.93	114.35
4	5-S	7512	CIT	O4-C5-C4	3.97	126.93	114.35
4	6-S	7512	CIT	O4-C5-C4	3.97	126.93	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7-S	7512	CIT	O4-C5-C4	3.97	126.93	114.35
4	8-S	7512	CIT	O4-C5-C4	3.97	126.93	114.35
4	9-S	7512	CIT	O4-C5-C4	3.97	126.93	114.35
4	10-S	7512	CIT	O4-C5-C4	3.97	126.93	114.35
4	1-W	7520	CIT	O4-C5-C4	3.97	126.93	114.35
4	2-W	7520	CIT	O4-C5-C4	3.97	126.93	114.35
4	3-W	7520	CIT	O4-C5-C4	3.97	126.93	114.35
4	4-W	7520	CIT	O4-C5-C4	3.97	126.93	114.35
4	5-W	7520	CIT	O4-C5-C4	3.97	126.93	114.35
4	6-W	7520	CIT	O4-C5-C4	3.97	126.93	114.35
4	7-W	7520	CIT	O4-C5-C4	3.97	126.93	114.35
4	8-W	7520	CIT	O4-C5-C4	3.97	126.93	114.35
4	9-W	7520	CIT	O4-C5-C4	3.97	126.93	114.35
4	10-W	7520	CIT	O4-C5-C4	3.97	126.93	114.35
4	1-A	7476	CIT	O4-C5-C4	3.97	126.92	114.35
4	2-A	7476	CIT	O4-C5-C4	3.97	126.92	114.35
4	3-A	7476	CIT	O4-C5-C4	3.97	126.92	114.35
4	4-A	7476	CIT	O4-C5-C4	3.97	126.92	114.35
4	5-A	7476	CIT	O4-C5-C4	3.97	126.92	114.35
4	6-A	7476	CIT	O4-C5-C4	3.97	126.92	114.35
4	7-A	7476	CIT	O4-C5-C4	3.97	126.92	114.35
4	8-A	7476	CIT	O4-C5-C4	3.97	126.92	114.35
4	9-A	7476	CIT	O4-C5-C4	3.97	126.92	114.35
4	10-A	7476	CIT	O4-C5-C4	3.97	126.92	114.35
4	1-P	7506	CIT	O4-C5-C4	3.97	126.92	114.35
4	2-P	7506	CIT	O4-C5-C4	3.97	126.92	114.35
4	3-P	7506	CIT	O4-C5-C4	3.97	126.92	114.35
4	4-P	7506	CIT	O4-C5-C4	3.97	126.92	114.35
4	5-P	7506	CIT	O4-C5-C4	3.97	126.92	114.35
4	6-P	7506	CIT	O4-C5-C4	3.97	126.92	114.35
4	7-P	7506	CIT	O4-C5-C4	3.97	126.92	114.35
4	8-P	7506	CIT	O4-C5-C4	3.97	126.92	114.35
4	9-P	7506	CIT	O4-C5-C4	3.97	126.92	114.35
4	10-P	7506	CIT	O4-C5-C4	3.97	126.92	114.35
4	1-I	7492	CIT	O4-C5-C4	3.97	126.91	114.35
4	2-I	7492	CIT	O4-C5-C4	3.97	126.91	114.35
4	3-I	7492	CIT	O4-C5-C4	3.97	126.91	114.35
4	4-I	7492	CIT	O4-C5-C4	3.97	126.91	114.35
4	5-I	7492	CIT	O4-C5-C4	3.97	126.91	114.35
4	6-I	7492	CIT	O4-C5-C4	3.97	126.91	114.35
4	7-I	7492	CIT	O4-C5-C4	3.97	126.91	114.35
4	8-I	7492	CIT	O4-C5-C4	3.97	126.91	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9-I	7492	CIT	O4-C5-C4	3.97	126.91	114.35
4	10-I	7492	CIT	O4-C5-C4	3.97	126.91	114.35
4	1-H	7490	CIT	O4-C5-C4	3.97	126.91	114.35
4	2-H	7490	CIT	O4-C5-C4	3.97	126.91	114.35
4	3-H	7490	CIT	O4-C5-C4	3.97	126.91	114.35
4	4-H	7490	CIT	O4-C5-C4	3.97	126.91	114.35
4	5-H	7490	CIT	O4-C5-C4	3.97	126.91	114.35
4	6-H	7490	CIT	O4-C5-C4	3.97	126.91	114.35
4	7-H	7490	CIT	O4-C5-C4	3.97	126.91	114.35
4	8-H	7490	CIT	O4-C5-C4	3.97	126.91	114.35
4	9-H	7490	CIT	O4-C5-C4	3.97	126.91	114.35
4	10-H	7490	CIT	O4-C5-C4	3.97	126.91	114.35
4	1-Q	7508	CIT	O4-C5-C4	3.96	126.91	114.35
4	2-Q	7508	CIT	O4-C5-C4	3.96	126.91	114.35
4	3-Q	7508	CIT	O4-C5-C4	3.96	126.91	114.35
4	4-Q	7508	CIT	O4-C5-C4	3.96	126.91	114.35
4	5-Q	7508	CIT	O4-C5-C4	3.96	126.91	114.35
4	6-Q	7508	CIT	O4-C5-C4	3.96	126.91	114.35
4	7-Q	7508	CIT	O4-C5-C4	3.96	126.91	114.35
4	8-Q	7508	CIT	O4-C5-C4	3.96	126.91	114.35
4	9-Q	7508	CIT	O4-C5-C4	3.96	126.91	114.35
4	10-Q	7508	CIT	O4-C5-C4	3.96	126.91	114.35
4	1-N	7502	CIT	O4-C5-C4	3.96	126.90	114.35
4	2-N	7502	CIT	O4-C5-C4	3.96	126.90	114.35
4	3-N	7502	CIT	O4-C5-C4	3.96	126.90	114.35
4	4-N	7502	CIT	O4-C5-C4	3.96	126.90	114.35
4	5-N	7502	CIT	O4-C5-C4	3.96	126.90	114.35
4	6-N	7502	CIT	O4-C5-C4	3.96	126.90	114.35
4	7-N	7502	CIT	O4-C5-C4	3.96	126.90	114.35
4	8-N	7502	CIT	O4-C5-C4	3.96	126.90	114.35
4	9-N	7502	CIT	O4-C5-C4	3.96	126.90	114.35
4	10-N	7502	CIT	O4-C5-C4	3.96	126.90	114.35
4	1-J	7494	CIT	O4-C5-C4	3.96	126.90	114.35
4	2-J	7494	CIT	O4-C5-C4	3.96	126.90	114.35
4	3-J	7494	CIT	O4-C5-C4	3.96	126.90	114.35
4	4-J	7494	CIT	O4-C5-C4	3.96	126.90	114.35
4	5-J	7494	CIT	O4-C5-C4	3.96	126.90	114.35
4	6-J	7494	CIT	O4-C5-C4	3.96	126.90	114.35
4	7-J	7494	CIT	O4-C5-C4	3.96	126.90	114.35
4	8-J	7494	CIT	O4-C5-C4	3.96	126.90	114.35
4	9-J	7494	CIT	O4-C5-C4	3.96	126.90	114.35
4	10-J	7494	CIT	O4-C5-C4	3.96	126.90	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-L	7498	CIT	O4-C5-C4	3.96	126.90	114.35
4	2-L	7498	CIT	O4-C5-C4	3.96	126.90	114.35
4	3-L	7498	CIT	O4-C5-C4	3.96	126.90	114.35
4	4-L	7498	CIT	O4-C5-C4	3.96	126.90	114.35
4	5-L	7498	CIT	O4-C5-C4	3.96	126.90	114.35
4	6-L	7498	CIT	O4-C5-C4	3.96	126.90	114.35
4	7-L	7498	CIT	O4-C5-C4	3.96	126.90	114.35
4	8-L	7498	CIT	O4-C5-C4	3.96	126.90	114.35
4	9-L	7498	CIT	O4-C5-C4	3.96	126.90	114.35
4	10-L	7498	CIT	O4-C5-C4	3.96	126.90	114.35
4	1-U	7516	CIT	O4-C5-C4	3.96	126.90	114.35
4	2-U	7516	CIT	O4-C5-C4	3.96	126.90	114.35
4	3-U	7516	CIT	O4-C5-C4	3.96	126.90	114.35
4	4-U	7516	CIT	O4-C5-C4	3.96	126.90	114.35
4	5-U	7516	CIT	O4-C5-C4	3.96	126.90	114.35
4	6-U	7516	CIT	O4-C5-C4	3.96	126.90	114.35
4	7-U	7516	CIT	O4-C5-C4	3.96	126.90	114.35
4	8-U	7516	CIT	O4-C5-C4	3.96	126.90	114.35
4	9-U	7516	CIT	O4-C5-C4	3.96	126.90	114.35
4	10-U	7516	CIT	O4-C5-C4	3.96	126.90	114.35
4	1-V	7518	CIT	O4-C5-C4	3.96	126.90	114.35
4	2-V	7518	CIT	O4-C5-C4	3.96	126.90	114.35
4	3-V	7518	CIT	O4-C5-C4	3.96	126.90	114.35
4	4-V	7518	CIT	O4-C5-C4	3.96	126.90	114.35
4	5-V	7518	CIT	O4-C5-C4	3.96	126.90	114.35
4	6-V	7518	CIT	O4-C5-C4	3.96	126.90	114.35
4	7-V	7518	CIT	O4-C5-C4	3.96	126.90	114.35
4	8-V	7518	CIT	O4-C5-C4	3.96	126.90	114.35
4	9-V	7518	CIT	O4-C5-C4	3.96	126.90	114.35
4	10-V	7518	CIT	O4-C5-C4	3.96	126.90	114.35
4	1-F	7486	CIT	O4-C5-C4	3.96	126.89	114.35
4	2-F	7486	CIT	O4-C5-C4	3.96	126.89	114.35
4	3-F	7486	CIT	O4-C5-C4	3.96	126.89	114.35
4	4-F	7486	CIT	O4-C5-C4	3.96	126.89	114.35
4	5-F	7486	CIT	O4-C5-C4	3.96	126.89	114.35
4	6-F	7486	CIT	O4-C5-C4	3.96	126.89	114.35
4	7-F	7486	CIT	O4-C5-C4	3.96	126.89	114.35
4	8-F	7486	CIT	O4-C5-C4	3.96	126.89	114.35
4	9-F	7486	CIT	O4-C5-C4	3.96	126.89	114.35
4	10-F	7486	CIT	O4-C5-C4	3.96	126.89	114.35
4	1-T	7514	CIT	O4-C5-C4	3.96	126.89	114.35
4	2-T	7514	CIT	O4-C5-C4	3.96	126.89	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-T	7514	CIT	O4-C5-C4	3.96	126.89	114.35
4	4-T	7514	CIT	O4-C5-C4	3.96	126.89	114.35
4	5-T	7514	CIT	O4-C5-C4	3.96	126.89	114.35
4	6-T	7514	CIT	O4-C5-C4	3.96	126.89	114.35
4	7-T	7514	CIT	O4-C5-C4	3.96	126.89	114.35
4	8-T	7514	CIT	O4-C5-C4	3.96	126.89	114.35
4	9-T	7514	CIT	O4-C5-C4	3.96	126.89	114.35
4	10-T	7514	CIT	O4-C5-C4	3.96	126.89	114.35
4	1-R	7510	CIT	O4-C5-C4	3.96	126.88	114.35
4	2-R	7510	CIT	O4-C5-C4	3.96	126.88	114.35
4	3-R	7510	CIT	O4-C5-C4	3.96	126.88	114.35
4	4-R	7510	CIT	O4-C5-C4	3.96	126.88	114.35
4	5-R	7510	CIT	O4-C5-C4	3.96	126.88	114.35
4	6-R	7510	CIT	O4-C5-C4	3.96	126.88	114.35
4	7-R	7510	CIT	O4-C5-C4	3.96	126.88	114.35
4	8-R	7510	CIT	O4-C5-C4	3.96	126.88	114.35
4	9-R	7510	CIT	O4-C5-C4	3.96	126.88	114.35
4	10-R	7510	CIT	O4-C5-C4	3.96	126.88	114.35
4	1-C	7480	CIT	O4-C5-C4	3.95	126.86	114.35
4	2-C	7480	CIT	O4-C5-C4	3.95	126.86	114.35
4	3-C	7480	CIT	O4-C5-C4	3.95	126.86	114.35
4	4-C	7480	CIT	O4-C5-C4	3.95	126.86	114.35
4	5-C	7480	CIT	O4-C5-C4	3.95	126.86	114.35
4	6-C	7480	CIT	O4-C5-C4	3.95	126.86	114.35
4	7-C	7480	CIT	O4-C5-C4	3.95	126.86	114.35
4	8-C	7480	CIT	O4-C5-C4	3.95	126.86	114.35
4	9-C	7480	CIT	O4-C5-C4	3.95	126.86	114.35
4	10-C	7480	CIT	O4-C5-C4	3.95	126.86	114.35
3	1-T	7513	AMP	N9-C8-N7	3.63	119.08	113.94
3	2-T	7513	AMP	N9-C8-N7	3.63	119.08	113.94
3	3-T	7513	AMP	N9-C8-N7	3.63	119.08	113.94
3	4-T	7513	AMP	N9-C8-N7	3.63	119.08	113.94
3	5-T	7513	AMP	N9-C8-N7	3.63	119.08	113.94
3	6-T	7513	AMP	N9-C8-N7	3.63	119.08	113.94
3	7-T	7513	AMP	N9-C8-N7	3.63	119.08	113.94
3	8-T	7513	AMP	N9-C8-N7	3.63	119.08	113.94
3	9-T	7513	AMP	N9-C8-N7	3.63	119.08	113.94
3	10-T	7513	AMP	N9-C8-N7	3.63	119.08	113.94
3	1-C	7479	AMP	N9-C8-N7	3.62	119.07	113.94
3	2-C	7479	AMP	N9-C8-N7	3.62	119.07	113.94
3	3-C	7479	AMP	N9-C8-N7	3.62	119.07	113.94
3	4-C	7479	AMP	N9-C8-N7	3.62	119.07	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-C	7479	AMP	N9-C8-N7	3.62	119.07	113.94
3	6-C	7479	AMP	N9-C8-N7	3.62	119.07	113.94
3	7-C	7479	AMP	N9-C8-N7	3.62	119.07	113.94
3	8-C	7479	AMP	N9-C8-N7	3.62	119.07	113.94
3	9-C	7479	AMP	N9-C8-N7	3.62	119.07	113.94
3	10-C	7479	AMP	N9-C8-N7	3.62	119.07	113.94
3	1-E	7483	AMP	N9-C8-N7	3.61	119.06	113.94
3	2-E	7483	AMP	N9-C8-N7	3.61	119.06	113.94
3	3-E	7483	AMP	N9-C8-N7	3.61	119.06	113.94
3	4-E	7483	AMP	N9-C8-N7	3.61	119.06	113.94
3	5-E	7483	AMP	N9-C8-N7	3.61	119.06	113.94
3	6-E	7483	AMP	N9-C8-N7	3.61	119.06	113.94
3	7-E	7483	AMP	N9-C8-N7	3.61	119.06	113.94
3	8-E	7483	AMP	N9-C8-N7	3.61	119.06	113.94
3	9-E	7483	AMP	N9-C8-N7	3.61	119.06	113.94
3	10-E	7483	AMP	N9-C8-N7	3.61	119.06	113.94
3	1-P	7505	AMP	N9-C8-N7	3.60	119.05	113.94
3	2-P	7505	AMP	N9-C8-N7	3.60	119.05	113.94
3	3-P	7505	AMP	N9-C8-N7	3.60	119.05	113.94
3	4-P	7505	AMP	N9-C8-N7	3.60	119.05	113.94
3	5-P	7505	AMP	N9-C8-N7	3.60	119.05	113.94
3	6-P	7505	AMP	N9-C8-N7	3.60	119.05	113.94
3	7-P	7505	AMP	N9-C8-N7	3.60	119.05	113.94
3	8-P	7505	AMP	N9-C8-N7	3.60	119.05	113.94
3	9-P	7505	AMP	N9-C8-N7	3.60	119.05	113.94
3	10-P	7505	AMP	N9-C8-N7	3.60	119.05	113.94
3	1-I	7491	AMP	N9-C8-N7	3.60	119.04	113.94
3	2-I	7491	AMP	N9-C8-N7	3.60	119.04	113.94
3	3-I	7491	AMP	N9-C8-N7	3.60	119.04	113.94
3	4-I	7491	AMP	N9-C8-N7	3.60	119.04	113.94
3	5-I	7491	AMP	N9-C8-N7	3.60	119.04	113.94
3	6-I	7491	AMP	N9-C8-N7	3.60	119.04	113.94
3	7-I	7491	AMP	N9-C8-N7	3.60	119.04	113.94
3	8-I	7491	AMP	N9-C8-N7	3.60	119.04	113.94
3	9-I	7491	AMP	N9-C8-N7	3.60	119.04	113.94
3	10-I	7491	AMP	N9-C8-N7	3.60	119.04	113.94
3	1-R	7509	AMP	N9-C8-N7	3.60	119.04	113.94
3	2-R	7509	AMP	N9-C8-N7	3.60	119.04	113.94
3	3-R	7509	AMP	N9-C8-N7	3.60	119.04	113.94
3	4-R	7509	AMP	N9-C8-N7	3.60	119.04	113.94
3	5-R	7509	AMP	N9-C8-N7	3.60	119.04	113.94
3	6-R	7509	AMP	N9-C8-N7	3.60	119.04	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-R	7509	AMP	N9-C8-N7	3.60	119.04	113.94
3	8-R	7509	AMP	N9-C8-N7	3.60	119.04	113.94
3	9-R	7509	AMP	N9-C8-N7	3.60	119.04	113.94
3	10-R	7509	AMP	N9-C8-N7	3.60	119.04	113.94
3	1-U	7515	AMP	N9-C8-N7	3.59	119.03	113.94
3	2-U	7515	AMP	N9-C8-N7	3.59	119.03	113.94
3	3-U	7515	AMP	N9-C8-N7	3.59	119.03	113.94
3	4-U	7515	AMP	N9-C8-N7	3.59	119.03	113.94
3	5-U	7515	AMP	N9-C8-N7	3.59	119.03	113.94
3	6-U	7515	AMP	N9-C8-N7	3.59	119.03	113.94
3	7-U	7515	AMP	N9-C8-N7	3.59	119.03	113.94
3	8-U	7515	AMP	N9-C8-N7	3.59	119.03	113.94
3	9-U	7515	AMP	N9-C8-N7	3.59	119.03	113.94
3	10-U	7515	AMP	N9-C8-N7	3.59	119.03	113.94
3	1-S	7511	AMP	N9-C8-N7	3.59	119.03	113.94
3	2-S	7511	AMP	N9-C8-N7	3.59	119.03	113.94
3	3-S	7511	AMP	N9-C8-N7	3.59	119.03	113.94
3	4-S	7511	AMP	N9-C8-N7	3.59	119.03	113.94
3	5-S	7511	AMP	N9-C8-N7	3.59	119.03	113.94
3	6-S	7511	AMP	N9-C8-N7	3.59	119.03	113.94
3	7-S	7511	AMP	N9-C8-N7	3.59	119.03	113.94
3	8-S	7511	AMP	N9-C8-N7	3.59	119.03	113.94
3	9-S	7511	AMP	N9-C8-N7	3.59	119.03	113.94
3	10-S	7511	AMP	N9-C8-N7	3.59	119.03	113.94
3	1-F	7485	AMP	N9-C8-N7	3.59	119.02	113.94
3	2-F	7485	AMP	N9-C8-N7	3.59	119.02	113.94
3	3-F	7485	AMP	N9-C8-N7	3.59	119.02	113.94
3	4-F	7485	AMP	N9-C8-N7	3.59	119.02	113.94
3	5-F	7485	AMP	N9-C8-N7	3.59	119.02	113.94
3	6-F	7485	AMP	N9-C8-N7	3.59	119.02	113.94
3	7-F	7485	AMP	N9-C8-N7	3.59	119.02	113.94
3	8-F	7485	AMP	N9-C8-N7	3.59	119.02	113.94
3	9-F	7485	AMP	N9-C8-N7	3.59	119.02	113.94
3	10-F	7485	AMP	N9-C8-N7	3.59	119.02	113.94
3	1-K	7495	AMP	N9-C8-N7	3.59	119.02	113.94
3	2-K	7495	AMP	N9-C8-N7	3.59	119.02	113.94
3	3-K	7495	AMP	N9-C8-N7	3.59	119.02	113.94
3	4-K	7495	AMP	N9-C8-N7	3.59	119.02	113.94
3	5-K	7495	AMP	N9-C8-N7	3.59	119.02	113.94
3	6-K	7495	AMP	N9-C8-N7	3.59	119.02	113.94
3	7-K	7495	AMP	N9-C8-N7	3.59	119.02	113.94
3	8-K	7495	AMP	N9-C8-N7	3.59	119.02	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-K	7495	AMP	N9-C8-N7	3.59	119.02	113.94
3	10-K	7495	AMP	N9-C8-N7	3.59	119.02	113.94
3	1-G	7487	AMP	N9-C8-N7	3.58	119.02	113.94
3	2-G	7487	AMP	N9-C8-N7	3.58	119.02	113.94
3	3-G	7487	AMP	N9-C8-N7	3.58	119.02	113.94
3	4-G	7487	AMP	N9-C8-N7	3.58	119.02	113.94
3	5-G	7487	AMP	N9-C8-N7	3.58	119.02	113.94
3	6-G	7487	AMP	N9-C8-N7	3.58	119.02	113.94
3	7-G	7487	AMP	N9-C8-N7	3.58	119.02	113.94
3	8-G	7487	AMP	N9-C8-N7	3.58	119.02	113.94
3	9-G	7487	AMP	N9-C8-N7	3.58	119.02	113.94
3	10-G	7487	AMP	N9-C8-N7	3.58	119.02	113.94
3	1-A	7475	AMP	N9-C8-N7	3.58	119.02	113.94
3	2-A	7475	AMP	N9-C8-N7	3.58	119.02	113.94
3	3-A	7475	AMP	N9-C8-N7	3.58	119.02	113.94
3	4-A	7475	AMP	N9-C8-N7	3.58	119.02	113.94
3	5-A	7475	AMP	N9-C8-N7	3.58	119.02	113.94
3	6-A	7475	AMP	N9-C8-N7	3.58	119.02	113.94
3	7-A	7475	AMP	N9-C8-N7	3.58	119.02	113.94
3	8-A	7475	AMP	N9-C8-N7	3.58	119.02	113.94
3	9-A	7475	AMP	N9-C8-N7	3.58	119.02	113.94
3	10-A	7475	AMP	N9-C8-N7	3.58	119.02	113.94
3	1-M	7499	AMP	N9-C8-N7	3.58	119.02	113.94
3	2-M	7499	AMP	N9-C8-N7	3.58	119.02	113.94
3	3-M	7499	AMP	N9-C8-N7	3.58	119.02	113.94
3	4-M	7499	AMP	N9-C8-N7	3.58	119.02	113.94
3	5-M	7499	AMP	N9-C8-N7	3.58	119.02	113.94
3	6-M	7499	AMP	N9-C8-N7	3.58	119.02	113.94
3	7-M	7499	AMP	N9-C8-N7	3.58	119.02	113.94
3	8-M	7499	AMP	N9-C8-N7	3.58	119.02	113.94
3	9-M	7499	AMP	N9-C8-N7	3.58	119.02	113.94
3	10-M	7499	AMP	N9-C8-N7	3.58	119.02	113.94
3	1-V	7517	AMP	N9-C8-N7	3.58	119.02	113.94
3	2-V	7517	AMP	N9-C8-N7	3.58	119.02	113.94
3	3-V	7517	AMP	N9-C8-N7	3.58	119.02	113.94
3	4-V	7517	AMP	N9-C8-N7	3.58	119.02	113.94
3	5-V	7517	AMP	N9-C8-N7	3.58	119.02	113.94
3	6-V	7517	AMP	N9-C8-N7	3.58	119.02	113.94
3	7-V	7517	AMP	N9-C8-N7	3.58	119.02	113.94
3	8-V	7517	AMP	N9-C8-N7	3.58	119.02	113.94
3	9-V	7517	AMP	N9-C8-N7	3.58	119.02	113.94
3	10-V	7517	AMP	N9-C8-N7	3.58	119.02	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-N	7501	AMP	N9-C8-N7	3.58	119.01	113.94
3	2-N	7501	AMP	N9-C8-N7	3.58	119.01	113.94
3	3-N	7501	AMP	N9-C8-N7	3.58	119.01	113.94
3	4-N	7501	AMP	N9-C8-N7	3.58	119.01	113.94
3	5-N	7501	AMP	N9-C8-N7	3.58	119.01	113.94
3	6-N	7501	AMP	N9-C8-N7	3.58	119.01	113.94
3	7-N	7501	AMP	N9-C8-N7	3.58	119.01	113.94
3	8-N	7501	AMP	N9-C8-N7	3.58	119.01	113.94
3	9-N	7501	AMP	N9-C8-N7	3.58	119.01	113.94
3	10-N	7501	AMP	N9-C8-N7	3.58	119.01	113.94
3	1-D	7481	AMP	N9-C8-N7	3.58	119.01	113.94
3	2-D	7481	AMP	N9-C8-N7	3.58	119.01	113.94
3	3-D	7481	AMP	N9-C8-N7	3.58	119.01	113.94
3	4-D	7481	AMP	N9-C8-N7	3.58	119.01	113.94
3	5-D	7481	AMP	N9-C8-N7	3.58	119.01	113.94
3	6-D	7481	AMP	N9-C8-N7	3.58	119.01	113.94
3	7-D	7481	AMP	N9-C8-N7	3.58	119.01	113.94
3	8-D	7481	AMP	N9-C8-N7	3.58	119.01	113.94
3	9-D	7481	AMP	N9-C8-N7	3.58	119.01	113.94
3	10-D	7481	AMP	N9-C8-N7	3.58	119.01	113.94
3	1-O	7503	AMP	N9-C8-N7	3.58	119.01	113.94
3	2-O	7503	AMP	N9-C8-N7	3.58	119.01	113.94
3	3-O	7503	AMP	N9-C8-N7	3.58	119.01	113.94
3	4-O	7503	AMP	N9-C8-N7	3.58	119.01	113.94
3	5-O	7503	AMP	N9-C8-N7	3.58	119.01	113.94
3	6-O	7503	AMP	N9-C8-N7	3.58	119.01	113.94
3	7-O	7503	AMP	N9-C8-N7	3.58	119.01	113.94
3	8-O	7503	AMP	N9-C8-N7	3.58	119.01	113.94
3	9-O	7503	AMP	N9-C8-N7	3.58	119.01	113.94
3	10-O	7503	AMP	N9-C8-N7	3.58	119.01	113.94
3	1-W	7519	AMP	N9-C8-N7	3.57	119.00	113.94
3	2-W	7519	AMP	N9-C8-N7	3.57	119.00	113.94
3	3-W	7519	AMP	N9-C8-N7	3.57	119.00	113.94
3	4-W	7519	AMP	N9-C8-N7	3.57	119.00	113.94
3	5-W	7519	AMP	N9-C8-N7	3.57	119.00	113.94
3	6-W	7519	AMP	N9-C8-N7	3.57	119.00	113.94
3	7-W	7519	AMP	N9-C8-N7	3.57	119.00	113.94
3	8-W	7519	AMP	N9-C8-N7	3.57	119.00	113.94
3	9-W	7519	AMP	N9-C8-N7	3.57	119.00	113.94
3	10-W	7519	AMP	N9-C8-N7	3.57	119.00	113.94
3	1-X	7521	AMP	N9-C8-N7	3.57	118.99	113.94
3	2-X	7521	AMP	N9-C8-N7	3.57	118.99	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-X	7521	AMP	N9-C8-N7	3.57	118.99	113.94
3	4-X	7521	AMP	N9-C8-N7	3.57	118.99	113.94
3	5-X	7521	AMP	N9-C8-N7	3.57	118.99	113.94
3	6-X	7521	AMP	N9-C8-N7	3.57	118.99	113.94
3	7-X	7521	AMP	N9-C8-N7	3.57	118.99	113.94
3	8-X	7521	AMP	N9-C8-N7	3.57	118.99	113.94
3	9-X	7521	AMP	N9-C8-N7	3.57	118.99	113.94
3	10-X	7521	AMP	N9-C8-N7	3.57	118.99	113.94
3	1-Q	7507	AMP	N9-C8-N7	3.56	118.99	113.94
3	2-Q	7507	AMP	N9-C8-N7	3.56	118.99	113.94
3	3-Q	7507	AMP	N9-C8-N7	3.56	118.99	113.94
3	4-Q	7507	AMP	N9-C8-N7	3.56	118.99	113.94
3	5-Q	7507	AMP	N9-C8-N7	3.56	118.99	113.94
3	6-Q	7507	AMP	N9-C8-N7	3.56	118.99	113.94
3	7-Q	7507	AMP	N9-C8-N7	3.56	118.99	113.94
3	8-Q	7507	AMP	N9-C8-N7	3.56	118.99	113.94
3	9-Q	7507	AMP	N9-C8-N7	3.56	118.99	113.94
3	10-Q	7507	AMP	N9-C8-N7	3.56	118.99	113.94
3	1-L	7497	AMP	N9-C8-N7	3.56	118.99	113.94
3	2-L	7497	AMP	N9-C8-N7	3.56	118.99	113.94
3	3-L	7497	AMP	N9-C8-N7	3.56	118.99	113.94
3	4-L	7497	AMP	N9-C8-N7	3.56	118.99	113.94
3	5-L	7497	AMP	N9-C8-N7	3.56	118.99	113.94
3	6-L	7497	AMP	N9-C8-N7	3.56	118.99	113.94
3	7-L	7497	AMP	N9-C8-N7	3.56	118.99	113.94
3	8-L	7497	AMP	N9-C8-N7	3.56	118.99	113.94
3	9-L	7497	AMP	N9-C8-N7	3.56	118.99	113.94
3	10-L	7497	AMP	N9-C8-N7	3.56	118.99	113.94
3	1-B	7477	AMP	C4'-O4'-C1'	-3.56	101.61	109.47
3	2-B	7477	AMP	C4'-O4'-C1'	-3.56	101.61	109.47
3	3-B	7477	AMP	C4'-O4'-C1'	-3.56	101.61	109.47
3	4-B	7477	AMP	C4'-O4'-C1'	-3.56	101.61	109.47
3	5-B	7477	AMP	C4'-O4'-C1'	-3.56	101.61	109.47
3	6-B	7477	AMP	C4'-O4'-C1'	-3.56	101.61	109.47
3	7-B	7477	AMP	C4'-O4'-C1'	-3.56	101.61	109.47
3	8-B	7477	AMP	C4'-O4'-C1'	-3.56	101.61	109.47
3	9-B	7477	AMP	C4'-O4'-C1'	-3.56	101.61	109.47
3	10-B	7477	AMP	C4'-O4'-C1'	-3.56	101.61	109.47
3	1-B	7477	AMP	N9-C8-N7	3.55	118.98	113.94
3	2-B	7477	AMP	N9-C8-N7	3.55	118.98	113.94
3	3-B	7477	AMP	N9-C8-N7	3.55	118.98	113.94
3	4-B	7477	AMP	N9-C8-N7	3.55	118.98	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-B	7477	AMP	N9-C8-N7	3.55	118.98	113.94
3	6-B	7477	AMP	N9-C8-N7	3.55	118.98	113.94
3	7-B	7477	AMP	N9-C8-N7	3.55	118.98	113.94
3	8-B	7477	AMP	N9-C8-N7	3.55	118.98	113.94
3	9-B	7477	AMP	N9-C8-N7	3.55	118.98	113.94
3	10-B	7477	AMP	N9-C8-N7	3.55	118.98	113.94
3	1-J	7493	AMP	N9-C8-N7	3.55	118.98	113.94
3	2-J	7493	AMP	N9-C8-N7	3.55	118.98	113.94
3	3-J	7493	AMP	N9-C8-N7	3.55	118.98	113.94
3	4-J	7493	AMP	N9-C8-N7	3.55	118.98	113.94
3	5-J	7493	AMP	N9-C8-N7	3.55	118.98	113.94
3	6-J	7493	AMP	N9-C8-N7	3.55	118.98	113.94
3	7-J	7493	AMP	N9-C8-N7	3.55	118.98	113.94
3	8-J	7493	AMP	N9-C8-N7	3.55	118.98	113.94
3	9-J	7493	AMP	N9-C8-N7	3.55	118.98	113.94
3	10-J	7493	AMP	N9-C8-N7	3.55	118.98	113.94
3	1-K	7495	AMP	C4'-O4'-C1'	-3.55	101.62	109.47
3	2-K	7495	AMP	C4'-O4'-C1'	-3.55	101.62	109.47
3	3-K	7495	AMP	C4'-O4'-C1'	-3.55	101.62	109.47
3	4-K	7495	AMP	C4'-O4'-C1'	-3.55	101.62	109.47
3	5-K	7495	AMP	C4'-O4'-C1'	-3.55	101.62	109.47
3	6-K	7495	AMP	C4'-O4'-C1'	-3.55	101.62	109.47
3	7-K	7495	AMP	C4'-O4'-C1'	-3.55	101.62	109.47
3	8-K	7495	AMP	C4'-O4'-C1'	-3.55	101.62	109.47
3	9-K	7495	AMP	C4'-O4'-C1'	-3.55	101.62	109.47
3	10-K	7495	AMP	C4'-O4'-C1'	-3.55	101.62	109.47
3	1-H	7489	AMP	N9-C8-N7	3.55	118.97	113.94
3	2-H	7489	AMP	N9-C8-N7	3.55	118.97	113.94
3	3-H	7489	AMP	N9-C8-N7	3.55	118.97	113.94
3	4-H	7489	AMP	N9-C8-N7	3.55	118.97	113.94
3	5-H	7489	AMP	N9-C8-N7	3.55	118.97	113.94
3	6-H	7489	AMP	N9-C8-N7	3.55	118.97	113.94
3	7-H	7489	AMP	N9-C8-N7	3.55	118.97	113.94
3	8-H	7489	AMP	N9-C8-N7	3.55	118.97	113.94
3	9-H	7489	AMP	N9-C8-N7	3.55	118.97	113.94
3	10-H	7489	AMP	N9-C8-N7	3.55	118.97	113.94
3	1-H	7489	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	2-H	7489	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	3-H	7489	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	4-H	7489	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	5-H	7489	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	6-H	7489	AMP	C4'-O4'-C1'	-3.54	101.64	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-H	7489	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	8-H	7489	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	9-H	7489	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	10-H	7489	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	1-Q	7507	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	2-Q	7507	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	3-Q	7507	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	4-Q	7507	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	5-Q	7507	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	6-Q	7507	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	7-Q	7507	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	8-Q	7507	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	9-Q	7507	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	10-Q	7507	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	1-O	7503	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	2-O	7503	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	3-O	7503	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	4-O	7503	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	5-O	7503	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	6-O	7503	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	7-O	7503	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	8-O	7503	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	9-O	7503	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	10-O	7503	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	1-S	7511	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	2-S	7511	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	3-S	7511	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	4-S	7511	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	5-S	7511	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	6-S	7511	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	7-S	7511	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	8-S	7511	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	9-S	7511	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	10-S	7511	AMP	C4'-O4'-C1'	-3.54	101.64	109.47
3	1-D	7481	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	2-D	7481	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	3-D	7481	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	4-D	7481	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	5-D	7481	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	6-D	7481	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	7-D	7481	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	8-D	7481	AMP	C4'-O4'-C1'	-3.54	101.65	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-D	7481	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	10-D	7481	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	1-R	7509	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	2-R	7509	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	3-R	7509	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	4-R	7509	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	5-R	7509	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	6-R	7509	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	7-R	7509	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	8-R	7509	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	9-R	7509	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	10-R	7509	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	1-X	7521	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	2-X	7521	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	3-X	7521	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	4-X	7521	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	5-X	7521	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	6-X	7521	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	7-X	7521	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	8-X	7521	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	9-X	7521	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	10-X	7521	AMP	C4'-O4'-C1'	-3.54	101.65	109.47
3	1-M	7499	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	2-M	7499	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	3-M	7499	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	4-M	7499	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	5-M	7499	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	6-M	7499	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	7-M	7499	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	8-M	7499	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	9-M	7499	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	10-M	7499	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	1-W	7519	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	2-W	7519	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	3-W	7519	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	4-W	7519	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	5-W	7519	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	6-W	7519	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	7-W	7519	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	8-W	7519	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	9-W	7519	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	10-W	7519	AMP	C4'-O4'-C1'	-3.54	101.66	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-G	7487	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	2-G	7487	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	3-G	7487	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	4-G	7487	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	5-G	7487	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	6-G	7487	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	7-G	7487	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	8-G	7487	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	9-G	7487	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	10-G	7487	AMP	C4'-O4'-C1'	-3.54	101.66	109.47
3	1-A	7475	AMP	C4'-O4'-C1'	-3.53	101.66	109.47
3	2-A	7475	AMP	C4'-O4'-C1'	-3.53	101.66	109.47
3	3-A	7475	AMP	C4'-O4'-C1'	-3.53	101.66	109.47
3	4-A	7475	AMP	C4'-O4'-C1'	-3.53	101.66	109.47
3	5-A	7475	AMP	C4'-O4'-C1'	-3.53	101.66	109.47
3	6-A	7475	AMP	C4'-O4'-C1'	-3.53	101.66	109.47
3	7-A	7475	AMP	C4'-O4'-C1'	-3.53	101.66	109.47
3	8-A	7475	AMP	C4'-O4'-C1'	-3.53	101.66	109.47
3	9-A	7475	AMP	C4'-O4'-C1'	-3.53	101.66	109.47
3	10-A	7475	AMP	C4'-O4'-C1'	-3.53	101.66	109.47
3	1-L	7497	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	2-L	7497	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	3-L	7497	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	4-L	7497	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	5-L	7497	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	6-L	7497	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	7-L	7497	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	8-L	7497	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	9-L	7497	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	10-L	7497	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	1-C	7479	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	2-C	7479	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	3-C	7479	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	4-C	7479	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	5-C	7479	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	6-C	7479	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	7-C	7479	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	8-C	7479	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	9-C	7479	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	10-C	7479	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	1-P	7505	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	2-P	7505	AMP	C4'-O4'-C1'	-3.53	101.67	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-P	7505	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	4-P	7505	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	5-P	7505	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	6-P	7505	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	7-P	7505	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	8-P	7505	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	9-P	7505	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	10-P	7505	AMP	C4'-O4'-C1'	-3.53	101.67	109.47
3	1-N	7501	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	2-N	7501	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	3-N	7501	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	4-N	7501	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	5-N	7501	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	6-N	7501	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	7-N	7501	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	8-N	7501	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	9-N	7501	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	10-N	7501	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	1-U	7515	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	2-U	7515	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	3-U	7515	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	4-U	7515	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	5-U	7515	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	6-U	7515	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	7-U	7515	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	8-U	7515	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	9-U	7515	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	10-U	7515	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	1-T	7513	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	2-T	7513	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	3-T	7513	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	4-T	7513	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	5-T	7513	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	6-T	7513	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	7-T	7513	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	8-T	7513	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	9-T	7513	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	10-T	7513	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	1-B	7477	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	2-B	7477	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	3-B	7477	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	4-B	7477	AMP	C5'-C4'-C3'	-3.53	102.52	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-B	7477	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	6-B	7477	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	7-B	7477	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	8-B	7477	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	9-B	7477	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	10-B	7477	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	1-N	7501	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	2-N	7501	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	3-N	7501	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	4-N	7501	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	5-N	7501	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	6-N	7501	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	7-N	7501	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	8-N	7501	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	9-N	7501	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	10-N	7501	AMP	C5'-C4'-C3'	-3.53	102.52	115.21
3	1-I	7491	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	2-I	7491	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	3-I	7491	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	4-I	7491	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	5-I	7491	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	6-I	7491	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	7-I	7491	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	8-I	7491	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	9-I	7491	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	10-I	7491	AMP	C4'-O4'-C1'	-3.53	101.68	109.47
3	1-D	7481	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	2-D	7481	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	3-D	7481	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	4-D	7481	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	5-D	7481	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	6-D	7481	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	7-D	7481	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	8-D	7481	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	9-D	7481	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	10-D	7481	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	1-G	7487	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	2-G	7487	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	3-G	7487	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	4-G	7487	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	5-G	7487	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	6-G	7487	AMP	C5'-C4'-C3'	-3.52	102.52	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-G	7487	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	8-G	7487	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	9-G	7487	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	10-G	7487	AMP	C5'-C4'-C3'	-3.52	102.52	115.21
3	1-K	7495	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	2-K	7495	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	3-K	7495	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	4-K	7495	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	5-K	7495	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	6-K	7495	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	7-K	7495	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	8-K	7495	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	9-K	7495	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	10-K	7495	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	1-J	7493	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	2-J	7493	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	3-J	7493	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	4-J	7493	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	5-J	7493	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	6-J	7493	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	7-J	7493	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	8-J	7493	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	9-J	7493	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	10-J	7493	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	1-J	7493	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	2-J	7493	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	3-J	7493	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	4-J	7493	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	5-J	7493	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	6-J	7493	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	7-J	7493	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	8-J	7493	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	9-J	7493	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	10-J	7493	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	1-F	7485	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	2-F	7485	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	3-F	7485	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	4-F	7485	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	5-F	7485	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	6-F	7485	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	7-F	7485	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	8-F	7485	AMP	C4'-O4'-C1'	-3.52	101.69	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-F	7485	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	10-F	7485	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	1-F	7485	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	2-F	7485	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	3-F	7485	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	4-F	7485	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	5-F	7485	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	6-F	7485	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	7-F	7485	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	8-F	7485	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	9-F	7485	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	10-F	7485	AMP	C5'-C4'-C3'	-3.52	102.53	115.21
3	1-V	7517	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	2-V	7517	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	3-V	7517	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	4-V	7517	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	5-V	7517	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	6-V	7517	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	7-V	7517	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	8-V	7517	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	9-V	7517	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	10-V	7517	AMP	C4'-O4'-C1'	-3.52	101.69	109.47
3	1-Q	7507	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	2-Q	7507	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	3-Q	7507	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	4-Q	7507	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	5-Q	7507	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	6-Q	7507	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	7-Q	7507	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	8-Q	7507	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	9-Q	7507	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	10-Q	7507	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	1-O	7503	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	2-O	7503	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	3-O	7503	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	4-O	7503	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	5-O	7503	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	6-O	7503	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	7-O	7503	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	8-O	7503	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	9-O	7503	AMP	C5'-C4'-C3'	-3.52	102.54	115.21
3	10-O	7503	AMP	C5'-C4'-C3'	-3.52	102.54	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-E	7483	AMP	C4'-O4'-C1'	-3.52	101.70	109.47
3	2-E	7483	AMP	C4'-O4'-C1'	-3.52	101.70	109.47
3	3-E	7483	AMP	C4'-O4'-C1'	-3.52	101.70	109.47
3	4-E	7483	AMP	C4'-O4'-C1'	-3.52	101.70	109.47
3	5-E	7483	AMP	C4'-O4'-C1'	-3.52	101.70	109.47
3	6-E	7483	AMP	C4'-O4'-C1'	-3.52	101.70	109.47
3	7-E	7483	AMP	C4'-O4'-C1'	-3.52	101.70	109.47
3	8-E	7483	AMP	C4'-O4'-C1'	-3.52	101.70	109.47
3	9-E	7483	AMP	C4'-O4'-C1'	-3.52	101.70	109.47
3	10-E	7483	AMP	C4'-O4'-C1'	-3.52	101.70	109.47
3	1-A	7475	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	2-A	7475	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	3-A	7475	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	4-A	7475	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	5-A	7475	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	6-A	7475	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	7-A	7475	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	8-A	7475	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	9-A	7475	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	10-A	7475	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	1-L	7497	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	2-L	7497	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	3-L	7497	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	4-L	7497	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	5-L	7497	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	6-L	7497	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	7-L	7497	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	8-L	7497	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	9-L	7497	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	10-L	7497	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	1-H	7489	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	2-H	7489	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	3-H	7489	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	4-H	7489	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	5-H	7489	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	6-H	7489	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	7-H	7489	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	8-H	7489	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	9-H	7489	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	10-H	7489	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	1-S	7511	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	2-S	7511	AMP	C5'-C4'-C3'	-3.52	102.55	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-S	7511	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	4-S	7511	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	5-S	7511	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	6-S	7511	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	7-S	7511	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	8-S	7511	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	9-S	7511	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	10-S	7511	AMP	C5'-C4'-C3'	-3.52	102.55	115.21
3	1-I	7491	AMP	C5'-C4'-C3'	-3.51	102.56	115.21
3	2-I	7491	AMP	C5'-C4'-C3'	-3.51	102.56	115.21
3	3-I	7491	AMP	C5'-C4'-C3'	-3.51	102.56	115.21
3	4-I	7491	AMP	C5'-C4'-C3'	-3.51	102.56	115.21
3	5-I	7491	AMP	C5'-C4'-C3'	-3.51	102.56	115.21
3	6-I	7491	AMP	C5'-C4'-C3'	-3.51	102.56	115.21
3	7-I	7491	AMP	C5'-C4'-C3'	-3.51	102.56	115.21
3	8-I	7491	AMP	C5'-C4'-C3'	-3.51	102.56	115.21
3	9-I	7491	AMP	C5'-C4'-C3'	-3.51	102.56	115.21
3	10-I	7491	AMP	C5'-C4'-C3'	-3.51	102.56	115.21
3	1-E	7483	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	2-E	7483	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	3-E	7483	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	4-E	7483	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	5-E	7483	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	6-E	7483	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	7-E	7483	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	8-E	7483	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	9-E	7483	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	10-E	7483	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	1-U	7515	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	2-U	7515	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	3-U	7515	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	4-U	7515	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	5-U	7515	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	6-U	7515	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	7-U	7515	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	8-U	7515	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	9-U	7515	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	10-U	7515	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	1-V	7517	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	2-V	7517	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	3-V	7517	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	4-V	7517	AMP	C5'-C4'-C3'	-3.51	102.57	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-V	7517	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	6-V	7517	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	7-V	7517	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	8-V	7517	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	9-V	7517	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	10-V	7517	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	1-W	7519	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	2-W	7519	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	3-W	7519	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	4-W	7519	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	5-W	7519	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	6-W	7519	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	7-W	7519	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	8-W	7519	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	9-W	7519	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	10-W	7519	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	1-X	7521	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	2-X	7521	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	3-X	7521	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	4-X	7521	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	5-X	7521	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	6-X	7521	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	7-X	7521	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	8-X	7521	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	9-X	7521	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	10-X	7521	AMP	C5'-C4'-C3'	-3.51	102.57	115.21
3	1-M	7499	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	2-M	7499	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	3-M	7499	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	4-M	7499	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	5-M	7499	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	6-M	7499	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	7-M	7499	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	8-M	7499	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	9-M	7499	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	10-M	7499	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	1-P	7505	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	2-P	7505	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	3-P	7505	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	4-P	7505	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	5-P	7505	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	6-P	7505	AMP	C5'-C4'-C3'	-3.51	102.58	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-P	7505	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	8-P	7505	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	9-P	7505	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	10-P	7505	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	1-T	7513	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	2-T	7513	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	3-T	7513	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	4-T	7513	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	5-T	7513	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	6-T	7513	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	7-T	7513	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	8-T	7513	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	9-T	7513	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	10-T	7513	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	1-C	7479	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	2-C	7479	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	3-C	7479	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	4-C	7479	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	5-C	7479	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	6-C	7479	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	7-C	7479	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	8-C	7479	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	9-C	7479	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	10-C	7479	AMP	C5'-C4'-C3'	-3.51	102.58	115.21
3	1-R	7509	AMP	C5'-C4'-C3'	-3.51	102.59	115.21
3	2-R	7509	AMP	C5'-C4'-C3'	-3.51	102.59	115.21
3	3-R	7509	AMP	C5'-C4'-C3'	-3.51	102.59	115.21
3	4-R	7509	AMP	C5'-C4'-C3'	-3.51	102.59	115.21
3	5-R	7509	AMP	C5'-C4'-C3'	-3.51	102.59	115.21
3	6-R	7509	AMP	C5'-C4'-C3'	-3.51	102.59	115.21
3	7-R	7509	AMP	C5'-C4'-C3'	-3.51	102.59	115.21
3	8-R	7509	AMP	C5'-C4'-C3'	-3.51	102.59	115.21
3	9-R	7509	AMP	C5'-C4'-C3'	-3.51	102.59	115.21
3	10-R	7509	AMP	C5'-C4'-C3'	-3.51	102.59	115.21
3	1-P	7505	AMP	C4-N9-C1'	3.32	134.40	126.63
3	2-P	7505	AMP	C4-N9-C1'	3.32	134.40	126.63
3	3-P	7505	AMP	C4-N9-C1'	3.32	134.40	126.63
3	4-P	7505	AMP	C4-N9-C1'	3.32	134.40	126.63
3	5-P	7505	AMP	C4-N9-C1'	3.32	134.40	126.63
3	6-P	7505	AMP	C4-N9-C1'	3.32	134.40	126.63
3	7-P	7505	AMP	C4-N9-C1'	3.32	134.40	126.63
3	8-P	7505	AMP	C4-N9-C1'	3.32	134.40	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-P	7505	AMP	C4-N9-C1'	3.32	134.40	126.63
3	10-P	7505	AMP	C4-N9-C1'	3.32	134.40	126.63
3	1-L	7497	AMP	C4-N9-C1'	3.32	134.39	126.63
3	2-L	7497	AMP	C4-N9-C1'	3.32	134.39	126.63
3	3-L	7497	AMP	C4-N9-C1'	3.32	134.39	126.63
3	4-L	7497	AMP	C4-N9-C1'	3.32	134.39	126.63
3	5-L	7497	AMP	C4-N9-C1'	3.32	134.39	126.63
3	6-L	7497	AMP	C4-N9-C1'	3.32	134.39	126.63
3	7-L	7497	AMP	C4-N9-C1'	3.32	134.39	126.63
3	8-L	7497	AMP	C4-N9-C1'	3.32	134.39	126.63
3	9-L	7497	AMP	C4-N9-C1'	3.32	134.39	126.63
3	10-L	7497	AMP	C4-N9-C1'	3.32	134.39	126.63
3	1-D	7481	AMP	C4-N9-C1'	3.31	134.37	126.63
3	2-D	7481	AMP	C4-N9-C1'	3.31	134.37	126.63
3	3-D	7481	AMP	C4-N9-C1'	3.31	134.37	126.63
3	4-D	7481	AMP	C4-N9-C1'	3.31	134.37	126.63
3	5-D	7481	AMP	C4-N9-C1'	3.31	134.37	126.63
3	6-D	7481	AMP	C4-N9-C1'	3.31	134.37	126.63
3	7-D	7481	AMP	C4-N9-C1'	3.31	134.37	126.63
3	8-D	7481	AMP	C4-N9-C1'	3.31	134.37	126.63
3	9-D	7481	AMP	C4-N9-C1'	3.31	134.37	126.63
3	10-D	7481	AMP	C4-N9-C1'	3.31	134.37	126.63
3	1-U	7515	AMP	C4-N9-C1'	3.31	134.37	126.63
3	2-U	7515	AMP	C4-N9-C1'	3.31	134.37	126.63
3	3-U	7515	AMP	C4-N9-C1'	3.31	134.37	126.63
3	4-U	7515	AMP	C4-N9-C1'	3.31	134.37	126.63
3	5-U	7515	AMP	C4-N9-C1'	3.31	134.37	126.63
3	6-U	7515	AMP	C4-N9-C1'	3.31	134.37	126.63
3	7-U	7515	AMP	C4-N9-C1'	3.31	134.37	126.63
3	8-U	7515	AMP	C4-N9-C1'	3.31	134.37	126.63
3	9-U	7515	AMP	C4-N9-C1'	3.31	134.37	126.63
3	10-U	7515	AMP	C4-N9-C1'	3.31	134.37	126.63
3	1-N	7501	AMP	C4-N9-C1'	3.30	134.35	126.63
3	2-N	7501	AMP	C4-N9-C1'	3.30	134.35	126.63
3	3-N	7501	AMP	C4-N9-C1'	3.30	134.35	126.63
3	4-N	7501	AMP	C4-N9-C1'	3.30	134.35	126.63
3	5-N	7501	AMP	C4-N9-C1'	3.30	134.35	126.63
3	6-N	7501	AMP	C4-N9-C1'	3.30	134.35	126.63
3	7-N	7501	AMP	C4-N9-C1'	3.30	134.35	126.63
3	8-N	7501	AMP	C4-N9-C1'	3.30	134.35	126.63
3	9-N	7501	AMP	C4-N9-C1'	3.30	134.35	126.63
3	10-N	7501	AMP	C4-N9-C1'	3.30	134.35	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-V	7517	AMP	C4-N9-C1'	3.30	134.35	126.63
3	2-V	7517	AMP	C4-N9-C1'	3.30	134.35	126.63
3	3-V	7517	AMP	C4-N9-C1'	3.30	134.35	126.63
3	4-V	7517	AMP	C4-N9-C1'	3.30	134.35	126.63
3	5-V	7517	AMP	C4-N9-C1'	3.30	134.35	126.63
3	6-V	7517	AMP	C4-N9-C1'	3.30	134.35	126.63
3	7-V	7517	AMP	C4-N9-C1'	3.30	134.35	126.63
3	8-V	7517	AMP	C4-N9-C1'	3.30	134.35	126.63
3	9-V	7517	AMP	C4-N9-C1'	3.30	134.35	126.63
3	10-V	7517	AMP	C4-N9-C1'	3.30	134.35	126.63
3	1-O	7503	AMP	C4-N9-C1'	3.30	134.35	126.63
3	2-O	7503	AMP	C4-N9-C1'	3.30	134.35	126.63
3	3-O	7503	AMP	C4-N9-C1'	3.30	134.35	126.63
3	4-O	7503	AMP	C4-N9-C1'	3.30	134.35	126.63
3	5-O	7503	AMP	C4-N9-C1'	3.30	134.35	126.63
3	6-O	7503	AMP	C4-N9-C1'	3.30	134.35	126.63
3	7-O	7503	AMP	C4-N9-C1'	3.30	134.35	126.63
3	8-O	7503	AMP	C4-N9-C1'	3.30	134.35	126.63
3	9-O	7503	AMP	C4-N9-C1'	3.30	134.35	126.63
3	10-O	7503	AMP	C4-N9-C1'	3.30	134.35	126.63
3	1-W	7519	AMP	C4-N9-C1'	3.30	134.35	126.63
3	2-W	7519	AMP	C4-N9-C1'	3.30	134.35	126.63
3	3-W	7519	AMP	C4-N9-C1'	3.30	134.35	126.63
3	4-W	7519	AMP	C4-N9-C1'	3.30	134.35	126.63
3	5-W	7519	AMP	C4-N9-C1'	3.30	134.35	126.63
3	6-W	7519	AMP	C4-N9-C1'	3.30	134.35	126.63
3	7-W	7519	AMP	C4-N9-C1'	3.30	134.35	126.63
3	8-W	7519	AMP	C4-N9-C1'	3.30	134.35	126.63
3	9-W	7519	AMP	C4-N9-C1'	3.30	134.35	126.63
3	10-W	7519	AMP	C4-N9-C1'	3.30	134.35	126.63
3	1-Q	7507	AMP	C4-N9-C1'	3.30	134.35	126.63
3	2-Q	7507	AMP	C4-N9-C1'	3.30	134.35	126.63
3	3-Q	7507	AMP	C4-N9-C1'	3.30	134.35	126.63
3	4-Q	7507	AMP	C4-N9-C1'	3.30	134.35	126.63
3	5-Q	7507	AMP	C4-N9-C1'	3.30	134.35	126.63
3	6-Q	7507	AMP	C4-N9-C1'	3.30	134.35	126.63
3	7-Q	7507	AMP	C4-N9-C1'	3.30	134.35	126.63
3	8-Q	7507	AMP	C4-N9-C1'	3.30	134.35	126.63
3	9-Q	7507	AMP	C4-N9-C1'	3.30	134.35	126.63
3	10-Q	7507	AMP	C4-N9-C1'	3.30	134.35	126.63
3	1-B	7477	AMP	C4-N9-C1'	3.30	134.35	126.63
3	2-B	7477	AMP	C4-N9-C1'	3.30	134.35	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-B	7477	AMP	C4-N9-C1'	3.30	134.35	126.63
3	4-B	7477	AMP	C4-N9-C1'	3.30	134.35	126.63
3	5-B	7477	AMP	C4-N9-C1'	3.30	134.35	126.63
3	6-B	7477	AMP	C4-N9-C1'	3.30	134.35	126.63
3	7-B	7477	AMP	C4-N9-C1'	3.30	134.35	126.63
3	8-B	7477	AMP	C4-N9-C1'	3.30	134.35	126.63
3	9-B	7477	AMP	C4-N9-C1'	3.30	134.35	126.63
3	10-B	7477	AMP	C4-N9-C1'	3.30	134.35	126.63
3	1-E	7483	AMP	C4-N9-C1'	3.30	134.35	126.63
3	2-E	7483	AMP	C4-N9-C1'	3.30	134.35	126.63
3	3-E	7483	AMP	C4-N9-C1'	3.30	134.35	126.63
3	4-E	7483	AMP	C4-N9-C1'	3.30	134.35	126.63
3	5-E	7483	AMP	C4-N9-C1'	3.30	134.35	126.63
3	6-E	7483	AMP	C4-N9-C1'	3.30	134.35	126.63
3	7-E	7483	AMP	C4-N9-C1'	3.30	134.35	126.63
3	8-E	7483	AMP	C4-N9-C1'	3.30	134.35	126.63
3	9-E	7483	AMP	C4-N9-C1'	3.30	134.35	126.63
3	10-E	7483	AMP	C4-N9-C1'	3.30	134.35	126.63
3	1-F	7485	AMP	C4-N9-C1'	3.30	134.34	126.63
3	2-F	7485	AMP	C4-N9-C1'	3.30	134.34	126.63
3	3-F	7485	AMP	C4-N9-C1'	3.30	134.34	126.63
3	4-F	7485	AMP	C4-N9-C1'	3.30	134.34	126.63
3	5-F	7485	AMP	C4-N9-C1'	3.30	134.34	126.63
3	6-F	7485	AMP	C4-N9-C1'	3.30	134.34	126.63
3	7-F	7485	AMP	C4-N9-C1'	3.30	134.34	126.63
3	8-F	7485	AMP	C4-N9-C1'	3.30	134.34	126.63
3	9-F	7485	AMP	C4-N9-C1'	3.30	134.34	126.63
3	10-F	7485	AMP	C4-N9-C1'	3.30	134.34	126.63
3	1-J	7493	AMP	C4-N9-C1'	3.30	134.34	126.63
3	2-J	7493	AMP	C4-N9-C1'	3.30	134.34	126.63
3	3-J	7493	AMP	C4-N9-C1'	3.30	134.34	126.63
3	4-J	7493	AMP	C4-N9-C1'	3.30	134.34	126.63
3	5-J	7493	AMP	C4-N9-C1'	3.30	134.34	126.63
3	6-J	7493	AMP	C4-N9-C1'	3.30	134.34	126.63
3	7-J	7493	AMP	C4-N9-C1'	3.30	134.34	126.63
3	8-J	7493	AMP	C4-N9-C1'	3.30	134.34	126.63
3	9-J	7493	AMP	C4-N9-C1'	3.30	134.34	126.63
3	10-J	7493	AMP	C4-N9-C1'	3.30	134.34	126.63
3	1-A	7475	AMP	C4-N9-C1'	3.29	134.34	126.63
3	2-A	7475	AMP	C4-N9-C1'	3.29	134.34	126.63
3	3-A	7475	AMP	C4-N9-C1'	3.29	134.34	126.63
3	4-A	7475	AMP	C4-N9-C1'	3.29	134.34	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-A	7475	AMP	C4-N9-C1'	3.29	134.34	126.63
3	6-A	7475	AMP	C4-N9-C1'	3.29	134.34	126.63
3	7-A	7475	AMP	C4-N9-C1'	3.29	134.34	126.63
3	8-A	7475	AMP	C4-N9-C1'	3.29	134.34	126.63
3	9-A	7475	AMP	C4-N9-C1'	3.29	134.34	126.63
3	10-A	7475	AMP	C4-N9-C1'	3.29	134.34	126.63
3	1-G	7487	AMP	C4-N9-C1'	3.29	134.33	126.63
3	2-G	7487	AMP	C4-N9-C1'	3.29	134.33	126.63
3	3-G	7487	AMP	C4-N9-C1'	3.29	134.33	126.63
3	4-G	7487	AMP	C4-N9-C1'	3.29	134.33	126.63
3	5-G	7487	AMP	C4-N9-C1'	3.29	134.33	126.63
3	6-G	7487	AMP	C4-N9-C1'	3.29	134.33	126.63
3	7-G	7487	AMP	C4-N9-C1'	3.29	134.33	126.63
3	8-G	7487	AMP	C4-N9-C1'	3.29	134.33	126.63
3	9-G	7487	AMP	C4-N9-C1'	3.29	134.33	126.63
3	10-G	7487	AMP	C4-N9-C1'	3.29	134.33	126.63
3	1-T	7513	AMP	C4-N9-C1'	3.29	134.33	126.63
3	2-T	7513	AMP	C4-N9-C1'	3.29	134.33	126.63
3	3-T	7513	AMP	C4-N9-C1'	3.29	134.33	126.63
3	4-T	7513	AMP	C4-N9-C1'	3.29	134.33	126.63
3	5-T	7513	AMP	C4-N9-C1'	3.29	134.33	126.63
3	6-T	7513	AMP	C4-N9-C1'	3.29	134.33	126.63
3	7-T	7513	AMP	C4-N9-C1'	3.29	134.33	126.63
3	8-T	7513	AMP	C4-N9-C1'	3.29	134.33	126.63
3	9-T	7513	AMP	C4-N9-C1'	3.29	134.33	126.63
3	10-T	7513	AMP	C4-N9-C1'	3.29	134.33	126.63
3	1-H	7489	AMP	C4-N9-C1'	3.29	134.32	126.63
3	2-H	7489	AMP	C4-N9-C1'	3.29	134.32	126.63
3	3-H	7489	AMP	C4-N9-C1'	3.29	134.32	126.63
3	4-H	7489	AMP	C4-N9-C1'	3.29	134.32	126.63
3	5-H	7489	AMP	C4-N9-C1'	3.29	134.32	126.63
3	6-H	7489	AMP	C4-N9-C1'	3.29	134.32	126.63
3	7-H	7489	AMP	C4-N9-C1'	3.29	134.32	126.63
3	8-H	7489	AMP	C4-N9-C1'	3.29	134.32	126.63
3	9-H	7489	AMP	C4-N9-C1'	3.29	134.32	126.63
3	10-H	7489	AMP	C4-N9-C1'	3.29	134.32	126.63
3	1-S	7511	AMP	C4-N9-C1'	3.29	134.32	126.63
3	2-S	7511	AMP	C4-N9-C1'	3.29	134.32	126.63
3	3-S	7511	AMP	C4-N9-C1'	3.29	134.32	126.63
3	4-S	7511	AMP	C4-N9-C1'	3.29	134.32	126.63
3	5-S	7511	AMP	C4-N9-C1'	3.29	134.32	126.63
3	6-S	7511	AMP	C4-N9-C1'	3.29	134.32	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-S	7511	AMP	C4-N9-C1'	3.29	134.32	126.63
3	8-S	7511	AMP	C4-N9-C1'	3.29	134.32	126.63
3	9-S	7511	AMP	C4-N9-C1'	3.29	134.32	126.63
3	10-S	7511	AMP	C4-N9-C1'	3.29	134.32	126.63
3	1-K	7495	AMP	C4-N9-C1'	3.29	134.32	126.63
3	2-K	7495	AMP	C4-N9-C1'	3.29	134.32	126.63
3	3-K	7495	AMP	C4-N9-C1'	3.29	134.32	126.63
3	4-K	7495	AMP	C4-N9-C1'	3.29	134.32	126.63
3	5-K	7495	AMP	C4-N9-C1'	3.29	134.32	126.63
3	6-K	7495	AMP	C4-N9-C1'	3.29	134.32	126.63
3	7-K	7495	AMP	C4-N9-C1'	3.29	134.32	126.63
3	8-K	7495	AMP	C4-N9-C1'	3.29	134.32	126.63
3	9-K	7495	AMP	C4-N9-C1'	3.29	134.32	126.63
3	10-K	7495	AMP	C4-N9-C1'	3.29	134.32	126.63
3	1-M	7499	AMP	C4-N9-C1'	3.28	134.31	126.63
3	2-M	7499	AMP	C4-N9-C1'	3.28	134.31	126.63
3	3-M	7499	AMP	C4-N9-C1'	3.28	134.31	126.63
3	4-M	7499	AMP	C4-N9-C1'	3.28	134.31	126.63
3	5-M	7499	AMP	C4-N9-C1'	3.28	134.31	126.63
3	6-M	7499	AMP	C4-N9-C1'	3.28	134.31	126.63
3	7-M	7499	AMP	C4-N9-C1'	3.28	134.31	126.63
3	8-M	7499	AMP	C4-N9-C1'	3.28	134.31	126.63
3	9-M	7499	AMP	C4-N9-C1'	3.28	134.31	126.63
3	10-M	7499	AMP	C4-N9-C1'	3.28	134.31	126.63
3	1-I	7491	AMP	C4-N9-C1'	3.28	134.31	126.63
3	2-I	7491	AMP	C4-N9-C1'	3.28	134.31	126.63
3	3-I	7491	AMP	C4-N9-C1'	3.28	134.31	126.63
3	4-I	7491	AMP	C4-N9-C1'	3.28	134.31	126.63
3	5-I	7491	AMP	C4-N9-C1'	3.28	134.31	126.63
3	6-I	7491	AMP	C4-N9-C1'	3.28	134.31	126.63
3	7-I	7491	AMP	C4-N9-C1'	3.28	134.31	126.63
3	8-I	7491	AMP	C4-N9-C1'	3.28	134.31	126.63
3	9-I	7491	AMP	C4-N9-C1'	3.28	134.31	126.63
3	10-I	7491	AMP	C4-N9-C1'	3.28	134.31	126.63
3	1-R	7509	AMP	C4-N9-C1'	3.28	134.30	126.63
3	2-R	7509	AMP	C4-N9-C1'	3.28	134.30	126.63
3	3-R	7509	AMP	C4-N9-C1'	3.28	134.30	126.63
3	4-R	7509	AMP	C4-N9-C1'	3.28	134.30	126.63
3	5-R	7509	AMP	C4-N9-C1'	3.28	134.30	126.63
3	6-R	7509	AMP	C4-N9-C1'	3.28	134.30	126.63
3	7-R	7509	AMP	C4-N9-C1'	3.28	134.30	126.63
3	8-R	7509	AMP	C4-N9-C1'	3.28	134.30	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-R	7509	AMP	C4-N9-C1'	3.28	134.30	126.63
3	10-R	7509	AMP	C4-N9-C1'	3.28	134.30	126.63
3	1-C	7479	AMP	C4-N9-C1'	3.27	134.29	126.63
3	2-C	7479	AMP	C4-N9-C1'	3.27	134.29	126.63
3	3-C	7479	AMP	C4-N9-C1'	3.27	134.29	126.63
3	4-C	7479	AMP	C4-N9-C1'	3.27	134.29	126.63
3	5-C	7479	AMP	C4-N9-C1'	3.27	134.29	126.63
3	6-C	7479	AMP	C4-N9-C1'	3.27	134.29	126.63
3	7-C	7479	AMP	C4-N9-C1'	3.27	134.29	126.63
3	8-C	7479	AMP	C4-N9-C1'	3.27	134.29	126.63
3	9-C	7479	AMP	C4-N9-C1'	3.27	134.29	126.63
3	10-C	7479	AMP	C4-N9-C1'	3.27	134.29	126.63
3	1-X	7521	AMP	C4-N9-C1'	3.27	134.29	126.63
3	2-X	7521	AMP	C4-N9-C1'	3.27	134.29	126.63
3	3-X	7521	AMP	C4-N9-C1'	3.27	134.29	126.63
3	4-X	7521	AMP	C4-N9-C1'	3.27	134.29	126.63
3	5-X	7521	AMP	C4-N9-C1'	3.27	134.29	126.63
3	6-X	7521	AMP	C4-N9-C1'	3.27	134.29	126.63
3	7-X	7521	AMP	C4-N9-C1'	3.27	134.29	126.63
3	8-X	7521	AMP	C4-N9-C1'	3.27	134.29	126.63
3	9-X	7521	AMP	C4-N9-C1'	3.27	134.29	126.63
3	10-X	7521	AMP	C4-N9-C1'	3.27	134.29	126.63
3	1-N	7501	AMP	C4-C5-N7	2.82	113.81	110.58
3	2-N	7501	AMP	C4-C5-N7	2.82	113.81	110.58
3	3-N	7501	AMP	C4-C5-N7	2.82	113.81	110.58
3	4-N	7501	AMP	C4-C5-N7	2.82	113.81	110.58
3	5-N	7501	AMP	C4-C5-N7	2.82	113.81	110.58
3	6-N	7501	AMP	C4-C5-N7	2.82	113.81	110.58
3	7-N	7501	AMP	C4-C5-N7	2.82	113.81	110.58
3	8-N	7501	AMP	C4-C5-N7	2.82	113.81	110.58
3	9-N	7501	AMP	C4-C5-N7	2.82	113.81	110.58
3	10-N	7501	AMP	C4-C5-N7	2.82	113.81	110.58
3	1-H	7489	AMP	C4-C5-N7	2.80	113.79	110.58
3	2-H	7489	AMP	C4-C5-N7	2.80	113.79	110.58
3	3-H	7489	AMP	C4-C5-N7	2.80	113.79	110.58
3	4-H	7489	AMP	C4-C5-N7	2.80	113.79	110.58
3	5-H	7489	AMP	C4-C5-N7	2.80	113.79	110.58
3	6-H	7489	AMP	C4-C5-N7	2.80	113.79	110.58
3	7-H	7489	AMP	C4-C5-N7	2.80	113.79	110.58
3	8-H	7489	AMP	C4-C5-N7	2.80	113.79	110.58
3	9-H	7489	AMP	C4-C5-N7	2.80	113.79	110.58
3	10-H	7489	AMP	C4-C5-N7	2.80	113.79	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-X	7521	AMP	C4-C5-N7	2.80	113.78	110.58
3	2-X	7521	AMP	C4-C5-N7	2.80	113.78	110.58
3	3-X	7521	AMP	C4-C5-N7	2.80	113.78	110.58
3	4-X	7521	AMP	C4-C5-N7	2.80	113.78	110.58
3	5-X	7521	AMP	C4-C5-N7	2.80	113.78	110.58
3	6-X	7521	AMP	C4-C5-N7	2.80	113.78	110.58
3	7-X	7521	AMP	C4-C5-N7	2.80	113.78	110.58
3	8-X	7521	AMP	C4-C5-N7	2.80	113.78	110.58
3	9-X	7521	AMP	C4-C5-N7	2.80	113.78	110.58
3	10-X	7521	AMP	C4-C5-N7	2.80	113.78	110.58
3	1-E	7483	AMP	C4-C5-N7	2.80	113.78	110.58
3	2-E	7483	AMP	C4-C5-N7	2.80	113.78	110.58
3	3-E	7483	AMP	C4-C5-N7	2.80	113.78	110.58
3	4-E	7483	AMP	C4-C5-N7	2.80	113.78	110.58
3	5-E	7483	AMP	C4-C5-N7	2.80	113.78	110.58
3	6-E	7483	AMP	C4-C5-N7	2.80	113.78	110.58
3	7-E	7483	AMP	C4-C5-N7	2.80	113.78	110.58
3	8-E	7483	AMP	C4-C5-N7	2.80	113.78	110.58
3	9-E	7483	AMP	C4-C5-N7	2.80	113.78	110.58
3	10-E	7483	AMP	C4-C5-N7	2.80	113.78	110.58
3	1-J	7493	AMP	C4-C5-N7	2.80	113.78	110.58
3	2-J	7493	AMP	C4-C5-N7	2.80	113.78	110.58
3	3-J	7493	AMP	C4-C5-N7	2.80	113.78	110.58
3	4-J	7493	AMP	C4-C5-N7	2.80	113.78	110.58
3	5-J	7493	AMP	C4-C5-N7	2.80	113.78	110.58
3	6-J	7493	AMP	C4-C5-N7	2.80	113.78	110.58
3	7-J	7493	AMP	C4-C5-N7	2.80	113.78	110.58
3	8-J	7493	AMP	C4-C5-N7	2.80	113.78	110.58
3	9-J	7493	AMP	C4-C5-N7	2.80	113.78	110.58
3	10-J	7493	AMP	C4-C5-N7	2.80	113.78	110.58
3	1-K	7495	AMP	C4-C5-N7	2.78	113.76	110.58
3	2-K	7495	AMP	C4-C5-N7	2.78	113.76	110.58
3	3-K	7495	AMP	C4-C5-N7	2.78	113.76	110.58
3	4-K	7495	AMP	C4-C5-N7	2.78	113.76	110.58
3	5-K	7495	AMP	C4-C5-N7	2.78	113.76	110.58
3	6-K	7495	AMP	C4-C5-N7	2.78	113.76	110.58
3	7-K	7495	AMP	C4-C5-N7	2.78	113.76	110.58
3	8-K	7495	AMP	C4-C5-N7	2.78	113.76	110.58
3	9-K	7495	AMP	C4-C5-N7	2.78	113.76	110.58
3	10-K	7495	AMP	C4-C5-N7	2.78	113.76	110.58
3	1-M	7499	AMP	C4-C5-N7	2.78	113.76	110.58
3	2-M	7499	AMP	C4-C5-N7	2.78	113.76	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-M	7499	AMP	C4-C5-N7	2.78	113.76	110.58
3	4-M	7499	AMP	C4-C5-N7	2.78	113.76	110.58
3	5-M	7499	AMP	C4-C5-N7	2.78	113.76	110.58
3	6-M	7499	AMP	C4-C5-N7	2.78	113.76	110.58
3	7-M	7499	AMP	C4-C5-N7	2.78	113.76	110.58
3	8-M	7499	AMP	C4-C5-N7	2.78	113.76	110.58
3	9-M	7499	AMP	C4-C5-N7	2.78	113.76	110.58
3	10-M	7499	AMP	C4-C5-N7	2.78	113.76	110.58
3	1-A	7475	AMP	C4-C5-N7	2.78	113.76	110.58
3	2-A	7475	AMP	C4-C5-N7	2.78	113.76	110.58
3	3-A	7475	AMP	C4-C5-N7	2.78	113.76	110.58
3	4-A	7475	AMP	C4-C5-N7	2.78	113.76	110.58
3	5-A	7475	AMP	C4-C5-N7	2.78	113.76	110.58
3	6-A	7475	AMP	C4-C5-N7	2.78	113.76	110.58
3	7-A	7475	AMP	C4-C5-N7	2.78	113.76	110.58
3	8-A	7475	AMP	C4-C5-N7	2.78	113.76	110.58
3	9-A	7475	AMP	C4-C5-N7	2.78	113.76	110.58
3	10-A	7475	AMP	C4-C5-N7	2.78	113.76	110.58
3	1-D	7481	AMP	C4-C5-N7	2.77	113.75	110.58
3	2-D	7481	AMP	C4-C5-N7	2.77	113.75	110.58
3	3-D	7481	AMP	C4-C5-N7	2.77	113.75	110.58
3	4-D	7481	AMP	C4-C5-N7	2.77	113.75	110.58
3	5-D	7481	AMP	C4-C5-N7	2.77	113.75	110.58
3	6-D	7481	AMP	C4-C5-N7	2.77	113.75	110.58
3	7-D	7481	AMP	C4-C5-N7	2.77	113.75	110.58
3	8-D	7481	AMP	C4-C5-N7	2.77	113.75	110.58
3	9-D	7481	AMP	C4-C5-N7	2.77	113.75	110.58
3	10-D	7481	AMP	C4-C5-N7	2.77	113.75	110.58
3	1-R	7509	AMP	C4-C5-N7	2.77	113.75	110.58
3	2-R	7509	AMP	C4-C5-N7	2.77	113.75	110.58
3	3-R	7509	AMP	C4-C5-N7	2.77	113.75	110.58
3	4-R	7509	AMP	C4-C5-N7	2.77	113.75	110.58
3	5-R	7509	AMP	C4-C5-N7	2.77	113.75	110.58
3	6-R	7509	AMP	C4-C5-N7	2.77	113.75	110.58
3	7-R	7509	AMP	C4-C5-N7	2.77	113.75	110.58
3	8-R	7509	AMP	C4-C5-N7	2.77	113.75	110.58
3	9-R	7509	AMP	C4-C5-N7	2.77	113.75	110.58
3	10-R	7509	AMP	C4-C5-N7	2.77	113.75	110.58
3	1-O	7503	AMP	C4-C5-N7	2.77	113.75	110.58
3	2-O	7503	AMP	C4-C5-N7	2.77	113.75	110.58
3	3-O	7503	AMP	C4-C5-N7	2.77	113.75	110.58
3	4-O	7503	AMP	C4-C5-N7	2.77	113.75	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-O	7503	AMP	C4-C5-N7	2.77	113.75	110.58
3	6-O	7503	AMP	C4-C5-N7	2.77	113.75	110.58
3	7-O	7503	AMP	C4-C5-N7	2.77	113.75	110.58
3	8-O	7503	AMP	C4-C5-N7	2.77	113.75	110.58
3	9-O	7503	AMP	C4-C5-N7	2.77	113.75	110.58
3	10-O	7503	AMP	C4-C5-N7	2.77	113.75	110.58
3	1-T	7513	AMP	C4-C5-N7	2.77	113.75	110.58
3	2-T	7513	AMP	C4-C5-N7	2.77	113.75	110.58
3	3-T	7513	AMP	C4-C5-N7	2.77	113.75	110.58
3	4-T	7513	AMP	C4-C5-N7	2.77	113.75	110.58
3	5-T	7513	AMP	C4-C5-N7	2.77	113.75	110.58
3	6-T	7513	AMP	C4-C5-N7	2.77	113.75	110.58
3	7-T	7513	AMP	C4-C5-N7	2.77	113.75	110.58
3	8-T	7513	AMP	C4-C5-N7	2.77	113.75	110.58
3	9-T	7513	AMP	C4-C5-N7	2.77	113.75	110.58
3	10-T	7513	AMP	C4-C5-N7	2.77	113.75	110.58
3	1-V	7517	AMP	C4-C5-N7	2.77	113.75	110.58
3	2-V	7517	AMP	C4-C5-N7	2.77	113.75	110.58
3	3-V	7517	AMP	C4-C5-N7	2.77	113.75	110.58
3	4-V	7517	AMP	C4-C5-N7	2.77	113.75	110.58
3	5-V	7517	AMP	C4-C5-N7	2.77	113.75	110.58
3	6-V	7517	AMP	C4-C5-N7	2.77	113.75	110.58
3	7-V	7517	AMP	C4-C5-N7	2.77	113.75	110.58
3	8-V	7517	AMP	C4-C5-N7	2.77	113.75	110.58
3	9-V	7517	AMP	C4-C5-N7	2.77	113.75	110.58
3	10-V	7517	AMP	C4-C5-N7	2.77	113.75	110.58
3	1-C	7479	AMP	C4-C5-N7	2.77	113.75	110.58
3	2-C	7479	AMP	C4-C5-N7	2.77	113.75	110.58
3	3-C	7479	AMP	C4-C5-N7	2.77	113.75	110.58
3	4-C	7479	AMP	C4-C5-N7	2.77	113.75	110.58
3	5-C	7479	AMP	C4-C5-N7	2.77	113.75	110.58
3	6-C	7479	AMP	C4-C5-N7	2.77	113.75	110.58
3	7-C	7479	AMP	C4-C5-N7	2.77	113.75	110.58
3	8-C	7479	AMP	C4-C5-N7	2.77	113.75	110.58
3	9-C	7479	AMP	C4-C5-N7	2.77	113.75	110.58
3	10-C	7479	AMP	C4-C5-N7	2.77	113.75	110.58
3	1-G	7487	AMP	C4-C5-N7	2.77	113.75	110.58
3	2-G	7487	AMP	C4-C5-N7	2.77	113.75	110.58
3	3-G	7487	AMP	C4-C5-N7	2.77	113.75	110.58
3	4-G	7487	AMP	C4-C5-N7	2.77	113.75	110.58
3	5-G	7487	AMP	C4-C5-N7	2.77	113.75	110.58
3	6-G	7487	AMP	C4-C5-N7	2.77	113.75	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-G	7487	AMP	C4-C5-N7	2.77	113.75	110.58
3	8-G	7487	AMP	C4-C5-N7	2.77	113.75	110.58
3	9-G	7487	AMP	C4-C5-N7	2.77	113.75	110.58
3	10-G	7487	AMP	C4-C5-N7	2.77	113.75	110.58
3	1-W	7519	AMP	C4-C5-N7	2.77	113.75	110.58
3	2-W	7519	AMP	C4-C5-N7	2.77	113.75	110.58
3	3-W	7519	AMP	C4-C5-N7	2.77	113.75	110.58
3	4-W	7519	AMP	C4-C5-N7	2.77	113.75	110.58
3	5-W	7519	AMP	C4-C5-N7	2.77	113.75	110.58
3	6-W	7519	AMP	C4-C5-N7	2.77	113.75	110.58
3	7-W	7519	AMP	C4-C5-N7	2.77	113.75	110.58
3	8-W	7519	AMP	C4-C5-N7	2.77	113.75	110.58
3	9-W	7519	AMP	C4-C5-N7	2.77	113.75	110.58
3	10-W	7519	AMP	C4-C5-N7	2.77	113.75	110.58
3	1-L	7497	AMP	C4-C5-N7	2.76	113.74	110.58
3	2-L	7497	AMP	C4-C5-N7	2.76	113.74	110.58
3	3-L	7497	AMP	C4-C5-N7	2.76	113.74	110.58
3	4-L	7497	AMP	C4-C5-N7	2.76	113.74	110.58
3	5-L	7497	AMP	C4-C5-N7	2.76	113.74	110.58
3	6-L	7497	AMP	C4-C5-N7	2.76	113.74	110.58
3	7-L	7497	AMP	C4-C5-N7	2.76	113.74	110.58
3	8-L	7497	AMP	C4-C5-N7	2.76	113.74	110.58
3	9-L	7497	AMP	C4-C5-N7	2.76	113.74	110.58
3	10-L	7497	AMP	C4-C5-N7	2.76	113.74	110.58
3	1-Q	7507	AMP	C4-C5-N7	2.76	113.74	110.58
3	2-Q	7507	AMP	C4-C5-N7	2.76	113.74	110.58
3	3-Q	7507	AMP	C4-C5-N7	2.76	113.74	110.58
3	4-Q	7507	AMP	C4-C5-N7	2.76	113.74	110.58
3	5-Q	7507	AMP	C4-C5-N7	2.76	113.74	110.58
3	6-Q	7507	AMP	C4-C5-N7	2.76	113.74	110.58
3	7-Q	7507	AMP	C4-C5-N7	2.76	113.74	110.58
3	8-Q	7507	AMP	C4-C5-N7	2.76	113.74	110.58
3	9-Q	7507	AMP	C4-C5-N7	2.76	113.74	110.58
3	10-Q	7507	AMP	C4-C5-N7	2.76	113.74	110.58
3	1-P	7505	AMP	C4-C5-N7	2.76	113.74	110.58
3	2-P	7505	AMP	C4-C5-N7	2.76	113.74	110.58
3	3-P	7505	AMP	C4-C5-N7	2.76	113.74	110.58
3	4-P	7505	AMP	C4-C5-N7	2.76	113.74	110.58
3	5-P	7505	AMP	C4-C5-N7	2.76	113.74	110.58
3	6-P	7505	AMP	C4-C5-N7	2.76	113.74	110.58
3	7-P	7505	AMP	C4-C5-N7	2.76	113.74	110.58
3	8-P	7505	AMP	C4-C5-N7	2.76	113.74	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-P	7505	AMP	C4-C5-N7	2.76	113.74	110.58
3	10-P	7505	AMP	C4-C5-N7	2.76	113.74	110.58
3	1-U	7515	AMP	C4-C5-N7	2.76	113.74	110.58
3	2-U	7515	AMP	C4-C5-N7	2.76	113.74	110.58
3	3-U	7515	AMP	C4-C5-N7	2.76	113.74	110.58
3	4-U	7515	AMP	C4-C5-N7	2.76	113.74	110.58
3	5-U	7515	AMP	C4-C5-N7	2.76	113.74	110.58
3	6-U	7515	AMP	C4-C5-N7	2.76	113.74	110.58
3	7-U	7515	AMP	C4-C5-N7	2.76	113.74	110.58
3	8-U	7515	AMP	C4-C5-N7	2.76	113.74	110.58
3	9-U	7515	AMP	C4-C5-N7	2.76	113.74	110.58
3	10-U	7515	AMP	C4-C5-N7	2.76	113.74	110.58
3	1-I	7491	AMP	C4-C5-N7	2.75	113.73	110.58
3	2-I	7491	AMP	C4-C5-N7	2.75	113.73	110.58
3	3-I	7491	AMP	C4-C5-N7	2.75	113.73	110.58
3	4-I	7491	AMP	C4-C5-N7	2.75	113.73	110.58
3	5-I	7491	AMP	C4-C5-N7	2.75	113.73	110.58
3	6-I	7491	AMP	C4-C5-N7	2.75	113.73	110.58
3	7-I	7491	AMP	C4-C5-N7	2.75	113.73	110.58
3	8-I	7491	AMP	C4-C5-N7	2.75	113.73	110.58
3	9-I	7491	AMP	C4-C5-N7	2.75	113.73	110.58
3	10-I	7491	AMP	C4-C5-N7	2.75	113.73	110.58
3	1-F	7485	AMP	C4-C5-N7	2.75	113.73	110.58
3	2-F	7485	AMP	C4-C5-N7	2.75	113.73	110.58
3	3-F	7485	AMP	C4-C5-N7	2.75	113.73	110.58
3	4-F	7485	AMP	C4-C5-N7	2.75	113.73	110.58
3	5-F	7485	AMP	C4-C5-N7	2.75	113.73	110.58
3	6-F	7485	AMP	C4-C5-N7	2.75	113.73	110.58
3	7-F	7485	AMP	C4-C5-N7	2.75	113.73	110.58
3	8-F	7485	AMP	C4-C5-N7	2.75	113.73	110.58
3	9-F	7485	AMP	C4-C5-N7	2.75	113.73	110.58
3	10-F	7485	AMP	C4-C5-N7	2.75	113.73	110.58
3	1-B	7477	AMP	C4-C5-N7	2.75	113.73	110.58
3	2-B	7477	AMP	C4-C5-N7	2.75	113.73	110.58
3	3-B	7477	AMP	C4-C5-N7	2.75	113.73	110.58
3	4-B	7477	AMP	C4-C5-N7	2.75	113.73	110.58
3	5-B	7477	AMP	C4-C5-N7	2.75	113.73	110.58
3	6-B	7477	AMP	C4-C5-N7	2.75	113.73	110.58
3	7-B	7477	AMP	C4-C5-N7	2.75	113.73	110.58
3	8-B	7477	AMP	C4-C5-N7	2.75	113.73	110.58
3	9-B	7477	AMP	C4-C5-N7	2.75	113.73	110.58
3	10-B	7477	AMP	C4-C5-N7	2.75	113.73	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-S	7511	AMP	C4-C5-N7	2.74	113.72	110.58
3	2-S	7511	AMP	C4-C5-N7	2.74	113.72	110.58
3	3-S	7511	AMP	C4-C5-N7	2.74	113.72	110.58
3	4-S	7511	AMP	C4-C5-N7	2.74	113.72	110.58
3	5-S	7511	AMP	C4-C5-N7	2.74	113.72	110.58
3	6-S	7511	AMP	C4-C5-N7	2.74	113.72	110.58
3	7-S	7511	AMP	C4-C5-N7	2.74	113.72	110.58
3	8-S	7511	AMP	C4-C5-N7	2.74	113.72	110.58
3	9-S	7511	AMP	C4-C5-N7	2.74	113.72	110.58
3	10-S	7511	AMP	C4-C5-N7	2.74	113.72	110.58
4	1-K	7496	CIT	O4-C5-O3	-2.56	116.75	123.33
4	2-K	7496	CIT	O4-C5-O3	-2.56	116.75	123.33
4	3-K	7496	CIT	O4-C5-O3	-2.56	116.75	123.33
4	4-K	7496	CIT	O4-C5-O3	-2.56	116.75	123.33
4	5-K	7496	CIT	O4-C5-O3	-2.56	116.75	123.33
4	6-K	7496	CIT	O4-C5-O3	-2.56	116.75	123.33
4	7-K	7496	CIT	O4-C5-O3	-2.56	116.75	123.33
4	8-K	7496	CIT	O4-C5-O3	-2.56	116.75	123.33
4	9-K	7496	CIT	O4-C5-O3	-2.56	116.75	123.33
4	10-K	7496	CIT	O4-C5-O3	-2.56	116.75	123.33
4	1-Q	7508	CIT	O4-C5-O3	-2.55	116.77	123.33
4	2-Q	7508	CIT	O4-C5-O3	-2.55	116.77	123.33
4	3-Q	7508	CIT	O4-C5-O3	-2.55	116.77	123.33
4	4-Q	7508	CIT	O4-C5-O3	-2.55	116.77	123.33
4	5-Q	7508	CIT	O4-C5-O3	-2.55	116.77	123.33
4	6-Q	7508	CIT	O4-C5-O3	-2.55	116.77	123.33
4	7-Q	7508	CIT	O4-C5-O3	-2.55	116.77	123.33
4	8-Q	7508	CIT	O4-C5-O3	-2.55	116.77	123.33
4	9-Q	7508	CIT	O4-C5-O3	-2.55	116.77	123.33
4	10-Q	7508	CIT	O4-C5-O3	-2.55	116.77	123.33
4	1-E	7484	CIT	O4-C5-O3	-2.55	116.77	123.33
4	2-E	7484	CIT	O4-C5-O3	-2.55	116.77	123.33
4	3-E	7484	CIT	O4-C5-O3	-2.55	116.77	123.33
4	4-E	7484	CIT	O4-C5-O3	-2.55	116.77	123.33
4	5-E	7484	CIT	O4-C5-O3	-2.55	116.77	123.33
4	6-E	7484	CIT	O4-C5-O3	-2.55	116.77	123.33
4	7-E	7484	CIT	O4-C5-O3	-2.55	116.77	123.33
4	8-E	7484	CIT	O4-C5-O3	-2.55	116.77	123.33
4	9-E	7484	CIT	O4-C5-O3	-2.55	116.77	123.33
4	10-E	7484	CIT	O4-C5-O3	-2.55	116.77	123.33
4	1-M	7500	CIT	O4-C5-O3	-2.55	116.77	123.33
4	2-M	7500	CIT	O4-C5-O3	-2.55	116.77	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-M	7500	CIT	O4-C5-O3	-2.55	116.77	123.33
4	4-M	7500	CIT	O4-C5-O3	-2.55	116.77	123.33
4	5-M	7500	CIT	O4-C5-O3	-2.55	116.77	123.33
4	6-M	7500	CIT	O4-C5-O3	-2.55	116.77	123.33
4	7-M	7500	CIT	O4-C5-O3	-2.55	116.77	123.33
4	8-M	7500	CIT	O4-C5-O3	-2.55	116.77	123.33
4	9-M	7500	CIT	O4-C5-O3	-2.55	116.77	123.33
4	10-M	7500	CIT	O4-C5-O3	-2.55	116.77	123.33
4	1-B	7478	CIT	O4-C5-O3	-2.55	116.77	123.33
4	2-B	7478	CIT	O4-C5-O3	-2.55	116.77	123.33
4	3-B	7478	CIT	O4-C5-O3	-2.55	116.77	123.33
4	4-B	7478	CIT	O4-C5-O3	-2.55	116.77	123.33
4	5-B	7478	CIT	O4-C5-O3	-2.55	116.77	123.33
4	6-B	7478	CIT	O4-C5-O3	-2.55	116.77	123.33
4	7-B	7478	CIT	O4-C5-O3	-2.55	116.77	123.33
4	8-B	7478	CIT	O4-C5-O3	-2.55	116.77	123.33
4	9-B	7478	CIT	O4-C5-O3	-2.55	116.77	123.33
4	10-B	7478	CIT	O4-C5-O3	-2.55	116.77	123.33
4	1-S	7512	CIT	O4-C5-O3	-2.55	116.77	123.33
4	2-S	7512	CIT	O4-C5-O3	-2.55	116.77	123.33
4	3-S	7512	CIT	O4-C5-O3	-2.55	116.77	123.33
4	4-S	7512	CIT	O4-C5-O3	-2.55	116.77	123.33
4	5-S	7512	CIT	O4-C5-O3	-2.55	116.77	123.33
4	6-S	7512	CIT	O4-C5-O3	-2.55	116.77	123.33
4	7-S	7512	CIT	O4-C5-O3	-2.55	116.77	123.33
4	8-S	7512	CIT	O4-C5-O3	-2.55	116.77	123.33
4	9-S	7512	CIT	O4-C5-O3	-2.55	116.77	123.33
4	10-S	7512	CIT	O4-C5-O3	-2.55	116.77	123.33
4	1-L	7498	CIT	O4-C5-O3	-2.55	116.78	123.33
4	2-L	7498	CIT	O4-C5-O3	-2.55	116.78	123.33
4	3-L	7498	CIT	O4-C5-O3	-2.55	116.78	123.33
4	4-L	7498	CIT	O4-C5-O3	-2.55	116.78	123.33
4	5-L	7498	CIT	O4-C5-O3	-2.55	116.78	123.33
4	6-L	7498	CIT	O4-C5-O3	-2.55	116.78	123.33
4	7-L	7498	CIT	O4-C5-O3	-2.55	116.78	123.33
4	8-L	7498	CIT	O4-C5-O3	-2.55	116.78	123.33
4	9-L	7498	CIT	O4-C5-O3	-2.55	116.78	123.33
4	10-L	7498	CIT	O4-C5-O3	-2.55	116.78	123.33
4	1-O	7504	CIT	O4-C5-O3	-2.55	116.78	123.33
4	2-O	7504	CIT	O4-C5-O3	-2.55	116.78	123.33
4	3-O	7504	CIT	O4-C5-O3	-2.55	116.78	123.33
4	4-O	7504	CIT	O4-C5-O3	-2.55	116.78	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5-O	7504	CIT	O4-C5-O3	-2.55	116.78	123.33
4	6-O	7504	CIT	O4-C5-O3	-2.55	116.78	123.33
4	7-O	7504	CIT	O4-C5-O3	-2.55	116.78	123.33
4	8-O	7504	CIT	O4-C5-O3	-2.55	116.78	123.33
4	9-O	7504	CIT	O4-C5-O3	-2.55	116.78	123.33
4	10-O	7504	CIT	O4-C5-O3	-2.55	116.78	123.33
4	1-I	7492	CIT	O4-C5-O3	-2.55	116.78	123.33
4	2-I	7492	CIT	O4-C5-O3	-2.55	116.78	123.33
4	3-I	7492	CIT	O4-C5-O3	-2.55	116.78	123.33
4	4-I	7492	CIT	O4-C5-O3	-2.55	116.78	123.33
4	5-I	7492	CIT	O4-C5-O3	-2.55	116.78	123.33
4	6-I	7492	CIT	O4-C5-O3	-2.55	116.78	123.33
4	7-I	7492	CIT	O4-C5-O3	-2.55	116.78	123.33
4	8-I	7492	CIT	O4-C5-O3	-2.55	116.78	123.33
4	9-I	7492	CIT	O4-C5-O3	-2.55	116.78	123.33
4	10-I	7492	CIT	O4-C5-O3	-2.55	116.78	123.33
4	1-W	7520	CIT	O4-C5-O3	-2.55	116.78	123.33
4	2-W	7520	CIT	O4-C5-O3	-2.55	116.78	123.33
4	3-W	7520	CIT	O4-C5-O3	-2.55	116.78	123.33
4	4-W	7520	CIT	O4-C5-O3	-2.55	116.78	123.33
4	5-W	7520	CIT	O4-C5-O3	-2.55	116.78	123.33
4	6-W	7520	CIT	O4-C5-O3	-2.55	116.78	123.33
4	7-W	7520	CIT	O4-C5-O3	-2.55	116.78	123.33
4	8-W	7520	CIT	O4-C5-O3	-2.55	116.78	123.33
4	9-W	7520	CIT	O4-C5-O3	-2.55	116.78	123.33
4	10-W	7520	CIT	O4-C5-O3	-2.55	116.78	123.33
4	1-N	7502	CIT	O4-C5-O3	-2.55	116.78	123.33
4	2-N	7502	CIT	O4-C5-O3	-2.55	116.78	123.33
4	3-N	7502	CIT	O4-C5-O3	-2.55	116.78	123.33
4	4-N	7502	CIT	O4-C5-O3	-2.55	116.78	123.33
4	5-N	7502	CIT	O4-C5-O3	-2.55	116.78	123.33
4	6-N	7502	CIT	O4-C5-O3	-2.55	116.78	123.33
4	7-N	7502	CIT	O4-C5-O3	-2.55	116.78	123.33
4	8-N	7502	CIT	O4-C5-O3	-2.55	116.78	123.33
4	9-N	7502	CIT	O4-C5-O3	-2.55	116.78	123.33
4	10-N	7502	CIT	O4-C5-O3	-2.55	116.78	123.33
4	1-H	7490	CIT	O4-C5-O3	-2.55	116.78	123.33
4	2-H	7490	CIT	O4-C5-O3	-2.55	116.78	123.33
4	3-H	7490	CIT	O4-C5-O3	-2.55	116.78	123.33
4	4-H	7490	CIT	O4-C5-O3	-2.55	116.78	123.33
4	5-H	7490	CIT	O4-C5-O3	-2.55	116.78	123.33
4	6-H	7490	CIT	O4-C5-O3	-2.55	116.78	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7-H	7490	CIT	O4-C5-O3	-2.55	116.78	123.33
4	8-H	7490	CIT	O4-C5-O3	-2.55	116.78	123.33
4	9-H	7490	CIT	O4-C5-O3	-2.55	116.78	123.33
4	10-H	7490	CIT	O4-C5-O3	-2.55	116.78	123.33
4	1-P	7506	CIT	O4-C5-O3	-2.55	116.78	123.33
4	2-P	7506	CIT	O4-C5-O3	-2.55	116.78	123.33
4	3-P	7506	CIT	O4-C5-O3	-2.55	116.78	123.33
4	4-P	7506	CIT	O4-C5-O3	-2.55	116.78	123.33
4	5-P	7506	CIT	O4-C5-O3	-2.55	116.78	123.33
4	6-P	7506	CIT	O4-C5-O3	-2.55	116.78	123.33
4	7-P	7506	CIT	O4-C5-O3	-2.55	116.78	123.33
4	8-P	7506	CIT	O4-C5-O3	-2.55	116.78	123.33
4	9-P	7506	CIT	O4-C5-O3	-2.55	116.78	123.33
4	10-P	7506	CIT	O4-C5-O3	-2.55	116.78	123.33
4	1-V	7518	CIT	O4-C5-O3	-2.55	116.78	123.33
4	2-V	7518	CIT	O4-C5-O3	-2.55	116.78	123.33
4	3-V	7518	CIT	O4-C5-O3	-2.55	116.78	123.33
4	4-V	7518	CIT	O4-C5-O3	-2.55	116.78	123.33
4	5-V	7518	CIT	O4-C5-O3	-2.55	116.78	123.33
4	6-V	7518	CIT	O4-C5-O3	-2.55	116.78	123.33
4	7-V	7518	CIT	O4-C5-O3	-2.55	116.78	123.33
4	8-V	7518	CIT	O4-C5-O3	-2.55	116.78	123.33
4	9-V	7518	CIT	O4-C5-O3	-2.55	116.78	123.33
4	10-V	7518	CIT	O4-C5-O3	-2.55	116.78	123.33
4	1-D	7482	CIT	O4-C5-O3	-2.54	116.79	123.33
4	2-D	7482	CIT	O4-C5-O3	-2.54	116.79	123.33
4	3-D	7482	CIT	O4-C5-O3	-2.54	116.79	123.33
4	4-D	7482	CIT	O4-C5-O3	-2.54	116.79	123.33
4	5-D	7482	CIT	O4-C5-O3	-2.54	116.79	123.33
4	6-D	7482	CIT	O4-C5-O3	-2.54	116.79	123.33
4	7-D	7482	CIT	O4-C5-O3	-2.54	116.79	123.33
4	8-D	7482	CIT	O4-C5-O3	-2.54	116.79	123.33
4	9-D	7482	CIT	O4-C5-O3	-2.54	116.79	123.33
4	10-D	7482	CIT	O4-C5-O3	-2.54	116.79	123.33
4	1-A	7476	CIT	O4-C5-O3	-2.54	116.79	123.33
4	2-A	7476	CIT	O4-C5-O3	-2.54	116.79	123.33
4	3-A	7476	CIT	O4-C5-O3	-2.54	116.79	123.33
4	4-A	7476	CIT	O4-C5-O3	-2.54	116.79	123.33
4	5-A	7476	CIT	O4-C5-O3	-2.54	116.79	123.33
4	6-A	7476	CIT	O4-C5-O3	-2.54	116.79	123.33
4	7-A	7476	CIT	O4-C5-O3	-2.54	116.79	123.33
4	8-A	7476	CIT	O4-C5-O3	-2.54	116.79	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9-A	7476	CIT	O4-C5-O3	-2.54	116.79	123.33
4	10-A	7476	CIT	O4-C5-O3	-2.54	116.79	123.33
4	1-J	7494	CIT	O4-C5-O3	-2.54	116.79	123.33
4	2-J	7494	CIT	O4-C5-O3	-2.54	116.79	123.33
4	3-J	7494	CIT	O4-C5-O3	-2.54	116.79	123.33
4	4-J	7494	CIT	O4-C5-O3	-2.54	116.79	123.33
4	5-J	7494	CIT	O4-C5-O3	-2.54	116.79	123.33
4	6-J	7494	CIT	O4-C5-O3	-2.54	116.79	123.33
4	7-J	7494	CIT	O4-C5-O3	-2.54	116.79	123.33
4	8-J	7494	CIT	O4-C5-O3	-2.54	116.79	123.33
4	9-J	7494	CIT	O4-C5-O3	-2.54	116.79	123.33
4	10-J	7494	CIT	O4-C5-O3	-2.54	116.79	123.33
4	1-U	7516	CIT	O4-C5-O3	-2.54	116.80	123.33
4	2-U	7516	CIT	O4-C5-O3	-2.54	116.80	123.33
4	3-U	7516	CIT	O4-C5-O3	-2.54	116.80	123.33
4	4-U	7516	CIT	O4-C5-O3	-2.54	116.80	123.33
4	5-U	7516	CIT	O4-C5-O3	-2.54	116.80	123.33
4	6-U	7516	CIT	O4-C5-O3	-2.54	116.80	123.33
4	7-U	7516	CIT	O4-C5-O3	-2.54	116.80	123.33
4	8-U	7516	CIT	O4-C5-O3	-2.54	116.80	123.33
4	9-U	7516	CIT	O4-C5-O3	-2.54	116.80	123.33
4	10-U	7516	CIT	O4-C5-O3	-2.54	116.80	123.33
4	1-X	7522	CIT	O4-C5-O3	-2.54	116.80	123.33
4	2-X	7522	CIT	O4-C5-O3	-2.54	116.80	123.33
4	3-X	7522	CIT	O4-C5-O3	-2.54	116.80	123.33
4	4-X	7522	CIT	O4-C5-O3	-2.54	116.80	123.33
4	5-X	7522	CIT	O4-C5-O3	-2.54	116.80	123.33
4	6-X	7522	CIT	O4-C5-O3	-2.54	116.80	123.33
4	7-X	7522	CIT	O4-C5-O3	-2.54	116.80	123.33
4	8-X	7522	CIT	O4-C5-O3	-2.54	116.80	123.33
4	9-X	7522	CIT	O4-C5-O3	-2.54	116.80	123.33
4	10-X	7522	CIT	O4-C5-O3	-2.54	116.80	123.33
4	1-G	7488	CIT	O4-C5-O3	-2.54	116.81	123.33
4	2-G	7488	CIT	O4-C5-O3	-2.54	116.81	123.33
4	3-G	7488	CIT	O4-C5-O3	-2.54	116.81	123.33
4	4-G	7488	CIT	O4-C5-O3	-2.54	116.81	123.33
4	5-G	7488	CIT	O4-C5-O3	-2.54	116.81	123.33
4	6-G	7488	CIT	O4-C5-O3	-2.54	116.81	123.33
4	7-G	7488	CIT	O4-C5-O3	-2.54	116.81	123.33
4	8-G	7488	CIT	O4-C5-O3	-2.54	116.81	123.33
4	9-G	7488	CIT	O4-C5-O3	-2.54	116.81	123.33
4	10-G	7488	CIT	O4-C5-O3	-2.54	116.81	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-T	7514	CIT	O4-C5-O3	-2.53	116.82	123.33
4	2-T	7514	CIT	O4-C5-O3	-2.53	116.82	123.33
4	3-T	7514	CIT	O4-C5-O3	-2.53	116.82	123.33
4	4-T	7514	CIT	O4-C5-O3	-2.53	116.82	123.33
4	5-T	7514	CIT	O4-C5-O3	-2.53	116.82	123.33
4	6-T	7514	CIT	O4-C5-O3	-2.53	116.82	123.33
4	7-T	7514	CIT	O4-C5-O3	-2.53	116.82	123.33
4	8-T	7514	CIT	O4-C5-O3	-2.53	116.82	123.33
4	9-T	7514	CIT	O4-C5-O3	-2.53	116.82	123.33
4	10-T	7514	CIT	O4-C5-O3	-2.53	116.82	123.33
4	1-F	7486	CIT	O4-C5-O3	-2.53	116.82	123.33
4	2-F	7486	CIT	O4-C5-O3	-2.53	116.82	123.33
4	3-F	7486	CIT	O4-C5-O3	-2.53	116.82	123.33
4	4-F	7486	CIT	O4-C5-O3	-2.53	116.82	123.33
4	5-F	7486	CIT	O4-C5-O3	-2.53	116.82	123.33
4	6-F	7486	CIT	O4-C5-O3	-2.53	116.82	123.33
4	7-F	7486	CIT	O4-C5-O3	-2.53	116.82	123.33
4	8-F	7486	CIT	O4-C5-O3	-2.53	116.82	123.33
4	9-F	7486	CIT	O4-C5-O3	-2.53	116.82	123.33
4	10-F	7486	CIT	O4-C5-O3	-2.53	116.82	123.33
4	1-R	7510	CIT	O4-C5-O3	-2.53	116.83	123.33
4	2-R	7510	CIT	O4-C5-O3	-2.53	116.83	123.33
4	3-R	7510	CIT	O4-C5-O3	-2.53	116.83	123.33
4	4-R	7510	CIT	O4-C5-O3	-2.53	116.83	123.33
4	5-R	7510	CIT	O4-C5-O3	-2.53	116.83	123.33
4	6-R	7510	CIT	O4-C5-O3	-2.53	116.83	123.33
4	7-R	7510	CIT	O4-C5-O3	-2.53	116.83	123.33
4	8-R	7510	CIT	O4-C5-O3	-2.53	116.83	123.33
4	9-R	7510	CIT	O4-C5-O3	-2.53	116.83	123.33
4	10-R	7510	CIT	O4-C5-O3	-2.53	116.83	123.33
4	1-H	7490	CIT	O5-C6-C3	-2.53	117.20	122.09
4	2-H	7490	CIT	O5-C6-C3	-2.53	117.20	122.09
4	3-H	7490	CIT	O5-C6-C3	-2.53	117.20	122.09
4	4-H	7490	CIT	O5-C6-C3	-2.53	117.20	122.09
4	5-H	7490	CIT	O5-C6-C3	-2.53	117.20	122.09
4	6-H	7490	CIT	O5-C6-C3	-2.53	117.20	122.09
4	7-H	7490	CIT	O5-C6-C3	-2.53	117.20	122.09
4	8-H	7490	CIT	O5-C6-C3	-2.53	117.20	122.09
4	9-H	7490	CIT	O5-C6-C3	-2.53	117.20	122.09
4	10-H	7490	CIT	O5-C6-C3	-2.53	117.20	122.09
4	1-X	7522	CIT	O5-C6-C3	-2.52	117.20	122.09
4	2-X	7522	CIT	O5-C6-C3	-2.52	117.20	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-X	7522	CIT	O5-C6-C3	-2.52	117.20	122.09
4	4-X	7522	CIT	O5-C6-C3	-2.52	117.20	122.09
4	5-X	7522	CIT	O5-C6-C3	-2.52	117.20	122.09
4	6-X	7522	CIT	O5-C6-C3	-2.52	117.20	122.09
4	7-X	7522	CIT	O5-C6-C3	-2.52	117.20	122.09
4	8-X	7522	CIT	O5-C6-C3	-2.52	117.20	122.09
4	9-X	7522	CIT	O5-C6-C3	-2.52	117.20	122.09
4	10-X	7522	CIT	O5-C6-C3	-2.52	117.20	122.09
4	1-C	7480	CIT	O4-C5-O3	-2.52	116.84	123.33
4	2-C	7480	CIT	O4-C5-O3	-2.52	116.84	123.33
4	3-C	7480	CIT	O4-C5-O3	-2.52	116.84	123.33
4	4-C	7480	CIT	O4-C5-O3	-2.52	116.84	123.33
4	5-C	7480	CIT	O4-C5-O3	-2.52	116.84	123.33
4	6-C	7480	CIT	O4-C5-O3	-2.52	116.84	123.33
4	7-C	7480	CIT	O4-C5-O3	-2.52	116.84	123.33
4	8-C	7480	CIT	O4-C5-O3	-2.52	116.84	123.33
4	9-C	7480	CIT	O4-C5-O3	-2.52	116.84	123.33
4	10-C	7480	CIT	O4-C5-O3	-2.52	116.84	123.33
4	1-D	7482	CIT	O5-C6-C3	-2.52	117.20	122.09
4	2-D	7482	CIT	O5-C6-C3	-2.52	117.20	122.09
4	3-D	7482	CIT	O5-C6-C3	-2.52	117.20	122.09
4	4-D	7482	CIT	O5-C6-C3	-2.52	117.20	122.09
4	5-D	7482	CIT	O5-C6-C3	-2.52	117.20	122.09
4	6-D	7482	CIT	O5-C6-C3	-2.52	117.20	122.09
4	7-D	7482	CIT	O5-C6-C3	-2.52	117.20	122.09
4	8-D	7482	CIT	O5-C6-C3	-2.52	117.20	122.09
4	9-D	7482	CIT	O5-C6-C3	-2.52	117.20	122.09
4	10-D	7482	CIT	O5-C6-C3	-2.52	117.20	122.09
4	1-I	7492	CIT	O5-C6-C3	-2.52	117.21	122.09
4	2-I	7492	CIT	O5-C6-C3	-2.52	117.21	122.09
4	3-I	7492	CIT	O5-C6-C3	-2.52	117.21	122.09
4	4-I	7492	CIT	O5-C6-C3	-2.52	117.21	122.09
4	5-I	7492	CIT	O5-C6-C3	-2.52	117.21	122.09
4	6-I	7492	CIT	O5-C6-C3	-2.52	117.21	122.09
4	7-I	7492	CIT	O5-C6-C3	-2.52	117.21	122.09
4	8-I	7492	CIT	O5-C6-C3	-2.52	117.21	122.09
4	9-I	7492	CIT	O5-C6-C3	-2.52	117.21	122.09
4	10-I	7492	CIT	O5-C6-C3	-2.52	117.21	122.09
4	1-R	7510	CIT	O5-C6-C3	-2.52	117.22	122.09
4	2-R	7510	CIT	O5-C6-C3	-2.52	117.22	122.09
4	3-R	7510	CIT	O5-C6-C3	-2.52	117.22	122.09
4	4-R	7510	CIT	O5-C6-C3	-2.52	117.22	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5-R	7510	CIT	O5-C6-C3	-2.52	117.22	122.09
4	6-R	7510	CIT	O5-C6-C3	-2.52	117.22	122.09
4	7-R	7510	CIT	O5-C6-C3	-2.52	117.22	122.09
4	8-R	7510	CIT	O5-C6-C3	-2.52	117.22	122.09
4	9-R	7510	CIT	O5-C6-C3	-2.52	117.22	122.09
4	10-R	7510	CIT	O5-C6-C3	-2.52	117.22	122.09
4	1-M	7500	CIT	O5-C6-C3	-2.51	117.22	122.09
4	2-M	7500	CIT	O5-C6-C3	-2.51	117.22	122.09
4	3-M	7500	CIT	O5-C6-C3	-2.51	117.22	122.09
4	4-M	7500	CIT	O5-C6-C3	-2.51	117.22	122.09
4	5-M	7500	CIT	O5-C6-C3	-2.51	117.22	122.09
4	6-M	7500	CIT	O5-C6-C3	-2.51	117.22	122.09
4	7-M	7500	CIT	O5-C6-C3	-2.51	117.22	122.09
4	8-M	7500	CIT	O5-C6-C3	-2.51	117.22	122.09
4	9-M	7500	CIT	O5-C6-C3	-2.51	117.22	122.09
4	10-M	7500	CIT	O5-C6-C3	-2.51	117.22	122.09
4	1-E	7484	CIT	O5-C6-C3	-2.51	117.22	122.09
4	2-E	7484	CIT	O5-C6-C3	-2.51	117.22	122.09
4	3-E	7484	CIT	O5-C6-C3	-2.51	117.22	122.09
4	4-E	7484	CIT	O5-C6-C3	-2.51	117.22	122.09
4	5-E	7484	CIT	O5-C6-C3	-2.51	117.22	122.09
4	6-E	7484	CIT	O5-C6-C3	-2.51	117.22	122.09
4	7-E	7484	CIT	O5-C6-C3	-2.51	117.22	122.09
4	8-E	7484	CIT	O5-C6-C3	-2.51	117.22	122.09
4	9-E	7484	CIT	O5-C6-C3	-2.51	117.22	122.09
4	10-E	7484	CIT	O5-C6-C3	-2.51	117.22	122.09
4	1-U	7516	CIT	O5-C6-C3	-2.51	117.23	122.09
4	2-U	7516	CIT	O5-C6-C3	-2.51	117.23	122.09
4	3-U	7516	CIT	O5-C6-C3	-2.51	117.23	122.09
4	4-U	7516	CIT	O5-C6-C3	-2.51	117.23	122.09
4	5-U	7516	CIT	O5-C6-C3	-2.51	117.23	122.09
4	6-U	7516	CIT	O5-C6-C3	-2.51	117.23	122.09
4	7-U	7516	CIT	O5-C6-C3	-2.51	117.23	122.09
4	8-U	7516	CIT	O5-C6-C3	-2.51	117.23	122.09
4	9-U	7516	CIT	O5-C6-C3	-2.51	117.23	122.09
4	10-U	7516	CIT	O5-C6-C3	-2.51	117.23	122.09
4	1-S	7512	CIT	O5-C6-C3	-2.51	117.24	122.09
4	2-S	7512	CIT	O5-C6-C3	-2.51	117.24	122.09
4	3-S	7512	CIT	O5-C6-C3	-2.51	117.24	122.09
4	4-S	7512	CIT	O5-C6-C3	-2.51	117.24	122.09
4	5-S	7512	CIT	O5-C6-C3	-2.51	117.24	122.09
4	6-S	7512	CIT	O5-C6-C3	-2.51	117.24	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7-S	7512	CIT	O5-C6-C3	-2.51	117.24	122.09
4	8-S	7512	CIT	O5-C6-C3	-2.51	117.24	122.09
4	9-S	7512	CIT	O5-C6-C3	-2.51	117.24	122.09
4	10-S	7512	CIT	O5-C6-C3	-2.51	117.24	122.09
4	1-Q	7508	CIT	O5-C6-C3	-2.50	117.24	122.09
4	2-Q	7508	CIT	O5-C6-C3	-2.50	117.24	122.09
4	3-Q	7508	CIT	O5-C6-C3	-2.50	117.24	122.09
4	4-Q	7508	CIT	O5-C6-C3	-2.50	117.24	122.09
4	5-Q	7508	CIT	O5-C6-C3	-2.50	117.24	122.09
4	6-Q	7508	CIT	O5-C6-C3	-2.50	117.24	122.09
4	7-Q	7508	CIT	O5-C6-C3	-2.50	117.24	122.09
4	8-Q	7508	CIT	O5-C6-C3	-2.50	117.24	122.09
4	9-Q	7508	CIT	O5-C6-C3	-2.50	117.24	122.09
4	10-Q	7508	CIT	O5-C6-C3	-2.50	117.24	122.09
4	1-G	7488	CIT	O5-C6-C3	-2.50	117.24	122.09
4	2-G	7488	CIT	O5-C6-C3	-2.50	117.24	122.09
4	3-G	7488	CIT	O5-C6-C3	-2.50	117.24	122.09
4	4-G	7488	CIT	O5-C6-C3	-2.50	117.24	122.09
4	5-G	7488	CIT	O5-C6-C3	-2.50	117.24	122.09
4	6-G	7488	CIT	O5-C6-C3	-2.50	117.24	122.09
4	7-G	7488	CIT	O5-C6-C3	-2.50	117.24	122.09
4	8-G	7488	CIT	O5-C6-C3	-2.50	117.24	122.09
4	9-G	7488	CIT	O5-C6-C3	-2.50	117.24	122.09
4	10-G	7488	CIT	O5-C6-C3	-2.50	117.24	122.09
4	1-J	7494	CIT	O5-C6-C3	-2.50	117.24	122.09
4	2-J	7494	CIT	O5-C6-C3	-2.50	117.24	122.09
4	3-J	7494	CIT	O5-C6-C3	-2.50	117.24	122.09
4	4-J	7494	CIT	O5-C6-C3	-2.50	117.24	122.09
4	5-J	7494	CIT	O5-C6-C3	-2.50	117.24	122.09
4	6-J	7494	CIT	O5-C6-C3	-2.50	117.24	122.09
4	7-J	7494	CIT	O5-C6-C3	-2.50	117.24	122.09
4	8-J	7494	CIT	O5-C6-C3	-2.50	117.24	122.09
4	9-J	7494	CIT	O5-C6-C3	-2.50	117.24	122.09
4	10-J	7494	CIT	O5-C6-C3	-2.50	117.24	122.09
4	1-A	7476	CIT	O5-C6-C3	-2.50	117.25	122.09
4	2-A	7476	CIT	O5-C6-C3	-2.50	117.25	122.09
4	3-A	7476	CIT	O5-C6-C3	-2.50	117.25	122.09
4	4-A	7476	CIT	O5-C6-C3	-2.50	117.25	122.09
4	5-A	7476	CIT	O5-C6-C3	-2.50	117.25	122.09
4	6-A	7476	CIT	O5-C6-C3	-2.50	117.25	122.09
4	7-A	7476	CIT	O5-C6-C3	-2.50	117.25	122.09
4	8-A	7476	CIT	O5-C6-C3	-2.50	117.25	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9-A	7476	CIT	O5-C6-C3	-2.50	117.25	122.09
4	10-A	7476	CIT	O5-C6-C3	-2.50	117.25	122.09
4	1-L	7498	CIT	O5-C6-C3	-2.50	117.25	122.09
4	2-L	7498	CIT	O5-C6-C3	-2.50	117.25	122.09
4	3-L	7498	CIT	O5-C6-C3	-2.50	117.25	122.09
4	4-L	7498	CIT	O5-C6-C3	-2.50	117.25	122.09
4	5-L	7498	CIT	O5-C6-C3	-2.50	117.25	122.09
4	6-L	7498	CIT	O5-C6-C3	-2.50	117.25	122.09
4	7-L	7498	CIT	O5-C6-C3	-2.50	117.25	122.09
4	8-L	7498	CIT	O5-C6-C3	-2.50	117.25	122.09
4	9-L	7498	CIT	O5-C6-C3	-2.50	117.25	122.09
4	10-L	7498	CIT	O5-C6-C3	-2.50	117.25	122.09
4	1-K	7496	CIT	O5-C6-C3	-2.50	117.25	122.09
4	2-K	7496	CIT	O5-C6-C3	-2.50	117.25	122.09
4	3-K	7496	CIT	O5-C6-C3	-2.50	117.25	122.09
4	4-K	7496	CIT	O5-C6-C3	-2.50	117.25	122.09
4	5-K	7496	CIT	O5-C6-C3	-2.50	117.25	122.09
4	6-K	7496	CIT	O5-C6-C3	-2.50	117.25	122.09
4	7-K	7496	CIT	O5-C6-C3	-2.50	117.25	122.09
4	8-K	7496	CIT	O5-C6-C3	-2.50	117.25	122.09
4	9-K	7496	CIT	O5-C6-C3	-2.50	117.25	122.09
4	10-K	7496	CIT	O5-C6-C3	-2.50	117.25	122.09
4	1-C	7480	CIT	O5-C6-C3	-2.50	117.25	122.09
4	2-C	7480	CIT	O5-C6-C3	-2.50	117.25	122.09
4	3-C	7480	CIT	O5-C6-C3	-2.50	117.25	122.09
4	4-C	7480	CIT	O5-C6-C3	-2.50	117.25	122.09
4	5-C	7480	CIT	O5-C6-C3	-2.50	117.25	122.09
4	6-C	7480	CIT	O5-C6-C3	-2.50	117.25	122.09
4	7-C	7480	CIT	O5-C6-C3	-2.50	117.25	122.09
4	8-C	7480	CIT	O5-C6-C3	-2.50	117.25	122.09
4	9-C	7480	CIT	O5-C6-C3	-2.50	117.25	122.09
4	10-C	7480	CIT	O5-C6-C3	-2.50	117.25	122.09
4	1-N	7502	CIT	O5-C6-C3	-2.50	117.26	122.09
4	2-N	7502	CIT	O5-C6-C3	-2.50	117.26	122.09
4	3-N	7502	CIT	O5-C6-C3	-2.50	117.26	122.09
4	4-N	7502	CIT	O5-C6-C3	-2.50	117.26	122.09
4	5-N	7502	CIT	O5-C6-C3	-2.50	117.26	122.09
4	6-N	7502	CIT	O5-C6-C3	-2.50	117.26	122.09
4	7-N	7502	CIT	O5-C6-C3	-2.50	117.26	122.09
4	8-N	7502	CIT	O5-C6-C3	-2.50	117.26	122.09
4	9-N	7502	CIT	O5-C6-C3	-2.50	117.26	122.09
4	10-N	7502	CIT	O5-C6-C3	-2.50	117.26	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-O	7504	CIT	O5-C6-C3	-2.49	117.26	122.09
4	2-O	7504	CIT	O5-C6-C3	-2.49	117.26	122.09
4	3-O	7504	CIT	O5-C6-C3	-2.49	117.26	122.09
4	4-O	7504	CIT	O5-C6-C3	-2.49	117.26	122.09
4	5-O	7504	CIT	O5-C6-C3	-2.49	117.26	122.09
4	6-O	7504	CIT	O5-C6-C3	-2.49	117.26	122.09
4	7-O	7504	CIT	O5-C6-C3	-2.49	117.26	122.09
4	8-O	7504	CIT	O5-C6-C3	-2.49	117.26	122.09
4	9-O	7504	CIT	O5-C6-C3	-2.49	117.26	122.09
4	10-O	7504	CIT	O5-C6-C3	-2.49	117.26	122.09
4	1-V	7518	CIT	O5-C6-C3	-2.49	117.26	122.09
4	2-V	7518	CIT	O5-C6-C3	-2.49	117.26	122.09
4	3-V	7518	CIT	O5-C6-C3	-2.49	117.26	122.09
4	4-V	7518	CIT	O5-C6-C3	-2.49	117.26	122.09
4	5-V	7518	CIT	O5-C6-C3	-2.49	117.26	122.09
4	6-V	7518	CIT	O5-C6-C3	-2.49	117.26	122.09
4	7-V	7518	CIT	O5-C6-C3	-2.49	117.26	122.09
4	8-V	7518	CIT	O5-C6-C3	-2.49	117.26	122.09
4	9-V	7518	CIT	O5-C6-C3	-2.49	117.26	122.09
4	10-V	7518	CIT	O5-C6-C3	-2.49	117.26	122.09
4	1-B	7478	CIT	O5-C6-C3	-2.49	117.27	122.09
4	2-B	7478	CIT	O5-C6-C3	-2.49	117.27	122.09
4	3-B	7478	CIT	O5-C6-C3	-2.49	117.27	122.09
4	4-B	7478	CIT	O5-C6-C3	-2.49	117.27	122.09
4	5-B	7478	CIT	O5-C6-C3	-2.49	117.27	122.09
4	6-B	7478	CIT	O5-C6-C3	-2.49	117.27	122.09
4	7-B	7478	CIT	O5-C6-C3	-2.49	117.27	122.09
4	8-B	7478	CIT	O5-C6-C3	-2.49	117.27	122.09
4	9-B	7478	CIT	O5-C6-C3	-2.49	117.27	122.09
4	10-B	7478	CIT	O5-C6-C3	-2.49	117.27	122.09
4	1-F	7486	CIT	O5-C6-C3	-2.49	117.27	122.09
4	2-F	7486	CIT	O5-C6-C3	-2.49	117.27	122.09
4	3-F	7486	CIT	O5-C6-C3	-2.49	117.27	122.09
4	4-F	7486	CIT	O5-C6-C3	-2.49	117.27	122.09
4	5-F	7486	CIT	O5-C6-C3	-2.49	117.27	122.09
4	6-F	7486	CIT	O5-C6-C3	-2.49	117.27	122.09
4	7-F	7486	CIT	O5-C6-C3	-2.49	117.27	122.09
4	8-F	7486	CIT	O5-C6-C3	-2.49	117.27	122.09
4	9-F	7486	CIT	O5-C6-C3	-2.49	117.27	122.09
4	10-F	7486	CIT	O5-C6-C3	-2.49	117.27	122.09
4	1-T	7514	CIT	O5-C6-C3	-2.49	117.27	122.09
4	2-T	7514	CIT	O5-C6-C3	-2.49	117.27	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-T	7514	CIT	O5-C6-C3	-2.49	117.27	122.09
4	4-T	7514	CIT	O5-C6-C3	-2.49	117.27	122.09
4	5-T	7514	CIT	O5-C6-C3	-2.49	117.27	122.09
4	6-T	7514	CIT	O5-C6-C3	-2.49	117.27	122.09
4	7-T	7514	CIT	O5-C6-C3	-2.49	117.27	122.09
4	8-T	7514	CIT	O5-C6-C3	-2.49	117.27	122.09
4	9-T	7514	CIT	O5-C6-C3	-2.49	117.27	122.09
4	10-T	7514	CIT	O5-C6-C3	-2.49	117.27	122.09
4	1-P	7506	CIT	O5-C6-C3	-2.49	117.28	122.09
4	2-P	7506	CIT	O5-C6-C3	-2.49	117.28	122.09
4	3-P	7506	CIT	O5-C6-C3	-2.49	117.28	122.09
4	4-P	7506	CIT	O5-C6-C3	-2.49	117.28	122.09
4	5-P	7506	CIT	O5-C6-C3	-2.49	117.28	122.09
4	6-P	7506	CIT	O5-C6-C3	-2.49	117.28	122.09
4	7-P	7506	CIT	O5-C6-C3	-2.49	117.28	122.09
4	8-P	7506	CIT	O5-C6-C3	-2.49	117.28	122.09
4	9-P	7506	CIT	O5-C6-C3	-2.49	117.28	122.09
4	10-P	7506	CIT	O5-C6-C3	-2.49	117.28	122.09
4	1-W	7520	CIT	O5-C6-C3	-2.48	117.29	122.09
4	2-W	7520	CIT	O5-C6-C3	-2.48	117.29	122.09
4	3-W	7520	CIT	O5-C6-C3	-2.48	117.29	122.09
4	4-W	7520	CIT	O5-C6-C3	-2.48	117.29	122.09
4	5-W	7520	CIT	O5-C6-C3	-2.48	117.29	122.09
4	6-W	7520	CIT	O5-C6-C3	-2.48	117.29	122.09
4	7-W	7520	CIT	O5-C6-C3	-2.48	117.29	122.09
4	8-W	7520	CIT	O5-C6-C3	-2.48	117.29	122.09
4	9-W	7520	CIT	O5-C6-C3	-2.48	117.29	122.09
4	10-W	7520	CIT	O5-C6-C3	-2.48	117.29	122.09
3	1-C	7479	AMP	C5-C4-N3	-2.46	123.33	126.72
3	2-C	7479	AMP	C5-C4-N3	-2.46	123.33	126.72
3	3-C	7479	AMP	C5-C4-N3	-2.46	123.33	126.72
3	4-C	7479	AMP	C5-C4-N3	-2.46	123.33	126.72
3	5-C	7479	AMP	C5-C4-N3	-2.46	123.33	126.72
3	6-C	7479	AMP	C5-C4-N3	-2.46	123.33	126.72
3	7-C	7479	AMP	C5-C4-N3	-2.46	123.33	126.72
3	8-C	7479	AMP	C5-C4-N3	-2.46	123.33	126.72
3	9-C	7479	AMP	C5-C4-N3	-2.46	123.33	126.72
3	10-C	7479	AMP	C5-C4-N3	-2.46	123.33	126.72
3	1-P	7505	AMP	C5-C4-N3	-2.46	123.33	126.72
3	2-P	7505	AMP	C5-C4-N3	-2.46	123.33	126.72
3	3-P	7505	AMP	C5-C4-N3	-2.46	123.33	126.72
3	4-P	7505	AMP	C5-C4-N3	-2.46	123.33	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-P	7505	AMP	C5-C4-N3	-2.46	123.33	126.72
3	6-P	7505	AMP	C5-C4-N3	-2.46	123.33	126.72
3	7-P	7505	AMP	C5-C4-N3	-2.46	123.33	126.72
3	8-P	7505	AMP	C5-C4-N3	-2.46	123.33	126.72
3	9-P	7505	AMP	C5-C4-N3	-2.46	123.33	126.72
3	10-P	7505	AMP	C5-C4-N3	-2.46	123.33	126.72
3	1-U	7515	AMP	C5-C4-N3	-2.44	123.35	126.72
3	2-U	7515	AMP	C5-C4-N3	-2.44	123.35	126.72
3	3-U	7515	AMP	C5-C4-N3	-2.44	123.35	126.72
3	4-U	7515	AMP	C5-C4-N3	-2.44	123.35	126.72
3	5-U	7515	AMP	C5-C4-N3	-2.44	123.35	126.72
3	6-U	7515	AMP	C5-C4-N3	-2.44	123.35	126.72
3	7-U	7515	AMP	C5-C4-N3	-2.44	123.35	126.72
3	8-U	7515	AMP	C5-C4-N3	-2.44	123.35	126.72
3	9-U	7515	AMP	C5-C4-N3	-2.44	123.35	126.72
3	10-U	7515	AMP	C5-C4-N3	-2.44	123.35	126.72
3	1-F	7485	AMP	C5-C4-N3	-2.44	123.36	126.72
3	2-F	7485	AMP	C5-C4-N3	-2.44	123.36	126.72
3	3-F	7485	AMP	C5-C4-N3	-2.44	123.36	126.72
3	4-F	7485	AMP	C5-C4-N3	-2.44	123.36	126.72
3	5-F	7485	AMP	C5-C4-N3	-2.44	123.36	126.72
3	6-F	7485	AMP	C5-C4-N3	-2.44	123.36	126.72
3	7-F	7485	AMP	C5-C4-N3	-2.44	123.36	126.72
3	8-F	7485	AMP	C5-C4-N3	-2.44	123.36	126.72
3	9-F	7485	AMP	C5-C4-N3	-2.44	123.36	126.72
3	10-F	7485	AMP	C5-C4-N3	-2.44	123.36	126.72
3	1-S	7511	AMP	C5-C4-N3	-2.44	123.36	126.72
3	2-S	7511	AMP	C5-C4-N3	-2.44	123.36	126.72
3	3-S	7511	AMP	C5-C4-N3	-2.44	123.36	126.72
3	4-S	7511	AMP	C5-C4-N3	-2.44	123.36	126.72
3	5-S	7511	AMP	C5-C4-N3	-2.44	123.36	126.72
3	6-S	7511	AMP	C5-C4-N3	-2.44	123.36	126.72
3	7-S	7511	AMP	C5-C4-N3	-2.44	123.36	126.72
3	8-S	7511	AMP	C5-C4-N3	-2.44	123.36	126.72
3	9-S	7511	AMP	C5-C4-N3	-2.44	123.36	126.72
3	10-S	7511	AMP	C5-C4-N3	-2.44	123.36	126.72
3	1-V	7517	AMP	C5-C4-N3	-2.44	123.36	126.72
3	2-V	7517	AMP	C5-C4-N3	-2.44	123.36	126.72
3	3-V	7517	AMP	C5-C4-N3	-2.44	123.36	126.72
3	4-V	7517	AMP	C5-C4-N3	-2.44	123.36	126.72
3	5-V	7517	AMP	C5-C4-N3	-2.44	123.36	126.72
3	6-V	7517	AMP	C5-C4-N3	-2.44	123.36	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-V	7517	AMP	C5-C4-N3	-2.44	123.36	126.72
3	8-V	7517	AMP	C5-C4-N3	-2.44	123.36	126.72
3	9-V	7517	AMP	C5-C4-N3	-2.44	123.36	126.72
3	10-V	7517	AMP	C5-C4-N3	-2.44	123.36	126.72
3	1-L	7497	AMP	C5-C4-N3	-2.44	123.36	126.72
3	2-L	7497	AMP	C5-C4-N3	-2.44	123.36	126.72
3	3-L	7497	AMP	C5-C4-N3	-2.44	123.36	126.72
3	4-L	7497	AMP	C5-C4-N3	-2.44	123.36	126.72
3	5-L	7497	AMP	C5-C4-N3	-2.44	123.36	126.72
3	6-L	7497	AMP	C5-C4-N3	-2.44	123.36	126.72
3	7-L	7497	AMP	C5-C4-N3	-2.44	123.36	126.72
3	8-L	7497	AMP	C5-C4-N3	-2.44	123.36	126.72
3	9-L	7497	AMP	C5-C4-N3	-2.44	123.36	126.72
3	10-L	7497	AMP	C5-C4-N3	-2.44	123.36	126.72
3	1-B	7477	AMP	C5-C4-N3	-2.44	123.36	126.72
3	2-B	7477	AMP	C5-C4-N3	-2.44	123.36	126.72
3	3-B	7477	AMP	C5-C4-N3	-2.44	123.36	126.72
3	4-B	7477	AMP	C5-C4-N3	-2.44	123.36	126.72
3	5-B	7477	AMP	C5-C4-N3	-2.44	123.36	126.72
3	6-B	7477	AMP	C5-C4-N3	-2.44	123.36	126.72
3	7-B	7477	AMP	C5-C4-N3	-2.44	123.36	126.72
3	8-B	7477	AMP	C5-C4-N3	-2.44	123.36	126.72
3	9-B	7477	AMP	C5-C4-N3	-2.44	123.36	126.72
3	10-B	7477	AMP	C5-C4-N3	-2.44	123.36	126.72
3	1-R	7509	AMP	C5-C4-N3	-2.43	123.37	126.72
3	2-R	7509	AMP	C5-C4-N3	-2.43	123.37	126.72
3	3-R	7509	AMP	C5-C4-N3	-2.43	123.37	126.72
3	4-R	7509	AMP	C5-C4-N3	-2.43	123.37	126.72
3	5-R	7509	AMP	C5-C4-N3	-2.43	123.37	126.72
3	6-R	7509	AMP	C5-C4-N3	-2.43	123.37	126.72
3	7-R	7509	AMP	C5-C4-N3	-2.43	123.37	126.72
3	8-R	7509	AMP	C5-C4-N3	-2.43	123.37	126.72
3	9-R	7509	AMP	C5-C4-N3	-2.43	123.37	126.72
3	10-R	7509	AMP	C5-C4-N3	-2.43	123.37	126.72
3	1-M	7499	AMP	C5-C4-N3	-2.43	123.37	126.72
3	2-M	7499	AMP	C5-C4-N3	-2.43	123.37	126.72
3	3-M	7499	AMP	C5-C4-N3	-2.43	123.37	126.72
3	4-M	7499	AMP	C5-C4-N3	-2.43	123.37	126.72
3	5-M	7499	AMP	C5-C4-N3	-2.43	123.37	126.72
3	6-M	7499	AMP	C5-C4-N3	-2.43	123.37	126.72
3	7-M	7499	AMP	C5-C4-N3	-2.43	123.37	126.72
3	8-M	7499	AMP	C5-C4-N3	-2.43	123.37	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-M	7499	AMP	C5-C4-N3	-2.43	123.37	126.72
3	10-M	7499	AMP	C5-C4-N3	-2.43	123.37	126.72
3	1-O	7503	AMP	C5-C4-N3	-2.43	123.37	126.72
3	2-O	7503	AMP	C5-C4-N3	-2.43	123.37	126.72
3	3-O	7503	AMP	C5-C4-N3	-2.43	123.37	126.72
3	4-O	7503	AMP	C5-C4-N3	-2.43	123.37	126.72
3	5-O	7503	AMP	C5-C4-N3	-2.43	123.37	126.72
3	6-O	7503	AMP	C5-C4-N3	-2.43	123.37	126.72
3	7-O	7503	AMP	C5-C4-N3	-2.43	123.37	126.72
3	8-O	7503	AMP	C5-C4-N3	-2.43	123.37	126.72
3	9-O	7503	AMP	C5-C4-N3	-2.43	123.37	126.72
3	10-O	7503	AMP	C5-C4-N3	-2.43	123.37	126.72
3	1-H	7489	AMP	C5-C4-N3	-2.43	123.37	126.72
3	2-H	7489	AMP	C5-C4-N3	-2.43	123.37	126.72
3	3-H	7489	AMP	C5-C4-N3	-2.43	123.37	126.72
3	4-H	7489	AMP	C5-C4-N3	-2.43	123.37	126.72
3	5-H	7489	AMP	C5-C4-N3	-2.43	123.37	126.72
3	6-H	7489	AMP	C5-C4-N3	-2.43	123.37	126.72
3	7-H	7489	AMP	C5-C4-N3	-2.43	123.37	126.72
3	8-H	7489	AMP	C5-C4-N3	-2.43	123.37	126.72
3	9-H	7489	AMP	C5-C4-N3	-2.43	123.37	126.72
3	10-H	7489	AMP	C5-C4-N3	-2.43	123.37	126.72
3	1-W	7519	AMP	C5-C4-N3	-2.43	123.37	126.72
3	2-W	7519	AMP	C5-C4-N3	-2.43	123.37	126.72
3	3-W	7519	AMP	C5-C4-N3	-2.43	123.37	126.72
3	4-W	7519	AMP	C5-C4-N3	-2.43	123.37	126.72
3	5-W	7519	AMP	C5-C4-N3	-2.43	123.37	126.72
3	6-W	7519	AMP	C5-C4-N3	-2.43	123.37	126.72
3	7-W	7519	AMP	C5-C4-N3	-2.43	123.37	126.72
3	8-W	7519	AMP	C5-C4-N3	-2.43	123.37	126.72
3	9-W	7519	AMP	C5-C4-N3	-2.43	123.37	126.72
3	10-W	7519	AMP	C5-C4-N3	-2.43	123.37	126.72
3	1-D	7481	AMP	C5-C4-N3	-2.43	123.38	126.72
3	2-D	7481	AMP	C5-C4-N3	-2.43	123.38	126.72
3	3-D	7481	AMP	C5-C4-N3	-2.43	123.38	126.72
3	4-D	7481	AMP	C5-C4-N3	-2.43	123.38	126.72
3	5-D	7481	AMP	C5-C4-N3	-2.43	123.38	126.72
3	6-D	7481	AMP	C5-C4-N3	-2.43	123.38	126.72
3	7-D	7481	AMP	C5-C4-N3	-2.43	123.38	126.72
3	8-D	7481	AMP	C5-C4-N3	-2.43	123.38	126.72
3	9-D	7481	AMP	C5-C4-N3	-2.43	123.38	126.72
3	10-D	7481	AMP	C5-C4-N3	-2.43	123.38	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-K	7495	AMP	C5-C4-N3	-2.43	123.38	126.72
3	2-K	7495	AMP	C5-C4-N3	-2.43	123.38	126.72
3	3-K	7495	AMP	C5-C4-N3	-2.43	123.38	126.72
3	4-K	7495	AMP	C5-C4-N3	-2.43	123.38	126.72
3	5-K	7495	AMP	C5-C4-N3	-2.43	123.38	126.72
3	6-K	7495	AMP	C5-C4-N3	-2.43	123.38	126.72
3	7-K	7495	AMP	C5-C4-N3	-2.43	123.38	126.72
3	8-K	7495	AMP	C5-C4-N3	-2.43	123.38	126.72
3	9-K	7495	AMP	C5-C4-N3	-2.43	123.38	126.72
3	10-K	7495	AMP	C5-C4-N3	-2.43	123.38	126.72
3	1-A	7475	AMP	C5-C4-N3	-2.42	123.38	126.72
3	2-A	7475	AMP	C5-C4-N3	-2.42	123.38	126.72
3	3-A	7475	AMP	C5-C4-N3	-2.42	123.38	126.72
3	4-A	7475	AMP	C5-C4-N3	-2.42	123.38	126.72
3	5-A	7475	AMP	C5-C4-N3	-2.42	123.38	126.72
3	6-A	7475	AMP	C5-C4-N3	-2.42	123.38	126.72
3	7-A	7475	AMP	C5-C4-N3	-2.42	123.38	126.72
3	8-A	7475	AMP	C5-C4-N3	-2.42	123.38	126.72
3	9-A	7475	AMP	C5-C4-N3	-2.42	123.38	126.72
3	10-A	7475	AMP	C5-C4-N3	-2.42	123.38	126.72
3	1-T	7513	AMP	C5-C4-N3	-2.42	123.38	126.72
3	2-T	7513	AMP	C5-C4-N3	-2.42	123.38	126.72
3	3-T	7513	AMP	C5-C4-N3	-2.42	123.38	126.72
3	4-T	7513	AMP	C5-C4-N3	-2.42	123.38	126.72
3	5-T	7513	AMP	C5-C4-N3	-2.42	123.38	126.72
3	6-T	7513	AMP	C5-C4-N3	-2.42	123.38	126.72
3	7-T	7513	AMP	C5-C4-N3	-2.42	123.38	126.72
3	8-T	7513	AMP	C5-C4-N3	-2.42	123.38	126.72
3	9-T	7513	AMP	C5-C4-N3	-2.42	123.38	126.72
3	10-T	7513	AMP	C5-C4-N3	-2.42	123.38	126.72
3	1-G	7487	AMP	C5-C4-N3	-2.42	123.38	126.72
3	2-G	7487	AMP	C5-C4-N3	-2.42	123.38	126.72
3	3-G	7487	AMP	C5-C4-N3	-2.42	123.38	126.72
3	4-G	7487	AMP	C5-C4-N3	-2.42	123.38	126.72
3	5-G	7487	AMP	C5-C4-N3	-2.42	123.38	126.72
3	6-G	7487	AMP	C5-C4-N3	-2.42	123.38	126.72
3	7-G	7487	AMP	C5-C4-N3	-2.42	123.38	126.72
3	8-G	7487	AMP	C5-C4-N3	-2.42	123.38	126.72
3	9-G	7487	AMP	C5-C4-N3	-2.42	123.38	126.72
3	10-G	7487	AMP	C5-C4-N3	-2.42	123.38	126.72
3	1-I	7491	AMP	C5-C4-N3	-2.42	123.38	126.72
3	2-I	7491	AMP	C5-C4-N3	-2.42	123.38	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-I	7491	AMP	C5-C4-N3	-2.42	123.38	126.72
3	4-I	7491	AMP	C5-C4-N3	-2.42	123.38	126.72
3	5-I	7491	AMP	C5-C4-N3	-2.42	123.38	126.72
3	6-I	7491	AMP	C5-C4-N3	-2.42	123.38	126.72
3	7-I	7491	AMP	C5-C4-N3	-2.42	123.38	126.72
3	8-I	7491	AMP	C5-C4-N3	-2.42	123.38	126.72
3	9-I	7491	AMP	C5-C4-N3	-2.42	123.38	126.72
3	10-I	7491	AMP	C5-C4-N3	-2.42	123.38	126.72
3	1-Q	7507	AMP	C5-C4-N3	-2.42	123.39	126.72
3	2-Q	7507	AMP	C5-C4-N3	-2.42	123.39	126.72
3	3-Q	7507	AMP	C5-C4-N3	-2.42	123.39	126.72
3	4-Q	7507	AMP	C5-C4-N3	-2.42	123.39	126.72
3	5-Q	7507	AMP	C5-C4-N3	-2.42	123.39	126.72
3	6-Q	7507	AMP	C5-C4-N3	-2.42	123.39	126.72
3	7-Q	7507	AMP	C5-C4-N3	-2.42	123.39	126.72
3	8-Q	7507	AMP	C5-C4-N3	-2.42	123.39	126.72
3	9-Q	7507	AMP	C5-C4-N3	-2.42	123.39	126.72
3	10-Q	7507	AMP	C5-C4-N3	-2.42	123.39	126.72
3	1-J	7493	AMP	C5-C4-N3	-2.42	123.39	126.72
3	2-J	7493	AMP	C5-C4-N3	-2.42	123.39	126.72
3	3-J	7493	AMP	C5-C4-N3	-2.42	123.39	126.72
3	4-J	7493	AMP	C5-C4-N3	-2.42	123.39	126.72
3	5-J	7493	AMP	C5-C4-N3	-2.42	123.39	126.72
3	6-J	7493	AMP	C5-C4-N3	-2.42	123.39	126.72
3	7-J	7493	AMP	C5-C4-N3	-2.42	123.39	126.72
3	8-J	7493	AMP	C5-C4-N3	-2.42	123.39	126.72
3	9-J	7493	AMP	C5-C4-N3	-2.42	123.39	126.72
3	10-J	7493	AMP	C5-C4-N3	-2.42	123.39	126.72
3	1-E	7483	AMP	C5-C4-N3	-2.42	123.39	126.72
3	2-E	7483	AMP	C5-C4-N3	-2.42	123.39	126.72
3	3-E	7483	AMP	C5-C4-N3	-2.42	123.39	126.72
3	4-E	7483	AMP	C5-C4-N3	-2.42	123.39	126.72
3	5-E	7483	AMP	C5-C4-N3	-2.42	123.39	126.72
3	6-E	7483	AMP	C5-C4-N3	-2.42	123.39	126.72
3	7-E	7483	AMP	C5-C4-N3	-2.42	123.39	126.72
3	8-E	7483	AMP	C5-C4-N3	-2.42	123.39	126.72
3	9-E	7483	AMP	C5-C4-N3	-2.42	123.39	126.72
3	10-E	7483	AMP	C5-C4-N3	-2.42	123.39	126.72
3	1-N	7501	AMP	C5-C4-N3	-2.41	123.40	126.72
3	2-N	7501	AMP	C5-C4-N3	-2.41	123.40	126.72
3	3-N	7501	AMP	C5-C4-N3	-2.41	123.40	126.72
3	4-N	7501	AMP	C5-C4-N3	-2.41	123.40	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-N	7501	AMP	C5-C4-N3	-2.41	123.40	126.72
3	6-N	7501	AMP	C5-C4-N3	-2.41	123.40	126.72
3	7-N	7501	AMP	C5-C4-N3	-2.41	123.40	126.72
3	8-N	7501	AMP	C5-C4-N3	-2.41	123.40	126.72
3	9-N	7501	AMP	C5-C4-N3	-2.41	123.40	126.72
3	10-N	7501	AMP	C5-C4-N3	-2.41	123.40	126.72
3	1-X	7521	AMP	C5-C4-N3	-2.39	123.42	126.72
3	2-X	7521	AMP	C5-C4-N3	-2.39	123.42	126.72
3	3-X	7521	AMP	C5-C4-N3	-2.39	123.42	126.72
3	4-X	7521	AMP	C5-C4-N3	-2.39	123.42	126.72
3	5-X	7521	AMP	C5-C4-N3	-2.39	123.42	126.72
3	6-X	7521	AMP	C5-C4-N3	-2.39	123.42	126.72
3	7-X	7521	AMP	C5-C4-N3	-2.39	123.42	126.72
3	8-X	7521	AMP	C5-C4-N3	-2.39	123.42	126.72
3	9-X	7521	AMP	C5-C4-N3	-2.39	123.42	126.72
3	10-X	7521	AMP	C5-C4-N3	-2.39	123.42	126.72
4	1-X	7522	CIT	O3-C5-C4	-2.38	116.22	122.95
4	2-X	7522	CIT	O3-C5-C4	-2.38	116.22	122.95
4	3-X	7522	CIT	O3-C5-C4	-2.38	116.22	122.95
4	4-X	7522	CIT	O3-C5-C4	-2.38	116.22	122.95
4	5-X	7522	CIT	O3-C5-C4	-2.38	116.22	122.95
4	6-X	7522	CIT	O3-C5-C4	-2.38	116.22	122.95
4	7-X	7522	CIT	O3-C5-C4	-2.38	116.22	122.95
4	8-X	7522	CIT	O3-C5-C4	-2.38	116.22	122.95
4	9-X	7522	CIT	O3-C5-C4	-2.38	116.22	122.95
4	10-X	7522	CIT	O3-C5-C4	-2.38	116.22	122.95
4	1-D	7482	CIT	O3-C5-C4	-2.36	116.25	122.95
4	2-D	7482	CIT	O3-C5-C4	-2.36	116.25	122.95
4	3-D	7482	CIT	O3-C5-C4	-2.36	116.25	122.95
4	4-D	7482	CIT	O3-C5-C4	-2.36	116.25	122.95
4	5-D	7482	CIT	O3-C5-C4	-2.36	116.25	122.95
4	6-D	7482	CIT	O3-C5-C4	-2.36	116.25	122.95
4	7-D	7482	CIT	O3-C5-C4	-2.36	116.25	122.95
4	8-D	7482	CIT	O3-C5-C4	-2.36	116.25	122.95
4	9-D	7482	CIT	O3-C5-C4	-2.36	116.25	122.95
4	10-D	7482	CIT	O3-C5-C4	-2.36	116.25	122.95
4	1-G	7488	CIT	O3-C5-C4	-2.36	116.26	122.95
4	2-G	7488	CIT	O3-C5-C4	-2.36	116.26	122.95
4	3-G	7488	CIT	O3-C5-C4	-2.36	116.26	122.95
4	4-G	7488	CIT	O3-C5-C4	-2.36	116.26	122.95
4	5-G	7488	CIT	O3-C5-C4	-2.36	116.26	122.95
4	6-G	7488	CIT	O3-C5-C4	-2.36	116.26	122.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7-G	7488	CIT	O3-C5-C4	-2.36	116.26	122.95
4	8-G	7488	CIT	O3-C5-C4	-2.36	116.26	122.95
4	9-G	7488	CIT	O3-C5-C4	-2.36	116.26	122.95
4	10-G	7488	CIT	O3-C5-C4	-2.36	116.26	122.95
4	1-O	7504	CIT	O3-C5-C4	-2.36	116.26	122.95
4	2-O	7504	CIT	O3-C5-C4	-2.36	116.26	122.95
4	3-O	7504	CIT	O3-C5-C4	-2.36	116.26	122.95
4	4-O	7504	CIT	O3-C5-C4	-2.36	116.26	122.95
4	5-O	7504	CIT	O3-C5-C4	-2.36	116.26	122.95
4	6-O	7504	CIT	O3-C5-C4	-2.36	116.26	122.95
4	7-O	7504	CIT	O3-C5-C4	-2.36	116.26	122.95
4	8-O	7504	CIT	O3-C5-C4	-2.36	116.26	122.95
4	9-O	7504	CIT	O3-C5-C4	-2.36	116.26	122.95
4	10-O	7504	CIT	O3-C5-C4	-2.36	116.26	122.95
4	1-M	7500	CIT	O3-C5-C4	-2.36	116.26	122.95
4	2-M	7500	CIT	O3-C5-C4	-2.36	116.26	122.95
4	3-M	7500	CIT	O3-C5-C4	-2.36	116.26	122.95
4	4-M	7500	CIT	O3-C5-C4	-2.36	116.26	122.95
4	5-M	7500	CIT	O3-C5-C4	-2.36	116.26	122.95
4	6-M	7500	CIT	O3-C5-C4	-2.36	116.26	122.95
4	7-M	7500	CIT	O3-C5-C4	-2.36	116.26	122.95
4	8-M	7500	CIT	O3-C5-C4	-2.36	116.26	122.95
4	9-M	7500	CIT	O3-C5-C4	-2.36	116.26	122.95
4	10-M	7500	CIT	O3-C5-C4	-2.36	116.26	122.95
4	1-E	7484	CIT	O3-C5-C4	-2.36	116.27	122.95
4	2-E	7484	CIT	O3-C5-C4	-2.36	116.27	122.95
4	3-E	7484	CIT	O3-C5-C4	-2.36	116.27	122.95
4	4-E	7484	CIT	O3-C5-C4	-2.36	116.27	122.95
4	5-E	7484	CIT	O3-C5-C4	-2.36	116.27	122.95
4	6-E	7484	CIT	O3-C5-C4	-2.36	116.27	122.95
4	7-E	7484	CIT	O3-C5-C4	-2.36	116.27	122.95
4	8-E	7484	CIT	O3-C5-C4	-2.36	116.27	122.95
4	9-E	7484	CIT	O3-C5-C4	-2.36	116.27	122.95
4	10-E	7484	CIT	O3-C5-C4	-2.36	116.27	122.95
4	1-B	7478	CIT	O3-C5-C4	-2.36	116.28	122.95
4	2-B	7478	CIT	O3-C5-C4	-2.36	116.28	122.95
4	3-B	7478	CIT	O3-C5-C4	-2.36	116.28	122.95
4	4-B	7478	CIT	O3-C5-C4	-2.36	116.28	122.95
4	5-B	7478	CIT	O3-C5-C4	-2.36	116.28	122.95
4	6-B	7478	CIT	O3-C5-C4	-2.36	116.28	122.95
4	7-B	7478	CIT	O3-C5-C4	-2.36	116.28	122.95
4	8-B	7478	CIT	O3-C5-C4	-2.36	116.28	122.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9-B	7478	CIT	O3-C5-C4	-2.36	116.28	122.95
4	10-B	7478	CIT	O3-C5-C4	-2.36	116.28	122.95
4	1-K	7496	CIT	O3-C5-C4	-2.36	116.28	122.95
4	2-K	7496	CIT	O3-C5-C4	-2.36	116.28	122.95
4	3-K	7496	CIT	O3-C5-C4	-2.36	116.28	122.95
4	4-K	7496	CIT	O3-C5-C4	-2.36	116.28	122.95
4	5-K	7496	CIT	O3-C5-C4	-2.36	116.28	122.95
4	6-K	7496	CIT	O3-C5-C4	-2.36	116.28	122.95
4	7-K	7496	CIT	O3-C5-C4	-2.36	116.28	122.95
4	8-K	7496	CIT	O3-C5-C4	-2.36	116.28	122.95
4	9-K	7496	CIT	O3-C5-C4	-2.36	116.28	122.95
4	10-K	7496	CIT	O3-C5-C4	-2.36	116.28	122.95
4	1-A	7476	CIT	O3-C5-C4	-2.35	116.29	122.95
4	2-A	7476	CIT	O3-C5-C4	-2.35	116.29	122.95
4	3-A	7476	CIT	O3-C5-C4	-2.35	116.29	122.95
4	4-A	7476	CIT	O3-C5-C4	-2.35	116.29	122.95
4	5-A	7476	CIT	O3-C5-C4	-2.35	116.29	122.95
4	6-A	7476	CIT	O3-C5-C4	-2.35	116.29	122.95
4	7-A	7476	CIT	O3-C5-C4	-2.35	116.29	122.95
4	8-A	7476	CIT	O3-C5-C4	-2.35	116.29	122.95
4	9-A	7476	CIT	O3-C5-C4	-2.35	116.29	122.95
4	10-A	7476	CIT	O3-C5-C4	-2.35	116.29	122.95
4	1-F	7486	CIT	O3-C5-C4	-2.35	116.29	122.95
4	2-F	7486	CIT	O3-C5-C4	-2.35	116.29	122.95
4	3-F	7486	CIT	O3-C5-C4	-2.35	116.29	122.95
4	4-F	7486	CIT	O3-C5-C4	-2.35	116.29	122.95
4	5-F	7486	CIT	O3-C5-C4	-2.35	116.29	122.95
4	6-F	7486	CIT	O3-C5-C4	-2.35	116.29	122.95
4	7-F	7486	CIT	O3-C5-C4	-2.35	116.29	122.95
4	8-F	7486	CIT	O3-C5-C4	-2.35	116.29	122.95
4	9-F	7486	CIT	O3-C5-C4	-2.35	116.29	122.95
4	10-F	7486	CIT	O3-C5-C4	-2.35	116.29	122.95
4	1-R	7510	CIT	O3-C5-C4	-2.35	116.29	122.95
4	2-R	7510	CIT	O3-C5-C4	-2.35	116.29	122.95
4	3-R	7510	CIT	O3-C5-C4	-2.35	116.29	122.95
4	4-R	7510	CIT	O3-C5-C4	-2.35	116.29	122.95
4	5-R	7510	CIT	O3-C5-C4	-2.35	116.29	122.95
4	6-R	7510	CIT	O3-C5-C4	-2.35	116.29	122.95
4	7-R	7510	CIT	O3-C5-C4	-2.35	116.29	122.95
4	8-R	7510	CIT	O3-C5-C4	-2.35	116.29	122.95
4	9-R	7510	CIT	O3-C5-C4	-2.35	116.29	122.95
4	10-R	7510	CIT	O3-C5-C4	-2.35	116.29	122.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-T	7514	CIT	O3-C5-C4	-2.35	116.29	122.95
4	2-T	7514	CIT	O3-C5-C4	-2.35	116.29	122.95
4	3-T	7514	CIT	O3-C5-C4	-2.35	116.29	122.95
4	4-T	7514	CIT	O3-C5-C4	-2.35	116.29	122.95
4	5-T	7514	CIT	O3-C5-C4	-2.35	116.29	122.95
4	6-T	7514	CIT	O3-C5-C4	-2.35	116.29	122.95
4	7-T	7514	CIT	O3-C5-C4	-2.35	116.29	122.95
4	8-T	7514	CIT	O3-C5-C4	-2.35	116.29	122.95
4	9-T	7514	CIT	O3-C5-C4	-2.35	116.29	122.95
4	10-T	7514	CIT	O3-C5-C4	-2.35	116.29	122.95
4	1-W	7520	CIT	O3-C5-C4	-2.35	116.29	122.95
4	2-W	7520	CIT	O3-C5-C4	-2.35	116.29	122.95
4	3-W	7520	CIT	O3-C5-C4	-2.35	116.29	122.95
4	4-W	7520	CIT	O3-C5-C4	-2.35	116.29	122.95
4	5-W	7520	CIT	O3-C5-C4	-2.35	116.29	122.95
4	6-W	7520	CIT	O3-C5-C4	-2.35	116.29	122.95
4	7-W	7520	CIT	O3-C5-C4	-2.35	116.29	122.95
4	8-W	7520	CIT	O3-C5-C4	-2.35	116.29	122.95
4	9-W	7520	CIT	O3-C5-C4	-2.35	116.29	122.95
4	10-W	7520	CIT	O3-C5-C4	-2.35	116.29	122.95
4	1-C	7480	CIT	O3-C5-C4	-2.35	116.30	122.95
4	2-C	7480	CIT	O3-C5-C4	-2.35	116.30	122.95
4	3-C	7480	CIT	O3-C5-C4	-2.35	116.30	122.95
4	4-C	7480	CIT	O3-C5-C4	-2.35	116.30	122.95
4	5-C	7480	CIT	O3-C5-C4	-2.35	116.30	122.95
4	6-C	7480	CIT	O3-C5-C4	-2.35	116.30	122.95
4	7-C	7480	CIT	O3-C5-C4	-2.35	116.30	122.95
4	8-C	7480	CIT	O3-C5-C4	-2.35	116.30	122.95
4	9-C	7480	CIT	O3-C5-C4	-2.35	116.30	122.95
4	10-C	7480	CIT	O3-C5-C4	-2.35	116.30	122.95
4	1-S	7512	CIT	O3-C5-C4	-2.35	116.30	122.95
4	2-S	7512	CIT	O3-C5-C4	-2.35	116.30	122.95
4	3-S	7512	CIT	O3-C5-C4	-2.35	116.30	122.95
4	4-S	7512	CIT	O3-C5-C4	-2.35	116.30	122.95
4	5-S	7512	CIT	O3-C5-C4	-2.35	116.30	122.95
4	6-S	7512	CIT	O3-C5-C4	-2.35	116.30	122.95
4	7-S	7512	CIT	O3-C5-C4	-2.35	116.30	122.95
4	8-S	7512	CIT	O3-C5-C4	-2.35	116.30	122.95
4	9-S	7512	CIT	O3-C5-C4	-2.35	116.30	122.95
4	10-S	7512	CIT	O3-C5-C4	-2.35	116.30	122.95
4	1-P	7506	CIT	O3-C5-C4	-2.35	116.30	122.95
4	2-P	7506	CIT	O3-C5-C4	-2.35	116.30	122.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-P	7506	CIT	O3-C5-C4	-2.35	116.30	122.95
4	4-P	7506	CIT	O3-C5-C4	-2.35	116.30	122.95
4	5-P	7506	CIT	O3-C5-C4	-2.35	116.30	122.95
4	6-P	7506	CIT	O3-C5-C4	-2.35	116.30	122.95
4	7-P	7506	CIT	O3-C5-C4	-2.35	116.30	122.95
4	8-P	7506	CIT	O3-C5-C4	-2.35	116.30	122.95
4	9-P	7506	CIT	O3-C5-C4	-2.35	116.30	122.95
4	10-P	7506	CIT	O3-C5-C4	-2.35	116.30	122.95
4	1-J	7494	CIT	O3-C5-C4	-2.35	116.31	122.95
4	2-J	7494	CIT	O3-C5-C4	-2.35	116.31	122.95
4	3-J	7494	CIT	O3-C5-C4	-2.35	116.31	122.95
4	4-J	7494	CIT	O3-C5-C4	-2.35	116.31	122.95
4	5-J	7494	CIT	O3-C5-C4	-2.35	116.31	122.95
4	6-J	7494	CIT	O3-C5-C4	-2.35	116.31	122.95
4	7-J	7494	CIT	O3-C5-C4	-2.35	116.31	122.95
4	8-J	7494	CIT	O3-C5-C4	-2.35	116.31	122.95
4	9-J	7494	CIT	O3-C5-C4	-2.35	116.31	122.95
4	10-J	7494	CIT	O3-C5-C4	-2.35	116.31	122.95
4	1-H	7490	CIT	O3-C5-C4	-2.35	116.31	122.95
4	2-H	7490	CIT	O3-C5-C4	-2.35	116.31	122.95
4	3-H	7490	CIT	O3-C5-C4	-2.35	116.31	122.95
4	4-H	7490	CIT	O3-C5-C4	-2.35	116.31	122.95
4	5-H	7490	CIT	O3-C5-C4	-2.35	116.31	122.95
4	6-H	7490	CIT	O3-C5-C4	-2.35	116.31	122.95
4	7-H	7490	CIT	O3-C5-C4	-2.35	116.31	122.95
4	8-H	7490	CIT	O3-C5-C4	-2.35	116.31	122.95
4	9-H	7490	CIT	O3-C5-C4	-2.35	116.31	122.95
4	10-H	7490	CIT	O3-C5-C4	-2.35	116.31	122.95
4	1-I	7492	CIT	O3-C5-C4	-2.35	116.31	122.95
4	2-I	7492	CIT	O3-C5-C4	-2.35	116.31	122.95
4	3-I	7492	CIT	O3-C5-C4	-2.35	116.31	122.95
4	4-I	7492	CIT	O3-C5-C4	-2.35	116.31	122.95
4	5-I	7492	CIT	O3-C5-C4	-2.35	116.31	122.95
4	6-I	7492	CIT	O3-C5-C4	-2.35	116.31	122.95
4	7-I	7492	CIT	O3-C5-C4	-2.35	116.31	122.95
4	8-I	7492	CIT	O3-C5-C4	-2.35	116.31	122.95
4	9-I	7492	CIT	O3-C5-C4	-2.35	116.31	122.95
4	10-I	7492	CIT	O3-C5-C4	-2.35	116.31	122.95
4	1-U	7516	CIT	O3-C5-C4	-2.35	116.31	122.95
4	2-U	7516	CIT	O3-C5-C4	-2.35	116.31	122.95
4	3-U	7516	CIT	O3-C5-C4	-2.35	116.31	122.95
4	4-U	7516	CIT	O3-C5-C4	-2.35	116.31	122.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5-U	7516	CIT	O3-C5-C4	-2.35	116.31	122.95
4	6-U	7516	CIT	O3-C5-C4	-2.35	116.31	122.95
4	7-U	7516	CIT	O3-C5-C4	-2.35	116.31	122.95
4	8-U	7516	CIT	O3-C5-C4	-2.35	116.31	122.95
4	9-U	7516	CIT	O3-C5-C4	-2.35	116.31	122.95
4	10-U	7516	CIT	O3-C5-C4	-2.35	116.31	122.95
4	1-N	7502	CIT	O3-C5-C4	-2.34	116.31	122.95
4	2-N	7502	CIT	O3-C5-C4	-2.34	116.31	122.95
4	3-N	7502	CIT	O3-C5-C4	-2.34	116.31	122.95
4	4-N	7502	CIT	O3-C5-C4	-2.34	116.31	122.95
4	5-N	7502	CIT	O3-C5-C4	-2.34	116.31	122.95
4	6-N	7502	CIT	O3-C5-C4	-2.34	116.31	122.95
4	7-N	7502	CIT	O3-C5-C4	-2.34	116.31	122.95
4	8-N	7502	CIT	O3-C5-C4	-2.34	116.31	122.95
4	9-N	7502	CIT	O3-C5-C4	-2.34	116.31	122.95
4	10-N	7502	CIT	O3-C5-C4	-2.34	116.31	122.95
4	1-V	7518	CIT	O3-C5-C4	-2.34	116.32	122.95
4	2-V	7518	CIT	O3-C5-C4	-2.34	116.32	122.95
4	3-V	7518	CIT	O3-C5-C4	-2.34	116.32	122.95
4	4-V	7518	CIT	O3-C5-C4	-2.34	116.32	122.95
4	5-V	7518	CIT	O3-C5-C4	-2.34	116.32	122.95
4	6-V	7518	CIT	O3-C5-C4	-2.34	116.32	122.95
4	7-V	7518	CIT	O3-C5-C4	-2.34	116.32	122.95
4	8-V	7518	CIT	O3-C5-C4	-2.34	116.32	122.95
4	9-V	7518	CIT	O3-C5-C4	-2.34	116.32	122.95
4	10-V	7518	CIT	O3-C5-C4	-2.34	116.32	122.95
4	1-L	7498	CIT	O3-C5-C4	-2.34	116.32	122.95
4	2-L	7498	CIT	O3-C5-C4	-2.34	116.32	122.95
4	3-L	7498	CIT	O3-C5-C4	-2.34	116.32	122.95
4	4-L	7498	CIT	O3-C5-C4	-2.34	116.32	122.95
4	5-L	7498	CIT	O3-C5-C4	-2.34	116.32	122.95
4	6-L	7498	CIT	O3-C5-C4	-2.34	116.32	122.95
4	7-L	7498	CIT	O3-C5-C4	-2.34	116.32	122.95
4	8-L	7498	CIT	O3-C5-C4	-2.34	116.32	122.95
4	9-L	7498	CIT	O3-C5-C4	-2.34	116.32	122.95
4	10-L	7498	CIT	O3-C5-C4	-2.34	116.32	122.95
4	1-Q	7508	CIT	O3-C5-C4	-2.34	116.33	122.95
4	2-Q	7508	CIT	O3-C5-C4	-2.34	116.33	122.95
4	3-Q	7508	CIT	O3-C5-C4	-2.34	116.33	122.95
4	4-Q	7508	CIT	O3-C5-C4	-2.34	116.33	122.95
4	5-Q	7508	CIT	O3-C5-C4	-2.34	116.33	122.95
4	6-Q	7508	CIT	O3-C5-C4	-2.34	116.33	122.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7-Q	7508	CIT	O3-C5-C4	-2.34	116.33	122.95
4	8-Q	7508	CIT	O3-C5-C4	-2.34	116.33	122.95
4	9-Q	7508	CIT	O3-C5-C4	-2.34	116.33	122.95
4	10-Q	7508	CIT	O3-C5-C4	-2.34	116.33	122.95
3	1-D	7481	AMP	O3P-P-O5'	2.30	112.68	106.67
3	2-D	7481	AMP	O3P-P-O5'	2.30	112.68	106.67
3	3-D	7481	AMP	O3P-P-O5'	2.30	112.68	106.67
3	4-D	7481	AMP	O3P-P-O5'	2.30	112.68	106.67
3	5-D	7481	AMP	O3P-P-O5'	2.30	112.68	106.67
3	6-D	7481	AMP	O3P-P-O5'	2.30	112.68	106.67
3	7-D	7481	AMP	O3P-P-O5'	2.30	112.68	106.67
3	8-D	7481	AMP	O3P-P-O5'	2.30	112.68	106.67
3	9-D	7481	AMP	O3P-P-O5'	2.30	112.68	106.67
3	10-D	7481	AMP	O3P-P-O5'	2.30	112.68	106.67
3	1-V	7517	AMP	O3P-P-O5'	2.30	112.66	106.67
3	2-V	7517	AMP	O3P-P-O5'	2.30	112.66	106.67
3	3-V	7517	AMP	O3P-P-O5'	2.30	112.66	106.67
3	4-V	7517	AMP	O3P-P-O5'	2.30	112.66	106.67
3	5-V	7517	AMP	O3P-P-O5'	2.30	112.66	106.67
3	6-V	7517	AMP	O3P-P-O5'	2.30	112.66	106.67
3	7-V	7517	AMP	O3P-P-O5'	2.30	112.66	106.67
3	8-V	7517	AMP	O3P-P-O5'	2.30	112.66	106.67
3	9-V	7517	AMP	O3P-P-O5'	2.30	112.66	106.67
3	10-V	7517	AMP	O3P-P-O5'	2.30	112.66	106.67
3	1-P	7505	AMP	O3P-P-O5'	2.30	112.66	106.67
3	2-P	7505	AMP	O3P-P-O5'	2.30	112.66	106.67
3	3-P	7505	AMP	O3P-P-O5'	2.30	112.66	106.67
3	4-P	7505	AMP	O3P-P-O5'	2.30	112.66	106.67
3	5-P	7505	AMP	O3P-P-O5'	2.30	112.66	106.67
3	6-P	7505	AMP	O3P-P-O5'	2.30	112.66	106.67
3	7-P	7505	AMP	O3P-P-O5'	2.30	112.66	106.67
3	8-P	7505	AMP	O3P-P-O5'	2.30	112.66	106.67
3	9-P	7505	AMP	O3P-P-O5'	2.30	112.66	106.67
3	10-P	7505	AMP	O3P-P-O5'	2.30	112.66	106.67
3	1-H	7489	AMP	O3P-P-O5'	2.30	112.66	106.67
3	2-H	7489	AMP	O3P-P-O5'	2.30	112.66	106.67
3	3-H	7489	AMP	O3P-P-O5'	2.30	112.66	106.67
3	4-H	7489	AMP	O3P-P-O5'	2.30	112.66	106.67
3	5-H	7489	AMP	O3P-P-O5'	2.30	112.66	106.67
3	6-H	7489	AMP	O3P-P-O5'	2.30	112.66	106.67
3	7-H	7489	AMP	O3P-P-O5'	2.30	112.66	106.67
3	8-H	7489	AMP	O3P-P-O5'	2.30	112.66	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-H	7489	AMP	O3P-P-O5'	2.30	112.66	106.67
3	10-H	7489	AMP	O3P-P-O5'	2.30	112.66	106.67
3	1-C	7479	AMP	O3P-P-O5'	2.29	112.65	106.67
3	2-C	7479	AMP	O3P-P-O5'	2.29	112.65	106.67
3	3-C	7479	AMP	O3P-P-O5'	2.29	112.65	106.67
3	4-C	7479	AMP	O3P-P-O5'	2.29	112.65	106.67
3	5-C	7479	AMP	O3P-P-O5'	2.29	112.65	106.67
3	6-C	7479	AMP	O3P-P-O5'	2.29	112.65	106.67
3	7-C	7479	AMP	O3P-P-O5'	2.29	112.65	106.67
3	8-C	7479	AMP	O3P-P-O5'	2.29	112.65	106.67
3	9-C	7479	AMP	O3P-P-O5'	2.29	112.65	106.67
3	10-C	7479	AMP	O3P-P-O5'	2.29	112.65	106.67
3	1-S	7511	AMP	O3P-P-O5'	2.29	112.65	106.67
3	2-S	7511	AMP	O3P-P-O5'	2.29	112.65	106.67
3	3-S	7511	AMP	O3P-P-O5'	2.29	112.65	106.67
3	4-S	7511	AMP	O3P-P-O5'	2.29	112.65	106.67
3	5-S	7511	AMP	O3P-P-O5'	2.29	112.65	106.67
3	6-S	7511	AMP	O3P-P-O5'	2.29	112.65	106.67
3	7-S	7511	AMP	O3P-P-O5'	2.29	112.65	106.67
3	8-S	7511	AMP	O3P-P-O5'	2.29	112.65	106.67
3	9-S	7511	AMP	O3P-P-O5'	2.29	112.65	106.67
3	10-S	7511	AMP	O3P-P-O5'	2.29	112.65	106.67
3	1-G	7487	AMP	O3P-P-O5'	2.29	112.64	106.67
3	2-G	7487	AMP	O3P-P-O5'	2.29	112.64	106.67
3	3-G	7487	AMP	O3P-P-O5'	2.29	112.64	106.67
3	4-G	7487	AMP	O3P-P-O5'	2.29	112.64	106.67
3	5-G	7487	AMP	O3P-P-O5'	2.29	112.64	106.67
3	6-G	7487	AMP	O3P-P-O5'	2.29	112.64	106.67
3	7-G	7487	AMP	O3P-P-O5'	2.29	112.64	106.67
3	8-G	7487	AMP	O3P-P-O5'	2.29	112.64	106.67
3	9-G	7487	AMP	O3P-P-O5'	2.29	112.64	106.67
3	10-G	7487	AMP	O3P-P-O5'	2.29	112.64	106.67
3	1-F	7485	AMP	O3P-P-O5'	2.29	112.64	106.67
3	2-F	7485	AMP	O3P-P-O5'	2.29	112.64	106.67
3	3-F	7485	AMP	O3P-P-O5'	2.29	112.64	106.67
3	4-F	7485	AMP	O3P-P-O5'	2.29	112.64	106.67
3	5-F	7485	AMP	O3P-P-O5'	2.29	112.64	106.67
3	6-F	7485	AMP	O3P-P-O5'	2.29	112.64	106.67
3	7-F	7485	AMP	O3P-P-O5'	2.29	112.64	106.67
3	8-F	7485	AMP	O3P-P-O5'	2.29	112.64	106.67
3	9-F	7485	AMP	O3P-P-O5'	2.29	112.64	106.67
3	10-F	7485	AMP	O3P-P-O5'	2.29	112.64	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-E	7483	AMP	O3P-P-O5'	2.29	112.64	106.67
3	2-E	7483	AMP	O3P-P-O5'	2.29	112.64	106.67
3	3-E	7483	AMP	O3P-P-O5'	2.29	112.64	106.67
3	4-E	7483	AMP	O3P-P-O5'	2.29	112.64	106.67
3	5-E	7483	AMP	O3P-P-O5'	2.29	112.64	106.67
3	6-E	7483	AMP	O3P-P-O5'	2.29	112.64	106.67
3	7-E	7483	AMP	O3P-P-O5'	2.29	112.64	106.67
3	8-E	7483	AMP	O3P-P-O5'	2.29	112.64	106.67
3	9-E	7483	AMP	O3P-P-O5'	2.29	112.64	106.67
3	10-E	7483	AMP	O3P-P-O5'	2.29	112.64	106.67
3	1-I	7491	AMP	O3P-P-O5'	2.29	112.64	106.67
3	2-I	7491	AMP	O3P-P-O5'	2.29	112.64	106.67
3	3-I	7491	AMP	O3P-P-O5'	2.29	112.64	106.67
3	4-I	7491	AMP	O3P-P-O5'	2.29	112.64	106.67
3	5-I	7491	AMP	O3P-P-O5'	2.29	112.64	106.67
3	6-I	7491	AMP	O3P-P-O5'	2.29	112.64	106.67
3	7-I	7491	AMP	O3P-P-O5'	2.29	112.64	106.67
3	8-I	7491	AMP	O3P-P-O5'	2.29	112.64	106.67
3	9-I	7491	AMP	O3P-P-O5'	2.29	112.64	106.67
3	10-I	7491	AMP	O3P-P-O5'	2.29	112.64	106.67
3	1-A	7475	AMP	O3P-P-O5'	2.29	112.63	106.67
3	2-A	7475	AMP	O3P-P-O5'	2.29	112.63	106.67
3	3-A	7475	AMP	O3P-P-O5'	2.29	112.63	106.67
3	4-A	7475	AMP	O3P-P-O5'	2.29	112.63	106.67
3	5-A	7475	AMP	O3P-P-O5'	2.29	112.63	106.67
3	6-A	7475	AMP	O3P-P-O5'	2.29	112.63	106.67
3	7-A	7475	AMP	O3P-P-O5'	2.29	112.63	106.67
3	8-A	7475	AMP	O3P-P-O5'	2.29	112.63	106.67
3	9-A	7475	AMP	O3P-P-O5'	2.29	112.63	106.67
3	10-A	7475	AMP	O3P-P-O5'	2.29	112.63	106.67
3	1-R	7509	AMP	O3P-P-O5'	2.29	112.63	106.67
3	2-R	7509	AMP	O3P-P-O5'	2.29	112.63	106.67
3	3-R	7509	AMP	O3P-P-O5'	2.29	112.63	106.67
3	4-R	7509	AMP	O3P-P-O5'	2.29	112.63	106.67
3	5-R	7509	AMP	O3P-P-O5'	2.29	112.63	106.67
3	6-R	7509	AMP	O3P-P-O5'	2.29	112.63	106.67
3	7-R	7509	AMP	O3P-P-O5'	2.29	112.63	106.67
3	8-R	7509	AMP	O3P-P-O5'	2.29	112.63	106.67
3	9-R	7509	AMP	O3P-P-O5'	2.29	112.63	106.67
3	10-R	7509	AMP	O3P-P-O5'	2.29	112.63	106.67
3	1-J	7493	AMP	O3P-P-O5'	2.29	112.63	106.67
3	2-J	7493	AMP	O3P-P-O5'	2.29	112.63	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-J	7493	AMP	O3P-P-O5'	2.29	112.63	106.67
3	4-J	7493	AMP	O3P-P-O5'	2.29	112.63	106.67
3	5-J	7493	AMP	O3P-P-O5'	2.29	112.63	106.67
3	6-J	7493	AMP	O3P-P-O5'	2.29	112.63	106.67
3	7-J	7493	AMP	O3P-P-O5'	2.29	112.63	106.67
3	8-J	7493	AMP	O3P-P-O5'	2.29	112.63	106.67
3	9-J	7493	AMP	O3P-P-O5'	2.29	112.63	106.67
3	10-J	7493	AMP	O3P-P-O5'	2.29	112.63	106.67
3	1-B	7477	AMP	O3P-P-O5'	2.28	112.63	106.67
3	2-B	7477	AMP	O3P-P-O5'	2.28	112.63	106.67
3	3-B	7477	AMP	O3P-P-O5'	2.28	112.63	106.67
3	4-B	7477	AMP	O3P-P-O5'	2.28	112.63	106.67
3	5-B	7477	AMP	O3P-P-O5'	2.28	112.63	106.67
3	6-B	7477	AMP	O3P-P-O5'	2.28	112.63	106.67
3	7-B	7477	AMP	O3P-P-O5'	2.28	112.63	106.67
3	8-B	7477	AMP	O3P-P-O5'	2.28	112.63	106.67
3	9-B	7477	AMP	O3P-P-O5'	2.28	112.63	106.67
3	10-B	7477	AMP	O3P-P-O5'	2.28	112.63	106.67
3	1-K	7495	AMP	O3P-P-O5'	2.28	112.62	106.67
3	2-K	7495	AMP	O3P-P-O5'	2.28	112.62	106.67
3	3-K	7495	AMP	O3P-P-O5'	2.28	112.62	106.67
3	4-K	7495	AMP	O3P-P-O5'	2.28	112.62	106.67
3	5-K	7495	AMP	O3P-P-O5'	2.28	112.62	106.67
3	6-K	7495	AMP	O3P-P-O5'	2.28	112.62	106.67
3	7-K	7495	AMP	O3P-P-O5'	2.28	112.62	106.67
3	8-K	7495	AMP	O3P-P-O5'	2.28	112.62	106.67
3	9-K	7495	AMP	O3P-P-O5'	2.28	112.62	106.67
3	10-K	7495	AMP	O3P-P-O5'	2.28	112.62	106.67
3	1-O	7503	AMP	O3P-P-O5'	2.28	112.62	106.67
3	2-O	7503	AMP	O3P-P-O5'	2.28	112.62	106.67
3	3-O	7503	AMP	O3P-P-O5'	2.28	112.62	106.67
3	4-O	7503	AMP	O3P-P-O5'	2.28	112.62	106.67
3	5-O	7503	AMP	O3P-P-O5'	2.28	112.62	106.67
3	6-O	7503	AMP	O3P-P-O5'	2.28	112.62	106.67
3	7-O	7503	AMP	O3P-P-O5'	2.28	112.62	106.67
3	8-O	7503	AMP	O3P-P-O5'	2.28	112.62	106.67
3	9-O	7503	AMP	O3P-P-O5'	2.28	112.62	106.67
3	10-O	7503	AMP	O3P-P-O5'	2.28	112.62	106.67
3	1-Q	7507	AMP	O3P-P-O5'	2.28	112.62	106.67
3	2-Q	7507	AMP	O3P-P-O5'	2.28	112.62	106.67
3	3-Q	7507	AMP	O3P-P-O5'	2.28	112.62	106.67
3	4-Q	7507	AMP	O3P-P-O5'	2.28	112.62	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-Q	7507	AMP	O3P-P-O5'	2.28	112.62	106.67
3	6-Q	7507	AMP	O3P-P-O5'	2.28	112.62	106.67
3	7-Q	7507	AMP	O3P-P-O5'	2.28	112.62	106.67
3	8-Q	7507	AMP	O3P-P-O5'	2.28	112.62	106.67
3	9-Q	7507	AMP	O3P-P-O5'	2.28	112.62	106.67
3	10-Q	7507	AMP	O3P-P-O5'	2.28	112.62	106.67
3	1-N	7501	AMP	O3P-P-O5'	2.28	112.61	106.67
3	2-N	7501	AMP	O3P-P-O5'	2.28	112.61	106.67
3	3-N	7501	AMP	O3P-P-O5'	2.28	112.61	106.67
3	4-N	7501	AMP	O3P-P-O5'	2.28	112.61	106.67
3	5-N	7501	AMP	O3P-P-O5'	2.28	112.61	106.67
3	6-N	7501	AMP	O3P-P-O5'	2.28	112.61	106.67
3	7-N	7501	AMP	O3P-P-O5'	2.28	112.61	106.67
3	8-N	7501	AMP	O3P-P-O5'	2.28	112.61	106.67
3	9-N	7501	AMP	O3P-P-O5'	2.28	112.61	106.67
3	10-N	7501	AMP	O3P-P-O5'	2.28	112.61	106.67
4	1-S	7512	CIT	O7-C3-C6	-2.28	105.73	108.96
4	2-S	7512	CIT	O7-C3-C6	-2.28	105.73	108.96
4	3-S	7512	CIT	O7-C3-C6	-2.28	105.73	108.96
4	4-S	7512	CIT	O7-C3-C6	-2.28	105.73	108.96
4	5-S	7512	CIT	O7-C3-C6	-2.28	105.73	108.96
4	6-S	7512	CIT	O7-C3-C6	-2.28	105.73	108.96
4	7-S	7512	CIT	O7-C3-C6	-2.28	105.73	108.96
4	8-S	7512	CIT	O7-C3-C6	-2.28	105.73	108.96
4	9-S	7512	CIT	O7-C3-C6	-2.28	105.73	108.96
4	10-S	7512	CIT	O7-C3-C6	-2.28	105.73	108.96
4	1-U	7516	CIT	O7-C3-C6	-2.28	105.73	108.96
4	2-U	7516	CIT	O7-C3-C6	-2.28	105.73	108.96
4	3-U	7516	CIT	O7-C3-C6	-2.28	105.73	108.96
4	4-U	7516	CIT	O7-C3-C6	-2.28	105.73	108.96
4	5-U	7516	CIT	O7-C3-C6	-2.28	105.73	108.96
4	6-U	7516	CIT	O7-C3-C6	-2.28	105.73	108.96
4	7-U	7516	CIT	O7-C3-C6	-2.28	105.73	108.96
4	8-U	7516	CIT	O7-C3-C6	-2.28	105.73	108.96
4	9-U	7516	CIT	O7-C3-C6	-2.28	105.73	108.96
4	10-U	7516	CIT	O7-C3-C6	-2.28	105.73	108.96
3	1-T	7513	AMP	O3P-P-O5'	2.28	112.60	106.67
3	2-T	7513	AMP	O3P-P-O5'	2.28	112.60	106.67
3	3-T	7513	AMP	O3P-P-O5'	2.28	112.60	106.67
3	4-T	7513	AMP	O3P-P-O5'	2.28	112.60	106.67
3	5-T	7513	AMP	O3P-P-O5'	2.28	112.60	106.67
3	6-T	7513	AMP	O3P-P-O5'	2.28	112.60	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-T	7513	AMP	O3P-P-O5'	2.28	112.60	106.67
3	8-T	7513	AMP	O3P-P-O5'	2.28	112.60	106.67
3	9-T	7513	AMP	O3P-P-O5'	2.28	112.60	106.67
3	10-T	7513	AMP	O3P-P-O5'	2.28	112.60	106.67
3	1-L	7497	AMP	O3P-P-O5'	2.28	112.60	106.67
3	2-L	7497	AMP	O3P-P-O5'	2.28	112.60	106.67
3	3-L	7497	AMP	O3P-P-O5'	2.28	112.60	106.67
3	4-L	7497	AMP	O3P-P-O5'	2.28	112.60	106.67
3	5-L	7497	AMP	O3P-P-O5'	2.28	112.60	106.67
3	6-L	7497	AMP	O3P-P-O5'	2.28	112.60	106.67
3	7-L	7497	AMP	O3P-P-O5'	2.28	112.60	106.67
3	8-L	7497	AMP	O3P-P-O5'	2.28	112.60	106.67
3	9-L	7497	AMP	O3P-P-O5'	2.28	112.60	106.67
3	10-L	7497	AMP	O3P-P-O5'	2.28	112.60	106.67
3	1-U	7515	AMP	O3P-P-O5'	2.28	112.60	106.67
3	2-U	7515	AMP	O3P-P-O5'	2.28	112.60	106.67
3	3-U	7515	AMP	O3P-P-O5'	2.28	112.60	106.67
3	4-U	7515	AMP	O3P-P-O5'	2.28	112.60	106.67
3	5-U	7515	AMP	O3P-P-O5'	2.28	112.60	106.67
3	6-U	7515	AMP	O3P-P-O5'	2.28	112.60	106.67
3	7-U	7515	AMP	O3P-P-O5'	2.28	112.60	106.67
3	8-U	7515	AMP	O3P-P-O5'	2.28	112.60	106.67
3	9-U	7515	AMP	O3P-P-O5'	2.28	112.60	106.67
3	10-U	7515	AMP	O3P-P-O5'	2.28	112.60	106.67
3	1-W	7519	AMP	O3P-P-O5'	2.27	112.60	106.67
3	2-W	7519	AMP	O3P-P-O5'	2.27	112.60	106.67
3	3-W	7519	AMP	O3P-P-O5'	2.27	112.60	106.67
3	4-W	7519	AMP	O3P-P-O5'	2.27	112.60	106.67
3	5-W	7519	AMP	O3P-P-O5'	2.27	112.60	106.67
3	6-W	7519	AMP	O3P-P-O5'	2.27	112.60	106.67
3	7-W	7519	AMP	O3P-P-O5'	2.27	112.60	106.67
3	8-W	7519	AMP	O3P-P-O5'	2.27	112.60	106.67
3	9-W	7519	AMP	O3P-P-O5'	2.27	112.60	106.67
3	10-W	7519	AMP	O3P-P-O5'	2.27	112.60	106.67
3	1-X	7521	AMP	O3P-P-O5'	2.27	112.59	106.67
3	2-X	7521	AMP	O3P-P-O5'	2.27	112.59	106.67
3	3-X	7521	AMP	O3P-P-O5'	2.27	112.59	106.67
3	4-X	7521	AMP	O3P-P-O5'	2.27	112.59	106.67
3	5-X	7521	AMP	O3P-P-O5'	2.27	112.59	106.67
3	6-X	7521	AMP	O3P-P-O5'	2.27	112.59	106.67
3	7-X	7521	AMP	O3P-P-O5'	2.27	112.59	106.67
3	8-X	7521	AMP	O3P-P-O5'	2.27	112.59	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-X	7521	AMP	O3P-P-O5'	2.27	112.59	106.67
3	10-X	7521	AMP	O3P-P-O5'	2.27	112.59	106.67
3	1-M	7499	AMP	O3P-P-O5'	2.26	112.57	106.67
3	2-M	7499	AMP	O3P-P-O5'	2.26	112.57	106.67
3	3-M	7499	AMP	O3P-P-O5'	2.26	112.57	106.67
3	4-M	7499	AMP	O3P-P-O5'	2.26	112.57	106.67
3	5-M	7499	AMP	O3P-P-O5'	2.26	112.57	106.67
3	6-M	7499	AMP	O3P-P-O5'	2.26	112.57	106.67
3	7-M	7499	AMP	O3P-P-O5'	2.26	112.57	106.67
3	8-M	7499	AMP	O3P-P-O5'	2.26	112.57	106.67
3	9-M	7499	AMP	O3P-P-O5'	2.26	112.57	106.67
3	10-M	7499	AMP	O3P-P-O5'	2.26	112.57	106.67
4	1-K	7496	CIT	O7-C3-C6	-2.26	105.75	108.96
4	2-K	7496	CIT	O7-C3-C6	-2.26	105.75	108.96
4	3-K	7496	CIT	O7-C3-C6	-2.26	105.75	108.96
4	4-K	7496	CIT	O7-C3-C6	-2.26	105.75	108.96
4	5-K	7496	CIT	O7-C3-C6	-2.26	105.75	108.96
4	6-K	7496	CIT	O7-C3-C6	-2.26	105.75	108.96
4	7-K	7496	CIT	O7-C3-C6	-2.26	105.75	108.96
4	8-K	7496	CIT	O7-C3-C6	-2.26	105.75	108.96
4	9-K	7496	CIT	O7-C3-C6	-2.26	105.75	108.96
4	10-K	7496	CIT	O7-C3-C6	-2.26	105.75	108.96
4	1-H	7490	CIT	O7-C3-C6	-2.26	105.75	108.96
4	2-H	7490	CIT	O7-C3-C6	-2.26	105.75	108.96
4	3-H	7490	CIT	O7-C3-C6	-2.26	105.75	108.96
4	4-H	7490	CIT	O7-C3-C6	-2.26	105.75	108.96
4	5-H	7490	CIT	O7-C3-C6	-2.26	105.75	108.96
4	6-H	7490	CIT	O7-C3-C6	-2.26	105.75	108.96
4	7-H	7490	CIT	O7-C3-C6	-2.26	105.75	108.96
4	8-H	7490	CIT	O7-C3-C6	-2.26	105.75	108.96
4	9-H	7490	CIT	O7-C3-C6	-2.26	105.75	108.96
4	10-H	7490	CIT	O7-C3-C6	-2.26	105.75	108.96
4	1-J	7494	CIT	O7-C3-C6	-2.26	105.75	108.96
4	2-J	7494	CIT	O7-C3-C6	-2.26	105.75	108.96
4	3-J	7494	CIT	O7-C3-C6	-2.26	105.75	108.96
4	4-J	7494	CIT	O7-C3-C6	-2.26	105.75	108.96
4	5-J	7494	CIT	O7-C3-C6	-2.26	105.75	108.96
4	6-J	7494	CIT	O7-C3-C6	-2.26	105.75	108.96
4	7-J	7494	CIT	O7-C3-C6	-2.26	105.75	108.96
4	8-J	7494	CIT	O7-C3-C6	-2.26	105.75	108.96
4	9-J	7494	CIT	O7-C3-C6	-2.26	105.75	108.96
4	10-J	7494	CIT	O7-C3-C6	-2.26	105.75	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-D	7482	CIT	O7-C3-C6	-2.26	105.75	108.96
4	2-D	7482	CIT	O7-C3-C6	-2.26	105.75	108.96
4	3-D	7482	CIT	O7-C3-C6	-2.26	105.75	108.96
4	4-D	7482	CIT	O7-C3-C6	-2.26	105.75	108.96
4	5-D	7482	CIT	O7-C3-C6	-2.26	105.75	108.96
4	6-D	7482	CIT	O7-C3-C6	-2.26	105.75	108.96
4	7-D	7482	CIT	O7-C3-C6	-2.26	105.75	108.96
4	8-D	7482	CIT	O7-C3-C6	-2.26	105.75	108.96
4	9-D	7482	CIT	O7-C3-C6	-2.26	105.75	108.96
4	10-D	7482	CIT	O7-C3-C6	-2.26	105.75	108.96
4	1-R	7510	CIT	O7-C3-C6	-2.26	105.75	108.96
4	2-R	7510	CIT	O7-C3-C6	-2.26	105.75	108.96
4	3-R	7510	CIT	O7-C3-C6	-2.26	105.75	108.96
4	4-R	7510	CIT	O7-C3-C6	-2.26	105.75	108.96
4	5-R	7510	CIT	O7-C3-C6	-2.26	105.75	108.96
4	6-R	7510	CIT	O7-C3-C6	-2.26	105.75	108.96
4	7-R	7510	CIT	O7-C3-C6	-2.26	105.75	108.96
4	8-R	7510	CIT	O7-C3-C6	-2.26	105.75	108.96
4	9-R	7510	CIT	O7-C3-C6	-2.26	105.75	108.96
4	10-R	7510	CIT	O7-C3-C6	-2.26	105.75	108.96
4	1-I	7492	CIT	O7-C3-C6	-2.25	105.76	108.96
4	2-I	7492	CIT	O7-C3-C6	-2.25	105.76	108.96
4	3-I	7492	CIT	O7-C3-C6	-2.25	105.76	108.96
4	4-I	7492	CIT	O7-C3-C6	-2.25	105.76	108.96
4	5-I	7492	CIT	O7-C3-C6	-2.25	105.76	108.96
4	6-I	7492	CIT	O7-C3-C6	-2.25	105.76	108.96
4	7-I	7492	CIT	O7-C3-C6	-2.25	105.76	108.96
4	8-I	7492	CIT	O7-C3-C6	-2.25	105.76	108.96
4	9-I	7492	CIT	O7-C3-C6	-2.25	105.76	108.96
4	10-I	7492	CIT	O7-C3-C6	-2.25	105.76	108.96
4	1-T	7514	CIT	O7-C3-C6	-2.25	105.77	108.96
4	2-T	7514	CIT	O7-C3-C6	-2.25	105.77	108.96
4	3-T	7514	CIT	O7-C3-C6	-2.25	105.77	108.96
4	4-T	7514	CIT	O7-C3-C6	-2.25	105.77	108.96
4	5-T	7514	CIT	O7-C3-C6	-2.25	105.77	108.96
4	6-T	7514	CIT	O7-C3-C6	-2.25	105.77	108.96
4	7-T	7514	CIT	O7-C3-C6	-2.25	105.77	108.96
4	8-T	7514	CIT	O7-C3-C6	-2.25	105.77	108.96
4	9-T	7514	CIT	O7-C3-C6	-2.25	105.77	108.96
4	10-T	7514	CIT	O7-C3-C6	-2.25	105.77	108.96
4	1-C	7480	CIT	O7-C3-C6	-2.25	105.77	108.96
4	2-C	7480	CIT	O7-C3-C6	-2.25	105.77	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-C	7480	CIT	O7-C3-C6	-2.25	105.77	108.96
4	4-C	7480	CIT	O7-C3-C6	-2.25	105.77	108.96
4	5-C	7480	CIT	O7-C3-C6	-2.25	105.77	108.96
4	6-C	7480	CIT	O7-C3-C6	-2.25	105.77	108.96
4	7-C	7480	CIT	O7-C3-C6	-2.25	105.77	108.96
4	8-C	7480	CIT	O7-C3-C6	-2.25	105.77	108.96
4	9-C	7480	CIT	O7-C3-C6	-2.25	105.77	108.96
4	10-C	7480	CIT	O7-C3-C6	-2.25	105.77	108.96
4	1-A	7476	CIT	O7-C3-C6	-2.25	105.77	108.96
4	2-A	7476	CIT	O7-C3-C6	-2.25	105.77	108.96
4	3-A	7476	CIT	O7-C3-C6	-2.25	105.77	108.96
4	4-A	7476	CIT	O7-C3-C6	-2.25	105.77	108.96
4	5-A	7476	CIT	O7-C3-C6	-2.25	105.77	108.96
4	6-A	7476	CIT	O7-C3-C6	-2.25	105.77	108.96
4	7-A	7476	CIT	O7-C3-C6	-2.25	105.77	108.96
4	8-A	7476	CIT	O7-C3-C6	-2.25	105.77	108.96
4	9-A	7476	CIT	O7-C3-C6	-2.25	105.77	108.96
4	10-A	7476	CIT	O7-C3-C6	-2.25	105.77	108.96
4	1-P	7506	CIT	O7-C3-C6	-2.24	105.78	108.96
4	2-P	7506	CIT	O7-C3-C6	-2.24	105.78	108.96
4	3-P	7506	CIT	O7-C3-C6	-2.24	105.78	108.96
4	4-P	7506	CIT	O7-C3-C6	-2.24	105.78	108.96
4	5-P	7506	CIT	O7-C3-C6	-2.24	105.78	108.96
4	6-P	7506	CIT	O7-C3-C6	-2.24	105.78	108.96
4	7-P	7506	CIT	O7-C3-C6	-2.24	105.78	108.96
4	8-P	7506	CIT	O7-C3-C6	-2.24	105.78	108.96
4	9-P	7506	CIT	O7-C3-C6	-2.24	105.78	108.96
4	10-P	7506	CIT	O7-C3-C6	-2.24	105.78	108.96
4	1-X	7522	CIT	O7-C3-C6	-2.24	105.78	108.96
4	2-X	7522	CIT	O7-C3-C6	-2.24	105.78	108.96
4	3-X	7522	CIT	O7-C3-C6	-2.24	105.78	108.96
4	4-X	7522	CIT	O7-C3-C6	-2.24	105.78	108.96
4	5-X	7522	CIT	O7-C3-C6	-2.24	105.78	108.96
4	6-X	7522	CIT	O7-C3-C6	-2.24	105.78	108.96
4	7-X	7522	CIT	O7-C3-C6	-2.24	105.78	108.96
4	8-X	7522	CIT	O7-C3-C6	-2.24	105.78	108.96
4	9-X	7522	CIT	O7-C3-C6	-2.24	105.78	108.96
4	10-X	7522	CIT	O7-C3-C6	-2.24	105.78	108.96
4	1-V	7518	CIT	O7-C3-C6	-2.24	105.78	108.96
4	2-V	7518	CIT	O7-C3-C6	-2.24	105.78	108.96
4	3-V	7518	CIT	O7-C3-C6	-2.24	105.78	108.96
4	4-V	7518	CIT	O7-C3-C6	-2.24	105.78	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5-V	7518	CIT	O7-C3-C6	-2.24	105.78	108.96
4	6-V	7518	CIT	O7-C3-C6	-2.24	105.78	108.96
4	7-V	7518	CIT	O7-C3-C6	-2.24	105.78	108.96
4	8-V	7518	CIT	O7-C3-C6	-2.24	105.78	108.96
4	9-V	7518	CIT	O7-C3-C6	-2.24	105.78	108.96
4	10-V	7518	CIT	O7-C3-C6	-2.24	105.78	108.96
4	1-G	7488	CIT	O7-C3-C6	-2.24	105.78	108.96
4	2-G	7488	CIT	O7-C3-C6	-2.24	105.78	108.96
4	3-G	7488	CIT	O7-C3-C6	-2.24	105.78	108.96
4	4-G	7488	CIT	O7-C3-C6	-2.24	105.78	108.96
4	5-G	7488	CIT	O7-C3-C6	-2.24	105.78	108.96
4	6-G	7488	CIT	O7-C3-C6	-2.24	105.78	108.96
4	7-G	7488	CIT	O7-C3-C6	-2.24	105.78	108.96
4	8-G	7488	CIT	O7-C3-C6	-2.24	105.78	108.96
4	9-G	7488	CIT	O7-C3-C6	-2.24	105.78	108.96
4	10-G	7488	CIT	O7-C3-C6	-2.24	105.78	108.96
4	1-M	7500	CIT	O7-C3-C6	-2.24	105.78	108.96
4	2-M	7500	CIT	O7-C3-C6	-2.24	105.78	108.96
4	3-M	7500	CIT	O7-C3-C6	-2.24	105.78	108.96
4	4-M	7500	CIT	O7-C3-C6	-2.24	105.78	108.96
4	5-M	7500	CIT	O7-C3-C6	-2.24	105.78	108.96
4	6-M	7500	CIT	O7-C3-C6	-2.24	105.78	108.96
4	7-M	7500	CIT	O7-C3-C6	-2.24	105.78	108.96
4	8-M	7500	CIT	O7-C3-C6	-2.24	105.78	108.96
4	9-M	7500	CIT	O7-C3-C6	-2.24	105.78	108.96
4	10-M	7500	CIT	O7-C3-C6	-2.24	105.78	108.96
4	1-F	7486	CIT	O7-C3-C6	-2.24	105.79	108.96
4	2-F	7486	CIT	O7-C3-C6	-2.24	105.79	108.96
4	3-F	7486	CIT	O7-C3-C6	-2.24	105.79	108.96
4	4-F	7486	CIT	O7-C3-C6	-2.24	105.79	108.96
4	5-F	7486	CIT	O7-C3-C6	-2.24	105.79	108.96
4	6-F	7486	CIT	O7-C3-C6	-2.24	105.79	108.96
4	7-F	7486	CIT	O7-C3-C6	-2.24	105.79	108.96
4	8-F	7486	CIT	O7-C3-C6	-2.24	105.79	108.96
4	9-F	7486	CIT	O7-C3-C6	-2.24	105.79	108.96
4	10-F	7486	CIT	O7-C3-C6	-2.24	105.79	108.96
4	1-W	7520	CIT	O7-C3-C6	-2.23	105.79	108.96
4	2-W	7520	CIT	O7-C3-C6	-2.23	105.79	108.96
4	3-W	7520	CIT	O7-C3-C6	-2.23	105.79	108.96
4	4-W	7520	CIT	O7-C3-C6	-2.23	105.79	108.96
4	5-W	7520	CIT	O7-C3-C6	-2.23	105.79	108.96
4	6-W	7520	CIT	O7-C3-C6	-2.23	105.79	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7-W	7520	CIT	O7-C3-C6	-2.23	105.79	108.96
4	8-W	7520	CIT	O7-C3-C6	-2.23	105.79	108.96
4	9-W	7520	CIT	O7-C3-C6	-2.23	105.79	108.96
4	10-W	7520	CIT	O7-C3-C6	-2.23	105.79	108.96
4	1-E	7484	CIT	O7-C3-C6	-2.23	105.79	108.96
4	2-E	7484	CIT	O7-C3-C6	-2.23	105.79	108.96
4	3-E	7484	CIT	O7-C3-C6	-2.23	105.79	108.96
4	4-E	7484	CIT	O7-C3-C6	-2.23	105.79	108.96
4	5-E	7484	CIT	O7-C3-C6	-2.23	105.79	108.96
4	6-E	7484	CIT	O7-C3-C6	-2.23	105.79	108.96
4	7-E	7484	CIT	O7-C3-C6	-2.23	105.79	108.96
4	8-E	7484	CIT	O7-C3-C6	-2.23	105.79	108.96
4	9-E	7484	CIT	O7-C3-C6	-2.23	105.79	108.96
4	10-E	7484	CIT	O7-C3-C6	-2.23	105.79	108.96
4	1-Q	7508	CIT	O7-C3-C6	-2.23	105.79	108.96
4	2-Q	7508	CIT	O7-C3-C6	-2.23	105.79	108.96
4	3-Q	7508	CIT	O7-C3-C6	-2.23	105.79	108.96
4	4-Q	7508	CIT	O7-C3-C6	-2.23	105.79	108.96
4	5-Q	7508	CIT	O7-C3-C6	-2.23	105.79	108.96
4	6-Q	7508	CIT	O7-C3-C6	-2.23	105.79	108.96
4	7-Q	7508	CIT	O7-C3-C6	-2.23	105.79	108.96
4	8-Q	7508	CIT	O7-C3-C6	-2.23	105.79	108.96
4	9-Q	7508	CIT	O7-C3-C6	-2.23	105.79	108.96
4	10-Q	7508	CIT	O7-C3-C6	-2.23	105.79	108.96
4	1-B	7478	CIT	O7-C3-C6	-2.23	105.80	108.96
4	2-B	7478	CIT	O7-C3-C6	-2.23	105.80	108.96
4	3-B	7478	CIT	O7-C3-C6	-2.23	105.80	108.96
4	4-B	7478	CIT	O7-C3-C6	-2.23	105.80	108.96
4	5-B	7478	CIT	O7-C3-C6	-2.23	105.80	108.96
4	6-B	7478	CIT	O7-C3-C6	-2.23	105.80	108.96
4	7-B	7478	CIT	O7-C3-C6	-2.23	105.80	108.96
4	8-B	7478	CIT	O7-C3-C6	-2.23	105.80	108.96
4	9-B	7478	CIT	O7-C3-C6	-2.23	105.80	108.96
4	10-B	7478	CIT	O7-C3-C6	-2.23	105.80	108.96
4	1-N	7502	CIT	O7-C3-C6	-2.22	105.81	108.96
4	2-N	7502	CIT	O7-C3-C6	-2.22	105.81	108.96
4	3-N	7502	CIT	O7-C3-C6	-2.22	105.81	108.96
4	4-N	7502	CIT	O7-C3-C6	-2.22	105.81	108.96
4	5-N	7502	CIT	O7-C3-C6	-2.22	105.81	108.96
4	6-N	7502	CIT	O7-C3-C6	-2.22	105.81	108.96
4	7-N	7502	CIT	O7-C3-C6	-2.22	105.81	108.96
4	8-N	7502	CIT	O7-C3-C6	-2.22	105.81	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9-N	7502	CIT	O7-C3-C6	-2.22	105.81	108.96
4	10-N	7502	CIT	O7-C3-C6	-2.22	105.81	108.96
4	1-L	7498	CIT	O7-C3-C6	-2.22	105.81	108.96
4	2-L	7498	CIT	O7-C3-C6	-2.22	105.81	108.96
4	3-L	7498	CIT	O7-C3-C6	-2.22	105.81	108.96
4	4-L	7498	CIT	O7-C3-C6	-2.22	105.81	108.96
4	5-L	7498	CIT	O7-C3-C6	-2.22	105.81	108.96
4	6-L	7498	CIT	O7-C3-C6	-2.22	105.81	108.96
4	7-L	7498	CIT	O7-C3-C6	-2.22	105.81	108.96
4	8-L	7498	CIT	O7-C3-C6	-2.22	105.81	108.96
4	9-L	7498	CIT	O7-C3-C6	-2.22	105.81	108.96
4	10-L	7498	CIT	O7-C3-C6	-2.22	105.81	108.96
4	1-O	7504	CIT	O7-C3-C6	-2.21	105.82	108.96
4	2-O	7504	CIT	O7-C3-C6	-2.21	105.82	108.96
4	3-O	7504	CIT	O7-C3-C6	-2.21	105.82	108.96
4	4-O	7504	CIT	O7-C3-C6	-2.21	105.82	108.96
4	5-O	7504	CIT	O7-C3-C6	-2.21	105.82	108.96
4	6-O	7504	CIT	O7-C3-C6	-2.21	105.82	108.96
4	7-O	7504	CIT	O7-C3-C6	-2.21	105.82	108.96
4	8-O	7504	CIT	O7-C3-C6	-2.21	105.82	108.96
4	9-O	7504	CIT	O7-C3-C6	-2.21	105.82	108.96
4	10-O	7504	CIT	O7-C3-C6	-2.21	105.82	108.96
4	1-D	7482	CIT	O2-C1-O1	2.15	128.85	123.33
4	2-D	7482	CIT	O2-C1-O1	2.15	128.85	123.33
4	3-D	7482	CIT	O2-C1-O1	2.15	128.85	123.33
4	4-D	7482	CIT	O2-C1-O1	2.15	128.85	123.33
4	5-D	7482	CIT	O2-C1-O1	2.15	128.85	123.33
4	6-D	7482	CIT	O2-C1-O1	2.15	128.85	123.33
4	7-D	7482	CIT	O2-C1-O1	2.15	128.85	123.33
4	8-D	7482	CIT	O2-C1-O1	2.15	128.85	123.33
4	9-D	7482	CIT	O2-C1-O1	2.15	128.85	123.33
4	10-D	7482	CIT	O2-C1-O1	2.15	128.85	123.33
4	1-M	7500	CIT	O2-C1-O1	2.14	128.85	123.33
4	2-M	7500	CIT	O2-C1-O1	2.14	128.85	123.33
4	3-M	7500	CIT	O2-C1-O1	2.14	128.85	123.33
4	4-M	7500	CIT	O2-C1-O1	2.14	128.85	123.33
4	5-M	7500	CIT	O2-C1-O1	2.14	128.85	123.33
4	6-M	7500	CIT	O2-C1-O1	2.14	128.85	123.33
4	7-M	7500	CIT	O2-C1-O1	2.14	128.85	123.33
4	8-M	7500	CIT	O2-C1-O1	2.14	128.85	123.33
4	9-M	7500	CIT	O2-C1-O1	2.14	128.85	123.33
4	10-M	7500	CIT	O2-C1-O1	2.14	128.85	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-B	7478	CIT	O2-C1-O1	2.14	128.84	123.33
4	2-B	7478	CIT	O2-C1-O1	2.14	128.84	123.33
4	3-B	7478	CIT	O2-C1-O1	2.14	128.84	123.33
4	4-B	7478	CIT	O2-C1-O1	2.14	128.84	123.33
4	5-B	7478	CIT	O2-C1-O1	2.14	128.84	123.33
4	6-B	7478	CIT	O2-C1-O1	2.14	128.84	123.33
4	7-B	7478	CIT	O2-C1-O1	2.14	128.84	123.33
4	8-B	7478	CIT	O2-C1-O1	2.14	128.84	123.33
4	9-B	7478	CIT	O2-C1-O1	2.14	128.84	123.33
4	10-B	7478	CIT	O2-C1-O1	2.14	128.84	123.33
4	1-E	7484	CIT	O2-C1-O1	2.14	128.84	123.33
4	2-E	7484	CIT	O2-C1-O1	2.14	128.84	123.33
4	3-E	7484	CIT	O2-C1-O1	2.14	128.84	123.33
4	4-E	7484	CIT	O2-C1-O1	2.14	128.84	123.33
4	5-E	7484	CIT	O2-C1-O1	2.14	128.84	123.33
4	6-E	7484	CIT	O2-C1-O1	2.14	128.84	123.33
4	7-E	7484	CIT	O2-C1-O1	2.14	128.84	123.33
4	8-E	7484	CIT	O2-C1-O1	2.14	128.84	123.33
4	9-E	7484	CIT	O2-C1-O1	2.14	128.84	123.33
4	10-E	7484	CIT	O2-C1-O1	2.14	128.84	123.33
4	1-T	7514	CIT	O2-C1-O1	2.14	128.83	123.33
4	2-T	7514	CIT	O2-C1-O1	2.14	128.83	123.33
4	3-T	7514	CIT	O2-C1-O1	2.14	128.83	123.33
4	4-T	7514	CIT	O2-C1-O1	2.14	128.83	123.33
4	5-T	7514	CIT	O2-C1-O1	2.14	128.83	123.33
4	6-T	7514	CIT	O2-C1-O1	2.14	128.83	123.33
4	7-T	7514	CIT	O2-C1-O1	2.14	128.83	123.33
4	8-T	7514	CIT	O2-C1-O1	2.14	128.83	123.33
4	9-T	7514	CIT	O2-C1-O1	2.14	128.83	123.33
4	10-T	7514	CIT	O2-C1-O1	2.14	128.83	123.33
4	1-G	7488	CIT	O2-C1-O1	2.14	128.83	123.33
4	2-G	7488	CIT	O2-C1-O1	2.14	128.83	123.33
4	3-G	7488	CIT	O2-C1-O1	2.14	128.83	123.33
4	4-G	7488	CIT	O2-C1-O1	2.14	128.83	123.33
4	5-G	7488	CIT	O2-C1-O1	2.14	128.83	123.33
4	6-G	7488	CIT	O2-C1-O1	2.14	128.83	123.33
4	7-G	7488	CIT	O2-C1-O1	2.14	128.83	123.33
4	8-G	7488	CIT	O2-C1-O1	2.14	128.83	123.33
4	9-G	7488	CIT	O2-C1-O1	2.14	128.83	123.33
4	10-G	7488	CIT	O2-C1-O1	2.14	128.83	123.33
4	1-F	7486	CIT	O2-C1-O1	2.14	128.83	123.33
4	2-F	7486	CIT	O2-C1-O1	2.14	128.83	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-F	7486	CIT	O2-C1-O1	2.14	128.83	123.33
4	4-F	7486	CIT	O2-C1-O1	2.14	128.83	123.33
4	5-F	7486	CIT	O2-C1-O1	2.14	128.83	123.33
4	6-F	7486	CIT	O2-C1-O1	2.14	128.83	123.33
4	7-F	7486	CIT	O2-C1-O1	2.14	128.83	123.33
4	8-F	7486	CIT	O2-C1-O1	2.14	128.83	123.33
4	9-F	7486	CIT	O2-C1-O1	2.14	128.83	123.33
4	10-F	7486	CIT	O2-C1-O1	2.14	128.83	123.33
4	1-Q	7508	CIT	O2-C1-O1	2.13	128.82	123.33
4	2-Q	7508	CIT	O2-C1-O1	2.13	128.82	123.33
4	3-Q	7508	CIT	O2-C1-O1	2.13	128.82	123.33
4	4-Q	7508	CIT	O2-C1-O1	2.13	128.82	123.33
4	5-Q	7508	CIT	O2-C1-O1	2.13	128.82	123.33
4	6-Q	7508	CIT	O2-C1-O1	2.13	128.82	123.33
4	7-Q	7508	CIT	O2-C1-O1	2.13	128.82	123.33
4	8-Q	7508	CIT	O2-C1-O1	2.13	128.82	123.33
4	9-Q	7508	CIT	O2-C1-O1	2.13	128.82	123.33
4	10-Q	7508	CIT	O2-C1-O1	2.13	128.82	123.33
4	1-U	7516	CIT	O2-C1-O1	2.13	128.82	123.33
4	2-U	7516	CIT	O2-C1-O1	2.13	128.82	123.33
4	3-U	7516	CIT	O2-C1-O1	2.13	128.82	123.33
4	4-U	7516	CIT	O2-C1-O1	2.13	128.82	123.33
4	5-U	7516	CIT	O2-C1-O1	2.13	128.82	123.33
4	6-U	7516	CIT	O2-C1-O1	2.13	128.82	123.33
4	7-U	7516	CIT	O2-C1-O1	2.13	128.82	123.33
4	8-U	7516	CIT	O2-C1-O1	2.13	128.82	123.33
4	9-U	7516	CIT	O2-C1-O1	2.13	128.82	123.33
4	10-U	7516	CIT	O2-C1-O1	2.13	128.82	123.33
4	1-I	7492	CIT	O2-C1-O1	2.13	128.81	123.33
4	2-I	7492	CIT	O2-C1-O1	2.13	128.81	123.33
4	3-I	7492	CIT	O2-C1-O1	2.13	128.81	123.33
4	4-I	7492	CIT	O2-C1-O1	2.13	128.81	123.33
4	5-I	7492	CIT	O2-C1-O1	2.13	128.81	123.33
4	6-I	7492	CIT	O2-C1-O1	2.13	128.81	123.33
4	7-I	7492	CIT	O2-C1-O1	2.13	128.81	123.33
4	8-I	7492	CIT	O2-C1-O1	2.13	128.81	123.33
4	9-I	7492	CIT	O2-C1-O1	2.13	128.81	123.33
4	10-I	7492	CIT	O2-C1-O1	2.13	128.81	123.33
4	1-K	7496	CIT	O2-C1-O1	2.13	128.80	123.33
4	2-K	7496	CIT	O2-C1-O1	2.13	128.80	123.33
4	3-K	7496	CIT	O2-C1-O1	2.13	128.80	123.33
4	4-K	7496	CIT	O2-C1-O1	2.13	128.80	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5-K	7496	CIT	O2-C1-O1	2.13	128.80	123.33
4	6-K	7496	CIT	O2-C1-O1	2.13	128.80	123.33
4	7-K	7496	CIT	O2-C1-O1	2.13	128.80	123.33
4	8-K	7496	CIT	O2-C1-O1	2.13	128.80	123.33
4	9-K	7496	CIT	O2-C1-O1	2.13	128.80	123.33
4	10-K	7496	CIT	O2-C1-O1	2.13	128.80	123.33
4	1-A	7476	CIT	O2-C1-O1	2.13	128.80	123.33
4	2-A	7476	CIT	O2-C1-O1	2.13	128.80	123.33
4	3-A	7476	CIT	O2-C1-O1	2.13	128.80	123.33
4	4-A	7476	CIT	O2-C1-O1	2.13	128.80	123.33
4	5-A	7476	CIT	O2-C1-O1	2.13	128.80	123.33
4	6-A	7476	CIT	O2-C1-O1	2.13	128.80	123.33
4	7-A	7476	CIT	O2-C1-O1	2.13	128.80	123.33
4	8-A	7476	CIT	O2-C1-O1	2.13	128.80	123.33
4	9-A	7476	CIT	O2-C1-O1	2.13	128.80	123.33
4	10-A	7476	CIT	O2-C1-O1	2.13	128.80	123.33
4	1-R	7510	CIT	O2-C1-O1	2.12	128.80	123.33
4	2-R	7510	CIT	O2-C1-O1	2.12	128.80	123.33
4	3-R	7510	CIT	O2-C1-O1	2.12	128.80	123.33
4	4-R	7510	CIT	O2-C1-O1	2.12	128.80	123.33
4	5-R	7510	CIT	O2-C1-O1	2.12	128.80	123.33
4	6-R	7510	CIT	O2-C1-O1	2.12	128.80	123.33
4	7-R	7510	CIT	O2-C1-O1	2.12	128.80	123.33
4	8-R	7510	CIT	O2-C1-O1	2.12	128.80	123.33
4	9-R	7510	CIT	O2-C1-O1	2.12	128.80	123.33
4	10-R	7510	CIT	O2-C1-O1	2.12	128.80	123.33
4	1-W	7520	CIT	O2-C1-O1	2.12	128.79	123.33
4	2-W	7520	CIT	O2-C1-O1	2.12	128.79	123.33
4	3-W	7520	CIT	O2-C1-O1	2.12	128.79	123.33
4	4-W	7520	CIT	O2-C1-O1	2.12	128.79	123.33
4	5-W	7520	CIT	O2-C1-O1	2.12	128.79	123.33
4	6-W	7520	CIT	O2-C1-O1	2.12	128.79	123.33
4	7-W	7520	CIT	O2-C1-O1	2.12	128.79	123.33
4	8-W	7520	CIT	O2-C1-O1	2.12	128.79	123.33
4	9-W	7520	CIT	O2-C1-O1	2.12	128.79	123.33
4	10-W	7520	CIT	O2-C1-O1	2.12	128.79	123.33
4	1-H	7490	CIT	O2-C1-O1	2.12	128.79	123.33
4	2-H	7490	CIT	O2-C1-O1	2.12	128.79	123.33
4	3-H	7490	CIT	O2-C1-O1	2.12	128.79	123.33
4	4-H	7490	CIT	O2-C1-O1	2.12	128.79	123.33
4	5-H	7490	CIT	O2-C1-O1	2.12	128.79	123.33
4	6-H	7490	CIT	O2-C1-O1	2.12	128.79	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7-H	7490	CIT	O2-C1-O1	2.12	128.79	123.33
4	8-H	7490	CIT	O2-C1-O1	2.12	128.79	123.33
4	9-H	7490	CIT	O2-C1-O1	2.12	128.79	123.33
4	10-H	7490	CIT	O2-C1-O1	2.12	128.79	123.33
4	1-N	7502	CIT	O2-C1-O1	2.12	128.78	123.33
4	2-N	7502	CIT	O2-C1-O1	2.12	128.78	123.33
4	3-N	7502	CIT	O2-C1-O1	2.12	128.78	123.33
4	4-N	7502	CIT	O2-C1-O1	2.12	128.78	123.33
4	5-N	7502	CIT	O2-C1-O1	2.12	128.78	123.33
4	6-N	7502	CIT	O2-C1-O1	2.12	128.78	123.33
4	7-N	7502	CIT	O2-C1-O1	2.12	128.78	123.33
4	8-N	7502	CIT	O2-C1-O1	2.12	128.78	123.33
4	9-N	7502	CIT	O2-C1-O1	2.12	128.78	123.33
4	10-N	7502	CIT	O2-C1-O1	2.12	128.78	123.33
4	1-O	7504	CIT	O2-C1-O1	2.12	128.78	123.33
4	2-O	7504	CIT	O2-C1-O1	2.12	128.78	123.33
4	3-O	7504	CIT	O2-C1-O1	2.12	128.78	123.33
4	4-O	7504	CIT	O2-C1-O1	2.12	128.78	123.33
4	5-O	7504	CIT	O2-C1-O1	2.12	128.78	123.33
4	6-O	7504	CIT	O2-C1-O1	2.12	128.78	123.33
4	7-O	7504	CIT	O2-C1-O1	2.12	128.78	123.33
4	8-O	7504	CIT	O2-C1-O1	2.12	128.78	123.33
4	9-O	7504	CIT	O2-C1-O1	2.12	128.78	123.33
4	10-O	7504	CIT	O2-C1-O1	2.12	128.78	123.33
4	1-P	7506	CIT	O2-C1-O1	2.12	128.78	123.33
4	2-P	7506	CIT	O2-C1-O1	2.12	128.78	123.33
4	3-P	7506	CIT	O2-C1-O1	2.12	128.78	123.33
4	4-P	7506	CIT	O2-C1-O1	2.12	128.78	123.33
4	5-P	7506	CIT	O2-C1-O1	2.12	128.78	123.33
4	6-P	7506	CIT	O2-C1-O1	2.12	128.78	123.33
4	7-P	7506	CIT	O2-C1-O1	2.12	128.78	123.33
4	8-P	7506	CIT	O2-C1-O1	2.12	128.78	123.33
4	9-P	7506	CIT	O2-C1-O1	2.12	128.78	123.33
4	10-P	7506	CIT	O2-C1-O1	2.12	128.78	123.33
4	1-L	7498	CIT	O2-C1-O1	2.12	128.78	123.33
4	2-L	7498	CIT	O2-C1-O1	2.12	128.78	123.33
4	3-L	7498	CIT	O2-C1-O1	2.12	128.78	123.33
4	4-L	7498	CIT	O2-C1-O1	2.12	128.78	123.33
4	5-L	7498	CIT	O2-C1-O1	2.12	128.78	123.33
4	6-L	7498	CIT	O2-C1-O1	2.12	128.78	123.33
4	7-L	7498	CIT	O2-C1-O1	2.12	128.78	123.33
4	8-L	7498	CIT	O2-C1-O1	2.12	128.78	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9-L	7498	CIT	O2-C1-O1	2.12	128.78	123.33
4	10-L	7498	CIT	O2-C1-O1	2.12	128.78	123.33
4	1-J	7494	CIT	O2-C1-O1	2.12	128.78	123.33
4	2-J	7494	CIT	O2-C1-O1	2.12	128.78	123.33
4	3-J	7494	CIT	O2-C1-O1	2.12	128.78	123.33
4	4-J	7494	CIT	O2-C1-O1	2.12	128.78	123.33
4	5-J	7494	CIT	O2-C1-O1	2.12	128.78	123.33
4	6-J	7494	CIT	O2-C1-O1	2.12	128.78	123.33
4	7-J	7494	CIT	O2-C1-O1	2.12	128.78	123.33
4	8-J	7494	CIT	O2-C1-O1	2.12	128.78	123.33
4	9-J	7494	CIT	O2-C1-O1	2.12	128.78	123.33
4	10-J	7494	CIT	O2-C1-O1	2.12	128.78	123.33
4	1-V	7518	CIT	O2-C1-O1	2.12	128.78	123.33
4	2-V	7518	CIT	O2-C1-O1	2.12	128.78	123.33
4	3-V	7518	CIT	O2-C1-O1	2.12	128.78	123.33
4	4-V	7518	CIT	O2-C1-O1	2.12	128.78	123.33
4	5-V	7518	CIT	O2-C1-O1	2.12	128.78	123.33
4	6-V	7518	CIT	O2-C1-O1	2.12	128.78	123.33
4	7-V	7518	CIT	O2-C1-O1	2.12	128.78	123.33
4	8-V	7518	CIT	O2-C1-O1	2.12	128.78	123.33
4	9-V	7518	CIT	O2-C1-O1	2.12	128.78	123.33
4	10-V	7518	CIT	O2-C1-O1	2.12	128.78	123.33
4	1-X	7522	CIT	O2-C1-O1	2.11	128.76	123.33
4	2-X	7522	CIT	O2-C1-O1	2.11	128.76	123.33
4	3-X	7522	CIT	O2-C1-O1	2.11	128.76	123.33
4	4-X	7522	CIT	O2-C1-O1	2.11	128.76	123.33
4	5-X	7522	CIT	O2-C1-O1	2.11	128.76	123.33
4	6-X	7522	CIT	O2-C1-O1	2.11	128.76	123.33
4	7-X	7522	CIT	O2-C1-O1	2.11	128.76	123.33
4	8-X	7522	CIT	O2-C1-O1	2.11	128.76	123.33
4	9-X	7522	CIT	O2-C1-O1	2.11	128.76	123.33
4	10-X	7522	CIT	O2-C1-O1	2.11	128.76	123.33
4	1-C	7480	CIT	O2-C1-O1	2.11	128.76	123.33
4	2-C	7480	CIT	O2-C1-O1	2.11	128.76	123.33
4	3-C	7480	CIT	O2-C1-O1	2.11	128.76	123.33
4	4-C	7480	CIT	O2-C1-O1	2.11	128.76	123.33
4	5-C	7480	CIT	O2-C1-O1	2.11	128.76	123.33
4	6-C	7480	CIT	O2-C1-O1	2.11	128.76	123.33
4	7-C	7480	CIT	O2-C1-O1	2.11	128.76	123.33
4	8-C	7480	CIT	O2-C1-O1	2.11	128.76	123.33
4	9-C	7480	CIT	O2-C1-O1	2.11	128.76	123.33
4	10-C	7480	CIT	O2-C1-O1	2.11	128.76	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-S	7512	CIT	O2-C1-O1	2.11	128.75	123.33
4	2-S	7512	CIT	O2-C1-O1	2.11	128.75	123.33
4	3-S	7512	CIT	O2-C1-O1	2.11	128.75	123.33
4	4-S	7512	CIT	O2-C1-O1	2.11	128.75	123.33
4	5-S	7512	CIT	O2-C1-O1	2.11	128.75	123.33
4	6-S	7512	CIT	O2-C1-O1	2.11	128.75	123.33
4	7-S	7512	CIT	O2-C1-O1	2.11	128.75	123.33
4	8-S	7512	CIT	O2-C1-O1	2.11	128.75	123.33
4	9-S	7512	CIT	O2-C1-O1	2.11	128.75	123.33
4	10-S	7512	CIT	O2-C1-O1	2.11	128.75	123.33
4	1-U	7516	CIT	O6-C6-C3	2.05	117.07	113.14
4	2-U	7516	CIT	O6-C6-C3	2.05	117.07	113.14
4	3-U	7516	CIT	O6-C6-C3	2.05	117.07	113.14
4	4-U	7516	CIT	O6-C6-C3	2.05	117.07	113.14
4	5-U	7516	CIT	O6-C6-C3	2.05	117.07	113.14
4	6-U	7516	CIT	O6-C6-C3	2.05	117.07	113.14
4	7-U	7516	CIT	O6-C6-C3	2.05	117.07	113.14
4	8-U	7516	CIT	O6-C6-C3	2.05	117.07	113.14
4	9-U	7516	CIT	O6-C6-C3	2.05	117.07	113.14
4	10-U	7516	CIT	O6-C6-C3	2.05	117.07	113.14
4	1-S	7512	CIT	O6-C6-C3	2.05	117.06	113.14
4	2-S	7512	CIT	O6-C6-C3	2.05	117.06	113.14
4	3-S	7512	CIT	O6-C6-C3	2.05	117.06	113.14
4	4-S	7512	CIT	O6-C6-C3	2.05	117.06	113.14
4	5-S	7512	CIT	O6-C6-C3	2.05	117.06	113.14
4	6-S	7512	CIT	O6-C6-C3	2.05	117.06	113.14
4	7-S	7512	CIT	O6-C6-C3	2.05	117.06	113.14
4	8-S	7512	CIT	O6-C6-C3	2.05	117.06	113.14
4	9-S	7512	CIT	O6-C6-C3	2.05	117.06	113.14
4	10-S	7512	CIT	O6-C6-C3	2.05	117.06	113.14
4	1-I	7492	CIT	O6-C6-C3	2.04	117.06	113.14
4	2-I	7492	CIT	O6-C6-C3	2.04	117.06	113.14
4	3-I	7492	CIT	O6-C6-C3	2.04	117.06	113.14
4	4-I	7492	CIT	O6-C6-C3	2.04	117.06	113.14
4	5-I	7492	CIT	O6-C6-C3	2.04	117.06	113.14
4	6-I	7492	CIT	O6-C6-C3	2.04	117.06	113.14
4	7-I	7492	CIT	O6-C6-C3	2.04	117.06	113.14
4	8-I	7492	CIT	O6-C6-C3	2.04	117.06	113.14
4	9-I	7492	CIT	O6-C6-C3	2.04	117.06	113.14
4	10-I	7492	CIT	O6-C6-C3	2.04	117.06	113.14
4	1-R	7510	CIT	O6-C6-C3	2.04	117.05	113.14
4	2-R	7510	CIT	O6-C6-C3	2.04	117.05	113.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-R	7510	CIT	O6-C6-C3	2.04	117.05	113.14
4	4-R	7510	CIT	O6-C6-C3	2.04	117.05	113.14
4	5-R	7510	CIT	O6-C6-C3	2.04	117.05	113.14
4	6-R	7510	CIT	O6-C6-C3	2.04	117.05	113.14
4	7-R	7510	CIT	O6-C6-C3	2.04	117.05	113.14
4	8-R	7510	CIT	O6-C6-C3	2.04	117.05	113.14
4	9-R	7510	CIT	O6-C6-C3	2.04	117.05	113.14
4	10-R	7510	CIT	O6-C6-C3	2.04	117.05	113.14
4	1-J	7494	CIT	O6-C6-C3	2.04	117.05	113.14
4	2-J	7494	CIT	O6-C6-C3	2.04	117.05	113.14
4	3-J	7494	CIT	O6-C6-C3	2.04	117.05	113.14
4	4-J	7494	CIT	O6-C6-C3	2.04	117.05	113.14
4	5-J	7494	CIT	O6-C6-C3	2.04	117.05	113.14
4	6-J	7494	CIT	O6-C6-C3	2.04	117.05	113.14
4	7-J	7494	CIT	O6-C6-C3	2.04	117.05	113.14
4	8-J	7494	CIT	O6-C6-C3	2.04	117.05	113.14
4	9-J	7494	CIT	O6-C6-C3	2.04	117.05	113.14
4	10-J	7494	CIT	O6-C6-C3	2.04	117.05	113.14
4	1-K	7496	CIT	O6-C6-C3	2.03	117.04	113.14
4	2-K	7496	CIT	O6-C6-C3	2.03	117.04	113.14
4	3-K	7496	CIT	O6-C6-C3	2.03	117.04	113.14
4	4-K	7496	CIT	O6-C6-C3	2.03	117.04	113.14
4	5-K	7496	CIT	O6-C6-C3	2.03	117.04	113.14
4	6-K	7496	CIT	O6-C6-C3	2.03	117.04	113.14
4	7-K	7496	CIT	O6-C6-C3	2.03	117.04	113.14
4	8-K	7496	CIT	O6-C6-C3	2.03	117.04	113.14
4	9-K	7496	CIT	O6-C6-C3	2.03	117.04	113.14
4	10-K	7496	CIT	O6-C6-C3	2.03	117.04	113.14
4	1-D	7482	CIT	O6-C6-C3	2.03	117.04	113.14
4	2-D	7482	CIT	O6-C6-C3	2.03	117.04	113.14
4	3-D	7482	CIT	O6-C6-C3	2.03	117.04	113.14
4	4-D	7482	CIT	O6-C6-C3	2.03	117.04	113.14
4	5-D	7482	CIT	O6-C6-C3	2.03	117.04	113.14
4	6-D	7482	CIT	O6-C6-C3	2.03	117.04	113.14
4	7-D	7482	CIT	O6-C6-C3	2.03	117.04	113.14
4	8-D	7482	CIT	O6-C6-C3	2.03	117.04	113.14
4	9-D	7482	CIT	O6-C6-C3	2.03	117.04	113.14
4	10-D	7482	CIT	O6-C6-C3	2.03	117.04	113.14
4	1-V	7518	CIT	O6-C6-C3	2.03	117.03	113.14
4	2-V	7518	CIT	O6-C6-C3	2.03	117.03	113.14
4	3-V	7518	CIT	O6-C6-C3	2.03	117.03	113.14
4	4-V	7518	CIT	O6-C6-C3	2.03	117.03	113.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5-V	7518	CIT	O6-C6-C3	2.03	117.03	113.14
4	6-V	7518	CIT	O6-C6-C3	2.03	117.03	113.14
4	7-V	7518	CIT	O6-C6-C3	2.03	117.03	113.14
4	8-V	7518	CIT	O6-C6-C3	2.03	117.03	113.14
4	9-V	7518	CIT	O6-C6-C3	2.03	117.03	113.14
4	10-V	7518	CIT	O6-C6-C3	2.03	117.03	113.14
4	1-C	7480	CIT	O6-C6-C3	2.02	117.02	113.14
4	2-C	7480	CIT	O6-C6-C3	2.02	117.02	113.14
4	3-C	7480	CIT	O6-C6-C3	2.02	117.02	113.14
4	4-C	7480	CIT	O6-C6-C3	2.02	117.02	113.14
4	5-C	7480	CIT	O6-C6-C3	2.02	117.02	113.14
4	6-C	7480	CIT	O6-C6-C3	2.02	117.02	113.14
4	7-C	7480	CIT	O6-C6-C3	2.02	117.02	113.14
4	8-C	7480	CIT	O6-C6-C3	2.02	117.02	113.14
4	9-C	7480	CIT	O6-C6-C3	2.02	117.02	113.14
4	10-C	7480	CIT	O6-C6-C3	2.02	117.02	113.14
4	1-O	7504	CIT	O6-C6-C3	2.02	117.02	113.14
4	2-O	7504	CIT	O6-C6-C3	2.02	117.02	113.14
4	3-O	7504	CIT	O6-C6-C3	2.02	117.02	113.14
4	4-O	7504	CIT	O6-C6-C3	2.02	117.02	113.14
4	5-O	7504	CIT	O6-C6-C3	2.02	117.02	113.14
4	6-O	7504	CIT	O6-C6-C3	2.02	117.02	113.14
4	7-O	7504	CIT	O6-C6-C3	2.02	117.02	113.14
4	8-O	7504	CIT	O6-C6-C3	2.02	117.02	113.14
4	9-O	7504	CIT	O6-C6-C3	2.02	117.02	113.14
4	10-O	7504	CIT	O6-C6-C3	2.02	117.02	113.14
4	1-T	7514	CIT	O6-C6-C3	2.02	117.02	113.14
4	2-T	7514	CIT	O6-C6-C3	2.02	117.02	113.14
4	3-T	7514	CIT	O6-C6-C3	2.02	117.02	113.14
4	4-T	7514	CIT	O6-C6-C3	2.02	117.02	113.14
4	5-T	7514	CIT	O6-C6-C3	2.02	117.02	113.14
4	6-T	7514	CIT	O6-C6-C3	2.02	117.02	113.14
4	7-T	7514	CIT	O6-C6-C3	2.02	117.02	113.14
4	8-T	7514	CIT	O6-C6-C3	2.02	117.02	113.14
4	9-T	7514	CIT	O6-C6-C3	2.02	117.02	113.14
4	10-T	7514	CIT	O6-C6-C3	2.02	117.02	113.14
4	1-F	7486	CIT	O6-C6-C3	2.02	117.02	113.14
4	2-F	7486	CIT	O6-C6-C3	2.02	117.02	113.14
4	3-F	7486	CIT	O6-C6-C3	2.02	117.02	113.14
4	4-F	7486	CIT	O6-C6-C3	2.02	117.02	113.14
4	5-F	7486	CIT	O6-C6-C3	2.02	117.02	113.14
4	6-F	7486	CIT	O6-C6-C3	2.02	117.02	113.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7-F	7486	CIT	O6-C6-C3	2.02	117.02	113.14
4	8-F	7486	CIT	O6-C6-C3	2.02	117.02	113.14
4	9-F	7486	CIT	O6-C6-C3	2.02	117.02	113.14
4	10-F	7486	CIT	O6-C6-C3	2.02	117.02	113.14
4	1-G	7488	CIT	O6-C6-C3	2.02	117.02	113.14
4	2-G	7488	CIT	O6-C6-C3	2.02	117.02	113.14
4	3-G	7488	CIT	O6-C6-C3	2.02	117.02	113.14
4	4-G	7488	CIT	O6-C6-C3	2.02	117.02	113.14
4	5-G	7488	CIT	O6-C6-C3	2.02	117.02	113.14
4	6-G	7488	CIT	O6-C6-C3	2.02	117.02	113.14
4	7-G	7488	CIT	O6-C6-C3	2.02	117.02	113.14
4	8-G	7488	CIT	O6-C6-C3	2.02	117.02	113.14
4	9-G	7488	CIT	O6-C6-C3	2.02	117.02	113.14
4	10-G	7488	CIT	O6-C6-C3	2.02	117.02	113.14
4	1-P	7506	CIT	O6-C6-C3	2.02	117.02	113.14
4	2-P	7506	CIT	O6-C6-C3	2.02	117.02	113.14
4	3-P	7506	CIT	O6-C6-C3	2.02	117.02	113.14
4	4-P	7506	CIT	O6-C6-C3	2.02	117.02	113.14
4	5-P	7506	CIT	O6-C6-C3	2.02	117.02	113.14
4	6-P	7506	CIT	O6-C6-C3	2.02	117.02	113.14
4	7-P	7506	CIT	O6-C6-C3	2.02	117.02	113.14
4	8-P	7506	CIT	O6-C6-C3	2.02	117.02	113.14
4	9-P	7506	CIT	O6-C6-C3	2.02	117.02	113.14
4	10-P	7506	CIT	O6-C6-C3	2.02	117.02	113.14
4	1-Q	7508	CIT	O6-C6-C3	2.02	117.02	113.14
4	2-Q	7508	CIT	O6-C6-C3	2.02	117.02	113.14
4	3-Q	7508	CIT	O6-C6-C3	2.02	117.02	113.14
4	4-Q	7508	CIT	O6-C6-C3	2.02	117.02	113.14
4	5-Q	7508	CIT	O6-C6-C3	2.02	117.02	113.14
4	6-Q	7508	CIT	O6-C6-C3	2.02	117.02	113.14
4	7-Q	7508	CIT	O6-C6-C3	2.02	117.02	113.14
4	8-Q	7508	CIT	O6-C6-C3	2.02	117.02	113.14
4	9-Q	7508	CIT	O6-C6-C3	2.02	117.02	113.14
4	10-Q	7508	CIT	O6-C6-C3	2.02	117.02	113.14
4	1-H	7490	CIT	O6-C6-C3	2.02	117.01	113.14
4	2-H	7490	CIT	O6-C6-C3	2.02	117.01	113.14
4	3-H	7490	CIT	O6-C6-C3	2.02	117.01	113.14
4	4-H	7490	CIT	O6-C6-C3	2.02	117.01	113.14
4	5-H	7490	CIT	O6-C6-C3	2.02	117.01	113.14
4	6-H	7490	CIT	O6-C6-C3	2.02	117.01	113.14
4	7-H	7490	CIT	O6-C6-C3	2.02	117.01	113.14
4	8-H	7490	CIT	O6-C6-C3	2.02	117.01	113.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9-H	7490	CIT	O6-C6-C3	2.02	117.01	113.14
4	10-H	7490	CIT	O6-C6-C3	2.02	117.01	113.14
4	1-A	7476	CIT	O6-C6-C3	2.02	117.01	113.14
4	2-A	7476	CIT	O6-C6-C3	2.02	117.01	113.14
4	3-A	7476	CIT	O6-C6-C3	2.02	117.01	113.14
4	4-A	7476	CIT	O6-C6-C3	2.02	117.01	113.14
4	5-A	7476	CIT	O6-C6-C3	2.02	117.01	113.14
4	6-A	7476	CIT	O6-C6-C3	2.02	117.01	113.14
4	7-A	7476	CIT	O6-C6-C3	2.02	117.01	113.14
4	8-A	7476	CIT	O6-C6-C3	2.02	117.01	113.14
4	9-A	7476	CIT	O6-C6-C3	2.02	117.01	113.14
4	10-A	7476	CIT	O6-C6-C3	2.02	117.01	113.14
4	1-M	7500	CIT	O6-C6-C3	2.01	117.00	113.14
4	2-M	7500	CIT	O6-C6-C3	2.01	117.00	113.14
4	3-M	7500	CIT	O6-C6-C3	2.01	117.00	113.14
4	4-M	7500	CIT	O6-C6-C3	2.01	117.00	113.14
4	5-M	7500	CIT	O6-C6-C3	2.01	117.00	113.14
4	6-M	7500	CIT	O6-C6-C3	2.01	117.00	113.14
4	7-M	7500	CIT	O6-C6-C3	2.01	117.00	113.14
4	8-M	7500	CIT	O6-C6-C3	2.01	117.00	113.14
4	9-M	7500	CIT	O6-C6-C3	2.01	117.00	113.14
4	10-M	7500	CIT	O6-C6-C3	2.01	117.00	113.14
4	1-E	7484	CIT	O6-C6-C3	2.01	117.00	113.14
4	2-E	7484	CIT	O6-C6-C3	2.01	117.00	113.14
4	3-E	7484	CIT	O6-C6-C3	2.01	117.00	113.14
4	4-E	7484	CIT	O6-C6-C3	2.01	117.00	113.14
4	5-E	7484	CIT	O6-C6-C3	2.01	117.00	113.14
4	6-E	7484	CIT	O6-C6-C3	2.01	117.00	113.14
4	7-E	7484	CIT	O6-C6-C3	2.01	117.00	113.14
4	8-E	7484	CIT	O6-C6-C3	2.01	117.00	113.14
4	9-E	7484	CIT	O6-C6-C3	2.01	117.00	113.14
4	10-E	7484	CIT	O6-C6-C3	2.01	117.00	113.14
4	1-B	7478	CIT	O6-C6-C3	2.01	116.99	113.14
4	2-B	7478	CIT	O6-C6-C3	2.01	116.99	113.14
4	3-B	7478	CIT	O6-C6-C3	2.01	116.99	113.14
4	4-B	7478	CIT	O6-C6-C3	2.01	116.99	113.14
4	5-B	7478	CIT	O6-C6-C3	2.01	116.99	113.14
4	6-B	7478	CIT	O6-C6-C3	2.01	116.99	113.14
4	7-B	7478	CIT	O6-C6-C3	2.01	116.99	113.14
4	8-B	7478	CIT	O6-C6-C3	2.01	116.99	113.14
4	9-B	7478	CIT	O6-C6-C3	2.01	116.99	113.14
4	10-B	7478	CIT	O6-C6-C3	2.01	116.99	113.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-X	7522	CIT	O6-C6-C3	2.00	116.98	113.14
4	2-X	7522	CIT	O6-C6-C3	2.00	116.98	113.14
4	3-X	7522	CIT	O6-C6-C3	2.00	116.98	113.14
4	4-X	7522	CIT	O6-C6-C3	2.00	116.98	113.14
4	5-X	7522	CIT	O6-C6-C3	2.00	116.98	113.14
4	6-X	7522	CIT	O6-C6-C3	2.00	116.98	113.14
4	7-X	7522	CIT	O6-C6-C3	2.00	116.98	113.14
4	8-X	7522	CIT	O6-C6-C3	2.00	116.98	113.14
4	9-X	7522	CIT	O6-C6-C3	2.00	116.98	113.14
4	10-X	7522	CIT	O6-C6-C3	2.00	116.98	113.14

There are no chirality outliers.

All (2160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1-A	7475	AMP	C5'-O5'-P-O2P
3	1-A	7475	AMP	C5'-O5'-P-O3P
3	2-A	7475	AMP	C5'-O5'-P-O2P
3	2-A	7475	AMP	C5'-O5'-P-O3P
3	3-A	7475	AMP	C5'-O5'-P-O2P
3	3-A	7475	AMP	C5'-O5'-P-O3P
3	4-A	7475	AMP	C5'-O5'-P-O2P
3	4-A	7475	AMP	C5'-O5'-P-O3P
3	5-A	7475	AMP	C5'-O5'-P-O2P
3	5-A	7475	AMP	C5'-O5'-P-O3P
3	6-A	7475	AMP	C5'-O5'-P-O2P
3	6-A	7475	AMP	C5'-O5'-P-O3P
3	7-A	7475	AMP	C5'-O5'-P-O2P
3	7-A	7475	AMP	C5'-O5'-P-O3P
3	8-A	7475	AMP	C5'-O5'-P-O2P
3	8-A	7475	AMP	C5'-O5'-P-O3P
3	9-A	7475	AMP	C5'-O5'-P-O2P
3	9-A	7475	AMP	C5'-O5'-P-O3P
3	10-A	7475	AMP	C5'-O5'-P-O2P
3	10-A	7475	AMP	C5'-O5'-P-O3P
3	1-B	7477	AMP	C5'-O5'-P-O2P
3	1-B	7477	AMP	C5'-O5'-P-O3P
3	2-B	7477	AMP	C5'-O5'-P-O2P
3	2-B	7477	AMP	C5'-O5'-P-O3P
3	3-B	7477	AMP	C5'-O5'-P-O2P
3	3-B	7477	AMP	C5'-O5'-P-O3P
3	4-B	7477	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	4-B	7477	AMP	C5'-O5'-P-O3P
3	5-B	7477	AMP	C5'-O5'-P-O2P
3	5-B	7477	AMP	C5'-O5'-P-O3P
3	6-B	7477	AMP	C5'-O5'-P-O2P
3	6-B	7477	AMP	C5'-O5'-P-O3P
3	7-B	7477	AMP	C5'-O5'-P-O2P
3	7-B	7477	AMP	C5'-O5'-P-O3P
3	8-B	7477	AMP	C5'-O5'-P-O2P
3	8-B	7477	AMP	C5'-O5'-P-O3P
3	9-B	7477	AMP	C5'-O5'-P-O2P
3	9-B	7477	AMP	C5'-O5'-P-O3P
3	10-B	7477	AMP	C5'-O5'-P-O2P
3	10-B	7477	AMP	C5'-O5'-P-O3P
3	1-C	7479	AMP	C5'-O5'-P-O2P
3	1-C	7479	AMP	C5'-O5'-P-O3P
3	2-C	7479	AMP	C5'-O5'-P-O2P
3	2-C	7479	AMP	C5'-O5'-P-O3P
3	3-C	7479	AMP	C5'-O5'-P-O2P
3	3-C	7479	AMP	C5'-O5'-P-O3P
3	4-C	7479	AMP	C5'-O5'-P-O2P
3	4-C	7479	AMP	C5'-O5'-P-O3P
3	5-C	7479	AMP	C5'-O5'-P-O2P
3	5-C	7479	AMP	C5'-O5'-P-O3P
3	6-C	7479	AMP	C5'-O5'-P-O2P
3	6-C	7479	AMP	C5'-O5'-P-O3P
3	7-C	7479	AMP	C5'-O5'-P-O2P
3	7-C	7479	AMP	C5'-O5'-P-O3P
3	8-C	7479	AMP	C5'-O5'-P-O2P
3	8-C	7479	AMP	C5'-O5'-P-O3P
3	9-C	7479	AMP	C5'-O5'-P-O2P
3	9-C	7479	AMP	C5'-O5'-P-O3P
3	10-C	7479	AMP	C5'-O5'-P-O2P
3	10-C	7479	AMP	C5'-O5'-P-O3P
3	1-D	7481	AMP	C5'-O5'-P-O2P
3	1-D	7481	AMP	C5'-O5'-P-O3P
3	2-D	7481	AMP	C5'-O5'-P-O2P
3	2-D	7481	AMP	C5'-O5'-P-O3P
3	3-D	7481	AMP	C5'-O5'-P-O2P
3	3-D	7481	AMP	C5'-O5'-P-O3P
3	4-D	7481	AMP	C5'-O5'-P-O2P
3	4-D	7481	AMP	C5'-O5'-P-O3P
3	5-D	7481	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	5-D	7481	AMP	C5'-O5'-P-O3P
3	6-D	7481	AMP	C5'-O5'-P-O2P
3	6-D	7481	AMP	C5'-O5'-P-O3P
3	7-D	7481	AMP	C5'-O5'-P-O2P
3	7-D	7481	AMP	C5'-O5'-P-O3P
3	8-D	7481	AMP	C5'-O5'-P-O2P
3	8-D	7481	AMP	C5'-O5'-P-O3P
3	9-D	7481	AMP	C5'-O5'-P-O2P
3	9-D	7481	AMP	C5'-O5'-P-O3P
3	10-D	7481	AMP	C5'-O5'-P-O2P
3	10-D	7481	AMP	C5'-O5'-P-O3P
3	1-E	7483	AMP	C5'-O5'-P-O2P
3	1-E	7483	AMP	C5'-O5'-P-O3P
3	2-E	7483	AMP	C5'-O5'-P-O2P
3	2-E	7483	AMP	C5'-O5'-P-O3P
3	3-E	7483	AMP	C5'-O5'-P-O2P
3	3-E	7483	AMP	C5'-O5'-P-O3P
3	4-E	7483	AMP	C5'-O5'-P-O2P
3	4-E	7483	AMP	C5'-O5'-P-O3P
3	5-E	7483	AMP	C5'-O5'-P-O2P
3	5-E	7483	AMP	C5'-O5'-P-O3P
3	6-E	7483	AMP	C5'-O5'-P-O2P
3	6-E	7483	AMP	C5'-O5'-P-O3P
3	7-E	7483	AMP	C5'-O5'-P-O2P
3	7-E	7483	AMP	C5'-O5'-P-O3P
3	8-E	7483	AMP	C5'-O5'-P-O2P
3	8-E	7483	AMP	C5'-O5'-P-O3P
3	9-E	7483	AMP	C5'-O5'-P-O2P
3	9-E	7483	AMP	C5'-O5'-P-O3P
3	10-E	7483	AMP	C5'-O5'-P-O2P
3	10-E	7483	AMP	C5'-O5'-P-O3P
3	1-F	7485	AMP	C5'-O5'-P-O2P
3	1-F	7485	AMP	C5'-O5'-P-O3P
3	2-F	7485	AMP	C5'-O5'-P-O2P
3	2-F	7485	AMP	C5'-O5'-P-O3P
3	3-F	7485	AMP	C5'-O5'-P-O2P
3	3-F	7485	AMP	C5'-O5'-P-O3P
3	4-F	7485	AMP	C5'-O5'-P-O2P
3	4-F	7485	AMP	C5'-O5'-P-O3P
3	5-F	7485	AMP	C5'-O5'-P-O2P
3	5-F	7485	AMP	C5'-O5'-P-O3P
3	6-F	7485	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	6-F	7485	AMP	C5'-O5'-P-O3P
3	7-F	7485	AMP	C5'-O5'-P-O2P
3	7-F	7485	AMP	C5'-O5'-P-O3P
3	8-F	7485	AMP	C5'-O5'-P-O2P
3	8-F	7485	AMP	C5'-O5'-P-O3P
3	9-F	7485	AMP	C5'-O5'-P-O2P
3	9-F	7485	AMP	C5'-O5'-P-O3P
3	10-F	7485	AMP	C5'-O5'-P-O2P
3	10-F	7485	AMP	C5'-O5'-P-O3P
3	1-G	7487	AMP	C5'-O5'-P-O2P
3	1-G	7487	AMP	C5'-O5'-P-O3P
3	2-G	7487	AMP	C5'-O5'-P-O2P
3	2-G	7487	AMP	C5'-O5'-P-O3P
3	3-G	7487	AMP	C5'-O5'-P-O2P
3	3-G	7487	AMP	C5'-O5'-P-O3P
3	4-G	7487	AMP	C5'-O5'-P-O2P
3	4-G	7487	AMP	C5'-O5'-P-O3P
3	5-G	7487	AMP	C5'-O5'-P-O2P
3	5-G	7487	AMP	C5'-O5'-P-O3P
3	6-G	7487	AMP	C5'-O5'-P-O2P
3	6-G	7487	AMP	C5'-O5'-P-O3P
3	7-G	7487	AMP	C5'-O5'-P-O2P
3	7-G	7487	AMP	C5'-O5'-P-O3P
3	8-G	7487	AMP	C5'-O5'-P-O2P
3	8-G	7487	AMP	C5'-O5'-P-O3P
3	9-G	7487	AMP	C5'-O5'-P-O2P
3	9-G	7487	AMP	C5'-O5'-P-O3P
3	10-G	7487	AMP	C5'-O5'-P-O2P
3	10-G	7487	AMP	C5'-O5'-P-O3P
3	1-H	7489	AMP	C5'-O5'-P-O2P
3	1-H	7489	AMP	C5'-O5'-P-O3P
3	2-H	7489	AMP	C5'-O5'-P-O2P
3	2-H	7489	AMP	C5'-O5'-P-O3P
3	3-H	7489	AMP	C5'-O5'-P-O2P
3	3-H	7489	AMP	C5'-O5'-P-O3P
3	4-H	7489	AMP	C5'-O5'-P-O2P
3	4-H	7489	AMP	C5'-O5'-P-O3P
3	5-H	7489	AMP	C5'-O5'-P-O2P
3	5-H	7489	AMP	C5'-O5'-P-O3P
3	6-H	7489	AMP	C5'-O5'-P-O2P
3	6-H	7489	AMP	C5'-O5'-P-O3P
3	7-H	7489	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	7-H	7489	AMP	C5'-O5'-P-O3P
3	8-H	7489	AMP	C5'-O5'-P-O2P
3	8-H	7489	AMP	C5'-O5'-P-O3P
3	9-H	7489	AMP	C5'-O5'-P-O2P
3	9-H	7489	AMP	C5'-O5'-P-O3P
3	10-H	7489	AMP	C5'-O5'-P-O2P
3	10-H	7489	AMP	C5'-O5'-P-O3P
3	1-I	7491	AMP	C5'-O5'-P-O2P
3	1-I	7491	AMP	C5'-O5'-P-O3P
3	2-I	7491	AMP	C5'-O5'-P-O2P
3	2-I	7491	AMP	C5'-O5'-P-O3P
3	3-I	7491	AMP	C5'-O5'-P-O2P
3	3-I	7491	AMP	C5'-O5'-P-O3P
3	4-I	7491	AMP	C5'-O5'-P-O2P
3	4-I	7491	AMP	C5'-O5'-P-O3P
3	5-I	7491	AMP	C5'-O5'-P-O2P
3	5-I	7491	AMP	C5'-O5'-P-O3P
3	6-I	7491	AMP	C5'-O5'-P-O2P
3	6-I	7491	AMP	C5'-O5'-P-O3P
3	7-I	7491	AMP	C5'-O5'-P-O2P
3	7-I	7491	AMP	C5'-O5'-P-O3P
3	8-I	7491	AMP	C5'-O5'-P-O2P
3	8-I	7491	AMP	C5'-O5'-P-O3P
3	9-I	7491	AMP	C5'-O5'-P-O2P
3	9-I	7491	AMP	C5'-O5'-P-O3P
3	10-I	7491	AMP	C5'-O5'-P-O2P
3	10-I	7491	AMP	C5'-O5'-P-O3P
3	1-J	7493	AMP	C5'-O5'-P-O2P
3	1-J	7493	AMP	C5'-O5'-P-O3P
3	2-J	7493	AMP	C5'-O5'-P-O2P
3	2-J	7493	AMP	C5'-O5'-P-O3P
3	3-J	7493	AMP	C5'-O5'-P-O2P
3	3-J	7493	AMP	C5'-O5'-P-O3P
3	4-J	7493	AMP	C5'-O5'-P-O2P
3	4-J	7493	AMP	C5'-O5'-P-O3P
3	5-J	7493	AMP	C5'-O5'-P-O2P
3	5-J	7493	AMP	C5'-O5'-P-O3P
3	6-J	7493	AMP	C5'-O5'-P-O2P
3	6-J	7493	AMP	C5'-O5'-P-O3P
3	7-J	7493	AMP	C5'-O5'-P-O2P
3	7-J	7493	AMP	C5'-O5'-P-O3P
3	8-J	7493	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	8-J	7493	AMP	C5'-O5'-P-O3P
3	9-J	7493	AMP	C5'-O5'-P-O2P
3	9-J	7493	AMP	C5'-O5'-P-O3P
3	10-J	7493	AMP	C5'-O5'-P-O2P
3	10-J	7493	AMP	C5'-O5'-P-O3P
3	1-K	7495	AMP	C5'-O5'-P-O2P
3	1-K	7495	AMP	C5'-O5'-P-O3P
3	2-K	7495	AMP	C5'-O5'-P-O2P
3	2-K	7495	AMP	C5'-O5'-P-O3P
3	3-K	7495	AMP	C5'-O5'-P-O2P
3	3-K	7495	AMP	C5'-O5'-P-O3P
3	4-K	7495	AMP	C5'-O5'-P-O2P
3	4-K	7495	AMP	C5'-O5'-P-O3P
3	5-K	7495	AMP	C5'-O5'-P-O2P
3	5-K	7495	AMP	C5'-O5'-P-O3P
3	6-K	7495	AMP	C5'-O5'-P-O2P
3	6-K	7495	AMP	C5'-O5'-P-O3P
3	7-K	7495	AMP	C5'-O5'-P-O2P
3	7-K	7495	AMP	C5'-O5'-P-O3P
3	8-K	7495	AMP	C5'-O5'-P-O2P
3	8-K	7495	AMP	C5'-O5'-P-O3P
3	9-K	7495	AMP	C5'-O5'-P-O2P
3	9-K	7495	AMP	C5'-O5'-P-O3P
3	10-K	7495	AMP	C5'-O5'-P-O2P
3	10-K	7495	AMP	C5'-O5'-P-O3P
3	1-L	7497	AMP	C5'-O5'-P-O2P
3	1-L	7497	AMP	C5'-O5'-P-O3P
3	2-L	7497	AMP	C5'-O5'-P-O2P
3	2-L	7497	AMP	C5'-O5'-P-O3P
3	3-L	7497	AMP	C5'-O5'-P-O2P
3	3-L	7497	AMP	C5'-O5'-P-O3P
3	4-L	7497	AMP	C5'-O5'-P-O2P
3	4-L	7497	AMP	C5'-O5'-P-O3P
3	5-L	7497	AMP	C5'-O5'-P-O2P
3	5-L	7497	AMP	C5'-O5'-P-O3P
3	6-L	7497	AMP	C5'-O5'-P-O2P
3	6-L	7497	AMP	C5'-O5'-P-O3P
3	7-L	7497	AMP	C5'-O5'-P-O2P
3	7-L	7497	AMP	C5'-O5'-P-O3P
3	8-L	7497	AMP	C5'-O5'-P-O2P
3	8-L	7497	AMP	C5'-O5'-P-O3P
3	9-L	7497	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	9-L	7497	AMP	C5'-O5'-P-O3P
3	10-L	7497	AMP	C5'-O5'-P-O2P
3	10-L	7497	AMP	C5'-O5'-P-O3P
3	1-M	7499	AMP	C5'-O5'-P-O2P
3	1-M	7499	AMP	C5'-O5'-P-O3P
3	2-M	7499	AMP	C5'-O5'-P-O2P
3	2-M	7499	AMP	C5'-O5'-P-O3P
3	3-M	7499	AMP	C5'-O5'-P-O2P
3	3-M	7499	AMP	C5'-O5'-P-O3P
3	4-M	7499	AMP	C5'-O5'-P-O2P
3	4-M	7499	AMP	C5'-O5'-P-O3P
3	5-M	7499	AMP	C5'-O5'-P-O2P
3	5-M	7499	AMP	C5'-O5'-P-O3P
3	6-M	7499	AMP	C5'-O5'-P-O2P
3	6-M	7499	AMP	C5'-O5'-P-O3P
3	7-M	7499	AMP	C5'-O5'-P-O2P
3	7-M	7499	AMP	C5'-O5'-P-O3P
3	8-M	7499	AMP	C5'-O5'-P-O2P
3	8-M	7499	AMP	C5'-O5'-P-O3P
3	9-M	7499	AMP	C5'-O5'-P-O2P
3	9-M	7499	AMP	C5'-O5'-P-O3P
3	10-M	7499	AMP	C5'-O5'-P-O2P
3	10-M	7499	AMP	C5'-O5'-P-O3P
3	1-N	7501	AMP	C5'-O5'-P-O2P
3	1-N	7501	AMP	C5'-O5'-P-O3P
3	2-N	7501	AMP	C5'-O5'-P-O2P
3	2-N	7501	AMP	C5'-O5'-P-O3P
3	3-N	7501	AMP	C5'-O5'-P-O2P
3	3-N	7501	AMP	C5'-O5'-P-O3P
3	4-N	7501	AMP	C5'-O5'-P-O2P
3	4-N	7501	AMP	C5'-O5'-P-O3P
3	5-N	7501	AMP	C5'-O5'-P-O2P
3	5-N	7501	AMP	C5'-O5'-P-O3P
3	6-N	7501	AMP	C5'-O5'-P-O2P
3	6-N	7501	AMP	C5'-O5'-P-O3P
3	7-N	7501	AMP	C5'-O5'-P-O2P
3	7-N	7501	AMP	C5'-O5'-P-O3P
3	8-N	7501	AMP	C5'-O5'-P-O2P
3	8-N	7501	AMP	C5'-O5'-P-O3P
3	9-N	7501	AMP	C5'-O5'-P-O2P
3	9-N	7501	AMP	C5'-O5'-P-O3P
3	10-N	7501	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	10-N	7501	AMP	C5'-O5'-P-O3P
3	1-O	7503	AMP	C5'-O5'-P-O2P
3	1-O	7503	AMP	C5'-O5'-P-O3P
3	2-O	7503	AMP	C5'-O5'-P-O2P
3	2-O	7503	AMP	C5'-O5'-P-O3P
3	3-O	7503	AMP	C5'-O5'-P-O2P
3	3-O	7503	AMP	C5'-O5'-P-O3P
3	4-O	7503	AMP	C5'-O5'-P-O2P
3	4-O	7503	AMP	C5'-O5'-P-O3P
3	5-O	7503	AMP	C5'-O5'-P-O2P
3	5-O	7503	AMP	C5'-O5'-P-O3P
3	6-O	7503	AMP	C5'-O5'-P-O2P
3	6-O	7503	AMP	C5'-O5'-P-O3P
3	7-O	7503	AMP	C5'-O5'-P-O2P
3	7-O	7503	AMP	C5'-O5'-P-O3P
3	8-O	7503	AMP	C5'-O5'-P-O2P
3	8-O	7503	AMP	C5'-O5'-P-O3P
3	9-O	7503	AMP	C5'-O5'-P-O2P
3	9-O	7503	AMP	C5'-O5'-P-O3P
3	10-O	7503	AMP	C5'-O5'-P-O2P
3	10-O	7503	AMP	C5'-O5'-P-O3P
3	1-P	7505	AMP	C5'-O5'-P-O2P
3	1-P	7505	AMP	C5'-O5'-P-O3P
3	2-P	7505	AMP	C5'-O5'-P-O2P
3	2-P	7505	AMP	C5'-O5'-P-O3P
3	3-P	7505	AMP	C5'-O5'-P-O2P
3	3-P	7505	AMP	C5'-O5'-P-O3P
3	4-P	7505	AMP	C5'-O5'-P-O2P
3	4-P	7505	AMP	C5'-O5'-P-O3P
3	5-P	7505	AMP	C5'-O5'-P-O2P
3	5-P	7505	AMP	C5'-O5'-P-O3P
3	6-P	7505	AMP	C5'-O5'-P-O2P
3	6-P	7505	AMP	C5'-O5'-P-O3P
3	7-P	7505	AMP	C5'-O5'-P-O2P
3	7-P	7505	AMP	C5'-O5'-P-O3P
3	8-P	7505	AMP	C5'-O5'-P-O2P
3	8-P	7505	AMP	C5'-O5'-P-O3P
3	9-P	7505	AMP	C5'-O5'-P-O2P
3	9-P	7505	AMP	C5'-O5'-P-O3P
3	10-P	7505	AMP	C5'-O5'-P-O2P
3	10-P	7505	AMP	C5'-O5'-P-O3P
3	1-Q	7507	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	1-Q	7507	AMP	C5'-O5'-P-O3P
3	2-Q	7507	AMP	C5'-O5'-P-O2P
3	2-Q	7507	AMP	C5'-O5'-P-O3P
3	3-Q	7507	AMP	C5'-O5'-P-O2P
3	3-Q	7507	AMP	C5'-O5'-P-O3P
3	4-Q	7507	AMP	C5'-O5'-P-O2P
3	4-Q	7507	AMP	C5'-O5'-P-O3P
3	5-Q	7507	AMP	C5'-O5'-P-O2P
3	5-Q	7507	AMP	C5'-O5'-P-O3P
3	6-Q	7507	AMP	C5'-O5'-P-O2P
3	6-Q	7507	AMP	C5'-O5'-P-O3P
3	7-Q	7507	AMP	C5'-O5'-P-O2P
3	7-Q	7507	AMP	C5'-O5'-P-O3P
3	8-Q	7507	AMP	C5'-O5'-P-O2P
3	8-Q	7507	AMP	C5'-O5'-P-O3P
3	9-Q	7507	AMP	C5'-O5'-P-O2P
3	9-Q	7507	AMP	C5'-O5'-P-O3P
3	10-Q	7507	AMP	C5'-O5'-P-O2P
3	10-Q	7507	AMP	C5'-O5'-P-O3P
3	1-R	7509	AMP	C5'-O5'-P-O2P
3	1-R	7509	AMP	C5'-O5'-P-O3P
3	2-R	7509	AMP	C5'-O5'-P-O2P
3	2-R	7509	AMP	C5'-O5'-P-O3P
3	3-R	7509	AMP	C5'-O5'-P-O2P
3	3-R	7509	AMP	C5'-O5'-P-O3P
3	4-R	7509	AMP	C5'-O5'-P-O2P
3	4-R	7509	AMP	C5'-O5'-P-O3P
3	5-R	7509	AMP	C5'-O5'-P-O2P
3	5-R	7509	AMP	C5'-O5'-P-O3P
3	6-R	7509	AMP	C5'-O5'-P-O2P
3	6-R	7509	AMP	C5'-O5'-P-O3P
3	7-R	7509	AMP	C5'-O5'-P-O2P
3	7-R	7509	AMP	C5'-O5'-P-O3P
3	8-R	7509	AMP	C5'-O5'-P-O2P
3	8-R	7509	AMP	C5'-O5'-P-O3P
3	9-R	7509	AMP	C5'-O5'-P-O2P
3	9-R	7509	AMP	C5'-O5'-P-O3P
3	10-R	7509	AMP	C5'-O5'-P-O2P
3	10-R	7509	AMP	C5'-O5'-P-O3P
3	1-S	7511	AMP	C5'-O5'-P-O2P
3	1-S	7511	AMP	C5'-O5'-P-O3P
3	2-S	7511	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	2-S	7511	AMP	C5'-O5'-P-O3P
3	3-S	7511	AMP	C5'-O5'-P-O2P
3	3-S	7511	AMP	C5'-O5'-P-O3P
3	4-S	7511	AMP	C5'-O5'-P-O2P
3	4-S	7511	AMP	C5'-O5'-P-O3P
3	5-S	7511	AMP	C5'-O5'-P-O2P
3	5-S	7511	AMP	C5'-O5'-P-O3P
3	6-S	7511	AMP	C5'-O5'-P-O2P
3	6-S	7511	AMP	C5'-O5'-P-O3P
3	7-S	7511	AMP	C5'-O5'-P-O2P
3	7-S	7511	AMP	C5'-O5'-P-O3P
3	8-S	7511	AMP	C5'-O5'-P-O2P
3	8-S	7511	AMP	C5'-O5'-P-O3P
3	9-S	7511	AMP	C5'-O5'-P-O2P
3	9-S	7511	AMP	C5'-O5'-P-O3P
3	10-S	7511	AMP	C5'-O5'-P-O2P
3	10-S	7511	AMP	C5'-O5'-P-O3P
3	1-T	7513	AMP	C5'-O5'-P-O2P
3	1-T	7513	AMP	C5'-O5'-P-O3P
3	2-T	7513	AMP	C5'-O5'-P-O2P
3	2-T	7513	AMP	C5'-O5'-P-O3P
3	3-T	7513	AMP	C5'-O5'-P-O2P
3	3-T	7513	AMP	C5'-O5'-P-O3P
3	4-T	7513	AMP	C5'-O5'-P-O2P
3	4-T	7513	AMP	C5'-O5'-P-O3P
3	5-T	7513	AMP	C5'-O5'-P-O2P
3	5-T	7513	AMP	C5'-O5'-P-O3P
3	6-T	7513	AMP	C5'-O5'-P-O2P
3	6-T	7513	AMP	C5'-O5'-P-O3P
3	7-T	7513	AMP	C5'-O5'-P-O2P
3	7-T	7513	AMP	C5'-O5'-P-O3P
3	8-T	7513	AMP	C5'-O5'-P-O2P
3	8-T	7513	AMP	C5'-O5'-P-O3P
3	9-T	7513	AMP	C5'-O5'-P-O2P
3	9-T	7513	AMP	C5'-O5'-P-O3P
3	10-T	7513	AMP	C5'-O5'-P-O2P
3	10-T	7513	AMP	C5'-O5'-P-O3P
3	1-U	7515	AMP	C5'-O5'-P-O2P
3	1-U	7515	AMP	C5'-O5'-P-O3P
3	2-U	7515	AMP	C5'-O5'-P-O2P
3	2-U	7515	AMP	C5'-O5'-P-O3P
3	3-U	7515	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	3-U	7515	AMP	C5'-O5'-P-O3P
3	4-U	7515	AMP	C5'-O5'-P-O2P
3	4-U	7515	AMP	C5'-O5'-P-O3P
3	5-U	7515	AMP	C5'-O5'-P-O2P
3	5-U	7515	AMP	C5'-O5'-P-O3P
3	6-U	7515	AMP	C5'-O5'-P-O2P
3	6-U	7515	AMP	C5'-O5'-P-O3P
3	7-U	7515	AMP	C5'-O5'-P-O2P
3	7-U	7515	AMP	C5'-O5'-P-O3P
3	8-U	7515	AMP	C5'-O5'-P-O2P
3	8-U	7515	AMP	C5'-O5'-P-O3P
3	9-U	7515	AMP	C5'-O5'-P-O2P
3	9-U	7515	AMP	C5'-O5'-P-O3P
3	10-U	7515	AMP	C5'-O5'-P-O2P
3	10-U	7515	AMP	C5'-O5'-P-O3P
3	1-V	7517	AMP	C5'-O5'-P-O2P
3	1-V	7517	AMP	C5'-O5'-P-O3P
3	2-V	7517	AMP	C5'-O5'-P-O2P
3	2-V	7517	AMP	C5'-O5'-P-O3P
3	3-V	7517	AMP	C5'-O5'-P-O2P
3	3-V	7517	AMP	C5'-O5'-P-O3P
3	4-V	7517	AMP	C5'-O5'-P-O2P
3	4-V	7517	AMP	C5'-O5'-P-O3P
3	5-V	7517	AMP	C5'-O5'-P-O2P
3	5-V	7517	AMP	C5'-O5'-P-O3P
3	6-V	7517	AMP	C5'-O5'-P-O2P
3	6-V	7517	AMP	C5'-O5'-P-O3P
3	7-V	7517	AMP	C5'-O5'-P-O2P
3	7-V	7517	AMP	C5'-O5'-P-O3P
3	8-V	7517	AMP	C5'-O5'-P-O2P
3	8-V	7517	AMP	C5'-O5'-P-O3P
3	9-V	7517	AMP	C5'-O5'-P-O2P
3	9-V	7517	AMP	C5'-O5'-P-O3P
3	10-V	7517	AMP	C5'-O5'-P-O2P
3	10-V	7517	AMP	C5'-O5'-P-O3P
3	1-W	7519	AMP	C5'-O5'-P-O2P
3	1-W	7519	AMP	C5'-O5'-P-O3P
3	2-W	7519	AMP	C5'-O5'-P-O2P
3	2-W	7519	AMP	C5'-O5'-P-O3P
3	3-W	7519	AMP	C5'-O5'-P-O2P
3	3-W	7519	AMP	C5'-O5'-P-O3P
3	4-W	7519	AMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	4-W	7519	AMP	C5'-O5'-P-O3P
3	5-W	7519	AMP	C5'-O5'-P-O2P
3	5-W	7519	AMP	C5'-O5'-P-O3P
3	6-W	7519	AMP	C5'-O5'-P-O2P
3	6-W	7519	AMP	C5'-O5'-P-O3P
3	7-W	7519	AMP	C5'-O5'-P-O2P
3	7-W	7519	AMP	C5'-O5'-P-O3P
3	8-W	7519	AMP	C5'-O5'-P-O2P
3	8-W	7519	AMP	C5'-O5'-P-O3P
3	9-W	7519	AMP	C5'-O5'-P-O2P
3	9-W	7519	AMP	C5'-O5'-P-O3P
3	10-W	7519	AMP	C5'-O5'-P-O2P
3	10-W	7519	AMP	C5'-O5'-P-O3P
3	1-X	7521	AMP	C5'-O5'-P-O2P
3	1-X	7521	AMP	C5'-O5'-P-O3P
3	2-X	7521	AMP	C5'-O5'-P-O2P
3	2-X	7521	AMP	C5'-O5'-P-O3P
3	3-X	7521	AMP	C5'-O5'-P-O2P
3	3-X	7521	AMP	C5'-O5'-P-O3P
3	4-X	7521	AMP	C5'-O5'-P-O2P
3	4-X	7521	AMP	C5'-O5'-P-O3P
3	5-X	7521	AMP	C5'-O5'-P-O2P
3	5-X	7521	AMP	C5'-O5'-P-O3P
3	6-X	7521	AMP	C5'-O5'-P-O2P
3	6-X	7521	AMP	C5'-O5'-P-O3P
3	7-X	7521	AMP	C5'-O5'-P-O2P
3	7-X	7521	AMP	C5'-O5'-P-O3P
3	8-X	7521	AMP	C5'-O5'-P-O2P
3	8-X	7521	AMP	C5'-O5'-P-O3P
3	9-X	7521	AMP	C5'-O5'-P-O2P
3	9-X	7521	AMP	C5'-O5'-P-O3P
3	10-X	7521	AMP	C5'-O5'-P-O2P
3	10-X	7521	AMP	C5'-O5'-P-O3P
3	1-A	7475	AMP	C5'-O5'-P-O1P
3	2-A	7475	AMP	C5'-O5'-P-O1P
3	3-A	7475	AMP	C5'-O5'-P-O1P
3	4-A	7475	AMP	C5'-O5'-P-O1P
3	5-A	7475	AMP	C5'-O5'-P-O1P
3	6-A	7475	AMP	C5'-O5'-P-O1P
3	7-A	7475	AMP	C5'-O5'-P-O1P
3	8-A	7475	AMP	C5'-O5'-P-O1P
3	9-A	7475	AMP	C5'-O5'-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	10-A	7475	AMP	C5'-O5'-P-O1P
3	1-B	7477	AMP	C5'-O5'-P-O1P
3	2-B	7477	AMP	C5'-O5'-P-O1P
3	3-B	7477	AMP	C5'-O5'-P-O1P
3	4-B	7477	AMP	C5'-O5'-P-O1P
3	5-B	7477	AMP	C5'-O5'-P-O1P
3	6-B	7477	AMP	C5'-O5'-P-O1P
3	7-B	7477	AMP	C5'-O5'-P-O1P
3	8-B	7477	AMP	C5'-O5'-P-O1P
3	9-B	7477	AMP	C5'-O5'-P-O1P
3	10-B	7477	AMP	C5'-O5'-P-O1P
3	1-C	7479	AMP	C5'-O5'-P-O1P
3	2-C	7479	AMP	C5'-O5'-P-O1P
3	3-C	7479	AMP	C5'-O5'-P-O1P
3	4-C	7479	AMP	C5'-O5'-P-O1P
3	5-C	7479	AMP	C5'-O5'-P-O1P
3	6-C	7479	AMP	C5'-O5'-P-O1P
3	7-C	7479	AMP	C5'-O5'-P-O1P
3	8-C	7479	AMP	C5'-O5'-P-O1P
3	9-C	7479	AMP	C5'-O5'-P-O1P
3	10-C	7479	AMP	C5'-O5'-P-O1P
3	1-D	7481	AMP	C5'-O5'-P-O1P
3	2-D	7481	AMP	C5'-O5'-P-O1P
3	3-D	7481	AMP	C5'-O5'-P-O1P
3	4-D	7481	AMP	C5'-O5'-P-O1P
3	5-D	7481	AMP	C5'-O5'-P-O1P
3	6-D	7481	AMP	C5'-O5'-P-O1P
3	7-D	7481	AMP	C5'-O5'-P-O1P
3	8-D	7481	AMP	C5'-O5'-P-O1P
3	9-D	7481	AMP	C5'-O5'-P-O1P
3	10-D	7481	AMP	C5'-O5'-P-O1P
3	1-E	7483	AMP	C5'-O5'-P-O1P
3	2-E	7483	AMP	C5'-O5'-P-O1P
3	3-E	7483	AMP	C5'-O5'-P-O1P
3	4-E	7483	AMP	C5'-O5'-P-O1P
3	5-E	7483	AMP	C5'-O5'-P-O1P
3	6-E	7483	AMP	C5'-O5'-P-O1P
3	7-E	7483	AMP	C5'-O5'-P-O1P
3	8-E	7483	AMP	C5'-O5'-P-O1P
3	9-E	7483	AMP	C5'-O5'-P-O1P
3	10-E	7483	AMP	C5'-O5'-P-O1P
3	1-F	7485	AMP	C5'-O5'-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	2-F	7485	AMP	C5'-O5'-P-O1P
3	3-F	7485	AMP	C5'-O5'-P-O1P
3	4-F	7485	AMP	C5'-O5'-P-O1P
3	5-F	7485	AMP	C5'-O5'-P-O1P
3	6-F	7485	AMP	C5'-O5'-P-O1P
3	7-F	7485	AMP	C5'-O5'-P-O1P
3	8-F	7485	AMP	C5'-O5'-P-O1P
3	9-F	7485	AMP	C5'-O5'-P-O1P
3	10-F	7485	AMP	C5'-O5'-P-O1P
3	1-G	7487	AMP	C5'-O5'-P-O1P
3	2-G	7487	AMP	C5'-O5'-P-O1P
3	3-G	7487	AMP	C5'-O5'-P-O1P
3	4-G	7487	AMP	C5'-O5'-P-O1P
3	5-G	7487	AMP	C5'-O5'-P-O1P
3	6-G	7487	AMP	C5'-O5'-P-O1P
3	7-G	7487	AMP	C5'-O5'-P-O1P
3	8-G	7487	AMP	C5'-O5'-P-O1P
3	9-G	7487	AMP	C5'-O5'-P-O1P
3	10-G	7487	AMP	C5'-O5'-P-O1P
3	1-H	7489	AMP	C5'-O5'-P-O1P
3	2-H	7489	AMP	C5'-O5'-P-O1P
3	3-H	7489	AMP	C5'-O5'-P-O1P
3	4-H	7489	AMP	C5'-O5'-P-O1P
3	5-H	7489	AMP	C5'-O5'-P-O1P
3	6-H	7489	AMP	C5'-O5'-P-O1P
3	7-H	7489	AMP	C5'-O5'-P-O1P
3	8-H	7489	AMP	C5'-O5'-P-O1P
3	9-H	7489	AMP	C5'-O5'-P-O1P
3	10-H	7489	AMP	C5'-O5'-P-O1P
3	1-I	7491	AMP	C5'-O5'-P-O1P
3	2-I	7491	AMP	C5'-O5'-P-O1P
3	3-I	7491	AMP	C5'-O5'-P-O1P
3	4-I	7491	AMP	C5'-O5'-P-O1P
3	5-I	7491	AMP	C5'-O5'-P-O1P
3	6-I	7491	AMP	C5'-O5'-P-O1P
3	7-I	7491	AMP	C5'-O5'-P-O1P
3	8-I	7491	AMP	C5'-O5'-P-O1P
3	9-I	7491	AMP	C5'-O5'-P-O1P
3	10-I	7491	AMP	C5'-O5'-P-O1P
3	1-J	7493	AMP	C5'-O5'-P-O1P
3	2-J	7493	AMP	C5'-O5'-P-O1P
3	3-J	7493	AMP	C5'-O5'-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	4-J	7493	AMP	C5'-O5'-P-O1P
3	5-J	7493	AMP	C5'-O5'-P-O1P
3	6-J	7493	AMP	C5'-O5'-P-O1P
3	7-J	7493	AMP	C5'-O5'-P-O1P
3	8-J	7493	AMP	C5'-O5'-P-O1P
3	9-J	7493	AMP	C5'-O5'-P-O1P
3	10-J	7493	AMP	C5'-O5'-P-O1P
3	1-K	7495	AMP	C5'-O5'-P-O1P
3	2-K	7495	AMP	C5'-O5'-P-O1P
3	3-K	7495	AMP	C5'-O5'-P-O1P
3	4-K	7495	AMP	C5'-O5'-P-O1P
3	5-K	7495	AMP	C5'-O5'-P-O1P
3	6-K	7495	AMP	C5'-O5'-P-O1P
3	7-K	7495	AMP	C5'-O5'-P-O1P
3	8-K	7495	AMP	C5'-O5'-P-O1P
3	9-K	7495	AMP	C5'-O5'-P-O1P
3	10-K	7495	AMP	C5'-O5'-P-O1P
3	1-L	7497	AMP	C5'-O5'-P-O1P
3	2-L	7497	AMP	C5'-O5'-P-O1P
3	3-L	7497	AMP	C5'-O5'-P-O1P
3	4-L	7497	AMP	C5'-O5'-P-O1P
3	5-L	7497	AMP	C5'-O5'-P-O1P
3	6-L	7497	AMP	C5'-O5'-P-O1P
3	7-L	7497	AMP	C5'-O5'-P-O1P
3	8-L	7497	AMP	C5'-O5'-P-O1P
3	9-L	7497	AMP	C5'-O5'-P-O1P
3	10-L	7497	AMP	C5'-O5'-P-O1P
3	1-M	7499	AMP	C5'-O5'-P-O1P
3	2-M	7499	AMP	C5'-O5'-P-O1P
3	3-M	7499	AMP	C5'-O5'-P-O1P
3	4-M	7499	AMP	C5'-O5'-P-O1P
3	5-M	7499	AMP	C5'-O5'-P-O1P
3	6-M	7499	AMP	C5'-O5'-P-O1P
3	7-M	7499	AMP	C5'-O5'-P-O1P
3	8-M	7499	AMP	C5'-O5'-P-O1P
3	9-M	7499	AMP	C5'-O5'-P-O1P
3	10-M	7499	AMP	C5'-O5'-P-O1P
3	1-N	7501	AMP	C5'-O5'-P-O1P
3	2-N	7501	AMP	C5'-O5'-P-O1P
3	3-N	7501	AMP	C5'-O5'-P-O1P
3	4-N	7501	AMP	C5'-O5'-P-O1P
3	5-N	7501	AMP	C5'-O5'-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	6-N	7501	AMP	C5'-O5'-P-O1P
3	7-N	7501	AMP	C5'-O5'-P-O1P
3	8-N	7501	AMP	C5'-O5'-P-O1P
3	9-N	7501	AMP	C5'-O5'-P-O1P
3	10-N	7501	AMP	C5'-O5'-P-O1P
3	1-O	7503	AMP	C5'-O5'-P-O1P
3	2-O	7503	AMP	C5'-O5'-P-O1P
3	3-O	7503	AMP	C5'-O5'-P-O1P
3	4-O	7503	AMP	C5'-O5'-P-O1P
3	5-O	7503	AMP	C5'-O5'-P-O1P
3	6-O	7503	AMP	C5'-O5'-P-O1P
3	7-O	7503	AMP	C5'-O5'-P-O1P
3	8-O	7503	AMP	C5'-O5'-P-O1P
3	9-O	7503	AMP	C5'-O5'-P-O1P
3	10-O	7503	AMP	C5'-O5'-P-O1P
3	1-P	7505	AMP	C5'-O5'-P-O1P
3	2-P	7505	AMP	C5'-O5'-P-O1P
3	3-P	7505	AMP	C5'-O5'-P-O1P
3	4-P	7505	AMP	C5'-O5'-P-O1P
3	5-P	7505	AMP	C5'-O5'-P-O1P
3	6-P	7505	AMP	C5'-O5'-P-O1P
3	7-P	7505	AMP	C5'-O5'-P-O1P
3	8-P	7505	AMP	C5'-O5'-P-O1P
3	9-P	7505	AMP	C5'-O5'-P-O1P
3	10-P	7505	AMP	C5'-O5'-P-O1P
3	1-Q	7507	AMP	C5'-O5'-P-O1P
3	2-Q	7507	AMP	C5'-O5'-P-O1P
3	3-Q	7507	AMP	C5'-O5'-P-O1P
3	4-Q	7507	AMP	C5'-O5'-P-O1P
3	5-Q	7507	AMP	C5'-O5'-P-O1P
3	6-Q	7507	AMP	C5'-O5'-P-O1P
3	7-Q	7507	AMP	C5'-O5'-P-O1P
3	8-Q	7507	AMP	C5'-O5'-P-O1P
3	9-Q	7507	AMP	C5'-O5'-P-O1P
3	10-Q	7507	AMP	C5'-O5'-P-O1P
3	1-R	7509	AMP	C5'-O5'-P-O1P
3	2-R	7509	AMP	C5'-O5'-P-O1P
3	3-R	7509	AMP	C5'-O5'-P-O1P
3	4-R	7509	AMP	C5'-O5'-P-O1P
3	5-R	7509	AMP	C5'-O5'-P-O1P
3	6-R	7509	AMP	C5'-O5'-P-O1P
3	7-R	7509	AMP	C5'-O5'-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	8-R	7509	AMP	C5'-O5'-P-O1P
3	9-R	7509	AMP	C5'-O5'-P-O1P
3	10-R	7509	AMP	C5'-O5'-P-O1P
3	1-S	7511	AMP	C5'-O5'-P-O1P
3	2-S	7511	AMP	C5'-O5'-P-O1P
3	3-S	7511	AMP	C5'-O5'-P-O1P
3	4-S	7511	AMP	C5'-O5'-P-O1P
3	5-S	7511	AMP	C5'-O5'-P-O1P
3	6-S	7511	AMP	C5'-O5'-P-O1P
3	7-S	7511	AMP	C5'-O5'-P-O1P
3	8-S	7511	AMP	C5'-O5'-P-O1P
3	9-S	7511	AMP	C5'-O5'-P-O1P
3	10-S	7511	AMP	C5'-O5'-P-O1P
3	1-T	7513	AMP	C5'-O5'-P-O1P
3	2-T	7513	AMP	C5'-O5'-P-O1P
3	3-T	7513	AMP	C5'-O5'-P-O1P
3	4-T	7513	AMP	C5'-O5'-P-O1P
3	5-T	7513	AMP	C5'-O5'-P-O1P
3	6-T	7513	AMP	C5'-O5'-P-O1P
3	7-T	7513	AMP	C5'-O5'-P-O1P
3	8-T	7513	AMP	C5'-O5'-P-O1P
3	9-T	7513	AMP	C5'-O5'-P-O1P
3	10-T	7513	AMP	C5'-O5'-P-O1P
3	1-U	7515	AMP	C5'-O5'-P-O1P
3	2-U	7515	AMP	C5'-O5'-P-O1P
3	3-U	7515	AMP	C5'-O5'-P-O1P
3	4-U	7515	AMP	C5'-O5'-P-O1P
3	5-U	7515	AMP	C5'-O5'-P-O1P
3	6-U	7515	AMP	C5'-O5'-P-O1P
3	7-U	7515	AMP	C5'-O5'-P-O1P
3	8-U	7515	AMP	C5'-O5'-P-O1P
3	9-U	7515	AMP	C5'-O5'-P-O1P
3	10-U	7515	AMP	C5'-O5'-P-O1P
3	1-V	7517	AMP	C5'-O5'-P-O1P
3	2-V	7517	AMP	C5'-O5'-P-O1P
3	3-V	7517	AMP	C5'-O5'-P-O1P
3	4-V	7517	AMP	C5'-O5'-P-O1P
3	5-V	7517	AMP	C5'-O5'-P-O1P
3	6-V	7517	AMP	C5'-O5'-P-O1P
3	7-V	7517	AMP	C5'-O5'-P-O1P
3	8-V	7517	AMP	C5'-O5'-P-O1P
3	9-V	7517	AMP	C5'-O5'-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	10-V	7517	AMP	C5'-O5'-P-O1P
3	1-W	7519	AMP	C5'-O5'-P-O1P
3	2-W	7519	AMP	C5'-O5'-P-O1P
3	3-W	7519	AMP	C5'-O5'-P-O1P
3	4-W	7519	AMP	C5'-O5'-P-O1P
3	5-W	7519	AMP	C5'-O5'-P-O1P
3	6-W	7519	AMP	C5'-O5'-P-O1P
3	7-W	7519	AMP	C5'-O5'-P-O1P
3	8-W	7519	AMP	C5'-O5'-P-O1P
3	9-W	7519	AMP	C5'-O5'-P-O1P
3	10-W	7519	AMP	C5'-O5'-P-O1P
3	1-X	7521	AMP	C5'-O5'-P-O1P
3	2-X	7521	AMP	C5'-O5'-P-O1P
3	3-X	7521	AMP	C5'-O5'-P-O1P
3	4-X	7521	AMP	C5'-O5'-P-O1P
3	5-X	7521	AMP	C5'-O5'-P-O1P
3	6-X	7521	AMP	C5'-O5'-P-O1P
3	7-X	7521	AMP	C5'-O5'-P-O1P
3	8-X	7521	AMP	C5'-O5'-P-O1P
3	9-X	7521	AMP	C5'-O5'-P-O1P
3	10-X	7521	AMP	C5'-O5'-P-O1P
3	1-A	7475	AMP	C2'-C1'-N9-C4
3	2-A	7475	AMP	C2'-C1'-N9-C4
3	3-A	7475	AMP	C2'-C1'-N9-C4
3	4-A	7475	AMP	C2'-C1'-N9-C4
3	5-A	7475	AMP	C2'-C1'-N9-C4
3	6-A	7475	AMP	C2'-C1'-N9-C4
3	7-A	7475	AMP	C2'-C1'-N9-C4
3	8-A	7475	AMP	C2'-C1'-N9-C4
3	9-A	7475	AMP	C2'-C1'-N9-C4
3	10-A	7475	AMP	C2'-C1'-N9-C4
3	1-B	7477	AMP	C2'-C1'-N9-C4
3	2-B	7477	AMP	C2'-C1'-N9-C4
3	3-B	7477	AMP	C2'-C1'-N9-C4
3	4-B	7477	AMP	C2'-C1'-N9-C4
3	5-B	7477	AMP	C2'-C1'-N9-C4
3	6-B	7477	AMP	C2'-C1'-N9-C4
3	7-B	7477	AMP	C2'-C1'-N9-C4
3	8-B	7477	AMP	C2'-C1'-N9-C4
3	9-B	7477	AMP	C2'-C1'-N9-C4
3	10-B	7477	AMP	C2'-C1'-N9-C4
3	1-C	7479	AMP	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	2-C	7479	AMP	C2'-C1'-N9-C4
3	3-C	7479	AMP	C2'-C1'-N9-C4
3	4-C	7479	AMP	C2'-C1'-N9-C4
3	5-C	7479	AMP	C2'-C1'-N9-C4
3	6-C	7479	AMP	C2'-C1'-N9-C4
3	7-C	7479	AMP	C2'-C1'-N9-C4
3	8-C	7479	AMP	C2'-C1'-N9-C4
3	9-C	7479	AMP	C2'-C1'-N9-C4
3	10-C	7479	AMP	C2'-C1'-N9-C4
3	1-D	7481	AMP	C2'-C1'-N9-C4
3	2-D	7481	AMP	C2'-C1'-N9-C4
3	3-D	7481	AMP	C2'-C1'-N9-C4
3	4-D	7481	AMP	C2'-C1'-N9-C4
3	5-D	7481	AMP	C2'-C1'-N9-C4
3	6-D	7481	AMP	C2'-C1'-N9-C4
3	7-D	7481	AMP	C2'-C1'-N9-C4
3	8-D	7481	AMP	C2'-C1'-N9-C4
3	9-D	7481	AMP	C2'-C1'-N9-C4
3	10-D	7481	AMP	C2'-C1'-N9-C4
3	1-E	7483	AMP	C2'-C1'-N9-C4
3	2-E	7483	AMP	C2'-C1'-N9-C4
3	3-E	7483	AMP	C2'-C1'-N9-C4
3	4-E	7483	AMP	C2'-C1'-N9-C4
3	5-E	7483	AMP	C2'-C1'-N9-C4
3	6-E	7483	AMP	C2'-C1'-N9-C4
3	7-E	7483	AMP	C2'-C1'-N9-C4
3	8-E	7483	AMP	C2'-C1'-N9-C4
3	9-E	7483	AMP	C2'-C1'-N9-C4
3	10-E	7483	AMP	C2'-C1'-N9-C4
3	1-F	7485	AMP	C2'-C1'-N9-C4
3	2-F	7485	AMP	C2'-C1'-N9-C4
3	3-F	7485	AMP	C2'-C1'-N9-C4
3	4-F	7485	AMP	C2'-C1'-N9-C4
3	5-F	7485	AMP	C2'-C1'-N9-C4
3	6-F	7485	AMP	C2'-C1'-N9-C4
3	7-F	7485	AMP	C2'-C1'-N9-C4
3	8-F	7485	AMP	C2'-C1'-N9-C4
3	9-F	7485	AMP	C2'-C1'-N9-C4
3	10-F	7485	AMP	C2'-C1'-N9-C4
3	1-G	7487	AMP	C2'-C1'-N9-C4
3	2-G	7487	AMP	C2'-C1'-N9-C4
3	3-G	7487	AMP	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	4-G	7487	AMP	C2'-C1'-N9-C4
3	5-G	7487	AMP	C2'-C1'-N9-C4
3	6-G	7487	AMP	C2'-C1'-N9-C4
3	7-G	7487	AMP	C2'-C1'-N9-C4
3	8-G	7487	AMP	C2'-C1'-N9-C4
3	9-G	7487	AMP	C2'-C1'-N9-C4
3	10-G	7487	AMP	C2'-C1'-N9-C4
3	1-H	7489	AMP	C2'-C1'-N9-C4
3	2-H	7489	AMP	C2'-C1'-N9-C4
3	3-H	7489	AMP	C2'-C1'-N9-C4
3	4-H	7489	AMP	C2'-C1'-N9-C4
3	5-H	7489	AMP	C2'-C1'-N9-C4
3	6-H	7489	AMP	C2'-C1'-N9-C4
3	7-H	7489	AMP	C2'-C1'-N9-C4
3	8-H	7489	AMP	C2'-C1'-N9-C4
3	9-H	7489	AMP	C2'-C1'-N9-C4
3	10-H	7489	AMP	C2'-C1'-N9-C4
3	1-I	7491	AMP	C2'-C1'-N9-C4
3	2-I	7491	AMP	C2'-C1'-N9-C4
3	3-I	7491	AMP	C2'-C1'-N9-C4
3	4-I	7491	AMP	C2'-C1'-N9-C4
3	5-I	7491	AMP	C2'-C1'-N9-C4
3	6-I	7491	AMP	C2'-C1'-N9-C4
3	7-I	7491	AMP	C2'-C1'-N9-C4
3	8-I	7491	AMP	C2'-C1'-N9-C4
3	9-I	7491	AMP	C2'-C1'-N9-C4
3	10-I	7491	AMP	C2'-C1'-N9-C4
3	1-J	7493	AMP	C2'-C1'-N9-C4
3	2-J	7493	AMP	C2'-C1'-N9-C4
3	3-J	7493	AMP	C2'-C1'-N9-C4
3	4-J	7493	AMP	C2'-C1'-N9-C4
3	5-J	7493	AMP	C2'-C1'-N9-C4
3	6-J	7493	AMP	C2'-C1'-N9-C4
3	7-J	7493	AMP	C2'-C1'-N9-C4
3	8-J	7493	AMP	C2'-C1'-N9-C4
3	9-J	7493	AMP	C2'-C1'-N9-C4
3	10-J	7493	AMP	C2'-C1'-N9-C4
3	1-K	7495	AMP	C2'-C1'-N9-C4
3	2-K	7495	AMP	C2'-C1'-N9-C4
3	3-K	7495	AMP	C2'-C1'-N9-C4
3	4-K	7495	AMP	C2'-C1'-N9-C4
3	5-K	7495	AMP	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	6-K	7495	AMP	C2'-C1'-N9-C4
3	7-K	7495	AMP	C2'-C1'-N9-C4
3	8-K	7495	AMP	C2'-C1'-N9-C4
3	9-K	7495	AMP	C2'-C1'-N9-C4
3	10-K	7495	AMP	C2'-C1'-N9-C4
3	1-L	7497	AMP	C2'-C1'-N9-C4
3	2-L	7497	AMP	C2'-C1'-N9-C4
3	3-L	7497	AMP	C2'-C1'-N9-C4
3	4-L	7497	AMP	C2'-C1'-N9-C4
3	5-L	7497	AMP	C2'-C1'-N9-C4
3	6-L	7497	AMP	C2'-C1'-N9-C4
3	7-L	7497	AMP	C2'-C1'-N9-C4
3	8-L	7497	AMP	C2'-C1'-N9-C4
3	9-L	7497	AMP	C2'-C1'-N9-C4
3	10-L	7497	AMP	C2'-C1'-N9-C4
3	1-M	7499	AMP	C2'-C1'-N9-C4
3	2-M	7499	AMP	C2'-C1'-N9-C4
3	3-M	7499	AMP	C2'-C1'-N9-C4
3	4-M	7499	AMP	C2'-C1'-N9-C4
3	5-M	7499	AMP	C2'-C1'-N9-C4
3	6-M	7499	AMP	C2'-C1'-N9-C4
3	7-M	7499	AMP	C2'-C1'-N9-C4
3	8-M	7499	AMP	C2'-C1'-N9-C4
3	9-M	7499	AMP	C2'-C1'-N9-C4
3	10-M	7499	AMP	C2'-C1'-N9-C4
3	1-N	7501	AMP	C2'-C1'-N9-C4
3	2-N	7501	AMP	C2'-C1'-N9-C4
3	3-N	7501	AMP	C2'-C1'-N9-C4
3	4-N	7501	AMP	C2'-C1'-N9-C4
3	5-N	7501	AMP	C2'-C1'-N9-C4
3	6-N	7501	AMP	C2'-C1'-N9-C4
3	7-N	7501	AMP	C2'-C1'-N9-C4
3	8-N	7501	AMP	C2'-C1'-N9-C4
3	9-N	7501	AMP	C2'-C1'-N9-C4
3	10-N	7501	AMP	C2'-C1'-N9-C4
3	1-O	7503	AMP	C2'-C1'-N9-C4
3	2-O	7503	AMP	C2'-C1'-N9-C4
3	3-O	7503	AMP	C2'-C1'-N9-C4
3	4-O	7503	AMP	C2'-C1'-N9-C4
3	5-O	7503	AMP	C2'-C1'-N9-C4
3	6-O	7503	AMP	C2'-C1'-N9-C4
3	7-O	7503	AMP	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	8-O	7503	AMP	C2'-C1'-N9-C4
3	9-O	7503	AMP	C2'-C1'-N9-C4
3	10-O	7503	AMP	C2'-C1'-N9-C4
3	1-P	7505	AMP	C2'-C1'-N9-C4
3	2-P	7505	AMP	C2'-C1'-N9-C4
3	3-P	7505	AMP	C2'-C1'-N9-C4
3	4-P	7505	AMP	C2'-C1'-N9-C4
3	5-P	7505	AMP	C2'-C1'-N9-C4
3	6-P	7505	AMP	C2'-C1'-N9-C4
3	7-P	7505	AMP	C2'-C1'-N9-C4
3	8-P	7505	AMP	C2'-C1'-N9-C4
3	9-P	7505	AMP	C2'-C1'-N9-C4
3	10-P	7505	AMP	C2'-C1'-N9-C4
3	1-Q	7507	AMP	C2'-C1'-N9-C4
3	2-Q	7507	AMP	C2'-C1'-N9-C4
3	3-Q	7507	AMP	C2'-C1'-N9-C4
3	4-Q	7507	AMP	C2'-C1'-N9-C4
3	5-Q	7507	AMP	C2'-C1'-N9-C4
3	6-Q	7507	AMP	C2'-C1'-N9-C4
3	7-Q	7507	AMP	C2'-C1'-N9-C4
3	8-Q	7507	AMP	C2'-C1'-N9-C4
3	9-Q	7507	AMP	C2'-C1'-N9-C4
3	10-Q	7507	AMP	C2'-C1'-N9-C4
3	1-R	7509	AMP	C2'-C1'-N9-C4
3	2-R	7509	AMP	C2'-C1'-N9-C4
3	3-R	7509	AMP	C2'-C1'-N9-C4
3	4-R	7509	AMP	C2'-C1'-N9-C4
3	5-R	7509	AMP	C2'-C1'-N9-C4
3	6-R	7509	AMP	C2'-C1'-N9-C4
3	7-R	7509	AMP	C2'-C1'-N9-C4
3	8-R	7509	AMP	C2'-C1'-N9-C4
3	9-R	7509	AMP	C2'-C1'-N9-C4
3	10-R	7509	AMP	C2'-C1'-N9-C4
3	1-S	7511	AMP	C2'-C1'-N9-C4
3	2-S	7511	AMP	C2'-C1'-N9-C4
3	3-S	7511	AMP	C2'-C1'-N9-C4
3	4-S	7511	AMP	C2'-C1'-N9-C4
3	5-S	7511	AMP	C2'-C1'-N9-C4
3	6-S	7511	AMP	C2'-C1'-N9-C4
3	7-S	7511	AMP	C2'-C1'-N9-C4
3	8-S	7511	AMP	C2'-C1'-N9-C4
3	9-S	7511	AMP	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	10-S	7511	AMP	C2'-C1'-N9-C4
3	1-T	7513	AMP	C2'-C1'-N9-C4
3	2-T	7513	AMP	C2'-C1'-N9-C4
3	3-T	7513	AMP	C2'-C1'-N9-C4
3	4-T	7513	AMP	C2'-C1'-N9-C4
3	5-T	7513	AMP	C2'-C1'-N9-C4
3	6-T	7513	AMP	C2'-C1'-N9-C4
3	7-T	7513	AMP	C2'-C1'-N9-C4
3	8-T	7513	AMP	C2'-C1'-N9-C4
3	9-T	7513	AMP	C2'-C1'-N9-C4
3	10-T	7513	AMP	C2'-C1'-N9-C4
3	1-U	7515	AMP	C2'-C1'-N9-C4
3	2-U	7515	AMP	C2'-C1'-N9-C4
3	3-U	7515	AMP	C2'-C1'-N9-C4
3	4-U	7515	AMP	C2'-C1'-N9-C4
3	5-U	7515	AMP	C2'-C1'-N9-C4
3	6-U	7515	AMP	C2'-C1'-N9-C4
3	7-U	7515	AMP	C2'-C1'-N9-C4
3	8-U	7515	AMP	C2'-C1'-N9-C4
3	9-U	7515	AMP	C2'-C1'-N9-C4
3	10-U	7515	AMP	C2'-C1'-N9-C4
3	1-V	7517	AMP	C2'-C1'-N9-C4
3	2-V	7517	AMP	C2'-C1'-N9-C4
3	3-V	7517	AMP	C2'-C1'-N9-C4
3	4-V	7517	AMP	C2'-C1'-N9-C4
3	5-V	7517	AMP	C2'-C1'-N9-C4
3	6-V	7517	AMP	C2'-C1'-N9-C4
3	7-V	7517	AMP	C2'-C1'-N9-C4
3	8-V	7517	AMP	C2'-C1'-N9-C4
3	9-V	7517	AMP	C2'-C1'-N9-C4
3	10-V	7517	AMP	C2'-C1'-N9-C4
3	1-W	7519	AMP	C2'-C1'-N9-C4
3	2-W	7519	AMP	C2'-C1'-N9-C4
3	3-W	7519	AMP	C2'-C1'-N9-C4
3	4-W	7519	AMP	C2'-C1'-N9-C4
3	5-W	7519	AMP	C2'-C1'-N9-C4
3	6-W	7519	AMP	C2'-C1'-N9-C4
3	7-W	7519	AMP	C2'-C1'-N9-C4
3	8-W	7519	AMP	C2'-C1'-N9-C4
3	9-W	7519	AMP	C2'-C1'-N9-C4
3	10-W	7519	AMP	C2'-C1'-N9-C4
3	1-X	7521	AMP	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	2-X	7521	AMP	C2'-C1'-N9-C4
3	3-X	7521	AMP	C2'-C1'-N9-C4
3	4-X	7521	AMP	C2'-C1'-N9-C4
3	5-X	7521	AMP	C2'-C1'-N9-C4
3	6-X	7521	AMP	C2'-C1'-N9-C4
3	7-X	7521	AMP	C2'-C1'-N9-C4
3	8-X	7521	AMP	C2'-C1'-N9-C4
3	9-X	7521	AMP	C2'-C1'-N9-C4
3	10-X	7521	AMP	C2'-C1'-N9-C4
3	1-A	7475	AMP	C2'-C1'-N9-C8
3	2-A	7475	AMP	C2'-C1'-N9-C8
3	3-A	7475	AMP	C2'-C1'-N9-C8
3	4-A	7475	AMP	C2'-C1'-N9-C8
3	5-A	7475	AMP	C2'-C1'-N9-C8
3	6-A	7475	AMP	C2'-C1'-N9-C8
3	7-A	7475	AMP	C2'-C1'-N9-C8
3	8-A	7475	AMP	C2'-C1'-N9-C8
3	9-A	7475	AMP	C2'-C1'-N9-C8
3	10-A	7475	AMP	C2'-C1'-N9-C8
3	1-B	7477	AMP	C2'-C1'-N9-C8
3	2-B	7477	AMP	C2'-C1'-N9-C8
3	3-B	7477	AMP	C2'-C1'-N9-C8
3	4-B	7477	AMP	C2'-C1'-N9-C8
3	5-B	7477	AMP	C2'-C1'-N9-C8
3	6-B	7477	AMP	C2'-C1'-N9-C8
3	7-B	7477	AMP	C2'-C1'-N9-C8
3	8-B	7477	AMP	C2'-C1'-N9-C8
3	9-B	7477	AMP	C2'-C1'-N9-C8
3	10-B	7477	AMP	C2'-C1'-N9-C8
3	1-C	7479	AMP	C2'-C1'-N9-C8
3	2-C	7479	AMP	C2'-C1'-N9-C8
3	3-C	7479	AMP	C2'-C1'-N9-C8
3	4-C	7479	AMP	C2'-C1'-N9-C8
3	5-C	7479	AMP	C2'-C1'-N9-C8
3	6-C	7479	AMP	C2'-C1'-N9-C8
3	7-C	7479	AMP	C2'-C1'-N9-C8
3	8-C	7479	AMP	C2'-C1'-N9-C8
3	9-C	7479	AMP	C2'-C1'-N9-C8
3	10-C	7479	AMP	C2'-C1'-N9-C8
3	1-D	7481	AMP	C2'-C1'-N9-C8
3	2-D	7481	AMP	C2'-C1'-N9-C8
3	3-D	7481	AMP	C2'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	4-D	7481	AMP	C2'-C1'-N9-C8
3	5-D	7481	AMP	C2'-C1'-N9-C8
3	6-D	7481	AMP	C2'-C1'-N9-C8
3	7-D	7481	AMP	C2'-C1'-N9-C8
3	8-D	7481	AMP	C2'-C1'-N9-C8
3	9-D	7481	AMP	C2'-C1'-N9-C8
3	10-D	7481	AMP	C2'-C1'-N9-C8
3	1-E	7483	AMP	C2'-C1'-N9-C8
3	2-E	7483	AMP	C2'-C1'-N9-C8
3	3-E	7483	AMP	C2'-C1'-N9-C8
3	4-E	7483	AMP	C2'-C1'-N9-C8
3	5-E	7483	AMP	C2'-C1'-N9-C8
3	6-E	7483	AMP	C2'-C1'-N9-C8
3	7-E	7483	AMP	C2'-C1'-N9-C8
3	8-E	7483	AMP	C2'-C1'-N9-C8
3	9-E	7483	AMP	C2'-C1'-N9-C8
3	10-E	7483	AMP	C2'-C1'-N9-C8
3	1-F	7485	AMP	C2'-C1'-N9-C8
3	2-F	7485	AMP	C2'-C1'-N9-C8
3	3-F	7485	AMP	C2'-C1'-N9-C8
3	4-F	7485	AMP	C2'-C1'-N9-C8
3	5-F	7485	AMP	C2'-C1'-N9-C8
3	6-F	7485	AMP	C2'-C1'-N9-C8
3	7-F	7485	AMP	C2'-C1'-N9-C8
3	8-F	7485	AMP	C2'-C1'-N9-C8
3	9-F	7485	AMP	C2'-C1'-N9-C8
3	10-F	7485	AMP	C2'-C1'-N9-C8
3	1-G	7487	AMP	C2'-C1'-N9-C8
3	2-G	7487	AMP	C2'-C1'-N9-C8
3	3-G	7487	AMP	C2'-C1'-N9-C8
3	4-G	7487	AMP	C2'-C1'-N9-C8
3	5-G	7487	AMP	C2'-C1'-N9-C8
3	6-G	7487	AMP	C2'-C1'-N9-C8
3	7-G	7487	AMP	C2'-C1'-N9-C8
3	8-G	7487	AMP	C2'-C1'-N9-C8
3	9-G	7487	AMP	C2'-C1'-N9-C8
3	10-G	7487	AMP	C2'-C1'-N9-C8
3	1-H	7489	AMP	C2'-C1'-N9-C8
3	2-H	7489	AMP	C2'-C1'-N9-C8
3	3-H	7489	AMP	C2'-C1'-N9-C8
3	4-H	7489	AMP	C2'-C1'-N9-C8
3	5-H	7489	AMP	C2'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	6-H	7489	AMP	C2'-C1'-N9-C8
3	7-H	7489	AMP	C2'-C1'-N9-C8
3	8-H	7489	AMP	C2'-C1'-N9-C8
3	9-H	7489	AMP	C2'-C1'-N9-C8
3	10-H	7489	AMP	C2'-C1'-N9-C8
3	1-I	7491	AMP	C2'-C1'-N9-C8
3	2-I	7491	AMP	C2'-C1'-N9-C8
3	3-I	7491	AMP	C2'-C1'-N9-C8
3	4-I	7491	AMP	C2'-C1'-N9-C8
3	5-I	7491	AMP	C2'-C1'-N9-C8
3	6-I	7491	AMP	C2'-C1'-N9-C8
3	7-I	7491	AMP	C2'-C1'-N9-C8
3	8-I	7491	AMP	C2'-C1'-N9-C8
3	9-I	7491	AMP	C2'-C1'-N9-C8
3	10-I	7491	AMP	C2'-C1'-N9-C8
3	1-J	7493	AMP	C2'-C1'-N9-C8
3	2-J	7493	AMP	C2'-C1'-N9-C8
3	3-J	7493	AMP	C2'-C1'-N9-C8
3	4-J	7493	AMP	C2'-C1'-N9-C8
3	5-J	7493	AMP	C2'-C1'-N9-C8
3	6-J	7493	AMP	C2'-C1'-N9-C8
3	7-J	7493	AMP	C2'-C1'-N9-C8
3	8-J	7493	AMP	C2'-C1'-N9-C8
3	9-J	7493	AMP	C2'-C1'-N9-C8
3	10-J	7493	AMP	C2'-C1'-N9-C8
3	1-K	7495	AMP	C2'-C1'-N9-C8
3	2-K	7495	AMP	C2'-C1'-N9-C8
3	3-K	7495	AMP	C2'-C1'-N9-C8
3	4-K	7495	AMP	C2'-C1'-N9-C8
3	5-K	7495	AMP	C2'-C1'-N9-C8
3	6-K	7495	AMP	C2'-C1'-N9-C8
3	7-K	7495	AMP	C2'-C1'-N9-C8
3	8-K	7495	AMP	C2'-C1'-N9-C8
3	9-K	7495	AMP	C2'-C1'-N9-C8
3	10-K	7495	AMP	C2'-C1'-N9-C8
3	1-L	7497	AMP	C2'-C1'-N9-C8
3	2-L	7497	AMP	C2'-C1'-N9-C8
3	3-L	7497	AMP	C2'-C1'-N9-C8
3	4-L	7497	AMP	C2'-C1'-N9-C8
3	5-L	7497	AMP	C2'-C1'-N9-C8
3	6-L	7497	AMP	C2'-C1'-N9-C8
3	7-L	7497	AMP	C2'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	8-L	7497	AMP	C2'-C1'-N9-C8
3	9-L	7497	AMP	C2'-C1'-N9-C8
3	10-L	7497	AMP	C2'-C1'-N9-C8
3	1-M	7499	AMP	C2'-C1'-N9-C8
3	2-M	7499	AMP	C2'-C1'-N9-C8
3	3-M	7499	AMP	C2'-C1'-N9-C8
3	4-M	7499	AMP	C2'-C1'-N9-C8
3	5-M	7499	AMP	C2'-C1'-N9-C8
3	6-M	7499	AMP	C2'-C1'-N9-C8
3	7-M	7499	AMP	C2'-C1'-N9-C8
3	8-M	7499	AMP	C2'-C1'-N9-C8
3	9-M	7499	AMP	C2'-C1'-N9-C8
3	10-M	7499	AMP	C2'-C1'-N9-C8
3	1-N	7501	AMP	C2'-C1'-N9-C8
3	2-N	7501	AMP	C2'-C1'-N9-C8
3	3-N	7501	AMP	C2'-C1'-N9-C8
3	4-N	7501	AMP	C2'-C1'-N9-C8
3	5-N	7501	AMP	C2'-C1'-N9-C8
3	6-N	7501	AMP	C2'-C1'-N9-C8
3	7-N	7501	AMP	C2'-C1'-N9-C8
3	8-N	7501	AMP	C2'-C1'-N9-C8
3	9-N	7501	AMP	C2'-C1'-N9-C8
3	10-N	7501	AMP	C2'-C1'-N9-C8
3	1-O	7503	AMP	C2'-C1'-N9-C8
3	2-O	7503	AMP	C2'-C1'-N9-C8
3	3-O	7503	AMP	C2'-C1'-N9-C8
3	4-O	7503	AMP	C2'-C1'-N9-C8
3	5-O	7503	AMP	C2'-C1'-N9-C8
3	6-O	7503	AMP	C2'-C1'-N9-C8
3	7-O	7503	AMP	C2'-C1'-N9-C8
3	8-O	7503	AMP	C2'-C1'-N9-C8
3	9-O	7503	AMP	C2'-C1'-N9-C8
3	10-O	7503	AMP	C2'-C1'-N9-C8
3	1-P	7505	AMP	C2'-C1'-N9-C8
3	2-P	7505	AMP	C2'-C1'-N9-C8
3	3-P	7505	AMP	C2'-C1'-N9-C8
3	4-P	7505	AMP	C2'-C1'-N9-C8
3	5-P	7505	AMP	C2'-C1'-N9-C8
3	6-P	7505	AMP	C2'-C1'-N9-C8
3	7-P	7505	AMP	C2'-C1'-N9-C8
3	8-P	7505	AMP	C2'-C1'-N9-C8
3	9-P	7505	AMP	C2'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	10-P	7505	AMP	C2'-C1'-N9-C8
3	1-Q	7507	AMP	C2'-C1'-N9-C8
3	2-Q	7507	AMP	C2'-C1'-N9-C8
3	3-Q	7507	AMP	C2'-C1'-N9-C8
3	4-Q	7507	AMP	C2'-C1'-N9-C8
3	5-Q	7507	AMP	C2'-C1'-N9-C8
3	6-Q	7507	AMP	C2'-C1'-N9-C8
3	7-Q	7507	AMP	C2'-C1'-N9-C8
3	8-Q	7507	AMP	C2'-C1'-N9-C8
3	9-Q	7507	AMP	C2'-C1'-N9-C8
3	10-Q	7507	AMP	C2'-C1'-N9-C8
3	1-R	7509	AMP	C2'-C1'-N9-C8
3	2-R	7509	AMP	C2'-C1'-N9-C8
3	3-R	7509	AMP	C2'-C1'-N9-C8
3	4-R	7509	AMP	C2'-C1'-N9-C8
3	5-R	7509	AMP	C2'-C1'-N9-C8
3	6-R	7509	AMP	C2'-C1'-N9-C8
3	7-R	7509	AMP	C2'-C1'-N9-C8
3	8-R	7509	AMP	C2'-C1'-N9-C8
3	9-R	7509	AMP	C2'-C1'-N9-C8
3	10-R	7509	AMP	C2'-C1'-N9-C8
3	1-S	7511	AMP	C2'-C1'-N9-C8
3	2-S	7511	AMP	C2'-C1'-N9-C8
3	3-S	7511	AMP	C2'-C1'-N9-C8
3	4-S	7511	AMP	C2'-C1'-N9-C8
3	5-S	7511	AMP	C2'-C1'-N9-C8
3	6-S	7511	AMP	C2'-C1'-N9-C8
3	7-S	7511	AMP	C2'-C1'-N9-C8
3	8-S	7511	AMP	C2'-C1'-N9-C8
3	9-S	7511	AMP	C2'-C1'-N9-C8
3	10-S	7511	AMP	C2'-C1'-N9-C8
3	1-T	7513	AMP	C2'-C1'-N9-C8
3	2-T	7513	AMP	C2'-C1'-N9-C8
3	3-T	7513	AMP	C2'-C1'-N9-C8
3	4-T	7513	AMP	C2'-C1'-N9-C8
3	5-T	7513	AMP	C2'-C1'-N9-C8
3	6-T	7513	AMP	C2'-C1'-N9-C8
3	7-T	7513	AMP	C2'-C1'-N9-C8
3	8-T	7513	AMP	C2'-C1'-N9-C8
3	9-T	7513	AMP	C2'-C1'-N9-C8
3	10-T	7513	AMP	C2'-C1'-N9-C8
3	1-U	7515	AMP	C2'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	2-U	7515	AMP	C2'-C1'-N9-C8
3	3-U	7515	AMP	C2'-C1'-N9-C8
3	4-U	7515	AMP	C2'-C1'-N9-C8
3	5-U	7515	AMP	C2'-C1'-N9-C8
3	6-U	7515	AMP	C2'-C1'-N9-C8
3	7-U	7515	AMP	C2'-C1'-N9-C8
3	8-U	7515	AMP	C2'-C1'-N9-C8
3	9-U	7515	AMP	C2'-C1'-N9-C8
3	10-U	7515	AMP	C2'-C1'-N9-C8
3	1-V	7517	AMP	C2'-C1'-N9-C8
3	2-V	7517	AMP	C2'-C1'-N9-C8
3	3-V	7517	AMP	C2'-C1'-N9-C8
3	4-V	7517	AMP	C2'-C1'-N9-C8
3	5-V	7517	AMP	C2'-C1'-N9-C8
3	6-V	7517	AMP	C2'-C1'-N9-C8
3	7-V	7517	AMP	C2'-C1'-N9-C8
3	8-V	7517	AMP	C2'-C1'-N9-C8
3	9-V	7517	AMP	C2'-C1'-N9-C8
3	10-V	7517	AMP	C2'-C1'-N9-C8
3	1-W	7519	AMP	C2'-C1'-N9-C8
3	2-W	7519	AMP	C2'-C1'-N9-C8
3	3-W	7519	AMP	C2'-C1'-N9-C8
3	4-W	7519	AMP	C2'-C1'-N9-C8
3	5-W	7519	AMP	C2'-C1'-N9-C8
3	6-W	7519	AMP	C2'-C1'-N9-C8
3	7-W	7519	AMP	C2'-C1'-N9-C8
3	8-W	7519	AMP	C2'-C1'-N9-C8
3	9-W	7519	AMP	C2'-C1'-N9-C8
3	10-W	7519	AMP	C2'-C1'-N9-C8
3	1-X	7521	AMP	C2'-C1'-N9-C8
3	2-X	7521	AMP	C2'-C1'-N9-C8
3	3-X	7521	AMP	C2'-C1'-N9-C8
3	4-X	7521	AMP	C2'-C1'-N9-C8
3	5-X	7521	AMP	C2'-C1'-N9-C8
3	6-X	7521	AMP	C2'-C1'-N9-C8
3	7-X	7521	AMP	C2'-C1'-N9-C8
3	8-X	7521	AMP	C2'-C1'-N9-C8
3	9-X	7521	AMP	C2'-C1'-N9-C8
3	10-X	7521	AMP	C2'-C1'-N9-C8
4	1-A	7476	CIT	C1-C2-C3-O7
4	2-A	7476	CIT	C1-C2-C3-O7
4	3-A	7476	CIT	C1-C2-C3-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	4-A	7476	CIT	C1-C2-C3-O7
4	5-A	7476	CIT	C1-C2-C3-O7
4	6-A	7476	CIT	C1-C2-C3-O7
4	7-A	7476	CIT	C1-C2-C3-O7
4	8-A	7476	CIT	C1-C2-C3-O7
4	9-A	7476	CIT	C1-C2-C3-O7
4	10-A	7476	CIT	C1-C2-C3-O7
4	1-B	7478	CIT	C1-C2-C3-O7
4	2-B	7478	CIT	C1-C2-C3-O7
4	3-B	7478	CIT	C1-C2-C3-O7
4	4-B	7478	CIT	C1-C2-C3-O7
4	5-B	7478	CIT	C1-C2-C3-O7
4	6-B	7478	CIT	C1-C2-C3-O7
4	7-B	7478	CIT	C1-C2-C3-O7
4	8-B	7478	CIT	C1-C2-C3-O7
4	9-B	7478	CIT	C1-C2-C3-O7
4	10-B	7478	CIT	C1-C2-C3-O7
4	1-C	7480	CIT	C1-C2-C3-O7
4	2-C	7480	CIT	C1-C2-C3-O7
4	3-C	7480	CIT	C1-C2-C3-O7
4	4-C	7480	CIT	C1-C2-C3-O7
4	5-C	7480	CIT	C1-C2-C3-O7
4	6-C	7480	CIT	C1-C2-C3-O7
4	7-C	7480	CIT	C1-C2-C3-O7
4	8-C	7480	CIT	C1-C2-C3-O7
4	9-C	7480	CIT	C1-C2-C3-O7
4	10-C	7480	CIT	C1-C2-C3-O7
4	1-D	7482	CIT	C1-C2-C3-O7
4	2-D	7482	CIT	C1-C2-C3-O7
4	3-D	7482	CIT	C1-C2-C3-O7
4	4-D	7482	CIT	C1-C2-C3-O7
4	5-D	7482	CIT	C1-C2-C3-O7
4	6-D	7482	CIT	C1-C2-C3-O7
4	7-D	7482	CIT	C1-C2-C3-O7
4	8-D	7482	CIT	C1-C2-C3-O7
4	9-D	7482	CIT	C1-C2-C3-O7
4	10-D	7482	CIT	C1-C2-C3-O7
4	1-E	7484	CIT	C1-C2-C3-O7
4	2-E	7484	CIT	C1-C2-C3-O7
4	3-E	7484	CIT	C1-C2-C3-O7
4	4-E	7484	CIT	C1-C2-C3-O7
4	5-E	7484	CIT	C1-C2-C3-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	6-E	7484	CIT	C1-C2-C3-O7
4	7-E	7484	CIT	C1-C2-C3-O7
4	8-E	7484	CIT	C1-C2-C3-O7
4	9-E	7484	CIT	C1-C2-C3-O7
4	10-E	7484	CIT	C1-C2-C3-O7
4	1-F	7486	CIT	C1-C2-C3-O7
4	2-F	7486	CIT	C1-C2-C3-O7
4	3-F	7486	CIT	C1-C2-C3-O7
4	4-F	7486	CIT	C1-C2-C3-O7
4	5-F	7486	CIT	C1-C2-C3-O7
4	6-F	7486	CIT	C1-C2-C3-O7
4	7-F	7486	CIT	C1-C2-C3-O7
4	8-F	7486	CIT	C1-C2-C3-O7
4	9-F	7486	CIT	C1-C2-C3-O7
4	10-F	7486	CIT	C1-C2-C3-O7
4	1-G	7488	CIT	C1-C2-C3-O7
4	2-G	7488	CIT	C1-C2-C3-O7
4	3-G	7488	CIT	C1-C2-C3-O7
4	4-G	7488	CIT	C1-C2-C3-O7
4	5-G	7488	CIT	C1-C2-C3-O7
4	6-G	7488	CIT	C1-C2-C3-O7
4	7-G	7488	CIT	C1-C2-C3-O7
4	8-G	7488	CIT	C1-C2-C3-O7
4	9-G	7488	CIT	C1-C2-C3-O7
4	10-G	7488	CIT	C1-C2-C3-O7
4	1-H	7490	CIT	C1-C2-C3-O7
4	2-H	7490	CIT	C1-C2-C3-O7
4	3-H	7490	CIT	C1-C2-C3-O7
4	4-H	7490	CIT	C1-C2-C3-O7
4	5-H	7490	CIT	C1-C2-C3-O7
4	6-H	7490	CIT	C1-C2-C3-O7
4	7-H	7490	CIT	C1-C2-C3-O7
4	8-H	7490	CIT	C1-C2-C3-O7
4	9-H	7490	CIT	C1-C2-C3-O7
4	10-H	7490	CIT	C1-C2-C3-O7
4	1-I	7492	CIT	C1-C2-C3-O7
4	2-I	7492	CIT	C1-C2-C3-O7
4	3-I	7492	CIT	C1-C2-C3-O7
4	4-I	7492	CIT	C1-C2-C3-O7
4	5-I	7492	CIT	C1-C2-C3-O7
4	6-I	7492	CIT	C1-C2-C3-O7
4	7-I	7492	CIT	C1-C2-C3-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	8-I	7492	CIT	C1-C2-C3-O7
4	9-I	7492	CIT	C1-C2-C3-O7
4	10-I	7492	CIT	C1-C2-C3-O7
4	1-J	7494	CIT	C1-C2-C3-O7
4	2-J	7494	CIT	C1-C2-C3-O7
4	3-J	7494	CIT	C1-C2-C3-O7
4	4-J	7494	CIT	C1-C2-C3-O7
4	5-J	7494	CIT	C1-C2-C3-O7
4	6-J	7494	CIT	C1-C2-C3-O7
4	7-J	7494	CIT	C1-C2-C3-O7
4	8-J	7494	CIT	C1-C2-C3-O7
4	9-J	7494	CIT	C1-C2-C3-O7
4	10-J	7494	CIT	C1-C2-C3-O7
4	1-K	7496	CIT	C1-C2-C3-O7
4	2-K	7496	CIT	C1-C2-C3-O7
4	3-K	7496	CIT	C1-C2-C3-O7
4	4-K	7496	CIT	C1-C2-C3-O7
4	5-K	7496	CIT	C1-C2-C3-O7
4	6-K	7496	CIT	C1-C2-C3-O7
4	7-K	7496	CIT	C1-C2-C3-O7
4	8-K	7496	CIT	C1-C2-C3-O7
4	9-K	7496	CIT	C1-C2-C3-O7
4	10-K	7496	CIT	C1-C2-C3-O7
4	1-L	7498	CIT	C1-C2-C3-O7
4	2-L	7498	CIT	C1-C2-C3-O7
4	3-L	7498	CIT	C1-C2-C3-O7
4	4-L	7498	CIT	C1-C2-C3-O7
4	5-L	7498	CIT	C1-C2-C3-O7
4	6-L	7498	CIT	C1-C2-C3-O7
4	7-L	7498	CIT	C1-C2-C3-O7
4	8-L	7498	CIT	C1-C2-C3-O7
4	9-L	7498	CIT	C1-C2-C3-O7
4	10-L	7498	CIT	C1-C2-C3-O7
4	1-M	7500	CIT	C1-C2-C3-O7
4	2-M	7500	CIT	C1-C2-C3-O7
4	3-M	7500	CIT	C1-C2-C3-O7
4	4-M	7500	CIT	C1-C2-C3-O7
4	5-M	7500	CIT	C1-C2-C3-O7
4	6-M	7500	CIT	C1-C2-C3-O7
4	7-M	7500	CIT	C1-C2-C3-O7
4	8-M	7500	CIT	C1-C2-C3-O7
4	9-M	7500	CIT	C1-C2-C3-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	10-M	7500	CIT	C1-C2-C3-O7
4	1-N	7502	CIT	C1-C2-C3-O7
4	2-N	7502	CIT	C1-C2-C3-O7
4	3-N	7502	CIT	C1-C2-C3-O7
4	4-N	7502	CIT	C1-C2-C3-O7
4	5-N	7502	CIT	C1-C2-C3-O7
4	6-N	7502	CIT	C1-C2-C3-O7
4	7-N	7502	CIT	C1-C2-C3-O7
4	8-N	7502	CIT	C1-C2-C3-O7
4	9-N	7502	CIT	C1-C2-C3-O7
4	10-N	7502	CIT	C1-C2-C3-O7
4	1-O	7504	CIT	C1-C2-C3-O7
4	2-O	7504	CIT	C1-C2-C3-O7
4	3-O	7504	CIT	C1-C2-C3-O7
4	4-O	7504	CIT	C1-C2-C3-O7
4	5-O	7504	CIT	C1-C2-C3-O7
4	6-O	7504	CIT	C1-C2-C3-O7
4	7-O	7504	CIT	C1-C2-C3-O7
4	8-O	7504	CIT	C1-C2-C3-O7
4	9-O	7504	CIT	C1-C2-C3-O7
4	10-O	7504	CIT	C1-C2-C3-O7
4	1-P	7506	CIT	C1-C2-C3-O7
4	2-P	7506	CIT	C1-C2-C3-O7
4	3-P	7506	CIT	C1-C2-C3-O7
4	4-P	7506	CIT	C1-C2-C3-O7
4	5-P	7506	CIT	C1-C2-C3-O7
4	6-P	7506	CIT	C1-C2-C3-O7
4	7-P	7506	CIT	C1-C2-C3-O7
4	8-P	7506	CIT	C1-C2-C3-O7
4	9-P	7506	CIT	C1-C2-C3-O7
4	10-P	7506	CIT	C1-C2-C3-O7
4	1-Q	7508	CIT	C1-C2-C3-O7
4	2-Q	7508	CIT	C1-C2-C3-O7
4	3-Q	7508	CIT	C1-C2-C3-O7
4	4-Q	7508	CIT	C1-C2-C3-O7
4	5-Q	7508	CIT	C1-C2-C3-O7
4	6-Q	7508	CIT	C1-C2-C3-O7
4	7-Q	7508	CIT	C1-C2-C3-O7
4	8-Q	7508	CIT	C1-C2-C3-O7
4	9-Q	7508	CIT	C1-C2-C3-O7
4	10-Q	7508	CIT	C1-C2-C3-O7
4	1-R	7510	CIT	C1-C2-C3-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	2-R	7510	CIT	C1-C2-C3-O7
4	3-R	7510	CIT	C1-C2-C3-O7
4	4-R	7510	CIT	C1-C2-C3-O7
4	5-R	7510	CIT	C1-C2-C3-O7
4	6-R	7510	CIT	C1-C2-C3-O7
4	7-R	7510	CIT	C1-C2-C3-O7
4	8-R	7510	CIT	C1-C2-C3-O7
4	9-R	7510	CIT	C1-C2-C3-O7
4	10-R	7510	CIT	C1-C2-C3-O7
4	1-S	7512	CIT	C1-C2-C3-O7
4	2-S	7512	CIT	C1-C2-C3-O7
4	3-S	7512	CIT	C1-C2-C3-O7
4	4-S	7512	CIT	C1-C2-C3-O7
4	5-S	7512	CIT	C1-C2-C3-O7
4	6-S	7512	CIT	C1-C2-C3-O7
4	7-S	7512	CIT	C1-C2-C3-O7
4	8-S	7512	CIT	C1-C2-C3-O7
4	9-S	7512	CIT	C1-C2-C3-O7
4	10-S	7512	CIT	C1-C2-C3-O7
4	1-T	7514	CIT	C1-C2-C3-O7
4	2-T	7514	CIT	C1-C2-C3-O7
4	3-T	7514	CIT	C1-C2-C3-O7
4	4-T	7514	CIT	C1-C2-C3-O7
4	5-T	7514	CIT	C1-C2-C3-O7
4	6-T	7514	CIT	C1-C2-C3-O7
4	7-T	7514	CIT	C1-C2-C3-O7
4	8-T	7514	CIT	C1-C2-C3-O7
4	9-T	7514	CIT	C1-C2-C3-O7
4	10-T	7514	CIT	C1-C2-C3-O7
4	1-U	7516	CIT	C1-C2-C3-O7
4	2-U	7516	CIT	C1-C2-C3-O7
4	3-U	7516	CIT	C1-C2-C3-O7
4	4-U	7516	CIT	C1-C2-C3-O7
4	5-U	7516	CIT	C1-C2-C3-O7
4	6-U	7516	CIT	C1-C2-C3-O7
4	7-U	7516	CIT	C1-C2-C3-O7
4	8-U	7516	CIT	C1-C2-C3-O7
4	9-U	7516	CIT	C1-C2-C3-O7
4	10-U	7516	CIT	C1-C2-C3-O7
4	1-V	7518	CIT	C1-C2-C3-O7
4	2-V	7518	CIT	C1-C2-C3-O7
4	3-V	7518	CIT	C1-C2-C3-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	4-V	7518	CIT	C1-C2-C3-O7
4	5-V	7518	CIT	C1-C2-C3-O7
4	6-V	7518	CIT	C1-C2-C3-O7
4	7-V	7518	CIT	C1-C2-C3-O7
4	8-V	7518	CIT	C1-C2-C3-O7
4	9-V	7518	CIT	C1-C2-C3-O7
4	10-V	7518	CIT	C1-C2-C3-O7
4	1-W	7520	CIT	C1-C2-C3-O7
4	2-W	7520	CIT	C1-C2-C3-O7
4	3-W	7520	CIT	C1-C2-C3-O7
4	4-W	7520	CIT	C1-C2-C3-O7
4	5-W	7520	CIT	C1-C2-C3-O7
4	6-W	7520	CIT	C1-C2-C3-O7
4	7-W	7520	CIT	C1-C2-C3-O7
4	8-W	7520	CIT	C1-C2-C3-O7
4	9-W	7520	CIT	C1-C2-C3-O7
4	10-W	7520	CIT	C1-C2-C3-O7
4	1-X	7522	CIT	C1-C2-C3-O7
4	2-X	7522	CIT	C1-C2-C3-O7
4	3-X	7522	CIT	C1-C2-C3-O7
4	4-X	7522	CIT	C1-C2-C3-O7
4	5-X	7522	CIT	C1-C2-C3-O7
4	6-X	7522	CIT	C1-C2-C3-O7
4	7-X	7522	CIT	C1-C2-C3-O7
4	8-X	7522	CIT	C1-C2-C3-O7
4	9-X	7522	CIT	C1-C2-C3-O7
4	10-X	7522	CIT	C1-C2-C3-O7
4	1-A	7476	CIT	O7-C3-C4-C5
4	2-A	7476	CIT	O7-C3-C4-C5
4	3-A	7476	CIT	O7-C3-C4-C5
4	4-A	7476	CIT	O7-C3-C4-C5
4	5-A	7476	CIT	O7-C3-C4-C5
4	6-A	7476	CIT	O7-C3-C4-C5
4	7-A	7476	CIT	O7-C3-C4-C5
4	8-A	7476	CIT	O7-C3-C4-C5
4	9-A	7476	CIT	O7-C3-C4-C5
4	10-A	7476	CIT	O7-C3-C4-C5
4	1-B	7478	CIT	O7-C3-C4-C5
4	2-B	7478	CIT	O7-C3-C4-C5
4	3-B	7478	CIT	O7-C3-C4-C5
4	4-B	7478	CIT	O7-C3-C4-C5
4	5-B	7478	CIT	O7-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	6-B	7478	CIT	O7-C3-C4-C5
4	7-B	7478	CIT	O7-C3-C4-C5
4	8-B	7478	CIT	O7-C3-C4-C5
4	9-B	7478	CIT	O7-C3-C4-C5
4	10-B	7478	CIT	O7-C3-C4-C5
4	1-C	7480	CIT	O7-C3-C4-C5
4	2-C	7480	CIT	O7-C3-C4-C5
4	3-C	7480	CIT	O7-C3-C4-C5
4	4-C	7480	CIT	O7-C3-C4-C5
4	5-C	7480	CIT	O7-C3-C4-C5
4	6-C	7480	CIT	O7-C3-C4-C5
4	7-C	7480	CIT	O7-C3-C4-C5
4	8-C	7480	CIT	O7-C3-C4-C5
4	9-C	7480	CIT	O7-C3-C4-C5
4	10-C	7480	CIT	O7-C3-C4-C5
4	1-D	7482	CIT	O7-C3-C4-C5
4	2-D	7482	CIT	O7-C3-C4-C5
4	3-D	7482	CIT	O7-C3-C4-C5
4	4-D	7482	CIT	O7-C3-C4-C5
4	5-D	7482	CIT	O7-C3-C4-C5
4	6-D	7482	CIT	O7-C3-C4-C5
4	7-D	7482	CIT	O7-C3-C4-C5
4	8-D	7482	CIT	O7-C3-C4-C5
4	9-D	7482	CIT	O7-C3-C4-C5
4	10-D	7482	CIT	O7-C3-C4-C5
4	1-E	7484	CIT	O7-C3-C4-C5
4	2-E	7484	CIT	O7-C3-C4-C5
4	3-E	7484	CIT	O7-C3-C4-C5
4	4-E	7484	CIT	O7-C3-C4-C5
4	5-E	7484	CIT	O7-C3-C4-C5
4	6-E	7484	CIT	O7-C3-C4-C5
4	7-E	7484	CIT	O7-C3-C4-C5
4	8-E	7484	CIT	O7-C3-C4-C5
4	9-E	7484	CIT	O7-C3-C4-C5
4	10-E	7484	CIT	O7-C3-C4-C5
4	1-F	7486	CIT	O7-C3-C4-C5
4	2-F	7486	CIT	O7-C3-C4-C5
4	3-F	7486	CIT	O7-C3-C4-C5
4	4-F	7486	CIT	O7-C3-C4-C5
4	5-F	7486	CIT	O7-C3-C4-C5
4	6-F	7486	CIT	O7-C3-C4-C5
4	7-F	7486	CIT	O7-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	8-F	7486	CIT	O7-C3-C4-C5
4	9-F	7486	CIT	O7-C3-C4-C5
4	10-F	7486	CIT	O7-C3-C4-C5
4	1-G	7488	CIT	O7-C3-C4-C5
4	2-G	7488	CIT	O7-C3-C4-C5
4	3-G	7488	CIT	O7-C3-C4-C5
4	4-G	7488	CIT	O7-C3-C4-C5
4	5-G	7488	CIT	O7-C3-C4-C5
4	6-G	7488	CIT	O7-C3-C4-C5
4	7-G	7488	CIT	O7-C3-C4-C5
4	8-G	7488	CIT	O7-C3-C4-C5
4	9-G	7488	CIT	O7-C3-C4-C5
4	10-G	7488	CIT	O7-C3-C4-C5
4	1-H	7490	CIT	O7-C3-C4-C5
4	2-H	7490	CIT	O7-C3-C4-C5
4	3-H	7490	CIT	O7-C3-C4-C5
4	4-H	7490	CIT	O7-C3-C4-C5
4	5-H	7490	CIT	O7-C3-C4-C5
4	6-H	7490	CIT	O7-C3-C4-C5
4	7-H	7490	CIT	O7-C3-C4-C5
4	8-H	7490	CIT	O7-C3-C4-C5
4	9-H	7490	CIT	O7-C3-C4-C5
4	10-H	7490	CIT	O7-C3-C4-C5
4	1-I	7492	CIT	O7-C3-C4-C5
4	2-I	7492	CIT	O7-C3-C4-C5
4	3-I	7492	CIT	O7-C3-C4-C5
4	4-I	7492	CIT	O7-C3-C4-C5
4	5-I	7492	CIT	O7-C3-C4-C5
4	6-I	7492	CIT	O7-C3-C4-C5
4	7-I	7492	CIT	O7-C3-C4-C5
4	8-I	7492	CIT	O7-C3-C4-C5
4	9-I	7492	CIT	O7-C3-C4-C5
4	10-I	7492	CIT	O7-C3-C4-C5
4	1-J	7494	CIT	O7-C3-C4-C5
4	2-J	7494	CIT	O7-C3-C4-C5
4	3-J	7494	CIT	O7-C3-C4-C5
4	4-J	7494	CIT	O7-C3-C4-C5
4	5-J	7494	CIT	O7-C3-C4-C5
4	6-J	7494	CIT	O7-C3-C4-C5
4	7-J	7494	CIT	O7-C3-C4-C5
4	8-J	7494	CIT	O7-C3-C4-C5
4	9-J	7494	CIT	O7-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	10-J	7494	CIT	O7-C3-C4-C5
4	1-K	7496	CIT	O7-C3-C4-C5
4	2-K	7496	CIT	O7-C3-C4-C5
4	3-K	7496	CIT	O7-C3-C4-C5
4	4-K	7496	CIT	O7-C3-C4-C5
4	5-K	7496	CIT	O7-C3-C4-C5
4	6-K	7496	CIT	O7-C3-C4-C5
4	7-K	7496	CIT	O7-C3-C4-C5
4	8-K	7496	CIT	O7-C3-C4-C5
4	9-K	7496	CIT	O7-C3-C4-C5
4	10-K	7496	CIT	O7-C3-C4-C5
4	1-L	7498	CIT	O7-C3-C4-C5
4	2-L	7498	CIT	O7-C3-C4-C5
4	3-L	7498	CIT	O7-C3-C4-C5
4	4-L	7498	CIT	O7-C3-C4-C5
4	5-L	7498	CIT	O7-C3-C4-C5
4	6-L	7498	CIT	O7-C3-C4-C5
4	7-L	7498	CIT	O7-C3-C4-C5
4	8-L	7498	CIT	O7-C3-C4-C5
4	9-L	7498	CIT	O7-C3-C4-C5
4	10-L	7498	CIT	O7-C3-C4-C5
4	1-M	7500	CIT	O7-C3-C4-C5
4	2-M	7500	CIT	O7-C3-C4-C5
4	3-M	7500	CIT	O7-C3-C4-C5
4	4-M	7500	CIT	O7-C3-C4-C5
4	5-M	7500	CIT	O7-C3-C4-C5
4	6-M	7500	CIT	O7-C3-C4-C5
4	7-M	7500	CIT	O7-C3-C4-C5
4	8-M	7500	CIT	O7-C3-C4-C5
4	9-M	7500	CIT	O7-C3-C4-C5
4	10-M	7500	CIT	O7-C3-C4-C5
4	1-N	7502	CIT	O7-C3-C4-C5
4	2-N	7502	CIT	O7-C3-C4-C5
4	3-N	7502	CIT	O7-C3-C4-C5
4	4-N	7502	CIT	O7-C3-C4-C5
4	5-N	7502	CIT	O7-C3-C4-C5
4	6-N	7502	CIT	O7-C3-C4-C5
4	7-N	7502	CIT	O7-C3-C4-C5
4	8-N	7502	CIT	O7-C3-C4-C5
4	9-N	7502	CIT	O7-C3-C4-C5
4	10-N	7502	CIT	O7-C3-C4-C5
4	1-O	7504	CIT	O7-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	2-O	7504	CIT	O7-C3-C4-C5
4	3-O	7504	CIT	O7-C3-C4-C5
4	4-O	7504	CIT	O7-C3-C4-C5
4	5-O	7504	CIT	O7-C3-C4-C5
4	6-O	7504	CIT	O7-C3-C4-C5
4	7-O	7504	CIT	O7-C3-C4-C5
4	8-O	7504	CIT	O7-C3-C4-C5
4	9-O	7504	CIT	O7-C3-C4-C5
4	10-O	7504	CIT	O7-C3-C4-C5
4	1-P	7506	CIT	O7-C3-C4-C5
4	2-P	7506	CIT	O7-C3-C4-C5
4	3-P	7506	CIT	O7-C3-C4-C5
4	4-P	7506	CIT	O7-C3-C4-C5
4	5-P	7506	CIT	O7-C3-C4-C5
4	6-P	7506	CIT	O7-C3-C4-C5
4	7-P	7506	CIT	O7-C3-C4-C5
4	8-P	7506	CIT	O7-C3-C4-C5
4	9-P	7506	CIT	O7-C3-C4-C5
4	10-P	7506	CIT	O7-C3-C4-C5
4	1-Q	7508	CIT	O7-C3-C4-C5
4	2-Q	7508	CIT	O7-C3-C4-C5
4	3-Q	7508	CIT	O7-C3-C4-C5
4	4-Q	7508	CIT	O7-C3-C4-C5
4	5-Q	7508	CIT	O7-C3-C4-C5
4	6-Q	7508	CIT	O7-C3-C4-C5
4	7-Q	7508	CIT	O7-C3-C4-C5
4	8-Q	7508	CIT	O7-C3-C4-C5
4	9-Q	7508	CIT	O7-C3-C4-C5
4	10-Q	7508	CIT	O7-C3-C4-C5
4	1-R	7510	CIT	O7-C3-C4-C5
4	2-R	7510	CIT	O7-C3-C4-C5
4	3-R	7510	CIT	O7-C3-C4-C5
4	4-R	7510	CIT	O7-C3-C4-C5
4	5-R	7510	CIT	O7-C3-C4-C5
4	6-R	7510	CIT	O7-C3-C4-C5
4	7-R	7510	CIT	O7-C3-C4-C5
4	8-R	7510	CIT	O7-C3-C4-C5
4	9-R	7510	CIT	O7-C3-C4-C5
4	10-R	7510	CIT	O7-C3-C4-C5
4	1-S	7512	CIT	O7-C3-C4-C5
4	2-S	7512	CIT	O7-C3-C4-C5
4	3-S	7512	CIT	O7-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	4-S	7512	CIT	O7-C3-C4-C5
4	5-S	7512	CIT	O7-C3-C4-C5
4	6-S	7512	CIT	O7-C3-C4-C5
4	7-S	7512	CIT	O7-C3-C4-C5
4	8-S	7512	CIT	O7-C3-C4-C5
4	9-S	7512	CIT	O7-C3-C4-C5
4	10-S	7512	CIT	O7-C3-C4-C5
4	1-T	7514	CIT	O7-C3-C4-C5
4	2-T	7514	CIT	O7-C3-C4-C5
4	3-T	7514	CIT	O7-C3-C4-C5
4	4-T	7514	CIT	O7-C3-C4-C5
4	5-T	7514	CIT	O7-C3-C4-C5
4	6-T	7514	CIT	O7-C3-C4-C5
4	7-T	7514	CIT	O7-C3-C4-C5
4	8-T	7514	CIT	O7-C3-C4-C5
4	9-T	7514	CIT	O7-C3-C4-C5
4	10-T	7514	CIT	O7-C3-C4-C5
4	1-U	7516	CIT	O7-C3-C4-C5
4	2-U	7516	CIT	O7-C3-C4-C5
4	3-U	7516	CIT	O7-C3-C4-C5
4	4-U	7516	CIT	O7-C3-C4-C5
4	5-U	7516	CIT	O7-C3-C4-C5
4	6-U	7516	CIT	O7-C3-C4-C5
4	7-U	7516	CIT	O7-C3-C4-C5
4	8-U	7516	CIT	O7-C3-C4-C5
4	9-U	7516	CIT	O7-C3-C4-C5
4	10-U	7516	CIT	O7-C3-C4-C5
4	1-V	7518	CIT	O7-C3-C4-C5
4	2-V	7518	CIT	O7-C3-C4-C5
4	3-V	7518	CIT	O7-C3-C4-C5
4	4-V	7518	CIT	O7-C3-C4-C5
4	5-V	7518	CIT	O7-C3-C4-C5
4	6-V	7518	CIT	O7-C3-C4-C5
4	7-V	7518	CIT	O7-C3-C4-C5
4	8-V	7518	CIT	O7-C3-C4-C5
4	9-V	7518	CIT	O7-C3-C4-C5
4	10-V	7518	CIT	O7-C3-C4-C5
4	1-W	7520	CIT	O7-C3-C4-C5
4	2-W	7520	CIT	O7-C3-C4-C5
4	3-W	7520	CIT	O7-C3-C4-C5
4	4-W	7520	CIT	O7-C3-C4-C5
4	5-W	7520	CIT	O7-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	6-W	7520	CIT	O7-C3-C4-C5
4	7-W	7520	CIT	O7-C3-C4-C5
4	8-W	7520	CIT	O7-C3-C4-C5
4	9-W	7520	CIT	O7-C3-C4-C5
4	10-W	7520	CIT	O7-C3-C4-C5
4	1-X	7522	CIT	O7-C3-C4-C5
4	2-X	7522	CIT	O7-C3-C4-C5
4	3-X	7522	CIT	O7-C3-C4-C5
4	4-X	7522	CIT	O7-C3-C4-C5
4	5-X	7522	CIT	O7-C3-C4-C5
4	6-X	7522	CIT	O7-C3-C4-C5
4	7-X	7522	CIT	O7-C3-C4-C5
4	8-X	7522	CIT	O7-C3-C4-C5
4	9-X	7522	CIT	O7-C3-C4-C5
4	10-X	7522	CIT	O7-C3-C4-C5
4	1-A	7476	CIT	C1-C2-C3-C4
4	2-A	7476	CIT	C1-C2-C3-C4
4	3-A	7476	CIT	C1-C2-C3-C4
4	4-A	7476	CIT	C1-C2-C3-C4
4	5-A	7476	CIT	C1-C2-C3-C4
4	6-A	7476	CIT	C1-C2-C3-C4
4	7-A	7476	CIT	C1-C2-C3-C4
4	8-A	7476	CIT	C1-C2-C3-C4
4	9-A	7476	CIT	C1-C2-C3-C4
4	10-A	7476	CIT	C1-C2-C3-C4
4	1-B	7478	CIT	C1-C2-C3-C4
4	2-B	7478	CIT	C1-C2-C3-C4
4	3-B	7478	CIT	C1-C2-C3-C4
4	4-B	7478	CIT	C1-C2-C3-C4
4	5-B	7478	CIT	C1-C2-C3-C4
4	6-B	7478	CIT	C1-C2-C3-C4
4	7-B	7478	CIT	C1-C2-C3-C4
4	8-B	7478	CIT	C1-C2-C3-C4
4	9-B	7478	CIT	C1-C2-C3-C4
4	10-B	7478	CIT	C1-C2-C3-C4
4	1-C	7480	CIT	C1-C2-C3-C4
4	2-C	7480	CIT	C1-C2-C3-C4
4	3-C	7480	CIT	C1-C2-C3-C4
4	4-C	7480	CIT	C1-C2-C3-C4
4	5-C	7480	CIT	C1-C2-C3-C4
4	6-C	7480	CIT	C1-C2-C3-C4
4	7-C	7480	CIT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	8-C	7480	CIT	C1-C2-C3-C4
4	9-C	7480	CIT	C1-C2-C3-C4
4	10-C	7480	CIT	C1-C2-C3-C4
4	1-D	7482	CIT	C1-C2-C3-C4
4	2-D	7482	CIT	C1-C2-C3-C4
4	3-D	7482	CIT	C1-C2-C3-C4
4	4-D	7482	CIT	C1-C2-C3-C4
4	5-D	7482	CIT	C1-C2-C3-C4
4	6-D	7482	CIT	C1-C2-C3-C4
4	7-D	7482	CIT	C1-C2-C3-C4
4	8-D	7482	CIT	C1-C2-C3-C4
4	9-D	7482	CIT	C1-C2-C3-C4
4	10-D	7482	CIT	C1-C2-C3-C4
4	1-E	7484	CIT	C1-C2-C3-C4
4	2-E	7484	CIT	C1-C2-C3-C4
4	3-E	7484	CIT	C1-C2-C3-C4
4	4-E	7484	CIT	C1-C2-C3-C4
4	5-E	7484	CIT	C1-C2-C3-C4
4	6-E	7484	CIT	C1-C2-C3-C4
4	7-E	7484	CIT	C1-C2-C3-C4
4	8-E	7484	CIT	C1-C2-C3-C4
4	9-E	7484	CIT	C1-C2-C3-C4
4	10-E	7484	CIT	C1-C2-C3-C4
4	1-F	7486	CIT	C1-C2-C3-C4
4	2-F	7486	CIT	C1-C2-C3-C4
4	3-F	7486	CIT	C1-C2-C3-C4
4	4-F	7486	CIT	C1-C2-C3-C4
4	5-F	7486	CIT	C1-C2-C3-C4
4	6-F	7486	CIT	C1-C2-C3-C4
4	7-F	7486	CIT	C1-C2-C3-C4
4	8-F	7486	CIT	C1-C2-C3-C4
4	9-F	7486	CIT	C1-C2-C3-C4
4	10-F	7486	CIT	C1-C2-C3-C4
4	1-G	7488	CIT	C1-C2-C3-C4
4	2-G	7488	CIT	C1-C2-C3-C4
4	3-G	7488	CIT	C1-C2-C3-C4
4	4-G	7488	CIT	C1-C2-C3-C4
4	5-G	7488	CIT	C1-C2-C3-C4
4	6-G	7488	CIT	C1-C2-C3-C4
4	7-G	7488	CIT	C1-C2-C3-C4
4	8-G	7488	CIT	C1-C2-C3-C4
4	9-G	7488	CIT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	10-G	7488	CIT	C1-C2-C3-C4
4	1-H	7490	CIT	C1-C2-C3-C4
4	2-H	7490	CIT	C1-C2-C3-C4
4	3-H	7490	CIT	C1-C2-C3-C4
4	4-H	7490	CIT	C1-C2-C3-C4
4	5-H	7490	CIT	C1-C2-C3-C4
4	6-H	7490	CIT	C1-C2-C3-C4
4	7-H	7490	CIT	C1-C2-C3-C4
4	8-H	7490	CIT	C1-C2-C3-C4
4	9-H	7490	CIT	C1-C2-C3-C4
4	10-H	7490	CIT	C1-C2-C3-C4
4	1-I	7492	CIT	C1-C2-C3-C4
4	2-I	7492	CIT	C1-C2-C3-C4
4	3-I	7492	CIT	C1-C2-C3-C4
4	4-I	7492	CIT	C1-C2-C3-C4
4	5-I	7492	CIT	C1-C2-C3-C4
4	6-I	7492	CIT	C1-C2-C3-C4
4	7-I	7492	CIT	C1-C2-C3-C4
4	8-I	7492	CIT	C1-C2-C3-C4
4	9-I	7492	CIT	C1-C2-C3-C4
4	10-I	7492	CIT	C1-C2-C3-C4
4	1-J	7494	CIT	C1-C2-C3-C4
4	2-J	7494	CIT	C1-C2-C3-C4
4	3-J	7494	CIT	C1-C2-C3-C4
4	4-J	7494	CIT	C1-C2-C3-C4
4	5-J	7494	CIT	C1-C2-C3-C4
4	6-J	7494	CIT	C1-C2-C3-C4
4	7-J	7494	CIT	C1-C2-C3-C4
4	8-J	7494	CIT	C1-C2-C3-C4
4	9-J	7494	CIT	C1-C2-C3-C4
4	10-J	7494	CIT	C1-C2-C3-C4
4	1-K	7496	CIT	C1-C2-C3-C4
4	2-K	7496	CIT	C1-C2-C3-C4
4	3-K	7496	CIT	C1-C2-C3-C4
4	4-K	7496	CIT	C1-C2-C3-C4
4	5-K	7496	CIT	C1-C2-C3-C4
4	6-K	7496	CIT	C1-C2-C3-C4
4	7-K	7496	CIT	C1-C2-C3-C4
4	8-K	7496	CIT	C1-C2-C3-C4
4	9-K	7496	CIT	C1-C2-C3-C4
4	10-K	7496	CIT	C1-C2-C3-C4
4	1-L	7498	CIT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	2-L	7498	CIT	C1-C2-C3-C4
4	3-L	7498	CIT	C1-C2-C3-C4
4	4-L	7498	CIT	C1-C2-C3-C4
4	5-L	7498	CIT	C1-C2-C3-C4
4	6-L	7498	CIT	C1-C2-C3-C4
4	7-L	7498	CIT	C1-C2-C3-C4
4	8-L	7498	CIT	C1-C2-C3-C4
4	9-L	7498	CIT	C1-C2-C3-C4
4	10-L	7498	CIT	C1-C2-C3-C4
4	1-M	7500	CIT	C1-C2-C3-C4
4	2-M	7500	CIT	C1-C2-C3-C4
4	3-M	7500	CIT	C1-C2-C3-C4
4	4-M	7500	CIT	C1-C2-C3-C4
4	5-M	7500	CIT	C1-C2-C3-C4
4	6-M	7500	CIT	C1-C2-C3-C4
4	7-M	7500	CIT	C1-C2-C3-C4
4	8-M	7500	CIT	C1-C2-C3-C4
4	9-M	7500	CIT	C1-C2-C3-C4
4	10-M	7500	CIT	C1-C2-C3-C4
4	1-N	7502	CIT	C1-C2-C3-C4
4	2-N	7502	CIT	C1-C2-C3-C4
4	3-N	7502	CIT	C1-C2-C3-C4
4	4-N	7502	CIT	C1-C2-C3-C4
4	5-N	7502	CIT	C1-C2-C3-C4
4	6-N	7502	CIT	C1-C2-C3-C4
4	7-N	7502	CIT	C1-C2-C3-C4
4	8-N	7502	CIT	C1-C2-C3-C4
4	9-N	7502	CIT	C1-C2-C3-C4
4	10-N	7502	CIT	C1-C2-C3-C4
4	1-O	7504	CIT	C1-C2-C3-C4
4	2-O	7504	CIT	C1-C2-C3-C4
4	3-O	7504	CIT	C1-C2-C3-C4
4	4-O	7504	CIT	C1-C2-C3-C4
4	5-O	7504	CIT	C1-C2-C3-C4
4	6-O	7504	CIT	C1-C2-C3-C4
4	7-O	7504	CIT	C1-C2-C3-C4
4	8-O	7504	CIT	C1-C2-C3-C4
4	9-O	7504	CIT	C1-C2-C3-C4
4	10-O	7504	CIT	C1-C2-C3-C4
4	1-P	7506	CIT	C1-C2-C3-C4
4	2-P	7506	CIT	C1-C2-C3-C4
4	3-P	7506	CIT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	4-P	7506	CIT	C1-C2-C3-C4
4	5-P	7506	CIT	C1-C2-C3-C4
4	6-P	7506	CIT	C1-C2-C3-C4
4	7-P	7506	CIT	C1-C2-C3-C4
4	8-P	7506	CIT	C1-C2-C3-C4
4	9-P	7506	CIT	C1-C2-C3-C4
4	10-P	7506	CIT	C1-C2-C3-C4
4	1-Q	7508	CIT	C1-C2-C3-C4
4	2-Q	7508	CIT	C1-C2-C3-C4
4	3-Q	7508	CIT	C1-C2-C3-C4
4	4-Q	7508	CIT	C1-C2-C3-C4
4	5-Q	7508	CIT	C1-C2-C3-C4
4	6-Q	7508	CIT	C1-C2-C3-C4
4	7-Q	7508	CIT	C1-C2-C3-C4
4	8-Q	7508	CIT	C1-C2-C3-C4
4	9-Q	7508	CIT	C1-C2-C3-C4
4	10-Q	7508	CIT	C1-C2-C3-C4
4	1-R	7510	CIT	C1-C2-C3-C4
4	2-R	7510	CIT	C1-C2-C3-C4
4	3-R	7510	CIT	C1-C2-C3-C4
4	4-R	7510	CIT	C1-C2-C3-C4
4	5-R	7510	CIT	C1-C2-C3-C4
4	6-R	7510	CIT	C1-C2-C3-C4
4	7-R	7510	CIT	C1-C2-C3-C4
4	8-R	7510	CIT	C1-C2-C3-C4
4	9-R	7510	CIT	C1-C2-C3-C4
4	10-R	7510	CIT	C1-C2-C3-C4
4	1-S	7512	CIT	C1-C2-C3-C4
4	2-S	7512	CIT	C1-C2-C3-C4
4	3-S	7512	CIT	C1-C2-C3-C4
4	4-S	7512	CIT	C1-C2-C3-C4
4	5-S	7512	CIT	C1-C2-C3-C4
4	6-S	7512	CIT	C1-C2-C3-C4
4	7-S	7512	CIT	C1-C2-C3-C4
4	8-S	7512	CIT	C1-C2-C3-C4
4	9-S	7512	CIT	C1-C2-C3-C4
4	10-S	7512	CIT	C1-C2-C3-C4
4	1-T	7514	CIT	C1-C2-C3-C4
4	2-T	7514	CIT	C1-C2-C3-C4
4	3-T	7514	CIT	C1-C2-C3-C4
4	4-T	7514	CIT	C1-C2-C3-C4
4	5-T	7514	CIT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	6-T	7514	CIT	C1-C2-C3-C4
4	7-T	7514	CIT	C1-C2-C3-C4
4	8-T	7514	CIT	C1-C2-C3-C4
4	9-T	7514	CIT	C1-C2-C3-C4
4	10-T	7514	CIT	C1-C2-C3-C4
4	1-U	7516	CIT	C1-C2-C3-C4
4	2-U	7516	CIT	C1-C2-C3-C4
4	3-U	7516	CIT	C1-C2-C3-C4
4	4-U	7516	CIT	C1-C2-C3-C4
4	5-U	7516	CIT	C1-C2-C3-C4
4	6-U	7516	CIT	C1-C2-C3-C4
4	7-U	7516	CIT	C1-C2-C3-C4
4	8-U	7516	CIT	C1-C2-C3-C4
4	9-U	7516	CIT	C1-C2-C3-C4
4	10-U	7516	CIT	C1-C2-C3-C4
4	1-V	7518	CIT	C1-C2-C3-C4
4	2-V	7518	CIT	C1-C2-C3-C4
4	3-V	7518	CIT	C1-C2-C3-C4
4	4-V	7518	CIT	C1-C2-C3-C4
4	5-V	7518	CIT	C1-C2-C3-C4
4	6-V	7518	CIT	C1-C2-C3-C4
4	7-V	7518	CIT	C1-C2-C3-C4
4	8-V	7518	CIT	C1-C2-C3-C4
4	9-V	7518	CIT	C1-C2-C3-C4
4	10-V	7518	CIT	C1-C2-C3-C4
4	1-W	7520	CIT	C1-C2-C3-C4
4	2-W	7520	CIT	C1-C2-C3-C4
4	3-W	7520	CIT	C1-C2-C3-C4
4	4-W	7520	CIT	C1-C2-C3-C4
4	5-W	7520	CIT	C1-C2-C3-C4
4	6-W	7520	CIT	C1-C2-C3-C4
4	7-W	7520	CIT	C1-C2-C3-C4
4	8-W	7520	CIT	C1-C2-C3-C4
4	9-W	7520	CIT	C1-C2-C3-C4
4	10-W	7520	CIT	C1-C2-C3-C4
4	1-X	7522	CIT	C1-C2-C3-C4
4	2-X	7522	CIT	C1-C2-C3-C4
4	3-X	7522	CIT	C1-C2-C3-C4
4	4-X	7522	CIT	C1-C2-C3-C4
4	5-X	7522	CIT	C1-C2-C3-C4
4	6-X	7522	CIT	C1-C2-C3-C4
4	7-X	7522	CIT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	8-X	7522	CIT	C1-C2-C3-C4
4	9-X	7522	CIT	C1-C2-C3-C4
4	10-X	7522	CIT	C1-C2-C3-C4
3	1-A	7475	AMP	O4'-C1'-N9-C8
3	2-A	7475	AMP	O4'-C1'-N9-C8
3	3-A	7475	AMP	O4'-C1'-N9-C8
3	4-A	7475	AMP	O4'-C1'-N9-C8
3	5-A	7475	AMP	O4'-C1'-N9-C8
3	6-A	7475	AMP	O4'-C1'-N9-C8
3	7-A	7475	AMP	O4'-C1'-N9-C8
3	8-A	7475	AMP	O4'-C1'-N9-C8
3	9-A	7475	AMP	O4'-C1'-N9-C8
3	10-A	7475	AMP	O4'-C1'-N9-C8
3	1-B	7477	AMP	O4'-C1'-N9-C8
3	2-B	7477	AMP	O4'-C1'-N9-C8
3	3-B	7477	AMP	O4'-C1'-N9-C8
3	4-B	7477	AMP	O4'-C1'-N9-C8
3	5-B	7477	AMP	O4'-C1'-N9-C8
3	6-B	7477	AMP	O4'-C1'-N9-C8
3	7-B	7477	AMP	O4'-C1'-N9-C8
3	8-B	7477	AMP	O4'-C1'-N9-C8
3	9-B	7477	AMP	O4'-C1'-N9-C8
3	10-B	7477	AMP	O4'-C1'-N9-C8
3	1-C	7479	AMP	O4'-C1'-N9-C8
3	2-C	7479	AMP	O4'-C1'-N9-C8
3	3-C	7479	AMP	O4'-C1'-N9-C8
3	4-C	7479	AMP	O4'-C1'-N9-C8
3	5-C	7479	AMP	O4'-C1'-N9-C8
3	6-C	7479	AMP	O4'-C1'-N9-C8
3	7-C	7479	AMP	O4'-C1'-N9-C8
3	8-C	7479	AMP	O4'-C1'-N9-C8
3	9-C	7479	AMP	O4'-C1'-N9-C8
3	10-C	7479	AMP	O4'-C1'-N9-C8
3	1-D	7481	AMP	O4'-C1'-N9-C8
3	2-D	7481	AMP	O4'-C1'-N9-C8
3	3-D	7481	AMP	O4'-C1'-N9-C8
3	4-D	7481	AMP	O4'-C1'-N9-C8
3	5-D	7481	AMP	O4'-C1'-N9-C8
3	6-D	7481	AMP	O4'-C1'-N9-C8
3	7-D	7481	AMP	O4'-C1'-N9-C8
3	8-D	7481	AMP	O4'-C1'-N9-C8
3	9-D	7481	AMP	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	10-D	7481	AMP	O4'-C1'-N9-C8
3	1-E	7483	AMP	O4'-C1'-N9-C8
3	2-E	7483	AMP	O4'-C1'-N9-C8
3	3-E	7483	AMP	O4'-C1'-N9-C8
3	4-E	7483	AMP	O4'-C1'-N9-C8
3	5-E	7483	AMP	O4'-C1'-N9-C8
3	6-E	7483	AMP	O4'-C1'-N9-C8
3	7-E	7483	AMP	O4'-C1'-N9-C8
3	8-E	7483	AMP	O4'-C1'-N9-C8
3	9-E	7483	AMP	O4'-C1'-N9-C8
3	10-E	7483	AMP	O4'-C1'-N9-C8
3	1-F	7485	AMP	O4'-C1'-N9-C8
3	2-F	7485	AMP	O4'-C1'-N9-C8
3	3-F	7485	AMP	O4'-C1'-N9-C8
3	4-F	7485	AMP	O4'-C1'-N9-C8
3	5-F	7485	AMP	O4'-C1'-N9-C8
3	6-F	7485	AMP	O4'-C1'-N9-C8
3	7-F	7485	AMP	O4'-C1'-N9-C8
3	8-F	7485	AMP	O4'-C1'-N9-C8
3	9-F	7485	AMP	O4'-C1'-N9-C8
3	10-F	7485	AMP	O4'-C1'-N9-C8
3	1-G	7487	AMP	O4'-C1'-N9-C8
3	2-G	7487	AMP	O4'-C1'-N9-C8
3	3-G	7487	AMP	O4'-C1'-N9-C8
3	4-G	7487	AMP	O4'-C1'-N9-C8
3	5-G	7487	AMP	O4'-C1'-N9-C8
3	6-G	7487	AMP	O4'-C1'-N9-C8
3	7-G	7487	AMP	O4'-C1'-N9-C8
3	8-G	7487	AMP	O4'-C1'-N9-C8
3	9-G	7487	AMP	O4'-C1'-N9-C8
3	10-G	7487	AMP	O4'-C1'-N9-C8
3	1-H	7489	AMP	O4'-C1'-N9-C8
3	2-H	7489	AMP	O4'-C1'-N9-C8
3	3-H	7489	AMP	O4'-C1'-N9-C8
3	4-H	7489	AMP	O4'-C1'-N9-C8
3	5-H	7489	AMP	O4'-C1'-N9-C8
3	6-H	7489	AMP	O4'-C1'-N9-C8
3	7-H	7489	AMP	O4'-C1'-N9-C8
3	8-H	7489	AMP	O4'-C1'-N9-C8
3	9-H	7489	AMP	O4'-C1'-N9-C8
3	10-H	7489	AMP	O4'-C1'-N9-C8
3	1-I	7491	AMP	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	2-I	7491	AMP	O4'-C1'-N9-C8
3	3-I	7491	AMP	O4'-C1'-N9-C8
3	4-I	7491	AMP	O4'-C1'-N9-C8
3	5-I	7491	AMP	O4'-C1'-N9-C8
3	6-I	7491	AMP	O4'-C1'-N9-C8
3	7-I	7491	AMP	O4'-C1'-N9-C8
3	8-I	7491	AMP	O4'-C1'-N9-C8
3	9-I	7491	AMP	O4'-C1'-N9-C8
3	10-I	7491	AMP	O4'-C1'-N9-C8
3	1-J	7493	AMP	O4'-C1'-N9-C8
3	2-J	7493	AMP	O4'-C1'-N9-C8
3	3-J	7493	AMP	O4'-C1'-N9-C8
3	4-J	7493	AMP	O4'-C1'-N9-C8
3	5-J	7493	AMP	O4'-C1'-N9-C8
3	6-J	7493	AMP	O4'-C1'-N9-C8
3	7-J	7493	AMP	O4'-C1'-N9-C8
3	8-J	7493	AMP	O4'-C1'-N9-C8
3	9-J	7493	AMP	O4'-C1'-N9-C8
3	10-J	7493	AMP	O4'-C1'-N9-C8
3	1-K	7495	AMP	O4'-C1'-N9-C8
3	2-K	7495	AMP	O4'-C1'-N9-C8
3	3-K	7495	AMP	O4'-C1'-N9-C8
3	4-K	7495	AMP	O4'-C1'-N9-C8
3	5-K	7495	AMP	O4'-C1'-N9-C8
3	6-K	7495	AMP	O4'-C1'-N9-C8
3	7-K	7495	AMP	O4'-C1'-N9-C8
3	8-K	7495	AMP	O4'-C1'-N9-C8
3	9-K	7495	AMP	O4'-C1'-N9-C8
3	10-K	7495	AMP	O4'-C1'-N9-C8
3	1-L	7497	AMP	O4'-C1'-N9-C8
3	2-L	7497	AMP	O4'-C1'-N9-C8
3	3-L	7497	AMP	O4'-C1'-N9-C8
3	4-L	7497	AMP	O4'-C1'-N9-C8
3	5-L	7497	AMP	O4'-C1'-N9-C8
3	6-L	7497	AMP	O4'-C1'-N9-C8
3	7-L	7497	AMP	O4'-C1'-N9-C8
3	8-L	7497	AMP	O4'-C1'-N9-C8
3	9-L	7497	AMP	O4'-C1'-N9-C8
3	10-L	7497	AMP	O4'-C1'-N9-C8
3	1-M	7499	AMP	O4'-C1'-N9-C8
3	2-M	7499	AMP	O4'-C1'-N9-C8
3	3-M	7499	AMP	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	4-M	7499	AMP	O4'-C1'-N9-C8
3	5-M	7499	AMP	O4'-C1'-N9-C8
3	6-M	7499	AMP	O4'-C1'-N9-C8
3	7-M	7499	AMP	O4'-C1'-N9-C8
3	8-M	7499	AMP	O4'-C1'-N9-C8
3	9-M	7499	AMP	O4'-C1'-N9-C8
3	10-M	7499	AMP	O4'-C1'-N9-C8
3	1-N	7501	AMP	O4'-C1'-N9-C8
3	2-N	7501	AMP	O4'-C1'-N9-C8
3	3-N	7501	AMP	O4'-C1'-N9-C8
3	4-N	7501	AMP	O4'-C1'-N9-C8
3	5-N	7501	AMP	O4'-C1'-N9-C8
3	6-N	7501	AMP	O4'-C1'-N9-C8
3	7-N	7501	AMP	O4'-C1'-N9-C8
3	8-N	7501	AMP	O4'-C1'-N9-C8
3	9-N	7501	AMP	O4'-C1'-N9-C8
3	10-N	7501	AMP	O4'-C1'-N9-C8
3	1-O	7503	AMP	O4'-C1'-N9-C8
3	2-O	7503	AMP	O4'-C1'-N9-C8
3	3-O	7503	AMP	O4'-C1'-N9-C8
3	4-O	7503	AMP	O4'-C1'-N9-C8
3	5-O	7503	AMP	O4'-C1'-N9-C8
3	6-O	7503	AMP	O4'-C1'-N9-C8
3	7-O	7503	AMP	O4'-C1'-N9-C8
3	8-O	7503	AMP	O4'-C1'-N9-C8
3	9-O	7503	AMP	O4'-C1'-N9-C8
3	10-O	7503	AMP	O4'-C1'-N9-C8
3	1-P	7505	AMP	O4'-C1'-N9-C8
3	2-P	7505	AMP	O4'-C1'-N9-C8
3	3-P	7505	AMP	O4'-C1'-N9-C8
3	4-P	7505	AMP	O4'-C1'-N9-C8
3	5-P	7505	AMP	O4'-C1'-N9-C8
3	6-P	7505	AMP	O4'-C1'-N9-C8
3	7-P	7505	AMP	O4'-C1'-N9-C8
3	8-P	7505	AMP	O4'-C1'-N9-C8
3	9-P	7505	AMP	O4'-C1'-N9-C8
3	10-P	7505	AMP	O4'-C1'-N9-C8
3	1-Q	7507	AMP	O4'-C1'-N9-C8
3	2-Q	7507	AMP	O4'-C1'-N9-C8
3	3-Q	7507	AMP	O4'-C1'-N9-C8
3	4-Q	7507	AMP	O4'-C1'-N9-C8
3	5-Q	7507	AMP	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	6-Q	7507	AMP	O4'-C1'-N9-C8
3	7-Q	7507	AMP	O4'-C1'-N9-C8
3	8-Q	7507	AMP	O4'-C1'-N9-C8
3	9-Q	7507	AMP	O4'-C1'-N9-C8
3	10-Q	7507	AMP	O4'-C1'-N9-C8
3	1-R	7509	AMP	O4'-C1'-N9-C8
3	2-R	7509	AMP	O4'-C1'-N9-C8
3	3-R	7509	AMP	O4'-C1'-N9-C8
3	4-R	7509	AMP	O4'-C1'-N9-C8
3	5-R	7509	AMP	O4'-C1'-N9-C8
3	6-R	7509	AMP	O4'-C1'-N9-C8
3	7-R	7509	AMP	O4'-C1'-N9-C8
3	8-R	7509	AMP	O4'-C1'-N9-C8
3	9-R	7509	AMP	O4'-C1'-N9-C8
3	10-R	7509	AMP	O4'-C1'-N9-C8
3	1-S	7511	AMP	O4'-C1'-N9-C8
3	2-S	7511	AMP	O4'-C1'-N9-C8
3	3-S	7511	AMP	O4'-C1'-N9-C8
3	4-S	7511	AMP	O4'-C1'-N9-C8
3	5-S	7511	AMP	O4'-C1'-N9-C8
3	6-S	7511	AMP	O4'-C1'-N9-C8
3	7-S	7511	AMP	O4'-C1'-N9-C8
3	8-S	7511	AMP	O4'-C1'-N9-C8
3	9-S	7511	AMP	O4'-C1'-N9-C8
3	10-S	7511	AMP	O4'-C1'-N9-C8
3	1-T	7513	AMP	O4'-C1'-N9-C8
3	2-T	7513	AMP	O4'-C1'-N9-C8
3	3-T	7513	AMP	O4'-C1'-N9-C8
3	4-T	7513	AMP	O4'-C1'-N9-C8
3	5-T	7513	AMP	O4'-C1'-N9-C8
3	6-T	7513	AMP	O4'-C1'-N9-C8
3	7-T	7513	AMP	O4'-C1'-N9-C8
3	8-T	7513	AMP	O4'-C1'-N9-C8
3	9-T	7513	AMP	O4'-C1'-N9-C8
3	10-T	7513	AMP	O4'-C1'-N9-C8
3	1-U	7515	AMP	O4'-C1'-N9-C8
3	2-U	7515	AMP	O4'-C1'-N9-C8
3	3-U	7515	AMP	O4'-C1'-N9-C8
3	4-U	7515	AMP	O4'-C1'-N9-C8
3	5-U	7515	AMP	O4'-C1'-N9-C8
3	6-U	7515	AMP	O4'-C1'-N9-C8
3	7-U	7515	AMP	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

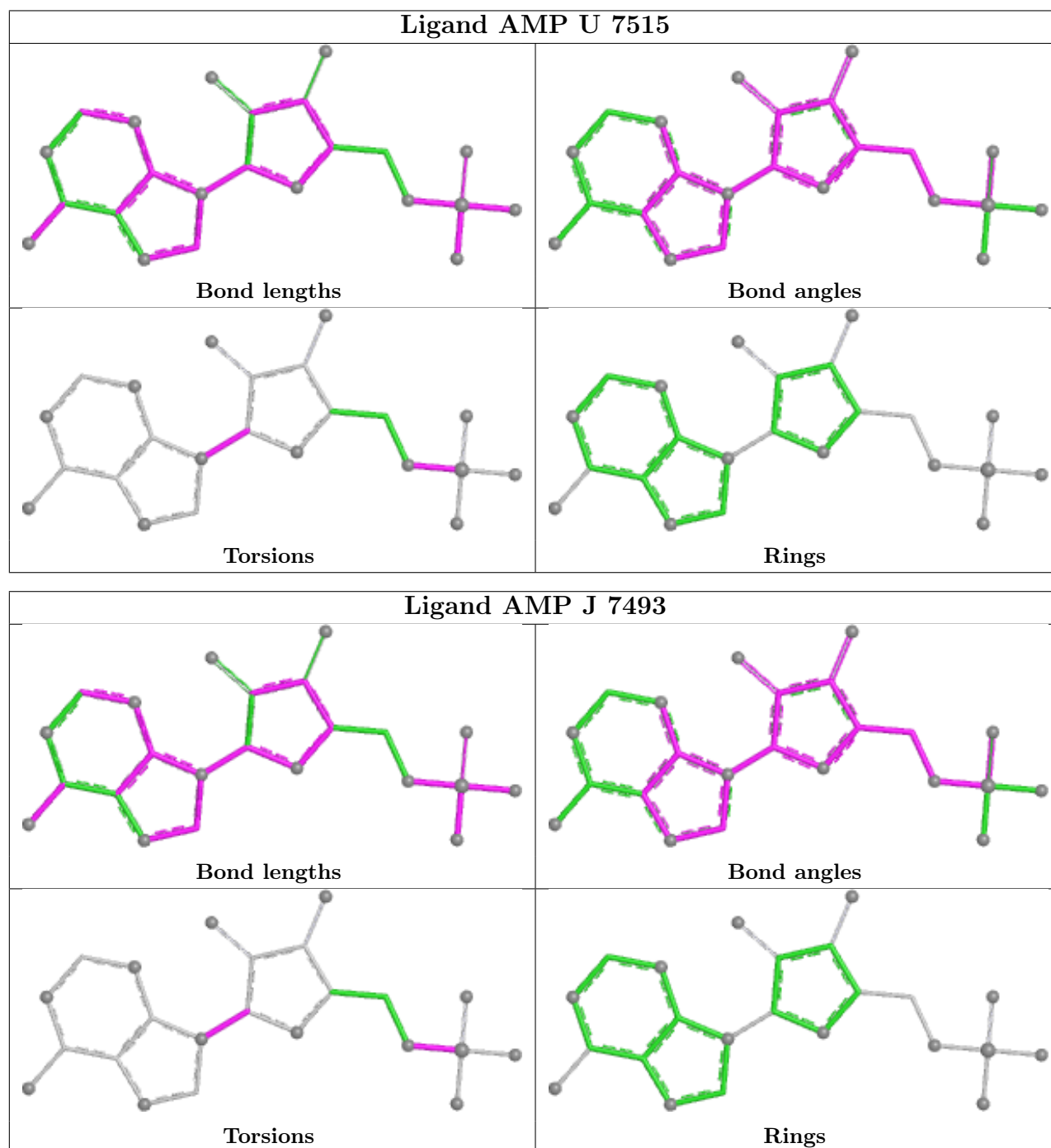
Mol	Chain	Res	Type	Atoms
3	8-U	7515	AMP	O4'-C1'-N9-C8
3	9-U	7515	AMP	O4'-C1'-N9-C8
3	10-U	7515	AMP	O4'-C1'-N9-C8
3	1-V	7517	AMP	O4'-C1'-N9-C8
3	2-V	7517	AMP	O4'-C1'-N9-C8
3	3-V	7517	AMP	O4'-C1'-N9-C8
3	4-V	7517	AMP	O4'-C1'-N9-C8
3	5-V	7517	AMP	O4'-C1'-N9-C8
3	6-V	7517	AMP	O4'-C1'-N9-C8
3	7-V	7517	AMP	O4'-C1'-N9-C8
3	8-V	7517	AMP	O4'-C1'-N9-C8
3	9-V	7517	AMP	O4'-C1'-N9-C8
3	10-V	7517	AMP	O4'-C1'-N9-C8
3	1-W	7519	AMP	O4'-C1'-N9-C8
3	2-W	7519	AMP	O4'-C1'-N9-C8
3	3-W	7519	AMP	O4'-C1'-N9-C8
3	4-W	7519	AMP	O4'-C1'-N9-C8
3	5-W	7519	AMP	O4'-C1'-N9-C8
3	6-W	7519	AMP	O4'-C1'-N9-C8
3	7-W	7519	AMP	O4'-C1'-N9-C8
3	8-W	7519	AMP	O4'-C1'-N9-C8
3	9-W	7519	AMP	O4'-C1'-N9-C8
3	10-W	7519	AMP	O4'-C1'-N9-C8
3	1-X	7521	AMP	O4'-C1'-N9-C8
3	2-X	7521	AMP	O4'-C1'-N9-C8
3	3-X	7521	AMP	O4'-C1'-N9-C8
3	4-X	7521	AMP	O4'-C1'-N9-C8
3	5-X	7521	AMP	O4'-C1'-N9-C8
3	6-X	7521	AMP	O4'-C1'-N9-C8
3	7-X	7521	AMP	O4'-C1'-N9-C8
3	8-X	7521	AMP	O4'-C1'-N9-C8
3	9-X	7521	AMP	O4'-C1'-N9-C8
3	10-X	7521	AMP	O4'-C1'-N9-C8

There are no ring outliers.

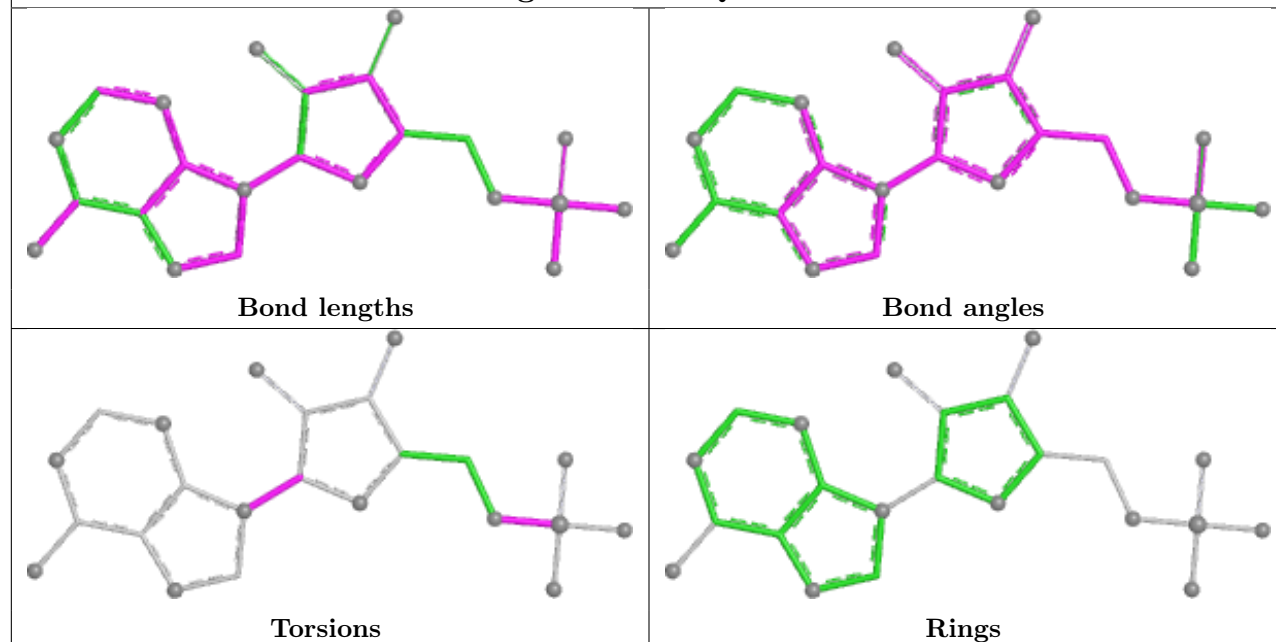
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

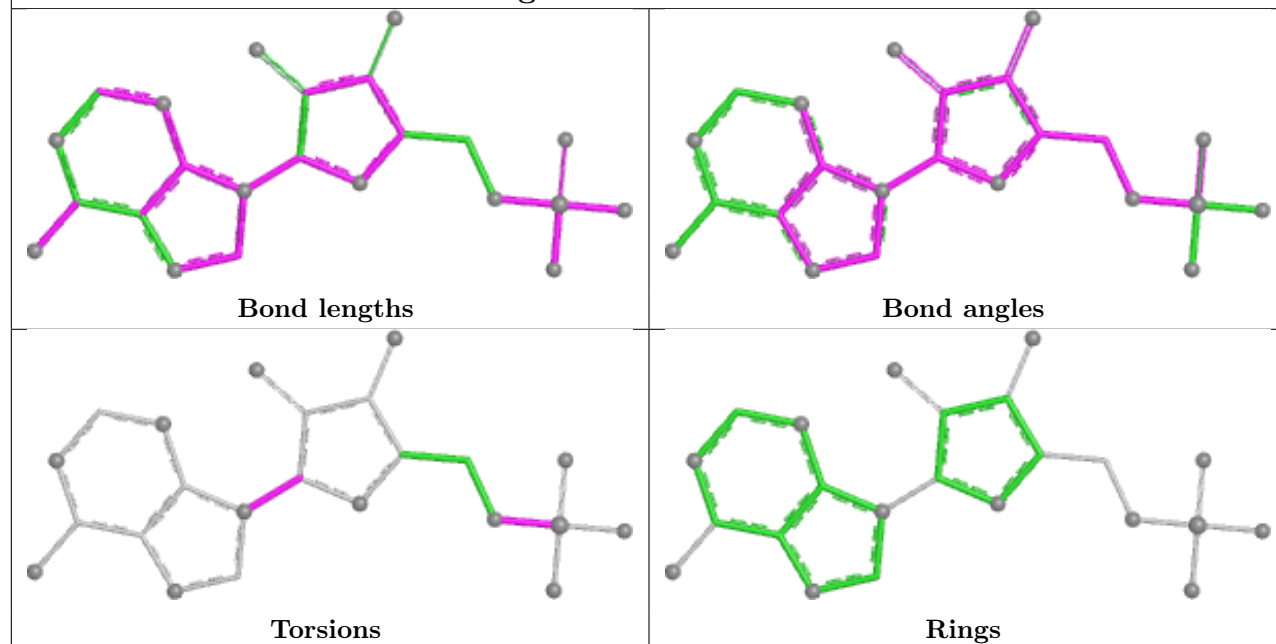
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



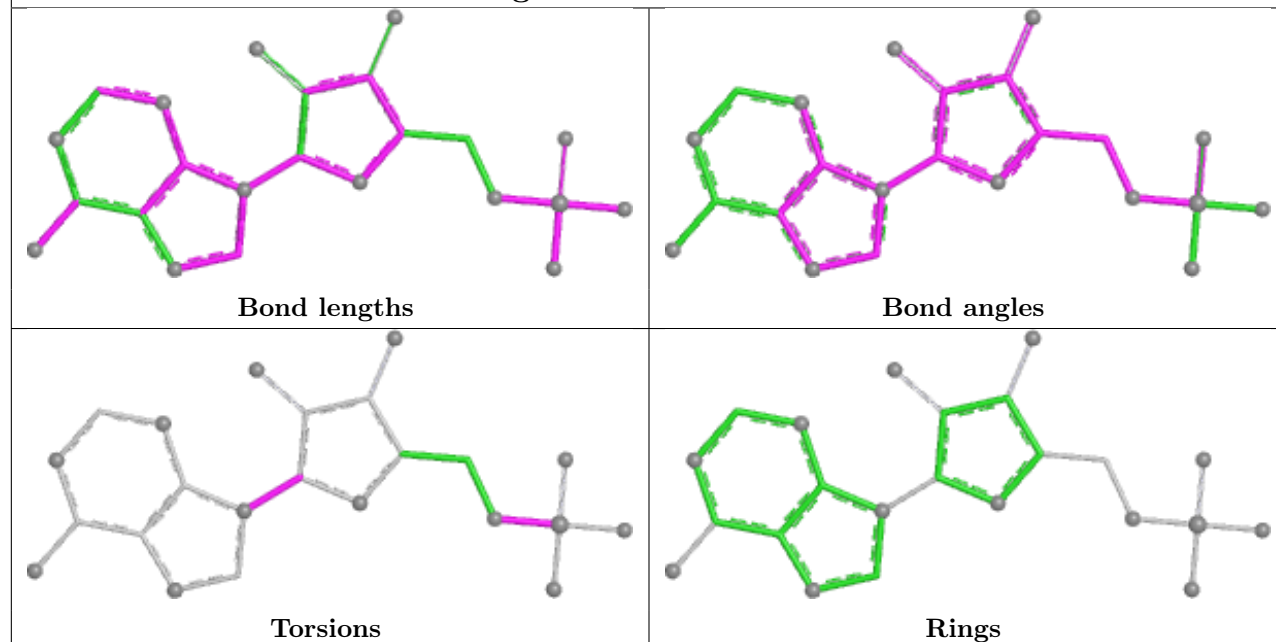
Ligand AMP Q 7507



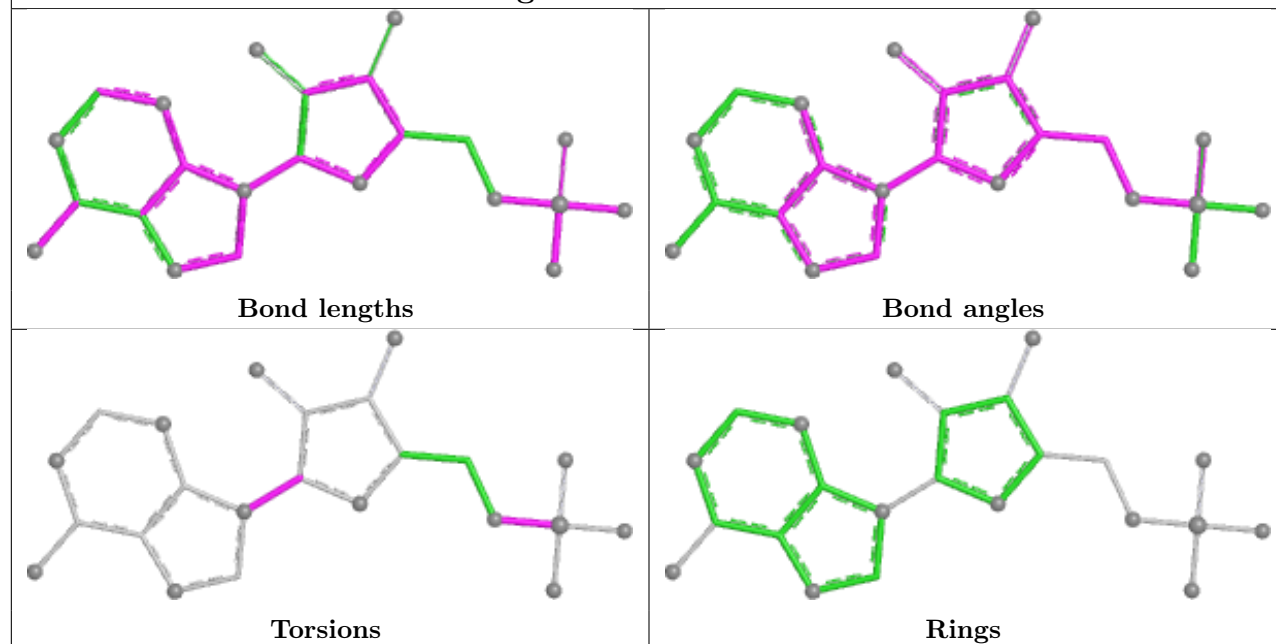
Ligand AMP P 7505



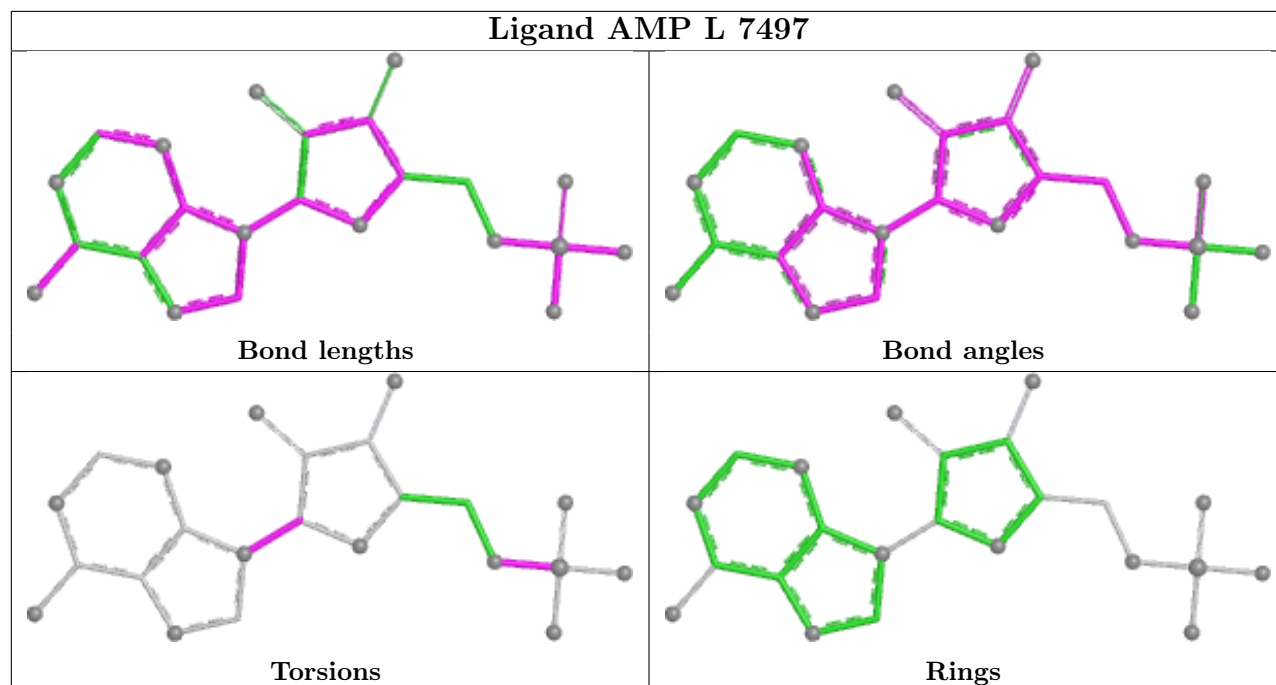
Ligand AMP W 7519



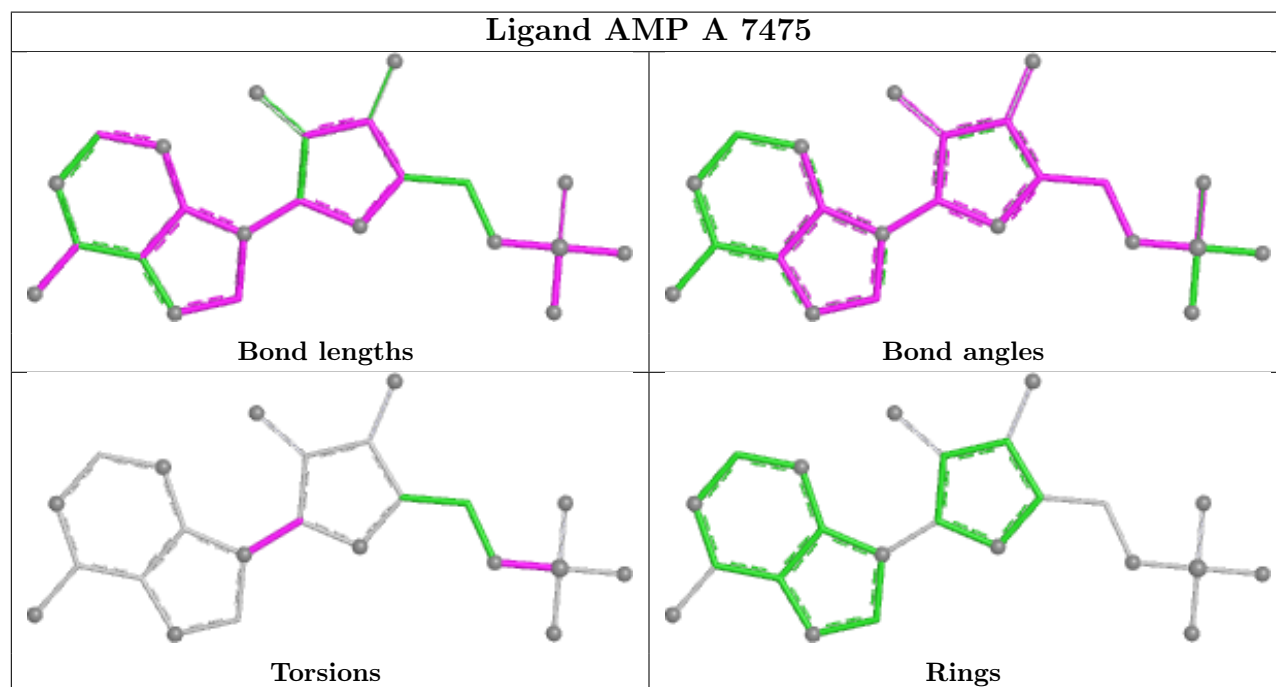
Ligand AMP D 7481



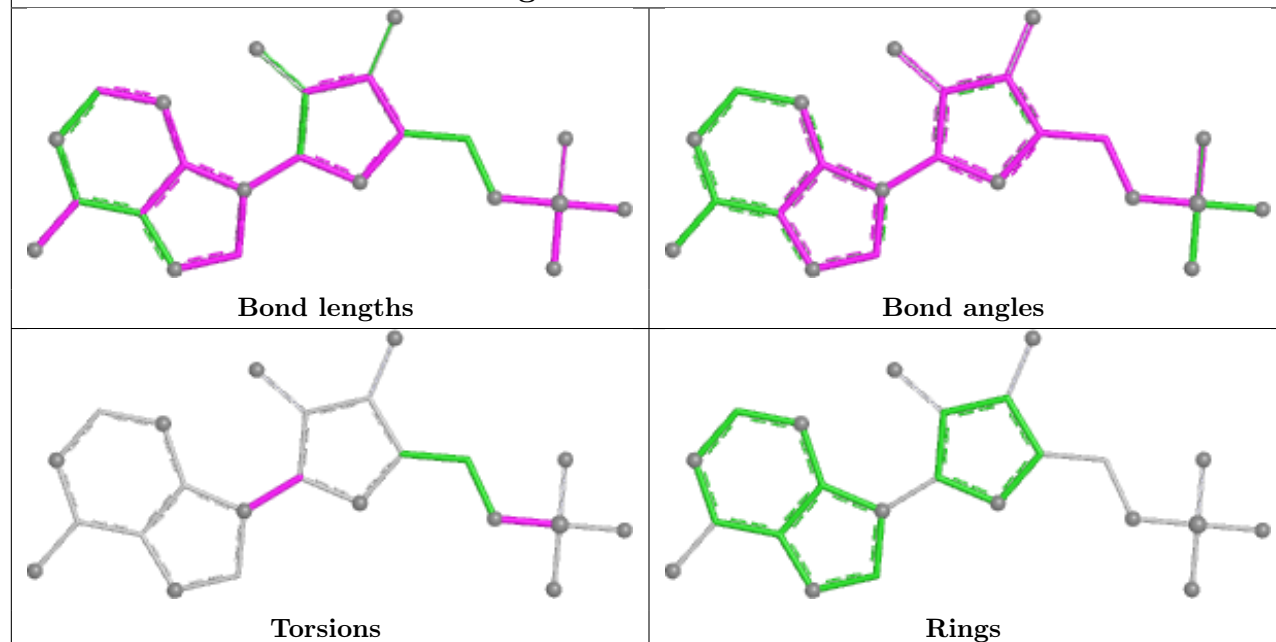
Ligand AMP L 7497



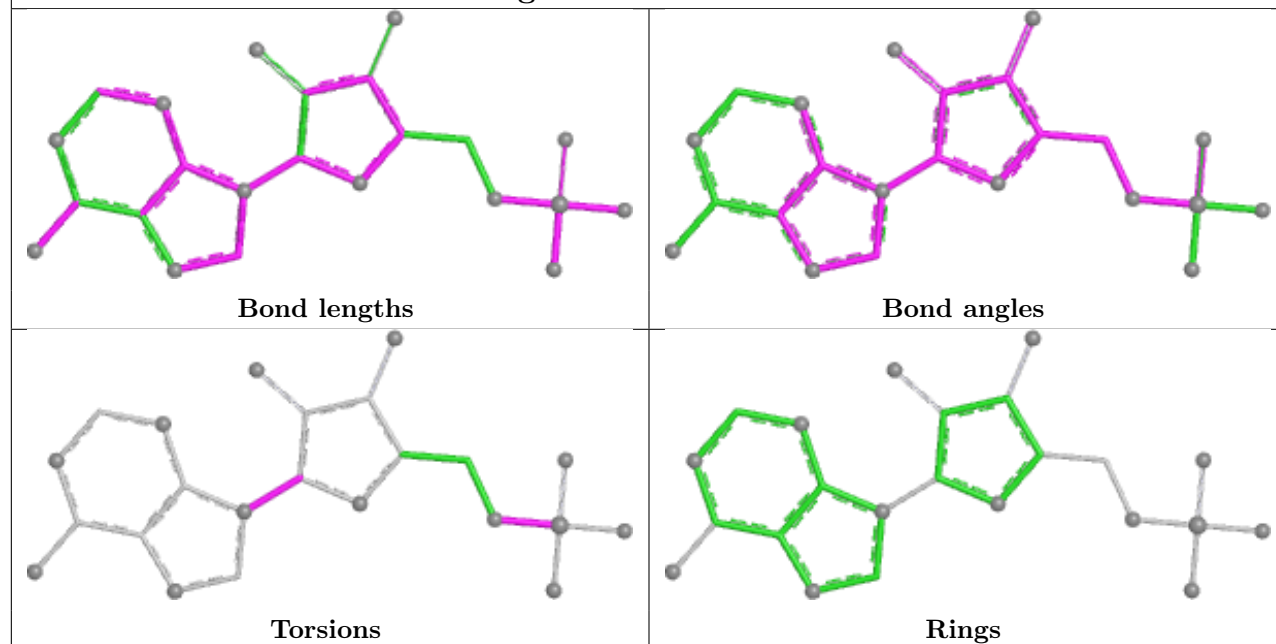
Ligand AMP A 7475



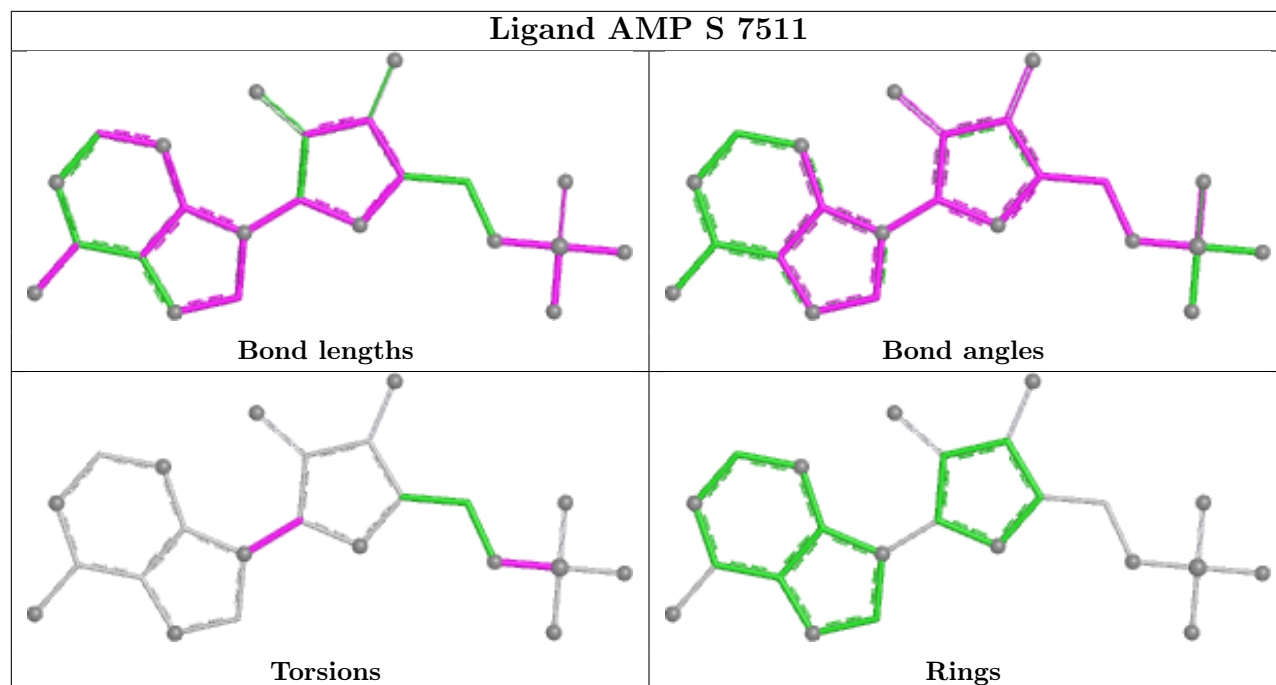
Ligand AMP T 7513



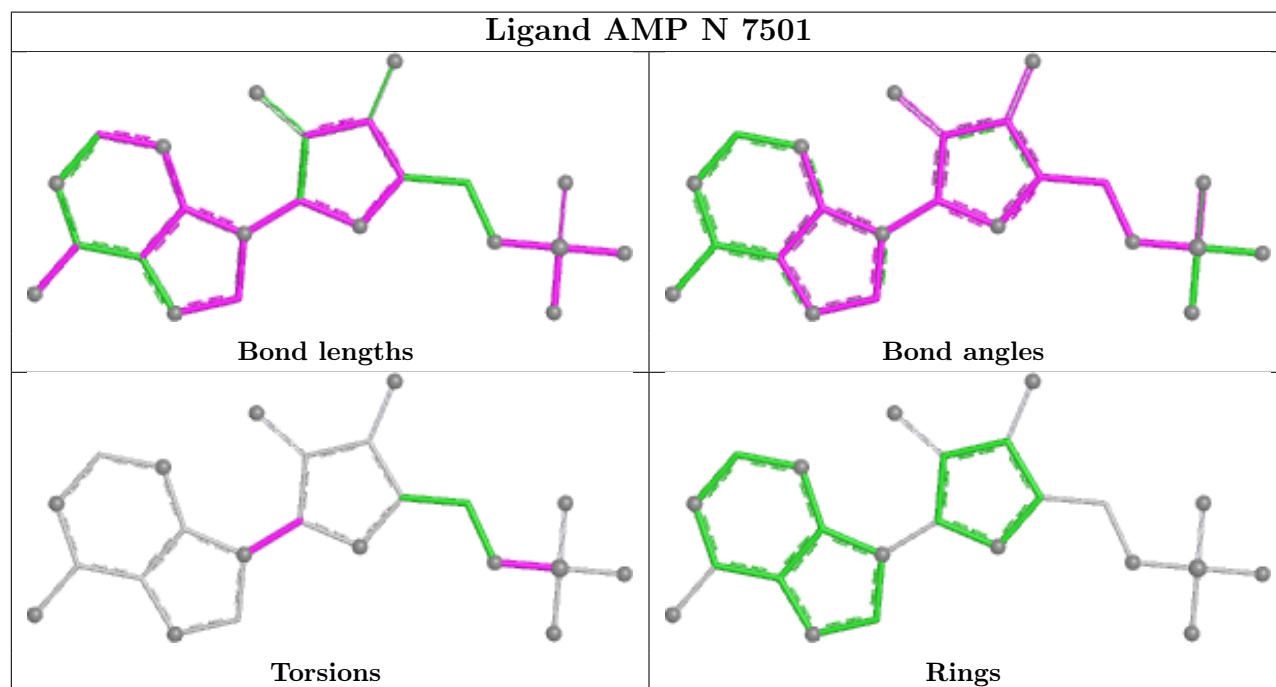
Ligand AMP B 7477



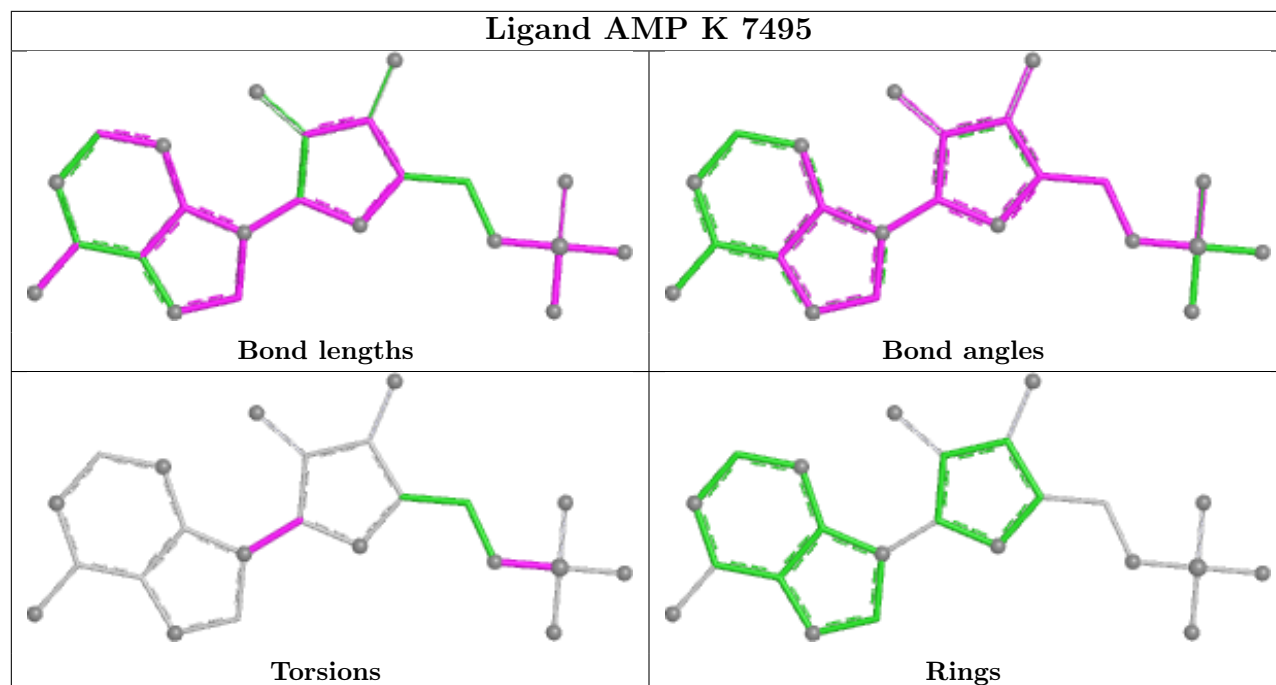
Ligand AMP S 7511



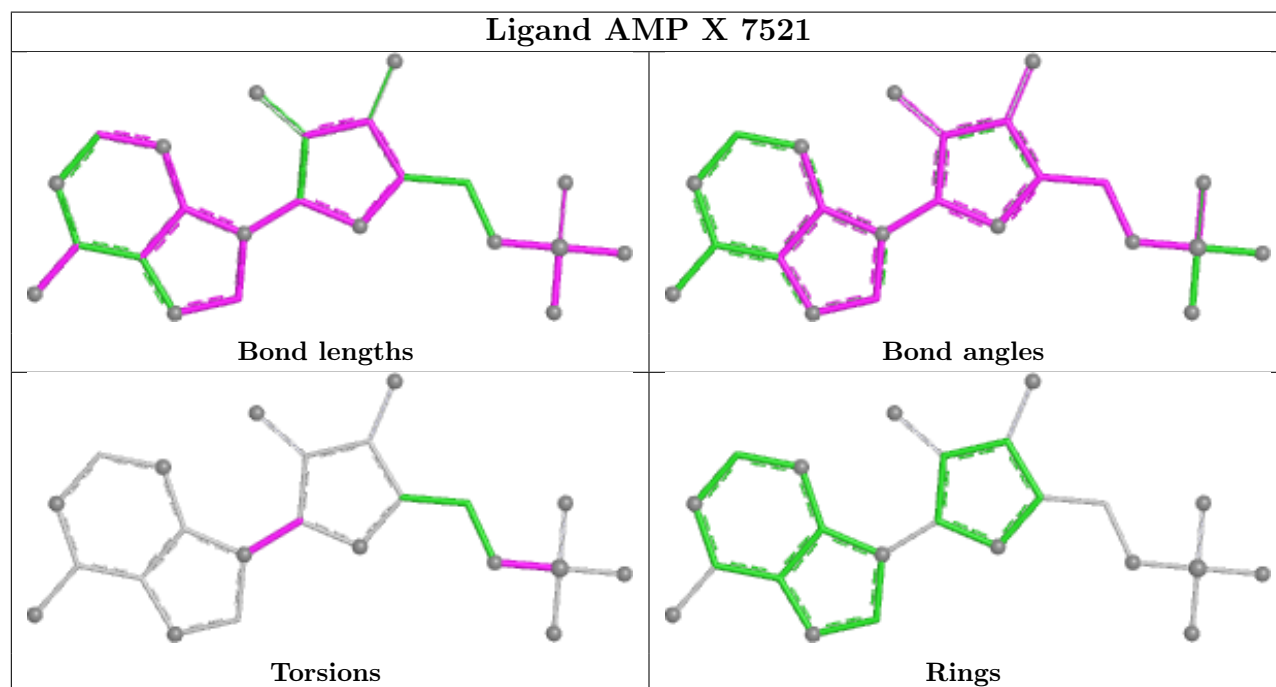
Ligand AMP N 7501



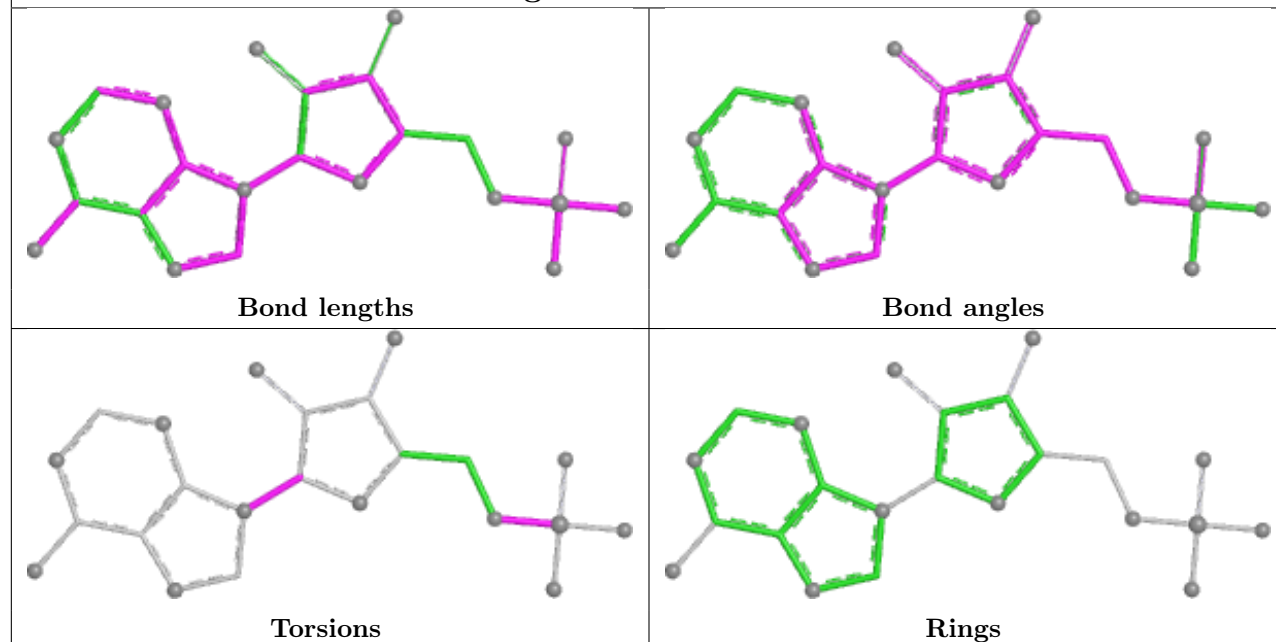
Ligand AMP K 7495



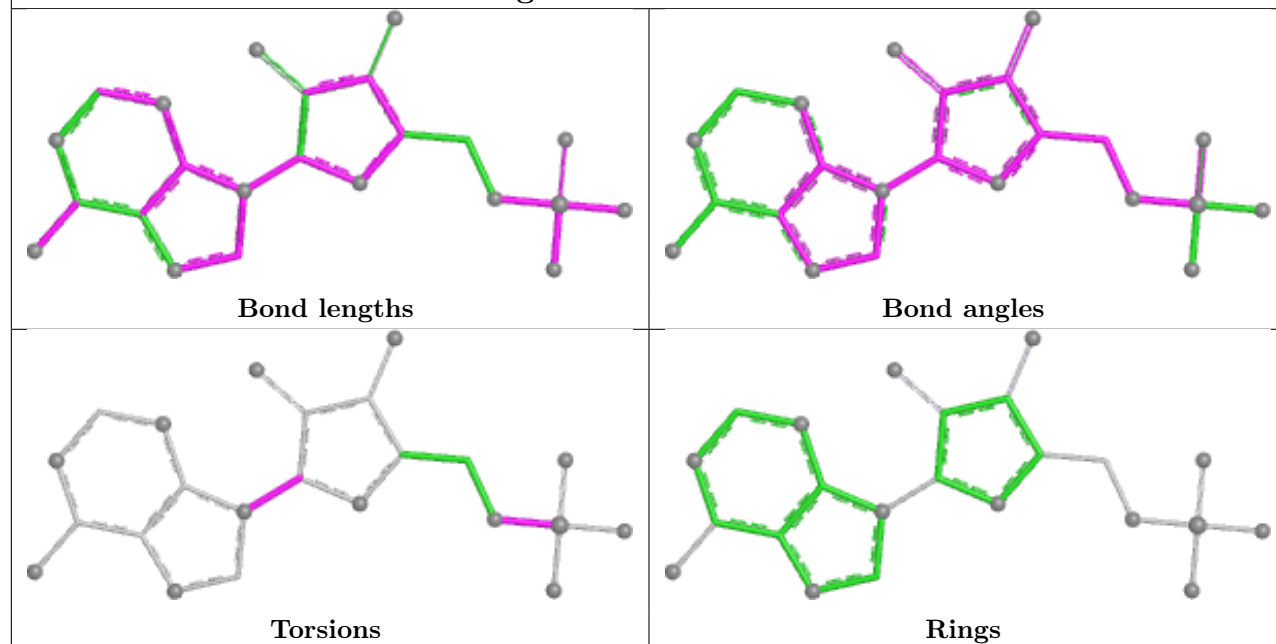
Ligand AMP X 7521



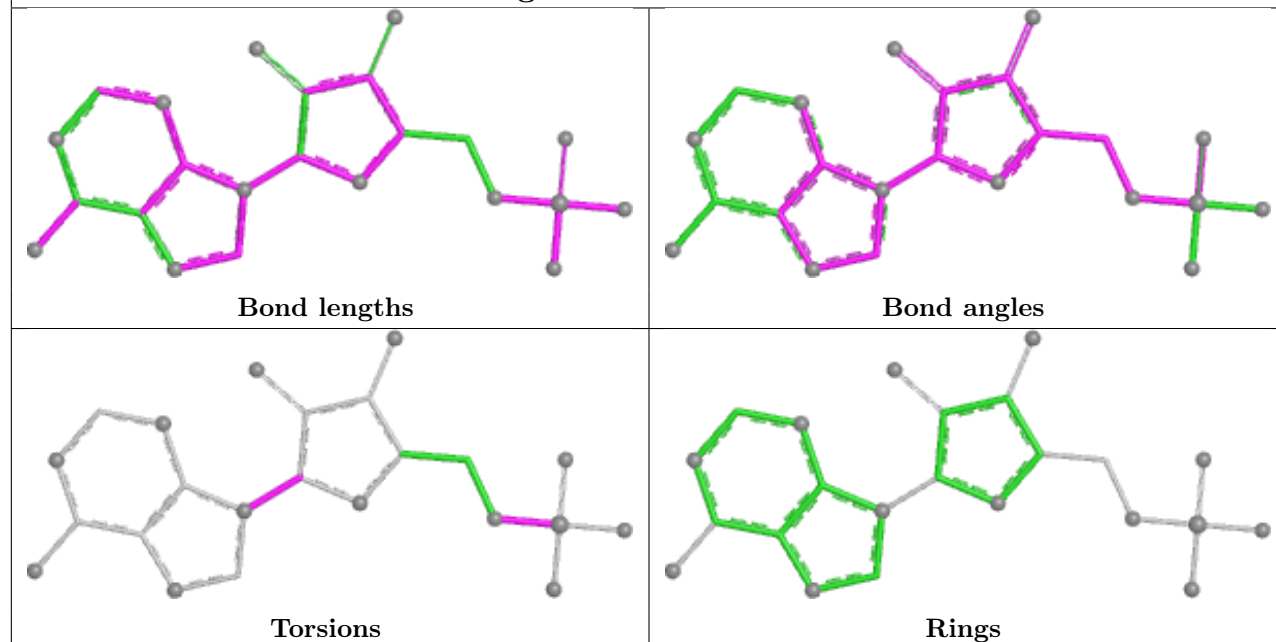
Ligand AMP I 7491



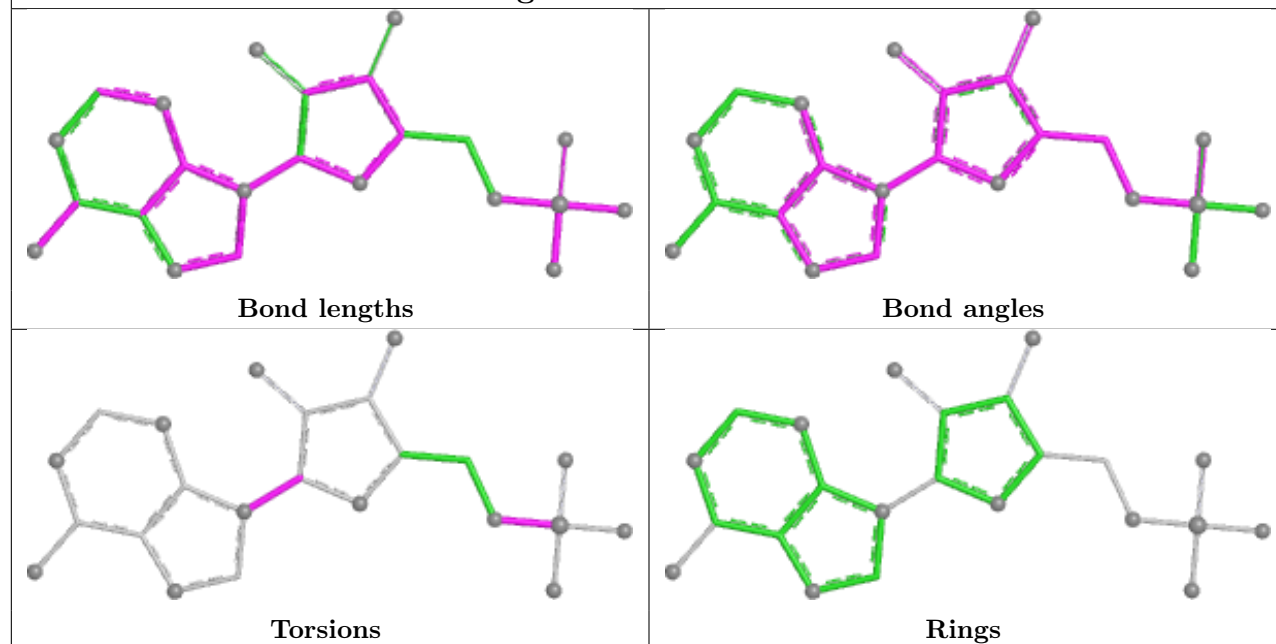
Ligand AMP H 7489



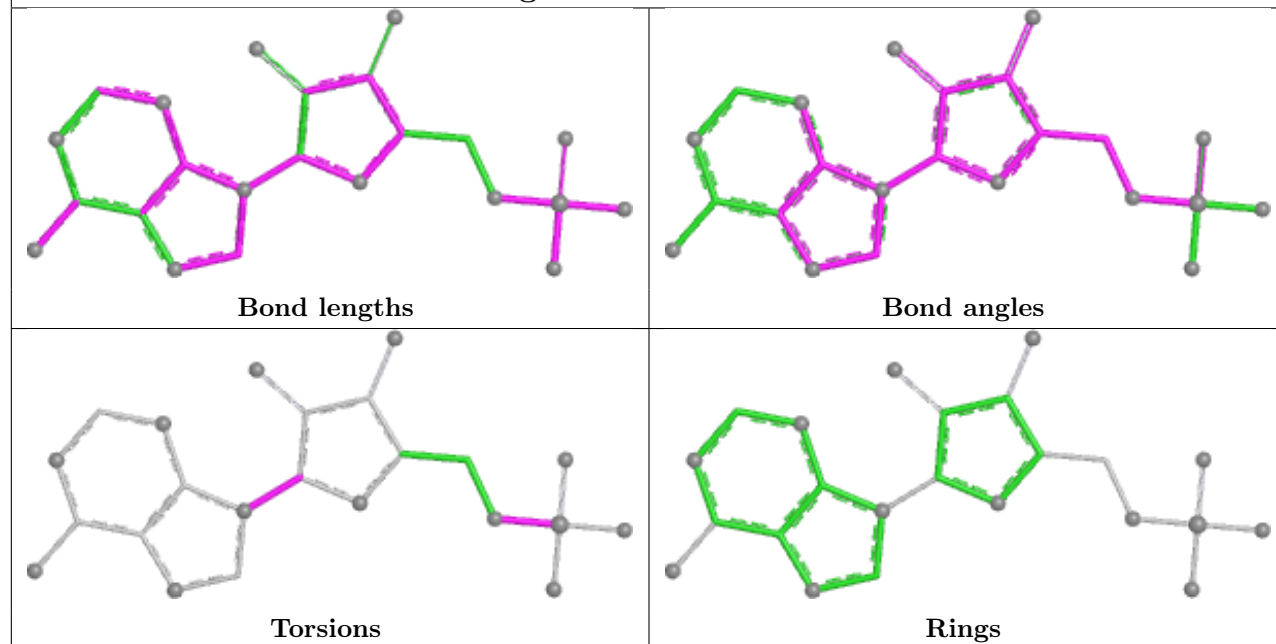
Ligand AMP C 7479



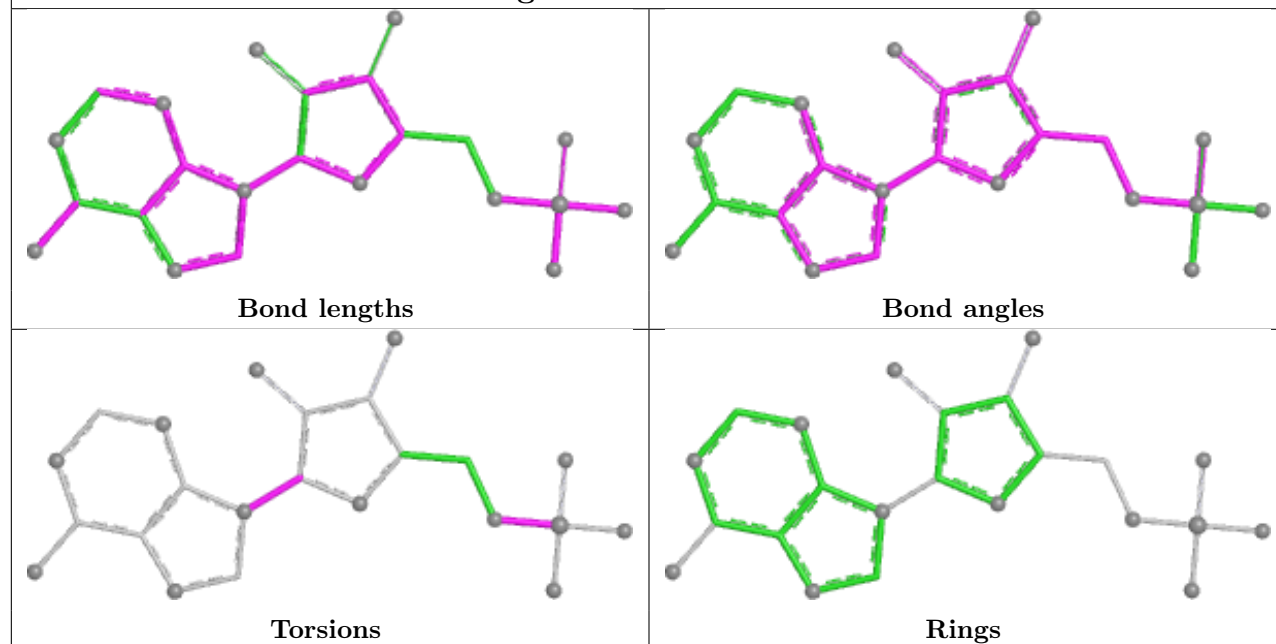
Ligand AMP V 7517



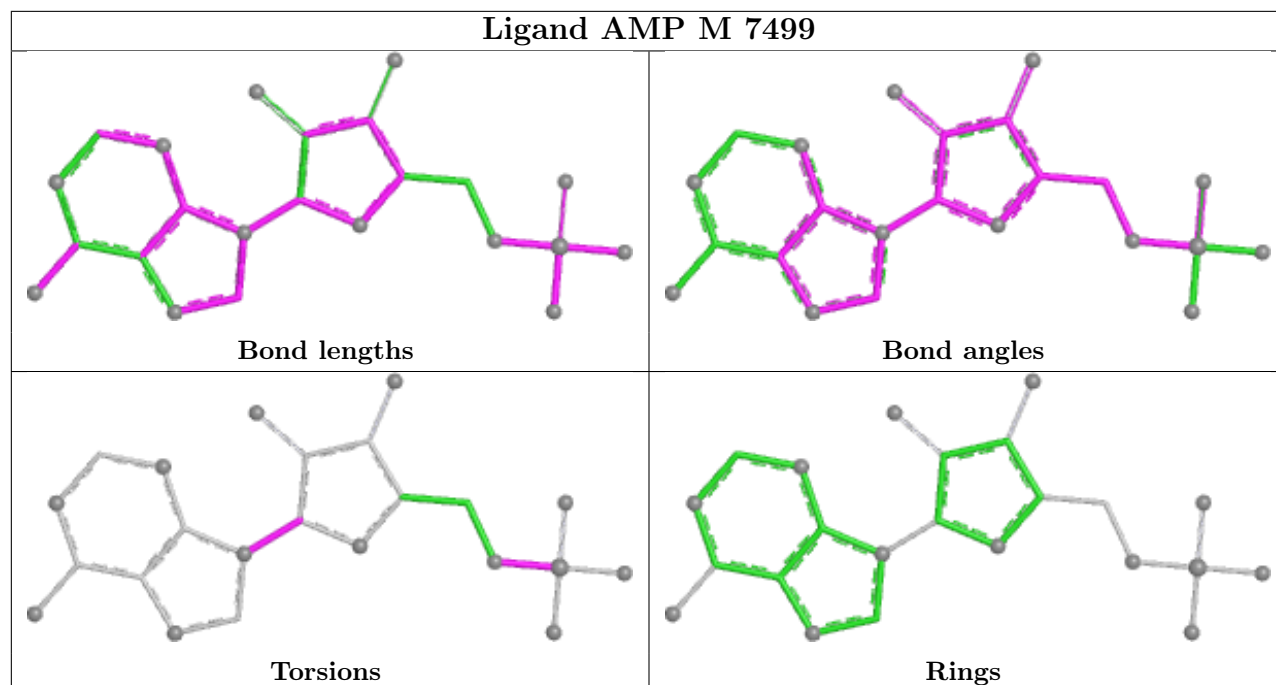
Ligand AMP F 7485



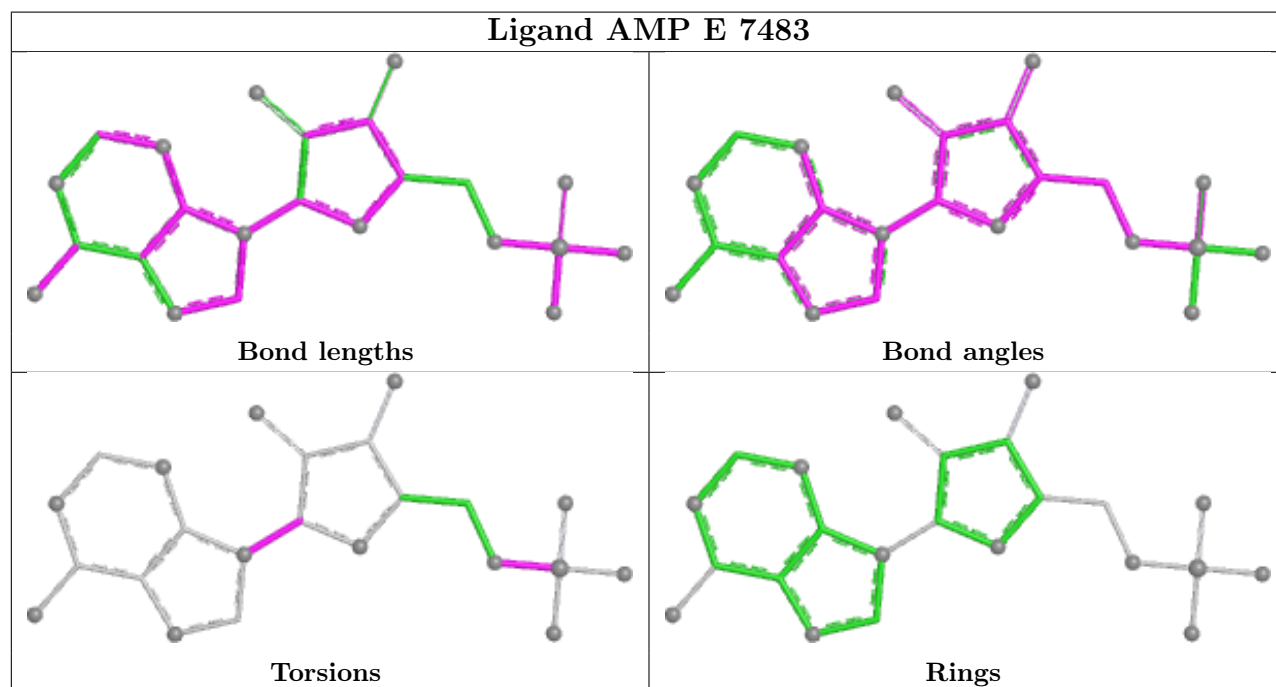
Ligand AMP R 7509

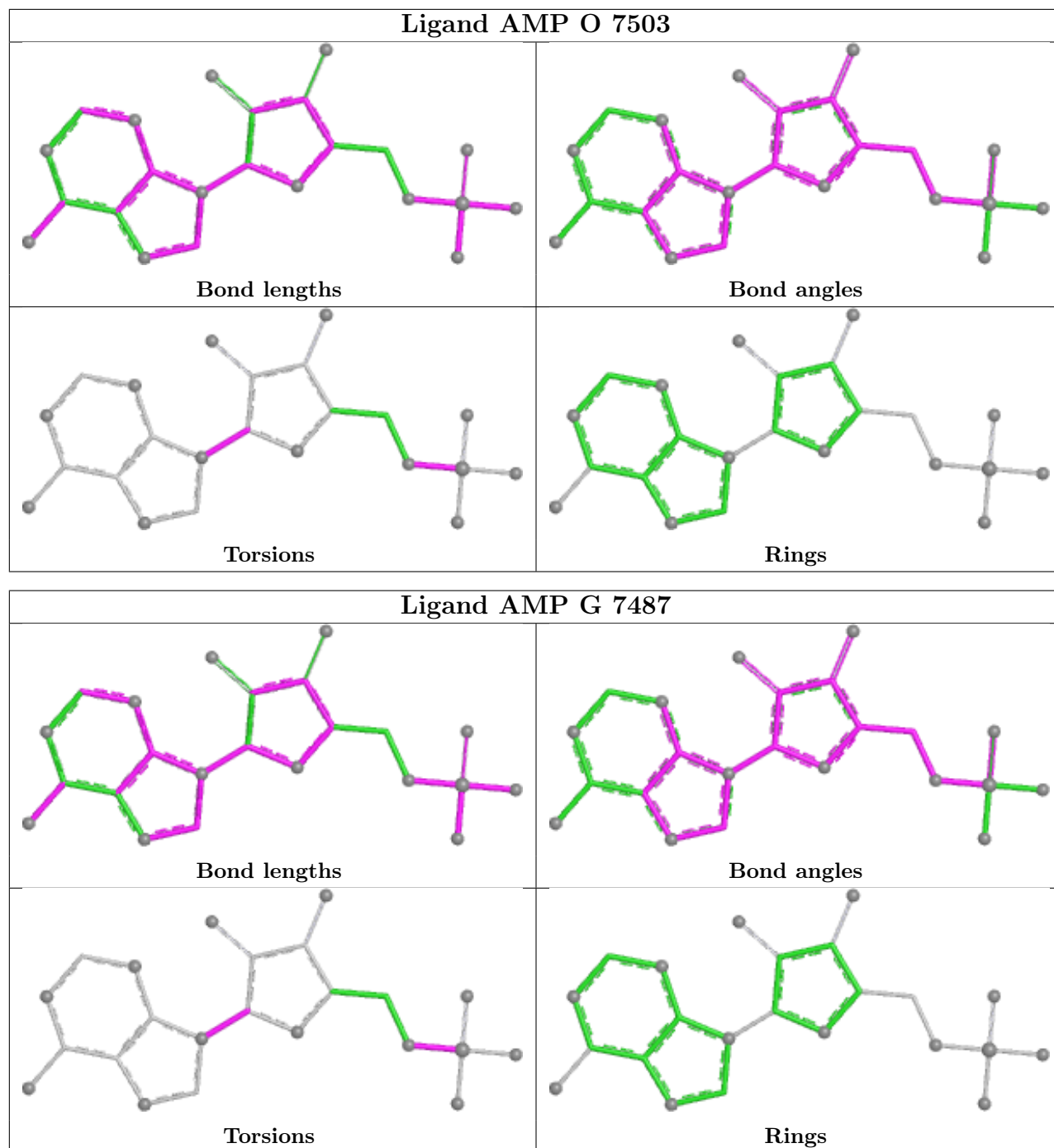


Ligand AMP M 7499



Ligand AMP E 7483





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	477/477 (100%)	2.41	203 (42%) 0 0	1, 2, 4, 5	477 (100%)
1	1-B	477/477 (100%)	2.40	202 (42%) 0 0	1, 2, 4, 5	477 (100%)
1	1-C	477/477 (100%)	2.17	190 (39%) 1 0	1, 2, 4, 5	477 (100%)
1	1-D	477/477 (100%)	2.50	214 (44%) 0 0	1, 2, 4, 5	477 (100%)
1	1-E	477/477 (100%)	2.37	210 (44%) 0 0	1, 2, 4, 5	477 (100%)
1	1-F	477/477 (100%)	2.63	230 (48%) 0 0	1, 2, 4, 5	477 (100%)
1	1-G	477/477 (100%)	2.76	235 (49%) 0 0	1, 2, 4, 5	477 (100%)
1	1-H	477/477 (100%)	2.33	203 (42%) 0 0	1, 2, 4, 5	477 (100%)
1	1-I	477/477 (100%)	2.19	188 (39%) 1 0	1, 2, 4, 5	477 (100%)
1	1-J	477/477 (100%)	2.35	197 (41%) 0 0	1, 2, 4, 5	477 (100%)
1	1-K	477/477 (100%)	2.42	212 (44%) 0 0	1, 2, 4, 5	477 (100%)
1	1-L	477/477 (100%)	2.75	251 (52%) 0 0	1, 2, 4, 5	477 (100%)
1	1-M	477/477 (100%)	2.36	206 (43%) 0 0	1, 2, 4, 5	477 (100%)
1	1-N	477/477 (100%)	2.43	209 (43%) 0 0	1, 2, 4, 5	477 (100%)
1	1-O	477/477 (100%)	2.19	193 (40%) 0 0	1, 2, 4, 5	477 (100%)
1	1-P	477/477 (100%)	2.62	229 (48%) 0 0	1, 2, 4, 5	477 (100%)
1	1-Q	477/477 (100%)	2.46	214 (44%) 0 0	1, 2, 4, 5	477 (100%)
1	1-R	477/477 (100%)	2.64	229 (48%) 0 0	1, 2, 4, 5	477 (100%)
1	1-S	477/477 (100%)	2.77	229 (48%) 0 0	1, 2, 4, 5	477 (100%)
1	1-T	477/477 (100%)	2.37	207 (43%) 0 0	1, 2, 4, 5	477 (100%)
1	1-U	477/477 (100%)	2.20	203 (42%) 0 0	1, 2, 4, 5	477 (100%)
1	1-V	477/477 (100%)	2.30	196 (41%) 0 0	1, 2, 4, 5	477 (100%)
1	1-W	477/477 (100%)	2.43	203 (42%) 0 0	1, 2, 4, 5	477 (100%)
1	1-X	477/477 (100%)	2.58	219 (45%) 0 0	1, 2, 4, 5	477 (100%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2-A	0/477	-	-	-	-
1	2-B	0/477	-	-	-	-
1	2-C	0/477	-	-	-	-
1	2-D	0/477	-	-	-	-
1	2-E	0/477	-	-	-	-
1	2-F	0/477	-	-	-	-
1	2-G	0/477	-	-	-	-
1	2-H	0/477	-	-	-	-
1	2-I	0/477	-	-	-	-
1	2-J	0/477	-	-	-	-
1	2-K	0/477	-	-	-	-
1	2-L	0/477	-	-	-	-
1	2-M	0/477	-	-	-	-
1	2-N	0/477	-	-	-	-
1	2-O	0/477	-	-	-	-
1	2-P	0/477	-	-	-	-
1	2-Q	0/477	-	-	-	-
1	2-R	0/477	-	-	-	-
1	2-S	0/477	-	-	-	-
1	2-T	0/477	-	-	-	-
1	2-U	0/477	-	-	-	-
1	2-V	0/477	-	-	-	-
1	2-W	0/477	-	-	-	-
1	2-X	0/477	-	-	-	-
1	3-A	0/477	-	-	-	-
1	3-B	0/477	-	-	-	-
1	3-C	0/477	-	-	-	-
1	3-D	0/477	-	-	-	-
1	3-E	0/477	-	-	-	-
1	3-F	0/477	-	-	-	-
1	3-G	0/477	-	-	-	-
1	3-H	0/477	-	-	-	-
1	3-I	0/477	-	-	-	-
1	3-J	0/477	-	-	-	-
1	3-K	0/477	-	-	-	-
1	3-L	0/477	-	-	-	-
1	3-M	0/477	-	-	-	-
1	3-N	0/477	-	-	-	-
1	3-O	0/477	-	-	-	-
1	3-P	0/477	-	-	-	-
1	3-Q	0/477	-	-	-	-
1	3-R	0/477	-	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	3-S	0/477	-	-	-	-
1	3-T	0/477	-	-	-	-
1	3-U	0/477	-	-	-	-
1	3-V	0/477	-	-	-	-
1	3-W	0/477	-	-	-	-
1	3-X	0/477	-	-	-	-
1	4-A	0/477	-	-	-	-
1	4-B	0/477	-	-	-	-
1	4-C	0/477	-	-	-	-
1	4-D	0/477	-	-	-	-
1	4-E	0/477	-	-	-	-
1	4-F	0/477	-	-	-	-
1	4-G	0/477	-	-	-	-
1	4-H	0/477	-	-	-	-
1	4-I	0/477	-	-	-	-
1	4-J	0/477	-	-	-	-
1	4-K	0/477	-	-	-	-
1	4-L	0/477	-	-	-	-
1	4-M	0/477	-	-	-	-
1	4-N	0/477	-	-	-	-
1	4-O	0/477	-	-	-	-
1	4-P	0/477	-	-	-	-
1	4-Q	0/477	-	-	-	-
1	4-R	0/477	-	-	-	-
1	4-S	0/477	-	-	-	-
1	4-T	0/477	-	-	-	-
1	4-U	0/477	-	-	-	-
1	4-V	0/477	-	-	-	-
1	4-W	0/477	-	-	-	-
1	4-X	0/477	-	-	-	-
1	5-A	0/477	-	-	-	-
1	5-B	0/477	-	-	-	-
1	5-C	0/477	-	-	-	-
1	5-D	0/477	-	-	-	-
1	5-E	0/477	-	-	-	-
1	5-F	0/477	-	-	-	-
1	5-G	0/477	-	-	-	-
1	5-H	0/477	-	-	-	-
1	5-I	0/477	-	-	-	-
1	5-J	0/477	-	-	-	-
1	5-K	0/477	-	-	-	-
1	5-L	0/477	-	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	5-M	0/477	-	-	-	-
1	5-N	0/477	-	-	-	-
1	5-O	0/477	-	-	-	-
1	5-P	0/477	-	-	-	-
1	5-Q	0/477	-	-	-	-
1	5-R	0/477	-	-	-	-
1	5-S	0/477	-	-	-	-
1	5-T	0/477	-	-	-	-
1	5-U	0/477	-	-	-	-
1	5-V	0/477	-	-	-	-
1	5-W	0/477	-	-	-	-
1	5-X	0/477	-	-	-	-
1	6-A	0/477	-	-	-	-
1	6-B	0/477	-	-	-	-
1	6-C	0/477	-	-	-	-
1	6-D	0/477	-	-	-	-
1	6-E	0/477	-	-	-	-
1	6-F	0/477	-	-	-	-
1	6-G	0/477	-	-	-	-
1	6-H	0/477	-	-	-	-
1	6-I	0/477	-	-	-	-
1	6-J	0/477	-	-	-	-
1	6-K	0/477	-	-	-	-
1	6-L	0/477	-	-	-	-
1	6-M	0/477	-	-	-	-
1	6-N	0/477	-	-	-	-
1	6-O	0/477	-	-	-	-
1	6-P	0/477	-	-	-	-
1	6-Q	0/477	-	-	-	-
1	6-R	0/477	-	-	-	-
1	6-S	0/477	-	-	-	-
1	6-T	0/477	-	-	-	-
1	6-U	0/477	-	-	-	-
1	6-V	0/477	-	-	-	-
1	6-W	0/477	-	-	-	-
1	6-X	0/477	-	-	-	-
1	7-A	0/477	-	-	-	-
1	7-B	0/477	-	-	-	-
1	7-C	0/477	-	-	-	-
1	7-D	0/477	-	-	-	-
1	7-E	0/477	-	-	-	-
1	7-F	0/477	-	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	7-G	0/477	-	-	-	-
1	7-H	0/477	-	-	-	-
1	7-I	0/477	-	-	-	-
1	7-J	0/477	-	-	-	-
1	7-K	0/477	-	-	-	-
1	7-L	0/477	-	-	-	-
1	7-M	0/477	-	-	-	-
1	7-N	0/477	-	-	-	-
1	7-O	0/477	-	-	-	-
1	7-P	0/477	-	-	-	-
1	7-Q	0/477	-	-	-	-
1	7-R	0/477	-	-	-	-
1	7-S	0/477	-	-	-	-
1	7-T	0/477	-	-	-	-
1	7-U	0/477	-	-	-	-
1	7-V	0/477	-	-	-	-
1	7-W	0/477	-	-	-	-
1	7-X	0/477	-	-	-	-
1	8-A	0/477	-	-	-	-
1	8-B	0/477	-	-	-	-
1	8-C	0/477	-	-	-	-
1	8-D	0/477	-	-	-	-
1	8-E	0/477	-	-	-	-
1	8-F	0/477	-	-	-	-
1	8-G	0/477	-	-	-	-
1	8-H	0/477	-	-	-	-
1	8-I	0/477	-	-	-	-
1	8-J	0/477	-	-	-	-
1	8-K	0/477	-	-	-	-
1	8-L	0/477	-	-	-	-
1	8-M	0/477	-	-	-	-
1	8-N	0/477	-	-	-	-
1	8-O	0/477	-	-	-	-
1	8-P	0/477	-	-	-	-
1	8-Q	0/477	-	-	-	-
1	8-R	0/477	-	-	-	-
1	8-S	0/477	-	-	-	-
1	8-T	0/477	-	-	-	-
1	8-U	0/477	-	-	-	-
1	8-V	0/477	-	-	-	-
1	8-W	0/477	-	-	-	-
1	8-X	0/477	-	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	9-A	0/477	-	-	-	-
1	9-B	0/477	-	-	-	-
1	9-C	0/477	-	-	-	-
1	9-D	0/477	-	-	-	-
1	9-E	0/477	-	-	-	-
1	9-F	0/477	-	-	-	-
1	9-G	0/477	-	-	-	-
1	9-H	0/477	-	-	-	-
1	9-I	0/477	-	-	-	-
1	9-J	0/477	-	-	-	-
1	9-K	0/477	-	-	-	-
1	9-L	0/477	-	-	-	-
1	9-M	0/477	-	-	-	-
1	9-N	0/477	-	-	-	-
1	9-O	0/477	-	-	-	-
1	9-P	0/477	-	-	-	-
1	9-Q	0/477	-	-	-	-
1	9-R	0/477	-	-	-	-
1	9-S	0/477	-	-	-	-
1	9-T	0/477	-	-	-	-
1	9-U	0/477	-	-	-	-
1	9-V	0/477	-	-	-	-
1	9-W	0/477	-	-	-	-
1	9-X	0/477	-	-	-	-
1	10-A	0/477	-	-	-	-
1	10-B	0/477	-	-	-	-
1	10-C	0/477	-	-	-	-
1	10-D	0/477	-	-	-	-
1	10-E	0/477	-	-	-	-
1	10-F	0/477	-	-	-	-
1	10-G	0/477	-	-	-	-
1	10-H	0/477	-	-	-	-
1	10-I	0/477	-	-	-	-
1	10-J	0/477	-	-	-	-
1	10-K	0/477	-	-	-	-
1	10-L	0/477	-	-	-	-
1	10-M	0/477	-	-	-	-
1	10-N	0/477	-	-	-	-
1	10-O	0/477	-	-	-	-
1	10-P	0/477	-	-	-	-
1	10-Q	0/477	-	-	-	-
1	10-R	0/477	-	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	10-S	0/477	-	-	-	-
1	10-T	0/477	-	-	-	-
1	10-U	0/477	-	-	-	-
1	10-V	0/477	-	-	-	-
1	10-W	0/477	-	-	-	-
1	10-X	0/477	-	-	-	-
All	All	11448/114480 (10%)	2.44	5072 (44%) 0 0	1, 2, 4, 5	11448 (100%)

All (5072) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	325	GLY	15.9
1	1-P	328	ALA	15.6
1	1-R	166	ALA	14.8
1	1-X	64	ASP	14.8
1	1-A	60	ILE	14.4
1	1-O	95	PHE	13.6
1	1-L	349	GLY	13.3
1	1-A	328	ALA	13.3
1	1-G	95	PHE	12.9
1	1-H	56	GLY	12.8
1	1-L	95	PHE	12.3
1	1-E	178	GLY	12.3
1	1-L	64	ASP	12.2
1	1-Q	54	ILE	12.1
1	1-R	62	GLU	12.1
1	1-I	56	GLY	12.1
1	1-X	166	ALA	11.9
1	1-X	601	THR	11.9
1	1-T	179	TYR	11.8
1	1-D	350	SER	11.7
1	1-G	97	LEU	11.7
1	1-R	95	PHE	11.6
1	1-T	328	ALA	11.5
1	1-L	57	PHE	11.5
1	1-X	96	THR	11.5
1	1-S	95	PHE	11.5
1	1-G	93	ASP	11.5
1	1-N	178	GLY	11.5
1	1-M	95	PHE	11.4
1	1-P	349	GLY	11.4
1	1-V	59	SER	11.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-H	179	TYR	11.4
1	1-J	349	GLY	11.3
1	1-F	62	GLU	11.3
1	1-L	60	ILE	11.2
1	1-X	60	ILE	11.2
1	1-W	349	GLY	11.2
1	1-G	349	GLY	11.2
1	1-F	95	PHE	11.1
1	1-G	350	SER	11.1
1	1-I	166	ALA	11.1
1	1-D	403	GLU	11.0
1	1-L	96	THR	11.0
1	1-L	396	LEU	11.0
1	1-H	328	ALA	11.0
1	1-F	56	GLY	11.0
1	1-H	325	GLY	11.0
1	1-G	396	LEU	10.9
1	1-L	350	SER	10.9
1	1-F	166	ALA	10.8
1	1-J	166	ALA	10.8
1	1-S	338	ASN	10.8
1	1-L	51	GLY	10.7
1	1-R	396	LEU	10.7
1	1-S	601	THR	10.7
1	1-Q	95	PHE	10.7
1	1-P	325	GLY	10.6
1	1-A	95	PHE	10.6
1	1-X	95	PHE	10.6
1	1-L	405	ALA	10.6
1	1-B	54	ILE	10.6
1	1-E	60	ILE	10.6
1	1-T	95	PHE	10.6
1	1-H	178	GLY	10.6
1	1-J	601	THR	10.5
1	1-Q	63	SER	10.5
1	1-D	349	GLY	10.5
1	1-S	54	ILE	10.5
1	1-G	166	ALA	10.4
1	1-D	62	GLU	10.4
1	1-P	350	SER	10.3
1	1-G	338	ASN	10.3
1	1-W	396	LEU	10.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-S	94	PRO	10.3
1	1-P	396	LEU	10.3
1	1-R	57	PHE	10.2
1	1-H	95	PHE	10.2
1	1-F	396	LEU	10.2
1	1-L	338	ASN	10.2
1	1-O	166	ALA	10.2
1	1-G	94	PRO	10.2
1	1-R	61	HIS	10.2
1	1-T	57	PHE	10.1
1	1-B	178	GLY	10.1
1	1-E	404	ALA	10.1
1	1-B	61	HIS	10.1
1	1-S	61	HIS	10.1
1	1-C	166	ALA	10.1
1	1-L	601	THR	10.1
1	1-B	404	ALA	10.1
1	1-M	61	HIS	10.1
1	1-O	54	ILE	10.1
1	1-Q	60	ILE	10.0
1	1-W	61	HIS	10.0
1	1-J	59	SER	10.0
1	1-J	350	SER	10.0
1	1-B	166	ALA	10.0
1	1-G	54	ILE	10.0
1	1-S	397	TYR	10.0
1	1-X	63	SER	10.0
1	1-A	61	HIS	9.9
1	1-X	396	LEU	9.9
1	1-J	54	ILE	9.9
1	1-T	404	ALA	9.8
1	1-R	325	GLY	9.8
1	1-T	56	GLY	9.8
1	1-M	60	ILE	9.8
1	1-G	335	SER	9.8
1	1-J	396	LEU	9.8
1	1-R	383	LYS	9.7
1	1-R	349	GLY	9.7
1	1-P	54	ILE	9.7
1	1-T	60	ILE	9.7
1	1-E	166	ALA	9.7
1	1-V	326	TYR	9.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-F	601	THR	9.7
1	1-X	54	ILE	9.6
1	1-G	326	TYR	9.6
1	1-D	54	ILE	9.6
1	1-D	95	PHE	9.6
1	1-J	95	PHE	9.6
1	1-W	326	TYR	9.6
1	1-N	601	THR	9.6
1	1-L	166	ALA	9.6
1	1-D	61	HIS	9.5
1	1-A	178	GLY	9.5
1	1-V	60	ILE	9.5
1	1-E	179	TYR	9.5
1	1-N	55	ARG	9.5
1	1-G	325	GLY	9.5
1	1-Q	56	GLY	9.5
1	1-W	63	SER	9.5
1	1-T	54	ILE	9.5
1	1-S	93	ASP	9.5
1	1-Q	166	ALA	9.4
1	1-S	350	SER	9.4
1	1-H	54	ILE	9.4
1	1-B	601	THR	9.4
1	1-Q	328	ALA	9.4
1	1-C	178	GLY	9.4
1	1-G	601	THR	9.4
1	1-D	94	PRO	9.4
1	1-S	166	ALA	9.4
1	1-W	166	ALA	9.4
1	1-F	178	GLY	9.4
1	1-E	54	ILE	9.4
1	1-W	55	ARG	9.4
1	1-K	351	PRO	9.3
1	1-P	97	LEU	9.3
1	1-J	424	ASP	9.3
1	1-W	402	GLU	9.3
1	1-D	166	ALA	9.3
1	1-H	58	GLN	9.3
1	1-C	326	TYR	9.3
1	1-L	177	GLY	9.3
1	1-E	63	SER	9.3
1	1-N	54	ILE	9.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	62	GLU	9.3
1	1-D	58	GLN	9.3
1	1-R	601	THR	9.3
1	1-V	95	PHE	9.3
1	1-K	179	TYR	9.3
1	1-S	326	TYR	9.3
1	1-F	57	PHE	9.2
1	1-F	383	LYS	9.2
1	1-W	60	ILE	9.2
1	1-U	56	GLY	9.2
1	1-K	58	GLN	9.2
1	1-W	58	GLN	9.2
1	1-S	97	LEU	9.2
1	1-I	54	ILE	9.2
1	1-P	402	GLU	9.2
1	1-I	177	GLY	9.2
1	1-A	398	GLU	9.2
1	1-U	396	LEU	9.1
1	1-S	51	GLY	9.1
1	1-M	54	ILE	9.1
1	1-F	58	GLN	9.1
1	1-S	335	SER	9.1
1	1-X	398	GLU	9.1
1	1-P	94	PRO	9.1
1	1-U	166	ALA	9.1
1	1-G	348	THR	9.1
1	1-S	62	GLU	9.1
1	1-L	49	PHE	9.1
1	1-W	95	PHE	9.1
1	1-L	54	ILE	9.1
1	1-T	326	TYR	9.1
1	1-T	166	ALA	9.1
1	1-D	325	GLY	9.1
1	1-X	178	GLY	9.1
1	1-B	57	PHE	9.1
1	1-D	396	LEU	9.0
1	1-S	399	LEU	9.0
1	1-T	325	GLY	9.0
1	1-S	398	GLU	9.0
1	1-F	326	TYR	9.0
1	1-X	56	GLY	9.0
1	1-S	328	ALA	9.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-X	405	ALA	9.0
1	1-P	403	GLU	9.0
1	1-X	57	PHE	8.9
1	1-S	400	PRO	8.9
1	1-W	179	TYR	8.9
1	1-I	396	LEU	8.9
1	1-M	166	ALA	8.9
1	1-P	177	GLY	8.9
1	1-R	60	ILE	8.9
1	1-O	326	TYR	8.9
1	1-G	61	HIS	8.9
1	1-Q	405	ALA	8.9
1	1-G	351	PRO	8.9
1	1-O	178	GLY	8.9
1	1-C	179	TYR	8.8
1	1-G	328	ALA	8.8
1	1-F	349	GLY	8.8
1	1-E	64	ASP	8.8
1	1-K	399	LEU	8.8
1	1-M	328	ALA	8.8
1	1-A	63	SER	8.8
1	1-G	405	ALA	8.8
1	1-L	63	SER	8.8
1	1-X	350	SER	8.8
1	1-K	61	HIS	8.8
1	1-Q	179	TYR	8.8
1	1-Q	326	TYR	8.8
1	1-P	61	HIS	8.7
1	1-D	338	ASN	8.7
1	1-G	399	LEU	8.7
1	1-F	424	ASP	8.7
1	1-E	62	GLU	8.7
1	1-T	62	GLU	8.7
1	1-T	178	GLY	8.7
1	1-F	61	HIS	8.7
1	1-K	396	LEU	8.7
1	1-S	50	ASP	8.7
1	1-V	166	ALA	8.7
1	1-K	349	GLY	8.7
1	1-S	177	GLY	8.7
1	1-A	350	SER	8.7
1	1-D	60	ILE	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-O	396	LEU	8.7
1	1-H	326	TYR	8.7
1	1-Q	178	GLY	8.6
1	1-F	405	ALA	8.6
1	1-F	397	TYR	8.6
1	1-A	54	ILE	8.6
1	1-P	348	THR	8.6
1	1-E	328	ALA	8.6
1	1-N	328	ALA	8.6
1	1-S	348	THR	8.6
1	1-T	58	GLN	8.6
1	1-F	60	ILE	8.6
1	1-N	179	TYR	8.6
1	1-N	166	ALA	8.5
1	1-X	326	TYR	8.5
1	1-B	59	SER	8.5
1	1-R	395	ASP	8.5
1	1-L	398	GLU	8.5
1	1-J	64	ASP	8.5
1	1-Q	64	ASP	8.5
1	1-J	328	ALA	8.5
1	1-V	396	LEU	8.5
1	1-F	55	ARG	8.5
1	1-O	57	PHE	8.5
1	1-O	62	GLU	8.5
1	1-G	424	ASP	8.4
1	1-J	56	GLY	8.4
1	1-S	406	SER	8.4
1	1-P	60	ILE	8.4
1	1-S	58	GLN	8.4
1	1-E	326	TYR	8.4
1	1-L	326	TYR	8.4
1	1-I	95	PHE	8.4
1	1-R	338	ASN	8.4
1	1-J	61	HIS	8.4
1	1-L	179	TYR	8.4
1	1-H	177	GLY	8.4
1	1-L	56	GLY	8.4
1	1-B	60	ILE	8.3
1	1-S	60	ILE	8.3
1	1-S	396	LEU	8.3
1	1-W	57	PHE	8.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-F	338	ASN	8.3
1	1-F	402	GLU	8.3
1	1-E	59	SER	8.3
1	1-V	350	SER	8.3
1	1-K	95	PHE	8.3
1	1-N	95	PHE	8.3
1	1-W	401	PRO	8.3
1	1-W	350	SER	8.3
1	1-K	327	GLU	8.3
1	1-W	177	GLY	8.3
1	1-W	178	GLY	8.3
1	1-U	326	TYR	8.3
1	1-C	404	ALA	8.3
1	1-A	401	PRO	8.3
1	1-B	94	PRO	8.3
1	1-K	60	ILE	8.2
1	1-H	166	ALA	8.2
1	1-E	350	SER	8.2
1	1-Q	59	SER	8.2
1	1-R	58	GLN	8.2
1	1-J	60	ILE	8.2
1	1-P	166	ALA	8.2
1	1-D	402	GLU	8.2
1	1-X	62	GLU	8.2
1	1-K	54	ILE	8.2
1	1-V	54	ILE	8.2
1	1-F	337	ARG	8.2
1	1-A	402	GLU	8.2
1	1-Q	62	GLU	8.2
1	1-B	53	SER	8.2
1	1-E	95	PHE	8.2
1	1-F	59	SER	8.2
1	1-S	347	ILE	8.2
1	1-L	65	MET	8.2
1	1-G	403	GLU	8.2
1	1-B	177	GLY	8.1
1	1-E	57	PHE	8.1
1	1-B	401	PRO	8.1
1	1-N	326	TYR	8.1
1	1-R	327	GLU	8.1
1	1-F	335	SER	8.1
1	1-P	401	PRO	8.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-W	59	SER	8.1
1	1-S	179	TYR	8.1
1	1-P	424	ASP	8.1
1	1-K	166	ALA	8.1
1	1-J	179	TYR	8.1
1	1-J	326	TYR	8.1
1	1-K	325	GLY	8.1
1	1-L	178	GLY	8.1
1	1-S	325	GLY	8.1
1	1-W	399	LEU	8.1
1	1-R	59	SER	8.1
1	1-C	327	GLU	8.1
1	1-X	55	ARG	8.0
1	1-B	349	GLY	8.0
1	1-D	178	GLY	8.0
1	1-N	56	GLY	8.0
1	1-Q	51	GLY	8.0
1	1-W	351	PRO	8.0
1	1-H	53	SER	8.0
1	1-U	62	GLU	8.0
1	1-D	326	TYR	8.0
1	1-M	325	GLY	8.0
1	1-X	349	GLY	8.0
1	1-V	327	GLU	8.0
1	1-W	504	ASN	8.0
1	1-X	49	PHE	8.0
1	1-I	404	ALA	8.0
1	1-K	350	SER	8.0
1	1-S	405	ALA	8.0
1	1-J	55	ARG	8.0
1	1-F	54	ILE	8.0
1	1-G	402	GLU	8.0
1	1-K	402	GLU	8.0
1	1-H	404	ALA	8.0
1	1-N	60	ILE	7.9
1	1-X	402	GLU	7.9
1	1-R	424	ASP	7.9
1	1-M	53	SER	7.9
1	1-W	338	ASN	7.9
1	1-A	56	GLY	7.9
1	1-K	178	GLY	7.9
1	1-R	177	GLY	7.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-H	62	GLU	7.9
1	1-D	328	ALA	7.9
1	1-V	402	GLU	7.9
1	1-I	63	SER	7.9
1	1-K	55	ARG	7.9
1	1-M	326	TYR	7.9
1	1-A	62	GLU	7.8
1	1-M	398	GLU	7.8
1	1-B	326	TYR	7.8
1	1-L	328	ALA	7.8
1	1-O	179	TYR	7.8
1	1-J	62	GLU	7.8
1	1-F	325	GLY	7.8
1	1-H	176	LYS	7.8
1	1-N	177	GLY	7.8
1	1-R	178	GLY	7.8
1	1-B	58	GLN	7.8
1	1-J	53	SER	7.8
1	1-T	601	THR	7.8
1	1-F	97	LEU	7.8
1	1-U	349	GLY	7.8
1	1-C	328	ALA	7.8
1	1-B	396	LEU	7.8
1	1-E	424	ASP	7.8
1	1-M	62	GLU	7.7
1	1-F	350	SER	7.7
1	1-L	59	SER	7.7
1	1-M	349	GLY	7.7
1	1-F	385	LYS	7.7
1	1-G	57	PHE	7.7
1	1-L	55	ARG	7.7
1	1-N	327	GLU	7.7
1	1-B	179	TYR	7.7
1	1-C	335	SER	7.7
1	1-W	53	SER	7.7
1	1-J	178	GLY	7.7
1	1-V	424	ASP	7.7
1	1-K	405	ALA	7.7
1	1-G	406	SER	7.7
1	1-P	52	SER	7.7
1	1-U	178	GLY	7.7
1	1-H	402	GLU	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-U	95	PHE	7.7
1	1-V	601	THR	7.7
1	1-P	95	PHE	7.6
1	1-D	56	GLY	7.6
1	1-R	179	TYR	7.6
1	1-N	62	GLU	7.6
1	1-W	62	GLU	7.6
1	1-G	504	ASN	7.6
1	1-F	177	GLY	7.6
1	1-M	405	ALA	7.6
1	1-O	401	PRO	7.6
1	1-Q	404	ALA	7.6
1	1-N	58	GLN	7.6
1	1-P	55	ARG	7.6
1	1-P	56	GLY	7.6
1	1-J	327	GLU	7.6
1	1-G	56	GLY	7.6
1	1-O	349	GLY	7.6
1	1-G	60	ILE	7.6
1	1-M	601	THR	7.6
1	1-G	398	GLU	7.6
1	1-I	62	GLU	7.6
1	1-S	403	GLU	7.6
1	1-M	401	PRO	7.5
1	1-S	395	ASP	7.5
1	1-S	208	LYS	7.5
1	1-P	337	ARG	7.5
1	1-G	62	GLU	7.5
1	1-A	283	TYR	7.5
1	1-N	94	PRO	7.5
1	1-P	395	ASP	7.5
1	1-L	58	GLN	7.5
1	1-N	61	HIS	7.5
1	1-M	402	GLU	7.5
1	1-U	327	GLU	7.5
1	1-U	398	GLU	7.5
1	1-G	397	TYR	7.5
1	1-O	94	PRO	7.5
1	1-V	399	LEU	7.5
1	1-F	602	GLU	7.5
1	1-Q	350	SER	7.5
1	1-Q	401	PRO	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-V	179	TYR	7.5
1	1-A	166	ALA	7.5
1	1-K	63	SER	7.5
1	1-R	97	LEU	7.4
1	1-N	398	GLU	7.4
1	1-R	54	ILE	7.4
1	1-X	65	MET	7.4
1	1-A	96	THR	7.4
1	1-B	400	PRO	7.4
1	1-J	94	PRO	7.4
1	1-M	404	ALA	7.4
1	1-E	396	LEU	7.4
1	1-X	397	TYR	7.4
1	1-P	504	ASN	7.4
1	1-K	401	PRO	7.4
1	1-L	351	PRO	7.4
1	1-U	94	PRO	7.4
1	1-G	58	GLN	7.4
1	1-M	396	LEU	7.4
1	1-O	58	GLN	7.4
1	1-R	402	GLU	7.4
1	1-P	338	ASN	7.4
1	1-H	401	PRO	7.4
1	1-F	64	ASP	7.4
1	1-L	399	LEU	7.4
1	1-I	398	GLU	7.4
1	1-W	54	ILE	7.4
1	1-O	63	SER	7.3
1	1-R	350	SER	7.3
1	1-M	395	ASP	7.3
1	1-R	399	LEU	7.3
1	1-B	55	ARG	7.3
1	1-R	385	LYS	7.3
1	1-J	402	GLU	7.3
1	1-S	424	ASP	7.3
1	1-K	177	GLY	7.3
1	1-M	56	GLY	7.3
1	1-S	503	GLY	7.3
1	1-R	397	TYR	7.3
1	1-C	401	PRO	7.3
1	1-E	601	THR	7.3
1	1-R	63	SER	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	395	ASP	7.3
1	1-E	349	GLY	7.3
1	1-S	178	GLY	7.3
1	1-K	62	GLU	7.3
1	1-D	55	ARG	7.3
1	1-S	337	ARG	7.3
1	1-C	95	PHE	7.3
1	1-L	325	GLY	7.3
1	1-D	504	ASN	7.2
1	1-Q	337	ARG	7.2
1	1-L	395	ASP	7.2
1	1-G	503	GLY	7.2
1	1-Q	424	ASP	7.2
1	1-T	177	GLY	7.2
1	1-V	325	GLY	7.2
1	1-X	325	GLY	7.2
1	1-N	57	PHE	7.2
1	1-R	94	PRO	7.2
1	1-I	326	TYR	7.2
1	1-F	52	SER	7.2
1	1-R	64	ASP	7.2
1	1-V	328	ALA	7.2
1	1-E	53	SER	7.2
1	1-L	289	GLY	7.2
1	1-N	287	TYR	7.1
1	1-B	350	SER	7.1
1	1-E	405	ALA	7.1
1	1-R	50	ASP	7.1
1	1-L	62	GLU	7.1
1	1-M	57	PHE	7.1
1	1-N	405	ALA	7.1
1	1-P	50	ASP	7.1
1	1-X	53	SER	7.1
1	1-X	395	ASP	7.1
1	1-V	337	ARG	7.1
1	1-M	97	LEU	7.1
1	1-G	179	TYR	7.1
1	1-R	335	SER	7.1
1	1-C	349	GLY	7.1
1	1-H	57	PHE	7.1
1	1-T	49	PHE	7.1
1	1-P	399	LEU	7.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-O	601	THR	7.1
1	1-B	328	ALA	7.1
1	1-R	328	ALA	7.1
1	1-K	398	GLU	7.1
1	1-C	60	ILE	7.1
1	1-V	57	PHE	7.0
1	1-D	397	TYR	7.0
1	1-J	351	PRO	7.0
1	1-P	179	TYR	7.0
1	1-H	65	MET	7.0
1	1-N	53	SER	7.0
1	1-I	60	ILE	7.0
1	1-F	339	ARG	7.0
1	1-C	94	PRO	7.0
1	1-U	401	PRO	7.0
1	1-J	325	GLY	7.0
1	1-G	55	ARG	7.0
1	1-K	601	THR	7.0
1	1-V	62	GLU	7.0
1	1-I	178	GLY	7.0
1	1-K	49	PHE	7.0
1	1-S	57	PHE	7.0
1	1-C	398	GLU	7.0
1	1-Q	177	GLY	7.0
1	1-U	54	ILE	6.9
1	1-A	179	TYR	6.9
1	1-C	397	TYR	6.9
1	1-N	396	LEU	6.9
1	1-F	395	ASP	6.9
1	1-G	177	GLY	6.9
1	1-X	177	GLY	6.9
1	1-A	326	TYR	6.9
1	1-H	55	ARG	6.9
1	1-C	62	GLU	6.9
1	1-P	412	THR	6.9
1	1-V	404	ALA	6.9
1	1-S	63	SER	6.9
1	1-P	326	TYR	6.9
1	1-L	402	GLU	6.9
1	1-T	402	GLU	6.9
1	1-U	338	ASN	6.9
1	1-X	328	ALA	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-R	337	ARG	6.9
1	1-X	174	ARG	6.9
1	1-T	176	LYS	6.9
1	1-R	326	TYR	6.9
1	1-T	398	GLU	6.9
1	1-R	401	PRO	6.9
1	1-W	64	ASP	6.9
1	1-M	59	SER	6.8
1	1-Q	403	GLU	6.8
1	1-D	177	GLY	6.8
1	1-G	395	ASP	6.8
1	1-A	53	SER	6.8
1	1-C	396	LEU	6.8
1	1-X	403	GLU	6.8
1	1-P	57	PHE	6.8
1	1-F	94	PRO	6.8
1	1-P	58	GLN	6.8
1	1-D	337	ARG	6.8
1	1-R	339	ARG	6.8
1	1-O	328	ALA	6.8
1	1-D	406	SER	6.8
1	1-L	61	HIS	6.8
1	1-L	324	PRO	6.8
1	1-H	208	LYS	6.8
1	1-M	58	GLN	6.8
1	1-M	178	GLY	6.8
1	1-N	382	ILE	6.8
1	1-S	53	SER	6.8
1	1-A	57	PHE	6.8
1	1-B	337	ARG	6.8
1	1-I	58	GLN	6.8
1	1-R	348	THR	6.8
1	1-T	96	THR	6.8
1	1-I	349	GLY	6.7
1	1-V	178	GLY	6.7
1	1-B	97	LEU	6.7
1	1-T	59	SER	6.7
1	1-V	61	HIS	6.7
1	1-N	176	LYS	6.7
1	1-E	58	GLN	6.7
1	1-J	287	TYR	6.7
1	1-R	51	GLY	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-O	395	ASP	6.7
1	1-O	398	GLU	6.7
1	1-S	401	PRO	6.7
1	1-T	287	TYR	6.7
1	1-C	56	GLY	6.7
1	1-E	403	GLU	6.7
1	1-E	61	HIS	6.7
1	1-P	335	SER	6.7
1	1-J	58	GLN	6.7
1	1-Q	601	THR	6.7
1	1-U	283	TYR	6.7
1	1-P	405	ALA	6.7
1	1-C	55	ARG	6.7
1	1-D	401	PRO	6.7
1	1-D	327	GLU	6.6
1	1-P	283	TYR	6.6
1	1-V	401	PRO	6.6
1	1-O	59	SER	6.6
1	1-K	286	THR	6.6
1	1-H	349	GLY	6.6
1	1-U	177	GLY	6.6
1	1-V	56	GLY	6.6
1	1-U	399	LEU	6.6
1	1-P	287	TYR	6.6
1	1-T	55	ARG	6.6
1	1-V	334	TYR	6.6
1	1-D	351	PRO	6.6
1	1-S	327	GLU	6.6
1	1-S	402	GLU	6.6
1	1-E	56	GLY	6.6
1	1-R	56	GLY	6.6
1	1-Q	396	LEU	6.6
1	1-U	60	ILE	6.6
1	1-R	279	ALA	6.6
1	1-S	404	ALA	6.6
1	1-K	64	ASP	6.6
1	1-N	39	ASP	6.6
1	1-F	179	TYR	6.6
1	1-G	400	PRO	6.6
1	1-P	406	SER	6.6
1	1-S	383	LYS	6.6
1	1-V	398	GLU	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	601	THR	6.6
1	1-K	56	GLY	6.6
1	1-R	504	ASN	6.6
1	1-W	56	GLY	6.6
1	1-X	348	THR	6.6
1	1-H	60	ILE	6.6
1	1-Q	399	LEU	6.6
1	1-C	64	ASP	6.6
1	1-I	61	HIS	6.6
1	1-G	283	TYR	6.6
1	1-G	334	TYR	6.6
1	1-F	401	PRO	6.6
1	1-T	65	MET	6.6
1	1-U	350	SER	6.6
1	1-O	55	ARG	6.5
1	1-U	55	ARG	6.5
1	1-X	175	HIS	6.5
1	1-D	405	ALA	6.5
1	1-G	50	ASP	6.5
1	1-W	395	ASP	6.5
1	1-C	59	SER	6.5
1	1-U	57	PHE	6.5
1	1-K	504	ASN	6.5
1	1-V	64	ASP	6.5
1	1-I	59	SER	6.5
1	1-X	59	SER	6.5
1	1-C	61	HIS	6.5
1	1-G	412	THR	6.5
1	1-I	97	LEU	6.5
1	1-J	338	ASN	6.5
1	1-U	329	PRO	6.5
1	1-J	337	ARG	6.5
1	1-L	334	TYR	6.5
1	1-I	327	GLU	6.5
1	1-K	57	PHE	6.5
1	1-O	56	GLY	6.5
1	1-S	349	GLY	6.5
1	1-O	176	LYS	6.5
1	1-B	403	GLU	6.5
1	1-Q	327	GLU	6.5
1	1-D	283	TYR	6.5
1	1-A	335	SER	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-L	382	ILE	6.4
1	1-B	62	GLU	6.4
1	1-M	403	GLU	6.4
1	1-P	98	GLU	6.4
1	1-S	98	GLU	6.4
1	1-D	179	TYR	6.4
1	1-M	283	TYR	6.4
1	1-I	350	SER	6.4
1	1-N	349	GLY	6.4
1	1-X	338	ASN	6.4
1	1-F	328	ALA	6.4
1	1-K	328	ALA	6.4
1	1-L	337	ARG	6.4
1	1-B	398	GLU	6.4
1	1-T	399	LEU	6.4
1	1-N	63	SER	6.4
1	1-W	325	GLY	6.4
1	1-X	58	GLN	6.4
1	1-K	94	PRO	6.4
1	1-D	93	ASP	6.4
1	1-B	325	GLY	6.4
1	1-C	405	ALA	6.4
1	1-E	177	GLY	6.3
1	1-N	49	PHE	6.3
1	1-O	397	TYR	6.3
1	1-K	53	SER	6.3
1	1-K	59	SER	6.3
1	1-Q	53	SER	6.3
1	1-L	401	PRO	6.3
1	1-P	96	THR	6.3
1	1-P	398	GLU	6.3
1	1-Q	395	ASP	6.3
1	1-V	51	GLY	6.3
1	1-E	334	TYR	6.3
1	1-D	335	SER	6.3
1	1-L	53	SER	6.3
1	1-M	350	SER	6.3
1	1-S	52	SER	6.3
1	1-A	269	HIS	6.3
1	1-F	399	LEU	6.3
1	1-I	55	ARG	6.3
1	1-X	66	LEU	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	56	GLY	6.3
1	1-J	602	GLU	6.3
1	1-L	602	GLU	6.3
1	1-Q	398	GLU	6.3
1	1-F	167	ASP	6.3
1	1-R	93	ASP	6.3
1	1-B	399	LEU	6.3
1	1-K	97	LEU	6.3
1	1-W	327	GLU	6.3
1	1-G	59	SER	6.3
1	1-H	63	SER	6.3
1	1-N	59	SER	6.3
1	1-R	410	THR	6.3
1	1-B	424	ASP	6.3
1	1-K	395	ASP	6.3
1	1-V	55	ARG	6.3
1	1-P	49	PHE	6.2
1	1-A	348	THR	6.2
1	1-V	63	SER	6.2
1	1-S	283	TYR	6.2
1	1-A	64	ASP	6.2
1	1-J	412	THR	6.2
1	1-R	384	ASN	6.2
1	1-F	334	TYR	6.2
1	1-G	287	TYR	6.2
1	1-L	397	TYR	6.2
1	1-L	403	GLU	6.2
1	1-M	51	GLY	6.2
1	1-Q	57	PHE	6.2
1	1-T	350	SER	6.2
1	1-W	337	ARG	6.2
1	1-T	97	LEU	6.2
1	1-F	165	GLU	6.2
1	1-S	55	ARG	6.2
1	1-K	338	ASN	6.2
1	1-F	50	ASP	6.2
1	1-F	394	LYS	6.2
1	1-H	398	GLU	6.1
1	1-S	351	PRO	6.1
1	1-O	405	ALA	6.1
1	1-G	63	SER	6.1
1	1-V	52	SER	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-Q	394	LYS	6.1
1	1-F	403	GLU	6.1
1	1-Q	402	GLU	6.1
1	1-X	399	LEU	6.1
1	1-N	325	GLY	6.1
1	1-L	504	ASN	6.1
1	1-D	424	ASP	6.1
1	1-E	395	ASP	6.1
1	1-A	58	GLN	6.1
1	1-O	402	GLU	6.1
1	1-U	402	GLU	6.1
1	1-P	397	TYR	6.1
1	1-V	351	PRO	6.1
1	1-E	337	ARG	6.1
1	1-M	175	HIS	6.1
1	1-M	49	PHE	6.1
1	1-D	601	THR	6.1
1	1-F	279	ALA	6.1
1	1-N	404	ALA	6.1
1	1-A	59	SER	6.1
1	1-E	327	GLU	6.1
1	1-G	98	GLU	6.1
1	1-K	397	TYR	6.1
1	1-H	337	ARG	6.1
1	1-T	61	HIS	6.1
1	1-G	49	PHE	6.1
1	1-J	57	PHE	6.1
1	1-G	404	ALA	6.1
1	1-I	348	THR	6.1
1	1-U	601	THR	6.1
1	1-W	601	THR	6.1
1	1-N	424	ASP	6.1
1	1-U	504	ASN	6.1
1	1-E	335	SER	6.1
1	1-X	335	SER	6.1
1	1-P	65	MET	6.0
1	1-O	61	HIS	6.0
1	1-Q	96	THR	6.0
1	1-A	327	GLU	6.0
1	1-G	393	ASP	6.0
1	1-D	53	SER	6.0
1	1-N	350	SER	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-W	283	TYR	6.0
1	1-B	49	PHE	6.0
1	1-D	412	THR	6.0
1	1-G	602	GLU	6.0
1	1-V	167	ASP	6.0
1	1-X	424	ASP	6.0
1	1-I	399	LEU	6.0
1	1-S	339	ARG	6.0
1	1-I	401	PRO	6.0
1	1-I	325	GLY	6.0
1	1-V	349	GLY	6.0
1	1-J	334	TYR	6.0
1	1-V	283	TYR	6.0
1	1-X	179	TYR	6.0
1	1-B	602	GLU	6.0
1	1-R	398	GLU	6.0
1	1-J	96	THR	6.0
1	1-R	405	ALA	6.0
1	1-B	336	GLN	6.0
1	1-D	395	ASP	6.0
1	1-D	399	LEU	6.0
1	1-G	383	LYS	6.0
1	1-V	176	LYS	6.0
1	1-M	179	TYR	6.0
1	1-W	403	GLU	6.0
1	1-A	424	ASP	5.9
1	1-N	93	ASP	5.9
1	1-N	208	LYS	5.9
1	1-P	93	ASP	5.9
1	1-S	384	ASN	5.9
1	1-C	54	ILE	5.9
1	1-U	174	ARG	5.9
1	1-S	59	SER	5.9
1	1-A	55	ARG	5.9
1	1-J	176	LYS	5.9
1	1-V	287	TYR	5.9
1	1-U	58	GLN	5.9
1	1-X	383	LYS	5.9
1	1-C	97	LEU	5.9
1	1-B	292	ASP	5.9
1	1-T	401	PRO	5.9
1	1-V	93	ASP	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-G	384	ASN	5.9
1	1-L	52	SER	5.9
1	1-Q	345	ILE	5.9
1	1-N	602	GLU	5.9
1	1-R	334	TYR	5.9
1	1-V	397	TYR	5.9
1	1-H	49	PHE	5.9
1	1-I	405	ALA	5.9
1	1-M	293	THR	5.9
1	1-W	328	ALA	5.9
1	1-A	94	PRO	5.9
1	1-C	391	PRO	5.9
1	1-F	384	ASN	5.9
1	1-I	52	SER	5.9
1	1-G	51	GLY	5.9
1	1-S	56	GLY	5.9
1	1-S	413	GLN	5.9
1	1-L	404	ALA	5.8
1	1-U	397	TYR	5.8
1	1-M	424	ASP	5.8
1	1-X	93	ASP	5.8
1	1-B	52	SER	5.8
1	1-U	337	ARG	5.8
1	1-X	337	ARG	5.8
1	1-B	327	GLU	5.8
1	1-F	404	ALA	5.8
1	1-W	94	PRO	5.8
1	1-H	287	TYR	5.8
1	1-D	64	ASP	5.8
1	1-B	335	SER	5.8
1	1-E	289	GLY	5.8
1	1-D	398	GLU	5.8
1	1-E	401	PRO	5.8
1	1-B	95	PHE	5.8
1	1-S	412	THR	5.8
1	1-M	397	TYR	5.8
1	1-P	64	ASP	5.8
1	1-W	397	TYR	5.8
1	1-A	337	ARG	5.8
1	1-G	208	LYS	5.8
1	1-A	403	GLU	5.8
1	1-I	324	PRO	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	175	HIS	5.8
1	1-X	43	PHE	5.8
1	1-G	1	THR	5.8
1	1-K	326	TYR	5.8
1	1-G	327	GLU	5.8
1	1-K	403	GLU	5.8
1	1-D	52	SER	5.8
1	1-J	401	PRO	5.7
1	1-H	405	ALA	5.7
1	1-S	92	HIS	5.7
1	1-I	504	ASN	5.7
1	1-S	504	ASN	5.7
1	1-X	334	TYR	5.7
1	1-G	178	GLY	5.7
1	1-H	350	SER	5.7
1	1-M	65	MET	5.7
1	1-G	401	PRO	5.7
1	1-P	388	PRO	5.7
1	1-P	339	ARG	5.7
1	1-W	175	HIS	5.7
1	1-G	423	ALA	5.7
1	1-U	405	ALA	5.7
1	1-C	57	PHE	5.7
1	1-P	601	THR	5.7
1	1-W	167	ASP	5.7
1	1-L	431	GLY	5.7
1	1-M	63	SER	5.7
1	1-V	53	SER	5.7
1	1-N	383	LYS	5.7
1	1-D	97	LEU	5.7
1	1-L	94	PRO	5.7
1	1-K	175	HIS	5.7
1	1-P	404	ALA	5.7
1	1-D	348	THR	5.7
1	1-E	402	GLU	5.7
1	1-F	327	GLU	5.7
1	1-N	395	ASP	5.7
1	1-Q	293	THR	5.7
1	1-C	289	GLY	5.7
1	1-O	350	SER	5.7
1	1-X	394	LYS	5.7
1	1-P	324	PRO	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-Q	174	ARG	5.7
1	1-W	339	ARG	5.7
1	1-V	602	GLU	5.7
1	1-V	405	ALA	5.7
1	1-R	167	ASP	5.7
1	1-K	283	TYR	5.7
1	1-F	53	SER	5.7
1	1-G	53	SER	5.7
1	1-J	406	SER	5.7
1	1-U	61	HIS	5.6
1	1-X	61	HIS	5.6
1	1-X	351	PRO	5.7
1	1-C	403	GLU	5.6
1	1-K	285	GLU	5.6
1	1-L	93	ASP	5.6
1	1-O	177	GLY	5.6
1	1-T	334	TYR	5.6
1	1-F	406	SER	5.6
1	1-O	351	PRO	5.6
1	1-T	329	PRO	5.6
1	1-J	405	ALA	5.6
1	1-W	405	ALA	5.6
1	1-A	49	PHE	5.6
1	1-I	57	PHE	5.6
1	1-C	395	ASP	5.6
1	1-B	338	ASN	5.6
1	1-O	325	GLY	5.6
1	1-E	55	ARG	5.6
1	1-J	43	PHE	5.6
1	1-P	394	LYS	5.6
1	1-W	49	PHE	5.6
1	1-W	208	LYS	5.6
1	1-K	424	ASP	5.6
1	1-C	58	GLN	5.6
1	1-G	337	ARG	5.6
1	1-Q	382	ILE	5.6
1	1-R	154	ILE	5.6
1	1-B	324	PRO	5.6
1	1-E	175	HIS	5.6
1	1-M	269	HIS	5.6
1	1-M	335	SER	5.6
1	1-F	398	GLU	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	405	ALA	5.6
1	1-G	43	PHE	5.6
1	1-T	336	GLN	5.6
1	1-X	51	GLY	5.6
1	1-V	384	ASN	5.6
1	1-B	269	HIS	5.6
1	1-P	269	HIS	5.6
1	1-Q	66	LEU	5.5
1	1-A	336	GLN	5.5
1	1-H	93	ASP	5.5
1	1-A	97	LEU	5.5
1	1-H	396	LEU	5.5
1	1-H	399	LEU	5.5
1	1-L	327	GLU	5.5
1	1-N	97	LEU	5.5
1	1-U	97	LEU	5.5
1	1-I	397	TYR	5.5
1	1-K	348	THR	5.5
1	1-V	395	ASP	5.5
1	1-W	277	ASP	5.5
1	1-F	154	ILE	5.5
1	1-P	351	PRO	5.5
1	1-T	400	PRO	5.5
1	1-T	403	GLU	5.5
1	1-R	66	LEU	5.5
1	1-V	335	SER	5.5
1	1-I	179	TYR	5.5
1	1-M	337	ARG	5.5
1	1-Q	279	ALA	5.5
1	1-D	50	ASP	5.5
1	1-T	395	ASP	5.5
1	1-C	329	PRO	5.5
1	1-G	52	SER	5.5
1	1-I	287	TYR	5.5
1	1-Q	287	TYR	5.5
1	1-R	287	TYR	5.5
1	1-B	50	ASP	5.5
1	1-C	167	ASP	5.5
1	1-D	57	PHE	5.5
1	1-R	293	THR	5.5
1	1-Q	175	HIS	5.5
1	1-A	176	LYS	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-M	176	LYS	5.5
1	1-X	384	ASN	5.5
1	1-D	65	MET	5.4
1	1-L	406	SER	5.4
1	1-N	335	SER	5.4
1	1-T	53	SER	5.4
1	1-L	283	TYR	5.4
1	1-A	293	THR	5.4
1	1-I	49	PHE	5.4
1	1-J	503	GLY	5.4
1	1-Q	381	GLY	5.4
1	1-N	401	PRO	5.4
1	1-Q	94	PRO	5.4
1	1-X	401	PRO	5.4
1	1-G	174	ARG	5.4
1	1-W	174	ARG	5.4
1	1-D	63	SER	5.4
1	1-G	96	THR	5.4
1	1-T	293	THR	5.4
1	1-T	393	ASP	5.4
1	1-P	329	PRO	5.4
1	1-C	350	SER	5.4
1	1-C	176	LYS	5.4
1	1-T	405	ALA	5.4
1	1-A	93	ASP	5.4
1	1-A	349	GLY	5.4
1	1-B	334	TYR	5.4
1	1-D	98	GLU	5.4
1	1-S	602	GLU	5.4
1	1-X	602	GLU	5.4
1	1-H	96	THR	5.4
1	1-W	348	THR	5.4
1	1-R	55	ARG	5.4
1	1-M	208	LYS	5.4
1	1-B	63	SER	5.4
1	1-V	406	SER	5.4
1	1-E	325	GLY	5.4
1	1-U	51	GLY	5.4
1	1-C	50	ASP	5.4
1	1-N	351	PRO	5.4
1	1-N	391	PRO	5.4
1	1-S	96	THR	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-X	167	ASP	5.4
1	1-C	334	TYR	5.4
1	1-T	337	ARG	5.4
1	1-X	504	ASN	5.3
1	1-D	271	HIS	5.3
1	1-M	406	SER	5.3
1	1-W	335	SER	5.3
1	1-V	289	GLY	5.3
1	1-F	292	ASP	5.3
1	1-H	64	ASP	5.3
1	1-J	44	ASP	5.3
1	1-E	49	PHE	5.3
1	1-A	334	TYR	5.3
1	1-V	97	LEU	5.3
1	1-L	384	ASN	5.3
1	1-L	383	LYS	5.3
1	1-E	336	GLN	5.3
1	1-C	353	ALA	5.3
1	1-G	339	ARG	5.3
1	1-I	337	ARG	5.3
1	1-F	65	MET	5.3
1	1-S	65	MET	5.3
1	1-H	324	PRO	5.3
1	1-J	400	PRO	5.3
1	1-N	324	PRO	5.3
1	1-B	93	ASP	5.3
1	1-H	395	ASP	5.3
1	1-Q	50	ASP	5.3
1	1-U	382	ILE	5.3
1	1-E	397	TYR	5.3
1	1-T	397	TYR	5.3
1	1-R	394	LYS	5.3
1	1-K	404	ALA	5.3
1	1-A	347	ILE	5.3
1	1-D	347	ILE	5.3
1	1-R	382	ILE	5.3
1	1-X	50	ASP	5.3
1	1-F	1	THR	5.3
1	1-D	394	LYS	5.3
1	1-M	334	TYR	5.3
1	1-G	92	HIS	5.3
1	1-H	391	PRO	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-J	404	ALA	5.3
1	1-U	325	GLY	5.3
1	1-P	347	ILE	5.3
1	1-Q	167	ASP	5.3
1	1-S	345	ILE	5.3
1	1-T	64	ASP	5.3
1	1-F	348	THR	5.3
1	1-C	49	PHE	5.2
1	1-A	397	TYR	5.2
1	1-B	287	TYR	5.2
1	1-C	287	TYR	5.2
1	1-R	283	TYR	5.2
1	1-S	334	TYR	5.2
1	1-A	175	HIS	5.2
1	1-D	207	GLU	5.2
1	1-D	339	ARG	5.2
1	1-L	174	ARG	5.2
1	1-N	337	ARG	5.2
1	1-W	602	GLU	5.2
1	1-A	324	PRO	5.2
1	1-J	292	ASP	5.2
1	1-C	173	VAL	5.2
1	1-F	283	TYR	5.2
1	1-H	327	GLU	5.2
1	1-I	402	GLU	5.2
1	1-V	403	GLU	5.2
1	1-B	383	LYS	5.2
1	1-H	400	PRO	5.2
1	1-U	324	PRO	5.2
1	1-F	93	ASP	5.2
1	1-R	292	ASP	5.2
1	1-L	339	ARG	5.2
1	1-L	426	GLU	5.2
1	1-V	426	GLU	5.2
1	1-Q	334	TYR	5.2
1	1-O	289	GLY	5.2
1	1-I	407	ILE	5.2
1	1-F	39	ASP	5.2
1	1-L	50	ASP	5.2
1	1-T	44	ASP	5.2
1	1-U	64	ASP	5.2
1	1-W	424	ASP	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-G	65	MET	5.2
1	1-A	208	LYS	5.2
1	1-V	208	LYS	5.2
1	1-T	94	PRO	5.2
1	1-Q	325	GLY	5.2
1	1-G	347	ILE	5.2
1	1-T	335	SER	5.2
1	1-H	50	ASP	5.1
1	1-S	44	ASP	5.1
1	1-T	208	LYS	5.1
1	1-S	329	PRO	5.1
1	1-L	46	GLY	5.1
1	1-R	390	ALA	5.1
1	1-A	50	ASP	5.1
1	1-E	167	ASP	5.1
1	1-F	174	ARG	5.1
1	1-G	336	GLN	5.1
1	1-N	402	GLU	5.1
1	1-X	327	GLU	5.1
1	1-B	65	MET	5.1
1	1-B	208	LYS	5.1
1	1-K	337	ARG	5.1
1	1-O	60	ILE	5.1
1	1-V	339	ARG	5.1
1	1-Q	52	SER	5.1
1	1-U	406	SER	5.1
1	1-F	49	PHE	5.1
1	1-G	269	HIS	5.1
1	1-T	269	HIS	5.1
1	1-J	504	ASN	5.1
1	1-X	94	PRO	5.1
1	1-B	397	TYR	5.1
1	1-L	287	TYR	5.1
1	1-N	334	TYR	5.1
1	1-J	177	GLY	5.1
1	1-Q	349	GLY	5.1
1	1-L	66	LEU	5.1
1	1-B	167	ASP	5.1
1	1-I	93	ASP	5.1
1	1-P	208	LYS	5.1
1	1-S	176	LYS	5.1
1	1-V	175	HIS	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-D	324	PRO	5.1
1	1-V	94	PRO	5.1
1	1-H	209	GLY	5.1
1	1-O	287	TYR	5.1
1	1-S	500	GLY	5.1
1	1-S	9	ALA	5.1
1	1-E	3	ASP	5.0
1	1-Q	3	ASP	5.0
1	1-T	50	ASP	5.0
1	1-D	59	SER	5.0
1	1-M	348	THR	5.0
1	1-N	504	ASN	5.0
1	1-G	262	GLY	5.0
1	1-H	330	ILE	5.0
1	1-W	292	ASP	5.0
1	1-C	53	SER	5.0
1	1-L	348	THR	5.0
1	1-O	1	THR	5.0
1	1-T	412	THR	5.0
1	1-W	410	THR	5.0
1	1-X	52	SER	5.0
1	1-P	43	PHE	5.0
1	1-W	43	PHE	5.0
1	1-E	208	LYS	5.0
1	1-D	602	GLU	5.0
1	1-T	602	GLU	5.0
1	1-W	404	ALA	5.0
1	1-X	426	GLU	5.0
1	1-I	64	ASP	5.0
1	1-L	424	ASP	5.0
1	1-O	324	PRO	5.0
1	1-Q	339	ARG	5.0
1	1-C	65	MET	5.0
1	1-S	128	ALA	5.0
1	1-J	93	ASP	5.0
1	1-J	395	ASP	5.0
1	1-S	287	TYR	5.0
1	1-S	292	ASP	5.0
1	1-A	338	ASN	5.0
1	1-H	97	LEU	5.0
1	1-T	66	LEU	5.0
1	1-T	349	GLY	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-V	58	GLN	5.0
1	1-D	269	HIS	4.9
1	1-N	279	ALA	4.9
1	1-R	423	ALA	4.9
1	1-E	287	TYR	4.9
1	1-F	287	TYR	4.9
1	1-K	292	ASP	4.9
1	1-J	348	THR	4.9
1	1-M	55	ARG	4.9
1	1-F	324	PRO	4.9
1	1-F	400	PRO	4.9
1	1-H	2	PRO	4.9
1	1-I	338	ASN	4.9
1	1-O	65	MET	4.9
1	1-O	327	GLU	4.9
1	1-P	178	GLY	4.9
1	1-Q	407	ILE	4.9
1	1-O	167	ASP	4.9
1	1-Q	55	ARG	4.9
1	1-E	176	LYS	4.9
1	1-H	601	THR	4.9
1	1-N	397	TYR	4.9
1	1-Q	348	THR	4.9
1	1-R	406	SER	4.9
1	1-E	94	PRO	4.9
1	1-G	324	PRO	4.9
1	1-G	282	MET	4.9
1	1-Q	58	GLN	4.9
1	1-M	44	ASP	4.9
1	1-Q	208	LYS	4.9
1	1-T	93	ASP	4.9
1	1-C	406	SER	4.9
1	1-R	52	SER	4.9
1	1-T	43	PHE	4.9
1	1-U	59	SER	4.9
1	1-G	175	HIS	4.9
1	1-P	51	GLY	4.9
1	1-S	269	HIS	4.9
1	1-P	128	ALA	4.9
1	1-U	328	ALA	4.9
1	1-X	467	ASP	4.9
1	1-J	1	THR	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	59	SER	4.9
1	1-M	207	GLU	4.9
1	1-J	175	HIS	4.9
1	1-Q	61	HIS	4.9
1	1-S	332	LEU	4.9
1	1-T	396	LEU	4.9
1	1-W	97	LEU	4.9
1	1-C	177	GLY	4.9
1	1-J	51	GLY	4.9
1	1-E	345	ILE	4.8
1	1-O	337	ARG	4.8
1	1-S	423	ALA	4.8
1	1-H	424	ASP	4.8
1	1-N	393	ASP	4.8
1	1-X	45	ASP	4.8
1	1-E	293	THR	4.8
1	1-G	99	PRO	4.8
1	1-M	94	PRO	4.8
1	1-M	351	PRO	4.8
1	1-D	49	PHE	4.8
1	1-I	334	TYR	4.8
1	1-J	426	GLU	4.8
1	1-T	327	GLU	4.8
1	1-D	413	GLN	4.8
1	1-A	504	ASN	4.8
1	1-B	176	LYS	4.8
1	1-H	339	ARG	4.8
1	1-J	174	ARG	4.8
1	1-M	174	ARG	4.8
1	1-T	383	LYS	4.8
1	1-B	329	PRO	4.8
1	1-B	391	PRO	4.8
1	1-W	388	PRO	4.8
1	1-B	129	GLU	4.8
1	1-M	602	GLU	4.8
1	1-V	387	GLU	4.8
1	1-K	335	SER	4.8
1	1-P	117	SER	4.8
1	1-A	396	LEU	4.8
1	1-C	399	LEU	4.8
1	1-D	173	VAL	4.8
1	1-H	61	HIS	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-N	269	HIS	4.8
1	1-J	339	ARG	4.8
1	1-O	504	ASN	4.8
1	1-S	174	ARG	4.8
1	1-V	177	GLY	4.8
1	1-G	388	PRO	4.8
1	1-U	400	PRO	4.8
1	1-G	286	THR	4.8
1	1-I	601	THR	4.8
1	1-W	426	GLU	4.8
1	1-C	63	SER	4.8
1	1-E	43	PHE	4.8
1	1-F	175	HIS	4.8
1	1-O	97	LEU	4.8
1	1-N	50	ASP	4.8
1	1-P	467	ASP	4.8
1	1-R	403	GLU	4.8
1	1-S	293	THR	4.8
1	1-S	49	PHE	4.8
1	1-M	399	LEU	4.8
1	1-O	399	LEU	4.8
1	1-Q	406	SER	4.8
1	1-H	203	GLY	4.7
1	1-J	397	TYR	4.8
1	1-M	287	TYR	4.8
1	1-N	289	GLY	4.7
1	1-S	262	GLY	4.7
1	1-J	324	PRO	4.7
1	1-A	602	GLU	4.7
1	1-E	398	GLU	4.7
1	1-R	602	GLU	4.7
1	1-S	167	ASP	4.7
1	1-T	424	ASP	4.7
1	1-R	176	LYS	4.7
1	1-C	1	THR	4.7
1	1-F	413	GLN	4.7
1	1-J	269	HIS	4.7
1	1-C	52	SER	4.7
1	1-H	338	ASN	4.7
1	1-O	500	GLY	4.7
1	1-H	334	TYR	4.7
1	1-K	334	TYR	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	382	ILE	4.7
1	1-X	382	ILE	4.7
1	1-C	288	ALA	4.7
1	1-J	387	GLU	4.7
1	1-N	426	GLU	4.7
1	1-R	324	PRO	4.7
1	1-M	383	LYS	4.7
1	1-Q	383	LYS	4.7
1	1-R	208	LYS	4.7
1	1-W	393	ASP	4.7
1	1-I	96	THR	4.7
1	1-K	43	PHE	4.7
1	1-O	53	SER	4.7
1	1-A	177	GLY	4.7
1	1-K	503	GLY	4.7
1	1-I	347	ILE	4.7
1	1-J	283	TYR	4.7
1	1-N	283	TYR	4.7
1	1-A	400	PRO	4.7
1	1-B	385	LYS	4.7
1	1-B	402	GLU	4.7
1	1-J	398	GLU	4.7
1	1-E	393	ASP	4.7
1	1-K	50	ASP	4.7
1	1-N	292	ASP	4.7
1	1-O	93	ASP	4.7
1	1-N	412	THR	4.7
1	1-C	392	VAL	4.7
1	1-C	325	GLY	4.7
1	1-T	51	GLY	4.7
1	1-A	382	ILE	4.7
1	1-B	386	ILE	4.7
1	1-M	382	ILE	4.7
1	1-X	347	ILE	4.7
1	1-U	65	MET	4.7
1	1-X	287	TYR	4.7
1	1-R	387	GLU	4.7
1	1-W	207	GLU	4.7
1	1-L	344	ARG	4.7
1	1-V	269	HIS	4.7
1	1-X	293	THR	4.7
1	1-J	97	LEU	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-G	173	VAL	4.6
1	1-B	51	GLY	4.6
1	1-H	406	SER	4.6
1	1-J	335	SER	4.6
1	1-R	386	ILE	4.6
1	1-I	94	PRO	4.6
1	1-S	324	PRO	4.6
1	1-E	348	THR	4.6
1	1-J	49	PHE	4.6
1	1-R	43	PHE	4.6
1	1-H	503	GLY	4.6
1	1-G	117	SER	4.6
1	1-J	65	MET	4.6
1	1-C	402	GLU	4.6
1	1-M	285	GLU	4.6
1	1-R	420	ARG	4.6
1	1-D	400	PRO	4.6
1	1-D	404	ALA	4.6
1	1-M	279	ALA	4.6
1	1-Q	171	TYR	4.6
1	1-N	175	HIS	4.6
1	1-D	96	THR	4.6
1	1-N	293	THR	4.6
1	1-W	293	THR	4.6
1	1-W	332	LEU	4.6
1	1-A	65	MET	4.6
1	1-E	65	MET	4.6
1	1-F	127	GLY	4.6
1	1-X	431	GLY	4.6
1	1-C	338	ASN	4.6
1	1-E	602	GLU	4.6
1	1-G	273	SER	4.6
1	1-I	335	SER	4.6
1	1-I	329	PRO	4.6
1	1-I	388	PRO	4.6
1	1-U	351	PRO	4.6
1	1-H	397	TYR	4.6
1	1-P	413	GLN	4.6
1	1-K	44	ASP	4.6
1	1-B	293	THR	4.6
1	1-C	339	ARG	4.6
1	1-K	262	GLY	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	503	GLY	4.6
1	1-E	407	ILE	4.6
1	1-K	154	ILE	4.6
1	1-F	329	PRO	4.6
1	1-L	388	PRO	4.6
1	1-E	269	HIS	4.6
1	1-H	336	GLN	4.6
1	1-R	413	GLN	4.6
1	1-C	93	ASP	4.6
1	1-G	292	ASP	4.6
1	1-F	293	THR	4.6
1	1-M	420	ARG	4.5
1	1-N	420	ARG	4.5
1	1-W	98	GLU	4.5
1	1-W	165	GLU	4.5
1	1-M	324	PRO	4.5
1	1-B	405	ALA	4.5
1	1-N	288	ALA	4.5
1	1-X	279	ALA	4.5
1	1-U	394	LYS	4.5
1	1-W	394	LYS	4.5
1	1-P	44	ASP	4.5
1	1-U	334	TYR	4.5
1	1-U	395	ASP	4.5
1	1-A	207	GLU	4.5
1	1-E	426	GLU	4.5
1	1-Q	426	GLU	4.5
1	1-Q	289	GLY	4.5
1	1-H	94	PRO	4.5
1	1-U	53	SER	4.5
1	1-O	175	HIS	4.5
1	1-D	423	ALA	4.5
1	1-V	279	ALA	4.5
1	1-O	208	LYS	4.5
1	1-I	66	LEU	4.5
1	1-S	284	ASP	4.5
1	1-E	171	TYR	4.5
1	1-E	339	ARG	4.5
1	1-R	174	ARG	4.5
1	1-J	285	GLU	4.5
1	1-S	289	GLY	4.5
1	1-U	49	PHE	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-F	382	ILE	4.5
1	1-W	400	PRO	4.5
1	1-R	53	SER	4.5
1	1-T	504	ASN	4.5
1	1-V	504	ASN	4.5
1	1-N	10	LYS	4.5
1	1-R	128	ALA	4.5
1	1-R	163	ALA	4.5
1	1-C	174	ARG	4.5
1	1-P	174	ARG	4.5
1	1-X	283	TYR	4.5
1	1-J	127	GLY	4.5
1	1-I	120	ILE	4.5
1	1-K	330	ILE	4.5
1	1-P	425	HIS	4.5
1	1-U	175	HIS	4.5
1	1-W	271	HIS	4.5
1	1-H	59	SER	4.5
1	1-N	41	SER	4.5
1	1-A	404	ALA	4.5
1	1-L	48	ALA	4.5
1	1-L	279	ALA	4.5
1	1-B	395	ASP	4.5
1	1-G	277	ASP	4.5
1	1-O	64	ASP	4.5
1	1-U	424	ASP	4.5
1	1-P	602	GLU	4.5
1	1-M	1	THR	4.4
1	1-R	1	THR	4.4
1	1-E	381	GLY	4.4
1	1-R	503	GLY	4.4
1	1-D	176	LYS	4.4
1	1-Q	40	LYS	4.4
1	1-T	175	HIS	4.4
1	1-G	413	GLN	4.4
1	1-A	406	SER	4.4
1	1-E	101	SER	4.4
1	1-L	117	SER	4.4
1	1-N	399	LEU	4.4
1	1-K	207	GLU	4.4
1	1-C	601	THR	4.4
1	1-V	293	THR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-J	289	GLY	4.4
1	1-M	177	GLY	4.4
1	1-S	127	GLY	4.4
1	1-G	91	VAL	4.4
1	1-H	269	HIS	4.4
1	1-J	388	PRO	4.4
1	1-K	388	PRO	4.4
1	1-R	269	HIS	4.4
1	1-R	351	PRO	4.4
1	1-V	49	PHE	4.4
1	1-E	504	ASN	4.4
1	1-J	399	LEU	4.4
1	1-X	332	LEU	4.4
1	1-A	167	ASP	4.4
1	1-W	383	LYS	4.4
1	1-X	412	THR	4.4
1	1-G	329	PRO	4.4
1	1-H	289	GLY	4.4
1	1-I	400	PRO	4.4
1	1-O	329	PRO	4.4
1	1-R	262	GLY	4.4
1	1-Q	269	HIS	4.4
1	1-V	388	PRO	4.4
1	1-C	345	ILE	4.4
1	1-D	334	TYR	4.4
1	1-S	333	VAL	4.4
1	1-O	49	PHE	4.4
1	1-M	504	ASN	4.4
1	1-S	353	ALA	4.4
1	1-X	68	LEU	4.4
1	1-B	98	GLU	4.4
1	1-A	365	GLY	4.4
1	1-G	296	HIS	4.4
1	1-J	278	GLY	4.4
1	1-S	286	THR	4.4
1	1-Q	329	PRO	4.4
1	1-E	382	ILE	4.4
1	1-J	347	ILE	4.4
1	1-N	154	ILE	4.4
1	1-C	337	ARG	4.4
1	1-B	384	ASN	4.4
1	1-A	279	ALA	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	291	SER	4.4
1	1-I	279	ALA	4.4
1	1-T	63	SER	4.4
1	1-D	426	GLU	4.4
1	1-G	72	GLU	4.4
1	1-H	379	LEU	4.4
1	1-U	207	GLU	4.4
1	1-E	467	ASP	4.4
1	1-K	324	PRO	4.3
1	1-B	413	GLN	4.3
1	1-M	43	PHE	4.3
1	1-P	297	TYR	4.3
1	1-A	384	ASN	4.3
1	1-G	387	GLU	4.3
1	1-M	183	ALA	4.3
1	1-M	332	LEU	4.3
1	1-S	285	GLU	4.3
1	1-I	208	LYS	4.3
1	1-Q	335	SER	4.3
1	1-U	332	LEU	4.3
1	1-H	167	ASP	4.3
1	1-V	467	ASP	4.3
1	1-W	44	ASP	4.3
1	1-P	420	ARG	4.3
1	1-W	324	PRO	4.3
1	1-V	412	THR	4.3
1	1-W	96	THR	4.3
1	1-A	386	ILE	4.3
1	1-D	345	ILE	4.3
1	1-N	333	VAL	4.3
1	1-I	176	LYS	4.3
1	1-N	403	GLU	4.3
1	1-S	352	LYS	4.3
1	1-R	175	HIS	4.3
1	1-U	339	ARG	4.3
1	1-X	324	PRO	4.3
1	1-Q	413	GLN	4.3
1	1-U	348	THR	4.3
1	1-M	330	ILE	4.3
1	1-P	154	ILE	4.3
1	1-O	173	VAL	4.3
1	1-U	384	ASN	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-Q	305	ALA	4.3
1	1-I	53	SER	4.3
1	1-V	340	SER	4.3
1	1-A	339	ARG	4.3
1	1-T	174	ARG	4.3
1	1-U	391	PRO	4.3
1	1-I	127	GLY	4.3
1	1-E	347	ILE	4.3
1	1-K	603	LYS	4.3
1	1-K	208	LYS	4.3
1	1-N	43	PHE	4.3
1	1-T	207	GLU	4.3
1	1-O	334	TYR	4.3
1	1-X	404	ALA	4.3
1	1-B	406	SER	4.3
1	1-D	359	ARG	4.3
1	1-G	355	ARG	4.3
1	1-O	52	SER	4.3
1	1-O	339	ARG	4.3
1	1-U	344	ARG	4.3
1	1-H	51	GLY	4.2
1	1-A	330	ILE	4.2
1	1-D	208	LYS	4.2
1	1-J	286	THR	4.2
1	1-R	165	GLU	4.2
1	1-S	12	GLU	4.2
1	1-F	66	LEU	4.2
1	1-L	332	LEU	4.2
1	1-L	353	ALA	4.2
1	1-O	338	ASN	4.2
1	1-T	283	TYR	4.2
1	1-U	287	TYR	4.2
1	1-X	48	ALA	4.2
1	1-N	339	ARG	4.2
1	1-P	340	SER	4.2
1	1-I	424	ASP	4.2
1	1-L	167	ASP	4.2
1	1-O	50	ASP	4.2
1	1-T	324	PRO	4.2
1	1-L	381	GLY	4.2
1	1-R	345	ILE	4.2
1	1-V	154	ILE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-W	398	GLU	4.2
1	1-V	43	PHE	4.2
1	1-T	359	ARG	4.2
1	1-K	48	ALA	4.2
1	1-Q	338	ASN	4.2
1	1-T	338	ASN	4.2
1	1-U	404	ALA	4.2
1	1-N	52	SER	4.2
1	1-O	406	SER	4.2
1	1-F	388	PRO	4.2
1	1-C	424	ASP	4.2
1	1-E	413	GLN	4.2
1	1-M	93	ASP	4.2
1	1-W	176	LYS	4.2
1	1-D	1	THR	4.2
1	1-H	1	THR	4.2
1	1-J	382	ILE	4.2
1	1-O	412	THR	4.2
1	1-P	345	ILE	4.2
1	1-R	330	ILE	4.2
1	1-P	327	GLU	4.2
1	1-W	412	THR	4.2
1	1-K	206	LEU	4.2
1	1-N	290	LEU	4.2
1	1-P	344	ARG	4.2
1	1-O	279	ALA	4.2
1	1-D	175	HIS	4.2
1	1-D	329	PRO	4.2
1	1-D	352	LYS	4.2
1	1-I	351	PRO	4.2
1	1-K	383	LYS	4.2
1	1-N	385	LYS	4.2
1	1-P	99	PRO	4.2
1	1-W	501	SER	4.2
1	1-X	329	PRO	4.2
1	1-G	167	ASP	4.2
1	1-L	45	ASP	4.2
1	1-S	3	ASP	4.2
1	1-T	389	GLN	4.2
1	1-A	127	GLY	4.2
1	1-O	262	GLY	4.2
1	1-G	165	GLU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-M	72	GLU	4.2
1	1-M	96	THR	4.2
1	1-O	96	THR	4.2
1	1-K	468	VAL	4.2
1	1-Q	333	VAL	4.2
1	1-I	420	ARG	4.2
1	1-K	420	ARG	4.2
1	1-U	420	ARG	4.2
1	1-L	6	PHE	4.2
1	1-B	288	ALA	4.2
1	1-I	269	HIS	4.2
1	1-L	37	ALA	4.2
1	1-L	269	HIS	4.2
1	1-N	65	MET	4.2
1	1-Q	288	ALA	4.2
1	1-W	353	ALA	4.2
1	1-G	391	PRO	4.1
1	1-P	63	SER	4.1
1	1-Q	283	TYR	4.1
1	1-Q	397	TYR	4.1
1	1-W	406	SER	4.1
1	1-G	44	ASP	4.1
1	1-M	327	GLU	4.1
1	1-U	426	GLU	4.1
1	1-O	345	ILE	4.1
1	1-E	96	THR	4.1
1	1-O	410	THR	4.1
1	1-N	174	ARG	4.1
1	1-F	43	PHE	4.1
1	1-A	383	LYS	4.1
1	1-D	385	LYS	4.1
1	1-G	603	LYS	4.1
1	1-L	176	LYS	4.1
1	1-P	383	LYS	4.1
1	1-N	338	ASN	4.1
1	1-D	336	GLN	4.1
1	1-B	393	ASP	4.1
1	1-C	283	TYR	4.1
1	1-K	287	TYR	4.1
1	1-P	53	SER	4.1
1	1-U	44	ASP	4.1
1	1-A	262	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-I	98	GLU	4.1
1	1-C	420	ARG	4.1
1	1-X	339	ARG	4.1
1	1-X	344	ARG	4.1
1	1-I	1	THR	4.1
1	1-L	286	THR	4.1
1	1-C	394	LYS	4.1
1	1-Q	176	LYS	4.1
1	1-A	288	ALA	4.1
1	1-G	353	ALA	4.1
1	1-K	391	PRO	4.1
1	1-M	336	GLN	4.1
1	1-N	280	PRO	4.1
1	1-T	99	PRO	4.1
1	1-V	324	PRO	4.1
1	1-H	403	GLU	4.1
1	1-L	285	GLU	4.1
1	1-Q	101	SER	4.1
1	1-U	63	SER	4.1
1	1-H	46	GLY	4.1
1	1-R	297	TYR	4.1
1	1-T	381	GLY	4.1
1	1-W	334	TYR	4.1
1	1-F	412	THR	4.1
1	1-G	293	THR	4.1
1	1-V	348	THR	4.1
1	1-E	42	VAL	4.1
1	1-L	394	LYS	4.1
1	1-V	383	LYS	4.1
1	1-D	296	HIS	4.1
1	1-L	175	HIS	4.1
1	1-N	336	GLN	4.1
1	1-N	384	ASN	4.1
1	1-V	336	GLN	4.1
1	1-M	426	GLU	4.1
1	1-Q	72	GLU	4.1
1	1-B	3	ASP	4.1
1	1-F	63	SER	4.1
1	1-G	420	ARG	4.1
1	1-I	262	GLY	4.1
1	1-K	339	ARG	4.1
1	1-W	51	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	385	LYS	4.1
1	1-B	1	THR	4.1
1	1-C	410	THR	4.1
1	1-N	96	THR	4.1
1	1-O	42	VAL	4.1
1	1-R	271	HIS	4.1
1	1-J	280	PRO	4.0
1	1-R	404	ALA	4.0
1	1-T	163	ALA	4.0
1	1-U	388	PRO	4.0
1	1-D	285	GLU	4.0
1	1-R	129	GLU	4.0
1	1-K	174	ARG	4.0
1	1-D	167	ASP	4.0
1	1-F	386	ILE	4.0
1	1-T	382	ILE	4.0
1	1-U	330	ILE	4.0
1	1-D	293	THR	4.0
1	1-K	410	THR	4.0
1	1-Q	65	MET	4.0
1	1-V	92	HIS	4.0
1	1-C	413	GLN	4.0
1	1-F	336	GLN	4.0
1	1-M	400	PRO	4.0
1	1-Q	324	PRO	4.0
1	1-B	339	ARG	4.0
1	1-E	174	ARG	4.0
1	1-E	285	GLU	4.0
1	1-X	285	GLU	4.0
1	1-E	394	LYS	4.0
1	1-F	51	GLY	4.0
1	1-H	284	ASP	4.0
1	1-H	393	ASP	4.0
1	1-M	167	ASP	4.0
1	1-N	394	LYS	4.0
1	1-R	467	ASP	4.0
1	1-X	39	ASP	4.0
1	1-K	117	SER	4.0
1	1-K	345	ILE	4.0
1	1-Q	117	SER	4.0
1	1-S	117	SER	4.0
1	1-C	412	THR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-K	412	THR	4.0
1	1-N	206	LEU	4.0
1	1-Q	290	LEU	4.0
1	1-W	1	THR	4.0
1	1-W	287	TYR	4.0
1	1-M	392	VAL	4.0
1	1-Q	392	VAL	4.0
1	1-O	413	GLN	4.0
1	1-Q	49	PHE	4.0
1	1-T	388	PRO	4.0
1	1-B	165	GLU	4.0
1	1-F	387	GLU	4.0
1	1-I	328	ALA	4.0
1	1-R	72	GLU	4.0
1	1-V	338	ASN	4.0
1	1-G	394	LYS	4.0
1	1-L	127	GLY	4.0
1	1-M	127	GLY	4.0
1	1-Q	292	ASP	4.0
1	1-O	335	SER	4.0
1	1-A	1	THR	4.0
1	1-D	123	THR	4.0
1	1-B	392	VAL	4.0
1	1-A	174	ARG	4.0
1	1-D	187	GLN	4.0
1	1-D	388	PRO	4.0
1	1-X	400	PRO	4.0
1	1-C	602	GLU	4.0
1	1-O	165	GLU	4.0
1	1-M	394	LYS	4.0
1	1-O	404	ALA	4.0
1	1-K	222	ASN	4.0
1	1-Q	504	ASN	4.0
1	1-B	127	GLY	4.0
1	1-J	167	ASP	4.0
1	1-L	467	ASP	4.0
1	1-U	93	ASP	4.0
1	1-W	503	GLY	4.0
1	1-X	262	GLY	4.0
1	1-W	154	ILE	4.0
1	1-H	335	SER	4.0
1	1-J	52	SER	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-R	92	HIS	4.0
1	1-E	399	LEU	4.0
1	1-R	96	THR	4.0
1	1-U	1	THR	4.0
1	1-G	323	VAL	4.0
1	1-J	173	VAL	4.0
1	1-M	339	ARG	4.0
1	1-O	426	GLU	3.9
1	1-Q	388	PRO	4.0
1	1-Q	400	PRO	4.0
1	1-W	329	PRO	4.0
1	1-X	413	GLN	4.0
1	1-C	207	GLU	3.9
1	1-G	129	GLU	3.9
1	1-X	165	GLU	3.9
1	1-E	40	LYS	3.9
1	1-E	288	ALA	3.9
1	1-F	353	ALA	3.9
1	1-F	504	ASN	3.9
1	1-B	64	ASP	3.9
1	1-E	282	MET	3.9
1	1-H	44	ASP	3.9
1	1-R	282	MET	3.9
1	1-S	282	MET	3.9
1	1-P	330	ILE	3.9
1	1-V	345	ILE	3.9
1	1-H	175	HIS	3.9
1	1-A	286	THR	3.9
1	1-H	293	THR	3.9
1	1-J	392	VAL	3.9
1	1-R	91	VAL	3.9
1	1-G	352	LYS	3.9
1	1-G	426	GLU	3.9
1	1-N	98	GLU	3.9
1	1-P	400	PRO	3.9
1	1-S	99	PRO	3.9
1	1-R	225	PHE	3.9
1	1-D	128	ALA	3.9
1	1-E	384	ASN	3.9
1	1-R	264	ASN	3.9
1	1-A	503	GLY	3.9
1	1-G	381	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-X	503	GLY	3.9
1	1-U	292	ASP	3.9
1	1-I	92	HIS	3.9
1	1-N	425	HIS	3.9
1	1-F	273	SER	3.9
1	1-Q	97	LEU	3.9
1	1-T	501	SER	3.9
1	1-B	420	ARG	3.9
1	1-C	293	THR	3.9
1	1-L	293	THR	3.9
1	1-N	429	THR	3.9
1	1-C	351	PRO	3.9
1	1-E	391	PRO	3.9
1	1-O	391	PRO	3.9
1	1-R	400	PRO	3.9
1	1-S	323	VAL	3.9
1	1-T	333	VAL	3.9
1	1-L	128	ALA	3.9
1	1-D	262	GLY	3.9
1	1-G	64	ASP	3.9
1	1-T	345	ILE	3.9
1	1-X	3	ASP	3.9
1	1-S	66	LEU	3.9
1	1-X	97	LEU	3.9
1	1-I	406	SER	3.9
1	1-J	63	SER	3.9
1	1-K	406	SER	3.9
1	1-P	176	LYS	3.9
1	1-E	1	THR	3.9
1	1-O	293	THR	3.9
1	1-T	286	THR	3.9
1	1-F	351	PRO	3.9
1	1-G	333	VAL	3.9
1	1-V	171	TYR	3.9
1	1-B	43	PHE	3.9
1	1-H	6	PHE	3.9
1	1-J	48	ALA	3.9
1	1-L	43	PHE	3.9
1	1-C	282	MET	3.9
1	1-N	37	ALA	3.9
1	1-B	504	ASN	3.9
1	1-P	384	ASN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-Q	384	ASN	3.9
1	1-H	365	GLY	3.9
1	1-A	292	ASP	3.9
1	1-M	393	ASP	3.9
1	1-N	167	ASP	3.9
1	1-U	386	ILE	3.9
1	1-V	344	ARG	3.9
1	1-G	176	LYS	3.9
1	1-O	40	LYS	3.9
1	1-C	285	GLU	3.9
1	1-H	602	GLU	3.9
1	1-K	426	GLU	3.9
1	1-R	98	GLU	3.9
1	1-S	387	GLU	3.9
1	1-V	391	PRO	3.9
1	1-G	42	VAL	3.9
1	1-X	91	VAL	3.9
1	1-H	283	TYR	3.8
1	1-M	377	ALA	3.8
1	1-P	334	TYR	3.8
1	1-B	262	GLY	3.8
1	1-M	500	GLY	3.8
1	1-W	384	ASN	3.8
1	1-A	393	ASP	3.8
1	1-C	154	ILE	3.8
1	1-C	382	ILE	3.8
1	1-K	176	LYS	3.8
1	1-N	355	ARG	3.8
1	1-K	284	ASP	3.8
1	1-P	167	ASP	3.8
1	1-R	393	ASP	3.8
1	1-U	407	ILE	3.8
1	1-W	39	ASP	3.8
1	1-A	98	GLU	3.8
1	1-C	129	GLU	3.8
1	1-P	426	GLU	3.8
1	1-L	336	GLN	3.8
1	1-L	280	PRO	3.8
1	1-T	351	PRO	3.8
1	1-R	286	THR	3.8
1	1-L	323	VAL	3.8
1	1-P	423	ALA	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-I	339	ARG	3.8
1	1-G	431	GLY	3.8
1	1-K	7	LYS	3.8
1	1-S	271	HIS	3.8
1	1-S	344	ARG	3.8
1	1-N	381	GLY	3.8
1	1-F	345	ILE	3.8
1	1-T	407	ILE	3.8
1	1-L	68	LEU	3.8
1	1-N	66	LEU	3.8
1	1-U	413	GLN	3.8
1	1-P	155	SER	3.8
1	1-X	406	SER	3.8
1	1-O	348	THR	3.8
1	1-U	410	THR	3.8
1	1-K	323	VAL	3.8
1	1-A	43	PHE	3.8
1	1-C	208	LYS	3.8
1	1-M	163	ALA	3.8
1	1-O	383	LYS	3.8
1	1-P	225	PHE	3.8
1	1-U	130	ALA	3.8
1	1-W	295	ARG	3.8
1	1-C	347	ILE	3.8
1	1-D	154	ILE	3.8
1	1-U	154	ILE	3.8
1	1-E	281	LEU	3.8
1	1-I	602	GLU	3.8
1	1-N	332	LEU	3.8
1	1-Q	98	GLU	3.8
1	1-S	206	LEU	3.8
1	1-Q	336	GLN	3.8
1	1-E	400	PRO	3.8
1	1-V	400	PRO	3.8
1	1-G	155	SER	3.8
1	1-L	335	SER	3.8
1	1-R	501	SER	3.8
1	1-V	392	VAL	3.8
1	1-G	344	ARG	3.8
1	1-O	420	ARG	3.8
1	1-P	603	LYS	3.8
1	1-G	279	ALA	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-H	128	ALA	3.8
1	1-O	269	HIS	3.8
1	1-P	271	HIS	3.8
1	1-W	279	ALA	3.8
1	1-V	500	GLY	3.8
1	1-H	384	ASN	3.8
1	1-N	285	GLU	3.8
1	1-S	426	GLU	3.8
1	1-U	403	GLU	3.8
1	1-O	380	ASP	3.8
1	1-Q	39	ASP	3.8
1	1-Q	393	ASP	3.8
1	1-V	292	ASP	3.8
1	1-O	306	PRO	3.8
1	1-W	280	PRO	3.8
1	1-V	65	MET	3.8
1	1-Q	1	THR	3.7
1	1-R	273	SER	3.7
1	1-D	383	LYS	3.7
1	1-H	40	LYS	3.7
1	1-I	394	LYS	3.7
1	1-E	270	CYS	3.7
1	1-B	425	HIS	3.7
1	1-L	271	HIS	3.7
1	1-H	43	PHE	3.7
1	1-X	288	ALA	3.7
1	1-T	46	GLY	3.7
1	1-J	72	GLU	3.7
1	1-U	179	TYR	3.7
1	1-W	345	ILE	3.7
1	1-H	292	ASP	3.7
1	1-N	409	GLN	3.7
1	1-V	3	ASP	3.7
1	1-Q	502	PRO	3.7
1	1-R	329	PRO	3.7
1	1-B	410	THR	3.7
1	1-F	410	THR	3.7
1	1-H	412	THR	3.7
1	1-I	392	VAL	3.7
1	1-M	52	SER	3.7
1	1-N	1	THR	3.7
1	1-P	286	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-R	412	THR	3.7
1	1-X	269	HIS	3.7
1	1-R	305	ALA	3.7
1	1-R	49	PHE	3.7
1	1-H	98	GLU	3.7
1	1-P	365	GLY	3.7
1	1-Q	602	GLU	3.7
1	1-U	500	GLY	3.7
1	1-X	15	GLU	3.7
1	1-A	399	LEU	3.7
1	1-D	330	ILE	3.7
1	1-L	67	LEU	3.7
1	1-L	413	GLN	3.7
1	1-E	292	ASP	3.7
1	1-S	277	ASP	3.7
1	1-H	306	PRO	3.7
1	1-U	208	LYS	3.7
1	1-T	52	SER	3.7
1	1-V	288	ALA	3.7
1	1-A	72	GLU	3.7
1	1-F	342	CYS	3.7
1	1-O	403	GLU	3.7
1	1-Q	270	CYS	3.7
1	1-X	129	GLU	3.7
1	1-G	500	GLY	3.7
1	1-K	51	GLY	3.7
1	1-C	290	LEU	3.7
1	1-G	154	ILE	3.7
1	1-G	330	ILE	3.7
1	1-G	332	LEU	3.7
1	1-H	332	LEU	3.7
1	1-L	290	LEU	3.7
1	1-T	409	GLN	3.7
1	1-W	221	ILE	3.7
1	1-G	264	ASN	3.7
1	1-J	384	ASN	3.7
1	1-E	44	ASP	3.7
1	1-O	424	ASP	3.7
1	1-V	280	PRO	3.7
1	1-W	4	ASP	3.7
1	1-W	391	PRO	3.7
1	1-B	10	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-F	10	LYS	3.7
1	1-G	100	TYR	3.7
1	1-A	420	ARG	3.7
1	1-H	174	ARG	3.7
1	1-R	344	ARG	3.7
1	1-G	392	VAL	3.7
1	1-P	429	THR	3.7
1	1-F	269	HIS	3.7
1	1-O	92	HIS	3.7
1	1-U	52	SER	3.7
1	1-E	207	GLU	3.7
1	1-X	377	ALA	3.7
1	1-C	300	GLY	3.7
1	1-D	43	PHE	3.7
1	1-U	127	GLY	3.7
1	1-X	289	GLY	3.7
1	1-C	270	CYS	3.7
1	1-D	332	LEU	3.7
1	1-S	187	GLN	3.7
1	1-W	347	ILE	3.7
1	1-C	504	ASN	3.7
1	1-D	603	LYS	3.7
1	1-K	394	LYS	3.7
1	1-L	208	LYS	3.7
1	1-M	338	ASN	3.7
1	1-N	264	ASN	3.7
1	1-W	352	LYS	3.7
1	1-E	388	PRO	3.7
1	1-Q	467	ASP	3.7
1	1-S	355	ARG	3.7
1	1-V	174	ARG	3.7
1	1-D	287	TYR	3.7
1	1-C	96	THR	3.6
1	1-C	269	HIS	3.6
1	1-D	425	HIS	3.6
1	1-H	392	VAL	3.6
1	1-K	96	THR	3.6
1	1-T	1	THR	3.6
1	1-U	173	VAL	3.6
1	1-V	333	VAL	3.6
1	1-X	429	THR	3.6
1	1-D	155	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-G	41	SER	3.6
1	1-K	357	GLU	3.6
1	1-B	163	ALA	3.6
1	1-D	353	ALA	3.6
1	1-N	423	ALA	3.6
1	1-F	381	GLY	3.6
1	1-M	262	GLY	3.6
1	1-U	289	GLY	3.6
1	1-A	66	LEU	3.6
1	1-F	208	LYS	3.6
1	1-L	97	LEU	3.6
1	1-P	332	LEU	3.6
1	1-R	352	LYS	3.6
1	1-V	394	LYS	3.6
1	1-A	351	PRO	3.6
1	1-D	264	ASN	3.6
1	1-E	329	PRO	3.6
1	1-R	411	PRO	3.6
1	1-S	64	ASP	3.6
1	1-S	393	ASP	3.6
1	1-J	425	HIS	3.6
1	1-M	286	THR	3.6
1	1-S	173	VAL	3.6
1	1-W	173	VAL	3.6
1	1-Q	207	GLU	3.6
1	1-A	353	ALA	3.6
1	1-C	279	ALA	3.6
1	1-M	423	ALA	3.6
1	1-W	341	ALA	3.6
1	1-J	24	LEU	3.6
1	1-J	413	GLN	3.6
1	1-O	282	MET	3.6
1	1-Q	43	PHE	3.6
1	1-B	355	ARG	3.6
1	1-J	386	ILE	3.6
1	1-R	388	PRO	3.6
1	1-K	454	ASN	3.6
1	1-F	284	ASP	3.6
1	1-K	167	ASP	3.6
1	1-S	4	ASP	3.6
1	1-W	50	ASP	3.6
1	1-A	296	HIS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-L	125	TYR	3.6
1	1-L	297	TYR	3.6
1	1-S	296	HIS	3.6
1	1-N	286	THR	3.6
1	1-S	1	THR	3.6
1	1-C	426	GLU	3.6
1	1-K	387	GLU	3.6
1	1-U	392	VAL	3.6
1	1-M	36	SER	3.6
1	1-D	10	LYS	3.6
1	1-F	332	LEU	3.6
1	1-G	127	GLY	3.6
1	1-P	295	ARG	3.6
1	1-Q	503	GLY	3.6
1	1-X	67	LEU	3.6
1	1-O	382	ILE	3.6
1	1-G	284	ASP	3.6
1	1-N	343	VAL	3.6
1	1-P	410	THR	3.6
1	1-S	129	GLU	3.6
1	1-E	182	VAL	3.6
1	1-Q	173	VAL	3.6
1	1-X	410	THR	3.6
1	1-F	40	LYS	3.6
1	1-J	383	LYS	3.6
1	1-T	117	SER	3.6
1	1-U	501	SER	3.6
1	1-U	340	SER	3.6
1	1-S	336	GLN	3.6
1	1-U	423	ALA	3.6
1	1-V	420	ARG	3.6
1	1-I	332	LEU	3.6
1	1-K	66	LEU	3.6
1	1-M	66	LEU	3.6
1	1-N	209	GLY	3.6
1	1-W	68	LEU	3.6
1	1-B	120	ILE	3.6
1	1-I	280	PRO	3.6
1	1-S	382	ILE	3.6
1	1-X	391	PRO	3.6
1	1-L	39	ASP	3.6
1	1-L	393	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-O	393	ASP	3.6
1	1-S	331	ASN	3.6
1	1-T	167	ASP	3.6
1	1-C	92	HIS	3.5
1	1-A	270	CYS	3.5
1	1-O	10	LYS	3.5
1	1-B	96	THR	3.5
1	1-L	392	VAL	3.5
1	1-L	412	THR	3.5
1	1-T	173	VAL	3.5
1	1-B	174	ARG	3.5
1	1-D	344	ARG	3.5
1	1-G	187	GLN	3.5
1	1-A	206	LEU	3.5
1	1-C	423	ALA	3.5
1	1-I	381	GLY	3.5
1	1-M	381	GLY	3.5
1	1-D	225	PHE	3.5
1	1-G	345	ILE	3.5
1	1-K	386	ILE	3.5
1	1-P	27	ILE	3.5
1	1-R	347	ILE	3.5
1	1-W	445	PHE	3.5
1	1-G	331	ASN	3.5
1	1-I	284	ASP	3.5
1	1-I	395	ASP	3.5
1	1-J	467	ASP	3.5
1	1-M	50	ASP	3.5
1	1-M	64	ASP	3.5
1	1-U	3	ASP	3.5
1	1-V	4	ASP	3.5
1	1-J	208	LYS	3.5
1	1-T	10	LYS	3.5
1	1-X	276	LYS	3.5
1	1-N	173	VAL	3.5
1	1-Q	164	THR	3.5
1	1-R	123	THR	3.5
1	1-S	297	TYR	3.5
1	1-A	356	LEU	3.5
1	1-S	501	SER	3.5
1	1-D	51	GLY	3.5
1	1-E	275	TRP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-H	279	ALA	3.5
1	1-M	365	GLY	3.5
1	1-U	381	GLY	3.5
1	1-N	400	PRO	3.5
1	1-P	280	PRO	3.5
1	1-S	388	PRO	3.5
1	1-I	330	ILE	3.5
1	1-S	221	ILE	3.5
1	1-I	384	ASN	3.5
1	1-N	296	HIS	3.5
1	1-V	50	ASP	3.5
1	1-V	425	HIS	3.5
1	1-F	426	GLU	3.5
1	1-J	403	GLU	3.5
1	1-T	98	GLU	3.5
1	1-B	348	THR	3.5
1	1-C	348	THR	3.5
1	1-E	410	THR	3.5
1	1-U	286	THR	3.5
1	1-W	118	THR	3.5
1	1-X	164	THR	3.5
1	1-N	413	GLN	3.5
1	1-O	187	GLN	3.5
1	1-T	413	GLN	3.5
1	1-B	427	TYR	3.5
1	1-H	47	LEU	3.5
1	1-H	66	LEU	3.5
1	1-B	278	GLY	3.5
1	1-F	423	ALA	3.5
1	1-J	340	SER	3.5
1	1-O	46	GLY	3.5
1	1-Q	41	SER	3.5
1	1-K	329	PRO	3.5
1	1-E	330	ILE	3.5
1	1-H	345	ILE	3.5
1	1-M	347	ILE	3.5
1	1-H	383	LYS	3.5
1	1-K	352	LYS	3.5
1	1-S	40	LYS	3.5
1	1-X	271	HIS	3.5
1	1-A	222	ASN	3.5
1	1-C	384	ASN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-D	284	ASP	3.5
1	1-F	4	ASP	3.5
1	1-K	11	ASP	3.5
1	1-M	264	ASN	3.5
1	1-I	207	GLU	3.5
1	1-J	129	GLU	3.5
1	1-L	165	GLU	3.5
1	1-V	285	GLU	3.5
1	1-W	344	ARG	3.5
1	1-R	65	MET	3.5
1	1-L	173	VAL	3.5
1	1-V	332	LEU	3.5
1	1-G	289	GLY	3.5
1	1-L	114	TYR	3.5
1	1-E	231	ALA	3.5
1	1-H	288	ALA	3.5
1	1-H	423	ALA	3.5
1	1-L	340	SER	3.5
1	1-P	273	SER	3.5
1	1-Q	36	SER	3.5
1	1-Q	431	GLY	3.5
1	1-R	341	ALA	3.5
1	1-T	502	PRO	3.5
1	1-F	407	ILE	3.5
1	1-J	345	ILE	3.5
1	1-N	330	ILE	3.5
1	1-T	330	ILE	3.5
1	1-V	347	ILE	3.5
1	1-B	40	LYS	3.5
1	1-C	10	LYS	3.5
1	1-E	338	ASN	3.4
1	1-H	72	GLU	3.4
1	1-N	331	ASN	3.4
1	1-P	207	GLU	3.4
1	1-X	355	ARG	3.4
1	1-I	428	LEU	3.4
1	1-X	438	LEU	3.4
1	1-B	46	GLY	3.4
1	1-B	209	GLY	3.4
1	1-B	280	PRO	3.4
1	1-D	503	GLY	3.4
1	1-I	51	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-M	270	CYS	3.4
1	1-R	280	PRO	3.4
1	1-T	289	GLY	3.4
1	1-A	287	TYR	3.4
1	1-G	385	LYS	3.4
1	1-H	221	ILE	3.4
1	1-K	155	SER	3.4
1	1-K	407	ILE	3.4
1	1-N	406	SER	3.4
1	1-O	154	ILE	3.4
1	1-H	303	HIS	3.4
1	1-S	225	PHE	3.4
1	1-W	269	HIS	3.4
1	1-A	467	ASP	3.4
1	1-B	277	ASP	3.4
1	1-F	295	ARG	3.4
1	1-H	504	ASN	3.4
1	1-I	3	ASP	3.4
1	1-I	44	ASP	3.4
1	1-X	420	ARG	3.4
1	1-R	389	GLN	3.4
1	1-X	286	THR	3.4
1	1-H	502	PRO	3.4
1	1-H	346	PRO	3.4
1	1-J	391	PRO	3.4
1	1-L	385	LYS	3.4
1	1-C	127	GLY	3.4
1	1-F	500	GLY	3.4
1	1-F	262	GLY	3.4
1	1-B	279	ALA	3.4
1	1-E	163	ALA	3.4
1	1-M	37	ALA	3.4
1	1-B	330	ILE	3.4
1	1-J	330	ILE	3.4
1	1-L	154	ILE	3.4
1	1-M	407	ILE	3.4
1	1-X	345	ILE	3.4
1	1-C	12	GLU	3.4
1	1-C	43	PHE	3.4
1	1-F	285	GLU	3.4
1	1-M	98	GLU	3.4
1	1-P	355	ARG	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-U	602	GLU	3.4
1	1-A	44	ASP	3.4
1	1-N	282	MET	3.4
1	1-Q	44	ASP	3.4
1	1-B	264	ASN	3.4
1	1-P	331	ASN	3.4
1	1-M	413	GLN	3.4
1	1-F	91	VAL	3.4
1	1-B	332	LEU	3.4
1	1-C	383	LYS	3.4
1	1-F	276	LYS	3.4
1	1-I	312	THR	3.4
1	1-N	348	THR	3.4
1	1-P	118	THR	3.4
1	1-W	286	THR	3.4
1	1-M	388	PRO	3.4
1	1-H	127	GLY	3.4
1	1-J	262	GLY	3.4
1	1-A	163	ALA	3.4
1	1-F	390	ALA	3.4
1	1-L	9	ALA	3.4
1	1-N	128	ALA	3.4
1	1-X	116	ILE	3.4
1	1-G	359	ARG	3.4
1	1-N	207	GLU	3.4
1	1-P	100	TYR	3.4
1	1-P	129	GLU	3.4
1	1-R	285	GLU	3.4
1	1-S	165	GLU	3.4
1	1-T	165	GLU	3.4
1	1-C	44	ASP	3.4
1	1-E	50	ASP	3.4
1	1-J	50	ASP	3.4
1	1-X	292	ASP	3.4
1	1-R	436	ASN	3.4
1	1-I	409	GLN	3.4
1	1-I	413	GLN	3.4
1	1-B	173	VAL	3.4
1	1-P	392	VAL	3.4
1	1-R	42	VAL	3.4
1	1-R	68	LEU	3.4
1	1-O	388	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-R	391	PRO	3.4
1	1-E	262	GLY	3.4
1	1-K	127	GLY	3.4
1	1-G	288	ALA	3.4
1	1-N	347	ILE	3.4
1	1-O	174	ARG	3.4
1	1-Q	294	ALA	3.4
1	1-T	347	ILE	3.4
1	1-F	12	GLU	3.4
1	1-P	285	GLU	3.4
1	1-B	41	SER	3.4
1	1-B	340	SER	3.4
1	1-X	501	SER	3.4
1	1-D	297	TYR	3.3
1	1-K	93	ASP	3.3
1	1-A	264	ASN	3.3
1	1-L	222	ASN	3.3
1	1-X	264	ASN	3.3
1	1-A	352	LYS	3.3
1	1-Q	5	VAL	3.3
1	1-Q	391	PRO	3.3
1	1-S	5	VAL	3.3
1	1-T	348	THR	3.3
1	1-C	262	GLY	3.3
1	1-E	500	GLY	3.3
1	1-H	381	GLY	3.3
1	1-I	175	HIS	3.3
1	1-L	432	GLY	3.3
1	1-N	359	ARG	3.3
1	1-Q	344	ARG	3.3
1	1-V	127	GLY	3.3
1	1-H	165	GLU	3.3
1	1-I	285	GLU	3.3
1	1-I	403	GLU	3.3
1	1-O	128	ALA	3.3
1	1-O	285	GLU	3.3
1	1-U	387	GLU	3.3
1	1-B	101	SER	3.3
1	1-V	270	CYS	3.3
1	1-Q	284	ASP	3.3
1	1-R	277	ASP	3.3
1	1-U	393	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-V	39	ASP	3.3
1	1-F	409	GLN	3.3
1	1-Q	409	GLN	3.3
1	1-W	222	ASN	3.3
1	1-C	66	LEU	3.3
1	1-O	332	LEU	3.3
1	1-S	68	LEU	3.3
1	1-J	164	THR	3.3
1	1-O	118	THR	3.3
1	1-O	182	VAL	3.3
1	1-X	118	THR	3.3
1	1-C	211	HIS	3.3
1	1-C	278	GLY	3.3
1	1-M	278	GLY	3.3
1	1-M	289	GLY	3.3
1	1-P	296	HIS	3.3
1	1-V	207	GLU	3.3
1	1-I	288	ALA	3.3
1	1-P	353	ALA	3.3
1	1-S	407	ILE	3.3
1	1-U	347	ILE	3.3
1	1-X	128	ALA	3.3
1	1-X	353	ALA	3.3
1	1-K	65	MET	3.3
1	1-F	155	SER	3.3
1	1-K	52	SER	3.3
1	1-E	38	PHE	3.3
1	1-S	13	LYS	3.3
1	1-S	385	LYS	3.3
1	1-T	352	LYS	3.3
1	1-I	292	ASP	3.3
1	1-K	393	ASP	3.3
1	1-W	284	ASP	3.3
1	1-E	306	PRO	3.3
1	1-J	290	LEU	3.3
1	1-J	306	PRO	3.3
1	1-O	281	LEU	3.3
1	1-Q	332	LEU	3.3
1	1-R	332	LEU	3.3
1	1-T	281	LEU	3.3
1	1-J	359	ARG	3.3
1	1-A	412	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	92	HIS	3.3
1	1-P	91	VAL	3.3
1	1-D	129	GLU	3.3
1	1-E	98	GLU	3.3
1	1-I	72	GLU	3.3
1	1-O	207	GLU	3.3
1	1-U	92	HIS	3.3
1	1-U	98	GLU	3.3
1	1-V	129	GLU	3.3
1	1-V	410	THR	3.3
1	1-X	1	THR	3.3
1	1-K	381	GLY	3.3
1	1-Q	500	GLY	3.3
1	1-Q	378	GLY	3.3
1	1-H	154	ILE	3.3
1	1-O	37	ALA	3.3
1	1-P	282	MET	3.3
1	1-T	394	LYS	3.3
1	1-G	340	SER	3.3
1	1-D	393	ASP	3.3
1	1-E	248	GLN	3.3
1	1-K	467	ASP	3.3
1	1-N	467	ASP	3.3
1	1-R	409	GLN	3.3
1	1-B	270	CYS	3.3
1	1-D	384	ASN	3.3
1	1-F	421	LEU	3.3
1	1-H	388	PRO	3.3
1	1-I	344	ARG	3.3
1	1-L	359	ARG	3.3
1	1-N	344	ARG	3.3
1	1-Q	351	PRO	3.3
1	1-V	355	ARG	3.3
1	1-W	67	LEU	3.3
1	1-A	343	VAL	3.3
1	1-B	285	GLU	3.3
1	1-H	207	GLU	3.3
1	1-O	72	GLU	3.3
1	1-P	387	GLU	3.3
1	1-R	422	GLU	3.3
1	1-U	269	HIS	3.3
1	1-A	289	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-C	51	GLY	3.3
1	1-E	250	GLY	3.3
1	1-Q	127	GLY	3.3
1	1-R	127	GLY	3.3
1	1-T	503	GLY	3.3
1	1-W	65	MET	3.3
1	1-B	347	ILE	3.3
1	1-D	386	ILE	3.3
1	1-K	347	ILE	3.3
1	1-P	352	LYS	3.3
1	1-V	40	LYS	3.3
1	1-N	155	SER	3.2
1	1-K	409	GLN	3.2
1	1-P	409	GLN	3.2
1	1-P	434	PHE	3.2
1	1-X	187	GLN	3.2
1	1-O	39	ASP	3.2
1	1-G	125	TYR	3.2
1	1-H	359	ARG	3.2
1	1-B	2	PRO	3.2
1	1-D	99	PRO	3.2
1	1-L	379	LEU	3.2
1	1-M	342	CYS	3.2
1	1-I	165	GLU	3.2
1	1-V	173	VAL	3.2
1	1-X	282	MET	3.2
1	1-X	323	VAL	3.2
1	1-F	118	THR	3.2
1	1-F	278	GLY	3.2
1	1-N	51	GLY	3.2
1	1-F	352	LYS	3.2
1	1-L	288	ALA	3.2
1	1-W	423	ALA	3.2
1	1-X	163	ALA	3.2
1	1-P	187	GLN	3.2
1	1-D	174	ARG	3.2
1	1-U	50	ASP	3.2
1	1-W	93	ASP	3.2
1	1-E	351	PRO	3.2
1	1-F	68	LEU	3.2
1	1-H	290	LEU	3.2
1	1-L	502	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	67	LEU	3.2
1	1-T	297	TYR	3.2
1	1-U	66	LEU	3.2
1	1-H	129	GLU	3.2
1	1-J	440	GLU	3.2
1	1-N	342	CYS	3.2
1	1-H	333	VAL	3.2
1	1-P	13	LYS	3.2
1	1-V	10	LYS	3.2
1	1-X	208	LYS	3.2
1	1-X	333	VAL	3.2
1	1-B	412	THR	3.2
1	1-D	127	GLY	3.2
1	1-F	96	THR	3.2
1	1-J	431	GLY	3.2
1	1-K	164	THR	3.2
1	1-N	500	GLY	3.2
1	1-R	265	GLY	3.2
1	1-R	300	GLY	3.2
1	1-B	423	ALA	3.2
1	1-S	163	ALA	3.2
1	1-V	413	GLN	3.2
1	1-D	340	SER	3.2
1	1-D	444	SER	3.2
1	1-M	344	ARG	3.2
1	1-Q	6	PHE	3.2
1	1-Q	420	ARG	3.2
1	1-S	41	SER	3.2
1	1-B	284	ASP	3.2
1	1-F	222	ASN	3.2
1	1-F	92	HIS	3.2
1	1-F	428	LEU	3.2
1	1-G	206	LEU	3.2
1	1-K	165	GLU	3.2
1	1-K	290	LEU	3.2
1	1-S	306	PRO	3.2
1	1-K	296	HIS	3.2
1	1-L	387	GLU	3.2
1	1-T	72	GLU	3.2
1	1-U	165	GLU	3.2
1	1-V	290	LEU	3.2
1	1-M	282	MET	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-S	125	TYR	3.2
1	1-E	127	GLY	3.2
1	1-F	42	VAL	3.2
1	1-K	289	GLY	3.2
1	1-P	173	VAL	3.2
1	1-S	164	THR	3.2
1	1-U	262	GLY	3.2
1	1-B	154	ILE	3.2
1	1-B	407	ILE	3.2
1	1-P	116	ILE	3.2
1	1-P	418	ILE	3.2
1	1-D	9	ALA	3.2
1	1-A	413	GLN	3.2
1	1-G	272	GLN	3.2
1	1-H	413	GLN	3.2
1	1-J	336	GLN	3.2
1	1-K	344	ARG	3.2
1	1-L	355	ARG	3.2
1	1-V	359	ARG	3.2
1	1-D	117	SER	3.2
1	1-F	117	SER	3.2
1	1-Q	273	SER	3.2
1	1-A	385	LYS	3.2
1	1-B	66	LEU	3.2
1	1-E	129	GLU	3.2
1	1-I	383	LYS	3.2
1	1-Q	165	GLU	3.2
1	1-S	10	LYS	3.2
1	1-S	175	HIS	3.2
1	1-W	290	LEU	3.2
1	1-X	115	LEU	3.2
1	1-Q	282	MET	3.2
1	1-X	170	GLY	3.2
1	1-I	154	ILE	3.2
1	1-K	1	THR	3.2
1	1-L	164	THR	3.2
1	1-Q	342	CYS	3.2
1	1-R	407	ILE	3.2
1	1-A	423	ALA	3.1
1	1-E	423	ALA	3.1
1	1-F	163	ALA	3.1
1	1-L	423	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-R	355	ARG	3.1
1	1-W	409	GLN	3.1
1	1-H	101	SER	3.1
1	1-N	36	SER	3.1
1	1-O	43	PHE	3.1
1	1-D	467	ASP	3.1
1	1-A	502	PRO	3.1
1	1-C	72	GLU	3.1
1	1-J	39	ASP	3.1
1	1-J	394	LYS	3.1
1	1-R	340	SER	3.1
1	1-K	602	GLU	3.1
1	1-K	400	PRO	3.1
1	1-L	12	GLU	3.1
1	1-N	12	GLU	3.1
1	1-Q	93	ASP	3.1
1	1-S	394	LYS	3.1
1	1-V	603	LYS	3.1
1	1-N	388	PRO	3.1
1	1-B	282	MET	3.1
1	1-G	68	LEU	3.1
1	1-G	115	LEU	3.1
1	1-R	24	LEU	3.1
1	1-V	271	HIS	3.1
1	1-K	384	ASN	3.1
1	1-A	323	VAL	3.1
1	1-A	381	GLY	3.1
1	1-J	171	TYR	3.1
1	1-K	417	VAL	3.1
1	1-P	433	VAL	3.1
1	1-T	209	GLY	3.1
1	1-W	289	GLY	3.1
1	1-W	392	VAL	3.1
1	1-A	205	ILE	3.1
1	1-H	118	THR	3.1
1	1-G	163	ALA	3.1
1	1-W	355	ARG	3.1
1	1-A	10	LYS	3.1
1	1-R	276	LYS	3.1
1	1-G	440	GLU	3.1
1	1-J	98	GLU	3.1
1	1-N	129	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-M	391	PRO	3.1
1	1-N	277	ASP	3.1
1	1-O	501	SER	3.1
1	1-P	444	SER	3.1
1	1-W	285	GLU	3.1
1	1-D	282	MET	3.1
1	1-R	306	PRO	3.1
1	1-L	438	LEU	3.1
1	1-O	290	LEU	3.1
1	1-D	381	GLY	3.1
1	1-M	42	VAL	3.1
1	1-O	51	GLY	3.1
1	1-E	283	TYR	3.1
1	1-F	344	ARG	3.1
1	1-G	164	THR	3.1
1	1-L	75	ARG	3.1
1	1-M	154	ILE	3.1
1	1-M	427	TYR	3.1
1	1-N	120	ILE	3.1
1	1-O	330	ILE	3.1
1	1-O	429	THR	3.1
1	1-P	164	THR	3.1
1	1-W	420	ARG	3.1
1	1-G	310	ALA	3.1
1	1-L	187	GLN	3.1
1	1-S	279	ALA	3.1
1	1-U	305	ALA	3.1
1	1-W	390	ALA	3.1
1	1-I	270	CYS	3.1
1	1-N	352	LYS	3.1
1	1-V	7	LYS	3.1
1	1-X	176	LYS	3.1
1	1-B	426	GLU	3.1
1	1-O	98	GLU	3.1
1	1-O	129	GLU	3.1
1	1-H	99	PRO	3.1
1	1-K	92	HIS	3.1
1	1-N	329	PRO	3.1
1	1-Q	180	PHE	3.1
1	1-S	467	ASP	3.1
1	1-U	43	PHE	3.1
1	1-W	6	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-X	388	PRO	3.1
1	1-E	66	LEU	3.1
1	1-F	24	LEU	3.1
1	1-I	39	ASP	3.1
1	1-J	501	SER	3.1
1	1-P	206	LEU	3.1
1	1-V	44	ASP	3.1
1	1-X	44	ASP	3.1
1	1-X	206	LEU	3.1
1	1-R	157	TRP	3.1
1	1-C	355	ARG	3.1
1	1-G	295	ARG	3.1
1	1-J	295	ARG	3.1
1	1-L	503	GLY	3.1
1	1-N	127	GLY	3.1
1	1-T	127	GLY	3.1
1	1-K	392	VAL	3.1
1	1-O	392	VAL	3.1
1	1-A	123	THR	3.1
1	1-H	382	ILE	3.1
1	1-J	410	THR	3.1
1	1-U	345	ILE	3.1
1	1-M	297	TYR	3.1
1	1-P	171	TYR	3.1
1	1-A	394	LYS	3.1
1	1-H	276	LYS	3.1
1	1-I	128	ALA	3.1
1	1-Q	128	ALA	3.1
1	1-X	130	ALA	3.1
1	1-F	207	GLU	3.1
1	1-G	285	GLU	3.1
1	1-F	425	HIS	3.1
1	1-X	425	HIS	3.1
1	1-D	206	LEU	3.1
1	1-E	284	ASP	3.1
1	1-I	43	PHE	3.1
1	1-L	122	ASP	3.1
1	1-P	274	LEU	3.1
1	1-L	444	SER	3.1
1	1-S	36	SER	3.1
1	1-O	185	ASN	3.1
1	1-J	344	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	503	GLY	3.1
1	1-F	431	GLY	3.1
1	1-F	213	VAL	3.1
1	1-G	382	ILE	3.1
1	1-J	433	VAL	3.1
1	1-P	386	ILE	3.1
1	1-S	91	VAL	3.1
1	1-A	110	LYS	3.0
1	1-A	164	THR	3.0
1	1-A	409	GLN	3.0
1	1-D	409	GLN	3.0
1	1-H	394	LYS	3.0
1	1-N	603	LYS	3.0
1	1-P	1	THR	3.0
1	1-B	377	ALA	3.0
1	1-C	341	ALA	3.0
1	1-F	297	TYR	3.0
1	1-F	341	ALA	3.0
1	1-L	35	ALA	3.0
1	1-S	16	TYR	3.0
1	1-S	124	ALA	3.0
1	1-X	423	ALA	3.0
1	1-A	440	GLU	3.0
1	1-H	212	GLU	3.0
1	1-B	175	HIS	3.0
1	1-D	44	ASP	3.0
1	1-E	93	ASP	3.0
1	1-E	180	PHE	3.0
1	1-S	43	PHE	3.0
1	1-U	281	LEU	3.0
1	1-V	38	PHE	3.0
1	1-V	67	LEU	3.0
1	1-F	467	ASP	3.0
1	1-J	393	ASP	3.0
1	1-K	501	SER	3.0
1	1-O	101	SER	3.0
1	1-V	501	SER	3.0
1	1-W	340	SER	3.0
1	1-F	264	ASN	3.0
1	1-J	355	ARG	3.0
1	1-L	275	TRP	3.0
1	1-P	262	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-R	365	GLY	3.0
1	1-B	345	ILE	3.0
1	1-D	5	VAL	3.0
1	1-E	120	ILE	3.0
1	1-L	333	VAL	3.0
1	1-S	330	ILE	3.0
1	1-T	392	VAL	3.0
1	1-E	389	GLN	3.0
1	1-O	389	GLN	3.0
1	1-R	336	GLN	3.0
1	1-G	429	THR	3.0
1	1-Q	286	THR	3.0
1	1-U	293	THR	3.0
1	1-A	390	ALA	3.0
1	1-N	305	ALA	3.0
1	1-O	48	ALA	3.0
1	1-U	163	ALA	3.0
1	1-A	285	GLU	3.0
1	1-B	207	GLU	3.0
1	1-L	72	GLU	3.0
1	1-M	165	GLU	3.0
1	1-Q	129	GLU	3.0
1	1-X	72	GLU	3.0
1	1-E	92	HIS	3.0
1	1-F	271	HIS	3.0
1	1-T	425	HIS	3.0
1	1-E	280	PRO	3.0
1	1-E	324	PRO	3.0
1	1-H	329	PRO	3.0
1	1-D	274	LEU	3.0
1	1-M	8	LEU	3.0
1	1-N	438	LEU	3.0
1	1-Q	24	LEU	3.0
1	1-D	277	ASP	3.0
1	1-F	152	ASP	3.0
1	1-I	50	ASP	3.0
1	1-J	180	PHE	3.0
1	1-J	277	ASP	3.0
1	1-S	342	CYS	3.0
1	1-T	277	ASP	3.0
1	1-X	6	PHE	3.0
1	1-D	295	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-E	344	ARG	3.0
1	1-Q	359	ARG	3.0
1	1-R	295	ARG	3.0
1	1-T	339	ARG	3.0
1	1-F	176	LYS	3.0
1	1-I	385	LYS	3.0
1	1-U	10	LYS	3.0
1	1-B	300	GLY	3.0
1	1-H	500	GLY	3.0
1	1-O	278	GLY	3.0
1	1-Q	262	GLY	3.0
1	1-R	431	GLY	3.0
1	1-T	262	GLY	3.0
1	1-V	278	GLY	3.0
1	1-B	333	VAL	3.0
1	1-C	389	GLN	3.0
1	1-F	333	VAL	3.0
1	1-H	275	TRP	3.0
1	1-M	120	ILE	3.0
1	1-N	275	TRP	3.0
1	1-Q	154	ILE	3.0
1	1-S	392	VAL	3.0
1	1-W	336	GLN	3.0
1	1-X	275	TRP	3.0
1	1-A	118	THR	3.0
1	1-L	118	THR	3.0
1	1-A	130	ALA	3.0
1	1-A	165	GLU	3.0
1	1-A	282	MET	3.0
1	1-F	288	ALA	3.0
1	1-I	15	GLU	3.0
1	1-K	98	GLU	3.0
1	1-K	129	GLU	3.0
1	1-M	162	ALA	3.0
1	1-G	271	HIS	3.0
1	1-G	297	TYR	3.0
1	1-C	502	PRO	3.0
1	1-C	306	PRO	3.0
1	1-F	391	PRO	3.0
1	1-I	391	PRO	3.0
1	1-L	400	PRO	3.0
1	1-B	290	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-H	206	LEU	3.0
1	1-D	38	PHE	3.0
1	1-F	44	ASP	3.0
1	1-G	416	ASP	3.0
1	1-K	152	ASP	3.0
1	1-L	292	ASP	3.0
1	1-L	434	PHE	3.0
1	1-P	292	ASP	3.0
1	1-T	406	SER	3.0
1	1-C	222	ASN	3.0
1	1-H	331	ASN	3.0
1	1-L	185	ASN	3.0
1	1-Q	264	ASN	3.0
1	1-B	381	GLY	3.0
1	1-P	203	GLY	3.0
1	1-R	289	GLY	3.0
1	1-G	386	ILE	3.0
1	1-Q	347	ILE	3.0
1	1-F	129	GLU	3.0
1	1-K	275	TRP	3.0
1	1-L	84	THR	3.0
1	1-Q	412	THR	3.0
1	1-E	35	ALA	3.0
1	1-O	162	ALA	3.0
1	1-Q	108	ALA	3.0
1	1-R	211	HIS	3.0
1	1-U	353	ALA	3.0
1	1-L	329	PRO	3.0
1	1-V	502	PRO	3.0
1	1-V	306	PRO	3.0
1	1-B	8	LEU	3.0
1	1-B	356	LEU	3.0
1	1-E	229	LEU	3.0
1	1-E	355	ARG	3.0
1	1-M	290	LEU	3.0
1	1-S	67	LEU	3.0
1	1-B	276	LYS	3.0
1	1-C	3	ASP	3.0
1	1-J	4	ASP	3.0
1	1-K	385	LYS	3.0
1	1-F	434	PHE	3.0
1	1-N	11	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-N	64	ASP	3.0
1	1-E	273	SER	3.0
1	1-G	270	CYS	3.0
1	1-Q	363	SER	3.0
1	1-U	270	CYS	3.0
1	1-X	117	SER	3.0
1	1-X	270	CYS	3.0
1	1-O	331	ASN	3.0
1	1-A	500	GLY	3.0
1	1-F	289	GLY	3.0
1	1-N	389	GLN	3.0
1	1-P	336	GLN	3.0
1	1-S	365	GLY	3.0
1	1-A	154	ILE	2.9
1	1-B	12	GLU	2.9
1	1-D	91	VAL	2.9
1	1-W	330	ILE	2.9
1	1-K	72	GLU	2.9
1	1-U	129	GLU	2.9
1	1-W	282	MET	2.9
1	1-F	286	THR	2.9
1	1-H	429	THR	2.9
1	1-K	429	THR	2.9
1	1-M	164	THR	2.9
1	1-T	441	THR	2.9
1	1-D	377	ALA	2.9
1	1-D	463	ALA	2.9
1	1-O	183	ALA	2.9
1	1-C	359	ARG	2.9
1	1-M	329	PRO	2.9
1	1-P	306	PRO	2.9
1	1-C	332	LEU	2.9
1	1-I	354	LYS	2.9
1	1-L	115	LEU	2.9
1	1-O	171	TYR	2.9
1	1-Q	281	LEU	2.9
1	1-B	44	ASP	2.9
1	1-H	39	ASP	2.9
1	1-H	152	ASP	2.9
1	1-I	167	ASP	2.9
1	1-N	380	ASP	2.9
1	1-T	39	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-T	311	PHE	2.9
1	1-U	277	ASP	2.9
1	1-W	380	ASP	2.9
1	1-X	393	ASP	2.9
1	1-J	41	SER	2.9
1	1-L	291	SER	2.9
1	1-T	340	SER	2.9
1	1-W	273	SER	2.9
1	1-B	500	GLY	2.9
1	1-G	365	GLY	2.9
1	1-G	409	GLN	2.9
1	1-J	270	CYS	2.9
1	1-M	409	GLN	2.9
1	1-T	264	ASN	2.9
1	1-V	432	GLY	2.9
1	1-D	357	GLU	2.9
1	1-F	116	ILE	2.9
1	1-U	221	ILE	2.9
1	1-E	392	VAL	2.9
1	1-G	433	VAL	2.9
1	1-J	333	VAL	2.9
1	1-L	343	VAL	2.9
1	1-P	417	VAL	2.9
1	1-V	165	GLU	2.9
1	1-A	92	HIS	2.9
1	1-A	425	HIS	2.9
1	1-F	164	THR	2.9
1	1-I	410	THR	2.9
1	1-P	293	THR	2.9
1	1-V	286	THR	2.9
1	1-W	296	HIS	2.9
1	1-D	130	ALA	2.9
1	1-E	420	ARG	2.9
1	1-K	295	ARG	2.9
1	1-K	353	ALA	2.9
1	1-M	128	ALA	2.9
1	1-R	288	ALA	2.9
1	1-T	423	ALA	2.9
1	1-D	40	LYS	2.9
1	1-J	275	TRP	2.9
1	1-S	276	LYS	2.9
1	1-U	7	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-V	385	LYS	2.9
1	1-D	421	LEU	2.9
1	1-G	290	LEU	2.9
1	1-I	290	LEU	2.9
1	1-T	332	LEU	2.9
1	1-A	465	TYR	2.9
1	1-I	283	TYR	2.9
1	1-W	125	TYR	2.9
1	1-A	284	ASP	2.9
1	1-G	152	ASP	2.9
1	1-H	277	ASP	2.9
1	1-K	45	ASP	2.9
1	1-M	292	ASP	2.9
1	1-C	501	SER	2.9
1	1-D	41	SER	2.9
1	1-F	41	SER	2.9
1	1-M	155	SER	2.9
1	1-O	307	SER	2.9
1	1-X	336	GLN	2.9
1	1-G	432	GLY	2.9
1	1-H	282	MET	2.9
1	1-P	289	GLY	2.9
1	1-X	222	ASN	2.9
1	1-X	365	GLY	2.9
1	1-A	426	GLU	2.9
1	1-C	165	GLU	2.9
1	1-G	12	GLU	2.9
1	1-L	212	GLU	2.9
1	1-R	12	GLU	2.9
1	1-F	120	ILE	2.9
1	1-T	386	ILE	2.9
1	1-X	407	ILE	2.9
1	1-V	323	VAL	2.9
1	1-W	42	VAL	2.9
1	1-B	344	ARG	2.9
1	1-I	293	THR	2.9
1	1-I	412	THR	2.9
1	1-M	412	THR	2.9
1	1-S	420	ARG	2.9
1	1-U	164	THR	2.9
1	1-F	99	PRO	2.9
1	1-H	377	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-I	341	ALA	2.9
1	1-L	2	PRO	2.9
1	1-S	108	ALA	2.9
1	1-S	463	ALA	2.9
1	1-W	13	LYS	2.9
1	1-E	438	LEU	2.9
1	1-R	302	LEU	2.9
1	1-A	4	ASP	2.9
1	1-C	284	ASP	2.9
1	1-D	380	ASP	2.9
1	1-F	427	TYR	2.9
1	1-K	4	ASP	2.9
1	1-P	393	ASP	2.9
1	1-U	4	ASP	2.9
1	1-S	6	PHE	2.9
1	1-H	389	GLN	2.9
1	1-Q	187	GLN	2.9
1	1-D	72	GLU	2.9
1	1-E	36	SER	2.9
1	1-E	52	SER	2.9
1	1-F	98	GLU	2.9
1	1-H	426	GLU	2.9
1	1-I	222	ASN	2.9
1	1-L	365	GLY	2.9
1	1-N	365	GLY	2.9
1	1-P	127	GLY	2.9
1	1-S	431	GLY	2.9
1	1-W	387	GLU	2.9
1	1-A	120	ILE	2.9
1	1-E	154	ILE	2.9
1	1-M	386	ILE	2.9
1	1-O	347	ILE	2.9
1	1-X	154	ILE	2.9
1	1-D	343	VAL	2.9
1	1-D	355	ARG	2.9
1	1-O	355	ARG	2.9
1	1-Q	425	HIS	2.9
1	1-X	42	VAL	2.9
1	1-D	164	THR	2.9
1	1-I	286	THR	2.9
1	1-E	108	ALA	2.9
1	1-J	353	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-V	71	PRO	2.9
1	1-E	290	LEU	2.9
1	1-F	67	LEU	2.9
1	1-L	301	LEU	2.9
1	1-P	66	LEU	2.9
1	1-M	275	TRP	2.9
1	1-O	275	TRP	2.9
1	1-K	39	ASP	2.9
1	1-L	44	ASP	2.9
1	1-P	4	ASP	2.9
1	1-P	380	ASP	2.9
1	1-I	100	TYR	2.9
1	1-Q	125	TYR	2.9
1	1-F	422	GLU	2.9
1	1-K	12	GLU	2.9
1	1-S	15	GLU	2.9
1	1-X	207	GLU	2.9
1	1-O	381	GLY	2.9
1	1-D	101	SER	2.8
1	1-P	222	ASN	2.8
1	1-S	264	ASN	2.8
1	1-S	360	SER	2.8
1	1-E	425	HIS	2.8
1	1-F	330	ILE	2.8
1	1-F	347	ILE	2.8
1	1-T	331	ASN	2.8
1	1-J	603	LYS	2.8
1	1-O	394	LYS	2.8
1	1-T	40	LYS	2.8
1	1-X	40	LYS	2.8
1	1-S	14	VAL	2.8
1	1-C	286	THR	2.8
1	1-S	408	PRO	2.8
1	1-T	391	PRO	2.8
1	1-V	342	CYS	2.8
1	1-W	270	CYS	2.8
1	1-E	48	ALA	2.8
1	1-E	279	ALA	2.8
1	1-F	128	ALA	2.8
1	1-G	130	ALA	2.8
1	1-H	390	ALA	2.8
1	1-M	288	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-N	163	ALA	2.8
1	1-Q	48	ALA	2.8
1	1-C	67	LEU	2.8
1	1-C	274	LEU	2.8
1	1-H	356	LEU	2.8
1	1-R	274	LEU	2.8
1	1-U	290	LEU	2.8
1	1-W	206	LEU	2.8
1	1-A	275	TRP	2.8
1	1-B	275	TRP	2.8
1	1-D	272	GLN	2.8
1	1-E	187	GLN	2.8
1	1-H	467	ASP	2.8
1	1-I	122	ASP	2.8
1	1-K	282	MET	2.8
1	1-K	413	GLN	2.8
1	1-M	39	ASP	2.8
1	1-M	389	GLN	2.8
1	1-S	45	ASP	2.8
1	1-T	380	ASP	2.8
1	1-D	434	PHE	2.8
1	1-R	426	GLU	2.8
1	1-N	125	TYR	2.8
1	1-T	171	TYR	2.8
1	1-X	16	TYR	2.8
1	1-G	40	LYS	2.8
1	1-H	262	GLY	2.8
1	1-S	295	ARG	2.8
1	1-T	431	GLY	2.8
1	1-A	407	ILE	2.8
1	1-C	444	SER	2.8
1	1-I	117	SER	2.8
1	1-J	155	SER	2.8
1	1-P	264	ASN	2.8
1	1-S	386	ILE	2.8
1	1-S	425	HIS	2.8
1	1-U	101	SER	2.8
1	1-W	92	HIS	2.8
1	1-L	42	VAL	2.8
1	1-X	173	VAL	2.8
1	1-O	280	PRO	2.8
1	1-U	2	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-D	429	THR	2.8
1	1-R	429	THR	2.8
1	1-V	96	THR	2.8
1	1-W	164	THR	2.8
1	1-I	423	ALA	2.8
1	1-N	390	ALA	2.8
1	1-S	294	ALA	2.8
1	1-V	353	ALA	2.8
1	1-K	68	LEU	2.8
1	1-Q	47	LEU	2.8
1	1-S	379	LEU	2.8
1	1-U	206	LEU	2.8
1	1-W	66	LEU	2.8
1	1-W	342	CYS	2.8
1	1-F	45	ASP	2.8
1	1-H	409	GLN	2.8
1	1-M	15	GLU	2.8
1	1-P	3	ASP	2.8
1	1-Q	285	GLU	2.8
1	1-T	292	ASP	2.8
1	1-W	129	GLU	2.8
1	1-W	152	ASP	2.8
1	1-C	385	LYS	2.8
1	1-F	420	ARG	2.8
1	1-J	420	ARG	2.8
1	1-K	143	ARG	2.8
1	1-Q	31	PHE	2.8
1	1-F	365	GLY	2.8
1	1-N	427	TYR	2.8
1	1-Q	92	HIS	2.8
1	1-T	125	TYR	2.8
1	1-L	116	ILE	2.8
1	1-M	298	ILE	2.8
1	1-R	298	ILE	2.8
1	1-X	291	SER	2.8
1	1-B	468	VAL	2.8
1	1-D	392	VAL	2.8
1	1-I	502	PRO	2.8
1	1-R	346	PRO	2.8
1	1-E	162	ALA	2.8
1	1-Q	121	ALA	2.8
1	1-T	341	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-U	128	ALA	2.8
1	1-W	356	LEU	2.8
1	1-L	270	CYS	2.8
1	1-L	342	CYS	2.8
1	1-C	336	GLN	2.8
1	1-C	45	ASP	2.8
1	1-C	277	ASP	2.8
1	1-C	295	ARG	2.8
1	1-L	352	LYS	2.8
1	1-T	129	GLU	2.8
1	1-R	75	ARG	2.8
1	1-T	354	LYS	2.8
1	1-W	276	LYS	2.8
1	1-K	277	ASP	2.8
1	1-R	122	ASP	2.8
1	1-B	445	PHE	2.8
1	1-C	500	GLY	2.8
1	1-F	211	HIS	2.8
1	1-I	38	PHE	2.8
1	1-L	38	PHE	2.8
1	1-N	230	HIS	2.8
1	1-O	127	GLY	2.8
1	1-O	425	HIS	2.8
1	1-W	225	PHE	2.8
1	1-H	278	GLY	2.8
1	1-Q	275	TRP	2.8
1	1-W	381	GLY	2.8
1	1-C	114	TYR	2.8
1	1-H	125	TYR	2.8
1	1-L	347	ILE	2.8
1	1-R	120	ILE	2.8
1	1-V	120	ILE	2.8
1	1-W	386	ILE	2.8
1	1-T	155	SER	2.8
1	1-W	117	SER	2.8
1	1-X	444	SER	2.8
1	1-I	173	VAL	2.8
1	1-D	308	LEU	2.8
1	1-G	128	ALA	2.8
1	1-G	379	LEU	2.8
1	1-I	274	LEU	2.8
1	1-L	121	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	379	LEU	2.8
1	1-Q	37	ALA	2.8
1	1-Q	410	THR	2.8
1	1-R	301	LEU	2.8
1	1-A	40	LYS	2.8
1	1-I	359	ARG	2.8
1	1-J	207	GLU	2.8
1	1-K	40	LYS	2.8
1	1-L	295	ARG	2.8
1	1-M	10	LYS	2.8
1	1-Q	352	LYS	2.8
1	1-S	603	LYS	2.8
1	1-S	409	GLN	2.8
1	1-U	187	GLN	2.8
1	1-V	12	GLU	2.8
1	1-M	4	ASP	2.8
1	1-Q	4	ASP	2.8
1	1-W	467	ASP	2.8
1	1-Q	211	HIS	2.8
1	1-S	304	HIS	2.8
1	1-E	365	GLY	2.7
1	1-F	225	PHE	2.8
1	1-L	418	ILE	2.7
1	1-O	298	ILE	2.7
1	1-V	298	ILE	2.7
1	1-F	313	ASN	2.7
1	1-G	280	PRO	2.7
1	1-H	351	PRO	2.7
1	1-J	436	ASN	2.7
1	1-K	16	TYR	2.7
1	1-K	331	ASN	2.7
1	1-U	157	TRP	2.7
1	1-P	125	TYR	2.7
1	1-E	155	SER	2.7
1	1-R	117	SER	2.7
1	1-A	82	ALA	2.7
1	1-C	164	THR	2.7
1	1-C	302	LEU	2.7
1	1-D	286	THR	2.7
1	1-E	164	THR	2.7
1	1-E	206	LEU	2.7
1	1-E	286	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-R	290	LEU	2.7
1	1-U	429	THR	2.7
1	1-X	290	LEU	2.7
1	1-V	37	ALA	2.7
1	1-W	37	ALA	2.7
1	1-X	82	ALA	2.7
1	1-H	603	LYS	2.7
1	1-R	83	LYS	2.7
1	1-I	129	GLU	2.7
1	1-Q	12	GLU	2.7
1	1-P	342	CYS	2.7
1	1-X	342	CYS	2.7
1	1-A	3	ASP	2.7
1	1-D	292	ASP	2.7
1	1-E	39	ASP	2.7
1	1-I	296	HIS	2.7
1	1-L	296	HIS	2.7
1	1-N	4	ASP	2.7
1	1-R	425	HIS	2.7
1	1-U	39	ASP	2.7
1	1-D	6	PHE	2.7
1	1-J	250	GLY	2.7
1	1-U	278	GLY	2.7
1	1-W	180	PHE	2.7
1	1-I	116	ILE	2.7
1	1-B	351	PRO	2.7
1	1-E	264	ASN	2.7
1	1-F	411	PRO	2.7
1	1-M	306	PRO	2.7
1	1-R	222	ASN	2.7
1	1-B	125	TYR	2.7
1	1-H	297	TYR	2.7
1	1-H	340	SER	2.7
1	1-L	91	VAL	2.7
1	1-M	101	SER	2.7
1	1-R	333	VAL	2.7
1	1-U	297	TYR	2.7
1	1-W	16	TYR	2.7
1	1-A	379	LEU	2.7
1	1-L	302	LEU	2.7
1	1-B	390	ALA	2.7
1	1-H	164	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-J	282	MET	2.7
1	1-L	276	LYS	2.7
1	1-L	410	THR	2.7
1	1-M	429	THR	2.7
1	1-Q	423	ALA	2.7
1	1-T	429	THR	2.7
1	1-U	176	LYS	2.7
1	1-U	279	ALA	2.7
1	1-A	359	ARG	2.7
1	1-I	295	ARG	2.7
1	1-K	359	ARG	2.7
1	1-S	102	ARG	2.7
1	1-V	295	ARG	2.7
1	1-I	387	GLU	2.7
1	1-J	357	GLU	2.7
1	1-K	15	GLU	2.7
1	1-S	207	GLU	2.7
1	1-H	187	GLN	2.7
1	1-W	187	GLN	2.7
1	1-N	271	HIS	2.7
1	1-V	211	HIS	2.7
1	1-E	152	ASP	2.7
1	1-G	3	ASP	2.7
1	1-I	277	ASP	2.7
1	1-K	342	CYS	2.7
1	1-L	3	ASP	2.7
1	1-L	445	PHE	2.7
1	1-O	365	GLY	2.7
1	1-X	38	PHE	2.7
1	1-F	27	ILE	2.7
1	1-I	382	ILE	2.7
1	1-L	407	ILE	2.7
1	1-S	154	ILE	2.7
1	1-D	391	PRO	2.7
1	1-M	184	PRO	2.7
1	1-H	222	ASN	2.7
1	1-A	91	VAL	2.7
1	1-C	323	VAL	2.7
1	1-A	290	LEU	2.7
1	1-B	603	LYS	2.7
1	1-I	343	VAL	2.7
1	1-M	340	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-M	343	VAL	2.7
1	1-S	273	SER	2.7
1	1-T	468	VAL	2.7
1	1-E	297	TYR	2.7
1	1-V	275	TRP	2.7
1	1-W	274	LEU	2.7
1	1-X	157	TRP	2.7
1	1-E	128	ALA	2.7
1	1-Q	124	ALA	2.7
1	1-X	102	ARG	2.7
1	1-M	422	GLU	2.7
1	1-N	72	GLU	2.7
1	1-O	602	GLU	2.7
1	1-Q	272	GLN	2.7
1	1-L	211	HIS	2.7
1	1-S	303	HIS	2.7
1	1-U	122	ASP	2.7
1	1-W	3	ASP	2.7
1	1-A	51	GLY	2.7
1	1-D	209	GLY	2.7
1	1-E	51	GLY	2.7
1	1-F	432	GLY	2.7
1	1-T	500	GLY	2.7
1	1-W	217	GLY	2.7
1	1-X	278	GLY	2.7
1	1-A	38	PHE	2.7
1	1-M	502	PRO	2.7
1	1-O	502	PRO	2.7
1	1-U	99	PRO	2.7
1	1-V	346	PRO	2.7
1	1-X	306	PRO	2.7
1	1-C	264	ASN	2.7
1	1-G	185	ASN	2.7
1	1-L	603	LYS	2.7
1	1-L	110	LYS	2.7
1	1-L	264	ASN	2.7
1	1-P	10	LYS	2.7
1	1-Q	603	LYS	2.7
1	1-Q	10	LYS	2.7
1	1-C	68	LEU	2.7
1	1-D	376	MET	2.7
1	1-E	173	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-L	282	MET	2.7
1	1-E	340	SER	2.7
1	1-N	68	LEU	2.7
1	1-X	356	LEU	2.7
1	1-X	433	VAL	2.7
1	1-B	387	GLU	2.7
1	1-K	279	ALA	2.7
1	1-K	288	ALA	2.7
1	1-L	32	THR	2.7
1	1-M	410	THR	2.7
1	1-N	165	GLU	2.7
1	1-P	288	ALA	2.7
1	1-P	305	ALA	2.7
1	1-V	98	GLU	2.7
1	1-W	162	ALA	2.7
1	1-F	187	GLN	2.7
1	1-U	336	GLN	2.7
1	1-K	271	HIS	2.7
1	1-L	425	HIS	2.7
1	1-T	271	HIS	2.7
1	1-A	39	ASP	2.6
1	1-B	467	ASP	2.6
1	1-C	292	ASP	2.6
1	1-G	467	ASP	2.6
1	1-Q	277	ASP	2.6
1	1-S	39	ASP	2.6
1	1-W	265	GLY	2.6
1	1-W	365	GLY	2.6
1	1-X	500	GLY	2.6
1	1-G	407	ILE	2.6
1	1-J	38	PHE	2.6
1	1-K	6	PHE	2.6
1	1-K	382	ILE	2.6
1	1-O	342	CYS	2.6
1	1-R	603	LYS	2.6
1	1-V	180	PHE	2.6
1	1-W	603	LYS	2.6
1	1-D	420	ARG	2.6
1	1-I	174	ARG	2.6
1	1-L	102	ARG	2.6
1	1-U	282	MET	2.6
1	1-B	67	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-I	333	VAL	2.6
1	1-K	173	VAL	2.6
1	1-O	24	LEU	2.6
1	1-T	47	LEU	2.6
1	1-W	281	LEU	2.6
1	1-C	155	SER	2.6
1	1-L	415	SER	2.6
1	1-N	291	SER	2.6
1	1-O	117	SER	2.6
1	1-R	155	SER	2.6
1	1-S	72	GLU	2.6
1	1-S	440	GLU	2.6
1	1-W	72	GLU	2.6
1	1-A	48	ALA	2.6
1	1-A	297	TYR	2.6
1	1-B	118	THR	2.6
1	1-B	286	THR	2.6
1	1-B	409	GLN	2.6
1	1-B	466	TYR	2.6
1	1-G	389	GLN	2.6
1	1-I	163	ALA	2.6
1	1-O	288	ALA	2.6
1	1-S	37	ALA	2.6
1	1-T	48	ALA	2.6
1	1-V	423	ALA	2.6
1	1-W	171	TYR	2.6
1	1-M	92	HIS	2.6
1	1-E	4	ASP	2.6
1	1-A	603	LYS	2.6
1	1-F	503	GLY	2.6
1	1-G	378	GLY	2.6
1	1-L	156	GLY	2.6
1	1-N	44	ASP	2.6
1	1-P	40	LYS	2.6
1	1-P	432	GLY	2.6
1	1-T	45	ASP	2.6
1	1-A	345	ILE	2.6
1	1-A	408	PRO	2.6
1	1-E	6	PHE	2.6
1	1-S	120	ILE	2.6
1	1-X	107	ILE	2.6
1	1-A	355	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-G	102	ARG	2.6
1	1-I	282	MET	2.6
1	1-L	420	ARG	2.6
1	1-P	102	ARG	2.6
1	1-P	359	ARG	2.6
1	1-U	342	CYS	2.6
1	1-L	356	LEU	2.6
1	1-N	88	ASN	2.6
1	1-O	115	LEU	2.6
1	1-Q	206	LEU	2.6
1	1-C	5	VAL	2.6
1	1-D	387	GLU	2.6
1	1-E	333	VAL	2.6
1	1-N	323	VAL	2.6
1	1-E	406	SER	2.6
1	1-I	273	SER	2.6
1	1-N	340	SER	2.6
1	1-P	360	SER	2.6
1	1-H	163	ALA	2.6
1	1-L	163	ALA	2.6
1	1-L	429	THR	2.6
1	1-Q	463	ALA	2.6
1	1-R	353	ALA	2.6
1	1-U	96	THR	2.6
1	1-V	231	ALA	2.6
1	1-A	303	HIS	2.6
1	1-C	297	TYR	2.6
1	1-C	303	HIS	2.6
1	1-H	425	HIS	2.6
1	1-J	296	HIS	2.6
1	1-L	427	TYR	2.6
1	1-P	230	HIS	2.6
1	1-S	100	TYR	2.6
1	1-L	13	LYS	2.6
1	1-N	40	LYS	2.6
1	1-C	393	ASP	2.6
1	1-G	119	GLY	2.6
1	1-H	431	GLY	2.6
1	1-J	3	ASP	2.6
1	1-L	380	ASP	2.6
1	1-R	44	ASP	2.6
1	1-S	209	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-T	265	GLY	2.6
1	1-X	284	ASP	2.6
1	1-K	99	PRO	2.6
1	1-M	346	PRO	2.6
1	1-Q	411	PRO	2.6
1	1-M	345	ILE	2.6
1	1-T	355	ARG	2.6
1	1-W	382	ILE	2.6
1	1-X	359	ARG	2.6
1	1-B	206	LEU	2.6
1	1-B	421	LEU	2.6
1	1-E	97	LEU	2.6
1	1-E	332	LEU	2.6
1	1-F	356	LEU	2.6
1	1-J	332	LEU	2.6
1	1-M	387	GLU	2.6
1	1-R	8	LEU	2.6
1	1-B	331	ASN	2.6
1	1-G	417	VAL	2.6
1	1-K	106	ASN	2.6
1	1-N	222	ASN	2.6
1	1-R	342	CYS	2.6
1	1-P	182	VAL	2.6
1	1-F	389	GLN	2.6
1	1-H	52	SER	2.6
1	1-K	444	SER	2.6
1	1-W	155	SER	2.6
1	1-L	312	THR	2.6
1	1-N	162	ALA	2.6
1	1-M	296	HIS	2.6
1	1-N	92	HIS	2.6
1	1-O	211	HIS	2.6
1	1-D	100	TYR	2.6
1	1-G	114	TYR	2.6
1	1-I	125	TYR	2.6
1	1-X	297	TYR	2.6
1	1-O	385	LYS	2.6
1	1-C	275	TRP	2.6
1	1-D	500	GLY	2.6
1	1-E	184	PRO	2.6
1	1-F	419	ASP	2.6
1	1-G	380	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-I	203	GLY	2.6
1	1-K	355	ARG	2.6
1	1-L	391	PRO	2.6
1	1-R	500	GLY	2.6
1	1-U	45	ASP	2.6
1	1-G	120	ILE	2.6
1	1-J	154	ILE	2.6
1	1-V	439	ILE	2.6
1	1-I	225	PHE	2.6
1	1-J	21	PHE	2.6
1	1-S	180	PHE	2.6
1	1-D	15	GLU	2.6
1	1-E	12	GLU	2.6
1	1-J	12	GLU	2.6
1	1-K	375	LEU	2.6
1	1-L	112	GLU	2.6
1	1-L	206	LEU	2.6
1	1-L	308	LEU	2.6
1	1-P	72	GLU	2.6
1	1-M	384	ASN	2.6
1	1-P	449	ASN	2.6
1	1-Q	454	ASN	2.6
1	1-T	384	ASN	2.6
1	1-D	270	CYS	2.6
1	1-G	342	CYS	2.6
1	1-A	211	HIS	2.6
1	1-C	175	HIS	2.6
1	1-F	144	ALA	2.6
1	1-G	360	SER	2.6
1	1-H	348	THR	2.6
1	1-J	92	HIS	2.6
1	1-J	163	ALA	2.6
1	1-K	269	HIS	2.6
1	1-K	390	ALA	2.6
1	1-P	501	SER	2.6
1	1-T	390	ALA	2.6
1	1-X	41	SER	2.6
1	1-N	164	THR	2.6
1	1-L	10	LYS	2.6
1	1-L	40	LYS	2.6
1	1-K	460	TYR	2.6
1	1-M	295	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-O	75	ARG	2.5
1	1-S	359	ARG	2.5
1	1-T	420	ARG	2.5
1	1-S	275	TRP	2.5
1	1-B	4	ASP	2.5
1	1-B	263	ASP	2.5
1	1-D	45	ASP	2.5
1	1-D	365	GLY	2.5
1	1-F	46	GLY	2.5
1	1-K	190	ASP	2.5
1	1-S	419	ASP	2.5
1	1-V	393	ASP	2.5
1	1-G	221	ILE	2.5
1	1-G	298	ILE	2.5
1	1-A	180	PHE	2.5
1	1-D	440	GLU	2.5
1	1-F	72	GLU	2.5
1	1-K	434	PHE	2.5
1	1-J	67	LEU	2.5
1	1-J	206	LEU	2.5
1	1-N	356	LEU	2.5
1	1-O	66	LEU	2.5
1	1-U	47	LEU	2.5
1	1-U	274	LEU	2.5
1	1-V	66	LEU	2.5
1	1-X	281	LEU	2.5
1	1-B	343	VAL	2.5
1	1-K	5	VAL	2.5
1	1-K	389	GLN	2.5
1	1-L	182	VAL	2.5
1	1-C	296	HIS	2.5
1	1-C	342	CYS	2.5
1	1-F	162	ALA	2.5
1	1-G	501	SER	2.5
1	1-K	41	SER	2.5
1	1-K	108	ALA	2.5
1	1-L	390	ALA	2.5
1	1-M	444	SER	2.5
1	1-N	353	ALA	2.5
1	1-S	444	SER	2.5
1	1-E	125	TYR	2.5
1	1-K	125	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-X	171	TYR	2.5
1	1-A	391	PRO	2.5
1	1-E	181	PRO	2.5
1	1-F	300	GLY	2.5
1	1-L	306	PRO	2.5
1	1-N	122	ASP	2.5
1	1-N	278	GLY	2.5
1	1-Q	280	PRO	2.5
1	1-V	284	ASP	2.5
1	1-X	122	ASP	2.5
1	1-X	217	GLY	2.5
1	1-H	347	ILE	2.5
1	1-N	116	ILE	2.5
1	1-V	382	ILE	2.5
1	1-X	87	ILE	2.5
1	1-X	205	ILE	2.5
1	1-A	129	GLU	2.5
1	1-H	357	GLU	2.5
1	1-T	440	GLU	2.5
1	1-D	379	LEU	2.5
1	1-G	47	LEU	2.5
1	1-H	38	PHE	2.5
1	1-U	67	LEU	2.5
1	1-W	413	GLN	2.5
1	1-C	352	LYS	2.5
1	1-C	425	HIS	2.5
1	1-F	296	HIS	2.5
1	1-G	354	LYS	2.5
1	1-J	88	ASN	2.5
1	1-K	264	ASN	2.5
1	1-M	5	VAL	2.5
1	1-O	222	ASN	2.5
1	1-Q	213	VAL	2.5
1	1-R	110	LYS	2.5
1	1-G	111	ALA	2.5
1	1-H	144	ALA	2.5
1	1-T	288	ALA	2.5
1	1-X	373	ALA	2.5
1	1-C	429	THR	2.5
1	1-E	444	SER	2.5
1	1-F	101	SER	2.5
1	1-M	123	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	123	THR	2.5
1	1-W	363	SER	2.5
1	1-U	295	ARG	2.5
1	1-I	65	MET	2.5
1	1-F	71	PRO	2.5
1	1-F	171	TYR	2.5
1	1-G	223	TYR	2.5
1	1-I	2	PRO	2.5
1	1-I	69	PRO	2.5
1	1-K	306	PRO	2.5
1	1-M	16	TYR	2.5
1	1-P	346	PRO	2.5
1	1-W	99	PRO	2.5
1	1-C	216	GLY	2.5
1	1-E	170	GLY	2.5
1	1-J	500	GLY	2.5
1	1-S	432	GLY	2.5
1	1-C	98	GLU	2.5
1	1-F	122	ASP	2.5
1	1-N	345	ILE	2.5
1	1-O	387	GLU	2.5
1	1-X	263	ASP	2.5
1	1-K	116	ILE	2.5
1	1-R	205	ILE	2.5
1	1-C	434	PHE	2.5
1	1-M	421	LEU	2.5
1	1-P	68	LEU	2.5
1	1-R	38	PHE	2.5
1	1-S	38	PHE	2.5
1	1-E	383	LYS	2.5
1	1-J	10	LYS	2.5
1	1-J	352	LYS	2.5
1	1-M	352	LYS	2.5
1	1-D	323	VAL	2.5
1	1-R	454	ASN	2.5
1	1-V	185	ASN	2.5
1	1-W	213	VAL	2.5
1	1-W	333	VAL	2.5
1	1-E	359	ARG	2.5
1	1-I	355	ARG	2.5
1	1-J	128	ALA	2.5
1	1-L	232	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-O	344	ARG	2.5
1	1-Q	35	ALA	2.5
1	1-Q	231	ALA	2.5
1	1-R	359	ARG	2.5
1	1-A	36	SER	2.5
1	1-A	340	SER	2.5
1	1-E	501	SER	2.5
1	1-J	318	SER	2.5
1	1-L	1	THR	2.5
1	1-N	363	SER	2.5
1	1-O	286	THR	2.5
1	1-R	101	SER	2.5
1	1-T	291	SER	2.5
1	1-U	441	THR	2.5
1	1-V	101	SER	2.5
1	1-V	441	THR	2.5
1	1-F	78	PRO	2.5
1	1-J	34	PRO	2.5
1	1-L	181	PRO	2.5
1	1-I	500	GLY	2.5
1	1-I	503	GLY	2.5
1	1-N	46	GLY	2.5
1	1-O	503	GLY	2.5
1	1-O	3	ASP	2.5
1	1-O	44	ASP	2.5
1	1-O	283	TYR	2.5
1	1-P	357	GLU	2.5
1	1-S	171	TYR	2.5
1	1-T	387	GLU	2.5
1	1-T	432	GLY	2.5
1	1-B	297	TYR	2.5
1	1-C	4	ASP	2.5
1	1-D	39	ASP	2.5
1	1-G	39	ASP	2.5
1	1-H	122	ASP	2.5
1	1-I	345	ILE	2.5
1	1-L	330	ILE	2.5
1	1-Q	330	ILE	2.5
1	1-T	284	ASP	2.5
1	1-W	120	ILE	2.5
1	1-D	66	LEU	2.5
1	1-D	68	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-H	67	LEU	2.5
1	1-L	47	LEU	2.5
1	1-L	281	LEU	2.5
1	1-M	67	LEU	2.5
1	1-Q	274	LEU	2.5
1	1-U	68	LEU	2.5
1	1-G	180	PHE	2.5
1	1-I	336	GLN	2.5
1	1-K	336	GLN	2.5
1	1-O	180	PHE	2.5
1	1-T	6	PHE	2.5
1	1-A	304	HIS	2.5
1	1-D	92	HIS	2.5
1	1-E	213	VAL	2.5
1	1-F	454	ASN	2.5
1	1-H	343	VAL	2.5
1	1-I	42	VAL	2.5
1	1-T	185	ASN	2.5
1	1-U	355	ARG	2.5
1	1-A	124	ALA	2.5
1	1-B	128	ALA	2.5
1	1-D	48	ALA	2.5
1	1-E	183	ALA	2.5
1	1-K	37	ALA	2.5
1	1-M	353	ALA	2.5
1	1-M	463	ALA	2.5
1	1-T	128	ALA	2.5
1	1-W	35	ALA	2.5
1	1-J	123	THR	2.5
1	1-J	372	SER	2.5
1	1-L	123	THR	2.5
1	1-L	441	THR	2.5
1	1-V	1	THR	2.5
1	1-V	155	SER	2.5
1	1-W	41	SER	2.5
1	1-X	441	THR	2.5
1	1-A	99	PRO	2.4
1	1-F	306	PRO	2.4
1	1-H	280	PRO	2.4
1	1-P	270	CYS	2.4
1	1-C	365	GLY	2.4
1	1-D	165	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-G	357	GLU	2.4
1	1-P	209	GLY	2.4
1	1-P	422	GLU	2.4
1	1-R	378	GLY	2.4
1	1-U	46	GLY	2.4
1	1-U	72	GLU	2.4
1	1-B	283	TYR	2.4
1	1-D	171	TYR	2.4
1	1-F	125	TYR	2.4
1	1-J	407	ILE	2.4
1	1-N	114	TYR	2.4
1	1-N	171	TYR	2.4
1	1-Q	114	TYR	2.4
1	1-R	152	ASP	2.4
1	1-S	116	ILE	2.4
1	1-T	385	LYS	2.4
1	1-U	603	LYS	2.4
1	1-U	383	LYS	2.4
1	1-V	152	ASP	2.4
1	1-B	308	LEU	2.4
1	1-F	274	LEU	2.4
1	1-G	356	LEU	2.4
1	1-J	68	LEU	2.4
1	1-N	67	LEU	2.4
1	1-P	356	LEU	2.4
1	1-S	421	LEU	2.4
1	1-V	356	LEU	2.4
1	1-L	409	GLN	2.4
1	1-G	126	PHE	2.4
1	1-J	271	HIS	2.4
1	1-N	445	PHE	2.4
1	1-S	211	HIS	2.4
1	1-U	225	PHE	2.4
1	1-U	303	HIS	2.4
1	1-A	295	ARG	2.4
1	1-Q	247	TRP	2.4
1	1-F	173	VAL	2.4
1	1-F	331	ASN	2.4
1	1-H	313	ASN	2.4
1	1-K	213	VAL	2.4
1	1-K	343	VAL	2.4
1	1-O	343	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	343	VAL	2.4
1	1-X	453	VAL	2.4
1	1-E	9	ALA	2.4
1	1-G	183	ALA	2.4
1	1-I	48	ALA	2.4
1	1-K	35	ALA	2.4
1	1-T	37	ALA	2.4
1	1-X	390	ALA	2.4
1	1-K	293	THR	2.4
1	1-N	118	THR	2.4
1	1-S	123	THR	2.4
1	1-E	117	SER	2.4
1	1-E	291	SER	2.4
1	1-J	142	SER	2.4
1	1-L	501	SER	2.4
1	1-X	36	SER	2.4
1	1-B	34	PRO	2.4
1	1-B	411	PRO	2.4
1	1-C	388	PRO	2.4
1	1-C	400	PRO	2.4
1	1-D	280	PRO	2.4
1	1-P	391	PRO	2.4
1	1-G	212	GLU	2.4
1	1-M	129	GLU	2.4
1	1-M	440	GLU	2.4
1	1-O	15	GLU	2.4
1	1-Q	15	GLU	2.4
1	1-R	207	GLU	2.4
1	1-W	357	GLU	2.4
1	1-X	98	GLU	2.4
1	1-C	431	GLY	2.4
1	1-D	216	GLY	2.4
1	1-E	503	GLY	2.4
1	1-F	603	LYS	2.4
1	1-M	431	GLY	2.4
1	1-O	209	GLY	2.4
1	1-A	45	ASP	2.4
1	1-H	4	ASP	2.4
1	1-I	107	ILE	2.4
1	1-M	122	ASP	2.4
1	1-P	419	ASP	2.4
1	1-R	45	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-U	467	ASP	2.4
1	1-V	277	ASP	2.4
1	1-X	386	ILE	2.4
1	1-E	272	GLN	2.4
1	1-E	421	LEU	2.4
1	1-F	16	TYR	2.4
1	1-F	223	TYR	2.4
1	1-F	290	LEU	2.4
1	1-K	67	LEU	2.4
1	1-U	428	LEU	2.4
1	1-S	230	HIS	2.4
1	1-U	230	HIS	2.4
1	1-C	38	PHE	2.4
1	1-D	102	ARG	2.4
1	1-E	75	ARG	2.4
1	1-N	295	ARG	2.4
1	1-O	38	PHE	2.4
1	1-P	126	PHE	2.4
1	1-T	295	ARG	2.4
1	1-U	359	ARG	2.4
1	1-W	359	ARG	2.4
1	1-X	225	PHE	2.4
1	1-D	157	TRP	2.4
1	1-N	392	VAL	2.4
1	1-U	275	TRP	2.4
1	1-F	74	ALA	2.4
1	1-J	231	ALA	2.4
1	1-O	390	ALA	2.4
1	1-Q	353	ALA	2.4
1	1-R	37	ALA	2.4
1	1-R	130	ALA	2.4
1	1-S	288	ALA	2.4
1	1-U	121	ALA	2.4
1	1-U	124	ALA	2.4
1	1-U	463	ALA	2.4
1	1-J	118	THR	2.4
1	1-N	410	THR	2.4
1	1-A	388	PRO	2.4
1	1-F	408	PRO	2.4
1	1-C	13	LYS	2.4
1	1-I	603	LYS	2.4
1	1-L	207	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-N	360	SER	2.4
1	1-Q	306	PRO	2.4
1	1-R	99	PRO	2.4
1	1-S	346	PRO	2.4
1	1-U	155	SER	2.4
1	1-U	408	PRO	2.4
1	1-W	291	SER	2.4
1	1-X	69	PRO	2.4
1	1-P	354	LYS	2.4
1	1-V	354	LYS	2.4
1	1-B	289	GLY	2.4
1	1-D	431	GLY	2.4
1	1-S	46	GLY	2.4
1	1-W	216	GLY	2.4
1	1-X	127	GLY	2.4
1	1-E	122	ASP	2.4
1	1-L	298	ILE	2.4
1	1-P	382	ILE	2.4
1	1-R	4	ASP	2.4
1	1-X	234	ASP	2.4
1	1-X	298	ILE	2.4
1	1-M	115	LEU	2.4
1	1-B	295	ARG	2.4
1	1-D	211	HIS	2.4
1	1-O	359	ARG	2.4
1	1-Q	271	HIS	2.4
1	1-T	296	HIS	2.4
1	1-V	230	HIS	2.4
1	1-X	109	ARG	2.4
1	1-A	427	TYR	2.4
1	1-D	125	TYR	2.4
1	1-H	223	TYR	2.4
1	1-J	100	TYR	2.4
1	1-N	100	TYR	2.4
1	1-Q	16	TYR	2.4
1	1-U	427	TYR	2.4
1	1-V	297	TYR	2.4
1	1-X	125	TYR	2.4
1	1-G	90	PHE	2.4
1	1-A	453	VAL	2.4
1	1-S	42	VAL	2.4
1	1-X	392	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-L	88	ASN	2.4
1	1-P	185	ASN	2.4
1	1-I	183	ALA	2.4
1	1-L	183	ALA	2.4
1	1-Q	163	ALA	2.4
1	1-T	294	ALA	2.4
1	1-V	124	ALA	2.4
1	1-B	388	PRO	2.4
1	1-B	422	GLU	2.4
1	1-C	2	PRO	2.4
1	1-E	165	GLU	2.4
1	1-E	312	THR	2.4
1	1-I	83	LYS	2.4
1	1-N	123	THR	2.4
1	1-R	164	THR	2.4
1	1-S	83	LYS	2.4
1	1-S	312	THR	2.4
1	1-O	99	PRO	2.4
1	1-O	400	PRO	2.4
1	1-R	2	PRO	2.4
1	1-X	12	GLU	2.4
1	1-S	266	SER	2.4
1	1-D	299	GLY	2.4
1	1-H	432	GLY	2.4
1	1-I	289	GLY	2.4
1	1-T	365	GLY	2.4
1	1-U	156	GLY	2.4
1	1-W	170	GLY	2.4
1	1-X	418	ILE	2.4
1	1-E	24	LEU	2.4
1	1-E	409	GLN	2.4
1	1-F	379	LEU	2.4
1	1-G	211	HIS	2.4
1	1-G	425	HIS	2.4
1	1-H	24	LEU	2.4
1	1-H	344	ARG	2.4
1	1-H	355	ARG	2.4
1	1-M	3	ASP	2.4
1	1-M	277	ASP	2.4
1	1-O	248	GLN	2.4
1	1-P	428	LEU	2.4
1	1-R	39	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-S	11	ASP	2.4
1	1-U	284	ASP	2.4
1	1-H	342	CYS	2.4
1	1-N	270	CYS	2.4
1	1-N	188	TYR	2.4
1	1-O	311	PHE	2.4
1	1-Q	297	TYR	2.4
1	1-S	90	PHE	2.4
1	1-G	5	VAL	2.4
1	1-X	468	VAL	2.4
1	1-S	222	ASN	2.4
1	1-W	264	ASN	2.4
1	1-E	37	ALA	2.4
1	1-H	385	LYS	2.4
1	1-O	352	LYS	2.4
1	1-Q	183	ALA	2.4
1	1-Q	310	ALA	2.4
1	1-T	279	ALA	2.4
1	1-V	81	ALA	2.4
1	1-E	72	GLU	2.4
1	1-A	259	PRO	2.3
1	1-C	157	TRP	2.4
1	1-D	306	PRO	2.3
1	1-F	312	THR	2.3
1	1-I	275	TRP	2.4
1	1-L	411	PRO	2.3
1	1-A	444	SER	2.3
1	1-B	378	GLY	2.3
1	1-R	209	GLY	2.3
1	1-S	265	GLY	2.3
1	1-X	432	GLY	2.3
1	1-A	271	HIS	2.3
1	1-B	39	ASP	2.3
1	1-B	229	LEU	2.3
1	1-D	228	LEU	2.3
1	1-I	221	ILE	2.3
1	1-K	47	LEU	2.3
1	1-L	87	ILE	2.3
1	1-N	386	ILE	2.3
1	1-P	205	ILE	2.3
1	1-P	407	ILE	2.3
1	1-Q	87	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-R	187	GLN	2.3
1	1-I	380	ASP	2.3
1	1-O	467	ASP	2.3
1	1-R	421	LEU	2.3
1	1-S	85	LEU	2.3
1	1-W	428	LEU	2.3
1	1-A	268	MET	2.3
1	1-C	125	TYR	2.3
1	1-F	6	PHE	2.3
1	1-F	38	PHE	2.3
1	1-A	392	VAL	2.3
1	1-B	394	LYS	2.3
1	1-E	385	LYS	2.3
1	1-G	453	VAL	2.3
1	1-H	91	VAL	2.3
1	1-K	13	LYS	2.3
1	1-N	91	VAL	2.3
1	1-R	173	VAL	2.3
1	1-W	110	LYS	2.3
1	1-P	113	ASN	2.3
1	1-R	185	ASN	2.3
1	1-U	185	ASN	2.3
1	1-V	436	ASN	2.3
1	1-A	162	ALA	2.3
1	1-C	37	ALA	2.3
1	1-E	15	GLU	2.3
1	1-H	48	ALA	2.3
1	1-L	162	ALA	2.3
1	1-B	457	PRO	2.3
1	1-C	346	PRO	2.3
1	1-O	314	PRO	2.3
1	1-U	306	PRO	2.3
1	1-E	429	THR	2.3
1	1-K	123	THR	2.3
1	1-P	441	THR	2.3
1	1-B	36	SER	2.3
1	1-D	36	SER	2.3
1	1-O	41	SER	2.3
1	1-O	142	SER	2.3
1	1-P	101	SER	2.3
1	1-Q	355	ARG	2.3
1	1-T	142	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-U	291	SER	2.3
1	1-W	52	SER	2.3
1	1-D	289	GLY	2.3
1	1-E	209	GLY	2.3
1	1-K	300	GLY	2.3
1	1-B	68	LEU	2.3
1	1-D	407	ILE	2.3
1	1-F	221	ILE	2.3
1	1-M	68	LEU	2.3
1	1-M	438	LEU	2.3
1	1-N	115	LEU	2.3
1	1-N	421	LEU	2.3
1	1-O	116	ILE	2.3
1	1-O	230	HIS	2.3
1	1-P	107	ILE	2.3
1	1-U	8	LEU	2.3
1	1-U	271	HIS	2.3
1	1-V	248	GLN	2.3
1	1-G	66	LEU	2.3
1	1-G	308	LEU	2.3
1	1-I	67	LEU	2.3
1	1-I	379	LEU	2.3
1	1-Q	67	LEU	2.3
1	1-R	464	LEU	2.3
1	1-X	221	ILE	2.3
1	1-F	393	ASP	2.3
1	1-M	45	ASP	2.3
1	1-P	122	ASP	2.3
1	1-J	374	MET	2.3
1	1-B	38	PHE	2.3
1	1-F	7	LYS	2.3
1	1-G	6	PHE	2.3
1	1-G	358	PHE	2.3
1	1-H	354	LYS	2.3
1	1-O	270	CYS	2.3
1	1-W	354	LYS	2.3
1	1-X	434	PHE	2.3
1	1-B	323	VAL	2.3
1	1-E	5	VAL	2.3
1	1-G	16	TYR	2.3
1	1-J	427	TYR	2.3
1	1-L	171	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-S	453	VAL	2.3
1	1-X	114	TYR	2.3
1	1-F	131	GLU	2.3
1	1-L	129	GLU	2.3
1	1-W	15	GLU	2.3
1	1-D	222	ASN	2.3
1	1-F	436	ASN	2.3
1	1-I	264	ASN	2.3
1	1-J	264	ASN	2.3
1	1-E	294	ALA	2.3
1	1-G	121	ALA	2.3
1	1-J	502	PRO	2.3
1	1-K	259	PRO	2.3
1	1-M	69	PRO	2.3
1	1-P	81	ALA	2.3
1	1-S	48	ALA	2.3
1	1-J	293	THR	2.3
1	1-K	118	THR	2.3
1	1-V	84	THR	2.3
1	1-B	359	ARG	2.3
1	1-C	273	SER	2.3
1	1-G	157	TRP	2.3
1	1-H	265	GLY	2.3
1	1-K	147	SER	2.3
1	1-L	262	GLY	2.3
1	1-N	157	TRP	2.3
1	1-Q	340	SER	2.3
1	1-S	157	TRP	2.3
1	1-C	230	HIS	2.3
1	1-M	271	HIS	2.3
1	1-X	296	HIS	2.3
1	1-C	386	ILE	2.3
1	1-D	290	LEU	2.3
1	1-E	386	ILE	2.3
1	1-G	274	LEU	2.3
1	1-L	386	ILE	2.3
1	1-Q	120	ILE	2.3
1	1-R	379	LEU	2.3
1	1-U	85	LEU	2.3
1	1-V	386	ILE	2.3
1	1-X	330	ILE	2.3
1	1-X	379	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-I	45	ASP	2.3
1	1-L	284	ASP	2.3
1	1-Q	45	ASP	2.3
1	1-R	3	ASP	2.3
1	1-V	380	ASP	2.3
1	1-J	13	LYS	2.3
1	1-L	194	LYS	2.3
1	1-U	83	LYS	2.3
1	1-L	126	PHE	2.3
1	1-A	16	TYR	2.3
1	1-A	42	VAL	2.3
1	1-D	460	TYR	2.3
1	1-F	14	VAL	2.3
1	1-H	173	VAL	2.3
1	1-H	285	GLU	2.3
1	1-I	426	GLU	2.3
1	1-J	323	VAL	2.3
1	1-K	333	VAL	2.3
1	1-K	430	GLU	2.3
1	1-M	451	GLU	2.3
1	1-P	150	GLU	2.3
1	1-R	114	TYR	2.3
1	1-S	238	TYR	2.3
1	1-T	213	VAL	2.3
1	1-V	91	VAL	2.3
1	1-A	35	ALA	2.3
1	1-E	310	ALA	2.3
1	1-F	121	ALA	2.3
1	1-H	264	ASN	2.3
1	1-I	37	ALA	2.3
1	1-J	288	ALA	2.3
1	1-L	436	ASN	2.3
1	1-N	48	ALA	2.3
1	1-P	408	PRO	2.3
1	1-Q	346	PRO	2.3
1	1-U	280	PRO	2.3
1	1-X	111	ALA	2.3
1	1-C	344	ARG	2.3
1	1-G	75	ARG	2.3
1	1-A	160	THR	2.3
1	1-B	312	THR	2.3
1	1-T	118	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	46	GLY	2.3
1	1-A	187	GLN	2.3
1	1-C	381	GLY	2.3
1	1-N	501	SER	2.3
1	1-N	304	HIS	2.3
1	1-S	119	GLY	2.3
1	1-T	272	GLN	2.3
1	1-V	262	GLY	2.3
1	1-X	46	GLY	2.3
1	1-I	147	SER	2.3
1	1-U	139	SER	2.3
1	1-U	363	SER	2.3
1	1-D	107	ILE	2.3
1	1-G	67	LEU	2.3
1	1-G	275	TRP	2.3
1	1-J	322	LEU	2.3
1	1-L	345	ILE	2.3
1	1-M	221	ILE	2.3
1	1-M	356	LEU	2.3
1	1-N	298	ILE	2.3
1	1-Q	76	ILE	2.3
1	1-Q	464	LEU	2.3
1	1-T	154	ILE	2.3
1	1-T	274	LEU	2.3
1	1-V	330	ILE	2.3
1	1-F	282	MET	2.3
1	1-A	190	ASP	2.3
1	1-E	380	ASP	2.3
1	1-G	13	LYS	2.3
1	1-H	352	LYS	2.3
1	1-M	380	ASP	2.3
1	1-T	152	ASP	2.3
1	1-U	152	ASP	2.3
1	1-F	31	PHE	2.3
1	1-H	225	PHE	2.3
1	1-L	225	PHE	2.3
1	1-S	126	PHE	2.3
1	1-T	426	GLU	2.3
1	1-V	6	PHE	2.3
1	1-X	387	GLU	2.3
1	1-O	213	VAL	2.3
1	1-B	502	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-C	280	PRO	2.3
1	1-D	342	CYS	2.3
1	1-J	125	TYR	2.3
1	1-K	102	ARG	2.3
1	1-S	69	PRO	2.3
1	1-V	99	PRO	2.3
1	1-C	163	ALA	2.2
1	1-C	390	ALA	2.2
1	1-J	279	ALA	2.2
1	1-M	9	ALA	2.2
1	1-Q	185	ASN	2.2
1	1-U	460	TYR	2.3
1	1-V	48	ALA	2.2
1	1-A	441	THR	2.2
1	1-I	118	THR	2.2
1	1-N	84	THR	2.2
1	1-R	312	THR	2.2
1	1-A	209	GLY	2.2
1	1-G	300	GLY	2.2
1	1-I	303	HIS	2.2
1	1-K	425	HIS	2.2
1	1-L	230	HIS	2.2
1	1-N	161	GLY	2.2
1	1-Q	365	GLY	2.2
1	1-R	272	GLN	2.2
1	1-R	381	GLY	2.2
1	1-U	425	HIS	2.2
1	1-A	27	ILE	2.2
1	1-A	421	LEU	2.2
1	1-G	281	LEU	2.2
1	1-G	438	LEU	2.2
1	1-K	274	LEU	2.2
1	1-K	332	LEU	2.2
1	1-M	415	SER	2.2
1	1-N	101	SER	2.2
1	1-P	47	LEU	2.2
1	1-R	281	LEU	2.2
1	1-R	439	ILE	2.2
1	1-T	24	LEU	2.2
1	1-T	379	LEU	2.2
1	1-V	352	LYS	2.2
1	1-V	444	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-W	36	SER	2.2
1	1-W	421	LEU	2.2
1	1-X	110	LYS	2.2
1	1-X	385	LYS	2.2
1	1-C	152	ASP	2.2
1	1-E	45	ASP	2.2
1	1-R	284	ASP	2.2
1	1-E	358	PHE	2.2
1	1-I	445	PHE	2.2
1	1-L	180	PHE	2.2
1	1-N	225	PHE	2.2
1	1-X	311	PHE	2.2
1	1-A	344	ARG	2.2
1	1-E	91	VAL	2.2
1	1-H	417	VAL	2.2
1	1-I	75	ARG	2.2
1	1-J	14	VAL	2.2
1	1-L	213	VAL	2.2
1	1-L	417	VAL	2.2
1	1-M	355	ARG	2.2
1	1-T	169	ARG	2.2
1	1-T	323	VAL	2.2
1	1-V	411	PRO	2.2
1	1-W	346	PRO	2.2
1	1-W	417	VAL	2.2
1	1-A	121	ALA	2.2
1	1-D	305	ALA	2.2
1	1-G	48	ALA	2.2
1	1-O	35	ALA	2.2
1	1-P	341	ALA	2.2
1	1-D	427	TYR	2.2
1	1-G	238	TYR	2.2
1	1-A	410	THR	2.2
1	1-C	409	GLN	2.2
1	1-J	211	HIS	2.2
1	1-M	187	GLN	2.2
1	1-U	409	GLN	2.2
1	1-V	187	GLN	2.2
1	1-B	7	LYS	2.2
1	1-L	209	GLY	2.2
1	1-N	354	LYS	2.2
1	1-Q	385	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-U	251	LYS	2.2
1	1-G	421	LEU	2.2
1	1-M	274	LEU	2.2
1	1-P	290	LEU	2.2
1	1-P	308	LEU	2.2
1	1-S	24	LEU	2.2
1	1-S	290	LEU	2.2
1	1-W	47	LEU	2.2
1	1-W	301	LEU	2.2
1	1-F	291	SER	2.2
1	1-H	363	SER	2.2
1	1-I	155	SER	2.2
1	1-K	87	ILE	2.2
1	1-M	41	SER	2.2
1	1-T	418	ILE	2.2
1	1-U	87	ILE	2.2
1	1-U	120	ILE	2.2
1	1-U	273	SER	2.2
1	1-W	407	ILE	2.2
1	1-H	380	ASP	2.2
1	1-Q	122	ASP	2.2
1	1-R	263	ASP	2.2
1	1-A	387	GLU	2.2
1	1-L	220	GLU	2.2
1	1-M	212	GLU	2.2
1	1-V	72	GLU	2.2
1	1-K	80	ARG	2.2
1	1-O	295	ARG	2.2
1	1-J	225	PHE	2.2
1	1-Q	38	PHE	2.2
1	1-Q	311	PHE	2.2
1	1-T	38	PHE	2.2
1	1-A	333	VAL	2.2
1	1-B	17	VAL	2.2
1	1-F	5	VAL	2.2
1	1-K	502	PRO	2.2
1	1-N	69	PRO	2.2
1	1-N	99	PRO	2.2
1	1-T	280	PRO	2.2
1	1-U	343	VAL	2.2
1	1-V	343	VAL	2.2
1	1-W	343	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-X	343	VAL	2.2
1	1-A	463	ALA	2.2
1	1-B	454	ASN	2.2
1	1-D	288	ALA	2.2
1	1-H	162	ALA	2.2
1	1-P	463	ALA	2.2
1	1-R	81	ALA	2.2
1	1-S	81	ALA	2.2
1	1-T	162	ALA	2.2
1	1-X	294	ALA	2.2
1	1-D	13	LYS	2.2
1	1-E	303	HIS	2.2
1	1-I	352	LYS	2.2
1	1-P	304	HIS	2.2
1	1-A	342	CYS	2.2
1	1-K	312	THR	2.2
1	1-R	270	CYS	2.2
1	1-X	123	THR	2.2
1	1-X	224	GLN	2.2
1	1-D	67	LEU	2.2
1	1-H	8	LEU	2.2
1	1-K	431	GLY	2.2
1	1-M	503	GLY	2.2
1	1-P	119	GLY	2.2
1	1-T	206	LEU	2.2
1	1-V	161	GLY	2.2
1	1-X	308	LEU	2.2
1	1-B	205	ILE	2.2
1	1-B	439	ILE	2.2
1	1-D	33	ILE	2.2
1	1-N	205	ILE	2.2
1	1-T	27	ILE	2.2
1	1-A	501	SER	2.2
1	1-D	501	SER	2.2
1	1-F	444	SER	2.2
1	1-L	36	SER	2.2
1	1-O	155	SER	2.2
1	1-T	41	SER	2.2
1	1-U	335	SER	2.2
1	1-V	41	SER	2.2
1	1-X	101	SER	2.2
1	1-B	152	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-D	4	ASP	2.2
1	1-O	284	ASP	2.2
1	1-O	292	ASP	2.2
1	1-P	103	ASP	2.2
1	1-W	45	ASP	2.2
1	1-E	357	GLU	2.2
1	1-L	451	GLU	2.2
1	1-F	442	TRP	2.2
1	1-T	157	TRP	2.2
1	1-I	99	PRO	2.2
1	1-O	445	PHE	2.2
1	1-P	2	PRO	2.2
1	1-P	38	PHE	2.2
1	1-Q	126	PHE	2.2
1	1-S	314	PRO	2.2
1	1-S	391	PRO	2.2
1	1-X	126	PHE	2.2
1	1-A	468	VAL	2.2
1	1-L	433	VAL	2.2
1	1-T	417	VAL	2.2
1	1-C	603	LYS	2.2
1	1-G	81	ALA	2.2
1	1-H	82	ALA	2.2
1	1-H	92	HIS	2.2
1	1-I	353	ALA	2.2
1	1-J	354	LYS	2.2
1	1-M	390	ALA	2.2
1	1-P	231	ALA	2.2
1	1-Q	390	ALA	2.2
1	1-R	7	LYS	2.2
1	1-R	40	LYS	2.2
1	1-J	454	ASN	2.2
1	1-M	425	HIS	2.2
1	1-R	82	ALA	2.2
1	1-S	305	ALA	2.2
1	1-V	341	ALA	2.2
1	1-W	185	ASN	2.2
1	1-W	454	ASN	2.2
1	1-L	272	GLN	2.2
1	1-A	332	LEU	2.2
1	1-B	47	LEU	2.2
1	1-B	146	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-D	203	GLY	2.2
1	1-E	466	TYR	2.2
1	1-F	149	TYR	2.2
1	1-M	312	THR	2.2
1	1-O	149	TYR	2.2
1	1-P	312	THR	2.2
1	1-S	308	LEU	2.2
1	1-T	427	TYR	2.2
1	1-U	118	THR	2.2
1	1-U	412	THR	2.2
1	1-F	270	CYS	2.2
1	1-H	274	LEU	2.2
1	1-J	8	LEU	2.2
1	1-J	365	GLY	2.2
1	1-J	464	LEU	2.2
1	1-P	421	LEU	2.2
1	1-Q	68	LEU	2.2
1	1-R	428	LEU	2.2
1	1-X	464	LEU	2.2
1	1-C	330	ILE	2.2
1	1-E	41	SER	2.2
1	1-F	137	SER	2.2
1	1-H	155	SER	2.2
1	1-H	291	SER	2.2
1	1-J	291	SER	2.2
1	1-D	212	GLU	2.2
1	1-E	416	ASP	2.2
1	1-F	380	ASP	2.2
1	1-Q	212	GLU	2.2
1	1-R	380	ASP	2.2
1	1-R	419	ASP	2.2
1	1-U	167	ASP	2.2
1	1-V	102	ARG	2.2
1	1-D	2	PRO	2.2
1	1-U	502	PRO	2.2
1	1-A	6	PHE	2.2
1	1-F	13	LYS	2.2
1	1-G	225	PHE	2.2
1	1-R	320	LYS	2.2
1	1-M	91	VAL	2.1
1	1-P	468	VAL	2.1
1	1-G	230	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-E	331	ASN	2.1
1	1-J	81	ALA	2.1
1	1-K	153	ALA	2.1
1	1-K	187	GLN	2.1
1	1-K	377	ALA	2.1
1	1-M	222	ASN	2.1
1	1-O	264	ASN	2.1
1	1-O	409	GLN	2.1
1	1-R	377	ALA	2.1
1	1-U	296	HIS	2.1
1	1-V	222	ASN	2.1
1	1-A	47	LEU	2.1
1	1-A	429	THR	2.1
1	1-A	438	LEU	2.1
1	1-C	281	LEU	2.1
1	1-C	312	THR	2.1
1	1-C	421	LEU	2.1
1	1-E	85	LEU	2.1
1	1-F	209	GLY	2.1
1	1-F	299	GLY	2.1
1	1-J	66	LEU	2.1
1	1-K	281	LEU	2.1
1	1-M	206	LEU	2.1
1	1-P	381	GLY	2.1
1	1-S	47	LEU	2.1
1	1-V	85	LEU	2.1
1	1-V	206	LEU	2.1
1	1-W	267	GLY	2.1
1	1-D	27	ILE	2.1
1	1-E	188	TYR	2.1
1	1-H	298	ILE	2.1
1	1-O	439	ILE	2.1
1	1-P	16	TYR	2.1
1	1-E	451	GLU	2.1
1	1-A	52	SER	2.1
1	1-I	41	SER	2.1
1	1-K	109	ARG	2.1
1	1-U	430	GLU	2.1
1	1-G	45	ASP	2.1
1	1-I	393	ASP	2.1
1	1-L	202	SER	2.1
1	1-L	227	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-M	273	SER	2.1
1	1-N	152	ASP	2.1
1	1-Q	11	ASP	2.1
1	1-R	11	ASP	2.1
1	1-R	291	SER	2.1
1	1-U	266	SER	2.1
1	1-W	122	ASP	2.1
1	1-C	324	PRO	2.1
1	1-J	110	LYS	2.1
1	1-N	502	PRO	2.1
1	1-T	603	LYS	2.1
1	1-G	445	PHE	2.1
1	1-H	311	PHE	2.1
1	1-M	157	TRP	2.1
1	1-S	434	PHE	2.1
1	1-S	445	PHE	2.1
1	1-D	333	VAL	2.1
1	1-D	433	VAL	2.1
1	1-G	189	VAL	2.1
1	1-K	91	VAL	2.1
1	1-T	343	VAL	2.1
1	1-U	304	HIS	2.1
1	1-W	425	HIS	2.1
1	1-G	144	ALA	2.1
1	1-P	279	ALA	2.1
1	1-V	121	ALA	2.1
1	1-W	288	ALA	2.1
1	1-D	454	ASN	2.1
1	1-E	185	ASN	2.1
1	1-K	436	ASN	2.1
1	1-S	185	ASN	2.1
1	1-B	375	LEU	2.1
1	1-B	431	GLY	2.1
1	1-B	435	THR	2.1
1	1-E	441	THR	2.1
1	1-F	378	GLY	2.1
1	1-H	438	LEU	2.1
1	1-I	123	THR	2.1
1	1-I	217	GLY	2.1
1	1-M	432	GLY	2.1
1	1-O	206	LEU	2.1
1	1-Q	115	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-Q	118	THR	2.1
1	1-T	356	LEU	2.1
1	1-V	46	GLY	2.1
1	1-A	418	ILE	2.1
1	1-F	298	ILE	2.1
1	1-O	200	ILE	2.1
1	1-O	443	ILE	2.1
1	1-S	205	ILE	2.1
1	1-F	359	ARG	2.1
1	1-H	295	ARG	2.1
1	1-H	440	GLU	2.1
1	1-L	109	ARG	2.1
1	1-L	240	TYR	2.1
1	1-N	440	GLU	2.1
1	1-R	212	GLU	2.1
1	1-U	451	GLU	2.1
1	1-J	342	CYS	2.1
1	1-C	101	SER	2.1
1	1-C	419	ASP	2.1
1	1-D	363	SER	2.1
1	1-J	36	SER	2.1
1	1-N	70	ASP	2.1
1	1-P	263	ASP	2.1
1	1-P	284	ASP	2.1
1	1-T	419	ASP	2.1
1	1-U	307	SER	2.1
1	1-V	36	SER	2.1
1	1-X	340	SER	2.1
1	1-G	10	LYS	2.1
1	1-M	385	LYS	2.1
1	1-J	99	PRO	2.1
1	1-J	346	PRO	2.1
1	1-N	408	PRO	2.1
1	1-Q	78	PRO	2.1
1	1-S	502	PRO	2.1
1	1-J	126	PHE	2.1
1	1-M	180	PHE	2.1
1	1-Q	304	HIS	2.1
1	1-T	180	PHE	2.1
1	1-X	374	MET	2.1
1	1-B	433	VAL	2.1
1	1-C	91	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-C	333	VAL	2.1
1	1-J	187	GLN	2.1
1	1-M	173	VAL	2.1
1	1-N	316	VAL	2.1
1	1-R	5	VAL	2.1
1	1-B	35	ALA	2.1
1	1-B	121	ALA	2.1
1	1-E	157	TRP	2.1
1	1-F	310	ALA	2.1
1	1-K	9	ALA	2.1
1	1-L	442	TRP	2.1
1	1-P	130	ALA	2.1
1	1-S	111	ALA	2.1
1	1-V	163	ALA	2.1
1	1-W	130	ALA	2.1
1	1-S	313	ASN	2.1
1	1-F	301	LEU	2.1
1	1-H	421	LEU	2.1
1	1-A	312	THR	2.1
1	1-G	312	THR	2.1
1	1-K	432	GLY	2.1
1	1-M	196	LEU	2.1
1	1-N	322	LEU	2.1
1	1-O	260	LEU	2.1
1	1-P	302	LEU	2.1
1	1-R	119	GLY	2.1
1	1-V	80	ARG	2.1
1	1-W	102	ARG	2.1
1	1-A	221	ILE	2.1
1	1-B	116	ILE	2.1
1	1-B	418	ILE	2.1
1	1-F	134	ILE	2.1
1	1-H	407	ILE	2.1
1	1-J	298	ILE	2.1
1	1-K	443	ILE	2.1
1	1-L	33	ILE	2.1
1	1-T	422	GLU	2.1
1	1-A	223	TYR	2.1
1	1-C	100	TYR	2.1
1	1-E	16	TYR	2.1
1	1-E	149	TYR	2.1
1	1-H	100	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-I	460	TYR	2.1
1	1-K	100	TYR	2.1
1	1-O	460	TYR	2.1
1	1-Q	223	TYR	2.1
1	1-R	427	TYR	2.1
1	1-T	149	TYR	2.1
1	1-A	117	SER	2.1
1	1-D	190	ASP	2.1
1	1-J	385	LYS	2.1
1	1-L	4	ASP	2.1
1	1-L	354	LYS	2.1
1	1-D	273	SER	2.1
1	1-H	270	CYS	2.1
1	1-K	340	SER	2.1
1	1-U	117	SER	2.1
1	1-X	211	HIS	2.1
1	1-F	358	PHE	2.1
1	1-H	272	GLN	2.1
1	1-P	31	PHE	2.1
1	1-W	272	GLN	2.1
1	1-I	5	VAL	2.1
1	1-Q	42	VAL	2.1
1	1-T	189	VAL	2.1
1	1-U	91	VAL	2.1
1	1-U	433	VAL	2.1
1	1-W	5	VAL	2.1
1	1-X	182	VAL	2.1
1	1-G	463	ALA	2.1
1	1-P	183	ALA	2.1
1	1-T	9	ALA	2.1
1	1-T	130	ALA	2.1
1	1-U	111	ALA	2.1
1	1-X	37	ALA	2.1
1	1-B	102	ARG	2.1
1	1-C	102	ARG	2.1
1	1-D	301	LEU	2.1
1	1-J	222	ASN	2.1
1	1-K	301	LEU	2.1
1	1-K	421	LEU	2.1
1	1-L	113	ASN	2.1
1	1-M	428	LEU	2.1
1	1-P	237	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	275	TRP	2.1
1	1-T	226	ASN	2.1
1	1-T	322	LEU	2.1
1	1-H	156	GLY	2.1
1	1-N	503	GLY	2.1
1	1-P	431	GLY	2.1
1	1-R	278	GLY	2.1
1	1-U	102	ARG	2.1
1	1-W	500	GLY	2.1
1	1-W	203	GLY	2.1
1	1-B	72	GLU	2.1
1	1-I	73	THR	2.1
1	1-I	435	THR	2.1
1	1-O	440	GLU	2.1
1	1-S	410	THR	2.1
1	1-U	15	GLU	2.1
1	1-X	451	GLU	2.1
1	1-K	205	ILE	2.1
1	1-R	221	ILE	2.1
1	1-T	76	ILE	2.1
1	1-T	221	ILE	2.1
1	1-G	7	LYS	2.1
1	1-U	110	LYS	2.1
1	1-C	467	ASP	2.1
1	1-I	16	TYR	2.1
1	1-J	284	ASP	2.1
1	1-M	149	TYR	2.1
1	1-O	297	TYR	2.1
1	1-R	125	TYR	2.1
1	1-U	125	TYR	2.1
1	1-V	125	TYR	2.1
1	1-V	437	ASP	2.1
1	1-A	41	SER	2.1
1	1-F	340	SER	2.1
1	1-I	340	SER	2.1
1	1-O	36	SER	2.1
1	1-T	101	SER	2.1
1	1-T	266	SER	2.1
1	1-F	69	PRO	2.1
1	1-G	367	PRO	2.1
1	1-L	71	PRO	2.1
1	1-T	2	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-T	71	PRO	2.1
1	1-T	270	CYS	2.1
1	1-V	184	PRO	2.1
1	1-L	374	MET	2.1
1	1-M	374	MET	2.1
1	1-N	374	MET	2.1
1	1-D	303	HIS	2.1
1	1-O	303	HIS	2.1
1	1-Q	303	HIS	2.1
1	1-C	187	GLN	2.0
1	1-V	389	GLN	2.0
1	1-D	468	VAL	2.0
1	1-G	204	PHE	2.0
1	1-H	453	VAL	2.0
1	1-K	42	VAL	2.0
1	1-R	89	PHE	2.0
1	1-R	433	VAL	2.0
1	1-R	445	PHE	2.0
1	1-U	323	VAL	2.0
1	1-A	102	ARG	2.0
1	1-B	183	ALA	2.0
1	1-E	295	ARG	2.0
1	1-G	20	ARG	2.0
1	1-N	75	ARG	2.0
1	1-P	294	ALA	2.0
1	1-Q	295	ARG	2.0
1	1-S	75	ARG	2.0
1	1-V	463	ALA	2.0
1	1-W	48	ALA	2.0
1	1-E	301	LEU	2.0
1	1-E	302	LEU	2.0
1	1-F	85	LEU	2.0
1	1-G	301	LEU	2.0
1	1-I	168	ASN	2.0
1	1-O	8	LEU	2.0
1	1-Q	438	LEU	2.0
1	1-R	206	LEU	2.0
1	1-R	313	ASN	2.0
1	1-R	331	ASN	2.0
1	1-T	313	ASN	2.0
1	1-U	264	ASN	2.0
1	1-V	264	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-X	454	ASN	2.0
1	1-D	150	GLU	2.0
1	1-D	267	GLY	2.0
1	1-D	432	GLY	2.0
1	1-I	365	GLY	2.0
1	1-L	157	TRP	2.0
1	1-L	216	GLY	2.0
1	1-S	170	GLY	2.0
1	1-W	157	TRP	2.0
1	1-X	265	GLY	2.0
1	1-B	164	THR	2.0
1	1-C	116	ILE	2.0
1	1-D	410	THR	2.0
1	1-E	10	LYS	2.0
1	1-G	87	ILE	2.0
1	1-G	123	THR	2.0
1	1-G	276	LYS	2.0
1	1-G	410	THR	2.0
1	1-J	205	ILE	2.0
1	1-K	354	LYS	2.0
1	1-L	221	ILE	2.0
1	1-M	84	THR	2.0
1	1-O	13	LYS	2.0
1	1-O	276	LYS	2.0
1	1-P	110	LYS	2.0
1	1-Q	298	ILE	2.0
1	1-R	10	LYS	2.0
1	1-W	40	LYS	2.0
1	1-B	122	ASP	2.0
1	1-B	190	ASP	2.0
1	1-C	380	ASP	2.0
1	1-G	233	ASP	2.0
1	1-B	78	PRO	2.0
1	1-E	502	PRO	2.0
1	1-F	346	PRO	2.0
1	1-F	459	PRO	2.0
1	1-G	427	TYR	2.0
1	1-H	465	TYR	2.0
1	1-I	297	TYR	2.0
1	1-N	45	ASP	2.0
1	1-P	181	PRO	2.0
1	1-Q	71	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-R	188	TYR	2.0
1	1-T	467	ASP	2.0
1	1-C	376	MET	2.0
1	1-G	36	SER	2.0
1	1-I	501	SER	2.0
1	1-M	501	SER	2.0
1	1-N	117	SER	2.0
1	1-U	346	PRO	2.0
1	1-C	271	HIS	2.0
1	1-I	304	HIS	2.0
1	1-R	248	GLN	2.0
1	1-F	343	VAL	2.0
1	1-J	42	VAL	2.0
1	1-K	90	PHE	2.0
1	1-L	189	VAL	2.0
1	1-L	453	VAL	2.0
1	1-M	17	VAL	2.0
1	1-M	189	VAL	2.0
1	1-N	42	VAL	2.0
1	1-P	5	VAL	2.0
1	1-V	445	PHE	2.0
1	1-C	128	ALA	2.0
1	1-C	294	ALA	2.0
1	1-D	183	ALA	2.0
1	1-E	130	ALA	2.0
1	1-F	294	ALA	2.0
1	1-G	124	ALA	2.0
1	1-H	464	LEU	2.0
1	1-I	191	LEU	2.0
1	1-L	322	LEU	2.0
1	1-L	377	ALA	2.0
1	1-M	305	ALA	2.0
1	1-C	40	LYS	2.0
1	1-D	422	GLU	2.0
1	1-E	222	ASN	2.0
1	1-F	250	GLY	2.0
1	1-F	320	LYS	2.0
1	1-H	10	LYS	2.0
1	1-J	7	LYS	2.0
1	1-K	10	LYS	2.0
1	1-L	430	GLU	2.0
1	1-O	302	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-P	12	GLU	2.0
1	1-P	229	LEU	2.0
1	1-P	375	LEU	2.0
1	1-T	8	LEU	2.0
1	1-T	68	LEU	2.0
1	1-V	115	LEU	2.0
1	1-V	281	LEU	2.0
1	1-X	274	LEU	2.0
1	1-M	366	ASN	2.0
1	1-N	250	GLY	2.0
1	1-O	384	ASN	2.0
1	1-P	26	GLY	2.0
1	1-S	299	GLY	2.0
1	1-U	222	ASN	2.0
1	1-W	300	GLY	2.0
1	1-A	107	ILE	2.0
1	1-I	386	ILE	2.0
1	1-L	205	ILE	2.0
1	1-J	157	TRP	2.0
1	1-T	442	TRP	2.0
1	1-A	329	PRO	2.0
1	1-B	71	PRO	2.0
1	1-B	346	PRO	2.0
1	1-J	122	ASP	2.0
1	1-M	152	ASP	2.0
1	1-T	346	PRO	2.0
1	1-C	340	SER	2.0
1	1-G	363	SER	2.0
1	1-H	171	TYR	2.0
1	1-H	215	SER	2.0
1	1-K	297	TYR	2.0
1	1-L	101	SER	2.0
1	1-L	360	SER	2.0
1	1-M	465	TYR	2.0
1	1-O	296	HIS	2.0
1	1-P	92	HIS	2.0
1	1-P	427	TYR	2.0
1	1-P	466	TYR	2.0
1	1-Q	296	HIS	2.0
1	1-Q	427	TYR	2.0
1	1-R	230	HIS	2.0
1	1-T	92	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-X	155	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	1-D	7481	23/23	0.40	0.20	24,24,24,24	23
2	MN	2-A	470	1/1	-	-	24,24,24,24	1
2	MN	3-A	470	1/1	-	-	24,24,24,24	1
2	MN	4-A	470	1/1	-	-	24,24,24,24	1
2	MN	5-A	470	1/1	-	-	24,24,24,24	1
2	MN	6-A	470	1/1	-	-	24,24,24,24	1
2	MN	7-A	470	1/1	-	-	24,24,24,24	1
2	MN	8-A	470	1/1	-	-	24,24,24,24	1
2	MN	9-A	470	1/1	-	-	24,24,24,24	1
2	MN	10-A	470	1/1	-	-	24,24,24,24	1
3	AMP	1-K	7495	23/23	0.40	0.20	24,24,24,24	23
2	MN	2-B	470	1/1	-	-	24,24,24,24	1
2	MN	3-B	470	1/1	-	-	24,24,24,24	1
2	MN	4-B	470	1/1	-	-	24,24,24,24	1
2	MN	5-B	470	1/1	-	-	24,24,24,24	1
2	MN	6-B	470	1/1	-	-	24,24,24,24	1
2	MN	7-B	470	1/1	-	-	24,24,24,24	1
2	MN	8-B	470	1/1	-	-	24,24,24,24	1
2	MN	9-B	470	1/1	-	-	24,24,24,24	1
2	MN	10-B	470	1/1	-	-	24,24,24,24	1
4	CIT	1-E	7484	13/13	0.41	0.31	24,24,24,24	13
2	MN	2-C	470	1/1	-	-	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	3-C	470	1/1	-	-	24,24,24,24	1
2	MN	4-C	470	1/1	-	-	24,24,24,24	1
2	MN	5-C	470	1/1	-	-	24,24,24,24	1
2	MN	6-C	470	1/1	-	-	24,24,24,24	1
2	MN	7-C	470	1/1	-	-	24,24,24,24	1
2	MN	8-C	470	1/1	-	-	24,24,24,24	1
2	MN	9-C	470	1/1	-	-	24,24,24,24	1
2	MN	10-C	470	1/1	-	-	24,24,24,24	1
3	AMP	1-I	7491	23/23	0.43	0.19	24,24,24,24	23
2	MN	2-D	470	1/1	-	-	24,24,24,24	1
2	MN	3-D	470	1/1	-	-	24,24,24,24	1
2	MN	4-D	470	1/1	-	-	24,24,24,24	1
2	MN	5-D	470	1/1	-	-	24,24,24,24	1
2	MN	6-D	470	1/1	-	-	24,24,24,24	1
2	MN	7-D	470	1/1	-	-	24,24,24,24	1
2	MN	8-D	470	1/1	-	-	24,24,24,24	1
2	MN	9-D	470	1/1	-	-	24,24,24,24	1
2	MN	10-D	470	1/1	-	-	24,24,24,24	1
3	AMP	1-N	7501	23/23	0.45	0.19	24,24,24,24	23
2	MN	2-E	470	1/1	-	-	24,24,24,24	1
2	MN	3-E	470	1/1	-	-	24,24,24,24	1
2	MN	4-E	470	1/1	-	-	24,24,24,24	1
2	MN	5-E	470	1/1	-	-	24,24,24,24	1
2	MN	6-E	470	1/1	-	-	24,24,24,24	1
2	MN	7-E	470	1/1	-	-	24,24,24,24	1
2	MN	8-E	470	1/1	-	-	24,24,24,24	1
2	MN	9-E	470	1/1	-	-	24,24,24,24	1
2	MN	10-E	470	1/1	-	-	24,24,24,24	1
3	AMP	1-P	7505	23/23	0.45	0.19	24,24,24,24	23
2	MN	2-F	470	1/1	-	-	24,24,24,24	1
2	MN	3-F	470	1/1	-	-	24,24,24,24	1
2	MN	4-F	470	1/1	-	-	24,24,24,24	1
2	MN	5-F	470	1/1	-	-	24,24,24,24	1
2	MN	6-F	470	1/1	-	-	24,24,24,24	1
2	MN	7-F	470	1/1	-	-	24,24,24,24	1
2	MN	8-F	470	1/1	-	-	24,24,24,24	1
2	MN	9-F	470	1/1	-	-	24,24,24,24	1
2	MN	10-F	470	1/1	-	-	24,24,24,24	1
3	AMP	1-J	7493	23/23	0.45	0.20	24,24,24,24	23
2	MN	2-G	470	1/1	-	-	24,24,24,24	1
2	MN	3-G	470	1/1	-	-	24,24,24,24	1
2	MN	4-G	470	1/1	-	-	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	5-G	470	1/1	-	-	24,24,24,24	1
2	MN	6-G	470	1/1	-	-	24,24,24,24	1
2	MN	7-G	470	1/1	-	-	24,24,24,24	1
2	MN	8-G	470	1/1	-	-	24,24,24,24	1
2	MN	9-G	470	1/1	-	-	24,24,24,24	1
2	MN	10-G	470	1/1	-	-	24,24,24,24	1
3	AMP	1-A	7475	23/23	0.46	0.19	24,24,24,24	23
2	MN	2-H	470	1/1	-	-	24,24,24,24	1
2	MN	3-H	470	1/1	-	-	24,24,24,24	1
2	MN	4-H	470	1/1	-	-	24,24,24,24	1
2	MN	5-H	470	1/1	-	-	24,24,24,24	1
2	MN	6-H	470	1/1	-	-	24,24,24,24	1
2	MN	7-H	470	1/1	-	-	24,24,24,24	1
2	MN	8-H	470	1/1	-	-	24,24,24,24	1
2	MN	9-H	470	1/1	-	-	24,24,24,24	1
2	MN	10-H	470	1/1	-	-	24,24,24,24	1
3	AMP	1-H	7489	23/23	0.46	0.20	24,24,24,24	23
2	MN	2-I	470	1/1	-	-	24,24,24,24	1
2	MN	3-I	470	1/1	-	-	24,24,24,24	1
2	MN	4-I	470	1/1	-	-	24,24,24,24	1
2	MN	5-I	470	1/1	-	-	24,24,24,24	1
2	MN	6-I	470	1/1	-	-	24,24,24,24	1
2	MN	7-I	470	1/1	-	-	24,24,24,24	1
2	MN	8-I	470	1/1	-	-	24,24,24,24	1
2	MN	9-I	470	1/1	-	-	24,24,24,24	1
2	MN	10-I	470	1/1	-	-	24,24,24,24	1
3	AMP	1-V	7517	23/23	0.48	0.18	24,24,24,24	23
2	MN	2-J	470	1/1	-	-	24,24,24,24	1
2	MN	3-J	470	1/1	-	-	24,24,24,24	1
2	MN	4-J	470	1/1	-	-	24,24,24,24	1
2	MN	5-J	470	1/1	-	-	24,24,24,24	1
2	MN	6-J	470	1/1	-	-	24,24,24,24	1
2	MN	7-J	470	1/1	-	-	24,24,24,24	1
2	MN	8-J	470	1/1	-	-	24,24,24,24	1
2	MN	9-J	470	1/1	-	-	24,24,24,24	1
2	MN	10-J	470	1/1	-	-	24,24,24,24	1
3	AMP	1-F	7485	23/23	0.51	0.18	24,24,24,24	23
2	MN	2-K	470	1/1	-	-	24,24,24,24	1
2	MN	3-K	470	1/1	-	-	24,24,24,24	1
2	MN	4-K	470	1/1	-	-	24,24,24,24	1
2	MN	5-K	470	1/1	-	-	24,24,24,24	1
2	MN	6-K	470	1/1	-	-	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	7-K	470	1/1	-	-	24,24,24,24	1
2	MN	8-K	470	1/1	-	-	24,24,24,24	1
2	MN	9-K	470	1/1	-	-	24,24,24,24	1
2	MN	10-K	470	1/1	-	-	24,24,24,24	1
3	AMP	1-R	7509	23/23	0.51	0.20	24,24,24,24	23
2	MN	2-L	470	1/1	-	-	24,24,24,24	1
2	MN	3-L	470	1/1	-	-	24,24,24,24	1
2	MN	4-L	470	1/1	-	-	24,24,24,24	1
2	MN	5-L	470	1/1	-	-	24,24,24,24	1
2	MN	6-L	470	1/1	-	-	24,24,24,24	1
2	MN	7-L	470	1/1	-	-	24,24,24,24	1
2	MN	8-L	470	1/1	-	-	24,24,24,24	1
2	MN	9-L	470	1/1	-	-	24,24,24,24	1
2	MN	10-L	470	1/1	-	-	24,24,24,24	1
3	AMP	1-G	7487	23/23	0.52	0.17	24,24,24,24	23
2	MN	2-M	470	1/1	-	-	24,24,24,24	1
2	MN	3-M	470	1/1	-	-	24,24,24,24	1
2	MN	4-M	470	1/1	-	-	24,24,24,24	1
2	MN	5-M	470	1/1	-	-	24,24,24,24	1
2	MN	6-M	470	1/1	-	-	24,24,24,24	1
2	MN	7-M	470	1/1	-	-	24,24,24,24	1
2	MN	8-M	470	1/1	-	-	24,24,24,24	1
2	MN	9-M	470	1/1	-	-	24,24,24,24	1
2	MN	10-M	470	1/1	-	-	24,24,24,24	1
4	CIT	1-B	7478	13/13	0.52	0.27	24,24,24,24	13
2	MN	2-N	470	1/1	-	-	24,24,24,24	1
2	MN	3-N	470	1/1	-	-	24,24,24,24	1
2	MN	4-N	470	1/1	-	-	24,24,24,24	1
2	MN	5-N	470	1/1	-	-	24,24,24,24	1
2	MN	6-N	470	1/1	-	-	24,24,24,24	1
2	MN	7-N	470	1/1	-	-	24,24,24,24	1
2	MN	8-N	470	1/1	-	-	24,24,24,24	1
2	MN	9-N	470	1/1	-	-	24,24,24,24	1
2	MN	10-N	470	1/1	-	-	24,24,24,24	1
3	AMP	1-B	7477	23/23	0.52	0.17	24,24,24,24	23
2	MN	2-O	470	1/1	-	-	24,24,24,24	1
2	MN	3-O	470	1/1	-	-	24,24,24,24	1
2	MN	4-O	470	1/1	-	-	24,24,24,24	1
2	MN	5-O	470	1/1	-	-	24,24,24,24	1
2	MN	6-O	470	1/1	-	-	24,24,24,24	1
2	MN	7-O	470	1/1	-	-	24,24,24,24	1
2	MN	8-O	470	1/1	-	-	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	9-O	470	1/1	-	-	24,24,24,24	1
2	MN	10-O	470	1/1	-	-	24,24,24,24	1
4	CIT	1-T	7514	13/13	0.52	0.26	24,24,24,24	13
2	MN	2-P	470	1/1	-	-	24,24,24,24	1
2	MN	3-P	470	1/1	-	-	24,24,24,24	1
2	MN	4-P	470	1/1	-	-	24,24,24,24	1
2	MN	5-P	470	1/1	-	-	24,24,24,24	1
2	MN	6-P	470	1/1	-	-	24,24,24,24	1
2	MN	7-P	470	1/1	-	-	24,24,24,24	1
2	MN	8-P	470	1/1	-	-	24,24,24,24	1
2	MN	9-P	470	1/1	-	-	24,24,24,24	1
2	MN	10-P	470	1/1	-	-	24,24,24,24	1
3	AMP	1-E	7483	23/23	0.53	0.17	24,24,24,24	23
2	MN	2-Q	470	1/1	-	-	24,24,24,24	1
2	MN	3-Q	470	1/1	-	-	24,24,24,24	1
2	MN	4-Q	470	1/1	-	-	24,24,24,24	1
2	MN	5-Q	470	1/1	-	-	24,24,24,24	1
2	MN	6-Q	470	1/1	-	-	24,24,24,24	1
2	MN	7-Q	470	1/1	-	-	24,24,24,24	1
2	MN	8-Q	470	1/1	-	-	24,24,24,24	1
2	MN	9-Q	470	1/1	-	-	24,24,24,24	1
2	MN	10-Q	470	1/1	-	-	24,24,24,24	1
3	AMP	1-U	7515	23/23	0.53	0.17	24,24,24,24	23
2	MN	2-R	470	1/1	-	-	24,24,24,24	1
2	MN	3-R	470	1/1	-	-	24,24,24,24	1
2	MN	4-R	470	1/1	-	-	24,24,24,24	1
2	MN	5-R	470	1/1	-	-	24,24,24,24	1
2	MN	6-R	470	1/1	-	-	24,24,24,24	1
2	MN	7-R	470	1/1	-	-	24,24,24,24	1
2	MN	8-R	470	1/1	-	-	24,24,24,24	1
2	MN	9-R	470	1/1	-	-	24,24,24,24	1
2	MN	10-R	470	1/1	-	-	24,24,24,24	1
3	AMP	1-O	7503	23/23	0.54	0.17	24,24,24,24	23
2	MN	2-S	470	1/1	-	-	24,24,24,24	1
2	MN	3-S	470	1/1	-	-	24,24,24,24	1
2	MN	4-S	470	1/1	-	-	24,24,24,24	1
2	MN	5-S	470	1/1	-	-	24,24,24,24	1
2	MN	6-S	470	1/1	-	-	24,24,24,24	1
2	MN	7-S	470	1/1	-	-	24,24,24,24	1
2	MN	8-S	470	1/1	-	-	24,24,24,24	1
2	MN	9-S	470	1/1	-	-	24,24,24,24	1
2	MN	10-S	470	1/1	-	-	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	1-W	7519	23/23	0.54	0.18	24,24,24,24	23
2	MN	2-T	470	1/1	-	-	24,24,24,24	1
2	MN	3-T	470	1/1	-	-	24,24,24,24	1
2	MN	4-T	470	1/1	-	-	24,24,24,24	1
2	MN	5-T	470	1/1	-	-	24,24,24,24	1
2	MN	6-T	470	1/1	-	-	24,24,24,24	1
2	MN	7-T	470	1/1	-	-	24,24,24,24	1
2	MN	8-T	470	1/1	-	-	24,24,24,24	1
2	MN	9-T	470	1/1	-	-	24,24,24,24	1
2	MN	10-T	470	1/1	-	-	24,24,24,24	1
3	AMP	1-L	7497	23/23	0.54	0.19	24,24,24,24	23
2	MN	2-U	470	1/1	-	-	24,24,24,24	1
2	MN	3-U	470	1/1	-	-	24,24,24,24	1
2	MN	4-U	470	1/1	-	-	24,24,24,24	1
2	MN	5-U	470	1/1	-	-	24,24,24,24	1
2	MN	6-U	470	1/1	-	-	24,24,24,24	1
2	MN	7-U	470	1/1	-	-	24,24,24,24	1
2	MN	8-U	470	1/1	-	-	24,24,24,24	1
2	MN	9-U	470	1/1	-	-	24,24,24,24	1
2	MN	10-U	470	1/1	-	-	24,24,24,24	1
3	AMP	1-M	7499	23/23	0.54	0.17	24,24,24,24	23
2	MN	2-V	470	1/1	-	-	24,24,24,24	1
2	MN	3-V	470	1/1	-	-	24,24,24,24	1
2	MN	4-V	470	1/1	-	-	24,24,24,24	1
2	MN	5-V	470	1/1	-	-	24,24,24,24	1
2	MN	6-V	470	1/1	-	-	24,24,24,24	1
2	MN	7-V	470	1/1	-	-	24,24,24,24	1
2	MN	8-V	470	1/1	-	-	24,24,24,24	1
2	MN	9-V	470	1/1	-	-	24,24,24,24	1
2	MN	10-V	470	1/1	-	-	24,24,24,24	1
4	CIT	1-I	7492	13/13	0.54	0.25	24,24,24,24	13
2	MN	2-W	470	1/1	-	-	24,24,24,24	1
2	MN	3-W	470	1/1	-	-	24,24,24,24	1
2	MN	4-W	470	1/1	-	-	24,24,24,24	1
2	MN	5-W	470	1/1	-	-	24,24,24,24	1
2	MN	6-W	470	1/1	-	-	24,24,24,24	1
2	MN	7-W	470	1/1	-	-	24,24,24,24	1
2	MN	8-W	470	1/1	-	-	24,24,24,24	1
2	MN	9-W	470	1/1	-	-	24,24,24,24	1
2	MN	10-W	470	1/1	-	-	24,24,24,24	1
3	AMP	1-C	7479	23/23	0.54	0.18	24,24,24,24	23
2	MN	2-X	470	1/1	-	-	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	3-X	470	1/1	-	-	24,24,24,24	1
2	MN	4-X	470	1/1	-	-	24,24,24,24	1
2	MN	5-X	470	1/1	-	-	24,24,24,24	1
2	MN	6-X	470	1/1	-	-	24,24,24,24	1
2	MN	7-X	470	1/1	-	-	24,24,24,24	1
2	MN	8-X	470	1/1	-	-	24,24,24,24	1
2	MN	9-X	470	1/1	-	-	24,24,24,24	1
2	MN	10-X	470	1/1	-	-	24,24,24,24	1
4	CIT	1-L	7498	13/13	0.55	0.26	24,24,24,24	13
3	AMP	2-A	7475	23/23	-	-	24,24,24,24	23
3	AMP	3-A	7475	23/23	-	-	24,24,24,24	23
3	AMP	4-A	7475	23/23	-	-	24,24,24,24	23
3	AMP	5-A	7475	23/23	-	-	24,24,24,24	23
3	AMP	6-A	7475	23/23	-	-	24,24,24,24	23
3	AMP	7-A	7475	23/23	-	-	24,24,24,24	23
3	AMP	8-A	7475	23/23	-	-	24,24,24,24	23
3	AMP	9-A	7475	23/23	-	-	24,24,24,24	23
3	AMP	10-A	7475	23/23	-	-	24,24,24,24	23
3	AMP	1-Q	7507	23/23	0.56	0.16	24,24,24,24	23
3	AMP	2-B	7477	23/23	-	-	24,24,24,24	23
3	AMP	3-B	7477	23/23	-	-	24,24,24,24	23
3	AMP	4-B	7477	23/23	-	-	24,24,24,24	23
3	AMP	5-B	7477	23/23	-	-	24,24,24,24	23
3	AMP	6-B	7477	23/23	-	-	24,24,24,24	23
3	AMP	7-B	7477	23/23	-	-	24,24,24,24	23
3	AMP	8-B	7477	23/23	-	-	24,24,24,24	23
3	AMP	9-B	7477	23/23	-	-	24,24,24,24	23
3	AMP	10-B	7477	23/23	-	-	24,24,24,24	23
4	CIT	1-N	7502	13/13	0.56	0.23	24,24,24,24	13
3	AMP	2-C	7479	23/23	-	-	24,24,24,24	23
3	AMP	3-C	7479	23/23	-	-	24,24,24,24	23
3	AMP	4-C	7479	23/23	-	-	24,24,24,24	23
3	AMP	5-C	7479	23/23	-	-	24,24,24,24	23
3	AMP	6-C	7479	23/23	-	-	24,24,24,24	23
3	AMP	7-C	7479	23/23	-	-	24,24,24,24	23
3	AMP	8-C	7479	23/23	-	-	24,24,24,24	23
3	AMP	9-C	7479	23/23	-	-	24,24,24,24	23
3	AMP	10-C	7479	23/23	-	-	24,24,24,24	23
4	CIT	1-Q	7508	13/13	0.56	0.27	24,24,24,24	13
3	AMP	2-D	7481	23/23	-	-	24,24,24,24	23
3	AMP	3-D	7481	23/23	-	-	24,24,24,24	23
3	AMP	4-D	7481	23/23	-	-	24,24,24,24	23

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	5-D	7481	23/23	-	-	24,24,24,24	23
3	AMP	6-D	7481	23/23	-	-	24,24,24,24	23
3	AMP	7-D	7481	23/23	-	-	24,24,24,24	23
3	AMP	8-D	7481	23/23	-	-	24,24,24,24	23
3	AMP	9-D	7481	23/23	-	-	24,24,24,24	23
3	AMP	10-D	7481	23/23	-	-	24,24,24,24	23
3	AMP	1-S	7511	23/23	0.56	0.17	24,24,24,24	23
3	AMP	2-E	7483	23/23	-	-	24,24,24,24	23
3	AMP	3-E	7483	23/23	-	-	24,24,24,24	23
3	AMP	4-E	7483	23/23	-	-	24,24,24,24	23
3	AMP	5-E	7483	23/23	-	-	24,24,24,24	23
3	AMP	6-E	7483	23/23	-	-	24,24,24,24	23
3	AMP	7-E	7483	23/23	-	-	24,24,24,24	23
3	AMP	8-E	7483	23/23	-	-	24,24,24,24	23
3	AMP	9-E	7483	23/23	-	-	24,24,24,24	23
3	AMP	10-E	7483	23/23	-	-	24,24,24,24	23
4	CIT	1-F	7486	13/13	0.57	0.29	24,24,24,24	13
3	AMP	2-F	7485	23/23	-	-	24,24,24,24	23
3	AMP	3-F	7485	23/23	-	-	24,24,24,24	23
3	AMP	4-F	7485	23/23	-	-	24,24,24,24	23
3	AMP	5-F	7485	23/23	-	-	24,24,24,24	23
3	AMP	6-F	7485	23/23	-	-	24,24,24,24	23
3	AMP	7-F	7485	23/23	-	-	24,24,24,24	23
3	AMP	8-F	7485	23/23	-	-	24,24,24,24	23
3	AMP	9-F	7485	23/23	-	-	24,24,24,24	23
3	AMP	10-F	7485	23/23	-	-	24,24,24,24	23
4	CIT	1-O	7504	13/13	0.58	0.26	24,24,24,24	13
3	AMP	2-G	7487	23/23	-	-	24,24,24,24	23
3	AMP	3-G	7487	23/23	-	-	24,24,24,24	23
3	AMP	4-G	7487	23/23	-	-	24,24,24,24	23
3	AMP	5-G	7487	23/23	-	-	24,24,24,24	23
3	AMP	6-G	7487	23/23	-	-	24,24,24,24	23
3	AMP	7-G	7487	23/23	-	-	24,24,24,24	23
3	AMP	8-G	7487	23/23	-	-	24,24,24,24	23
3	AMP	9-G	7487	23/23	-	-	24,24,24,24	23
3	AMP	10-G	7487	23/23	-	-	24,24,24,24	23
4	CIT	1-C	7480	13/13	0.58	0.28	24,24,24,24	13
3	AMP	2-H	7489	23/23	-	-	24,24,24,24	23
3	AMP	3-H	7489	23/23	-	-	24,24,24,24	23
3	AMP	4-H	7489	23/23	-	-	24,24,24,24	23
3	AMP	5-H	7489	23/23	-	-	24,24,24,24	23
3	AMP	6-H	7489	23/23	-	-	24,24,24,24	23

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	7-H	7489	23/23	-	-	24,24,24,24	23
3	AMP	8-H	7489	23/23	-	-	24,24,24,24	23
3	AMP	9-H	7489	23/23	-	-	24,24,24,24	23
3	AMP	10-H	7489	23/23	-	-	24,24,24,24	23
3	AMP	1-T	7513	23/23	0.58	0.18	24,24,24,24	23
3	AMP	2-I	7491	23/23	-	-	24,24,24,24	23
3	AMP	3-I	7491	23/23	-	-	24,24,24,24	23
3	AMP	4-I	7491	23/23	-	-	24,24,24,24	23
3	AMP	5-I	7491	23/23	-	-	24,24,24,24	23
3	AMP	6-I	7491	23/23	-	-	24,24,24,24	23
3	AMP	7-I	7491	23/23	-	-	24,24,24,24	23
3	AMP	8-I	7491	23/23	-	-	24,24,24,24	23
3	AMP	9-I	7491	23/23	-	-	24,24,24,24	23
3	AMP	10-I	7491	23/23	-	-	24,24,24,24	23
4	CIT	1-S	7512	13/13	0.59	0.24	24,24,24,24	13
3	AMP	2-J	7493	23/23	-	-	24,24,24,24	23
3	AMP	3-J	7493	23/23	-	-	24,24,24,24	23
3	AMP	4-J	7493	23/23	-	-	24,24,24,24	23
3	AMP	5-J	7493	23/23	-	-	24,24,24,24	23
3	AMP	6-J	7493	23/23	-	-	24,24,24,24	23
3	AMP	7-J	7493	23/23	-	-	24,24,24,24	23
3	AMP	8-J	7493	23/23	-	-	24,24,24,24	23
3	AMP	9-J	7493	23/23	-	-	24,24,24,24	23
3	AMP	10-J	7493	23/23	-	-	24,24,24,24	23
4	CIT	1-H	7490	13/13	0.63	0.23	24,24,24,24	13
3	AMP	2-K	7495	23/23	-	-	24,24,24,24	23
3	AMP	3-K	7495	23/23	-	-	24,24,24,24	23
3	AMP	4-K	7495	23/23	-	-	24,24,24,24	23
3	AMP	5-K	7495	23/23	-	-	24,24,24,24	23
3	AMP	6-K	7495	23/23	-	-	24,24,24,24	23
3	AMP	7-K	7495	23/23	-	-	24,24,24,24	23
3	AMP	8-K	7495	23/23	-	-	24,24,24,24	23
3	AMP	9-K	7495	23/23	-	-	24,24,24,24	23
3	AMP	10-K	7495	23/23	-	-	24,24,24,24	23
4	CIT	1-G	7488	13/13	0.63	0.24	24,24,24,24	13
3	AMP	2-L	7497	23/23	-	-	24,24,24,24	23
3	AMP	3-L	7497	23/23	-	-	24,24,24,24	23
3	AMP	4-L	7497	23/23	-	-	24,24,24,24	23
3	AMP	5-L	7497	23/23	-	-	24,24,24,24	23
3	AMP	6-L	7497	23/23	-	-	24,24,24,24	23
3	AMP	7-L	7497	23/23	-	-	24,24,24,24	23
3	AMP	8-L	7497	23/23	-	-	24,24,24,24	23

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	9-L	7497	23/23	-	-	24,24,24,24	23
3	AMP	10-L	7497	23/23	-	-	24,24,24,24	23
4	CIT	1-V	7518	13/13	0.64	0.20	24,24,24,24	13
3	AMP	2-M	7499	23/23	-	-	24,24,24,24	23
3	AMP	3-M	7499	23/23	-	-	24,24,24,24	23
3	AMP	4-M	7499	23/23	-	-	24,24,24,24	23
3	AMP	5-M	7499	23/23	-	-	24,24,24,24	23
3	AMP	6-M	7499	23/23	-	-	24,24,24,24	23
3	AMP	7-M	7499	23/23	-	-	24,24,24,24	23
3	AMP	8-M	7499	23/23	-	-	24,24,24,24	23
3	AMP	9-M	7499	23/23	-	-	24,24,24,24	23
3	AMP	10-M	7499	23/23	-	-	24,24,24,24	23
4	CIT	1-U	7516	13/13	0.65	0.25	24,24,24,24	13
3	AMP	2-N	7501	23/23	-	-	24,24,24,24	23
3	AMP	3-N	7501	23/23	-	-	24,24,24,24	23
3	AMP	4-N	7501	23/23	-	-	24,24,24,24	23
3	AMP	5-N	7501	23/23	-	-	24,24,24,24	23
3	AMP	6-N	7501	23/23	-	-	24,24,24,24	23
3	AMP	7-N	7501	23/23	-	-	24,24,24,24	23
3	AMP	8-N	7501	23/23	-	-	24,24,24,24	23
3	AMP	9-N	7501	23/23	-	-	24,24,24,24	23
3	AMP	10-N	7501	23/23	-	-	24,24,24,24	23
4	CIT	1-M	7500	13/13	0.65	0.21	24,24,24,24	13
3	AMP	2-O	7503	23/23	-	-	24,24,24,24	23
3	AMP	3-O	7503	23/23	-	-	24,24,24,24	23
3	AMP	4-O	7503	23/23	-	-	24,24,24,24	23
3	AMP	5-O	7503	23/23	-	-	24,24,24,24	23
3	AMP	6-O	7503	23/23	-	-	24,24,24,24	23
3	AMP	7-O	7503	23/23	-	-	24,24,24,24	23
3	AMP	8-O	7503	23/23	-	-	24,24,24,24	23
3	AMP	9-O	7503	23/23	-	-	24,24,24,24	23
3	AMP	10-O	7503	23/23	-	-	24,24,24,24	23
4	CIT	1-A	7476	13/13	0.66	0.18	24,24,24,24	13
3	AMP	2-P	7505	23/23	-	-	24,24,24,24	23
3	AMP	3-P	7505	23/23	-	-	24,24,24,24	23
3	AMP	4-P	7505	23/23	-	-	24,24,24,24	23
3	AMP	5-P	7505	23/23	-	-	24,24,24,24	23
3	AMP	6-P	7505	23/23	-	-	24,24,24,24	23
3	AMP	7-P	7505	23/23	-	-	24,24,24,24	23
3	AMP	8-P	7505	23/23	-	-	24,24,24,24	23
3	AMP	9-P	7505	23/23	-	-	24,24,24,24	23
3	AMP	10-P	7505	23/23	-	-	24,24,24,24	23

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CIT	1-R	7510	13/13	0.66	0.25	24,24,24,24	13
3	AMP	2-Q	7507	23/23	-	-	24,24,24,24	23
3	AMP	3-Q	7507	23/23	-	-	24,24,24,24	23
3	AMP	4-Q	7507	23/23	-	-	24,24,24,24	23
3	AMP	5-Q	7507	23/23	-	-	24,24,24,24	23
3	AMP	6-Q	7507	23/23	-	-	24,24,24,24	23
3	AMP	7-Q	7507	23/23	-	-	24,24,24,24	23
3	AMP	8-Q	7507	23/23	-	-	24,24,24,24	23
3	AMP	9-Q	7507	23/23	-	-	24,24,24,24	23
3	AMP	10-Q	7507	23/23	-	-	24,24,24,24	23
3	AMP	1-X	7521	23/23	0.66	0.15	24,24,24,24	23
3	AMP	2-R	7509	23/23	-	-	24,24,24,24	23
3	AMP	3-R	7509	23/23	-	-	24,24,24,24	23
3	AMP	4-R	7509	23/23	-	-	24,24,24,24	23
3	AMP	5-R	7509	23/23	-	-	24,24,24,24	23
3	AMP	6-R	7509	23/23	-	-	24,24,24,24	23
3	AMP	7-R	7509	23/23	-	-	24,24,24,24	23
3	AMP	8-R	7509	23/23	-	-	24,24,24,24	23
3	AMP	9-R	7509	23/23	-	-	24,24,24,24	23
3	AMP	10-R	7509	23/23	-	-	24,24,24,24	23
2	MN	1-L	470	1/1	0.68	0.32	24,24,24,24	1
3	AMP	2-S	7511	23/23	-	-	24,24,24,24	23
3	AMP	3-S	7511	23/23	-	-	24,24,24,24	23
3	AMP	4-S	7511	23/23	-	-	24,24,24,24	23
3	AMP	5-S	7511	23/23	-	-	24,24,24,24	23
3	AMP	6-S	7511	23/23	-	-	24,24,24,24	23
3	AMP	7-S	7511	23/23	-	-	24,24,24,24	23
3	AMP	8-S	7511	23/23	-	-	24,24,24,24	23
3	AMP	9-S	7511	23/23	-	-	24,24,24,24	23
3	AMP	10-S	7511	23/23	-	-	24,24,24,24	23
2	MN	1-G	470	1/1	0.68	0.46	24,24,24,24	1
3	AMP	2-T	7513	23/23	-	-	24,24,24,24	23
3	AMP	3-T	7513	23/23	-	-	24,24,24,24	23
3	AMP	4-T	7513	23/23	-	-	24,24,24,24	23
3	AMP	5-T	7513	23/23	-	-	24,24,24,24	23
3	AMP	6-T	7513	23/23	-	-	24,24,24,24	23
3	AMP	7-T	7513	23/23	-	-	24,24,24,24	23
3	AMP	8-T	7513	23/23	-	-	24,24,24,24	23
3	AMP	9-T	7513	23/23	-	-	24,24,24,24	23
3	AMP	10-T	7513	23/23	-	-	24,24,24,24	23
4	CIT	1-D	7482	13/13	0.68	0.18	24,24,24,24	13
3	AMP	2-U	7515	23/23	-	-	24,24,24,24	23

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	3-U	7515	23/23	-	-	24,24,24,24	23
3	AMP	4-U	7515	23/23	-	-	24,24,24,24	23
3	AMP	5-U	7515	23/23	-	-	24,24,24,24	23
3	AMP	6-U	7515	23/23	-	-	24,24,24,24	23
3	AMP	7-U	7515	23/23	-	-	24,24,24,24	23
3	AMP	8-U	7515	23/23	-	-	24,24,24,24	23
3	AMP	9-U	7515	23/23	-	-	24,24,24,24	23
3	AMP	10-U	7515	23/23	-	-	24,24,24,24	23
4	CIT	1-P	7506	13/13	0.69	0.17	24,24,24,24	13
3	AMP	2-V	7517	23/23	-	-	24,24,24,24	23
3	AMP	3-V	7517	23/23	-	-	24,24,24,24	23
3	AMP	4-V	7517	23/23	-	-	24,24,24,24	23
3	AMP	5-V	7517	23/23	-	-	24,24,24,24	23
3	AMP	6-V	7517	23/23	-	-	24,24,24,24	23
3	AMP	7-V	7517	23/23	-	-	24,24,24,24	23
3	AMP	8-V	7517	23/23	-	-	24,24,24,24	23
3	AMP	9-V	7517	23/23	-	-	24,24,24,24	23
3	AMP	10-V	7517	23/23	-	-	24,24,24,24	23
4	CIT	1-W	7520	13/13	0.69	0.21	24,24,24,24	13
3	AMP	2-W	7519	23/23	-	-	24,24,24,24	23
3	AMP	3-W	7519	23/23	-	-	24,24,24,24	23
3	AMP	4-W	7519	23/23	-	-	24,24,24,24	23
3	AMP	5-W	7519	23/23	-	-	24,24,24,24	23
3	AMP	6-W	7519	23/23	-	-	24,24,24,24	23
3	AMP	7-W	7519	23/23	-	-	24,24,24,24	23
3	AMP	8-W	7519	23/23	-	-	24,24,24,24	23
3	AMP	9-W	7519	23/23	-	-	24,24,24,24	23
3	AMP	10-W	7519	23/23	-	-	24,24,24,24	23
4	CIT	1-X	7522	13/13	0.69	0.22	24,24,24,24	13
3	AMP	2-X	7521	23/23	-	-	24,24,24,24	23
3	AMP	3-X	7521	23/23	-	-	24,24,24,24	23
3	AMP	4-X	7521	23/23	-	-	24,24,24,24	23
3	AMP	5-X	7521	23/23	-	-	24,24,24,24	23
3	AMP	6-X	7521	23/23	-	-	24,24,24,24	23
3	AMP	7-X	7521	23/23	-	-	24,24,24,24	23
3	AMP	8-X	7521	23/23	-	-	24,24,24,24	23
3	AMP	9-X	7521	23/23	-	-	24,24,24,24	23
3	AMP	10-X	7521	23/23	-	-	24,24,24,24	23
4	CIT	1-J	7494	13/13	0.70	0.18	24,24,24,24	13
4	CIT	2-A	7476	13/13	-	-	24,24,24,24	13
4	CIT	3-A	7476	13/13	-	-	24,24,24,24	13
4	CIT	4-A	7476	13/13	-	-	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CIT	5-A	7476	13/13	-	-	24,24,24,24	13
4	CIT	6-A	7476	13/13	-	-	24,24,24,24	13
4	CIT	7-A	7476	13/13	-	-	24,24,24,24	13
4	CIT	8-A	7476	13/13	-	-	24,24,24,24	13
4	CIT	9-A	7476	13/13	-	-	24,24,24,24	13
4	CIT	10-A	7476	13/13	-	-	24,24,24,24	13
4	CIT	1-K	7496	13/13	0.71	0.22	24,24,24,24	13
4	CIT	2-B	7478	13/13	-	-	24,24,24,24	13
4	CIT	3-B	7478	13/13	-	-	24,24,24,24	13
4	CIT	4-B	7478	13/13	-	-	24,24,24,24	13
4	CIT	5-B	7478	13/13	-	-	24,24,24,24	13
4	CIT	6-B	7478	13/13	-	-	24,24,24,24	13
4	CIT	7-B	7478	13/13	-	-	24,24,24,24	13
4	CIT	8-B	7478	13/13	-	-	24,24,24,24	13
4	CIT	9-B	7478	13/13	-	-	24,24,24,24	13
4	CIT	10-B	7478	13/13	-	-	24,24,24,24	13
2	MN	1-D	470	1/1	0.72	0.26	24,24,24,24	1
4	CIT	2-C	7480	13/13	-	-	24,24,24,24	13
4	CIT	3-C	7480	13/13	-	-	24,24,24,24	13
4	CIT	4-C	7480	13/13	-	-	24,24,24,24	13
4	CIT	5-C	7480	13/13	-	-	24,24,24,24	13
4	CIT	6-C	7480	13/13	-	-	24,24,24,24	13
4	CIT	7-C	7480	13/13	-	-	24,24,24,24	13
4	CIT	8-C	7480	13/13	-	-	24,24,24,24	13
4	CIT	9-C	7480	13/13	-	-	24,24,24,24	13
4	CIT	10-C	7480	13/13	-	-	24,24,24,24	13
2	MN	1-E	470	1/1	0.74	0.36	24,24,24,24	1
4	CIT	2-D	7482	13/13	-	-	24,24,24,24	13
4	CIT	3-D	7482	13/13	-	-	24,24,24,24	13
4	CIT	4-D	7482	13/13	-	-	24,24,24,24	13
4	CIT	5-D	7482	13/13	-	-	24,24,24,24	13
4	CIT	6-D	7482	13/13	-	-	24,24,24,24	13
4	CIT	7-D	7482	13/13	-	-	24,24,24,24	13
4	CIT	8-D	7482	13/13	-	-	24,24,24,24	13
4	CIT	9-D	7482	13/13	-	-	24,24,24,24	13
4	CIT	10-D	7482	13/13	-	-	24,24,24,24	13
2	MN	1-A	470	1/1	0.75	0.32	24,24,24,24	1
4	CIT	2-E	7484	13/13	-	-	24,24,24,24	13
4	CIT	3-E	7484	13/13	-	-	24,24,24,24	13
4	CIT	4-E	7484	13/13	-	-	24,24,24,24	13
4	CIT	5-E	7484	13/13	-	-	24,24,24,24	13
4	CIT	6-E	7484	13/13	-	-	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CIT	7-E	7484	13/13	-	-	24,24,24,24	13
4	CIT	8-E	7484	13/13	-	-	24,24,24,24	13
4	CIT	9-E	7484	13/13	-	-	24,24,24,24	13
4	CIT	10-E	7484	13/13	-	-	24,24,24,24	13
2	MN	1-X	470	1/1	0.75	0.35	24,24,24,24	1
4	CIT	2-F	7486	13/13	-	-	24,24,24,24	13
4	CIT	3-F	7486	13/13	-	-	24,24,24,24	13
4	CIT	4-F	7486	13/13	-	-	24,24,24,24	13
4	CIT	5-F	7486	13/13	-	-	24,24,24,24	13
4	CIT	6-F	7486	13/13	-	-	24,24,24,24	13
4	CIT	7-F	7486	13/13	-	-	24,24,24,24	13
4	CIT	8-F	7486	13/13	-	-	24,24,24,24	13
4	CIT	9-F	7486	13/13	-	-	24,24,24,24	13
4	CIT	10-F	7486	13/13	-	-	24,24,24,24	13
2	MN	1-N	470	1/1	0.78	0.29	24,24,24,24	1
4	CIT	2-G	7488	13/13	-	-	24,24,24,24	13
4	CIT	3-G	7488	13/13	-	-	24,24,24,24	13
4	CIT	4-G	7488	13/13	-	-	24,24,24,24	13
4	CIT	5-G	7488	13/13	-	-	24,24,24,24	13
4	CIT	6-G	7488	13/13	-	-	24,24,24,24	13
4	CIT	7-G	7488	13/13	-	-	24,24,24,24	13
4	CIT	8-G	7488	13/13	-	-	24,24,24,24	13
4	CIT	9-G	7488	13/13	-	-	24,24,24,24	13
4	CIT	10-G	7488	13/13	-	-	24,24,24,24	13
2	MN	1-V	470	1/1	0.82	0.30	24,24,24,24	1
4	CIT	2-H	7490	13/13	-	-	24,24,24,24	13
4	CIT	3-H	7490	13/13	-	-	24,24,24,24	13
4	CIT	4-H	7490	13/13	-	-	24,24,24,24	13
4	CIT	5-H	7490	13/13	-	-	24,24,24,24	13
4	CIT	6-H	7490	13/13	-	-	24,24,24,24	13
4	CIT	7-H	7490	13/13	-	-	24,24,24,24	13
4	CIT	8-H	7490	13/13	-	-	24,24,24,24	13
4	CIT	9-H	7490	13/13	-	-	24,24,24,24	13
4	CIT	10-H	7490	13/13	-	-	24,24,24,24	13
2	MN	1-O	470	1/1	0.83	0.43	24,24,24,24	1
4	CIT	2-I	7492	13/13	-	-	24,24,24,24	13
4	CIT	3-I	7492	13/13	-	-	24,24,24,24	13
4	CIT	4-I	7492	13/13	-	-	24,24,24,24	13
4	CIT	5-I	7492	13/13	-	-	24,24,24,24	13
4	CIT	6-I	7492	13/13	-	-	24,24,24,24	13
4	CIT	7-I	7492	13/13	-	-	24,24,24,24	13
4	CIT	8-I	7492	13/13	-	-	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CIT	9-I	7492	13/13	-	-	24,24,24,24	13
4	CIT	10-I	7492	13/13	-	-	24,24,24,24	13
2	MN	1-H	470	1/1	0.84	0.28	24,24,24,24	1
4	CIT	2-J	7494	13/13	-	-	24,24,24,24	13
4	CIT	3-J	7494	13/13	-	-	24,24,24,24	13
4	CIT	4-J	7494	13/13	-	-	24,24,24,24	13
4	CIT	5-J	7494	13/13	-	-	24,24,24,24	13
4	CIT	6-J	7494	13/13	-	-	24,24,24,24	13
4	CIT	7-J	7494	13/13	-	-	24,24,24,24	13
4	CIT	8-J	7494	13/13	-	-	24,24,24,24	13
4	CIT	9-J	7494	13/13	-	-	24,24,24,24	13
4	CIT	10-J	7494	13/13	-	-	24,24,24,24	13
2	MN	1-M	470	1/1	0.84	0.31	24,24,24,24	1
4	CIT	2-K	7496	13/13	-	-	24,24,24,24	13
4	CIT	3-K	7496	13/13	-	-	24,24,24,24	13
4	CIT	4-K	7496	13/13	-	-	24,24,24,24	13
4	CIT	5-K	7496	13/13	-	-	24,24,24,24	13
4	CIT	6-K	7496	13/13	-	-	24,24,24,24	13
4	CIT	7-K	7496	13/13	-	-	24,24,24,24	13
4	CIT	8-K	7496	13/13	-	-	24,24,24,24	13
4	CIT	9-K	7496	13/13	-	-	24,24,24,24	13
4	CIT	10-K	7496	13/13	-	-	24,24,24,24	13
2	MN	1-I	470	1/1	0.84	0.34	24,24,24,24	1
4	CIT	2-L	7498	13/13	-	-	24,24,24,24	13
4	CIT	3-L	7498	13/13	-	-	24,24,24,24	13
4	CIT	4-L	7498	13/13	-	-	24,24,24,24	13
4	CIT	5-L	7498	13/13	-	-	24,24,24,24	13
4	CIT	6-L	7498	13/13	-	-	24,24,24,24	13
4	CIT	7-L	7498	13/13	-	-	24,24,24,24	13
4	CIT	8-L	7498	13/13	-	-	24,24,24,24	13
4	CIT	9-L	7498	13/13	-	-	24,24,24,24	13
4	CIT	10-L	7498	13/13	-	-	24,24,24,24	13
2	MN	1-T	470	1/1	0.85	0.27	24,24,24,24	1
4	CIT	2-M	7500	13/13	-	-	24,24,24,24	13
4	CIT	3-M	7500	13/13	-	-	24,24,24,24	13
4	CIT	4-M	7500	13/13	-	-	24,24,24,24	13
4	CIT	5-M	7500	13/13	-	-	24,24,24,24	13
4	CIT	6-M	7500	13/13	-	-	24,24,24,24	13
4	CIT	7-M	7500	13/13	-	-	24,24,24,24	13
4	CIT	8-M	7500	13/13	-	-	24,24,24,24	13
4	CIT	9-M	7500	13/13	-	-	24,24,24,24	13
4	CIT	10-M	7500	13/13	-	-	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	1-S	470	1/1	0.86	0.34	24,24,24,24	1
4	CIT	2-N	7502	13/13	-	-	24,24,24,24	13
4	CIT	3-N	7502	13/13	-	-	24,24,24,24	13
4	CIT	4-N	7502	13/13	-	-	24,24,24,24	13
4	CIT	5-N	7502	13/13	-	-	24,24,24,24	13
4	CIT	6-N	7502	13/13	-	-	24,24,24,24	13
4	CIT	7-N	7502	13/13	-	-	24,24,24,24	13
4	CIT	8-N	7502	13/13	-	-	24,24,24,24	13
4	CIT	9-N	7502	13/13	-	-	24,24,24,24	13
4	CIT	10-N	7502	13/13	-	-	24,24,24,24	13
2	MN	1-J	470	1/1	0.86	0.34	24,24,24,24	1
4	CIT	2-O	7504	13/13	-	-	24,24,24,24	13
4	CIT	3-O	7504	13/13	-	-	24,24,24,24	13
4	CIT	4-O	7504	13/13	-	-	24,24,24,24	13
4	CIT	5-O	7504	13/13	-	-	24,24,24,24	13
4	CIT	6-O	7504	13/13	-	-	24,24,24,24	13
4	CIT	7-O	7504	13/13	-	-	24,24,24,24	13
4	CIT	8-O	7504	13/13	-	-	24,24,24,24	13
4	CIT	9-O	7504	13/13	-	-	24,24,24,24	13
4	CIT	10-O	7504	13/13	-	-	24,24,24,24	13
2	MN	1-B	470	1/1	0.88	0.25	24,24,24,24	1
4	CIT	2-P	7506	13/13	-	-	24,24,24,24	13
4	CIT	3-P	7506	13/13	-	-	24,24,24,24	13
4	CIT	4-P	7506	13/13	-	-	24,24,24,24	13
4	CIT	5-P	7506	13/13	-	-	24,24,24,24	13
4	CIT	6-P	7506	13/13	-	-	24,24,24,24	13
4	CIT	7-P	7506	13/13	-	-	24,24,24,24	13
4	CIT	8-P	7506	13/13	-	-	24,24,24,24	13
4	CIT	9-P	7506	13/13	-	-	24,24,24,24	13
4	CIT	10-P	7506	13/13	-	-	24,24,24,24	13
2	MN	1-U	470	1/1	0.88	0.40	24,24,24,24	1
4	CIT	2-Q	7508	13/13	-	-	24,24,24,24	13
4	CIT	3-Q	7508	13/13	-	-	24,24,24,24	13
4	CIT	4-Q	7508	13/13	-	-	24,24,24,24	13
4	CIT	5-Q	7508	13/13	-	-	24,24,24,24	13
4	CIT	6-Q	7508	13/13	-	-	24,24,24,24	13
4	CIT	7-Q	7508	13/13	-	-	24,24,24,24	13
4	CIT	8-Q	7508	13/13	-	-	24,24,24,24	13
4	CIT	9-Q	7508	13/13	-	-	24,24,24,24	13
4	CIT	10-Q	7508	13/13	-	-	24,24,24,24	13
2	MN	1-W	470	1/1	0.89	0.28	24,24,24,24	1
4	CIT	2-R	7510	13/13	-	-	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CIT	3-R	7510	13/13	-	-	24,24,24,24	13
4	CIT	4-R	7510	13/13	-	-	24,24,24,24	13
4	CIT	5-R	7510	13/13	-	-	24,24,24,24	13
4	CIT	6-R	7510	13/13	-	-	24,24,24,24	13
4	CIT	7-R	7510	13/13	-	-	24,24,24,24	13
4	CIT	8-R	7510	13/13	-	-	24,24,24,24	13
4	CIT	9-R	7510	13/13	-	-	24,24,24,24	13
4	CIT	10-R	7510	13/13	-	-	24,24,24,24	13
2	MN	1-C	470	1/1	0.89	0.26	24,24,24,24	1
4	CIT	2-S	7512	13/13	-	-	24,24,24,24	13
4	CIT	3-S	7512	13/13	-	-	24,24,24,24	13
4	CIT	4-S	7512	13/13	-	-	24,24,24,24	13
4	CIT	5-S	7512	13/13	-	-	24,24,24,24	13
4	CIT	6-S	7512	13/13	-	-	24,24,24,24	13
4	CIT	7-S	7512	13/13	-	-	24,24,24,24	13
4	CIT	8-S	7512	13/13	-	-	24,24,24,24	13
4	CIT	9-S	7512	13/13	-	-	24,24,24,24	13
4	CIT	10-S	7512	13/13	-	-	24,24,24,24	13
2	MN	1-R	470	1/1	0.90	0.26	24,24,24,24	1
4	CIT	2-T	7514	13/13	-	-	24,24,24,24	13
4	CIT	3-T	7514	13/13	-	-	24,24,24,24	13
4	CIT	4-T	7514	13/13	-	-	24,24,24,24	13
4	CIT	5-T	7514	13/13	-	-	24,24,24,24	13
4	CIT	6-T	7514	13/13	-	-	24,24,24,24	13
4	CIT	7-T	7514	13/13	-	-	24,24,24,24	13
4	CIT	8-T	7514	13/13	-	-	24,24,24,24	13
4	CIT	9-T	7514	13/13	-	-	24,24,24,24	13
4	CIT	10-T	7514	13/13	-	-	24,24,24,24	13
2	MN	1-Q	470	1/1	0.92	0.32	24,24,24,24	1
4	CIT	2-U	7516	13/13	-	-	24,24,24,24	13
4	CIT	3-U	7516	13/13	-	-	24,24,24,24	13
4	CIT	4-U	7516	13/13	-	-	24,24,24,24	13
4	CIT	5-U	7516	13/13	-	-	24,24,24,24	13
4	CIT	6-U	7516	13/13	-	-	24,24,24,24	13
4	CIT	7-U	7516	13/13	-	-	24,24,24,24	13
4	CIT	8-U	7516	13/13	-	-	24,24,24,24	13
4	CIT	9-U	7516	13/13	-	-	24,24,24,24	13
4	CIT	10-U	7516	13/13	-	-	24,24,24,24	13
2	MN	1-K	470	1/1	0.92	0.31	24,24,24,24	1
4	CIT	2-V	7518	13/13	-	-	24,24,24,24	13
4	CIT	3-V	7518	13/13	-	-	24,24,24,24	13
4	CIT	4-V	7518	13/13	-	-	24,24,24,24	13

Continued on next page...

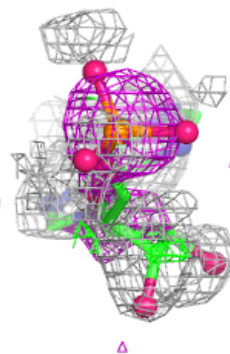
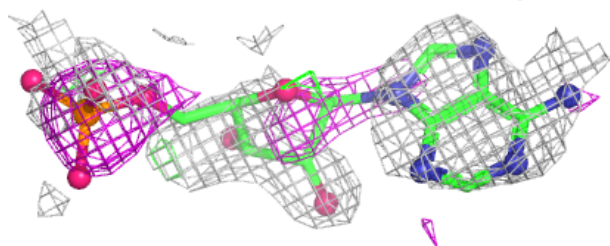
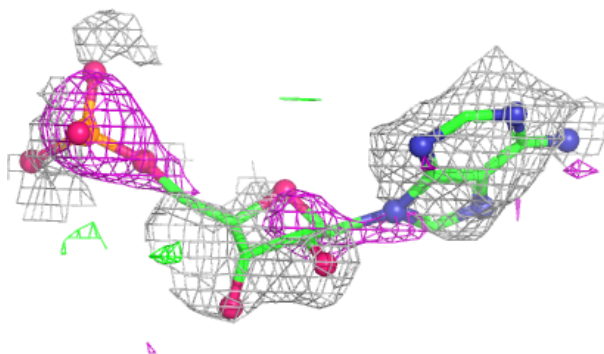
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CIT	5-V	7518	13/13	-	-	24,24,24,24	13
4	CIT	6-V	7518	13/13	-	-	24,24,24,24	13
4	CIT	7-V	7518	13/13	-	-	24,24,24,24	13
4	CIT	8-V	7518	13/13	-	-	24,24,24,24	13
4	CIT	9-V	7518	13/13	-	-	24,24,24,24	13
4	CIT	10-V	7518	13/13	-	-	24,24,24,24	13
2	MN	1-P	470	1/1	0.94	0.25	24,24,24,24	1
4	CIT	2-W	7520	13/13	-	-	24,24,24,24	13
4	CIT	3-W	7520	13/13	-	-	24,24,24,24	13
4	CIT	4-W	7520	13/13	-	-	24,24,24,24	13
4	CIT	5-W	7520	13/13	-	-	24,24,24,24	13
4	CIT	6-W	7520	13/13	-	-	24,24,24,24	13
4	CIT	7-W	7520	13/13	-	-	24,24,24,24	13
4	CIT	8-W	7520	13/13	-	-	24,24,24,24	13
4	CIT	9-W	7520	13/13	-	-	24,24,24,24	13
4	CIT	10-W	7520	13/13	-	-	24,24,24,24	13
2	MN	1-F	470	1/1	0.96	0.40	24,24,24,24	1
4	CIT	2-X	7522	13/13	-	-	24,24,24,24	13
4	CIT	3-X	7522	13/13	-	-	24,24,24,24	13
4	CIT	4-X	7522	13/13	-	-	24,24,24,24	13
4	CIT	5-X	7522	13/13	-	-	24,24,24,24	13
4	CIT	6-X	7522	13/13	-	-	24,24,24,24	13
4	CIT	7-X	7522	13/13	-	-	24,24,24,24	13
4	CIT	8-X	7522	13/13	-	-	24,24,24,24	13
4	CIT	9-X	7522	13/13	-	-	24,24,24,24	13
4	CIT	10-X	7522	13/13	-	-	24,24,24,24	13

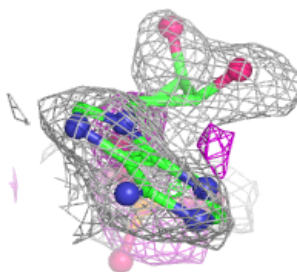
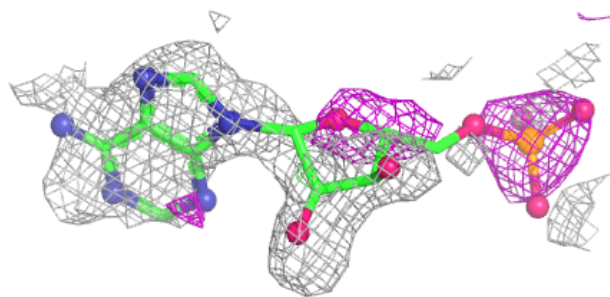
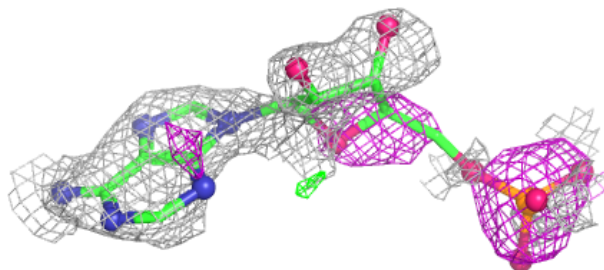
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AMP D 7481:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

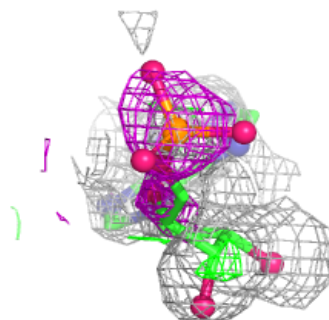
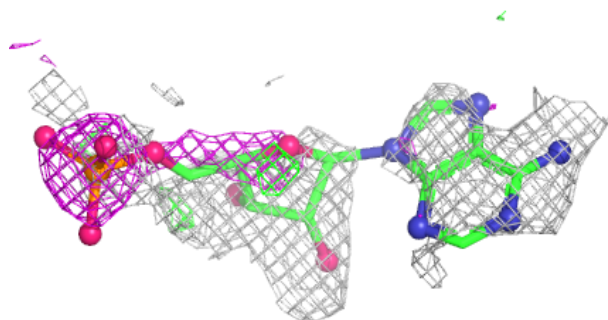
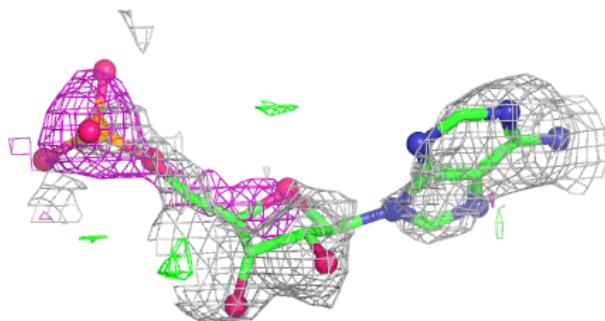
**Electron density around AMP K 7495:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

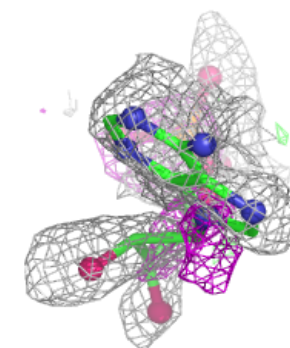
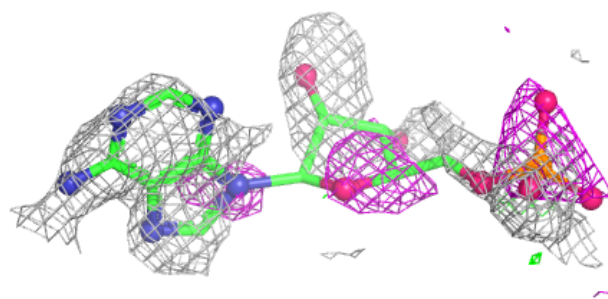
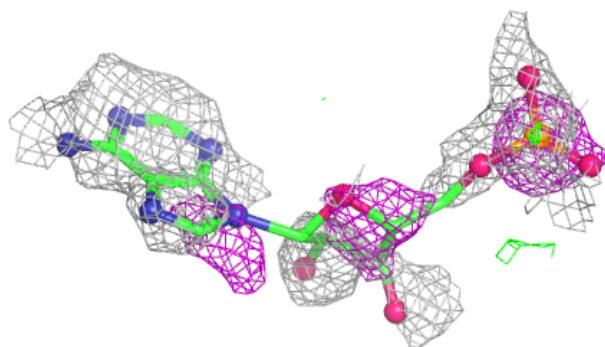


Electron density around AMP I 7491:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

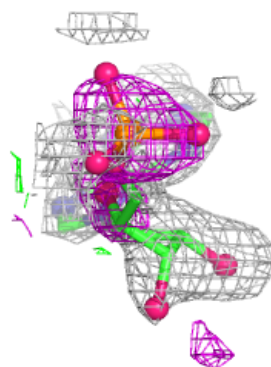
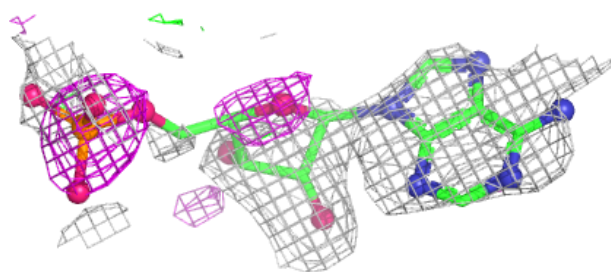
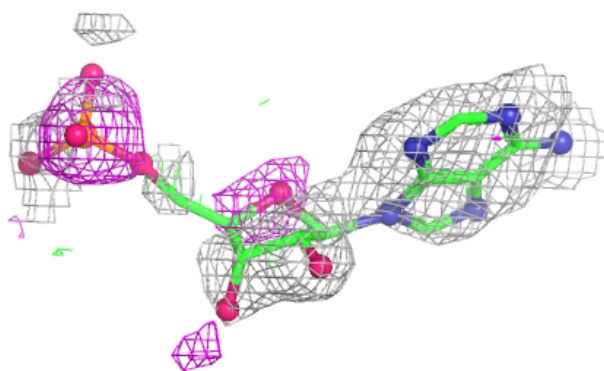
**Electron density around AMP N 7501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

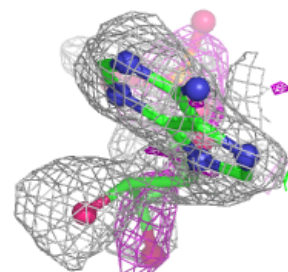
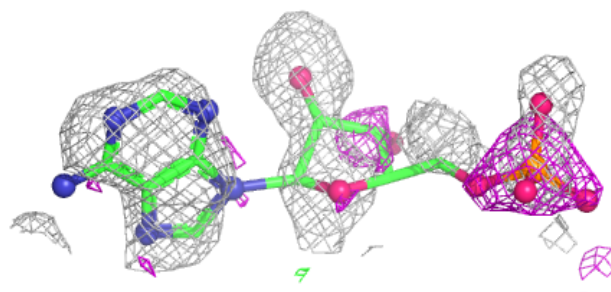
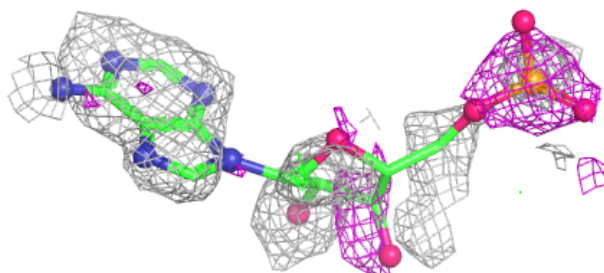


Electron density around AMP P 7505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

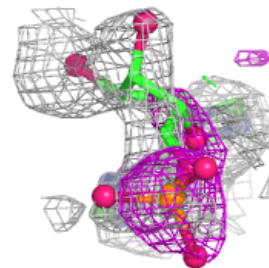
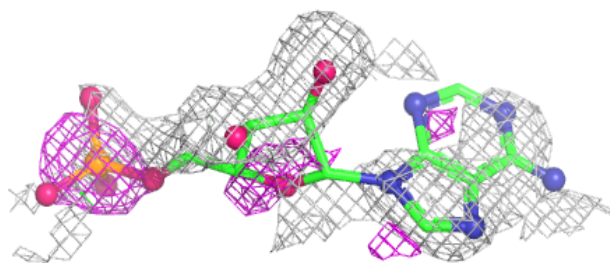
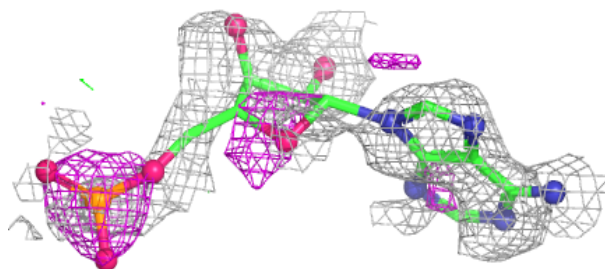
**Electron density around AMP J 7493:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

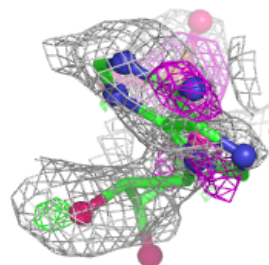
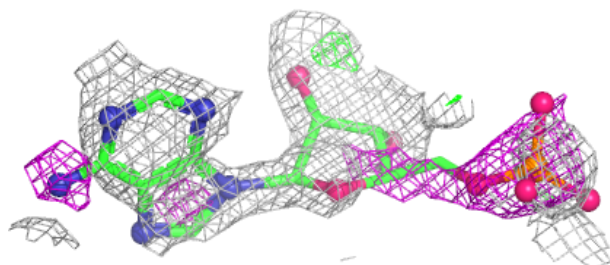
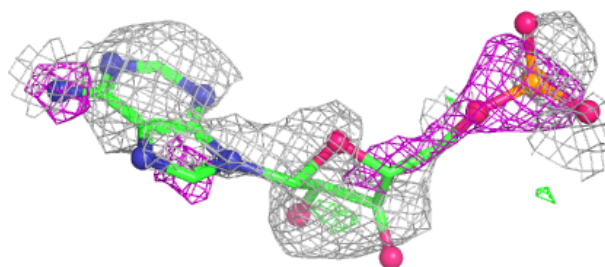


Electron density around AMP A 7475:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

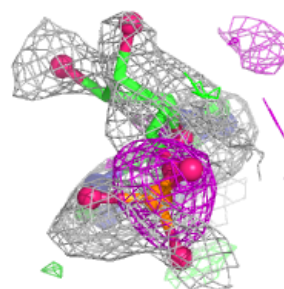
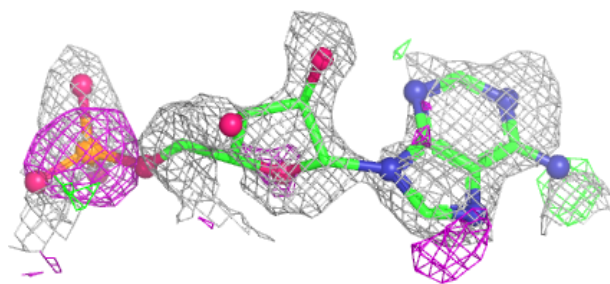
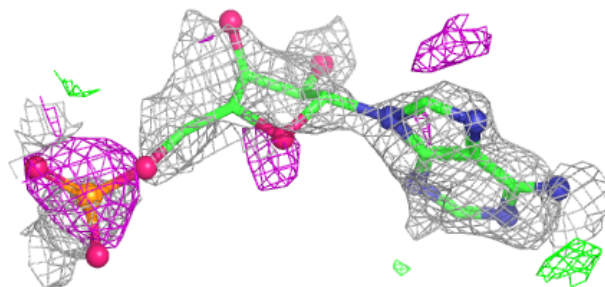
**Electron density around AMP H 7489:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

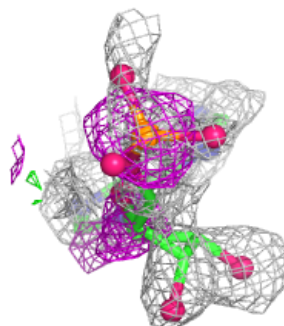
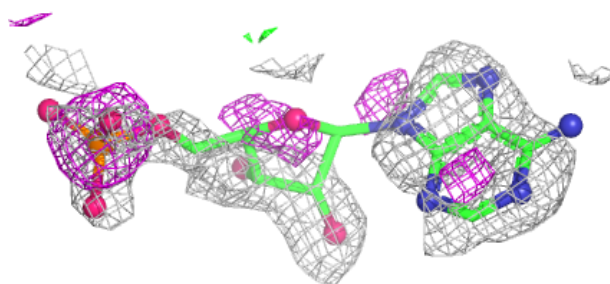
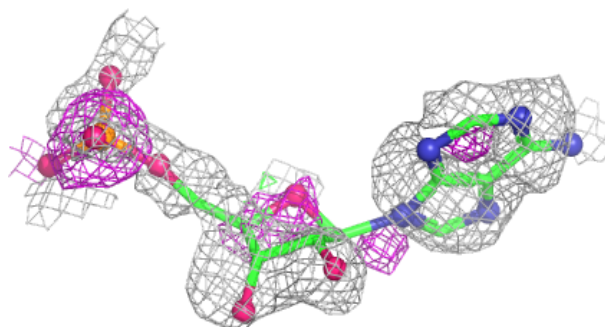


Electron density around AMP V 7517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

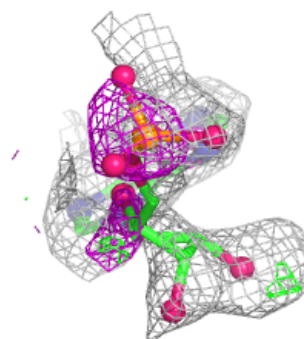
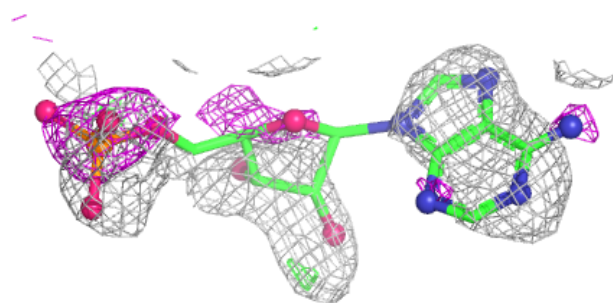
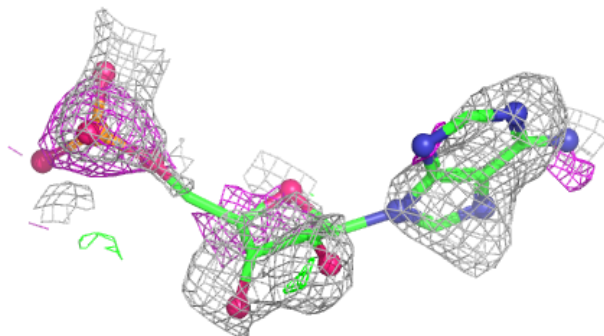
**Electron density around AMP F 7485:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

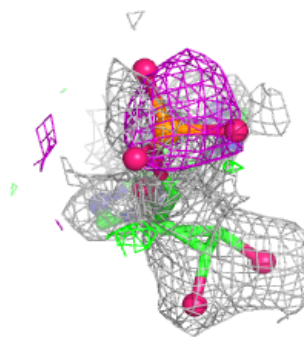
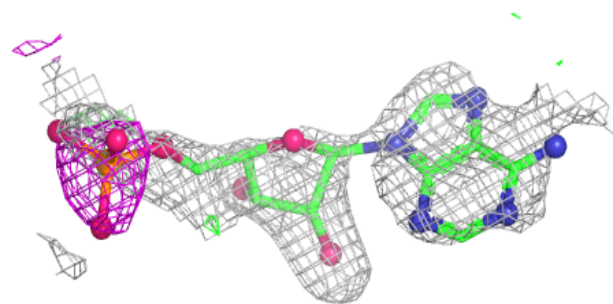
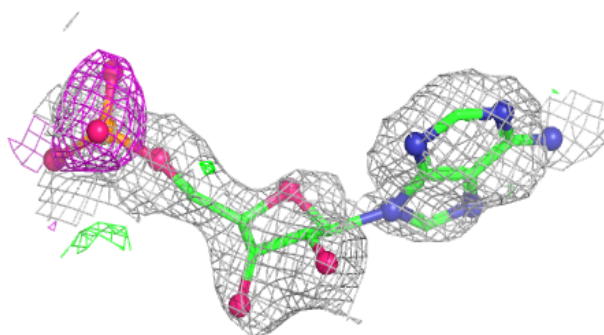


Electron density around AMP R 7509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

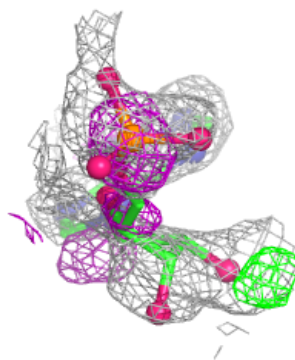
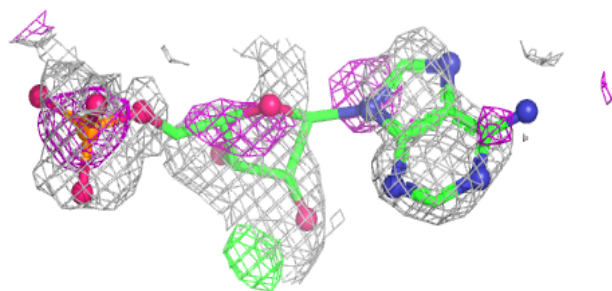
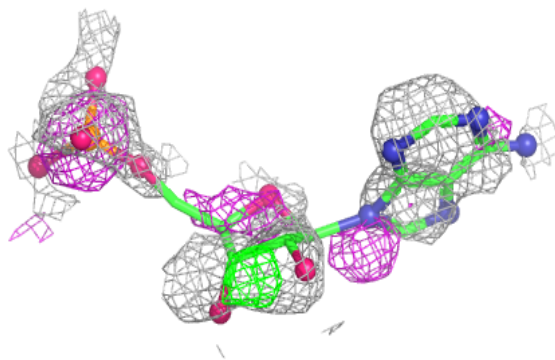
**Electron density around AMP G 7487:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

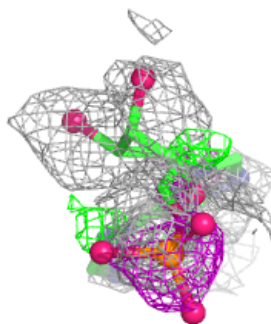
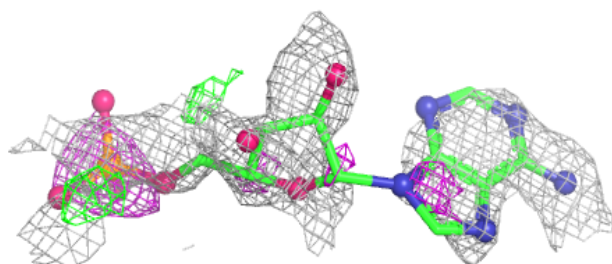
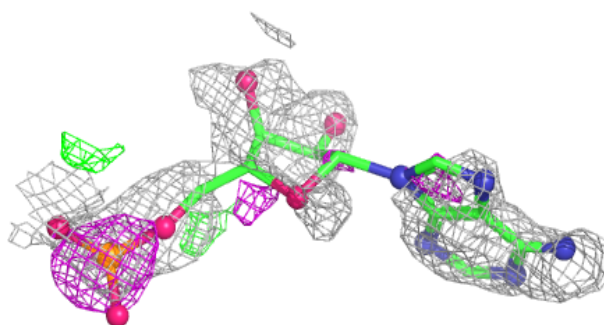


Electron density around AMP B 7477:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

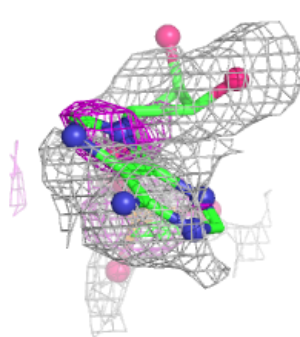
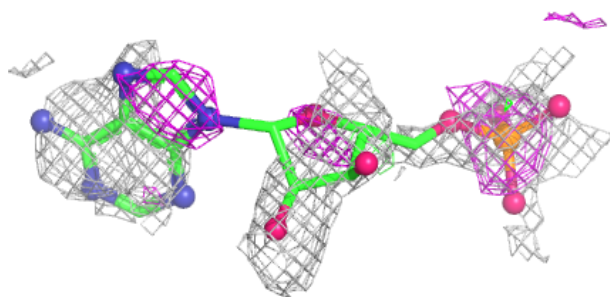
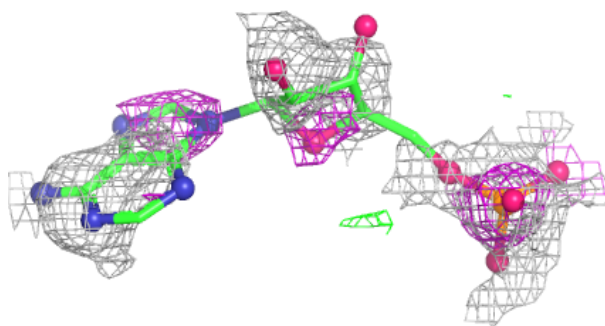
**Electron density around AMP E 7483:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

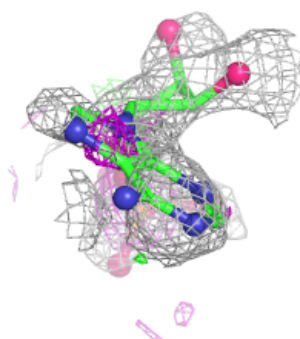
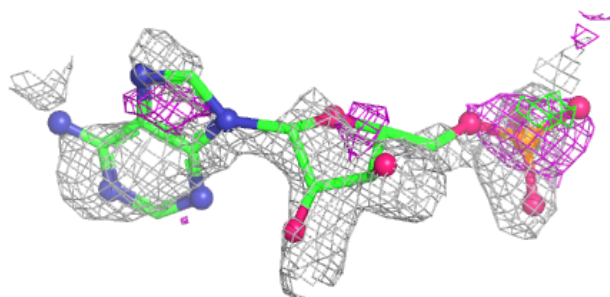
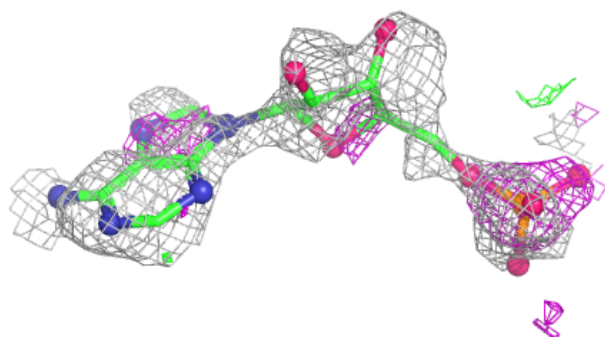


Electron density around AMP U 7515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

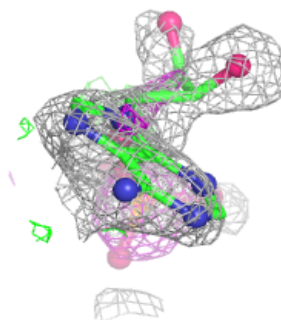
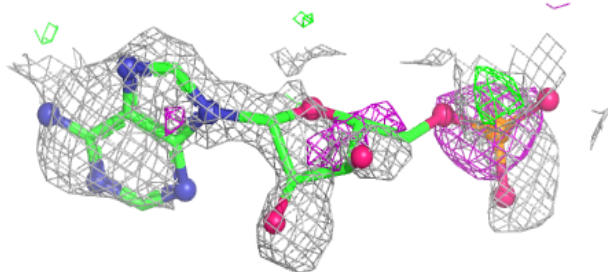
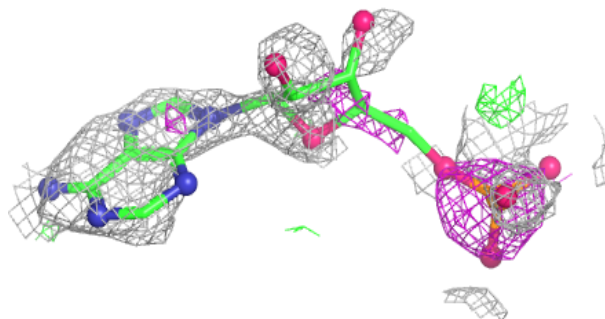
**Electron density around AMP O 7503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

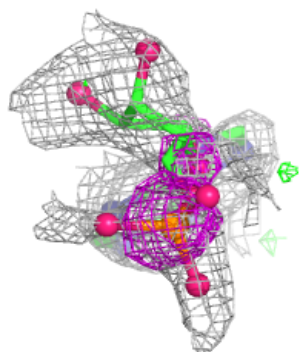
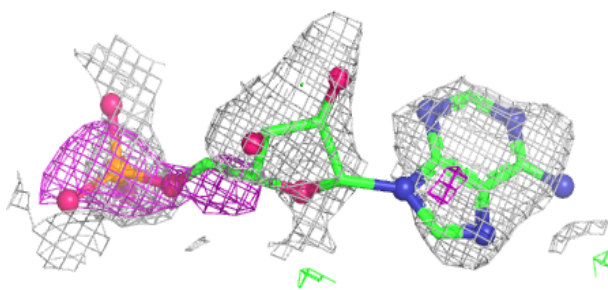
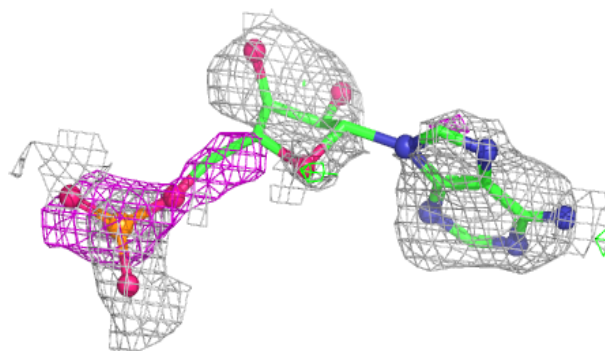


Electron density around AMP W 7519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

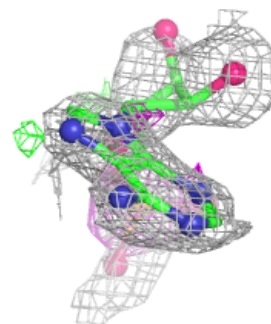
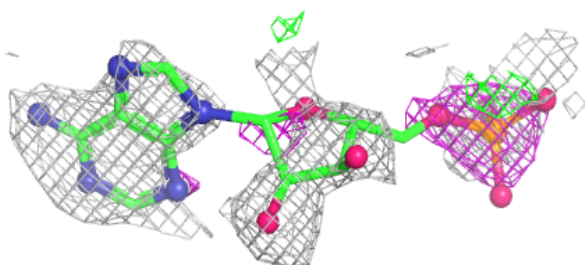
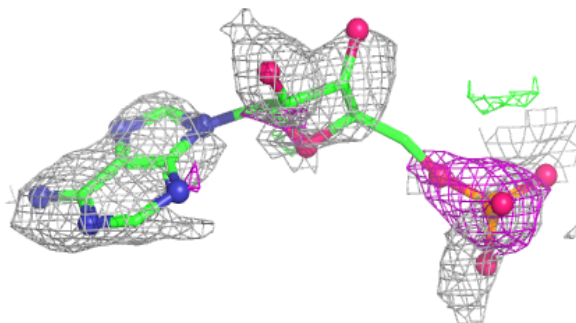
**Electron density around AMP L 7497:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

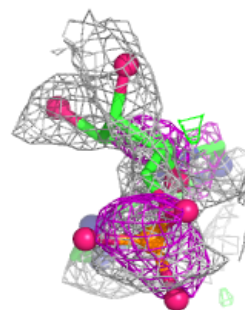
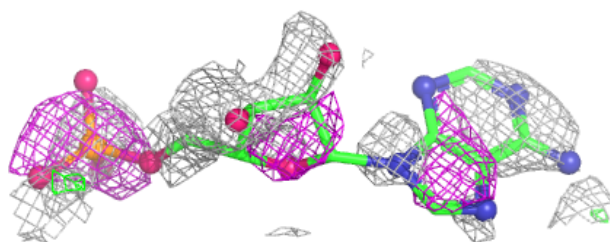
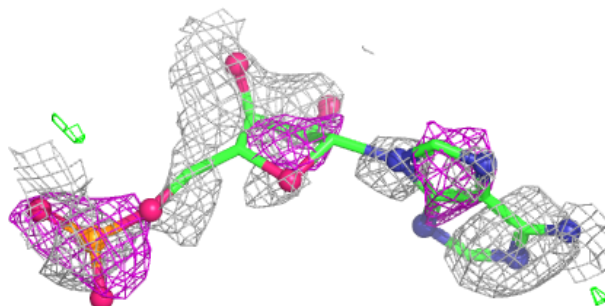


Electron density around AMP M 7499:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

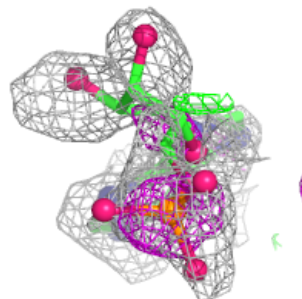
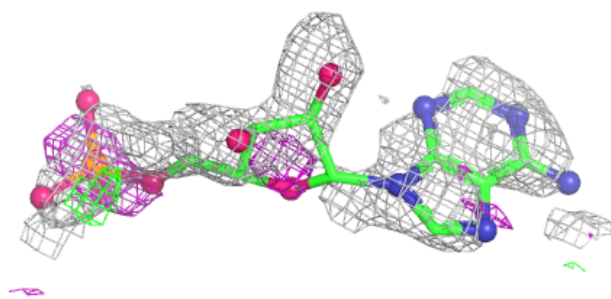
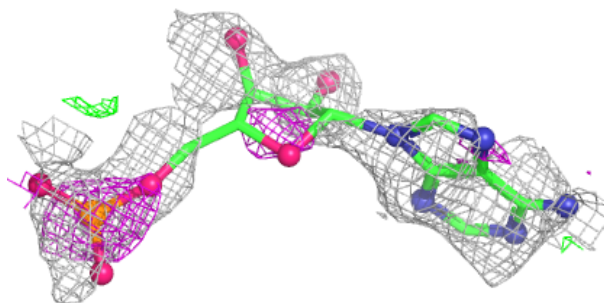
**Electron density around AMP C 7479:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

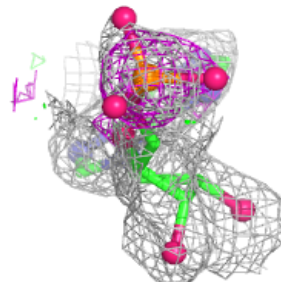
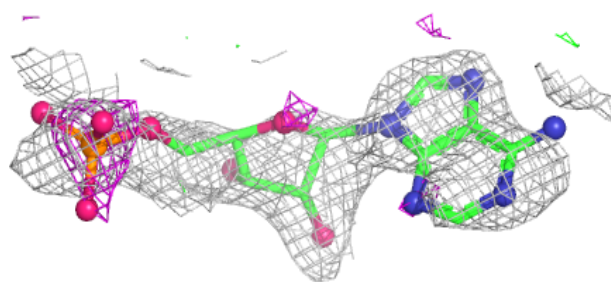
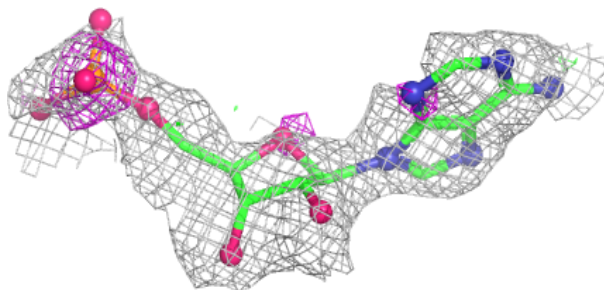


Electron density around AMP Q 7507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

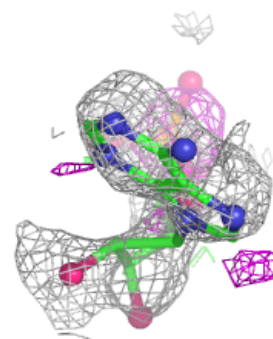
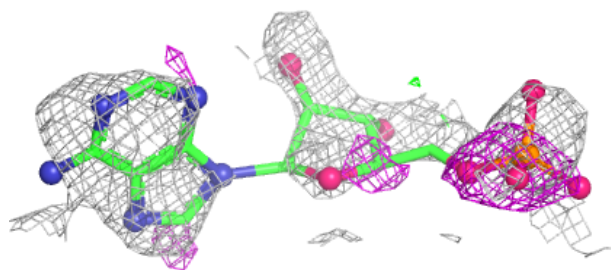
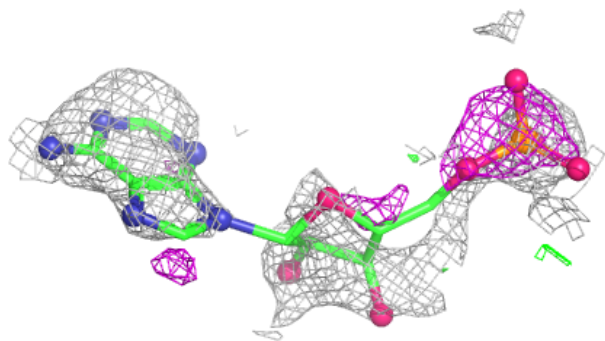
**Electron density around AMP S 7511:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

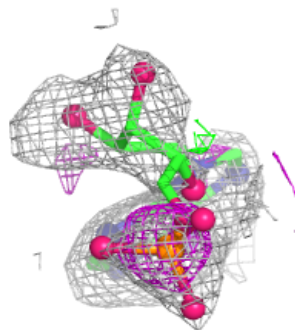
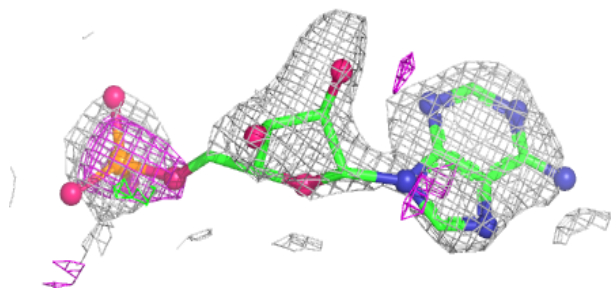
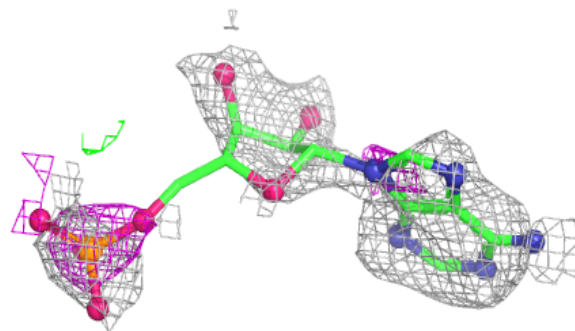


Electron density around AMP T 7513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AMP X 7521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.