



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:20 PM UTC

PDB ID : 3EPC / pdb_00003epc
EMDB ID : EMD-1570
Title : CryoEM structure of poliovirus receptor bound to poliovirus type 1
Authors : Zhang, P.; Mueller, S.; Morais, M.C.; Bator, C.M.; Bowman, V.D.; Hafenstein, S.; Wimmer, E.; Rossmann, M.G.
Deposited on : 2008-09-29
Resolution : 8.00 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

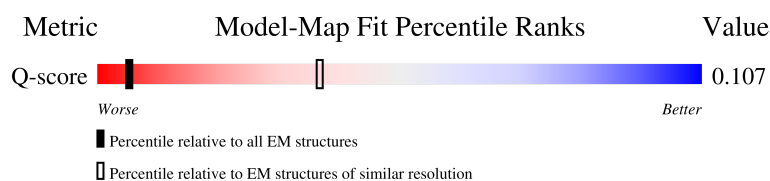
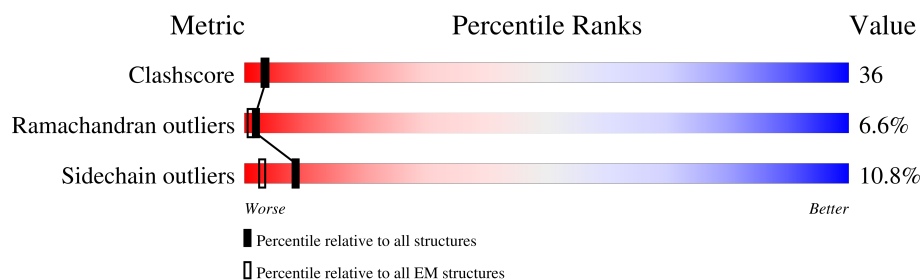
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	213	18% 38% 42% 15% 6%
2	1	283	• 57% 34% 6%
3	2	268	• 62% 29% •
4	4	68	6% 47% 31% 9% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	3	235	

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
6	SPH	1	0	X	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Poliovirus receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	213	Total	C	N	O	S	0	0
			1638	1038	281	310	9		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	105	ASP	ASN	engineered mutation	UNP P15151
R	120	SER	ASN	engineered mutation	UNP P15151
R	188	GLN	ASN	engineered mutation	UNP P15151
R	218	GLN	ASN	engineered mutation	UNP P15151
R	237	SER	ASN	engineered mutation	UNP P15151

- Molecule 2 is a protein called Protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	283	Total	C	N	O	S	0	0
			2222	1416	378	423	5		

- Molecule 3 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	268	Total	C	N	O	S	0	0
			2085	1317	358	396	14		

- Molecule 4 is a protein called Protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	63	Total	C	N	O	S	0	1
			477	293	82	101	1		

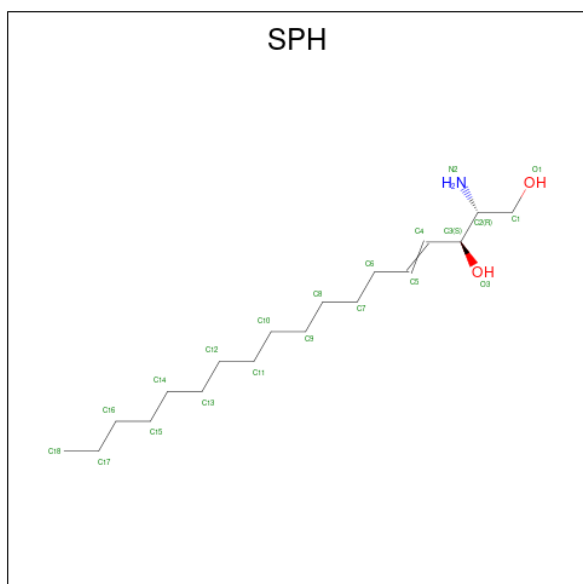
- Molecule 5 is a protein called Protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	235	Total	C	N	O	S	0	0
			1834	1169	299	349	17		

There is a discrepancy between the modelled and reference sequences:

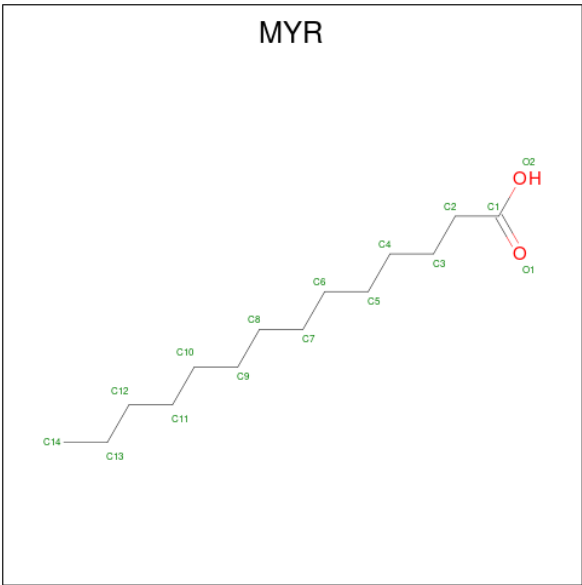
Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	SEE REMARK 999	UNP P03300

- Molecule 6 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
6	1	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 7 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).

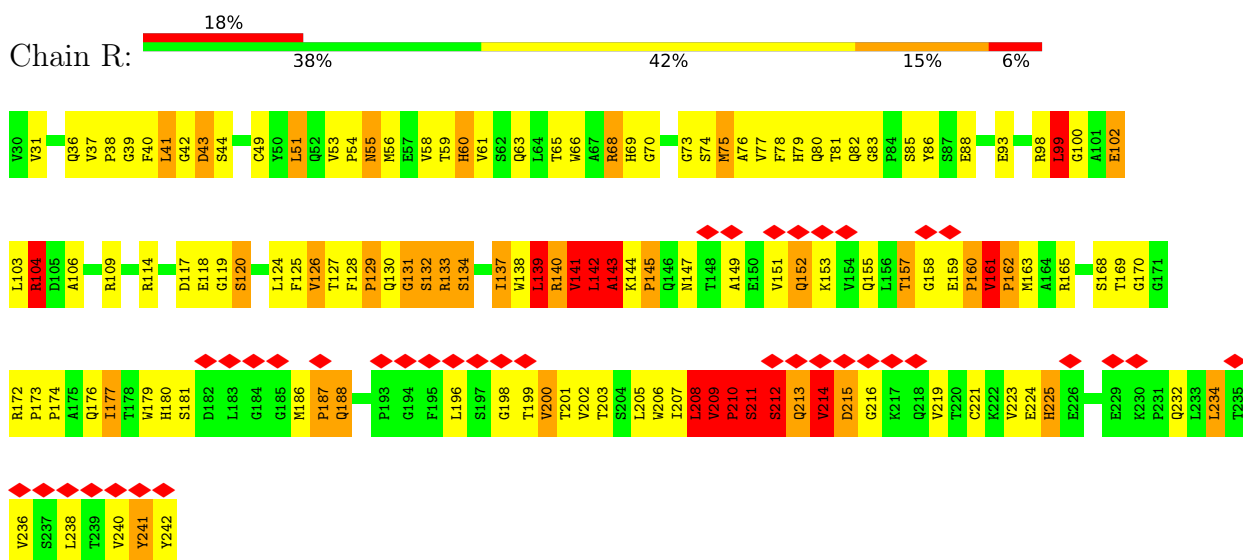


Mol	Chain	Residues	Atoms			AltConf
7	4	1	Total	C	O	0
			15	14	1	

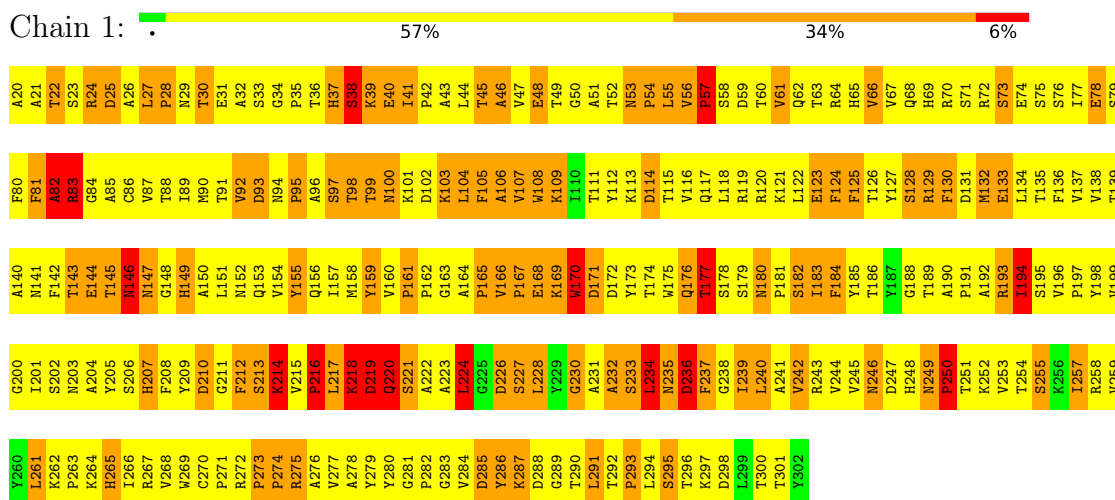
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Poliovirus receptor

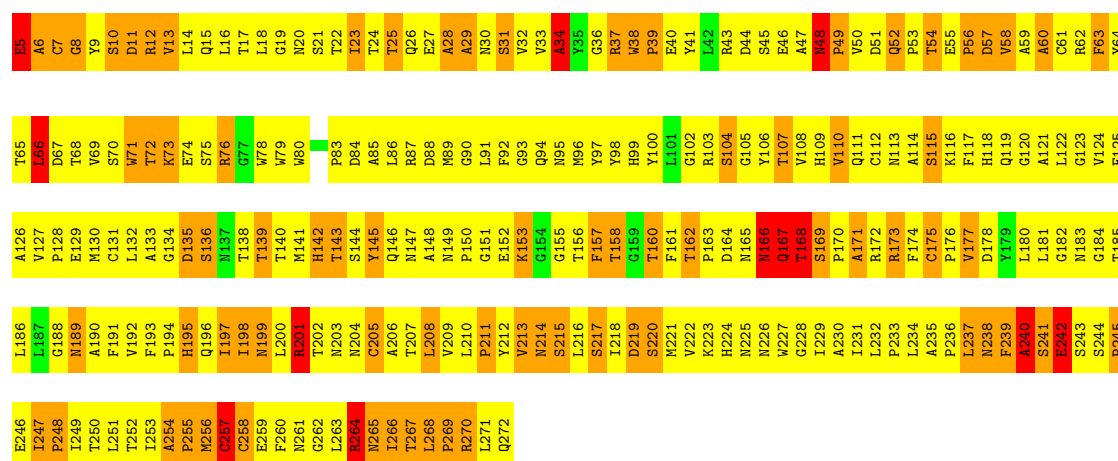


• Molecule 2: Protein VP1



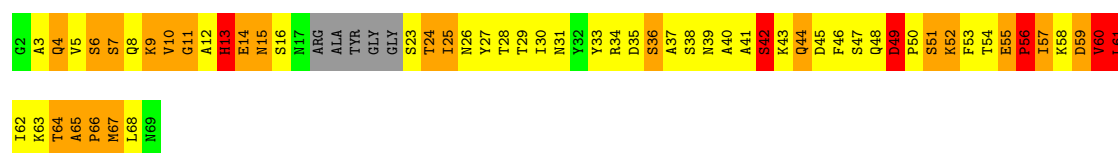
• Molecule 3: Protein VP2

Chain 2:  62% 29%



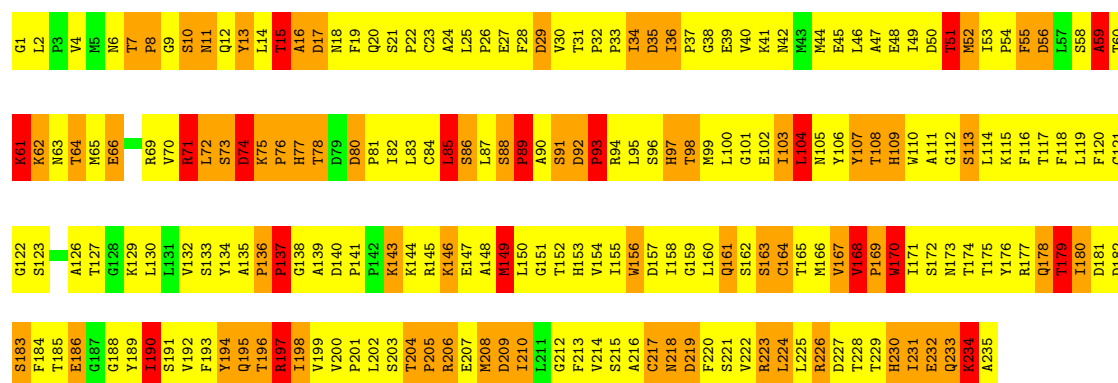
• Molecule 4: Protein VP4

Chain 4:  6% 47% 31% 9% 7%



• Molecule 5: Protein VP3

Chain 3:  6% 57% 29% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	857	Depositor
Maximum defocus (nm)	2126	Depositor
Magnification	47000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	32.252	Depositor
Minimum map value	-6.836	Depositor
Average map value	1.633	Depositor
Map value standard deviation	5.404	Depositor
Recommended contour level	7.03	Depositor
Map size ($\text{\AA}$)	575.05005, 575.05005, 575.05005	wwPDB
Map dimensions	217, 217, 217	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.65, 2.65, 2.65	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SPH, MYR

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	R	0.60	1/1678 (0.1%)	1.10	11/2289 (0.5%)
2	1	3.03	364/2285 (15.9%)	2.83	285/3124 (9.1%)
3	2	3.01	322/2142 (15.0%)	2.88	291/2928 (9.9%)
4	4	3.02	82/484 (16.9%)	2.92	68/653 (10.4%)
5	3	3.00	272/1881 (14.5%)	2.79	223/2562 (8.7%)
All	All	2.71	1041/8470 (12.3%)	2.59	878/11556 (7.6%)

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	R	1	6

All (1041) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	151	GLY	N-CA	11.45	1.53	1.44
2	1	196	VAL	N-CA	9.60	1.53	1.45
3	2	245	PRO	C-N	-9.35	1.22	1.33
5	3	159	GLY	N-CA	9.24	1.53	1.45
5	3	196	THR	CA-C	8.83	1.60	1.52
5	3	1	GLY	N-CA	8.82	1.59	1.45
2	1	283	GLY	N-CA	8.65	1.52	1.44
4	4	14	GLU	N-CA	8.62	1.56	1.46
2	1	20	ALA	N-CA	8.38	1.62	1.46
2	1	93	ASP	C-N	-8.27	1.22	1.33
3	2	237	LEU	C-N	-8.24	1.22	1.33
4	4	23	SER	N-CA	8.19	1.61	1.46
4	4	47	SER	C-N	-7.99	1.21	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	273	PRO	CA-C	7.97	1.59	1.52
2	1	195	SER	C-N	-7.96	1.25	1.33
3	2	30	ASN	C-N	-7.95	1.22	1.33
5	3	196	THR	N-CA	7.93	1.54	1.46
5	3	53	ILE	N-CA	7.91	1.52	1.46
3	2	246	GLU	C-N	-7.84	1.24	1.33
2	1	80	PHE	N-CA	7.84	1.55	1.46
3	2	235	ALA	N-CA	7.77	1.54	1.46
2	1	146	ASN	C-N	-7.75	1.22	1.33
5	3	141	PRO	CA-C	7.74	1.59	1.52
2	1	124	PHE	C-O	-7.68	1.14	1.24
5	3	136	PRO	CA-C	7.67	1.59	1.52
2	1	272	ARG	CA-C	7.59	1.60	1.52
5	3	231	ILE	C-N	-7.58	1.23	1.33
3	2	263	LEU	C-N	-7.52	1.25	1.33
2	1	124	PHE	N-CA	7.45	1.56	1.46
3	2	6	ALA	N-CA	7.44	1.55	1.46
3	2	217	SER	N-CA	7.44	1.55	1.46
2	1	202	SER	N-CA	7.41	1.54	1.45
3	2	127	VAL	N-CA	7.41	1.52	1.46
2	1	149	HIS	C-N	-7.40	1.24	1.33
2	1	163	GLY	CA-C	7.39	1.59	1.52
5	3	195	GLN	N-CA	7.35	1.55	1.46
2	1	292	THR	N-CA	7.31	1.53	1.46
2	1	161	PRO	CA-C	7.30	1.58	1.52
3	2	92	PHE	N-CA	7.28	1.55	1.46
3	2	169	SER	N-CA	7.26	1.54	1.46
5	3	70	VAL	CA-C	7.25	1.59	1.53
2	1	115	THR	N-CA	7.25	1.54	1.45
5	3	204	THR	CA-C	7.25	1.59	1.52
3	2	162	THR	N-CA	7.24	1.54	1.46
3	2	118	HIS	C-N	-7.23	1.23	1.33
2	1	163	GLY	N-CA	7.22	1.53	1.45
3	2	59	ALA	N-CA	7.21	1.55	1.46
3	2	175	CYS	N-CA	7.16	1.53	1.46
2	1	72	ARG	N-CA	7.14	1.54	1.46
5	3	148	ALA	N-CA	7.13	1.54	1.46
2	1	79	SER	N-CA	7.12	1.54	1.46
3	2	235	ALA	CA-C	7.09	1.60	1.52
5	3	47	ALA	N-CA	7.09	1.55	1.46
5	3	32	PRO	CA-C	7.09	1.58	1.52
4	4	13	HIS	C-N	-7.04	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	218	ILE	C-N	-7.04	1.25	1.33
5	3	184	PHE	N-CA	7.04	1.54	1.46
2	1	73	SER	N-CA	7.04	1.54	1.46
2	1	76	SER	N-CA	7.03	1.54	1.45
3	2	117	PHE	N-CA	7.01	1.55	1.46
5	3	28	PHE	N-CA	7.01	1.55	1.46
2	1	125	PHE	N-CA	6.99	1.54	1.46
4	4	37	ALA	N-CA	6.99	1.54	1.46
3	2	235	ALA	C-N	-6.99	1.24	1.33
5	3	51	THR	N-CA	6.98	1.54	1.46
2	1	212	PHE	N-CA	6.96	1.54	1.45
3	2	240	ALA	N-CA	6.96	1.55	1.46
2	1	114	ASP	N-CA	6.96	1.55	1.46
2	1	43	ALA	N-CA	6.95	1.55	1.46
2	1	96	ALA	N-CA	6.95	1.54	1.46
5	3	98	THR	N-CA	6.95	1.54	1.45
2	1	171	ASP	N-CA	6.95	1.53	1.46
3	2	94	GLN	N-CA	6.95	1.54	1.46
2	1	237	PHE	N-CA	6.94	1.54	1.46
2	1	295	SER	N-CA	6.93	1.53	1.45
2	1	99	THR	C-N	-6.93	1.24	1.34
3	2	248	PRO	C-N	-6.92	1.23	1.33
3	2	185	THR	N-CA	6.91	1.54	1.45
3	2	133	ALA	N-CA	6.90	1.54	1.46
2	1	196	VAL	CA-C	6.90	1.58	1.52
3	2	148	ALA	N-CA	6.90	1.55	1.46
2	1	148	GLY	CA-C	6.89	1.59	1.52
2	1	243	ARG	C-N	-6.88	1.26	1.33
5	3	120	PHE	N-CA	6.88	1.55	1.46
2	1	232	ALA	N-CA	6.87	1.55	1.46
5	3	183	SER	N-CA	6.87	1.54	1.46
3	2	45	SER	N-CA	6.86	1.54	1.46
3	2	238	ASN	C-N	-6.86	1.24	1.33
3	2	105	GLY	N-CA	6.84	1.53	1.45
2	1	82	ALA	N-CA	6.84	1.55	1.46
2	1	105	PHE	N-CA	6.82	1.54	1.46
3	2	177	VAL	N-CA	6.82	1.53	1.46
3	2	270	ARG	CA-C	6.82	1.60	1.53
3	2	105	GLY	C-N	-6.82	1.24	1.33
5	3	177	ARG	N-CA	6.80	1.53	1.45
3	2	146	GLN	N-CA	6.79	1.54	1.46
3	2	29	ALA	N-CA	6.78	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	180	ASN	CA-C	6.78	1.60	1.53
2	1	207	HIS	N-CA	6.77	1.54	1.46
5	3	175	THR	N-CA	6.77	1.54	1.46
2	1	202	SER	CA-C	6.76	1.60	1.52
3	2	60	ALA	CA-C	6.75	1.60	1.52
3	2	190	ALA	N-CA	6.75	1.54	1.46
5	3	64	THR	N-CA	6.75	1.54	1.45
2	1	78	GLU	CA-C	6.74	1.61	1.52
2	1	85	ALA	N-CA	6.74	1.54	1.46
5	3	206	ARG	N-CA	6.73	1.55	1.46
2	1	284	VAL	N-CA	6.71	1.53	1.46
3	2	85	ALA	N-CA	6.71	1.54	1.46
3	2	93	GLY	CA-C	6.71	1.59	1.52
3	2	138	THR	N-CA	6.71	1.54	1.46
2	1	119	ARG	N-CA	6.70	1.54	1.46
2	1	33	SER	N-CA	6.70	1.54	1.46
2	1	64	ARG	N-CA	6.69	1.53	1.45
2	1	208	PHE	N-CA	6.69	1.54	1.46
3	2	139	THR	N-CA	6.69	1.54	1.45
2	1	126	THR	N-CA	6.68	1.54	1.46
2	1	51	ALA	N-CA	6.68	1.53	1.45
3	2	196	GLN	C-N	-6.68	1.25	1.33
3	2	242	GLU	CA-C	6.68	1.60	1.52
3	2	171	ALA	N-CA	6.68	1.54	1.46
2	1	96	ALA	CA-C	6.67	1.61	1.52
3	2	252	THR	N-CA	6.67	1.54	1.46
3	2	211	PRO	N-CA	6.66	1.54	1.46
3	2	88	ASP	N-CA	6.66	1.54	1.46
4	4	53	PHE	N-CA	6.66	1.54	1.46
3	2	168	THR	N-CA	6.65	1.54	1.46
5	3	84	CYS	N-CA	6.65	1.54	1.46
4	4	38	SER	N-CA	6.65	1.54	1.46
5	3	45	GLU	N-CA	6.65	1.54	1.46
2	1	300	THR	N-CA	6.64	1.53	1.46
5	3	127	THR	N-CA	6.64	1.53	1.45
5	3	132	VAL	N-CA	6.64	1.53	1.46
2	1	81	PHE	N-CA	6.63	1.54	1.46
3	2	6	ALA	C-O	-6.62	1.15	1.24
5	3	101	GLY	CA-C	6.62	1.59	1.51
2	1	97	SER	N-CA	6.61	1.54	1.46
4	4	12	ALA	CA-C	6.61	1.61	1.52
2	1	213	SER	N-CA	6.60	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	223	ALA	N-CA	6.59	1.54	1.46
5	3	15	THR	N-CA	6.58	1.54	1.46
3	2	191	PHE	N-CA	6.57	1.54	1.46
5	3	20	GLN	C-N	-6.57	1.24	1.34
3	2	172	ARG	C-N	-6.57	1.25	1.33
5	3	58	SER	N-CA	6.55	1.54	1.46
2	1	78	GLU	N-CA	6.54	1.54	1.46
2	1	222	ALA	N-CA	6.54	1.54	1.46
5	3	122	GLY	N-CA	6.54	1.53	1.45
2	1	281	GLY	C-N	-6.54	1.26	1.34
2	1	23	SER	N-CA	6.53	1.54	1.46
4	4	40	ALA	C-N	-6.53	1.24	1.33
2	1	227	SER	N-CA	6.53	1.54	1.46
5	3	217	CYS	N-CA	6.52	1.54	1.45
5	3	24	ALA	N-CA	6.51	1.54	1.46
3	2	239	PHE	N-CA	6.50	1.54	1.46
4	4	36	SER	N-CA	6.50	1.54	1.46
2	1	178	SER	N-CA	6.50	1.54	1.46
5	3	86	SER	N-CA	6.49	1.54	1.46
3	2	126	ALA	N-CA	6.49	1.54	1.46
3	2	234	LEU	N-CA	6.49	1.54	1.46
5	3	102	GLU	N-CA	6.49	1.54	1.46
5	3	186	GLU	N-CA	6.48	1.54	1.46
2	1	233	SER	N-CA	6.48	1.54	1.46
4	4	12	ALA	N-CA	6.48	1.55	1.46
3	2	11	ASP	N-CA	6.48	1.54	1.46
5	3	232	GLU	C-N	-6.47	1.24	1.33
2	1	251	THR	N-CA	6.47	1.54	1.46
5	3	219	ASP	N-CA	6.46	1.54	1.46
4	4	54	THR	N-CA	6.46	1.54	1.46
2	1	179	SER	N-CA	6.46	1.54	1.46
3	2	93	GLY	N-CA	6.45	1.53	1.45
5	3	207	GLU	C-N	-6.45	1.25	1.33
4	4	8	GLN	CA-C	6.45	1.61	1.52
2	1	172	ASP	N-CA	6.44	1.54	1.45
5	3	101	GLY	N-CA	6.44	1.53	1.45
5	3	147	GLU	N-CA	6.44	1.54	1.46
5	3	207	GLU	CA-C	6.43	1.60	1.52
3	2	44	ASP	N-CA	6.43	1.54	1.46
5	3	151	GLY	CA-C	6.43	1.59	1.52
2	1	120	ARG	N-CA	6.42	1.54	1.46
5	3	123	SER	N-CA	6.42	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	142	PHE	N-CA	6.41	1.53	1.46
3	2	60	ALA	N-CA	6.41	1.54	1.46
2	1	204	ALA	N-CA	6.41	1.54	1.46
3	2	39	PRO	C-N	-6.41	1.25	1.33
5	3	16	ALA	N-CA	6.40	1.54	1.46
3	2	215	SER	N-CA	6.40	1.54	1.46
4	4	62	ILE	N-CA	6.40	1.53	1.46
3	2	119	GLN	N-CA	6.39	1.53	1.45
5	3	180	ILE	N-CA	6.39	1.53	1.46
2	1	148	GLY	N-CA	6.39	1.53	1.45
2	1	40	GLU	C-N	-6.38	1.26	1.33
3	2	115	SER	N-CA	6.37	1.53	1.46
3	2	128	PRO	N-CA	6.37	1.54	1.47
5	3	90	ALA	N-CA	6.36	1.54	1.46
5	3	220	PHE	N-CA	6.36	1.54	1.46
5	3	161	GLN	N-CA	6.36	1.54	1.46
2	1	244	VAL	CA-C	6.35	1.59	1.53
3	2	24	THR	C-N	-6.35	1.25	1.33
5	3	94	ARG	N-CA	6.35	1.54	1.46
2	1	267	ARG	CA-C	6.35	1.60	1.52
5	3	118	PHE	N-CA	6.34	1.53	1.46
3	2	198	ILE	CA-C	6.34	1.58	1.52
5	3	55	PHE	N-CA	6.34	1.54	1.46
2	1	22	THR	N-CA	6.33	1.53	1.46
5	3	59	ALA	N-CA	6.33	1.54	1.46
2	1	189	THR	N-CA	6.33	1.53	1.45
5	3	185	THR	N-CA	6.33	1.53	1.46
2	1	128	SER	C-N	-6.32	1.25	1.33
2	1	301	THR	N-CA	6.32	1.53	1.46
2	1	32	ALA	N-CA	6.31	1.54	1.46
2	1	176	GLN	N-CA	6.31	1.54	1.46
2	1	140	ALA	N-CA	6.31	1.53	1.45
3	2	34	ALA	N-CA	6.31	1.54	1.46
5	3	10	SER	N-CA	6.31	1.54	1.46
2	1	290	THR	N-CA	6.30	1.54	1.46
2	1	220	GLN	N-CA	6.30	1.53	1.46
2	1	21	ALA	N-CA	6.30	1.54	1.46
2	1	219	ASP	N-CA	6.30	1.54	1.46
5	3	176	TYR	CA-C	6.30	1.60	1.52
2	1	192	ALA	N-CA	6.28	1.54	1.46
3	2	243	SER	N-CA	6.28	1.54	1.46
2	1	56	VAL	CA-C	6.27	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	119	GLN	CA-C	6.26	1.60	1.52
5	3	48	GLU	N-CA	6.26	1.54	1.46
5	3	53	ILE	CA-C	6.26	1.58	1.53
5	3	88	SER	N-CA	6.26	1.54	1.46
5	3	182	ASP	N-CA	6.24	1.53	1.46
5	3	179	THR	N-CA	6.24	1.54	1.46
4	4	64	THR	N-CA	6.24	1.54	1.46
3	2	206	ALA	N-CA	6.23	1.53	1.46
5	3	135	ALA	N-CA	6.23	1.53	1.46
3	2	129	GLU	CA-C	6.23	1.61	1.53
5	3	164	CYS	N-CA	6.23	1.53	1.46
5	3	214	VAL	C-N	-6.22	1.25	1.33
3	2	257	CYS	N-CA	6.22	1.54	1.46
3	2	157	PHE	C-N	-6.21	1.25	1.33
5	3	64	THR	CA-C	6.21	1.60	1.52
3	2	5	GLU	N-CA	6.21	1.58	1.46
2	1	58	SER	N-CA	6.20	1.54	1.46
3	2	43	ARG	N-CA	6.20	1.53	1.46
4	4	48	GLN	N-CA	6.20	1.53	1.45
2	1	276	ALA	N-CA	6.20	1.54	1.46
5	3	188	GLY	CA-C	6.19	1.58	1.52
2	1	168	GLU	N-CA	6.18	1.54	1.46
3	2	255	PRO	N-CA	6.18	1.54	1.47
2	1	150	ALA	N-CA	6.17	1.53	1.46
2	1	83	ARG	N-CA	6.17	1.53	1.46
3	2	61	CYS	N-CA	6.17	1.54	1.46
4	4	34	ARG	N-CA	6.17	1.54	1.46
5	3	73	SER	N-CA	6.16	1.53	1.46
5	3	213	PHE	N-CA	6.16	1.53	1.46
2	1	48	GLU	N-CA	6.16	1.54	1.46
3	2	167	GLN	N-CA	6.16	1.54	1.46
2	1	267	ARG	N-CA	6.15	1.53	1.46
3	2	247	ILE	C-N	-6.15	1.25	1.33
2	1	26	ALA	N-CA	6.15	1.54	1.46
2	1	71	SER	N-CA	6.14	1.53	1.45
2	1	277	VAL	N-CA	6.13	1.53	1.46
3	2	222	VAL	N-CA	6.13	1.53	1.46
3	2	144	SER	N-CA	6.13	1.53	1.46
2	1	59	ASP	N-CA	6.13	1.54	1.46
3	2	6	ALA	CA-C	6.13	1.61	1.52
3	2	206	ALA	CA-C	6.13	1.59	1.52
2	1	61	VAL	N-CA	6.13	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	3	ALA	N-CA	6.12	1.53	1.46
2	1	127	TYR	CA-C	6.12	1.60	1.52
3	2	196	GLN	N-CA	6.12	1.53	1.45
3	2	230	ALA	N-CA	6.12	1.53	1.46
2	1	281	GLY	N-CA	6.12	1.53	1.44
2	1	75	SER	N-CA	6.12	1.54	1.46
4	4	41	ALA	N-CA	6.11	1.53	1.46
5	3	172	SER	N-CA	6.11	1.53	1.45
3	2	201	ARG	N-CA	6.11	1.54	1.46
2	1	201	ILE	N-CA	6.11	1.53	1.46
3	2	40	GLU	N-CA	6.11	1.53	1.45
5	3	103	ILE	N-CA	6.11	1.53	1.46
5	3	168	VAL	CA-C	6.10	1.59	1.52
5	3	181	ASP	N-CA	6.10	1.54	1.46
2	1	40	GLU	N-CA	6.10	1.53	1.46
3	2	114	ALA	N-CA	6.10	1.54	1.46
5	3	229	THR	N-CA	6.10	1.54	1.46
3	2	76	ARG	N-CA	6.09	1.54	1.46
5	3	111	ALA	N-CA	6.08	1.53	1.45
5	3	91	SER	N-CA	6.08	1.53	1.46
2	1	233	SER	CA-C	6.08	1.60	1.52
2	1	247	ASP	N-CA	6.08	1.53	1.46
5	3	174	THR	N-CA	6.07	1.54	1.46
5	3	108	THR	N-CA	6.06	1.54	1.46
5	3	215	SER	N-CA	6.06	1.53	1.45
2	1	92	VAL	N-CA	6.06	1.53	1.46
5	3	82	ILE	N-CA	6.06	1.54	1.46
3	2	31	SER	N-CA	6.05	1.53	1.46
5	3	178	GLN	N-CA	6.05	1.53	1.46
2	1	195	SER	N-CA	6.05	1.53	1.46
2	1	52	THR	N-CA	6.05	1.53	1.46
2	1	92	VAL	C-N	-6.05	1.25	1.33
5	3	177	ARG	CA-C	6.05	1.60	1.52
2	1	111	THR	N-CA	6.04	1.53	1.46
3	2	209	VAL	CA-C	6.04	1.59	1.53
2	1	115	THR	CA-C	6.04	1.60	1.52
2	1	117	GLN	N-CA	6.04	1.53	1.46
3	2	26	GLN	N-CA	6.04	1.54	1.46
5	3	147	GLU	CA-C	6.04	1.60	1.52
2	1	215	VAL	CA-C	6.03	1.59	1.52
5	3	9	GLY	CA-C	6.03	1.59	1.51
3	2	157	PHE	N-CA	6.03	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	131	ASP	N-CA	6.03	1.53	1.46
3	2	158	THR	N-CA	6.03	1.53	1.46
4	4	42	SER	N-CA	6.02	1.53	1.46
2	1	275	ARG	N-CA	6.02	1.53	1.46
3	2	140	THR	N-CA	6.02	1.53	1.45
3	2	57	ASP	CA-C	6.02	1.58	1.53
2	1	211	GLY	CA-C	6.01	1.58	1.51
5	3	191	SER	N-CA	6.01	1.53	1.45
2	1	129	ARG	N-CA	6.01	1.53	1.46
3	2	240	ALA	CA-C	6.01	1.60	1.52
5	3	45	GLU	CA-C	6.01	1.60	1.52
3	2	113	ASN	C-N	-6.01	1.25	1.33
4	4	11	GLY	N-CA	6.01	1.54	1.45
5	3	157	ASP	N-CA	6.01	1.53	1.46
3	2	21	SER	N-CA	6.00	1.53	1.46
5	3	60	THR	N-CA	6.00	1.53	1.46
1	R	211	SER	C-N	-6.00	1.25	1.33
2	1	241	ALA	N-CA	6.00	1.54	1.46
3	2	260	PHE	N-CA	6.00	1.53	1.46
5	3	146	LYS	N-CA	6.00	1.53	1.46
4	4	35	ASP	N-CA	6.00	1.53	1.46
3	2	110	VAL	N-CA	5.99	1.53	1.46
3	2	87	ARG	N-CA	5.99	1.53	1.46
3	2	131	CYS	N-CA	5.99	1.53	1.46
3	2	72	THR	N-CA	5.99	1.53	1.45
5	3	163	SER	N-CA	5.99	1.52	1.45
5	3	194	TYR	CA-C	5.99	1.60	1.52
4	4	24	THR	N-CA	5.99	1.53	1.46
5	3	222	VAL	N-CA	5.98	1.52	1.46
2	1	121	LYS	N-CA	5.98	1.53	1.46
3	2	114	ALA	C-N	-5.97	1.26	1.33
5	3	78	THR	N-CA	5.97	1.53	1.46
3	2	7	CYS	N-CA	5.97	1.54	1.46
2	1	25	ASP	N-CA	5.97	1.53	1.46
5	3	19	PHE	N-CA	5.97	1.53	1.45
2	1	164	ALA	CA-C	5.97	1.59	1.53
3	2	12	ARG	N-CA	5.96	1.53	1.46
2	1	166	VAL	CA-C	5.96	1.59	1.52
3	2	47	ALA	N-CA	5.96	1.53	1.46
3	2	62	ARG	N-CA	5.96	1.54	1.46
4	4	44	GLN	N-CA	5.96	1.54	1.46
5	3	74	ASP	N-CA	5.96	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	251	THR	CA-C	5.96	1.60	1.52
2	1	190	ALA	N-CA	5.96	1.54	1.46
2	1	231	ALA	N-CA	5.96	1.53	1.46
5	3	234	LYS	N-CA	5.96	1.53	1.46
3	2	188	GLY	CA-C	5.95	1.59	1.51
5	3	12	GLN	N-CA	5.95	1.53	1.45
3	2	152	GLU	N-CA	5.95	1.53	1.46
3	2	174	PHE	N-CA	5.94	1.53	1.46
3	2	10	SER	N-CA	5.94	1.53	1.45
3	2	196	GLN	CA-C	5.94	1.59	1.52
5	3	164	CYS	CA-C	5.93	1.59	1.52
2	1	40	GLU	CA-C	5.93	1.60	1.52
3	2	125	PHE	N-CA	5.93	1.53	1.46
5	3	96	SER	N-CA	5.93	1.53	1.46
3	2	134	GLY	N-CA	5.92	1.52	1.45
4	4	9	LYS	N-CA	5.92	1.53	1.46
2	1	24	ARG	N-CA	5.92	1.53	1.46
3	2	40	GLU	CA-C	5.92	1.59	1.52
3	2	244	SER	N-CA	5.92	1.52	1.46
3	2	180	LEU	N-CA	5.91	1.53	1.46
2	1	221	SER	N-CA	5.91	1.53	1.46
5	3	21	SER	CA-C	5.91	1.58	1.52
3	2	46	GLU	N-CA	5.91	1.53	1.46
5	3	145	ARG	N-CA	5.91	1.53	1.46
5	3	33	PRO	C-N	-5.91	1.25	1.33
2	1	60	THR	N-CA	5.90	1.54	1.45
2	1	162	PRO	C-N	-5.89	1.28	1.34
2	1	184	PHE	N-CA	5.89	1.54	1.46
5	3	134	TYR	CA-C	5.89	1.59	1.52
4	4	53	PHE	CA-C	5.89	1.59	1.52
3	2	255	PRO	CA-C	5.89	1.59	1.52
2	1	135	THR	N-CA	5.88	1.53	1.46
3	2	52	GLN	CA-C	5.88	1.60	1.52
3	2	43	ARG	CA-C	5.88	1.60	1.52
2	1	176	GLN	CA-C	5.88	1.60	1.52
2	1	190	ALA	CA-C	5.88	1.60	1.52
2	1	250	PRO	N-CA	5.88	1.54	1.47
2	1	101	LYS	N-CA	5.88	1.53	1.46
2	1	26	ALA	CA-C	5.88	1.60	1.52
2	1	49	THR	N-CA	5.87	1.54	1.46
3	2	143	THR	N-CA	5.87	1.53	1.46
2	1	50	GLY	N-CA	5.87	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	198	TYR	CA-C	5.87	1.60	1.52
4	4	60	VAL	N-CA	5.87	1.53	1.46
3	2	135	ASP	N-CA	5.87	1.53	1.46
5	3	201	PRO	C-N	-5.87	1.26	1.33
3	2	121	ALA	N-CA	5.86	1.53	1.46
4	4	39	ASN	C-N	-5.86	1.25	1.33
4	4	51	SER	N-CA	5.86	1.53	1.46
5	3	169	PRO	N-CA	5.86	1.53	1.47
5	3	26	PRO	N-CA	5.86	1.54	1.47
3	2	19	GLY	N-CA	5.86	1.54	1.45
3	2	111	GLN	N-CA	5.86	1.53	1.46
2	1	25	ASP	CA-C	5.86	1.60	1.52
2	1	133	GLU	CA-C	5.86	1.60	1.53
4	4	40	ALA	N-CA	5.86	1.53	1.45
5	3	100	LEU	N-CA	5.85	1.53	1.46
5	3	39	GLU	CA-C	5.85	1.60	1.52
5	3	197	ARG	N-CA	5.84	1.53	1.46
5	3	226	ARG	N-CA	5.84	1.53	1.45
3	2	15	GLN	CA-C	5.83	1.60	1.53
2	1	255	SER	N-CA	5.83	1.53	1.45
2	1	174	THR	N-CA	5.83	1.53	1.46
3	2	52	GLN	N-CA	5.83	1.54	1.46
2	1	34	GLY	N-CA	5.82	1.52	1.44
5	3	186	GLU	CA-C	5.82	1.60	1.52
5	3	148	ALA	CA-C	5.82	1.60	1.52
2	1	211	GLY	N-CA	5.82	1.52	1.45
2	1	186	THR	N-CA	5.81	1.53	1.46
5	3	162	SER	N-CA	5.81	1.53	1.46
3	2	65	THR	N-CA	5.80	1.53	1.46
5	3	139	ALA	N-CA	5.80	1.54	1.46
2	1	205	TYR	CA-C	5.80	1.60	1.52
5	3	88	SER	CA-C	5.80	1.60	1.52
2	1	258	ARG	N-CA	5.80	1.53	1.46
3	2	116	LYS	N-CA	5.79	1.53	1.46
4	4	15	ASN	CA-C	5.79	1.60	1.52
2	1	204	ALA	CA-C	5.79	1.60	1.52
2	1	279	TYR	CA-C	5.79	1.59	1.52
5	3	227	ASP	N-CA	5.79	1.53	1.46
2	1	283	GLY	CA-C	5.79	1.58	1.52
4	4	14	GLU	CA-C	5.79	1.60	1.52
3	2	70	SER	N-CA	5.78	1.53	1.46
3	2	267	THR	N-CA	5.78	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	58	LYS	N-CA	5.78	1.53	1.46
3	2	62	ARG	CA-C	5.78	1.60	1.52
2	1	182	SER	N-CA	5.78	1.53	1.46
3	2	103	ARG	N-CA	5.78	1.53	1.46
2	1	35	PRO	N-CA	5.77	1.54	1.47
3	2	18	LEU	N-CA	5.77	1.53	1.46
3	2	84	ASP	N-CA	5.77	1.53	1.46
3	2	192	VAL	N-CA	5.77	1.54	1.46
3	2	242	GLU	N-CA	5.77	1.53	1.46
2	1	120	ARG	CA-C	5.77	1.60	1.52
3	2	126	ALA	CA-C	5.77	1.60	1.52
3	2	195	HIS	C-N	-5.77	1.26	1.33
3	2	69	VAL	CA-C	5.77	1.59	1.52
2	1	70	ARG	N-CA	5.76	1.53	1.46
2	1	193	ARG	N-CA	5.76	1.53	1.46
2	1	164	ALA	N-CA	5.76	1.54	1.45
3	2	100	TYR	N-CA	5.76	1.53	1.46
3	2	151	GLY	C-N	-5.75	1.26	1.33
3	2	118	HIS	CA-C	5.75	1.60	1.52
2	1	130	PHE	N-CA	5.73	1.52	1.46
3	2	49	PRO	N-CA	5.73	1.54	1.47
3	2	211	PRO	CA-C	5.73	1.59	1.52
2	1	139	THR	N-CA	5.73	1.53	1.46
5	3	4	VAL	N-CA	5.73	1.52	1.46
5	3	17	ASP	N-CA	5.73	1.53	1.45
2	1	48	GLU	CA-C	5.72	1.60	1.52
3	2	25	THR	N-CA	5.72	1.53	1.46
5	3	112	GLY	N-CA	5.72	1.51	1.45
5	3	158	ILE	N-CA	5.72	1.53	1.46
3	2	24	THR	N-CA	5.72	1.52	1.46
3	2	242	GLU	C-N	-5.72	1.26	1.34
2	1	83	ARG	CA-C	5.71	1.59	1.52
3	2	128	PRO	CA-C	5.71	1.59	1.52
2	1	227	SER	CA-C	5.70	1.59	1.52
3	2	139	THR	CA-C	5.70	1.59	1.52
3	2	160	THR	N-CA	5.70	1.53	1.46
2	1	274	PRO	N-CA	5.70	1.54	1.47
4	4	65	ALA	N-CA	5.70	1.54	1.45
2	1	129	ARG	CA-C	5.69	1.59	1.52
5	3	98	THR	CA-C	5.69	1.60	1.52
4	4	29	THR	N-CA	5.69	1.52	1.46
5	3	193	PHE	N-CA	5.69	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	208	PHE	CA-C	5.69	1.59	1.52
5	3	41	LYS	N-CA	5.69	1.53	1.45
5	3	102	GLU	CA-C	5.68	1.60	1.52
2	1	99	THR	CA-C	5.68	1.60	1.52
2	1	179	SER	CA-C	5.68	1.59	1.52
5	3	126	ALA	N-CA	5.68	1.53	1.46
3	2	169	SER	CA-C	5.68	1.59	1.52
2	1	249	ASN	CA-C	5.68	1.58	1.52
3	2	75	SER	N-CA	5.67	1.53	1.46
2	1	85	ALA	CA-C	5.67	1.59	1.52
2	1	103	LYS	N-CA	5.67	1.53	1.46
2	1	234	LEU	N-CA	5.67	1.53	1.46
5	3	92	ASP	N-CA	5.67	1.54	1.46
5	3	204	THR	N-CA	5.67	1.54	1.45
2	1	283	GLY	C-N	-5.66	1.28	1.34
2	1	91	THR	C-N	-5.66	1.26	1.33
3	2	59	ALA	CA-C	5.66	1.60	1.52
3	2	64	TYR	CA-C	5.66	1.59	1.52
5	3	78	THR	CA-C	5.66	1.59	1.52
3	2	234	LEU	C-N	-5.66	1.27	1.33
5	3	27	GLU	N-CA	5.65	1.53	1.46
5	3	152	THR	N-CA	5.65	1.53	1.46
5	3	168	VAL	N-CA	5.65	1.53	1.46
2	1	264	LYS	N-CA	5.65	1.52	1.45
3	2	173	ARG	N-CA	5.65	1.53	1.45
5	3	20	GLN	N-CA	5.65	1.53	1.45
5	3	116	PHE	N-CA	5.65	1.53	1.46
5	3	112	GLY	CA-C	5.65	1.58	1.52
5	3	36	ILE	CA-C	5.65	1.58	1.52
5	3	47	ALA	CA-C	5.65	1.60	1.52
2	1	69	HIS	N-CA	5.64	1.53	1.46
2	1	127	TYR	C-N	-5.64	1.26	1.33
2	1	236	ASP	N-CA	5.64	1.53	1.46
2	1	115	THR	C-N	-5.64	1.26	1.33
2	1	140	ALA	C-N	-5.64	1.26	1.33
2	1	278	ALA	N-CA	5.64	1.53	1.46
5	3	180	ILE	CA-C	5.64	1.59	1.52
5	3	195	GLN	CA-C	5.64	1.60	1.52
5	3	176	TYR	C-N	-5.64	1.25	1.33
2	1	146	ASN	CA-C	5.63	1.60	1.52
2	1	63	THR	N-CA	5.63	1.52	1.45
2	1	102	ASP	N-CA	5.63	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	5	VAL	N-CA	5.63	1.53	1.46
4	4	55	GLU	N-CA	5.63	1.54	1.46
2	1	284	VAL	CA-C	5.63	1.58	1.52
3	2	71	TRP	N-CA	5.63	1.53	1.46
5	3	85	LEU	N-CA	5.63	1.53	1.46
5	3	133	SER	N-CA	5.63	1.52	1.45
3	2	175	CYS	CA-C	5.63	1.59	1.53
3	2	218	ILE	N-CA	5.62	1.53	1.46
5	3	143	LYS	N-CA	5.62	1.53	1.45
5	3	66	GLU	N-CA	5.62	1.53	1.46
4	4	55	GLU	CA-C	5.62	1.59	1.52
2	1	128	SER	N-CA	5.62	1.53	1.45
3	2	151	GLY	CA-C	5.62	1.59	1.52
5	3	37	PRO	N-CA	5.62	1.54	1.47
3	2	218	ILE	CA-C	5.61	1.59	1.52
2	1	143	THR	N-CA	5.61	1.53	1.46
2	1	47	VAL	N-CA	5.61	1.53	1.46
3	2	202	THR	N-CA	5.61	1.53	1.46
3	2	220	SER	N-CA	5.61	1.53	1.46
5	3	25	LEU	N-CA	5.61	1.52	1.46
2	1	27	LEU	C-N	-5.60	1.26	1.33
2	1	56	VAL	N-CA	5.60	1.53	1.46
2	1	67	VAL	N-CA	5.59	1.53	1.46
2	1	62	GLN	N-CA	5.59	1.53	1.46
5	3	216	ALA	N-CA	5.59	1.53	1.46
3	2	264	ARG	CA-C	5.58	1.60	1.53
5	3	160	LEU	N-CA	5.58	1.53	1.46
2	1	275	ARG	CA-C	5.58	1.60	1.52
3	2	209	VAL	N-CA	5.58	1.53	1.46
3	2	108	VAL	N-CA	5.58	1.52	1.46
5	3	201	PRO	N-CA	5.58	1.54	1.47
5	3	32	PRO	C-N	-5.58	1.26	1.33
5	3	34	ILE	N-CA	5.58	1.52	1.46
3	2	67	ASP	N-CA	5.58	1.53	1.46
5	3	97	HIS	N-CA	5.58	1.53	1.46
2	1	28	PRO	N-CA	5.57	1.53	1.47
2	1	245	VAL	N-CA	5.57	1.53	1.46
3	2	174	PHE	C-N	-5.57	1.26	1.33
5	3	23	CYS	N-CA	5.57	1.53	1.46
3	2	249	ILE	CA-C	5.57	1.59	1.52
5	3	144	LYS	N-CA	5.57	1.52	1.46
3	2	217	SER	C-N	-5.57	1.27	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	194	PRO	N-CA	5.56	1.54	1.47
2	1	86	CYS	N-CA	5.56	1.53	1.46
2	1	265	HIS	N-CA	5.56	1.55	1.46
2	1	167	PRO	N-CA	5.56	1.53	1.47
3	2	73	LYS	N-CA	5.56	1.53	1.46
5	3	174	THR	CA-C	5.56	1.59	1.52
3	2	126	ALA	C-N	-5.56	1.28	1.33
4	4	48	GLN	CA-C	5.56	1.59	1.52
5	3	29	ASP	N-CA	5.56	1.53	1.46
5	3	203	SER	N-CA	5.56	1.54	1.46
2	1	23	SER	CA-C	5.56	1.60	1.52
3	2	118	HIS	N-CA	5.56	1.52	1.45
2	1	244	VAL	N-CA	5.55	1.53	1.46
3	2	36	GLY	N-CA	5.55	1.53	1.45
2	1	268	VAL	N-CA	5.55	1.52	1.46
2	1	79	SER	CA-C	5.55	1.59	1.52
5	3	230	HIS	C-N	-5.55	1.27	1.33
2	1	137	VAL	CA-C	5.55	1.58	1.53
3	2	164	ASP	N-CA	5.55	1.53	1.46
2	1	254	THR	N-CA	5.54	1.53	1.46
5	3	107	TYR	CA-C	5.54	1.59	1.52
5	3	84	CYS	CA-C	5.54	1.59	1.52
3	2	217	SER	CA-C	5.54	1.59	1.52
5	3	77	HIS	C-N	-5.54	1.26	1.33
2	1	76	SER	CA-C	5.54	1.60	1.52
3	2	22	THR	N-CA	5.54	1.52	1.46
3	2	99	HIS	N-CA	5.54	1.52	1.46
2	1	125	PHE	CA-C	5.54	1.59	1.52
3	2	33	VAL	N-CA	5.54	1.53	1.46
3	2	80	TRP	C-N	-5.54	1.25	1.33
3	2	148	ALA	CA-C	5.54	1.60	1.52
4	4	37	ALA	CA-C	5.54	1.60	1.52
3	2	24	THR	CA-C	5.53	1.59	1.52
5	3	8	PRO	N-CA	5.53	1.54	1.47
2	1	98	THR	N-CA	5.53	1.53	1.46
4	4	41	ALA	CA-C	5.53	1.60	1.52
2	1	36	THR	N-CA	5.53	1.52	1.46
5	3	42	ASN	CA-C	5.53	1.58	1.52
5	3	9	GLY	N-CA	5.52	1.53	1.44
2	1	97	SER	CA-C	5.52	1.60	1.52
5	3	161	GLN	CA-C	5.52	1.60	1.52
2	1	288	ASP	N-CA	5.52	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	212	TYR	CA-C	5.52	1.60	1.52
4	4	6	SER	N-CA	5.52	1.53	1.45
4	4	7	SER	N-CA	5.52	1.53	1.46
5	3	76	PRO	N-CA	5.52	1.53	1.47
5	3	26	PRO	CA-C	5.51	1.59	1.52
4	4	46	PHE	N-CA	5.51	1.52	1.46
2	1	248	HIS	N-CA	5.51	1.52	1.46
3	2	136	SER	N-CA	5.51	1.52	1.46
5	3	51	THR	CA-C	5.51	1.59	1.52
3	2	270	ARG	N-CA	5.50	1.53	1.46
2	1	36	THR	C-N	-5.50	1.26	1.33
2	1	220	GLN	CA-C	5.50	1.59	1.52
3	2	193	PHE	N-CA	5.50	1.54	1.46
3	2	68	THR	N-CA	5.50	1.53	1.46
5	3	221	SER	N-CA	5.50	1.52	1.45
2	1	30	THR	N-CA	5.49	1.53	1.46
2	1	156	GLN	CA-C	5.49	1.60	1.53
2	1	192	ALA	CA-C	5.49	1.59	1.52
5	3	46	LEU	N-CA	5.49	1.53	1.46
3	2	188	GLY	N-CA	5.49	1.53	1.45
5	3	33	PRO	N-CA	5.48	1.53	1.47
4	4	4	GLN	N-CA	5.48	1.54	1.46
3	2	55	GLU	N-CA	5.48	1.53	1.46
2	1	33	SER	CA-C	5.47	1.58	1.52
3	2	74	GLU	N-CA	5.47	1.53	1.46
5	3	40	VAL	N-CA	5.47	1.53	1.46
2	1	139	THR	CA-C	5.47	1.59	1.52
5	3	62	LYS	N-CA	5.47	1.52	1.46
2	1	74	GLU	N-CA	5.46	1.53	1.46
2	1	32	ALA	C-N	-5.46	1.26	1.33
2	1	77	ILE	N-CA	5.46	1.53	1.46
5	3	228	THR	N-CA	5.46	1.53	1.45
2	1	150	ALA	CA-C	5.46	1.59	1.52
2	1	162	PRO	N-CA	5.46	1.54	1.47
3	2	94	GLN	CA-C	5.46	1.59	1.52
2	1	137	VAL	N-CA	5.46	1.53	1.46
2	1	200	GLY	CA-C	5.46	1.58	1.52
2	1	248	HIS	CA-C	5.46	1.59	1.52
3	2	264	ARG	N-CA	5.46	1.54	1.46
3	2	265	ASN	C-N	-5.45	1.27	1.33
4	4	9	LYS	CA-C	5.45	1.60	1.52
4	4	44	GLN	CA-C	5.45	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	21	SER	CA-C	5.45	1.59	1.52
3	2	119	GLN	C-N	-5.45	1.26	1.33
3	2	146	GLN	CA-C	5.45	1.59	1.52
3	2	30	ASN	CA-C	5.45	1.60	1.52
4	4	50	PRO	N-CA	5.44	1.54	1.47
2	1	131	ASP	C-N	-5.44	1.25	1.33
5	3	106	TYR	CA-C	5.44	1.60	1.52
5	3	230	HIS	N-CA	5.44	1.53	1.46
2	1	100	ASN	N-CA	5.44	1.53	1.46
2	1	210	ASP	N-CA	5.44	1.53	1.46
2	1	271	PRO	N-CA	5.44	1.53	1.47
3	2	107	THR	CA-C	5.43	1.60	1.53
3	2	121	ALA	CA-C	5.43	1.59	1.52
2	1	35	PRO	CA-C	5.43	1.59	1.52
2	1	166	VAL	N-CA	5.43	1.53	1.46
4	4	52	LYS	N-CA	5.43	1.53	1.46
2	1	195	SER	CA-C	5.43	1.59	1.52
2	1	119	ARG	CA-C	5.42	1.59	1.52
2	1	122	LEU	N-CA	5.42	1.52	1.46
2	1	32	ALA	CA-C	5.42	1.60	1.52
2	1	274	PRO	CA-C	5.42	1.58	1.52
2	1	57	PRO	N-CA	5.42	1.54	1.47
2	1	289	GLY	N-CA	5.42	1.53	1.45
3	2	133	ALA	CA-C	5.41	1.59	1.52
3	2	58	VAL	N-CA	5.41	1.53	1.46
2	1	197	PRO	N-CA	5.41	1.54	1.47
4	4	60	VAL	CA-C	5.41	1.59	1.52
5	3	111	ALA	CA-C	5.41	1.59	1.52
2	1	259	VAL	N-CA	5.41	1.52	1.46
2	1	188	GLY	N-CA	5.40	1.53	1.45
3	2	28	ALA	N-CA	5.40	1.53	1.46
2	1	87	VAL	N-CA	5.40	1.53	1.46
2	1	107	VAL	CA-C	5.40	1.59	1.52
3	2	51	ASP	N-CA	5.40	1.53	1.46
4	4	13	HIS	N-CA	5.40	1.52	1.46
2	1	178	SER	CA-C	5.40	1.60	1.52
2	1	168	GLU	CA-C	5.39	1.59	1.52
2	1	269	TRP	N-CA	5.39	1.52	1.45
5	3	93	PRO	N-CA	5.39	1.54	1.47
5	3	202	LEU	N-CA	5.39	1.53	1.45
2	1	118	LEU	N-CA	5.39	1.52	1.46
5	3	140	ASP	CA-C	5.39	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	182	GLY	N-CA	5.39	1.53	1.45
2	1	111	THR	CA-C	5.39	1.59	1.52
2	1	157	ILE	N-CA	5.38	1.53	1.46
3	2	49	PRO	C-N	-5.38	1.28	1.34
3	2	163	PRO	N-CA	5.38	1.53	1.47
5	3	10	SER	CA-C	5.38	1.59	1.52
5	3	54	PRO	N-CA	5.38	1.54	1.47
2	1	170	TRP	N-CA	5.37	1.53	1.46
4	4	66	PRO	N-CA	5.37	1.54	1.47
3	2	29	ALA	CA-C	5.37	1.60	1.53
3	2	141	MET	N-CA	5.37	1.53	1.46
2	1	216	PRO	N-CA	5.36	1.54	1.47
5	3	223	ARG	N-CA	5.36	1.53	1.46
2	1	54	PRO	N-CA	5.36	1.54	1.47
2	1	68	GLN	N-CA	5.36	1.52	1.46
2	1	301	THR	CA-C	5.36	1.59	1.52
4	4	10	VAL	N-CA	5.36	1.52	1.46
4	4	36	SER	CA-C	5.36	1.59	1.52
4	4	41	ALA	C-N	-5.36	1.26	1.34
5	3	37	PRO	CA-C	5.36	1.59	1.52
3	2	127	VAL	CA-C	5.35	1.57	1.53
2	1	218	LYS	N-CA	5.35	1.53	1.46
3	2	96	MET	N-CA	5.35	1.52	1.46
4	4	8	GLN	N-CA	5.35	1.52	1.46
5	3	137	PRO	N-CA	5.35	1.54	1.47
2	1	241	ALA	CA-C	5.34	1.59	1.52
3	2	177	VAL	CA-C	5.34	1.59	1.52
2	1	286	TYR	C-N	-5.34	1.25	1.33
4	4	56	PRO	N-CA	5.34	1.54	1.47
5	3	50	ASP	N-CA	5.34	1.53	1.46
2	1	106	ALA	N-CA	5.34	1.52	1.46
2	1	226	ASP	N-CA	5.34	1.52	1.46
3	2	185	THR	CA-C	5.34	1.59	1.52
5	3	34	ILE	CA-C	5.33	1.58	1.52
2	1	145	THR	N-CA	5.33	1.53	1.46
2	1	153	GLN	N-CA	5.33	1.52	1.46
3	2	37	ARG	N-CA	5.33	1.53	1.46
3	2	171	ALA	CA-C	5.33	1.60	1.52
5	3	215	SER	CA-C	5.33	1.59	1.52
2	1	129	ARG	C-N	-5.33	1.27	1.33
2	1	43	ALA	CA-C	5.32	1.59	1.52
2	1	267	ARG	C-N	-5.32	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	76	ARG	CA-C	5.32	1.59	1.52
3	2	124	VAL	CA-C	5.32	1.58	1.53
3	2	132	LEU	N-CA	5.32	1.52	1.45
5	3	113	SER	N-CA	5.32	1.52	1.46
5	3	192	VAL	C-N	-5.32	1.26	1.33
2	1	281	GLY	CA-C	5.31	1.59	1.51
2	1	232	ALA	CA-C	5.31	1.59	1.52
3	2	63	PHE	N-CA	5.31	1.53	1.46
3	2	259	GLU	N-CA	5.31	1.52	1.46
3	2	201	ARG	CA-C	5.31	1.60	1.52
4	4	65	ALA	CA-C	5.31	1.59	1.52
5	3	16	ALA	CA-C	5.31	1.60	1.52
2	1	38	SER	N-CA	5.30	1.52	1.45
2	1	282	PRO	N-CA	5.30	1.54	1.47
5	3	217	CYS	CA-C	5.30	1.59	1.52
3	2	53	PRO	N-CA	5.30	1.53	1.47
5	3	114	LEU	C-N	-5.30	1.26	1.33
2	1	231	ALA	CA-C	5.30	1.59	1.52
3	2	184	GLY	N-CA	5.30	1.53	1.45
4	4	43	LYS	N-CA	5.30	1.53	1.46
5	3	222	VAL	C-N	-5.30	1.26	1.33
2	1	140	ALA	CA-C	5.30	1.59	1.52
3	2	252	THR	CA-C	5.30	1.59	1.52
2	1	293	PRO	N-CA	5.30	1.54	1.47
5	3	89	PRO	N-CA	5.30	1.54	1.47
5	3	145	ARG	CA-C	5.30	1.60	1.52
5	3	33	PRO	CA-C	5.29	1.59	1.52
5	3	109	HIS	N-CA	5.29	1.52	1.46
2	1	206	SER	CA-C	5.29	1.59	1.53
3	2	74	GLU	CA-C	5.29	1.59	1.52
2	1	144	GLU	N-CA	5.29	1.52	1.46
2	1	270	CYS	N-CA	5.29	1.53	1.46
2	1	89	ILE	CA-C	5.29	1.58	1.52
3	2	103	ARG	C-N	-5.29	1.26	1.33
3	2	123	GLY	N-CA	5.29	1.53	1.45
3	2	25	THR	CA-C	5.29	1.58	1.52
3	2	19	GLY	CA-C	5.29	1.59	1.52
3	2	161	PHE	C-N	-5.29	1.25	1.33
3	2	216	LEU	N-CA	5.29	1.52	1.45
5	3	86	SER	CA-C	5.28	1.59	1.52
3	2	124	VAL	N-CA	5.28	1.52	1.46
3	2	152	GLU	CA-C	5.28	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	12	GLN	CA-C	5.28	1.59	1.52
5	3	45	GLU	C-O	-5.28	1.17	1.24
3	2	85	ALA	CA-C	5.28	1.59	1.52
3	2	230	ALA	CA-C	5.28	1.59	1.52
3	2	224	HIS	N-CA	5.28	1.52	1.46
5	3	59	ALA	CA-C	5.28	1.59	1.52
5	3	114	LEU	N-CA	5.28	1.51	1.45
2	1	95	PRO	N-CA	5.28	1.54	1.47
4	4	59	ASP	N-CA	5.27	1.53	1.46
3	2	192	VAL	C-O	-5.27	1.17	1.24
4	4	8	GLN	C-N	-5.27	1.26	1.33
5	3	72	LEU	N-CA	5.27	1.52	1.45
2	1	160	VAL	N-CA	5.26	1.53	1.46
2	1	222	ALA	CA-C	5.26	1.59	1.52
3	2	220	SER	CA-C	5.26	1.59	1.52
3	2	262	GLY	N-CA	5.26	1.53	1.45
5	3	205	PRO	N-CA	5.26	1.54	1.47
2	1	230	GLY	N-CA	5.26	1.53	1.45
2	1	123	GLU	N-CA	5.26	1.53	1.46
3	2	164	ASP	CA-C	5.26	1.59	1.52
3	2	193	PHE	CA-C	5.26	1.60	1.53
4	4	38	SER	CA-C	5.26	1.59	1.52
4	4	25	ILE	CA-C	5.26	1.59	1.52
5	3	58	SER	CA-C	5.26	1.59	1.52
5	3	72	LEU	C-N	-5.26	1.27	1.33
3	2	250	THR	N-CA	5.25	1.52	1.46
3	2	258	CYS	N-CA	5.25	1.52	1.46
2	1	208	PHE	C-N	-5.25	1.26	1.33
2	1	243	ARG	CA-C	5.25	1.59	1.52
2	1	296	THR	C-N	-5.25	1.27	1.33
3	2	229	ILE	CA-C	5.25	1.58	1.53
5	3	171	ILE	N-CA	5.25	1.52	1.46
2	1	31	GLU	N-CA	5.25	1.52	1.46
2	1	218	LYS	CA-C	5.25	1.59	1.52
3	2	120	GLY	N-CA	5.25	1.51	1.45
3	2	236	PRO	N-CA	5.25	1.53	1.47
5	3	4	VAL	C-N	-5.25	1.26	1.33
2	1	271	PRO	C-N	-5.25	1.26	1.33
5	3	35	ASP	N-CA	5.25	1.52	1.46
4	4	3	ALA	CA-C	5.25	1.59	1.52
4	4	64	THR	CA-C	5.25	1.59	1.52
2	1	151	LEU	N-CA	5.24	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	230	GLY	CA-C	5.24	1.59	1.51
2	1	239	ILE	N-CA	5.24	1.51	1.46
3	2	213	VAL	N-CA	5.24	1.52	1.46
5	3	7	THR	N-CA	5.24	1.53	1.45
2	1	44	LEU	C-N	-5.24	1.26	1.33
2	1	246	ASN	CA-C	5.24	1.59	1.52
5	3	190	ILE	N-CA	5.24	1.52	1.46
3	2	56	PRO	N-CA	5.24	1.54	1.47
3	2	170	PRO	N-CA	5.24	1.53	1.47
3	2	123	GLY	CA-C	5.23	1.59	1.51
2	1	177	THR	N-CA	5.23	1.52	1.46
3	2	259	GLU	CA-C	5.23	1.58	1.52
2	1	37	HIS	N-CA	5.23	1.54	1.46
2	1	298	ASP	N-CA	5.23	1.52	1.46
2	1	88	THR	N-CA	5.23	1.52	1.46
3	2	219	ASP	N-CA	5.23	1.54	1.46
3	2	36	GLY	CA-C	5.23	1.59	1.51
2	1	263	PRO	N-CA	5.22	1.54	1.47
2	1	296	THR	N-CA	5.22	1.52	1.46
3	2	178	ASP	N-CA	5.22	1.52	1.46
4	4	11	GLY	CA-C	5.22	1.59	1.51
4	4	15	ASN	N-CA	5.22	1.52	1.46
4	4	62	ILE	CA-C	5.22	1.59	1.52
5	3	200	VAL	CA-C	5.22	1.58	1.52
3	2	45	SER	CA-C	5.22	1.59	1.52
3	2	92	PHE	CA-C	5.22	1.59	1.52
3	2	149	ASN	N-CA	5.22	1.52	1.46
3	2	69	VAL	N-CA	5.22	1.53	1.46
4	4	57	ILE	N-CA	5.22	1.52	1.46
2	1	93	ASP	N-CA	5.22	1.52	1.46
3	2	171	ALA	C-O	-5.22	1.17	1.24
2	1	25	ASP	C-N	-5.21	1.26	1.33
5	3	95	LEU	N-CA	5.21	1.52	1.46
2	1	150	ALA	C-N	-5.21	1.26	1.33
3	2	228	GLY	N-CA	5.21	1.52	1.45
2	1	21	ALA	CA-C	5.21	1.59	1.52
3	2	17	THR	N-CA	5.21	1.52	1.46
5	3	44	MET	N-CA	5.21	1.52	1.46
2	1	45	THR	N-CA	5.21	1.53	1.46
2	1	182	SER	CA-C	5.21	1.58	1.52
2	1	64	ARG	CA-C	5.21	1.60	1.53
2	1	82	ALA	CA-C	5.21	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	39	LYS	N-CA	5.21	1.52	1.46
2	1	84	GLY	N-CA	5.21	1.52	1.45
5	3	140	ASP	N-CA	5.20	1.53	1.46
5	3	104	LEU	N-CA	5.20	1.52	1.46
3	2	31	SER	CA-C	5.20	1.58	1.52
3	2	156	THR	N-CA	5.20	1.52	1.45
5	3	61	LYS	N-CA	5.20	1.52	1.46
2	1	125	PHE	C-N	-5.20	1.27	1.33
2	1	135	THR	CA-C	5.20	1.59	1.52
3	2	207	THR	N-CA	5.19	1.52	1.46
2	1	142	PHE	C-N	-5.19	1.25	1.33
3	2	223	LYS	N-CA	5.19	1.52	1.46
3	2	265	ASN	CA-C	5.19	1.59	1.52
3	2	103	ARG	CA-C	5.19	1.58	1.52
5	3	66	GLU	CA-C	5.19	1.59	1.52
2	1	213	SER	CA-C	5.18	1.59	1.52
5	3	220	PHE	C-N	-5.18	1.26	1.33
3	2	138	THR	CA-C	5.18	1.59	1.52
5	3	49	ILE	N-CA	5.18	1.52	1.46
5	3	165	THR	N-CA	5.18	1.52	1.46
3	2	228	GLY	CA-C	5.18	1.59	1.51
2	1	74	GLU	CA-C	5.18	1.59	1.52
5	3	39	GLU	N-CA	5.18	1.52	1.46
2	1	223	ALA	CA-C	5.18	1.59	1.52
3	2	253	ILE	N-CA	5.18	1.52	1.46
4	4	25	ILE	C-N	-5.18	1.26	1.33
5	3	27	GLU	CA-C	5.18	1.59	1.52
2	1	61	VAL	CA-C	5.17	1.59	1.52
2	1	272	ARG	N-CA	5.17	1.52	1.45
5	3	117	THR	N-CA	5.17	1.52	1.46
2	1	71	SER	CA-C	5.17	1.58	1.52
2	1	141	ASN	C-N	-5.17	1.26	1.33
2	1	175	TRP	N-CA	5.17	1.53	1.46
4	4	24	THR	CA-C	5.17	1.59	1.52
3	2	150	PRO	N-CA	5.16	1.54	1.47
5	3	23	CYS	CA-C	5.16	1.59	1.52
3	2	155	GLY	N-CA	5.16	1.52	1.45
5	3	190	ILE	CA-C	5.16	1.59	1.52
3	2	183	ASN	N-CA	5.16	1.51	1.46
5	3	80	ASP	C-N	-5.16	1.27	1.33
2	1	169	LYS	N-CA	5.16	1.52	1.46
3	2	168	THR	CA-C	5.16	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	156	TRP	NE1-CE2	-5.15	1.31	1.37
4	4	47	SER	N-CA	5.15	1.52	1.45
2	1	154	VAL	CA-C	5.15	1.59	1.52
2	1	181	PRO	N-CA	5.15	1.53	1.47
3	2	10	SER	CA-C	5.15	1.58	1.52
3	2	267	THR	CA-C	5.15	1.59	1.52
5	3	110	TRP	NE1-CE2	-5.15	1.31	1.37
2	1	42	PRO	N-CA	5.15	1.54	1.47
3	2	269	PRO	N-CA	5.15	1.53	1.47
4	4	7	SER	CA-C	5.15	1.59	1.52
2	1	273	PRO	C-N	-5.15	1.26	1.33
5	3	202	LEU	C-N	-5.15	1.26	1.33
2	1	30	THR	CA-C	5.14	1.59	1.52
3	2	28	ALA	C-N	-5.14	1.27	1.33
2	1	224	LEU	N-CA	5.14	1.52	1.46
5	3	177	ARG	C-N	-5.14	1.26	1.33
5	3	225	LEU	C-N	-5.14	1.27	1.33
2	1	124	PHE	CA-C	5.14	1.59	1.52
3	2	39	PRO	N-CA	5.14	1.53	1.47
5	3	81	PRO	N-CA	5.14	1.53	1.47
5	3	209	ASP	N-CA	5.14	1.52	1.46
3	2	54	THR	CA-C	5.14	1.59	1.52
5	3	126	ALA	CA-C	5.14	1.59	1.52
4	4	47	SER	CA-C	5.13	1.59	1.52
2	1	50	GLY	CA-C	5.13	1.58	1.51
3	2	80	TRP	NE1-CE2	-5.13	1.31	1.37
3	2	257	CYS	CA-C	5.13	1.59	1.52
4	4	34	ARG	CA-C	5.13	1.59	1.52
2	1	290	THR	CA-C	5.13	1.59	1.52
5	3	22	PRO	N-CA	5.13	1.53	1.47
5	3	170	TRP	NE1-CE2	-5.13	1.31	1.37
5	3	229	THR	CA-C	5.13	1.59	1.52
3	2	149	ASN	CA-C	5.13	1.58	1.53
3	2	153	LYS	N-CA	5.13	1.53	1.46
5	3	103	ILE	CA-C	5.12	1.59	1.52
2	1	200	GLY	N-CA	5.12	1.52	1.45
3	2	47	ALA	CA-C	5.12	1.59	1.52
5	3	106	TYR	N-CA	5.12	1.52	1.46
3	2	78	TRP	NE1-CE2	-5.12	1.31	1.37
3	2	192	VAL	CA-C	5.12	1.60	1.52
2	1	131	ASP	CA-C	5.12	1.59	1.52
2	1	218	LYS	C-O	-5.12	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	258	ARG	CA-C	5.12	1.59	1.52
3	2	115	SER	CA-C	5.12	1.59	1.52
2	1	271	PRO	CA-C	5.12	1.58	1.52
4	4	42	SER	CA-C	5.12	1.59	1.52
5	3	172	SER	CA-C	5.12	1.58	1.52
3	2	190	ALA	CA-C	5.12	1.60	1.52
4	4	29	THR	CA-C	5.12	1.58	1.52
4	4	49	ASP	CA-C	5.11	1.58	1.52
5	3	121	CYS	N-CA	5.11	1.53	1.46
3	2	38	TRP	NE1-CE2	-5.11	1.31	1.37
3	2	216	LEU	CA-C	5.11	1.58	1.52
5	3	123	SER	CA-C	5.11	1.59	1.52
5	3	8	PRO	CA-C	5.11	1.59	1.52
3	2	54	THR	N-CA	5.11	1.52	1.46
3	2	155	GLY	C-N	-5.11	1.26	1.33
2	1	81	PHE	CA-C	5.10	1.59	1.52
3	2	49	PRO	CA-C	5.10	1.59	1.52
2	1	28	PRO	CA-C	5.10	1.58	1.52
5	3	38	GLY	N-CA	5.10	1.52	1.45
2	1	167	PRO	CA-C	5.10	1.58	1.52
2	1	84	GLY	CA-C	5.10	1.59	1.51
3	2	13	VAL	N-CA	5.10	1.52	1.46
3	2	245	PRO	CA-C	5.10	1.58	1.52
5	3	92	ASP	CA-C	5.10	1.59	1.52
5	3	188	GLY	N-CA	5.10	1.52	1.45
3	2	104	SER	N-CA	5.09	1.52	1.46
5	3	216	ALA	CA-C	5.09	1.59	1.52
3	2	182	GLY	CA-C	5.09	1.59	1.51
2	1	55	LEU	C-N	-5.09	1.27	1.33
3	2	215	SER	CA-C	5.09	1.59	1.52
5	3	72	LEU	CA-C	5.09	1.59	1.52
5	3	156	TRP	N-CA	5.09	1.52	1.46
2	1	297	LYS	N-CA	5.09	1.52	1.46
5	3	207	GLU	N-CA	5.09	1.52	1.46
2	1	199	VAL	N-CA	5.08	1.52	1.46
5	3	173	ASN	CA-C	5.08	1.59	1.52
2	1	35	PRO	C-N	-5.08	1.26	1.33
3	2	227	TRP	NE1-CE2	-5.08	1.31	1.37
5	3	20	GLN	CA-C	5.08	1.59	1.53
2	1	191	PRO	N-CA	5.08	1.53	1.47
5	3	24	ALA	CA-C	5.08	1.59	1.52
2	1	51	ALA	CA-C	5.07	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	108	TRP	NE1-CE2	-5.07	1.31	1.37
4	4	35	ASP	CA-C	5.07	1.59	1.52
5	3	130	LEU	N-CA	5.07	1.51	1.45
3	2	71	TRP	NE1-CE2	-5.07	1.31	1.37
5	3	222	VAL	CA-C	5.07	1.58	1.52
3	2	136	SER	CA-C	5.07	1.58	1.52
3	2	173	ARG	CA-C	5.07	1.58	1.52
2	1	175	TRP	NE1-CE2	-5.06	1.31	1.37
3	2	8	GLY	N-CA	5.06	1.52	1.45
5	3	91	SER	CA-C	5.06	1.59	1.52
2	1	170	TRP	NE1-CE2	-5.05	1.31	1.37
5	3	173	ASN	N-CA	5.05	1.52	1.46
2	1	136	PHE	N-CA	5.05	1.53	1.46
2	1	269	TRP	NE1-CE2	-5.05	1.31	1.37
3	2	80	TRP	N-CA	5.05	1.52	1.45
5	3	4	VAL	CA-C	5.05	1.58	1.52
5	3	149	MET	N-CA	5.05	1.52	1.46
3	2	99	HIS	CA-C	5.05	1.58	1.52
5	3	49	ILE	CA-C	5.05	1.59	1.52
2	1	105	PHE	CA-C	5.05	1.58	1.52
5	3	226	ARG	CA-C	5.05	1.58	1.52
3	2	225	ASN	CA-C	5.04	1.59	1.53
4	4	67	MET	N-CA	5.04	1.52	1.46
2	1	52	THR	CA-C	5.04	1.59	1.52
3	2	79	TRP	NE1-CE2	-5.04	1.31	1.37
2	1	29	ASN	CA-C	5.04	1.59	1.52
2	1	165	PRO	N-CA	5.04	1.53	1.47
2	1	203	ASN	N-CA	5.04	1.53	1.46
4	4	45	ASP	N-CA	5.04	1.51	1.45
5	3	31	THR	CA-C	5.04	1.59	1.52
2	1	194	ILE	N-CA	5.04	1.51	1.46
3	2	202	THR	CA-C	5.04	1.58	1.52
2	1	277	VAL	CA-C	5.04	1.58	1.52
3	2	78	TRP	N-CA	5.04	1.52	1.45
2	1	160	VAL	CA-C	5.04	1.58	1.52
3	2	245	PRO	N-CA	5.04	1.53	1.47
2	1	243	ARG	N-CA	5.03	1.52	1.45
2	1	255	SER	CA-C	5.03	1.58	1.52
3	2	161	PHE	N-CA	5.03	1.52	1.46
5	3	138	GLY	N-CA	5.03	1.52	1.44
2	1	94	ASN	CA-C	5.03	1.58	1.52
2	1	128	SER	CA-C	5.03	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	40	ALA	CA-C	5.03	1.60	1.53
5	3	48	GLU	CA-C	5.03	1.59	1.52
2	1	65	HIS	N-CA	5.02	1.52	1.46
3	2	23	ILE	CA-C	5.02	1.58	1.52
5	3	199	VAL	C-N	-5.02	1.27	1.33
5	3	231	ILE	CA-C	5.02	1.58	1.52
3	2	226	ASN	N-CA	5.02	1.52	1.46
3	2	22	THR	CA-C	5.02	1.58	1.52
2	1	212	PHE	CA-C	5.01	1.58	1.52
3	2	61	CYS	CA-C	5.01	1.59	1.53
2	1	199	VAL	C-N	-5.01	1.28	1.33
3	2	90	GLY	N-CA	5.01	1.52	1.45
3	2	233	PRO	N-CA	5.01	1.53	1.47
5	3	21	SER	N-CA	5.01	1.53	1.46
2	1	62	GLN	CA-C	5.00	1.59	1.52
3	2	131	CYS	CA-C	5.00	1.59	1.52
5	3	56	ASP	N-CA	5.00	1.53	1.46
3	2	86	LEU	N-CA	5.00	1.52	1.46
3	2	262	GLY	CA-C	5.00	1.58	1.51
5	3	50	ASP	C-N	-5.00	1.26	1.33

All (878) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	127	VAL	N-CA-C	14.53	121.93	107.55
2	1	130	PHE	N-CA-C	13.48	128.81	108.46
2	1	272	ARG	O-C-N	13.03	131.13	121.88
3	2	127	VAL	O-C-N	11.72	128.75	121.37
3	2	125	PHE	N-CA-C	11.71	127.93	109.07
4	4	10	VAL	N-CA-C	11.13	123.04	108.12
3	2	63	PHE	N-CA-C	11.06	127.25	108.23
3	2	260	PHE	N-CA-C	11.04	127.39	109.40
1	R	211	SER	O-C-N	-10.94	108.97	123.19
5	3	21	SER	O-C-N	10.73	130.21	121.84
2	1	237	PHE	N-CA-C	10.66	126.90	111.87
5	3	193	PHE	N-CA-C	10.57	124.89	109.14
2	1	116	VAL	N-CA-C	10.56	122.78	111.58
5	3	53	ILE	N-CA-C	10.56	118.42	107.76
2	1	136	PHE	N-CA-C	10.48	127.25	107.75
3	2	174	PHE	N-CA-C	10.44	125.37	110.23
3	2	244	SER	O-C-N	10.38	129.92	121.20
1	R	209	VAL	CA-C-N	10.24	132.65	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	209	VAL	C-N-CA	10.24	132.65	119.84
5	3	19	PHE	N-CA-C	10.23	125.19	110.14
3	2	203	ASN	N-CA-C	10.16	126.13	108.75
3	2	226	ASN	N-CA-C	10.16	122.35	111.28
5	3	184	PHE	N-CA-C	10.07	122.26	111.28
4	4	46	PHE	N-CA-C	9.81	125.84	109.76
3	2	239	PHE	N-CA-C	9.72	125.19	108.76
5	3	220	PHE	N-CA-C	9.72	125.22	109.76
3	2	27	GLU	N-CA-C	9.58	121.93	110.44
3	2	169	SER	O-C-N	9.57	129.85	121.34
5	3	118	PHE	N-CA-C	9.56	124.31	108.73
2	1	94	ASN	O-C-N	9.52	129.26	121.17
2	1	106	ALA	N-CA-C	9.46	124.15	109.96
3	2	198	ILE	N-CA-C	9.39	116.26	106.21
5	3	213	PHE	N-CA-C	9.31	124.08	108.90
5	3	116	PHE	N-CA-C	9.17	124.12	107.99
3	2	205	CYS	N-CA-C	9.13	120.70	108.38
2	1	196	VAL	O-C-N	9.12	129.53	120.59
5	3	31	THR	O-C-N	9.12	129.41	121.20
1	R	37	VAL	N-CA-C	9.05	118.05	107.73
2	1	266	ILE	N-CA-C	8.94	122.45	108.87
3	2	232	LEU	O-C-N	8.87	129.99	121.66
3	2	247	ILE	O-C-N	8.81	131.15	121.10
3	2	193	PHE	N-CA-C	8.79	121.15	110.07
2	1	212	PHE	N-CA-C	8.78	123.72	109.85
4	4	26	ASN	N-CA-C	8.73	123.67	110.14
3	2	165	ASN	N-CA-C	8.68	123.87	113.28
2	1	180	ASN	O-C-N	8.62	130.17	121.30
2	1	138	VAL	N-CA-C	8.61	120.56	107.99
5	3	135	ALA	O-C-N	8.60	129.95	120.83
5	3	66	GLU	N-CA-C	8.49	121.67	111.82
3	2	152	GLU	N-CA-C	8.48	121.59	111.33
2	1	144	GLU	N-CA-C	8.48	123.06	109.24
5	3	232	GLU	N-CA-C	8.43	120.37	108.74
3	2	191	PHE	N-CA-C	8.41	122.64	112.38
2	1	104	LEU	N-CA-C	8.37	122.02	108.63
2	1	235	ASN	N-CA-C	8.32	120.93	109.54
3	2	183	ASN	N-CA-C	8.30	125.07	112.54
3	2	193	PHE	CB-CA-C	-8.25	97.24	108.87
3	2	195	HIS	N-CA-C	8.18	120.55	108.60
4	4	39	ASN	N-CA-C	8.17	121.46	110.35
2	1	184	PHE	N-CA-C	8.16	122.73	108.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	161	PHE	N-CA-C	8.16	122.26	108.23
2	1	78	GLU	O-C-N	8.14	130.46	122.07
3	2	32	VAL	N-CA-C	8.13	119.99	108.36
3	2	38	TRP	O-C-N	8.13	128.74	121.18
2	1	208	PHE	N-CA-C	8.10	123.06	108.48
3	2	13	VAL	N-CA-C	8.10	118.35	106.85
3	2	10	SER	N-CA-C	8.06	121.64	108.99
3	2	157	PHE	N-CA-C	8.04	122.39	110.48
5	3	133	SER	N-CA-C	8.04	122.73	109.95
4	4	31	ASN	N-CA-C	8.03	121.12	108.67
5	3	147	GLU	O-C-N	8.03	130.34	122.07
2	1	125	PHE	N-CA-C	8.02	122.69	109.06
2	1	31	GLU	N-CA-C	7.99	122.46	109.76
5	3	53	ILE	O-C-N	7.97	128.51	121.57
3	2	57	ASP	CB-CA-C	-7.97	107.37	116.54
3	2	210	LEU	O-C-N	7.91	128.63	121.35
5	3	2	LEU	O-C-N	7.90	128.19	121.31
3	2	241	SER	O-C-N	7.88	130.45	122.10
4	4	25	ILE	O-C-N	7.88	131.93	122.95
3	2	92	PHE	N-CA-C	7.82	119.80	111.28
3	2	176	PRO	CA-N-CD	-7.81	101.07	112.00
5	3	200	VAL	O-C-N	7.78	129.97	121.10
3	2	198	ILE	O-C-N	7.75	128.47	121.96
3	2	204	ASN	N-CA-C	7.74	120.61	111.71
4	4	8	GLN	O-C-N	7.74	132.54	123.02
2	1	245	VAL	O-C-N	7.74	129.72	121.90
5	3	6	ASN	N-CA-C	7.72	121.60	110.10
3	2	210	LEU	N-CA-C	7.72	119.97	109.24
3	2	149	ASN	O-C-N	7.68	128.41	121.42
5	3	204	THR	O-C-N	7.67	129.24	121.72
2	1	163	GLY	O-C-N	7.67	128.85	122.71
5	3	189	TYR	N-CA-C	7.67	121.40	108.90
2	1	38	SER	N-CA-C	7.66	121.53	109.81
2	1	141	ASN	N-CA-C	7.66	120.86	108.76
2	1	56	VAL	O-C-N	7.65	129.82	121.10
2	1	45	THR	N-CA-C	7.64	118.33	108.24
2	1	298	ASP	N-CA-C	7.59	121.23	110.23
2	1	215	VAL	O-C-N	7.59	129.75	121.10
5	3	71	ARG	N-CA-C	7.56	121.30	109.96
4	4	49	ASP	O-C-N	7.55	127.73	121.31
5	3	192	VAL	N-CA-C	7.55	118.68	108.11
5	3	158	ILE	N-CA-C	7.55	118.81	108.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	259	VAL	N-CA-C	7.54	119.49	107.73
3	2	246	GLU	N-CA-C	7.53	120.68	108.32
3	2	124	VAL	N-CA-C	7.53	118.67	107.15
4	4	5	VAL	N-CA-C	7.47	119.67	108.23
5	3	36	ILE	O-C-N	7.45	129.59	121.10
5	3	140	ASP	O-C-N	7.45	129.88	121.32
3	2	259	GLU	N-CA-C	7.43	121.69	109.06
2	1	105	PHE	N-CA-C	7.43	121.34	109.24
2	1	249	ASN	N-CA-C	7.42	120.31	109.04
3	2	52	GLN	O-C-N	7.42	129.85	121.32
5	3	7	THR	O-C-N	7.42	130.19	121.21
2	1	80	PHE	N-CA-C	7.40	120.28	111.33
2	1	242	VAL	N-CA-C	7.40	119.74	108.71
5	3	153	HIS	N-CA-C	7.40	119.98	108.96
2	1	79	SER	O-C-N	7.38	129.68	122.07
2	1	190	ALA	O-C-N	7.38	129.81	121.32
4	4	47	SER	O-C-N	7.38	131.33	123.06
5	3	167	VAL	N-CA-C	7.35	119.08	107.98
3	2	93	GLY	O-C-N	7.34	129.31	122.19
3	2	104	SER	N-CA-C	7.34	120.44	108.55
5	3	223	ARG	N-CA-C	7.33	118.86	108.74
5	3	232	GLU	O-C-N	7.33	131.50	122.92
5	3	199	VAL	N-CA-C	7.33	118.84	108.36
3	2	175	CYS	O-C-N	7.32	128.56	121.31
5	3	196	THR	O-C-N	7.32	128.96	121.79
4	4	10	VAL	CB-CA-C	-7.28	103.41	111.35
5	3	30	VAL	N-CA-C	7.27	119.19	109.37
5	3	25	LEU	O-C-N	7.26	128.50	121.31
3	2	136	SER	N-CA-C	7.26	120.75	109.07
5	3	70	VAL	CB-CA-C	-7.26	104.41	112.68
3	2	219	ASP	N-CA-C	7.25	117.84	108.34
3	2	174	PHE	CB-CA-C	-7.24	97.71	109.72
2	1	164	ALA	N-CA-C	7.24	119.02	109.83
3	2	254	ALA	O-C-N	7.23	130.74	121.12
2	1	119	ARG	O-C-N	7.23	129.61	122.09
5	3	101	GLY	O-C-N	7.23	129.28	122.13
5	3	167	VAL	CB-CA-C	-7.22	103.44	111.23
2	1	68	GLN	N-CA-C	7.21	120.19	109.59
2	1	93	ASP	N-CA-C	7.20	119.11	108.60
2	1	142	PHE	N-CA-C	7.19	120.75	109.96
3	2	50	VAL	N-CA-C	7.19	122.25	111.89
5	3	42	ASN	N-CA-C	7.19	120.49	108.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	34	GLY	O-C-N	7.18	128.95	121.77
2	1	141	ASN	O-C-N	7.18	131.53	123.48
3	2	94	GLN	O-C-N	7.18	129.47	122.07
3	2	261	ASN	N-CA-C	7.17	120.79	109.81
3	2	74	GLU	N-CA-C	7.17	121.26	112.23
2	1	166	VAL	O-C-N	7.17	129.27	121.10
2	1	268	VAL	N-CA-C	7.17	119.14	108.46
2	1	161	PRO	O-C-N	7.15	129.90	121.46
2	1	66	VAL	N-CA-C	7.13	119.22	107.24
5	3	126	ALA	N-CA-C	7.13	119.89	108.41
5	3	32	PRO	O-C-N	7.12	129.86	121.46
5	3	45	GLU	O-C-N	7.12	129.67	122.12
5	3	69	ARG	N-CA-C	7.11	120.36	108.20
5	3	214	VAL	N-CA-C	7.11	118.83	108.53
2	1	122	LEU	O-C-N	7.07	129.61	122.12
2	1	123	GLU	N-CA-C	7.07	121.49	113.01
4	4	63	LYS	N-CA-C	7.06	119.87	111.33
3	2	224	HIS	N-CA-C	7.06	120.69	108.76
5	3	39	GLU	N-CA-C	7.05	120.54	109.96
3	2	40	GLU	N-CA-C	7.04	120.04	108.99
2	1	249	ASN	O-C-N	7.02	129.15	121.36
2	1	164	ALA	O-C-N	7.02	129.29	121.43
3	2	113	ASN	N-CA-C	7.01	120.90	110.52
2	1	281	GLY	O-C-N	7.00	128.78	121.77
2	1	237	PHE	CB-CA-C	-6.99	100.23	111.28
1	R	104	ARG	N-CA-C	6.99	120.25	108.23
2	1	257	ILE	N-CA-C	6.98	117.49	106.88
5	3	18	ASN	N-CA-C	6.97	122.39	109.56
3	2	108	VAL	N-CA-C	6.94	118.47	107.98
2	1	273	PRO	O-C-N	6.94	129.65	121.46
1	R	53	VAL	N-CA-C	6.93	114.41	107.55
4	4	37	ALA	O-C-N	6.93	129.47	122.12
4	4	46	PHE	CA-CB-CG	-6.93	106.87	113.80
2	1	98	THR	N-CA-C	6.92	118.83	111.28
2	1	120	ARG	O-C-N	6.92	129.46	122.12
5	3	19	PHE	CB-CA-C	-6.92	98.05	110.36
5	3	55	PHE	N-CA-C	6.91	125.53	110.80
3	2	70	SER	N-CA-C	6.91	119.99	108.73
2	1	160	VAL	O-C-N	6.90	128.97	121.10
4	4	40	ALA	O-C-N	6.89	131.06	122.65
3	2	204	ASN	CB-CA-C	-6.89	97.89	110.63
3	2	266	ILE	N-CA-C	6.88	118.32	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	292	THR	O-C-N	6.88	128.12	121.31
5	3	102	GLU	N-CA-C	6.88	118.77	111.28
3	2	55	GLU	O-C-N	6.86	129.21	121.32
2	1	55	LEU	N-CA-C	6.86	119.67	110.35
4	4	57	ILE	N-CA-C	6.86	118.42	109.58
5	3	103	ILE	O-C-N	6.85	128.89	121.83
5	3	163	SER	N-CA-C	6.84	120.74	110.14
3	2	127	VAL	CB-CA-C	-6.83	102.98	111.04
2	1	180	ASN	N-CA-C	6.82	118.30	109.64
4	4	65	ALA	O-C-N	6.82	129.46	121.21
2	1	146	ASN	CB-CA-C	-6.81	96.86	110.42
3	2	47	ALA	N-CA-C	6.81	119.61	110.35
5	3	102	GLU	O-C-N	6.80	129.33	122.12
3	2	48	ASN	O-C-N	6.80	129.14	121.32
2	1	98	THR	O-C-N	6.76	129.29	122.12
3	2	117	PHE	N-CA-C	6.75	121.67	113.17
2	1	246	ASN	N-CA-C	6.74	120.00	110.23
5	3	168	VAL	O-C-N	6.73	128.78	121.10
5	3	231	ILE	O-C-N	6.73	129.65	123.19
2	1	231	ALA	N-CA-C	6.72	119.69	108.20
5	3	73	SER	N-CA-C	6.72	119.38	108.76
2	1	130	PHE	CB-CA-C	-6.71	98.91	109.72
3	2	230	ALA	N-CA-C	6.71	119.66	108.73
3	2	204	ASN	O-C-N	6.69	130.05	122.22
2	1	74	GLU	N-CA-C	6.68	120.69	112.54
4	4	53	PHE	N-CA-C	6.68	121.97	113.55
2	1	64	ARG	O-C-N	6.68	130.42	122.94
2	1	153	GLN	N-CA-C	6.66	120.14	110.28
2	1	85	ALA	N-CA-C	6.66	119.79	109.07
2	1	243	ARG	O-C-N	6.66	130.84	123.25
5	3	32	PRO	N-CA-C	6.66	118.82	110.70
3	2	58	VAL	O-C-N	6.66	128.62	121.90
5	3	195	GLN	O-C-N	6.66	129.01	122.09
3	2	146	GLN	O-C-N	6.65	128.92	122.07
4	4	14	GLU	CA-C-O	-6.65	114.50	121.55
3	2	213	VAL	N-CA-C	6.64	117.85	108.36
3	2	246	GLU	O-C-N	6.64	130.99	123.42
5	3	165	THR	N-CA-C	6.64	119.55	108.73
3	2	245	PRO	O-C-N	6.63	130.67	122.71
3	2	253	ILE	N-CA-C	6.62	118.32	108.46
5	3	139	ALA	N-CA-C	6.62	118.58	109.18
2	1	249	ASN	CB-CA-C	-6.60	102.33	109.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	162	THR	O-C-N	6.59	127.81	120.83
5	3	148	ALA	O-C-N	6.59	129.10	122.12
3	2	92	PHE	O-C-N	6.58	129.09	122.12
2	1	253	VAL	N-CA-C	6.58	117.74	107.28
4	4	6	SER	N-CA-C	6.58	119.40	109.41
5	3	183	SER	O-C-N	6.58	129.67	122.11
5	3	116	PHE	CB-CA-C	-6.57	100.14	111.30
5	3	156	TRP	N-CA-C	6.57	118.61	109.15
5	3	145	ARG	O-C-N	6.56	129.65	122.11
2	1	92	VAL	O-C-N	6.55	129.85	122.97
2	1	185	TYR	N-CA-C	6.55	119.78	109.96
5	3	111	ALA	N-CA-C	6.55	119.27	108.99
2	1	276	ALA	N-CA-C	6.54	120.52	112.54
2	1	239	ILE	N-CA-C	6.53	119.74	108.90
3	2	140	THR	N-CA-C	6.53	119.33	109.41
2	1	137	VAL	N-CA-C	6.52	117.13	107.15
3	2	168	THR	O-C-N	6.52	128.79	122.07
2	1	108	TRP	N-CA-C	6.51	119.14	108.52
3	2	63	PHE	CB-CA-C	-6.51	100.04	111.05
2	1	133	GLU	N-CA-C	6.50	119.84	107.75
5	3	216	ALA	N-CA-C	6.50	120.25	109.46
3	2	149	ASN	N-CA-C	6.49	120.78	108.97
5	3	233	GLN	N-CA-C	6.48	118.71	110.61
2	1	51	ALA	N-CA-C	6.48	120.60	110.17
2	1	42	PRO	O-C-N	6.47	129.17	122.18
2	1	48	GLU	O-C-N	6.47	129.58	122.20
2	1	29	ASN	N-CA-C	6.47	119.74	110.10
2	1	136	PHE	CB-CA-C	-6.47	100.44	111.31
2	1	46	ALA	N-CA-C	6.46	119.43	107.60
3	2	264	ARG	O-C-N	6.46	130.31	122.88
5	3	186	GLU	N-CA-C	6.46	119.59	110.23
5	3	154	VAL	N-CA-C	6.44	117.30	107.77
2	1	118	LEU	O-C-N	6.43	128.93	122.12
4	4	65	ALA	N-CA-C	6.43	118.82	110.40
3	2	110	VAL	N-CA-C	6.43	117.68	107.98
2	1	144	GLU	O-C-N	6.41	130.51	123.27
3	2	121	ALA	N-CA-C	6.41	119.42	108.02
2	1	66	VAL	O-C-N	6.40	129.24	123.03
5	3	34	ILE	O-C-N	6.40	129.67	123.14
5	3	141	PRO	O-C-N	6.40	129.01	121.46
5	3	184	PHE	CB-CA-C	-6.39	100.19	110.79
5	3	117	THR	N-CA-C	6.39	119.12	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	61	VAL	O-C-N	6.38	129.78	122.82
3	2	125	PHE	CB-CA-C	-6.38	98.68	109.72
4	4	55	GLU	O-C-N	6.38	128.66	121.32
4	4	46	PHE	O-C-N	6.38	130.66	123.19
5	3	88	SER	O-C-N	6.38	128.66	121.32
3	2	110	VAL	CB-CA-C	-6.38	104.34	111.23
2	1	102	ASP	N-CA-C	6.37	119.47	110.23
2	1	126	THR	N-CA-C	6.37	117.89	111.07
2	1	107	VAL	CB-CA-C	-6.37	104.02	111.09
5	3	11	ASN	O-C-N	6.37	128.56	121.87
3	2	120	GLY	O-C-N	6.36	128.88	122.65
2	1	270	CYS	O-C-N	6.35	128.63	121.32
3	2	92	PHE	CB-CA-C	-6.35	100.25	110.79
1	R	161	VAL	N-CA-C	6.35	122.60	108.88
2	1	25	ASP	O-C-N	6.34	130.49	123.01
5	3	184	PHE	O-C-N	6.34	128.84	122.12
2	1	121	LYS	O-C-N	6.34	128.60	122.07
5	3	30	VAL	O-C-N	6.33	129.12	122.67
4	4	25	ILE	CB-CA-C	-6.30	103.10	110.91
4	4	53	PHE	CB-CA-C	-6.30	99.58	109.34
3	2	9	TYR	N-CA-C	6.30	119.16	110.35
3	2	108	VAL	CB-CA-C	-6.28	104.45	111.23
5	3	160	LEU	O-C-N	6.28	129.33	122.11
4	4	3	ALA	N-CA-C	6.27	119.44	110.10
3	2	144	SER	N-CA-C	6.27	119.32	110.23
5	3	220	PHE	CB-CA-C	-6.27	99.63	109.84
5	3	147	GLU	N-CA-C	6.26	117.77	111.07
5	3	47	ALA	O-C-N	6.26	129.55	122.22
3	2	231	ILE	N-CA-C	6.26	116.67	106.72
3	2	171	ALA	O-C-N	6.25	130.46	122.33
2	1	81	PHE	N-CA-C	6.25	121.07	113.38
3	2	17	THR	N-CA-C	6.25	119.14	108.02
3	2	44	ASP	O-C-N	6.25	128.74	122.12
3	2	192	VAL	O-C-N	6.25	129.18	122.06
2	1	132	MET	N-CA-C	6.24	118.90	108.73
3	2	268	LEU	O-C-N	6.24	128.50	121.32
4	4	44	GLN	O-C-N	6.24	130.73	122.56
5	3	154	VAL	O-C-N	6.24	129.67	123.18
3	2	145	TYR	O-C-N	6.23	128.72	122.12
2	1	161	PRO	N-CA-C	6.23	118.30	110.70
2	1	41	ILE	O-C-N	6.20	128.17	121.10
3	2	225	ASN	N-CA-C	6.20	119.27	107.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	190	ALA	O-C-N	6.19	130.38	122.33
3	2	28	ALA	N-CA-C	6.19	120.36	109.96
3	2	199	ASN	N-CA-C	6.19	119.62	108.17
3	2	160	THR	N-CA-C	6.19	119.64	108.69
5	3	207	GLU	N-CA-C	6.19	119.22	108.76
3	2	37	ARG	N-CA-C	6.19	118.94	107.99
5	3	81	PRO	N-CA-C	6.18	120.55	111.03
4	4	30	ILE	N-CA-C	6.17	116.90	107.77
3	2	170	PRO	O-C-N	6.17	130.37	122.85
2	1	36	THR	N-CA-C	6.16	119.56	108.48
4	4	61	LEU	N-CA-C	6.16	119.27	109.24
3	2	266	ILE	O-C-N	6.15	128.75	122.79
5	3	100	LEU	O-C-N	6.14	128.39	122.07
3	2	161	PHE	CB-CA-C	-6.14	100.68	111.05
5	3	49	ILE	CB-CA-C	-6.14	103.53	110.96
3	2	111	GLN	N-CA-C	6.13	118.70	108.96
3	2	229	ILE	N-CA-C	6.12	116.52	107.15
2	1	252	LYS	N-CA-C	6.12	119.14	109.96
3	2	21	SER	N-CA-C	6.12	118.88	108.90
2	1	262	LYS	O-C-N	6.12	129.25	121.12
2	1	87	VAL	O-C-N	6.11	128.31	122.20
3	2	211	PRO	CA-C-O	-6.11	114.54	122.12
2	1	31	GLU	O-C-N	6.11	130.19	123.04
2	1	91	THR	N-CA-C	6.10	118.80	107.99
2	1	107	VAL	O-C-N	6.10	128.63	122.71
5	3	172	SER	N-CA-C	6.10	118.69	109.23
2	1	286	TYR	O-C-N	6.10	129.92	123.03
5	3	222	VAL	O-C-N	6.09	129.51	123.00
2	1	134	LEU	N-CA-C	6.08	118.21	108.41
1	R	75	MET	N-CA-C	6.08	119.42	108.48
3	2	100	TYR	O-C-N	6.08	128.33	122.07
5	3	207	GLU	O-C-N	6.08	130.42	123.31
3	2	198	ILE	CB-CA-C	-6.08	106.41	113.22
3	2	188	GLY	O-C-N	6.08	128.45	122.19
5	3	221	SER	N-CA-C	6.08	118.41	109.24
3	2	238	ASN	N-CA-C	6.06	119.38	108.48
2	1	80	PHE	O-C-N	6.05	128.53	122.12
2	1	196	VAL	CB-CA-C	-6.05	104.05	110.16
3	2	197	ILE	N-CA-C	6.04	116.56	107.80
5	3	113	SER	N-CA-C	6.04	119.49	109.46
3	2	152	GLU	O-C-N	6.04	128.52	122.12
5	3	53	ILE	CB-CA-C	-6.03	104.26	110.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	156	THR	N-CA-C	6.02	118.57	109.23
2	1	66	VAL	CB-CA-C	-6.02	103.57	110.73
2	1	76	SER	O-C-N	6.02	129.96	122.86
2	1	189	THR	O-C-N	6.02	129.80	123.06
3	2	222	VAL	CB-CA-C	-6.02	104.18	112.24
5	3	177	ARG	O-C-N	6.02	130.02	123.10
4	4	40	ALA	CA-C-O	-6.01	115.14	121.99
2	1	29	ASN	CB-CA-C	-6.01	100.53	109.90
5	3	119	LEU	N-CA-C	6.01	118.47	108.20
3	2	112	CYS	N-CA-C	6.00	118.58	107.60
5	3	98	THR	O-C-N	6.00	129.74	122.96
5	3	20	GLN	O-C-N	6.00	129.63	122.79
3	2	218	ILE	O-C-N	6.00	128.95	123.19
2	1	96	ALA	O-C-N	6.00	130.06	123.04
2	1	192	ALA	N-CA-C	6.00	118.69	110.24
5	3	77	HIS	N-CA-C	5.99	119.04	110.24
5	3	180	ILE	O-C-N	5.98	129.78	123.02
5	3	28	PHE	N-CA-C	5.98	123.53	110.80
3	2	79	TRP	N-CA-C	5.97	119.21	109.06
3	2	193	PHE	CA-C-O	-5.97	115.17	120.19
2	1	199	VAL	N-CA-C	5.97	121.75	109.34
2	1	253	VAL	CB-CA-C	-5.97	103.23	110.99
3	2	164	ASP	O-C-N	5.97	130.53	122.59
2	1	116	VAL	CB-CA-C	-5.96	104.44	111.94
5	3	70	VAL	O-C-N	5.95	128.97	122.36
2	1	99	THR	O-C-N	5.95	130.51	122.59
3	2	235	ALA	O-C-N	5.95	129.74	121.47
5	3	233	GLN	O-C-N	5.95	129.37	121.99
2	1	53	ASN	O-C-N	5.94	128.15	121.32
3	2	129	GLU	CB-CA-C	-5.94	103.46	111.89
5	3	92	ASP	O-C-N	5.94	128.15	121.32
5	3	167	VAL	O-C-N	5.93	129.15	122.68
5	3	202	LEU	CA-C-O	-5.93	115.78	122.01
2	1	80	PHE	CB-CA-C	-5.93	100.60	110.68
2	1	231	ALA	O-C-N	5.93	130.10	123.05
3	2	128	PRO	O-C-N	5.93	129.83	123.01
5	3	135	ALA	CB-CA-C	-5.92	104.29	110.33
2	1	27	LEU	O-C-N	5.92	128.41	121.66
2	1	285	ASP	N-CA-C	5.91	118.93	110.24
2	1	241	ALA	N-CA-C	5.91	118.39	107.99
2	1	244	VAL	O-C-N	5.91	129.53	122.62
2	1	220	GLN	N-CA-C	5.91	118.53	108.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	173	ARG	N-CA-C	5.90	118.15	109.24
5	3	226	ARG	N-CA-C	5.90	118.04	109.07
4	4	5	VAL	CB-CA-C	-5.90	103.83	110.96
4	4	46	PHE	CB-CA-C	-5.90	99.57	109.48
4	4	45	ASP	N-CA-C	5.89	119.66	110.17
5	3	115	LYS	N-CA-C	5.89	118.01	108.34
5	3	173	ASN	O-C-N	5.89	128.87	122.15
3	2	11	ASP	O-C-N	5.89	128.36	122.12
3	2	196	GLN	O-C-N	5.89	129.99	123.33
3	2	238	ASN	O-C-N	5.89	130.68	123.44
2	1	180	ASN	CB-CA-C	-5.88	100.22	109.52
5	3	46	LEU	O-C-N	5.88	128.86	122.15
2	1	193	ARG	N-CA-C	5.88	119.06	108.48
2	1	151	LEU	O-C-N	5.88	130.04	122.81
3	2	189	ASN	N-CA-C	5.87	120.44	113.28
3	2	244	SER	N-CA-C	5.86	118.03	109.30
2	1	194	ILE	O-C-N	5.86	129.68	123.00
3	2	142	HIS	N-CA-C	5.86	120.43	113.28
3	2	248	PRO	O-C-N	5.86	130.13	123.10
5	3	136	PRO	O-C-N	5.86	128.37	121.46
5	3	98	THR	CA-C-O	-5.85	114.74	121.47
3	2	23	ILE	O-C-N	5.85	129.32	123.18
2	1	183	ILE	O-C-N	5.84	130.54	122.88
2	1	208	PHE	CB-CA-C	-5.84	99.87	109.80
2	1	61	VAL	N-CA-C	5.84	117.48	108.44
3	2	43	ARG	O-C-N	5.84	129.99	122.81
3	2	249	ILE	O-C-N	5.84	129.78	122.66
4	4	13	HIS	N-CA-C	5.83	118.71	109.96
2	1	291	LEU	N-CA-C	5.83	120.09	113.15
5	3	151	GLY	O-C-N	5.82	129.34	123.11
4	4	38	SER	O-C-N	5.82	129.03	122.22
5	3	40	VAL	N-CA-C	5.81	117.37	108.71
3	2	236	PRO	O-C-N	5.81	130.27	122.89
3	2	236	PRO	N-CA-C	5.80	120.32	111.15
3	2	124	VAL	CB-CA-C	-5.80	104.39	111.88
5	3	114	LEU	O-C-N	5.80	129.59	123.03
5	3	70	VAL	N-CA-C	5.80	114.96	106.55
3	2	157	PHE	O-C-N	5.80	129.51	122.96
2	1	253	VAL	O-C-N	5.80	129.19	122.99
3	2	156	THR	O-C-N	5.79	129.99	123.27
3	2	68	THR	N-CA-C	5.79	118.59	109.96
3	2	45	SER	O-C-N	5.79	128.99	122.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	39	ASN	O-C-N	5.79	129.93	122.81
2	1	140	ALA	N-CA-C	5.79	118.99	109.85
2	1	173	TYR	N-CA-C	5.79	119.16	111.75
5	3	96	SER	O-C-N	5.79	128.79	122.20
3	2	133	ALA	N-CA-C	5.78	118.84	110.28
4	4	7	SER	N-CA-C	5.78	119.06	109.46
3	2	186	LEU	N-CA-C	5.78	118.58	109.96
2	1	40	GLU	N-CA-C	5.78	118.09	109.25
2	1	73	SER	O-C-N	5.78	129.19	122.20
3	2	151	GLY	O-C-N	5.78	129.03	122.67
5	3	226	ARG	O-C-N	5.78	129.84	123.25
3	2	163	PRO	N-CA-C	5.78	120.67	111.26
2	1	63	THR	N-CA-C	5.77	119.46	110.17
2	1	70	ARG	N-CA-C	5.77	118.59	110.23
3	2	239	PHE	O-C-N	5.77	130.06	123.31
2	1	206	SER	O-C-N	5.76	129.66	122.63
5	3	120	PHE	N-CA-C	5.75	123.06	110.80
2	1	130	PHE	O-C-N	5.75	129.85	123.52
5	3	210	ILE	O-C-N	5.75	129.83	123.10
5	3	112	GLY	O-C-N	5.75	128.81	123.35
2	1	29	ASN	O-C-N	5.75	130.08	122.95
5	3	136	PRO	N-CA-C	5.75	117.71	110.70
3	2	106	TYR	N-CA-C	5.75	118.57	108.75
5	3	135	ALA	N-CA-C	5.75	120.90	109.01
2	1	111	THR	N-CA-C	5.74	117.27	108.42
5	3	196	THR	CB-CA-C	-5.74	103.52	112.31
5	3	75	LYS	O-C-N	5.73	128.20	121.66
3	2	206	ALA	N-CA-C	5.73	117.74	108.34
5	3	132	VAL	N-CA-C	5.73	116.63	107.98
2	1	183	ILE	CB-CA-C	-5.72	103.24	111.19
2	1	128	SER	N-CA-C	5.72	117.88	109.24
5	3	16	ALA	O-C-N	5.71	129.48	122.34
2	1	150	ALA	O-C-N	5.71	130.46	123.44
5	3	213	PHE	CB-CA-C	-5.71	99.27	109.71
3	2	103	ARG	O-C-N	5.71	130.23	123.27
4	4	28	THR	N-CA-C	5.70	118.93	109.46
3	2	23	ILE	N-CA-C	5.70	116.15	108.17
4	4	12	ALA	N-CA-C	5.70	117.75	108.63
3	2	217	SER	O-C-N	5.70	128.16	122.12
2	1	124	PHE	CA-C-O	5.70	126.28	119.10
3	2	207	THR	N-CA-C	5.69	118.07	107.99
2	1	174	THR	O-C-N	5.69	128.69	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3	4	VAL	O-C-N	5.69	129.01	123.03
3	2	27	GLU	O-C-N	5.69	129.40	121.83
3	2	168	THR	CB-CA-C	-5.69	101.95	110.88
5	3	193	PHE	CB-CA-C	-5.69	97.99	110.67
5	3	215	SER	O-C-N	5.68	129.73	123.25
5	3	9	GLY	O-C-N	5.68	129.07	122.65
2	1	43	ALA	O-C-N	5.68	128.87	122.22
3	2	161	PHE	O-C-N	5.68	130.18	122.57
3	2	243	SER	O-C-N	5.68	129.25	122.27
2	1	33	SER	N-CA-C	5.68	117.66	108.41
5	3	182	ASP	N-CA-C	5.67	117.61	107.80
3	2	258	CYS	N-CA-C	5.67	118.78	109.76
3	2	46	GLU	O-C-N	5.66	129.42	122.34
3	2	59	ALA	O-C-N	5.66	128.84	122.22
3	2	234	LEU	O-C-N	5.66	128.12	122.12
5	3	118	PHE	CB-CA-C	-5.65	101.04	110.19
2	1	217	LEU	N-CA-C	5.64	117.42	108.67
3	2	254	ALA	CA-C-N	-5.64	114.14	119.90
3	2	254	ALA	C-N-CA	-5.64	114.14	119.90
2	1	137	VAL	CB-CA-C	-5.64	104.60	111.88
4	4	30	ILE	O-C-N	5.63	129.04	123.18
3	2	197	ILE	CA-C-N	-5.62	116.36	121.65
3	2	197	ILE	C-N-CA	-5.62	116.36	121.65
2	1	183	ILE	N-CA-C	5.62	115.69	107.37
5	3	127	THR	O-C-N	5.62	129.36	122.84
4	4	58	LYS	O-C-N	5.62	128.09	122.08
2	1	214	LYS	N-CA-C	5.61	117.93	109.23
2	1	205	TYR	O-C-N	5.61	129.79	123.06
5	3	146	LYS	O-C-N	5.61	128.99	122.20
5	3	214	VAL	O-C-N	5.61	128.86	123.14
3	2	29	ALA	O-C-N	5.60	130.26	122.08
3	2	206	ALA	O-C-N	5.60	129.82	123.27
3	2	14	LEU	N-CA-C	5.60	118.69	109.85
3	2	163	PRO	O-C-N	5.60	129.68	122.85
3	2	87	ARG	O-C-N	5.60	128.58	122.20
4	4	14	GLU	N-CA-C	5.59	117.96	110.35
2	1	277	VAL	O-C-N	5.59	128.98	123.00
3	2	64	TYR	O-C-N	5.59	129.56	123.13
2	1	223	ALA	O-C-N	5.59	128.57	122.20
2	1	200	GLY	O-C-N	5.59	128.59	122.84
3	2	211	PRO	O-C-N	5.59	129.96	123.14
5	3	82	ILE	O-C-N	5.59	128.11	121.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3	173	ASN	N-CA-C	5.58	117.45	111.36
4	4	41	ALA	O-C-N	5.58	129.89	123.02
5	3	97	HIS	CA-CB-CG	-5.58	108.22	113.80
2	1	295	SER	O-C-N	5.58	129.33	123.03
3	2	13	VAL	CB-CA-C	-5.57	104.29	111.53
3	2	214	ASN	N-CA-C	5.57	122.66	110.80
3	2	271	LEU	N-CA-C	5.57	119.82	113.19
3	2	265	ASN	CA-C-O	-5.57	115.49	121.56
3	2	12	ARG	O-C-N	5.56	129.11	122.27
3	2	72	THR	N-CA-C	5.56	118.14	109.52
2	1	283	GLY	O-C-N	5.55	128.75	122.86
2	1	147	ASN	O-C-N	5.55	129.97	122.59
2	1	95	PRO	O-C-N	5.55	130.13	122.64
3	2	89	MET	N-CA-C	5.54	117.74	107.99
3	2	107	THR	O-C-N	5.54	129.49	122.84
3	2	118	HIS	O-C-N	5.54	129.26	123.06
5	3	7	THR	N-CA-C	5.54	117.65	110.40
3	2	75	SER	N-CA-C	5.53	118.60	110.30
3	2	32	VAL	CB-CA-C	-5.53	103.32	110.84
3	2	170	PRO	N-CA-C	5.53	120.27	111.26
3	2	240	ALA	O-C-N	5.53	129.94	122.59
2	1	41	ILE	N-CA-C	5.53	120.82	108.88
3	2	91	LEU	N-CA-C	5.53	118.06	111.71
5	3	52	MET	N-CA-C	5.52	118.33	110.10
5	3	194	TYR	O-C-N	5.52	129.97	122.57
2	1	202	SER	O-C-N	5.52	130.22	123.10
5	3	197	ARG	NE-CZ-NH2	5.52	124.17	119.20
2	1	277	VAL	N-CA-C	5.52	117.85	108.86
3	2	253	ILE	O-C-N	5.51	129.00	123.10
3	2	6	ALA	O-C-N	5.51	129.49	122.33
3	2	237	LEU	O-C-N	5.51	129.67	123.06
5	3	96	SER	N-CA-C	5.51	118.80	111.75
3	2	108	VAL	O-C-N	5.49	128.66	122.68
3	2	113	ASN	O-C-N	5.49	129.09	122.94
5	3	169	PRO	N-CA-C	5.49	119.82	111.15
2	1	64	ARG	CA-C-O	-5.49	115.25	121.72
3	2	99	HIS	N-CA-C	5.48	118.42	109.59
5	3	121	CYS	N-CA-C	5.48	119.52	113.21
5	3	132	VAL	CB-CA-C	-5.48	105.31	111.23
5	3	188	GLY	O-C-N	5.48	128.06	122.85
2	1	22	THR	N-CA-C	5.48	118.39	110.28
2	1	71	SER	N-CA-C	5.48	118.16	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	102	ASP	O-C-N	5.47	129.60	122.87
2	1	261	LEU	N-CA-C	5.47	117.66	108.73
4	4	45	ASP	O-C-N	5.47	129.39	123.10
5	3	76	PRO	N-CA-C	5.47	119.68	111.14
1	R	208	LEU	CA-C-N	5.47	131.55	121.70
1	R	208	LEU	C-N-CA	5.47	131.55	121.70
3	2	65	THR	N-CA-C	5.47	117.22	108.41
4	4	48	GLN	O-C-N	5.47	129.97	123.24
5	3	44	MET	O-C-N	5.47	128.62	122.22
2	1	40	GLU	O-C-N	5.47	129.74	123.02
3	2	265	ASN	O-C-N	5.46	129.31	122.86
5	3	104	LEU	O-C-N	5.46	128.61	122.22
3	2	106	TYR	O-C-N	5.46	129.80	123.41
5	3	69	ARG	NE-CZ-NH2	5.46	124.11	119.20
2	1	154	VAL	CB-CA-C	-5.46	103.89	110.99
3	2	264	ARG	NE-CZ-NH2	5.46	124.11	119.20
5	3	154	VAL	CB-CA-C	-5.46	103.05	110.42
5	3	223	ARG	NE-CZ-NH2	5.46	124.11	119.20
3	2	115	SER	O-C-N	5.46	129.59	123.48
3	2	177	VAL	N-CA-C	5.46	116.62	108.54
5	3	105	ASN	N-CA-C	5.46	119.68	113.19
3	2	205	CYS	O-C-N	5.46	128.83	122.99
5	3	141	PRO	N-CA-C	5.46	117.36	110.70
5	3	216	ALA	O-C-N	5.45	129.44	123.22
2	1	224	LEU	O-C-N	5.45	127.98	122.09
2	1	26	ALA	O-C-N	5.45	129.60	123.06
3	2	46	GLU	N-CA-C	5.45	120.04	113.17
5	3	66	GLU	O-C-N	5.45	128.97	122.27
3	2	177	VAL	CB-CA-C	-5.44	104.71	111.08
3	2	60	ALA	O-C-N	5.44	129.39	122.10
3	2	226	ASN	O-C-N	5.44	127.89	122.12
2	1	267	ARG	NE-CZ-NH2	5.42	124.08	119.20
5	3	199	VAL	CB-CA-C	-5.42	103.46	110.84
5	3	109	HIS	N-CA-C	5.42	118.29	109.24
3	2	20	ASN	N-CA-C	5.42	119.60	113.15
3	2	54	THR	O-C-N	5.42	129.50	123.05
3	2	269	PRO	O-C-N	5.42	129.73	123.01
2	1	92	VAL	CB-CA-C	-5.41	103.78	111.19
5	3	217	CYS	O-C-N	5.41	129.25	122.86
4	4	64	THR	O-C-N	5.41	128.92	122.27
2	1	275	ARG	NE-CZ-NH2	5.41	124.07	119.20
3	2	119	GLN	O-C-N	5.41	130.36	123.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3	63	ASN	N-CA-C	5.41	119.04	111.90
3	2	229	ILE	O-C-N	5.41	128.94	122.62
3	2	43	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	1	267	ARG	O-C-N	5.40	129.86	123.27
5	3	39	GLU	O-C-N	5.40	129.57	122.93
2	1	154	VAL	N-CA-C	5.39	115.86	107.28
3	2	36	GLY	O-C-N	5.39	128.46	122.31
2	1	64	ARG	NE-CZ-NH2	5.39	124.05	119.20
3	2	40	GLU	O-C-N	5.39	129.42	123.33
5	3	226	ARG	NE-CZ-NH2	5.39	124.05	119.20
3	2	85	ALA	O-C-N	5.39	128.34	122.20
2	1	193	ARG	NE-CZ-NH2	5.38	124.05	119.20
2	1	138	VAL	CB-CA-C	-5.38	103.61	110.98
2	1	296	THR	N-CA-C	5.38	117.98	109.96
3	2	28	ALA	O-C-N	5.38	129.40	123.16
3	2	201	ARG	NE-CZ-NH2	5.38	124.04	119.20
3	2	147	ASN	N-CA-C	5.38	119.01	112.23
3	2	269	PRO	N-CA-C	5.38	119.76	111.21
2	1	129	ARG	NE-CZ-NH2	5.38	124.04	119.20
2	1	206	SER	N-CA-C	5.37	117.99	107.57
2	1	243	ARG	NE-CZ-NH2	5.37	124.04	119.20
5	3	228	THR	O-C-N	5.37	129.03	122.96
5	3	228	THR	N-CA-C	5.37	118.43	110.48
4	4	36	SER	O-C-N	5.37	129.74	122.59
5	3	201	PRO	O-C-N	5.37	129.89	122.64
2	1	129	ARG	O-C-N	5.37	130.15	123.28
3	2	250	THR	O-C-N	5.37	129.34	123.22
2	1	81	PHE	CB-CA-C	-5.37	100.31	109.65
3	2	22	THR	N-CA-C	5.37	117.83	108.76
3	2	222	VAL	N-CA-C	5.36	116.85	111.00
5	3	144	LYS	O-C-N	5.36	129.69	123.41
3	2	91	LEU	O-C-N	5.36	128.49	122.22
5	3	185	THR	O-C-N	5.36	128.95	122.35
4	4	43	LYS	O-C-N	5.36	129.72	122.59
2	1	72	ARG	O-C-N	5.36	128.94	122.35
2	1	89	ILE	CB-CA-C	-5.36	104.84	111.32
2	1	120	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	1	259	VAL	CB-CA-C	-5.36	104.45	111.25
4	4	34	ARG	NE-CZ-NH2	5.36	124.02	119.20
3	2	110	VAL	O-C-N	5.35	128.52	122.68
2	1	24	ARG	O-C-N	5.35	128.76	122.34
3	2	53	PRO	O-C-N	5.35	129.65	123.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	176	GLN	O-C-N	5.35	129.35	122.39
5	3	132	VAL	O-C-N	5.35	128.51	122.68
3	2	69	VAL	N-CA-C	5.35	116.89	109.45
3	2	103	ARG	NE-CZ-NH2	5.35	124.01	119.20
3	2	209	VAL	N-CA-C	5.35	115.33	107.15
3	2	225	ASN	CB-CA-C	-5.35	102.33	111.31
2	1	258	ARG	NE-CZ-NH2	5.34	124.01	119.20
5	3	206	ARG	NE-CZ-NH2	5.34	124.01	119.20
2	1	92	VAL	CA-C-O	-5.34	116.01	121.67
3	2	172	ARG	NE-CZ-NH2	5.34	124.00	119.20
5	3	176	TYR	O-C-N	5.34	129.36	123.33
5	3	177	ARG	NE-CZ-NH2	5.34	124.00	119.20
2	1	24	ARG	NE-CZ-NH2	5.33	124.00	119.20
3	2	37	ARG	NE-CZ-NH2	5.33	124.00	119.20
4	4	42	SER	O-C-N	5.33	128.28	122.20
5	3	145	ARG	NE-CZ-NH2	5.33	124.00	119.20
2	1	72	ARG	NE-CZ-NH2	5.33	124.00	119.20
3	2	62	ARG	NE-CZ-NH2	5.33	123.99	119.20
5	3	38	GLY	O-C-N	5.33	128.56	122.33
2	1	212	PHE	CB-CA-C	-5.32	99.33	109.66
3	2	256	MET	N-CA-C	5.32	117.91	109.50
2	1	76	SER	CA-C-O	-5.32	115.76	121.56
3	2	41	TYR	O-C-N	5.32	129.14	122.86
2	1	272	ARG	NE-CZ-NH2	5.32	123.98	119.20
2	1	287	LYS	N-CA-C	5.31	118.06	109.40
3	2	69	VAL	CB-CA-C	-5.31	104.16	111.49
3	2	197	ILE	O-C-N	5.31	129.31	123.10
3	2	104	SER	O-C-N	5.31	129.53	123.48
2	1	255	SER	N-CA-C	5.31	118.21	109.72
3	2	76	ARG	NE-CZ-NH2	5.31	123.98	119.20
5	3	111	ALA	O-C-N	5.31	129.33	123.33
2	1	114	ASP	O-C-N	5.31	128.43	122.22
3	2	62	ARG	O-C-N	5.31	129.84	122.78
5	3	209	ASP	O-C-N	5.31	129.40	123.19
3	2	254	ALA	N-CA-C	5.30	120.41	109.11
3	2	270	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	1	254	THR	O-C-N	5.30	129.27	123.22
2	1	70	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	1	63	THR	O-C-N	5.30	129.19	123.10
2	1	294	LEU	N-CA-C	5.30	117.91	110.23
4	4	27	TYR	O-C-N	5.30	129.51	123.31
5	3	117	THR	O-C-N	5.30	129.22	123.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	12	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	2	212	TYR	O-C-N	5.30	129.64	122.59
5	3	231	ILE	N-CA-C	5.30	114.84	108.06
3	2	95	ASN	O-C-N	5.29	128.78	122.27
5	3	71	ARG	NE-CZ-NH2	5.29	123.96	119.20
5	3	78	THR	O-C-N	5.29	129.82	123.36
5	3	126	ALA	O-C-N	5.29	129.28	122.93
2	1	119	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	1	300	THR	N-CA-C	5.29	118.75	112.72
5	3	191	SER	N-CA-C	5.28	118.17	109.72
3	2	87	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	1	218	LYS	O-C-N	5.28	129.61	122.59
2	1	184	PHE	CB-CA-C	-5.27	103.39	111.83
3	2	74	GLU	O-C-N	5.27	129.40	122.33
5	3	94	ARG	NE-CZ-NH2	5.27	123.94	119.20
2	1	247	ASP	O-C-N	5.27	129.29	122.81
4	4	4	GLN	N-CA-C	5.27	117.80	107.57
4	4	67	MET	O-C-N	5.27	128.17	122.11
3	2	32	VAL	O-C-N	5.27	128.88	123.03
5	3	55	PHE	CB-CA-C	-5.27	99.94	110.42
2	1	107	VAL	N-CA-C	5.27	115.99	106.61
3	2	128	PRO	CA-C-O	-5.27	115.59	121.23
3	2	173	ARG	NE-CZ-NH2	5.27	123.94	119.20
5	3	12	GLN	O-C-N	5.27	128.91	122.96
3	2	30	ASN	O-C-N	5.26	129.59	122.59
2	1	202	SER	CA-C-O	-5.26	115.19	121.56
3	2	25	THR	N-CA-C	5.26	117.18	108.13
3	2	109	HIS	N-CA-C	5.26	118.03	107.41
2	1	192	ALA	O-C-N	5.26	129.38	122.97
5	3	23	CYS	N-CA-C	5.26	116.82	108.67
5	3	33	PRO	O-C-N	5.26	129.68	123.06
5	3	198	ILE	O-C-N	5.26	129.14	122.57
4	4	35	ASP	O-C-N	5.25	129.17	123.13
2	1	126	THR	O-C-N	5.25	127.48	122.07
5	3	199	VAL	O-C-N	5.25	128.85	123.03
2	1	123	GLU	O-C-N	5.24	129.70	122.46
3	2	259	GLU	O-C-N	5.24	129.68	123.33
5	3	178	GLN	O-C-N	5.24	129.16	123.04
2	1	154	VAL	O-C-N	5.23	128.59	122.99
5	3	42	ASN	CB-CA-C	-5.23	102.60	110.24
2	1	173	TYR	O-C-N	5.23	128.16	122.20
3	2	157	PHE	CB-CA-C	-5.23	99.84	109.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	85	ALA	N-CA-C	5.22	118.44	111.75
2	1	52	THR	N-CA-C	5.22	117.24	108.73
2	1	137	VAL	O-C-N	5.22	128.73	122.62
5	3	64	THR	O-C-N	5.22	129.23	123.33
5	3	40	VAL	O-C-N	5.22	128.46	122.93
5	3	197	ARG	O-C-N	5.22	129.53	122.59
3	2	51	ASP	O-C-N	5.21	129.16	123.01
4	4	25	ILE	N-CA-C	5.21	116.09	108.58
2	1	37	HIS	O-C-N	5.21	129.06	122.28
2	1	99	THR	CB-CA-C	-5.21	100.05	110.42
2	1	83	ARG	NE-CZ-NH2	5.21	123.89	119.20
5	3	81	PRO	O-C-N	5.21	129.00	123.01
2	1	53	ASN	N-CA-C	5.21	121.32	109.81
5	3	174	THR	O-C-N	5.21	129.20	123.16
5	3	164	CYS	O-C-N	5.20	129.36	123.27
3	2	158	THR	N-CA-C	5.20	117.44	109.07
3	2	256	MET	O-C-N	5.20	129.64	123.24
5	3	49	ILE	O-C-N	5.20	129.28	122.94
2	1	78	GLU	CB-CA-C	-5.20	102.72	110.88
2	1	135	THR	O-C-N	5.20	129.41	123.27
2	1	89	ILE	N-CA-C	5.20	114.98	106.72
2	1	218	LYS	CB-CA-C	-5.19	100.09	110.42
4	4	39	ASN	CB-CA-C	-5.19	100.33	109.62
5	3	116	PHE	O-C-N	5.19	129.27	122.68
2	1	78	GLU	N-CA-C	5.19	116.62	111.07
3	2	166	ASN	N-CA-C	5.19	121.85	110.80
4	4	29	THR	N-CA-C	5.19	117.36	108.90
5	3	58	SER	O-C-N	5.19	129.19	122.81
5	3	152	THR	O-C-N	5.19	129.49	122.59
3	2	66	LEU	O-C-N	5.18	128.97	122.65
2	1	148	GLY	O-C-N	5.18	129.71	122.82
3	2	58	VAL	N-CA-C	5.18	118.31	111.17
2	1	35	PRO	O-C-N	5.17	129.17	122.91
2	1	152	ASN	N-CA-C	5.17	121.82	110.80
5	3	4	VAL	N-CA-C	5.17	116.81	108.85
5	3	77	HIS	CA-CB-CG	-5.17	108.63	113.80
5	3	231	ILE	CB-CA-C	-5.17	103.83	111.80
5	3	90	ALA	N-CA-C	5.17	119.67	112.90
3	2	233	PRO	O-C-N	5.17	129.62	122.64
5	3	76	PRO	O-C-N	5.17	129.28	123.03
2	1	227	SER	N-CA-C	5.17	116.69	108.79
4	4	59	ASP	N-CA-C	5.17	117.08	107.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	95	ASN	N-CA-C	5.16	117.81	111.82
4	4	60	VAL	CB-CA-C	-5.16	102.83	111.29
2	1	274	PRO	O-C-N	5.16	129.54	122.99
4	4	33	TYR	N-CA-C	5.16	118.48	110.17
3	2	147	ASN	O-C-N	5.16	129.24	122.33
4	4	7	SER	O-C-N	5.16	129.10	123.22
2	1	47	VAL	O-C-N	5.16	129.02	122.57
2	1	131	ASP	O-C-N	5.16	129.34	122.95
3	2	87	ARG	N-CA-C	5.16	118.35	111.75
5	3	80	ASP	N-CA-C	5.16	116.33	109.93
2	1	113	LYS	N-CA-C	5.15	119.72	113.38
2	1	22	THR	O-C-N	5.15	129.18	122.89
4	4	35	ASP	N-CA-C	5.15	117.15	108.96
3	2	33	VAL	O-C-N	5.15	129.00	122.57
3	2	208	LEU	N-CA-C	5.15	117.10	107.99
5	3	213	PHE	O-C-N	5.15	129.42	123.30
2	1	227	SER	O-C-N	5.14	128.92	123.42
2	1	232	ALA	O-C-N	5.14	129.43	122.59
3	2	129	GLU	O-C-N	5.14	128.93	122.55
2	1	28	PRO	N-CA-C	5.14	119.64	111.26
2	1	244	VAL	CB-CA-C	-5.14	105.25	111.88
2	1	182	SER	N-CA-C	5.14	117.77	109.40
2	1	246	ASN	O-C-N	5.14	129.19	122.87
3	2	209	VAL	CB-CA-C	-5.14	105.25	111.88
5	3	110	TRP	N-CA-C	5.13	117.81	109.24
5	3	123	SER	N-CA-C	5.13	117.74	110.50
2	1	226	ASP	N-CA-C	5.13	118.31	110.20
3	2	50	VAL	O-C-N	5.13	127.91	122.06
4	4	63	LYS	O-C-N	5.13	127.56	122.12
2	1	28	PRO	O-C-N	5.13	129.11	122.85
2	1	195	SER	O-C-N	5.12	129.18	123.19
2	1	197	PRO	O-C-N	5.12	129.55	122.64
3	2	258	CYS	O-C-N	5.12	129.03	123.04
3	2	242	GLU	O-C-N	5.12	129.24	122.89
4	4	57	ILE	O-C-N	5.11	128.18	122.61
2	1	242	VAL	CB-CA-C	-5.11	103.77	110.98
3	2	31	SER	O-C-N	5.11	129.51	123.33
2	1	133	GLU	O-C-N	5.11	129.15	122.87
5	3	192	VAL	O-C-N	5.11	128.78	123.26
2	1	139	THR	O-C-N	5.11	129.38	123.30
2	1	148	GLY	CA-C-O	-5.11	115.60	122.24
4	4	15	ASN	O-C-N	5.10	129.38	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	240	LEU	O-C-N	5.10	129.14	122.87
3	2	53	PRO	N-CA-C	5.10	119.32	111.21
3	2	264	ARG	CA-C-O	-5.10	115.61	120.56
5	3	103	ILE	CB-CA-C	-5.10	105.18	112.22
2	1	71	SER	O-C-N	5.10	129.51	123.24
2	1	224	LEU	N-CA-C	5.10	116.64	111.14
3	2	149	ASN	CB-CA-C	-5.10	102.82	110.87
2	1	186	THR	N-CA-C	5.10	116.91	108.20
5	3	13	TYR	N-CA-C	5.09	117.70	107.41
5	3	220	PHE	O-C-N	5.09	129.00	123.04
1	R	209	VAL	N-CA-C	5.09	125.25	111.00
2	1	23	SER	O-C-N	5.08	129.35	122.59
3	2	124	VAL	O-C-N	5.08	128.56	122.62
2	1	167	PRO	N-CA-C	5.07	119.53	111.26
3	2	168	THR	N-CA-C	5.07	116.50	111.07
4	4	34	ARG	O-C-N	5.07	128.51	122.27
4	4	59	ASP	O-C-N	5.07	129.12	122.68
3	2	115	SER	N-CA-C	5.07	116.76	108.76
2	1	177	THR	O-C-N	5.06	129.32	122.59
2	1	241	ALA	O-C-N	5.06	129.11	122.68
5	3	172	SER	O-C-N	5.06	129.14	123.27
2	1	269	TRP	N-CA-C	5.06	117.85	109.85
3	2	173	ARG	O-C-N	5.06	129.29	123.17
2	1	50	GLY	O-C-N	5.06	128.62	122.60
2	1	142	PHE	O-C-N	5.06	129.15	122.93
2	1	223	ALA	N-CA-C	5.05	118.22	111.75
2	1	273	PRO	N-CA-C	5.05	116.86	110.70
2	1	251	THR	O-C-N	5.05	128.97	123.22
2	1	258	ARG	O-C-N	5.05	129.38	122.82
5	3	61	LYS	O-C-N	5.04	128.79	122.23
2	1	181	PRO	O-C-N	5.04	129.44	122.64
2	1	159	TYR	O-C-N	5.04	128.97	122.93
5	3	221	SER	O-C-N	5.03	129.26	123.17
2	1	155	TYR	O-C-N	5.03	128.94	123.01
3	2	71	TRP	N-CA-C	5.03	116.96	108.96
3	2	194	PRO	O-C-N	5.03	129.43	122.64
2	1	51	ALA	O-C-N	5.03	128.88	123.10
2	1	228	LEU	N-CA-C	5.03	117.59	110.10
2	1	238	GLY	O-C-N	5.03	128.73	122.95
2	1	243	ARG	N-CA-C	5.02	116.71	109.07
3	2	267	THR	N-CA-C	5.02	116.46	108.67
3	2	126	ALA	N-CA-C	5.02	116.83	107.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	230	ALA	O-C-N	5.02	128.94	123.22
5	3	27	GLU	O-C-N	5.02	129.27	122.59
5	3	80	ASP	O-C-N	5.02	128.47	121.64
3	2	16	LEU	O-C-N	5.02	128.94	123.22
3	2	199	ASN	CB-CA-C	-5.02	103.13	111.41
2	1	82	ALA	O-C-N	5.02	129.26	122.59
2	1	89	ILE	O-C-N	5.02	128.78	122.66
2	1	204	ALA	O-C-N	5.01	129.26	122.59
2	1	135	THR	N-CA-C	5.01	116.69	108.52
3	2	102	GLY	O-C-N	5.01	129.22	122.70
3	2	191	PHE	O-C-N	5.01	128.90	122.39
5	3	86	SER	N-CA-C	5.01	117.73	109.76
5	3	227	ASP	O-C-N	5.01	129.09	122.93
3	2	88	ASP	O-C-N	5.01	128.21	122.25
3	2	195	HIS	CA-CB-CG	-5.01	108.79	113.80
4	4	28	THR	O-C-N	5.01	128.93	123.22
3	2	12	ARG	N-CA-C	5.00	117.62	111.82
2	1	97	SER	O-C-N	5.00	129.24	122.59
3	2	209	VAL	O-C-N	5.00	128.47	122.62
5	3	69	ARG	O-C-N	5.00	129.00	123.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	R	141	VAL	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	140	ARG	Peptide
1	R	143	ALA	Peptide
1	R	210	PRO	Peptide
1	R	211	SER	Peptide
1	R	212	SER	Mainchain
1	R	213	GLN	Peptide

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	R	1638	0	1617	248	0
2	1	2222	0	2173	208	0
3	2	2085	0	2000	104	0
4	4	477	0	457	37	0
5	3	1834	0	1815	132	0
6	1	21	0	36	27	0
7	4	15	0	27	1	0
All	All	8292	0	8125	592	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 36.

All (592) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:130:GLN:NE2	2:1:105:PHE:CE1	1.75	1.52
1:R:128:PHE:HE2	2:1:108:TRP:NE1	1.18	1.40
1:R:130:GLN:CG	2:1:105:PHE:O	1.70	1.37
1:R:130:GLN:NE2	2:1:105:PHE:CZ	1.97	1.32
3:2:5:GLU:CG	3:2:7:CYS:HB3	1.58	1.32
1:R:132:SER:OG	2:1:107:VAL:HG11	1.37	1.22
2:1:132:MET:CE	6:1:0:SPH:H81	1.69	1.22
1:R:128:PHE:CE2	2:1:108:TRP:NE1	2.05	1.22
1:R:73:GLY:HA3	5:3:97:HIS:CD2	1.77	1.19
2:1:177:THR:HG21	2:1:182:SER:OG	1.40	1.19
2:1:182:SER:H	5:3:15:THR:CG2	1.58	1.16
3:2:5:GLU:HG2	3:2:7:CYS:HB3	1.19	1.15
1:R:114:ARG:HH12	5:3:59:ALA:HB1	1.03	1.14
1:R:132:SER:OG	2:1:107:VAL:CG1	1.94	1.14
3:2:48:ASN:HB3	3:2:49:PRO:HD3	1.18	1.14
1:R:75:MET:CE	5:3:92:ASP:HA	1.73	1.14
1:R:75:MET:HE2	5:3:92:ASP:HA	1.27	1.14
2:1:182:SER:H	5:3:15:THR:HG21	1.10	1.14
2:1:237:PHE:CE2	6:1:0:SPH:H71	1.82	1.14
3:2:5:GLU:CG	3:2:7:CYS:CB	2.25	1.13
1:R:161:VAL:HB	1:R:163:MET:HB2	1.21	1.13
1:R:43:ASP:HB2	1:R:44:SER:CA	1.79	1.12
1:R:75:MET:HE2	5:3:92:ASP:CA	1.80	1.11
1:R:83:GLY:HA3	2:1:226:ASP:O	1.50	1.11
1:R:114:ARG:NH1	5:3:59:ALA:CB	2.13	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:132:MET:HE1	6:1:0:SPH:H81	1.16	1.10
1:R:130:GLN:HG3	2:1:105:PHE:C	1.76	1.08
1:R:130:GLN:HB2	2:1:106:ALA:HA	1.34	1.08
1:R:162:PRO:HD2	1:R:163:MET:HA	1.30	1.08
1:R:130:GLN:HA	2:1:107:VAL:HB	1.29	1.07
3:2:48:ASN:HB3	3:2:49:PRO:CD	1.86	1.06
1:R:43:ASP:CB	1:R:44:SER:HA	1.85	1.06
1:R:128:PHE:CE1	2:1:114:ASP:OD1	1.76	1.05
1:R:98:ARG:HD3	1:R:104:ARG:HH21	1.21	1.04
5:3:167:VAL:O	5:3:169:PRO:HD3	1.57	1.03
3:2:5:GLU:HG3	3:2:7:CYS:HB3	1.41	1.02
3:2:5:GLU:HG3	3:2:7:CYS:CB	1.90	1.01
1:R:98:ARG:HD3	1:R:104:ARG:NH2	1.75	1.01
1:R:75:MET:CE	5:3:92:ASP:CG	2.33	1.01
1:R:114:ARG:HH12	5:3:59:ALA:CB	1.71	1.00
1:R:54:PRO:HA	1:R:55:ASN:HB2	1.44	1.00
1:R:128:PHE:CE2	2:1:108:TRP:CD1	2.50	1.00
1:R:130:GLN:HG3	2:1:105:PHE:O	0.82	0.99
3:2:37:ARG:O	3:2:211:PRO:HG3	1.64	0.98
1:R:82:GLN:HB2	2:1:228:LEU:H	1.28	0.98
1:R:177:ILE:HD12	1:R:205:LEU:HB2	1.45	0.98
1:R:114:ARG:NH1	5:3:59:ALA:HB1	1.75	0.98
3:2:5:GLU:CD	3:2:7:CYS:H	1.72	0.96
2:1:22:THR:HG22	2:1:24:ARG:H	1.32	0.94
3:2:5:GLU:HG3	3:2:7:CYS:CA	1.99	0.93
1:R:75:MET:HE2	5:3:92:ASP:CB	1.97	0.93
1:R:141:VAL:HG23	1:R:141:VAL:O	1.68	0.93
3:2:5:GLU:OE2	3:2:7:CYS:HB2	1.66	0.93
1:R:132:SER:HB2	2:1:166:VAL:HG11	1.49	0.93
1:R:129:PRO:O	2:1:107:VAL:O	1.87	0.92
1:R:142:LEU:HD23	1:R:172:ARG:HB3	1.52	0.92
1:R:68:ARG:HD2	1:R:76:ALA:HB3	1.52	0.92
1:R:130:GLN:HE21	2:1:105:PHE:HE1	1.04	0.92
1:R:99:LEU:HD23	3:2:142:HIS:NE2	1.85	0.91
5:3:83:LEU:HD12	5:3:83:LEU:O	1.69	0.91
1:R:75:MET:CE	5:3:92:ASP:CA	2.33	0.91
2:1:144:GLU:C	2:1:146:ASN:H	1.79	0.91
2:1:56:VAL:HB	2:1:57:PRO:HD2	1.52	0.90
1:R:128:PHE:CD2	2:1:108:TRP:CD1	2.60	0.89
2:1:132:MET:HE1	6:1:0:SPH:C8	2.01	0.89
1:R:162:PRO:CD	1:R:163:MET:HA	2.03	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:142:LEU:CD2	1:R:172:ARG:HB3	2.03	0.88
1:R:43:ASP:HB2	1:R:44:SER:HA	0.91	0.87
5:3:71:ARG:NH1	5:3:209:ASP:OD2	2.07	0.87
3:2:267:THR:O	3:2:269:PRO:HD3	1.75	0.87
2:1:112:TYR:HE2	6:1:0:SPH:HO3	0.90	0.86
5:3:149:MET:HE2	5:3:150:LEU:CD2	2.06	0.86
3:2:168:THR:CG2	3:2:169:SER:N	2.35	0.86
2:1:144:GLU:O	2:1:146:ASN:N	2.09	0.86
3:2:168:THR:HG22	3:2:169:SER:N	1.90	0.85
1:R:75:MET:HE2	5:3:92:ASP:CG	2.02	0.85
3:2:270:ARG:O	3:2:270:ARG:HG2	1.73	0.85
2:1:182:SER:N	5:3:15:THR:CG2	2.40	0.84
2:1:237:PHE:CE2	6:1:0:SPH:C7	2.61	0.84
3:2:5:GLU:HG3	3:2:7:CYS:N	1.93	0.83
1:R:128:PHE:HE2	2:1:108:TRP:CD1	1.93	0.83
1:R:132:SER:CB	2:1:166:VAL:HG11	2.06	0.83
1:R:73:GLY:HA3	5:3:97:HIS:NE2	1.92	0.83
1:R:83:GLY:HA3	2:1:226:ASP:C	2.04	0.83
1:R:132:SER:HB2	2:1:166:VAL:CG1	2.09	0.83
1:R:128:PHE:HE1	2:1:114:ASP:OD1	1.52	0.82
3:2:34:ALA:HB3	3:2:211:PRO:HD2	1.61	0.82
1:R:130:GLN:HA	2:1:107:VAL:CB	2.10	0.82
2:1:193:ARG:NH1	5:3:8:PRO:HG2	1.94	0.82
1:R:82:GLN:CB	2:1:228:LEU:H	1.92	0.82
1:R:130:GLN:CD	2:1:105:PHE:CE1	2.57	0.82
5:3:232:GLU:OE1	5:3:234:LYS:HG2	1.78	0.81
2:1:182:SER:N	5:3:15:THR:HG21	1.94	0.81
1:R:54:PRO:CA	1:R:55:ASN:HB2	2.11	0.81
3:2:166:ASN:O	3:2:166:ASN:OD1	1.97	0.80
1:R:130:GLN:HG2	2:1:107:VAL:HG23	1.63	0.79
2:1:132:MET:HE2	6:1:0:SPH:H81	1.61	0.79
1:R:82:GLN:CB	2:1:228:LEU:N	2.46	0.79
4:4:14:GLU:HG2	4:4:16:SER:HB2	1.63	0.79
2:1:158:MET:SD	2:1:177:THR:HG23	2.22	0.79
1:R:75:MET:CG	5:3:91:SER:O	2.30	0.79
1:R:141:VAL:O	1:R:141:VAL:CG2	2.30	0.79
5:3:149:MET:HE2	5:3:150:LEU:HG	1.63	0.79
1:R:130:GLN:CB	2:1:106:ALA:HA	2.14	0.78
2:1:219:ASP:O	2:1:219:ASP:OD2	2.01	0.78
1:R:75:MET:HG3	5:3:91:SER:O	1.83	0.78
5:3:149:MET:HE2	5:3:150:LEU:CG	2.13	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:215:ASP:O	1:R:238:LEU:HB3	1.85	0.77
2:1:237:PHE:CZ	6:1:0:SPH:H71	2.20	0.77
1:R:143:ALA:O	1:R:225:HIS:NE2	2.17	0.77
2:1:27:LEU:HB3	2:1:28:PRO:HD2	1.66	0.77
1:R:128:PHE:HD2	2:1:108:TRP:HD1	1.33	0.76
4:4:14:GLU:C	4:4:16:SER:H	1.94	0.76
1:R:128:PHE:CD2	2:1:108:TRP:HD1	2.01	0.76
2:1:132:MET:CE	6:1:0:SPH:C8	2.58	0.76
1:R:130:GLN:CA	2:1:107:VAL:H	2.00	0.75
5:3:7:THR:HB	5:3:8:PRO:HD2	1.67	0.75
1:R:63:GLN:HG2	1:R:81:THR:HA	1.69	0.75
1:R:99:LEU:HG	2:1:226:ASP:OD1	1.87	0.75
5:3:149:MET:CE	5:3:150:LEU:CD2	2.65	0.74
3:2:242:GLU:OE2	3:2:242:GLU:N	2.19	0.74
1:R:140:ARG:O	1:R:141:VAL:HB	1.87	0.74
1:R:173:PRO:HG2	1:R:225:HIS:HE1	1.52	0.74
5:3:71:ARG:HH12	5:3:209:ASP:CG	1.95	0.74
2:1:109:LYS:HA	2:1:239:ILE:HG22	1.71	0.73
4:4:14:GLU:HG2	4:4:16:SER:H	1.50	0.73
4:4:14:GLU:HG2	4:4:16:SER:N	2.03	0.73
4:4:14:GLU:CG	4:4:16:SER:HB2	2.19	0.73
1:R:142:LEU:O	1:R:143:ALA:HB2	1.86	0.73
3:2:5:GLU:HG2	3:2:7:CYS:CB	2.04	0.73
2:1:182:SER:H	5:3:15:THR:HG22	1.52	0.72
5:3:71:ARG:HB2	5:3:71:ARG:CZ	2.19	0.72
5:3:74:ASP:HA	5:3:198:ILE:O	1.89	0.72
1:R:80:GLN:HG2	1:R:98:ARG:HG2	1.71	0.72
1:R:40:PHE:CZ	1:R:144:LYS:HB3	2.24	0.72
3:2:5:GLU:OE1	3:2:5:GLU:CA	2.38	0.72
3:2:168:THR:HG22	3:2:169:SER:H	1.54	0.71
1:R:73:GLY:CA	5:3:97:HIS:NE2	2.52	0.71
2:1:45:THR:OG1	4:4:67:MET:HE2	1.90	0.71
5:3:210:ILE:O	5:3:210:ILE:HG13	1.89	0.71
3:2:5:GLU:CG	3:2:7:CYS:H	2.02	0.71
3:2:38:TRP:CD1	3:2:39:PRO:HD2	2.26	0.71
5:3:149:MET:HE2	5:3:150:LEU:HD23	1.70	0.71
1:R:85:SER:HB2	2:1:214:LYS:HZ1	1.54	0.71
1:R:128:PHE:O	2:1:108:TRP:HA	1.90	0.71
2:1:22:THR:HG22	2:1:24:ARG:N	2.03	0.71
1:R:128:PHE:HB3	1:R:129:PRO:HD3	1.70	0.71
3:2:5:GLU:OE1	3:2:5:GLU:HA	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:10:VAL:CG2	4:4:25:ILE:HD12	2.22	0.70
1:R:124:LEU:HA	1:R:134:SER:HB2	1.74	0.70
4:4:14:GLU:CD	4:4:16:SER:HB2	2.15	0.70
1:R:41:LEU:CB	1:R:142:LEU:O	2.40	0.70
1:R:104:ARG:HD2	1:R:106:ALA:HB2	1.74	0.70
5:3:232:GLU:OE1	5:3:234:LYS:CG	2.39	0.69
1:R:73:GLY:CA	5:3:97:HIS:CD2	2.69	0.69
3:2:34:ALA:HB3	3:2:211:PRO:CD	2.22	0.69
4:4:10:VAL:HG12	4:4:13:HIS:CE1	2.27	0.69
1:R:68:ARG:HD2	1:R:76:ALA:CB	2.21	0.69
1:R:165:ARG:HG3	1:R:206:TRP:HB3	1.73	0.69
5:3:195:GLN:OE1	5:3:195:GLN:HA	1.92	0.69
5:3:234:LYS:O	5:3:235:ALA:HB3	1.91	0.69
1:R:132:SER:CB	2:1:107:VAL:HG11	2.23	0.69
4:4:42:SER:OG	4:4:44:GLN:HB2	1.92	0.69
4:4:65:ALA:HB1	4:4:66:PRO:HD2	1.73	0.69
5:3:196:THR:O	5:3:197:ARG:HB3	1.93	0.68
1:R:75:MET:O	5:3:93:PRO:HG3	1.93	0.68
5:3:97:HIS:CE1	5:3:230:HIS:ND1	2.60	0.68
2:1:103:LYS:HD3	2:1:170:TRP:CD2	2.27	0.68
3:2:12:ARG:HA	3:2:28:ALA:O	1.93	0.68
2:1:112:TYR:HE2	6:1:0:SPH:O3	1.71	0.68
4:4:61:LEU:O	4:4:61:LEU:HG	1.93	0.68
3:2:5:GLU:OE1	3:2:6:ALA:N	2.27	0.68
5:3:149:MET:CE	5:3:150:LEU:HD23	2.24	0.68
1:R:75:MET:CG	5:3:92:ASP:HA	2.24	0.67
1:R:99:LEU:O	3:2:142:HIS:CD2	2.47	0.67
5:3:234:LYS:O	5:3:235:ALA:CB	2.40	0.67
1:R:130:GLN:CB	2:1:107:VAL:H	2.08	0.67
5:3:97:HIS:CE1	5:3:230:HIS:CE1	2.83	0.67
1:R:98:ARG:HG3	1:R:99:LEU:H	1.60	0.67
2:1:132:MET:HE1	6:1:0:SPH:H101	1.75	0.66
1:R:40:PHE:CE1	1:R:143:ALA:HB1	2.31	0.66
3:2:5:GLU:CG	3:2:7:CYS:N	2.58	0.66
1:R:173:PRO:HG2	1:R:225:HIS:CE1	2.30	0.66
1:R:75:MET:HE1	5:3:92:ASP:CG	2.20	0.65
1:R:130:GLN:HA	2:1:107:VAL:N	2.11	0.65
1:R:59:THR:HG23	1:R:127:THR:HG23	1.77	0.65
1:R:142:LEU:O	1:R:143:ALA:CB	2.44	0.65
3:2:110:VAL:HG22	3:2:251:LEU:HD12	1.77	0.65
2:1:177:THR:CG2	2:1:182:SER:OG	2.33	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:240:VAL:O	1:R:241:TYR:HD2	1.79	0.65
2:1:132:MET:HE1	6:1:0:SPH:C10	2.27	0.65
2:1:22:THR:HB	2:1:25:ASP:OD1	1.97	0.64
3:2:5:GLU:CD	3:2:7:CYS:HB2	2.22	0.64
3:2:264:ARG:HD3	5:3:136:PRO:O	1.98	0.64
3:2:38:TRP:CG	3:2:39:PRO:HD2	2.32	0.64
1:R:157:THR:OG1	1:R:158:GLY:HA2	1.97	0.64
2:1:90:MET:CE	2:1:240:LEU:O	2.46	0.64
2:1:176:GLN:HE22	5:3:233:GLN:NE2	1.95	0.64
1:R:159:GLU:N	1:R:160:PRO:HD3	2.13	0.64
2:1:182:SER:N	5:3:15:THR:HG22	2.11	0.64
1:R:215:ASP:O	1:R:238:LEU:CB	2.45	0.64
5:3:83:LEU:HD12	5:3:83:LEU:C	2.23	0.63
1:R:83:GLY:H	2:1:227:SER:HA	1.62	0.63
2:1:159:TYR:HB2	6:1:0:SPH:H162	1.79	0.63
2:1:249:ASN:CG	2:1:250:PRO:HD2	2.22	0.63
2:1:159:TYR:O	2:1:161:PRO:HD3	1.98	0.63
1:R:130:GLN:CA	2:1:107:VAL:HB	2.17	0.63
2:1:237:PHE:CZ	6:1:0:SPH:H4	2.33	0.63
3:2:5:GLU:CD	3:2:7:CYS:CB	2.71	0.63
3:2:143:THR:HG23	3:2:173:ARG:HA	1.79	0.63
1:R:40:PHE:HZ	1:R:144:LYS:HB3	1.64	0.62
4:4:60:VAL:HG12	4:4:60:VAL:O	1.98	0.62
4:4:57:ILE:HD11	4:4:61:LEU:HB3	1.81	0.62
5:3:85:LEU:CD2	5:3:86:SER:N	2.62	0.62
1:R:215:ASP:HB3	1:R:216:GLY:CA	2.30	0.62
5:3:77:HIS:HE1	5:3:194:TYR:O	1.83	0.62
5:3:85:LEU:HD22	5:3:86:SER:N	2.13	0.62
1:R:149:ALA:HB2	1:R:234:LEU:HD12	1.81	0.62
3:2:5:GLU:CD	3:2:7:CYS:N	2.53	0.62
2:1:103:LYS:HD3	2:1:170:TRP:CG	2.34	0.61
2:1:213:SER:O	5:3:183:SER:HB3	2.00	0.61
2:1:237:PHE:CE2	6:1:0:SPH:C4	2.83	0.61
1:R:66:TRP:HB2	1:R:78:PHE:HB3	1.81	0.61
2:1:90:MET:HE1	2:1:240:LEU:O	2.00	0.61
3:2:5:GLU:C	3:2:7:CYS:N	2.57	0.61
2:1:128:SER:HB3	2:1:207:HIS:CE1	2.35	0.61
3:2:63:PHE:CD1	3:2:254:ALA:HB2	2.36	0.61
1:R:114:ARG:NH1	5:3:59:ALA:HB3	2.10	0.61
1:R:131:GLY:H	2:1:107:VAL:HB	1.66	0.61
1:R:139:LEU:HD22	1:R:140:ARG:HG3	1.80	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:218:LYS:C	2:1:220:GLN:H	2.08	0.61
2:1:218:LYS:O	2:1:220:GLN:N	2.34	0.61
4:4:42:SER:C	4:4:44:GLN:H	2.07	0.60
4:4:55:GLU:N	4:4:56:PRO:HD3	2.15	0.60
5:3:75:LYS:HB2	5:3:76:PRO:HD2	1.81	0.60
2:1:92:VAL:HG12	2:1:106:ALA:H	1.66	0.60
1:R:82:GLN:HB3	2:1:228:LEU:N	2.15	0.60
1:R:85:SER:HB2	2:1:214:LYS:NZ	2.17	0.60
1:R:151:VAL:HA	1:R:163:MET:O	2.01	0.60
3:2:267:THR:HG22	3:2:269:PRO:HD3	1.84	0.60
1:R:86:TYR:CE1	2:1:224:LEU:CD1	2.85	0.59
1:R:162:PRO:HD3	1:R:209:VAL:O	2.01	0.59
2:1:133:GLU:O	2:1:133:GLU:HG2	2.01	0.59
1:R:181:SER:HB3	1:R:219:VAL:HG23	1.85	0.59
4:4:10:VAL:HG21	4:4:25:ILE:HD12	1.82	0.59
1:R:130:GLN:HA	2:1:107:VAL:H	1.63	0.59
1:R:130:GLN:CD	2:1:105:PHE:O	2.45	0.59
5:3:208:MET:HE2	5:3:208:MET:H	1.67	0.59
1:R:132:SER:H	2:1:107:VAL:HG11	1.66	0.59
3:2:239:PHE:CD2	3:2:240:ALA:N	2.71	0.59
1:R:162:PRO:HD3	1:R:208:LEU:H	1.67	0.59
1:R:83:GLY:N	2:1:227:SER:HA	2.18	0.59
3:2:264:ARG:NH1	5:3:137:PRO:O	2.35	0.59
1:R:215:ASP:HB3	1:R:216:GLY:HA2	1.85	0.58
1:R:143:ALA:O	1:R:225:HIS:CE1	2.56	0.58
1:R:41:LEU:HB2	1:R:142:LEU:O	2.03	0.58
1:R:188:GLN:HB3	1:R:208:LEU:O	2.04	0.58
2:1:104:LEU:O	2:1:104:LEU:HG	2.02	0.58
5:3:87:LEU:HD13	5:3:190:ILE:HD11	1.86	0.58
5:3:88:SER:HB3	5:3:91:SER:OG	2.03	0.58
1:R:68:ARG:HG2	1:R:70:GLY:HA3	1.85	0.58
1:R:128:PHE:HE2	2:1:108:TRP:HE1	0.62	0.58
1:R:214:VAL:HG22	1:R:215:ASP:H	1.67	0.58
5:3:77:HIS:CE1	5:3:194:TYR:O	2.57	0.58
2:1:176:GLN:HE22	5:3:233:GLN:HE21	1.50	0.57
1:R:75:MET:CE	5:3:92:ASP:CB	2.70	0.57
4:4:10:VAL:CG1	4:4:13:HIS:CE1	2.87	0.57
1:R:99:LEU:CG	2:1:226:ASP:OD1	2.53	0.57
1:R:85:SER:CB	2:1:214:LYS:HZ1	2.18	0.57
1:R:130:GLN:CB	2:1:107:VAL:N	2.68	0.57
3:2:25:THR:HG23	3:2:25:THR:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:40:PHE:HZ	1:R:144:LYS:HD3	1.70	0.57
1:R:65:THR:HB	1:R:124:LEU:HG	1.86	0.56
1:R:151:VAL:HG21	1:R:238:LEU:HA	1.86	0.56
2:1:176:GLN:NE2	5:3:233:GLN:NE2	2.53	0.56
1:R:75:MET:HG2	5:3:91:SER:O	2.06	0.56
1:R:75:MET:HG2	5:3:92:ASP:HA	1.87	0.56
1:R:98:ARG:C	1:R:100:GLY:H	2.13	0.56
1:R:130:GLN:HA	2:1:107:VAL:CA	2.35	0.56
3:2:195:HIS:HA	3:2:208:LEU:HD21	1.87	0.56
5:3:178:GLN:C	5:3:180:ILE:H	2.14	0.56
1:R:82:GLN:HB2	2:1:228:LEU:N	2.04	0.56
1:R:131:GLY:HA2	1:R:133:ARG:HD3	1.86	0.56
1:R:117:ASP:HB2	1:R:141:VAL:CG1	2.36	0.56
1:R:130:GLN:HG2	2:1:107:VAL:N	2.21	0.56
5:3:34:ILE:O	5:3:36:ILE:N	2.39	0.56
2:1:216:PRO:HG2	3:2:145:TYR:CD1	2.41	0.56
5:3:218:ASN:HD22	5:3:219:ASP:N	2.03	0.56
1:R:130:GLN:CB	2:1:105:PHE:O	2.52	0.55
1:R:41:LEU:HB3	1:R:142:LEU:O	2.05	0.55
1:R:130:GLN:CA	2:1:107:VAL:N	2.69	0.55
1:R:163:MET:HE3	1:R:206:TRP:HB2	1.86	0.55
1:R:172:ARG:HA	1:R:201:THR:H	1.70	0.55
1:R:130:GLN:HE21	2:1:107:VAL:HG23	1.71	0.55
2:1:218:LYS:C	2:1:220:GLN:N	2.65	0.55
1:R:42:GLY:N	1:R:43:ASP:HA	2.22	0.55
5:3:204:THR:CG2	5:3:205:PRO:HD2	2.36	0.54
1:R:120:SER:HB3	1:R:138:TRP:CG	2.42	0.54
2:1:261:LEU:C	2:1:261:LEU:HD23	2.31	0.54
3:2:166:ASN:OD1	3:2:168:THR:HG22	2.06	0.54
5:3:73:SER:HA	5:3:208:MET:CE	2.38	0.54
1:R:99:LEU:CD2	3:2:142:HIS:NE2	2.66	0.54
4:4:42:SER:HG	4:4:44:GLN:HB2	1.71	0.54
1:R:41:LEU:HB2	1:R:141:VAL:O	2.07	0.54
2:1:237:PHE:CD2	6:1:0:SPH:C7	2.91	0.54
1:R:41:LEU:HD22	1:R:42:GLY:H	1.72	0.54
1:R:147:ASN:ND2	1:R:223:VAL:HG21	2.22	0.54
3:2:5:GLU:CG	3:2:7:CYS:HB2	2.34	0.54
3:2:60:ALA:O	3:2:255:PRO:HG2	2.08	0.54
1:R:80:GLN:CG	1:R:98:ARG:HG2	2.38	0.53
1:R:152:GLN:O	1:R:163:MET:HB3	2.08	0.53
3:2:256:MET:O	3:2:258:CYS:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:10:VAL:HG11	4:4:13:HIS:ND1	2.23	0.53
5:3:55:PHE:HE1	5:3:212:GLY:HA3	1.73	0.53
5:3:83:LEU:O	5:3:83:LEU:CD1	2.50	0.53
5:3:104:LEU:O	5:3:179:THR:HG21	2.08	0.53
1:R:36:GLN:NE2	1:R:137:ILE:HG13	2.23	0.53
3:2:110:VAL:HG22	3:2:251:LEU:CD1	2.39	0.53
5:3:107:TYR:O	5:3:179:THR:HG21	2.08	0.53
2:1:193:ARG:CZ	5:3:8:PRO:HG2	2.38	0.53
1:R:49:CYS:HB2	1:R:66:TRP:HZ2	1.73	0.53
1:R:117:ASP:CB	1:R:141:VAL:HG13	2.38	0.53
1:R:161:VAL:HB	1:R:163:MET:CB	2.14	0.53
3:2:267:THR:C	3:2:269:PRO:HD3	2.33	0.53
2:1:280:TYR:HB3	2:1:285:ASP:O	2.09	0.53
1:R:40:PHE:CZ	1:R:144:LYS:CB	2.92	0.52
1:R:129:PRO:C	2:1:107:VAL:O	2.52	0.52
4:4:14:GLU:HG2	4:4:16:SER:CB	2.37	0.52
2:1:112:TYR:CD2	6:1:0:SPH:H5	2.43	0.52
1:R:127:THR:HG22	1:R:129:PRO:HD2	1.91	0.52
2:1:38:SER:OG	2:1:39:LYS:N	2.41	0.52
2:1:45:THR:OG1	2:1:46:ALA:N	2.38	0.52
2:1:81:PHE:C	2:1:83:ARG:H	2.17	0.52
2:1:105:PHE:O	2:1:105:PHE:CD1	2.62	0.52
2:1:183:ILE:HD11	2:1:194:ILE:HG12	1.91	0.52
2:1:218:LYS:HD3	3:2:268:LEU:HB3	1.91	0.52
3:2:98:TYR:CE1	3:2:266:ILE:HD12	2.45	0.52
3:2:122:LEU:HB2	3:2:198:ILE:HB	1.90	0.52
5:3:85:LEU:CD2	5:3:85:LEU:C	2.82	0.52
1:R:80:GLN:O	1:R:98:ARG:NH2	2.42	0.52
4:4:14:GLU:C	4:4:16:SER:N	2.64	0.52
5:3:13:TYR:C	5:3:13:TYR:CD2	2.86	0.52
1:R:73:GLY:N	1:R:74:SER:HA	2.25	0.51
1:R:134:SER:O	2:1:168:GLU:HG2	2.10	0.51
3:2:136:SER:OG	3:2:139:THR:HG22	2.10	0.51
1:R:117:ASP:CB	1:R:141:VAL:CG1	2.88	0.51
2:1:291:LEU:C	2:1:293:PRO:HD3	2.35	0.51
5:3:73:SER:C	5:3:75:LYS:H	2.19	0.51
2:1:209:TYR:O	2:1:230:GLY:HA2	2.10	0.51
4:4:13:HIS:CD2	4:4:13:HIS:H	2.27	0.51
3:2:219:ASP:CG	3:2:220:SER:H	2.15	0.51
2:1:112:TYR:HD2	6:1:0:SPH:H5	1.76	0.51
2:1:169:LYS:C	2:1:171:ASP:H	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:85:LEU:HD22	5:3:85:LEU:C	2.36	0.51
1:R:41:LEU:N	1:R:142:LEU:O	2.43	0.51
2:1:95:PRO:HD2	2:1:103:LYS:HG3	1.93	0.51
2:1:158:MET:SD	2:1:177:THR:CG2	2.96	0.51
3:2:71:TRP:CD1	3:2:71:TRP:C	2.88	0.51
5:3:89:PRO:HB2	5:3:104:LEU:CD2	2.41	0.51
3:2:13:VAL:HA	3:2:25:THR:O	2.10	0.51
1:R:98:ARG:CG	1:R:99:LEU:H	2.24	0.51
4:4:10:VAL:CG1	4:4:13:HIS:ND1	2.74	0.50
1:R:187:PRO:O	1:R:188:GLN:HG3	2.11	0.50
3:2:198:ILE:O	3:2:198:ILE:HG22	2.11	0.50
4:4:55:GLU:N	4:4:56:PRO:CD	2.74	0.50
2:1:22:THR:CG2	2:1:24:ARG:H	2.16	0.50
5:3:14:LEU:O	5:3:16:ALA:N	2.44	0.50
5:3:129:LYS:O	5:3:195:GLN:HB3	2.12	0.50
1:R:169:THR:HA	1:R:202:VAL:HG23	1.93	0.50
2:1:169:LYS:C	2:1:171:ASP:N	2.69	0.50
2:1:237:PHE:CD2	6:1:0:SPH:H71	2.40	0.50
4:4:10:VAL:HG22	4:4:25:ILE:HD12	1.93	0.50
4:4:24:THR:HG23	4:4:24:THR:O	2.10	0.50
5:3:156:TRP:CD1	5:3:156:TRP:C	2.89	0.50
1:R:241:TYR:HA	1:R:242:TYR:C	2.37	0.50
1:R:93:GLU:HB3	1:R:109:ARG:HB3	1.92	0.50
3:2:239:PHE:O	3:2:240:ALA:C	2.55	0.49
3:2:256:MET:O	3:2:257:CYS:C	2.55	0.49
1:R:130:GLN:CG	2:1:105:PHE:CD1	2.95	0.49
2:1:48:GLU:HA	3:2:197:ILE:HB	1.94	0.49
1:R:158:GLY:HA3	1:R:159:GLU:HB3	1.94	0.49
2:1:159:TYR:CB	6:1:0:SPH:H162	2.42	0.49
3:2:5:GLU:C	3:2:7:CYS:H	2.18	0.49
1:R:85:SER:CB	2:1:214:LYS:NZ	2.75	0.49
2:1:144:GLU:C	2:1:146:ASN:N	2.50	0.49
2:1:233:SER:C	2:1:235:ASN:N	2.69	0.49
5:3:87:LEU:HD13	5:3:190:ILE:CD1	2.43	0.49
1:R:102:GLU:HG3	1:R:104:ARG:NH1	2.28	0.49
1:R:145:PRO:HA	1:R:170:GLY:O	2.12	0.49
3:2:5:GLU:OE1	3:2:5:GLU:C	2.55	0.49
5:3:89:PRO:HB2	5:3:104:LEU:HD23	1.95	0.49
1:R:155:GLN:NE2	1:R:212:SER:H	2.10	0.48
2:1:30:THR:HB	2:1:66:VAL:HB	1.95	0.48
5:3:155:ILE:HG22	5:3:155:ILE:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:53:ASN:C	2:1:55:LEU:H	2.22	0.48
5:3:183:SER:O	5:3:186:GLU:HG2	2.13	0.48
1:R:86:TYR:CE1	2:1:224:LEU:HD12	2.47	0.48
3:2:213:VAL:O	3:2:214:ASN:HB2	2.12	0.48
5:3:166:MET:HE3	5:3:168:VAL:CG2	2.43	0.48
1:R:54:PRO:CA	1:R:55:ASN:CB	2.87	0.48
3:2:110:VAL:O	3:2:205:CYS:HB2	2.13	0.48
3:2:256:MET:C	3:2:258:CYS:N	2.71	0.48
1:R:60:HIS:O	1:R:128:PHE:N	2.26	0.48
2:1:169:LYS:O	2:1:171:ASP:N	2.46	0.48
4:4:42:SER:C	4:4:44:GLN:N	2.72	0.48
2:1:130:PHE:O	2:1:130:PHE:CD1	2.66	0.48
3:2:66:LEU:N	3:2:66:LEU:HD23	2.29	0.48
1:R:130:GLN:HB2	2:1:107:VAL:H	1.78	0.48
1:R:128:PHE:HB3	1:R:129:PRO:CD	2.43	0.47
5:3:109:HIS:HB2	5:3:223:ARG:HG2	1.95	0.47
5:3:156:TRP:CD1	5:3:164:CYS:HB2	2.49	0.47
1:R:86:TYR:CE1	2:1:224:LEU:HD11	2.48	0.47
2:1:78:GLU:OE1	2:1:265:HIS:N	2.47	0.47
2:1:237:PHE:CZ	6:1:0:SPH:C4	2.96	0.47
5:3:74:ASP:CG	5:3:206:ARG:HE	2.22	0.47
2:1:105:PHE:O	2:1:105:PHE:CG	2.68	0.47
2:1:105:PHE:C	2:1:105:PHE:CD1	2.91	0.47
1:R:180:HIS:HA	1:R:186:MET:HG3	1.96	0.47
2:1:103:LYS:NZ	2:1:246:ASN:O	2.47	0.47
3:2:76:ARG:HB2	3:2:157:PHE:O	2.14	0.47
1:R:98:ARG:CD	1:R:104:ARG:NH2	2.64	0.47
2:1:237:PHE:HE2	6:1:0:SPH:C4	2.26	0.47
1:R:75:MET:CE	5:3:92:ASP:OD2	2.63	0.47
2:1:90:MET:CE	2:1:242:VAL:HG23	2.45	0.47
3:2:48:ASN:CB	3:2:49:PRO:CD	2.65	0.47
5:3:14:LEU:O	5:3:14:LEU:HG	2.13	0.47
5:3:233:GLN:O	5:3:235:ALA:N	2.47	0.47
1:R:98:ARG:O	1:R:99:LEU:HD22	2.15	0.47
1:R:179:TRP:CZ3	1:R:219:VAL:HG22	2.49	0.47
2:1:233:SER:O	2:1:235:ASN:N	2.48	0.47
1:R:99:LEU:O	3:2:142:HIS:HD2	1.94	0.47
1:R:186:MET:O	1:R:188:GLN:N	2.48	0.47
3:2:97:TYR:CE1	3:2:269:PRO:HG3	2.50	0.47
5:3:56:ASP:OD1	5:3:61:LYS:HE3	2.14	0.47
1:R:161:VAL:HG12	1:R:208:LEU:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:224:GLU:O	1:R:225:HIS:CB	2.62	0.47
1:R:38:PRO:HA	1:R:39:GLY:HA3	1.66	0.46
4:4:14:GLU:O	4:4:16:SER:N	2.48	0.46
1:R:75:MET:HG2	5:3:91:SER:C	2.41	0.46
1:R:152:GLN:HB2	1:R:153:LYS:HA	1.97	0.46
2:1:124:PHE:CE1	2:1:274:PRO:HG3	2.50	0.46
2:1:184:PHE:HB2	5:3:13:TYR:HB3	1.97	0.46
3:2:214:ASN:OD1	3:2:215:SER:N	2.48	0.46
1:R:170:GLY:HA2	1:R:200:VAL:HG13	1.96	0.46
3:2:54:THR:O	3:2:56:PRO:HD3	2.16	0.46
5:3:233:GLN:O	5:3:234:LYS:C	2.59	0.46
1:R:75:MET:SD	5:3:92:ASP:HA	2.52	0.46
1:R:130:GLN:CG	2:1:106:ALA:HA	2.45	0.46
1:R:132:SER:HB2	2:1:166:VAL:HG13	1.97	0.46
3:2:71:TRP:CD1	3:2:72:THR:N	2.84	0.46
5:3:85:LEU:HD23	5:3:86:SER:N	2.31	0.46
1:R:117:ASP:HB2	1:R:141:VAL:HG13	1.96	0.46
7:4:1:MYR:H71	7:4:1:MYR:H101	1.66	0.46
1:R:40:PHE:CZ	1:R:144:LYS:HD3	2.50	0.46
1:R:132:SER:N	2:1:107:VAL:HG11	2.31	0.46
1:R:133:ARG:HB2	2:1:167:PRO:O	2.16	0.46
2:1:93:ASP:OD2	2:1:93:ASP:C	2.58	0.46
3:2:83:PRO:HG3	3:2:221:MET:HE2	1.97	0.46
1:R:117:ASP:HB3	1:R:141:VAL:HG13	1.98	0.46
1:R:133:ARG:HG3	2:1:168:GLU:HA	1.97	0.46
1:R:157:THR:OG1	1:R:158:GLY:CA	2.64	0.46
5:3:231:ILE:HG13	5:3:232:GLU:N	2.30	0.46
1:R:130:GLN:CG	2:1:107:VAL:N	2.79	0.45
2:1:45:THR:HG1	4:4:67:MET:HE2	1.79	0.45
2:1:22:THR:HB	2:1:25:ASP:CG	2.41	0.45
2:1:123:GLU:C	2:1:125:PHE:H	2.22	0.45
1:R:188:GLN:O	1:R:207:ILE:HG22	2.16	0.45
1:R:240:VAL:O	1:R:241:TYR:CD2	2.64	0.45
5:3:98:THR:O	5:3:99:MET:C	2.59	0.45
2:1:159:TYR:CG	6:1:0:SPH:H142	2.51	0.45
4:4:49:ASP:OD1	4:4:51:SER:HB2	2.17	0.45
2:1:217:LEU:O	2:1:218:LYS:C	2.59	0.45
5:3:87:LEU:HG	5:3:87:LEU:O	2.17	0.45
1:R:99:LEU:HD23	3:2:142:HIS:CE1	2.49	0.45
2:1:128:SER:HB3	2:1:207:HIS:NE2	2.31	0.45
1:R:130:GLN:HG3	2:1:105:PHE:CD1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:131:GLY:N	2:1:107:VAL:HB	2.28	0.45
2:1:132:MET:HE2	6:1:0:SPH:C8	2.40	0.45
2:1:235:ASN:O	2:1:236:ASP:C	2.60	0.45
5:3:166:MET:HE3	5:3:168:VAL:HG22	1.98	0.45
1:R:172:ARG:O	1:R:174:PRO:HD3	2.17	0.44
2:1:27:LEU:HB3	2:1:28:PRO:CD	2.40	0.44
5:3:62:LYS:O	5:3:64:THR:HG23	2.17	0.44
1:R:130:GLN:HG2	2:1:106:ALA:C	2.42	0.44
1:R:130:GLN:CD	2:1:105:PHE:CZ	2.83	0.44
2:1:237:PHE:HZ	6:1:0:SPH:H4	1.77	0.44
1:R:142:LEU:HB3	1:R:143:ALA:H	1.49	0.44
3:2:219:ASP:OD1	3:2:220:SER:N	2.37	0.44
5:3:204:THR:HG23	5:3:205:PRO:HD2	2.00	0.44
1:R:104:ARG:HD3	1:R:104:ARG:HA	1.57	0.44
1:R:130:GLN:HE22	1:R:133:ARG:HD2	1.82	0.44
2:1:107:VAL:O	2:1:107:VAL:HG12	2.16	0.44
2:1:161:PRO:HG2	5:3:226:ARG:HB2	1.98	0.43
2:1:286:TYR:OH	3:2:175:CYS:O	2.33	0.43
3:2:29:ALA:HA	4:4:68:LEU:HD21	2.00	0.43
1:R:31:VAL:HG12	1:R:51:LEU:HD11	1.98	0.43
1:R:41:LEU:H	1:R:143:ALA:HB2	1.83	0.43
1:R:82:GLN:O	1:R:98:ARG:HG3	2.18	0.43
1:R:162:PRO:HB2	1:R:238:LEU:HG	2.00	0.43
3:2:158:THR:O	3:2:177:VAL:HA	2.18	0.43
5:3:14:LEU:C	5:3:16:ALA:N	2.76	0.43
5:3:195:GLN:OE1	5:3:195:GLN:CA	2.64	0.43
5:3:51:THR:HG21	5:3:99:MET:H	1.82	0.43
5:3:218:ASN:HD22	5:3:219:ASP:H	1.67	0.43
1:R:65:THR:HA	1:R:78:PHE:O	2.18	0.43
4:4:55:GLU:C	4:4:57:ILE:H	2.26	0.43
1:R:69:HIS:N	1:R:70:GLY:HA3	2.33	0.43
2:1:56:VAL:HB	2:1:57:PRO:CD	2.36	0.43
2:1:233:SER:O	2:1:234:LEU:C	2.61	0.43
2:1:234:LEU:HD23	2:1:234:LEU:HA	1.87	0.43
3:2:166:ASN:O	3:2:168:THR:N	2.51	0.43
5:3:190:ILE:O	5:3:190:ILE:HG22	2.18	0.43
1:R:207:ILE:HA	1:R:208:LEU:HB3	2.00	0.43
2:1:123:GLU:C	2:1:125:PHE:N	2.77	0.43
3:2:5:GLU:HG3	3:2:8:GLY:N	2.34	0.43
1:R:31:VAL:HG11	1:R:134:SER:HA	2.01	0.43
2:1:38:SER:HG	2:1:40:GLU:H	1.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:56:VAL:O	2:1:57:PRO:C	2.62	0.43
2:1:176:GLN:NE2	5:3:233:GLN:HE21	2.15	0.43
2:1:219:ASP:OD2	2:1:219:ASP:C	2.62	0.43
3:2:5:GLU:HG3	3:2:7:CYS:C	2.44	0.43
3:2:107:THR:O	3:2:107:THR:HG22	2.16	0.43
3:2:135:ASP:OD2	3:2:171:ALA:HB3	2.19	0.43
5:3:149:MET:O	5:3:149:MET:HG2	2.02	0.43
1:R:168:SER:HB3	1:R:203:THR:HG23	2.01	0.42
1:R:177:ILE:HG22	1:R:223:VAL:HG22	2.00	0.42
2:1:81:PHE:O	2:1:83:ARG:N	2.34	0.42
2:1:273:PRO:HB3	3:2:189:ASN:HB2	2.01	0.42
3:2:168:THR:HG23	3:2:169:SER:N	2.26	0.42
3:2:219:ASP:CG	3:2:220:SER:N	2.76	0.42
1:R:114:ARG:HH11	5:3:59:ALA:CB	2.18	0.42
2:1:78:GLU:O	2:1:82:ALA:N	2.52	0.42
5:3:113:SER:O	5:3:217:CYS:HB2	2.19	0.42
5:3:170:TRP:O	5:3:170:TRP:CG	2.71	0.42
1:R:144:LYS:HA	1:R:145:PRO:HD3	1.89	0.42
3:2:104:SER:HB3	3:2:221:MET:HE1	2.01	0.42
5:3:233:GLN:O	5:3:233:GLN:HG2	2.19	0.42
5:3:10:SER:O	5:3:11:ASN:HB2	2.19	0.42
1:R:114:ARG:NH1	5:3:59:ALA:HB2	2.24	0.42
1:R:142:LEU:HD21	1:R:172:ARG:HB3	1.97	0.42
2:1:177:THR:HG22	2:1:180:ASN:HB2	2.01	0.42
3:2:5:GLU:O	3:2:7:CYS:N	2.53	0.42
5:3:196:THR:O	5:3:197:ARG:CB	2.63	0.42
4:4:61:LEU:O	4:4:61:LEU:CG	2.62	0.42
1:R:159:GLU:H	1:R:160:PRO:HD3	1.82	0.42
2:1:37:HIS:CD2	2:1:37:HIS:O	2.73	0.42
2:1:98:THR:O	2:1:99:THR:C	2.62	0.42
3:2:57:ASP:CG	3:2:58:VAL:H	2.28	0.42
1:R:79:HIS:CD2	2:1:234:LEU:HD12	2.54	0.42
1:R:133:ARG:HB2	2:1:168:GLU:HA	2.02	0.42
1:R:221:CYS:HB3	1:R:234:LEU:HG	2.02	0.42
5:3:14:LEU:HB3	5:3:17:ASP:HB3	2.02	0.42
3:2:5:GLU:CD	3:2:5:GLU:C	2.87	0.42
3:2:198:ILE:HD13	3:2:205:CYS:HA	2.01	0.42
2:1:24:ARG:O	2:1:24:ARG:HG3	2.20	0.41
2:1:155:TYR:N	2:1:155:TYR:CD2	2.86	0.41
2:1:249:ASN:O	2:1:250:PRO:C	2.63	0.41
3:2:71:TRP:CE2	3:2:237:LEU:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:59:ASP:O	4:4:60:VAL:C	2.63	0.41
2:1:237:PHE:CG	6:1:0:SPH:H92	2.55	0.41
3:2:199:ASN:O	3:2:201:ARG:N	2.52	0.41
1:R:142:LEU:HD23	1:R:173:PRO:HD3	2.03	0.41
3:2:264:ARG:HB2	3:2:265:ASN:H	1.74	0.41
4:4:65:ALA:HB1	4:4:66:PRO:CD	2.45	0.41
5:3:108:THR:HB	5:3:224:LEU:HB3	2.02	0.41
1:R:157:THR:CB	1:R:158:GLY:HA2	2.50	0.41
2:1:212:PHE:CD1	2:1:212:PHE:N	2.87	0.41
1:R:76:ALA:H	1:R:77:VAL:HG23	1.85	0.41
2:1:257:ILE:HD12	2:1:257:ILE:N	2.36	0.41
5:3:136:PRO:O	5:3:137:PRO:O	2.39	0.41
1:R:126:VAL:HA	1:R:132:SER:HA	2.03	0.41
2:1:90:MET:HE1	2:1:242:VAL:HG23	2.03	0.41
4:4:4:GLN:O	4:4:4:GLN:HG3	2.21	0.41
1:R:210:PRO:HB2	1:R:211:SER:H	1.68	0.41
3:2:23:ILE:HD12	3:2:63:PHE:CZ	2.56	0.41
3:2:247:ILE:HA	3:2:248:PRO:HD3	1.92	0.41
5:3:136:PRO:HA	5:3:137:PRO:HD3	1.95	0.41
1:R:186:MET:N	1:R:187:PRO:CD	2.84	0.40
1:R:125:PHE:CD1	1:R:125:PHE:N	2.89	0.40
5:3:64:THR:C	5:3:66:GLU:N	2.79	0.40
5:3:78:THR:C	5:3:80:ASP:H	2.29	0.40
1:R:40:PHE:HZ	1:R:144:LYS:CB	2.29	0.40
1:R:118:GLU:HA	1:R:119:GLY:HA3	1.89	0.40
2:1:57:PRO:O	2:1:61:VAL:HG22	2.22	0.40
2:1:182:SER:O	5:3:15:THR:HG22	2.22	0.40
3:2:181:LEU:HG	3:2:181:LEU:O	2.21	0.40
1:R:69:HIS:CD2	1:R:120:SER:OG	2.75	0.40
2:1:93:ASP:CG	2:1:104:LEU:HB3	2.47	0.40
3:2:242:GLU:O	3:2:245:PRO:HD3	2.21	0.40
5:3:71:ARG:HG3	5:3:72:LEU:N	2.36	0.40
2:1:132:MET:HE1	6:1:0:SPH:C9	2.51	0.40
3:2:104:SER:HB2	3:2:258:CYS:HB2	2.02	0.40

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 PDB entries followed by that with respect to all EM entries.

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	R	211/213 (99%)	136 (64%)	50 (24%)	25 (12%)	0	4
2	1	281/283 (99%)	222 (79%)	43 (15%)	16 (6%)	1	14
3	2	266/268 (99%)	222 (84%)	36 (14%)	8 (3%)	3	23
4	4	59/68 (87%)	47 (80%)	7 (12%)	5 (8%)	0	9
5	3	233/235 (99%)	180 (77%)	38 (16%)	15 (6%)	1	12
All	All	1050/1067 (98%)	807 (77%)	174 (17%)	69 (7%)	2	12

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	55	ASN
1	R	99	LEU
1	R	143	ALA
1	R	188	GLN
1	R	210	PRO
1	R	212	SER
2	1	82	ALA
2	1	145	THR
2	1	219	ASP
3	2	200	LEU
3	2	257	CYS
5	3	15	THR
5	3	29	ASP
5	3	35	ASP
5	3	137	PRO
5	3	197	ARG
1	R	139	LEU
1	R	141	VAL
1	R	198	GLY
2	1	146	ASN
2	1	170	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	234	LEU
2	1	236	ASP
3	2	130	MET
3	2	167	GLN
4	4	15	ASN
5	3	170	TRP
5	3	179	THR
5	3	234	LYS
1	R	56	MET
1	R	88	GLU
1	R	131	GLY
1	R	134	SER
1	R	160	PRO
1	R	161	VAL
1	R	187	PRO
1	R	215	ASP
2	1	210	ASP
2	1	232	ALA
3	2	240	ALA
5	3	168	VAL
1	R	142	LEU
1	R	225	HIS
1	R	232	GLN
2	1	54	PRO
2	1	57	PRO
2	1	165	PRO
2	1	218	LYS
2	1	275	ARG
3	2	48	ASN
3	2	166	ASN
4	4	60	VAL
5	3	65	MET
2	1	216	PRO
3	2	34	ALA
4	4	9	LYS
5	3	59	ALA
5	3	74	ASP
5	3	89	PRO
5	3	161	GLN
4	4	56	PRO
1	R	162	PRO
1	R	209	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	250	PRO
1	R	145	PRO
5	3	93	PRO
1	R	129	PRO
1	R	214	VAL
4	4	11	GLY

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 PDB entries followed by that with respect to all EM entries.

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	R	185/185 (100%)	153 (83%)	32 (17%)	2	9
2	1	245/245 (100%)	224 (91%)	21 (9%)	10	29
3	2	228/228 (100%)	207 (91%)	21 (9%)	8	27
4	4	54/57 (95%)	44 (82%)	10 (18%)	1	8
5	3	210/210 (100%)	194 (92%)	16 (8%)	12	33
All	All	922/925 (100%)	822 (89%)	100 (11%)	8	21

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	41	LEU
1	R	43	ASP
1	R	51	LEU
1	R	58	VAL
1	R	60	HIS
1	R	61	VAL
1	R	68	ARG
1	R	99	LEU
1	R	102	GLU
1	R	103	LEU
1	R	104	ARG
1	R	120	SER
1	R	126	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	132	SER
1	R	133	ARG
1	R	137	ILE
1	R	139	LEU
1	R	141	VAL
1	R	142	LEU
1	R	152	GLN
1	R	157	THR
1	R	176	GLN
1	R	177	ILE
1	R	196	LEU
1	R	199	THR
1	R	200	VAL
1	R	208	LEU
1	R	213	GLN
1	R	214	VAL
1	R	234	LEU
1	R	236	VAL
1	R	241	TYR
2	1	38	SER
2	1	41	ILE
2	1	73	SER
2	1	83	ARG
2	1	97	SER
2	1	100	ASN
2	1	109	LYS
2	1	129	ARG
2	1	143	THR
2	1	146	ASN
2	1	147	ASN
2	1	149	HIS
2	1	177	THR
2	1	194	ILE
2	1	214	LYS
2	1	220	GLN
2	1	221	SER
2	1	224	LEU
2	1	255	SER
2	1	287	LYS
2	1	295	SER
3	2	5	GLU
3	2	10	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2	11	ASP
3	2	31	SER
3	2	48	ASN
3	2	52	GLN
3	2	66	LEU
3	2	73	LYS
3	2	115	SER
3	2	153	LYS
3	2	160	THR
3	2	162	THR
3	2	167	GLN
3	2	168	THR
3	2	201	ARG
3	2	217	SER
3	2	238	ASN
3	2	241	SER
3	2	242	GLU
3	2	264	ARG
3	2	272	GLN
4	4	6	SER
4	4	7	SER
4	4	13	HIS
4	4	36	SER
4	4	42	SER
4	4	49	ASP
4	4	52	LYS
4	4	60	VAL
4	4	61	LEU
4	4	64	THR
5	3	51	THR
5	3	52	MET
5	3	61	LYS
5	3	71	ARG
5	3	85	LEU
5	3	103	ILE
5	3	104	LEU
5	3	143	LYS
5	3	146	LYS
5	3	149	MET
5	3	163	SER
5	3	190	ILE
5	3	197	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	3	208	MET
5	3	218	ASN
5	3	224	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	36	GLN
1	R	55	ASN
1	R	69	HIS
1	R	80	GLN
1	R	130	GLN
1	R	155	GLN
1	R	232	GLN
2	1	37	HIS
2	1	69	HIS
2	1	149	HIS
2	1	152	ASN
2	1	220	GLN
3	2	48	ASN
3	2	95	ASN
3	2	165	ASN
3	2	238	ASN
3	2	261	ASN
4	4	13	HIS
4	4	26	ASN
4	4	31	ASN
4	4	39	ASN
5	3	6	ASN
5	3	218	ASN
5	3	233	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
6	SPH	1	0	-	19,20,20	1.44	2 (10%)	18,21,21	1.71	2 (11%)
7	MYR	4	1	4	14,14,15	1.01	1 (7%)	13,13,15	0.93	0

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
6	SPH	1	0	-	2/2/2/4	12/21/21/21	-
7	MYR	4	1	4	-	7/12/12/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	0	SPH	C4-C5	5.40	1.53	1.31
7	4	1	MYR	O2-C1	-3.39	1.24	1.42
6	1	0	SPH	C3-C4	2.11	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	1	0	SPH	C3-C4-C5	-5.87	112.52	124.69
6	1	0	SPH	C6-C5-C4	-2.71	113.38	125.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	1	0	SPH	C3
6	1	0	SPH	C2

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1	0	SPH	O1-C1-C2-N2
6	1	0	SPH	O1-C1-C2-C3
6	1	0	SPH	C1-C2-C3-O3
6	1	0	SPH	N2-C2-C3-C4
6	1	0	SPH	C2-C3-C4-C5
6	1	0	SPH	O3-C3-C4-C5
7	4	1	MYR	C7-C8-C9-C10
7	4	1	MYR	C10-C11-C12-C13
7	4	1	MYR	C5-C6-C7-C8
7	4	1	MYR	C6-C7-C8-C9
6	1	0	SPH	C11-C12-C13-C14
7	4	1	MYR	C11-C12-C13-C14
6	1	0	SPH	C4-C5-C6-C7
6	1	0	SPH	C1-C2-C3-C4
7	4	1	MYR	C9-C10-C11-C12
6	1	0	SPH	C7-C8-C9-C10
7	4	1	MYR	C1-C2-C3-C4
6	1	0	SPH	N2-C2-C3-O3
6	1	0	SPH	C10-C11-C12-C13

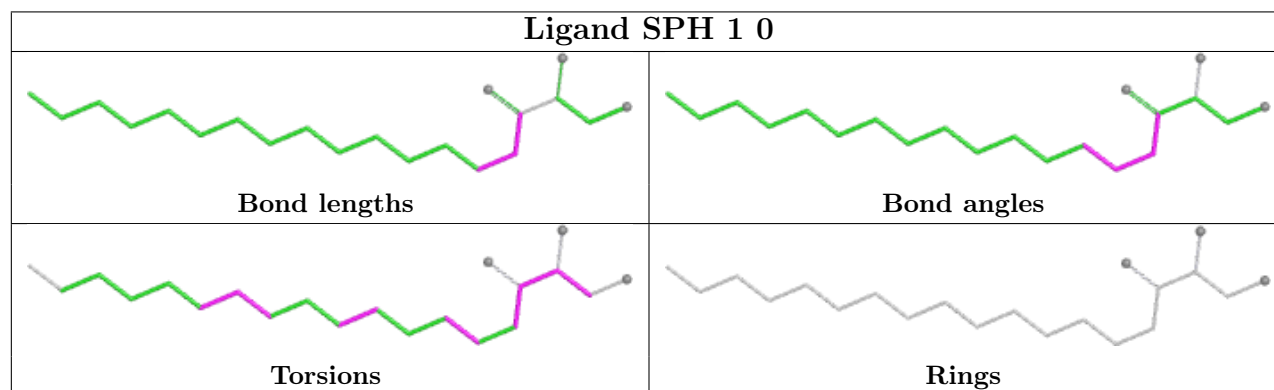
There are no ring outliers.

2 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	0	SPH	27	0
7	4	1	MYR	1	0

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.



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.

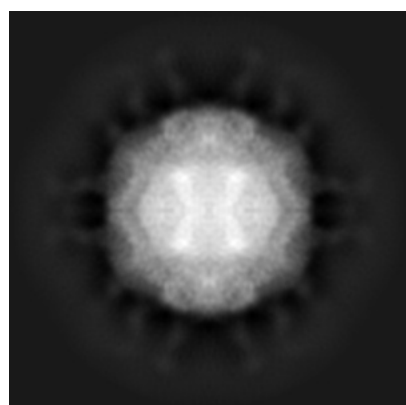
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1570. These allow visual inspection of the internal detail of the map and identification of artifacts.

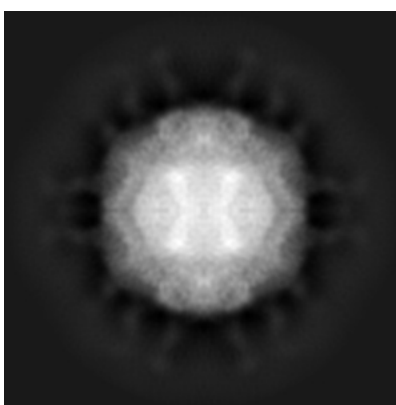
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

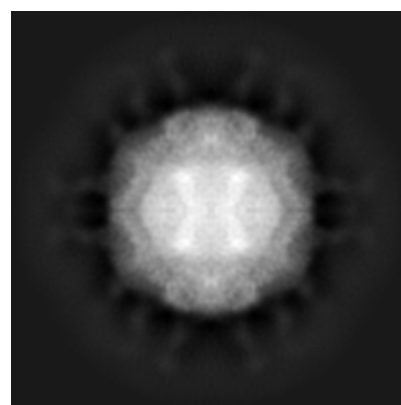
6.1.1 Primary map



X



Y

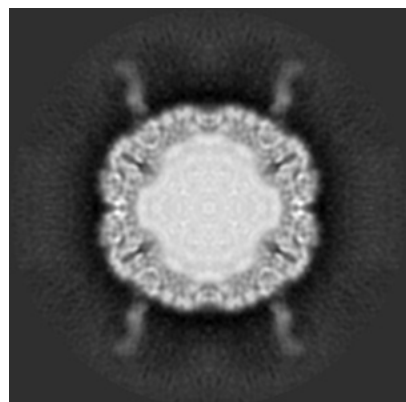


Z

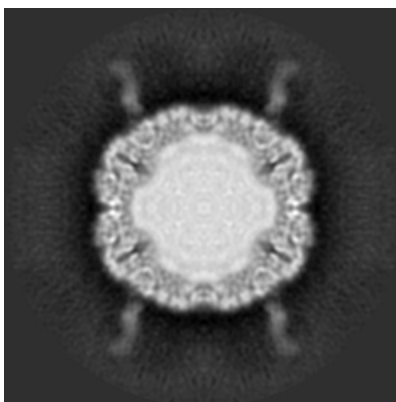
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

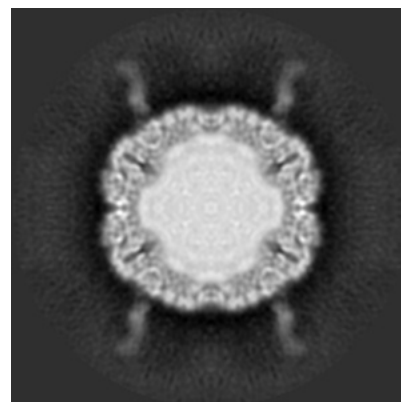
6.2.1 Primary map



X Index: 108



Y Index: 108

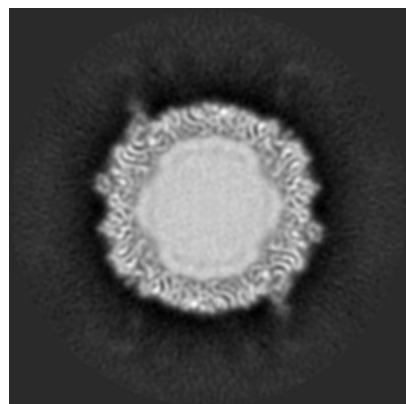


Z Index: 108

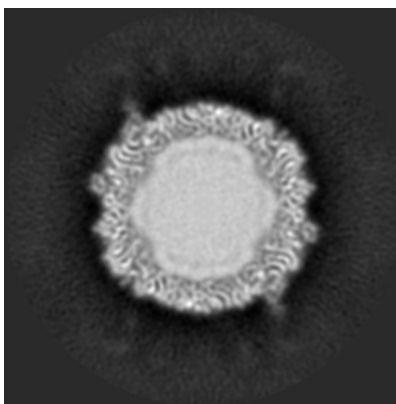
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

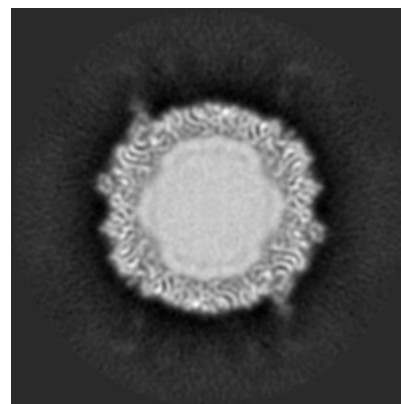
6.3.1 Primary map



X Index: 114



Y Index: 114

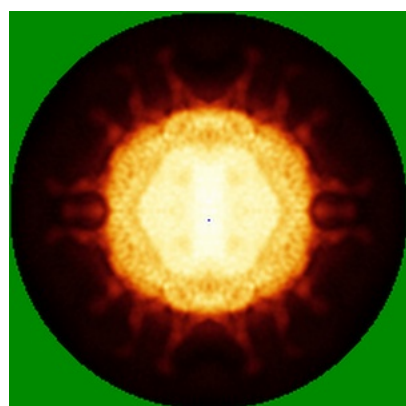


Z Index: 114

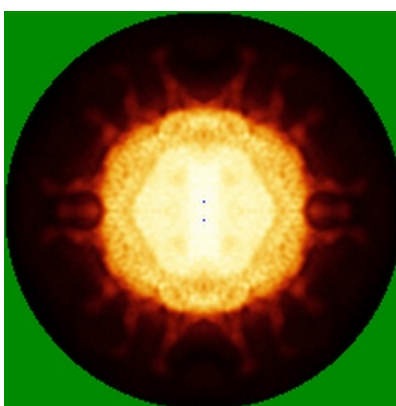
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

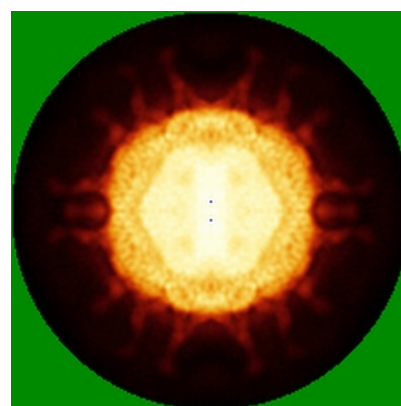
6.4.1 Primary map



X



Y

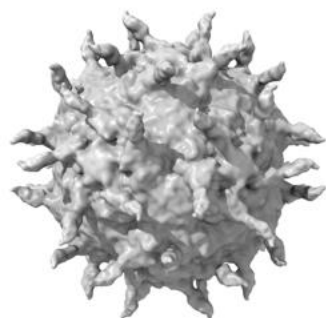


Z

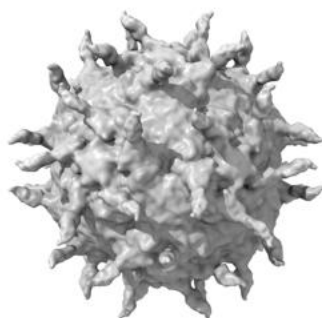
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

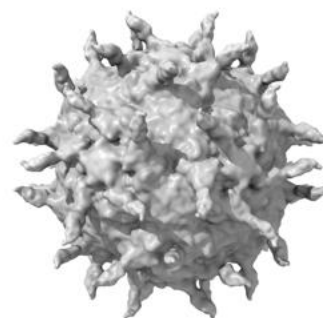
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

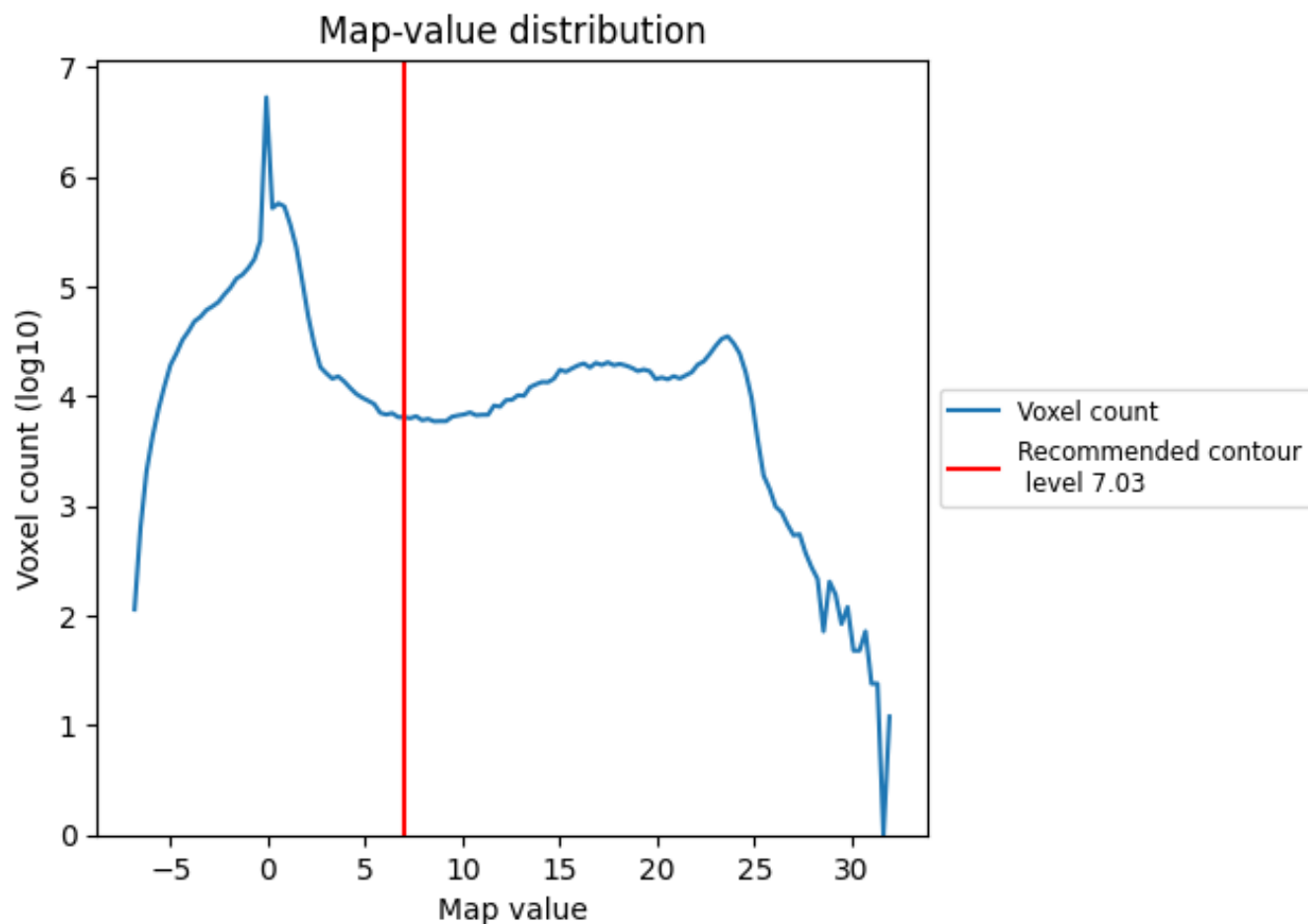
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

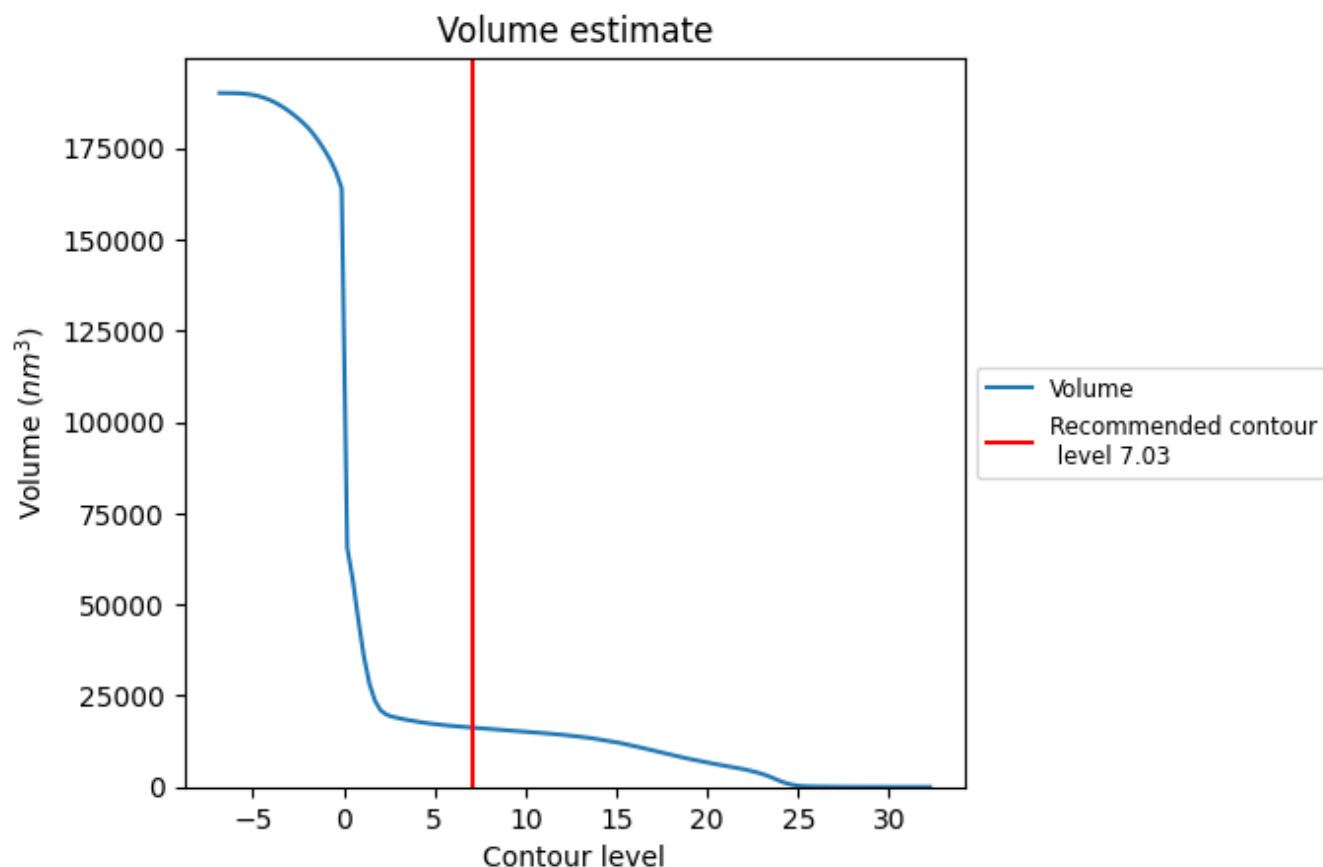
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

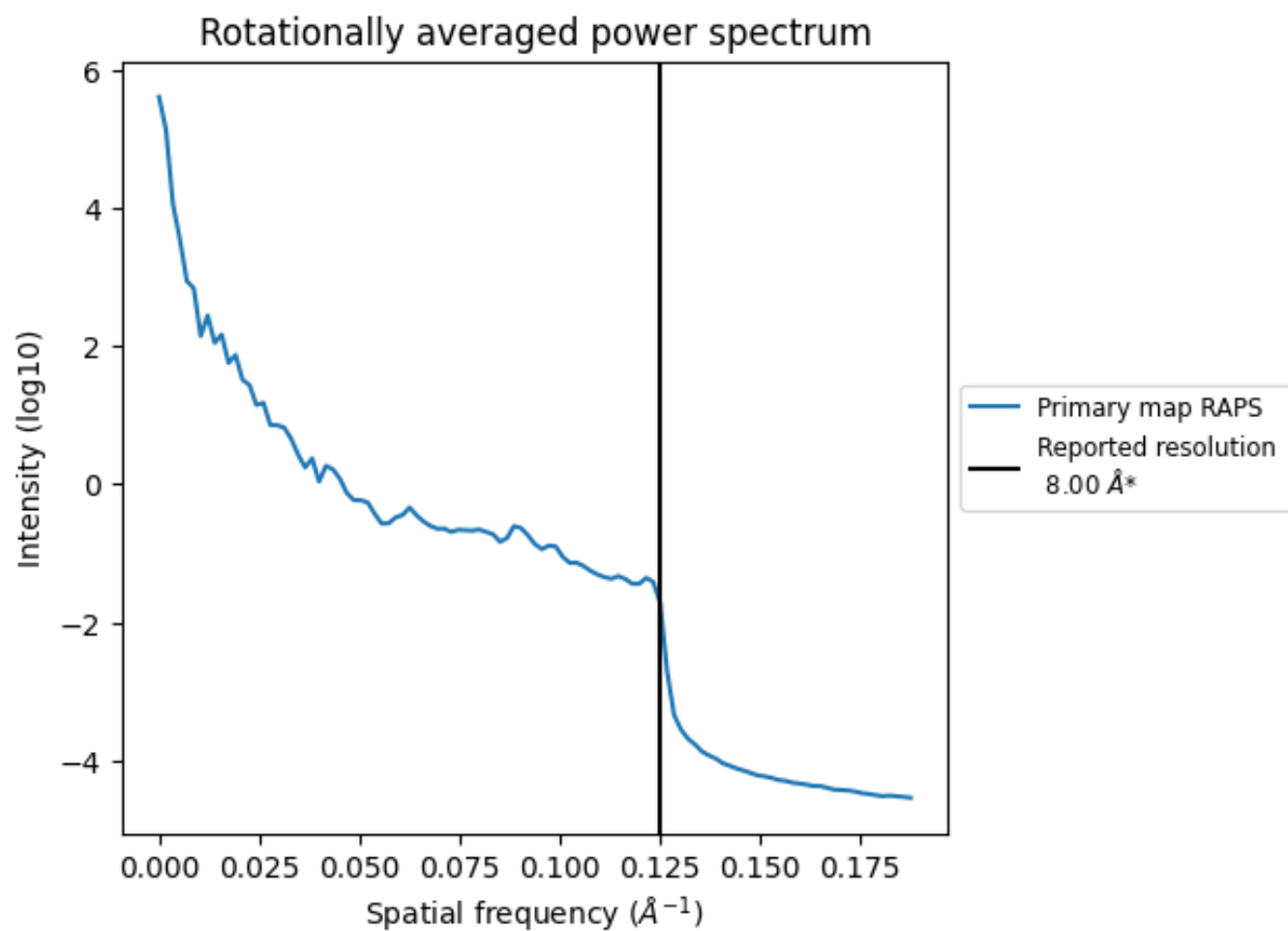
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 16285 nm^3 ; this corresponds to an approximate mass of 14711 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.125 Å⁻¹

8 Fourier-Shell correlation

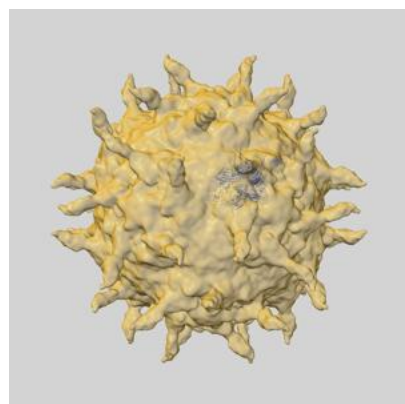
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

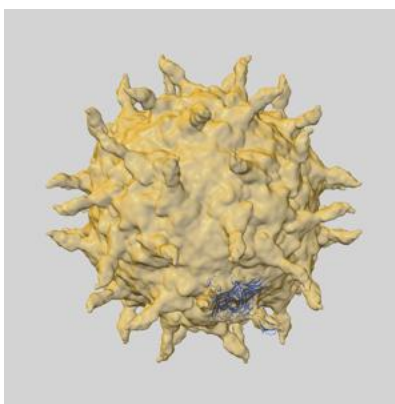
This section contains information regarding the fit between EMDB map EMD-1570 and PDB model 3EPC. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

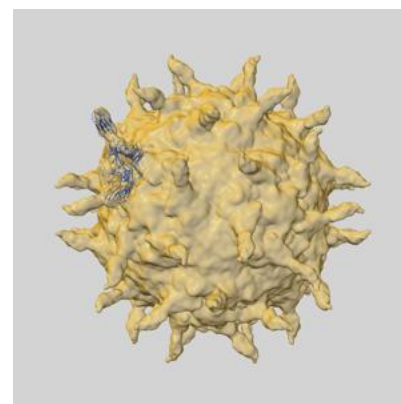
9.1.1 Map-model overlay [i](#)



X

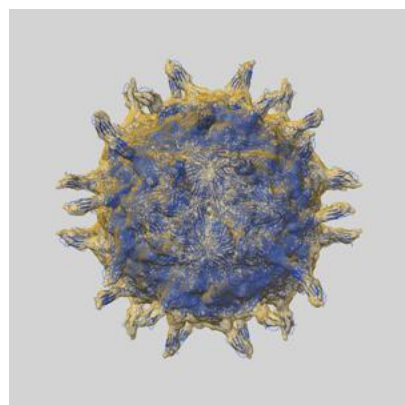


Y

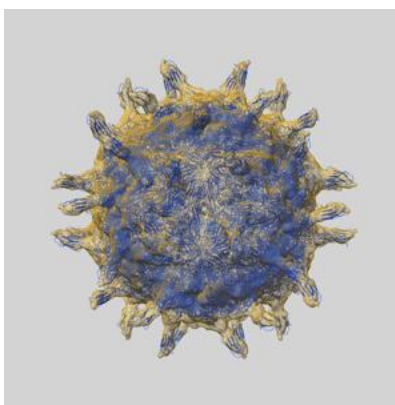


Z

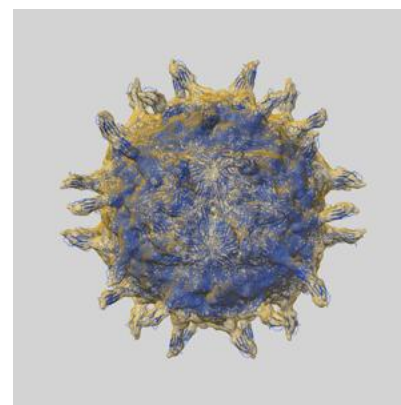
9.1.2 Map-model assembly overlay [i](#)



X



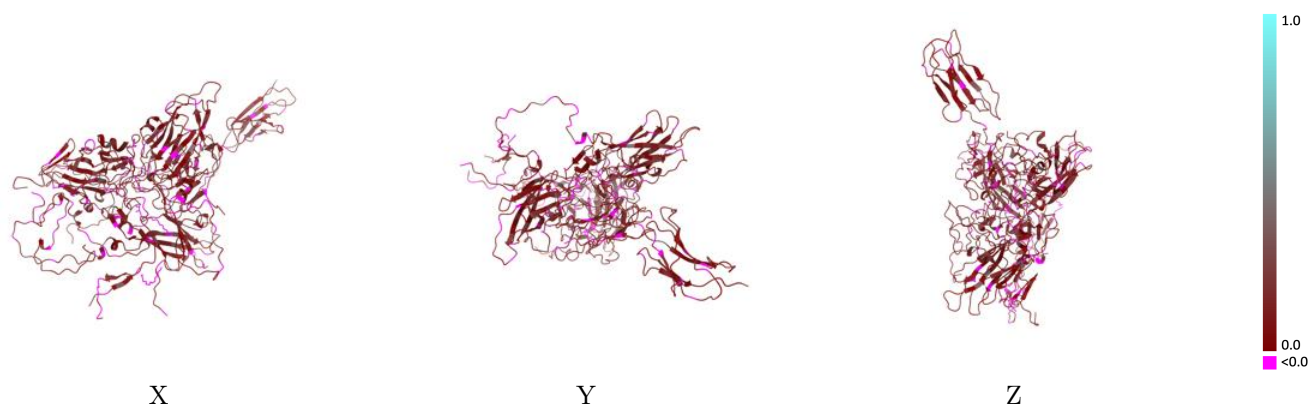
Y



Z

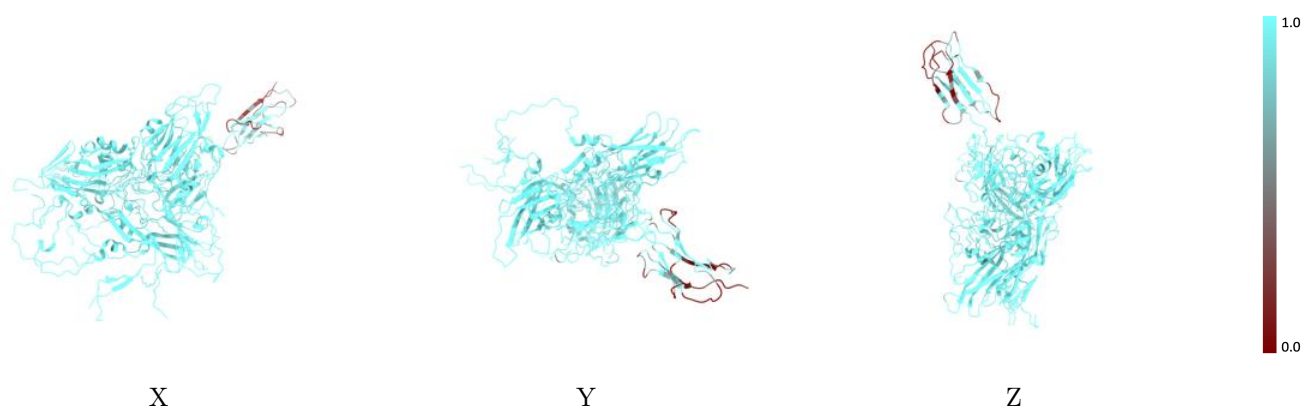
The images above show the 3D surface view of the map at the recommended contour level 7.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



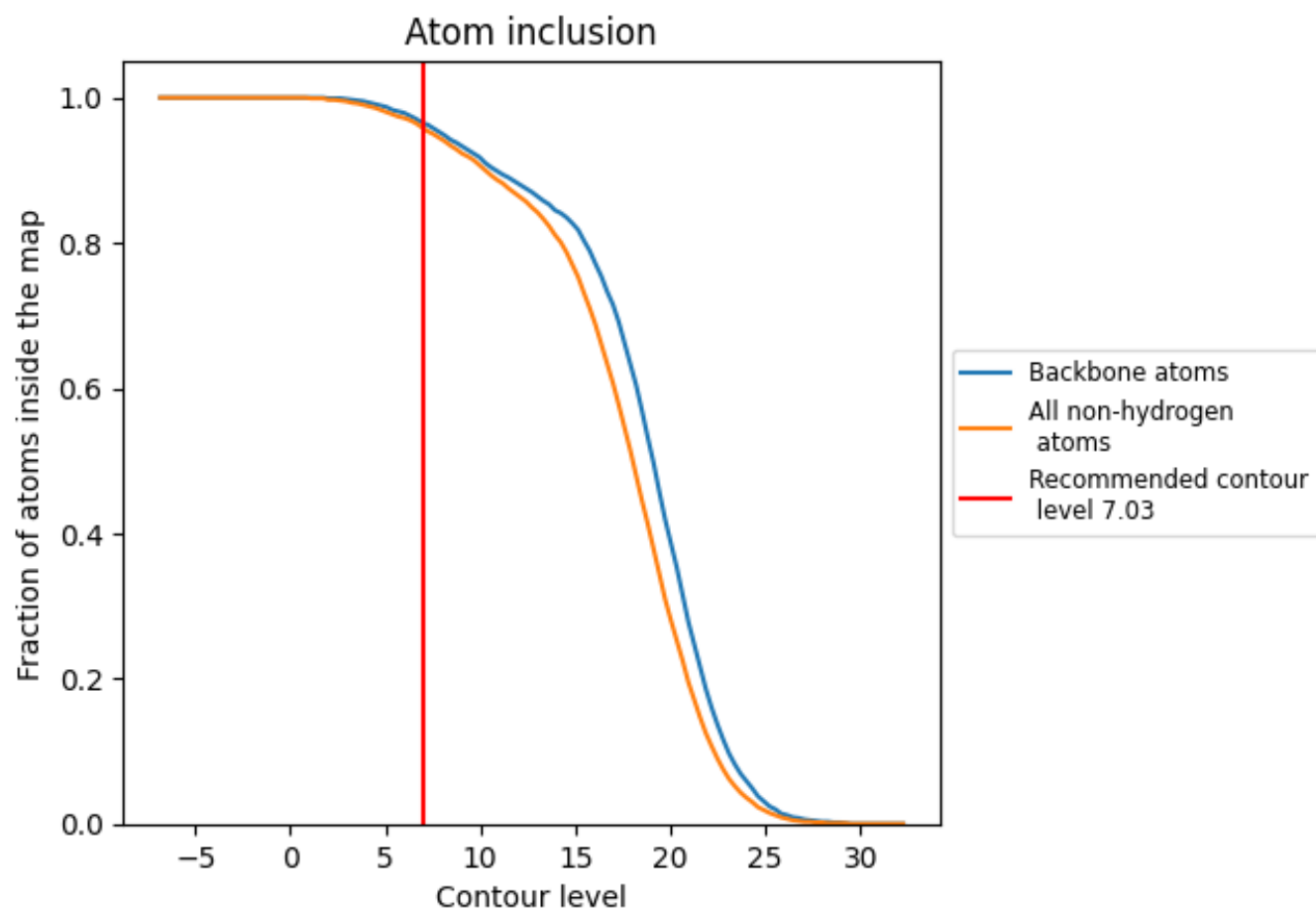
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (7.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9570	0.1070
1	1.0000	0.1020
2	0.9970	0.1100
3	1.0000	0.1130
4	0.9940	0.0580
R	0.7890	0.1170

