



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:56 AM UTC

PDB ID : 5WQL / pdb_00005wql
Title : Structure of a PDZ-protease bound to a substrate-binding adaptor
Authors : Su, M.Y.; Chang, C.I.
Deposited on : 2016-11-27
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

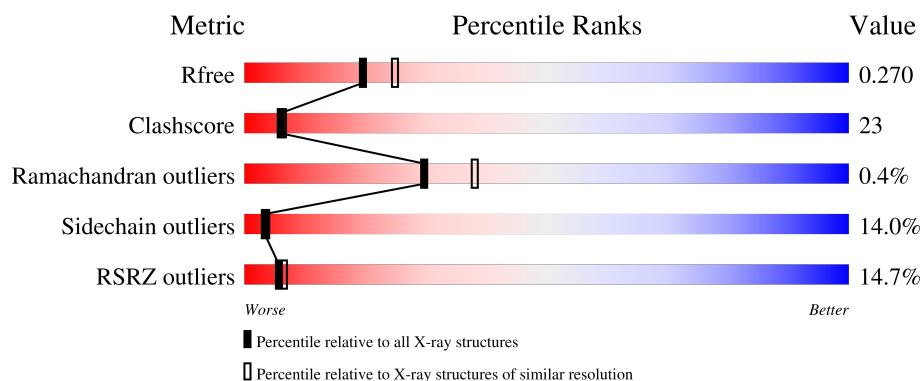
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	278	 38% 53% 6% •
1	B	278	 36% 55% 5% •
2	C	682	 20% 52% 31% 11% 5%
2	D	682	 17% 47% 33% 13% • 5%
3	F	6	 67% 17% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	6	 67% 33%
4	E	4	 75% 25%
5	G	4	 25% 50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15704 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Lipoprotein NlpI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	268	Total	C	N	O	S	0	0	0
			2176	1387	362	424	3			
1	A	270	Total	C	N	O	S	0	0	0
			2190	1395	364	427	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	GLY	-	expression tag	UNP P0AFB1
B	18	HIS	-	expression tag	UNP P0AFB1
B	19	MET	-	expression tag	UNP P0AFB1
A	17	GLY	-	expression tag	UNP P0AFB1
A	18	HIS	-	expression tag	UNP P0AFB1
A	19	MET	-	expression tag	UNP P0AFB1

- Molecule 2 is a protein called Tail-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	648	Total	C	N	O	S	0	0	0
			5140	3233	897	998	12			
2	D	647	Total	C	N	O	S	0	0	0
			5139	3233	899	995	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	477	ALA	LYS	engineered mutation	UNP P23865
D	477	ALA	LYS	engineered mutation	UNP P23865

- Molecule 3 is a protein called ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	6	Total	C	N	O	0	0	0
			30	18	6	6			
3	H	6	Total	C	N	O	0	0	0
			30	18	6	6			

- Molecule 4 is a protein called ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			21	12	4	5			

- Molecule 5 is a protein called LEU-SER-ARG-SER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	4	Total	C	N	O	0	0	0
			32	18	7	7			

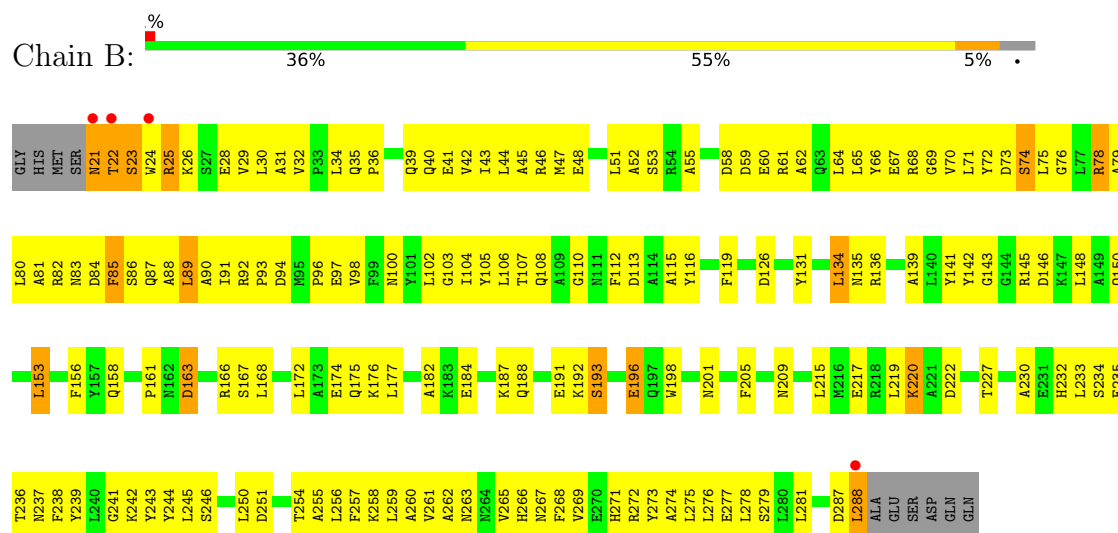
- Molecule 6 is water.

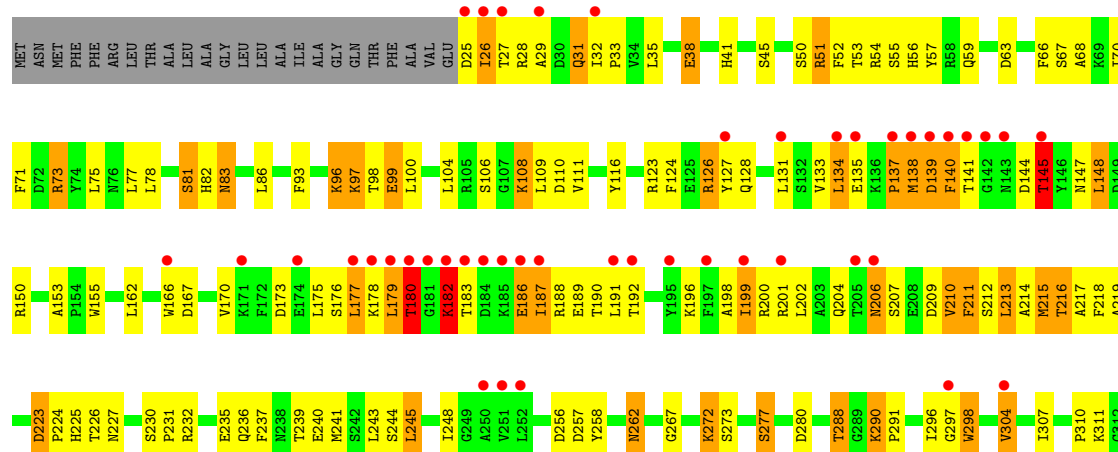
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	251	Total	O	0	0
			251	251		
6	A	250	Total	O	0	0
			250	250		
6	C	203	Total	O	0	0
			203	203		
6	D	241	Total	O	0	0
			241	241		
6	F	1	Total	O	0	0
			1	1		

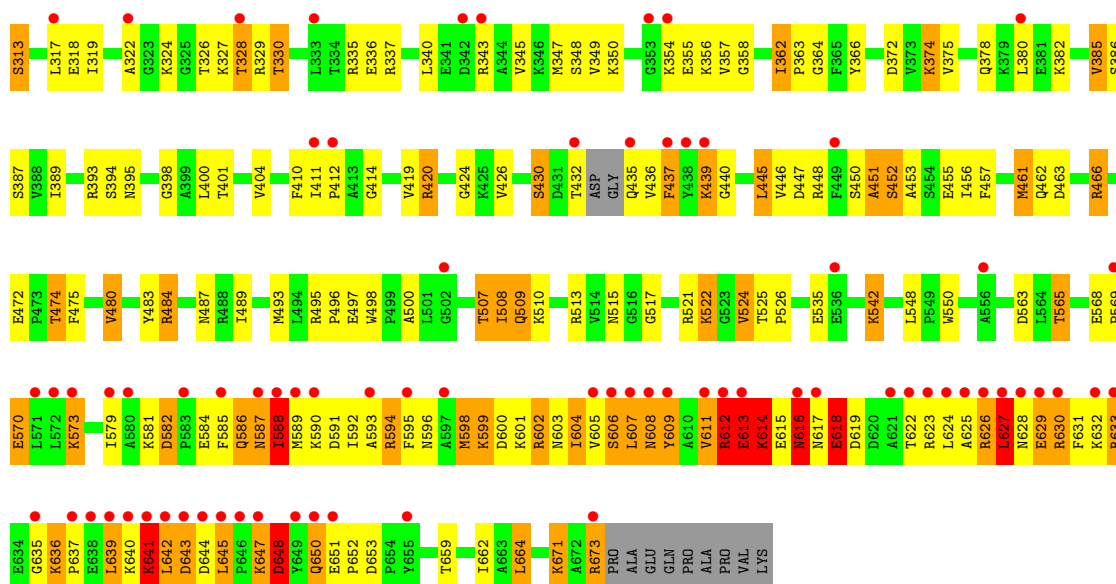
3 Residue-property plots

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

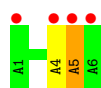
• Molecule 1: Lipoprotein NlpI



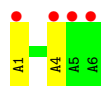




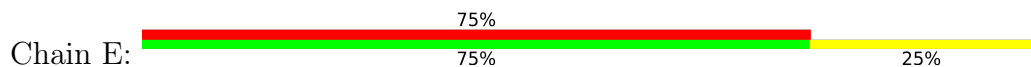
• Molecule 3: ALA-ALA-ALA-ALA-ALA-ALA



• Molecule 3: ALA-ALA-ALA-ALA-ALA-ALA



• Molecule 4: ALA-ALA-ALA-ALA



• Molecule 5: LEU-SER-ARG-SER



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.59Å 146.73Å 148.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	104.35 – 2.30 104.35 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.3 (104.35-2.30) 90.3 (104.35-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.217 , 0.271 0.220 , 0.270	Depositor DCC
R_{free} test set	5472 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15704	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2069e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	A	2.30	137/2236 (6.1%)	1.26	14/3034 (0.5%)
1	B	2.25	134/2222 (6.0%)	1.22	7/3016 (0.2%)
2	C	1.67	43/5227 (0.8%)	1.18	34/7059 (0.5%)
2	D	1.69	46/5225 (0.9%)	1.33	65/7054 (0.9%)
3	F	1.85	0/29	1.64	1/39 (2.6%)
3	H	1.46	0/29	1.57	0/39
4	E	1.23	0/20	0.91	0/25
5	G	1.11	0/31	1.26	1/38 (2.6%)
All	All	1.87	360/15019 (2.4%)	1.25	122/20304 (0.6%)

All (360) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ARG	C-O	-10.00	1.16	1.25
1	A	232	HIS	C-O	-8.54	1.14	1.24
1	A	260	ALA	C-O	-7.91	1.15	1.24
1	B	241	GLY	C-O	-7.71	1.14	1.23
1	B	267	ASN	C-O	-7.29	1.14	1.24
1	A	217	GLU	C-O	-7.27	1.15	1.24
1	A	277	GLU	C-O	-7.19	1.15	1.24
1	A	236	THR	C-O	-7.18	1.15	1.24
1	A	238	PHE	C-O	-7.17	1.15	1.24
1	A	205	PHE	C-O	-7.14	1.15	1.24
1	B	259	LEU	C-O	-7.14	1.15	1.24
1	A	100	ASN	C-O	-7.10	1.16	1.24
1	A	44	LEU	C-O	-7.08	1.15	1.24
1	B	60	GLU	C-O	-7.08	1.15	1.24
1	B	236	THR	C-O	-7.08	1.16	1.24
1	A	266	HIS	C-O	-7.03	1.15	1.24
1	B	48	GLU	C-O	-7.01	1.16	1.24
1	B	106	LEU	C-O	-6.97	1.16	1.24
1	A	90	ALA	C-O	-6.97	1.16	1.24
2	C	229	LEU	C-O	-6.93	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	TYR	C-O	-6.89	1.16	1.24
1	A	203	VAL	C-O	-6.86	1.16	1.24
1	A	275	LEU	C-O	-6.85	1.16	1.24
1	B	32	VAL	C-O	-6.84	1.15	1.24
1	A	32	VAL	C-O	-6.83	1.15	1.24
1	A	210	ILE	C-O	-6.81	1.17	1.24
1	A	115	ALA	C-O	-6.79	1.16	1.24
1	A	272	ARG	C-O	-6.78	1.16	1.24
1	B	139	ALA	C-O	-6.78	1.16	1.24
1	A	79	ALA	C-O	-6.78	1.16	1.24
1	A	259	LEU	C-O	-6.78	1.16	1.24
1	A	92	ARG	C-O	-6.74	1.18	1.24
1	A	261	VAL	C-O	-6.72	1.16	1.24
1	B	86	SER	C-O	-6.68	1.16	1.24
1	B	71	LEU	C-O	-6.64	1.16	1.24
1	B	62	ALA	C-O	-6.58	1.16	1.24
1	A	46	ARG	C-O	-6.58	1.16	1.24
1	B	112	PHE	C-O	-6.56	1.16	1.24
1	B	205	PHE	C-O	-6.54	1.16	1.24
1	B	271	HIS	C-O	-6.53	1.16	1.24
1	B	69	GLY	C-O	-6.52	1.16	1.23
1	A	219	LEU	C-O	-6.52	1.16	1.24
1	B	90	ALA	C-O	-6.51	1.16	1.24
1	B	273	TYR	C-O	-6.51	1.15	1.24
1	B	255	ALA	C-O	-6.50	1.16	1.24
1	B	242	LYS	C-O	-6.49	1.16	1.24
1	B	272	ARG	C-O	-6.45	1.16	1.24
1	A	143	GLY	C-O	-6.44	1.15	1.23
1	A	207	LEU	C-O	-6.42	1.15	1.24
1	A	105	TYR	C-O	-6.40	1.16	1.24
1	B	261	VAL	C-O	-6.37	1.16	1.24
2	C	480	VAL	C-O	-6.37	1.17	1.24
1	B	104	ILE	C-O	-6.36	1.16	1.24
2	D	235	GLU	C-O	-6.30	1.16	1.24
1	A	87	GLN	C-O	-6.29	1.16	1.24
1	A	229	LEU	C-O	-6.29	1.16	1.24
2	C	225	HIS	C-O	-6.27	1.16	1.24
1	A	47	MET	C-O	-6.27	1.16	1.24
1	B	68	ARG	C-O	-6.27	1.16	1.24
1	B	91	ILE	C-O	-6.25	1.17	1.24
1	A	69	GLY	C-O	-6.24	1.16	1.23
1	A	239	TYR	C-O	-6.24	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ARG	C-O	-6.24	1.16	1.24
2	D	456	ILE	C-O	-6.24	1.17	1.24
1	A	163	ASP	C-O	-6.22	1.16	1.24
1	A	270	GLU	C-O	-6.22	1.16	1.24
1	A	114	ALA	C-O	-6.21	1.16	1.24
1	B	108	GLN	C-O	-6.16	1.16	1.24
1	A	252	SER	C-O	-6.16	1.17	1.24
1	A	255	ALA	C-O	-6.16	1.17	1.24
1	B	167	SER	C-O	-6.15	1.16	1.24
1	B	51	LEU	C-O	-6.15	1.16	1.24
1	B	70	VAL	C-O	-6.15	1.17	1.24
1	B	66	TYR	C-O	-6.15	1.17	1.24
1	B	35	GLN	C-O	-6.14	1.17	1.24
1	B	64	LEU	C-O	-6.13	1.17	1.24
2	D	211	PHE	C-O	-6.12	1.17	1.24
1	B	52	ALA	C-O	-6.12	1.16	1.24
2	D	362	ILE	C-O	-6.12	1.17	1.24
2	C	54	ARG	C-O	-6.12	1.14	1.23
2	C	55	SER	C-O	-6.12	1.15	1.24
1	A	164	PRO	C-O	-6.11	1.16	1.24
2	D	70	ILE	C-O	-6.11	1.17	1.24
1	B	235	GLU	C-O	-6.10	1.17	1.24
1	B	238	PHE	C-O	-6.10	1.17	1.24
1	A	97	GLU	C-O	-6.09	1.17	1.24
1	A	222	ASP	C-O	-6.09	1.16	1.24
1	A	201	ASN	C-O	-6.07	1.17	1.24
1	B	232	HIS	C-O	-6.04	1.17	1.24
1	B	227	THR	C-O	-6.04	1.17	1.24
1	B	100	ASN	C-O	-6.03	1.17	1.24
1	B	254	THR	C-O	-6.03	1.17	1.24
1	A	240	LEU	C-O	-6.03	1.17	1.24
1	B	102	LEU	C-O	-6.03	1.17	1.24
1	B	83	ASN	C-O	-6.02	1.17	1.24
1	A	276	LEU	C-O	-6.02	1.17	1.24
1	B	143	GLY	C-O	-5.99	1.16	1.23
1	A	172	LEU	C-O	-5.99	1.17	1.24
1	B	263	ASN	C-O	-5.99	1.16	1.24
2	D	52	PHE	C-O	-5.99	1.17	1.24
1	B	275	LEU	C-O	-5.98	1.17	1.24
1	B	233	LEU	C-O	-5.97	1.17	1.24
1	A	71	LEU	C-O	-5.97	1.17	1.24
1	A	253	ALA	C-O	-5.96	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	608	ASN	CA-C	-5.95	1.45	1.52
2	D	419	VAL	C-O	-5.94	1.18	1.24
1	B	45	ALA	C-O	-5.93	1.17	1.24
1	A	93	PRO	C-O	-5.93	1.16	1.24
1	A	258	LYS	C-O	-5.92	1.17	1.24
1	A	62	ALA	C-O	-5.92	1.17	1.24
1	B	44	LEU	C-O	-5.92	1.17	1.24
1	B	72	TYR	C-O	-5.92	1.17	1.24
1	A	85	PHE	C-O	-5.91	1.17	1.24
1	A	117	GLU	C-O	-5.91	1.17	1.24
1	B	250	LEU	C-O	-5.90	1.17	1.24
2	C	237	PHE	C-O	-5.89	1.17	1.24
1	A	204	GLU	C-O	-5.89	1.17	1.24
1	A	280	LEU	C-O	-5.89	1.17	1.24
1	B	89	LEU	C-O	-5.88	1.17	1.24
1	A	75	LEU	C-O	-5.88	1.15	1.23
1	B	41	GLU	C-O	-5.88	1.17	1.24
1	A	101	TYR	C-O	-5.88	1.17	1.24
1	B	260	ALA	C-O	-5.87	1.17	1.24
1	A	254	THR	C-O	-5.86	1.17	1.24
2	C	51	ARG	C-O	-5.86	1.17	1.24
1	B	142	TYR	C-O	-5.85	1.16	1.24
1	A	81	ALA	C-O	-5.85	1.17	1.24
2	C	396	GLY	C-O	-5.85	1.17	1.24
2	D	457	PHE	C-O	-5.85	1.17	1.24
1	B	53	SER	C-O	-5.84	1.16	1.23
1	A	68	ARG	C-O	-5.84	1.17	1.24
1	B	96	PRO	C-O	-5.84	1.16	1.24
1	A	99	PHE	C-O	-5.84	1.16	1.24
1	A	187	LYS	C-O	-5.83	1.17	1.24
1	A	104	ILE	C-O	-5.83	1.17	1.24
1	A	106	LEU	C-O	-5.83	1.17	1.24
1	B	107	THR	C-O	-5.82	1.17	1.24
1	B	141	TYR	C-O	-5.81	1.17	1.24
1	A	220	LYS	C-O	-5.78	1.17	1.24
2	C	61	ASP	CA-C	-5.78	1.45	1.52
1	B	75	LEU	C-O	-5.77	1.16	1.24
1	A	141	TYR	C-O	-5.77	1.17	1.24
1	A	242	LYS	C-O	-5.77	1.17	1.24
1	A	103	GLY	C-O	-5.77	1.16	1.23
2	D	256	ASP	C-O	-5.77	1.19	1.24
1	B	276	LEU	C-O	-5.76	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	505	GLN	C-O	-5.76	1.17	1.24
1	A	70	VAL	C-O	-5.76	1.17	1.24
2	D	219	ALA	C-O	-5.76	1.17	1.24
1	B	47	MET	C-O	-5.75	1.17	1.24
1	A	131	TYR	C-O	-5.75	1.16	1.24
2	C	455	GLU	C-O	-5.75	1.17	1.24
1	A	216	MET	C-O	-5.75	1.17	1.24
1	A	198	TRP	C-O	-5.75	1.17	1.24
2	D	116	TYR	C-O	-5.74	1.17	1.24
1	B	29	VAL	C-O	-5.74	1.18	1.24
1	A	138	ILE	C-O	-5.74	1.17	1.24
2	C	43	THR	C-O	-5.73	1.17	1.24
2	C	56	HIS	C-O	-5.73	1.16	1.23
2	D	215	MET	C-O	-5.73	1.17	1.24
2	D	401	THR	C-O	-5.73	1.17	1.24
1	B	161	PRO	C-O	-5.72	1.16	1.24
1	B	67	GLU	C-O	-5.72	1.17	1.24
2	D	480	VAL	C-O	-5.72	1.17	1.24
1	A	110	GLY	C-O	-5.71	1.16	1.24
1	A	267	ASN	C-O	-5.71	1.16	1.24
1	B	256	LEU	C-O	-5.71	1.17	1.24
1	A	122	VAL	C-O	-5.71	1.17	1.24
1	A	171	TYR	C-O	-5.71	1.17	1.24
1	B	265	VAL	C-O	-5.71	1.16	1.23
1	B	278	LEU	C-O	-5.70	1.17	1.24
1	A	139	ALA	C-O	-5.70	1.17	1.24
2	D	63	ASP	C-O	-5.70	1.17	1.23
1	A	64	LEU	C-O	-5.70	1.17	1.24
1	A	227	THR	C-O	-5.69	1.17	1.24
1	B	115	ALA	C-O	-5.68	1.17	1.24
1	A	264	ASN	C-O	-5.68	1.15	1.23
1	B	76	GLY	C-O	-5.68	1.16	1.24
1	B	277	GLU	C-O	-5.68	1.17	1.24
2	C	233	ASN	C-O	-5.66	1.17	1.24
1	B	281	LEU	C-O	-5.66	1.17	1.24
1	B	78	ARG	CZ-NH2	-5.66	1.26	1.33
1	A	95	MET	C-O	-5.65	1.18	1.24
1	A	218	ARG	C-O	-5.64	1.17	1.24
1	A	162	ASN	C-O	-5.64	1.16	1.24
1	A	89	LEU	C-O	-5.62	1.17	1.24
1	A	200	TRP	C-O	-5.61	1.17	1.24
1	B	84	ASP	C-O	-5.61	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	GLY	C-O	-5.61	1.16	1.24
2	C	100	LEU	C-O	-5.60	1.17	1.24
2	D	239	THR	C-O	-5.60	1.17	1.24
1	A	142	TYR	C-O	-5.60	1.17	1.24
2	C	419	VAL	C-O	-5.60	1.18	1.24
1	A	212	GLU	C-O	-5.59	1.17	1.24
1	A	262	ALA	C-O	-5.59	1.16	1.24
1	B	262	ALA	C-O	-5.59	1.17	1.24
1	A	196	GLU	C-O	-5.59	1.17	1.24
2	D	462	GLN	C-O	-5.59	1.17	1.24
1	B	222	ASP	C-O	-5.58	1.17	1.24
1	B	46	ARG	C-O	-5.58	1.17	1.24
1	B	134	LEU	C-O	-5.58	1.17	1.24
2	C	229	LEU	CA-C	-5.57	1.46	1.52
2	C	232	ARG	C-O	-5.57	1.17	1.24
1	B	244	TYR	C-O	-5.56	1.17	1.24
1	B	65	LEU	C-O	-5.55	1.17	1.24
1	A	168	LEU	C-O	-5.55	1.17	1.24
2	D	213	LEU	C-O	-5.55	1.17	1.24
2	C	364	GLY	C-O	-5.54	1.18	1.23
2	C	483	TYR	C-O	-5.53	1.17	1.24
1	B	73	ASP	C-O	-5.52	1.17	1.24
1	B	74	SER	C-O	-5.52	1.16	1.24
1	B	136	ARG	C-O	-5.51	1.17	1.24
2	C	452	SER	C-O	-5.50	1.17	1.24
1	B	257	PHE	C-O	-5.50	1.17	1.24
2	D	225	HIS	C-O	-5.49	1.16	1.24
1	A	167	SER	C-O	-5.49	1.17	1.24
1	A	48	GLU	C-O	-5.49	1.17	1.24
1	B	97	GLU	C-O	-5.48	1.17	1.24
1	B	269	VAL	C-O	-5.48	1.17	1.24
1	A	88	ALA	C-O	-5.47	1.17	1.24
1	A	226	ASN	C-O	-5.47	1.17	1.24
1	B	230	ALA	C-O	-5.46	1.17	1.24
2	D	508	ILE	C-O	-5.46	1.18	1.24
1	B	82	ARG	C-O	-5.45	1.17	1.24
1	A	125	LEU	C-O	-5.44	1.17	1.24
1	B	234	SER	C-O	-5.44	1.17	1.24
1	B	126	ASP	N-CA	-5.43	1.42	1.46
2	C	547	ALA	C-O	-5.43	1.17	1.23
2	D	232	ARG	C-O	-5.42	1.17	1.24
1	B	279	SER	C-O	-5.42	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	ALA	C-O	-5.42	1.17	1.24
1	A	36	PRO	C-O	-5.42	1.17	1.23
1	A	59	ASP	C-O	-5.41	1.17	1.24
1	A	134	LEU	C-O	-5.40	1.17	1.24
2	D	51	ARG	C-O	-5.40	1.17	1.24
1	B	215	LEU	C-O	-5.40	1.17	1.24
2	D	489	ILE	C-O	-5.40	1.17	1.24
1	B	81	ALA	C-O	-5.39	1.17	1.24
1	A	233	LEU	C-O	-5.39	1.17	1.24
2	C	45	SER	C-O	-5.39	1.17	1.24
1	B	30	LEU	C-O	-5.39	1.17	1.23
1	A	234	SER	C-O	-5.38	1.18	1.24
1	B	135	ASN	C-O	-5.38	1.17	1.24
1	B	172	LEU	C-O	-5.38	1.17	1.24
2	C	479	THR	C-O	-5.38	1.17	1.23
2	D	483	TYR	C-O	-5.38	1.17	1.24
1	B	79	ALA	C-O	-5.38	1.17	1.24
1	A	206	TYR	C-O	-5.37	1.17	1.24
2	D	226	THR	C-O	-5.37	1.17	1.24
1	A	51	LEU	C-O	-5.36	1.17	1.24
1	B	40	GLN	C-O	-5.36	1.18	1.24
2	D	182	LYS	N-CA	-5.36	1.39	1.46
2	D	446	VAL	C-O	-5.35	1.18	1.23
1	B	43	ILE	C-O	-5.34	1.18	1.24
1	A	78	ARG	C-O	-5.34	1.17	1.24
1	A	72	TYR	C-O	-5.33	1.17	1.24
2	C	273	SER	N-CA	-5.32	1.40	1.46
1	B	34	LEU	C-O	-5.31	1.17	1.23
1	B	93	PRO	C-O	-5.31	1.17	1.24
2	D	372	ASP	C-O	-5.30	1.18	1.24
1	B	58	ASP	C-O	-5.30	1.18	1.24
1	A	149	ALA	C-O	-5.30	1.18	1.24
1	A	243	TYR	C-O	-5.29	1.18	1.24
2	C	226	THR	C-O	-5.28	1.17	1.24
2	D	54	ARG	C-O	-5.27	1.16	1.23
1	A	123	LEU	C-O	-5.26	1.17	1.24
1	A	265	VAL	C-O	-5.26	1.17	1.23
2	D	498	TRP	CA-C	-5.26	1.47	1.53
2	C	49	THR	C-O	-5.26	1.18	1.24
2	C	46	GLU	C-O	-5.25	1.18	1.24
1	A	107	THR	C-O	-5.25	1.18	1.24
1	A	225	ASP	C-O	-5.25	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	TYR	C-O	-5.25	1.17	1.24
2	C	239	THR	C-O	-5.24	1.18	1.24
1	B	274	ALA	C-O	-5.24	1.18	1.24
2	D	45	SER	C-O	-5.24	1.18	1.24
1	A	121	SER	C-O	-5.23	1.18	1.24
1	A	231	GLU	C-O	-5.23	1.18	1.24
1	A	161	PRO	C-O	-5.23	1.17	1.24
1	B	239	TYR	C-O	-5.22	1.17	1.24
1	B	268	PHE	C-O	-5.22	1.17	1.23
2	D	55	SER	C-O	-5.22	1.17	1.24
2	D	104	LEU	C-O	-5.22	1.18	1.24
1	B	148	LEU	C-O	-5.21	1.18	1.24
1	A	96	PRO	C-O	-5.21	1.17	1.24
1	B	209	ASN	C-O	-5.20	1.18	1.24
1	A	278	LEU	C-O	-5.19	1.18	1.24
1	B	31	ALA	C-O	-5.19	1.17	1.23
1	B	131	TYR	C-O	-5.18	1.17	1.24
1	A	154	LEU	C-O	-5.18	1.18	1.24
1	A	186	LEU	C-O	-5.18	1.18	1.24
2	C	78	LEU	C-O	-5.18	1.18	1.24
2	C	493	MET	C-O	-5.18	1.18	1.24
2	D	214	ALA	C-O	-5.18	1.18	1.24
1	B	59	ASP	C-O	-5.18	1.18	1.24
1	A	140	LEU	C-O	-5.17	1.18	1.24
2	D	664	LEU	C-O	-5.17	1.18	1.24
1	A	30	LEU	C-O	-5.17	1.17	1.23
1	B	201	ASN	C-O	-5.17	1.18	1.24
1	B	119	PHE	C-O	-5.17	1.18	1.24
1	A	91	ILE	C-O	-5.16	1.18	1.24
2	C	436	VAL	C-O	-5.16	1.18	1.24
1	A	86	SER	C-O	-5.15	1.18	1.24
2	C	224	PRO	C-O	-5.15	1.17	1.24
1	B	243	TYR	C-O	-5.15	1.18	1.24
1	B	88	ALA	C-O	-5.14	1.18	1.24
1	A	214	THR	C-O	-5.14	1.18	1.24
1	B	55	ALA	C-O	-5.14	1.17	1.24
2	D	66	PHE	C-O	-5.14	1.18	1.24
1	B	251	ASP	C-O	-5.13	1.18	1.24
1	B	258	LYS	C-O	-5.13	1.18	1.24
2	D	106	SER	C-O	-5.13	1.18	1.24
1	A	180	LYS	C-O	-5.13	1.18	1.24
2	D	137	PRO	CA-C	-5.12	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	LEU	C-O	-5.12	1.18	1.24
1	B	80	LEU	C-O	-5.12	1.18	1.24
1	B	237	ASN	C-O	-5.12	1.18	1.24
1	A	39	GLN	C-O	-5.12	1.18	1.24
1	A	223	ALA	C-O	-5.12	1.17	1.23
1	A	215	LEU	C-O	-5.10	1.18	1.24
2	D	614	LYS	C-O	-5.10	1.18	1.24
1	B	42	VAL	C-O	-5.10	1.18	1.24
2	C	456	ILE	C-O	-5.10	1.18	1.24
1	B	39	GLN	C-O	-5.10	1.18	1.24
2	C	508	ILE	C-O	-5.10	1.18	1.24
2	D	487	ASN	C-O	-5.10	1.17	1.23
1	A	183	LYS	C-O	-5.09	1.18	1.24
1	B	78	ARG	C-O	-5.09	1.18	1.24
2	C	201	ARG	C-O	-5.09	1.18	1.24
1	B	36	PRO	C-O	-5.09	1.18	1.23
1	B	85	PHE	C-O	-5.08	1.18	1.24
2	D	404	VAL	C-O	-5.08	1.18	1.24
1	B	28	GLU	C-O	-5.08	1.17	1.23
1	B	163	ASP	C-O	-5.08	1.18	1.24
1	A	118	ALA	C-O	-5.08	1.18	1.24
1	B	150	GLN	C-O	-5.07	1.18	1.24
2	C	504	VAL	C-O	-5.07	1.19	1.24
1	A	263	ASN	C-O	-5.07	1.17	1.24
2	C	64	GLN	C-O	-5.07	1.18	1.24
1	A	157	TYR	C-O	-5.07	1.18	1.24
1	A	119	PHE	C-O	-5.06	1.18	1.24
2	C	59	GLN	C-O	-5.06	1.18	1.24
1	B	110	GLY	C-O	-5.06	1.17	1.24
1	B	87	GLN	C-O	-5.06	1.18	1.24
1	B	168	LEU	C-O	-5.05	1.18	1.24
1	A	230	ALA	C-O	-5.05	1.18	1.24
1	A	126	ASP	C-O	-5.05	1.17	1.24
2	C	112	PHE	C-O	-5.05	1.18	1.24
2	C	428	GLU	C-O	-5.05	1.18	1.24
1	B	153	LEU	C-O	-5.04	1.18	1.24
1	B	61	ARG	C-O	-5.04	1.18	1.24
2	C	98	THR	C-O	-5.04	1.17	1.24
2	D	98	THR	C-O	-5.04	1.17	1.24
2	D	218	PHE	C-O	-5.04	1.18	1.24
1	A	251	ASP	C-O	-5.03	1.18	1.24
1	B	103	GLY	C-O	-5.03	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	ASP	C-O	-5.03	1.18	1.24
2	D	73	ARG	C-O	-5.02	1.18	1.24
2	D	50	SER	C-O	-5.00	1.18	1.24
2	C	73	ARG	C-O	-5.00	1.18	1.24

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	139	ASP	N-CA-C	13.76	126.30	111.03
2	D	140	PHE	N-CA-C	12.64	130.01	109.40
2	D	635	GLY	N-CA-C	11.38	126.38	112.73
1	B	196	GLU	N-CA-C	10.04	122.30	111.36
2	D	606	SER	N-CA-C	9.68	121.43	111.07
1	A	196	GLU	N-CA-C	9.52	121.43	111.14
1	B	22	THR	N-CA-C	-9.19	100.57	114.16
2	D	83	ASN	N-CA-C	9.18	125.66	113.72
2	C	157	LYS	N-CA-C	8.41	121.57	111.82
2	D	648	ASP	N-CA-C	-8.39	94.91	108.41
1	B	78	ARG	N-CA-C	8.26	120.36	111.36
2	C	568	GLU	N-CA-C	8.14	123.54	112.55
2	D	643	ASP	N-CA-C	-8.10	100.45	110.65
2	D	625	ALA	N-CA-C	8.07	123.19	112.13
2	D	618	GLU	N-CA-C	-7.99	102.53	111.71
2	D	288	THR	N-CA-C	7.82	119.81	111.28
2	D	180	THR	N-CA-C	-7.81	102.08	111.69
2	D	522	LYS	N-CA-C	7.66	119.71	111.36
2	D	628	ASN	N-CA-C	7.66	119.70	111.36
2	D	440	GLY	N-CA-C	7.65	121.18	112.00
2	D	639	LEU	N-CA-C	7.65	121.69	108.76
1	B	146	ASP	N-CA-C	7.60	119.56	111.28
2	C	413	ALA	N-CA-C	7.21	120.84	110.24
2	D	298	TRP	N-CA-C	7.17	121.18	109.85
2	D	614	LYS	N-CA-C	-7.02	103.56	111.07
1	A	146	ASP	N-CA-C	6.97	118.88	111.28
2	C	242	SER	N-CA-C	6.96	119.89	111.82
2	C	320	LEU	N-CA-C	-6.92	98.53	109.04
2	D	612	ARG	CA-C-N	6.89	134.70	121.54
2	D	612	ARG	C-N-CA	6.89	134.70	121.54
2	C	383	GLN	N-CA-C	-6.87	94.97	107.75
2	D	568	GLU	N-CA-C	6.84	122.87	113.16
2	D	273	SER	N-CA-C	6.73	118.61	111.28
2	C	290	LYS	N-CA-C	6.72	120.75	109.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	273	SER	N-CA-C	-6.58	96.16	107.61
1	A	112	PHE	N-CA-C	6.56	118.43	111.28
2	C	227	ASN	N-CA-C	6.45	118.97	109.24
2	D	227	ASN	N-CA-C	6.43	118.95	109.24
2	D	319	ILE	N-CA-C	6.41	117.15	108.17
1	A	267	ASN	N-CA-C	6.40	120.92	113.18
2	D	616	ASN	N-CA-C	6.38	117.90	111.07
2	D	81	SER	N-CA-C	-6.33	98.95	109.46
2	D	474	THR	N-CA-C	6.32	118.03	110.19
2	D	627	LEU	N-CA-C	-6.30	104.46	111.71
2	D	613	GLU	CA-C-N	-6.29	112.26	120.44
2	D	613	GLU	C-N-CA	-6.29	112.26	120.44
2	D	206	ASN	CB-CA-C	-6.28	99.44	109.80
2	C	252	LEU	N-CA-C	6.27	119.00	110.35
2	D	262	ASN	N-CA-C	6.22	118.14	111.36
2	D	613	GLU	N-CA-CB	6.22	121.00	110.49
2	D	451	ALA	N-CA-C	6.18	118.58	109.24
2	D	53	THR	N-CA-C	6.14	118.95	111.82
2	D	248	ILE	N-CA-C	6.11	118.77	112.90
2	D	612	ARG	N-CA-C	-6.09	100.63	109.59
3	F	5	ALA	N-CA-C	6.08	118.65	109.23
2	C	324	LYS	N-CA-C	6.07	118.34	108.08
2	C	467	ALA	N-CA-C	6.07	118.18	109.14
2	C	189	GLU	N-CA-C	6.04	123.66	110.80
2	D	139	ASP	CA-C-N	-6.02	113.91	122.94
2	D	139	ASP	C-N-CA	-6.02	113.91	122.94
2	C	326	THR	N-CA-C	6.01	119.31	110.30
2	D	466	ARG	N-CA-C	6.01	117.63	111.14
2	C	223	ASP	N-CA-C	5.96	113.58	108.22
2	D	588	ILE	N-CA-C	-5.94	104.94	110.53
2	C	53	THR	N-CA-C	5.94	117.83	111.36
2	C	139	ASP	CB-CA-C	-5.93	101.76	110.95
2	C	410	PHE	CA-C-N	-5.93	118.17	123.33
2	C	410	PHE	C-N-CA	-5.93	118.17	123.33
2	D	611	VAL	N-CA-C	5.91	116.10	110.42
2	D	613	GLU	N-CA-C	-5.89	98.26	110.80
2	D	635	GLY	CA-C-N	5.88	132.28	121.70
2	D	635	GLY	C-N-CA	5.88	132.28	121.70
2	D	93	PHE	N-CA-C	5.82	118.56	111.82
2	D	110	ASP	N-CA-C	5.78	117.25	111.07
2	D	244	SER	N-CA-C	5.78	118.06	108.99
2	C	475	PHE	N-CA-C	5.75	118.33	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	255	ASP	N-CA-C	-5.73	102.31	111.02
2	D	322	ALA	N-CA-C	5.72	119.36	112.38
1	B	193	SER	N-CA-C	5.70	117.89	110.53
2	D	509	GLN	N-CA-C	5.70	117.52	108.79
1	A	235	GLU	CB-CA-C	-5.68	101.96	110.88
1	B	266	HIS	N-CA-C	5.65	117.44	111.28
1	A	53	SER	N-CA-C	-5.62	101.32	110.20
2	D	641	LYS	N-CA-C	-5.62	104.53	111.33
2	C	194	ARG	CB-CA-C	-5.60	102.09	110.88
2	D	635	GLY	CA-C-O	-5.59	114.99	120.75
2	D	653	ASP	CA-C-N	5.57	125.24	119.05
2	D	653	ASP	C-N-CA	5.57	125.24	119.05
1	A	222	ASP	N-CA-C	5.57	117.43	111.36
2	C	474	THR	N-CA-C	5.51	117.95	110.35
2	D	582	ASP	N-CA-C	5.49	117.38	109.48
2	D	489	ILE	N-CA-C	5.40	117.81	111.05
2	D	97	LYS	N-CA-C	5.39	118.96	112.38
1	A	55	ALA	N-CA-C	5.36	118.04	111.82
2	D	139	ASP	N-CA-C	-5.32	99.61	108.34
2	C	41	HIS	N-CA-C	5.32	117.08	111.28
2	C	244	SER	N-CA-C	5.32	117.90	109.50
1	A	266	HIS	N-CA-C	5.31	117.06	111.28
2	C	451	ALA	N-CA-C	5.30	117.24	109.24
2	C	222	ILE	N-CA-C	5.29	115.39	110.42
1	A	32	VAL	N-CA-C	-5.29	103.77	108.95
2	C	529	ILE	N-CA-C	5.29	115.71	107.99
2	D	592	ILE	N-CA-C	5.28	115.50	110.53
2	D	258	TYR	N-CA-C	5.27	117.98	109.40
1	A	273	TYR	CB-CA-C	5.25	120.76	110.67
5	G	2	SER	N-CA-C	5.22	117.13	108.20
2	C	300	LEU	N-CA-C	5.21	116.96	111.28
2	D	167	ASP	N-CA-C	-5.21	105.50	111.07
2	D	83	ASN	CB-CA-C	-5.19	100.83	109.55
2	D	145	THR	N-CA-C	5.19	118.18	110.14
1	A	130	ASN	N-CA-C	5.17	116.91	111.28
1	B	22	THR	CB-CA-C	5.16	118.31	110.37
2	D	598	MET	N-CA-C	5.13	119.50	112.88
1	A	91	ILE	N-CA-C	5.12	115.35	110.53
2	C	258	TYR	N-CA-C	5.10	117.56	109.50
2	D	223	ASP	CB-CA-C	5.10	116.95	110.22
1	A	177	LEU	N-CA-C	5.07	116.66	111.03
2	C	307	ILE	N-CA-C	5.04	115.76	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	27	THR	N-CA-C	5.03	119.02	112.13
2	C	97	LYS	N-CA-C	5.03	117.49	111.71
2	D	307	ILE	N-CA-C	5.02	115.25	110.53
2	D	587	ASN	N-CA-CB	5.02	118.72	110.39

There are no chirality outliers.

There are no planarity outliers.

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	A	2190	0	2114	25	0
1	B	2176	0	2100	25	0
2	C	5140	0	5151	273	0
2	D	5139	0	5156	347	0
3	F	30	0	32	2	0
3	H	30	0	32	5	0
4	E	21	0	22	1	0
5	G	32	0	36	2	0
6	A	250	0	0	2	0
6	B	251	0	0	4	0
6	C	203	0	0	5	0
6	D	241	0	0	5	0
6	F	1	0	0	0	0
All	All	15704	0	14643	669	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 23.

All (669) 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)
2:D:640:LYS:HG3	2:D:643:ASP:CB	1.34	1.56
2:D:640:LYS:CG	2:D:643:ASP:HB2	1.29	1.53
2:D:393:ARG:HH11	2:D:445:LEU:CD1	1.55	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:LEU:CD2	2:D:179:LEU:HD11	1.73	1.17
2:C:264:MET:HE2	2:C:271:ALA:HA	1.27	1.15
2:C:292:MET:HE2	2:C:318:GLU:HB2	1.29	1.15
2:C:292:MET:CE	2:C:318:GLU:HB2	1.77	1.14
2:C:608:ASN:HB3	2:C:611:VAL:CG1	1.76	1.14
2:D:455:GLU:HG2	2:D:474:THR:HG21	1.14	1.13
2:C:139:ASP:HB3	2:C:141:THR:HG22	1.16	1.12
2:D:175:LEU:HD23	2:D:179:LEU:CD1	1.78	1.12
2:D:175:LEU:HD21	2:D:179:LEU:HD11	1.19	1.11
2:D:175:LEU:CD2	2:D:179:LEU:CD1	2.28	1.11
2:D:175:LEU:HD23	2:D:179:LEU:HD12	1.24	1.11
2:D:26:ILE:HG23	2:D:31:GLN:HB3	1.32	1.09
2:D:182:LYS:HZ3	2:D:186:GLU:HG3	1.04	1.09
2:D:28:ARG:HD3	2:D:31:GLN:HE22	1.18	1.09
2:D:393:ARG:HH11	2:D:445:LEU:HD11	1.04	1.08
2:C:567:PHE:CD1	2:C:669:LEU:HD13	1.87	1.08
2:D:126:ARG:HG2	2:D:166:TRP:CE2	1.88	1.07
2:D:461:MET:CE	2:D:466:ARG:HG2	1.85	1.06
2:C:139:ASP:HB3	2:C:141:THR:CG2	1.85	1.06
2:C:563:ASP:OD1	2:C:565:THR:HG22	1.54	1.06
2:C:264:MET:CE	2:C:271:ALA:HA	1.85	1.06
2:C:283:VAL:HG23	2:C:296:ILE:CG1	1.85	1.06
2:D:182:LYS:NZ	2:D:186:GLU:HG3	1.70	1.06
2:C:139:ASP:CB	2:C:141:THR:HG22	1.86	1.05
2:D:633:ARG:HB2	2:D:633:ARG:HH21	1.15	1.05
2:C:283:VAL:HG23	2:C:296:ILE:HG13	1.33	1.04
2:D:614:LYS:O	2:D:618:GLU:HB3	1.59	1.03
2:C:290:LYS:HB3	2:C:291:PRO:HD2	1.41	1.02
2:D:177:LEU:HD21	2:D:190:THR:HG21	1.36	1.02
2:D:455:GLU:CG	2:D:474:THR:HG21	1.89	1.02
2:C:567:PHE:O	2:C:571:LEU:HD12	1.60	1.02
2:C:292:MET:CE	2:C:318:GLU:N	2.21	1.01
2:D:393:ARG:NH1	2:D:445:LEU:CD1	2.23	1.01
2:D:393:ARG:NH1	2:D:445:LEU:HD11	1.74	1.01
2:C:568:GLU:HB3	2:C:569:PRO:HD3	1.37	1.01
2:D:631:PHE:HA	2:D:637:PRO:CD	1.88	1.01
2:C:567:PHE:CD1	2:C:669:LEU:CD1	2.44	1.00
2:C:608:ASN:OD1	2:C:611:VAL:HG12	1.58	1.00
2:D:26:ILE:CG2	2:D:31:GLN:HB3	1.90	1.00
2:D:631:PHE:CD1	2:D:637:PRO:HG2	1.97	0.99
2:C:292:MET:HE1	2:C:318:GLU:N	1.77	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:631:PHE:CB	2:D:637:PRO:HD2	1.93	0.98
2:D:631:PHE:CA	2:D:637:PRO:HD2	1.94	0.98
2:C:608:ASN:HB3	2:C:611:VAL:HG11	1.43	0.98
2:D:631:PHE:HA	2:D:637:PRO:HD2	1.46	0.98
2:C:299:ARG:HG2	2:C:302:ASP:OD2	1.64	0.97
2:D:393:ARG:HD3	2:D:445:LEU:HD13	1.45	0.95
2:D:626:ARG:HH21	2:D:629:GLU:HG2	1.30	0.95
2:D:318:GLU:OE2	2:D:328:THR:HG23	1.66	0.95
1:A:22:THR:HB	1:A:25:ARG:NH1	1.81	0.94
2:D:126:ARG:HG2	2:D:166:TRP:NE1	1.83	0.94
2:C:292:MET:HE2	2:C:318:GLU:CB	1.97	0.93
2:D:642:LEU:HD13	2:D:644:ASP:HB2	1.50	0.93
2:C:26:ILE:HD12	2:C:26:ILE:H	1.29	0.93
2:C:197:PHE:CE2	2:C:256:ASP:HB3	2.04	0.93
2:C:197:PHE:CE1	2:C:200:ARG:NH2	2.37	0.92
2:D:134:LEU:HD23	2:D:188:ARG:HG2	1.49	0.92
2:D:474:THR:HG22	2:D:475:PHE:H	1.34	0.91
2:C:608:ASN:CG	2:C:611:VAL:HG12	1.96	0.90
2:D:461:MET:HE3	2:D:466:ARG:HG2	1.51	0.90
2:D:182:LYS:HZ3	2:D:186:GLU:CG	1.83	0.90
2:D:347:MET:HE3	2:D:380:LEU:HD21	1.50	0.90
2:C:26:ILE:HG22	2:C:31:GLN:HB3	1.53	0.89
2:C:609:TYR:CE2	2:C:613:GLU:HG3	2.08	0.89
2:D:579:ILE:HG22	2:D:585:PHE:CD2	2.08	0.89
2:D:640:LYS:CB	2:D:643:ASP:HB2	2.01	0.89
2:C:188:ARG:HH11	2:C:188:ARG:HG2	1.34	0.89
2:C:563:ASP:O	2:C:564:LEU:HD23	1.72	0.89
2:D:177:LEU:CD2	2:D:190:THR:HG21	2.02	0.88
2:D:26:ILE:HG23	2:D:31:GLN:CB	2.03	0.88
2:C:264:MET:CE	2:C:271:ALA:CA	2.51	0.88
1:A:22:THR:HB	1:A:25:ARG:HH12	1.36	0.88
2:D:633:ARG:HB2	2:D:633:ARG:NH2	1.89	0.88
2:C:538:GLU:OE1	2:C:538:GLU:N	2.05	0.87
2:C:264:MET:HE2	2:C:271:ALA:CA	2.04	0.87
2:C:343:ARG:O	2:C:363:PRO:HG2	1.75	0.87
2:D:650:GLN:O	2:D:650:GLN:NE2	2.08	0.87
2:C:608:ASN:CB	2:C:611:VAL:HG12	2.05	0.86
2:C:139:ASP:CG	2:C:141:THR:CG2	2.48	0.86
2:D:602:ARG:HB3	2:D:602:ARG:HH11	1.41	0.86
2:D:26:ILE:HD12	2:D:26:ILE:H	1.41	0.86
2:D:310:PRO:O	2:D:313:SER:HB2	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:563:ASP:C	2:C:564:LEU:HD23	2.01	0.85
2:C:382:LYS:HD2	2:C:383:GLN:HG2	1.59	0.85
2:C:347:MET:HE3	2:C:347:MET:O	1.75	0.84
2:D:587:ASN:O	2:D:591:ASP:HB2	1.78	0.84
2:D:521:ARG:O	2:D:542:LYS:HE2	1.77	0.84
2:D:126:ARG:CG	2:D:166:TRP:CE2	2.61	0.83
2:C:608:ASN:CB	2:C:611:VAL:CG1	2.56	0.83
2:C:608:ASN:HB3	2:C:611:VAL:HG12	1.58	0.83
2:C:175:LEU:O	2:C:175:LEU:HD12	1.79	0.82
2:D:570:GLU:HA	2:D:573:LYS:HE3	1.60	0.82
2:D:28:ARG:HD3	2:D:31:GLN:NE2	1.92	0.82
2:C:139:ASP:CB	2:C:141:THR:CG2	2.52	0.82
2:D:579:ILE:CG2	2:D:585:PHE:CD2	2.61	0.82
2:C:347:MET:HE3	2:C:347:MET:C	2.04	0.82
2:D:140:PHE:O	2:D:609:TYR:CD1	2.32	0.82
2:C:292:MET:HE3	2:C:318:GLU:HB2	1.61	0.82
2:C:264:MET:HE3	2:C:270:ALA:C	2.05	0.81
2:D:631:PHE:HB3	2:D:636:LYS:HB2	1.62	0.81
2:C:354:LYS:H	2:C:354:LYS:HD2	1.44	0.81
2:C:299:ARG:CG	2:C:302:ASP:OD2	2.28	0.80
2:D:126:ARG:CG	2:D:166:TRP:NE1	2.44	0.80
2:D:585:PHE:O	2:D:586:GLN:NE2	2.14	0.80
2:C:336:GLU:O	2:C:338:ILE:HD12	1.81	0.80
2:D:134:LEU:CD2	2:D:188:ARG:HG2	2.10	0.80
2:C:264:MET:CE	2:C:270:ALA:C	2.54	0.79
2:C:223:ASP:HB2	2:C:224:PRO:HD2	1.65	0.79
2:D:626:ARG:NH2	2:D:629:GLU:HG2	1.96	0.79
2:C:567:PHE:HD1	2:C:669:LEU:CD1	1.96	0.79
2:C:669:LEU:HD22	2:C:669:LEU:O	1.83	0.79
2:D:474:THR:HG22	2:D:475:PHE:N	1.98	0.79
2:D:175:LEU:HD12	2:D:609:TYR:CE1	2.19	0.78
2:D:450:SER:O	2:D:474:THR:HG23	1.83	0.78
2:C:292:MET:CE	2:C:318:GLU:H	1.96	0.78
2:D:461:MET:HE3	2:D:466:ARG:CG	2.13	0.78
2:D:484:ARG:HH21	2:D:484:ARG:HG3	1.47	0.78
2:C:166:TRP:O	2:C:170:VAL:HG13	1.83	0.78
2:D:318:GLU:OE2	2:D:328:THR:CG2	2.31	0.78
2:D:608:ASN:HB3	2:D:611:VAL:HG12	1.65	0.78
1:A:163:ASP:OD2	1:A:166:ARG:HD2	1.84	0.78
2:C:264:MET:CE	2:C:271:ALA:N	2.46	0.78
2:C:178:LYS:HE3	2:C:609:TYR:CE1	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:283:VAL:CG2	2:C:296:ILE:HG13	2.12	0.77
2:D:357:VAL:HG22	2:D:387:SER:HB2	1.66	0.77
2:D:627:LEU:HD12	2:D:627:LEU:H	1.50	0.77
2:D:29:ALA:O	2:D:32:ILE:HG22	1.84	0.77
2:D:177:LEU:HD13	2:D:191:LEU:CD1	2.15	0.77
2:D:563:ASP:OD1	2:D:565:THR:HG22	1.85	0.77
2:C:87:ALA:O	2:C:91:GLU:HG2	1.84	0.76
2:C:600:ASP:HB2	2:C:601:LYS:HD3	1.68	0.76
2:D:86:LEU:HD21	2:D:162:LEU:CD1	2.15	0.76
2:D:461:MET:CE	2:D:466:ARG:CG	2.64	0.76
2:D:614:LYS:O	2:D:618:GLU:CB	2.35	0.75
2:D:631:PHE:CG	2:D:637:PRO:HD2	2.22	0.75
2:C:283:VAL:HG21	2:C:296:ILE:HD11	1.68	0.75
2:D:627:LEU:H	2:D:627:LEU:CD1	1.96	0.75
2:C:128:GLN:HA	2:C:131:LEU:HD12	1.67	0.75
2:C:596:ASN:HA	2:C:599:LYS:HE3	1.69	0.75
2:C:292:MET:CE	2:C:318:GLU:CB	2.57	0.75
2:D:186:GLU:O	2:D:189:GLU:N	2.20	0.74
2:C:354:LYS:HD3	2:C:355:GLU:HG2	1.68	0.74
2:C:448:ARG:NH2	2:C:532:THR:CG2	2.50	0.74
2:D:642:LEU:HD12	2:D:642:LEU:O	1.88	0.74
2:C:139:ASP:OD2	2:C:141:THR:CG2	2.36	0.74
2:D:596:ASN:HA	2:D:599:LYS:HE2	1.70	0.74
2:D:134:LEU:HD21	2:D:188:ARG:HA	1.69	0.74
2:C:283:VAL:CG2	2:C:296:ILE:HD11	2.17	0.73
2:C:292:MET:HE1	2:C:317:LEU:C	2.13	0.73
2:C:651:GLU:HG3	2:C:652:PRO:HD2	1.70	0.73
6:C:803:HOH:O	3:H:1:ALA:HA	1.86	0.73
2:C:264:MET:HE3	2:C:271:ALA:N	2.03	0.73
2:D:393:ARG:HH11	2:D:445:LEU:HD13	1.52	0.73
2:D:150:ARG:HG2	2:D:150:ARG:HH11	1.53	0.73
2:D:393:ARG:CD	2:D:445:LEU:HD13	2.18	0.73
2:C:193:ARG:HH12	2:C:256:ASP:CG	1.97	0.73
2:D:639:LEU:O	2:D:640:LYS:HD3	1.89	0.73
2:D:175:LEU:O	2:D:179:LEU:HD12	1.89	0.72
2:C:608:ASN:O	2:C:611:VAL:HG13	1.88	0.72
2:C:290:LYS:HB3	2:C:291:PRO:CD	2.18	0.72
2:C:197:PHE:CZ	2:C:256:ASP:HB3	2.25	0.72
2:C:448:ARG:HH21	2:C:532:THR:HG22	1.53	0.72
2:D:137:PRO:C	2:D:138:MET:HG2	2.14	0.72
2:D:614:LYS:HD2	2:D:614:LYS:C	2.13	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:ILE:HD12	2:D:26:ILE:N	2.03	0.72
2:D:631:PHE:HA	2:D:637:PRO:HD3	1.71	0.72
2:C:568:GLU:HB3	2:C:569:PRO:CD	2.18	0.71
1:B:163:ASP:HB3	1:B:166:ARG:HG3	1.71	0.71
2:D:647:LYS:H	2:D:647:LYS:HD3	1.55	0.71
2:D:582:ASP:HB3	2:D:585:PHE:HB2	1.72	0.71
2:D:626:ARG:HD2	2:D:629:GLU:HB3	1.72	0.71
2:D:640:LYS:HG3	2:D:643:ASP:CG	2.14	0.71
2:C:281:LYS:HE2	2:C:322:ALA:HA	1.72	0.70
2:C:197:PHE:HE1	2:C:200:ARG:HH22	1.38	0.70
2:D:450:SER:O	2:D:474:THR:CG2	2.39	0.70
2:C:307:ILE:O	2:C:335:ARG:NH1	2.24	0.70
2:C:435:GLN:OE1	2:C:435:GLN:HA	1.90	0.70
1:A:63:GLN:NE2	1:A:67:GLU:OE2	2.22	0.70
2:C:144:ASP:OD2	2:C:171:LYS:NZ	2.23	0.70
2:D:177:LEU:CD1	2:D:191:LEU:HD11	2.20	0.70
2:C:26:ILE:HD12	2:C:26:ILE:N	2.04	0.70
2:C:448:ARG:NH2	2:C:532:THR:HG22	2.07	0.70
2:D:177:LEU:CD1	2:D:191:LEU:CD1	2.70	0.70
2:C:567:PHE:O	2:C:571:LEU:CD1	2.37	0.69
2:D:602:ARG:HB3	2:D:602:ARG:NH1	2.05	0.69
2:C:284:GLY:C	2:C:292:MET:HE3	2.17	0.69
2:D:420:ARG:HD3	2:D:424:GLY:HA2	1.74	0.69
2:D:144:ASP:O	2:D:607:LEU:HB2	1.93	0.69
2:C:563:ASP:CG	2:C:565:THR:HG22	2.18	0.69
2:C:578:ARG:HA	2:C:581:LYS:HE3	1.75	0.69
2:D:177:LEU:HD21	2:D:190:THR:CG2	2.17	0.69
2:D:186:GLU:HA	2:D:186:GLU:OE1	1.92	0.69
2:D:586:GLN:NE2	2:D:586:GLN:HA	2.07	0.69
2:D:175:LEU:HD23	2:D:175:LEU:C	2.18	0.69
2:D:522:LYS:HD2	2:D:550:TRP:CD1	2.28	0.69
2:C:283:VAL:CG2	2:C:296:ILE:CD1	2.72	0.68
2:C:178:LYS:HE3	2:C:609:TYR:CD1	2.28	0.68
2:D:150:ARG:HG2	2:D:150:ARG:NH1	2.07	0.68
2:D:175:LEU:HD23	2:D:175:LEU:O	1.93	0.68
2:D:201:ARG:HH12	2:D:202:LEU:HD23	1.58	0.68
2:C:200:ARG:NH2	2:C:257:ASP:OD2	2.27	0.68
2:D:86:LEU:HD21	2:D:162:LEU:HD12	1.74	0.68
2:D:389:ILE:CD1	2:D:659:THR:HG22	2.24	0.68
2:C:139:ASP:CG	2:C:141:THR:HG21	2.19	0.67
2:C:600:ASP:HB2	2:C:601:LYS:CD	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:TRP:O	1:B:26:LYS:N	2.28	0.67
2:C:283:VAL:HG23	2:C:296:ILE:CD1	2.24	0.67
2:C:448:ARG:HH21	2:C:532:THR:CG2	2.07	0.67
2:D:631:PHE:CD1	2:D:637:PRO:CG	2.76	0.67
1:A:22:THR:CB	1:A:25:ARG:HH12	2.07	0.67
2:D:497:GLU:OE1	2:D:497:GLU:N	2.23	0.67
2:D:133:VAL:HG11	2:D:170:VAL:HG11	1.74	0.67
2:C:342:ASP:OD2	5:G:3:ARG:NH2	2.28	0.66
1:B:191:GLU:OE1	1:B:191:GLU:HA	1.94	0.66
2:C:567:PHE:HD1	2:C:669:LEU:HD11	1.60	0.66
2:D:133:VAL:CG1	2:D:170:VAL:HG11	2.26	0.66
2:D:177:LEU:HD13	2:D:191:LEU:HD13	1.75	0.66
2:D:650:GLN:CD	2:D:650:GLN:H	2.03	0.66
1:B:176:LYS:HE3	6:B:413:HOH:O	1.96	0.66
2:D:631:PHE:O	2:D:636:LYS:HA	1.96	0.65
2:C:472:GLU:OE2	2:C:532:THR:CG2	2.44	0.65
2:D:389:ILE:HD13	2:D:659:THR:HG22	1.78	0.65
2:D:420:ARG:HG3	2:D:426:VAL:HG22	1.78	0.65
2:C:232:ARG:NH1	2:C:301:ASP:HB2	2.12	0.65
2:D:343:ARG:HE	2:D:363:PRO:HB2	1.61	0.65
1:A:78:ARG:NH2	6:A:303:HOH:O	2.29	0.65
2:C:139:ASP:OD2	2:C:141:THR:HG21	1.96	0.65
2:D:393:ARG:NH1	2:D:445:LEU:HD13	2.10	0.64
2:C:264:MET:HE1	2:C:270:ALA:O	1.96	0.64
2:C:310:PRO:O	2:C:313:SER:HB2	1.97	0.64
2:C:81:SER:O	2:C:83:ASN:N	2.30	0.64
2:D:624:LEU:HD21	2:D:642:LEU:HB2	1.79	0.64
2:D:182:LYS:HB3	2:D:187:ILE:CD1	2.27	0.64
2:D:484:ARG:HG3	2:D:484:ARG:NH2	2.09	0.64
2:D:587:ASN:O	2:D:591:ASP:CB	2.46	0.64
1:A:49:GLN:NE2	1:A:49:GLN:HA	2.13	0.64
2:C:178:LYS:CE	2:C:609:TYR:CD1	2.81	0.64
2:D:631:PHE:HB3	2:D:637:PRO:HD2	1.80	0.64
2:D:455:GLU:CD	2:D:474:THR:HG21	2.22	0.64
2:D:474:THR:CG2	2:D:475:PHE:H	2.09	0.64
2:C:188:ARG:HG2	2:C:188:ARG:NH1	2.12	0.64
2:D:26:ILE:CG2	2:D:31:GLN:CB	2.68	0.63
2:D:563:ASP:OD1	2:D:565:THR:CG2	2.45	0.63
2:C:223:ASP:HB2	2:C:224:PRO:CD	2.27	0.63
2:D:223:ASP:OD2	2:D:507:THR:HG21	1.98	0.63
2:C:188:ARG:HH11	2:C:188:ARG:CG	2.10	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:178:LYS:HD2	2:D:609:TYR:HE2	1.62	0.63
2:D:207:SER:O	2:D:210:VAL:HG13	1.99	0.63
2:D:126:ARG:HD3	2:D:166:TRP:CD1	2.33	0.62
2:D:237:PHE:CZ	2:D:241:MET:HE3	2.34	0.62
2:C:290:LYS:CB	2:C:291:PRO:HD2	2.23	0.62
2:C:584:GLU:O	2:C:588:ILE:HG13	1.98	0.62
2:D:223:ASP:HB2	2:D:224:PRO:HD3	1.80	0.62
2:D:267:GLY:O	2:D:272:LYS:HE2	2.00	0.62
2:D:461:MET:HE2	2:D:466:ARG:HG2	1.76	0.62
2:D:594:ARG:O	2:D:598:MET:HE3	1.98	0.62
2:D:126:ARG:HG2	2:D:166:TRP:CZ2	2.34	0.62
2:D:606:SER:HB3	2:D:612:ARG:HD3	1.81	0.62
2:C:452:SER:HB2	3:H:4:ALA:O	1.99	0.61
2:D:223:ASP:HB2	2:D:224:PRO:CD	2.30	0.61
2:C:252:LEU:HD11	2:C:307:ILE:HD13	1.82	0.61
2:C:256:ASP:C	2:C:258:TYR:H	2.08	0.61
2:D:212:SER:O	2:D:216:THR:HG23	2.01	0.61
2:D:623:ARG:O	2:D:627:LEU:HD11	2.01	0.61
2:D:452:SER:HB3	3:F:4:ALA:O	2.01	0.61
2:D:347:MET:HE3	2:D:380:LEU:CD2	2.28	0.61
1:B:22:THR:HA	1:B:24:TRP:CD1	2.36	0.60
2:C:292:MET:CE	2:C:318:GLU:CA	2.78	0.60
2:C:292:MET:HE2	2:C:318:GLU:CA	2.32	0.60
2:C:354:LYS:HD2	2:C:354:LYS:N	2.16	0.60
2:D:647:LYS:H	2:D:647:LYS:CD	2.12	0.60
2:D:182:LYS:HB3	2:D:187:ILE:HD11	1.83	0.60
2:D:627:LEU:HD12	2:D:627:LEU:N	2.16	0.60
2:C:81:SER:HB2	6:C:701:HOH:O	2.01	0.60
2:D:178:LYS:HD3	2:D:609:TYR:CD2	2.35	0.60
2:C:199:ILE:O	2:C:202:LEU:HB2	2.02	0.60
2:D:411:ILE:HD11	2:D:466:ARG:HB2	1.84	0.60
2:C:256:ASP:O	2:C:258:TYR:N	2.34	0.60
1:B:188:GLN:O	1:B:192:LYS:HB2	2.02	0.59
2:C:609:TYR:CZ	2:C:613:GLU:HG3	2.37	0.59
2:D:579:ILE:HG22	2:D:585:PHE:CG	2.37	0.59
2:D:631:PHE:HB3	2:D:636:LYS:CB	2.32	0.59
1:A:187:LYS:O	1:A:191:GLU:HG2	2.03	0.59
2:C:196:LYS:NZ	2:C:200:ARG:HE	2.01	0.59
2:C:472:GLU:OE2	2:C:532:THR:HG22	2.03	0.59
1:B:24:TRP:C	1:B:26:LYS:N	2.60	0.59
2:C:40:GLN:O	2:C:44:VAL:HG23	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:LYS:HG2	2:C:186:GLU:HG3	1.83	0.59
2:D:411:ILE:HG12	2:D:461:MET:HE1	1.85	0.59
2:C:369:LEU:O	2:C:373:VAL:HG23	2.02	0.59
2:C:236:GLN:O	2:C:240:GLU:HG3	2.03	0.59
2:D:145:THR:OG1	2:D:604:ILE:HG23	2.03	0.59
2:D:137:PRO:HA	2:D:188:ARG:HH22	1.68	0.59
1:B:78:ARG:NH1	6:B:303:HOH:O	2.35	0.58
2:C:183:THR:O	2:C:187:ILE:HG13	2.03	0.58
2:C:206:ASN:OD1	2:C:209:ASP:OD2	2.21	0.58
1:B:184:GLU:OE2	1:B:187:LYS:HE2	2.04	0.58
2:C:73:ARG:NH2	2:C:545:ASP:OD2	2.36	0.58
2:D:187:ILE:HD13	2:D:187:ILE:H	1.68	0.58
2:D:600:ASP:OD1	2:D:601:LYS:HG2	2.03	0.58
2:C:452:SER:CB	3:H:4:ALA:O	2.51	0.58
2:C:608:ASN:O	2:C:611:VAL:CG1	2.52	0.58
2:D:474:THR:OG1	2:D:524:VAL:HG13	2.04	0.58
2:D:182:LYS:HG3	2:D:186:GLU:HG3	1.86	0.57
2:D:223:ASP:CB	2:D:224:PRO:CD	2.82	0.57
2:C:264:MET:HE1	2:C:270:ALA:C	2.29	0.57
2:D:585:PHE:C	2:D:586:GLN:HE21	2.12	0.57
2:D:609:TYR:HD1	2:D:609:TYR:H	1.52	0.57
2:D:508:ILE:HG13	2:D:509:GLN:HG2	1.86	0.57
2:C:309:GLY:HA3	2:C:335:ARG:NE	2.20	0.57
2:D:148:LEU:HD12	2:D:603:ASN:O	2.04	0.57
2:C:64:GLN:HG2	2:C:98:THR:HB	1.87	0.56
2:D:513:ARG:HB2	2:D:515:ASN:HB2	1.86	0.56
1:B:24:TRP:C	1:B:26:LYS:H	2.13	0.56
2:C:283:VAL:CG2	2:C:296:ILE:CG1	2.70	0.56
2:C:645:LEU:HD12	2:C:646:PRO:HD2	1.86	0.56
2:D:178:LYS:HD2	2:D:609:TYR:CE2	2.41	0.56
1:B:198:TRP:CH2	1:B:219:LEU:HA	2.39	0.56
2:C:316:ARG:HG2	2:C:332:THR:OG1	2.06	0.56
2:D:144:ASP:O	2:D:607:LEU:CB	2.53	0.56
2:D:297:GLY:C	2:D:298:TRP:HD1	2.13	0.56
2:C:284:GLY:HA3	2:C:292:MET:HE3	1.87	0.56
2:D:461:MET:HE3	2:D:466:ARG:CB	2.35	0.56
2:C:290:LYS:CB	2:C:291:PRO:CD	2.82	0.56
2:C:328:THR:O	2:C:328:THR:HG23	2.05	0.56
2:D:313:SER:HB3	2:D:335:ARG:HD2	1.88	0.56
2:C:232:ARG:NH1	2:C:301:ASP:CB	2.69	0.56
2:D:177:LEU:HD13	2:D:191:LEU:HD11	1.84	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ASN:HB2	2:D:209:ASP:OD2	2.06	0.56
2:D:579:ILE:CG2	2:D:585:PHE:CE2	2.89	0.56
2:D:347:MET:HE1	2:D:349:VAL:HG23	1.87	0.56
2:D:644:ASP:O	2:D:645:LEU:HD12	2.06	0.56
1:B:21:ASN:N	6:B:304:HOH:O	2.39	0.55
2:C:292:MET:HE3	2:C:318:GLU:H	1.70	0.55
2:D:38:GLU:HB2	2:D:41:HIS:CE1	2.41	0.55
2:D:480:VAL:HB	2:D:509:GLN:HG3	1.86	0.55
2:D:579:ILE:HG21	2:D:585:PHE:CD2	2.41	0.55
2:C:342:ASP:OD1	2:C:342:ASP:N	2.30	0.55
2:D:81:SER:O	2:D:83:ASN:N	2.35	0.55
2:D:626:ARG:NH2	2:D:629:GLU:CG	2.66	0.55
2:D:212:SER:O	2:D:216:THR:CG2	2.55	0.55
2:D:73:ARG:HD2	2:D:217:ALA:O	2.06	0.55
2:D:631:PHE:CA	2:D:637:PRO:CD	2.63	0.55
2:C:652:PRO:O	2:C:654:PRO:HD3	2.05	0.55
2:D:178:LYS:HD3	2:D:609:TYR:HD2	1.72	0.55
2:D:640:LYS:HG3	2:D:643:ASP:CA	2.28	0.55
2:C:609:TYR:C	2:C:609:TYR:CD2	2.85	0.55
2:D:148:LEU:HD12	2:D:603:ASN:C	2.32	0.55
2:C:461:MET:HA	2:C:461:MET:HE2	1.88	0.54
1:A:22:THR:CG2	1:A:25:ARG:HH12	2.19	0.54
2:D:318:GLU:OE1	2:D:330:THR:HB	2.08	0.54
2:D:595:PHE:C	2:D:595:PHE:CD1	2.85	0.54
2:D:613:GLU:O	2:D:617:ASN:N	2.28	0.54
2:D:71:PHE:CE2	2:D:75:LEU:HD11	2.43	0.54
1:A:191:GLU:OE1	1:A:191:GLU:HA	2.07	0.54
2:C:188:ARG:O	2:C:192:THR:OG1	2.22	0.54
2:C:102:ASP:OD1	2:C:105:ARG:NH2	2.37	0.54
2:D:579:ILE:HG21	2:D:585:PHE:CE2	2.43	0.54
2:C:38:GLU:HB2	2:C:41:HIS:ND1	2.23	0.54
2:D:343:ARG:O	2:D:343:ARG:HG3	2.07	0.54
2:D:496:PRO:HD2	2:D:497:GLU:OE1	2.07	0.54
2:D:455:GLU:HG2	2:D:474:THR:CG2	2.09	0.54
2:D:374:LYS:HG2	2:D:437:PHE:CZ	2.43	0.53
2:D:599:LYS:HB3	2:D:602:ARG:NH2	2.22	0.53
2:D:614:LYS:O	2:D:614:LYS:HD2	2.09	0.53
2:C:279:GLY:O	2:C:281:LYS:HD3	2.08	0.53
2:D:126:ARG:CG	2:D:166:TRP:CD1	2.91	0.53
2:D:631:PHE:CE1	2:D:637:PRO:HG2	2.41	0.53
2:D:455:GLU:CD	2:D:474:THR:CG2	2.81	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:624:LEU:O	2:D:624:LEU:HG	2.08	0.53
2:C:146:TYR:CE1	2:C:169:LYS:HA	2.44	0.53
2:C:81:SER:O	2:C:82:HIS:C	2.51	0.53
2:C:590:LYS:HE2	2:C:590:LYS:O	2.09	0.53
2:C:175:LEU:HD12	2:C:175:LEU:C	2.34	0.53
2:D:173:ASP:O	2:D:177:LEU:HD12	2.09	0.53
2:D:38:GLU:HB2	2:D:41:HIS:ND1	2.24	0.52
1:A:49:GLN:HA	1:A:49:GLN:HE21	1.73	0.52
2:C:28:ARG:HG2	2:C:30:ASP:HB2	1.92	0.52
2:D:455:GLU:CG	2:D:474:THR:CG2	2.78	0.52
2:D:374:LYS:O	2:D:378:GLN:HG3	2.09	0.52
1:A:89:LEU:HG	1:A:98:VAL:HG11	1.91	0.52
2:C:631:PHE:CD1	2:C:636:LYS:HD3	2.44	0.52
2:D:82:HIS:ND1	2:D:153:ALA:O	2.39	0.52
2:C:336:GLU:O	2:C:338:ILE:CD1	2.55	0.52
2:D:187:ILE:CD1	2:D:187:ILE:N	2.72	0.52
2:C:420:ARG:NH1	2:C:553:ILE:HG22	2.25	0.52
2:C:601:LYS:HD3	2:C:601:LYS:N	2.25	0.52
2:C:456:ILE:HG13	2:C:511:PHE:CE1	2.45	0.52
2:C:530:MET:HB3	2:C:531:PRO:HD2	1.92	0.52
2:C:600:ASP:OD1	2:C:600:ASP:N	2.42	0.52
2:D:631:PHE:C	2:D:636:LYS:HB3	2.34	0.52
2:C:411:ILE:HD11	2:C:466:ARG:HB2	1.92	0.51
2:D:134:LEU:HD21	2:D:188:ARG:CA	2.40	0.51
2:D:245:LEU:HD23	2:D:340:LEU:HD21	1.92	0.51
2:D:651:GLU:HB3	2:D:652:PRO:HD2	1.91	0.51
2:D:177:LEU:O	2:D:180:THR:HB	2.09	0.51
2:C:284:GLY:CA	2:C:292:MET:HE3	2.39	0.51
1:A:156:PHE:CD2	1:A:166:ARG:HG2	2.46	0.51
2:C:177:LEU:O	2:C:180:THR:OG1	2.29	0.51
2:C:641:LYS:HG2	2:C:644:ASP:OD2	2.11	0.51
2:D:619:ASP:HA	2:D:622:THR:OG1	2.11	0.51
2:C:37:GLU:HB2	2:C:113:TYR:CE1	2.45	0.51
2:C:351:THR:HG23	2:C:356:LYS:HE3	1.93	0.51
2:D:134:LEU:CD2	2:D:188:ARG:CG	2.84	0.51
2:C:126:ARG:NE	2:C:126:ARG:HA	2.26	0.51
2:C:362:ILE:HD12	2:C:390:ILE:CG2	2.41	0.51
2:C:497:GLU:OE2	2:C:497:GLU:N	2.41	0.51
1:B:22:THR:HA	1:B:24:TRP:NE1	2.26	0.51
1:B:24:TRP:O	1:B:25:ARG:C	2.54	0.51
2:C:271:ALA:C	2:C:273:SER:H	2.18	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:HIS:CE1	2:D:507:THR:HG23	2.46	0.50
2:D:374:LYS:HG2	2:D:437:PHE:CE2	2.46	0.50
2:D:624:LEU:HD13	2:D:644:ASP:HA	1.92	0.50
2:C:145:THR:CA	2:C:607:LEU:HD12	2.41	0.50
2:C:269:PRO:HG3	2:C:336:GLU:HG2	1.93	0.50
2:C:585:PHE:O	2:C:589:MET:HG2	2.11	0.50
2:D:631:PHE:CD1	2:D:637:PRO:HD2	2.46	0.50
2:C:264:MET:HE1	2:C:271:ALA:HA	1.85	0.50
2:D:304:VAL:HG22	4:E:4:ALA:HB2	1.92	0.50
2:D:602:ARG:NH1	2:D:602:ARG:CB	2.72	0.50
2:D:673:ARG:O	6:D:701:HOH:O	2.20	0.50
2:C:188:ARG:NH1	2:C:188:ARG:CG	2.73	0.50
2:C:249:GLY:O	2:C:265:VAL:HG23	2.12	0.50
2:C:251:VAL:CG1	2:C:263:SER:OG	2.60	0.50
2:D:200:ARG:O	2:D:204:GLN:HG3	2.12	0.50
1:A:134:LEU:HB2	1:A:156:PHE:CD2	2.47	0.50
2:D:510:LYS:HD3	2:D:548:LEU:HD23	1.94	0.50
1:B:198:TRP:CH2	1:B:219:LEU:CA	2.95	0.50
2:D:277:SER:O	2:D:280:ASP:HB2	2.12	0.50
2:D:647:LYS:HD3	2:D:647:LYS:N	2.25	0.50
2:D:26:ILE:HA	2:D:31:GLN:OE1	2.12	0.49
2:D:86:LEU:HD21	2:D:162:LEU:HD11	1.91	0.49
2:D:178:LYS:CD	2:D:609:TYR:CE2	2.94	0.49
2:D:201:ARG:NH1	2:D:202:LEU:HD23	2.24	0.49
2:D:631:PHE:O	2:D:636:LYS:HB3	2.12	0.49
1:A:164:PRO:HB3	1:A:200:TRP:CD2	2.46	0.49
2:C:59:GLN:NE2	6:C:707:HOH:O	2.38	0.49
2:D:626:ARG:HG3	2:D:626:ARG:O	2.12	0.49
2:C:57:TYR:CD1	2:C:57:TYR:C	2.90	0.49
2:D:183:THR:HG23	2:D:186:GLU:HG2	1.93	0.49
2:C:256:ASP:C	2:C:258:TYR:N	2.70	0.49
2:D:398:GLY:N	3:F:5:ALA:HB2	2.28	0.49
1:B:85:PHE:HB3	1:B:98:VAL:HG13	1.95	0.49
2:D:343:ARG:O	2:D:363:PRO:HG2	2.12	0.49
2:D:177:LEU:CD2	2:D:190:THR:CG2	2.83	0.49
2:D:461:MET:HE3	2:D:466:ARG:HB3	1.95	0.49
2:D:586:GLN:NE2	6:D:704:HOH:O	2.30	0.49
2:D:133:VAL:HG11	2:D:170:VAL:CG1	2.42	0.48
2:D:420:ARG:CG	2:D:426:VAL:HG22	2.41	0.48
2:D:439:LYS:CA	2:D:439:LYS:HE2	2.42	0.48
2:D:593:ALA:O	2:D:596:ASN:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:356:LYS:HB2	2:C:385:VAL:HG23	1.96	0.48
2:D:223:ASP:OD2	2:D:507:THR:CG2	2.62	0.48
2:C:254:MET:HA	2:C:258:TYR:O	2.14	0.48
2:D:67:SER:OG	2:D:100:LEU:HB2	2.13	0.48
2:D:231:PRO:HG3	2:D:500:ALA:O	2.13	0.48
2:D:237:PHE:CZ	2:D:241:MET:CE	2.96	0.48
2:D:290:LYS:HB3	2:D:291:PRO:HD2	1.96	0.48
2:D:447:ASP:HA	2:D:472:GLU:HB2	1.94	0.48
2:D:515:ASN:HB3	2:D:517:GLY:H	1.77	0.48
2:D:141:THR:O	2:D:141:THR:OG1	2.27	0.48
2:D:177:LEU:HD11	2:D:191:LEU:HD11	1.94	0.48
2:D:187:ILE:CD1	2:D:187:ILE:H	2.25	0.48
2:D:345:VAL:HG23	2:D:362:ILE:HG12	1.95	0.48
2:D:599:LYS:O	2:D:602:ARG:HB2	2.13	0.48
2:C:466:ARG:HD2	2:C:466:ARG:O	2.14	0.48
2:D:26:ILE:HG23	2:D:31:GLN:CG	2.43	0.48
2:D:412:PRO:HA	2:D:436:VAL:HG23	1.95	0.48
2:C:133:VAL:HG23	2:C:136:LYS:HE3	1.95	0.48
2:C:139:ASP:HB3	2:C:141:THR:H	1.79	0.48
2:C:223:ASP:CB	2:C:224:PRO:CD	2.91	0.48
2:C:283:VAL:HG22	2:C:283:VAL:O	2.13	0.48
2:D:311:LYS:O	2:D:311:LYS:HG3	2.13	0.48
2:D:347:MET:CE	2:D:349:VAL:HG23	2.43	0.48
2:C:223:ASP:CB	2:C:224:PRO:HD2	2.41	0.48
2:D:177:LEU:HD11	2:D:191:LEU:CD1	2.42	0.48
2:D:389:ILE:HD13	2:D:659:THR:CG2	2.42	0.48
2:C:410:PHE:O	2:C:411:ILE:HD13	2.14	0.47
2:C:178:LYS:HE2	2:C:609:TYR:CD1	2.49	0.47
2:C:186:GLU:O	2:C:187:ILE:C	2.57	0.47
2:D:631:PHE:HD1	2:D:637:PRO:HG2	1.71	0.47
2:D:355:GLU:CD	2:D:664:LEU:HD22	2.39	0.47
2:C:109:LEU:HB3	2:C:112:PHE:HD2	1.79	0.47
2:D:127:TYR:CZ	2:D:198:ALA:HB1	2.50	0.47
2:D:640:LYS:CB	2:D:643:ASP:CB	2.84	0.47
1:A:286:ASP:C	1:A:288:LEU:H	2.22	0.47
1:B:89:LEU:HG	1:B:98:VAL:HG11	1.96	0.47
2:C:85:LEU:O	2:C:156:PRO:HD2	2.15	0.47
2:D:27:THR:C	2:D:28:ARG:HG3	2.40	0.47
2:D:614:LYS:C	2:D:614:LYS:CD	2.85	0.47
2:D:640:LYS:CG	2:D:643:ASP:CB	2.25	0.47
2:D:613:GLU:O	2:D:614:LYS:C	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:ASP:O	2:C:82:HIS:HD2	1.98	0.47
2:C:657:ASP:O	2:C:660:VAL:HB	2.14	0.47
2:D:236:GLN:O	2:D:240:GLU:HG3	2.14	0.47
2:C:146:TYR:HE1	2:C:169:LYS:HA	1.81	0.46
2:C:431:ASP:N	6:C:704:HOH:O	2.36	0.46
2:C:196:LYS:HZ1	2:C:200:ARG:HE	1.63	0.46
2:C:601:LYS:CD	2:C:601:LYS:N	2.79	0.46
2:D:542:LYS:HB3	2:D:542:LYS:HE3	1.40	0.46
2:D:586:GLN:NE2	2:D:586:GLN:CA	2.77	0.46
2:C:567:PHE:HB3	2:C:669:LEU:HD12	1.97	0.46
2:D:147:ASN:HA	2:D:603:ASN:O	2.16	0.46
2:D:148:LEU:HD12	2:D:603:ASN:HA	1.98	0.46
2:C:144:ASP:OD1	2:C:144:ASP:N	2.36	0.46
2:C:252:LEU:HD11	2:C:307:ILE:CD1	2.46	0.46
2:D:206:ASN:HB2	2:D:209:ASP:CG	2.40	0.46
2:C:189:GLU:O	2:C:189:GLU:HG2	2.16	0.46
2:D:461:MET:HE2	2:D:466:ARG:CG	2.41	0.46
2:D:521:ARG:O	2:D:542:LYS:CE	2.57	0.46
2:D:630:ARG:HE	2:D:630:ARG:HB3	1.45	0.46
2:C:568:GLU:CB	2:C:569:PRO:CD	2.88	0.46
2:C:300:LEU:HD12	2:C:300:LEU:O	2.16	0.45
2:D:175:LEU:CD2	2:D:175:LEU:C	2.85	0.45
1:B:23:SER:O	1:B:26:LYS:HB3	2.16	0.45
1:B:94:ASP:CG	2:D:493:MET:HE1	2.41	0.45
2:C:253:GLN:O	2:C:260:VAL:N	2.49	0.45
2:D:257:ASP:O	2:D:296:ILE:O	2.33	0.45
2:D:497:GLU:HG3	6:D:871:HOH:O	2.16	0.45
2:D:525:THR:HA	2:D:526:PRO:HD3	1.80	0.45
2:D:609:TYR:CD1	2:D:609:TYR:N	2.83	0.45
2:C:350:LYS:HD2	2:C:660:VAL:HG21	1.97	0.45
2:C:564:LEU:HD23	2:C:564:LEU:N	2.31	0.45
2:D:32:ILE:O	2:D:32:ILE:HG23	2.16	0.45
2:D:211:PHE:CE1	2:D:215:MET:HE3	2.51	0.45
2:C:411:ILE:HD12	2:C:411:ILE:HA	1.67	0.45
2:C:446:VAL:O	2:C:471:GLY:HA3	2.17	0.45
2:C:609:TYR:CE2	2:C:613:GLU:CG	2.92	0.45
2:D:642:LEU:HD13	2:D:644:ASP:CB	2.33	0.45
2:C:309:GLY:CA	2:C:335:ARG:HD2	2.47	0.45
2:C:358:GLY:O	2:C:388:VAL:HA	2.16	0.45
2:D:272:LYS:HB2	2:D:272:LYS:HE3	1.60	0.45
2:D:27:THR:OG1	2:D:28:ARG:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:ASP:OD1	2:D:144:ASP:N	2.49	0.45
2:D:608:ASN:HB3	2:D:611:VAL:CG1	2.40	0.45
2:C:67:SER:OG	2:C:100:LEU:HB2	2.16	0.45
2:C:452:SER:HB3	3:H:4:ALA:HB1	1.99	0.45
2:D:619:ASP:O	2:D:622:THR:OG1	2.31	0.45
2:C:177:LEU:HB3	2:C:182:LYS:HD2	2.00	0.44
2:C:100:LEU:HD23	2:C:100:LEU:HA	1.82	0.44
2:C:197:PHE:CZ	2:C:256:ASP:CB	2.99	0.44
2:C:279:GLY:C	2:C:322:ALA:HB2	2.42	0.44
2:D:642:LEU:HD12	2:D:644:ASP:H	1.83	0.44
2:C:564:LEU:HD13	2:C:666:LEU:HD11	1.98	0.44
2:C:624:LEU:HD11	2:C:639:LEU:HD12	1.98	0.44
2:D:626:ARG:NH2	2:D:629:GLU:CD	2.75	0.44
1:A:249:ASP:CG	1:A:252:SER:HB2	2.42	0.44
2:D:627:LEU:HA	2:D:630:ARG:HH21	1.83	0.44
1:B:220:LYS:HE3	6:B:472:HOH:O	2.18	0.44
1:A:198:TRP:CH2	1:A:219:LEU:HA	2.53	0.44
2:D:82:HIS:CD2	2:D:155:TRP:CH2	3.05	0.44
2:C:269:PRO:CG	2:C:336:GLU:HG2	2.48	0.44
1:B:288:LEU:HD22	1:B:288:LEU:HA	1.79	0.44
2:C:229:LEU:N	2:C:229:LEU:HD12	2.32	0.44
2:C:582:ASP:HA	2:C:583:PRO:HD3	1.74	0.44
2:D:245:LEU:CD2	2:D:340:LEU:HD21	2.47	0.44
2:C:388:VAL:HG23	2:C:438:TYR:OH	2.17	0.43
2:D:496:PRO:CD	2:D:497:GLU:OE1	2.66	0.43
2:C:134:LEU:HD23	2:C:134:LEU:HA	1.70	0.43
2:C:304:VAL:HG21	5:G:2:SER:OG	2.18	0.43
2:D:358:GLY:N	2:D:385:VAL:HG21	2.33	0.43
2:C:362:ILE:HD12	2:C:390:ILE:HG23	1.99	0.43
2:D:126:ARG:HG3	2:D:166:TRP:CE2	2.50	0.43
2:D:297:GLY:C	2:D:298:TRP:CD1	2.94	0.43
2:C:568:GLU:CB	2:C:569:PRO:HD3	2.23	0.43
2:D:59:GLN:NE2	6:D:710:HOH:O	2.32	0.43
2:D:124:PHE:CD1	2:D:199:ILE:HD13	2.53	0.43
1:B:22:THR:O	1:B:22:THR:HG22	2.17	0.43
2:C:26:ILE:CG2	2:C:31:GLN:HB3	2.37	0.43
2:D:178:LYS:CD	2:D:609:TYR:CD2	3.02	0.43
2:D:410:PHE:HB2	2:D:461:MET:CE	2.49	0.43
1:A:124:GLU:OE1	2:C:47:ARG:NH2	2.48	0.43
2:C:126:ARG:HB3	2:C:166:TRP:CE2	2.53	0.43
2:D:96:LYS:O	2:D:99:GLU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:LEU:HD22	2:D:366:TYR:CD1	2.54	0.43
2:C:81:SER:HB3	2:C:83:ASN:ND2	2.33	0.43
2:C:285:VAL:HG11	2:C:306:LEU:HB3	2.01	0.43
2:C:536:GLU:H	2:C:536:GLU:HG2	1.60	0.43
2:C:664:LEU:O	2:C:668:LYS:HB2	2.19	0.43
2:D:108:LYS:HA	2:D:108:LYS:HD3	1.64	0.43
2:D:183:THR:CG2	2:D:186:GLU:HG2	2.49	0.43
2:C:81:SER:C	2:C:83:ASN:N	2.77	0.42
2:D:640:LYS:HG3	2:D:643:ASP:HB2	0.51	0.42
2:C:140:PHE:HB3	2:C:609:TYR:HB2	1.99	0.42
2:D:68:ALA:HB1	2:D:97:LYS:HE2	2.00	0.42
2:C:47:ARG:CZ	2:C:488:ARG:HG3	2.49	0.42
2:D:99:GLU:OE1	6:D:702:HOH:O	2.21	0.42
2:D:606:SER:O	2:D:607:LEU:HB2	2.18	0.42
2:C:270:ALA:HA	2:C:276:ILE:HD11	2.02	0.42
2:C:563:ASP:OD1	2:C:564:LEU:N	2.53	0.42
2:D:642:LEU:HD12	2:D:642:LEU:C	2.43	0.42
2:C:197:PHE:CD1	2:C:200:ARG:NH2	2.83	0.42
2:D:31:GLN:O	2:D:33:PRO:HD3	2.19	0.42
2:D:631:PHE:CD1	2:D:637:PRO:CD	3.02	0.42
2:C:78:LEU:HD21	2:C:116:TYR:CD2	2.54	0.42
2:C:86:LEU:O	2:C:89:ASP:HB2	2.19	0.42
2:C:310:PRO:O	2:C:313:SER:CB	2.66	0.42
2:D:35:LEU:HD23	2:D:35:LEU:HA	1.89	0.42
1:B:174:GLU:HB3	1:B:182:ALA:HB2	2.02	0.42
2:C:127:TYR:HB3	2:C:199:ILE:HD11	2.02	0.42
2:C:138:MET:HB2	6:C:793:HOH:O	2.19	0.42
2:C:197:PHE:CZ	2:C:257:ASP:OD2	2.72	0.42
2:D:647:LYS:HB2	2:D:648:ASP:H	1.67	0.42
1:B:134:LEU:HB2	1:B:156:PHE:CD2	2.55	0.42
2:C:362:ILE:HA	2:C:363:PRO:HD3	1.85	0.42
2:D:175:LEU:HD21	2:D:179:LEU:CD1	2.05	0.42
1:A:237:ASN:HB2	1:A:260:ALA:HB2	2.01	0.42
2:D:126:ARG:CD	2:D:166:TRP:NE1	2.82	0.42
1:B:113:ASP:HA	1:B:116:TYR:CD2	2.55	0.42
2:C:26:ILE:H	2:C:26:ILE:CD1	2.09	0.42
2:D:148:LEU:CD1	2:D:603:ASN:HA	2.50	0.42
2:D:201:ARG:HH22	2:D:202:LEU:HD21	1.85	0.42
2:C:382:LYS:HB3	2:C:382:LYS:HE3	1.57	0.41
1:A:163:ASP:HB3	1:A:166:ARG:HD3	2.02	0.41
2:C:38:GLU:HB2	2:C:41:HIS:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:452:SER:HB3	2:D:453:ALA:H	1.60	0.41
2:D:569:PRO:O	2:D:573:LYS:HG2	2.20	0.41
2:D:175:LEU:HD12	2:D:609:TYR:CD1	2.55	0.41
1:A:111:ASN:ND2	6:A:314:HOH:O	2.49	0.41
2:C:206:ASN:CG	2:C:209:ASP:OD2	2.63	0.41
2:C:306:LEU:HD23	2:C:306:LEU:HA	1.60	0.41
2:C:642:LEU:HD12	2:C:642:LEU:O	2.20	0.41
2:D:230:SER:HB2	2:D:231:PRO:HD2	2.02	0.41
2:D:448:ARG:HE	2:D:448:ARG:HB3	1.66	0.41
2:C:590:LYS:HA	2:C:590:LYS:HD2	1.84	0.41
2:D:329:ARG:HH11	2:D:329:ARG:HD2	1.68	0.41
1:A:183:LYS:HE3	1:A:183:LYS:HB2	1.90	0.41
2:C:135:GLU:OE2	2:C:135:GLU:N	2.53	0.41
2:C:166:TRP:O	2:C:170:VAL:CG1	2.62	0.41
2:C:340:LEU:HA	2:C:340:LEU:HD23	1.81	0.41
2:D:57:TYR:CD1	2:D:57:TYR:C	2.98	0.41
2:D:410:PHE:HB2	2:D:461:MET:HE1	2.03	0.41
2:D:613:GLU:H	2:D:616:ASN:H	1.68	0.41
2:C:324:LYS:HB3	2:C:325:GLY:H	1.59	0.41
2:C:354:LYS:HD3	2:C:355:GLU:CG	2.45	0.41
2:D:86:LEU:CD2	2:D:162:LEU:HD11	2.50	0.41
2:D:414:GLY:O	2:D:430:SER:HB3	2.21	0.41
2:C:264:MET:HE3	2:C:270:ALA:CB	2.50	0.41
2:D:436:VAL:HG11	2:D:439:LYS:HG2	2.01	0.41
2:D:612:ARG:H	2:D:612:ARG:HG2	1.71	0.41
2:C:356:LYS:C	2:C:385:VAL:HG22	2.46	0.41
2:C:578:ARG:HA	2:C:581:LYS:CE	2.48	0.41
2:D:82:HIS:CD2	2:D:155:TRP:CZ3	3.09	0.41
2:D:455:GLU:OE1	2:D:474:THR:CG2	2.69	0.41
2:D:463:ASP:OD1	2:D:513:ARG:NH2	2.51	0.41
2:D:631:PHE:O	2:D:636:LYS:CA	2.65	0.41
2:C:273:SER:C	2:C:275:ALA:H	2.29	0.41
2:D:347:MET:HE2	2:D:348:SER:C	2.46	0.40
2:D:364:GLY:HA2	2:D:395:ASN:OD1	2.21	0.40
2:D:135:GLU:H	2:D:135:GLU:HG2	1.75	0.40
2:D:671:LYS:HD2	2:D:671:LYS:HA	1.51	0.40
2:C:452:SER:HB3	3:H:4:ALA:O	2.22	0.40
2:C:598:MET:HE3	2:C:598:MET:HB2	1.44	0.40
2:D:126:ARG:NE	2:D:126:ARG:HA	2.36	0.40
2:D:176:SER:HA	2:D:179:LEU:HD12	2.02	0.40
2:D:451:ALA:HA	2:D:455:GLU:HG3	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:584:GLU:O	2:D:588:ILE:HD12	2.20	0.40
2:D:641:LYS:HB2	2:D:641:LYS:HE3	1.49	0.40
2:C:356:LYS:HB3	2:C:356:LYS:HE2	1.28	0.40
2:C:388:VAL:HG23	2:C:438:TYR:CZ	2.57	0.40
2:C:609:TYR:CZ	2:C:613:GLU:CG	3.04	0.40
1:A:198:TRP:CH2	1:A:219:LEU:CA	3.04	0.40
1:A:235:GLU:HA	1:A:270:GLU:HG2	2.03	0.40
2:C:177:LEU:O	2:C:182:LYS:HB2	2.21	0.40
2:C:351:THR:CG2	2:C:356:LYS:HE3	2.51	0.40
2:D:640:LYS:O	2:D:641:LYS:C	2.65	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/278 (96%)	264 (98%)	4 (2%)	0	100	100
1	B	266/278 (96%)	261 (98%)	3 (1%)	2 (1%)	16	20
2	C	646/682 (95%)	631 (98%)	11 (2%)	4 (1%)	21	27
2	D	643/682 (94%)	621 (97%)	21 (3%)	1 (0%)	43	55
3	F	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
3	H	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
4	E	2/4 (50%)	2 (100%)	0	0	100	100
5	G	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1835/1940 (95%)	1787 (97%)	41 (2%)	7 (0%)	30	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	82	HIS
2	C	257	ASP
1	B	25	ARG
2	D	613	GLU
1	B	287	ASP
2	C	187	ILE
2	C	137	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/237 (98%)	222 (96%)	9 (4%)	28	43
1	B	229/237 (97%)	215 (94%)	14 (6%)	17	24
2	C	558/583 (96%)	474 (85%)	84 (15%)	3	3
2	D	558/583 (96%)	447 (80%)	111 (20%)	1	1
5	G	4/4 (100%)	1 (25%)	3 (75%)	0	0
All	All	1580/1644 (96%)	1359 (86%)	221 (14%)	3	3

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	21	ASN
1	B	23	SER
1	B	74	SER
1	B	145	ARG
1	B	153	LEU
1	B	158	GLN
1	B	175	GLN
1	B	177	LEU
1	B	193	SER
1	B	196	GLU
1	B	217	GLU
1	B	220	LYS
1	B	246	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	288	LEU
1	A	19	MET
1	A	53	SER
1	A	111	ASN
1	A	166	ARG
1	A	175	GLN
1	A	192	LYS
1	A	279	SER
1	A	283	GLN
1	A	288	LEU
2	C	26	ILE
2	C	31	GLN
2	C	34	VAL
2	C	37	GLU
2	C	81	SER
2	C	91	GLU
2	C	108	LYS
2	C	115	LEU
2	C	121	LYS
2	C	133	VAL
2	C	135	GLU
2	C	138	MET
2	C	141	THR
2	C	169	LYS
2	C	170	VAL
2	C	182	LYS
2	C	183	THR
2	C	186	GLU
2	C	188	ARG
2	C	193	ARG
2	C	201	ARG
2	C	239	THR
2	C	245	LEU
2	C	248	ILE
2	C	251	VAL
2	C	256	ASP
2	C	260	VAL
2	C	273	SER
2	C	276	ILE
2	C	277	SER
2	C	281	LYS
2	C	294	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	303	VAL
2	C	311	LYS
2	C	313	SER
2	C	318	GLU
2	C	324	LYS
2	C	329	ARG
2	C	342	ASP
2	C	343	ARG
2	C	346	LYS
2	C	347	MET
2	C	349	VAL
2	C	354	LYS
2	C	355	GLU
2	C	356	LYS
2	C	379	LYS
2	C	381	GLU
2	C	382	LYS
2	C	383	GLN
2	C	385	VAL
2	C	411	ILE
2	C	435	GLN
2	C	439	LYS
2	C	504	VAL
2	C	522	LYS
2	C	535	GLU
2	C	536	GLU
2	C	538	GLU
2	C	552	SER
2	C	559	VAL
2	C	560	LYS
2	C	565	THR
2	C	571	LEU
2	C	572	LEU
2	C	581	LYS
2	C	594	ARG
2	C	598	MET
2	C	600	ASP
2	C	601	LYS
2	C	611	VAL
2	C	612	ARG
2	C	613	GLU
2	C	614	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	615	GLU
2	C	618	GLU
2	C	636	LYS
2	C	639	LEU
2	C	641	LYS
2	C	647	LYS
2	C	668	LYS
2	C	669	LEU
2	C	670	GLU
2	C	671	LYS
2	D	25	ASP
2	D	26	ILE
2	D	31	GLN
2	D	38	GLU
2	D	51	ARG
2	D	77	LEU
2	D	78	LEU
2	D	96	LYS
2	D	99	GLU
2	D	108	LYS
2	D	109	LEU
2	D	111	VAL
2	D	123	ARG
2	D	126	ARG
2	D	128	GLN
2	D	131	LEU
2	D	134	LEU
2	D	138	MET
2	D	139	ASP
2	D	145	THR
2	D	148	LEU
2	D	177	LEU
2	D	179	LEU
2	D	180	THR
2	D	182	LYS
2	D	186	GLU
2	D	187	ILE
2	D	192	THR
2	D	196	LYS
2	D	199	ILE
2	D	210	VAL
2	D	213	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	216	THR
2	D	245	LEU
2	D	262	ASN
2	D	272	LYS
2	D	277	SER
2	D	288	THR
2	D	290	LYS
2	D	304	VAL
2	D	313	SER
2	D	317	LEU
2	D	324	LYS
2	D	326	THR
2	D	327	LYS
2	D	328	THR
2	D	330	THR
2	D	336	GLU
2	D	337	ARG
2	D	350	LYS
2	D	354	LYS
2	D	356	LYS
2	D	374	LYS
2	D	375	VAL
2	D	382	LYS
2	D	385	VAL
2	D	386	SER
2	D	394	SER
2	D	400	LEU
2	D	420	ARG
2	D	430	SER
2	D	432	THR
2	D	435	GLN
2	D	437	PHE
2	D	439	LYS
2	D	445	LEU
2	D	452	SER
2	D	461	MET
2	D	484	ARG
2	D	495	ARG
2	D	507	THR
2	D	524	VAL
2	D	535	GLU
2	D	542	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	565	THR
2	D	570	GLU
2	D	573	LYS
2	D	581	LYS
2	D	586	GLN
2	D	588	ILE
2	D	589	MET
2	D	590	LYS
2	D	594	ARG
2	D	599	LYS
2	D	602	ARG
2	D	604	ILE
2	D	605	VAL
2	D	607	LEU
2	D	609	TYR
2	D	612	ARG
2	D	613	GLU
2	D	614	LYS
2	D	615	GLU
2	D	616	ASN
2	D	618	GLU
2	D	626	ARG
2	D	627	LEU
2	D	629	GLU
2	D	630	ARG
2	D	632	LYS
2	D	633	ARG
2	D	636	LYS
2	D	641	LYS
2	D	642	LEU
2	D	645	LEU
2	D	647	LYS
2	D	648	ASP
2	D	650	GLN
2	D	662	ILE
2	D	671	LYS
2	D	673	ARG
5	G	1	LEU
5	G	3	ARG
5	G	4	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	GLN
1	B	175	GLN
1	B	189	HIS
1	A	49	GLN
1	A	83	ASN
1	A	100	ASN
1	A	111	ASN
1	A	135	ASN
1	A	197	GLN
1	A	232	HIS
1	A	283	GLN
2	C	418	GLN
2	D	59	GLN
2	D	435	GLN
2	D	586	GLN
2	D	628	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	270/278 (97%)	-0.17	3 (1%) 78 79	10, 20, 41, 90	0
1	B	268/278 (96%)	-0.07	4 (1%) 72 73	11, 21, 47, 113	0
2	C	648/682 (95%)	1.06	135 (20%) 2 3	18, 52, 96, 132	0
2	D	647/682 (94%)	1.04	118 (18%) 3 4	19, 45, 92, 117	0
3	F	6/6 (100%)	2.50	4 (66%) 0 0	35, 40, 59, 64	0
3	H	6/6 (100%)	3.05	4 (66%) 0 0	38, 42, 61, 70	0
4	E	4/4 (100%)	2.70	3 (75%) 0 0	38, 51, 59, 70	0
5	G	4/4 (100%)	1.43	1 (25%) 2 2	56, 64, 65, 69	0
All	All	1853/1940 (95%)	0.73	272 (14%) 6 6	10, 40, 91, 132	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	LEU	7.2
2	D	639	LEU	7.0
3	H	6	ALA	6.8
2	C	303	VAL	6.7
2	C	275	ALA	6.2
2	D	140	PHE	6.2
2	D	297	GLY	5.7
2	D	645	LEU	5.6
1	B	22	THR	5.4
2	D	642	LEU	5.3
2	C	29	ALA	5.3
2	C	672	ALA	5.2
2	C	254	MET	5.2
2	D	178	LYS	5.0
2	D	142	GLY	5.0
2	D	572	LEU	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	81	SER	4.9
2	D	127	TYR	4.8
2	C	283	VAL	4.8
2	C	138	MET	4.7
2	D	432	THR	4.7
2	C	328	THR	4.6
2	D	626	ARG	4.6
3	F	5	ALA	4.6
2	D	624	LEU	4.5
2	D	641	LYS	4.5
2	D	629	GLU	4.4
2	D	635	GLY	4.4
2	D	646	PRO	4.4
2	C	383	GLN	4.4
2	C	567	PHE	4.4
2	C	252	LEU	4.3
3	H	5	ALA	4.3
2	D	137	PRO	4.2
2	D	627	LEU	4.2
2	C	276	ILE	4.2
2	D	26	ILE	4.2
2	C	197	PHE	4.2
2	C	297	GLY	4.2
2	D	609	TYR	4.1
2	C	273	SER	4.1
2	D	588	ILE	4.1
2	D	134	LEU	4.1
2	D	630	ARG	4.0
2	D	587	ASN	4.0
3	F	6	ALA	4.0
4	E	3	ALA	4.0
2	C	295	VAL	3.9
2	D	251	VAL	3.8
2	C	413	ALA	3.8
2	D	637	PRO	3.8
2	C	177	LEU	3.8
1	B	21	ASN	3.7
2	C	320	LEU	3.6
2	C	278	VAL	3.6
2	C	259	THR	3.6
2	C	667	ALA	3.6
2	D	638	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	32	ILE	3.6
2	C	332	THR	3.6
2	C	26	ILE	3.5
1	A	288	LEU	3.5
2	C	182	LYS	3.5
2	D	644	ASP	3.5
2	D	185	LYS	3.5
2	C	385	VAL	3.4
2	D	611	VAL	3.4
2	C	289	GLY	3.4
2	C	323	GLY	3.4
2	C	317	LEU	3.4
2	C	333	LEU	3.4
2	C	258	TYR	3.4
2	C	257	ASP	3.4
2	D	579	ILE	3.3
2	C	191	LEU	3.3
2	D	197	PHE	3.3
2	D	595	PHE	3.3
2	D	589	MET	3.3
2	C	380	LEU	3.2
2	D	177	LEU	3.2
2	C	282	ILE	3.2
2	D	29	ALA	3.2
2	D	649	TYR	3.2
1	B	24	TRP	3.2
2	D	590	LYS	3.2
2	D	607	LEU	3.2
2	C	288	THR	3.2
2	D	183	THR	3.2
2	C	301	ASP	3.1
2	D	673	ARG	3.1
2	D	647	LYS	3.1
2	D	186	GLU	3.1
4	E	1	ALA	3.1
2	C	251	VAL	3.1
2	C	299	ARG	3.1
2	C	327	LYS	3.1
2	C	382	LYS	3.1
2	D	32	ILE	3.1
2	D	143	ASN	3.1
2	C	300	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	G	1	LEU	3.1
2	C	326	THR	3.0
2	C	25	ASP	3.0
2	C	140	PHE	3.0
2	D	181	GLY	3.0
2	C	188	ARG	3.0
2	C	329	ARG	3.0
2	C	668	LYS	3.0
2	D	625	ALA	3.0
2	C	265	VAL	2.9
2	C	352	VAL	2.9
2	C	134	LEU	2.9
2	C	598	MET	2.9
2	C	280	ASP	2.9
2	D	583	PRO	2.9
2	D	317	LEU	2.9
2	C	293	VAL	2.9
2	C	176	SER	2.8
2	C	562	GLY	2.8
2	C	322	ALA	2.8
2	D	593	ALA	2.8
4	E	2	ALA	2.8
2	D	643	ASP	2.8
2	C	669	LEU	2.8
2	C	274	LYS	2.8
2	C	324	LYS	2.8
2	C	201	ARG	2.8
2	D	437	PHE	2.8
2	C	31	GLN	2.8
2	D	191	LEU	2.8
2	D	328	THR	2.7
2	C	178	LYS	2.7
2	D	141	THR	2.7
2	C	291	PRO	2.7
2	D	439	LYS	2.7
2	C	566	ALA	2.7
2	C	196	LYS	2.7
2	D	182	LYS	2.6
2	C	351	THR	2.6
2	C	181	GLY	2.6
2	D	623	ARG	2.6
2	C	130	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	206	ASN	2.6
2	D	180	THR	2.6
2	D	380	LEU	2.6
2	D	640	LYS	2.6
2	C	577	ALA	2.6
2	C	597	ALA	2.6
3	H	4	ALA	2.6
2	D	633	ARG	2.6
2	C	384	ASN	2.6
2	D	449	PHE	2.6
2	D	205	THR	2.6
2	D	569	PRO	2.6
2	C	290	LYS	2.6
2	D	632	LYS	2.6
2	C	533	GLY	2.6
2	D	622	THR	2.6
2	C	260	VAL	2.6
2	D	571	LEU	2.5
2	C	612	ARG	2.5
2	D	171	LYS	2.5
2	D	438	TYR	2.5
2	C	131	LEU	2.5
2	C	607	LEU	2.5
3	F	1	ALA	2.5
2	C	432	THR	2.5
2	D	192	THR	2.5
2	D	166	TRP	2.5
2	C	331	VAL	2.5
2	D	252	LEU	2.5
2	C	30	ASP	2.5
2	C	139	ASP	2.5
2	C	137	PRO	2.5
2	D	585	PHE	2.5
2	D	606	SER	2.5
2	C	261	ILE	2.5
2	D	131	LEU	2.5
2	C	379	LYS	2.5
2	D	617	ASN	2.5
2	D	135	GLU	2.4
2	D	613	GLU	2.4
2	C	349	VAL	2.4
2	C	184	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	616	ASN	2.4
2	D	322	ALA	2.4
2	D	605	VAL	2.4
2	D	354	LYS	2.4
2	C	642	LEU	2.4
2	D	655	TYR	2.4
2	D	139	ASP	2.4
2	D	184	ASP	2.4
2	D	628	ASN	2.4
2	C	33	PRO	2.4
2	D	621	ALA	2.4
2	D	435	GLN	2.4
2	C	250	ALA	2.4
2	C	325	GLY	2.4
2	D	250	ALA	2.4
2	C	564	LEU	2.4
2	C	135	GLU	2.4
2	D	597	ALA	2.3
2	D	27	THR	2.3
2	C	296	ILE	2.3
2	C	315	VAL	2.3
2	C	185	LYS	2.3
2	D	195	TYR	2.3
2	D	556	ALA	2.3
2	C	321	PRO	2.3
2	C	284	GLY	2.3
2	C	438	TYR	2.3
1	A	53	SER	2.3
2	C	28	ARG	2.3
2	C	579	ILE	2.3
2	D	138	MET	2.3
2	D	580	ALA	2.3
2	C	192	THR	2.3
2	C	437	PHE	2.2
2	C	342	ASP	2.2
2	C	433	ASP	2.2
2	D	25	ASP	2.2
2	C	441	PRO	2.2
2	C	200	ARG	2.2
2	C	309	GLY	2.2
1	A	198	TRP	2.2
2	C	264	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	412	PRO	2.2
2	D	651	GLU	2.2
2	C	314	LYS	2.2
2	C	330	THR	2.2
2	D	304	VAL	2.2
2	C	255	ASP	2.2
2	D	145	THR	2.2
3	F	4	ALA	2.2
2	C	590	LYS	2.2
2	C	610	ALA	2.2
2	D	187	ILE	2.1
2	C	124	PHE	2.1
2	C	595	PHE	2.1
2	C	601	LYS	2.1
2	C	253	GLN	2.1
2	C	132	SER	2.1
2	C	647	LYS	2.1
2	C	666	LEU	2.1
2	D	199	ILE	2.1
2	D	411	ILE	2.1
2	D	342	ASP	2.1
2	C	304	VAL	2.1
2	D	353	GLY	2.1
2	C	572	LEU	2.1
2	D	174	GLU	2.1
2	C	127	TYR	2.1
2	D	502	GLY	2.1
2	D	612	ARG	2.1
2	C	270	ALA	2.1
3	H	1	ALA	2.1
2	D	536	GLU	2.1
2	C	306	LEU	2.1
2	D	608	ASN	2.1
2	C	436	VAL	2.1
2	C	605	VAL	2.1
2	D	343	ARG	2.1
2	D	650	GLN	2.0
2	C	639	LEU	2.0
2	D	333	LEU	2.0
2	D	201	ARG	2.0
2	C	434	GLY	2.0
2	C	136	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	298	TRP	2.0
2	D	179	LEU	2.0
2	C	573	LYS	2.0
2	D	573	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.