



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:09 PM EDT

PDB ID : 4R3O / pdb_00004r3o
Title : Human Constitutive 20S Proteasome
Authors : Sacchettini, J.C.; Harshbarger, W.H.
Deposited on : 2014-08-16
Resolution : 2.60 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

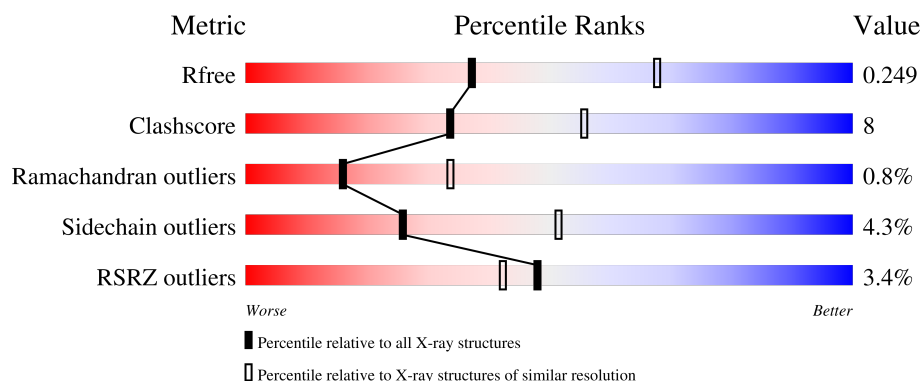
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	244	5% 75% 22% .
1	O	244	4% 82% 16% .
2	B	233	5% 82% 16% .
2	P	233	6% 81% 18% .
3	C	250	2% 84% 15% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	250	
4	D	243	
4	R	243	
5	E	234	
5	S	234	
6	F	238	
6	T	238	
7	G	245	
7	U	245	
8	H	202	
8	V	202	
9	I	220	
9	W	220	
10	J	204	
10	X	204	
11	K	199	
11	Y	199	
12	L	201	
12	Z	201	
13	1	213	
13	M	213	
14	2	217	
14	N	217	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 47831 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 Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1845	1171	309	352	13			
1	O	244	Total	C	N	O	S	0	0	0
			1845	1171	309	352	13			

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1707	1081	287	334	5			
2	P	233	Total	C	N	O	S	0	0	0
			1712	1085	287	334	6			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	250	Total	C	N	O	S	0	0	0
			1912	1204	329	371	8			
3	Q	250	Total	C	N	O	S	0	0	0
			1913	1203	330	372	8			

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1724	1068	312	339	5			
4	R	243	Total	C	N	O	S	0	0	0
			1691	1051	309	327	4			

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	S	234	Total	C	N	O	S	0	0	0
			1716	1102	290	313	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	T	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	U	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	V	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	W	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	Y	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	Z	201	Total	C	N	O	S	0	0	0
			1551	977	273	292	9			

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	213	Total	C	N	O	S	0	0	0
			1641	1036	282	313	10			
13	1	213	Total	C	N	O	S	0	0	0
			1644	1039	282	313	10			

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	217	Total	C	N	O	S	0	0	0
			1676	1057	287	320	12			
14	2	217	Total	C	N	O	S	0	0	0
			1678	1058	290	318	12			

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	O	0	0
			2	2		
15	D	4	Total	O	0	0
			4	4		

Continued on next page...

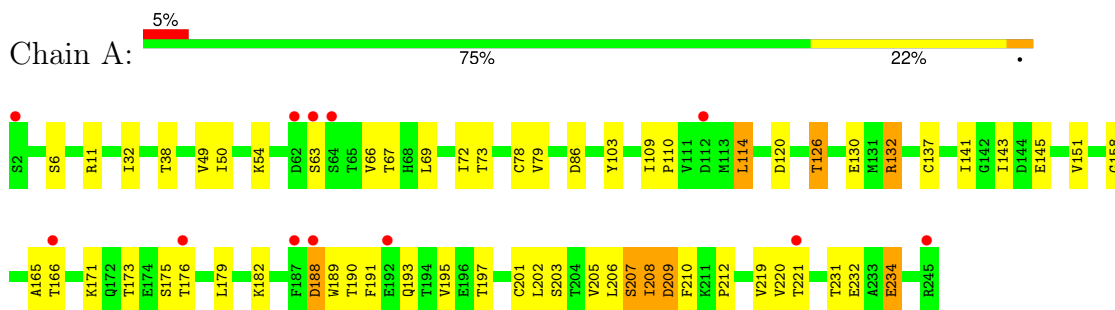
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	E	8	Total 8	O 8	0	0
15	F	19	Total 19	O 19	0	0
15	G	1	Total 1	O 1	0	0
15	K	9	Total 9	O 9	0	0
15	L	8	Total 8	O 8	0	0
15	M	34	Total 34	O 34	0	0
15	N	11	Total 11	O 11	0	0
15	O	1	Total 1	O 1	0	0
15	P	24	Total 24	O 24	0	0
15	Q	10	Total 10	O 10	0	0
15	R	5	Total 5	O 5	0	0
15	W	17	Total 17	O 17	0	0
15	X	25	Total 25	O 25	0	0
15	Y	3	Total 3	O 3	0	0
15	Z	4	Total 4	O 4	0	0

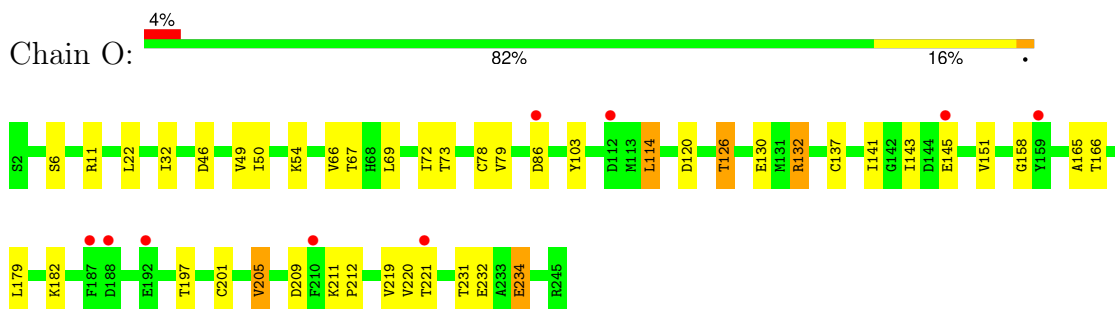
3 Residue-property plots [i](#)

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

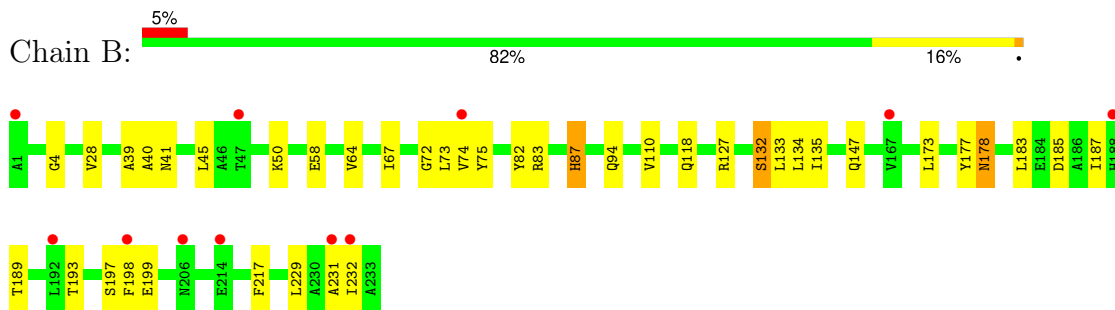
- Molecule 1: Proteasome subunit alpha type-6



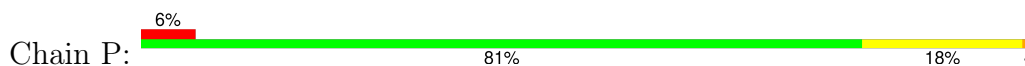
- Molecule 1: Proteasome subunit alpha type-6

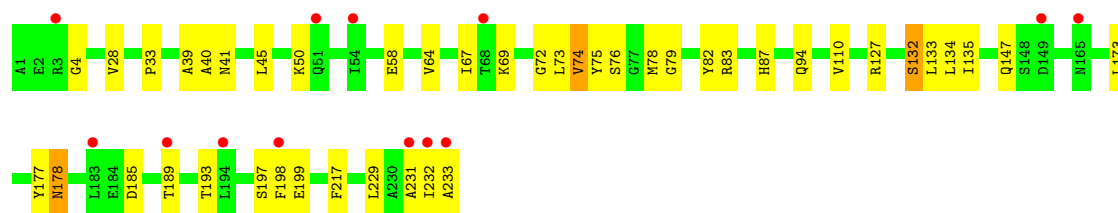


- Molecule 2: Proteasome subunit alpha type-2

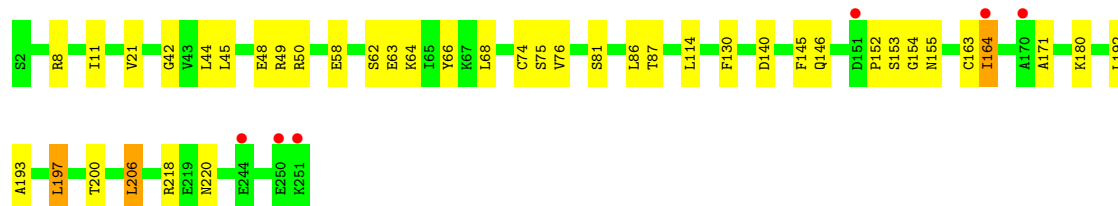
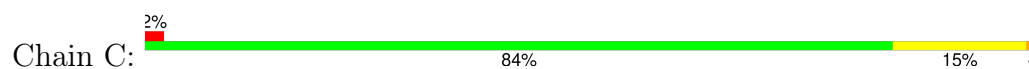


- Molecule 2: Proteasome subunit alpha type-2

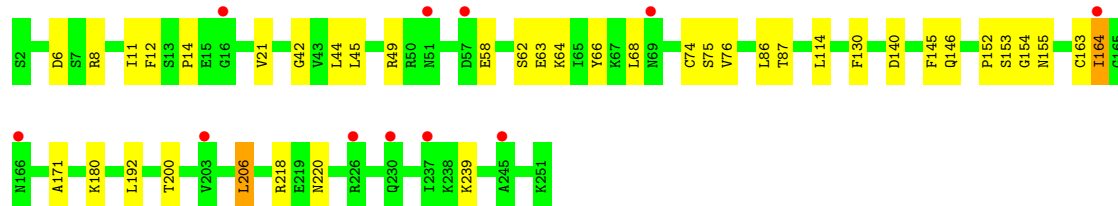
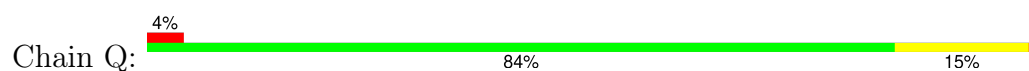




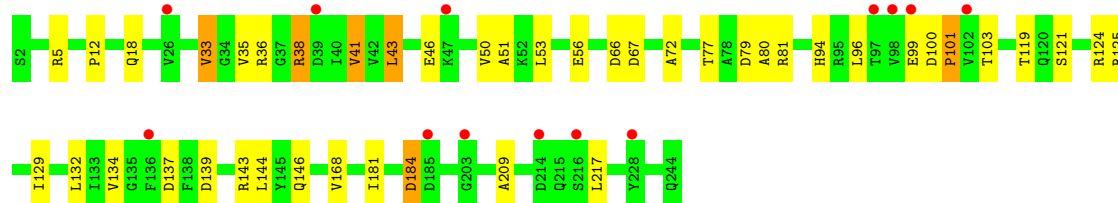
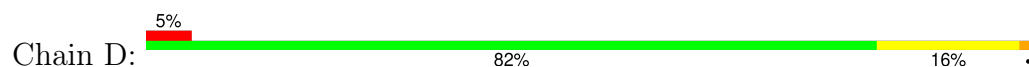
• Molecule 3: Proteasome subunit alpha type-4



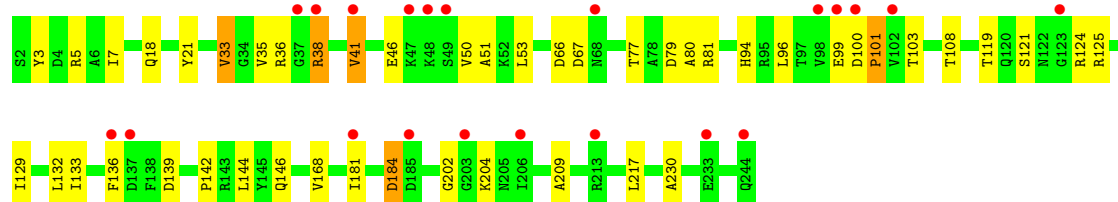
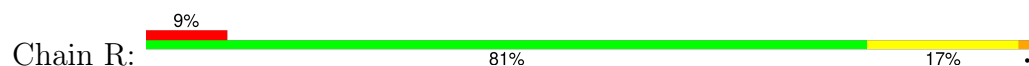
• Molecule 3: Proteasome subunit alpha type-4



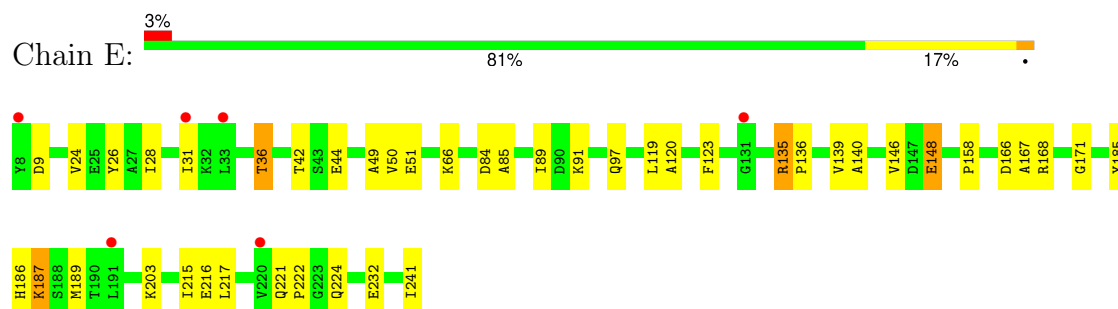
• Molecule 4: Proteasome subunit alpha type-7



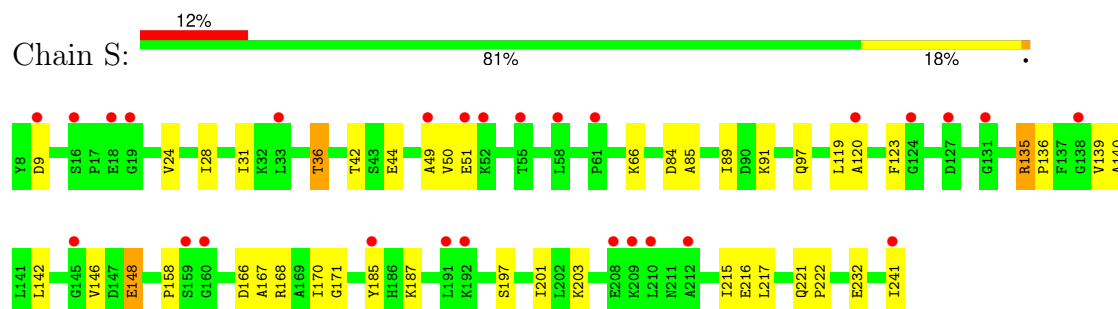
• Molecule 4: Proteasome subunit alpha type-7



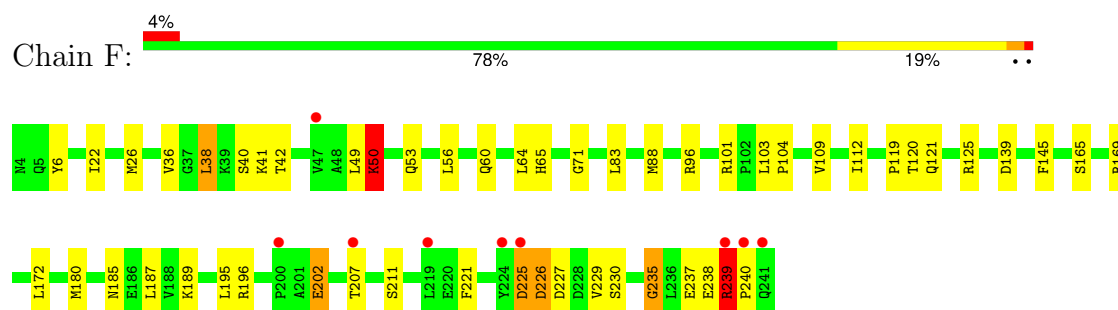
- Molecule 5: Proteasome subunit alpha type-5



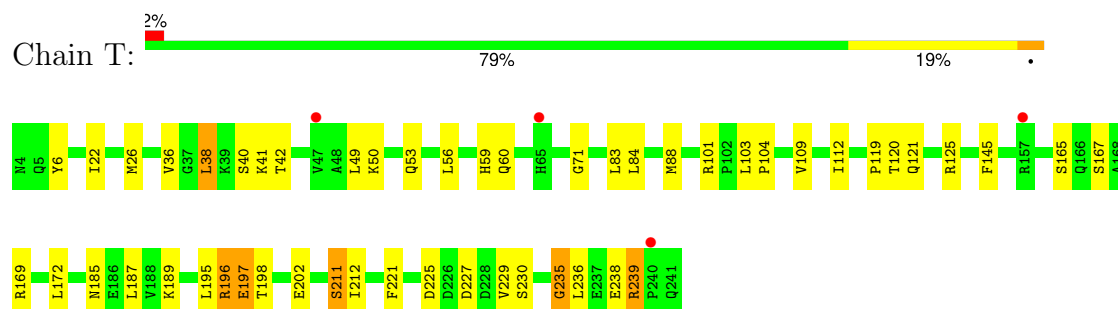
- Molecule 5: Proteasome subunit alpha type-5



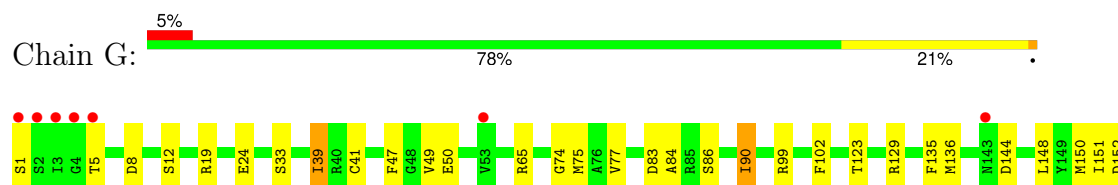
- Molecule 6: Proteasome subunit alpha type-1

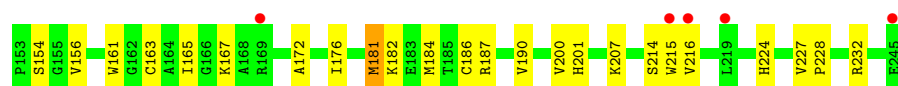


- Molecule 6: Proteasome subunit alpha type-1

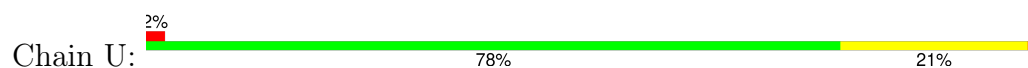


- Molecule 7: Proteasome subunit alpha type-3

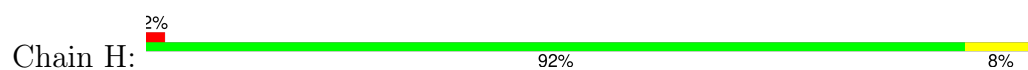




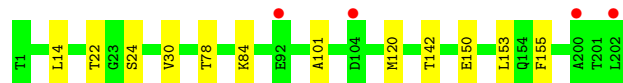
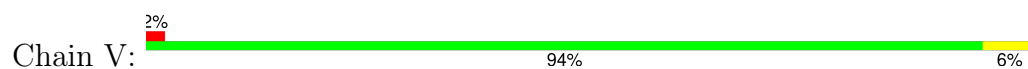
• Molecule 7: Proteasome subunit alpha type-3



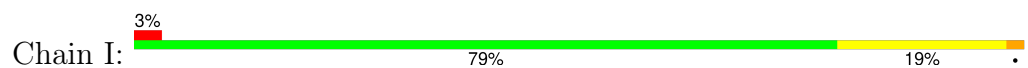
• Molecule 8: Proteasome subunit beta type-6



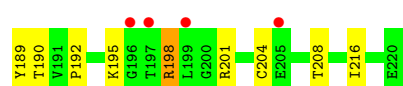
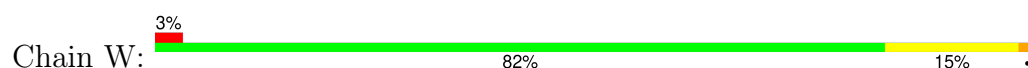
• Molecule 8: Proteasome subunit beta type-6



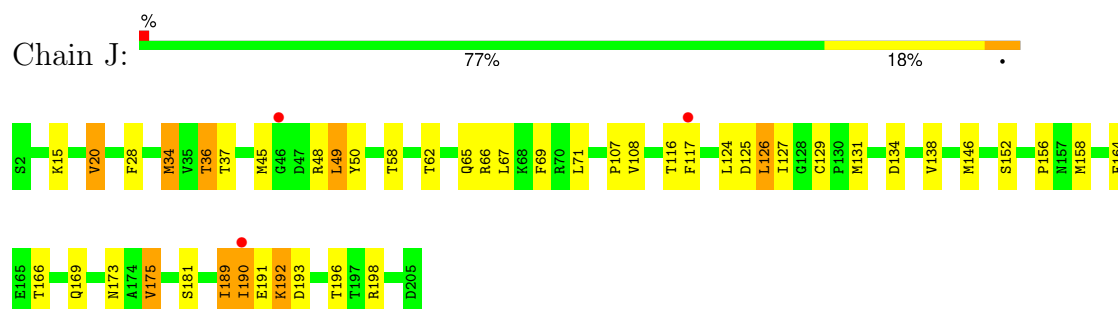
• Molecule 9: Proteasome subunit beta type-7



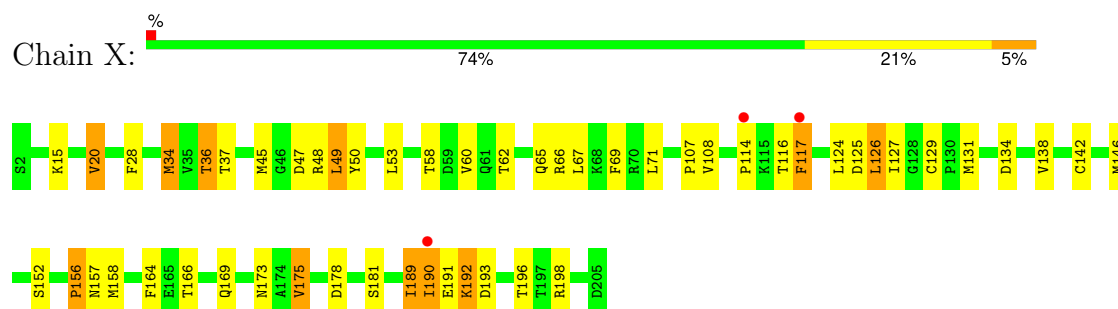
• Molecule 9: Proteasome subunit beta type-7



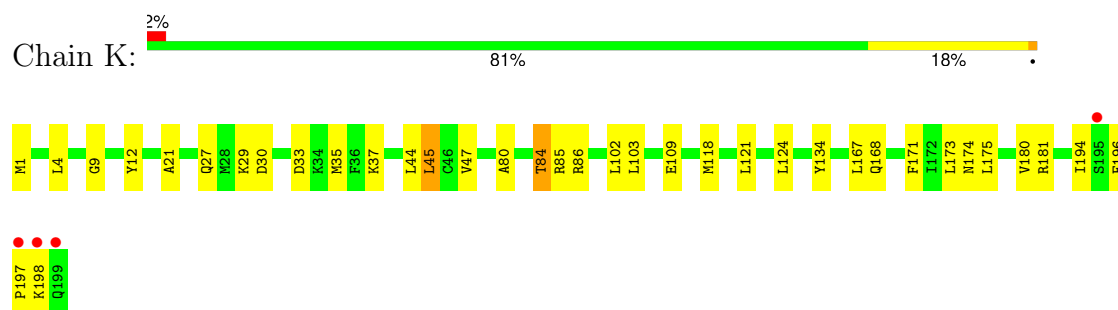
- Molecule 10: Proteasome subunit beta type-3



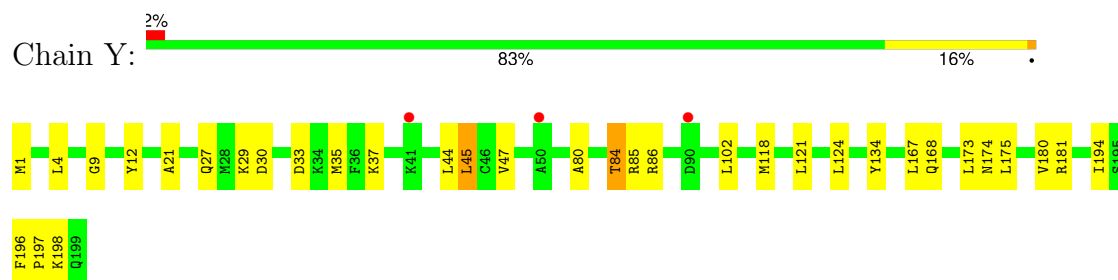
- Molecule 10: Proteasome subunit beta type-3



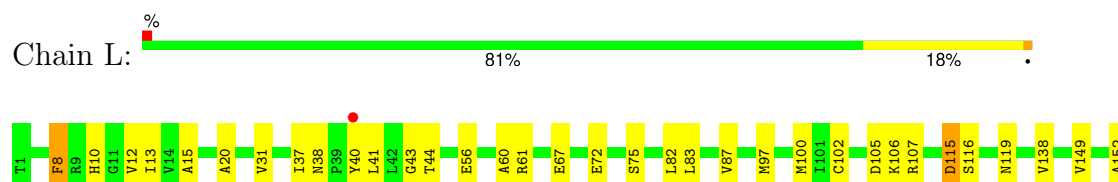
- Molecule 11: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-2

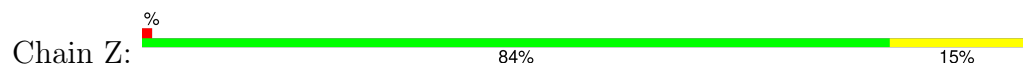


- Molecule 12: Proteasome subunit beta type-5

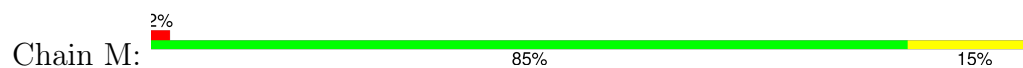




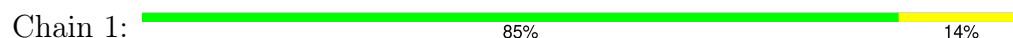
• Molecule 12: Proteasome subunit beta type-5



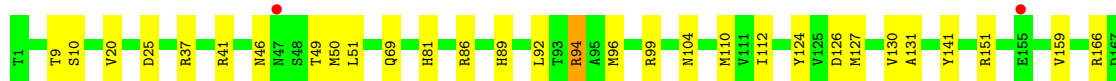
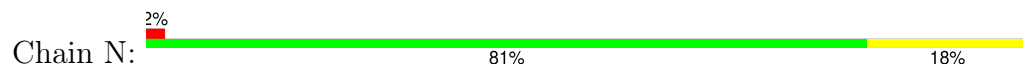
• Molecule 13: Proteasome subunit beta type-1



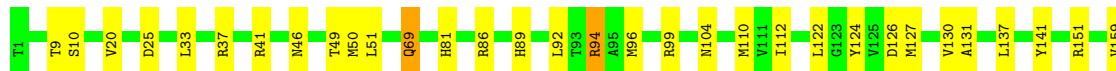
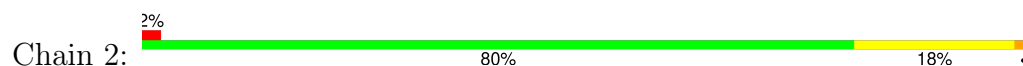
• Molecule 13: Proteasome subunit beta type-1

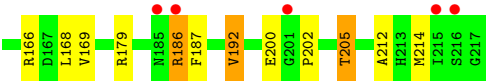


• Molecule 14: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.23Å 205.06Å 163.13Å 90.00° 106.37° 90.00°	Depositor
Resolution (Å)	36.34 – 2.60 36.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (36.34-2.60) 88.4 (36.34-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.45 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.204 , 0.244 0.217 , 0.249	Depositor DCC
R_{free} test set	11447 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	47831	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.33	0/1878	0.78	3/2549 (0.1%)
1	O	0.30	0/1878	0.74	0/2549
2	B	0.32	0/1742	0.74	0/2372
2	P	0.32	0/1747	0.74	0/2378
3	C	0.31	0/1942	0.73	0/2628
3	Q	0.31	0/1943	0.74	0/2629
4	D	0.30	0/1748	0.77	0/2386
4	R	0.30	0/1716	0.79	0/2347
5	E	0.32	0/1786	0.75	0/2419
5	S	0.31	0/1743	0.75	0/2333
6	F	0.37	1/1885 (0.1%)	0.77	2/2552 (0.1%)
6	T	0.33	0/1885	0.75	0/2552
7	G	0.34	0/1920	0.75	0/2591
7	U	0.34	0/1920	0.78	0/2591
8	H	0.35	0/1535	0.73	0/2078
8	V	0.34	0/1535	0.73	0/2078
9	I	0.40	1/1670 (0.1%)	0.82	2/2265 (0.1%)
9	W	0.35	0/1670	0.76	1/2265 (0.0%)
10	J	0.32	0/1614	0.75	0/2177
10	X	0.33	0/1614	0.75	0/2177
11	K	0.31	0/1603	0.72	0/2174
11	Y	0.31	0/1603	0.71	0/2174
12	L	0.37	0/1579	0.72	0/2134
12	Z	0.33	0/1582	0.71	0/2138
13	1	0.35	0/1674	0.72	0/2257
13	M	0.41	0/1671	0.74	0/2253
14	2	0.32	0/1711	0.76	0/2319
14	N	0.32	0/1709	0.76	0/2317
All	All	0.33	2/48503 (0.0%)	0.75	8/65682 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	188	PRO	N-CD	5.13	1.55	1.47
6	F	240	PRO	N-CD	5.05	1.54	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	187	ARG	C-N-CD	8.43	139.14	120.60
1	A	209	ASP	N-CA-C	-7.71	100.87	111.28
1	A	63	SER	CA-C-N	5.84	130.03	120.63
1	A	63	SER	C-N-CA	5.84	130.03	120.63
9	I	171	SER	CB-CA-C	-5.63	110.10	116.63
9	W	171	SER	CB-CA-C	-5.51	110.23	116.63
6	F	239	ARG	CA-C-N	-5.17	113.38	119.84
6	F	239	ARG	C-N-CA	-5.17	113.38	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1845	0	1805	52	0
1	O	1845	0	1805	28	0
2	B	1707	0	1591	27	0
2	P	1712	0	1605	35	0
3	C	1912	0	1851	21	0
3	Q	1913	0	1848	23	0
4	D	1724	0	1525	24	0
4	R	1691	0	1468	27	0
5	E	1759	0	1707	32	0
5	S	1716	0	1707	25	0
6	F	1850	0	1822	49	0
6	T	1850	0	1822	44	0
7	G	1885	0	1845	32	0
7	U	1885	0	1845	33	0
8	H	1509	0	1473	12	0
8	V	1509	0	1473	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1643	0	1644	41	0
9	W	1643	0	1644	35	0
10	J	1585	0	1598	30	0
10	X	1585	0	1598	36	0
11	K	1570	0	1547	25	0
11	Y	1570	0	1547	23	0
12	L	1548	0	1499	25	0
12	Z	1551	0	1508	22	0
13	1	1644	0	1627	20	0
13	M	1641	0	1618	26	0
14	2	1678	0	1640	30	0
14	N	1676	0	1633	32	0
15	A	2	0	0	0	0
15	D	4	0	0	0	0
15	E	8	0	0	6	0
15	F	19	0	0	9	0
15	G	1	0	0	0	0
15	K	9	0	0	1	0
15	L	8	0	0	1	0
15	M	34	0	0	3	0
15	N	11	0	0	0	0
15	O	1	0	0	0	0
15	P	24	0	0	10	0
15	Q	10	0	0	1	0
15	R	5	0	0	2	0
15	W	17	0	0	1	0
15	X	25	0	0	3	0
15	Y	3	0	0	0	0
15	Z	4	0	0	0	0
All	All	47831	0	46295	720	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 8.

All (720) 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)
9:W:187:ARG:HB3	9:W:188:PRO:CD	1.57	1.28
9:W:187:ARG:HB3	9:W:188:PRO:HD2	1.13	1.11
9:W:187:ARG:CB	9:W:188:PRO:CD	2.35	1.05
6:T:196:ARG:HD3	6:T:239:ARG:HE	1.21	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:189:LYS:HD3	15:F:317:HOH:O	1.63	0.99
6:F:96:ARG:HD2	13:M:73:LYS:HZ1	1.25	0.98
2:P:233:ALA:HB1	15:P:323:HOH:O	1.65	0.97
12:L:201:GLY:HA2	15:L:306:HOH:O	1.65	0.95
1:A:207:SER:O	1:A:208:ILE:HD13	1.68	0.93
6:F:96:ARG:HD2	13:M:73:LYS:NZ	1.84	0.92
6:F:180:MET:HG2	15:F:316:HOH:O	1.68	0.91
14:2:186:ARG:HE	14:2:202:PRO:HB3	1.36	0.91
1:A:203:SER:O	1:A:207:SER:N	2.04	0.90
12:L:38:ASN:ND2	12:L:40:TYR:CZ	2.40	0.90
9:I:32:SER:HB2	9:I:187:ARG:NH2	1.87	0.88
2:P:231:ALA:HA	15:P:307:HOH:O	1.75	0.87
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.54	0.87
9:I:32:SER:CA	9:I:187:ARG:HH21	1.90	0.84
9:W:187:ARG:CB	9:W:188:PRO:HD3	2.06	0.83
9:I:172:ASN:CG	9:I:191:VAL:HG22	2.03	0.83
1:A:171:LYS:HB3	1:A:205:VAL:HG21	1.59	0.83
6:F:207:THR:HB	6:F:226:ASP:O	1.79	0.82
9:I:32:SER:HA	9:I:187:ARG:HH21	1.45	0.82
5:E:186:HIS:HA	15:E:306:HOH:O	1.81	0.81
6:F:50:LYS:HE2	6:F:211:SER:OG	1.80	0.81
6:F:96:ARG:CD	13:M:73:LYS:HZ1	1.94	0.81
9:W:187:ARG:HG3	9:W:188:PRO:HD3	1.62	0.80
5:E:186:HIS:HB2	15:E:302:HOH:O	1.82	0.80
6:F:40:SER:HB3	15:F:307:HOH:O	1.81	0.80
1:A:67:THR:HG22	1:A:69:LEU:H	1.48	0.78
6:T:196:ARG:HD3	6:T:239:ARG:NE	1.96	0.78
6:T:239:ARG:HD2	6:T:239:ARG:O	1.82	0.78
1:A:171:LYS:HB3	1:A:205:VAL:CG2	2.12	0.78
9:I:172:ASN:OD1	9:I:191:VAL:HG13	1.83	0.78
2:P:110:VAL:HG22	2:P:135:ILE:HD12	1.66	0.78
2:B:110:VAL:HG22	2:B:135:ILE:HD12	1.66	0.77
9:W:187:ARG:CG	9:W:188:PRO:HD3	2.14	0.77
9:I:172:ASN:OD1	9:I:191:VAL:HG22	1.84	0.77
10:J:28:PHE:HB3	10:J:36:THR:HG22	1.65	0.77
6:T:239:ARG:H	6:T:239:ARG:NH1	1.80	0.77
1:O:67:THR:HG22	1:O:69:LEU:H	1.48	0.77
10:X:28:PHE:HB3	10:X:36:THR:HG22	1.66	0.76
11:Y:44:LEU:HD11	11:Y:102:LEU:HD12	1.67	0.76
11:K:44:LEU:HD11	11:K:102:LEU:HD12	1.67	0.75
3:Q:8:ARG:HB3	3:Q:11:ILE:HD12	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:204:LYS:CB	15:R:303:HOH:O	2.32	0.75
3:C:8:ARG:HB3	3:C:11:ILE:HD12	1.67	0.75
1:A:206:LEU:O	1:A:207:SER:OG	2.04	0.75
14:2:186:ARG:HE	14:2:202:PRO:CB	1.99	0.74
5:E:84:ASP:OD2	5:E:135:ARG:NH2	2.20	0.74
4:D:137:ASP:OD2	4:D:143:ARG:NH1	2.21	0.73
5:E:42:THR:HG22	5:E:44:GLU:H	1.53	0.73
5:S:42:THR:HG22	5:S:44:GLU:H	1.52	0.73
6:F:96:ARG:CD	13:M:73:LYS:NZ	2.50	0.72
12:Z:83:LEU:HD11	12:Z:97:MET:HE1	1.72	0.72
7:U:83:ASP:OD2	7:U:129:ARG:NH2	2.22	0.72
6:F:65:HIS:HB2	15:F:305:HOH:O	1.87	0.72
1:A:158:GLY:O	2:B:83:ARG:NH2	2.23	0.71
7:U:186:CYS:HB3	7:U:215:TRP:HZ3	1.54	0.71
7:G:83:ASP:OD2	7:G:129:ARG:NH2	2.23	0.71
6:F:237:GLU:CB	15:F:312:HOH:O	2.38	0.71
12:L:38:ASN:ND2	12:L:40:TYR:CE1	2.59	0.70
10:X:116:THR:O	10:X:192:LYS:NZ	2.23	0.70
10:J:116:THR:O	10:J:192:LYS:NZ	2.24	0.70
6:T:120:THR:O	7:U:129:ARG:NH1	2.24	0.70
9:I:32:SER:CB	9:I:187:ARG:NH2	2.54	0.70
6:T:104:PRO:HB3	14:2:81:HIS:HD2	1.56	0.70
6:T:196:ARG:CD	6:T:239:ARG:HE	2.00	0.69
10:X:65:GLN:OE1	11:Y:86:ARG:NH2	2.24	0.69
11:Y:33:ASP:OD2	11:Y:181:ARG:NH2	2.26	0.69
1:O:132:ARG:HG2	7:U:12:SER:HA	1.75	0.69
1:A:132:ARG:HG2	7:G:12:SER:HA	1.74	0.69
12:L:83:LEU:HD11	12:L:97:MET:HE1	1.75	0.69
2:P:69:LYS:HD2	15:P:314:HOH:O	1.93	0.69
7:U:1:SER:HA	7:U:19:ARG:HH12	1.56	0.69
6:F:104:PRO:HB3	14:N:81:HIS:HD2	1.58	0.69
7:G:1:SER:HA	7:G:19:ARG:HH12	1.57	0.68
11:K:33:ASP:OD2	11:K:181:ARG:NH2	2.25	0.68
1:A:202:LEU:O	1:A:205:VAL:CG1	2.42	0.68
1:A:202:LEU:O	1:A:205:VAL:HG12	1.94	0.67
2:P:67:ILE:HD11	2:P:73:LEU:HD12	1.74	0.67
12:L:115:ASP:HB2	12:L:119:ASN:HB2	1.76	0.67
6:F:120:THR:O	7:G:129:ARG:NH1	2.24	0.67
1:A:49:VAL:HG22	1:A:219:VAL:HG23	1.76	0.67
14:N:212:ALA:HA	8:V:30:VAL:HG21	1.75	0.67
2:B:67:ILE:HD11	2:B:73:LEU:HD12	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:GLN:HG3	9:I:65:LEU:HD13	1.78	0.66
10:J:45:MET:HE3	10:J:71:LEU:HD22	1.77	0.66
1:A:171:LYS:HG3	1:A:205:VAL:HG22	1.76	0.66
10:X:45:MET:HE3	10:X:71:LEU:HD22	1.77	0.66
6:F:225:ASP:O	6:F:226:ASP:HB2	1.93	0.66
14:N:51:LEU:HD11	14:N:110:MET:HB3	1.78	0.66
8:H:30:VAL:HG21	14:2:212:ALA:HA	1.76	0.66
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.78	0.66
14:2:51:LEU:HD13	14:2:112:ILE:HG12	1.76	0.66
9:I:172:ASN:OD1	9:I:191:VAL:CG1	2.44	0.66
12:Z:115:ASP:HB2	12:Z:119:ASN:HB2	1.78	0.66
14:2:51:LEU:HD11	14:2:110:MET:HB3	1.78	0.66
14:N:51:LEU:HD13	14:N:112:ILE:HG12	1.76	0.66
2:P:50:LYS:NZ	2:P:199:GLU:O	2.28	0.66
8:H:14:LEU:HD21	8:H:101:ALA:HB3	1.78	0.65
5:S:84:ASP:OD2	5:S:135:ARG:NH2	2.30	0.65
1:A:130:GLU:HG2	2:B:4:GLY:HA2	1.77	0.65
13:M:137:ALA:H	13:M:146:GLN:HE21	1.44	0.65
1:O:158:GLY:O	2:P:83:ARG:NH2	2.29	0.65
10:J:65:GLN:OE1	11:K:86:ARG:NH2	2.28	0.65
5:S:31:ILE:HD13	5:S:140:ALA:HB2	1.77	0.65
1:A:202:LEU:C	1:A:205:VAL:HG12	2.22	0.65
5:E:31:ILE:HD13	5:E:140:ALA:HB2	1.77	0.65
9:I:172:ASN:OD1	9:I:191:VAL:CG2	2.45	0.65
10:J:125:ASP:HB2	10:J:129:CYS:H	1.61	0.65
13:1:137:ALA:H	13:1:146:GLN:HE21	1.45	0.65
6:F:225:ASP:HA	6:F:229:VAL:HG23	1.78	0.64
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.78	0.64
1:A:201:CYS:O	1:A:205:VAL:HG12	1.98	0.64
2:P:94:GLN:HG3	9:W:65:LEU:HD13	1.80	0.64
9:I:32:SER:CA	9:I:187:ARG:NH2	2.61	0.64
1:O:49:VAL:HG22	1:O:219:VAL:HG23	1.79	0.64
5:E:49:ALA:HB2	5:E:217:LEU:HD23	1.80	0.64
11:K:1:MET:HE1	11:K:134:TYR:H	1.62	0.64
13:1:148:LEU:HD23	13:1:178:VAL:HG12	1.78	0.64
2:B:50:LYS:NZ	2:B:199:GLU:O	2.29	0.64
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.79	0.64
5:S:49:ALA:HB2	5:S:217:LEU:HD23	1.80	0.63
9:W:141:LYS:NZ	9:W:157:GLU:OE2	2.26	0.63
10:X:125:ASP:HB2	10:X:129:CYS:H	1.62	0.63
4:D:38:ARG:NE	4:D:181:ILE:O	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:148:LEU:HD23	13:M:178:VAL:HG12	1.79	0.63
6:T:167:SER:HB3	6:T:197:GLU:HG2	1.80	0.63
11:Y:1:MET:HE1	11:Y:134:TYR:H	1.63	0.63
4:R:38:ARG:NE	4:R:181:ILE:O	2.31	0.63
9:W:190:THR:HG22	9:W:192:PRO:HD3	1.81	0.62
11:Y:21:ALA:HB3	11:Y:29:LYS:HB3	1.80	0.62
6:F:196:ARG:HD3	6:F:239:ARG:CZ	2.29	0.62
12:L:38:ASN:HB2	12:L:41:LEU:HB2	1.82	0.62
6:F:225:ASP:HA	6:F:229:VAL:CG2	2.30	0.62
11:K:21:ALA:HB3	11:K:29:LYS:HB3	1.81	0.62
13:1:99:ARG:NH1	13:1:102:PHE:O	2.33	0.62
1:O:120:ASP:OD1	2:P:83:ARG:NH1	2.33	0.62
1:O:6:SER:HB2	1:O:11:ARG:HH11	1.62	0.61
14:2:9:THR:O	14:2:41:ARG:NH2	2.33	0.61
1:A:132:ARG:NH1	7:G:123:THR:O	2.33	0.61
14:N:9:THR:O	14:N:41:ARG:NH2	2.34	0.61
2:P:39:ALA:O	2:P:41:ASN:N	2.33	0.61
1:O:130:GLU:HG2	2:P:4:GLY:HA2	1.82	0.61
9:I:141:LYS:NZ	9:I:157:GLU:OE2	2.26	0.61
9:I:175:LEU:HD12	9:I:189:TYR:CE1	2.35	0.61
1:A:6:SER:HB2	1:A:11:ARG:HH11	1.63	0.61
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.83	0.61
7:U:227:VAL:O	7:U:232:ARG:NH1	2.34	0.61
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.83	0.61
10:J:34:MET:O	12:Z:166:ARG:NH1	2.34	0.61
13:M:99:ARG:NH1	13:M:102:PHE:O	2.33	0.61
6:F:180:MET:CG	15:F:316:HOH:O	2.37	0.60
6:T:104:PRO:HB3	14:2:81:HIS:CD2	2.36	0.60
1:O:132:ARG:NH1	7:U:123:THR:O	2.34	0.60
7:U:186:CYS:HB3	7:U:215:TRP:CZ3	2.36	0.60
6:F:189:LYS:CD	15:F:317:HOH:O	2.34	0.60
7:G:99:ARG:NH1	14:N:69:GLN:OE1	2.31	0.60
6:T:239:ARG:H	6:T:239:ARG:HH11	1.47	0.60
9:W:204:CYS:HB3	9:W:208:THR:HG21	1.84	0.60
12:Z:38:ASN:ND2	12:Z:40:TYR:CZ	2.66	0.60
2:B:39:ALA:O	2:B:41:ASN:N	2.35	0.60
9:I:32:SER:CB	9:I:187:ARG:HH21	2.15	0.60
1:A:203:SER:O	1:A:207:SER:CA	2.49	0.60
6:T:103:LEU:HD12	6:T:104:PRO:HD2	1.83	0.59
9:I:204:CYS:HB3	9:I:208:THR:HG21	1.84	0.59
10:X:47:ASP:HA	15:X:317:HOH:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:10:HIS:HD2	12:Z:149:VAL:HG23	1.67	0.59
3:C:62:SER:OG	3:C:63:GLU:N	2.35	0.59
5:E:168:ARG:NH1	6:F:53:GLN:OE1	2.35	0.59
6:T:36:VAL:HG13	6:T:172:LEU:HD11	1.84	0.59
12:L:166:ARG:NH1	10:X:34:MET:O	2.35	0.59
4:R:209:ALA:HB1	4:R:217:LEU:HD11	1.84	0.59
12:L:10:HIS:HD2	12:L:149:VAL:HG23	1.68	0.59
4:D:209:ALA:HB1	4:D:217:LEU:HD11	1.84	0.58
4:R:230:ALA:HA	15:R:301:HOH:O	2.02	0.58
11:Y:4:LEU:HD22	11:Y:45:LEU:HD12	1.85	0.58
11:K:4:LEU:HD22	11:K:45:LEU:HD12	1.84	0.58
6:F:237:GLU:O	6:F:239:ARG:N	2.37	0.58
9:I:174:ASP:CG	9:I:187:ARG:HG2	2.28	0.58
6:T:212:ILE:HD12	6:T:229:VAL:HG22	1.85	0.58
5:E:148:GLU:OE2	13:M:81:LYS:NZ	2.34	0.58
9:I:174:ASP:OD2	9:I:187:ARG:NE	2.36	0.58
12:L:97:MET:HB3	12:L:116:SER:HB3	1.86	0.58
3:Q:68:LEU:HD11	3:Q:74:CYS:HB3	1.86	0.58
6:F:40:SER:CB	15:F:307:HOH:O	2.43	0.58
6:F:104:PRO:HB3	14:N:81:HIS:CD2	2.38	0.58
2:P:74:VAL:HG23	2:P:134:LEU:HB2	1.86	0.58
1:O:126:THR:HG22	2:P:127:ARG:HH21	1.69	0.58
1:A:120:ASP:OD1	2:B:83:ARG:NH1	2.37	0.57
7:G:227:VAL:O	7:G:232:ARG:NH1	2.35	0.57
1:O:54:LYS:NZ	1:O:66:VAL:O	2.37	0.57
6:T:165:SER:OG	6:T:169:ARG:NH2	2.37	0.57
7:U:99:ARG:NH1	14:2:69:GLN:OE1	2.33	0.57
12:Z:38:ASN:HB2	12:Z:41:LEU:HB2	1.86	0.57
6:F:165:SER:OG	6:F:169:ARG:NH2	2.37	0.57
14:2:96:MET:HE3	14:2:127:MET:HA	1.86	0.57
3:C:68:LEU:HD11	3:C:74:CYS:HB3	1.86	0.57
6:T:121:GLN:HG3	7:U:129:ARG:HG3	1.87	0.57
10:X:189:ILE:HG23	10:X:196:THR:HB	1.85	0.57
6:T:239:ARG:O	6:T:239:ARG:NH1	2.32	0.57
2:B:74:VAL:HG23	2:B:134:LEU:HB2	1.86	0.57
6:F:36:VAL:HG13	6:F:172:LEU:HD11	1.85	0.57
5:S:148:GLU:OE2	13:1:81:LYS:NZ	2.37	0.57
4:D:80:ALA:HA	4:D:129:ILE:HD13	1.86	0.57
10:J:189:ILE:HG23	10:J:196:THR:HB	1.85	0.57
1:A:54:LYS:NZ	1:A:66:VAL:O	2.37	0.57
5:E:51:GLU:HA	5:E:215:ILE:HG22	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:20:VAL:HG12	10:J:190:ILE:HG12	1.86	0.57
4:R:119:THR:O	5:S:135:ARG:NH1	2.38	0.57
2:B:45:LEU:HD13	2:B:74:VAL:HG22	1.87	0.57
6:F:103:LEU:HD12	6:F:104:PRO:HD2	1.85	0.57
14:N:96:MET:HE3	14:N:127:MET:HA	1.87	0.57
6:T:196:ARG:C	6:T:198:THR:H	2.13	0.57
4:D:119:THR:O	5:E:135:ARG:NH1	2.38	0.56
13:1:63:THR:OG1	14:2:94:ARG:NH2	2.37	0.56
1:A:126:THR:HG22	2:B:127:ARG:HH21	1.70	0.56
3:C:154:GLY:O	4:D:81:ARG:NH2	2.36	0.56
13:M:38:ARG:NE	13:M:191:ASP:OD1	2.34	0.56
12:Z:97:MET:HB3	12:Z:116:SER:HB3	1.88	0.56
6:F:121:GLN:HG3	7:G:129:ARG:HG3	1.87	0.56
14:N:99:ARG:NH1	14:N:104:ASN:O	2.36	0.56
5:S:51:GLU:HA	5:S:215:ILE:HG22	1.88	0.56
9:W:6:VAL:HG23	9:W:124:TYR:HB3	1.87	0.56
13:M:38:ARG:HG3	15:M:305:HOH:O	2.04	0.56
13:1:38:ARG:NE	13:1:191:ASP:OD1	2.34	0.56
10:X:20:VAL:HG12	10:X:190:ILE:HG12	1.87	0.56
1:A:202:LEU:HA	1:A:205:VAL:CG1	2.36	0.56
6:T:227:ASP:O	6:T:230:SER:OG	2.24	0.56
11:Y:85:ARG:HG3	11:Y:124:LEU:HB2	1.88	0.56
1:A:182:LYS:HD3	1:A:197:THR:HG23	1.86	0.56
2:P:45:LEU:HD13	2:P:74:VAL:HG22	1.88	0.56
9:I:6:VAL:HG23	9:I:124:TYR:HB3	1.88	0.56
4:R:100:ASP:OD2	12:Z:107:ARG:NH2	2.39	0.56
4:R:80:ALA:HA	4:R:129:ILE:HD13	1.88	0.55
11:K:85:ARG:HG3	11:K:124:LEU:HB2	1.88	0.55
14:2:99:ARG:NH1	14:2:104:ASN:O	2.37	0.55
14:N:50:MET:HE2	14:N:192:VAL:HG22	1.88	0.55
1:A:132:ARG:HB3	7:G:12:SER:O	2.06	0.55
5:E:224:GLN:HB2	15:E:304:HOH:O	2.07	0.55
7:U:50:GLU:OE2	7:U:201:HIS:ND1	2.38	0.55
1:A:173:THR:O	1:A:176:THR:OG1	2.24	0.55
1:O:182:LYS:HD3	1:O:197:THR:HG23	1.87	0.55
2:P:76:SER:HA	15:P:310:HOH:O	2.05	0.55
5:S:168:ARG:NH1	6:T:53:GLN:OE1	2.40	0.55
9:W:189:TYR:O	9:W:190:THR:OG1	2.25	0.55
1:A:32:ILE:HD13	1:A:137:CYS:HB2	1.90	0.54
6:F:227:ASP:O	6:F:230:SER:OG	2.25	0.54
13:1:28:ARG:NE	13:1:191:ASP:OD2	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:155:ASN:OD1	4:R:77:THR:OG1	2.24	0.54
6:T:40:SER:HB3	6:T:187:LEU:HD22	1.90	0.54
7:U:152:ASP:OD1	7:U:154:SER:OG	2.25	0.54
9:I:144:PRO:HB3	14:2:214:MET:HE1	1.90	0.54
1:A:6:SER:HB2	1:A:11:ARG:NH1	2.22	0.54
13:1:191:ASP:O	13:1:212:LYS:NZ	2.38	0.54
7:G:50:GLU:OE2	7:G:201:HIS:ND1	2.39	0.54
5:E:232:GLU:OE2	5:E:232:GLU:N	2.38	0.54
5:E:36:THR:HA	5:E:171:GLY:HA3	1.90	0.53
14:N:185:ASN:OD1	14:N:205:THR:OG1	2.20	0.53
2:P:33:PRO:HB3	15:P:309:HOH:O	2.08	0.53
1:A:207:SER:O	1:A:208:ILE:CD1	2.50	0.53
6:F:225:ASP:N	6:F:225:ASP:OD2	2.38	0.53
12:L:105:ASP:OD1	12:L:106:LYS:N	2.40	0.53
6:F:40:SER:HB3	6:F:187:LEU:HD22	1.90	0.53
12:Z:105:ASP:OD1	12:Z:106:LYS:N	2.40	0.53
1:O:32:ILE:HD13	1:O:137:CYS:HB2	1.91	0.53
3:Q:239:LYS:HG3	15:Q:308:HOH:O	2.08	0.53
14:N:214:MET:HE1	9:W:144:PRO:HB3	1.91	0.53
4:D:184:ASP:OD1	4:D:184:ASP:N	2.40	0.53
1:O:6:SER:HB2	1:O:11:ARG:NH1	2.22	0.53
4:R:184:ASP:N	4:R:184:ASP:OD1	2.40	0.53
10:X:34:MET:HE3	10:X:37:THR:HG23	1.90	0.53
14:2:50:MET:HE2	14:2:192:VAL:HG22	1.91	0.53
6:F:225:ASP:CA	6:F:229:VAL:HG23	2.39	0.53
10:J:34:MET:HE3	10:J:37:THR:HG23	1.90	0.53
3:Q:154:GLY:O	4:R:81:ARG:NH2	2.36	0.53
12:Z:44:THR:HG21	12:Z:100:MET:HE3	1.91	0.53
1:O:103:TYR:O	9:W:81:ARG:NH1	2.42	0.52
3:Q:49:ARG:NH2	3:Q:58:GLU:OE2	2.31	0.52
13:M:63:THR:OG1	14:N:94:ARG:NH2	2.43	0.52
3:Q:62:SER:OG	3:Q:63:GLU:N	2.35	0.52
5:E:85:ALA:HB2	5:E:139:VAL:HG21	1.91	0.52
10:J:15:LYS:NZ	10:J:134:ASP:OD1	2.41	0.52
5:S:85:ALA:HB2	5:S:139:VAL:HG21	1.91	0.52
10:X:15:LYS:NZ	10:X:134:ASP:OD1	2.42	0.52
5:E:167:ALA:HB3	6:F:56:LEU:HD13	1.90	0.52
11:K:109:GLU:HA	15:K:201:HOH:O	2.10	0.52
10:X:45:MET:HE2	10:X:67:LEU:HG	1.90	0.52
11:K:1:MET:CE	11:K:134:TYR:H	2.23	0.52
3:Q:45:LEU:HD13	3:Q:75:SER:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:62:THR:OG1	11:K:85:ARG:NH2	2.43	0.52
8:V:84:LYS:HG3	8:V:120:MET:HB2	1.92	0.52
11:Y:1:MET:CE	11:Y:134:TYR:H	2.22	0.52
2:B:185:ASP:O	2:B:189:THR:HG22	2.10	0.52
3:C:45:LEU:HD13	3:C:75:SER:HB2	1.92	0.52
11:K:37:LYS:H	11:K:37:LYS:HD2	1.74	0.52
12:L:44:THR:HG21	12:L:100:MET:HE3	1.92	0.51
1:O:50:ILE:HG21	1:O:79:VAL:HB	1.92	0.51
3:C:49:ARG:NH2	3:C:58:GLU:OE2	2.31	0.51
14:N:177:TYR:CZ	14:N:185:ASN:HB2	2.45	0.51
7:U:47:PHE:HB2	7:U:214:SER:HB2	1.93	0.51
8:V:142:THR:HB	8:V:155:PHE:HE1	1.75	0.51
8:H:142:THR:HB	8:H:155:PHE:HE1	1.75	0.51
13:M:191:ASP:O	13:M:212:LYS:NZ	2.38	0.51
5:S:36:THR:HA	5:S:171:GLY:HA3	1.92	0.51
1:A:50:ILE:HG21	1:A:79:VAL:HB	1.93	0.51
7:G:186:CYS:O	7:G:190:VAL:HG23	2.10	0.51
9:W:56:THR:CG2	15:W:313:HOH:O	2.57	0.51
14:2:9:THR:OG1	14:2:10:SER:N	2.44	0.51
10:J:45:MET:HE2	10:J:67:LEU:HG	1.92	0.51
6:T:212:ILE:CD1	6:T:229:VAL:HG13	2.41	0.51
10:X:158:MET:HE1	10:X:166:THR:OG1	2.11	0.51
3:C:21:VAL:HG11	3:C:153:SER:HB3	1.93	0.51
7:G:47:PHE:HB2	7:G:214:SER:HB2	1.93	0.51
3:Q:21:VAL:HG11	3:Q:153:SER:HB3	1.93	0.51
6:T:196:ARG:CD	6:T:239:ARG:NE	2.67	0.51
7:U:136:MET:HE2	7:U:148:LEU:HD11	1.91	0.51
10:X:114:PRO:HG2	15:X:312:HOH:O	2.11	0.51
7:G:136:MET:HE2	7:G:148:LEU:HD11	1.91	0.51
13:1:16:ALA:HB2	13:1:121:VAL:HG23	1.93	0.51
5:E:224:GLN:CB	15:E:304:HOH:O	2.59	0.51
7:G:74:GLY:HA3	7:G:224:HIS:CD2	2.46	0.50
5:S:24:VAL:O	5:S:28:ILE:HG12	2.11	0.50
7:U:74:GLY:HA3	7:U:224:HIS:CD2	2.46	0.50
11:Y:37:LYS:H	11:Y:37:LYS:HD2	1.75	0.50
14:2:166:ARG:NH2	14:2:200:GLU:OE1	2.42	0.50
13:M:169:ASP:OD2	13:M:173:ARG:NH2	2.44	0.50
13:1:169:ASP:OD2	13:1:173:ARG:NH2	2.44	0.50
8:H:84:LYS:HG3	8:H:120:MET:HB2	1.94	0.50
9:I:20:ALA:HB3	9:I:28:ASP:HB3	1.94	0.50
11:K:80:ALA:O	11:K:84:THR:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:173:ILE:O	9:I:189:TYR:N	2.40	0.50
10:J:158:MET:HE1	10:J:166:THR:OG1	2.11	0.50
9:W:20:ALA:HB3	9:W:28:ASP:HB3	1.94	0.50
11:Y:80:ALA:O	11:Y:84:THR:HG23	2.11	0.50
4:D:12:PRO:HA	5:E:26:TYR:CD1	2.47	0.50
2:P:94:GLN:HE21	2:P:94:GLN:HA	1.77	0.50
5:E:24:VAL:O	5:E:28:ILE:HG12	2.12	0.49
7:G:152:ASP:OD1	7:G:154:SER:OG	2.25	0.49
9:I:190:THR:O	9:I:192:PRO:HD3	2.12	0.49
1:O:132:ARG:HB3	7:U:12:SER:O	2.12	0.49
2:P:185:ASP:O	2:P:189:THR:HG22	2.11	0.49
10:X:66:ARG:O	10:X:69:PHE:HB3	2.12	0.49
1:A:202:LEU:O	1:A:205:VAL:HG13	2.12	0.49
10:J:66:ARG:O	10:J:69:PHE:HB3	2.12	0.49
13:M:16:ALA:HB2	13:M:121:VAL:HG23	1.94	0.49
9:W:186:LEU:HD13	9:W:189:TYR:HD1	1.77	0.49
2:B:173:LEU:HD21	2:B:193:THR:HG21	1.94	0.49
9:I:216:ILE:HD13	10:J:196:THR:HG23	1.93	0.49
7:U:186:CYS:O	7:U:190:VAL:HG23	2.12	0.49
4:R:94:HIS:ND1	4:R:101:PRO:O	2.41	0.49
2:B:94:GLN:HA	2:B:94:GLN:HE21	1.76	0.49
4:D:94:HIS:ND1	4:D:101:PRO:O	2.42	0.49
7:G:86:SER:O	7:G:90:ILE:HD12	2.12	0.49
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.93	0.49
2:P:173:LEU:HD21	2:P:193:THR:HG21	1.94	0.49
5:S:232:GLU:OE2	5:S:232:GLU:N	2.38	0.49
2:P:94:GLN:HG2	15:P:319:HOH:O	2.12	0.49
1:A:72:ILE:HG21	1:A:114:LEU:HD11	1.94	0.48
9:W:216:ILE:HD13	10:X:196:THR:HG23	1.94	0.48
13:1:12:ILE:HD12	13:1:55:SER:HB2	1.95	0.48
4:D:66:ASP:OD1	4:D:67:ASP:N	2.41	0.48
10:J:107:PRO:HG2	10:J:124:LEU:HB2	1.95	0.48
6:T:40:SER:OG	6:T:41:LYS:N	2.45	0.48
6:T:41:LYS:HG3	6:T:42:THR:HG23	1.95	0.48
9:I:175:LEU:HD12	9:I:189:TYR:CD1	2.49	0.48
5:E:166:ASP:HB3	5:E:185:TYR:CE2	2.49	0.48
6:F:202:GLU:H	6:F:202:GLU:HG3	1.40	0.48
4:R:79:ASP:OD2	4:R:125:ARG:NH2	2.47	0.48
10:X:107:PRO:HG2	10:X:124:LEU:HB2	1.95	0.48
2:B:87:HIS:HD1	2:B:87:HIS:C	2.21	0.48
5:E:66:LYS:N	5:E:216:GLU:OE2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:3:ILE:HD13	8:H:46:SER:HB3	1.94	0.48
9:I:113:ILE:HG12	9:I:119:THR:HG22	1.94	0.48
13:M:12:ILE:HD12	13:M:55:SER:HB2	1.96	0.48
14:N:126:ASP:HB2	14:N:130:VAL:HB	1.94	0.48
5:S:66:LYS:N	5:S:216:GLU:OE2	2.45	0.48
6:F:40:SER:OG	6:F:41:LYS:N	2.46	0.48
14:N:9:THR:OG1	14:N:10:SER:N	2.45	0.48
6:F:71:GLY:HA3	6:F:221:PHE:CZ	2.49	0.48
13:M:28:ARG:NE	13:M:191:ASP:OD2	2.35	0.48
5:S:167:ALA:HB3	6:T:56:LEU:HD13	1.95	0.48
3:Q:86:LEU:HD22	3:Q:114:LEU:HD11	1.95	0.48
12:L:20:ALA:HB2	12:L:31:VAL:HG21	1.95	0.48
9:I:187:ARG:HA	9:I:188:PRO:HA	1.61	0.48
4:R:66:ASP:OD1	4:R:67:ASP:N	2.42	0.48
14:2:126:ASP:HB2	14:2:130:VAL:HB	1.95	0.48
4:D:79:ASP:OD2	4:D:125:ARG:NH2	2.47	0.47
6:F:64:LEU:HA	15:F:315:HOH:O	2.12	0.47
6:T:239:ARG:HH11	6:T:239:ARG:C	2.20	0.47
10:X:58:THR:OG1	11:Y:121:LEU:O	2.27	0.47
1:O:72:ILE:HG21	1:O:114:LEU:HD11	1.95	0.47
4:D:121:SER:HB2	4:D:124:ARG:HD2	1.96	0.47
6:F:41:LYS:HG3	6:F:42:THR:HG23	1.96	0.47
5:S:166:ASP:HB3	5:S:185:TYR:CE2	2.48	0.47
6:T:71:GLY:HA3	6:T:221:PHE:CZ	2.50	0.47
14:2:124:TYR:O	14:2:131:ALA:HA	2.14	0.47
1:A:165:ALA:HB1	1:A:179:LEU:HD13	1.95	0.47
14:N:177:TYR:CE1	14:N:185:ASN:HB2	2.48	0.47
1:O:165:ALA:HB1	1:O:179:LEU:HD13	1.95	0.47
5:E:31:ILE:HD11	5:E:158:PRO:CD	2.45	0.47
9:W:174:ASP:CG	9:W:187:ARG:O	2.57	0.47
4:D:100:ASP:OD2	12:L:107:ARG:NH2	2.47	0.47
4:D:132:LEU:HD22	4:D:144:LEU:HD11	1.97	0.47
14:N:141:TYR:HE2	8:V:24:SER:HB2	1.80	0.47
4:R:132:LEU:HD22	4:R:144:LEU:HD11	1.97	0.47
9:W:113:ILE:HG12	9:W:119:THR:HG22	1.95	0.47
13:1:145:LEU:HD22	13:1:178:VAL:HB	1.97	0.47
9:I:64:GLU:O	9:I:68:LEU:HB2	2.13	0.47
7:U:86:SER:O	7:U:90:ILE:HD12	2.14	0.47
9:W:64:GLU:O	9:W:68:LEU:HB2	2.14	0.47
10:X:62:THR:OG1	11:Y:85:ARG:NH2	2.45	0.47
14:N:124:TYR:O	14:N:131:ALA:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:33:PRO:CB	15:P:309:HOH:O	2.63	0.47
12:Z:38:ASN:ND2	12:Z:40:TYR:CE1	2.83	0.47
1:A:202:LEU:CA	1:A:205:VAL:HG12	2.45	0.47
7:G:215:TRP:HE1	7:G:228:PRO:HD2	1.80	0.47
6:T:211:SER:OG	6:T:225:ASP:OD1	2.32	0.47
1:A:175:SER:OG	1:A:201:CYS:SG	2.69	0.46
6:T:196:ARG:C	6:T:198:THR:N	2.72	0.46
5:S:31:ILE:HD11	5:S:158:PRO:CD	2.46	0.46
11:Y:168:GLN:NE2	11:Y:175:LEU:O	2.35	0.46
3:C:66:TYR:CG	3:C:87:THR:HG21	2.51	0.46
9:I:198:ARG:NH2	10:J:152:SER:O	2.49	0.46
13:M:35:ILE:O	14:N:151:ARG:NH2	2.42	0.46
1:O:50:ILE:HG12	1:O:141:ILE:HD13	1.98	0.46
11:K:35:MET:HG2	11:K:45:LEU:HD13	1.97	0.46
11:K:196:PHE:O	11:K:198:LYS:N	2.48	0.46
6:T:196:ARG:O	6:T:198:THR:N	2.48	0.46
7:U:215:TRP:HE1	7:U:228:PRO:HD2	1.80	0.46
1:A:143:ILE:HG12	1:A:220:VAL:HG22	1.97	0.46
2:P:231:ALA:CA	15:P:307:HOH:O	2.47	0.46
4:R:51:ALA:C	4:R:53:LEU:H	2.24	0.46
9:W:198:ARG:NH2	10:X:152:SER:O	2.47	0.46
3:C:130:PHE:O	3:C:152:PRO:HB3	2.16	0.46
8:H:24:SER:HB2	14:2:141:TYR:HE2	1.81	0.46
13:M:184:GLU:HG3	9:W:195:LYS:HE2	1.98	0.46
14:N:212:ALA:HA	8:V:30:VAL:CG2	2.44	0.46
4:D:51:ALA:C	4:D:53:LEU:H	2.24	0.46
4:R:121:SER:HB2	4:R:124:ARG:HD2	1.97	0.46
1:A:103:TYR:O	9:I:81:ARG:NH1	2.47	0.46
2:B:75:TYR:HB3	2:B:82:TYR:CD1	2.51	0.46
13:M:145:LEU:HD22	13:M:178:VAL:HB	1.98	0.46
13:1:38:ARG:NH2	13:1:212:LYS:O	2.49	0.46
3:C:86:LEU:HD22	3:C:114:LEU:HD11	1.98	0.46
7:G:136:MET:HE3	7:G:163:CYS:HB3	1.98	0.46
11:K:168:GLN:NE2	11:K:175:LEU:O	2.36	0.46
11:Y:196:PHE:O	11:Y:198:LYS:N	2.49	0.46
1:A:208:ILE:O	1:A:209:ASP:HB2	2.15	0.45
1:O:143:ILE:HG12	1:O:220:VAL:HG22	1.98	0.45
12:Z:40:TYR:CZ	12:Z:73:ARG:HG2	2.51	0.45
9:W:59:ILE:HD12	9:W:82:MET:HB3	1.97	0.45
7:U:49:VAL:HG11	7:U:65:ARG:HB2	1.98	0.45
5:S:123:PHE:CE2	5:S:136:PRO:HG3	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:185:ASN:OD1	6:T:189:LYS:HE3	2.17	0.45
10:X:114:PRO:CG	15:X:312:HOH:O	2.64	0.45
13:M:136:LYS:HA	13:M:146:GLN:NE2	2.31	0.45
3:Q:66:TYR:CG	3:Q:87:THR:HG21	2.51	0.45
1:A:203:SER:O	1:A:207:SER:HA	2.17	0.45
2:B:177:TYR:O	2:B:178:ASN:ND2	2.47	0.45
7:G:49:VAL:HG11	7:G:65:ARG:HB2	1.99	0.45
2:P:75:TYR:HB3	2:P:82:TYR:CD1	2.52	0.45
4:R:38:ARG:CZ	4:R:38:ARG:H	2.30	0.45
11:Y:35:MET:HG2	11:Y:45:LEU:HD13	1.98	0.45
1:A:38:THR:HG21	1:A:171:LYS:HB2	1.99	0.45
5:E:50:VAL:HG11	5:E:66:LYS:HB2	1.99	0.45
15:M:324:HOH:O	9:W:198:ARG:HA	2.15	0.45
14:N:89:HIS:HA	14:N:112:ILE:HD12	1.99	0.45
3:Q:130:PHE:O	3:Q:152:PRO:HB3	2.16	0.45
13:M:38:ARG:NH2	13:M:212:LYS:O	2.50	0.45
3:Q:14:PRO:HA	4:R:21:TYR:CE1	2.52	0.45
2:B:28:VAL:HG11	2:B:132:SER:HB2	1.99	0.44
3:C:11:ILE:HG23	4:D:18:GLN:HE22	1.81	0.44
13:M:160:ASN:O	13:M:160:ASN:ND2	2.47	0.44
4:D:38:ARG:CZ	4:D:38:ARG:H	2.31	0.44
12:L:37:ILE:HG23	12:L:60:ALA:HB2	1.99	0.44
13:1:136:LYS:HA	13:1:146:GLN:NE2	2.32	0.44
1:A:188:ASP:O	1:A:190:THR:HG23	2.17	0.44
7:G:215:TRP:CD1	7:G:227:VAL:HA	2.53	0.44
10:J:58:THR:OG1	11:K:121:LEU:O	2.30	0.44
5:S:50:VAL:HG11	5:S:66:LYS:HB2	1.99	0.44
1:A:50:ILE:HG12	1:A:141:ILE:HD13	2.00	0.44
11:K:118:MET:HE2	11:K:118:MET:HB3	1.88	0.44
2:P:231:ALA:CB	15:P:307:HOH:O	2.65	0.44
10:X:48:ARG:HA	10:X:190:ILE:HD12	1.98	0.44
2:B:118:GLN:HG3	3:C:81:SER:HB2	1.98	0.44
3:C:171:ALA:HB2	3:C:200:THR:HG21	1.99	0.44
2:P:28:VAL:HG11	2:P:132:SER:HB2	1.99	0.44
6:T:50:LYS:HB3	6:T:59:HIS:HB3	1.99	0.44
10:X:138:VAL:HG11	10:X:146:MET:HB3	2.00	0.44
12:Z:13:ILE:HG13	12:Z:152:ALA:HB1	2.00	0.44
1:A:171:LYS:HA	1:A:171:LYS:HD3	1.78	0.44
1:A:212:PRO:HB2	1:A:232:GLU:HG3	1.99	0.44
7:G:102:PHE:HD1	8:H:78:THR:HG23	1.81	0.44
14:N:187:PHE:CE1	14:N:205:THR:HG23	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:177:TYR:O	2:P:178:ASN:ND2	2.48	0.44
6:T:22:ILE:O	6:T:26:MET:HG2	2.17	0.44
7:U:136:MET:HE3	7:U:163:CYS:HB3	2.00	0.44
10:X:62:THR:O	10:X:66:ARG:HG3	2.17	0.44
10:X:126:LEU:HD13	10:X:127:ILE:HG23	1.99	0.44
14:2:89:HIS:HA	14:2:112:ILE:HD12	1.99	0.44
1:A:171:LYS:CG	1:A:205:VAL:HG22	2.45	0.44
4:D:36:ARG:HA	4:D:41:VAL:HG12	1.99	0.44
6:F:139:ASP:HB2	14:N:81:HIS:CE1	2.52	0.44
10:J:62:THR:O	10:J:66:ARG:HG3	2.18	0.44
14:N:166:ARG:NH2	14:N:200:GLU:OE1	2.42	0.44
7:U:33:SER:O	7:U:167:LYS:HG3	2.18	0.44
12:Z:38:ASN:ND2	12:Z:40:TYR:OH	2.50	0.44
12:Z:75:SER:HB2	12:Z:105:ASP:OD2	2.18	0.44
13:1:160:ASN:O	13:1:160:ASN:ND2	2.47	0.44
3:C:197:LEU:HD12	3:C:197:LEU:HA	1.80	0.44
4:D:33:VAL:HG11	4:D:168:VAL:HG11	1.99	0.44
5:E:146:VAL:HG11	5:E:222:PRO:HA	2.00	0.44
5:E:203:LYS:HE2	5:E:241:ILE:HD11	1.99	0.44
6:F:189:LYS:HE2	6:F:235:GLY:O	2.17	0.44
10:J:48:ARG:HA	10:J:190:ILE:HD12	1.98	0.44
1:O:201:CYS:O	1:O:205:VAL:HB	2.17	0.44
4:R:33:VAL:HG11	4:R:168:VAL:HG11	2.00	0.44
4:R:36:ARG:HA	4:R:41:VAL:HG12	1.99	0.44
5:S:203:LYS:HE2	5:S:241:ILE:HD11	1.99	0.44
9:W:3:ILE:HD11	9:W:127:MET:HB2	2.00	0.44
9:W:28:ASP:HB2	10:X:131:MET:SD	2.58	0.44
12:L:67:GLU:HA	12:L:72:GLU:O	2.17	0.44
14:N:110:MET:HE3	14:N:110:MET:HB2	1.91	0.44
6:T:88:MET:HE3	6:T:112:ILE:HD11	2.00	0.44
9:W:174:ASP:OD1	9:W:187:ARG:O	2.35	0.44
5:E:85:ALA:O	5:E:89:ILE:HG12	2.18	0.43
5:E:123:PHE:CE2	5:E:136:PRO:HG3	2.53	0.43
6:F:49:LEU:C	6:F:50:LYS:O	2.60	0.43
11:K:180:VAL:HG21	11:K:194:ILE:HG12	1.99	0.43
14:N:92:LEU:O	14:N:96:MET:HG2	2.18	0.43
7:U:215:TRP:CD1	7:U:227:VAL:HA	2.52	0.43
10:X:164:PHE:CE1	10:X:198:ARG:HD2	2.53	0.43
11:Y:1:MET:HE3	11:Y:1:MET:HB3	1.75	0.43
6:F:88:MET:HE3	6:F:112:ILE:HD11	2.00	0.43
6:F:119:PRO:HB3	6:F:125:ARG:HH11	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:59:ILE:HD12	9:I:82:MET:HB3	1.98	0.43
14:N:20:VAL:HB	14:N:192:VAL:HG23	1.99	0.43
2:P:72:GLY:HA3	2:P:217:PHE:CE1	2.53	0.43
3:C:140:ASP:OD2	3:C:146:GLN:NE2	2.41	0.43
4:D:43:LEU:HD12	4:D:72:ALA:HB2	1.99	0.43
7:G:75:MET:HE3	7:G:135:PHE:CG	2.54	0.43
8:H:24:SER:HB2	14:2:141:TYR:CE2	2.54	0.43
11:K:1:MET:N	11:K:173:LEU:HD13	2.33	0.43
14:N:141:TYR:CE2	8:V:24:SER:HB2	2.53	0.43
2:P:64:VAL:HG12	2:P:217:PHE:HZ	1.83	0.43
5:S:146:VAL:HG11	5:S:222:PRO:HA	2.01	0.43
11:Y:1:MET:N	11:Y:173:LEU:HD13	2.33	0.43
3:C:42:GLY:HA2	3:C:145:PHE:CE1	2.53	0.43
7:U:39:ILE:HD11	7:U:181:MET:HB3	2.00	0.43
10:X:169:GLN:O	10:X:173:ASN:ND2	2.49	0.43
14:2:20:VAL:HB	14:2:192:VAL:HG23	1.99	0.43
2:B:72:GLY:HA3	2:B:217:PHE:CE1	2.53	0.43
6:F:22:ILE:O	6:F:26:MET:HG2	2.18	0.43
6:F:185:ASN:OD1	6:F:189:LYS:HE3	2.19	0.43
10:J:138:VAL:HG11	10:J:146:MET:HB3	2.01	0.43
14:N:25:ASP:HA	14:N:187:PHE:HA	2.00	0.43
1:O:211:LYS:HE2	1:O:211:LYS:HB3	1.73	0.43
1:O:212:PRO:HB2	1:O:232:GLU:HG3	2.00	0.43
6:T:239:ARG:HH11	6:T:239:ARG:N	2.16	0.43
13:1:35:ILE:O	14:2:151:ARG:NH2	2.44	0.43
9:I:63:LEU:HD23	9:I:63:LEU:HA	1.80	0.43
12:L:13:ILE:HG13	12:L:152:ALA:HB1	2.01	0.43
3:Q:171:ALA:HB2	3:Q:200:THR:HG21	2.00	0.43
6:T:189:LYS:HE2	6:T:235:GLY:O	2.19	0.43
14:2:187:PHE:CE1	14:2:205:THR:HG23	2.54	0.43
12:L:160:ILE:O	12:L:164:THR:HG23	2.18	0.43
9:W:198:ARG:HH21	10:X:152:SER:C	2.27	0.43
10:X:116:THR:HB	10:X:117:PHE:H	1.63	0.43
12:L:75:SER:HB2	12:L:105:ASP:OD2	2.19	0.43
5:S:85:ALA:O	5:S:89:ILE:HG12	2.18	0.43
6:T:49:LEU:HB2	6:T:195:LEU:HD11	2.01	0.43
2:B:229:LEU:C	2:B:231:ALA:H	2.26	0.43
10:J:164:PHE:CE1	10:J:198:ARG:HD2	2.53	0.43
2:P:229:LEU:C	2:P:231:ALA:H	2.26	0.43
9:W:50:ALA:O	9:W:54:MET:HG2	2.19	0.43
10:X:138:VAL:HB	10:X:146:MET:HE3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:180:VAL:HG21	11:Y:194:ILE:HG12	2.00	0.43
6:F:6:TYR:OH	7:G:8:ASP:OD2	2.36	0.43
10:J:175:VAL:HG22	10:J:181:SER:HB3	2.01	0.43
13:1:181:SER:O	13:1:184:GLU:HB2	2.19	0.43
3:C:155:ASN:OD1	4:D:77:THR:OG1	2.31	0.42
3:Q:140:ASP:OD2	3:Q:146:GLN:NE2	2.41	0.42
14:2:92:LEU:O	14:2:96:MET:HG2	2.19	0.42
1:A:109:ILE:HA	1:A:110:PRO:HD3	1.92	0.42
1:A:188:ASP:O	1:A:190:THR:N	2.52	0.42
6:T:119:PRO:HB3	6:T:125:ARG:HH11	1.83	0.42
7:G:150:MET:HG3	7:G:163:CYS:SG	2.60	0.42
9:I:3:ILE:HD11	9:I:127:MET:HB2	2.01	0.42
9:I:139:GLU:OE1	14:2:179:ARG:NH2	2.42	0.42
11:K:30:ASP:OD1	11:K:30:ASP:N	2.52	0.42
2:P:197:SER:O	2:P:199:GLU:N	2.52	0.42
3:Q:6:ASP:OD2	4:R:3:TYR:OH	2.32	0.42
1:A:86:ASP:OD2	1:A:132:ARG:NH2	2.52	0.42
2:B:64:VAL:HG12	2:B:217:PHE:HZ	1.84	0.42
2:B:183:LEU:O	2:B:187:ILE:HG13	2.19	0.42
6:F:49:LEU:HB2	6:F:195:LEU:HD11	2.01	0.42
9:I:193:ASN:HB3	13:1:211:ARG:NH2	2.34	0.42
1:O:22:LEU:HD12	2:P:78:MET:HE1	2.01	0.42
6:T:6:TYR:OH	7:U:8:ASP:OD2	2.33	0.42
7:U:102:PHE:HD1	8:V:78:THR:HG23	1.84	0.42
1:A:191:PHE:CE1	1:A:219:VAL:HG21	2.54	0.42
5:E:224:GLN:HA	15:E:304:HOH:O	2.19	0.42
7:G:33:SER:O	7:G:167:LYS:HG3	2.19	0.42
7:G:77:VAL:HG11	7:G:84:ALA:HB1	2.00	0.42
9:I:175:LEU:HD12	9:I:189:TYR:CZ	2.55	0.42
10:J:138:VAL:HB	10:J:146:MET:HE3	2.00	0.42
12:L:38:ASN:ND2	12:L:40:TYR:OH	2.51	0.42
5:S:91:LYS:HE3	5:S:119:LEU:HD21	2.02	0.42
7:U:75:MET:HE3	7:U:135:PHE:CG	2.54	0.42
1:A:234:GLU:H	1:A:234:GLU:HG2	1.59	0.42
7:G:161:TRP:CE2	7:G:182:LYS:HE2	2.55	0.42
8:H:104:ASP:HA	8:H:105:PRO:HD3	1.94	0.42
9:I:28:ASP:HB2	10:J:131:MET:SD	2.60	0.42
14:N:179:ARG:NH2	9:W:139:GLU:OE1	2.44	0.42
7:U:77:VAL:HG11	7:U:84:ALA:HB1	2.01	0.42
3:C:48:GLU:OE2	3:C:50:ARG:NE	2.48	0.42
3:C:163:CYS:SG	3:C:164:ILE:N	2.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:196:ARG:CZ	6:T:239:ARG:HG2	2.49	0.42
6:T:212:ILE:HD11	6:T:229:VAL:HG13	2.01	0.42
10:X:175:VAL:HG22	10:X:181:SER:HB3	2.01	0.42
4:D:43:LEU:HD22	4:D:134:VAL:HG21	2.02	0.42
10:X:49:LEU:C	10:X:50:TYR:HD1	2.27	0.42
14:2:25:ASP:HA	14:2:187:PHE:HA	2.01	0.42
12:L:43:GLY:HA3	12:L:56:GLU:OE1	2.20	0.42
11:Y:30:ASP:OD1	11:Y:30:ASP:N	2.52	0.42
11:Y:167:LEU:HD23	11:Y:167:LEU:HA	1.90	0.42
5:E:97:GLN:HB3	12:L:61:ARG:HG3	2.01	0.42
1:O:46:ASP:OD1	1:O:46:ASP:N	2.53	0.42
1:O:234:GLU:H	1:O:234:GLU:HG2	1.60	0.42
3:Q:63:GLU:HG2	3:Q:64:LYS:HG3	2.02	0.42
7:U:150:MET:HG3	7:U:163:CYS:SG	2.60	0.42
10:J:169:GLN:O	10:J:173:ASN:ND2	2.51	0.41
7:U:161:TRP:CE2	7:U:182:LYS:HE2	2.55	0.41
14:2:122:LEU:HG	14:2:137:LEU:HD12	2.01	0.41
2:B:87:HIS:C	2:B:87:HIS:ND1	2.77	0.41
6:F:109:VAL:HG21	6:F:145:PHE:CG	2.55	0.41
7:G:39:ILE:HD11	7:G:181:MET:HB3	2.02	0.41
10:J:126:LEU:HD13	10:J:127:ILE:HG23	2.01	0.41
13:M:181:SER:O	13:M:184:GLU:HB2	2.21	0.41
2:P:133:LEU:O	2:P:147:GLN:HA	2.20	0.41
3:Q:163:CYS:SG	3:Q:164:ILE:N	2.93	0.41
11:Y:118:MET:HE2	11:Y:118:MET:HB3	1.88	0.41
2:B:133:LEU:O	2:B:147:GLN:HA	2.19	0.41
3:C:63:GLU:HG2	3:C:64:LYS:HG3	2.02	0.41
7:G:19:ARG:NH2	7:G:24:GLU:OE1	2.52	0.41
9:I:50:ALA:HB2	10:J:129:CYS:HB2	2.02	0.41
11:K:9:GLY:HA3	11:K:12:TYR:CE1	2.55	0.41
13:M:17:GLY:HA3	13:M:20:PHE:CE1	2.55	0.41
3:Q:11:ILE:HG23	4:R:18:GLN:HE22	1.84	0.41
6:T:109:VAL:HG21	6:T:145:PHE:CG	2.55	0.41
13:1:17:GLY:HA3	13:1:20:PHE:CE1	2.55	0.41
3:C:193:ALA:O	3:C:197:LEU:HB2	2.20	0.41
1:O:86:ASP:OD2	1:O:132:ARG:NH2	2.53	0.41
4:R:136:PHE:CZ	4:R:142:PRO:HB3	2.56	0.41
12:Z:38:ASN:C	12:Z:40:TYR:H	2.28	0.41
13:1:57:PHE:HB3	13:1:105:TYR:HB3	2.02	0.41
2:B:197:SER:O	2:B:199:GLU:N	2.53	0.41
10:J:49:LEU:C	10:J:50:TYR:HD1	2.27	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:69:LYS:CE	15:P:314:HOH:O	2.67	0.41
3:Q:42:GLY:HA2	3:Q:145:PHE:CE1	2.56	0.41
7:U:171:ALA:O	7:U:174:THR:OG1	2.29	0.41
9:W:68:LEU:HD12	9:W:68:LEU:HA	1.95	0.41
5:E:186:HIS:O	5:E:189:MET:HG3	2.21	0.41
5:E:187:LYS:N	15:E:306:HOH:O	2.53	0.41
6:F:38:LEU:HD13	6:F:187:LEU:HG	2.02	0.41
4:D:12:PRO:HA	5:E:26:TYR:CE1	2.56	0.41
13:M:82:ALA:HA	15:M:332:HOH:O	2.21	0.41
8:H:84:LYS:HB3	8:H:84:LYS:HE3	1.82	0.41
11:K:102:LEU:HG	11:K:118:MET:HB2	2.02	0.41
11:K:167:LEU:HD23	11:K:167:LEU:HA	1.92	0.41
13:M:57:PHE:HB3	13:M:105:TYR:HB3	2.02	0.41
3:Q:11:ILE:HG12	4:R:7:ILE:HG23	2.03	0.41
3:Q:164:ILE:HD13	3:Q:164:ILE:HA	1.90	0.41
4:R:108:THR:HG23	4:R:133:ILE:HD12	2.03	0.41
10:X:53:LEU:HB2	10:X:60:VAL:HG13	2.02	0.41
12:Z:12:VAL:HG11	12:Z:102:CYS:HB3	2.03	0.41
9:I:50:ALA:O	9:I:54:MET:HG2	2.20	0.41
9:I:172:ASN:CB	9:I:191:VAL:HG22	2.51	0.41
9:I:198:ARG:HH21	10:J:152:SER:C	2.29	0.41
12:L:8:PHE:CD1	12:L:8:PHE:N	2.89	0.41
12:L:8:PHE:HD1	12:L:8:PHE:H	1.69	0.41
12:L:12:VAL:HG11	12:L:102:CYS:HB3	2.03	0.41
12:L:15:ALA:HB2	12:L:176:LEU:HD13	2.03	0.41
2:P:94:GLN:HA	2:P:94:GLN:NE2	2.36	0.41
6:T:84:LEU:HD23	6:T:84:LEU:HA	1.93	0.41
7:U:19:ARG:NH2	7:U:24:GLU:OE1	2.53	0.41
12:Z:160:ILE:O	12:Z:164:THR:HG23	2.19	0.41
2:B:94:GLN:HA	2:B:94:GLN:NE2	2.36	0.41
6:F:71:GLY:HA3	6:F:221:PHE:CE1	2.56	0.41
7:G:172:ALA:O	7:G:176:ILE:HG13	2.21	0.41
3:Q:12:PHE:HB2	4:R:18:GLN:OE1	2.21	0.41
5:S:142:LEU:HG	5:S:170:ILE:HD13	2.03	0.41
7:U:185:THR:O	7:U:189:ILE:HG12	2.20	0.41
1:A:191:PHE:O	1:A:195:VAL:HG23	2.21	0.40
5:E:91:LYS:HE3	5:E:119:LEU:HD21	2.03	0.40
7:G:41:CYS:HB2	7:G:184:MET:O	2.20	0.40
7:G:151:ILE:HA	7:G:156:VAL:O	2.21	0.40
8:H:30:VAL:CG2	14:2:212:ALA:HA	2.45	0.40
4:R:96:LEU:HD23	4:R:96:LEU:HA	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:14:LEU:HD21	8:V:101:ALA:CB	2.50	0.40
8:V:84:LYS:HB3	8:V:84:LYS:HE3	1.82	0.40
12:Z:43:GLY:HA3	12:Z:56:GLU:OE1	2.21	0.40
6:T:38:LEU:HD13	6:T:187:LEU:HG	2.03	0.40
11:K:45:LEU:HB2	11:K:103:LEU:HB2	2.02	0.40
11:K:85:ARG:HA	11:K:118:MET:HE1	2.03	0.40
11:Y:9:GLY:HA3	11:Y:12:TYR:CE1	2.56	0.40
4:D:96:LEU:HA	4:D:96:LEU:HD23	1.88	0.40
9:W:65:LEU:HD12	9:W:65:LEU:HA	1.89	0.40
10:X:142:CYS:HB3	10:X:178:ASP:HB2	2.03	0.40
10:X:156:PRO:HB2	10:X:157:ASN:H	1.75	0.40
1:A:190:THR:H	1:A:193:GLN:HB3	1.86	0.40
8:H:134:TYR:CE1	14:2:33:LEU:HD13	2.56	0.40
14:N:25:ASP:O	14:N:41:ARG:HD3	2.22	0.40
2:P:79:GLY:O	2:P:82:TYR:HB3	2.22	0.40
5:S:97:GLN:HB3	12:Z:61:ARG:HG3	2.02	0.40
5:S:197:SER:O	5:S:201:ILE:HG13	2.22	0.40
11:Y:85:ARG:HA	11:Y:118:MET:HE1	2.03	0.40
12:Z:8:PHE:CD1	12:Z:8:PHE:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	242/244 (99%)	230 (95%)	7 (3%)	5 (2%)	5	11
1	O	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	30	51
2	B	231/233 (99%)	210 (91%)	18 (8%)	3 (1%)	9	21
2	P	231/233 (99%)	209 (90%)	19 (8%)	3 (1%)	9	21
3	C	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	30	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	30	51
4	D	241/243 (99%)	222 (92%)	16 (7%)	3 (1%)	10	23
4	R	241/243 (99%)	222 (92%)	15 (6%)	4 (2%)	7	15
5	E	232/234 (99%)	220 (95%)	10 (4%)	2 (1%)	14	30
5	S	232/234 (99%)	220 (95%)	10 (4%)	2 (1%)	14	30
6	F	236/238 (99%)	223 (94%)	9 (4%)	4 (2%)	7	15
6	T	236/238 (99%)	224 (95%)	9 (4%)	3 (1%)	9	21
7	G	243/245 (99%)	233 (96%)	8 (3%)	2 (1%)	16	34
7	U	243/245 (99%)	234 (96%)	7 (3%)	2 (1%)	16	34
8	H	200/202 (99%)	196 (98%)	4 (2%)	0	100	100
8	V	200/202 (99%)	196 (98%)	4 (2%)	0	100	100
9	I	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
9	W	218/220 (99%)	208 (95%)	8 (4%)	2 (1%)	14	30
10	J	202/204 (99%)	189 (94%)	11 (5%)	2 (1%)	12	28
10	X	202/204 (99%)	189 (94%)	11 (5%)	2 (1%)	12	28
11	K	197/199 (99%)	188 (95%)	7 (4%)	2 (1%)	12	28
11	Y	197/199 (99%)	188 (95%)	7 (4%)	2 (1%)	12	28
12	L	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
12	Z	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
13	1	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
13	M	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
14	2	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	24	46
14	N	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	24	46
All	All	6230/6286 (99%)	5913 (95%)	269 (4%)	48 (1%)	16	34

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	PRO
5	E	120	ALA
6	F	238	GLU
7	G	207	LYS
10	J	156	PRO
4	R	101	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	120	ALA
7	U	207	LYS
9	W	187	ARG
10	X	156	PRO
1	A	188	ASP
1	A	189	TRP
2	B	40	ALA
2	B	198	PHE
4	D	46	GLU
4	D	50	VAL
10	J	117	PHE
2	P	40	ALA
2	P	198	PHE
2	P	232	ILE
4	R	46	GLU
4	R	50	VAL
6	T	197	GLU
10	X	117	PHE
1	A	210	PHE
2	B	232	ILE
6	F	226	ASP
6	F	235	GLY
6	T	235	GLY
14	2	46	ASN
1	A	207	SER
6	F	50	LYS
11	K	197	PRO
14	N	46	ASN
6	T	238	GLU
11	Y	197	PRO
3	C	206	LEU
11	K	174	ASN
1	O	209	ASP
3	Q	206	LEU
5	S	187	LYS
9	W	188	PRO
11	Y	174	ASN
5	E	187	LYS
7	U	216	VAL
7	G	216	VAL
1	A	208	ILE
4	R	202	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 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	193/208 (93%)	183 (95%)	10 (5%)	21	44
1	O	193/208 (93%)	182 (94%)	11 (6%)	18	40
2	B	163/190 (86%)	159 (98%)	4 (2%)	42	69
2	P	165/190 (87%)	160 (97%)	5 (3%)	36	64
3	C	193/210 (92%)	184 (95%)	9 (5%)	23	48
3	Q	193/210 (92%)	185 (96%)	8 (4%)	27	54
4	D	152/207 (73%)	140 (92%)	12 (8%)	11	26
4	R	142/207 (69%)	132 (93%)	10 (7%)	14	31
5	E	189/196 (96%)	184 (97%)	5 (3%)	40	68
5	S	189/196 (96%)	184 (97%)	5 (3%)	40	68
6	F	198/204 (97%)	190 (96%)	8 (4%)	28	55
6	T	198/204 (97%)	189 (96%)	9 (4%)	24	50
7	G	195/202 (96%)	187 (96%)	8 (4%)	27	54
7	U	195/202 (96%)	186 (95%)	9 (5%)	24	49
8	H	155/157 (99%)	151 (97%)	4 (3%)	40	68
8	V	155/157 (99%)	152 (98%)	3 (2%)	50	75
9	I	177/181 (98%)	167 (94%)	10 (6%)	19	40
9	W	177/181 (98%)	169 (96%)	8 (4%)	24	50
10	J	172/173 (99%)	160 (93%)	12 (7%)	14	31
10	X	172/173 (99%)	160 (93%)	12 (7%)	14	31
11	K	164/170 (96%)	159 (97%)	5 (3%)	36	64
11	Y	164/170 (96%)	160 (98%)	4 (2%)	43	70
12	L	153/156 (98%)	148 (97%)	5 (3%)	33	61
12	Z	154/156 (99%)	148 (96%)	6 (4%)	28	55
13	1	175/178 (98%)	172 (98%)	3 (2%)	53	78
13	M	174/178 (98%)	170 (98%)	4 (2%)	44	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2	175/179 (98%)	164 (94%)	11 (6%)	16	36
14	N	175/179 (98%)	166 (95%)	9 (5%)	21	45
All	All	4900/5222 (94%)	4691 (96%)	209 (4%)	26	51

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	78	CYS
1	A	114	LEU
1	A	126	THR
1	A	132	ARG
1	A	145	GLU
1	A	166	THR
1	A	221	THR
1	A	231	THR
1	A	234	GLU
2	B	58	GLU
2	B	87	HIS
2	B	132	SER
2	B	178	ASN
3	C	44	LEU
3	C	76	VAL
3	C	164	ILE
3	C	180	LYS
3	C	192	LEU
3	C	197	LEU
3	C	206	LEU
3	C	218	ARG
3	C	220	ASN
4	D	5	ARG
4	D	33	VAL
4	D	35	VAL
4	D	38	ARG
4	D	41	VAL
4	D	43	LEU
4	D	56	GLU
4	D	99	GLU
4	D	103	THR
4	D	139	ASP
4	D	146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	184	ASP
5	E	9	ASP
5	E	36	THR
5	E	135	ARG
5	E	148	GLU
5	E	221	GLN
6	F	38	LEU
6	F	50	LYS
6	F	60	GLN
6	F	83	LEU
6	F	101	ARG
6	F	202	GLU
6	F	225	ASP
6	F	239	ARG
7	G	5	THR
7	G	39	ILE
7	G	90	ILE
7	G	144	ASP
7	G	165	ILE
7	G	181	MET
7	G	187	ARG
7	G	200	VAL
8	H	22	THR
8	H	46	SER
8	H	150	GLU
8	H	153	LEU
9	I	6	VAL
9	I	56	THR
9	I	65	LEU
9	I	77	VAL
9	I	132	LEU
9	I	186	LEU
9	I	187	ARG
9	I	194	LYS
9	I	198	ARG
9	I	201	ARG
10	J	20	VAL
10	J	34	MET
10	J	36	THR
10	J	49	LEU
10	J	108	VAL
10	J	126	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	175	VAL
10	J	189	ILE
10	J	190	ILE
10	J	191	GLU
10	J	192	LYS
10	J	193	ASP
11	K	27	GLN
11	K	45	LEU
11	K	47	VAL
11	K	84	THR
11	K	171	PHE
12	L	8	PHE
12	L	82	LEU
12	L	87	VAL
12	L	115	ASP
12	L	138	VAL
13	M	6	VAL
13	M	76	LYS
13	M	136	LYS
13	M	164	VAL
14	N	37	ARG
14	N	49	THR
14	N	86	ARG
14	N	94	ARG
14	N	159	VAL
14	N	168	LEU
14	N	169	VAL
14	N	192	VAL
14	N	205	THR
1	O	73	THR
1	O	78	CYS
1	O	114	LEU
1	O	126	THR
1	O	132	ARG
1	O	145	GLU
1	O	166	THR
1	O	205	VAL
1	O	221	THR
1	O	231	THR
1	O	234	GLU
2	P	58	GLU
2	P	74	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	87	HIS
2	P	132	SER
2	P	178	ASN
3	Q	44	LEU
3	Q	76	VAL
3	Q	164	ILE
3	Q	180	LYS
3	Q	192	LEU
3	Q	206	LEU
3	Q	218	ARG
3	Q	220	ASN
4	R	5	ARG
4	R	33	VAL
4	R	35	VAL
4	R	38	ARG
4	R	41	VAL
4	R	99	GLU
4	R	103	THR
4	R	139	ASP
4	R	146	GLN
4	R	184	ASP
5	S	9	ASP
5	S	36	THR
5	S	135	ARG
5	S	148	GLU
5	S	221	GLN
6	T	38	LEU
6	T	60	GLN
6	T	83	LEU
6	T	101	ARG
6	T	196	ARG
6	T	202	GLU
6	T	211	SER
6	T	236	LEU
6	T	239	ARG
7	U	5	THR
7	U	39	ILE
7	U	41	CYS
7	U	42	LYS
7	U	90	ILE
7	U	144	ASP
7	U	165	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	181	MET
7	U	200	VAL
8	V	22	THR
8	V	150	GLU
8	V	153	LEU
9	W	6	VAL
9	W	56	THR
9	W	65	LEU
9	W	77	VAL
9	W	132	LEU
9	W	187	ARG
9	W	198	ARG
9	W	201	ARG
10	X	20	VAL
10	X	34	MET
10	X	36	THR
10	X	49	LEU
10	X	108	VAL
10	X	126	LEU
10	X	175	VAL
10	X	189	ILE
10	X	190	ILE
10	X	191	GLU
10	X	192	LYS
10	X	193	ASP
11	Y	27	GLN
11	Y	45	LEU
11	Y	47	VAL
11	Y	84	THR
12	Z	8	PHE
12	Z	73	ARG
12	Z	82	LEU
12	Z	87	VAL
12	Z	115	ASP
12	Z	138	VAL
13	1	6	VAL
13	1	136	LYS
13	1	164	VAL
14	2	37	ARG
14	2	49	THR
14	2	69	GLN
14	2	86	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	2	94	ARG
14	2	159	VAL
14	2	168	LEU
14	2	169	VAL
14	2	186	ARG
14	2	192	VAL
14	2	205	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	75	ASN
1	A	238	HIS
2	B	94	GLN
3	C	102	GLN
3	C	240	HIS
4	D	92	GLN
4	D	154	HIS
5	E	41	GLN
5	E	97	GLN
5	E	152	GLN
5	E	221	GLN
7	G	170	GLN
9	I	80	ASN
9	I	193	ASN
10	J	33	GLN
12	L	10	HIS
12	L	119	ASN
13	M	131	GLN
13	M	146	GLN
13	M	152	GLN
14	N	81	HIS
14	N	89	HIS
14	N	188	GLN
1	O	68	HIS
1	O	75	ASN
3	Q	102	GLN
3	Q	240	HIS
4	R	154	HIS
5	S	41	GLN
5	S	97	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	152	GLN
5	S	221	GLN
7	U	170	GLN
9	W	80	ASN
9	W	193	ASN
10	X	33	GLN
12	Z	10	HIS
12	Z	38	ASN
12	Z	119	ASN
13	1	131	GLN
13	1	146	GLN
13	1	152	GLN
14	2	81	HIS
14	2	89	HIS
14	2	188	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 ⓘ

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	244/244 (100%)	0.55	12 (4%)	35 29	55, 89, 135, 176	0
1	O	244/244 (100%)	0.58	9 (3%)	45 39	57, 97, 148, 214	0
2	B	233/233 (100%)	0.51	11 (4%)	36 30	56, 83, 130, 210	0
2	P	233/233 (100%)	0.59	13 (5%)	30 24	57, 83, 129, 215	0
3	C	250/250 (100%)	0.45	6 (2%)	59 54	57, 87, 147, 232	0
3	Q	250/250 (100%)	0.48	11 (4%)	39 33	54, 89, 157, 228	0
4	D	243/243 (100%)	0.66	13 (5%)	32 26	55, 95, 177, 238	0
4	R	243/243 (100%)	0.85	21 (8%)	16 12	53, 98, 190, 261	0
5	E	234/234 (100%)	0.48	6 (2%)	57 51	51, 90, 134, 187	0
5	S	234/234 (100%)	0.80	27 (11%)	9 7	50, 91, 134, 178	0
6	F	238/238 (100%)	0.44	9 (3%)	44 38	50, 79, 125, 199	0
6	T	238/238 (100%)	0.43	4 (1%)	69 64	54, 82, 130, 246	0
7	G	245/245 (100%)	0.48	12 (4%)	35 29	59, 85, 131, 198	0
7	U	245/245 (100%)	0.51	6 (2%)	59 54	61, 92, 145, 222	0
8	H	202/202 (100%)	0.29	4 (1%)	65 60	53, 69, 111, 212	0
8	V	202/202 (100%)	0.30	4 (1%)	65 60	50, 70, 113, 171	0
9	I	220/220 (100%)	0.31	7 (3%)	50 44	51, 67, 109, 169	0
9	W	220/220 (100%)	0.27	7 (3%)	50 44	48, 67, 114, 157	0
10	J	204/204 (100%)	0.17	3 (1%)	72 68	47, 66, 99, 150	0
10	X	204/204 (100%)	0.22	3 (1%)	72 68	46, 65, 96, 141	0
11	K	199/199 (100%)	0.29	4 (2%)	65 60	47, 70, 103, 207	0
11	Y	199/199 (100%)	0.23	3 (1%)	72 68	49, 70, 101, 171	0
12	L	201/201 (100%)	0.22	2 (0%)	79 76	41, 66, 100, 140	0
12	Z	201/201 (100%)	0.20	2 (0%)	79 76	46, 66, 101, 177	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	213/213 (100%)	0.03	1 (0%) 87 85	42, 63, 92, 149	0
13	M	213/213 (100%)	0.15	4 (1%) 66 61	44, 61, 94, 137	0
14	2	217/217 (100%)	0.20	5 (2%) 61 55	42, 69, 101, 167	0
14	N	217/217 (100%)	0.13	4 (1%) 67 63	42, 64, 102, 192	0
All	All	6286/6286 (100%)	0.40	213 (3%) 48 42	41, 77, 135, 261	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	S	131	GLY	8.0
1	O	187	PHE	5.3
1	A	62	ASP	4.9
14	2	215	ILE	4.7
4	D	47	LYS	4.5
5	S	120	ALA	4.5
2	B	1	ALA	4.3
2	P	231	ALA	4.3
2	P	233	ALA	4.3
5	S	127	ASP	4.1
2	B	231	ALA	4.1
8	H	199	VAL	4.1
9	I	189	TYR	3.8
1	A	245	ARG	3.7
2	P	232	ILE	3.7
12	Z	40	TYR	3.6
5	S	124	GLY	3.6
4	R	48	LYS	3.6
14	N	215	ILE	3.6
7	U	3	ILE	3.6
4	D	203	GLY	3.5
8	H	200	ALA	3.5
7	G	3	ILE	3.4
6	F	240	PRO	3.4
5	S	191	LEU	3.4
5	S	160	GLY	3.3
1	A	63	SER	3.3
6	T	240	PRO	3.3
3	Q	166	ASN	3.3
1	A	192	GLU	3.3
12	L	40	TYR	3.3
5	S	19	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	S	145	GLY	3.2
1	A	221	THR	3.2
5	S	61	PRO	3.2
3	Q	245	ALA	3.2
10	X	117	PHE	3.2
13	M	213	ASP	3.2
4	R	137	ASP	3.1
7	G	216	VAL	3.1
4	D	216	SER	3.1
6	F	224	TYR	3.1
4	D	185	ASP	3.1
7	G	1	SER	3.1
9	W	188	PRO	3.1
3	Q	16	GLY	3.1
3	Q	203	VAL	3.1
4	R	102	VAL	3.1
5	S	241	ILE	3.0
9	I	190	THR	3.0
1	O	192	GLU	3.0
7	G	2	SER	3.0
3	Q	230	GLN	3.0
11	K	199	GLN	3.0
6	F	47	VAL	3.0
10	J	117	PHE	3.0
5	S	49	ALA	2.9
9	I	191	VAL	2.9
8	H	201	THR	2.9
1	A	187	PHE	2.9
4	D	136	PHE	2.9
8	V	92	GLU	2.9
11	K	198	LYS	2.9
7	G	4	GLY	2.9
3	C	170	ALA	2.9
5	S	33	LEU	2.9
14	2	216	SER	2.8
14	N	217	GLY	2.8
14	2	201	GLY	2.8
5	E	33	LEU	2.8
4	R	233	GLU	2.8
4	R	47	LYS	2.8
5	S	192	LYS	2.8
1	O	159	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	M	209	SER	2.8
5	S	58	LEU	2.8
3	Q	51	ASN	2.8
8	V	202	LEU	2.8
14	2	186	ARG	2.7
2	B	206	ASN	2.7
3	Q	57	ASP	2.7
4	R	206	ILE	2.6
7	G	219	LEU	2.6
5	S	209	LYS	2.6
1	A	64	SER	2.6
9	I	188	PRO	2.6
6	F	241	GLN	2.6
4	R	100	ASP	2.6
3	Q	237	ILE	2.6
2	P	51	GLN	2.6
7	U	2	SER	2.6
6	T	65	HIS	2.6
1	O	145	GLU	2.6
1	O	210	PHE	2.6
1	O	86	ASP	2.5
2	P	149	ASP	2.5
6	F	225	ASP	2.5
4	R	99	GLU	2.5
2	P	165	ASN	2.5
4	R	213	ARG	2.5
1	O	188	ASP	2.5
2	B	188	HIS	2.5
4	R	37	GLY	2.5
8	V	200	ALA	2.5
2	P	3	ARG	2.5
4	R	38	ARG	2.5
4	R	49	SER	2.5
4	R	185	ASP	2.5
9	W	205	GLU	2.5
7	U	235	ALA	2.5
7	G	5	THR	2.4
12	Z	185	ILE	2.4
2	P	68	THR	2.4
5	S	185	TYR	2.4
2	P	198	PHE	2.4
2	B	232	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	X	190	ILE	2.4
1	A	188	ASP	2.4
4	R	203	GLY	2.4
5	E	131	GLY	2.4
9	W	196	GLY	2.4
12	L	201	GLY	2.4
4	R	244	GLN	2.4
4	D	228	TYR	2.4
6	T	157	ARG	2.4
1	A	2	SER	2.4
2	B	214	GLU	2.4
9	W	104	ASP	2.4
11	K	197	PRO	2.4
6	T	47	VAL	2.4
3	C	164	ILE	2.3
5	S	18	GLU	2.3
13	M	34	SER	2.3
2	B	192	LEU	2.3
3	Q	69	ASN	2.3
4	R	68	ASN	2.3
8	V	104	ASP	2.3
11	Y	90	ASP	2.3
6	F	200	PRO	2.3
5	E	191	LEU	2.3
6	F	219	LEU	2.3
8	H	202	LEU	2.3
6	F	207	THR	2.3
11	Y	41	LYS	2.3
14	N	47	ASN	2.3
2	B	74	VAL	2.3
7	U	219	LEU	2.3
10	J	190	ILE	2.3
9	W	180	LYS	2.2
7	G	169	ARG	2.2
4	D	214	ASP	2.2
10	J	46	GLY	2.2
5	S	212	ALA	2.2
7	U	146	ALA	2.2
4	D	97	THR	2.2
9	I	197	THR	2.2
7	G	143	ASN	2.2
5	S	52	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	N	155	GLU	2.2
3	Q	226	ARG	2.2
5	E	8	TYR	2.2
3	C	251	LYS	2.2
4	D	39	ASP	2.2
5	S	16	SER	2.2
2	B	167	VAL	2.2
5	E	220	VAL	2.2
2	P	54	ILE	2.2
5	E	31	ILE	2.2
7	U	176	ILE	2.2
5	S	51	GLU	2.2
5	S	208	GLU	2.2
2	B	47	THR	2.2
5	S	210	LEU	2.2
9	W	199	LEU	2.2
1	O	112	ASP	2.2
4	R	98	VAL	2.2
5	S	159	SER	2.2
2	B	198	PHE	2.2
7	G	215	TRP	2.1
9	I	201	ARG	2.1
4	R	123	GLY	2.1
10	X	114	PRO	2.1
2	P	183	LEU	2.1
5	S	138	GLY	2.1
9	I	11	GLY	2.1
3	C	151	ASP	2.1
5	S	9	ASP	2.1
11	K	195	SER	2.1
4	D	99	GLU	2.1
5	S	55	THR	2.1
4	D	98	VAL	2.1
4	R	41	VAL	2.1
4	R	181	ILE	2.1
3	C	250	GLU	2.1
6	F	239	ARG	2.1
2	P	189	THR	2.1
9	W	197	THR	2.1
14	2	185	ASN	2.1
4	D	26	VAL	2.1
4	D	102	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	136	PHE	2.1
3	C	244	GLU	2.0
1	A	176	THR	2.0
2	P	194	LEU	2.0
1	A	112	ASP	2.0
7	G	245	GLU	2.0
11	Y	50	ALA	2.0
13	M	186	ASP	2.0
1	A	166	THR	2.0
1	O	221	THR	2.0
3	Q	164	ILE	2.0
7	G	53	VAL	2.0
13	1	1	ARG	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.