



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:12 AM UTC

PDB ID : 1IRU / pdb_00001iru
Title : Crystal Structure of the mammalian 20S proteasome at 2.75 Å resolution
Authors : Unno, M.; Mizushima, T.; Morimoto, Y.; Tomisugi, Y.; Tanaka, K.; Yasuoka, N.; Tsukihara, T.
Deposited on : 2001-10-24
Resolution : 2.75 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

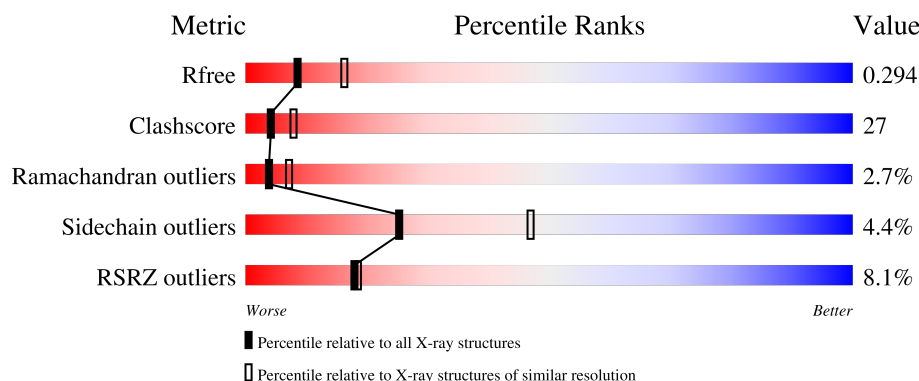
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	246	24% 50% 42% 7%
1	O	246	2% 49% 43% 7%
2	B	233	25% 48% 45% 7%
2	P	233	6% 49% 45% 6%
3	C	261	26% 44% 46% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	261	
4	D	248	
4	R	248	
5	E	241	
5	S	241	
6	F	263	
6	T	263	
7	G	254	
7	U	254	
8	H	205	
8	V	205	
9	I	234	
9	W	234	
10	J	205	
10	X	205	
11	K	201	
11	Y	201	
12	L	204	
12	Z	204	
13	1	213	
13	M	213	
14	2	219	
14	N	219	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 47757 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 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			
1	O	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			

- Molecule 2 is a protein called 20S proteasome.

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
			1707	1081	287	334	5			

- Molecule 3 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	Q	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			

- Molecule 4 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1665	1032	307	322	4			
4	R	243	Total	C	N	O	S	0	0	0
			1665	1032	307	322	4			

- Molecule 5 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	0	0
			1763	1104	290	358	11			
5	S	234	Total	C	N	O	S	0	0	0
			1763	1104	290	358	11			

- Molecule 6 is a protein called 20S proteasome.

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 20S proteasome.

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 20S proteasome.

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 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	220	Total	C	N	O	S	0	0	0
			1645	1034	282	317	12			
9	W	220	Total	C	N	O	S	0	0	0
			1645	1034	282	317	12			

- Molecule 10 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1585	1011	262	294	18			

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	1011	262	294	18			

- Molecule 11 is a protein called 20S proteasome.

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 20S proteasome.

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
			1548	974	273	292	9			

- Molecule 13 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			
13	1	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			

- Molecule 14 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	217	Total	C	N	O	S	0	0	0
			1671	1053	287	319	12			
14	2	217	Total	C	N	O	S	0	0	0
			1671	1053	287	319	12			

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		
15	B	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	1	Total 1	Mg 1	0	0
15	D	1	Total 1	Mg 1	0	0
15	G	3	Total 3	Mg 3	0	0
15	I	1	Total 1	Mg 1	0	0
15	J	4	Total 4	Mg 4	0	0
15	K	1	Total 1	Mg 1	0	0
15	M	2	Total 2	Mg 2	0	0
15	O	1	Total 1	Mg 1	0	0
15	P	1	Total 1	Mg 1	0	0
15	Q	1	Total 1	Mg 1	0	0
15	R	1	Total 1	Mg 1	0	0
15	U	3	Total 3	Mg 3	0	0
15	W	1	Total 1	Mg 1	0	0
15	X	4	Total 4	Mg 4	0	0
15	Y	1	Total 1	Mg 1	0	0
15	1	2	Total 2	Mg 2	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total 2	O 2	0	0
16	B	3	Total 3	O 3	0	0
16	C	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	F	6	Total O 6 6	0	0
16	G	4	Total O 4 4	0	0
16	H	7	Total O 7 7	0	0
16	I	6	Total O 6 6	0	0
16	J	1	Total O 1 1	0	0
16	K	6	Total O 6 6	0	0
16	L	8	Total O 8 8	0	0
16	M	10	Total O 10 10	0	0
16	N	9	Total O 9 9	0	0
16	O	7	Total O 7 7	0	0
16	P	6	Total O 6 6	0	0
16	Q	3	Total O 3 3	0	0
16	R	3	Total O 3 3	0	0
16	S	1	Total O 1 1	0	0
16	T	7	Total O 7 7	0	0
16	U	9	Total O 9 9	0	0
16	V	15	Total O 15 15	0	0
16	W	9	Total O 9 9	0	0
16	X	17	Total O 17 17	0	0
16	Y	3	Total O 3 3	0	0
16	Z	8	Total O 8 8	0	0

Continued on next page...

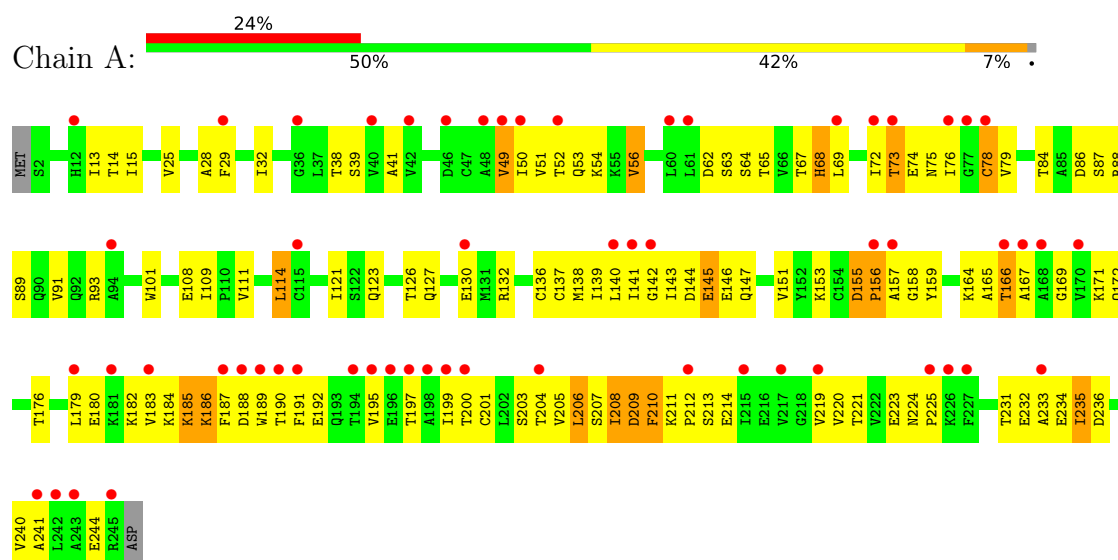
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	1	4	Total	O	0	0
			4	4		
16	2	8	Total	O	0	0
			8	8		

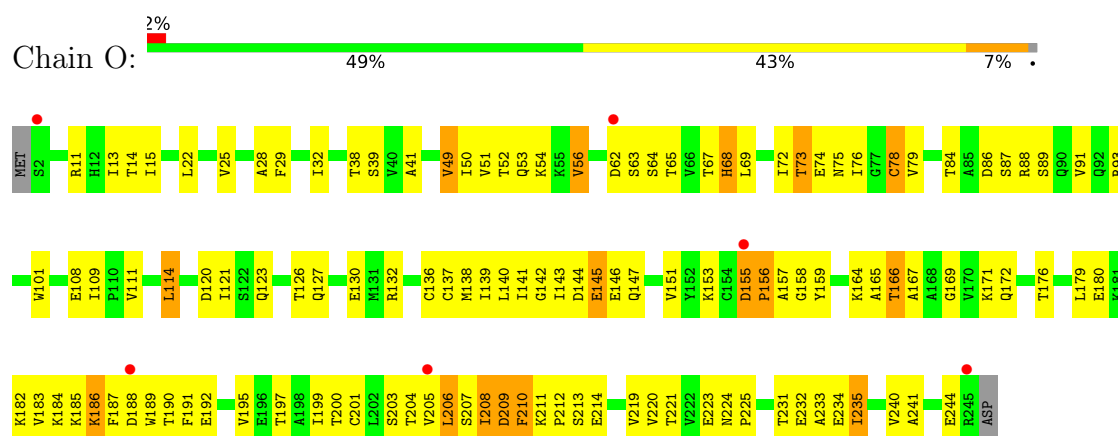
3 Residue-property plots

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: 20S proteasome

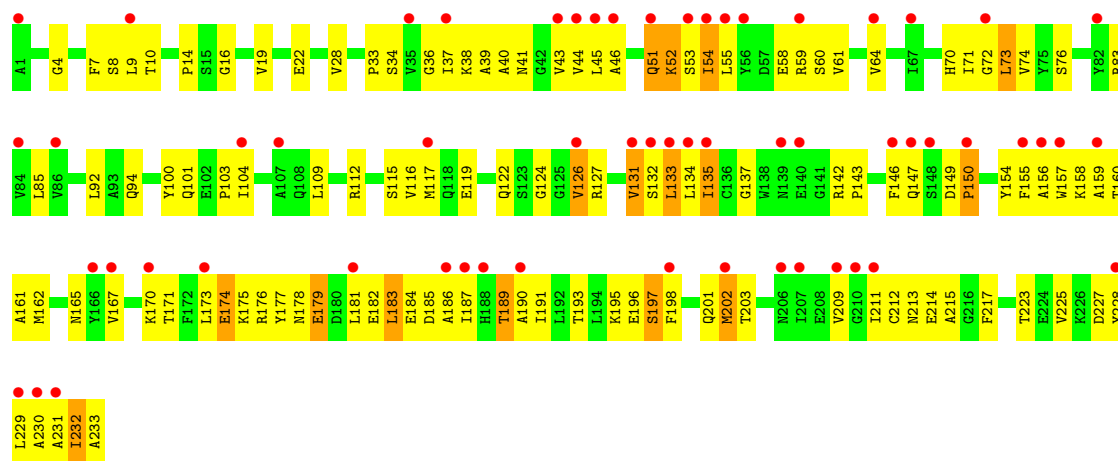


• Molecule 1: 20S proteasome

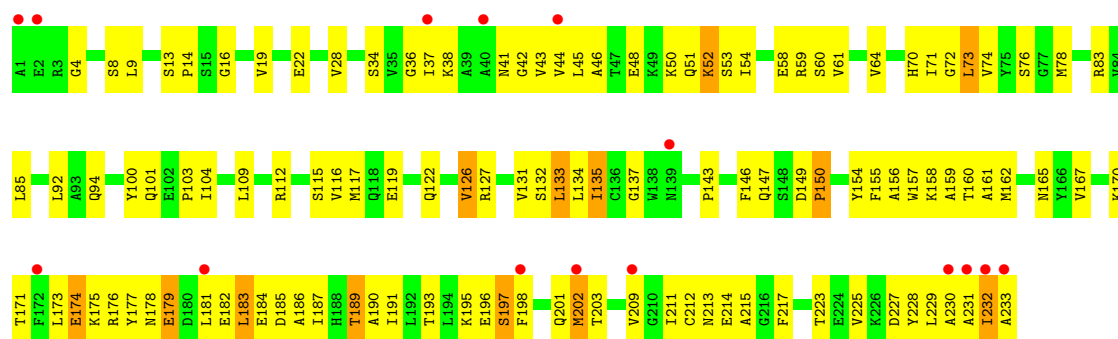


• Molecule 2: 20S proteasome

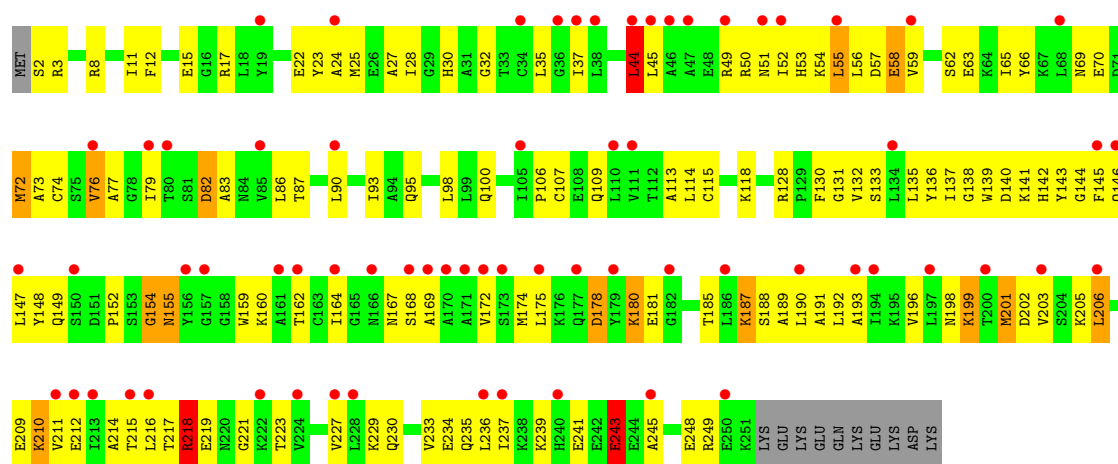
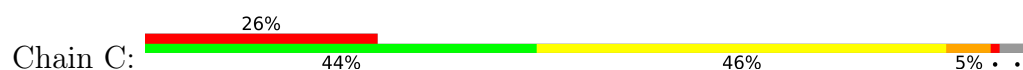




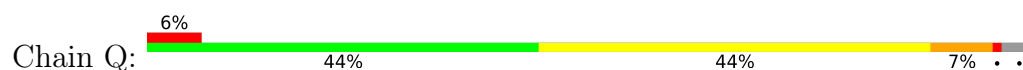
• Molecule 2: 20S proteasome

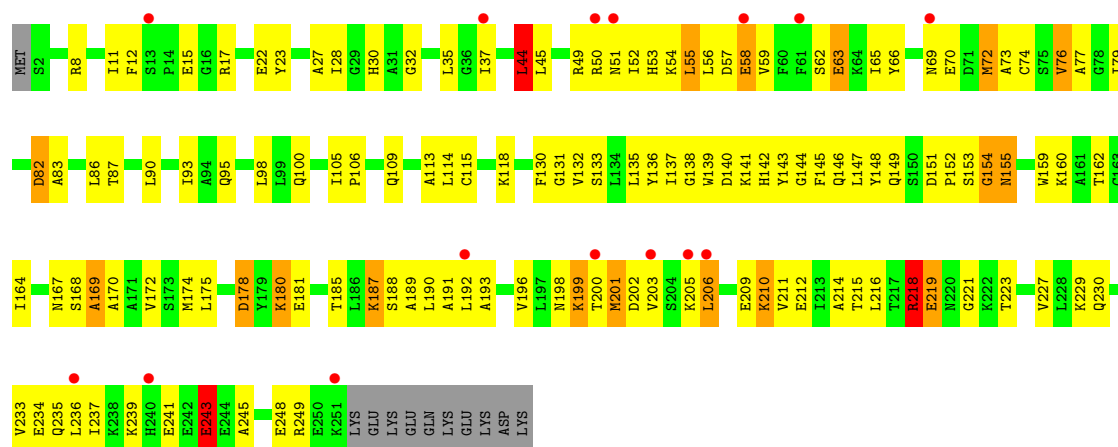


• Molecule 3: 20S proteasome

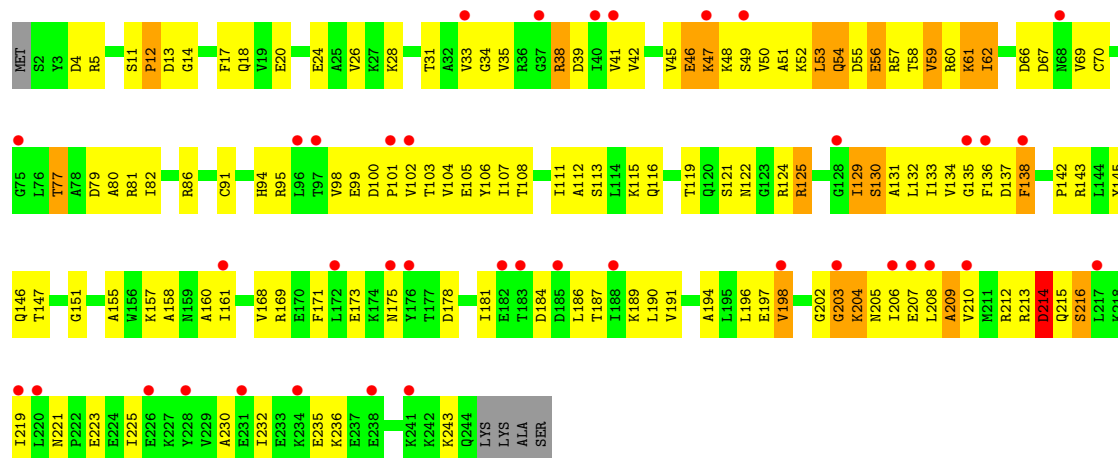
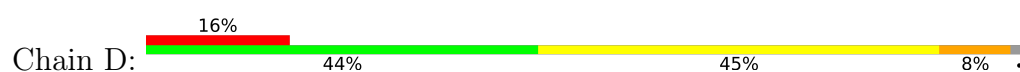


• Molecule 3: 20S proteasome

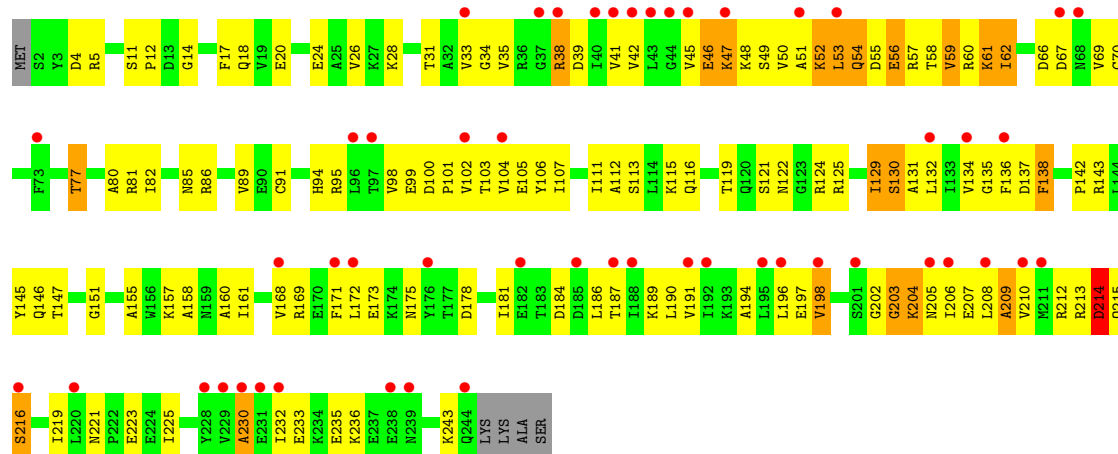
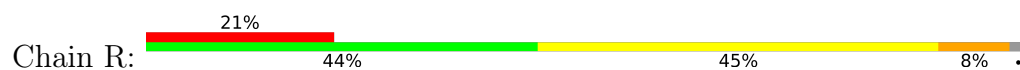




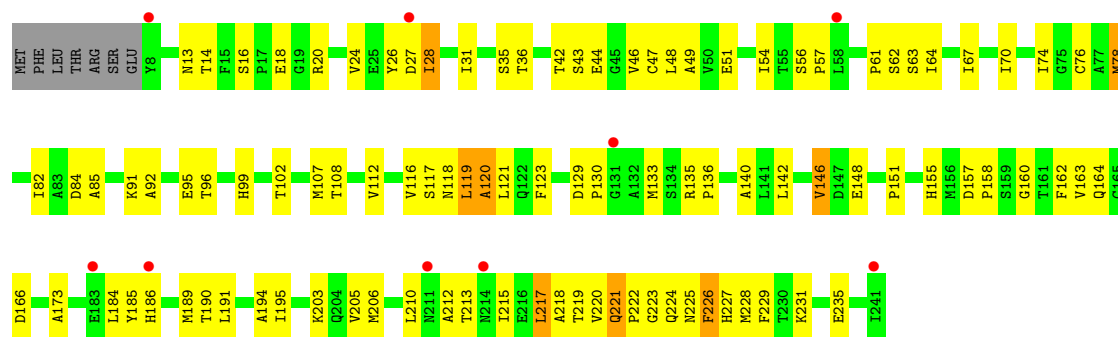
• Molecule 4: 20S proteasome



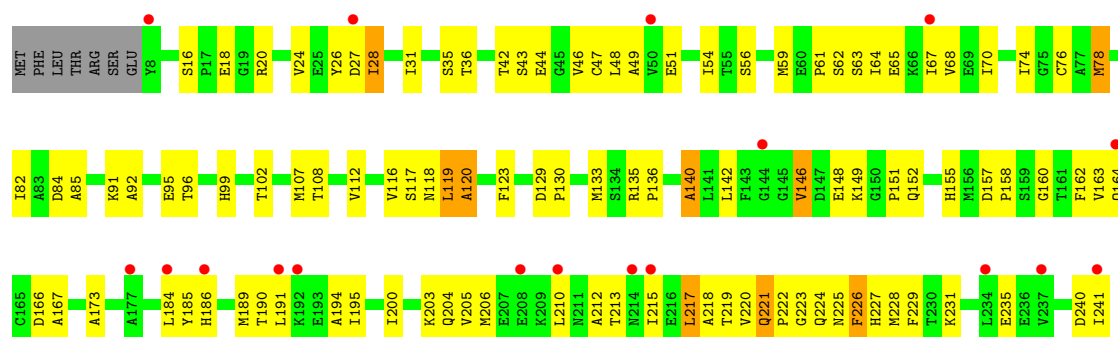
• Molecule 4: 20S proteasome



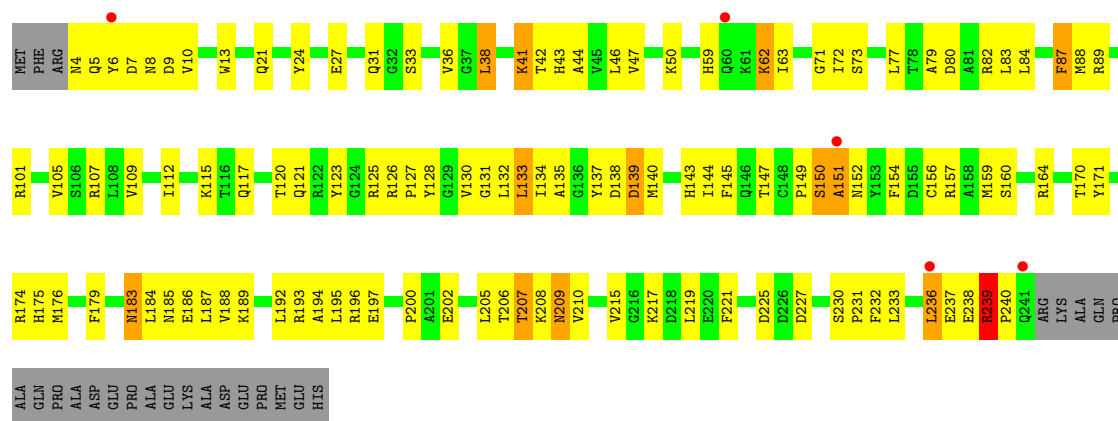
• Molecule 5: 20S proteasome



• Molecule 5: 20S proteasome

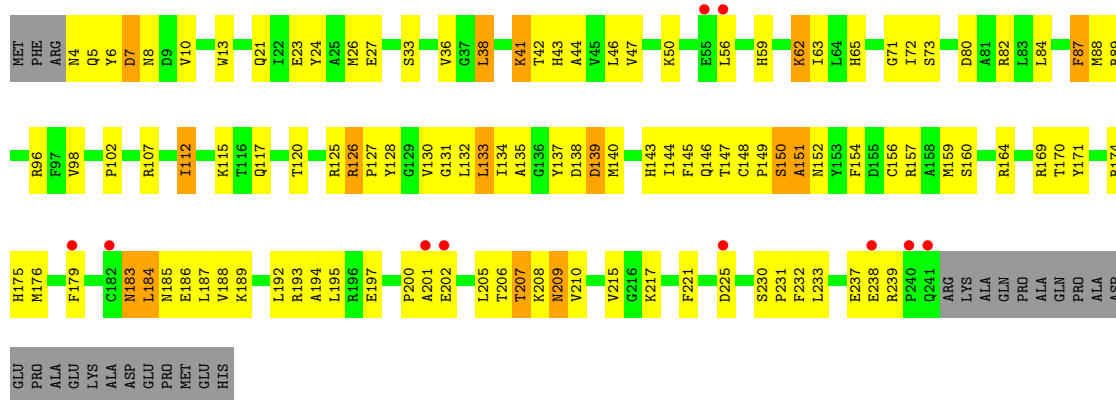


• Molecule 6: 20S proteasome

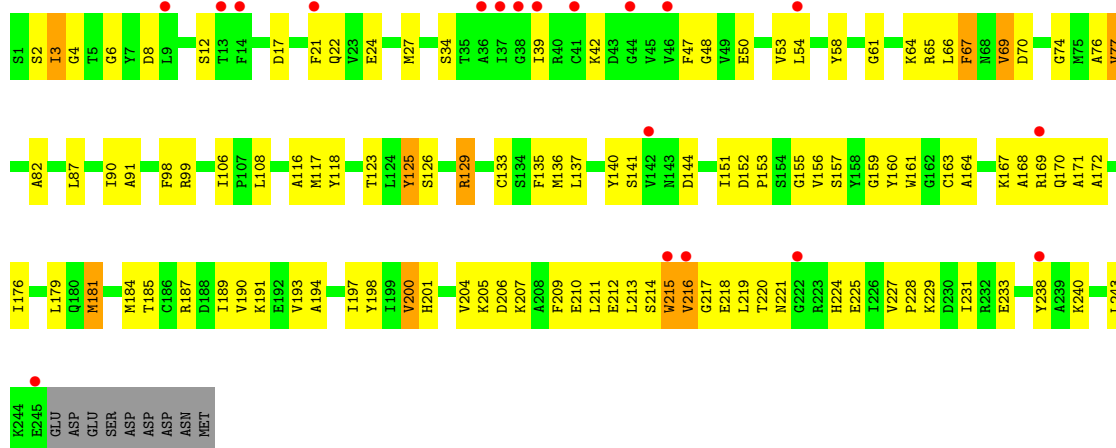


• Molecule 6: 20S proteasome

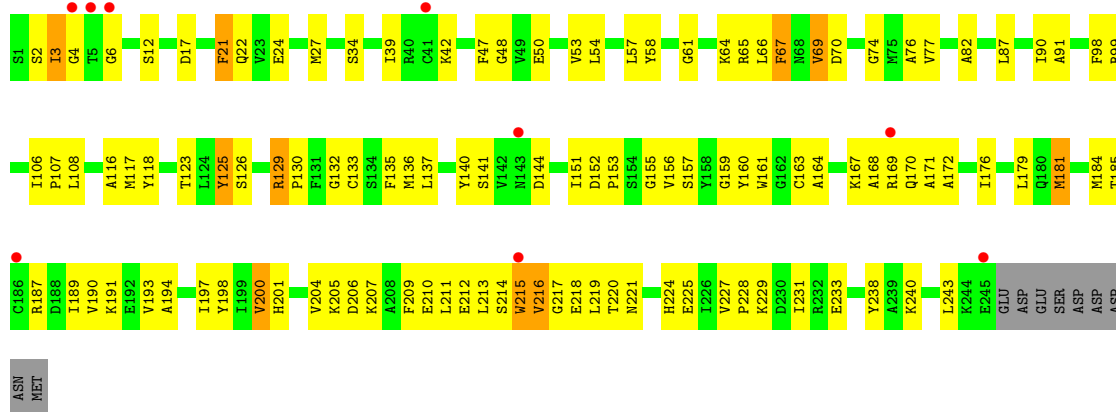




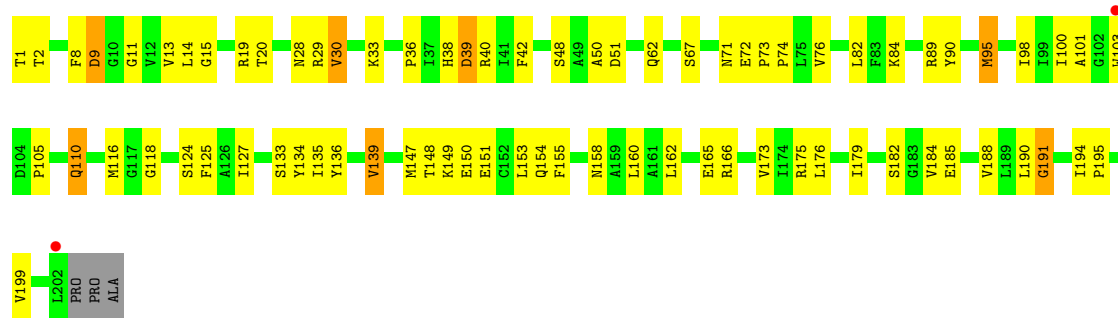
• Molecule 7: 20S proteasome



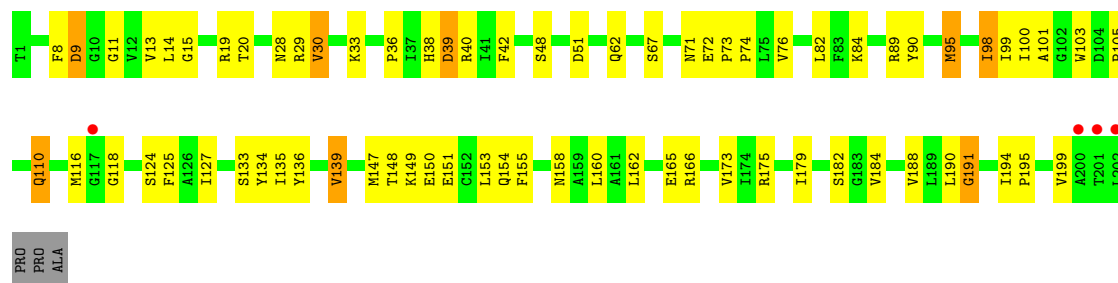
• Molecule 7: 20S proteasome



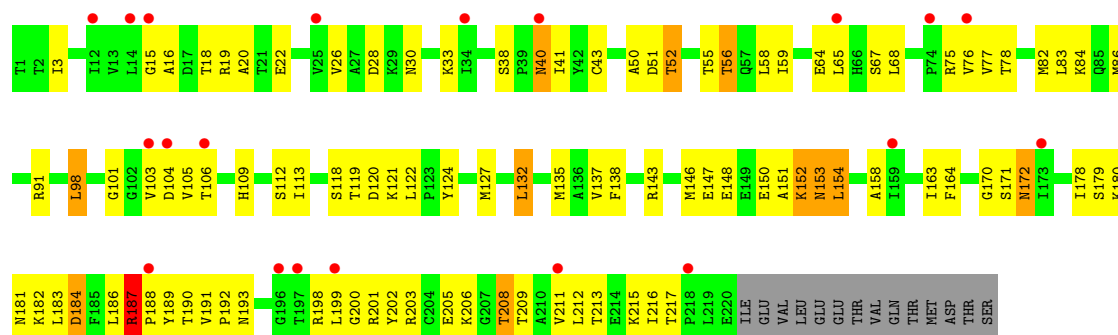
• Molecule 8: 20S proteasome



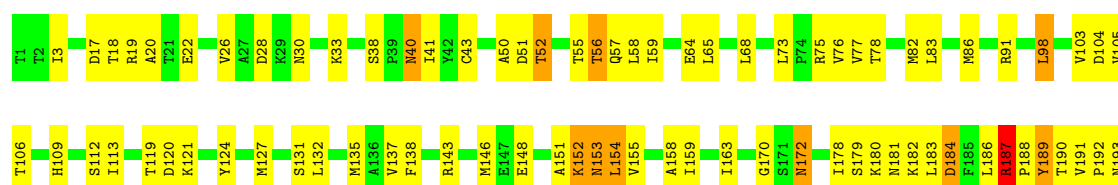
• Molecule 8: 20S proteasome



• Molecule 9: 20S proteasome

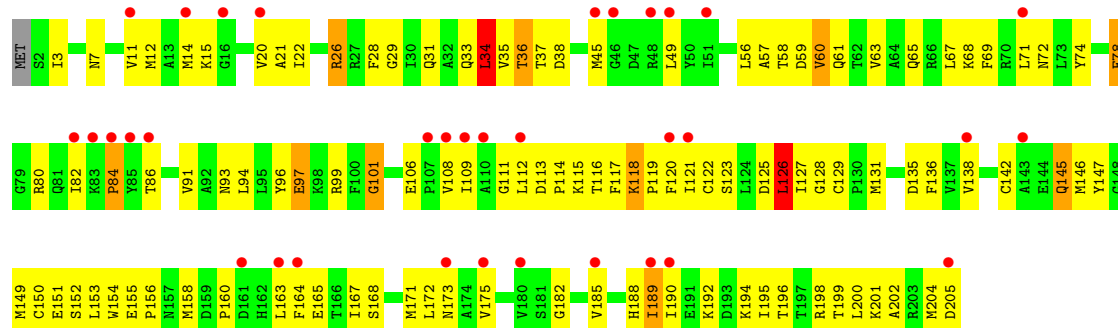
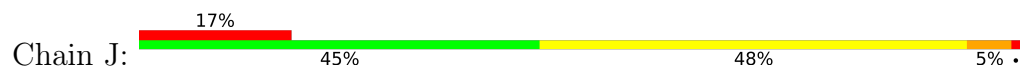


• Molecule 9: 20S proteasome

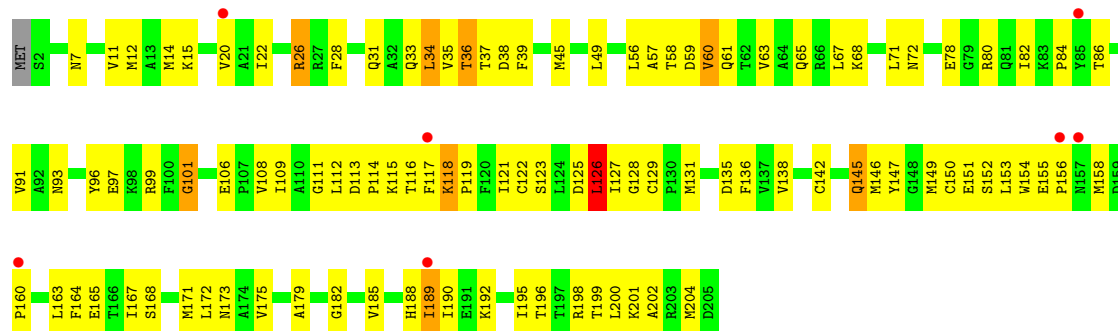




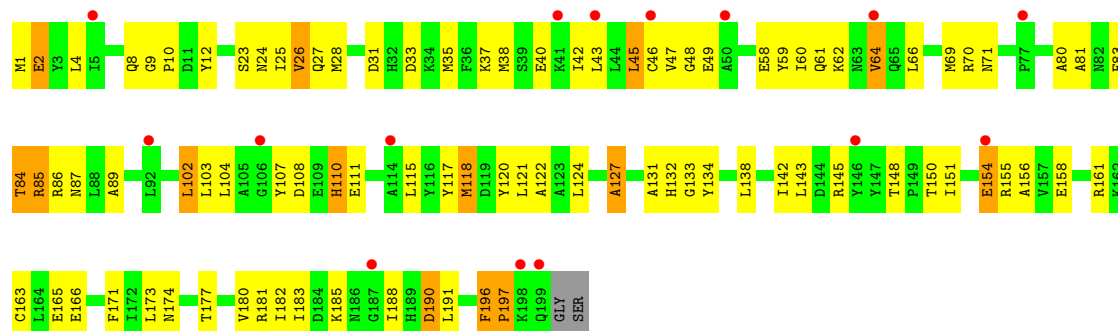
• Molecule 10: 20S proteasome



• Molecule 10: 20S proteasome

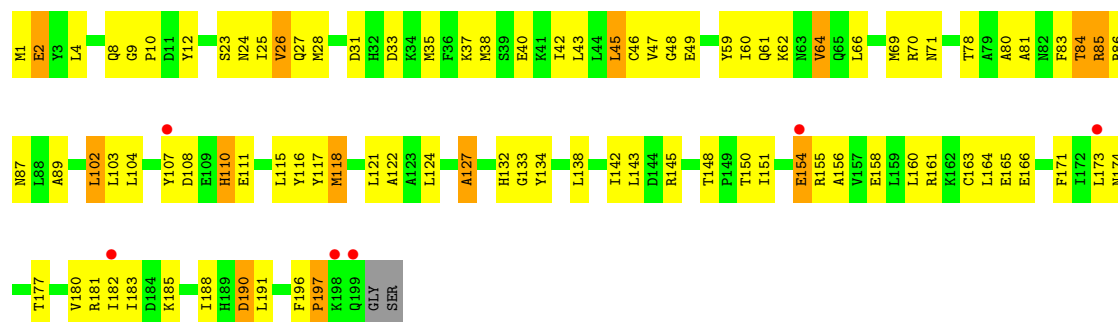


• Molecule 11: 20S proteasome

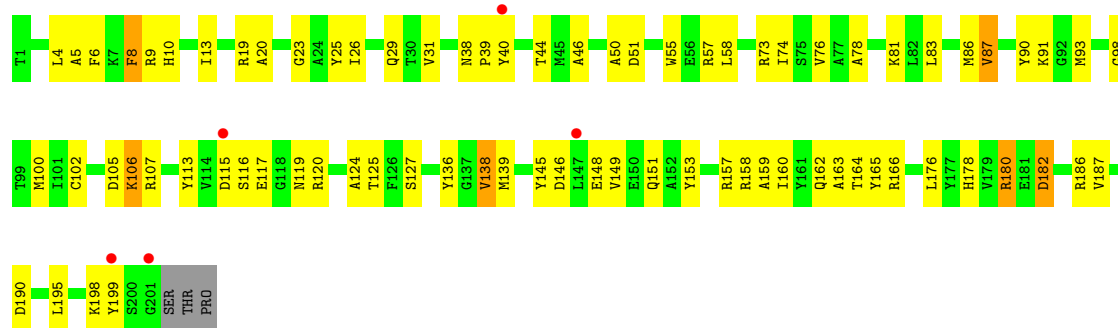


• Molecule 11: 20S proteasome

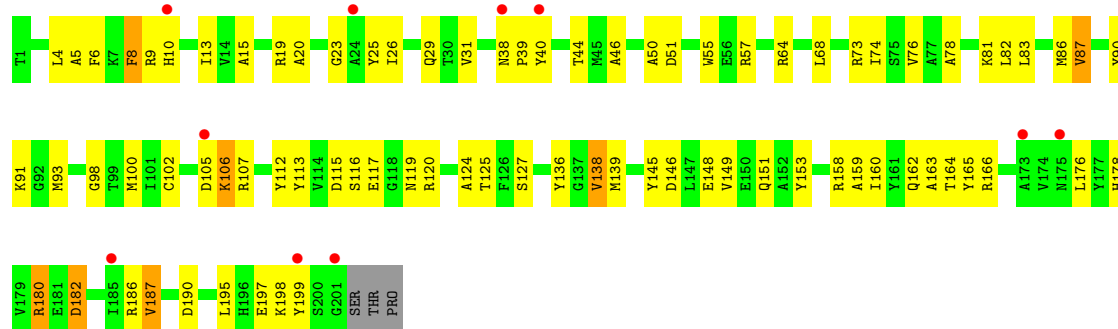




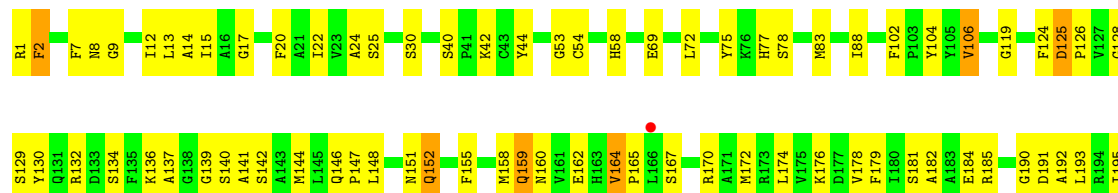
• Molecule 12: 20S proteasome



• Molecule 12: 20S proteasome

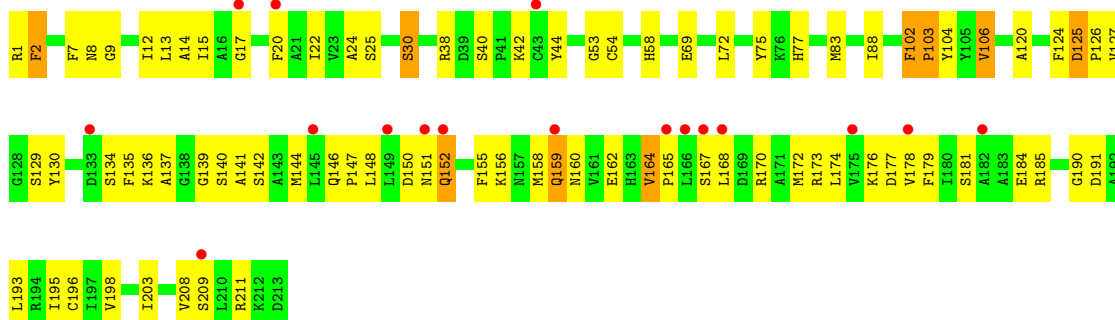


• Molecule 13: 20S proteasome

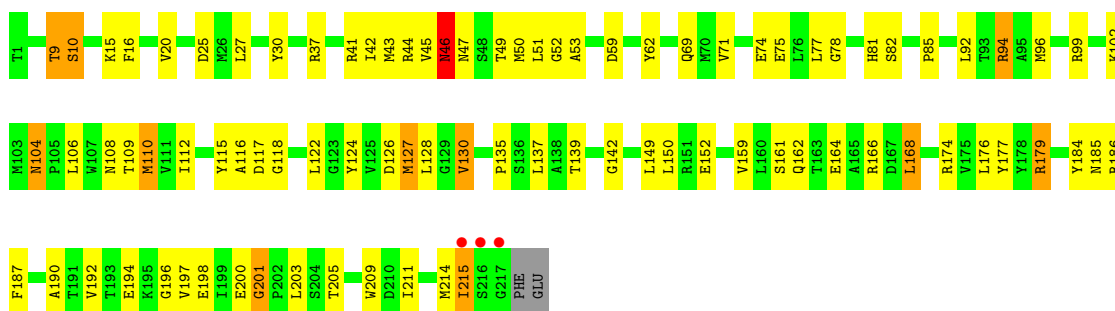




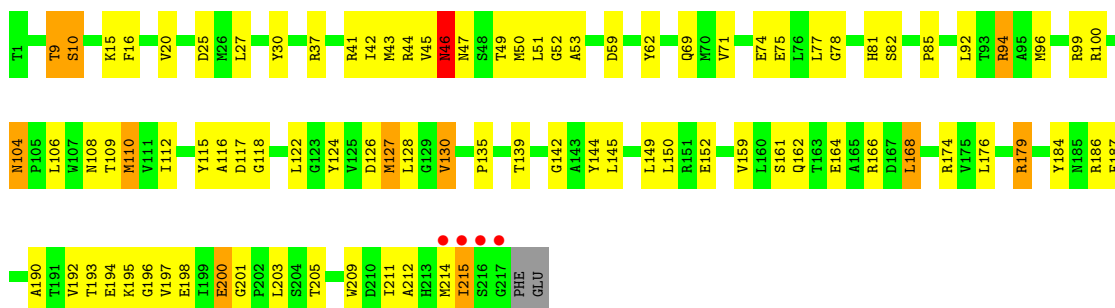
• Molecule 13: 20S proteasome



• Molecule 14: 20S proteasome



• Molecule 14: 20S proteasome



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	316.70Å 205.90Å 116.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.00 – 2.75 65.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (65.00-2.75) 96.1 (65.00-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.294 0.249 , 0.294	Depositor DCC
R_{free} test set	9420 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47757	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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 ⓘ

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

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	0.43	0/1875	1.03	13/2545 (0.5%)
1	O	0.51	0/1875	1.03	12/2545 (0.5%)
2	B	0.40	0/1742	0.95	4/2372 (0.2%)
2	P	0.47	0/1742	0.97	5/2372 (0.2%)
3	C	0.38	0/1931	0.98	10/2613 (0.4%)
3	Q	0.44	0/1931	0.99	11/2613 (0.4%)
4	D	0.42	0/1688	1.00	10/2310 (0.4%)
4	R	0.46	0/1688	1.02	13/2310 (0.6%)
5	E	0.51	0/1790	0.99	8/2424 (0.3%)
5	S	0.49	0/1790	0.98	9/2424 (0.4%)
6	F	0.49	0/1885	1.07	16/2552 (0.6%)
6	T	0.49	0/1885	1.06	14/2552 (0.5%)
7	G	0.47	0/1920	0.99	7/2591 (0.3%)
7	U	0.54	0/1920	1.01	8/2591 (0.3%)
8	H	0.54	0/1535	0.97	1/2078 (0.0%)
8	V	0.56	0/1535	0.97	1/2078 (0.0%)
9	I	0.49	0/1672	1.06	10/2267 (0.4%)
9	W	0.53	0/1672	1.07	10/2267 (0.4%)
10	J	0.48	0/1614	1.08	16/2178 (0.7%)
10	X	0.56	0/1614	1.11	13/2178 (0.6%)
11	K	0.50	0/1603	1.05	14/2174 (0.6%)
11	Y	0.53	0/1603	1.06	13/2174 (0.6%)
12	L	0.54	0/1579	1.00	5/2134 (0.2%)
12	Z	0.52	0/1579	1.00	5/2134 (0.2%)
13	1	0.49	0/1669	0.99	9/2250 (0.4%)
13	M	0.55	0/1669	1.00	9/2250 (0.4%)
14	2	0.53	0/1704	1.05	12/2311 (0.5%)
14	N	0.56	0/1704	1.05	12/2311 (0.5%)
All	All	0.50	0/48414	1.02	270/65598 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	2	0	1
14	N	0	1
All	All	0	2

There are no bond length outliers.

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	106	LYS	N-CA-C	-12.24	98.77	112.72
12	Z	106	LYS	N-CA-C	-12.02	99.01	112.72
9	W	105	VAL	N-CA-C	-10.99	97.22	112.50
9	I	105	VAL	N-CA-C	-10.90	97.35	112.50
9	W	187	ARG	CA-C-N	-9.99	108.39	119.98
9	W	187	ARG	C-N-CA	-9.99	108.39	119.98
3	C	70	GLU	N-CA-C	-9.94	101.28	113.50
9	I	187	ARG	CA-C-N	-9.87	108.53	119.98
9	I	187	ARG	C-N-CA	-9.87	108.53	119.98
3	Q	70	GLU	N-CA-C	-9.64	101.65	113.50
5	S	70	ILE	N-CA-C	-9.18	103.92	111.81
10	X	33	GLN	N-CA-C	9.17	123.28	109.25
6	T	225	ASP	N-CA-C	9.07	124.86	113.43
5	E	70	ILE	N-CA-C	-9.04	104.04	111.81
5	S	28	ILE	N-CA-C	-8.91	101.53	110.62
7	U	161	TRP	N-CA-C	-8.87	102.97	113.88
7	G	161	TRP	N-CA-C	-8.86	102.98	113.88
6	F	225	ASP	N-CA-C	8.77	124.48	113.43
5	E	28	ILE	N-CA-C	-8.65	101.80	110.62
12	Z	116	SER	N-CA-C	-8.55	102.55	113.16
12	L	116	SER	N-CA-C	-8.54	102.57	113.16
6	F	8	ASN	N-CA-C	8.50	123.84	113.38
10	X	80	ARG	N-CA-C	8.41	119.67	108.07
14	N	47	ASN	N-CA-C	8.40	122.62	112.38
10	J	80	ARG	N-CA-C	8.32	119.55	108.07
14	2	47	ASN	N-CA-C	8.30	122.50	112.38
10	J	33	GLN	N-CA-C	8.22	122.83	109.76
6	T	8	ASN	N-CA-C	8.07	123.31	113.38
2	P	158	LYS	N-CA-C	-7.98	103.00	112.89
10	X	78	GLU	N-CA-C	-7.92	100.07	110.53
1	A	164	LYS	N-CA-C	-7.90	102.28	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	LYS	N-CA-C	-7.89	103.10	112.89
3	Q	160	LYS	N-CA-C	-7.78	103.25	112.89
10	J	78	GLU	N-CA-C	-7.77	100.28	110.53
2	B	104	ILE	N-CA-C	7.72	116.52	108.95
13	M	102	PHE	CA-C-N	7.67	127.72	119.89
13	M	102	PHE	C-N-CA	7.67	127.72	119.89
11	K	196	PHE	CA-C-N	7.67	129.43	119.84
11	K	196	PHE	C-N-CA	7.67	129.43	119.84
11	K	127	ALA	CA-C-N	7.66	127.71	119.28
11	K	127	ALA	C-N-CA	7.66	127.71	119.28
11	Y	196	PHE	CA-C-N	7.66	129.42	119.84
11	Y	196	PHE	C-N-CA	7.66	129.42	119.84
13	1	102	PHE	CA-C-N	7.64	127.69	119.89
13	1	102	PHE	C-N-CA	7.64	127.69	119.89
6	F	150	SER	N-CA-C	-7.55	97.76	109.76
14	2	127	MET	N-CA-C	-7.55	104.07	113.28
3	C	160	LYS	N-CA-C	-7.52	103.57	112.89
13	1	125	ASP	N-CA-C	-7.51	101.30	110.31
6	T	150	SER	N-CA-C	-7.49	97.86	109.76
11	Y	127	ALA	CA-C-N	7.48	127.50	119.28
11	Y	127	ALA	C-N-CA	7.48	127.50	119.28
11	K	102	LEU	N-CA-C	7.47	120.09	108.96
1	A	235	ILE	N-CA-C	-7.45	103.59	110.82
1	O	235	ILE	N-CA-C	-7.33	103.64	110.53
11	Y	102	LEU	N-CA-C	7.32	119.86	108.96
14	2	109	THR	N-CA-C	-7.31	96.99	108.90
6	F	183	ASN	N-CA-C	-7.27	99.16	110.42
14	N	109	THR	N-CA-C	-7.26	96.49	108.76
6	F	157	ARG	N-CA-C	-7.26	103.39	112.90
5	E	119	LEU	N-CA-C	-7.25	104.33	113.02
6	T	183	ASN	N-CA-C	-7.23	99.22	110.42
2	P	104	ILE	N-CA-C	7.21	116.02	108.95
6	T	157	ARG	N-CA-C	-7.16	103.52	112.90
13	M	125	ASP	N-CA-C	-7.14	101.74	110.31
13	1	104	TYR	N-CA-C	-7.06	97.74	108.96
14	N	127	MET	N-CA-C	-7.04	104.70	113.28
5	S	119	LEU	N-CA-C	-7.02	104.60	113.02
1	O	164	LYS	N-CA-C	-6.96	103.13	111.69
14	2	179	ARG	N-CA-C	6.89	122.35	113.88
8	H	98	ILE	N-CA-C	6.80	119.23	108.89
7	G	6	GLY	N-CA-C	-6.72	105.51	114.25
10	J	163	LEU	N-CA-C	-6.71	103.75	112.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	163	LEU	N-CA-C	-6.70	103.77	112.68
7	U	6	GLY	N-CA-C	-6.67	105.58	114.25
14	N	106	LEU	N-CA-C	-6.64	96.84	108.20
1	O	49	VAL	N-CA-C	6.57	117.94	108.48
7	U	77	VAL	N-CA-C	6.56	119.22	108.99
12	L	87	VAL	N-CA-C	6.54	117.33	110.72
11	Y	2	GLU	N-CA-C	6.53	119.82	110.10
4	D	157	LYS	N-CA-C	-6.50	104.04	112.23
12	Z	87	VAL	N-CA-C	6.49	117.27	110.72
10	X	60	VAL	N-CA-C	-6.48	104.02	110.30
14	2	159	VAL	N-CA-C	6.46	116.94	107.37
4	R	157	LYS	N-CA-C	-6.45	104.10	112.23
9	I	154	LEU	N-CA-C	-6.45	104.33	111.36
8	V	98	ILE	N-CA-C	6.44	118.67	108.89
14	N	159	VAL	N-CA-C	6.43	116.88	107.37
14	2	106	LEU	N-CA-C	-6.42	97.22	108.20
10	J	101	GLY	CA-C-N	6.38	126.35	120.03
10	J	101	GLY	C-N-CA	6.38	126.35	120.03
1	A	49	VAL	N-CA-C	6.37	117.65	108.48
9	W	154	LEU	N-CA-C	-6.35	104.44	111.36
1	A	156	PRO	N-CA-C	-6.34	99.40	112.47
11	K	2	GLU	N-CA-C	6.33	119.54	110.10
10	J	60	VAL	N-CA-C	-6.31	104.18	110.30
7	G	77	VAL	N-CA-C	6.30	118.82	108.99
6	F	156	CYS	N-CA-C	6.25	119.73	109.85
1	O	156	PRO	N-CA-C	-6.23	99.64	112.47
5	S	212	ALA	N-CA-C	-6.22	105.45	113.16
6	T	156	CYS	N-CA-C	6.21	119.77	110.14
1	O	155	ASP	N-CA-C	6.14	119.61	110.39
3	Q	72	MET	N-CA-C	6.14	118.75	109.23
13	M	104	TYR	N-CA-C	-6.14	98.53	108.41
5	E	212	ALA	N-CA-C	-6.13	105.56	113.16
5	S	184	LEU	N-CA-C	6.05	120.83	112.90
1	A	155	ASP	N-CA-C	6.05	119.47	110.39
14	N	179	ARG	N-CA-C	6.05	121.71	113.97
14	2	53	ALA	N-CA-C	6.03	119.23	109.40
10	X	101	GLY	CA-C-N	6.02	125.99	120.03
10	X	101	GLY	C-N-CA	6.02	125.99	120.03
3	C	72	MET	N-CA-C	6.01	118.31	109.24
1	O	209	ASP	N-CA-C	-6.01	103.51	111.02
1	O	73	THR	N-CA-C	-6.00	100.30	109.65
5	E	184	LEU	N-CA-C	5.98	120.73	112.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	THR	N-CA-C	-5.96	100.36	109.65
6	T	41	LYS	N-CA-C	-5.95	105.33	113.30
6	F	128	TYR	N-CA-C	-5.93	101.50	110.28
6	T	128	TYR	N-CA-C	-5.92	101.53	110.28
1	A	209	ASP	N-CA-C	-5.91	103.64	111.02
7	G	126	SER	N-CA-C	-5.85	105.97	113.23
9	W	77	VAL	CB-CA-C	-5.85	104.38	112.04
4	R	236	LYS	N-CA-C	-5.83	106.79	112.97
14	N	53	ALA	N-CA-C	5.81	118.87	109.40
10	J	128	GLY	N-CA-C	5.81	123.62	115.43
10	J	106	GLU	CA-C-N	5.79	126.11	119.92
10	J	106	GLU	C-N-CA	5.79	126.11	119.92
7	U	126	SER	N-CA-C	-5.78	106.06	113.23
14	N	104	ASN	CA-C-N	5.78	125.75	120.03
14	N	104	ASN	C-N-CA	5.78	125.75	120.03
1	O	56	VAL	CA-C-N	5.76	125.47	119.82
1	O	56	VAL	C-N-CA	5.76	125.47	119.82
3	Q	218	ARG	N-CA-C	-5.75	103.11	110.53
13	1	106	VAL	N-CA-C	5.75	115.94	108.35
3	C	218	ARG	N-CA-C	-5.74	103.12	110.53
7	U	21	PHE	N-CA-C	5.74	118.31	111.71
10	X	126	LEU	N-CA-C	-5.73	106.14	113.01
4	D	236	LYS	N-CA-C	-5.72	106.91	112.97
2	B	73	LEU	N-CA-C	5.70	117.85	109.24
6	F	41	LYS	N-CA-C	-5.69	105.08	113.61
1	O	206	LEU	N-CA-C	-5.68	106.39	113.38
7	G	70	ASP	N-CA-C	-5.68	100.31	108.60
4	D	130	SER	N-CA-C	-5.64	101.39	110.14
7	U	70	ASP	N-CA-C	-5.63	100.38	108.60
2	P	73	LEU	N-CA-C	5.62	117.73	109.24
1	A	56	VAL	CA-C-N	5.62	125.33	119.82
1	A	56	VAL	C-N-CA	5.62	125.33	119.82
13	M	134	SER	N-CA-C	-5.62	104.78	111.69
6	T	112	ILE	N-CA-C	-5.61	104.89	110.62
5	S	74	ILE	N-CA-C	5.61	115.95	108.27
6	F	87	PHE	N-CA-C	-5.61	105.09	111.14
14	2	110	MET	N-CA-C	5.59	118.34	109.50
10	J	101	GLY	N-CA-C	-5.59	100.93	112.34
13	1	134	SER	N-CA-C	-5.59	104.82	111.69
5	E	16	SER	N-CA-C	-5.57	103.72	110.13
4	D	203	GLY	N-CA-C	-5.57	108.35	115.42
6	T	133	LEU	N-CA-C	-5.56	100.12	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	152	GLN	N-CA-C	5.55	117.14	111.14
1	A	68	HIS	N-CA-C	-5.54	104.43	113.19
10	X	106	GLU	CA-C-N	5.53	125.84	119.92
10	X	106	GLU	C-N-CA	5.53	125.84	119.92
11	K	64	VAL	N-CA-C	-5.52	104.98	111.00
10	X	101	GLY	N-CA-C	-5.52	101.08	112.34
13	M	106	VAL	N-CA-C	5.52	115.63	108.35
4	R	203	GLY	N-CA-C	-5.51	108.43	115.42
4	R	130	SER	N-CA-C	-5.49	101.63	110.14
10	X	179	ALA	N-CA-C	5.48	118.01	111.71
9	I	98	LEU	N-CA-C	5.47	118.47	109.72
3	Q	100	GLN	N-CA-C	5.46	117.24	111.28
14	N	110	MET	N-CA-C	5.46	118.12	109.50
14	N	130	VAL	N-CA-C	-5.45	101.70	108.89
10	J	34	LEU	N-CA-C	-5.45	102.82	110.50
13	M	152	GLN	N-CA-C	5.44	117.01	111.14
4	R	53	LEU	N-CA-C	-5.44	106.49	113.01
13	M	128	GLY	N-CA-C	5.43	121.99	114.92
1	A	206	LEU	N-CA-C	-5.43	106.71	113.38
1	O	208	ILE	N-CA-C	5.42	120.61	109.34
3	C	100	GLN	N-CA-C	5.41	117.18	111.28
4	R	125	ARG	CA-C-N	-5.41	115.16	120.52
4	R	125	ARG	C-N-CA	-5.41	115.16	120.52
11	Y	64	VAL	N-CA-C	-5.41	105.10	111.00
10	J	194	LYS	N-CA-C	5.41	116.48	108.86
11	K	26	VAL	N-CA-C	5.40	117.16	108.85
10	J	126	LEU	N-CA-C	-5.39	105.96	112.54
6	T	207	THR	N-CA-C	-5.39	106.77	113.19
1	A	208	ILE	N-CA-C	5.38	120.53	109.34
6	F	133	LEU	N-CA-C	-5.38	100.41	109.07
3	C	44	LEU	N-CA-C	5.37	117.14	109.14
11	Y	26	VAL	N-CA-C	5.37	117.12	108.85
13	1	127	VAL	N-CA-C	5.37	117.35	111.77
11	K	120	TYR	N-CA-C	-5.35	106.59	113.01
4	R	204	LYS	N-CA-C	-5.34	106.79	113.15
11	Y	46	CYS	N-CA-C	5.34	117.78	108.76
3	Q	154	GLY	N-CA-C	-5.33	106.33	115.08
6	T	87	PHE	N-CA-C	-5.33	105.38	111.14
11	Y	127	ALA	N-CA-C	5.33	114.99	108.11
5	S	16	SER	N-CA-C	-5.33	104.00	110.13
9	I	77	VAL	CB-CA-C	-5.32	105.07	112.04
6	F	205	LEU	N-CA-C	5.32	117.89	109.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	23	GLY	N-CA-C	-5.32	101.91	110.95
11	Y	154	GLU	N-CA-C	-5.32	105.15	111.69
3	Q	44	LEU	N-CA-C	5.31	117.49	109.41
4	D	204	LYS	N-CA-C	-5.31	106.83	113.15
11	K	127	ALA	N-CA-C	5.31	114.96	108.11
9	W	189	TYR	N-CA-C	-5.31	106.49	113.12
1	O	68	HIS	N-CA-C	-5.30	104.53	112.54
4	D	53	LEU	N-CA-C	-5.29	106.66	113.01
2	P	126	VAL	N-CA-C	5.28	117.22	108.99
11	Y	31	ASP	N-CA-C	5.27	115.97	108.54
3	C	154	GLY	N-CA-C	-5.27	106.44	115.08
10	X	128	GLY	N-CA-C	5.26	122.84	115.43
14	2	104	ASN	CA-C-N	5.25	125.23	120.03
14	2	104	ASN	C-N-CA	5.25	125.23	120.03
5	E	102	THR	N-CA-C	5.25	116.81	111.14
3	Q	76	VAL	N-CA-C	5.24	117.17	108.99
11	K	154	GLU	N-CA-C	-5.22	105.27	111.69
7	G	200	VAL	N-CA-C	5.21	115.93	110.62
4	D	94	HIS	N-CA-C	-5.21	106.88	113.18
5	E	74	ILE	N-CA-C	5.20	115.40	108.27
3	C	76	VAL	N-CA-C	5.20	117.10	108.99
9	W	98	LEU	N-CA-C	5.19	118.02	109.72
4	D	125	ARG	N-CA-C	-5.17	103.00	110.40
11	K	31	ASP	N-CA-C	5.17	115.83	108.54
11	K	46	CYS	N-CA-C	5.17	117.50	108.76
5	S	102	THR	N-CA-C	5.17	116.72	111.14
3	Q	63	GLU	N-CA-C	-5.16	108.00	114.56
6	F	239	ARG	CA-C-N	5.15	126.28	119.84
6	F	239	ARG	C-N-CA	5.15	126.28	119.84
7	U	125	TYR	N-CA-C	5.15	117.24	109.41
3	C	24	ALA	N-CA-C	-5.14	105.76	111.36
9	W	172	ASN	N-CA-C	5.14	117.16	110.53
3	Q	169	ALA	N-CA-C	-5.13	106.96	113.43
12	L	23	GLY	N-CA-C	-5.12	102.24	110.95
1	A	185	LYS	N-CA-C	-5.12	106.29	112.54
9	I	189	TYR	N-CA-C	-5.12	106.72	113.12
3	Q	249	ARG	N-CA-C	-5.12	106.88	113.02
12	L	58	LEU	N-CA-C	-5.11	105.71	111.28
5	S	140	ALA	N-CA-C	-5.11	100.71	109.24
13	M	78	SER	N-CA-C	5.11	116.93	111.36
6	T	205	LEU	N-CA-C	5.10	117.56	109.96
4	R	129	ILE	CB-CA-C	-5.10	104.71	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	102	LYS	N-CA-C	-5.09	106.66	112.92
10	J	3	ILE	N-CA-C	5.08	115.30	110.42
14	2	130	VAL	N-CA-C	-5.08	102.18	108.89
4	D	17	PHE	N-CA-C	5.07	117.20	111.11
9	I	122	LEU	CA-C-N	5.07	124.68	119.56
9	I	122	LEU	C-N-CA	5.07	124.68	119.56
3	C	249	ARG	N-CA-C	-5.06	106.95	113.02
11	Y	83	PHE	N-CA-C	-5.06	104.71	111.24
4	R	230	ALA	N-CA-C	-5.06	107.06	113.43
4	R	233	GLU	N-CA-C	-5.06	105.77	111.28
14	2	200	GLU	N-CA-C	5.06	117.48	109.24
6	F	219	LEU	N-CA-C	5.05	117.39	108.75
9	W	73	LEU	CA-C-N	5.05	125.05	119.89
9	W	73	LEU	C-N-CA	5.05	125.05	119.89
7	U	200	VAL	N-CA-C	5.05	115.77	110.62
11	K	83	PHE	N-CA-C	-5.05	104.73	111.24
13	1	103	PRO	N-CA-C	5.05	119.14	111.11
6	T	7	ASP	N-CA-C	5.04	119.69	113.50
12	Z	82	LEU	N-CA-C	-5.03	105.68	111.07
2	B	126	VAL	N-CA-C	5.03	117.25	108.95
6	F	207	THR	N-CA-C	-5.03	107.20	113.19
7	G	125	TYR	N-CA-C	5.03	117.06	109.41
4	D	129	ILE	CB-CA-C	-5.03	104.81	111.80
4	R	17	PHE	N-CA-C	5.03	117.14	111.11
9	I	172	ASN	N-CA-C	5.02	117.00	110.53
4	R	94	HIS	N-CA-C	-5.02	107.11	113.18
2	P	54	ILE	N-CA-C	-5.02	106.20	113.07
10	J	97	GLU	N-CA-C	-5.01	106.99	113.01
6	F	227	ASP	N-CA-C	-5.01	105.95	111.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	2	30	TYR	Sidechain
14	N	30	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1842	0	1803	107	0
1	O	1842	0	1803	113	0
2	B	1707	0	1591	103	0
2	P	1707	0	1591	110	0
3	C	1902	0	1835	150	0
3	Q	1902	0	1835	148	0
4	D	1665	0	1433	110	0
4	R	1665	0	1433	112	0
5	E	1763	0	1708	89	0
5	S	1763	0	1708	86	0
6	F	1850	0	1822	106	0
6	T	1850	0	1822	98	0
7	G	1885	0	1843	94	0
7	U	1885	0	1843	89	0
8	H	1509	0	1473	66	0
8	V	1509	0	1473	60	0
9	I	1645	0	1649	114	0
9	W	1645	0	1649	104	0
10	J	1585	0	1600	118	0
10	X	1585	0	1600	112	0
11	K	1570	0	1546	107	0
11	Y	1570	0	1546	104	0
12	L	1548	0	1499	81	0
12	Z	1548	0	1499	86	0
13	1	1639	0	1609	85	0
13	M	1639	0	1609	72	0
14	2	1671	0	1625	84	0
14	N	1671	0	1625	86	0
15	1	2	0	0	0	0
15	A	1	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	D	1	0	0	0	0
15	G	3	0	0	0	0
15	I	1	0	0	0	0
15	J	4	0	0	0	0
15	K	1	0	0	0	0
15	M	2	0	0	0	0
15	O	1	0	0	0	0
15	P	1	0	0	0	0
15	Q	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	R	1	0	0	0	0
15	U	3	0	0	0	0
15	W	1	0	0	0	0
15	X	4	0	0	0	0
15	Y	1	0	0	0	0
16	1	4	0	0	1	0
16	2	8	0	0	1	0
16	A	2	0	0	0	0
16	B	3	0	0	0	0
16	C	3	0	0	0	0
16	F	6	0	0	1	0
16	G	4	0	0	1	0
16	H	7	0	0	0	0
16	I	6	0	0	2	0
16	J	1	0	0	0	0
16	K	6	0	0	0	0
16	L	8	0	0	0	0
16	M	10	0	0	0	0
16	N	9	0	0	4	0
16	O	7	0	0	1	0
16	P	6	0	0	1	0
16	Q	3	0	0	1	0
16	R	3	0	0	0	0
16	S	1	0	0	0	0
16	T	7	0	0	1	0
16	U	9	0	0	0	0
16	V	15	0	0	0	0
16	W	9	0	0	0	0
16	X	17	0	0	0	0
16	Y	3	0	0	1	0
16	Z	8	0	0	0	0
All	All	47757	0	46072	2569	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 27.

All (2569) 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)
11:K:145:ARG:HE	12:Z:158:ARG:HD2	1.01	1.14
3:Q:180:LYS:H	3:Q:180:LYS:HD3	1.10	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:158:ARG:HD2	11:Y:145:ARG:HE	1.10	1.08
3:C:180:LYS:HD3	3:C:180:LYS:H	1.10	1.07
4:D:57:ARG:HA	4:D:60:ARG:HE	1.18	1.06
8:H:76:VAL:HB	8:H:110:GLN:HE21	1.17	1.05
5:E:99:HIS:HB2	5:E:107:MET:HE2	1.39	1.04
8:V:76:VAL:HB	8:V:110:GLN:HE21	1.22	1.04
4:R:57:ARG:HA	4:R:60:ARG:HE	1.19	1.04
14:2:49:THR:HG22	14:2:85:PRO:HG3	1.38	1.03
7:G:47:PHE:HB2	7:G:214:SER:HB2	1.39	1.03
5:S:99:HIS:HB2	5:S:107:MET:HE2	1.37	1.03
7:U:47:PHE:HB2	7:U:214:SER:HB2	1.42	1.01
11:Y:38:MET:HE1	11:Y:60:ILE:HG22	1.44	1.00
5:E:96:THR:HA	5:E:107:MET:HE3	1.44	1.00
11:Y:1:MET:HE1	11:Y:134:TYR:H	1.28	0.99
14:N:49:THR:HG22	14:N:85:PRO:HG3	1.40	0.98
4:R:38:ARG:HB2	4:R:38:ARG:HH11	1.28	0.98
10:J:7:ASN:ND2	10:J:57:ALA:H	1.61	0.97
11:K:145:ARG:HE	12:Z:158:ARG:CD	1.77	0.97
11:K:145:ARG:NE	12:Z:158:ARG:HD2	1.77	0.97
5:S:96:THR:HA	5:S:107:MET:HE3	1.45	0.97
10:X:7:ASN:ND2	10:X:57:ALA:H	1.63	0.96
11:K:38:MET:HE1	11:K:60:ILE:HG22	1.44	0.96
7:G:42:LYS:HE2	7:G:185:THR:HG22	1.46	0.95
1:A:126:THR:HG22	2:B:127:ARG:HH21	1.32	0.95
4:D:38:ARG:HB2	4:D:38:ARG:HH11	1.30	0.95
7:U:42:LYS:HE2	7:U:185:THR:HG22	1.45	0.95
1:A:67:THR:HG22	1:A:69:LEU:H	1.28	0.95
11:K:1:MET:HE1	11:K:134:TYR:H	1.30	0.94
13:M:8:ASN:HD22	13:M:58:HIS:H	1.14	0.94
1:O:67:THR:HG22	1:O:69:LEU:H	1.29	0.94
6:T:206:THR:H	6:T:209:ASN:HD21	1.02	0.93
13:1:8:ASN:HD22	13:1:58:HIS:H	1.13	0.93
9:I:40:ASN:H	9:I:40:ASN:HD22	1.16	0.93
14:N:211:ILE:HA	14:N:214:MET:HE3	1.51	0.93
6:F:206:THR:H	6:F:209:ASN:HD21	1.02	0.93
14:2:211:ILE:HA	14:2:214:MET:HE3	1.51	0.93
4:R:104:VAL:HG11	4:R:143:ARG:HB2	1.50	0.92
9:I:198:ARG:HH21	9:I:202:TYR:H	1.17	0.92
13:1:8:ASN:ND2	13:1:58:HIS:H	1.67	0.92
10:J:34:LEU:HD23	12:Z:166:ARG:HD3	1.51	0.92
1:O:126:THR:HG22	2:P:127:ARG:HH21	1.34	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:76:ILE:HD12	1:O:111:VAL:HG22	1.52	0.91
1:A:221:THR:HG22	1:A:223:GLU:H	1.35	0.91
9:W:40:ASN:H	9:W:40:ASN:HD22	1.15	0.91
8:H:76:VAL:HB	8:H:110:GLN:NE2	1.85	0.91
1:O:221:THR:HG22	1:O:223:GLU:H	1.33	0.91
10:X:145:GLN:HE21	10:X:145:GLN:H	0.93	0.90
12:L:19:ARG:HH21	12:L:29:GLN:HE22	1.18	0.90
13:M:8:ASN:ND2	13:M:58:HIS:H	1.69	0.90
10:J:145:GLN:HE21	10:J:145:GLN:H	0.93	0.89
4:D:104:VAL:HG11	4:D:143:ARG:HB2	1.51	0.89
1:A:76:ILE:HD12	1:A:111:VAL:HG22	1.52	0.89
11:Y:1:MET:CE	11:Y:134:TYR:H	1.86	0.89
12:Z:90:TYR:HA	12:Z:93:MET:HE3	1.55	0.89
7:U:34:SER:HB3	7:U:65:ARG:HH12	1.37	0.89
10:X:26:ARG:HB3	10:X:26:ARG:HH11	1.37	0.89
11:K:197:PRO:HB2	11:Y:197:PRO:HB2	1.55	0.88
6:F:13:TRP:H	7:G:22:GLN:HE22	1.12	0.88
8:V:76:VAL:HB	8:V:110:GLN:NE2	1.88	0.88
12:L:158:ARG:HD2	11:Y:145:ARG:NE	1.88	0.88
3:C:8:ARG:HB3	3:C:11:ILE:HD12	1.54	0.88
3:Q:8:ARG:HB3	3:Q:11:ILE:HD12	1.56	0.88
9:I:199:LEU:HD22	13:I:176:LYS:HD2	1.56	0.88
5:S:146:VAL:HG23	5:S:220:VAL:HG12	1.54	0.88
7:G:34:SER:HB3	7:G:65:ARG:HH12	1.38	0.88
5:E:206:MET:HE1	5:E:210:LEU:HD13	1.56	0.87
5:E:146:VAL:HG23	5:E:220:VAL:HG12	1.55	0.87
5:S:206:MET:HE1	5:S:210:LEU:HD13	1.56	0.87
9:W:198:ARG:HH21	9:W:202:TYR:H	1.17	0.87
12:L:90:TYR:HA	12:L:93:MET:HE3	1.57	0.87
10:J:26:ARG:HB3	10:J:26:ARG:HH11	1.39	0.87
11:Y:182:ILE:HD11	11:Y:191:LEU:HD11	1.56	0.86
14:2:51:LEU:HD13	14:2:112:ILE:HD13	1.56	0.86
11:K:81:ALA:HB2	11:K:104:LEU:HD23	1.57	0.86
9:I:190:THR:HG22	9:I:192:PRO:HD3	1.54	0.86
10:X:7:ASN:HD22	10:X:57:ALA:H	1.22	0.86
11:K:182:ILE:HD11	11:K:191:LEU:HD11	1.55	0.86
9:W:190:THR:HG22	9:W:192:PRO:HD3	1.58	0.86
11:K:1:MET:CE	11:K:134:TYR:H	1.89	0.85
5:E:99:HIS:CB	5:E:107:MET:HE2	2.06	0.85
10:J:145:GLN:HE21	10:J:145:GLN:N	1.75	0.85
10:J:160:PRO:HB3	10:J:189:ILE:HD11	1.56	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:99:HIS:CB	5:S:107:MET:HE2	2.07	0.85
9:I:75:ARG:HA	9:I:104:ASP:OD1	1.77	0.85
6:T:13:TRP:H	7:U:22:GLN:HE22	1.25	0.85
3:C:95:GLN:HE22	3:C:98:LEU:HD23	1.41	0.84
14:2:192:VAL:HG12	14:2:197:VAL:HG22	1.58	0.84
4:R:181:ILE:HA	4:R:186:LEU:HB3	1.60	0.84
5:S:210:LEU:HD11	5:S:215:ILE:HD13	1.59	0.84
11:K:151:ILE:HG13	11:K:155:ARG:HB2	1.59	0.84
12:L:158:ARG:CD	11:Y:145:ARG:HE	1.89	0.84
14:N:192:VAL:HG12	14:N:197:VAL:HG22	1.59	0.84
12:Z:19:ARG:HH21	12:Z:29:GLN:HE22	1.24	0.84
10:J:7:ASN:HD22	10:J:57:ALA:H	1.22	0.84
12:L:166:ARG:HD3	10:X:34:LEU:HD23	1.58	0.84
3:Q:180:LYS:H	3:Q:180:LYS:CD	1.89	0.84
10:X:160:PRO:HB3	10:X:189:ILE:HD11	1.59	0.84
8:H:14:LEU:HD21	8:H:101:ALA:HB3	1.60	0.84
11:K:151:ILE:HG13	11:K:155:ARG:CB	2.07	0.84
14:N:51:LEU:HD13	14:N:112:ILE:HD13	1.60	0.84
10:X:145:GLN:H	10:X:145:GLN:NE2	1.76	0.84
9:I:198:ARG:NH2	9:I:202:TYR:H	1.75	0.83
11:Y:151:ILE:HG13	11:Y:155:ARG:HB2	1.58	0.83
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.60	0.83
9:W:198:ARG:NH2	9:W:202:TYR:H	1.74	0.83
5:E:210:LEU:HD11	5:E:215:ILE:HD13	1.60	0.83
6:F:238:GLU:O	6:F:239:ARG:HB3	1.76	0.83
6:F:151:ALA:HB3	7:G:82:ALA:HB1	1.61	0.83
10:J:126:LEU:HD13	10:J:127:ILE:HG23	1.61	0.83
11:Y:151:ILE:HG13	11:Y:155:ARG:CB	2.08	0.82
9:W:205:GLU:O	9:W:208:THR:HG22	1.80	0.82
10:X:145:GLN:HE21	10:X:145:GLN:N	1.75	0.82
10:J:189:ILE:HG23	10:J:196:THR:HB	1.61	0.82
10:X:126:LEU:HD13	10:X:127:ILE:HG23	1.61	0.82
10:J:116:THR:O	10:J:192:LYS:HE2	1.79	0.81
2:P:213:ASN:HD21	2:P:215:ALA:HB3	1.45	0.81
3:Q:95:GLN:HE22	3:Q:98:LEU:HD23	1.43	0.81
9:W:75:ARG:HA	9:W:104:ASP:OD1	1.79	0.81
10:X:116:THR:O	10:X:192:LYS:HE2	1.79	0.81
2:B:213:ASN:HD21	2:B:215:ALA:HB3	1.44	0.81
4:D:181:ILE:HA	4:D:186:LEU:HB3	1.60	0.81
10:J:14:MET:HE3	10:J:167:ILE:HG13	1.63	0.81
3:C:239:LYS:O	3:C:239:LYS:HD3	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:196:ARG:HD3	6:F:239:ARG:HD3	1.63	0.81
10:J:145:GLN:H	10:J:145:GLN:NE2	1.77	0.81
3:Q:187:LYS:HA	3:Q:187:LYS:HE3	1.63	0.80
11:Y:81:ALA:HB2	11:Y:104:LEU:HD23	1.62	0.80
6:F:196:ARG:HH22	6:F:236:LEU:HD13	1.47	0.80
13:1:1:ARG:HG3	13:1:2:PHE:H	1.47	0.80
3:C:187:LYS:NZ	3:C:236:LEU:HD11	1.97	0.80
9:I:205:GLU:O	9:I:208:THR:HG22	1.82	0.80
10:J:37:THR:HG21	10:J:204:MET:HE1	1.63	0.80
3:C:180:LYS:HD3	3:C:180:LYS:N	1.95	0.80
13:M:1:ARG:HG3	13:M:2:PHE:H	1.46	0.80
3:Q:239:LYS:O	3:Q:239:LYS:HD3	1.82	0.80
10:X:37:THR:HG21	10:X:204:MET:HE1	1.62	0.80
4:D:57:ARG:HA	4:D:60:ARG:NE	1.96	0.80
5:S:117:SER:O	5:S:120:ALA:HB2	1.82	0.80
5:E:31:ILE:HD13	5:E:140:ALA:HB2	1.65	0.79
11:K:2:GLU:OE1	11:K:47:VAL:HG13	1.83	0.79
3:C:187:LYS:HA	3:C:187:LYS:HE3	1.64	0.79
11:K:80:ALA:O	11:K:84:THR:HG23	1.83	0.79
5:S:31:ILE:HD13	5:S:140:ALA:HB2	1.65	0.79
3:Q:187:LYS:NZ	3:Q:236:LEU:HD11	1.98	0.79
10:X:14:MET:HE3	10:X:167:ILE:HG13	1.63	0.79
11:Y:9:GLY:HA3	11:Y:12:TYR:CE2	2.17	0.79
3:C:180:LYS:H	3:C:180:LYS:CD	1.89	0.79
11:Y:80:ALA:O	11:Y:84:THR:HG23	1.82	0.78
4:R:57:ARG:HA	4:R:60:ARG:NE	1.96	0.78
6:T:206:THR:H	6:T:209:ASN:ND2	1.81	0.78
10:X:189:ILE:HG23	10:X:196:THR:HB	1.63	0.78
9:W:104:ASP:HB3	9:W:106:THR:H	1.49	0.78
12:L:6:PHE:HB2	12:L:125:THR:HG22	1.66	0.78
12:Z:138:VAL:HG21	12:Z:159:ALA:HA	1.65	0.78
11:K:9:GLY:HA3	11:K:12:TYR:CE2	2.19	0.78
14:2:46:ASN:C	14:2:46:ASN:HD22	1.91	0.78
14:N:46:ASN:C	14:N:46:ASN:HD22	1.90	0.78
3:C:79:ILE:HD13	3:C:131:GLY:HA3	1.66	0.78
4:R:38:ARG:HB2	4:R:38:ARG:NH1	1.98	0.78
6:T:230:SER:HB2	6:T:231:PRO:HD3	1.64	0.78
9:I:104:ASP:HB3	9:I:106:THR:H	1.48	0.77
5:E:117:SER:O	5:E:120:ALA:HB2	1.83	0.77
2:B:73:LEU:HD21	2:B:135:ILE:HG13	1.66	0.77
2:B:44:VAL:HG22	2:B:211:ILE:HG22	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:66:LEU:O	11:K:70:ARG:HG3	1.85	0.77
12:L:8:PHE:H	12:L:8:PHE:HD2	1.33	0.77
6:T:36:VAL:HG22	6:T:160:SER:HB2	1.67	0.77
4:D:136:PHE:HA	4:D:142:PRO:HA	1.67	0.77
12:L:19:ARG:HH21	12:L:29:GLN:NE2	1.81	0.77
1:A:73:THR:HG22	1:A:74:GLU:N	2.00	0.77
4:D:38:ARG:HB2	4:D:38:ARG:NH1	1.99	0.77
6:F:230:SER:HB2	6:F:231:PRO:HD3	1.66	0.77
2:P:44:VAL:HG22	2:P:211:ILE:HG22	1.65	0.77
6:T:151:ALA:HB3	7:U:82:ALA:HB1	1.67	0.77
12:L:138:VAL:HG21	12:L:159:ALA:HA	1.67	0.76
4:R:136:PHE:HA	4:R:142:PRO:HA	1.67	0.76
12:Z:8:PHE:H	12:Z:8:PHE:HD2	1.33	0.76
8:H:166:ARG:NE	14:2:37:ARG:HH21	1.84	0.76
1:O:73:THR:HG22	1:O:74:GLU:N	2.00	0.76
14:2:51:LEU:HD11	14:2:110:MET:HB3	1.68	0.76
9:W:198:ARG:HH21	9:W:202:TYR:N	1.84	0.76
12:Z:19:ARG:HH21	12:Z:29:GLN:NE2	1.84	0.76
6:F:206:THR:H	6:F:209:ASN:ND2	1.82	0.76
12:Z:6:PHE:HB2	12:Z:125:THR:HG22	1.68	0.75
3:Q:175:LEU:HD21	3:Q:196:VAL:HG21	1.68	0.75
11:Y:66:LEU:O	11:Y:70:ARG:HG3	1.87	0.75
1:O:200:THR:O	1:O:204:THR:HG23	1.87	0.75
11:K:45:LEU:HB2	11:K:103:LEU:HB2	1.69	0.75
10:X:20:VAL:HB	10:X:190:ILE:HD11	1.69	0.75
12:Z:76:VAL:HG23	12:Z:105:ASP:OD1	1.87	0.75
8:H:179:ILE:HG12	8:H:184:VAL:HG22	1.69	0.75
9:W:64:GLU:O	9:W:68:LEU:HB2	1.85	0.75
6:F:36:VAL:HG22	6:F:160:SER:HB2	1.67	0.75
14:N:37:ARG:HH21	8:V:166:ARG:NE	1.84	0.75
2:P:73:LEU:HD21	2:P:135:ILE:HG13	1.68	0.75
9:I:40:ASN:HD22	9:I:40:ASN:N	1.84	0.75
7:U:34:SER:HB3	7:U:65:ARG:NH1	2.02	0.75
3:Q:79:ILE:HD13	3:Q:131:GLY:HA3	1.67	0.74
9:W:40:ASN:HD22	9:W:40:ASN:N	1.83	0.74
11:Y:2:GLU:OE1	11:Y:47:VAL:HG13	1.87	0.74
14:2:15:LYS:HE2	14:2:135:PRO:HA	1.68	0.74
13:1:159:GLN:NE2	13:1:160:ASN:H	1.85	0.74
14:N:51:LEU:HD11	14:N:110:MET:HB3	1.69	0.74
6:T:237:GLU:C	6:T:239:ARG:H	1.93	0.74
11:Y:1:MET:HE1	11:Y:134:TYR:N	2.01	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:40:SER:O	13:M:42:LYS:HE3	1.87	0.74
5:S:96:THR:HA	5:S:107:MET:CE	2.17	0.74
7:U:136:MET:HE3	7:U:163:CYS:SG	2.27	0.74
5:E:96:THR:HA	5:E:107:MET:CE	2.15	0.74
11:Y:180:VAL:HG12	11:Y:191:LEU:HD12	1.70	0.74
2:P:64:VAL:HG22	2:P:74:VAL:HG12	1.70	0.74
10:X:45:MET:HE3	10:X:71:LEU:HD22	1.70	0.74
14:N:15:LYS:HE2	14:N:135:PRO:HA	1.68	0.73
1:A:130:GLU:HG2	2:B:4:GLY:HA2	1.70	0.73
3:C:175:LEU:HD21	3:C:196:VAL:HG21	1.69	0.73
8:V:179:ILE:HG12	8:V:184:VAL:HG22	1.68	0.73
9:I:198:ARG:HH21	9:I:202:TYR:N	1.85	0.73
7:G:34:SER:HB3	7:G:65:ARG:NH1	2.02	0.73
2:B:149:ASP:HB2	2:B:150:PRO:HD2	1.69	0.73
10:J:45:MET:HE3	10:J:71:LEU:HD22	1.69	0.73
9:W:40:ASN:H	9:W:40:ASN:ND2	1.87	0.73
12:L:76:VAL:HG23	12:L:105:ASP:OD1	1.86	0.73
3:Q:15:GLU:HB3	4:R:28:LYS:HZ3	1.54	0.73
2:P:182:GLU:HG2	2:P:183:LEU:H	1.53	0.73
12:Z:125:THR:HB	12:Z:139:MET:HE3	1.70	0.73
13:1:40:SER:O	13:1:42:LYS:HE3	1.87	0.73
13:M:159:GLN:NE2	13:M:160:ASN:H	1.87	0.73
3:Q:180:LYS:HD3	3:Q:180:LYS:N	1.95	0.73
2:B:37:ILE:HD12	2:B:190:ALA:HB2	1.70	0.72
2:B:182:GLU:HG2	2:B:183:LEU:H	1.53	0.72
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.71	0.72
9:I:64:GLU:O	9:I:68:LEU:HB2	1.88	0.72
11:K:1:MET:HE1	11:K:134:TYR:N	2.03	0.72
4:R:33:VAL:HG12	4:R:160:ALA:HB2	1.72	0.72
9:I:40:ASN:H	9:I:40:ASN:ND2	1.88	0.72
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.72	0.72
4:D:33:VAL:HG12	4:D:160:ALA:HB2	1.71	0.72
7:G:74:GLY:HA3	7:G:224:HIS:CD2	2.25	0.72
14:2:96:MET:HE3	14:2:127:MET:HA	1.72	0.72
12:Z:10:HIS:O	12:Z:178:HIS:HE1	1.73	0.72
2:B:165:ASN:HD22	2:B:197:SER:HB2	1.54	0.72
7:G:125:TYR:HB3	16:G:323:HOH:O	1.89	0.72
11:Y:45:LEU:HB2	11:Y:103:LEU:HB2	1.71	0.72
3:Q:35:LEU:HB2	3:Q:162:THR:O	1.90	0.72
2:B:228:TYR:HA	2:B:232:ILE:O	1.89	0.71
12:L:125:THR:HB	12:L:139:MET:HE3	1.70	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:73:THR:HG22	1:O:74:GLU:H	1.53	0.71
10:J:116:THR:HG22	10:J:117:PHE:N	2.05	0.71
11:Y:38:MET:CE	11:Y:60:ILE:HG22	2.20	0.71
10:J:12:MET:HE2	10:J:150:CYS:SG	2.30	0.71
2:P:37:ILE:HD12	2:P:190:ALA:HB2	1.72	0.71
10:X:58:THR:HG21	11:Y:121:LEU:O	1.91	0.71
1:A:73:THR:HG22	1:A:74:GLU:H	1.55	0.71
2:B:73:LEU:CD2	2:B:135:ILE:HG13	2.20	0.71
1:A:221:THR:HG22	1:A:223:GLU:N	2.06	0.71
12:L:125:THR:HB	12:L:139:MET:CE	2.20	0.71
10:X:12:MET:HE2	10:X:150:CYS:SG	2.30	0.71
2:P:228:TYR:HA	2:P:232:ILE:O	1.89	0.71
8:V:40:ARG:HH11	8:V:40:ARG:HG3	1.56	0.71
14:2:115:TYR:OH	14:2:118:GLY:HA2	1.91	0.71
2:P:149:ASP:HB2	2:P:150:PRO:HD2	1.72	0.71
10:X:116:THR:HG22	10:X:117:PHE:N	2.05	0.71
1:O:158:GLY:O	2:P:83:ARG:NH2	2.24	0.71
2:P:165:ASN:HD22	2:P:197:SER:HB2	1.56	0.71
3:C:35:LEU:HB2	3:C:162:THR:O	1.90	0.70
8:H:13:VAL:O	8:H:14:LEU:HD23	1.91	0.70
11:K:38:MET:HE1	11:K:60:ILE:CG2	2.21	0.70
11:Y:43:LEU:O	11:Y:104:LEU:HD12	1.91	0.70
6:F:62:LYS:O	6:F:73:SER:HA	1.91	0.70
10:J:20:VAL:HB	10:J:190:ILE:HD11	1.71	0.70
13:M:211:ARG:NH2	9:W:193:ASN:HB3	2.05	0.70
10:J:58:THR:HG21	11:K:121:LEU:O	1.92	0.70
1:O:221:THR:HG22	1:O:223:GLU:N	2.04	0.70
2:P:73:LEU:CD2	2:P:135:ILE:HG13	2.21	0.70
7:U:74:GLY:HA3	7:U:224:HIS:CD2	2.26	0.70
11:K:180:VAL:HG12	11:K:191:LEU:HD12	1.74	0.70
12:L:115:ASP:HB3	12:L:117:GLU:H	1.56	0.70
1:A:200:THR:O	1:A:204:THR:HG23	1.92	0.70
14:N:115:TYR:OH	14:N:118:GLY:HA2	1.92	0.70
6:T:62:LYS:O	6:T:73:SER:HA	1.92	0.70
2:B:39:ALA:C	2:B:41:ASN:H	2.00	0.70
2:P:64:VAL:HG22	2:P:74:VAL:CG1	2.22	0.70
12:Z:83:LEU:HA	12:Z:86:MET:HE3	1.72	0.70
9:I:187:ARG:HB3	9:I:188:PRO:CD	2.22	0.70
11:K:43:LEU:O	11:K:104:LEU:HD12	1.92	0.70
12:L:10:HIS:O	12:L:178:HIS:HE1	1.73	0.70
12:Z:125:THR:HB	12:Z:139:MET:CE	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:61:GLN:HE21	11:K:62:LYS:CE	2.05	0.69
10:X:93:ASN:O	10:X:97:GLU:HG3	1.92	0.69
14:2:49:THR:HG22	14:2:85:PRO:CG	2.20	0.69
9:I:3:ILE:HD11	9:I:127:MET:HB2	1.73	0.69
9:W:187:ARG:HB3	9:W:188:PRO:CD	2.21	0.69
2:B:64:VAL:HG22	2:B:74:VAL:HG12	1.72	0.69
3:C:76:VAL:HG13	3:C:132:VAL:HG13	1.73	0.69
13:1:1:ARG:CG	13:1:2:PHE:H	2.05	0.69
14:N:96:MET:HE3	14:N:127:MET:HA	1.74	0.69
11:Y:38:MET:HE1	11:Y:60:ILE:CG2	2.20	0.69
1:O:171:LYS:HB3	1:O:205:VAL:HG11	1.75	0.69
12:L:83:LEU:HA	12:L:86:MET:HE3	1.75	0.69
2:P:178:ASN:O	2:P:181:LEU:HG	1.93	0.69
10:J:93:ASN:O	10:J:97:GLU:HG3	1.93	0.69
1:A:171:LYS:HB3	1:A:205:VAL:HG11	1.74	0.68
7:G:136:MET:HE3	7:G:163:CYS:SG	2.33	0.68
5:E:24:VAL:O	5:E:28:ILE:HG12	1.94	0.68
10:J:125:ASP:HB2	10:J:129:CYS:H	1.58	0.68
12:L:44:THR:HG21	12:L:100:MET:HE3	1.75	0.68
13:M:1:ARG:CG	13:M:2:PHE:H	2.05	0.68
9:W:3:ILE:HD11	9:W:127:MET:HB2	1.75	0.68
12:Z:115:ASP:HB3	12:Z:117:GLU:H	1.58	0.68
3:C:187:LYS:HZ3	3:C:236:LEU:HD11	1.56	0.68
9:I:143:ARG:NH1	9:I:146:MET:HG2	2.09	0.68
10:J:68:LYS:NZ	10:J:72:ASN:HD21	1.92	0.68
8:H:40:ARG:HH11	8:H:40:ARG:HG3	1.59	0.68
4:R:42:VAL:HA	4:R:210:VAL:HG12	1.76	0.68
12:Z:44:THR:HG21	12:Z:100:MET:HE3	1.75	0.68
1:A:192:GLU:CD	1:A:192:GLU:H	2.01	0.68
2:B:178:ASN:O	2:B:181:LEU:HG	1.92	0.68
3:C:115:CYS:HB3	4:D:81:ARG:HH12	1.59	0.68
3:Q:45:LEU:HG	3:Q:137:ILE:HD13	1.76	0.68
14:N:135:PRO:HG2	16:N:220:HOH:O	1.93	0.68
6:F:159:MET:HG3	6:F:160:SER:N	2.10	0.67
11:K:38:MET:CE	11:K:60:ILE:HG22	2.19	0.67
7:U:167:LYS:HE3	7:U:206:ASP:OD2	1.94	0.67
1:A:231:THR:O	1:A:235:ILE:HG13	1.95	0.67
6:T:159:MET:HG3	6:T:160:SER:N	2.09	0.67
11:K:182:ILE:CD1	11:K:191:LEU:HD11	2.24	0.67
1:O:89:SER:HB2	7:U:117:MET:HE1	1.75	0.67
2:P:171:THR:HA	2:P:174:GLU:HB2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:105:ILE:HG22	16:Q:417:HOH:O	1.93	0.67
8:V:14:LEU:HD21	8:V:101:ALA:CB	2.24	0.67
10:J:114:PRO:O	10:J:115:LYS:HD2	1.94	0.67
1:O:231:THR:O	1:O:235:ILE:HG13	1.94	0.67
7:G:90:ILE:HD13	7:G:118:TYR:CE2	2.30	0.67
4:R:20:GLU:O	4:R:24:GLU:HG2	1.94	0.67
8:V:13:VAL:O	8:V:14:LEU:HD23	1.93	0.67
3:C:45:LEU:HG	3:C:137:ILE:HD13	1.76	0.67
10:J:36:THR:HG23	10:J:38:ASP:OD2	1.95	0.67
11:Y:182:ILE:CD1	11:Y:191:LEU:HD11	2.25	0.67
5:E:84:ASP:OD2	5:E:135:ARG:NH2	2.28	0.67
9:W:143:ARG:NH1	9:W:146:MET:HG2	2.10	0.67
2:B:171:THR:HA	2:B:174:GLU:HB2	1.77	0.66
3:Q:115:CYS:HB3	4:R:81:ARG:HH12	1.60	0.66
11:Y:24:ASN:ND2	11:Y:25:ILE:HG12	2.10	0.66
11:Y:183:ILE:HG12	11:Y:188:ILE:HG13	1.76	0.66
1:A:158:GLY:O	2:B:83:ARG:NH2	2.28	0.66
14:N:9:THR:HG22	16:N:223:HOH:O	1.93	0.66
5:S:24:VAL:O	5:S:28:ILE:HG12	1.96	0.66
10:X:190:ILE:HG22	10:X:195:ILE:CD1	2.25	0.66
14:2:51:LEU:HD13	14:2:112:ILE:CD1	2.24	0.66
9:W:58:LEU:HD23	9:W:86:MET:HE1	1.78	0.66
10:X:36:THR:HG23	10:X:38:ASP:OD2	1.96	0.66
10:X:65:GLN:NE2	11:Y:86:ARG:NH2	2.43	0.66
13:1:120:ALA:HA	16:1:420:HOH:O	1.96	0.66
4:D:42:VAL:HA	4:D:210:VAL:HG12	1.77	0.66
4:D:181:ILE:H	4:D:186:LEU:HD23	1.60	0.66
6:F:13:TRP:H	7:G:22:GLN:NE2	1.91	0.66
12:L:4:LEU:C	12:L:4:LEU:HD12	2.20	0.66
13:M:176:LYS:HD2	9:W:199:LEU:HD22	1.76	0.66
13:1:198:VAL:HG22	13:1:203:ILE:HG12	1.78	0.66
1:O:192:GLU:CD	1:O:192:GLU:H	2.02	0.66
3:Q:155:ASN:OD1	4:R:77:THR:HG21	1.96	0.66
10:X:114:PRO:O	10:X:115:LYS:HD2	1.95	0.66
10:X:125:ASP:HB2	10:X:129:CYS:H	1.59	0.66
3:C:239:LYS:HD3	3:C:239:LYS:C	2.20	0.66
7:G:167:LYS:HE3	7:G:206:ASP:OD2	1.96	0.66
3:Q:187:LYS:HZ3	3:Q:236:LEU:HD11	1.59	0.66
13:M:198:VAL:HG22	13:M:203:ILE:HG12	1.76	0.66
3:Q:154:GLY:O	4:R:81:ARG:NH2	2.29	0.66
6:T:89:ARG:NH1	13:1:77:HIS:HB3	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:125:ASP:HB2	13:1:126:PRO:HD2	1.78	0.66
10:J:190:ILE:HG22	10:J:195:ILE:CD1	2.26	0.66
2:B:149:ASP:HB2	2:B:150:PRO:CD	2.26	0.66
8:H:29:ARG:HD2	14:2:209:TRP:CZ3	2.31	0.66
1:O:130:GLU:HG2	2:P:4:GLY:HA2	1.78	0.66
4:R:31:THR:HB	4:R:46:GLU:CB	2.25	0.66
2:B:64:VAL:HG22	2:B:74:VAL:CG1	2.26	0.65
9:I:121:LYS:HD2	14:2:215:ILE:O	1.95	0.65
3:Q:76:VAL:HG13	3:Q:132:VAL:HG13	1.76	0.65
6:T:120:THR:O	7:U:129:ARG:NH1	2.28	0.65
8:V:147:MET:HE1	8:V:155:PHE:HB2	1.78	0.65
14:2:45:VAL:O	14:2:46:ASN:ND2	2.29	0.65
11:Y:61:GLN:HE21	11:Y:62:LYS:CE	2.09	0.65
9:I:52:THR:O	9:I:56:THR:HB	1.97	0.65
9:I:187:ARG:HB3	9:I:188:PRO:HD3	1.78	0.65
9:I:199:LEU:HD22	13:1:176:LYS:CD	2.26	0.65
1:A:86:ASP:O	1:A:89:SER:HB3	1.96	0.65
8:H:14:LEU:HD21	8:H:101:ALA:CB	2.26	0.65
2:P:187:ILE:O	2:P:191:ILE:HG13	1.97	0.65
5:S:84:ASP:OD2	5:S:135:ARG:NH2	2.29	0.65
6:F:139:ASP:OD1	14:N:81:HIS:CE1	2.50	0.65
4:R:98:VAL:HG12	4:R:99:GLU:N	2.12	0.65
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.77	0.65
1:A:155:ASP:HB3	1:A:157:ALA:H	1.61	0.65
3:C:155:ASN:OD1	4:D:77:THR:HG21	1.96	0.65
6:F:233:LEU:O	6:F:236:LEU:HG	1.96	0.65
1:O:54:LYS:O	1:O:56:VAL:HG23	1.96	0.65
5:S:129:ASP:HB3	5:S:130:PRO:HD2	1.79	0.65
1:A:182:LYS:HD3	1:A:197:THR:HG23	1.79	0.65
8:H:147:MET:HE1	8:H:155:PHE:HB2	1.79	0.65
1:O:211:LYS:HB3	1:O:212:PRO:HD2	1.79	0.65
3:Q:239:LYS:HD3	3:Q:239:LYS:C	2.22	0.65
9:W:52:THR:O	9:W:56:THR:HB	1.97	0.65
13:1:8:ASN:HD22	13:1:58:HIS:N	1.93	0.65
1:A:155:ASP:OD2	1:A:159:TYR:HB2	1.96	0.65
2:B:187:ILE:O	2:B:191:ILE:HG13	1.97	0.65
4:D:181:ILE:CB	4:D:187:THR:HA	2.27	0.65
1:O:179:LEU:O	1:O:183:VAL:HG23	1.97	0.65
4:R:181:ILE:H	4:R:186:LEU:HD23	1.62	0.65
10:X:68:LYS:NZ	10:X:72:ASN:HD21	1.94	0.65
12:L:6:PHE:CB	12:L:125:THR:HG22	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:155:ASP:HB3	1:O:157:ALA:H	1.62	0.64
2:P:149:ASP:HB2	2:P:150:PRO:CD	2.27	0.64
11:K:60:ILE:HG21	11:K:84:THR:HG22	1.79	0.64
7:U:185:THR:O	7:U:189:ILE:HG12	1.97	0.64
13:1:184:GLU:OE2	13:1:211:ARG:HD2	1.98	0.64
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.79	0.64
3:C:214:ALA:HB2	3:C:227:VAL:HG12	1.80	0.64
4:D:20:GLU:O	4:D:24:GLU:HG2	1.96	0.64
4:D:206:ILE:HG22	4:D:207:GLU:N	2.13	0.64
5:E:42:THR:HG21	5:E:190:THR:HA	1.78	0.64
3:C:174:MET:SD	3:C:196:VAL:HG22	2.37	0.64
14:N:209:TRP:CZ3	8:V:29:ARG:HD2	2.32	0.64
1:O:132:ARG:NH1	7:U:123:THR:O	2.31	0.64
3:Q:140:ASP:O	3:Q:142:HIS:N	2.31	0.64
4:R:181:ILE:CB	4:R:187:THR:HA	2.27	0.64
3:C:167:ASN:C	3:C:169:ALA:H	2.06	0.64
5:E:129:ASP:HB3	5:E:130:PRO:HD2	1.80	0.64
11:K:183:ILE:HG12	11:K:188:ILE:HG13	1.80	0.64
1:O:155:ASP:OD2	1:O:159:TYR:HB2	1.97	0.64
1:A:73:THR:HG22	1:A:75:ASN:H	1.62	0.64
3:C:154:GLY:O	4:D:81:ARG:NH2	2.30	0.64
14:N:51:LEU:HD13	14:N:112:ILE:CD1	2.28	0.64
9:W:22:GLU:HG3	9:W:22:GLU:O	1.98	0.64
4:D:31:THR:HB	4:D:46:GLU:CB	2.28	0.64
4:D:98:VAL:HG12	4:D:99:GLU:N	2.12	0.64
12:L:19:ARG:HE	12:L:29:GLN:NE2	1.94	0.64
5:S:49:ALA:HB2	5:S:217:LEU:CD2	2.28	0.64
10:J:65:GLN:NE2	11:K:86:ARG:NH2	2.45	0.64
11:K:24:ASN:ND2	11:K:25:ILE:HG12	2.12	0.64
7:U:90:ILE:HD13	7:U:118:TYR:CE2	2.33	0.64
9:W:206:LYS:HA	10:X:165:GLU:HG3	1.80	0.64
3:Q:167:ASN:C	3:Q:169:ALA:H	2.06	0.64
13:1:12:ILE:HD13	13:1:53:GLY:C	2.23	0.64
2:B:157:TRP:CE3	2:B:160:THR:HB	2.33	0.63
3:C:139:TRP:HA	3:C:144:GLY:O	1.98	0.63
8:H:30:VAL:O	8:H:30:VAL:CG1	2.47	0.63
10:J:68:LYS:HZ2	10:J:72:ASN:HD21	1.45	0.63
3:Q:174:MET:SD	3:Q:196:VAL:HG22	2.38	0.63
5:E:123:PHE:CE2	5:E:136:PRO:HG3	2.33	0.63
6:F:188:VAL:HG11	6:F:232:PHE:CD2	2.33	0.63
9:I:206:LYS:HA	10:J:165:GLU:HG3	1.78	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:125:ASP:HB2	13:M:126:PRO:HD2	1.80	0.63
13:M:211:ARG:HH21	9:W:193:ASN:HB3	1.63	0.63
3:Q:214:ALA:HB2	3:Q:227:VAL:HG12	1.78	0.63
9:W:59:ILE:HG13	9:W:83:LEU:CD2	2.28	0.63
3:Q:218:ARG:NH2	3:Q:221:GLY:O	2.32	0.63
5:S:42:THR:HG21	5:S:190:THR:HA	1.79	0.63
9:W:153:ASN:HD22	9:W:154:LEU:N	1.97	0.63
9:I:153:ASN:HD22	9:I:154:LEU:N	1.95	0.63
5:E:49:ALA:HB2	5:E:217:LEU:CD2	2.28	0.63
6:F:41:LYS:HG3	6:F:42:THR:HG23	1.81	0.63
9:I:152:LYS:HE3	9:I:186:LEU:CD1	2.29	0.63
14:N:45:VAL:O	14:N:46:ASN:ND2	2.32	0.63
1:O:182:LYS:HD3	1:O:197:THR:HG23	1.79	0.63
1:A:79:VAL:HG12	1:A:139:ILE:HB	1.81	0.63
1:A:201:CYS:O	1:A:205:VAL:HG23	1.98	0.63
4:D:39:ASP:HB2	4:D:184:ASP:OD1	1.99	0.63
9:I:58:LEU:HD23	9:I:86:MET:HE1	1.80	0.63
3:Q:209:GLU:C	3:Q:211:VAL:H	2.07	0.63
11:Y:60:ILE:HG21	11:Y:84:THR:HG22	1.80	0.63
1:A:179:LEU:O	1:A:183:VAL:HG23	1.99	0.63
2:B:36:GLY:O	2:B:159:ALA:HA	1.99	0.63
3:C:209:GLU:C	3:C:211:VAL:H	2.07	0.63
9:I:22:GLU:HG3	9:I:22:GLU:O	1.98	0.63
13:M:146:GLN:HB2	13:M:147:PRO:HD3	1.80	0.63
4:R:39:ASP:HB2	4:R:184:ASP:OD1	1.99	0.63
9:I:59:ILE:HG13	9:I:83:LEU:CD2	2.29	0.63
12:L:8:PHE:HD2	12:L:8:PHE:N	1.97	0.63
9:I:112:SER:OG	9:I:120:ASP:HB2	1.99	0.62
9:I:187:ARG:CG	9:I:188:PRO:HD3	2.29	0.62
12:Z:4:LEU:C	12:Z:4:LEU:HD12	2.24	0.62
4:D:91:CYS:HA	4:D:102:VAL:HG21	1.82	0.62
2:P:157:TRP:CE3	2:P:160:THR:HB	2.34	0.62
3:Q:139:TRP:HA	3:Q:144:GLY:O	1.99	0.62
8:V:95:MET:HG2	8:V:116:MET:HE1	1.81	0.62
6:F:120:THR:O	7:G:129:ARG:NH1	2.32	0.62
14:N:49:THR:HG22	14:N:85:PRO:CG	2.21	0.62
1:O:79:VAL:HG12	1:O:139:ILE:HB	1.81	0.62
5:S:191:LEU:O	5:S:195:ILE:HG13	1.99	0.62
6:T:41:LYS:HG3	6:T:42:THR:HG23	1.80	0.62
9:W:198:ARG:NH2	9:W:201:ARG:HA	2.14	0.62
1:A:89:SER:HB2	7:G:117:MET:HE1	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:185:THR:O	7:G:189:ILE:HG12	1.99	0.62
1:O:123:GLN:O	1:O:126:THR:HB	1.99	0.62
9:W:187:ARG:CG	9:W:188:PRO:HD3	2.30	0.62
8:H:95:MET:HG2	8:H:116:MET:HE1	1.80	0.62
1:O:73:THR:HG22	1:O:75:ASN:H	1.65	0.62
3:C:143:TYR:HB2	3:C:146:GLN:NE2	2.15	0.62
13:M:136:LYS:HA	13:M:146:GLN:HE22	1.64	0.62
11:Y:43:LEU:HD12	11:Y:183:ILE:HD11	1.81	0.62
1:O:86:ASP:O	1:O:89:SER:HB3	2.00	0.62
3:Q:8:ARG:HB3	3:Q:11:ILE:CD1	2.29	0.62
10:X:82:ILE:HD11	10:X:86:THR:HG22	1.82	0.62
2:B:229:LEU:C	2:B:231:ALA:H	2.08	0.62
7:U:220:THR:O	7:U:221:ASN:HB2	1.99	0.62
3:C:8:ARG:HB3	3:C:11:ILE:CD1	2.27	0.62
9:I:212:LEU:CD1	10:J:201:LYS:HA	2.30	0.62
4:R:206:ILE:HG22	4:R:207:GLU:N	2.13	0.62
14:N:74:GLU:CD	14:N:82:SER:HA	2.25	0.61
11:K:151:ILE:HG13	11:K:155:ARG:HB3	1.80	0.61
13:M:8:ASN:HD22	13:M:58:HIS:N	1.94	0.61
10:J:14:MET:HB2	10:J:167:ILE:HD12	1.82	0.61
12:Z:6:PHE:CB	12:Z:125:THR:HG22	2.30	0.61
1:O:201:CYS:O	1:O:205:VAL:HG23	2.01	0.61
2:P:36:GLY:O	2:P:159:ALA:HA	2.01	0.61
4:R:4:ASP:O	4:R:122:ASN:HB3	1.99	0.61
11:Y:37:LYS:HD2	11:Y:37:LYS:N	2.16	0.61
12:Z:19:ARG:HE	12:Z:29:GLN:NE2	1.98	0.61
2:B:39:ALA:O	2:B:41:ASN:N	2.34	0.61
2:P:229:LEU:C	2:P:231:ALA:H	2.08	0.61
6:T:71:GLY:HA3	6:T:221:PHE:CZ	2.36	0.61
1:A:206:LEU:O	1:A:208:ILE:HG13	2.00	0.61
6:F:73:SER:OG	6:F:133:LEU:HB2	2.00	0.61
9:W:212:LEU:CD1	10:X:201:LYS:HA	2.30	0.61
6:T:188:VAL:HG11	6:T:232:PHE:CD2	2.36	0.61
8:V:30:VAL:CG1	8:V:30:VAL:O	2.47	0.61
1:A:54:LYS:O	1:A:56:VAL:HG23	2.01	0.61
3:C:218:ARG:NH2	3:C:221:GLY:O	2.33	0.61
9:I:193:ASN:HB3	13:1:211:ARG:NH2	2.15	0.61
9:I:198:ARG:NH2	9:I:201:ARG:HA	2.15	0.61
13:M:184:GLU:OE2	13:M:211:ARG:HD2	1.99	0.61
2:P:135:ILE:H	2:P:135:ILE:HD12	1.66	0.61
13:1:137:ALA:H	13:1:146:GLN:NE2	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:201:MET:O	3:Q:203:VAL:N	2.34	0.61
13:1:146:GLN:HB2	13:1:147:PRO:HD3	1.81	0.61
2:B:72:GLY:HA3	2:B:217:PHE:CE1	2.36	0.61
4:D:131:ALA:O	4:D:146:GLN:HA	2.01	0.61
8:V:127:ILE:HD11	8:V:136:TYR:CE2	2.35	0.61
13:1:136:LYS:HA	13:1:146:GLN:HE22	1.64	0.61
5:E:166:ASP:HB3	5:E:185:TYR:CZ	2.36	0.60
11:K:37:LYS:HD2	11:K:37:LYS:N	2.15	0.60
11:K:85:ARG:HG3	11:K:124:LEU:HB2	1.82	0.60
1:A:136:CYS:O	1:A:156:PRO:HG3	2.01	0.60
8:H:89:ARG:HD3	8:H:90:TYR:CE1	2.36	0.60
2:P:135:ILE:HD12	2:P:135:ILE:N	2.16	0.60
11:Y:37:LYS:HD2	11:Y:37:LYS:H	1.66	0.60
13:M:12:ILE:HD13	13:M:53:GLY:C	2.26	0.60
1:O:172:GLN:O	1:O:176:THR:HG23	2.01	0.60
5:S:166:ASP:HB3	5:S:185:TYR:CZ	2.36	0.60
4:D:4:ASP:O	4:D:122:ASN:HB3	2.01	0.60
8:H:173:VAL:HG21	8:H:190:LEU:HD23	1.82	0.60
4:R:33:VAL:HG11	4:R:168:VAL:HG11	1.84	0.60
4:D:41:VAL:HG11	4:D:134:VAL:HG13	1.83	0.60
6:F:150:SER:O	6:F:152:ASN:N	2.33	0.60
4:R:131:ALA:O	4:R:146:GLN:HA	2.01	0.60
7:U:66:LEU:HD23	7:U:76:ALA:HA	1.84	0.60
1:A:172:GLN:O	1:A:176:THR:HG23	2.01	0.60
5:E:191:LEU:O	5:E:195:ILE:HG13	2.00	0.60
6:T:42:THR:OG1	6:T:43:HIS:HD2	1.85	0.60
6:T:169:ARG:HG2	7:U:57:LEU:CD1	2.31	0.60
3:C:138:GLY:HA2	3:C:216:LEU:HD13	1.83	0.60
1:A:155:ASP:C	1:A:157:ALA:H	2.10	0.60
2:B:34:SER:O	2:B:161:ALA:HA	2.02	0.60
5:E:203:LYS:HA	5:E:206:MET:HE3	1.83	0.60
13:M:137:ALA:H	13:M:146:GLN:NE2	2.00	0.60
1:O:141:ILE:CG2	1:O:151:VAL:HG22	2.31	0.60
9:W:213:THR:O	10:X:198:ARG:HA	2.02	0.60
11:Y:107:TYR:CE2	11:Y:185:LYS:HA	2.36	0.60
6:F:77:LEU:HA	16:F:264:HOH:O	2.00	0.60
4:R:91:CYS:HA	4:R:102:VAL:HG21	1.83	0.60
6:T:88:MET:HE3	6:T:112:ILE:HD11	1.82	0.60
10:J:82:ILE:HD11	10:J:86:THR:HG22	1.82	0.60
12:Z:8:PHE:HD2	12:Z:8:PHE:N	1.98	0.60
2:B:53:SER:C	2:B:55:LEU:H	2.10	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:33:VAL:HG11	4:D:168:VAL:HG11	1.84	0.59
3:Q:49:ARG:HD2	3:Q:212:GLU:OE1	2.02	0.59
1:A:142:GLY:HA2	1:A:220:VAL:HG21	1.83	0.59
8:H:127:ILE:HD11	8:H:136:TYR:CE2	2.38	0.59
5:S:27:ASP:OD2	5:S:28:ILE:N	2.36	0.59
6:T:73:SER:OG	6:T:133:LEU:HB2	2.01	0.59
6:T:206:THR:HG22	6:T:208:LYS:H	1.67	0.59
10:X:14:MET:HB2	10:X:167:ILE:HD12	1.84	0.59
1:A:123:GLN:O	1:A:126:THR:HB	2.03	0.59
1:A:141:ILE:CG2	1:A:151:VAL:HG22	2.31	0.59
3:C:201:MET:O	3:C:203:VAL:N	2.34	0.59
5:E:146:VAL:HG23	5:E:220:VAL:CG1	2.31	0.59
11:K:37:LYS:HD2	11:K:37:LYS:H	1.67	0.59
3:Q:143:TYR:HB2	3:Q:146:GLN:NE2	2.18	0.59
5:S:123:PHE:CE2	5:S:136:PRO:HG3	2.36	0.59
9:W:187:ARG:HG3	9:W:188:PRO:HD3	1.84	0.59
9:I:152:LYS:HE3	9:I:186:LEU:HD11	1.83	0.59
6:T:206:THR:N	6:T:209:ASN:HD21	1.87	0.59
8:V:89:ARG:HD3	8:V:90:TYR:CE1	2.36	0.59
12:Z:8:PHE:N	12:Z:8:PHE:CD2	2.69	0.59
14:2:115:TYR:HE2	14:2:194:GLU:HG2	1.67	0.59
3:C:115:CYS:HB3	4:D:81:ARG:NH1	2.17	0.59
3:C:143:TYR:HB2	3:C:146:GLN:CD	2.28	0.59
9:I:187:ARG:O	9:I:188:PRO:C	2.45	0.59
4:R:11:SER:HB3	4:R:12:PRO:HD2	1.84	0.59
4:R:58:THR:O	4:R:59:VAL:HB	2.02	0.59
7:U:151:ILE:N	7:U:151:ILE:HD12	2.17	0.59
2:B:39:ALA:C	2:B:41:ASN:N	2.58	0.59
9:I:187:ARG:HG3	9:I:188:PRO:HD3	1.83	0.59
12:L:8:PHE:N	12:L:8:PHE:CD2	2.69	0.59
5:E:27:ASP:OD2	5:E:28:ILE:N	2.36	0.59
5:E:146:VAL:CG2	5:E:220:VAL:HG12	2.31	0.59
7:G:215:TRP:HB2	7:G:225:GLU:O	2.03	0.59
2:P:185:ASP:O	2:P:189:THR:HG22	2.03	0.59
5:S:108:THR:O	5:S:112:VAL:HG23	2.03	0.59
6:T:150:SER:O	6:T:152:ASN:N	2.36	0.59
10:X:37:THR:CG2	10:X:204:MET:HE1	2.31	0.59
12:Z:138:VAL:CG2	12:Z:159:ALA:HA	2.32	0.59
2:B:195:LYS:C	2:B:197:SER:H	2.11	0.59
3:C:49:ARG:HD2	3:C:212:GLU:OE1	2.03	0.59
3:C:140:ASP:O	3:C:142:HIS:N	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:196:ARG:CD	6:F:239:ARG:HD3	2.31	0.59
10:J:151:GLU:HB2	13:1:181:SER:HB3	1.85	0.59
12:L:138:VAL:CG2	12:L:159:ALA:HA	2.33	0.59
14:N:115:TYR:HE2	14:N:194:GLU:HG2	1.68	0.59
10:X:113:ASP:HB3	10:X:116:THR:HB	1.85	0.59
2:B:227:ASP:HB3	2:B:233:ALA:HB1	1.85	0.59
7:G:184:MET:CB	7:G:189:ILE:HD11	2.32	0.59
3:Q:138:GLY:HA2	3:Q:216:LEU:HD13	1.85	0.59
7:U:184:MET:CB	7:U:189:ILE:HD11	2.32	0.59
2:P:227:ASP:HB3	2:P:233:ALA:HB1	1.84	0.59
3:Q:174:MET:HE1	3:Q:199:LYS:HG2	1.83	0.59
14:2:174:ARG:HE	14:2:205:THR:HG22	1.67	0.59
1:A:132:ARG:NH1	7:G:123:THR:O	2.36	0.58
2:B:185:ASP:O	2:B:189:THR:HG22	2.03	0.58
3:C:174:MET:HE1	3:C:199:LYS:HG2	1.85	0.58
6:F:71:GLY:HA3	6:F:221:PHE:CZ	2.38	0.58
10:J:136:PHE:CE2	10:J:150:CYS:HB3	2.38	0.58
14:N:215:ILE:O	9:W:121:LYS:HD2	2.03	0.58
2:P:43:VAL:HG12	2:P:44:VAL:N	2.18	0.58
8:V:162:LEU:O	8:V:165:GLU:HB3	2.03	0.58
1:A:145:GLU:HG2	1:A:146:GLU:N	2.17	0.58
7:G:151:ILE:HD12	7:G:151:ILE:N	2.19	0.58
1:O:206:LEU:O	1:O:208:ILE:HG13	2.02	0.58
6:F:196:ARG:NH2	6:F:236:LEU:HD13	2.16	0.58
11:K:23:SER:O	11:K:24:ASN:HB3	2.03	0.58
1:O:155:ASP:C	1:O:157:ALA:H	2.10	0.58
8:V:173:VAL:HG21	8:V:190:LEU:HD23	1.86	0.58
9:W:187:ARG:CB	9:W:188:PRO:HD3	2.33	0.58
12:Z:25:TYR:OH	13:1:146:GLN:HG3	2.03	0.58
3:C:140:ASP:OD1	3:C:142:HIS:HB2	2.03	0.58
8:H:30:VAL:HG21	14:2:211:ILE:HG13	1.85	0.58
13:M:164:VAL:HG23	13:M:165:PRO:HD2	1.84	0.58
2:P:44:VAL:HG21	2:P:187:ILE:HG12	1.86	0.58
9:I:187:ARG:CB	9:I:188:PRO:HD3	2.33	0.58
10:J:113:ASP:HB3	10:J:116:THR:HB	1.85	0.58
2:P:72:GLY:HA3	2:P:217:PHE:CE1	2.38	0.58
12:Z:148:GLU:HB2	12:Z:151:GLN:HG3	1.85	0.58
1:A:84:THR:HB	7:G:156:VAL:HG22	1.85	0.58
7:G:229:LYS:O	7:G:233:GLU:HG3	2.02	0.58
10:J:116:THR:HG22	10:J:117:PHE:H	1.67	0.58
14:2:192:VAL:CG1	14:2:197:VAL:HG22	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HB3	1:A:205:VAL:CG1	2.34	0.58
10:J:37:THR:CG2	10:J:204:MET:HE1	2.31	0.58
11:K:107:TYR:CE2	11:K:185:LYS:HA	2.37	0.58
14:N:71:VAL:HG21	16:N:221:HOH:O	2.03	0.58
1:O:144:ASP:HB3	1:O:147:GLN:HB2	1.86	0.58
2:P:195:LYS:C	2:P:197:SER:H	2.11	0.58
3:Q:175:LEU:CD2	3:Q:196:VAL:HG21	2.34	0.58
13:1:155:PHE:HA	13:1:158:MET:HE2	1.86	0.58
1:A:73:THR:CG2	1:A:74:GLU:N	2.67	0.58
2:B:165:ASN:ND2	2:B:197:SER:HB2	2.18	0.58
9:I:135:MET:HE3	14:2:179:ARG:CZ	2.33	0.58
12:L:148:GLU:HB2	12:L:151:GLN:HG3	1.86	0.58
14:N:142:GLY:HA2	14:N:176:LEU:HD21	1.86	0.58
9:I:153:ASN:ND2	9:I:154:LEU:N	2.52	0.58
1:O:145:GLU:HG2	1:O:146:GLU:N	2.18	0.58
6:T:98:VAL:HA	14:2:94:ARG:HG2	1.86	0.58
6:F:88:MET:HE3	6:F:112:ILE:HD11	1.85	0.58
14:2:99:ARG:HD2	14:2:104:ASN:O	2.03	0.58
14:2:142:GLY:HA2	14:2:176:LEU:HD21	1.85	0.58
10:J:172:LEU:HD22	10:J:202:ALA:HB2	1.85	0.57
1:O:142:GLY:HA2	1:O:220:VAL:HG21	1.86	0.57
4:R:196:LEU:C	4:R:198:VAL:H	2.12	0.57
8:V:173:VAL:HG23	8:V:190:LEU:HA	1.85	0.57
14:2:74:GLU:CD	14:2:82:SER:HA	2.28	0.57
4:D:80:ALA:HA	4:D:129:ILE:HD13	1.86	0.57
6:F:42:THR:OG1	6:F:43:HIS:HD2	1.86	0.57
14:N:174:ARG:HE	14:N:205:THR:HG22	1.67	0.57
1:O:73:THR:CG2	1:O:74:GLU:H	2.17	0.57
1:O:73:THR:CG2	1:O:74:GLU:N	2.67	0.57
5:S:49:ALA:HB2	5:S:217:LEU:HD22	1.86	0.57
1:A:138:MET:O	1:A:153:LYS:HA	2.04	0.57
5:E:31:ILE:HD11	5:E:158:PRO:HD3	1.87	0.57
5:E:217:LEU:HD13	5:E:218:ALA:N	2.18	0.57
6:F:171:TYR:OH	6:F:193:ARG:HD2	2.04	0.57
6:F:206:THR:HG22	6:F:208:LYS:H	1.69	0.57
3:Q:143:TYR:HB2	3:Q:146:GLN:CD	2.29	0.57
6:T:87:PHE:CE1	6:T:115:LYS:HD2	2.39	0.57
9:W:152:LYS:HE3	9:W:186:LEU:CD1	2.35	0.57
13:1:17:GLY:HA3	13:1:20:PHE:CE2	2.38	0.57
1:A:73:THR:CG2	1:A:74:GLU:H	2.17	0.57
2:B:135:ILE:HD12	2:B:135:ILE:N	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:ILE:HB	3:C:82:ASP:HB2	1.85	0.57
3:C:175:LEU:CD2	3:C:196:VAL:HG21	2.34	0.57
8:H:173:VAL:HG23	8:H:190:LEU:HA	1.85	0.57
9:I:213:THR:O	10:J:198:ARG:HA	2.03	0.57
13:M:17:GLY:HA3	13:M:20:PHE:CE2	2.40	0.57
1:O:171:LYS:HB3	1:O:205:VAL:CG1	2.33	0.57
5:S:47:CYS:O	5:S:48:LEU:HD23	2.04	0.57
6:T:171:TYR:OH	6:T:193:ARG:HD2	2.05	0.57
10:X:172:LEU:HD22	10:X:202:ALA:HB2	1.86	0.57
11:K:49:GLU:OE1	12:L:91:LYS:HE3	2.04	0.57
13:M:139:GLY:O	13:M:142:SER:HB2	2.05	0.57
13:1:164:VAL:HG23	13:1:165:PRO:HD2	1.85	0.57
14:2:9:THR:O	14:2:41:ARG:NH2	2.38	0.57
3:C:95:GLN:NE2	3:C:98:LEU:HD23	2.17	0.57
4:D:196:LEU:C	4:D:198:VAL:H	2.11	0.57
2:P:227:ASP:HB3	2:P:233:ALA:CB	2.35	0.57
3:Q:115:CYS:HB3	4:R:81:ARG:NH1	2.18	0.57
6:T:33:SER:OG	6:T:62:LYS:HE3	2.04	0.57
7:U:215:TRP:HB2	7:U:225:GLU:O	2.03	0.57
7:U:229:LYS:O	7:U:233:GLU:HG3	2.04	0.57
10:X:113:ASP:OD1	10:X:114:PRO:HD2	2.04	0.57
13:1:42:LYS:O	13:1:53:GLY:HA2	2.05	0.57
6:F:24:TYR:O	6:F:27:GLU:HB2	2.05	0.57
10:J:190:ILE:HG22	10:J:195:ILE:HD12	1.86	0.57
2:P:34:SER:O	2:P:161:ALA:HA	2.04	0.57
4:R:66:ASP:CA	11:Y:69:MET:HE2	2.34	0.57
9:W:112:SER:OG	9:W:120:ASP:HB2	2.04	0.57
9:W:137:VAL:HG21	9:W:158:ALA:HA	1.87	0.57
2:B:46:ALA:CB	2:B:209:VAL:HG12	2.35	0.57
2:B:213:ASN:ND2	2:B:215:ALA:HB3	2.18	0.57
5:E:47:CYS:O	5:E:48:LEU:HD23	2.05	0.57
7:G:220:THR:O	7:G:221:ASN:HB2	2.05	0.57
12:L:25:TYR:OH	13:M:146:GLN:HG3	2.04	0.57
4:R:202:GLY:C	4:R:204:LYS:H	2.12	0.57
10:X:116:THR:HG22	10:X:117:PHE:H	1.68	0.57
2:B:227:ASP:HB3	2:B:233:ALA:CB	2.35	0.57
3:C:8:ARG:CB	3:C:11:ILE:HD12	2.32	0.57
4:D:202:GLY:C	4:D:204:LYS:H	2.12	0.57
1:O:138:MET:O	1:O:153:LYS:HA	2.04	0.57
3:Q:79:ILE:HB	3:Q:82:ASP:HB2	1.86	0.57
3:Q:234:GLU:HA	3:Q:237:ILE:HB	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:41:VAL:HG11	4:R:134:VAL:HG13	1.86	0.57
9:W:78:THR:O	9:W:82:MET:HG3	2.04	0.57
9:W:106:THR:HG22	9:W:106:THR:O	2.05	0.57
11:Y:85:ARG:HG3	11:Y:124:LEU:HB2	1.87	0.57
13:1:139:GLY:O	13:1:142:SER:HB2	2.04	0.57
8:H:162:LEU:O	8:H:165:GLU:HB3	2.04	0.56
14:N:166:ARG:HH12	14:N:200:GLU:CD	2.13	0.56
4:D:58:THR:O	4:D:59:VAL:HB	2.05	0.56
5:E:108:THR:O	5:E:112:VAL:HG23	2.05	0.56
9:I:64:GLU:HB3	16:I:308:HOH:O	2.05	0.56
9:I:182:LYS:HD2	9:I:184:ASP:OD1	2.04	0.56
2:P:46:ALA:CB	2:P:209:VAL:HG12	2.35	0.56
8:V:30:VAL:O	8:V:30:VAL:HG12	2.04	0.56
11:Y:151:ILE:HG13	11:Y:155:ARG:HB3	1.83	0.56
6:F:206:THR:N	6:F:209:ASN:HD21	1.87	0.56
8:H:30:VAL:O	8:H:30:VAL:HG12	2.04	0.56
9:I:78:THR:O	9:I:82:MET:HG3	2.05	0.56
9:I:137:VAL:HG21	9:I:158:ALA:HA	1.87	0.56
5:S:217:LEU:HD13	5:S:218:ALA:N	2.20	0.56
8:V:84:LYS:HG2	8:V:118:GLY:O	2.05	0.56
11:Y:151:ILE:HD11	11:Y:156:ALA:N	2.20	0.56
2:B:8:SER:HB3	2:B:122:GLN:O	2.05	0.56
4:D:11:SER:HB3	4:D:12:PRO:HD2	1.86	0.56
5:E:14:THR:HG23	6:F:21:GLN:NE2	2.20	0.56
6:F:10:VAL:HG11	6:F:127:PRO:HD3	1.88	0.56
3:C:140:ASP:C	3:C:142:HIS:H	2.13	0.56
3:C:187:LYS:HZ1	3:C:236:LEU:HD11	1.70	0.56
14:N:192:VAL:CG1	14:N:197:VAL:HG22	2.35	0.56
3:Q:140:ASP:OD1	3:Q:142:HIS:HB2	2.04	0.56
4:R:51:ALA:O	4:R:53:LEU:N	2.32	0.56
4:R:232:ILE:HA	4:R:235:GLU:CB	2.35	0.56
1:A:144:ASP:HB3	1:A:147:GLN:HB2	1.86	0.56
3:C:234:GLU:HA	3:C:237:ILE:HB	1.88	0.56
8:H:84:LYS:HG2	8:H:118:GLY:O	2.05	0.56
13:M:155:PHE:HA	13:M:158:MET:HE2	1.86	0.56
3:Q:174:MET:HE1	3:Q:199:LYS:CG	2.35	0.56
5:S:203:LYS:HA	5:S:206:MET:HE3	1.86	0.56
8:V:135:ILE:O	8:V:139:VAL:HB	2.05	0.56
9:W:216:ILE:CD1	10:X:196:THR:HG23	2.36	0.56
14:2:166:ARG:HH12	14:2:200:GLU:CD	2.14	0.56
4:D:232:ILE:HA	4:D:235:GLU:CB	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:153:ASN:ND2	9:W:154:LEU:N	2.53	0.56
6:F:143:HIS:HB3	6:F:145:PHE:CE1	2.41	0.56
3:Q:149:GLN:CD	3:Q:164:ILE:HD11	2.30	0.56
1:A:67:THR:HG22	1:A:69:LEU:N	2.11	0.56
3:C:149:GLN:CD	3:C:164:ILE:HD11	2.30	0.56
3:C:174:MET:HE1	3:C:199:LYS:CG	2.36	0.56
10:J:113:ASP:OD1	10:J:114:PRO:HD2	2.06	0.56
11:K:43:LEU:HD12	11:K:183:ILE:HD11	1.86	0.56
1:O:65:THR:HG21	7:U:159:GLY:HA3	1.87	0.56
5:S:31:ILE:HD11	5:S:158:PRO:HD3	1.88	0.56
10:X:136:PHE:CE2	10:X:150:CYS:HB3	2.41	0.56
2:B:45:LEU:HD13	2:B:74:VAL:HG22	1.87	0.56
1:O:29:PHE:CZ	1:O:156:PRO:HD2	2.40	0.56
3:Q:8:ARG:CB	3:Q:11:ILE:HD12	2.34	0.56
3:C:136:TYR:HB2	3:C:148:TYR:HB2	1.88	0.55
4:D:51:ALA:O	4:D:53:LEU:N	2.34	0.55
4:D:57:ARG:CG	4:D:60:ARG:HH21	2.20	0.55
5:E:49:ALA:HB2	5:E:217:LEU:HD22	1.87	0.55
2:P:45:LEU:HD13	2:P:74:VAL:HG22	1.87	0.55
3:Q:95:GLN:NE2	3:Q:98:LEU:HD23	2.19	0.55
10:X:68:LYS:HZ2	10:X:72:ASN:HD21	1.54	0.55
11:Y:35:MET:HG2	11:Y:45:LEU:HD22	1.89	0.55
12:Z:46:ALA:HB3	12:Z:98:GLY:O	2.06	0.55
6:F:87:PHE:CE1	6:F:115:LYS:HD2	2.41	0.55
8:H:135:ILE:O	8:H:139:VAL:HB	2.07	0.55
13:M:42:LYS:O	13:M:53:GLY:HA2	2.06	0.55
14:N:9:THR:OG1	14:N:10:SER:N	2.32	0.55
4:R:80:ALA:HA	4:R:129:ILE:HD13	1.87	0.55
5:S:220:VAL:HG22	5:S:226:PHE:HA	1.88	0.55
7:U:42:LYS:HG2	7:U:184:MET:O	2.07	0.55
10:X:26:ARG:HB3	10:X:26:ARG:NH1	2.17	0.55
13:1:148:LEU:HD23	13:1:178:VAL:HG13	1.89	0.55
2:B:173:LEU:C	2:B:175:LYS:H	2.14	0.55
5:E:220:VAL:HG22	5:E:226:PHE:HA	1.88	0.55
9:I:193:ASN:HB3	13:1:211:ARG:HH21	1.71	0.55
1:O:50:ILE:CG2	1:O:79:VAL:HB	2.37	0.55
2:P:165:ASN:ND2	2:P:197:SER:HB2	2.19	0.55
3:Q:140:ASP:C	3:Q:142:HIS:H	2.13	0.55
9:W:187:ARG:O	9:W:188:PRO:C	2.43	0.55
13:1:148:LEU:HD23	13:1:178:VAL:CG1	2.36	0.55
6:F:159:MET:HE3	6:F:160:SER:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:40:TYR:HB3	12:L:73:ARG:CZ	2.37	0.55
2:P:92:LEU:HD13	2:P:112:ARG:HB3	1.88	0.55
5:S:146:VAL:CG2	5:S:220:VAL:HG12	2.31	0.55
1:A:50:ILE:CG2	1:A:79:VAL:HB	2.37	0.55
5:E:133:MET:HE2	5:E:133:MET:HA	1.89	0.55
11:K:151:ILE:HD11	11:K:156:ALA:N	2.21	0.55
1:O:79:VAL:CG1	1:O:139:ILE:HB	2.37	0.55
2:P:74:VAL:HG23	2:P:134:LEU:HB2	1.89	0.55
4:R:137:ASP:O	4:R:138:PHE:C	2.48	0.55
10:X:190:ILE:HG22	10:X:195:ILE:HD12	1.86	0.55
2:B:229:LEU:O	2:B:231:ALA:N	2.37	0.55
3:C:79:ILE:HD12	3:C:79:ILE:N	2.22	0.55
3:C:90:LEU:HG	3:C:114:LEU:HD22	1.88	0.55
9:I:212:LEU:HB2	10:J:199:THR:O	2.06	0.55
11:K:35:MET:HG2	11:K:45:LEU:HD22	1.88	0.55
3:Q:90:LEU:HG	3:Q:114:LEU:HD22	1.88	0.55
5:S:133:MET:HE2	5:S:133:MET:HA	1.89	0.55
6:T:237:GLU:C	6:T:239:ARG:N	2.64	0.55
9:W:187:ARG:CB	9:W:188:PRO:CD	2.85	0.55
9:W:215:LYS:HD3	9:W:216:ILE:N	2.22	0.55
14:2:9:THR:OG1	14:2:10:SER:N	2.33	0.55
6:F:33:SER:OG	6:F:62:LYS:HE3	2.07	0.55
9:I:143:ARG:O	9:I:146:MET:HG3	2.07	0.55
11:K:61:GLN:HE21	11:K:62:LYS:HE2	1.72	0.55
12:L:46:ALA:HB3	12:L:98:GLY:O	2.07	0.55
2:P:191:ILE:HG22	2:P:202:MET:CE	2.37	0.55
10:X:116:THR:CG2	10:X:117:PHE:N	2.70	0.55
5:E:173:ALA:CB	5:E:205:VAL:HB	2.37	0.55
13:M:148:LEU:HD23	13:M:178:VAL:CG1	2.37	0.55
3:Q:53:HIS:HE1	3:Q:55:LEU:HD12	1.72	0.55
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.88	0.55
1:A:79:VAL:CG1	1:A:139:ILE:HB	2.36	0.55
3:C:76:VAL:HG12	3:C:77:ALA:N	2.22	0.55
3:C:138:GLY:HA2	3:C:216:LEU:CD1	2.37	0.55
4:D:62:ILE:N	4:D:62:ILE:HD12	2.21	0.55
4:D:137:ASP:O	4:D:138:PHE:C	2.48	0.55
14:N:37:ARG:HH21	8:V:166:ARG:HE	1.53	0.55
2:P:229:LEU:O	2:P:231:ALA:N	2.38	0.55
3:Q:79:ILE:HD12	3:Q:79:ILE:N	2.22	0.55
5:S:146:VAL:HG23	5:S:220:VAL:CG1	2.31	0.55
6:T:107:ARG:NH2	14:2:74:GLU:HG3	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:154:GLN:HE21	8:V:158:ASN:HD21	1.53	0.55
1:A:29:PHE:CZ	1:A:156:PRO:HD2	2.42	0.55
4:D:66:ASP:CG	4:D:67:ASP:H	2.15	0.55
4:D:66:ASP:CA	11:K:69:MET:HE2	2.37	0.55
12:L:19:ARG:HE	12:L:29:GLN:HE21	1.54	0.55
1:O:84:THR:HB	7:U:156:VAL:HG22	1.88	0.55
1:O:136:CYS:O	1:O:156:PRO:HG3	2.07	0.55
11:Y:49:GLU:OE1	12:Z:91:LYS:HE3	2.07	0.55
1:A:65:THR:HG21	7:G:159:GLY:HA3	1.89	0.54
7:G:66:LEU:HD23	7:G:76:ALA:HA	1.88	0.54
8:H:38:HIS:CD2	8:H:74:PRO:HG3	2.41	0.54
2:P:173:LEU:C	2:P:175:LYS:H	2.13	0.54
6:T:209:ASN:HD22	6:T:209:ASN:H	1.56	0.54
1:A:50:ILE:HG21	1:A:79:VAL:HB	1.89	0.54
5:E:186:HIS:HB2	5:E:189:MET:HB3	1.89	0.54
7:G:50:GLU:OE2	7:G:201:HIS:HD2	1.90	0.54
9:I:187:ARG:CB	9:I:188:PRO:CD	2.85	0.54
14:N:126:ASP:HB3	14:N:128:LEU:H	1.72	0.54
3:Q:189:ALA:C	3:Q:191:ALA:N	2.65	0.54
4:R:66:ASP:CG	4:R:67:ASP:H	2.16	0.54
7:U:172:ALA:O	7:U:176:ILE:HG13	2.08	0.54
9:W:152:LYS:HE3	9:W:186:LEU:HD11	1.88	0.54
2:B:44:VAL:HG21	2:B:187:ILE:HG12	1.87	0.54
6:F:164:ARG:HH12	6:F:200:PRO:HG3	1.72	0.54
9:I:215:LYS:HD3	9:I:216:ILE:N	2.23	0.54
9:I:216:ILE:CD1	10:J:196:THR:HG23	2.37	0.54
13:M:148:LEU:HD23	13:M:178:VAL:HG13	1.88	0.54
14:N:71:VAL:O	14:N:75:GLU:HG3	2.07	0.54
3:Q:138:GLY:HA2	3:Q:216:LEU:CD1	2.38	0.54
6:T:143:HIS:HB3	6:T:145:PHE:CE1	2.42	0.54
6:T:164:ARG:HH12	6:T:200:PRO:HG3	1.71	0.54
9:W:143:ARG:O	9:W:146:MET:HG3	2.08	0.54
10:J:22:ILE:HG22	10:J:188:HIS:HB2	1.90	0.54
13:M:14:ALA:HA	13:M:22:ILE:O	2.08	0.54
4:R:57:ARG:CG	4:R:60:ARG:HH21	2.20	0.54
1:A:126:THR:CG2	2:B:127:ARG:HH21	2.14	0.54
10:J:116:THR:CG2	10:J:117:PHE:N	2.70	0.54
2:P:143:PRO:HG3	2:P:214:GLU:OE2	2.07	0.54
8:V:38:HIS:CD2	8:V:74:PRO:HG3	2.42	0.54
11:Y:23:SER:O	11:Y:24:ASN:HB3	2.06	0.54
14:2:94:ARG:HA	14:2:94:ARG:NE	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:HG22	1:A:53:GLN:N	2.23	0.54
7:G:172:ALA:O	7:G:176:ILE:HG13	2.07	0.54
8:H:36:PRO:HG3	8:H:42:PHE:CZ	2.43	0.54
14:N:94:ARG:NE	14:N:94:ARG:HA	2.22	0.54
4:R:62:ILE:HD12	4:R:62:ILE:N	2.23	0.54
6:T:24:TYR:O	6:T:27:GLU:HB2	2.07	0.54
6:T:139:ASP:OD1	14:2:81:HIS:CE1	2.61	0.54
12:Z:40:TYR:HB3	12:Z:73:ARG:CZ	2.37	0.54
2:B:135:ILE:HD12	2:B:135:ILE:H	1.71	0.54
5:E:225:ASN:O	5:E:226:PHE:C	2.51	0.54
14:N:186:ARG:HH12	8:V:199:VAL:HB	1.73	0.54
6:T:89:ARG:CZ	13:1:77:HIS:HB3	2.38	0.54
12:Z:160:ILE:O	12:Z:164:THR:HG23	2.08	0.54
6:F:209:ASN:HD22	6:F:209:ASN:H	1.56	0.54
8:H:154:GLN:HE21	8:H:158:ASN:HD21	1.56	0.54
9:I:76:VAL:HG21	9:I:109:HIS:HB2	1.89	0.54
11:K:60:ILE:CG2	11:K:84:THR:HG22	2.37	0.54
14:N:99:ARG:HD2	14:N:104:ASN:O	2.07	0.54
5:S:225:ASN:O	5:S:226:PHE:C	2.51	0.54
1:A:143:ILE:HD12	1:A:143:ILE:N	2.22	0.54
9:I:143:ARG:HH11	9:I:146:MET:HG2	1.73	0.54
9:I:216:ILE:HG22	9:I:217:THR:N	2.23	0.54
5:S:112:VAL:O	5:S:116:VAL:HG23	2.08	0.54
4:D:60:ARG:C	4:D:62:ILE:H	2.16	0.54
10:J:189:ILE:CG2	10:J:196:THR:HB	2.33	0.54
14:N:211:ILE:HG13	8:V:30:VAL:HG21	1.89	0.54
1:O:87:SER:O	1:O:91:VAL:HG23	2.08	0.54
1:O:213:SER:HB3	1:O:232:GLU:OE2	2.08	0.54
5:S:186:HIS:HB2	5:S:189:MET:HB3	1.89	0.54
14:2:192:VAL:HA	14:2:196:GLY:O	2.07	0.54
2:B:191:ILE:HG22	2:B:202:MET:CE	2.38	0.53
4:D:112:ALA:HB1	4:D:151:GLY:O	2.09	0.53
6:F:89:ARG:NH1	13:M:77:HIS:HB3	2.22	0.53
1:O:50:ILE:HG21	1:O:79:VAL:HB	1.88	0.53
6:F:183:ASN:OD1	6:F:186:GLU:HG3	2.09	0.53
9:I:106:THR:HG22	9:I:106:THR:O	2.08	0.53
10:J:142:CYS:SG	10:J:146:MET:HE2	2.48	0.53
3:Q:54:LYS:O	3:Q:55:LEU:HG	2.08	0.53
4:R:46:GLU:O	4:R:48:LYS:N	2.41	0.53
9:W:51:ASP:O	9:W:55:THR:HG23	2.09	0.53
11:Y:60:ILE:CG2	11:Y:84:THR:HG22	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:46:GLU:O	4:D:48:LYS:N	2.41	0.53
8:H:173:VAL:HG21	8:H:190:LEU:CD2	2.37	0.53
1:O:143:ILE:HD12	1:O:143:ILE:N	2.23	0.53
5:S:173:ALA:CB	5:S:205:VAL:HB	2.38	0.53
3:C:54:LYS:O	3:C:55:LEU:HG	2.09	0.53
3:C:76:VAL:CG1	3:C:132:VAL:HG13	2.38	0.53
8:H:13:VAL:HG11	8:H:153:LEU:HA	1.90	0.53
12:L:20:ALA:HB2	12:L:31:VAL:HG21	1.90	0.53
2:P:14:PRO:HG3	3:Q:23:TYR:CE1	2.43	0.53
2:P:48:GLU:CG	2:P:50:LYS:HG2	2.39	0.53
2:P:213:ASN:ND2	2:P:215:ALA:HB3	2.19	0.53
7:U:215:TRP:CE3	7:U:215:TRP:HA	2.44	0.53
9:W:153:ASN:ND2	9:W:153:ASN:C	2.67	0.53
5:E:54:ILE:HG22	5:E:56:SER:H	1.73	0.53
5:E:67:ILE:HG22	5:E:228:MET:HE1	1.90	0.53
5:E:78:MET:HE2	5:E:82:ILE:HG23	1.91	0.53
11:K:2:GLU:HB2	11:K:47:VAL:CG1	2.38	0.53
2:P:94:GLN:CG	9:W:65:LEU:HD13	2.38	0.53
3:Q:198:ASN:HA	3:Q:206:LEU:HD22	1.91	0.53
7:U:215:TRP:HA	7:U:215:TRP:HE3	1.73	0.53
5:E:35:SER:HB3	5:E:51:GLU:HG3	1.90	0.53
8:H:76:VAL:CB	8:H:110:GLN:HE21	2.04	0.53
4:R:95:ARG:O	4:R:98:VAL:O	2.26	0.53
5:S:35:SER:HB3	5:S:51:GLU:HG3	1.91	0.53
9:W:143:ARG:HH11	9:W:146:MET:HG2	1.74	0.53
3:C:95:GLN:NE2	3:C:95:GLN:HA	2.24	0.53
6:F:207:THR:HG22	6:F:233:LEU:HD12	1.90	0.53
8:H:166:ARG:HE	14:2:37:ARG:HH21	1.56	0.53
9:I:216:ILE:HG22	9:I:217:THR:H	1.73	0.53
11:K:143:LEU:HD21	11:K:163:CYS:SG	2.48	0.53
4:R:60:ARG:C	4:R:62:ILE:H	2.16	0.53
5:S:78:MET:HE2	5:S:82:ILE:HG23	1.90	0.53
11:Y:180:VAL:CG1	11:Y:191:LEU:HD12	2.39	0.53
2:B:143:PRO:HG3	2:B:214:GLU:OE2	2.09	0.53
3:C:188:SER:O	3:C:191:ALA:HB3	2.08	0.53
4:D:33:VAL:HG23	4:D:191:VAL:HG13	1.91	0.53
7:G:215:TRP:CE3	7:G:215:TRP:HA	2.44	0.53
7:G:240:LYS:O	7:G:243:LEU:HB3	2.08	0.53
7:U:184:MET:HB3	7:U:189:ILE:HD11	1.91	0.53
9:W:76:VAL:HG21	9:W:109:HIS:HB2	1.90	0.53
13:M:15:ILE:HD12	13:M:15:ILE:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:186:LYS:CB	1:O:189:TRP:HE1	2.22	0.53
2:P:201:GLN:O	2:P:203:THR:HG23	2.09	0.53
3:C:53:HIS:HE1	3:C:55:LEU:HD12	1.73	0.53
3:C:189:ALA:C	3:C:191:ALA:N	2.67	0.53
7:G:191:LYS:HB3	7:G:238:TYR:CD2	2.44	0.53
1:A:75:ASN:O	1:A:76:ILE:HD13	2.08	0.52
2:B:16:GLY:O	3:C:27:ALA:HB2	2.09	0.52
2:B:74:VAL:HG23	2:B:134:LEU:HB2	1.90	0.52
9:I:148:GLU:OE1	9:I:182:LYS:NZ	2.41	0.52
14:N:43:MET:HE3	14:N:45:VAL:CG2	2.39	0.52
2:P:64:VAL:HA	2:P:73:LEU:O	2.09	0.52
2:P:228:TYR:HA	2:P:233:ALA:HB3	1.91	0.52
5:S:78:MET:CE	5:S:82:ILE:HG23	2.39	0.52
9:W:182:LYS:HD2	9:W:184:ASP:OD1	2.08	0.52
9:W:212:LEU:HB2	10:X:199:THR:O	2.09	0.52
9:W:216:ILE:HG22	9:W:217:THR:N	2.24	0.52
2:B:64:VAL:HA	2:B:73:LEU:O	2.08	0.52
2:B:92:LEU:HD13	2:B:112:ARG:HB3	1.90	0.52
4:D:95:ARG:O	4:D:98:VAL:O	2.27	0.52
5:E:78:MET:CE	5:E:82:ILE:HG23	2.40	0.52
6:F:130:VAL:HG22	6:F:131:GLY:O	2.09	0.52
12:Z:10:HIS:O	12:Z:178:HIS:CE1	2.60	0.52
13:1:181:SER:O	13:1:184:GLU:HB2	2.09	0.52
1:A:186:LYS:CB	1:A:189:TRP:HE1	2.22	0.52
2:B:100:TYR:O	2:B:101:GLN:HB2	2.09	0.52
2:B:228:TYR:HA	2:B:233:ALA:HB3	1.91	0.52
3:C:147:LEU:HB3	3:C:159:TRP:O	2.09	0.52
4:D:59:VAL:HG22	4:D:59:VAL:O	2.09	0.52
5:E:78:MET:HG3	5:E:82:ILE:HD12	1.91	0.52
9:I:186:LEU:O	9:I:187:ARG:O	2.28	0.52
10:J:147:TYR:HB3	13:1:185:ARG:HG3	1.91	0.52
1:O:240:VAL:HG23	1:O:241:ALA:N	2.25	0.52
3:Q:95:GLN:NE2	3:Q:95:GLN:HA	2.24	0.52
3:Q:109:GLN:NE2	11:Y:71:ASN:HD21	2.08	0.52
4:R:33:VAL:CG1	4:R:168:VAL:HG11	2.39	0.52
8:V:154:GLN:HE21	8:V:158:ASN:ND2	2.07	0.52
2:B:173:LEU:C	2:B:175:LYS:N	2.67	0.52
3:C:236:LEU:HD22	3:C:236:LEU:N	2.24	0.52
12:Z:74:ILE:HG12	12:Z:78:ALA:HB3	1.91	0.52
3:C:15:GLU:HB3	4:D:28:LYS:HZ3	1.75	0.52
9:I:20:ALA:HB3	9:I:28:ASP:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:45:VAL:HA	16:N:221:HOH:O	2.09	0.52
3:Q:147:LEU:HB3	3:Q:159:TRP:O	2.08	0.52
8:V:13:VAL:HG11	8:V:153:LEU:HA	1.90	0.52
14:2:126:ASP:HB3	14:2:128:LEU:H	1.72	0.52
1:A:231:THR:HB	1:A:234:GLU:HG2	1.92	0.52
1:A:240:VAL:HG23	1:A:241:ALA:N	2.24	0.52
7:G:215:TRP:HA	7:G:215:TRP:HE3	1.73	0.52
10:J:109:ILE:HB	10:J:122:CYS:SG	2.49	0.52
11:K:40:GLU:O	11:K:188:ILE:HD13	2.10	0.52
12:L:19:ARG:NH2	12:L:29:GLN:NE2	2.54	0.52
1:O:75:ASN:O	1:O:76:ILE:HD13	2.09	0.52
3:Q:236:LEU:HD22	3:Q:236:LEU:N	2.25	0.52
6:T:10:VAL:HG11	6:T:127:PRO:HD3	1.90	0.52
7:U:99:ARG:HD2	14:2:69:GLN:HE21	1.74	0.52
9:W:20:ALA:HB3	9:W:28:ASP:HB3	1.91	0.52
10:X:58:THR:CG2	11:Y:121:LEU:O	2.57	0.52
11:Y:2:GLU:HB2	11:Y:47:VAL:CG1	2.39	0.52
1:A:143:ILE:HD13	1:A:220:VAL:HG22	1.91	0.52
5:E:189:MET:HE1	5:E:194:ALA:HA	1.91	0.52
6:F:185:ASN:O	6:F:189:LYS:HG3	2.10	0.52
2:P:51:GLN:O	2:P:52:LYS:O	2.28	0.52
3:Q:76:VAL:HG12	3:Q:77:ALA:N	2.24	0.52
3:Q:187:LYS:HZ1	3:Q:236:LEU:HD11	1.70	0.52
4:R:35:VAL:HG22	4:R:191:VAL:CG2	2.40	0.52
10:X:15:LYS:HE2	10:X:119:PRO:HG2	1.92	0.52
1:A:213:SER:HB3	1:A:232:GLU:OE2	2.09	0.52
2:B:201:GLN:O	2:B:203:THR:HG23	2.09	0.52
3:C:198:ASN:HA	3:C:206:LEU:HD22	1.91	0.52
7:G:184:MET:HB3	7:G:189:ILE:HD11	1.90	0.52
3:Q:37:ILE:H	3:Q:44:LEU:HD13	1.74	0.52
3:Q:188:SER:O	3:Q:191:ALA:HB3	2.08	0.52
4:R:59:VAL:HG22	4:R:59:VAL:O	2.10	0.52
7:U:240:LYS:O	7:U:243:LEU:HB3	2.10	0.52
8:V:173:VAL:HG21	8:V:190:LEU:CD2	2.40	0.52
10:X:117:PHE:CD1	10:X:118:LYS:N	2.78	0.52
2:B:190:ALA:O	2:B:193:THR:HG22	2.10	0.52
4:D:33:VAL:CG1	4:D:168:VAL:HG11	2.39	0.52
5:E:157:ASP:OD2	5:E:157:ASP:C	2.53	0.52
7:G:168:ALA:HB3	7:G:200:VAL:CG1	2.39	0.52
14:N:46:ASN:C	14:N:46:ASN:ND2	2.63	0.52
14:N:215:ILE:HD11	8:V:175:ARG:NH1	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:143:ILE:HD13	1:O:220:VAL:HG22	1.91	0.52
1:O:231:THR:HB	1:O:234:GLU:HG2	1.90	0.52
4:R:215:GLN:HG2	4:R:216:SER:N	2.24	0.52
7:U:50:GLU:OE2	7:U:201:HIS:HD2	1.92	0.52
7:U:184:MET:HB2	7:U:189:ILE:HD11	1.92	0.52
7:U:191:LYS:HB3	7:U:238:TYR:CD2	2.45	0.52
8:V:40:ARG:HG3	8:V:40:ARG:NH1	2.25	0.52
12:Z:162:GLN:O	12:Z:165:TYR:HB3	2.10	0.52
13:1:14:ALA:HA	13:1:22:ILE:O	2.10	0.52
1:A:93:ARG:CZ	1:A:121:ILE:HD13	2.40	0.52
9:I:153:ASN:ND2	9:I:153:ASN:C	2.66	0.52
3:Q:49:ARG:HG3	3:Q:63:GLU:OE1	2.10	0.52
3:Q:136:TYR:HB2	3:Q:148:TYR:HB2	1.91	0.52
5:S:54:ILE:HG22	5:S:56:SER:H	1.74	0.52
6:T:183:ASN:OD1	6:T:186:GLU:HG3	2.10	0.52
9:W:216:ILE:HG22	9:W:217:THR:H	1.75	0.52
10:X:168:SER:CB	10:X:200:LEU:HD11	2.40	0.52
10:X:189:ILE:CG2	10:X:196:THR:HB	2.36	0.52
9:I:146:MET:HE1	9:I:154:LEU:HD23	1.90	0.51
10:J:116:THR:CG2	10:J:117:PHE:H	2.23	0.51
12:L:74:ILE:HG12	12:L:78:ALA:HB3	1.91	0.51
3:Q:76:VAL:CG1	3:Q:132:VAL:HG13	2.40	0.51
9:W:186:LEU:O	9:W:187:ARG:O	2.28	0.51
10:X:22:ILE:HG22	10:X:188:HIS:HB2	1.91	0.51
10:X:65:GLN:HE21	11:Y:86:ARG:NH2	2.07	0.51
13:M:151:ASN:ND2	13:M:152:GLN:NE2	2.58	0.51
14:N:9:THR:O	14:N:41:ARG:NH2	2.43	0.51
1:O:67:THR:HG22	1:O:69:LEU:N	2.11	0.51
2:B:14:PRO:HG3	3:C:23:TYR:CE1	2.45	0.51
7:G:3:ILE:HD13	7:G:17:ASP:OD1	2.10	0.51
9:I:51:ASP:O	9:I:55:THR:HG23	2.11	0.51
11:K:35:MET:HG2	11:K:45:LEU:CD2	2.40	0.51
3:Q:229:LYS:O	3:Q:233:VAL:HG23	2.10	0.51
7:U:168:ALA:HB3	7:U:200:VAL:CG1	2.40	0.51
3:C:49:ARG:HG3	3:C:63:GLU:OE1	2.11	0.51
7:G:42:LYS:HG2	7:G:184:MET:O	2.10	0.51
11:K:102:LEU:HD11	11:K:118:MET:HE2	1.93	0.51
13:M:172:MET:O	13:M:176:LYS:HG3	2.11	0.51
14:N:49:THR:HG21	14:N:85:PRO:HA	1.92	0.51
1:O:52:THR:HG22	1:O:53:GLN:N	2.24	0.51
2:P:213:ASN:HD21	2:P:215:ALA:CB	2.20	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:157:ASP:OD2	5:S:157:ASP:C	2.53	0.51
13:1:83:MET:HE2	13:1:88:ILE:HA	1.92	0.51
2:B:133:LEU:O	2:B:147:GLN:HA	2.10	0.51
8:H:125:PHE:CZ	8:H:139:VAL:HG13	2.46	0.51
8:H:199:VAL:HB	14:2:186:ARG:HH12	1.75	0.51
9:I:143:ARG:HH11	9:I:143:ARG:HB2	1.76	0.51
9:I:203:ARG:HD2	9:I:205:GLU:OE2	2.11	0.51
10:J:26:ARG:HB3	10:J:26:ARG:NH1	2.18	0.51
10:J:114:PRO:C	10:J:115:LYS:HD2	2.36	0.51
10:J:117:PHE:CD1	10:J:118:LYS:N	2.78	0.51
11:K:121:LEU:O	11:K:122:ALA:HB3	2.11	0.51
1:O:32:ILE:HD13	1:O:137:CYS:HB2	1.91	0.51
2:P:112:ARG:HH11	2:P:112:ARG:HG3	1.76	0.51
9:W:208:THR:HG23	10:X:165:GLU:OE1	2.11	0.51
10:J:152:SER:O	10:J:153:LEU:HD23	2.11	0.51
11:K:171:PHE:CE2	11:K:173:LEU:HB2	2.45	0.51
3:Q:59:VAL:O	3:Q:59:VAL:HG12	2.10	0.51
6:F:107:ARG:NH2	14:N:74:GLU:HG3	2.25	0.51
13:M:83:MET:HE2	13:M:88:ILE:HA	1.92	0.51
2:P:100:TYR:O	2:P:101:GLN:HB2	2.11	0.51
7:U:53:VAL:HG23	7:U:209:PHE:HA	1.93	0.51
10:X:7:ASN:ND2	10:X:57:ALA:N	2.47	0.51
10:X:116:THR:CG2	10:X:117:PHE:H	2.24	0.51
10:X:142:CYS:SG	10:X:146:MET:HE2	2.50	0.51
2:B:112:ARG:HH11	2:B:112:ARG:HG3	1.75	0.51
3:C:37:ILE:H	3:C:44:LEU:HD13	1.75	0.51
12:L:195:LEU:O	12:L:199:TYR:HD1	1.94	0.51
4:R:206:ILE:HG22	4:R:207:GLU:H	1.75	0.51
9:W:146:MET:HE1	9:W:154:LEU:HD23	1.93	0.51
11:Y:61:GLN:HE21	11:Y:62:LYS:HE2	1.76	0.51
4:D:206:ILE:HG22	4:D:207:GLU:H	1.75	0.51
6:F:150:SER:C	6:F:152:ASN:H	2.19	0.51
10:J:113:ASP:CB	10:J:116:THR:HB	2.41	0.51
13:M:181:SER:O	13:M:184:GLU:HB2	2.10	0.51
3:Q:93:ILE:HD13	3:Q:113:ALA:HB1	1.93	0.51
3:Q:218:ARG:CZ	3:Q:221:GLY:O	2.57	0.51
5:S:78:MET:HG3	5:S:82:ILE:HD12	1.93	0.51
6:T:207:THR:HG22	6:T:233:LEU:HD12	1.92	0.51
14:2:46:ASN:C	14:2:46:ASN:ND2	2.64	0.51
4:D:215:GLN:HG2	4:D:216:SER:N	2.24	0.51
5:E:186:HIS:O	5:E:189:MET:HG2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:148:THR:C	8:H:150:GLU:N	2.67	0.51
14:N:192:VAL:HA	14:N:196:GLY:O	2.10	0.51
1:O:93:ARG:CZ	1:O:121:ILE:HD13	2.40	0.51
3:Q:245:ALA:O	3:Q:248:GLU:HG2	2.11	0.51
7:U:66:LEU:HD13	7:U:214:SER:OG	2.11	0.51
10:X:20:VAL:HB	10:X:190:ILE:CD1	2.40	0.51
11:Y:151:ILE:HD11	11:Y:156:ALA:HA	1.93	0.51
14:2:49:THR:HG21	14:2:85:PRO:HA	1.93	0.51
14:2:115:TYR:CE2	14:2:194:GLU:HG2	2.46	0.51
3:C:76:VAL:HG11	3:C:83:ALA:HB2	1.93	0.50
3:C:79:ILE:HD12	3:C:79:ILE:H	1.76	0.50
3:C:149:GLN:OE1	3:C:164:ILE:HD11	2.10	0.50
13:M:211:ARG:HH21	9:W:193:ASN:CB	2.25	0.50
14:N:179:ARG:CZ	9:W:135:MET:HE3	2.41	0.50
1:O:89:SER:CB	7:U:117:MET:HE1	2.40	0.50
2:P:71:ILE:HG22	2:P:72:GLY:N	2.26	0.50
5:S:167:ALA:HB3	6:T:56:LEU:HD13	1.93	0.50
6:T:159:MET:HE3	6:T:160:SER:O	2.10	0.50
8:V:148:THR:C	8:V:150:GLU:N	2.68	0.50
11:Y:24:ASN:ND2	11:Y:25:ILE:H	2.09	0.50
10:J:45:MET:HE2	10:J:67:LEU:HG	1.92	0.50
10:J:138:VAL:HG11	10:J:146:MET:HB3	1.93	0.50
11:K:59:TYR:HE2	11:K:87:ASN:OD1	1.93	0.50
4:R:33:VAL:HG23	4:R:191:VAL:HG13	1.93	0.50
4:R:115:LYS:O	4:R:119:THR:HG23	2.11	0.50
4:R:130:SER:HA	4:R:147:THR:O	2.11	0.50
11:Y:60:ILE:O	11:Y:64:VAL:HG23	2.11	0.50
3:C:218:ARG:CZ	3:C:221:GLY:O	2.59	0.50
7:G:216:VAL:HG13	7:G:216:VAL:O	2.11	0.50
8:H:154:GLN:HE21	8:H:158:ASN:ND2	2.10	0.50
2:P:190:ALA:O	2:P:193:THR:HG22	2.10	0.50
5:S:186:HIS:O	5:S:189:MET:HG2	2.11	0.50
8:V:103:TRP:CZ3	8:V:105:PRO:HG3	2.47	0.50
12:Z:19:ARG:NH2	12:Z:29:GLN:NE2	2.56	0.50
14:2:15:LYS:HB3	14:2:20:VAL:HG22	1.94	0.50
14:2:71:VAL:O	14:2:75:GLU:HG3	2.11	0.50
1:A:87:SER:O	1:A:91:VAL:HG23	2.12	0.50
4:D:33:VAL:HG12	4:D:160:ALA:CB	2.40	0.50
7:G:53:VAL:HG23	7:G:209:PHE:HA	1.93	0.50
4:R:112:ALA:HB1	4:R:151:GLY:O	2.11	0.50
5:S:18:GLU:CD	5:S:20:ARG:HH21	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:148:GLU:OE1	9:W:182:LYS:NZ	2.44	0.50
9:W:212:LEU:HD12	10:X:200:LEU:O	2.10	0.50
11:Y:59:TYR:HE2	11:Y:87:ASN:OD1	1.93	0.50
1:A:32:ILE:HD13	1:A:137:CYS:HB2	1.92	0.50
3:C:245:ALA:O	3:C:248:GLU:HG2	2.11	0.50
4:D:13:ASP:OD2	4:D:13:ASP:N	2.42	0.50
4:D:145:TYR:CE2	4:D:155:ALA:HB2	2.47	0.50
11:K:148:THR:O	11:K:151:ILE:HG22	2.11	0.50
12:L:166:ARG:NH1	10:X:34:LEU:HG	2.27	0.50
3:Q:149:GLN:OE1	3:Q:164:ILE:HD11	2.12	0.50
5:S:189:MET:HE1	5:S:194:ALA:HA	1.93	0.50
6:T:159:MET:HG3	6:T:160:SER:H	1.73	0.50
10:X:109:ILE:HB	10:X:122:CYS:SG	2.52	0.50
11:Y:12:TYR:N	11:Y:12:TYR:CD2	2.80	0.50
12:Z:195:LEU:O	12:Z:199:TYR:HD1	1.94	0.50
2:B:94:GLN:CG	9:I:65:LEU:HD13	2.42	0.50
3:C:218:ARG:NH2	3:C:223:THR:OG1	2.44	0.50
5:E:54:ILE:HD11	5:E:61:PRO:HB3	1.93	0.50
10:J:65:GLN:HE21	11:K:86:ARG:NH2	2.10	0.50
10:J:168:SER:CB	10:J:200:LEU:HD11	2.42	0.50
11:K:47:VAL:CG1	11:K:48:GLY:N	2.74	0.50
7:U:194:ALA:O	7:U:198:TYR:HD1	1.95	0.50
9:W:143:ARG:NH1	9:W:143:ARG:HB2	2.27	0.50
10:X:45:MET:HE2	10:X:67:LEU:HG	1.93	0.50
2:B:173:LEU:HD21	2:B:193:THR:HB	1.94	0.50
3:C:229:LYS:O	3:C:233:VAL:HG23	2.12	0.50
10:J:15:LYS:HE2	10:J:119:PRO:HG2	1.94	0.50
12:L:166:ARG:HH11	10:X:34:LEU:HG	1.77	0.50
1:O:54:LYS:O	1:O:54:LYS:HG2	2.12	0.50
6:T:10:VAL:HG12	6:T:21:GLN:CB	2.42	0.50
6:T:164:ARG:HH12	6:T:200:PRO:CG	2.24	0.50
9:W:143:ARG:HH11	9:W:143:ARG:HB2	1.75	0.50
10:X:113:ASP:CB	10:X:116:THR:HB	2.40	0.50
11:Y:155:ARG:NH2	11:Y:158:GLU:OE1	2.45	0.50
1:A:54:LYS:O	1:A:54:LYS:HG2	2.12	0.50
4:D:115:LYS:O	4:D:119:THR:HG23	2.12	0.50
7:G:184:MET:HB2	7:G:189:ILE:HD11	1.94	0.50
11:K:1:MET:N	11:K:173:LEU:HD13	2.27	0.50
12:L:10:HIS:O	12:L:178:HIS:CE1	2.60	0.50
12:L:162:GLN:O	12:L:165:TYR:HB3	2.11	0.50
2:P:173:LEU:HD21	2:P:193:THR:HB	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:105:GLU:O	4:R:106:TYR:C	2.55	0.50
5:S:67:ILE:HG22	5:S:228:MET:HE1	1.94	0.50
6:T:150:SER:C	6:T:152:ASN:H	2.20	0.50
10:X:114:PRO:C	10:X:115:LYS:HD2	2.36	0.50
11:Y:121:LEU:O	11:Y:122:ALA:HB3	2.12	0.50
11:Y:171:PHE:CE2	11:Y:173:LEU:HB2	2.47	0.50
13:1:172:MET:O	13:1:176:LYS:HG3	2.12	0.50
13:1:208:VAL:HG12	13:1:209:SER:N	2.27	0.50
4:D:35:VAL:HG22	4:D:191:VAL:CG2	2.42	0.50
9:I:143:ARG:NH1	9:I:143:ARG:HB2	2.27	0.50
10:J:7:ASN:ND2	10:J:57:ALA:N	2.45	0.50
10:X:12:MET:CE	10:X:150:CYS:SG	2.98	0.50
11:Y:148:THR:O	11:Y:151:ILE:HG22	2.12	0.50
3:C:59:VAL:O	3:C:59:VAL:HG12	2.11	0.49
4:D:105:GLU:O	4:D:106:TYR:C	2.56	0.49
9:I:202:TYR:O	9:I:203:ARG:C	2.54	0.49
9:I:212:LEU:HD12	10:J:200:LEU:O	2.12	0.49
2:P:162:MET:CB	16:P:417:HOH:O	2.60	0.49
3:Q:190:LEU:O	3:Q:193:ALA:HB3	2.12	0.49
6:T:107:ARG:HH22	14:2:74:GLU:CG	2.25	0.49
6:T:117:GLN:HA	6:T:151:ALA:HB2	1.94	0.49
6:T:130:VAL:HG22	6:T:131:GLY:O	2.12	0.49
7:U:3:ILE:HB	7:U:21:PHE:CZ	2.47	0.49
9:W:59:ILE:HG13	9:W:83:LEU:HG	1.94	0.49
11:Y:35:MET:HG2	11:Y:45:LEU:CD2	2.41	0.49
13:1:151:ASN:ND2	13:1:152:GLN:NE2	2.59	0.49
1:A:72:ILE:HG21	1:A:114:LEU:HD11	1.94	0.49
3:C:93:ILE:HD13	3:C:113:ALA:HB1	1.94	0.49
4:D:212:ARG:C	4:D:214:ASP:H	2.19	0.49
4:D:223:GLU:C	4:D:225:ILE:N	2.69	0.49
5:E:42:THR:HG22	5:E:43:SER:N	2.27	0.49
5:E:221:GLN:HG3	5:E:224:GLN:HB2	1.94	0.49
7:G:215:TRP:HB3	7:G:220:THR:HG21	1.94	0.49
13:M:44:TYR:HE2	13:M:69:GLU:OE2	1.95	0.49
4:R:145:TYR:CE2	4:R:155:ALA:HB2	2.47	0.49
8:V:36:PRO:HG3	8:V:42:PHE:CZ	2.46	0.49
14:2:50:MET:SD	14:2:192:VAL:HG13	2.52	0.49
2:B:73:LEU:HD23	2:B:135:ILE:HA	1.94	0.49
3:C:109:GLN:NE2	11:K:71:ASN:HD21	2.08	0.49
5:E:112:VAL:O	5:E:116:VAL:HG23	2.13	0.49
7:G:168:ALA:CB	7:G:200:VAL:HG13	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:2:GLU:HB2	11:K:47:VAL:HG11	1.94	0.49
12:L:38:ASN:HB3	12:L:39:PRO:HD2	1.95	0.49
2:P:94:GLN:HG3	9:W:65:LEU:HD13	1.94	0.49
2:P:133:LEU:O	2:P:147:GLN:HA	2.12	0.49
3:Q:74:CYS:HB2	3:Q:135:LEU:O	2.12	0.49
4:R:98:VAL:HG12	4:R:99:GLU:H	1.77	0.49
5:S:99:HIS:CD2	5:S:107:MET:HG3	2.46	0.49
11:Y:47:VAL:CG1	11:Y:48:GLY:N	2.75	0.49
11:Y:66:LEU:HG	11:Y:70:ARG:HD2	1.95	0.49
10:J:34:LEU:HG	12:Z:166:ARG:HH11	1.78	0.49
10:J:58:THR:CG2	11:K:121:LEU:O	2.59	0.49
11:K:47:VAL:HG12	11:K:48:GLY:N	2.27	0.49
11:K:161:ARG:O	11:K:165:GLU:HG3	2.12	0.49
1:O:11:ARG:HB2	16:O:407:HOH:O	2.12	0.49
3:Q:79:ILE:HD12	3:Q:79:ILE:H	1.76	0.49
5:S:54:ILE:HD11	5:S:61:PRO:HB3	1.94	0.49
6:T:38:LEU:N	6:T:38:LEU:HD12	2.28	0.49
6:T:107:ARG:HH22	14:2:74:GLU:HG3	1.77	0.49
7:U:215:TRP:HB3	7:U:220:THR:HG21	1.94	0.49
8:V:148:THR:HG23	8:V:151:GLU:OE2	2.11	0.49
13:1:15:ILE:HD12	13:1:15:ILE:N	2.27	0.49
10:J:172:LEU:HD23	10:J:185:VAL:HG21	1.95	0.49
11:K:180:VAL:CG1	11:K:191:LEU:HD12	2.42	0.49
12:L:125:THR:CB	12:L:139:MET:HE3	2.39	0.49
13:M:1:ARG:CG	13:M:2:PHE:N	2.75	0.49
1:O:72:ILE:HG21	1:O:114:LEU:HD11	1.94	0.49
3:Q:23:TYR:N	3:Q:23:TYR:CD2	2.80	0.49
4:R:212:ARG:C	4:R:214:ASP:H	2.19	0.49
6:T:185:ASN:O	6:T:189:LYS:HG3	2.13	0.49
11:Y:40:GLU:O	11:Y:188:ILE:HD13	2.12	0.49
1:A:88:ARG:HH11	1:A:88:ARG:HG3	1.77	0.49
3:C:190:LEU:O	3:C:193:ALA:HB3	2.13	0.49
5:E:189:MET:CE	5:E:194:ALA:HA	2.43	0.49
7:G:3:ILE:HB	7:G:21:PHE:CZ	2.47	0.49
5:S:166:ASP:HB3	5:S:185:TYR:CE2	2.47	0.49
7:U:152:ASP:HB2	7:U:153:PRO:HD2	1.94	0.49
8:V:8:PHE:CD1	8:V:8:PHE:C	2.90	0.49
2:B:213:ASN:HD21	2:B:215:ALA:CB	2.20	0.49
4:D:130:SER:HA	4:D:147:THR:O	2.13	0.49
8:H:48:SER:HB3	8:H:51:ASP:HB2	1.95	0.49
9:I:113:ILE:HG23	9:I:119:THR:HG22	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:HD13	11:K:45:LEU:HB3	1.95	0.49
3:Q:69:ASN:HB2	3:Q:72:MET:HB2	1.94	0.49
12:Z:6:PHE:HA	12:Z:124:ALA:O	2.12	0.49
1:A:123:GLN:HE22	1:A:127:GLN:NE2	2.10	0.49
9:I:135:MET:HE3	14:2:179:ARG:NH1	2.28	0.49
14:N:27:LEU:HD22	14:N:184:TYR:HB2	1.94	0.49
2:P:191:ILE:HG22	2:P:202:MET:HE1	1.94	0.49
3:Q:132:VAL:O	3:Q:152:PRO:HD3	2.13	0.49
4:R:33:VAL:HG12	4:R:160:ALA:CB	2.41	0.49
7:U:99:ARG:NH1	14:2:69:GLN:NE2	2.61	0.49
7:U:168:ALA:CB	7:U:200:VAL:HG13	2.43	0.49
11:Y:4:LEU:HD13	11:Y:45:LEU:HB3	1.95	0.49
2:B:52:LYS:C	2:B:54:ILE:H	2.20	0.49
5:E:46:VAL:HG23	5:E:151:PRO:HB3	1.95	0.49
7:G:194:ALA:O	7:G:198:TYR:HD1	1.96	0.49
8:H:100:ILE:HD12	8:H:100:ILE:N	2.27	0.49
8:H:148:THR:C	8:H:150:GLU:H	2.21	0.49
11:K:166:GLU:HA	11:K:166:GLU:OE1	2.12	0.49
12:L:105:ASP:C	12:L:107:ARG:H	2.21	0.49
5:S:210:LEU:CD1	5:S:215:ILE:HG21	2.42	0.49
7:U:135:PHE:CE1	7:U:151:ILE:HD13	2.47	0.49
10:X:7:ASN:HD22	10:X:57:ALA:N	2.02	0.49
10:X:152:SER:O	10:X:153:LEU:HD23	2.13	0.49
1:A:67:THR:HG22	1:A:68:HIS:N	2.28	0.49
6:F:164:ARG:HH12	6:F:200:PRO:CG	2.25	0.49
12:L:5:ALA:HA	12:L:13:ILE:O	2.13	0.49
1:O:195:VAL:O	1:O:199:ILE:HG12	2.13	0.49
3:Q:76:VAL:HG11	3:Q:83:ALA:HB2	1.94	0.49
5:S:221:GLN:HG3	5:S:224:GLN:HB2	1.94	0.49
7:U:216:VAL:HG13	7:U:216:VAL:O	2.13	0.49
11:Y:47:VAL:HG12	11:Y:48:GLY:N	2.28	0.49
11:Y:143:LEU:HD21	11:Y:163:CYS:SG	2.52	0.49
12:Z:19:ARG:HE	12:Z:29:GLN:HE21	1.60	0.49
2:B:191:ILE:HG22	2:B:202:MET:HE1	1.95	0.48
6:F:159:MET:HG3	6:F:160:SER:H	1.76	0.48
7:G:48:GLY:HA2	7:G:212:GLU:O	2.13	0.48
8:H:15:GLY:C	8:H:160:LEU:HD11	2.38	0.48
2:P:8:SER:HB3	2:P:122:GLN:O	2.13	0.48
3:Q:180:LYS:NZ	3:Q:188:SER:OG	2.46	0.48
4:R:223:GLU:C	4:R:225:ILE:H	2.19	0.48
6:T:194:ALA:O	6:T:197:GLU:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:112:LEU:HD23	10:X:119:PRO:HA	1.95	0.48
12:Z:125:THR:CB	12:Z:139:MET:HE3	2.39	0.48
2:B:94:GLN:HG3	9:I:65:LEU:HD13	1.95	0.48
6:F:107:ARG:HH22	14:N:74:GLU:HG3	1.77	0.48
11:K:155:ARG:NH2	11:K:158:GLU:OE1	2.45	0.48
3:Q:15:GLU:HB3	4:R:28:LYS:NZ	2.27	0.48
6:T:5:GLN:HG3	6:T:6:TYR:CD1	2.48	0.48
6:T:164:ARG:NH1	6:T:200:PRO:HG3	2.29	0.48
9:W:202:TYR:O	9:W:203:ARG:C	2.53	0.48
14:2:43:MET:HG2	14:2:44:ARG:N	2.28	0.48
6:F:46:LEU:HG	6:F:135:ALA:HB2	1.94	0.48
11:K:151:ILE:HD11	11:K:156:ALA:HA	1.94	0.48
14:N:43:MET:HG2	14:N:44:ARG:N	2.27	0.48
10:X:111:GLY:HA2	10:X:190:ILE:CD1	2.44	0.48
14:2:43:MET:HE3	14:2:45:VAL:CG2	2.42	0.48
3:C:79:ILE:HD13	3:C:131:GLY:CA	2.41	0.48
7:G:54:LEU:HB2	7:G:58:TYR:CE1	2.49	0.48
8:H:103:TRP:CZ3	8:H:105:PRO:HG3	2.48	0.48
11:K:60:ILE:HG21	11:K:84:THR:CG2	2.42	0.48
12:L:180:ARG:CB	12:L:180:ARG:HH11	2.26	0.48
12:L:182:ASP:OD2	12:L:182:ASP:N	2.37	0.48
5:S:46:VAL:HG23	5:S:151:PRO:HB3	1.94	0.48
7:U:3:ILE:HD13	7:U:17:ASP:OD1	2.13	0.48
12:Z:9:ARG:HH21	12:Z:146:ASP:HB3	1.77	0.48
13:1:44:TYR:HE2	13:1:69:GLU:OE2	1.96	0.48
10:J:12:MET:CE	10:J:150:CYS:SG	3.01	0.48
11:K:66:LEU:HG	11:K:70:ARG:HD2	1.96	0.48
14:N:50:MET:HE2	14:N:192:VAL:HG22	1.96	0.48
3:Q:82:ASP:OD2	3:Q:130:PHE:HA	2.13	0.48
4:R:223:GLU:C	4:R:225:ILE:N	2.69	0.48
7:U:215:TRP:CD1	7:U:228:PRO:HD3	2.48	0.48
12:Z:182:ASP:OD2	12:Z:182:ASP:N	2.37	0.48
3:C:62:SER:OG	3:C:63:GLU:N	2.47	0.48
3:C:86:LEU:HD22	3:C:114:LEU:HD11	1.95	0.48
5:E:210:LEU:CD1	5:E:215:ILE:HG21	2.44	0.48
6:F:194:ALA:O	6:F:197:GLU:HB2	2.14	0.48
9:I:212:LEU:HD12	10:J:201:LYS:HA	1.95	0.48
13:M:174:LEU:O	13:M:178:VAL:HG22	2.14	0.48
2:P:213:ASN:C	2:P:215:ALA:H	2.22	0.48
4:R:121:SER:HB2	4:R:124:ARG:HD2	1.95	0.48
5:S:231:LYS:O	5:S:235:GLU:HG2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:193:VAL:O	7:U:197:ILE:HG12	2.13	0.48
12:Z:5:ALA:HA	12:Z:13:ILE:O	2.14	0.48
2:B:179:GLU:C	2:B:181:LEU:H	2.21	0.48
3:C:15:GLU:HB3	4:D:28:LYS:NZ	2.29	0.48
5:E:166:ASP:HB3	5:E:185:TYR:CE2	2.48	0.48
6:F:10:VAL:HG12	6:F:21:GLN:CB	2.43	0.48
6:F:38:LEU:N	6:F:38:LEU:HD12	2.29	0.48
6:F:117:GLN:HA	6:F:151:ALA:HB2	1.94	0.48
1:O:220:VAL:HG23	1:O:225:PRO:O	2.14	0.48
9:W:212:LEU:HD12	10:X:201:LYS:HA	1.95	0.48
11:Y:60:ILE:HG21	11:Y:84:THR:CG2	2.44	0.48
14:2:27:LEU:HD22	14:2:184:TYR:HB2	1.95	0.48
14:N:50:MET:SD	14:N:192:VAL:HG13	2.53	0.48
3:Q:53:HIS:CE1	3:Q:55:LEU:HD12	2.49	0.48
4:R:46:GLU:O	4:R:47:LYS:C	2.57	0.48
7:U:24:GLU:HA	7:U:27:MET:HE3	1.96	0.48
4:D:46:GLU:O	4:D:47:LYS:C	2.57	0.48
5:E:95:GLU:C	5:E:107:MET:HE1	2.38	0.48
5:E:231:LYS:O	5:E:235:GLU:HG2	2.14	0.48
7:G:219:LEU:HD12	7:G:219:LEU:O	2.14	0.48
9:I:208:THR:HG23	10:J:165:GLU:OE1	2.13	0.48
10:J:112:LEU:HD23	10:J:119:PRO:HA	1.95	0.48
11:K:23:SER:HB2	11:K:28:MET:HE2	1.95	0.48
12:L:163:ALA:C	12:L:165:TYR:N	2.72	0.48
5:S:31:ILE:HD11	5:S:158:PRO:CD	2.43	0.48
8:V:125:PHE:CZ	8:V:139:VAL:HG13	2.49	0.48
11:Y:89:ALA:HB2	11:Y:122:ALA:CB	2.44	0.48
11:Y:166:GLU:OE1	11:Y:166:GLU:HA	2.14	0.48
3:C:23:TYR:CD2	3:C:23:TYR:N	2.81	0.48
4:D:223:GLU:C	4:D:225:ILE:H	2.20	0.48
6:F:164:ARG:NH1	6:F:200:PRO:HG3	2.29	0.48
7:G:215:TRP:CD1	7:G:228:PRO:HD3	2.49	0.48
12:L:160:ILE:O	12:L:164:THR:HG23	2.13	0.48
14:N:15:LYS:HB3	14:N:20:VAL:HG22	1.96	0.48
5:S:189:MET:CE	5:S:194:ALA:HA	2.44	0.48
13:1:124:PHE:CD2	13:1:130:TYR:HB3	2.49	0.48
13:1:190:GLY:O	13:1:191:ASP:HB2	2.13	0.48
1:A:88:ARG:HG3	1:A:88:ARG:NH1	2.28	0.47
1:A:231:THR:HG22	1:A:232:GLU:N	2.29	0.47
2:B:38:LYS:HA	2:B:43:VAL:HG22	1.96	0.47
2:B:137:GLY:HA2	2:B:212:CYS:SG	2.54	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:ILE:HD11	5:E:158:PRO:CD	2.44	0.47
6:F:5:GLN:HG3	6:F:6:TYR:CD1	2.49	0.47
10:J:67:LEU:HD22	10:J:91:VAL:HG22	1.96	0.47
10:J:111:GLY:HA2	10:J:190:ILE:CD1	2.44	0.47
10:J:205:ASP:O	12:Z:19:ARG:NH1	2.45	0.47
12:L:9:ARG:HH21	12:L:146:ASP:HB3	1.79	0.47
12:L:50:ALA:HB2	13:M:129:SER:HB2	1.94	0.47
14:N:115:TYR:CE2	14:N:194:GLU:HG2	2.47	0.47
1:O:41:ALA:HA	1:O:49:VAL:O	2.13	0.47
2:P:175:LYS:C	2:P:177:TYR:H	2.21	0.47
3:Q:139:TRP:CE2	3:Q:218:ARG:HD3	2.49	0.47
3:Q:180:LYS:HZ3	3:Q:188:SER:C	2.21	0.47
3:Q:185:THR:H	3:Q:188:SER:HG	1.61	0.47
4:R:98:VAL:CG1	4:R:99:GLU:N	2.77	0.47
6:T:46:LEU:HG	6:T:135:ALA:HB2	1.95	0.47
2:B:109:LEU:O	2:B:109:LEU:HG	2.14	0.47
3:C:74:CYS:HB2	3:C:135:LEU:O	2.13	0.47
4:D:35:VAL:O	4:D:41:VAL:HG13	2.14	0.47
7:G:99:ARG:HD2	14:N:69:GLN:HE21	1.78	0.47
7:G:193:VAL:O	7:G:197:ILE:HG12	2.14	0.47
8:H:30:VAL:HG13	14:2:212:ALA:HA	1.95	0.47
9:I:59:ILE:HG13	9:I:83:LEU:HG	1.95	0.47
10:J:109:ILE:O	10:J:121:ILE:HA	2.14	0.47
13:M:137:ALA:N	13:M:146:GLN:NE2	2.62	0.47
1:O:231:THR:HG22	1:O:232:GLU:N	2.29	0.47
8:V:148:THR:OG1	8:V:151:GLU:HG3	2.14	0.47
11:Y:1:MET:N	11:Y:173:LEU:HD13	2.29	0.47
11:Y:190:ASP:O	11:Y:191:LEU:HG	2.15	0.47
7:G:47:PHE:O	7:G:213:LEU:HA	2.14	0.47
7:G:152:ASP:HB2	7:G:153:PRO:HD2	1.96	0.47
10:J:34:LEU:HG	10:J:35:VAL:N	2.23	0.47
13:M:7:PHE:CZ	13:M:9:GLY:HA2	2.49	0.47
13:M:208:VAL:HG12	13:M:209:SER:N	2.29	0.47
2:P:179:GLU:C	2:P:181:LEU:H	2.22	0.47
5:S:78:MET:HG3	5:S:82:ILE:CD1	2.45	0.47
7:U:47:PHE:O	7:U:213:LEU:HA	2.15	0.47
9:W:203:ARG:HD2	9:W:205:GLU:OE2	2.13	0.47
11:Y:23:SER:HB2	11:Y:28:MET:HE2	1.96	0.47
1:A:52:THR:CG2	1:A:53:GLN:N	2.78	0.47
2:B:85:LEU:HD11	2:B:117:MET:HE3	1.96	0.47
10:J:149:MET:HE2	10:J:173:ASN:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:151:ASN:HD22	13:M:152:GLN:HE21	1.62	0.47
2:P:16:GLY:O	3:Q:27:ALA:HB2	2.13	0.47
4:R:35:VAL:O	4:R:41:VAL:HG13	2.13	0.47
4:R:212:ARG:O	4:R:214:ASP:N	2.48	0.47
6:T:169:ARG:HG2	7:U:57:LEU:HD12	1.95	0.47
8:V:148:THR:C	8:V:150:GLU:H	2.22	0.47
10:X:96:TYR:CE1	10:X:99:ARG:HD3	2.49	0.47
11:Y:24:ASN:CG	11:Y:25:ILE:H	2.22	0.47
13:1:137:ALA:N	13:1:146:GLN:NE2	2.61	0.47
1:A:41:ALA:HA	1:A:49:VAL:O	2.14	0.47
2:B:213:ASN:C	2:B:215:ALA:H	2.22	0.47
6:F:151:ALA:HB3	7:G:82:ALA:CB	2.40	0.47
10:J:123:SER:OG	10:J:131:MET:HE2	2.13	0.47
11:K:1:MET:H3	11:K:173:LEU:HD13	1.79	0.47
11:K:89:ALA:HB2	11:K:122:ALA:CB	2.45	0.47
13:M:12:ILE:HG12	13:M:25:SER:HB3	1.96	0.47
13:M:83:MET:CE	13:M:88:ILE:HA	2.45	0.47
1:O:67:THR:HG22	1:O:68:HIS:N	2.30	0.47
1:O:78:CYS:CB	1:O:140:LEU:HD23	2.44	0.47
2:P:59:ARG:O	2:P:61:VAL:N	2.47	0.47
2:P:182:GLU:HG2	2:P:183:LEU:N	2.26	0.47
3:Q:167:ASN:C	3:Q:169:ALA:N	2.72	0.47
3:Q:209:GLU:O	3:Q:211:VAL:N	2.48	0.47
4:R:42:VAL:CA	4:R:210:VAL:HG12	2.42	0.47
5:S:42:THR:HG22	5:S:43:SER:N	2.29	0.47
3:C:205:LYS:O	3:C:206:LEU:C	2.58	0.47
7:G:135:PHE:CE1	7:G:151:ILE:HD13	2.50	0.47
8:H:8:PHE:CD1	8:H:8:PHE:C	2.92	0.47
9:I:200:GLY:CA	13:1:173:ARG:HD3	2.44	0.47
12:L:4:LEU:CA	12:L:100:MET:HE1	2.45	0.47
12:L:40:TYR:HB3	12:L:73:ARG:NH2	2.29	0.47
2:P:173:LEU:C	2:P:175:LYS:N	2.66	0.47
3:Q:234:GLU:O	3:Q:237:ILE:HB	2.15	0.47
5:S:95:GLU:C	5:S:107:MET:HE1	2.38	0.47
2:B:7:PHE:O	2:B:124:GLY:HA2	2.15	0.47
2:B:71:ILE:HG22	2:B:72:GLY:N	2.29	0.47
3:C:82:ASP:OD2	3:C:130:PHE:HA	2.14	0.47
3:C:180:LYS:HZ3	3:C:188:SER:C	2.21	0.47
5:E:18:GLU:CD	5:E:20:ARG:HH21	2.22	0.47
5:E:24:VAL:HA	5:E:27:ASP:OD1	2.15	0.47
5:E:28:ILE:HD13	5:E:158:PRO:HD2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:HIS:CD2	5:E:107:MET:HG3	2.49	0.47
6:F:6:TYR:OH	7:G:8:ASP:OD2	2.24	0.47
8:H:1:THR:HG22	8:H:2:THR:N	2.30	0.47
8:H:148:THR:HG23	8:H:151:GLU:OE2	2.15	0.47
12:L:158:ARG:CG	12:L:199:TYR:HE2	2.28	0.47
14:N:77:LEU:O	14:N:78:GLY:C	2.57	0.47
2:P:73:LEU:HD23	2:P:135:ILE:HA	1.96	0.47
3:Q:159:TRP:CE3	4:R:54:GLN:HA	2.50	0.47
6:T:71:GLY:HA3	6:T:221:PHE:CE2	2.50	0.47
7:U:189:ILE:HG22	7:U:193:VAL:HG23	1.97	0.47
7:U:219:LEU:HD12	7:U:219:LEU:O	2.14	0.47
8:V:100:ILE:N	8:V:100:ILE:HD12	2.29	0.47
8:V:194:ILE:O	8:V:195:PRO:C	2.58	0.47
10:X:109:ILE:O	10:X:121:ILE:HA	2.14	0.47
12:Z:4:LEU:CA	12:Z:100:MET:HE1	2.44	0.47
12:Z:38:ASN:HB3	12:Z:39:PRO:HD2	1.96	0.47
12:Z:50:ALA:HB2	13:1:129:SER:HB2	1.95	0.47
12:Z:153:TYR:OH	12:Z:178:HIS:HD2	1.98	0.47
14:2:92:LEU:HD22	14:2:112:ILE:HD11	1.95	0.47
2:B:175:LYS:C	2:B:177:TYR:H	2.22	0.47
3:C:178:ASP:OD2	3:C:178:ASP:N	2.48	0.47
3:C:209:GLU:C	3:C:211:VAL:N	2.72	0.47
14:N:92:LEU:HD22	14:N:112:ILE:HD11	1.97	0.47
14:N:190:ALA:HA	14:N:198:GLU:O	2.14	0.47
1:O:101:TRP:CD2	1:O:109:ILE:HG13	2.50	0.47
1:O:120:ASP:OD1	2:P:83:ARG:NH1	2.48	0.47
2:P:217:PHE:CD2	2:P:217:PHE:C	2.93	0.47
7:U:54:LEU:HB2	7:U:58:TYR:CE1	2.50	0.47
10:X:172:LEU:HD23	10:X:185:VAL:HG21	1.97	0.47
12:Z:38:ASN:C	12:Z:40:TYR:H	2.22	0.47
3:C:3:ARG:NH2	6:F:9:ASP:OD1	2.37	0.47
7:G:189:ILE:HG22	7:G:193:VAL:HG23	1.97	0.47
12:L:6:PHE:HA	12:L:124:ALA:O	2.13	0.47
13:M:162:GLU:CD	13:M:162:GLU:H	2.22	0.47
9:W:43:CYS:SG	9:W:98:LEU:HB3	2.55	0.47
10:X:20:VAL:O	10:X:190:ILE:HG12	2.15	0.47
12:Z:10:HIS:CD2	12:Z:149:VAL:HG23	2.50	0.47
13:1:54:CYS:SG	13:1:106:VAL:HG13	2.55	0.47
14:2:50:MET:HE2	14:2:192:VAL:HG22	1.96	0.47
1:A:101:TRP:CD2	1:A:109:ILE:HG13	2.50	0.47
1:A:195:VAL:O	1:A:199:ILE:HG12	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:ALA:O	5:E:96:THR:HG23	2.15	0.47
6:F:50:LYS:HB3	6:F:59:HIS:HB3	1.96	0.47
6:F:117:GLN:CA	6:F:151:ALA:HB2	2.45	0.47
11:K:24:ASN:ND2	11:K:25:ILE:H	2.12	0.47
13:M:54:CYS:SG	13:M:106:VAL:HG13	2.55	0.47
1:O:221:THR:CG2	1:O:223:GLU:H	2.17	0.47
10:X:155:GLU:HB2	10:X:158:MET:HE3	1.96	0.47
14:2:59:ASP:O	14:2:62:TYR:HB3	2.15	0.47
1:A:67:THR:HG22	1:A:68:HIS:H	1.80	0.46
4:D:121:SER:HB2	4:D:124:ARG:HD2	1.97	0.46
5:E:51:GLU:HG3	5:E:51:GLU:O	2.15	0.46
7:G:66:LEU:HD13	7:G:214:SER:OG	2.14	0.46
9:I:103:VAL:HG23	9:I:178:ILE:HG22	1.97	0.46
9:I:124:TYR:CD1	9:I:138:PHE:HB3	2.50	0.46
3:Q:205:LYS:O	3:Q:206:LEU:C	2.58	0.46
3:Q:234:GLU:HG2	3:Q:237:ILE:HD12	1.97	0.46
11:Y:161:ARG:O	11:Y:165:GLU:HG3	2.15	0.46
12:Z:40:TYR:HB3	12:Z:73:ARG:NH2	2.30	0.46
12:Z:51:ASP:O	12:Z:55:TRP:HD1	1.99	0.46
12:Z:105:ASP:C	12:Z:107:ARG:H	2.20	0.46
13:1:162:GLU:H	13:1:162:GLU:CD	2.23	0.46
1:A:89:SER:CB	7:G:117:MET:HE1	2.46	0.46
1:A:208:ILE:O	1:A:209:ASP:C	2.56	0.46
3:C:139:TRP:CE2	3:C:218:ARG:HD3	2.50	0.46
3:C:180:LYS:NZ	3:C:188:SER:OG	2.48	0.46
4:D:206:ILE:CG2	4:D:207:GLU:N	2.78	0.46
5:E:13:ASN:OD1	6:F:126:ARG:HD3	2.15	0.46
7:G:179:LEU:O	7:G:181:MET:HE3	2.16	0.46
11:K:12:TYR:CD2	11:K:12:TYR:N	2.82	0.46
12:L:19:ARG:NH2	12:L:29:GLN:HE22	1.99	0.46
6:T:117:GLN:CA	6:T:151:ALA:HB2	2.45	0.46
2:B:46:ALA:HB2	2:B:209:VAL:HG12	1.97	0.46
3:C:209:GLU:O	3:C:211:VAL:N	2.48	0.46
3:C:234:GLU:O	3:C:237:ILE:HB	2.14	0.46
8:H:40:ARG:HG3	8:H:40:ARG:NH1	2.27	0.46
8:H:67:SER:O	8:H:71:ASN:N	2.48	0.46
10:J:20:VAL:HB	10:J:190:ILE:CD1	2.43	0.46
11:K:138:LEU:HD11	11:Y:26:VAL:HG12	1.96	0.46
1:O:208:ILE:O	1:O:209:ASP:C	2.58	0.46
7:U:12:SER:HB3	7:U:125:TYR:HA	1.98	0.46
8:V:67:SER:O	8:V:71:ASN:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:67:LEU:HD22	10:X:91:VAL:HG22	1.97	0.46
11:Y:2:GLU:HB2	11:Y:47:VAL:HG11	1.96	0.46
12:Z:180:ARG:CB	12:Z:180:ARG:HH11	2.27	0.46
14:2:42:ILE:HG22	14:2:43:MET:N	2.30	0.46
1:A:25:VAL:O	1:A:28:ALA:HB3	2.14	0.46
3:C:241:GLU:C	3:C:243:GLU:H	2.24	0.46
4:D:98:VAL:HG12	4:D:99:GLU:H	1.78	0.46
5:E:78:MET:HG3	5:E:82:ILE:CD1	2.45	0.46
11:K:1:MET:HE1	11:K:133:GLY:CA	2.46	0.46
14:N:42:ILE:HG22	14:N:43:MET:N	2.29	0.46
1:O:88:ARG:HH11	1:O:88:ARG:HG3	1.81	0.46
3:Q:174:MET:CE	3:Q:199:LYS:HG2	2.46	0.46
6:T:137:TYR:CE2	6:T:217:LYS:HA	2.51	0.46
6:T:138:ASP:C	6:T:140:MET:H	2.24	0.46
14:2:190:ALA:HA	14:2:198:GLU:O	2.15	0.46
1:A:78:CYS:CB	1:A:140:LEU:HD23	2.45	0.46
1:A:176:THR:O	1:A:180:GLU:HG2	2.15	0.46
1:A:220:VAL:HG23	1:A:225:PRO:O	2.15	0.46
3:C:159:TRP:CE3	4:D:54:GLN:HA	2.50	0.46
5:E:95:GLU:O	5:E:107:MET:HE1	2.15	0.46
9:I:200:GLY:HA2	13:1:173:ARG:HD3	1.97	0.46
12:L:4:LEU:HD12	12:L:4:LEU:O	2.16	0.46
13:M:14:ALA:C	13:M:15:ILE:HD12	2.39	0.46
14:N:43:MET:HE3	14:N:45:VAL:HG23	1.98	0.46
1:O:244:GLU:HA	1:O:244:GLU:OE2	2.16	0.46
2:P:137:GLY:HA2	2:P:212:CYS:SG	2.55	0.46
5:S:95:GLU:O	5:S:107:MET:HE1	2.15	0.46
6:T:84:LEU:O	6:T:88:MET:HG3	2.14	0.46
8:V:76:VAL:CB	8:V:110:GLN:HE21	2.09	0.46
3:C:167:ASN:C	3:C:169:ALA:N	2.72	0.46
4:D:203:GLY:C	4:D:205:ASN:H	2.22	0.46
6:F:138:ASP:C	6:F:140:MET:H	2.22	0.46
8:H:194:ILE:O	8:H:195:PRO:C	2.58	0.46
9:I:18:THR:HG23	9:I:172:ASN:O	2.15	0.46
9:I:182:LYS:HG2	9:I:183:LEU:N	2.31	0.46
9:I:190:THR:CG2	9:I:192:PRO:HD3	2.36	0.46
11:K:62:LYS:N	11:K:62:LYS:HD2	2.31	0.46
1:O:88:ARG:HG3	1:O:88:ARG:NH1	2.31	0.46
3:Q:241:GLU:C	3:Q:243:GLU:H	2.23	0.46
4:R:206:ILE:CG2	4:R:207:GLU:N	2.78	0.46
13:1:151:ASN:HD22	13:1:152:GLN:HE21	1.62	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:77:LEU:O	14:2:78:GLY:C	2.57	0.46
3:C:234:GLU:HG2	3:C:237:ILE:HD12	1.97	0.46
4:D:98:VAL:CG1	4:D:99:GLU:N	2.77	0.46
4:D:171:PHE:CE2	4:D:194:ALA:HA	2.51	0.46
4:D:212:ARG:O	4:D:214:ASP:N	2.49	0.46
9:I:19:ARG:HD3	9:I:26:VAL:HG22	1.98	0.46
10:J:7:ASN:HD22	10:J:56:LEU:HA	1.81	0.46
10:J:34:LEU:HD23	12:Z:166:ARG:CD	2.34	0.46
11:K:190:ASP:O	11:K:191:LEU:HG	2.15	0.46
13:M:24:ALA:HB1	13:M:193:LEU:HD11	1.98	0.46
3:Q:28:ILE:C	3:Q:30:HIS:H	2.24	0.46
3:Q:86:LEU:HD22	3:Q:114:LEU:HD11	1.98	0.46
5:S:92:ALA:O	5:S:96:THR:HG23	2.16	0.46
5:S:225:ASN:O	5:S:226:PHE:O	2.33	0.46
7:U:108:LEU:HD11	7:U:137:LEU:HB3	1.97	0.46
10:X:123:SER:OG	10:X:131:MET:HE2	2.15	0.46
10:X:175:VAL:HG11	10:X:182:GLY:HA2	1.98	0.46
3:C:53:HIS:CE1	3:C:55:LEU:HD12	2.50	0.46
3:C:218:ARG:HH21	3:C:223:THR:N	2.14	0.46
10:J:115:LYS:O	10:J:116:THR:OG1	2.32	0.46
14:N:124:TYR:HE1	14:N:139:THR:HG22	1.81	0.46
3:Q:66:TYR:O	3:Q:73:ALA:HA	2.16	0.46
11:Y:1:MET:HB2	16:Y:414:HOH:O	2.15	0.46
11:Y:154:GLU:HG3	11:Y:155:ARG:H	1.81	0.46
13:1:137:ALA:H	13:1:146:GLN:HE21	1.63	0.46
14:2:59:ASP:CB	14:2:108:ASN:HD21	2.29	0.46
6:F:107:ARG:HH22	14:N:74:GLU:CG	2.29	0.46
7:G:160:TYR:CD2	7:G:163:CYS:HB2	2.50	0.46
11:K:24:ASN:CG	11:K:25:ILE:H	2.23	0.46
3:Q:178:ASP:OD2	3:Q:178:ASP:N	2.47	0.46
3:Q:218:ARG:NH2	3:Q:223:THR:OG1	2.47	0.46
3:Q:218:ARG:HH21	3:Q:223:THR:N	2.14	0.46
6:T:159:MET:CG	6:T:160:SER:N	2.79	0.46
7:U:184:MET:HE2	7:U:189:ILE:HD13	1.98	0.46
11:Y:28:MET:HE1	12:Z:113:TYR:CE2	2.51	0.46
3:C:239:LYS:O	3:C:243:GLU:HB3	2.16	0.46
7:G:12:SER:HB3	7:G:125:TYR:HA	1.98	0.46
9:I:59:ILE:HG13	9:I:83:LEU:HD23	1.98	0.46
10:J:34:LEU:HG	12:Z:166:ARG:NH1	2.31	0.46
10:J:149:MET:HE3	10:J:153:LEU:HD11	1.98	0.46
11:K:60:ILE:O	11:K:64:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:10:HIS:CD2	12:L:149:VAL:HG23	2.51	0.46
14:N:92:LEU:O	14:N:96:MET:HG2	2.16	0.46
1:O:25:VAL:O	1:O:28:ALA:HB3	2.16	0.46
1:O:165:ALA:O	1:O:166:THR:HG23	2.16	0.46
2:P:48:GLU:HG2	2:P:50:LYS:HG2	1.96	0.46
3:Q:109:GLN:NE2	11:Y:71:ASN:ND2	2.64	0.46
4:R:203:GLY:C	4:R:205:ASN:H	2.22	0.46
5:S:160:GLY:O	6:T:82:ARG:NH2	2.49	0.46
9:W:113:ILE:HG23	9:W:119:THR:HG22	1.97	0.46
14:2:126:ASP:HB2	14:2:130:VAL:H	1.81	0.46
2:B:85:LEU:CD1	2:B:117:MET:HE3	2.46	0.45
3:C:28:ILE:C	3:C:30:HIS:H	2.24	0.45
3:C:132:VAL:O	3:C:152:PRO:HD3	2.15	0.45
7:G:24:GLU:HA	7:G:27:MET:HE3	1.97	0.45
8:H:11:GLY:HA3	8:H:179:ILE:O	2.16	0.45
10:J:96:TYR:CE1	10:J:99:ARG:HD3	2.50	0.45
12:L:38:ASN:C	12:L:40:TYR:H	2.24	0.45
14:N:179:ARG:NH1	9:W:135:MET:HE3	2.30	0.45
3:Q:239:LYS:O	3:Q:243:GLU:HB3	2.15	0.45
4:R:14:GLY:HA2	5:S:26:TYR:O	2.15	0.45
5:S:99:HIS:CG	5:S:107:MET:HG3	2.51	0.45
7:U:160:TYR:CD2	7:U:163:CYS:HB2	2.51	0.45
9:W:103:VAL:HG23	9:W:178:ILE:HG22	1.98	0.45
9:W:146:MET:HE3	9:W:151:ALA:HB2	1.98	0.45
9:W:182:LYS:HG2	9:W:183:LEU:N	2.31	0.45
12:Z:158:ARG:CG	12:Z:199:TYR:HE2	2.29	0.45
2:B:182:GLU:HG2	2:B:183:LEU:N	2.27	0.45
3:C:51:ASN:O	3:C:56:LEU:HD12	2.17	0.45
4:D:215:GLN:CG	4:D:216:SER:N	2.79	0.45
9:I:198:ARG:HH21	9:I:201:ARG:HA	1.81	0.45
10:J:155:GLU:HB2	10:J:158:MET:HE3	1.97	0.45
1:O:221:THR:O	1:O:224:ASN:C	2.59	0.45
6:T:176:MET:HA	6:T:179:PHE:CD1	2.51	0.45
9:W:59:ILE:HG13	9:W:83:LEU:HD23	1.98	0.45
9:W:124:TYR:CD1	9:W:138:PHE:HB3	2.52	0.45
13:1:24:ALA:HB1	13:1:193:LEU:HD11	1.99	0.45
2:B:217:PHE:C	2:B:217:PHE:CD2	2.94	0.45
3:C:69:ASN:HB2	3:C:72:MET:HB2	1.97	0.45
10:J:7:ASN:HD22	10:J:57:ALA:N	2.01	0.45
14:N:126:ASP:HB2	14:N:130:VAL:H	1.81	0.45
2:P:116:VAL:O	2:P:119:GLU:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:50:ARG:C	3:Q:52:ILE:H	2.25	0.45
5:S:91:LYS:HG3	5:S:119:LEU:HD11	1.98	0.45
8:V:11:GLY:HA3	8:V:179:ILE:O	2.16	0.45
11:Y:62:LYS:N	11:Y:62:LYS:HD2	2.31	0.45
11:Y:102:LEU:HD11	11:Y:118:MET:HE2	1.98	0.45
12:Z:57:ARG:HG3	12:Z:57:ARG:NH1	2.31	0.45
1:A:14:THR:O	2:B:127:ARG:HD3	2.16	0.45
2:B:51:GLN:O	2:B:53:SER:N	2.50	0.45
2:B:116:VAL:O	2:B:119:GLU:HB3	2.15	0.45
1:O:130:GLU:H	1:O:130:GLU:CD	2.23	0.45
2:P:85:LEU:HD11	2:P:117:MET:HE3	1.98	0.45
3:Q:189:ALA:C	3:Q:191:ALA:H	2.24	0.45
4:R:98:VAL:HG13	12:Z:78:ALA:CB	2.46	0.45
4:R:134:VAL:HG12	4:R:135:GLY:N	2.31	0.45
4:R:215:GLN:CG	4:R:216:SER:N	2.80	0.45
6:T:44:ALA:HB3	6:T:215:VAL:CG1	2.46	0.45
9:W:198:ARG:HH21	9:W:201:ARG:HA	1.80	0.45
13:1:13:LEU:HD12	13:1:14:ALA:H	1.80	0.45
1:A:180:GLU:O	1:A:184:LYS:HE2	2.17	0.45
2:B:59:ARG:O	2:B:61:VAL:N	2.49	0.45
3:C:109:GLN:NE2	11:K:71:ASN:ND2	2.65	0.45
4:D:98:VAL:HG13	12:L:78:ALA:CB	2.46	0.45
5:E:91:LYS:HG3	5:E:119:LEU:HD11	1.99	0.45
8:H:148:THR:OG1	8:H:151:GLU:HG3	2.16	0.45
11:K:89:ALA:HB2	11:K:122:ALA:HB1	1.99	0.45
11:K:134:TYR:HB2	11:K:171:PHE:CZ	2.51	0.45
14:N:20:VAL:HG11	14:N:122:LEU:HD13	1.98	0.45
2:P:46:ALA:HB2	2:P:209:VAL:HG12	1.98	0.45
6:T:174:ARG:C	6:T:175:HIS:HD2	2.25	0.45
7:U:187:ARG:CZ	7:U:231:ILE:HD12	2.46	0.45
8:V:8:PHE:O	8:V:9:ASP:C	2.60	0.45
8:V:15:GLY:C	8:V:160:LEU:HD11	2.41	0.45
11:Y:1:MET:HE1	11:Y:133:GLY:CA	2.45	0.45
11:Y:151:ILE:HD11	11:Y:156:ALA:CA	2.46	0.45
3:C:69:ASN:CB	3:C:72:MET:HB2	2.47	0.45
3:C:86:LEU:HD13	3:C:118:LYS:HD3	1.99	0.45
6:F:63:ILE:HA	6:F:72:ILE:O	2.17	0.45
6:F:71:GLY:HA3	6:F:221:PHE:CE2	2.51	0.45
6:F:84:LEU:O	6:F:88:MET:HG3	2.17	0.45
9:I:202:TYR:HE1	13:1:177:ASP:OD2	2.00	0.45
11:K:154:GLU:HG3	11:K:155:ARG:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:192:VAL:HG12	14:N:197:VAL:CG2	2.41	0.45
1:O:67:THR:HG22	1:O:68:HIS:H	1.82	0.45
2:P:190:ALA:O	2:P:193:THR:CG2	2.65	0.45
6:T:143:HIS:HB3	6:T:145:PHE:HE1	1.82	0.45
6:T:209:ASN:HD22	6:T:209:ASN:N	2.13	0.45
10:X:168:SER:OG	10:X:200:LEU:HD11	2.17	0.45
11:Y:134:TYR:HB2	11:Y:171:PHE:CZ	2.52	0.45
2:B:190:ALA:HA	2:B:193:THR:HG22	1.99	0.45
5:E:121:LEU:CD1	6:F:79:ALA:HB3	2.46	0.45
6:F:137:TYR:CE2	6:F:217:LYS:HA	2.52	0.45
7:G:108:LEU:HD11	7:G:137:LEU:HB3	1.98	0.45
8:H:72:GLU:HG2	8:H:73:PRO:HD2	1.98	0.45
10:J:20:VAL:O	10:J:190:ILE:HG12	2.17	0.45
11:K:61:GLN:NE2	11:K:62:LYS:HE2	2.32	0.45
13:M:124:PHE:CD2	13:M:130:TYR:HB3	2.52	0.45
14:N:43:MET:HE2	14:N:43:MET:HB3	1.77	0.45
1:O:143:ILE:CD1	1:O:220:VAL:HG13	2.47	0.45
2:P:186:ALA:HA	2:P:189:THR:CG2	2.46	0.45
3:Q:51:ASN:O	3:Q:56:LEU:HD12	2.16	0.45
4:R:171:PHE:CE2	4:R:194:ALA:HA	2.51	0.45
5:S:44:GLU:OE1	5:S:190:THR:HB	2.17	0.45
9:W:38:SER:OG	9:W:41:ILE:HB	2.17	0.45
10:X:125:ASP:HB3	10:X:127:ILE:H	1.82	0.45
5:E:121:LEU:HD12	6:F:79:ALA:HB3	1.98	0.45
6:F:143:HIS:HB3	6:F:145:PHE:HE1	1.80	0.45
3:Q:11:ILE:CG2	3:Q:12:PHE:N	2.79	0.45
5:S:118:ASN:C	5:S:120:ALA:H	2.25	0.45
7:U:215:TRP:O	7:U:224:HIS:HA	2.16	0.45
8:V:149:LYS:O	8:V:153:LEU:HB2	2.17	0.45
13:1:7:PHE:CZ	13:1:9:GLY:HA2	2.51	0.45
13:1:12:ILE:HG12	13:1:25:SER:HB3	1.98	0.45
1:A:244:GLU:OE2	1:A:244:GLU:HA	2.17	0.45
2:B:9:LEU:HB2	2:B:126:VAL:O	2.16	0.45
3:C:235:GLN:O	3:C:239:LYS:HB2	2.16	0.45
11:K:28:MET:HE1	12:L:113:TYR:CE2	2.52	0.45
13:M:72:LEU:CD2	13:M:83:MET:SD	3.04	0.45
1:O:210:PHE:HB2	1:O:214:GLU:HB2	1.98	0.45
4:R:155:ALA:H	5:S:63:SER:CB	2.29	0.45
8:V:188:VAL:HG12	8:V:190:LEU:HD23	1.99	0.45
9:W:19:ARG:HD3	9:W:26:VAL:HG22	1.99	0.45
14:2:20:VAL:HG11	14:2:122:LEU:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:59:ASP:HB2	14:2:108:ASN:HD21	1.82	0.45
2:B:160:THR:OG1	2:B:170:LYS:NZ	2.50	0.45
2:B:186:ALA:HA	2:B:189:THR:CG2	2.46	0.45
4:D:169:ARG:O	4:D:173:GLU:HG3	2.17	0.45
5:E:163:VAL:HG22	5:E:164:GLN:H	1.81	0.45
6:F:175:HIS:CD2	6:F:175:HIS:N	2.85	0.45
6:F:209:ASN:HD22	6:F:209:ASN:N	2.12	0.45
7:G:215:TRP:O	7:G:224:HIS:HA	2.17	0.45
10:J:122:CYS:HB2	10:J:131:MET:O	2.17	0.45
12:L:57:ARG:HG3	12:L:57:ARG:NH1	2.32	0.45
14:N:149:LEU:O	14:N:152:GLU:HB3	2.17	0.45
1:O:52:THR:CG2	1:O:53:GLN:N	2.79	0.45
1:O:62:ASP:C	1:O:64:SER:N	2.75	0.45
1:O:176:THR:O	1:O:180:GLU:HG2	2.17	0.45
2:P:190:ALA:HA	2:P:193:THR:HG22	1.99	0.45
3:Q:44:LEU:C	3:Q:44:LEU:HD22	2.42	0.45
8:V:72:GLU:HG2	8:V:73:PRO:HD2	1.98	0.45
9:W:18:THR:HG23	9:W:172:ASN:O	2.17	0.45
14:2:150:LEU:HD23	14:2:168:LEU:HD13	1.99	0.45
2:B:131:VAL:O	2:B:150:PRO:HD3	2.18	0.44
3:C:50:ARG:C	3:C:52:ILE:H	2.25	0.44
10:J:136:PHE:CZ	10:J:150:CYS:HB3	2.51	0.44
11:K:154:GLU:HG3	11:K:155:ARG:H	1.81	0.44
12:L:166:ARG:CD	10:X:34:LEU:HD23	2.39	0.44
4:R:11:SER:HB3	4:R:12:PRO:CD	2.47	0.44
4:R:55:ASP:O	4:R:56:GLU:C	2.60	0.44
5:S:51:GLU:HG3	5:S:51:GLU:O	2.16	0.44
6:T:50:LYS:HB3	6:T:59:HIS:HB3	1.99	0.44
6:T:230:SER:HB2	6:T:231:PRO:CD	2.43	0.44
7:U:74:GLY:HA3	7:U:224:HIS:NE2	2.33	0.44
7:U:106:ILE:HA	7:U:107:PRO:HD3	1.82	0.44
14:2:51:LEU:HD12	14:2:52:GLY:H	1.82	0.44
4:D:155:ALA:H	5:E:63:SER:CB	2.28	0.44
6:F:176:MET:HA	6:F:179:PHE:CD1	2.53	0.44
11:K:115:LEU:HB3	11:K:127:ALA:O	2.18	0.44
14:N:10:SER:HB3	14:N:139:THR:O	2.18	0.44
14:N:51:LEU:HD12	14:N:52:GLY:H	1.81	0.44
1:O:143:ILE:CD1	1:O:220:VAL:HG22	2.47	0.44
4:R:208:LEU:O	4:R:209:ALA:HB2	2.16	0.44
9:W:191:VAL:O	9:W:191:VAL:HG12	2.17	0.44
12:Z:163:ALA:C	12:Z:165:TYR:N	2.73	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:83:MET:CE	13:1:88:ILE:HA	2.46	0.44
13:1:174:LEU:O	13:1:178:VAL:HG22	2.18	0.44
13:1:179:PHE:CD2	13:1:193:LEU:HD13	2.51	0.44
14:2:144:TYR:HA	16:2:222:HOH:O	2.16	0.44
1:A:221:THR:O	1:A:224:ASN:C	2.60	0.44
2:B:146:PHE:CE2	2:B:156:ALA:HB2	2.53	0.44
4:D:134:VAL:HG12	4:D:135:GLY:N	2.32	0.44
7:G:69:VAL:HG11	7:G:91:ALA:HB1	1.98	0.44
9:I:193:ASN:CB	13:1:211:ARG:HH21	2.30	0.44
13:M:190:GLY:O	13:M:191:ASP:HB2	2.16	0.44
1:O:192:GLU:CD	1:O:192:GLU:N	2.74	0.44
2:P:37:ILE:O	2:P:43:VAL:HG13	2.18	0.44
3:Q:62:SER:OG	3:Q:63:GLU:N	2.48	0.44
3:Q:79:ILE:HD13	3:Q:131:GLY:CA	2.43	0.44
4:R:116:GLN:CD	4:R:116:GLN:C	2.85	0.44
10:X:68:LYS:HZ3	10:X:72:ASN:CG	2.25	0.44
10:X:68:LYS:HZ3	10:X:72:ASN:ND2	2.15	0.44
12:Z:186:ARG:CB	12:Z:186:ARG:HH11	2.30	0.44
1:A:141:ILE:HG22	1:A:151:VAL:HA	2.00	0.44
10:J:59:ASP:O	10:J:63:VAL:HG23	2.17	0.44
13:M:125:ASP:C	13:M:125:ASP:OD1	2.61	0.44
13:M:141:ALA:O	13:M:144:MET:N	2.43	0.44
1:O:14:THR:O	2:P:127:ARG:HD3	2.17	0.44
3:Q:15:GLU:HB2	3:Q:17:ARG:HG2	2.00	0.44
4:R:42:VAL:CB	4:R:210:VAL:HG12	2.47	0.44
7:U:189:ILE:O	7:U:190:VAL:C	2.60	0.44
11:Y:33:ASP:OD2	11:Y:181:ARG:NH2	2.50	0.44
1:A:231:THR:HG22	1:A:233:ALA:H	1.83	0.44
2:B:195:LYS:C	2:B:197:SER:N	2.76	0.44
3:C:11:ILE:CG2	3:C:12:PHE:N	2.80	0.44
3:C:66:TYR:O	3:C:73:ALA:HA	2.17	0.44
3:C:95:GLN:OE1	10:J:72:ASN:CB	2.66	0.44
3:C:234:GLU:HA	3:C:237:ILE:CG1	2.47	0.44
4:D:208:LEU:O	4:D:209:ALA:HB2	2.18	0.44
5:E:163:VAL:HG22	5:E:164:GLN:N	2.33	0.44
6:F:159:MET:CG	6:F:160:SER:N	2.79	0.44
7:G:54:LEU:HB2	7:G:58:TYR:CD1	2.52	0.44
7:G:66:LEU:HD12	7:G:212:GLU:HB3	1.99	0.44
7:G:187:ARG:CZ	7:G:231:ILE:HD12	2.48	0.44
7:G:189:ILE:O	7:G:190:VAL:C	2.60	0.44
10:J:68:LYS:HZ3	10:J:72:ASN:CG	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:94:LEU:HD23	10:J:94:LEU:C	2.43	0.44
12:L:153:TYR:OH	12:L:178:HIS:HD2	2.01	0.44
13:M:137:ALA:H	13:M:146:GLN:HE21	1.64	0.44
14:N:59:ASP:O	14:N:62:TYR:HB3	2.17	0.44
14:N:215:ILE:HD11	8:V:175:ARG:CZ	2.48	0.44
4:R:212:ARG:CB	4:R:215:GLN:HB3	2.48	0.44
7:U:48:GLY:HA2	7:U:212:GLU:O	2.16	0.44
10:X:138:VAL:HG11	10:X:146:MET:HB3	1.98	0.44
11:Y:89:ALA:HB2	11:Y:122:ALA:HB1	1.99	0.44
13:1:72:LEU:CD2	13:1:83:MET:SD	3.06	0.44
14:2:25:ASP:O	14:2:41:ARG:HD3	2.17	0.44
1:A:143:ILE:CD1	1:A:220:VAL:HG22	2.47	0.44
1:A:165:ALA:O	1:A:166:THR:HG23	2.17	0.44
1:A:210:PHE:HB2	1:A:214:GLU:HB2	2.00	0.44
4:D:42:VAL:CA	4:D:210:VAL:HG12	2.44	0.44
4:D:100:ASP:HB3	4:D:101:PRO:HD2	1.99	0.44
6:F:174:ARG:C	6:F:175:HIS:HD2	2.25	0.44
7:G:99:ARG:NH1	14:N:69:GLN:NE2	2.64	0.44
8:H:8:PHE:O	8:H:9:ASP:C	2.61	0.44
9:I:211:VAL:HG11	10:J:198:ARG:HD3	2.00	0.44
11:K:145:ARG:HH11	11:K:145:ARG:HG3	1.82	0.44
12:L:158:ARG:HG3	12:L:199:TYR:HE2	1.82	0.44
13:M:160:ASN:ND2	13:M:160:ASN:O	2.50	0.44
1:O:203:SER:O	1:O:207:SER:N	2.50	0.44
2:P:9:LEU:HB2	2:P:126:VAL:O	2.18	0.44
3:Q:234:GLU:HA	3:Q:237:ILE:CG1	2.47	0.44
5:S:157:ASP:HB2	5:S:158:PRO:CD	2.48	0.44
11:Y:154:GLU:HG3	11:Y:155:ARG:N	2.32	0.44
1:A:62:ASP:C	1:A:64:SER:N	2.76	0.44
3:C:174:MET:CE	3:C:199:LYS:HG2	2.47	0.44
5:E:160:GLY:O	6:F:82:ARG:NH2	2.50	0.44
8:H:149:LYS:O	8:H:153:LEU:HB2	2.18	0.44
9:I:205:GLU:O	9:I:206:LYS:C	2.61	0.44
11:K:42:ILE:CG2	11:K:104:LEU:HD11	2.48	0.44
11:K:145:ARG:HE	12:Z:158:ARG:NE	2.15	0.44
1:O:231:THR:HG22	1:O:233:ALA:H	1.82	0.44
2:P:109:LEU:O	2:P:109:LEU:HG	2.17	0.44
2:P:147:GLN:O	2:P:154:TYR:HA	2.18	0.44
3:Q:44:LEU:HB3	3:Q:215:THR:HG22	1.98	0.44
3:Q:95:GLN:OE1	10:X:72:ASN:CB	2.66	0.44
7:U:54:LEU:HB2	7:U:58:TYR:CD1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:136:PHE:CZ	10:X:150:CYS:HB3	2.53	0.44
12:Z:115:ASP:HB2	12:Z:119:ASN:HB2	1.98	0.44
13:1:160:ASN:O	13:1:160:ASN:ND2	2.51	0.44
3:C:189:ALA:C	3:C:191:ALA:H	2.25	0.44
5:E:62:SER:C	5:E:64:ILE:H	2.25	0.44
5:E:225:ASN:O	5:E:226:PHE:O	2.34	0.44
9:I:38:SER:OG	9:I:41:ILE:HB	2.18	0.44
10:J:11:VAL:HG12	10:J:108:VAL:HG21	1.99	0.44
11:K:151:ILE:HD11	11:K:156:ALA:CA	2.48	0.44
13:M:179:PHE:CD2	13:M:193:LEU:HD13	2.53	0.44
14:N:59:ASP:CB	14:N:108:ASN:HD21	2.31	0.44
14:N:150:LEU:HD23	14:N:168:LEU:HD13	2.00	0.44
1:O:84:THR:O	1:O:87:SER:HB2	2.18	0.44
1:O:185:LYS:O	1:O:186:LYS:C	2.61	0.44
3:Q:155:ASN:CG	4:R:77:THR:HG21	2.43	0.44
5:S:24:VAL:HA	5:S:27:ASP:OD1	2.17	0.44
5:S:62:SER:C	5:S:64:ILE:H	2.26	0.44
6:T:132:LEU:HB2	6:T:147:THR:OG1	2.18	0.44
1:A:142:GLY:HA2	1:A:220:VAL:HG11	2.00	0.44
1:A:183:VAL:HG12	1:A:183:VAL:O	2.18	0.44
1:A:185:LYS:O	1:A:186:LYS:C	2.61	0.44
4:D:14:GLY:HA2	5:E:26:TYR:O	2.18	0.44
9:I:146:MET:HE3	9:I:151:ALA:HB2	1.99	0.44
10:J:168:SER:OG	10:J:200:LEU:HD11	2.18	0.44
12:L:158:ARG:HG3	12:L:199:TYR:CE2	2.53	0.44
2:P:38:LYS:NZ	3:Q:57:ASP:OD2	2.50	0.44
2:P:85:LEU:CD1	2:P:117:MET:HE3	2.48	0.44
2:P:195:LYS:C	2:P:197:SER:N	2.76	0.44
11:Y:10:PRO:HD2	11:Y:12:TYR:HE2	1.83	0.44
14:2:124:TYR:HE1	14:2:139:THR:HG22	1.83	0.44
1:A:130:GLU:H	1:A:130:GLU:CD	2.26	0.43
2:B:147:GLN:O	2:B:154:TYR:HA	2.18	0.43
3:C:139:TRP:CD1	3:C:144:GLY:HA2	2.53	0.43
3:C:229:LYS:O	3:C:230:GLN:C	2.61	0.43
4:D:62:ILE:HD12	4:D:62:ILE:H	1.83	0.43
4:D:212:ARG:CB	4:D:215:GLN:HB3	2.46	0.43
6:F:44:ALA:HB3	6:F:215:VAL:CG1	2.47	0.43
7:G:140:TYR:CG	7:G:217:GLY:HA2	2.53	0.43
8:H:62:GLN:HB3	8:H:82:LEU:HD13	2.00	0.43
10:J:68:LYS:NZ	10:J:72:ASN:ND2	2.63	0.43
12:L:19:ARG:NE	12:L:29:GLN:NE2	2.64	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:76:VAL:HG23	12:L:105:ASP:CG	2.43	0.43
14:N:161:SER:O	14:N:162:GLN:C	2.60	0.43
4:R:209:ALA:CB	4:R:219:ILE:HA	2.48	0.43
10:X:11:VAL:HG12	10:X:108:VAL:HG21	2.00	0.43
11:Y:108:ASP:C	11:Y:110:HIS:H	2.26	0.43
11:Y:115:LEU:HB3	11:Y:127:ALA:O	2.18	0.43
13:1:12:ILE:HD13	13:1:53:GLY:CA	2.48	0.43
14:2:16:PHE:CZ	14:2:162:GLN:HG3	2.54	0.43
1:A:188:ASP:O	1:A:190:THR:HG23	2.17	0.43
1:A:191:PHE:HE1	1:A:219:VAL:HG21	1.83	0.43
2:B:190:ALA:O	2:B:193:THR:CG2	2.65	0.43
3:C:44:LEU:C	3:C:44:LEU:HD22	2.43	0.43
10:J:175:VAL:HG11	10:J:182:GLY:HA2	2.00	0.43
3:Q:69:ASN:CB	3:Q:72:MET:HB2	2.47	0.43
4:R:100:ASP:HB3	4:R:101:PRO:HD2	1.99	0.43
6:T:65:HIS:ND1	13:1:77:HIS:HE1	2.16	0.43
7:U:136:MET:HE3	7:U:163:CYS:CB	2.48	0.43
9:W:28:ASP:OD1	9:W:30:ASN:N	2.47	0.43
9:W:179:SER:O	9:W:181:ASN:N	2.52	0.43
10:X:57:ALA:O	10:X:61:GLN:HG3	2.18	0.43
11:Y:117:TYR:CE1	11:Y:132:HIS:CE1	3.07	0.43
12:Z:158:ARG:HD3	12:Z:199:TYR:HE2	1.83	0.43
13:1:14:ALA:C	13:1:15:ILE:HD12	2.42	0.43
14:2:49:THR:CG2	14:2:85:PRO:HA	2.48	0.43
7:G:141:SER:OG	7:G:144:ASP:HB2	2.19	0.43
7:G:168:ALA:HB1	7:G:171:ALA:HB3	2.00	0.43
9:I:191:VAL:O	9:I:191:VAL:HG12	2.17	0.43
12:L:51:ASP:O	12:L:55:TRP:HD1	2.01	0.43
4:R:34:GLY:O	4:R:158:ALA:HA	2.18	0.43
5:S:163:VAL:HG22	5:S:164:GLN:H	1.83	0.43
6:T:10:VAL:HG12	6:T:21:GLN:HB2	2.00	0.43
6:T:13:TRP:CH2	7:U:132:GLY:HA3	2.53	0.43
9:W:212:LEU:HD11	10:X:201:LYS:HA	2.01	0.43
12:Z:8:PHE:HB2	12:Z:145:TYR:O	2.19	0.43
3:C:15:GLU:HB2	3:C:17:ARG:HG2	2.00	0.43
3:C:44:LEU:HB3	3:C:215:THR:HG22	1.99	0.43
6:F:4:ASN:HA	6:F:7:ASP:OD2	2.18	0.43
14:N:49:THR:CG2	14:N:85:PRO:HA	2.48	0.43
1:O:141:ILE:HG22	1:O:151:VAL:HA	2.00	0.43
3:Q:235:GLN:O	3:Q:239:LYS:HB2	2.17	0.43
4:R:48:LYS:O	4:R:49:SER:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:24:ASN:CG	11:Y:25:ILE:N	2.76	0.43
1:A:143:ILE:CD1	1:A:220:VAL:HG13	2.48	0.43
1:A:240:VAL:CG2	1:A:241:ALA:N	2.82	0.43
3:C:32:GLY:HA2	3:C:50:ARG:HE	1.83	0.43
3:C:155:ASN:HD22	3:C:155:ASN:HA	1.61	0.43
3:C:155:ASN:CG	4:D:77:THR:HG21	2.43	0.43
3:C:210:LYS:O	3:C:211:VAL:HG13	2.19	0.43
4:D:155:ALA:HB3	5:E:63:SER:HB3	2.00	0.43
5:E:44:GLU:OE1	5:E:190:THR:HB	2.18	0.43
6:F:5:GLN:HG3	6:F:6:TYR:CE1	2.53	0.43
9:I:164:PHE:HB3	13:1:38:ARG:HH22	1.83	0.43
11:K:151:ILE:CG1	11:K:155:ARG:HB2	2.42	0.43
3:Q:86:LEU:HD13	3:Q:118:LYS:HD3	2.00	0.43
3:Q:229:LYS:O	3:Q:230:GLN:C	2.61	0.43
4:R:155:ALA:HB3	5:S:63:SER:HB3	1.99	0.43
9:W:151:ALA:C	9:W:153:ASN:N	2.76	0.43
13:1:1:ARG:CG	13:1:2:PHE:N	2.75	0.43
2:B:182:GLU:HB3	2:B:185:ASP:OD2	2.19	0.43
4:D:209:ALA:CB	4:D:219:ILE:HA	2.48	0.43
7:G:98:PHE:CE2	7:G:106:ILE:HA	2.53	0.43
8:H:188:VAL:HG12	8:H:190:LEU:HD23	2.01	0.43
11:K:117:TYR:CE1	11:K:132:HIS:CE1	3.07	0.43
11:K:148:THR:C	11:K:150:THR:H	2.26	0.43
3:Q:11:ILE:HG22	3:Q:12:PHE:N	2.33	0.43
9:W:50:ALA:HB2	10:X:129:CYS:HB2	2.00	0.43
9:W:59:ILE:HG13	9:W:83:LEU:CG	2.49	0.43
2:B:51:GLN:O	2:B:52:LYS:C	2.62	0.43
3:C:11:ILE:HG23	4:D:18:GLN:CD	2.44	0.43
7:G:61:GLY:O	7:G:64:LYS:HG3	2.18	0.43
7:G:77:VAL:HG12	7:G:135:PHE:HB3	2.01	0.43
12:L:19:ARG:NE	12:L:26:ILE:HD12	2.34	0.43
12:L:158:ARG:HD3	12:L:199:TYR:HE2	1.83	0.43
1:O:78:CYS:HB2	1:O:140:LEU:HD23	2.00	0.43
1:O:180:GLU:O	1:O:184:LYS:HE2	2.18	0.43
3:Q:62:SER:CB	3:Q:65:ILE:HB	2.49	0.43
3:Q:139:TRP:CD1	3:Q:144:GLY:HA2	2.54	0.43
3:Q:210:LYS:O	3:Q:211:VAL:HG13	2.18	0.43
6:T:71:GLY:HA3	6:T:221:PHE:CE1	2.53	0.43
12:Z:8:PHE:HA	12:Z:145:TYR:CD1	2.53	0.43
12:Z:38:ASN:C	12:Z:40:TYR:N	2.76	0.43
8:H:147:MET:HE1	8:H:155:PHE:CB	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:187:ARG:HA	9:I:187:ARG:HD2	1.86	0.43
13:M:13:LEU:HD12	13:M:14:ALA:H	1.82	0.43
13:M:75:TYR:CG	13:M:83:MET:HG3	2.54	0.43
13:M:162:GLU:O	13:M:162:GLU:HG2	2.19	0.43
13:M:211:ARG:NH2	9:W:193:ASN:CB	2.79	0.43
14:N:16:PHE:CZ	14:N:162:GLN:HG3	2.53	0.43
2:P:182:GLU:CG	2:P:183:LEU:H	2.27	0.43
2:P:227:ASP:C	2:P:229:LEU:N	2.77	0.43
4:R:4:ASP:C	4:R:122:ASN:HB3	2.44	0.43
4:R:169:ARG:O	4:R:173:GLU:HG3	2.18	0.43
6:T:148:CYS:O	6:T:150:SER:O	2.37	0.43
7:U:140:TYR:CG	7:U:217:GLY:HA2	2.53	0.43
10:X:7:ASN:HD22	10:X:56:LEU:HA	1.83	0.43
10:X:164:PHE:CE1	10:X:198:ARG:HD2	2.54	0.43
12:Z:186:ARG:HH11	12:Z:186:ARG:HB3	1.83	0.43
14:2:100:ARG:HD3	14:2:100:ARG:C	2.43	0.43
14:2:116:ALA:O	14:2:117:ASP:HB2	2.18	0.43
3:C:35:LEU:HD12	3:C:175:LEU:HD11	2.01	0.43
4:D:48:LYS:O	4:D:49:SER:C	2.61	0.43
4:D:69:VAL:HG12	4:D:70:CYS:N	2.33	0.43
4:D:82:ILE:O	4:D:86:ARG:HG3	2.19	0.43
5:E:27:ASP:OD2	5:E:27:ASP:C	2.62	0.43
7:G:74:GLY:HA3	7:G:224:HIS:NE2	2.33	0.43
8:H:19:ARG:O	8:H:33:LYS:NZ	2.52	0.43
12:L:105:ASP:HB3	12:L:106:LYS:H	1.57	0.43
13:M:176:LYS:CD	9:W:199:LEU:HD22	2.46	0.43
2:P:146:PHE:CE2	2:P:156:ALA:HB2	2.54	0.43
3:Q:234:GLU:HA	3:Q:237:ILE:HD12	2.01	0.43
4:R:132:LEU:HG	4:R:161:ILE:CD1	2.49	0.43
10:X:122:CYS:HB2	10:X:131:MET:O	2.18	0.43
12:Z:4:LEU:N	12:Z:100:MET:HE1	2.34	0.43
13:1:75:TYR:CD2	13:1:83:MET:HG3	2.54	0.43
1:A:51:VAL:O	1:A:51:VAL:HG13	2.19	0.43
4:D:42:VAL:CB	4:D:210:VAL:HG12	2.49	0.43
4:D:45:VAL:O	4:D:45:VAL:HG13	2.18	0.43
5:E:47:CYS:HB3	5:E:219:THR:HG22	2.00	0.43
7:G:187:ARG:HA	7:G:187:ARG:HD2	1.90	0.43
8:H:30:VAL:CG1	14:2:212:ALA:HA	2.49	0.43
8:H:50:ALA:N	9:I:118:SER:HB3	2.34	0.43
13:M:12:ILE:HD13	13:M:53:GLY:CA	2.49	0.43
3:Q:95:GLN:CA	3:Q:95:GLN:HE21	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:66:ASP:HA	11:Y:69:MET:HE2	2.01	0.43
6:T:4:ASN:HA	6:T:7:ASP:OD2	2.19	0.43
6:T:192:LEU:HD21	6:T:210:VAL:HG11	2.01	0.43
7:U:164:ALA:O	7:U:169:ARG:HG3	2.19	0.43
10:X:126:LEU:N	10:X:126:LEU:HD12	2.34	0.43
10:X:149:MET:HE2	10:X:173:ASN:HB2	1.99	0.43
4:D:202:GLY:C	4:D:204:LYS:N	2.77	0.42
5:E:47:CYS:CB	5:E:219:THR:HG22	2.49	0.42
5:E:118:ASN:C	5:E:120:ALA:H	2.26	0.42
6:F:10:VAL:HG12	6:F:21:GLN:HB3	2.00	0.42
8:H:20:THR:OG1	8:H:28:ASN:HB3	2.19	0.42
9:I:28:ASP:OD1	9:I:30:ASN:N	2.50	0.42
11:K:35:MET:CG	11:K:45:LEU:HD13	2.49	0.42
12:L:8:PHE:HA	12:L:145:TYR:CD1	2.54	0.42
13:M:75:TYR:CD2	13:M:83:MET:HG3	2.54	0.42
3:Q:35:LEU:HD12	3:Q:175:LEU:HD11	2.01	0.42
3:Q:218:ARG:O	3:Q:219:GLU:HG3	2.19	0.42
4:R:221:ASN:HD22	4:R:223:GLU:CB	2.32	0.42
5:S:155:HIS:O	5:S:162:PHE:HA	2.19	0.42
7:U:116:ALA:HB1	7:U:155:GLY:O	2.19	0.42
14:2:149:LEU:O	14:2:152:GLU:HB3	2.18	0.42
2:B:10:THR:O	3:C:128:ARG:HD3	2.19	0.42
3:C:2:SER:HB3	6:F:123:TYR:CE2	2.54	0.42
3:C:57:ASP:O	3:C:58:GLU:C	2.61	0.42
6:F:138:ASP:OD1	6:F:140:MET:HB2	2.19	0.42
7:G:90:ILE:CD1	7:G:118:TYR:CE2	3.00	0.42
9:I:163:ILE:HG23	9:I:170:GLY:HA2	2.01	0.42
11:K:66:LEU:HD21	11:K:70:ARG:HH11	1.84	0.42
12:L:81:LYS:HD3	12:L:120:ARG:NH1	2.34	0.42
14:N:25:ASP:O	14:N:41:ARG:HD3	2.19	0.42
2:P:182:GLU:HB3	2:P:185:ASP:OD2	2.18	0.42
3:Q:155:ASN:HD22	3:Q:155:ASN:HA	1.60	0.42
4:R:202:GLY:C	4:R:204:LYS:N	2.77	0.42
5:S:221:GLN:O	5:S:223:GLY:N	2.52	0.42
6:T:63:ILE:HA	6:T:72:ILE:O	2.19	0.42
13:1:151:ASN:ND2	13:1:152:GLN:HE21	2.18	0.42
1:A:88:ARG:NH2	7:G:157:SER:O	2.52	0.42
1:A:203:SER:O	1:A:207:SER:N	2.51	0.42
2:B:28:VAL:HG13	2:B:76:SER:O	2.18	0.42
2:B:142:ARG:HA	2:B:143:PRO:HD3	1.83	0.42
2:B:157:TRP:CD2	2:B:160:THR:HB	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:GLU:HA	3:C:237:ILE:HD12	2.02	0.42
9:I:113:ILE:HG12	9:I:119:THR:HG22	2.01	0.42
11:K:58:GLU:O	11:K:62:LYS:HD3	2.19	0.42
12:L:127:SER:HB3	12:L:136:TYR:CE1	2.54	0.42
13:M:151:ASN:ND2	13:M:152:GLN:HE21	2.17	0.42
1:O:240:VAL:CG2	1:O:241:ALA:N	2.82	0.42
3:Q:11:ILE:HG23	4:R:18:GLN:CD	2.44	0.42
4:R:52:LYS:C	4:R:54:GLN:H	2.27	0.42
5:S:163:VAL:HG22	5:S:164:GLN:N	2.34	0.42
7:U:42:LYS:HE2	7:U:185:THR:CG2	2.33	0.42
7:U:66:LEU:HD12	7:U:212:GLU:HB3	2.01	0.42
8:V:48:SER:HB3	8:V:51:ASP:HB2	2.01	0.42
9:W:209:THR:HG21	10:X:168:SER:HB3	2.02	0.42
13:1:136:LYS:HG3	13:1:137:ALA:N	2.35	0.42
13:1:195:ILE:HD12	13:1:195:ILE:N	2.34	0.42
14:2:10:SER:HB3	14:2:139:THR:O	2.19	0.42
1:A:39:SER:O	1:A:167:ALA:HA	2.18	0.42
2:B:33:PRO:HA	2:B:162:MET:O	2.19	0.42
3:C:11:ILE:HG23	4:D:18:GLN:NE2	2.34	0.42
3:C:11:ILE:HG22	3:C:12:PHE:N	2.34	0.42
3:C:95:GLN:CA	3:C:95:GLN:HE21	2.31	0.42
3:C:143:TYR:O	3:C:144:GLY:C	2.62	0.42
4:D:132:LEU:HG	4:D:161:ILE:CD1	2.50	0.42
6:F:38:LEU:HD22	6:F:187:LEU:CD1	2.49	0.42
6:F:44:ALA:HB3	6:F:215:VAL:HG13	2.02	0.42
6:F:236:LEU:HB3	6:F:237:GLU:H	1.36	0.42
9:I:68:LEU:HD12	9:I:68:LEU:HA	1.82	0.42
10:J:125:ASP:HB3	10:J:127:ILE:H	1.85	0.42
11:K:107:TYR:CD2	11:K:185:LYS:HA	2.54	0.42
11:K:108:ASP:HB3	11:K:111:GLU:HB2	2.02	0.42
12:L:8:PHE:HB2	12:L:145:TYR:O	2.19	0.42
12:L:38:ASN:C	12:L:40:TYR:N	2.78	0.42
12:L:180:ARG:HH11	12:L:180:ARG:HB2	1.84	0.42
5:S:47:CYS:HB3	5:S:219:THR:HG22	2.01	0.42
3:C:145:PHE:C	3:C:146:GLN:HG3	2.45	0.42
4:D:55:ASP:O	4:D:56:GLU:C	2.62	0.42
4:D:98:VAL:HG12	4:D:100:ASP:H	1.85	0.42
4:D:206:ILE:CG2	4:D:207:GLU:H	2.33	0.42
5:E:76:CYS:HA	5:E:142:LEU:O	2.19	0.42
9:I:151:ALA:C	9:I:153:ASN:N	2.76	0.42
1:O:22:LEU:CD1	2:P:78:MET:HE1	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:43:VAL:CG1	2:P:44:VAL:N	2.80	0.42
2:P:45:LEU:HD22	2:P:74:VAL:CG2	2.50	0.42
2:P:101:GLN:NE2	9:W:57:GLN:OE1	2.51	0.42
2:P:157:TRP:CD2	2:P:160:THR:HB	2.53	0.42
4:R:69:VAL:HG12	4:R:70:CYS:N	2.34	0.42
6:T:154:PHE:CD1	6:T:154:PHE:N	2.88	0.42
7:U:90:ILE:CD1	7:U:118:TYR:CE2	3.01	0.42
8:V:62:GLN:HB3	8:V:82:LEU:HD13	2.02	0.42
11:Y:66:LEU:HD21	11:Y:70:ARG:HH11	1.84	0.42
14:2:10:SER:HB3	14:2:142:GLY:H	1.85	0.42
3:C:17:ARG:HD2	3:C:22:GLU:OE2	2.20	0.42
5:E:56:SER:HA	5:E:57:PRO:HD3	1.89	0.42
6:F:13:TRP:NE1	7:G:129:ARG:HD2	2.34	0.42
6:F:206:THR:HG22	6:F:207:THR:N	2.34	0.42
7:G:164:ALA:O	7:G:169:ARG:HG3	2.20	0.42
9:I:143:ARG:NH1	9:I:150:GLU:OE1	2.53	0.42
2:P:178:ASN:OD1	2:P:179:GLU:N	2.51	0.42
3:Q:17:ARG:HD2	3:Q:22:GLU:OE2	2.20	0.42
4:R:45:VAL:HG13	4:R:45:VAL:O	2.19	0.42
4:R:98:VAL:HG12	4:R:100:ASP:H	1.84	0.42
5:S:65:GLU:OE1	5:S:68:VAL:HG12	2.19	0.42
6:T:5:GLN:HG3	6:T:6:TYR:CE1	2.54	0.42
7:U:129:ARG:HA	7:U:130:PRO:HD3	1.94	0.42
7:U:141:SER:OG	7:U:144:ASP:HB2	2.19	0.42
10:X:68:LYS:HZ3	10:X:72:ASN:HD21	1.67	0.42
11:Y:108:ASP:HB3	11:Y:111:GLU:HB2	2.00	0.42
12:Z:19:ARG:NE	12:Z:26:ILE:HD12	2.33	0.42
1:A:206:LEU:O	1:A:207:SER:C	2.62	0.42
3:C:140:ASP:C	3:C:142:HIS:N	2.77	0.42
4:D:116:GLN:C	4:D:116:GLN:CD	2.87	0.42
4:D:187:THR:C	4:D:189:LYS:H	2.27	0.42
4:D:221:ASN:HD22	4:D:223:GLU:CB	2.33	0.42
5:E:157:ASP:HB2	5:E:158:PRO:CD	2.50	0.42
1:O:206:LEU:O	1:O:207:SER:C	2.63	0.42
6:T:206:THR:HG22	6:T:207:THR:N	2.35	0.42
6:T:230:SER:CB	6:T:231:PRO:HD3	2.43	0.42
12:Z:76:VAL:HG23	12:Z:105:ASP:CG	2.45	0.42
12:Z:127:SER:HB3	12:Z:136:TYR:CE1	2.54	0.42
12:Z:158:ARG:HG3	12:Z:199:TYR:CE2	2.55	0.42
5:E:14:THR:HG23	6:F:21:GLN:HE22	1.83	0.42
9:I:67:SER:HA	16:I:307:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:38:THR:HA	1:O:169:GLY:HA3	2.02	0.42
1:O:101:TRP:CD1	1:O:101:TRP:C	2.97	0.42
1:O:188:ASP:O	1:O:190:THR:HG23	2.19	0.42
3:Q:32:GLY:HA2	3:Q:50:ARG:HE	1.85	0.42
4:R:129:ILE:O	4:R:129:ILE:HG13	2.17	0.42
4:R:187:THR:C	4:R:189:LYS:H	2.27	0.42
7:U:61:GLY:O	7:U:64:LYS:HG3	2.20	0.42
9:W:113:ILE:HG12	9:W:119:THR:HG22	2.02	0.42
9:W:211:VAL:HG11	10:X:198:ARG:HD3	2.01	0.42
9:W:216:ILE:HD13	10:X:196:THR:HG23	2.00	0.42
10:X:149:MET:HE3	10:X:153:LEU:HD11	2.01	0.42
11:Y:42:ILE:CG2	11:Y:104:LEU:HD11	2.50	0.42
13:1:20:PHE:CD1	13:1:168:LEU:HD13	2.55	0.42
13:1:75:TYR:CG	13:1:83:MET:HG3	2.55	0.42
1:A:13:ILE:HG13	1:A:15:ILE:HG23	2.01	0.42
3:C:192:LEU:O	3:C:196:VAL:HG23	2.19	0.42
7:G:87:LEU:HD23	7:G:87:LEU:HA	1.85	0.42
10:J:68:LYS:O	10:J:69:PHE:C	2.62	0.42
11:K:196:PHE:HA	11:K:197:PRO:HD3	1.77	0.42
13:M:141:ALA:O	13:M:142:SER:C	2.63	0.42
13:M:185:ARG:HG3	10:X:147:TYR:HB3	2.02	0.42
14:N:174:ARG:HE	14:N:205:THR:CG2	2.32	0.42
14:N:177:TYR:CD1	14:N:185:ASN:HB2	2.55	0.42
2:P:160:THR:OG1	2:P:170:LYS:NZ	2.52	0.42
3:Q:145:PHE:C	3:Q:146:GLN:HG3	2.45	0.42
4:R:26:VAL:HG22	4:R:129:ILE:HA	2.01	0.42
6:T:134:ILE:O	6:T:144:ILE:HA	2.19	0.42
9:W:3:ILE:CD1	9:W:127:MET:HB2	2.47	0.42
10:X:65:GLN:NE2	11:Y:86:ARG:HH21	2.17	0.42
10:X:126:LEU:HD12	10:X:126:LEU:H	1.85	0.42
11:Y:107:TYR:CD2	11:Y:185:LYS:HA	2.55	0.42
11:Y:142:ILE:O	11:Y:145:ARG:HB3	2.19	0.42
13:1:102:PHE:N	13:1:103:PRO:HD3	2.35	0.42
14:2:43:MET:HE3	14:2:45:VAL:HG23	2.01	0.42
14:2:193:THR:C	14:2:195:LYS:N	2.78	0.42
1:A:78:CYS:HB2	1:A:140:LEU:HD23	2.02	0.42
1:A:84:THR:O	1:A:87:SER:HB2	2.20	0.42
3:C:174:MET:HE1	3:C:199:LYS:CB	2.50	0.42
3:C:185:THR:H	3:C:188:SER:HG	1.62	0.42
6:F:121:GLN:HG3	7:G:129:ARG:HG3	2.02	0.42
8:H:133:SER:O	8:V:134:TYR:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:19:ARG:O	9:I:33:LYS:NZ	2.52	0.42
9:I:179:SER:O	9:I:181:ASN:N	2.53	0.42
9:I:209:THR:HG21	10:J:168:SER:HB3	2.01	0.42
13:M:195:ILE:N	13:M:195:ILE:HD12	2.34	0.42
2:P:171:THR:CA	2:P:174:GLU:HB2	2.47	0.42
4:R:107:ILE:O	4:R:111:ILE:HG13	2.20	0.42
8:V:38:HIS:ND1	8:V:39:ASP:N	2.68	0.42
8:V:98:ILE:HG22	8:V:99:ILE:N	2.35	0.42
13:1:14:ALA:O	13:1:135:PHE:HA	2.20	0.42
13:1:137:ALA:N	13:1:146:GLN:HE21	2.18	0.42
13:1:141:ALA:O	13:1:142:SER:C	2.63	0.42
2:B:232:ILE:O	2:B:233:ALA:HB3	2.20	0.41
4:D:34:GLY:O	4:D:158:ALA:HA	2.20	0.41
4:D:79:ASP:OD1	4:D:125:ARG:NH2	2.53	0.41
6:F:13:TRP:N	7:G:22:GLN:HE22	1.95	0.41
7:G:2:SER:O	7:G:3:ILE:C	2.63	0.41
8:H:38:HIS:O	8:H:39:ASP:C	2.62	0.41
9:I:212:LEU:HD11	10:J:201:LYS:HA	2.00	0.41
11:K:33:ASP:OD2	11:K:181:ARG:NH2	2.53	0.41
13:M:192:ALA:O	13:M:210:LEU:HD12	2.20	0.41
14:N:166:ARG:NH2	14:N:200:GLU:OE2	2.44	0.41
1:O:93:ARG:HG2	1:O:93:ARG:NH1	2.34	0.41
1:O:123:GLN:HE22	1:O:127:GLN:NE2	2.17	0.41
1:O:126:THR:CG2	2:P:127:ARG:HH21	2.19	0.41
3:Q:95:GLN:HA	3:Q:95:GLN:HE21	1.85	0.41
5:S:27:ASP:OD2	5:S:27:ASP:C	2.62	0.41
8:V:190:LEU:O	8:V:191:GLY:C	2.63	0.41
9:W:19:ARG:O	9:W:33:LYS:NZ	2.53	0.41
9:W:163:ILE:HG23	9:W:170:GLY:HA2	2.02	0.41
10:X:20:VAL:HB	10:X:190:ILE:CG1	2.50	0.41
10:X:190:ILE:HG22	10:X:195:ILE:HD13	1.99	0.41
12:Z:158:ARG:HG3	12:Z:199:TYR:HE2	1.84	0.41
13:1:150:ASP:HB3	13:1:156:LYS:HD2	2.02	0.41
4:D:4:ASP:C	4:D:122:ASN:HB3	2.44	0.41
4:D:129:ILE:O	4:D:129:ILE:HG13	2.17	0.41
9:I:43:CYS:SG	9:I:98:LEU:HB3	2.60	0.41
10:J:7:ASN:HA	10:J:29:GLY:O	2.21	0.41
12:L:186:ARG:CB	12:L:186:ARG:HH11	2.33	0.41
1:O:13:ILE:HG13	1:O:15:ILE:HG23	2.01	0.41
1:O:183:VAL:O	1:O:183:VAL:HG12	2.18	0.41
3:Q:192:LEU:O	3:Q:196:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:117:GLN:HB2	6:T:151:ALA:CB	2.50	0.41
7:U:210:GLU:HG2	7:U:211:LEU:N	2.35	0.41
7:U:227:VAL:HA	7:U:228:PRO:HD3	1.95	0.41
9:W:205:GLU:O	9:W:206:LYS:C	2.62	0.41
11:Y:78:THR:HG23	11:Y:116:TYR:OH	2.20	0.41
1:A:38:THR:HA	1:A:169:GLY:HA3	2.02	0.41
1:A:145:GLU:CG	1:A:146:GLU:N	2.83	0.41
2:B:134:LEU:HA	2:B:146:PHE:O	2.20	0.41
2:B:227:ASP:C	2:B:229:LEU:N	2.77	0.41
4:D:108:THR:HG23	4:D:133:ILE:HD12	2.02	0.41
5:E:99:HIS:CG	5:E:107:MET:HG3	2.54	0.41
8:H:148:THR:O	8:H:150:GLU:N	2.53	0.41
9:I:59:ILE:HG13	9:I:83:LEU:CG	2.50	0.41
10:J:190:ILE:HG22	10:J:195:ILE:HD13	2.00	0.41
1:O:88:ARG:NH2	7:U:157:SER:O	2.53	0.41
2:P:232:ILE:O	2:P:233:ALA:HB3	2.20	0.41
3:Q:140:ASP:OD1	3:Q:140:ASP:C	2.63	0.41
3:Q:174:MET:HE1	3:Q:199:LYS:CB	2.50	0.41
4:R:196:LEU:C	4:R:198:VAL:N	2.79	0.41
5:S:200:ILE:O	5:S:204:GLN:HG3	2.21	0.41
5:S:227:HIS:HE1	5:S:229:PHE:HA	1.85	0.41
7:U:179:LEU:O	7:U:181:MET:HE3	2.20	0.41
8:V:19:ARG:O	8:V:33:LYS:NZ	2.51	0.41
11:Y:35:MET:CG	11:Y:45:LEU:HD13	2.51	0.41
12:Z:15:ALA:HB2	12:Z:176:LEU:HD13	2.02	0.41
14:2:51:LEU:HD12	14:2:52:GLY:N	2.36	0.41
2:B:58:GLU:CD	2:B:58:GLU:H	2.28	0.41
2:B:70:HIS:CE1	2:B:103:PRO:HB3	2.56	0.41
2:B:223:THR:C	2:B:225:VAL:N	2.76	0.41
3:C:95:GLN:NE2	3:C:95:GLN:CA	2.83	0.41
7:G:136:MET:HE3	7:G:163:CYS:CB	2.49	0.41
8:H:38:HIS:ND1	8:H:39:ASP:N	2.67	0.41
11:K:26:VAL:HG12	11:Y:138:LEU:HD11	2.03	0.41
11:K:108:ASP:C	11:K:110:HIS:H	2.27	0.41
12:L:125:THR:HB	12:L:139:MET:HE1	1.99	0.41
13:M:12:ILE:O	13:M:137:ALA:HA	2.21	0.41
14:N:45:VAL:O	14:N:49:THR:O	2.38	0.41
14:N:122:LEU:HG	14:N:137:LEU:HD12	2.01	0.41
1:O:93:ARG:HG2	1:O:93:ARG:HH11	1.85	0.41
1:O:145:GLU:CG	1:O:146:GLU:N	2.83	0.41
2:P:191:ILE:HG22	2:P:202:MET:HE3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:57:ASP:O	3:Q:58:GLU:C	2.63	0.41
4:R:206:ILE:CG2	4:R:207:GLU:H	2.33	0.41
4:R:230:ALA:C	4:R:232:ILE:N	2.78	0.41
5:S:76:CYS:HA	5:S:142:LEU:O	2.20	0.41
5:S:78:MET:HE3	5:S:85:ALA:HB3	2.02	0.41
6:T:10:VAL:HG12	6:T:21:GLN:HB3	2.01	0.41
10:X:59:ASP:O	10:X:63:VAL:HG23	2.20	0.41
2:B:182:GLU:CG	2:B:183:LEU:H	2.27	0.41
5:E:189:MET:HE2	5:E:194:ALA:HB2	2.02	0.41
6:F:71:GLY:HA3	6:F:221:PHE:CE1	2.56	0.41
9:I:84:LYS:HE3	9:I:84:LYS:HB2	1.77	0.41
9:I:101:GLY:HA2	9:I:109:HIS:O	2.21	0.41
10:J:57:ALA:O	10:J:61:GLN:HG3	2.21	0.41
10:J:126:LEU:N	10:J:126:LEU:HD12	2.35	0.41
11:K:4:LEU:O	11:K:131:ALA:HA	2.21	0.41
12:L:115:ASP:HB2	12:L:119:ASN:HB2	2.02	0.41
14:N:59:ASP:HB2	14:N:108:ASN:HD21	1.85	0.41
1:O:142:GLY:HA2	1:O:220:VAL:HG11	2.01	0.41
2:P:58:GLU:CD	2:P:58:GLU:H	2.28	0.41
2:P:70:HIS:CE1	2:P:103:PRO:HB3	2.55	0.41
4:R:45:VAL:HG21	4:R:61:LYS:CB	2.51	0.41
4:R:52:LYS:HD3	4:R:52:LYS:HA	1.94	0.41
6:T:38:LEU:HD22	6:T:187:LEU:CD1	2.50	0.41
6:T:174:ARG:HG3	16:T:267:HOH:O	2.20	0.41
7:U:2:SER:O	7:U:3:ILE:C	2.64	0.41
7:U:152:ASP:OD2	7:U:152:ASP:C	2.62	0.41
9:W:179:SER:C	9:W:181:ASN:H	2.29	0.41
9:W:187:ARG:O	9:W:189:TYR:N	2.54	0.41
11:Y:148:THR:C	11:Y:150:THR:H	2.29	0.41
14:2:92:LEU:O	14:2:96:MET:HG2	2.21	0.41
1:A:32:ILE:HD11	1:A:156:PRO:HG2	2.03	0.41
3:C:136:TYR:O	3:C:147:LEU:HA	2.20	0.41
6:F:154:PHE:CD1	6:F:154:PHE:N	2.88	0.41
6:F:230:SER:HB2	6:F:231:PRO:CD	2.44	0.41
8:H:175:ARG:NH1	14:2:215:ILE:HD11	2.35	0.41
9:I:3:ILE:CD1	9:I:127:MET:HB2	2.46	0.41
9:I:171:SER:HB3	9:I:172:ASN:H	1.62	0.41
9:I:216:ILE:HD13	10:J:196:THR:HG23	2.02	0.41
11:K:24:ASN:CG	11:K:25:ILE:N	2.78	0.41
12:L:113:TYR:O	12:L:120:ARG:HA	2.21	0.41
14:N:51:LEU:HD12	14:N:52:GLY:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:13:SER:O	3:Q:23:TYR:HB3	2.21	0.41
2:P:173:LEU:O	2:P:175:LYS:N	2.54	0.41
3:Q:151:ASP:C	3:Q:153:SER:H	2.28	0.41
5:S:59:MET:SD	5:S:64:ILE:HD11	2.59	0.41
5:S:240:ASP:O	5:S:241:ILE:C	2.64	0.41
6:T:175:HIS:N	6:T:175:HIS:CD2	2.86	0.41
8:V:84:LYS:HE3	8:V:84:LYS:HB3	1.93	0.41
9:W:17:ASP:CG	9:W:33:LYS:HZ2	2.28	0.41
13:1:162:GLU:O	13:1:162:GLU:HG2	2.20	0.41
4:D:26:VAL:HG22	4:D:129:ILE:HA	2.01	0.41
5:E:155:HIS:O	5:E:162:PHE:HA	2.20	0.41
6:F:105:VAL:O	6:F:109:VAL:HG23	2.21	0.41
6:F:117:GLN:HB2	6:F:151:ALA:CB	2.50	0.41
7:G:67:PHE:CD1	7:G:67:PHE:N	2.88	0.41
7:G:76:ALA:O	7:G:135:PHE:HA	2.21	0.41
9:I:202:TYR:CE1	13:1:177:ASP:OD2	2.73	0.41
10:J:164:PHE:CD2	10:J:164:PHE:C	2.99	0.41
13:M:195:ILE:HG22	13:M:196:CYS:N	2.36	0.41
3:Q:243:GLU:CD	3:Q:243:GLU:C	2.89	0.41
4:R:168:VAL:O	4:R:172:LEU:HG	2.21	0.41
6:T:96:ARG:NH2	6:T:102:PRO:HB3	2.35	0.41
6:T:170:THR:O	6:T:174:ARG:HG3	2.21	0.41
6:T:237:GLU:O	6:T:239:ARG:N	2.51	0.41
7:U:99:ARG:NH1	14:2:69:GLN:HE22	2.18	0.41
8:V:20:THR:OG1	8:V:28:ASN:HB3	2.19	0.41
10:X:28:PHE:HB2	10:X:39:PHE:CG	2.56	0.41
10:X:168:SER:HB3	10:X:200:LEU:CD1	2.51	0.41
13:1:83:MET:HE2	13:1:88:ILE:CA	2.51	0.41
3:C:25:MET:O	3:C:28:ILE:HB	2.21	0.41
4:D:11:SER:HB3	4:D:12:PRO:CD	2.50	0.41
4:D:107:ILE:O	4:D:111:ILE:HG13	2.21	0.41
4:D:230:ALA:C	4:D:232:ILE:N	2.78	0.41
6:F:27:GLU:O	6:F:31:GLN:HG2	2.20	0.41
6:F:134:ILE:O	6:F:144:ILE:HA	2.21	0.41
7:G:227:VAL:HA	7:G:228:PRO:HD3	1.96	0.41
11:K:60:ILE:HD12	11:K:84:THR:HA	2.03	0.41
11:K:142:ILE:O	11:K:145:ARG:HB3	2.20	0.41
2:P:223:THR:C	2:P:225:VAL:N	2.77	0.41
7:U:87:LEU:HD23	7:U:87:LEU:HA	1.85	0.41
7:U:168:ALA:HB1	7:U:171:ALA:HB3	2.02	0.41
8:V:147:MET:HE1	8:V:155:PHE:CB	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:34:LEU:HG	10:X:35:VAL:N	2.22	0.41
12:Z:9:ARG:HH21	12:Z:146:ASP:CB	2.32	0.41
13:1:8:ASN:HA	13:1:30:SER:O	2.21	0.41
13:1:159:GLN:CD	13:1:160:ASN:N	2.78	0.41
14:2:25:ASP:HA	14:2:187:PHE:HB3	2.03	0.41
1:A:212:PRO:HB3	1:A:236:ASP:HB2	2.02	0.41
3:C:72:MET:CE	3:C:107:CYS:HA	2.51	0.41
4:D:66:ASP:CG	4:D:67:ASP:N	2.78	0.41
5:E:217:LEU:O	5:E:229:PHE:HB2	2.20	0.41
6:F:101:ARG:O	6:F:101:ARG:HG3	2.17	0.41
7:G:90:ILE:HD13	7:G:118:TYR:CD2	2.55	0.41
8:H:134:TYR:HA	8:V:133:SER:O	2.20	0.41
8:H:149:LYS:HZ1	8:H:185:GLU:CD	2.28	0.41
8:H:153:LEU:CD1	8:H:176:LEU:HD13	2.51	0.41
10:J:74:TYR:CE1	10:J:78:GLU:HG3	2.56	0.41
10:J:164:PHE:CE1	10:J:198:ARG:HD2	2.55	0.41
13:M:119:GLY:O	13:M:132:ARG:NH2	2.53	0.41
14:N:116:ALA:O	14:N:117:ASP:HB2	2.21	0.41
14:N:161:SER:OG	14:N:164:GLU:HG3	2.20	0.41
1:O:39:SER:O	1:O:167:ALA:HA	2.21	0.41
1:O:143:ILE:HD11	1:O:220:VAL:HG13	2.03	0.41
2:P:28:VAL:HG13	2:P:76:SER:O	2.21	0.41
2:P:227:ASP:O	2:P:228:TYR:C	2.63	0.41
3:Q:130:PHE:O	3:Q:152:PRO:HB3	2.21	0.41
3:Q:143:TYR:O	3:Q:144:GLY:C	2.63	0.41
4:R:85:ASN:O	4:R:89:VAL:HG23	2.20	0.41
4:R:175:ASN:HB2	4:R:190:LEU:HD11	2.03	0.41
5:S:28:ILE:HD13	5:S:158:PRO:HD2	2.01	0.41
6:T:43:HIS:ND1	6:T:184:LEU:HD13	2.36	0.41
6:T:159:MET:HE3	6:T:160:SER:H	1.85	0.41
7:U:69:VAL:HG11	7:U:91:ALA:HB1	2.03	0.41
7:U:98:PHE:CE2	7:U:106:ILE:HA	2.56	0.41
9:W:127:MET:C	9:W:131:SER:HB3	2.45	0.41
9:W:187:ARG:HD2	9:W:187:ARG:HA	1.85	0.41
10:X:22:ILE:CG2	10:X:188:HIS:HB2	2.51	0.41
10:X:65:GLN:NE2	11:Y:86:ARG:HH22	2.17	0.41
10:X:200:LEU:HD23	10:X:200:LEU:N	2.36	0.41
11:Y:151:ILE:CG1	11:Y:155:ARG:HB2	2.40	0.41
12:Z:4:LEU:HD12	12:Z:4:LEU:O	2.21	0.41
12:Z:4:LEU:HG	12:Z:160:ILE:HD11	2.03	0.41
12:Z:100:MET:HA	12:Z:112:TYR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:180:ARG:HH11	12:Z:180:ARG:HB2	1.85	0.41
13:1:141:ALA:O	13:1:144:MET:N	2.47	0.41
13:1:159:GLN:NE2	13:1:160:ASN:N	2.63	0.41
13:1:195:ILE:HG22	13:1:196:CYS:N	2.36	0.41
14:2:186:ARG:HA	14:2:203:LEU:O	2.21	0.41
3:C:44:LEU:HD13	3:C:44:LEU:H	1.86	0.41
3:C:87:THR:O	3:C:90:LEU:HB2	2.21	0.41
3:C:243:GLU:CD	3:C:243:GLU:C	2.89	0.41
5:E:78:MET:HE3	5:E:85:ALA:HB3	2.03	0.41
6:F:80:ASP:OD1	6:F:126:ARG:NH2	2.53	0.41
6:F:133:LEU:HD23	6:F:133:LEU:HA	1.97	0.41
7:G:152:ASP:OD2	7:G:152:ASP:C	2.64	0.41
9:I:50:ALA:HB2	10:J:129:CYS:HB2	2.03	0.41
10:J:68:LYS:HZ3	10:J:72:ASN:ND2	2.19	0.41
10:J:135:ASP:HA	10:J:154:TRP:CZ2	2.56	0.41
10:J:168:SER:HB3	10:J:200:LEU:CD1	2.51	0.41
10:J:201:LYS:HZ3	12:Z:197:GLU:CD	2.29	0.41
14:N:25:ASP:HA	14:N:187:PHE:HB3	2.02	0.41
1:O:191:PHE:HE1	1:O:219:VAL:HG21	1.85	0.41
2:P:227:ASP:O	2:P:229:LEU:N	2.54	0.41
5:S:149:LYS:HB2	5:S:152:GLN:NE2	2.36	0.41
6:T:138:ASP:OD1	6:T:140:MET:HB2	2.20	0.41
11:Y:160:LEU:HD11	11:Y:164:LEU:HD11	2.03	0.41
14:2:161:SER:O	14:2:162:GLN:C	2.62	0.41
3:C:130:PHE:O	3:C:152:PRO:HB3	2.20	0.40
3:C:140:ASP:OD1	3:C:140:ASP:C	2.64	0.40
3:C:241:GLU:O	3:C:243:GLU:N	2.45	0.40
4:D:171:PHE:CD2	4:D:194:ALA:HA	2.56	0.40
5:E:227:HIS:HE1	5:E:229:PHE:HA	1.86	0.40
6:F:47:VAL:CG1	6:F:195:LEU:HD22	2.52	0.40
6:F:159:MET:HE3	6:F:160:SER:H	1.86	0.40
5:S:47:CYS:CB	5:S:219:THR:HG22	2.50	0.40
7:U:67:PHE:CD1	7:U:67:PHE:N	2.88	0.40
9:W:106:THR:O	9:W:106:THR:CG2	2.69	0.40
11:Y:145:ARG:HH11	11:Y:145:ARG:HG3	1.86	0.40
14:2:161:SER:OG	14:2:164:GLU:HG3	2.21	0.40
3:C:62:SER:CB	3:C:65:ILE:HB	2.50	0.40
5:E:67:ILE:CG2	5:E:228:MET:HE1	2.51	0.40
5:E:221:GLN:O	5:E:223:GLY:N	2.54	0.40
6:F:132:LEU:HB2	6:F:147:THR:OG1	2.21	0.40
6:F:170:THR:O	6:F:174:ARG:HG3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:147:GLU:O	9:I:148:GLU:C	2.64	0.40
9:I:179:SER:C	9:I:181:ASN:H	2.29	0.40
11:K:10:PRO:HD2	11:K:12:TYR:HE2	1.85	0.40
11:K:145:ARG:HG3	11:K:145:ARG:NH1	2.36	0.40
12:L:9:ARG:HH21	12:L:146:ASP:CB	2.34	0.40
12:L:186:ARG:HH11	12:L:186:ARG:HB3	1.86	0.40
13:M:182:ALA:C	13:M:184:GLU:N	2.79	0.40
14:N:201:GLY:O	14:N:203:LEU:HG	2.21	0.40
3:Q:44:LEU:HD13	3:Q:44:LEU:H	1.86	0.40
3:Q:170:ALA:HB3	3:Q:200:THR:HG22	2.03	0.40
6:T:23:GLU:O	6:T:26:MET:HB2	2.21	0.40
6:T:47:VAL:CG1	6:T:195:LEU:HD22	2.52	0.40
9:W:155:VAL:O	9:W:159:ILE:HG12	2.21	0.40
13:I:125:ASP:OD1	13:I:125:ASP:C	2.64	0.40
3:C:245:ALA:HA	3:C:248:GLU:OE2	2.22	0.40
4:D:45:VAL:HG21	4:D:61:LYS:CB	2.52	0.40
6:F:192:LEU:HD21	6:F:210:VAL:HG11	2.02	0.40
7:G:116:ALA:HB1	7:G:155:GLY:O	2.20	0.40
7:G:210:GLU:HG2	7:G:211:LEU:N	2.36	0.40
8:H:101:ALA:HA	8:H:110:GLN:O	2.21	0.40
10:J:21:ALA:HA	10:J:188:HIS:O	2.21	0.40
10:J:45:MET:CE	10:J:67:LEU:HG	2.51	0.40
12:L:157:ARG:HH21	12:L:176:LEU:HD23	1.86	0.40
2:P:42:GLY:HA2	2:P:212:CYS:O	2.21	0.40
2:P:134:LEU:HA	2:P:146:PHE:O	2.21	0.40
3:Q:44:LEU:CD1	3:Q:44:LEU:N	2.85	0.40
4:R:62:ILE:HD12	4:R:62:ILE:H	1.84	0.40
4:R:82:ILE:O	4:R:86:ARG:HG3	2.22	0.40
6:T:80:ASP:OD1	6:T:126:ARG:NH2	2.54	0.40
6:T:132:LEU:O	6:T:146:GLN:HA	2.22	0.40
10:X:82:ILE:HD11	10:X:86:THR:CG2	2.51	0.40
12:Z:64:ARG:NH2	12:Z:68:LEU:HD21	2.37	0.40
12:Z:153:TYR:CD2	12:Z:187:VAL:HG11	2.55	0.40
3:C:44:LEU:N	3:C:44:LEU:CD1	2.84	0.40
3:C:145:PHE:HE2	3:C:217:THR:HA	1.86	0.40
4:D:175:ASN:HB2	4:D:190:LEU:HD11	2.03	0.40
7:G:168:ALA:CB	7:G:200:VAL:CG1	3.00	0.40
7:G:184:MET:HE2	7:G:189:ILE:HD13	2.02	0.40
8:H:190:LEU:O	8:H:191:GLY:C	2.64	0.40
9:I:15:GLY:O	9:I:16:ALA:HB2	2.20	0.40
10:J:28:PHE:HD2	10:J:36:THR:HB	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:65:GLN:NE2	11:K:86:ARG:HH21	2.17	0.40
10:J:84:PRO:HB3	10:J:120:PHE:CD2	2.57	0.40
10:J:136:PHE:HZ	10:J:151:GLU:OE2	2.05	0.40
1:O:51:VAL:O	1:O:51:VAL:HG13	2.19	0.40
3:Q:87:THR:O	3:Q:90:LEU:HB2	2.21	0.40
3:Q:167:ASN:O	3:Q:169:ALA:N	2.52	0.40
4:R:57:ARG:HG3	4:R:60:ARG:HH21	1.85	0.40
4:R:66:ASP:CG	4:R:67:ASP:N	2.79	0.40
12:Z:105:ASP:HB3	12:Z:106:LYS:H	1.57	0.40
14:2:45:VAL:O	14:2:49:THR:O	2.39	0.40
1:A:78:CYS:HB3	1:A:140:LEU:HD23	2.04	0.40
6:F:13:TRP:HD1	7:G:22:GLN:NE2	2.20	0.40
6:F:83:LEU:HD23	6:F:83:LEU:HA	1.96	0.40
9:I:132:LEU:O	14:2:145:LEU:HD23	2.21	0.40
13:M:136:LYS:HG3	13:M:137:ALA:N	2.36	0.40
3:Q:17:ARG:HB2	3:Q:22:GLU:OE2	2.21	0.40
3:Q:136:TYR:O	3:Q:147:LEU:HA	2.21	0.40
3:Q:241:GLU:O	3:Q:243:GLU:N	2.45	0.40
6:T:87:PHE:CD1	6:T:115:LYS:HD2	2.56	0.40
6:T:171:TYR:CD2	6:T:194:ALA:HB2	2.56	0.40
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.51	0.40
10:X:135:ASP:HA	10:X:154:TRP:CZ2	2.55	0.40
10:X:136:PHE:HZ	10:X:151:GLU:OE2	2.03	0.40
12:Z:81:LYS:HD3	12:Z:120:ARG:NH1	2.37	0.40
12:Z:125:THR:HB	12:Z:139:MET:HE1	2.00	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	242/246 (98%)	220 (91%)	19 (8%)	3 (1%)	10 20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	242/246 (98%)	220 (91%)	19 (8%)	3 (1%)	10	20
2	B	231/233 (99%)	185 (80%)	30 (13%)	16 (7%)	1	1
2	P	231/233 (99%)	188 (81%)	28 (12%)	15 (6%)	1	1
3	C	248/261 (95%)	201 (81%)	34 (14%)	13 (5%)	1	2
3	Q	248/261 (95%)	202 (82%)	33 (13%)	13 (5%)	1	2
4	D	241/248 (97%)	192 (80%)	33 (14%)	16 (7%)	1	1
4	R	241/248 (97%)	191 (79%)	34 (14%)	16 (7%)	1	1
5	E	232/241 (96%)	205 (88%)	24 (10%)	3 (1%)	9	18
5	S	232/241 (96%)	205 (88%)	24 (10%)	3 (1%)	9	18
6	F	236/263 (90%)	214 (91%)	16 (7%)	6 (2%)	4	8
6	T	236/263 (90%)	214 (91%)	17 (7%)	5 (2%)	5	11
7	G	243/254 (96%)	223 (92%)	14 (6%)	6 (2%)	4	8
7	U	243/254 (96%)	221 (91%)	16 (7%)	6 (2%)	4	8
8	H	200/205 (98%)	188 (94%)	9 (4%)	3 (2%)	8	15
8	V	200/205 (98%)	188 (94%)	9 (4%)	3 (2%)	8	15
9	I	218/234 (93%)	193 (88%)	21 (10%)	4 (2%)	6	13
9	W	218/234 (93%)	193 (88%)	21 (10%)	4 (2%)	6	13
10	J	202/205 (98%)	180 (89%)	18 (9%)	4 (2%)	6	11
10	X	202/205 (98%)	180 (89%)	18 (9%)	4 (2%)	6	11
11	K	197/201 (98%)	174 (88%)	20 (10%)	3 (2%)	8	15
11	Y	197/201 (98%)	174 (88%)	20 (10%)	3 (2%)	8	15
12	L	199/204 (98%)	180 (90%)	17 (8%)	2 (1%)	12	24
12	Z	199/204 (98%)	181 (91%)	16 (8%)	2 (1%)	12	24
13	1	211/213 (99%)	191 (90%)	19 (9%)	1 (0%)	24	43
13	M	211/213 (99%)	192 (91%)	18 (8%)	1 (0%)	24	43
14	2	215/219 (98%)	195 (91%)	16 (7%)	4 (2%)	6	12
14	N	215/219 (98%)	196 (91%)	15 (7%)	4 (2%)	6	12
All	All	6230/6454 (96%)	5486 (88%)	578 (9%)	166 (3%)	4	7

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	52	LYS
2	B	54	ILE
2	B	60	SER
2	B	179	GLU
2	B	183	LEU
2	B	232	ILE
3	C	58	GLU
3	C	141	LYS
3	C	206	LEU
4	D	46	GLU
4	D	47	LYS
4	D	59	VAL
4	D	198	VAL
4	D	213	ARG
4	D	243	LYS
5	E	120	ALA
5	E	226	PHE
6	F	151	ALA
6	F	236	LEU
7	G	204	VAL
7	G	207	LYS
7	G	216	VAL
8	H	9	ASP
9	I	187	ARG
14	N	46	ASN
2	P	52	LYS
2	P	60	SER
2	P	179	GLU
2	P	183	LEU
2	P	232	ILE
3	Q	58	GLU
3	Q	141	LYS
3	Q	206	LEU
4	R	46	GLU
4	R	47	LYS
4	R	59	VAL
4	R	198	VAL
4	R	213	ARG
4	R	243	LYS
5	S	120	ALA
5	S	226	PHE
6	T	151	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	204	VAL
7	U	207	LYS
7	U	216	VAL
8	V	9	ASP
9	W	187	ARG
14	2	46	ASN
1	A	186	LYS
2	B	19	VAL
2	B	176	ARG
2	B	198	PHE
2	B	230	ALA
3	C	181	GLU
3	C	201	MET
3	C	202	ASP
3	C	210	LYS
3	C	219	GLU
3	C	243	GLU
4	D	50	VAL
4	D	197	GLU
4	D	214	ASP
4	D	216	SER
8	H	191	GLY
9	I	180	LYS
10	J	101	GLY
11	K	110	HIS
12	L	187	VAL
14	N	201	GLY
1	O	186	LYS
2	P	19	VAL
2	P	41	ASN
2	P	176	ARG
2	P	198	PHE
2	P	230	ALA
3	Q	181	GLU
3	Q	201	MET
3	Q	202	ASP
3	Q	210	LYS
3	Q	219	GLU
3	Q	243	GLU
4	R	50	VAL
4	R	197	GLU
4	R	214	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	216	SER
8	V	191	GLY
9	W	180	LYS
10	X	101	GLY
11	Y	110	HIS
14	2	201	GLY
1	A	187	PHE
2	B	51	GLN
2	B	184	GLU
3	C	168	SER
4	D	54	GLN
4	D	56	GLU
4	D	61	LYS
7	G	4	GLY
9	I	91	ARG
9	I	152	LYS
10	J	171	MET
11	K	197	PRO
1	O	187	PHE
2	P	53	SER
2	P	184	GLU
3	Q	168	SER
4	R	52	LYS
4	R	54	GLN
4	R	56	GLU
7	U	4	GLY
9	W	91	ARG
9	W	152	LYS
11	Y	197	PRO
12	Z	187	VAL
1	A	63	SER
2	B	196	GLU
2	B	202	MET
4	D	52	LYS
4	D	138	PHE
6	F	139	ASP
6	F	184	LEU
7	G	205	LYS
13	M	2	PHE
14	N	9	THR
1	O	63	SER
2	P	196	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	202	MET
4	R	61	LYS
4	R	138	PHE
6	T	184	LEU
7	U	205	LYS
10	X	31	GLN
10	X	171	MET
12	Z	198	LYS
13	1	2	PHE
14	2	9	THR
2	B	197	SER
3	C	55	LEU
4	D	209	ALA
6	F	239	ARG
8	H	39	ASP
10	J	31	GLN
10	J	118	LYS
11	K	174	ASN
12	L	198	LYS
2	P	197	SER
3	Q	55	LEU
3	Q	199	LYS
4	R	209	ALA
6	T	139	ASP
6	T	238	GLU
10	X	118	LYS
11	Y	174	ASN
3	C	172	VAL
3	C	199	LYS
5	E	222	PRO
3	Q	172	VAL
5	S	222	PRO
6	T	201	ALA
8	V	39	ASP
6	F	240	PRO
14	N	215	ILE
14	2	215	ILE
7	G	3	ILE
7	U	3	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/210 (91%)	186 (97%)	6 (3%)	35	59
1	O	192/210 (91%)	186 (97%)	6 (3%)	35	59
2	B	163/190 (86%)	152 (93%)	11 (7%)	15	28
2	P	163/190 (86%)	152 (93%)	11 (7%)	15	28
3	C	191/221 (86%)	181 (95%)	10 (5%)	21	39
3	Q	191/221 (86%)	181 (95%)	10 (5%)	21	39
4	D	136/211 (64%)	127 (93%)	9 (7%)	15	29
4	R	136/211 (64%)	128 (94%)	8 (6%)	18	33
5	E	190/204 (93%)	183 (96%)	7 (4%)	30	54
5	S	190/204 (93%)	183 (96%)	7 (4%)	30	54
6	F	198/224 (88%)	192 (97%)	6 (3%)	36	60
6	T	198/224 (88%)	191 (96%)	7 (4%)	32	56
7	G	195/211 (92%)	186 (95%)	9 (5%)	24	45
7	U	195/211 (92%)	186 (95%)	9 (5%)	24	45
8	H	155/159 (98%)	149 (96%)	6 (4%)	28	51
8	V	155/159 (98%)	149 (96%)	6 (4%)	28	51
9	I	177/195 (91%)	170 (96%)	7 (4%)	28	50
9	W	177/195 (91%)	170 (96%)	7 (4%)	28	50
10	J	172/174 (99%)	162 (94%)	10 (6%)	18	34
10	X	172/174 (99%)	162 (94%)	10 (6%)	18	34
11	K	164/171 (96%)	156 (95%)	8 (5%)	22	43
11	Y	164/171 (96%)	156 (95%)	8 (5%)	22	43
12	L	153/159 (96%)	146 (95%)	7 (5%)	24	45
12	Z	153/159 (96%)	146 (95%)	7 (5%)	24	45
13	1	173/178 (97%)	167 (96%)	6 (4%)	32	56
13	M	173/178 (97%)	167 (96%)	6 (4%)	32	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2	174/181 (96%)	170 (98%)	4 (2%)	44	66
14	N	174/181 (96%)	170 (98%)	4 (2%)	44	66
All	All	4866/5376 (90%)	4654 (96%)	212 (4%)	25	47

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	CYS
1	A	108	GLU
1	A	114	LEU
1	A	145	GLU
1	A	166	THR
1	A	210	PHE
2	B	22	GLU
2	B	115	SER
2	B	131	VAL
2	B	132	SER
2	B	133	LEU
2	B	135	ILE
2	B	150	PRO
2	B	155	PHE
2	B	167	VAL
2	B	174	GLU
2	B	189	THR
3	C	44	LEU
3	C	82	ASP
3	C	106	PRO
3	C	133	SER
3	C	155	ASN
3	C	178	ASP
3	C	180	LYS
3	C	187	LYS
3	C	218	ARG
3	C	243	GLU
4	D	5	ARG
4	D	12	PRO
4	D	38	ARG
4	D	62	ILE
4	D	77	THR
4	D	103	THR
4	D	113	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	178	ASP
4	D	214	ASP
5	E	36	THR
5	E	78	MET
5	E	146	VAL
5	E	148	GLU
5	E	213	THR
5	E	217	LEU
5	E	221	GLN
6	F	38	LEU
6	F	62	LYS
6	F	125	ARG
6	F	149	PRO
6	F	202	GLU
6	F	209	ASN
7	G	39	ILE
7	G	67	PHE
7	G	69	VAL
7	G	129	ARG
7	G	133	CYS
7	G	170	GLN
7	G	181	MET
7	G	215	TRP
7	G	218	GLU
8	H	30	VAL
8	H	95	MET
8	H	110	GLN
8	H	124	SER
8	H	139	VAL
8	H	182	SER
9	I	40	ASN
9	I	52	THR
9	I	56	THR
9	I	132	LEU
9	I	153	ASN
9	I	184	ASP
9	I	208	THR
10	J	26	ARG
10	J	34	LEU
10	J	36	THR
10	J	49	LEU
10	J	60	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	84	PRO
10	J	126	LEU
10	J	145	GLN
10	J	156	PRO
10	J	189	ILE
11	K	8	GLN
11	K	27	GLN
11	K	45	LEU
11	K	84	THR
11	K	85	ARG
11	K	118	MET
11	K	177	THR
11	K	190	ASP
12	L	8	PHE
12	L	87	VAL
12	L	102	CYS
12	L	138	VAL
12	L	180	ARG
12	L	182	ASP
12	L	190	ASP
13	M	30	SER
13	M	140	SER
13	M	159	GLN
13	M	164	VAL
13	M	167	SER
13	M	170	ARG
14	N	10	SER
14	N	46	ASN
14	N	94	ARG
14	N	168	LEU
1	O	78	CYS
1	O	108	GLU
1	O	114	LEU
1	O	145	GLU
1	O	166	THR
1	O	210	PHE
2	P	22	GLU
2	P	115	SER
2	P	131	VAL
2	P	132	SER
2	P	133	LEU
2	P	135	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	150	PRO
2	P	155	PHE
2	P	167	VAL
2	P	174	GLU
2	P	189	THR
3	Q	44	LEU
3	Q	82	ASP
3	Q	106	PRO
3	Q	133	SER
3	Q	155	ASN
3	Q	178	ASP
3	Q	180	LYS
3	Q	187	LYS
3	Q	218	ARG
3	Q	243	GLU
4	R	5	ARG
4	R	38	ARG
4	R	62	ILE
4	R	77	THR
4	R	103	THR
4	R	113	SER
4	R	178	ASP
4	R	214	ASP
5	S	36	THR
5	S	78	MET
5	S	146	VAL
5	S	148	GLU
5	S	213	THR
5	S	217	LEU
5	S	221	GLN
6	T	38	LEU
6	T	62	LYS
6	T	125	ARG
6	T	126	ARG
6	T	149	PRO
6	T	202	GLU
6	T	209	ASN
7	U	39	ILE
7	U	67	PHE
7	U	69	VAL
7	U	129	ARG
7	U	133	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	170	GLN
7	U	181	MET
7	U	215	TRP
7	U	218	GLU
8	V	30	VAL
8	V	95	MET
8	V	110	GLN
8	V	124	SER
8	V	139	VAL
8	V	182	SER
9	W	40	ASN
9	W	52	THR
9	W	56	THR
9	W	132	LEU
9	W	153	ASN
9	W	184	ASP
9	W	208	THR
10	X	26	ARG
10	X	34	LEU
10	X	36	THR
10	X	49	LEU
10	X	60	VAL
10	X	84	PRO
10	X	126	LEU
10	X	145	GLN
10	X	156	PRO
10	X	189	ILE
11	Y	8	GLN
11	Y	27	GLN
11	Y	45	LEU
11	Y	84	THR
11	Y	85	ARG
11	Y	118	MET
11	Y	177	THR
11	Y	190	ASP
12	Z	8	PHE
12	Z	87	VAL
12	Z	102	CYS
12	Z	138	VAL
12	Z	180	ARG
12	Z	182	ASP
12	Z	190	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1	30	SER
13	1	140	SER
13	1	159	GLN
13	1	164	VAL
13	1	167	SER
13	1	170	ARG
14	2	10	SER
14	2	46	ASN
14	2	94	ARG
14	2	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (185) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	33	ASN
1	A	53	GLN
1	A	68	HIS
1	A	92	GLN
1	A	127	GLN
1	A	172	GLN
1	A	238	HIS
2	B	41	ASN
2	B	108	GLN
2	B	111	GLN
2	B	122	GLN
2	B	165	ASN
2	B	206	ASN
2	B	213	ASN
3	C	69	ASN
3	C	95	GLN
3	C	100	GLN
3	C	109	GLN
3	C	123	GLN
3	C	155	ASN
3	C	166	ASN
3	C	167	ASN
3	C	198	ASN
3	C	220	ASN
3	C	235	GLN
3	C	240	HIS
4	D	15	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	23	GLN
4	D	92	GLN
4	D	200	GLN
5	E	99	HIS
5	E	152	GLN
5	E	164	GLN
5	E	182	GLN
5	E	204	GLN
5	E	211	ASN
5	E	221	GLN
5	E	224	GLN
5	E	227	HIS
6	F	5	GLN
6	F	8	ASN
6	F	20	HIS
6	F	43	HIS
6	F	86	ASN
6	F	146	GLN
6	F	175	HIS
6	F	203	GLN
6	F	209	ASN
7	G	22	GLN
7	G	201	HIS
8	H	7	GLN
8	H	62	GLN
8	H	106	GLN
8	H	110	GLN
8	H	154	GLN
8	H	158	ASN
9	I	30	ASN
9	I	40	ASN
9	I	66	HIS
9	I	116	HIS
9	I	153	ASN
10	J	7	ASN
10	J	40	GLN
10	J	65	GLN
10	J	72	ASN
10	J	81	GLN
10	J	145	GLN
11	K	8	GLN
11	K	24	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	61	GLN
11	K	99	HIS
11	K	132	HIS
11	K	193	ASN
12	L	10	HIS
12	L	29	GLN
12	L	178	HIS
13	M	8	ASN
13	M	77	HIS
13	M	79	ASN
13	M	108	ASN
13	M	146	GLN
13	M	151	ASN
13	M	152	GLN
13	M	159	GLN
13	M	160	ASN
14	N	46	ASN
14	N	69	GLN
14	N	81	HIS
14	N	108	ASN
14	N	157	GLN
14	N	208	ASN
14	N	213	HIS
1	O	12	HIS
1	O	33	ASN
1	O	53	GLN
1	O	68	HIS
1	O	90	GLN
1	O	92	GLN
1	O	127	GLN
1	O	172	GLN
1	O	238	HIS
2	P	41	ASN
2	P	108	GLN
2	P	111	GLN
2	P	122	GLN
2	P	165	ASN
2	P	206	ASN
2	P	213	ASN
3	Q	69	ASN
3	Q	95	GLN
3	Q	100	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	109	GLN
3	Q	123	GLN
3	Q	155	ASN
3	Q	166	ASN
3	Q	167	ASN
3	Q	198	ASN
3	Q	220	ASN
3	Q	235	GLN
3	Q	240	HIS
4	R	15	HIS
4	R	23	GLN
4	R	92	GLN
4	R	200	GLN
5	S	99	HIS
5	S	152	GLN
5	S	164	GLN
5	S	182	GLN
5	S	204	GLN
5	S	211	ASN
5	S	221	GLN
5	S	224	GLN
5	S	227	HIS
6	T	5	GLN
6	T	8	ASN
6	T	43	HIS
6	T	86	ASN
6	T	146	GLN
6	T	166	GLN
6	T	175	HIS
6	T	203	GLN
6	T	209	ASN
7	U	22	GLN
7	U	201	HIS
8	V	7	GLN
8	V	62	GLN
8	V	106	GLN
8	V	110	GLN
8	V	154	GLN
8	V	158	ASN
9	W	30	ASN
9	W	40	ASN
9	W	66	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	W	116	HIS
9	W	153	ASN
9	W	165	ASN
10	X	7	ASN
10	X	40	GLN
10	X	65	GLN
10	X	72	ASN
10	X	81	GLN
10	X	145	GLN
11	Y	8	GLN
11	Y	24	ASN
11	Y	61	GLN
11	Y	99	HIS
11	Y	132	HIS
12	Z	10	HIS
12	Z	29	GLN
12	Z	178	HIS
13	1	8	ASN
13	1	77	HIS
13	1	79	ASN
13	1	108	ASN
13	1	146	GLN
13	1	151	ASN
13	1	152	GLN
13	1	159	GLN
14	2	46	ASN
14	2	69	GLN
14	2	108	ASN
14	2	157	GLN
14	2	208	ASN
14	2	213	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	244/246 (99%)	1.36	58 (23%) 2 1	56, 89, 120, 135	0
1	O	244/246 (99%)	0.20	6 (2%) 58 56	38, 56, 81, 100	0
2	B	233/233 (100%)	1.51	59 (25%) 1 1	62, 97, 133, 142	0
2	P	233/233 (100%)	0.61	15 (6%) 25 25	36, 67, 105, 129	0
3	C	250/261 (95%)	1.52	67 (26%) 1 1	59, 103, 142, 148	0
3	Q	250/261 (95%)	0.80	15 (6%) 27 28	37, 70, 123, 141	0
4	D	243/248 (97%)	1.23	39 (16%) 5 4	54, 93, 146, 163	0
4	R	243/248 (97%)	1.13	51 (20%) 2 2	40, 82, 134, 157	0
5	E	234/241 (97%)	0.40	9 (3%) 44 41	39, 64, 94, 110	0
5	S	234/241 (97%)	0.73	18 (7%) 19 19	39, 74, 102, 132	0
6	F	238/263 (90%)	0.35	5 (2%) 63 61	42, 63, 91, 124	0
6	T	238/263 (90%)	0.34	10 (4%) 40 39	37, 58, 95, 135	0
7	G	245/254 (96%)	0.84	19 (7%) 19 19	49, 74, 104, 118	0
7	U	245/254 (96%)	0.19	9 (3%) 45 42	35, 53, 89, 126	0
8	H	202/205 (98%)	0.47	2 (0%) 79 79	35, 60, 78, 94	0
8	V	202/205 (98%)	0.17	4 (1%) 65 63	33, 49, 70, 102	0
9	I	220/234 (94%)	1.01	20 (9%) 15 14	49, 71, 100, 115	0
9	W	220/234 (94%)	0.17	0 100 100	30, 53, 81, 99	0
10	J	204/205 (99%)	1.20	34 (16%) 4 4	49, 79, 101, 111	0
10	X	204/205 (99%)	0.33	7 (3%) 48 46	36, 52, 78, 97	0
11	K	199/201 (99%)	0.86	15 (7%) 20 20	49, 69, 93, 110	0
11	Y	199/201 (99%)	0.43	6 (3%) 52 50	36, 56, 80, 113	0
12	L	201/204 (98%)	0.24	5 (2%) 58 56	35, 53, 75, 108	0
12	Z	201/204 (98%)	0.72	10 (4%) 34 34	45, 65, 85, 106	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%)	0.73	17 (7%) 18 18	40, 70, 97, 112	0
13	M	213/213 (100%)	0.06	1 (0%) 87 87	31, 50, 73, 97	0
14	2	217/219 (99%)	0.33	4 (1%) 67 65	33, 55, 81, 109	0
14	N	217/219 (99%)	0.09	3 (1%) 73 73	33, 51, 70, 109	0
All	All	6286/6454 (97%)	0.65	508 (8%) 18 18	30, 66, 115, 163	0

All (508) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ALA	6.5
13	1	166	LEU	5.8
3	C	171	ALA	5.4
2	P	1	ALA	5.3
2	P	233	ALA	4.9
14	N	215	ILE	4.7
4	R	228	TYR	4.5
11	K	199	GLN	4.3
2	B	207	ILE	4.3
3	C	172	VAL	4.3
4	D	228	TYR	4.2
2	P	232	ILE	4.2
2	B	45	LEU	4.2
5	S	27	ASP	4.1
1	A	183	VAL	4.1
11	Y	199	GLN	4.0
8	H	202	LEU	4.0
2	B	53	SER	4.0
4	R	40	ILE	4.0
8	V	202	LEU	4.0
3	Q	203	VAL	4.0
3	C	51	ASN	3.9
4	R	136	PHE	3.9
11	Y	198	LYS	3.8
4	R	104	VAL	3.8
5	E	8	TYR	3.7
2	B	150	PRO	3.7
2	B	155	PHE	3.7
4	D	220	LEU	3.7
3	C	194	ILE	3.7
2	B	44	VAL	3.7
10	J	84	PRO	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2	215	ILE	3.7
6	T	241	GLN	3.7
4	D	102	VAL	3.6
1	A	42	VAL	3.6
4	R	232	ILE	3.6
7	G	36	ALA	3.6
1	A	245	ARG	3.5
4	D	49	SER	3.5
3	Q	200	THR	3.5
3	C	80	THR	3.5
5	S	214	ASN	3.5
13	1	182	ALA	3.5
4	R	41	VAL	3.5
1	A	141	ILE	3.4
4	R	220	LEU	3.4
10	J	51	ILE	3.4
4	D	176	TYR	3.4
1	A	200	THR	3.4
1	A	142	GLY	3.4
1	A	140	LEU	3.4
2	B	46	ALA	3.4
3	Q	206	LEU	3.4
2	B	210	GLY	3.4
4	D	207	GLU	3.4
2	B	67	ILE	3.3
12	Z	175	ASN	3.3
4	D	217	LEU	3.3
4	R	47	LYS	3.3
10	J	46	GLY	3.3
2	P	198	PHE	3.3
3	C	168	SER	3.3
3	C	236	LEU	3.3
4	R	44	GLY	3.3
3	C	206	LEU	3.2
1	A	50	ILE	3.2
2	B	167	VAL	3.2
3	C	228	LEU	3.2
6	T	238	GLU	3.2
7	U	215	TRP	3.2
10	X	117	PHE	3.2
1	A	78	CYS	3.2
12	L	201	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2	217	GLY	3.2
1	A	198	ALA	3.2
3	C	170	ALA	3.2
9	I	173	ILE	3.2
2	P	139	ASN	3.1
5	S	237	VAL	3.1
3	C	55	LEU	3.1
10	J	107	PRO	3.1
4	D	136	PHE	3.1
3	C	157	GLY	3.1
11	K	198	LYS	3.1
2	B	135	ILE	3.1
2	P	40	ALA	3.1
3	C	213	ILE	3.1
2	B	157	TRP	3.1
5	S	241	ILE	3.0
11	K	106	GLY	3.0
1	A	233	ALA	3.0
3	Q	58	GLU	3.0
2	B	35	VAL	3.0
1	A	242	LEU	3.0
2	B	173	LEU	3.0
5	S	234	LEU	3.0
5	E	214	ASN	3.0
7	G	169	ARG	3.0
3	C	36	GLY	3.0
1	A	241	ALA	3.0
1	A	227	PHE	3.0
3	Q	61	PHE	3.0
4	R	196	LEU	3.0
2	B	146	PHE	3.0
2	B	181	LEU	2.9
3	C	110	LEU	2.9
11	Y	173	LEU	2.9
10	J	20	VAL	2.9
3	C	216	LEU	2.9
7	U	245	GLU	2.9
9	I	197	THR	2.9
3	C	47	ALA	2.9
4	R	45	VAL	2.9
10	J	108	VAL	2.9
3	C	175	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	208	LEU	2.9
6	T	56	LEU	2.9
2	B	82	TYR	2.9
3	C	156	TYR	2.9
7	G	39	ILE	2.9
10	J	189	ILE	2.9
9	I	196	GLY	2.9
10	J	16	GLY	2.9
2	P	231	ALA	2.9
2	B	131	VAL	2.9
10	J	185	VAL	2.9
1	O	2	SER	2.9
14	2	216	SER	2.9
3	C	161	ALA	2.9
2	B	228	TYR	2.8
3	C	147	LEU	2.8
9	I	211	VAL	2.8
6	T	240	PRO	2.8
5	E	241	ILE	2.8
10	X	189	ILE	2.8
11	K	187	GLY	2.8
1	A	179	LEU	2.8
4	R	182	GLU	2.8
2	B	211	ILE	2.8
10	J	112	LEU	2.8
1	A	195	VAL	2.8
3	C	19	TYR	2.8
3	C	46	ALA	2.8
3	C	240	HIS	2.8
4	R	191	VAL	2.8
4	R	210	VAL	2.8
8	V	201	THR	2.8
9	I	199	LEU	2.7
10	J	49	LEU	2.7
1	A	217	VAL	2.7
3	C	76	VAL	2.7
3	Q	37	ILE	2.7
2	B	134	LEU	2.7
14	N	217	GLY	2.7
2	B	187	ILE	2.7
3	C	164	ILE	2.7
2	P	181	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	104	ASP	2.7
9	I	74	PRO	2.7
2	B	54	ILE	2.7
5	E	58	LEU	2.7
4	D	203	GLY	2.7
7	G	14	PHE	2.7
10	J	11	VAL	2.7
4	D	101	PRO	2.7
10	J	205	ASP	2.7
5	S	164	GLN	2.6
11	K	43	LEU	2.6
4	R	231	GLU	2.6
13	1	151	ASN	2.6
2	B	159	ALA	2.6
4	R	229	VAL	2.6
1	A	156	PRO	2.6
9	I	106	THR	2.6
13	1	165	PRO	2.6
1	A	188	ASP	2.6
2	B	104	ILE	2.6
4	D	219	ILE	2.6
10	J	45	MET	2.6
7	U	41	CYS	2.6
2	B	140	GLU	2.6
4	R	134	VAL	2.6
4	R	239	ASN	2.6
2	B	132	SER	2.6
12	Z	173	ALA	2.6
7	U	5	THR	2.6
2	P	37	ILE	2.6
3	C	37	ILE	2.6
4	R	188	ILE	2.6
1	A	61	LEU	2.6
3	C	190	LEU	2.6
9	I	15	GLY	2.6
1	A	48	ALA	2.6
1	A	219	VAL	2.6
1	O	205	VAL	2.6
2	B	186	ALA	2.6
3	C	59	VAL	2.6
6	T	201	ALA	2.6
3	C	162	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	187	THR	2.6
4	D	172	LEU	2.6
10	J	163	LEU	2.6
12	L	147	LEU	2.6
4	D	238	GLU	2.6
2	B	198	PHE	2.6
3	C	193	ALA	2.6
4	D	138	PHE	2.6
11	K	50	ALA	2.6
6	F	60	GLN	2.6
4	D	185	ASP	2.5
11	Y	107	TYR	2.5
3	C	250	GLU	2.5
1	A	212	PRO	2.5
1	A	225	PRO	2.5
2	B	64	VAL	2.5
9	I	76	VAL	2.5
4	R	244	GLN	2.5
10	J	110	ALA	2.5
2	B	206	ASN	2.5
9	I	12	ILE	2.5
5	E	186	HIS	2.5
5	S	8	TYR	2.5
10	X	85	TYR	2.5
1	A	40	VAL	2.5
2	B	86	VAL	2.5
3	C	111	VAL	2.5
4	D	41	VAL	2.5
4	D	175	ASN	2.5
12	Z	38	ASN	2.5
1	A	189	TRP	2.5
3	C	45	LEU	2.5
3	Q	236	LEU	2.5
5	E	27	ASP	2.5
13	1	168	LEU	2.5
4	D	75	GLY	2.5
10	X	160	PRO	2.5
3	C	24	ALA	2.5
1	A	190	THR	2.5
4	D	47	LYS	2.5
5	S	67	ILE	2.5
12	L	115	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	166	TYR	2.5
5	E	131	GLY	2.5
12	Z	40	TYR	2.5
3	C	211	VAL	2.5
2	B	156	ALA	2.5
5	E	211	ASN	2.4
4	D	96	LEU	2.4
4	R	195	LEU	2.4
9	I	34	ILE	2.4
9	I	65	LEU	2.4
10	J	121	ILE	2.4
4	R	42	VAL	2.4
13	1	159	GLN	2.4
3	Q	50	ARG	2.4
2	B	9	LEU	2.4
2	B	229	LEU	2.4
7	G	54	LEU	2.4
7	U	143	ASN	2.4
2	B	188	HIS	2.4
14	N	216	SER	2.4
1	A	115	CYS	2.4
1	O	188	ASP	2.4
4	R	67	ASP	2.4
3	C	212	GLU	2.4
4	D	231	GLU	2.4
7	U	4	GLY	2.4
2	B	37	ILE	2.4
5	S	215	ILE	2.4
13	1	149	LEU	2.4
2	B	139	ASN	2.4
6	T	182	CYS	2.4
4	R	211	MET	2.4
4	D	128	GLY	2.4
7	G	38	GLY	2.4
11	K	77	PRO	2.4
3	C	177	GLN	2.4
3	C	227	VAL	2.4
1	O	245	ARG	2.4
2	B	107	ALA	2.4
2	B	133	LEU	2.4
3	C	38	LEU	2.4
4	R	208	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	204	THR	2.4
3	C	215	THR	2.4
3	C	166	ASN	2.4
10	J	173	ASN	2.4
2	B	148	SER	2.4
2	P	2	GLU	2.4
1	O	155	ASP	2.4
4	D	37	GLY	2.4
4	D	135	GLY	2.4
5	S	144	GLY	2.4
2	B	59	ARG	2.4
1	A	167	ALA	2.4
2	B	230	ALA	2.4
2	P	172	PHE	2.4
4	R	230	ALA	2.4
4	R	132	LEU	2.3
1	A	73	THR	2.3
1	A	196	GLU	2.3
7	G	245	GLU	2.3
14	2	214	MET	2.3
1	O	62	ASP	2.3
13	1	43	CYS	2.3
2	B	72	GLY	2.3
6	F	241	GLN	2.3
10	J	180	VAL	2.3
2	B	190	ALA	2.3
7	G	21	PHE	2.3
12	Z	185	ILE	2.3
10	J	85	TYR	2.3
3	Q	69	ASN	2.3
11	K	154	GLU	2.3
4	R	201	SER	2.3
12	Z	201	GLY	2.3
4	D	33	VAL	2.3
1	A	191	PHE	2.3
6	F	236	LEU	2.3
1	A	199	ILE	2.3
3	C	200	THR	2.3
2	B	170	LYS	2.3
3	Q	251	LYS	2.3
2	P	44	VAL	2.3
1	A	243	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	231	ALA	2.3
10	J	109	ILE	2.3
1	A	197	THR	2.3
11	K	41	LYS	2.3
4	D	68	ASN	2.3
9	I	188	PRO	2.3
12	Z	105	ASP	2.3
4	R	33	VAL	2.3
4	R	43	LEU	2.3
3	C	79	ILE	2.2
11	K	114	ALA	2.2
12	Z	10	HIS	2.2
1	A	52	THR	2.2
9	I	40	ASN	2.2
10	X	156	PRO	2.2
13	1	209	SER	2.2
4	R	102	VAL	2.2
7	G	216	VAL	2.2
13	1	175	VAL	2.2
1	A	226	LYS	2.2
3	C	222	LYS	2.2
3	C	237	ILE	2.2
4	D	161	ILE	2.2
4	R	192	ILE	2.2
9	I	159	ILE	2.2
13	1	20	PHE	2.2
5	E	183	GLU	2.2
2	B	51	GLN	2.2
3	C	68	LEU	2.2
3	C	90	LEU	2.2
5	S	184	LEU	2.2
2	B	84	VAL	2.2
3	C	224	VAL	2.2
4	D	198	VAL	2.2
4	D	210	VAL	2.2
4	D	234	LYS	2.2
8	H	103	TRP	2.2
4	D	188	ILE	2.2
4	R	206	ILE	2.2
11	K	5	ILE	2.2
10	J	143	ALA	2.2
4	R	97	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	13	THR	2.2
7	G	238	TYR	2.2
12	Z	199	TYR	2.2
2	B	147	GLN	2.2
3	C	146	GLN	2.2
4	R	185	ASP	2.2
7	G	222	GLY	2.2
7	U	6	GLY	2.2
3	C	150	SER	2.2
10	J	71	LEU	2.2
13	1	167	SER	2.2
2	B	202	MET	2.2
3	C	203	VAL	2.2
4	R	198	VAL	2.2
7	G	46	VAL	2.2
1	A	76	ILE	2.2
1	A	187	PHE	2.2
10	J	164	PHE	2.2
11	Y	182	ILE	2.2
1	A	130	GLU	2.2
1	A	166	THR	2.2
1	A	194	THR	2.2
12	L	199	TYR	2.2
1	A	181	LYS	2.2
1	A	36	GLY	2.2
2	B	55	LEU	2.2
3	C	186	LEU	2.2
3	Q	192	LEU	2.2
1	A	12	HIS	2.2
2	B	126	VAL	2.2
3	C	85	VAL	2.2
4	D	206	ILE	2.2
10	J	82	ILE	2.2
4	R	238	GLU	2.1
7	U	186	CYS	2.1
4	D	241	LYS	2.1
4	R	68	ASN	2.1
1	A	60	LEU	2.1
2	P	202	MET	2.1
4	R	96	LEU	2.1
3	C	105	ILE	2.1
3	Q	240	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	29	PHE	2.1
3	C	169	ALA	2.1
6	F	151	ALA	2.1
8	V	200	ALA	2.1
12	Z	24	ALA	2.1
6	T	55	GLU	2.1
6	T	202	GLU	2.1
10	J	48	ARG	2.1
4	D	97	THR	2.1
10	J	86	THR	2.1
7	G	41	CYS	2.1
11	K	46	CYS	2.1
2	B	117	MET	2.1
12	L	40	TYR	2.1
13	M	166	LEU	2.1
13	1	145	LEU	2.1
3	C	182	GLY	2.1
7	G	44	GLY	2.1
1	A	72	ILE	2.1
2	P	209	VAL	2.1
10	X	20	VAL	2.1
3	Q	13	SER	2.1
10	J	120	PHE	2.1
1	A	168	ALA	2.1
2	P	230	ALA	2.1
3	C	245	ALA	2.1
4	R	51	ALA	2.1
4	D	182	GLU	2.1
4	D	226	GLU	2.1
4	D	183	THR	2.1
3	Q	205	LYS	2.1
5	S	192	LYS	2.1
10	J	83	LYS	2.1
4	R	53	LEU	2.1
5	S	210	LEU	2.1
9	I	14	LEU	2.1
3	C	34	CYS	2.1
3	C	179	TYR	2.1
4	R	176	TYR	2.1
5	S	186	HIS	2.1
8	V	117	GLY	2.1
1	A	170	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	209	VAL	2.1
3	C	52	ILE	2.1
9	I	103	VAL	2.1
13	1	178	VAL	2.1
4	R	171	PHE	2.1
6	T	179	PHE	2.1
10	J	161	ASP	2.1
1	A	94	ALA	2.1
3	C	173	SER	2.1
4	R	216	SER	2.1
7	U	169	ARG	2.1
7	G	215	TRP	2.1
3	C	134	LEU	2.1
3	C	197	LEU	2.1
7	G	9	LEU	2.1
11	K	92	LEU	2.1
4	R	205	ASN	2.1
2	B	56	TYR	2.1
7	G	37	ILE	2.1
1	A	49	VAL	2.1
5	S	50	VAL	2.1
10	J	138	VAL	2.1
4	R	73	PHE	2.1
4	R	38	ARG	2.0
6	T	225	ASP	2.0
13	1	133	ASP	2.0
5	S	208	GLU	2.0
11	Y	154	GLU	2.0
10	J	14	MET	2.0
3	C	44	LEU	2.0
4	R	172	LEU	2.0
5	S	191	LEU	2.0
13	1	152	GLN	2.0
4	D	40	ILE	2.0
13	1	17	GLY	2.0
2	B	43	VAL	2.0
10	J	175	VAL	2.0
11	K	64	VAL	2.0
3	C	145	PHE	2.0
1	A	46	ASP	2.0
1	A	157	ALA	2.0
5	S	177	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	218	PRO	2.0
1	A	69	LEU	2.0
1	A	77	GLY	2.0
1	A	215	ILE	2.0
3	Q	51	ASN	2.0
4	R	37	GLY	2.0
10	J	190	ILE	2.0
10	X	157	ASN	2.0
3	C	49	ARG	2.0
4	R	168	VAL	2.0
7	G	142	VAL	2.0
9	I	25	VAL	2.0
6	F	6	TYR	2.0
11	K	146	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	A	301	1/1	0.64	0.19	83,83,83,83	0
15	MG	K	313	1/1	0.67	0.19	77,77,77,77	0
15	MG	D	309	1/1	0.70	0.23	87,87,87,87	0
15	MG	I	306	1/1	0.76	0.24	87,87,87,87	0
15	MG	G	319	1/1	0.77	0.13	66,66,66,66	0
15	MG	X	404	1/1	0.77	0.24	70,70,70,70	0
15	MG	U	417	1/1	0.79	0.19	64,64,64,64	0
15	MG	Q	414	1/1	0.79	0.21	90,90,90,90	0
15	MG	1	418	1/1	0.82	0.20	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	O	401	1/1	0.85	0.16	57,57,57,57	0
15	MG	M	318	1/1	0.86	0.11	81,81,81,81	0
15	MG	C	314	1/1	0.86	0.12	76,76,76,76	0
15	MG	G	317	1/1	0.88	0.15	85,85,85,85	0
15	MG	J	304	1/1	0.89	0.08	56,56,56,56	0
15	MG	U	419	1/1	0.89	0.14	70,70,70,70	0
15	MG	J	315	1/1	0.89	0.10	69,69,69,69	0
15	MG	G	311	1/1	0.89	0.18	97,97,97,97	0
15	MG	B	316	1/1	0.90	0.09	84,84,84,84	0
15	MG	W	406	1/1	0.90	0.09	59,59,59,59	0
15	MG	X	415	1/1	0.91	0.11	59,59,59,59	0
15	MG	Y	413	1/1	0.91	0.17	51,51,51,51	0
15	MG	J	407	1/1	0.91	0.08	70,70,70,70	0
15	MG	I	410	1/1	0.92	0.09	66,66,66,66	0
15	MG	J	320	1/1	0.92	0.14	112,112,112,112	0
15	MG	X	420	1/1	0.93	0.18	77,77,77,77	0
15	MG	P	416	1/1	0.93	0.08	72,72,72,72	0
15	MG	M	310	1/1	0.94	0.07	67,67,67,67	0
15	MG	R	409	1/1	0.94	0.10	59,59,59,59	0
15	MG	U	411	1/1	0.94	0.15	76,76,76,76	0
15	MG	X	307	1/1	0.96	0.08	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.