



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 10:25 AM BST

PDB ID : 1G0U
Title : A GATED CHANNEL INTO THE PROTEASOME CORE PARTICLE
Authors : Groll, M.; Bajorek, M.; Kohler, A.; Moroder, L.; Rubin, D.M.; Huber, R.; Glickman, M.H.; Finley, D.
Deposited on : 2000-10-09
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

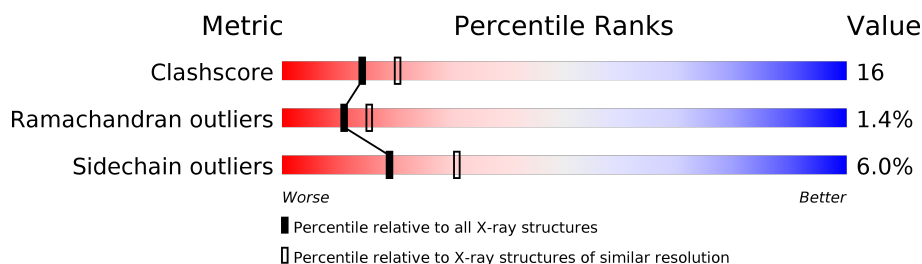
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

















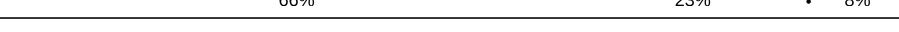

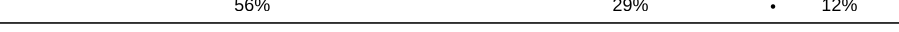

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	70% 28% .
1	O	250	67% 30% ..
2	B	245	58% 33% . .
2	P	245	64% 28% . .
3	C	243	61% 33% . .
3	Q	243	59% 33% 6% .
4	D	241	66% 28% . 5%
4	R	241	61% 31% . 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	234	
5	S	234	
6	F	248	
6	T	248	
7	G	252	
7	U	252	
8	H	222	
8	V	222	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	241	
12	Z	241	
13	1	266	
13	M	266	
14	2	196	
14	N	196	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51834 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEASOME COMPONENT Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1881	1200	308	370	3			
1	O	246	Total	C	N	O	S	0	0	0
			1881	1200	308	370	3			

- Molecule 2 is a protein called PROTEASOME COMPONENT Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1827	1157	303	364	3			
2	P	235	Total	C	N	O	S	0	0	0
			1827	1157	303	364	3			

- Molecule 3 is a protein called PROTEASOME COMPONENT PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1861	1163	325	369	4			
3	Q	238	Total	C	N	O	S	0	0	0
			1861	1163	325	369	4			

- Molecule 4 is a protein called PROTEASOME COMPONENT PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	230	Total	C	N	O	S	0	0	0
			1758	1100	293	358	7			
4	R	230	Total	C	N	O	S	0	0	0
			1758	1100	293	358	7			

- Molecule 5 is a protein called PROTEASOME COMPONENT PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	230	Total	C	N	O	S	0	0	0
			1755	1103	304	344	4			
5	S	230	Total	C	N	O	S	0	0	0
			1755	1103	304	344	4			

- Molecule 6 is a protein called PROTEASOME COMPONENT C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	242	Total	C	N	O	S	0	0	0
			1886	1199	328	355	4			
6	T	242	Total	C	N	O	S	0	0	0
			1886	1199	328	355	4			

- Molecule 7 is a protein called PROTEASOME COMPONENT C7-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	240	Total	C	N	O	S	0	0	0
			1897	1206	319	364	8			
7	U	240	Total	C	N	O	S	0	0	0
			1897	1206	319	364	8			

- Molecule 8 is a protein called PROTEASOME COMPONENT PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called PROTEASOME COMPONENT PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called PROTEASOME COMPONENT C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called PROTEASOME COMPONENT C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called PROTEASOME COMPONENT PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	2	Total	Mg	0	0
			2	2		
15	K	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total 1	Mg 1	0	0
15	I	2	Total 2	Mg 2	0	0
15	V	1	Total 1	Mg 1	0	0
15	W	2	Total 2	Mg 2	0	0
15	Z	2	Total 2	Mg 2	0	0
15	T	1	Total 1	Mg 1	0	0
15	N	1	Total 1	Mg 1	0	0
15	U	2	Total 2	Mg 2	0	0
15	2	1	Total 1	Mg 1	0	0
15	Y	1	Total 1	Mg 1	0	0
15	L	2	Total 2	Mg 2	0	0
15	F	1	Total 1	Mg 1	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	102	Total 102	O 102	0	0
16	B	74	Total 74	O 74	0	0
16	C	73	Total 73	O 73	0	0
16	D	82	Total 82	O 82	0	0
16	E	63	Total 63	O 63	0	0
16	F	97	Total 97	O 97	0	0
16	G	110	Total 110	O 110	0	0

Continued on next page...

Continued from previous page...

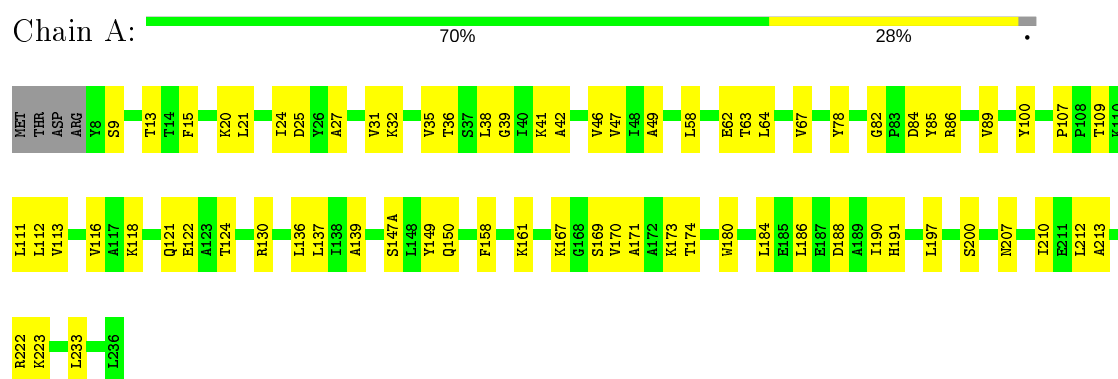
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	132	Total 132	O 132	0	0
16	I	107	Total 107	O 107	0	0
16	J	107	Total 107	O 107	0	0
16	K	107	Total 107	O 107	0	0
16	L	141	Total 141	O 141	0	0
16	M	151	Total 151	O 151	0	0
16	N	115	Total 115	O 115	0	0
16	O	98	Total 98	O 98	0	0
16	P	78	Total 78	O 78	0	0
16	Q	62	Total 62	O 62	0	0
16	R	79	Total 79	O 79	0	0
16	S	66	Total 66	O 66	0	0
16	T	94	Total 94	O 94	0	0
16	U	110	Total 110	O 110	0	0
16	V	131	Total 131	O 131	0	0
16	W	114	Total 114	O 114	0	0
16	X	110	Total 110	O 110	0	0
16	Y	104	Total 104	O 104	0	0
16	Z	137	Total 137	O 137	0	0
16	1	151	Total 151	O 151	0	0
16	2	113	Total 113	O 113	0	0

3 Residue-property plots [i](#)

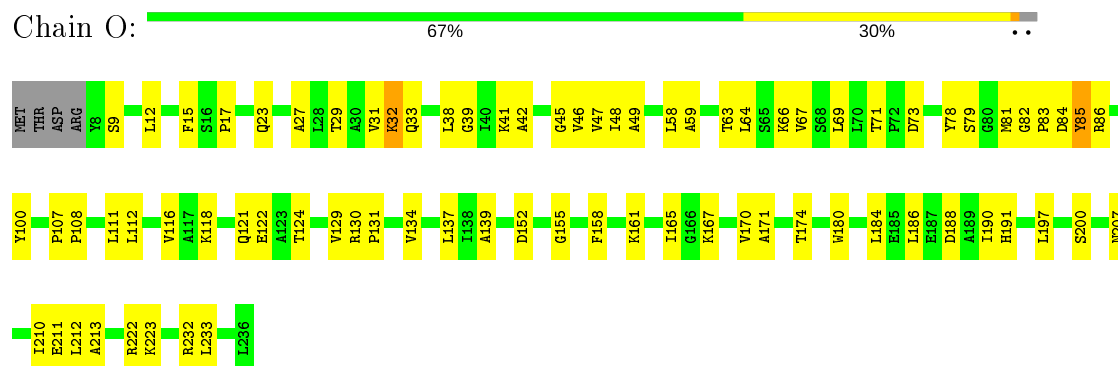
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

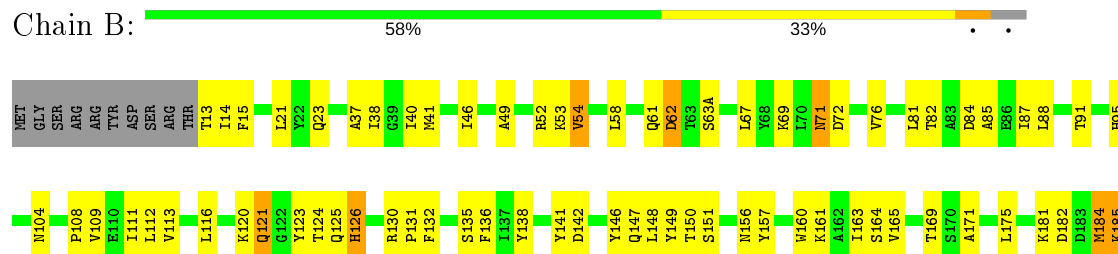
• Molecule 1: PROTEASOME COMPONENT Y7

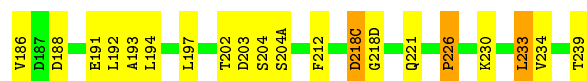


• Molecule 1: PROTEASOME COMPONENT Y7

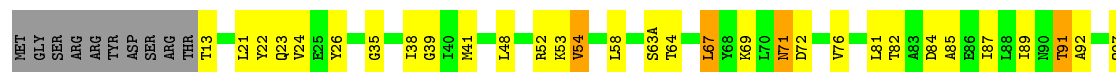


• Molecule 2: PROTEASOME COMPONENT Y13





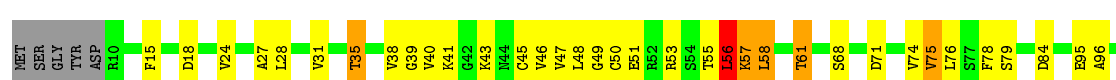
• Molecule 2: PROTEASOME COMPONENT Y13



• Molecule 3: PROTEASOME COMPONENT PRE6

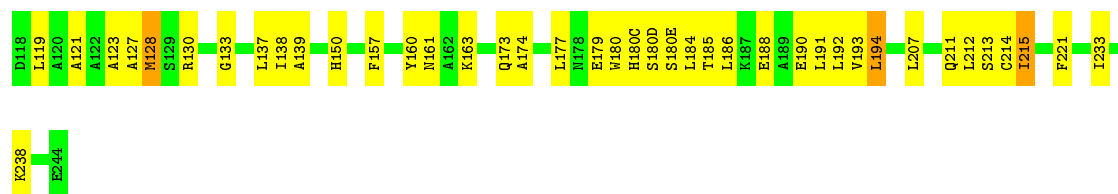


• Molecule 3: PROTEASOME COMPONENT PRE6

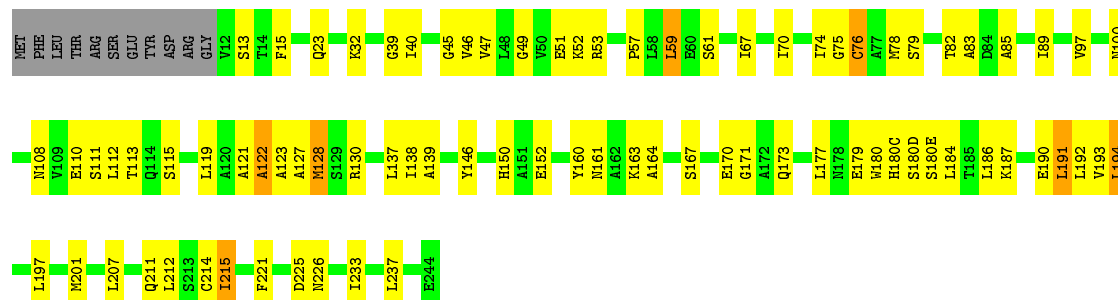


• Molecule 4: PROTEASOME COMPONENT PUP2

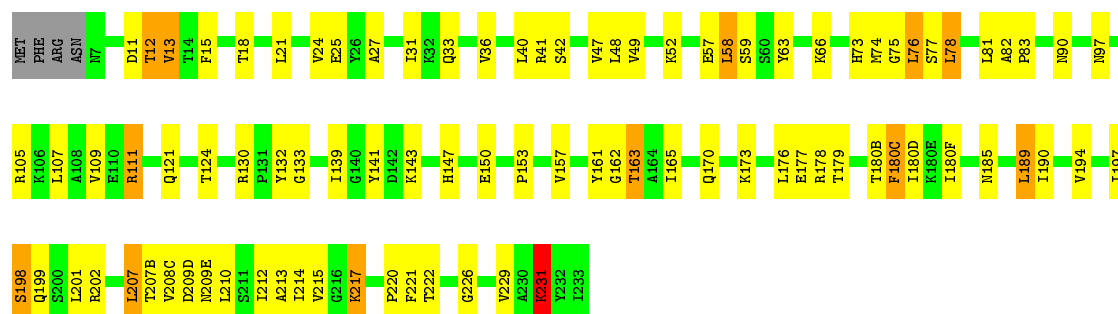




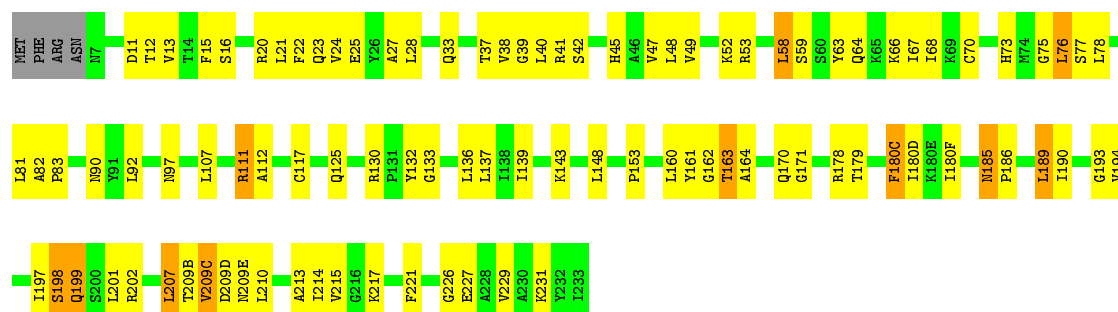
- Molecule 4: PROTEASOME COMPONENT PUP2



- Molecule 5: PROTEASOME COMPONENT PRE5

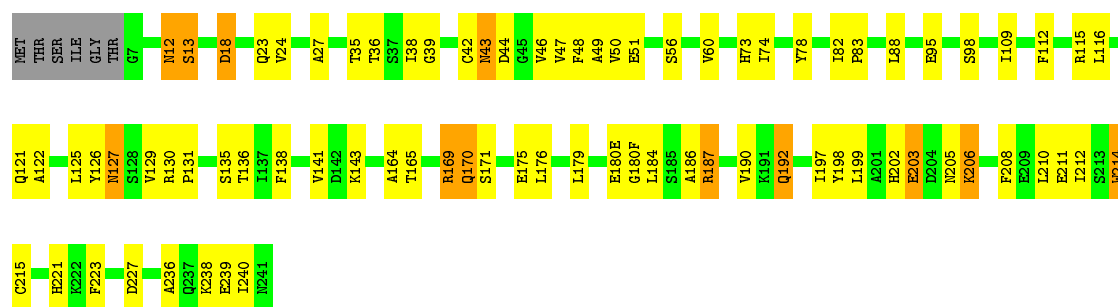


- Molecule 5: PROTEASOME COMPONENT PRE5



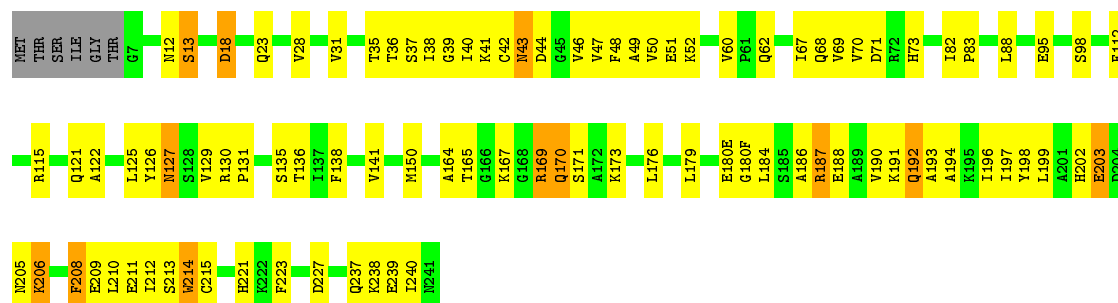
- Molecule 6: PROTEASOME COMPONENT C1





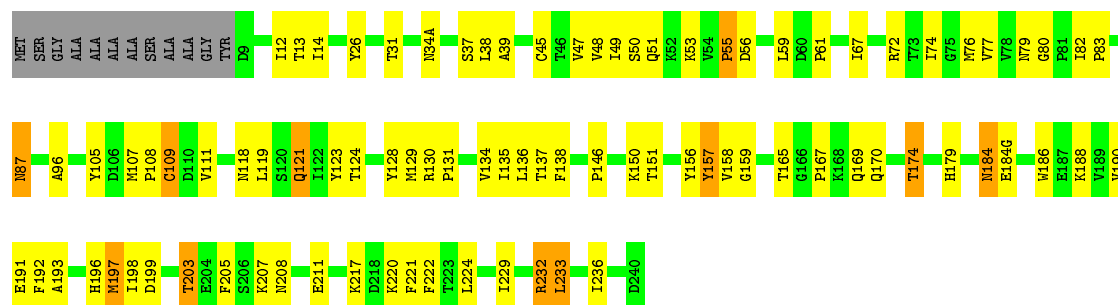
• Molecule 6: PROTEASOME COMPONENT C1

Chain T: 60% 33% 5%



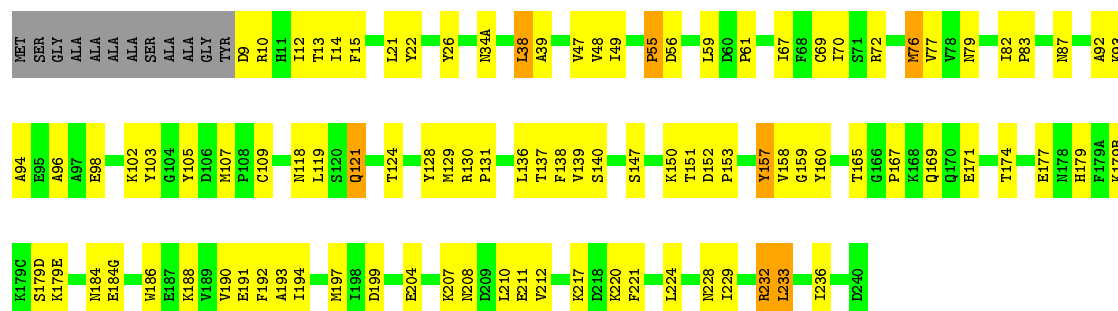
• Molecule 7: PROTEASOME COMPONENT C7-ALPHA

Chain G: 60% 31% 5%

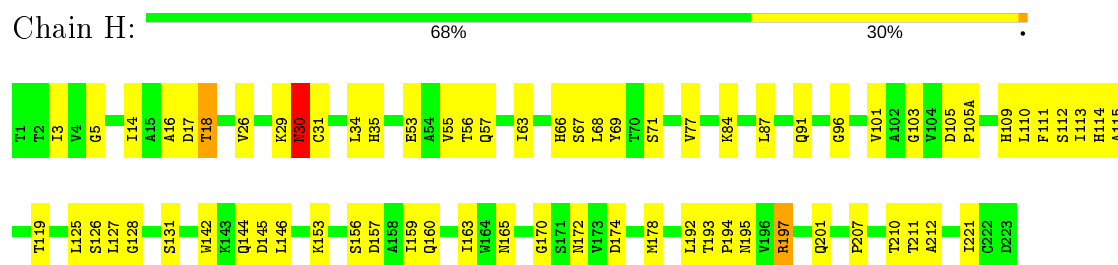


• Molecule 7: PROTEASOME COMPONENT C7-ALPHA

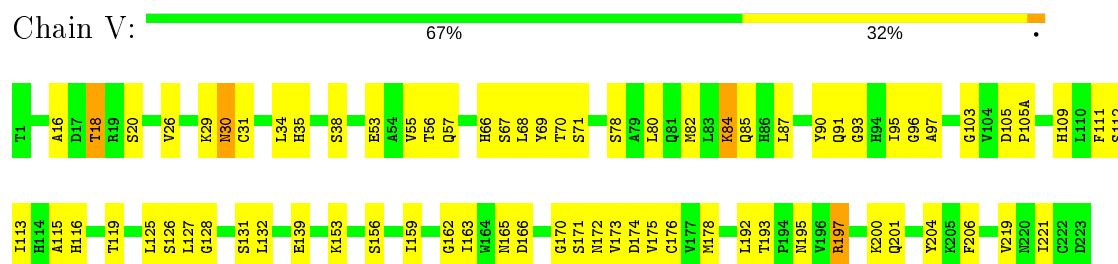
Chain U: 57% 36% 5%



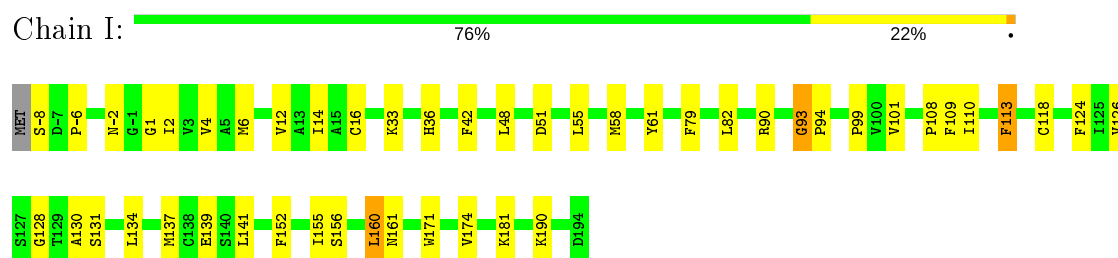
- Molecule 8: PROTEASOME COMPONENT PUP1



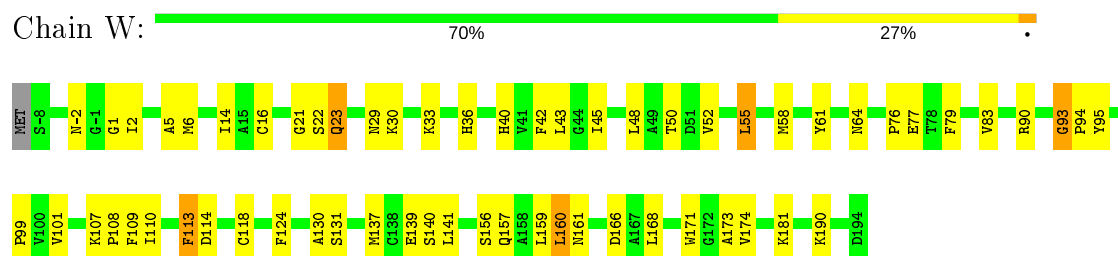
- Molecule 8: PROTEASOME COMPONENT PUP1



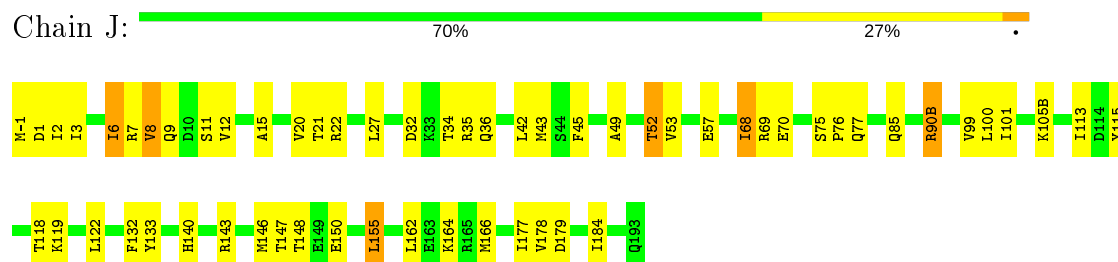
- Molecule 9: PROTEASOME COMPONENT PUP3



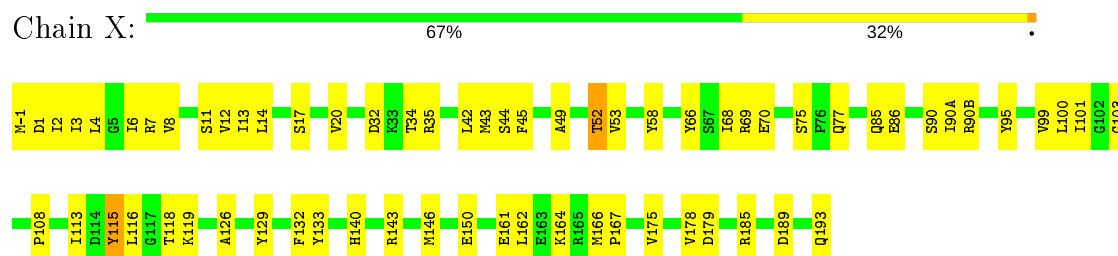
- Molecule 9: PROTEASOME COMPONENT PUP3



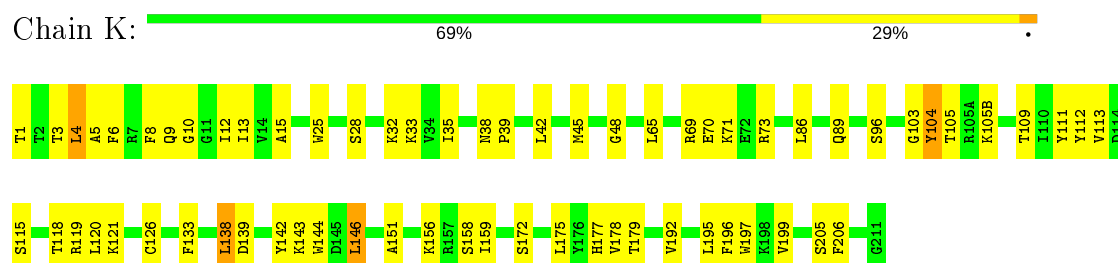
- Molecule 10: PROTEASOME COMPONENT C11



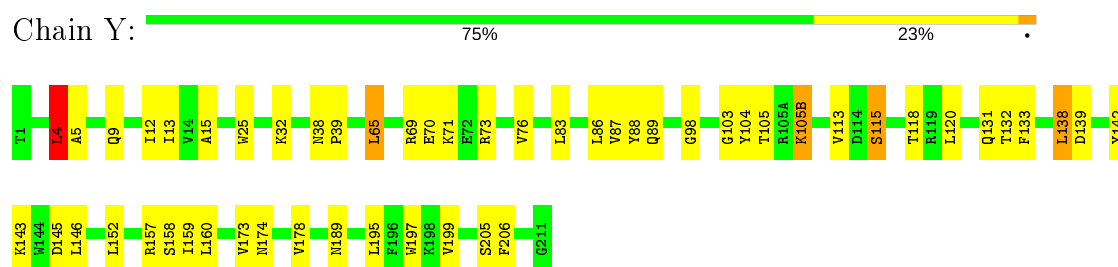
- Molecule 10: PROTEASOME COMPONENT C11



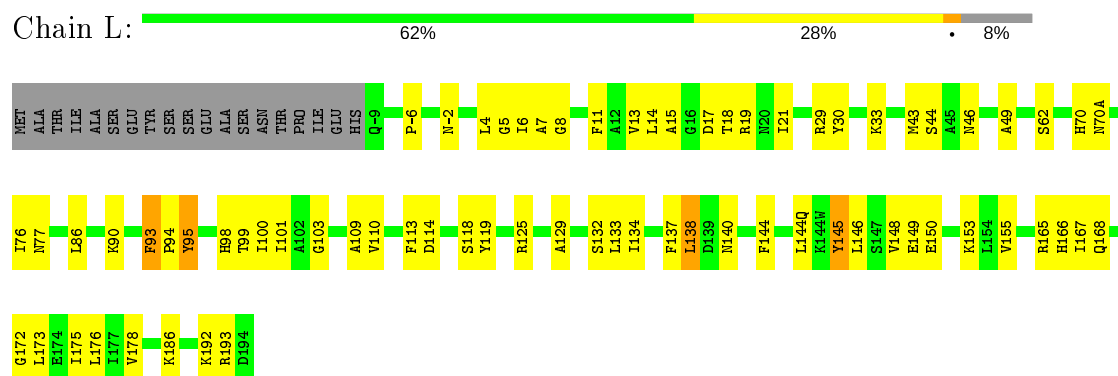
- Molecule 11: PROTEASOME COMPONENT PRE2



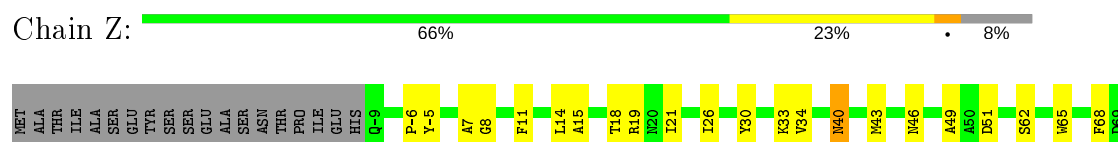
- Molecule 11: PROTEASOME COMPONENT PRE2

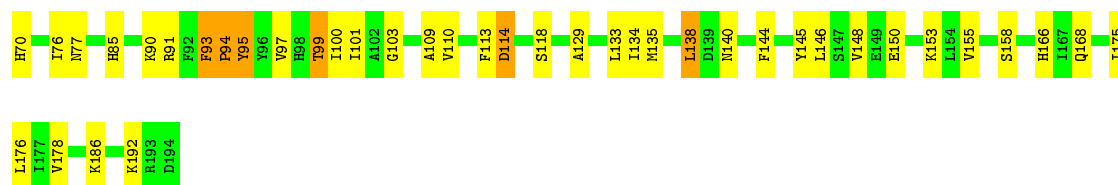


- Molecule 12: PROTEASOME COMPONENT C5



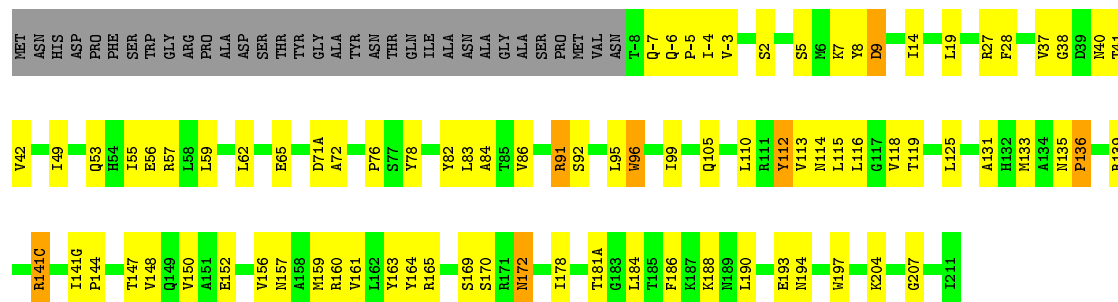
- Molecule 12: PROTEASOME COMPONENT C5





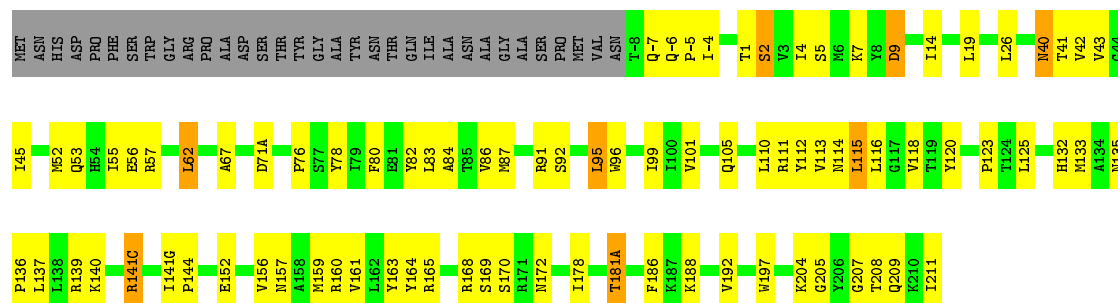
• Molecule 13: PROTEASOME COMPONENT PRE4

Chain M: 56% 29% 12%



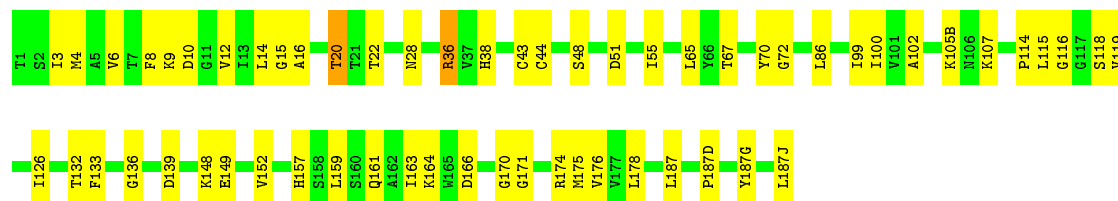
• Molecule 13: PROTEASOME COMPONENT PRE4

Chain 1: 55% 30% 12%



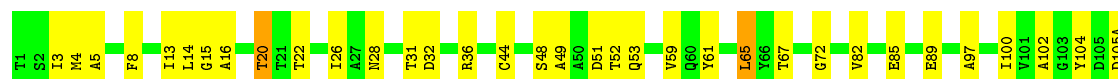
• Molecule 14: PROTEASOME COMPONENT PRE3

Chain N: 70% 29%



• Molecule 14: PROTEASOME COMPONENT PRE3

Chain 2: 63% 34%



K105B	M106	K107	G108	P114	L115	S118	V119	Y124	A125	I126	T132	F133	I134	Y135	G136	R143	M146	S147	K148	E149	E150	H157	S158	L159	S160	Q161	A162	I163	K164	M165	D166	G170	G171	R174	M175	V176	V177	L178	T179	A180	L187	I187A	F187B	Y187C	P187D	Y187G	L187J
-------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.18Å 301.10Å 144.10Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.250 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51834	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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	0.62	0/1918	0.78	1/2597 (0.0%)
1	O	0.58	0/1918	0.78	1/2597 (0.0%)
2	B	0.58	0/1856	0.75	0/2513
2	P	0.61	0/1856	0.76	0/2513
3	C	0.58	0/1889	0.75	1/2557 (0.0%)
3	Q	0.61	0/1889	0.77	1/2557 (0.0%)
4	D	0.63	0/1782	0.83	2/2404 (0.1%)
4	R	0.64	0/1782	0.81	2/2404 (0.1%)
5	E	0.52	0/1781	0.73	0/2407
5	S	0.54	0/1781	0.73	0/2407
6	F	0.56	0/1926	0.75	0/2599
6	T	0.60	0/1926	0.79	0/2599
7	G	0.61	0/1934	0.75	0/2618
7	U	0.62	0/1934	0.77	0/2618
8	H	0.61	0/1716	0.78	0/2326
8	V	0.61	0/1716	0.78	0/2326
9	I	0.64	0/1611	0.79	0/2174
9	W	0.67	0/1611	0.82	0/2174
10	J	0.61	0/1613	0.79	0/2173
10	X	0.64	0/1613	0.79	0/2173
11	K	0.62	0/1681	0.80	0/2274
11	Y	0.61	0/1681	0.78	2/2274 (0.1%)
12	L	0.63	0/1795	0.79	2/2420 (0.1%)
12	Z	0.63	0/1795	0.78	1/2420 (0.0%)
13	1	0.66	0/1855	0.82	1/2514 (0.0%)
13	M	0.63	0/1855	0.79	1/2514 (0.0%)
14	2	0.66	0/1541	0.78	0/2087
14	N	0.65	0/1541	0.78	0/2087
All	All	0.61	0/49796	0.78	15/67326 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
12	L	0	1
All	All	0	2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	128	MET	N-CA-C	-6.85	92.50	111.00
11	Y	4	LEU	CA-CB-CG	6.44	130.12	115.30
4	D	128	MET	N-CA-C	-6.08	94.59	111.00
13	M	95	LEU	N-CA-C	-5.95	94.93	111.00
12	L	95	TYR	N-CA-C	-5.92	95.03	111.00
1	O	137	LEU	N-CA-C	-5.85	95.20	111.00
3	C	56	LEU	CA-CB-CG	5.71	128.44	115.30
12	Z	95	TYR	N-CA-C	-5.37	96.49	111.00
11	Y	98	GLY	N-CA-C	-5.32	99.81	113.10
4	R	59	LEU	CA-CB-CG	5.24	127.36	115.30
4	D	127	ALA	N-CA-C	-5.24	96.86	111.00
3	Q	56	LEU	CA-CB-CG	5.21	127.29	115.30
13	1	95	LEU	N-CA-C	-5.17	97.03	111.00
12	L	98	HIS	N-CA-C	-5.15	97.11	111.00
1	A	137	LEU	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
1	O	85	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	1881	0	1893	50	0
1	O	1881	0	1893	61	0
2	B	1827	0	1824	67	0
2	P	1827	0	1824	58	0
3	C	1861	0	1873	79	0
3	Q	1861	0	1873	82	0
4	D	1758	0	1735	62	0
4	R	1758	0	1735	65	0
5	E	1755	0	1761	73	0
5	S	1755	0	1761	84	0
6	F	1886	0	1876	61	0
6	T	1886	0	1876	74	0
7	G	1897	0	1891	75	0
7	U	1897	0	1891	76	0
8	H	1685	0	1688	49	0
8	V	1685	0	1688	54	0
9	I	1581	0	1574	33	0
9	W	1581	0	1574	43	0
10	J	1585	0	1590	46	0
10	X	1585	0	1590	52	0
11	K	1644	0	1595	51	0
11	Y	1644	0	1595	38	0
12	L	1757	0	1711	62	0
12	Z	1757	0	1711	56	0
13	1	1824	0	1832	70	0
13	M	1824	0	1832	57	0
14	2	1512	0	1481	52	0
14	N	1512	0	1481	43	0
15	2	1	0	0	0	0
15	F	1	0	0	0	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	2	0	0	0	0
15	N	1	0	0	0	0
15	T	1	0	0	0	0
15	U	2	0	0	0	0
15	V	1	0	0	0	0
15	W	2	0	0	0	0
15	Y	1	0	0	0	0
15	Z	2	0	0	0	0
16	1	151	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	2	113	0	0	1	0
16	A	102	0	0	2	0
16	B	74	0	0	3	0
16	C	73	0	0	0	0
16	D	82	0	0	2	0
16	E	63	0	0	2	0
16	F	97	0	0	0	0
16	G	110	0	0	1	0
16	H	132	0	0	2	0
16	I	107	0	0	1	0
16	J	107	0	0	3	0
16	K	107	0	0	2	0
16	L	141	0	0	4	0
16	M	151	0	0	3	0
16	N	115	0	0	1	0
16	O	98	0	0	4	0
16	P	78	0	0	2	0
16	Q	62	0	0	2	0
16	R	79	0	0	4	0
16	S	66	0	0	3	0
16	T	94	0	0	1	0
16	U	110	0	0	2	0
16	V	131	0	0	1	0
16	W	114	0	0	2	0
16	X	110	0	0	4	0
16	Y	104	0	0	2	0
16	Z	137	0	0	4	0
All	All	51834	0	48648	1521	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 16.

All (1521) 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)
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.28	1.09
7:G:96:ALA:HA	7:G:107:MET:HE2	1.36	1.03
3:C:163:GLN:HE21	3:C:164:THR:H	1.09	1.01
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.10	0.99
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.48	0.95
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.29	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:PHE:H	4:D:23:GLN:HE22	1.16	0.94
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.53	0.90
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.54	0.90
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.34	0.89
11:K:105(B):LYS:HD2	11:K:105(B):LYS:H	1.37	0.89
8:V:172:ASN:HD22	8:V:193:THR:HA	1.39	0.88
11:Y:105(B):LYS:HD2	11:Y:105(B):LYS:H	1.39	0.86
13:1:133:MET:O	13:1:136:PRO:HD2	1.75	0.86
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.55	0.85
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.25	0.85
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.12	0.84
12:L:18:THR:CG2	12:L:30:TYR:HA	2.08	0.83
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.60	0.82
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.61	0.82
14:2:14:LEU:HD21	14:2:102:ALA:HB3	1.62	0.82
7:G:151:THR:HG22	7:G:157:TYR:CB	2.10	0.82
6:F:141:VAL:HG23	6:F:215:CYS:SG	2.21	0.81
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.63	0.81
13:1:141(C):ARG:HG3	13:1:141(C):ARG:HH11	1.45	0.81
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.44	0.81
7:U:121:GLN:O	7:U:124:THR:HB	1.81	0.81
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.63	0.80
3:C:15:PHE:N	4:D:23:GLN:HE22	1.78	0.80
4:R:130:ARG:HG3	4:R:130:ARG:HH11	1.45	0.80
8:V:26:VAL:HG11	8:V:29:LYS:HG2	1.63	0.80
2:B:202:THR:HG22	2:B:204:SER:H	1.46	0.80
3:C:163:GLN:NE2	3:C:164:THR:H	1.78	0.80
12:Z:-6:PRO:HB2	13:1:91:ARG:HH11	1.47	0.79
4:R:121:ALA:HB3	16:S:1158:HOH:O	1.81	0.79
4:D:121:ALA:HB3	16:D:298:HOH:O	1.83	0.78
14:2:157:HIS:CD2	14:2:187(J):LEU:HD13	2.19	0.78
7:G:76:MET:SD	7:G:138:PHE:CE2	2.77	0.78
7:U:59:LEU:O	7:U:61:PRO:HD3	1.83	0.78
6:F:186:ALA:O	6:F:190:VAL:HG23	1.84	0.78
7:G:96:ALA:HA	7:G:107:MET:CE	2.12	0.78
4:D:207:LEU:HD21	4:D:233:ILE:HG12	1.66	0.78
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.49	0.78
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.49	0.78
12:Z:18:THR:HG22	12:Z:30:TYR:HA	1.65	0.77
7:U:96:ALA:HA	7:U:107:MET:HE2	1.66	0.76
2:B:121:GLN:O	2:B:124:THR:HB	1.86	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.82	0.76
3:C:163:GLN:HE21	3:C:164:THR:N	1.84	0.76
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.68	0.76
10:J:43:MET:HG3	10:J:101:ILE:HG12	1.66	0.76
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.34	0.76
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.84	0.75
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.69	0.75
14:2:157:HIS:HD2	14:2:187(J):LEU:HD13	1.49	0.75
4:D:130:ARG:HH11	4:D:130:ARG:HG3	1.50	0.75
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.22	0.75
12:L:103:GLY:HA2	12:L:178:VAL:HG11	1.69	0.74
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.22	0.74
12:L:-6:PRO:HB2	13:M:91:ARG:HH11	1.51	0.74
2:P:202:THR:HG22	2:P:204:SER:H	1.52	0.74
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.69	0.74
5:E:226:GLY:O	5:E:229:VAL:HG22	1.88	0.74
12:Z:18:THR:CG2	12:Z:30:TYR:HA	2.18	0.74
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.68	0.73
4:D:46:VAL:HG11	4:D:139:ALA:HB1	1.69	0.73
6:F:13:SER:HB2	7:G:130:ARG:HB3	1.69	0.73
5:S:198:SER:HA	5:S:201:LEU:HG	1.70	0.73
5:S:73:HIS:HE1	5:S:107:LEU:O	1.71	0.73
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.03	0.73
6:T:186:ALA:O	6:T:190:VAL:HG23	1.88	0.73
1:O:108:PRO:HG2	1:O:111:LEU:HB2	1.71	0.72
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.71	0.72
3:C:15:PHE:H	4:D:23:GLN:NE2	1.84	0.72
2:P:121:GLN:O	2:P:124:THR:HB	1.88	0.72
7:G:82:ILE:HG22	7:G:83:PRO:HD3	1.71	0.72
8:H:172:ASN:HD22	8:H:193:THR:HA	1.53	0.72
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.36	0.72
12:Z:18:THR:HG21	12:Z:30:TYR:CD1	2.24	0.72
6:F:122:ALA:HA	6:F:125:LEU:HD12	1.70	0.72
7:G:77:VAL:HG12	7:G:137:THR:HB	1.69	0.72
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.72	0.72
8:H:26:VAL:HG11	8:H:29:LYS:HG2	1.71	0.72
11:K:12:ILE:HB	11:K:178:VAL:HB	1.72	0.72
11:K:142:TYR:O	11:K:143:LYS:HD2	1.89	0.72
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.69	0.72
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.70	0.72
13:M:141(C):ARG:HH11	13:M:141(C):ARG:HG3	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.56	0.71
2:B:120:LYS:HZ1	2:B:136:PHE:HD1	1.38	0.71
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.24	0.71
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.26	0.71
13:1:19:LEU:HD23	13:1:168:ARG:O	1.91	0.71
4:D:24:VAL:O	4:D:27:SER:HB3	1.91	0.71
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.54	0.71
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.06	0.71
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.73	0.70
10:J:2:ILE:HD13	10:J:162:LEU:HD13	1.73	0.70
1:O:27:ALA:O	1:O:31:VAL:HG23	1.90	0.70
4:R:207:LEU:HD21	4:R:233:ILE:HG12	1.72	0.70
13:1:5:SER:HB3	13:1:14:ILE:HG13	1.73	0.70
14:2:114:PRO:HD2	14:2:118:SER:O	1.92	0.70
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.74	0.70
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.40	0.70
5:S:143:LYS:HE3	13:1:78:TYR:OH	1.92	0.69
10:J:143:ARG:O	10:J:146:MET:HG3	1.91	0.69
6:F:170:GLN:H	6:F:170:GLN:CD	1.95	0.69
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.73	0.69
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.87	0.69
4:R:160:TYR:CD2	5:S:59:SER:HB3	2.27	0.69
12:L:153:LYS:HG2	8:V:201:GLN:HG2	1.75	0.69
14:N:114:PRO:HD2	14:N:118:SER:O	1.92	0.69
7:U:39:ALA:CB	7:U:48:VAL:HG12	2.21	0.69
5:S:132:TYR:O	5:S:153:PRO:HB3	1.92	0.69
12:L:18:THR:HG22	12:L:30:TYR:HA	1.73	0.69
7:U:96:ALA:HA	7:U:107:MET:CE	2.22	0.69
6:T:13:SER:HB2	7:U:130:ARG:HB3	1.73	0.69
3:Q:190:VAL:O	3:Q:194:VAL:HG23	1.92	0.68
1:A:197:LEU:HD23	1:A:210:ILE:HD12	1.74	0.68
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.75	0.68
2:B:40:ILE:HD12	2:B:193:ALA:HB2	1.76	0.68
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.59	0.68
5:E:21:LEU:O	5:E:25:GLU:HG3	1.93	0.68
12:Z:43:MET:HG3	12:Z:101:ILE:HG22	1.76	0.68
7:G:49:ILE:HD12	7:G:49:ILE:N	2.07	0.68
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.59	0.68
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.75	0.67
7:G:229:ILE:O	7:G:232:ARG:HB2	1.93	0.67
10:X:4:LEU:HD23	10:X:126:ALA:HB2	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:121:GLN:O	7:G:124:THR:HB	1.94	0.67
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.07	0.67
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.76	0.67
12:L:18:THR:HG21	12:L:30:TYR:CD1	2.29	0.67
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.59	0.67
5:S:77:SER:OG	5:S:137:LEU:HB2	1.94	0.67
6:T:141:VAL:HG23	6:T:215:CYS:SG	2.35	0.67
3:C:71:ASP:HA	10:J:68:ILE:HD11	1.77	0.67
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.60	0.67
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.76	0.67
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.94	0.67
5:E:73:HIS:HE1	5:E:107:LEU:O	1.76	0.67
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.60	0.67
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.75	0.67
10:X:45:PHE:HB3	10:X:99:VAL:HG12	1.76	0.66
10:J:15:ALA:HB2	10:J:155:LEU:HD11	1.76	0.66
4:D:97:VAL:HG21	11:K:65:LEU:CD1	2.25	0.66
1:A:121:GLN:O	1:A:124:THR:HB	1.95	0.66
7:G:39:ALA:CB	7:G:48:VAL:HG12	2.25	0.66
5:S:209(B):THR:H	5:S:209(E):ASN:HB2	1.60	0.66
7:G:184(G):GLU:HG2	7:G:188:LYS:HB3	1.76	0.66
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.77	0.66
12:L:-6:PRO:HB2	13:M:91:ARG:NH1	2.11	0.66
4:D:186:LEU:O	4:D:190:GLU:HG3	1.96	0.66
10:J:7:ARG:HB3	10:J:12:VAL:HG22	1.78	0.66
7:U:229:ILE:O	7:U:232:ARG:HB2	1.95	0.66
7:U:233:LEU:O	7:U:236:ILE:HG13	1.96	0.66
12:Z:103:GLY:HA2	12:Z:178:VAL:HG11	1.75	0.66
2:B:13:THR:HA	16:B:256:HOH:O	1.95	0.66
5:E:198:SER:HA	5:E:201:LEU:HG	1.78	0.66
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.78	0.66
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.77	0.65
13:1:80:PHE:CZ	13:1:111:ARG:HG2	2.32	0.65
4:D:177:LEU:HD22	5:E:58:LEU:HD22	1.77	0.65
10:J:43:MET:HG3	10:J:101:ILE:CG1	2.26	0.65
12:L:134:ILE:HG22	12:L:138:LEU:HD22	1.79	0.65
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.62	0.65
12:L:140:ASN:ND2	9:W:161:ASN:HD21	1.95	0.65
14:N:67:THR:HA	14:N:72:GLY:O	1.96	0.65
4:D:215:ILE:HG22	4:D:221:PHE:HD2	1.63	0.64
11:Y:5:ALA:HA	11:Y:13:ILE:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:141:PHE:HE2	3:Q:215:VAL:HG22	1.63	0.64
5:S:207:LEU:HA	5:S:209(E):ASN:HD22	1.63	0.64
7:G:184(G):GLU:HG2	7:G:188:LYS:CB	2.27	0.64
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.28	0.64
2:B:69:LYS:HG3	2:B:221:GLN:OE1	1.98	0.64
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.80	0.64
4:R:46:VAL:HG11	4:R:139:ALA:HB1	1.80	0.64
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.32	0.64
13:1:135:ASN:O	13:1:139:ARG:HG3	1.98	0.63
7:G:76:MET:SD	7:G:138:PHE:HE2	2.19	0.63
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.95	0.63
5:E:207:LEU:HA	5:E:209(E):ASN:HD22	1.62	0.63
6:T:221:HIS:HE1	6:T:223:PHE:CE1	2.15	0.63
13:1:4:ILE:HD11	13:1:159:MET:HG2	1.79	0.63
12:Z:19:ARG:HD2	12:Z:168:GLN:O	1.98	0.63
2:B:181:LYS:O	2:B:184:MET:HG3	1.97	0.63
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	1.79	0.63
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.29	0.63
3:C:185:THR:HB	3:C:188:GLU:HG2	1.81	0.63
2:P:13:THR:HA	16:P:1519:HOH:O	1.99	0.63
11:Y:138:LEU:HD13	11:Y:158:SER:OG	1.99	0.63
7:G:77:VAL:CG1	7:G:137:THR:HB	2.28	0.63
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.80	0.63
10:J:35:ARG:O	10:J:42:LEU:HD12	1.98	0.62
6:T:170:GLN:CD	6:T:170:GLN:H	2.02	0.62
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.81	0.62
6:T:126:TYR:HE1	7:U:129:MET:SD	2.21	0.62
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.63	0.62
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.81	0.62
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.81	0.62
12:Z:-6:PRO:HB2	13:1:91:ARG:NH1	2.13	0.62
12:L:18:THR:HG21	12:L:30:TYR:HD1	1.64	0.62
1:O:118:LYS:O	1:O:122:GLU:HG3	2.00	0.62
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.29	0.62
8:H:34:LEU:HD22	8:H:174:ASP:HB3	1.82	0.62
13:M:-6:GLN:O	13:M:-6:GLN:HG3	2.00	0.62
7:G:130:ARG:HG3	7:G:131:PRO:O	2.00	0.62
6:T:130:ARG:HG3	6:T:130:ARG:HH11	1.65	0.62
10:X:2:ILE:HD13	10:X:162:LEU:HD13	1.81	0.62
11:Y:113:VAL:HA	11:Y:118:THR:O	1.99	0.62
1:A:13:THR:HG22	1:A:21:LEU:HD22	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:26:VAL:CG1	8:V:29:LYS:HG2	2.29	0.62
1:A:112:LEU:O	1:A:116:VAL:HG23	2.00	0.61
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.65	0.61
5:S:41:ARG:NH1	5:S:42:SER:O	2.33	0.61
1:O:130:ARG:HD3	7:U:13:THR:O	2.00	0.61
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.46	0.61
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.46	0.61
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.82	0.61
2:P:99:TYR:HH	10:X:66:TYR:HH	1.45	0.61
1:A:186:LEU:O	1:A:190:ILE:HG13	2.00	0.61
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.36	0.61
4:R:215:ILE:HG22	4:R:221:PHE:HD2	1.64	0.61
6:F:127:ASN:HD22	6:F:127:ASN:C	2.04	0.61
7:G:233:LEU:O	7:G:236:ILE:HG13	2.01	0.61
1:O:45:GLY:HA3	1:O:186:LEU:HD13	1.81	0.61
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	1.81	0.61
11:K:142:TYR:C	11:K:143:LYS:HD2	2.21	0.61
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.35	0.61
7:U:49:ILE:N	7:U:49:ILE:HD12	2.16	0.61
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.82	0.61
5:E:143:LYS:HE3	13:M:78:TYR:OH	2.00	0.61
11:Y:73:ARG:NH2	11:Y:105:THR:HG22	2.16	0.61
2:P:120:LYS:HZ1	2:P:136:PHE:HD1	1.49	0.61
2:P:76:VAL:CG1	2:P:138:TYR:CD2	2.84	0.61
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.65	0.61
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.81	0.61
8:V:172:ASN:ND2	8:V:193:THR:HG22	2.16	0.60
1:O:197:LEU:CD2	1:O:210:ILE:HD12	2.30	0.60
12:Z:8:GLY:HA3	12:Z:11:PHE:CZ	2.35	0.60
9:I:4:VAL:HG23	9:I:126:VAL:HG12	1.84	0.60
13:M:157:ASN:ND2	13:M:160:ARG:HH11	2.00	0.60
4:R:197:LEU:O	4:R:201:MET:HG3	2.01	0.60
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.31	0.60
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.37	0.60
1:A:109:THR:O	1:A:113:VAL:HG23	2.01	0.60
5:S:15:PHE:H	6:T:23:GLN:HE22	1.48	0.60
12:Z:146:LEU:HD22	12:Z:150:GLU:HG2	1.83	0.60
2:B:14:ILE:HG22	3:C:12:LEU:HD13	1.82	0.60
16:B:245:HOH:O	10:J:85:GLN:HB2	2.01	0.60
5:S:226:GLY:O	5:S:229:VAL:HG22	2.02	0.60
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:171:GLY:O	14:2:187(D):PRO:HG3	2.02	0.60
7:G:108:PRO:HB2	7:G:111:VAL:HG23	1.83	0.60
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.83	0.60
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.01	0.60
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.83	0.60
2:B:150:THR:O	2:B:157:TYR:HA	2.02	0.60
3:Q:15:PHE:H	4:R:23:GLN:NE2	1.97	0.60
13:M:112:TYR:O	13:M:119:THR:HA	2.02	0.60
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.84	0.60
3:Q:68:SER:O	3:Q:75:VAL:HG12	2.00	0.59
13:1:186:PHE:HE1	13:1:188:LYS:HG3	1.66	0.59
13:1:57:ARG:HH11	13:1:57:ARG:HG2	1.66	0.59
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.37	0.59
13:M:7:LYS:HD2	13:M:141(G):ILE:HD13	1.84	0.59
14:2:159:LEU:O	14:2:163:ILE:HG13	2.02	0.59
3:Q:182:PRO:O	3:Q:184:ALA:N	2.36	0.59
4:D:39:GLY:HA2	4:D:47:VAL:O	2.02	0.59
4:D:46:VAL:O	4:D:214:CYS:HA	2.01	0.59
14:N:9:LYS:O	14:N:107:LYS:HD3	2.02	0.59
9:W:101:VAL:O	9:W:110:ILE:HA	2.03	0.59
1:O:79:SER:HB2	1:O:165:ILE:HD12	1.84	0.59
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.85	0.59
9:I:6:MET:HG2	9:I:124:PHE:HB3	1.83	0.59
5:S:210:LEU:HB3	5:S:229:VAL:HG21	1.84	0.59
3:C:39:GLY:HA2	3:C:47:VAL:O	2.02	0.59
5:E:132:TYR:O	5:E:153:PRO:HB3	2.02	0.59
10:J:132:PHE:HA	11:Y:133:PHE:CE1	2.38	0.59
11:K:138:LEU:HD13	11:K:158:SER:OG	2.02	0.59
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.38	0.59
2:B:163:ILE:HG13	2:B:164:SER:N	2.18	0.58
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.37	0.58
10:X:53:VAL:HB	16:Y:9089:HOH:O	2.03	0.58
7:U:69:CYS:O	7:U:93:LYS:HE2	2.02	0.58
13:1:152:GLU:O	13:1:156:VAL:HG23	2.03	0.58
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.84	0.58
3:C:14:ILE:HB	4:D:23:GLN:NE2	2.18	0.58
1:O:130:ARG:HH11	1:O:130:ARG:HG3	1.69	0.58
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.85	0.58
5:S:180(C):PHE:HA	5:S:180(F):ILE:HG13	1.85	0.58
12:L:140:ASN:ND2	9:W:161:ASN:ND2	2.51	0.58
13:M:152:GLU:O	13:M:156:VAL:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.85	0.58
5:S:67:ILE:HG21	5:S:213:ALA:HB2	1.86	0.58
10:X:43:MET:HG3	10:X:101:ILE:HG12	1.86	0.58
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.85	0.58
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.84	0.58
6:F:43:ASN:HD22	6:F:44:ASP:H	1.51	0.58
4:R:130:ARG:HG3	4:R:130:ARG:NH1	2.18	0.58
2:B:41:MET:HB2	2:B:148:LEU:HD22	1.84	0.58
8:V:78:SER:O	8:V:82:MET:HG3	2.03	0.58
11:K:5:ALA:HA	11:K:13:ILE:O	2.04	0.58
12:L:166:HIS:HD2	12:L:168:GLN:H	1.49	0.58
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.33	0.58
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.34	0.58
8:V:172:ASN:ND2	8:V:193:THR:HA	2.14	0.58
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.84	0.58
3:C:197:LEU:HD13	3:C:210:ILE:HG23	1.85	0.58
4:D:97:VAL:HG21	11:K:65:LEU:HD12	1.86	0.58
14:N:157:HIS:HD2	14:N:187(J):LEU:HD13	1.68	0.58
10:X:-1:MET:HG2	10:X:1:ASP:H	1.68	0.58
10:X:43:MET:HG3	10:X:101:ILE:CG1	2.33	0.58
3:C:57:LYS:O	3:C:58:LEU:HB2	2.03	0.57
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.33	0.57
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.38	0.57
14:N:55:ILE:HG23	14:N:86:LEU:HD12	1.86	0.57
3:Q:24:VAL:O	3:Q:27:ALA:HB3	2.04	0.57
6:T:210:LEU:HD12	6:T:211:GLU:H	1.69	0.57
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.39	0.57
11:K:172:SER:HA	11:K:192:VAL:HG23	1.87	0.57
12:L:176:LEU:HG	12:L:186:LYS:HG3	1.86	0.57
8:H:201:GLN:HG2	12:Z:153:LYS:HG2	1.86	0.57
13:1:157:ASN:HD22	13:1:160:ARG:NH1	2.01	0.57
1:A:118:LYS:O	1:A:122:GLU:HG3	2.03	0.57
13:M:113:VAL:HA	13:M:118:VAL:O	2.05	0.57
14:2:3:ILE:HG22	14:2:16:ALA:HB2	1.86	0.57
3:C:175:PHE:CZ	3:C:195:ARG:HB3	2.39	0.57
4:R:180(C):HIS:O	4:R:184:LEU:HD12	2.04	0.57
14:2:49:ALA:O	14:2:53:GLN:HG3	2.04	0.57
1:A:197:LEU:CD2	1:A:210:ILE:HD12	2.34	0.57
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.86	0.57
6:F:130:ARG:HH11	6:F:130:ARG:HG3	1.70	0.57
5:S:48:LEU:HB2	5:S:213:ALA:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:21:ILE:HG22	12:Z:26:ILE:HA	1.87	0.57
5:E:66:LYS:O	5:E:77:SER:HA	2.05	0.57
6:F:78:TYR:HB3	6:F:136:THR:HG23	1.86	0.57
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.86	0.57
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.03	0.57
3:Q:130:ARG:HG3	3:Q:130:ARG:HH11	1.70	0.57
14:N:187(D):PRO:HA	14:N:187(G):TYR:CE2	2.40	0.57
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.85	0.56
3:C:182:PRO:O	3:C:184:ALA:N	2.38	0.56
5:E:208(C):VAL:O	5:E:226:GLY:HA2	2.05	0.56
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.70	0.56
5:S:21:LEU:O	5:S:25:GLU:HG3	2.04	0.56
3:Q:141:PHE:CE2	3:Q:215:VAL:HG22	2.40	0.56
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.86	0.56
1:O:130:ARG:HH21	7:U:124:THR:CG2	2.18	0.56
2:P:76:VAL:HG11	2:P:138:TYR:CD2	2.40	0.56
3:Q:76:LEU:HD12	3:Q:138:ILE:CG1	2.35	0.56
3:Q:79:SER:OG	3:Q:165:ILE:HG13	2.05	0.56
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.39	0.56
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.88	0.56
8:V:103:GLY:HA2	8:V:178:MET:SD	2.46	0.56
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.87	0.56
3:C:156:ILE:HD12	4:D:83:ALA:HB2	1.85	0.56
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.40	0.56
1:O:188:ASP:O	1:O:191:HIS:HB3	2.05	0.56
9:W:156:SER:O	9:W:160:LEU:HB2	2.06	0.56
14:2:8:PHE:HA	16:2:2032:HOH:O	2.05	0.56
3:C:134:VAL:HG12	3:C:135:SER:N	2.20	0.56
14:N:133:PHE:HE2	14:N:166:ASP:HB2	1.69	0.56
1:O:42:ALA:HB1	1:O:184:LEU:O	2.06	0.56
5:E:81:LEU:HB2	5:E:133:GLY:O	2.06	0.56
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.40	0.56
7:G:179:HIS:NE2	7:G:192:PHE:HE2	2.04	0.56
13:M:53:GLN:O	13:M:56:GLU:HB2	2.06	0.56
8:V:116:HIS:HB2	16:V:2053:HOH:O	2.06	0.56
1:O:15:PHE:H	2:P:23:GLN:HE22	1.53	0.56
8:V:206:PHE:CZ	9:W:157:GLN:HG3	2.41	0.56
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.88	0.56
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.40	0.56
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.88	0.56
6:F:210:LEU:HD12	6:F:211:GLU:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	1.87	0.56
12:L:129:ALA:HB1	12:L:166:HIS:CE1	2.41	0.55
11:K:4:LEU:HD13	11:K:15:ALA:O	2.05	0.55
4:R:163:LYS:HG3	4:R:164:ALA:N	2.21	0.55
5:S:66:LYS:O	5:S:77:SER:HA	2.05	0.55
1:A:130:ARG:HH11	1:A:130:ARG:HG3	1.71	0.55
3:C:140:GLY:HA2	3:C:215:VAL:HG21	1.88	0.55
7:G:59:LEU:O	7:G:61:PRO:HD3	2.06	0.55
6:T:49:ALA:HA	6:T:211:GLU:O	2.07	0.55
8:V:126:SER:O	8:V:127:LEU:HD23	2.06	0.55
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.37	0.55
7:U:10:ARG:HG2	7:U:22:TYR:CD2	2.41	0.55
10:X:75:SER:HB2	16:X:2291:HOH:O	2.05	0.55
4:R:97:VAL:HG21	11:Y:65:LEU:CD1	2.37	0.55
1:A:15:PHE:H	2:B:23:GLN:HE22	1.54	0.55
5:E:207(B):THR:H	5:E:209(E):ASN:HB2	1.69	0.55
7:G:150:LYS:O	7:G:157:TYR:HA	2.06	0.55
11:Y:105(B):LYS:H	11:Y:105(B):LYS:CD	2.12	0.55
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.06	0.55
6:F:221:HIS:HE1	6:F:223:PHE:CE1	2.24	0.55
6:F:35:THR:HG21	6:F:51:GLU:O	2.07	0.55
7:G:79:ASN:OD1	7:G:165:THR:HB	2.07	0.55
6:T:127:ASN:HD22	6:T:127:ASN:C	2.09	0.55
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.37	0.55
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.37	0.55
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.07	0.55
7:G:207:LYS:HG3	7:G:208:ASN:OD1	2.07	0.55
7:G:198:ILE:HG23	7:G:203:THR:O	2.07	0.55
13:M:184:LEU:HD21	13:M:186:PHE:HB2	1.88	0.55
4:D:215:ILE:HG22	4:D:221:PHE:CD2	2.42	0.55
4:R:39:GLY:HA2	4:R:47:VAL:O	2.07	0.55
8:V:66:HIS:O	8:V:70:THR:HG23	2.07	0.55
4:D:160:TYR:CE1	4:D:163:LYS:HD3	2.42	0.54
10:X:143:ARG:O	10:X:146:MET:HG3	2.07	0.54
8:H:165:ASN:OD1	13:1:136:PRO:HA	2.08	0.54
10:J:178:VAL:HG22	10:J:184:ILE:HG12	1.89	0.54
3:Q:71:ASP:HA	10:X:68:ILE:HD11	1.89	0.54
7:U:136:LEU:O	7:U:150:LYS:HA	2.07	0.54
8:H:172:ASN:HB3	8:H:192:LEU:O	2.07	0.54
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.71	0.54
7:U:77:VAL:HG12	7:U:137:THR:HB	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:ILE:HG22	10:J:100:LEU:CD1	2.38	0.54
5:S:198:SER:HA	5:S:201:LEU:CG	2.38	0.54
7:U:179(D):SER:O	7:U:179(E):LYS:HB2	2.07	0.54
1:A:41:LYS:HG3	1:A:46:VAL:HG22	1.88	0.54
2:B:185:LYS:HD3	2:B:186:VAL:N	2.23	0.54
4:D:112:LEU:O	4:D:116:VAL:HG23	2.07	0.54
12:L:93:PHE:N	12:L:94:PRO:HD3	2.23	0.54
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.90	0.54
1:O:12:LEU:HD12	1:O:129:VAL:O	2.07	0.54
10:X:133:TYR:CZ	10:X:166:MET:HG3	2.43	0.54
3:C:35:THR:HB	3:C:51:GLU:HG3	1.89	0.54
11:K:8:PHE:HA	11:K:144:TRP:CE3	2.43	0.54
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.73	0.54
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.90	0.54
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.89	0.54
12:Z:133:LEU:HD12	12:Z:133:LEU:N	2.22	0.54
14:2:15:GLY:HA2	14:2:174:ARG:O	2.08	0.54
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.89	0.54
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.73	0.54
7:G:45:CYS:O	7:G:146:PRO:HB3	2.08	0.54
2:P:71:ASN:ND2	2:P:72:ASP:N	2.56	0.54
4:R:113:THR:HG23	4:R:138:ILE:HD12	1.89	0.54
5:S:52:LYS:HD2	5:S:63:TYR:O	2.08	0.54
2:P:87:ILE:O	2:P:91:THR:HG23	2.08	0.54
6:F:49:ALA:HA	6:F:211:GLU:O	2.08	0.54
13:M:57:ARG:HH11	13:M:57:ARG:HG2	1.72	0.54
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.90	0.54
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.90	0.54
9:W:79:PHE:O	9:W:83:VAL:HG23	2.08	0.54
16:R:2121:HOH:O	12:Z:70:HIS:HE1	1.90	0.54
3:C:151:THR:HG22	3:C:157:TYR:HB3	1.90	0.53
4:D:130:ARG:NH1	4:D:130:ARG:HG3	2.22	0.53
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.38	0.53
7:U:130:ARG:HG3	7:U:131:PRO:O	2.09	0.53
7:U:139:VAL:HA	7:U:147:SER:O	2.08	0.53
13:1:4:ILE:HD11	13:1:159:MET:SD	2.48	0.53
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.89	0.53
3:C:45:CYS:HA	3:C:141:PHE:HZ	1.73	0.53
1:O:78:TYR:CE2	1:O:82:GLY:HA2	2.44	0.53
6:T:38:ILE:HG22	6:T:164:ALA:HB1	1.89	0.53
6:T:43:ASN:HD22	6:T:44:ASP:N	2.06	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:128:GLY:O	8:V:131:SER:HB2	2.07	0.53
3:C:130:ARG:HH11	3:C:130:ARG:HG3	1.73	0.53
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.15	0.53
3:C:175:PHE:CD2	3:C:196:SER:HB3	2.44	0.53
5:E:150:GLU:O	5:E:157:VAL:HA	2.09	0.53
9:I:79:PHE:O	9:I:82:LEU:HB3	2.09	0.53
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.90	0.53
4:R:215:ILE:HG13	4:R:215:ILE:O	2.08	0.53
6:F:126:TYR:HE1	7:G:129:MET:SD	2.31	0.53
10:J:68:ILE:HG22	10:J:69:ARG:N	2.23	0.53
1:O:41:LYS:HG3	1:O:46:VAL:HG22	1.89	0.53
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.43	0.53
5:S:48:LEU:HD13	5:S:77:SER:HB3	1.91	0.53
7:U:9:ASP:HA	7:U:14:ILE:HD11	1.91	0.53
1:O:82:GLY:O	1:O:85:TYR:HB3	2.09	0.53
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.73	0.53
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.03	0.53
1:O:23:GLN:OE1	7:U:15:PHE:HB2	2.09	0.53
1:A:49:ALA:HB2	1:A:212:LEU:HG	1.91	0.53
3:C:57:LYS:HD2	3:C:58:LEU:N	2.24	0.53
5:E:180(C):PHE:HA	5:E:180(F):ILE:HG13	1.90	0.53
10:J:15:ALA:HB2	10:J:155:LEU:CD1	2.39	0.53
1:O:121:GLN:O	1:O:124:THR:HB	2.09	0.53
7:U:13:THR:HB	7:U:124:THR:O	2.09	0.53
6:F:39:GLY:HA2	6:F:47:VAL:O	2.09	0.53
3:Q:156:ILE:HD12	4:R:83:ALA:HB2	1.90	0.53
8:V:16:ALA:HA	8:V:159:ILE:HD12	1.91	0.53
13:1:53:GLN:O	13:1:56:GLU:HB2	2.09	0.53
4:D:46:VAL:HG11	4:D:139:ALA:CB	2.35	0.53
4:D:85:ALA:O	4:D:89:ILE:HG12	2.10	0.53
7:G:49:ILE:HD13	7:G:193:ALA:HB1	1.91	0.53
2:P:76:VAL:HG12	2:P:138:TYR:CD2	2.44	0.53
12:Z:166:HIS:HE1	16:Z:1689:HOH:O	1.92	0.53
13:1:141(C):ARG:CG	13:1:141(C):ARG:HH11	2.19	0.52
1:A:67:VAL:HG11	1:A:213:ALA:HB2	1.91	0.52
3:C:163:GLN:HG3	3:C:164:THR:N	2.24	0.52
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.24	0.52
13:1:113:VAL:HA	13:1:118:VAL:O	2.09	0.52
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.45	0.52
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.08	0.52
6:T:43:ASN:HD22	6:T:44:ASP:H	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.91	0.52
10:J:11:SER:HB3	10:J:179:ASP:HB3	1.92	0.52
11:K:48:GLY:N	11:K:96:SER:O	2.40	0.52
4:R:177:LEU:HD22	5:S:58:LEU:HD22	1.91	0.52
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.44	0.52
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.90	0.52
1:O:197:LEU:HD23	1:O:210:ILE:HD12	1.91	0.52
6:T:194:ALA:HA	6:T:210:LEU:HD21	1.91	0.52
10:X:129:TYR:HA	10:X:132:PHE:HD2	1.74	0.52
16:P:1497:HOH:O	10:X:85:GLN:HB2	2.10	0.52
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.90	0.52
10:J:45:PHE:HB3	10:J:99:VAL:HG12	1.90	0.52
14:N:36:ARG:HG2	14:N:38:HIS:O	2.10	0.52
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.40	0.52
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.91	0.52
6:F:192:GLN:HA	6:F:192:GLN:NE2	2.25	0.52
6:F:43:ASN:HD22	6:F:44:ASP:N	2.08	0.52
8:H:103:GLY:HA2	8:H:178:MET:SD	2.48	0.52
11:K:195:LEU:O	11:K:199:VAL:HG23	2.10	0.52
4:R:179:GLU:HB3	4:R:192:LEU:HD21	1.91	0.52
10:X:44:SER:OG	10:X:100:LEU:HB2	2.10	0.52
2:B:13:THR:O	3:C:130:ARG:HD3	2.10	0.52
5:E:74:MET:HE2	5:E:109:VAL:HG22	1.90	0.52
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.91	0.52
3:Q:40:VAL:HG23	3:Q:189:CYS:SG	2.50	0.52
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.75	0.52
14:N:4:MET:HB3	14:N:126:ILE:HG22	1.91	0.52
2:P:89:ILE:O	2:P:92:ALA:HB3	2.10	0.52
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.92	0.52
1:A:21:LEU:HD13	1:A:24:ILE:HD12	1.92	0.52
4:D:49:GLY:HA2	4:D:211:GLN:O	2.09	0.52
5:E:31:ILE:HD11	5:E:153:PRO:HD2	1.91	0.52
7:G:47:VAL:HG12	7:G:48:VAL:N	2.25	0.52
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.91	0.52
13:M:172:ASN:HA	13:M:190:LEU:O	2.10	0.52
6:T:238:LYS:NZ	6:T:239:GLU:HG3	2.24	0.52
13:M:147:THR:OG1	13:M:150:VAL:HG23	2.10	0.51
1:O:180:TRP:HA	1:O:184:LEU:HD11	1.92	0.51
3:Q:159:SER:O	4:R:59:LEU:HD22	2.10	0.51
5:S:16:SER:HB3	5:S:22:PHE:HE2	1.76	0.51
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:133:PHE:CE1	10:X:132:PHE:HA	2.46	0.51
12:L:15:ALA:HB1	12:L:173:LEU:HD11	1.92	0.51
4:R:112:LEU:O	4:R:115:SER:HB3	2.10	0.51
4:R:51:GLU:OE1	4:R:53:ARG:HB2	2.10	0.51
5:S:45:HIS:HB2	5:S:189:LEU:HD12	1.92	0.51
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.09	0.51
12:L:30:TYR:HB3	16:L:9110:HOH:O	2.10	0.51
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.44	0.51
7:U:67:ILE:HG12	7:U:77:VAL:HG23	1.93	0.51
9:W:159:LEU:HD23	9:W:173:ALA:HB1	1.92	0.51
5:E:48:LEU:HB2	5:E:213:ALA:HB3	1.92	0.51
6:F:180(E):GLU:HG3	6:F:180(F):GLY:H	1.75	0.51
13:M:161:VAL:O	13:M:164:TYR:HB2	2.10	0.51
6:T:122:ALA:HA	6:T:125:LEU:HD12	1.93	0.51
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.58	0.51
11:K:6:PHE:CE2	11:K:13:ILE:HB	2.46	0.51
14:N:157:HIS:CD2	14:N:187(J):LEU:HD13	2.46	0.51
5:S:47:VAL:HG23	5:S:189:LEU:HD13	1.92	0.51
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.50	0.51
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.46	0.51
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.39	0.51
7:G:48:VAL:HG23	7:G:48:VAL:O	2.10	0.51
6:T:203:GLU:HA	6:T:206:LYS:HB3	1.93	0.51
3:C:40:VAL:HA	3:C:162:ALA:HA	1.92	0.51
5:E:139:ILE:HA	5:E:147:HIS:O	2.11	0.51
5:E:194:VAL:O	5:E:197:ILE:HG22	2.11	0.51
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.25	0.51
1:A:13:THR:O	2:B:130:ARG:HD3	2.10	0.51
10:J:76:PRO:HD2	16:J:254:HOH:O	2.11	0.51
11:K:111:TYR:CE1	11:K:121:LYS:HB2	2.45	0.51
11:K:3:THR:O	11:K:126:CYS:HA	2.10	0.51
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.21	0.51
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.25	0.51
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.11	0.51
13:1:9:ASP:CB	13:1:144:PRO:HA	2.41	0.51
3:C:49:GLY:C	3:C:50:CYS:SG	2.89	0.51
10:J:7:ARG:CB	10:J:12:VAL:HG22	2.40	0.51
12:L:166:HIS:CD2	12:L:168:GLN:H	2.28	0.51
16:M:236:HOH:O	14:N:116:GLY:HA3	2.10	0.51
8:H:5:GLY:HA3	8:H:110:LEU:HD11	1.93	0.51
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:140:ASN:O	12:L:144:PHE:HA	2.10	0.51
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.94	0.51
13:1:45:ILE:HG23	13:1:99:ILE:HG12	1.93	0.50
8:H:128:GLY:O	8:H:131:SER:HB2	2.10	0.50
13:1:157:ASN:ND2	13:1:160:ARG:NH1	2.58	0.50
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.93	0.50
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.46	0.50
9:I:113:PHE:CD2	9:I:113:PHE:N	2.79	0.50
3:Q:49:GLY:C	3:Q:50:CYS:SG	2.90	0.50
6:T:237:GLN:O	6:T:240:ILE:HG22	2.10	0.50
6:T:36:THR:HA	6:T:165:THR:O	2.10	0.50
9:I:161:ASN:HD21	12:Z:140:ASN:ND2	2.09	0.50
6:F:36:THR:HG22	6:F:51:GLU:OE2	2.12	0.50
7:G:192:PHE:CD1	7:G:192:PHE:C	2.85	0.50
13:M:27:ARG:HD3	13:M:28:PHE:CE2	2.46	0.50
10:X:103:GLY:HA2	10:X:178:VAL:HG11	1.93	0.50
5:E:162:GLY:O	5:E:163:THR:HB	2.10	0.50
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.93	0.50
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.94	0.50
12:L:166:HIS:HD2	12:L:168:GLN:N	2.09	0.50
5:S:24:VAL:O	5:S:27:ALA:HB3	2.12	0.50
2:B:71:ASN:ND2	2:B:72:ASP:H	2.10	0.50
10:J:21:THR:O	10:J:22:ARG:HD3	2.12	0.50
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.46	0.50
9:W:22:SER:O	9:W:23:GLN:HB2	2.12	0.50
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.47	0.50
11:K:113:VAL:HA	11:K:118:THR:O	2.11	0.50
7:U:82:ILE:HG22	7:U:83:PRO:HD3	1.92	0.50
12:L:165:ARG:HA	8:V:26:VAL:HB	1.94	0.50
3:C:238:GLN:C	3:C:240:LYS:H	2.14	0.50
11:K:10:GLY:O	11:K:177:HIS:NE2	2.42	0.50
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.42	0.50
14:N:99:ILE:HG22	14:N:100:ILE:N	2.26	0.50
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.26	0.50
6:T:52:LYS:HD2	6:T:211:GLU:OE2	2.12	0.50
6:T:41:LYS:HA	6:T:46:VAL:HG12	1.93	0.50
4:D:180(C):HIS:O	4:D:184:LEU:HD12	2.12	0.50
10:J:-1:MET:HG2	10:J:1:ASP:H	1.76	0.50
9:W:77:GLU:H	9:W:77:GLU:CD	2.15	0.50
10:X:35:ARG:O	10:X:42:LEU:HD12	2.11	0.50
3:C:49:GLY:HA3	3:C:212:ILE:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:SER:O	4:D:59:LEU:HD22	2.11	0.49
10:J:113:ILE:HA	10:J:118:THR:O	2.12	0.49
3:Q:49:GLY:CA	3:Q:212:ILE:HD13	2.41	0.49
3:Q:28:LEU:O	3:Q:31:VAL:HB	2.12	0.49
10:X:146:MET:HE2	10:X:150:GLU:C	2.32	0.49
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.32	0.49
2:B:163:ILE:HG13	2:B:164:SER:H	1.78	0.49
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.11	0.49
1:O:84:ASP:CG	1:O:130:ARG:HH22	2.15	0.49
5:S:162:GLY:O	5:S:163:THR:HB	2.12	0.49
7:U:220:LYS:HG2	7:U:221:PHE:N	2.27	0.49
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.48	0.49
13:M:141(C):ARG:HH11	13:M:141(C):ARG:CG	2.24	0.49
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.94	0.49
1:O:67:VAL:HG11	1:O:213:ALA:HB2	1.94	0.49
3:Q:49:GLY:HA3	3:Q:212:ILE:HD13	1.94	0.49
4:R:32:LYS:O	4:R:167:SER:HA	2.12	0.49
7:U:49:ILE:HD13	7:U:193:ALA:HB1	1.94	0.49
8:V:132:LEU:N	8:V:132:LEU:HD12	2.27	0.49
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.12	0.49
5:E:179:THR:HG22	5:E:180(B):THR:HB	1.93	0.49
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.52	0.49
6:T:169:ARG:O	6:T:173:LYS:HG3	2.13	0.49
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.10	0.49
5:E:231:LYS:HD2	5:E:231:LYS:H	1.77	0.49
5:E:66:LYS:HD3	16:E:294:HOH:O	2.12	0.49
7:G:80:GLY:HA3	7:G:134:VAL:HG12	1.93	0.49
11:K:73:ARG:NH2	11:K:105:THR:HG22	2.28	0.49
13:M:186:PHE:HE1	13:M:188:LYS:HG3	1.77	0.49
2:B:194:LEU:HD13	2:B:233:LEU:HD12	1.94	0.49
4:D:215:ILE:O	4:D:215:ILE:HG13	2.13	0.49
5:E:76:LEU:O	5:E:76:LEU:HD23	2.13	0.49
2:P:71:ASN:ND2	2:P:72:ASP:H	2.11	0.49
7:U:158:VAL:HG22	7:U:159:GLY:N	2.27	0.49
12:Z:19:ARG:HG2	12:Z:21:ILE:HG23	1.94	0.49
13:1:55:ILE:HD13	13:1:99:ILE:HD11	1.93	0.49
4:D:207:LEU:CD2	4:D:233:ILE:HG12	2.40	0.49
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.46	0.49
8:H:26:VAL:CG1	8:H:29:LYS:HG2	2.40	0.49
2:P:163:ILE:HG13	2:P:164:SER:N	2.26	0.49
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:7:LYS:HD2	13:1:141(G):ILE:HD13	1.95	0.49
5:E:130:ARG:HH11	5:E:130:ARG:HG3	1.76	0.49
11:K:1:THR:HG23	11:K:33:LYS:NZ	2.28	0.49
2:P:39:GLY:O	2:P:148:LEU:HD21	2.12	0.49
13:1:19:LEU:HD11	13:1:26:LEU:HB3	1.95	0.49
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.95	0.49
1:A:147(A):SER:HB2	1:A:149:TYR:CE2	2.48	0.49
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.93	0.49
5:E:198:SER:HA	5:E:201:LEU:CD1	2.43	0.49
9:I:126:VAL:HG11	9:I:134:LEU:HB3	1.94	0.49
2:P:64:THR:HG21	16:W:9048:HOH:O	2.11	0.49
2:P:76:VAL:CG1	2:P:138:TYR:HD2	2.25	0.49
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.28	0.49
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	1.95	0.49
4:D:81:LEU:N	4:D:133:GLY:O	2.42	0.49
14:N:159:LEU:O	14:N:163:ILE:HG13	2.13	0.49
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.24	0.49
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.94	0.49
5:S:161:TYR:CD1	5:S:180(D):ILE:HD13	2.47	0.49
5:S:53:ARG:O	5:S:63:TYR:HA	2.13	0.49
5:S:77:SER:O	5:S:136:LEU:HA	2.13	0.49
4:D:215:ILE:CG2	4:D:221:PHE:HD2	2.25	0.48
16:A:265:HOH:O	8:H:69:TYR:HA	2.12	0.48
4:R:186:LEU:O	4:R:190:GLU:HG3	2.12	0.48
14:2:163:ILE:HD12	14:2:187(G):TYR:CE1	2.48	0.48
3:C:76:LEU:HD12	3:C:138:ILE:HG12	1.95	0.48
5:E:161:TYR:CD1	5:E:180(D):ILE:HD13	2.48	0.48
5:E:52:LYS:HE3	5:E:209(D):ASP:O	2.12	0.48
13:M:165:ARG:HD3	8:V:139:GLU:OE1	2.13	0.48
8:V:20:SER:HB2	8:V:31:CYS:SG	2.54	0.48
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.80	0.48
7:U:192:PHE:C	7:U:192:PHE:CD1	2.86	0.48
7:U:38:LEU:HD12	7:U:39:ALA:N	2.28	0.48
12:Z:100:ILE:HG22	12:Z:101:ILE:N	2.27	0.48
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.49	0.48
2:B:62:ASP:HA	2:B:226:PRO:HG2	1.95	0.48
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.13	0.48
7:G:136:LEU:O	7:G:150:LYS:HA	2.14	0.48
12:L:166:HIS:CD2	12:L:168:GLN:HB2	2.48	0.48
8:V:90:TYR:O	8:V:93:GLY:N	2.47	0.48
2:P:121:GLN:C	2:P:121:GLN:NE2	2.67	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:1998:HOH:O	8:V:69:TYR:HA	2.14	0.48
14:2:134:ILE:HD12	14:2:158:SER:HB3	1.93	0.48
1:A:85:TYR:O	1:A:89:VAL:HG23	2.14	0.48
2:B:141:TYR:CD1	2:B:142:ASP:N	2.82	0.48
2:B:46:ILE:CG2	2:B:148:LEU:HD13	2.44	0.48
2:B:71:ASN:ND2	2:B:72:ASP:N	2.62	0.48
3:C:172:VAL:CG2	3:C:196:SER:HB2	2.43	0.48
4:D:174:ALA:O	4:D:177:LEU:HB2	2.13	0.48
6:F:175:GLU:CD	6:F:199:LEU:HD23	2.34	0.48
6:F:35:THR:CG2	6:F:36:THR:N	2.77	0.48
5:S:52:LYS:HE3	5:S:209(D):ASP:O	2.14	0.48
7:U:186:TRP:O	7:U:190:VAL:HG23	2.13	0.48
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.14	0.48
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.48	0.48
16:A:272:HOH:O	7:G:128:TYR:HD2	1.97	0.48
8:H:34:LEU:HB2	16:H:373:HOH:O	2.12	0.48
4:R:49:GLY:HA2	4:R:211:GLN:O	2.13	0.48
5:S:130:ARG:HG3	5:S:130:ARG:HH11	1.77	0.48
6:T:136:THR:O	6:T:150:MET:HA	2.14	0.48
2:P:53:LYS:HG2	2:P:54:VAL:HG23	1.95	0.48
5:S:20:ARG:HB3	5:S:25:GLU:OE2	2.14	0.48
6:T:192:GLN:NE2	6:T:192:GLN:HA	2.29	0.48
14:2:14:LEU:O	14:2:175:MET:HA	2.14	0.48
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.69	0.48
3:C:232:TYR:O	3:C:236:ILE:HG13	2.12	0.48
5:E:190:ILE:HD13	5:E:212:ILE:HG21	1.96	0.48
11:K:103:GLY:O	11:K:109:THR:N	2.44	0.48
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.96	0.48
5:E:24:VAL:O	5:E:27:ALA:HB3	2.13	0.48
11:K:86:LEU:O	11:K:89:GLN:HB2	2.13	0.48
14:N:14:LEU:O	14:N:175:MET:HA	2.13	0.48
16:O:2073:HOH:O	7:U:128:TYR:HD2	1.96	0.48
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.96	0.48
8:V:175:VAL:HG12	8:V:176:CYS:N	2.29	0.48
12:Z:18:THR:O	12:Z:18:THR:HG22	2.13	0.48
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.29	0.47
2:B:15:PHE:H	3:C:23:GLN:HE22	1.62	0.47
3:C:24:VAL:O	3:C:27:ALA:HB3	2.13	0.47
5:E:52:LYS:HD2	5:E:63:TYR:O	2.13	0.47
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.96	0.47
14:N:3:ILE:HG22	14:N:16:ALA:HB1	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:38:ILE:HD11	6:T:193:ALA:HB1	1.96	0.47
7:U:79:ASN:OD1	7:U:165:THR:HB	2.13	0.47
11:Y:69:ARG:HB3	11:Y:70:GLU:OE2	2.14	0.47
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.96	0.47
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.49	0.47
4:D:173:GLN:O	4:D:177:LEU:HD23	2.14	0.47
8:H:18:THR:HG22	8:H:31:CYS:O	2.14	0.47
10:J:15:ALA:CB	10:J:155:LEU:HD11	2.44	0.47
11:K:42:LEU:HD12	11:K:178:VAL:CG2	2.44	0.47
3:Q:40:VAL:HA	3:Q:162:ALA:HA	1.96	0.47
3:Q:43:LYS:HG2	3:Q:43:LYS:O	2.13	0.47
3:Q:95:GLU:O	3:Q:95:GLU:HG3	2.15	0.47
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.44	0.47
9:W:113:PHE:HA	9:W:118:CYS:O	2.15	0.47
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.29	0.47
14:2:31:THR:HG22	14:2:32:ASP:N	2.29	0.47
5:E:198:SER:HA	5:E:201:LEU:CG	2.43	0.47
8:H:109:HIS:HB3	8:H:111:PHE:CE2	2.50	0.47
8:H:17:ASP:HA	8:H:172:ASN:O	2.14	0.47
12:L:43:MET:HG2	12:L:44:SER:N	2.29	0.47
4:R:173:GLN:O	4:R:177:LEU:HD23	2.14	0.47
5:S:148:LEU:HB3	5:S:160:LEU:O	2.14	0.47
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.45	0.47
7:G:26:TYR:CD1	7:G:26:TYR:N	2.82	0.47
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.95	0.47
12:L:18:THR:HG22	12:L:29:ARG:O	2.15	0.47
3:Q:115:TYR:O	3:Q:119:VAL:HG23	2.14	0.47
4:R:121:ALA:O	4:R:123:ALA:N	2.46	0.47
6:T:221:HIS:HE1	6:T:223:PHE:HE1	1.61	0.47
5:E:15:PHE:H	6:F:23:GLN:HE22	1.63	0.47
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.95	0.47
10:J:75:SER:HB2	16:J:254:HOH:O	2.14	0.47
1:O:66:LYS:HB2	1:O:211:GLU:OE2	2.15	0.47
4:R:207:LEU:HD23	4:R:207:LEU:O	2.14	0.47
7:U:194:ILE:HD13	7:U:210:LEU:HD12	1.97	0.47
13:1:157:ASN:HB3	16:1:1810:HOH:O	2.15	0.47
4:D:79:SER:HA	16:D:258:HOH:O	2.14	0.47
12:L:146:LEU:HD22	12:L:150:GLU:HG2	1.96	0.47
4:R:160:TYR:HA	5:S:59:SER:HA	1.96	0.47
1:A:82:GLY:O	1:A:85:TYR:HB3	2.14	0.47
4:D:112:LEU:C	4:D:112:LEU:HD13	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.15	0.47
6:T:38:ILE:HA	6:T:164:ALA:HA	1.96	0.47
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.97	0.47
14:2:14:LEU:N	14:2:14:LEU:HD12	2.30	0.47
14:2:175:MET:HE3	14:2:187(B):PHE:CE2	2.49	0.47
14:2:3:ILE:HD12	14:2:44:CYS:HB3	1.97	0.47
2:B:130:ARG:HG3	2:B:130:ARG:HH11	1.79	0.47
2:B:147:GLN:HB3	2:B:149:TYR:CE2	2.50	0.47
4:D:121:ALA:O	4:D:123:ALA:N	2.48	0.47
13:M:114:ASN:O	13:M:116:LEU:N	2.47	0.47
7:U:103:TYR:CE1	8:V:66:HIS:CD2	3.03	0.47
11:Y:159:ILE:HG21	11:Y:173:VAL:HG22	1.97	0.47
1:A:188:ASP:O	1:A:191:HIS:HB3	2.15	0.47
2:B:108:PRO:HD2	2:B:111:ILE:HD12	1.95	0.47
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.55	0.47
4:D:193:VAL:CG1	4:D:212:LEU:HD21	2.44	0.47
12:L:166:HIS:HE1	16:L:9022:HOH:O	1.97	0.47
1:O:186:LEU:O	1:O:190:ILE:HG13	2.15	0.47
3:Q:197:LEU:HD13	3:Q:210:ILE:HG23	1.96	0.47
3:Q:55:THR:HB	3:Q:56:LEU:HD22	1.97	0.47
4:R:112:LEU:C	4:R:112:LEU:HD13	2.35	0.47
4:R:85:ALA:O	4:R:89:ILE:HG12	2.15	0.47
5:S:161:TYR:HD1	5:S:180(D):ILE:HD13	1.80	0.47
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.15	0.47
8:H:3:ILE:O	8:H:3:ILE:HG13	2.15	0.47
9:I:14:ILE:O	9:I:14:ILE:HG23	2.15	0.47
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.50	0.47
3:Q:201:VAL:HG21	3:Q:210:ILE:HG12	1.96	0.47
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.97	0.47
7:U:140:SER:O	7:U:147:SER:N	2.47	0.47
13:1:43:VAL:HG22	13:1:101:VAL:HG22	1.97	0.47
13:1:91:ARG:HG3	13:1:92:SER:N	2.30	0.47
5:E:163:THR:N	5:E:176:LEU:HD13	2.29	0.47
5:E:33:GLN:HG2	5:E:33:GLN:O	2.15	0.47
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.50	0.47
2:P:163:ILE:HG13	2:P:164:SER:H	1.80	0.47
4:R:170:GLU:HG2	4:R:171:GLY:N	2.30	0.47
5:S:24:VAL:HG12	5:S:28:LEU:CD1	2.45	0.47
7:U:26:TYR:CD1	7:U:26:TYR:N	2.81	0.47
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.97	0.47
5:E:12:THR:HG21	5:E:124:THR:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:214:TRP:N	6:F:214:TRP:CD1	2.82	0.46
10:J:7:ARG:HA	10:J:12:VAL:HA	1.97	0.46
12:L:33:LYS:HE2	12:L:33:LYS:HB3	1.61	0.46
14:N:161:GLN:O	14:N:164:LYS:HB3	2.15	0.46
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.97	0.46
1:A:35:VAL:HG12	1:A:36:THR:N	2.30	0.46
1:A:39:GLY:HA2	1:A:47:VAL:O	2.15	0.46
13:M:135:ASN:HB2	13:M:136:PRO:HD3	1.97	0.46
1:O:38:LEU:O	1:O:48:ILE:HA	2.14	0.46
4:R:187:LYS:O	4:R:190:GLU:HB2	2.15	0.46
9:W:159:LEU:CD2	9:W:173:ALA:HB1	2.45	0.46
12:Z:15:ALA:HB2	12:Z:175:ILE:HG23	1.98	0.46
2:B:230:LYS:O	2:B:234:VAL:HG23	2.15	0.46
5:E:73:HIS:CE1	5:E:107:LEU:O	2.63	0.46
5:E:179:THR:O	5:E:179:THR:HG22	2.15	0.46
6:F:18:ASP:N	6:F:18:ASP:OD2	2.47	0.46
6:F:50:VAL:HG22	6:F:51:GLU:N	2.30	0.46
7:G:220:LYS:HG2	7:G:221:PHE:N	2.31	0.46
8:H:56:THR:HG22	8:H:57:GLN:N	2.30	0.46
9:I:101:VAL:O	9:I:110:ILE:HA	2.15	0.46
9:I:16:CYS:SG	9:I:174:VAL:HG12	2.55	0.46
14:N:163:ILE:CG2	14:N:170:GLY:HA2	2.45	0.46
1:O:38:LEU:HD12	1:O:38:LEU:C	2.36	0.46
3:Q:45:CYS:HA	3:Q:141:PHE:HZ	1.80	0.46
4:R:13:SER:HB2	5:S:130:ARG:HB3	1.98	0.46
10:J:113:ILE:CG1	10:J:119:LYS:HG3	2.34	0.46
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.44	0.46
11:K:197:TRP:CE2	9:W:190:LYS:HE3	2.49	0.46
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.09	0.46
4:R:79:SER:HA	16:R:1963:HOH:O	2.15	0.46
5:S:198:SER:HA	5:S:201:LEU:CD1	2.46	0.46
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.98	0.46
11:K:205:SER:HB2	10:X:140:HIS:HA	1.96	0.46
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.16	0.46
8:H:165:ASN:ND2	13:I:139:ARG:HH11	2.12	0.46
3:C:141:PHE:HE2	3:C:215:VAL:HG22	1.81	0.46
3:C:40:VAL:HG23	3:C:189:CYS:SG	2.56	0.46
4:D:76:CYS:HA	4:D:137:LEU:O	2.16	0.46
16:G:9067:HOH:O	8:H:66:HIS:HD2	1.99	0.46
14:N:15:GLY:HA2	14:N:174:ARG:O	2.13	0.46
1:O:111:LEU:HD23	1:O:111:LEU:HA	1.65	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:42:CYS:HB2	6:T:184:LEU:O	2.15	0.46
9:W:45:ILE:HG22	9:W:52:VAL:HG22	1.98	0.46
11:Y:32:LYS:HD2	11:Y:32:LYS:N	2.30	0.46
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.96	0.46
2:B:52:ARG:CZ	2:B:61:GLN:HG2	2.46	0.46
3:C:151:THR:HG22	3:C:157:TYR:CB	2.45	0.46
3:C:179:ASN:OD1	3:C:195:ARG:NH2	2.48	0.46
5:E:40:LEU:HA	5:E:162:GLY:HA2	1.97	0.46
8:H:172:ASN:ND2	8:H:193:THR:HG22	2.30	0.46
8:H:63:ILE:HD13	8:H:63:ILE:HA	1.81	0.46
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.16	0.46
13:M:133:MET:HG2	8:V:132:LEU:HB3	1.98	0.46
8:V:18:THR:HB	8:V:30:ASN:HA	1.97	0.46
10:J:164:LYS:HD3	11:Y:139:ASP:OD2	2.16	0.46
12:Z:43:MET:CG	12:Z:101:ILE:HG22	2.45	0.46
12:Z:175:ILE:C	12:Z:176:LEU:HD12	2.36	0.46
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.27	0.46
4:R:108:ASN:HB2	4:R:111:SER:OG	2.16	0.46
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.97	0.46
12:Z:51:ASP:OD1	12:Z:95:TYR:HA	2.15	0.46
6:F:36:THR:HA	6:F:165:THR:O	2.16	0.46
1:A:130:ARG:HD3	7:G:13:THR:O	2.15	0.46
13:M:157:ASN:HD22	13:M:160:ARG:NH1	2.14	0.46
5:S:125:GLN:O	5:S:125:GLN:HG2	2.15	0.46
6:T:39:GLY:HA2	6:T:47:VAL:O	2.16	0.46
5:S:161:TYR:CE2	6:T:60:VAL:HA	2.50	0.46
7:U:48:VAL:O	7:U:48:VAL:HG23	2.15	0.46
10:X:-1:MET:HG2	10:X:1:ASP:N	2.31	0.46
9:I:161:ASN:ND2	12:Z:140:ASN:ND2	2.63	0.46
14:2:104:TYR:CE1	14:2:180:ALA:HA	2.50	0.46
1:A:210:ILE:HA	1:A:210:ILE:HD13	1.75	0.46
1:A:78:TYR:CE2	1:A:82:GLY:HA2	2.51	0.46
3:C:183:PRO:CB	3:C:189:CYS:HA	2.46	0.46
7:G:123:TYR:N	7:G:123:TYR:CD1	2.83	0.46
8:H:144:GLN:O	8:H:145:ASP:HB2	2.16	0.46
8:H:192:LEU:HA	8:H:192:LEU:HD23	1.76	0.46
10:J:3:ILE:HG21	16:J:298:HOH:O	2.15	0.46
1:O:100:TYR:CE1	1:O:107:PRO:HA	2.51	0.46
3:Q:41:LYS:HG2	3:Q:161:SER:O	2.16	0.46
3:Q:238:GLN:C	3:Q:240:LYS:H	2.18	0.46
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:49:VAL:CG1	5:S:210:LEU:HD11	2.46	0.46
7:U:10:ARG:HG2	7:U:22:TYR:HD2	1.79	0.46
11:Y:143:LYS:O	11:Y:146:LEU:HD13	2.14	0.46
13:1:4:ILE:HD11	13:1:159:MET:CG	2.43	0.46
14:2:143:ARG:O	14:2:146:MET:HG3	2.16	0.46
2:B:123:TYR:CD1	2:B:132:PHE:HE1	2.34	0.46
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.16	0.46
14:N:8:PHE:HA	16:N:578:HOH:O	2.16	0.46
2:P:89:ILE:O	2:P:92:ALA:N	2.49	0.46
14:2:3:ILE:HG22	14:2:16:ALA:HB1	1.98	0.45
1:A:84:ASP:CG	1:A:130:ARG:HH22	2.18	0.45
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.46	0.45
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.98	0.45
8:H:142:TRP:CD1	8:H:146:LEU:HD11	2.51	0.45
12:L:5:GLY:HA2	12:L:13:VAL:O	2.16	0.45
4:R:46:VAL:O	4:R:214:CYS:HA	2.16	0.45
9:W:109:PHE:C	9:W:109:PHE:CD2	2.89	0.45
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.98	0.45
2:B:112:LEU:HD23	2:B:112:LEU:C	2.37	0.45
4:D:193:VAL:HG11	4:D:212:LEU:HD21	1.98	0.45
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.80	0.45
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.97	0.45
11:K:71:LYS:HG3	16:K:9064:HOH:O	2.16	0.45
12:L:19:ARG:HD2	12:L:168:GLN:O	2.16	0.45
1:O:69:LEU:HD23	1:O:69:LEU:C	2.37	0.45
2:P:202:THR:HG22	2:P:203:ASP:N	2.30	0.45
3:Q:140:GLY:HA2	3:Q:215:VAL:HG21	1.99	0.45
3:Q:96:ALA:HB3	16:Q:1480:HOH:O	2.15	0.45
9:W:113:PHE:CD2	9:W:113:PHE:N	2.83	0.45
2:B:37:ALA:HB3	2:B:165:VAL:CG2	2.47	0.45
2:B:14:ILE:CG2	3:C:12:LEU:HD13	2.46	0.45
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.43	0.45
5:E:78:LEU:O	5:E:78:LEU:HG	2.17	0.45
7:G:48:VAL:C	7:G:49:ILE:HD12	2.36	0.45
7:G:74:ILE:HD13	7:G:109:CYS:HA	1.99	0.45
10:J:3:ILE:HG22	10:J:100:LEU:HD12	1.98	0.45
14:N:171:GLY:O	14:N:187(D):PRO:HG3	2.16	0.45
1:O:58:LEU:HD23	1:O:58:LEU:HA	1.69	0.45
16:O:2144:HOH:O	2:P:82:THR:HG21	2.15	0.45
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.97	0.45
8:V:84:LYS:HG3	8:V:85:GLN:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:114:ASP:CG	9:W:118:CYS:HB3	2.37	0.45
1:A:169:SER:O	1:A:173:LYS:HG3	2.15	0.45
5:E:161:TYR:HD1	5:E:180(D):ILE:HD13	1.81	0.45
6:F:24:VAL:O	6:F:27:ALA:HB3	2.16	0.45
10:J:6:ILE:HG21	10:J:155:LEU:HD23	1.99	0.45
10:X:146:MET:CE	10:X:150:GLU:HB3	2.46	0.45
14:2:133:PHE:HE2	14:2:166:ASP:HB2	1.81	0.45
10:J:52:THR:CG2	10:J:53:VAL:N	2.79	0.45
12:L:133:LEU:N	12:L:133:LEU:HD12	2.32	0.45
12:L:76:ILE:HG23	12:L:77:ASN:N	2.32	0.45
2:P:112:LEU:HD23	2:P:112:LEU:C	2.36	0.45
3:Q:175:PHE:CZ	3:Q:195:ARG:HB3	2.51	0.45
8:V:34:LEU:HD22	8:V:174:ASP:HB3	1.98	0.45
9:W:6:MET:HG2	9:W:124:PHE:HB3	1.98	0.45
14:2:59:VAL:HG22	14:2:82:VAL:HG12	1.98	0.45
2:B:81:LEU:HB2	2:B:84:ASP:HB2	1.97	0.45
6:F:130:ARG:HG3	6:F:131:PRO:O	2.17	0.45
6:F:187:ARG:CG	6:F:187:ARG:HH11	2.29	0.45
7:G:49:ILE:CD1	7:G:49:ILE:N	2.75	0.45
12:L:4:LEU:HD23	12:L:155:VAL:HG22	1.98	0.45
13:M:163:TYR:HA	13:M:169:SER:OG	2.17	0.45
1:O:207:ASN:HA	1:O:233:LEU:CD1	2.47	0.45
4:R:233:ILE:O	4:R:237:LEU:HB3	2.16	0.45
6:T:180(E):GLU:HG3	6:T:180(F):GLY:H	1.81	0.45
1:O:81:MET:HE1	7:U:21:LEU:HD11	1.99	0.45
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.99	0.45
13:1:133:MET:C	13:1:136:PRO:HD2	2.37	0.45
9:I:16:CYS:SG	9:I:174:VAL:CG1	3.04	0.45
12:L:109:ALA:HA	16:L:9058:HOH:O	2.16	0.45
13:M:91:ARG:HG3	13:M:92:SER:N	2.32	0.45
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.17	0.45
3:Q:179:ASN:OD1	3:Q:195:ARG:NH2	2.50	0.45
5:S:194:VAL:O	5:S:197:ILE:HG22	2.16	0.45
6:T:187:ARG:CG	6:T:187:ARG:HH11	2.28	0.45
8:V:221:ILE:HG13	9:W:40:HIS:HA	1.97	0.45
13:1:1:THR:HG23	13:1:2:SER:N	2.31	0.45
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.27	0.45
10:J:53:VAL:HB	16:K:9042:HOH:O	2.16	0.45
13:M:9:ASP:CB	13:M:144:PRO:HA	2.46	0.45
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.98	0.45
2:B:161:LYS:HE3	3:C:59:GLN:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:190:GLU:O	4:D:194:LEU:HD22	2.17	0.45
12:L:148:VAL:HG13	12:L:149:GLU:N	2.32	0.45
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.52	0.45
6:T:214:TRP:CD1	6:T:214:TRP:N	2.84	0.45
8:V:53:GLU:OE2	8:V:57:GLN:HG3	2.17	0.45
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.81	0.45
6:F:127:ASN:ND2	6:F:127:ASN:C	2.70	0.45
8:H:77:VAL:HB	13:1:208:THR:HG22	1.99	0.45
13:M:-3:VAL:HG12	13:M:49:ILE:HG13	1.99	0.45
6:T:180(E):GLU:HG3	6:T:180(F):GLY:N	2.32	0.45
8:V:172:ASN:HB3	8:V:192:LEU:O	2.17	0.45
5:E:207:LEU:CD2	5:E:207:LEU:H	2.30	0.44
7:G:158:VAL:HG22	7:G:159:GLY:N	2.32	0.44
7:G:186:TRP:CZ3	7:G:224:LEU:HD21	2.52	0.44
11:K:69:ARG:HB3	11:K:70:GLU:OE2	2.17	0.44
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.98	0.44
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.99	0.44
8:V:67:SER:O	8:V:71:SER:N	2.50	0.44
13:1:82:TYR:O	13:1:86:VAL:HG23	2.17	0.44
5:E:47:VAL:HG12	5:E:48:LEU:N	2.33	0.44
6:F:130:ARG:CG	6:F:130:ARG:HH11	2.30	0.44
12:L:6:ILE:HB	12:L:13:VAL:HG22	2.00	0.44
2:P:136:PHE:O	2:P:150:THR:HA	2.17	0.44
2:P:38:ILE:O	2:P:48:LEU:HA	2.17	0.44
3:Q:130:ARG:NH1	3:Q:130:ARG:HG3	2.31	0.44
14:N:133:PHE:HA	14:2:132:THR:O	2.18	0.44
3:C:198:LEU:HD23	3:C:198:LEU:HA	1.82	0.44
4:R:76:CYS:HA	4:R:137:LEU:O	2.17	0.44
4:R:78:MET:SD	4:R:82:THR:HG22	2.58	0.44
7:U:207:LYS:HG3	7:U:208:ASN:OD1	2.17	0.44
7:U:39:ALA:HA	7:U:47:VAL:O	2.17	0.44
3:C:150:GLN:O	3:C:157:TYR:HA	2.18	0.44
3:C:25:GLU:O	3:C:28:LEU:HB2	2.18	0.44
5:E:40:LEU:HD23	5:E:40:LEU:N	2.32	0.44
6:F:35:THR:CG2	6:F:51:GLU:O	2.66	0.44
10:J:36:GLN:HG3	10:J:184:ILE:CD1	2.47	0.44
1:O:39:GLY:HA2	1:O:47:VAL:O	2.17	0.44
1:O:71:THR:O	1:O:73:ASP:N	2.50	0.44
11:K:139:ASP:OD2	10:X:164:LYS:HD3	2.17	0.44
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.99	0.44
12:Z:176:LEU:N	12:Z:176:LEU:HD12	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:VAL:CG1	2:B:138:TYR:CD2	3.01	0.44
2:B:95:HIS:HB2	16:B:274:HOH:O	2.18	0.44
3:C:197:LEU:HD13	3:C:210:ILE:CG2	2.48	0.44
7:G:31:THR:HG21	7:G:135:ILE:HG13	1.99	0.44
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.99	0.44
6:T:191:LYS:O	6:T:194:ALA:HB3	2.17	0.44
10:X:3:ILE:HG21	16:X:1456:HOH:O	2.17	0.44
13:1:9:ASP:HB3	13:1:144:PRO:HA	1.99	0.44
13:1:-7:GLN:HG3	13:1:96:TRP:CE3	2.53	0.44
2:B:87:ILE:O	2:B:91:THR:HG23	2.18	0.44
7:G:191:GLU:O	7:G:192:PHE:C	2.55	0.44
7:G:87:ASN:C	7:G:87:ASN:HD22	2.21	0.44
12:L:137:PHE:HZ	8:V:204:TYR:CE1	2.36	0.44
1:O:112:LEU:O	1:O:116:VAL:HG23	2.17	0.44
5:S:16:SER:HB3	5:S:22:PHE:CE2	2.52	0.44
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.53	0.44
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.98	0.44
8:V:18:THR:HG22	8:V:31:CYS:O	2.18	0.44
11:Y:131:GLN:HG3	11:Y:132:THR:N	2.32	0.44
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.48	0.44
14:2:52:THR:HG22	14:2:97:ALA:HB1	2.00	0.44
3:C:76:LEU:HA	3:C:137:LEU:O	2.18	0.44
4:D:113:THR:HG23	4:D:138:ILE:HD12	2.00	0.44
6:F:74:ILE:HD13	6:F:112:PHE:CD2	2.52	0.44
6:F:236:ALA:O	6:F:240:ILE:HB	2.17	0.44
6:F:238:LYS:NZ	6:F:239:GLU:HG3	2.33	0.44
9:I:190:LYS:HE3	11:Y:197:TRP:CE2	2.53	0.44
11:K:8:PHE:CE2	11:K:13:ILE:HG12	2.53	0.44
11:K:28:SER:HB2	12:L:125:ARG:HH22	1.83	0.44
13:M:131:ALA:O	13:M:135:ASN:HB2	2.17	0.44
13:M:82:TYR:O	13:M:86:VAL:HG23	2.17	0.44
1:O:130:ARG:NH1	1:O:131:PRO:O	2.51	0.44
1:A:136:LEU:O	1:A:150:GLN:HA	2.18	0.44
3:C:175:PHE:HZ	3:C:195:ARG:HB3	1.81	0.44
3:C:49:GLY:CA	3:C:212:ILE:HD13	2.48	0.44
6:F:169:ARG:HB3	6:F:169:ARG:HE	1.60	0.44
6:F:192:GLN:HA	6:F:192:GLN:HE21	1.83	0.44
6:F:38:ILE:HG13	6:F:38:ILE:O	2.18	0.44
6:F:48:PHE:CE2	6:F:138:PHE:HA	2.53	0.44
7:G:151:THR:HA	7:G:156:TYR:O	2.18	0.44
11:K:196:PHE:CE2	11:K:206:PHE:CD2	3.06	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:17:ASP:HA	12:L:172:GLY:O	2.18	0.44
12:L:43:MET:HG3	12:L:101:ILE:HG22	2.00	0.44
13:M:193:GLU:O	13:M:194:ASN:HB2	2.18	0.44
5:S:210:LEU:HA	5:S:210:LEU:HD12	1.79	0.44
2:B:136:PHE:O	2:B:150:THR:HA	2.18	0.44
3:C:38:VAL:O	3:C:48:LEU:HA	2.18	0.44
4:D:97:VAL:HG11	11:K:65:LEU:HD13	2.00	0.44
7:G:38:LEU:HD12	7:G:39:ALA:N	2.33	0.44
10:J:140:HIS:O	11:Y:205:SER:HB3	2.18	0.44
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.47	0.44
11:K:35:ILE:HD11	11:K:45:MET:CE	2.48	0.44
4:R:40:ILE:HD12	4:R:193:VAL:HG23	2.00	0.44
5:S:209(C):VAL:O	5:S:226:GLY:HA2	2.18	0.44
8:V:200:LYS:HE3	9:W:140:SER:O	2.18	0.44
9:W:58:MET:O	9:W:61:TYR:HB3	2.18	0.44
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.17	0.44
5:E:214:ILE:HG12	5:E:215:VAL:N	2.33	0.43
6:F:12:ASN:ND2	6:F:131:PRO:HD3	2.32	0.43
9:I:90:ARG:HA	9:I:90:ARG:HD3	1.85	0.43
10:J:8:VAL:HG23	10:J:9:GLN:N	2.32	0.43
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.46	0.43
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.33	0.43
3:Q:46:VAL:HB	3:Q:215:VAL:HG13	2.00	0.43
4:R:122:ALA:C	4:R:127:ALA:H	2.21	0.43
4:R:49:GLY:HA3	4:R:193:VAL:HG11	1.99	0.43
5:S:64:GLN:HA	16:S:2195:HOH:O	2.17	0.43
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.92	0.43
9:W:48:LEU:HG	9:W:50:THR:HG22	1.99	0.43
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.65	0.43
13:1:-5:PRO:HD3	13:1:96:TRP:CD2	2.53	0.43
2:B:126:HIS:CB	3:C:129:VAL:HG12	2.37	0.43
3:C:201:VAL:HG21	3:C:210:ILE:HG12	1.99	0.43
7:G:188:LYS:O	7:G:191:GLU:HB2	2.17	0.43
7:G:197:MET:HG2	7:G:205:PHE:CZ	2.53	0.43
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.54	0.43
11:K:32:LYS:HD2	11:K:32:LYS:N	2.33	0.43
2:P:218(C):ASP:HB3	2:P:218(D):GLY:H	1.63	0.43
5:S:190:ILE:O	5:S:193:GLY:N	2.52	0.43
5:S:209(B):THR:N	5:S:209(E):ASN:HB2	2.28	0.43
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.17	0.43
11:Y:25:TRP:HH2	12:Z:135:MET:HB2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:209:GLN:HG2	13:1:211:ILE:O	2.18	0.43
14:2:107:LYS:HG2	14:2:108:GLY:H	1.82	0.43
11:K:156:LYS:HB2	11:K:175:LEU:HD11	2.00	0.43
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.48	0.43
1:O:152:ASP:O	1:O:155:GLY:N	2.45	0.43
2:P:41:MET:HB2	2:P:148:LEU:HD22	2.00	0.43
4:R:70:ILE:HB	4:R:74:ILE:HG22	2.01	0.43
5:S:37:THR:O	5:S:164:ALA:HA	2.17	0.43
6:T:238:LYS:HZ1	6:T:239:GLU:HG3	1.82	0.43
6:T:38:ILE:HG13	6:T:38:ILE:O	2.16	0.43
6:T:69:VAL:HG12	16:1:2019:HOH:O	2.17	0.43
8:V:206:PHE:CE1	9:W:157:GLN:HG3	2.53	0.43
10:X:146:MET:HE2	10:X:150:GLU:HB3	1.99	0.43
10:X:43:MET:HG3	10:X:101:ILE:HG13	2.00	0.43
12:Z:49:ALA:HB1	16:1:2421:HOH:O	2.17	0.43
13:1:163:TYR:HA	13:1:169:SER:OG	2.18	0.43
5:E:49:VAL:CG1	5:E:210:LEU:HD11	2.49	0.43
6:F:46:VAL:HG23	6:F:48:PHE:CE1	2.53	0.43
12:L:100:ILE:HD11	12:L:125:ARG:HG3	2.00	0.43
13:M:112:TYR:CZ	13:M:114:ASN:HB3	2.52	0.43
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.67	0.43
5:S:107:LEU:HA	16:S:1845:HOH:O	2.17	0.43
6:T:136:THR:HG22	6:T:138:PHE:HD2	1.82	0.43
12:Z:155:VAL:O	12:Z:158:SER:HB2	2.19	0.43
13:1:160:ARG:HG3	13:1:192:VAL:CG1	2.49	0.43
14:2:163:ILE:HG21	14:2:187(G):TYR:HE1	1.83	0.43
1:A:27:ALA:O	1:A:31:VAL:HG23	2.18	0.43
5:E:173:LYS:O	5:E:177:GLU:HB2	2.19	0.43
6:F:180(E):GLU:HG3	6:F:180(F):GLY:N	2.33	0.43
8:H:157:ASP:O	8:H:160:GLN:N	2.51	0.43
11:K:38:ASN:OD1	11:K:38:ASN:C	2.56	0.43
1:O:29:THR:O	1:O:33:GLN:HG2	2.18	0.43
2:P:205:LEU:HA	2:P:205:LEU:HD12	1.83	0.43
3:Q:134:VAL:CG1	3:Q:135:SER:N	2.82	0.43
4:R:97:VAL:O	4:R:100:ASN:N	2.50	0.43
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.82	0.43
6:T:28:VAL:O	6:T:31:VAL:HB	2.19	0.43
7:U:55:PRO:HG2	7:U:56:ASP:H	1.83	0.43
10:X:14:LEU:O	10:X:175:VAL:HA	2.19	0.43
12:Z:49:ALA:HA	16:Z:1987:HOH:O	2.17	0.43
1:A:46:VAL:HG11	1:A:139:ALA:HB1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:TRP:CD1	2:B:160:TRP:N	2.86	0.43
9:I:42:PHE:N	9:I:42:PHE:CD1	2.86	0.43
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.34	0.43
11:Y:157:ARG:O	11:Y:160:LEU:HB3	2.19	0.43
13:1:137:LEU:O	13:1:140:LYS:HB2	2.18	0.43
13:1:181(A):THR:HB	16:1:1466:HOH:O	2.17	0.43
13:1:83:LEU:O	13:1:87:MET:HG2	2.18	0.43
14:2:147:SER:OG	14:2:150:GLU:HG3	2.18	0.43
14:2:67:THR:HA	14:2:72:GLY:O	2.19	0.43
3:C:38:VAL:HG22	3:C:39:GLY:N	2.32	0.43
5:E:13:VAL:HG13	5:E:13:VAL:O	2.19	0.43
5:E:48:LEU:HD13	5:E:77:SER:HB3	2.00	0.43
5:E:52:LYS:HB3	5:E:63:TYR:HB3	2.00	0.43
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.99	0.43
11:K:146:LEU:HD23	11:K:151:ALA:CA	2.48	0.43
11:K:172:SER:CA	11:K:192:VAL:HG23	2.48	0.43
12:L:113:PHE:N	12:L:113:PHE:CD1	2.87	0.43
12:L:49:ALA:HB1	16:M:300:HOH:O	2.18	0.43
14:N:99:ILE:CG2	14:N:100:ILE:N	2.81	0.43
5:S:38:VAL:HG22	5:S:164:ALA:HB2	2.00	0.43
6:T:40:ILE:HG12	6:T:176:LEU:HD11	2.00	0.43
9:W:43:LEU:HD21	9:W:45:ILE:HD11	2.00	0.43
3:C:52:ARG:HD2	3:C:208:LYS:O	2.19	0.43
7:G:96:ALA:CA	7:G:107:MET:HE2	2.27	0.43
11:K:25:TRP:CH2	12:L:132:SER:HA	2.54	0.43
13:M:5:SER:HB3	13:M:14:ILE:HG13	2.00	0.43
13:M:37:VAL:O	13:M:41:THR:HB	2.19	0.43
2:P:130:ARG:NH1	2:P:131:PRO:O	2.52	0.43
9:W:90:ARG:HD2	16:W:9098:HOH:O	2.18	0.43
12:Z:109:ALA:HA	16:Z:2081:HOH:O	2.18	0.43
13:1:165:ARG:HD2	13:1:165:ARG:N	2.34	0.43
2:B:141:TYR:C	2:B:141:TYR:CD1	2.92	0.43
2:B:188:ASP:O	2:B:191:GLU:HB3	2.18	0.43
13:M:9:ASP:HB3	13:M:144:PRO:HA	1.99	0.43
14:N:43:CYS:HA	14:N:100:ILE:O	2.19	0.43
6:T:40:ILE:HD12	6:T:193:ALA:HB2	2.00	0.43
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.57	0.43
2:B:141:TYR:CG	2:B:142:ASP:N	2.87	0.43
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.48	0.43
5:E:141:TYR:OH	5:E:217:LYS:HG3	2.18	0.43
13:M:164:TYR:O	14:2:26:ILE:HD12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:130:ARG:HG3	6:T:130:ARG:NH1	2.34	0.43
2:B:171:ALA:O	2:B:175:LEU:HG	2.19	0.42
4:D:37:ALA:C	4:D:38:ILE:HG13	2.40	0.42
13:M:55:ILE:HD13	13:M:99:ILE:HD11	2.01	0.42
13:M:-4:ILE:HG21	14:N:115:LEU:HB3	2.01	0.42
3:Q:121:GLN:HG3	16:R:1001:HOH:O	2.19	0.42
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.19	0.42
6:T:221:HIS:CE1	6:T:223:PHE:CE1	3.02	0.42
8:V:153:LYS:O	8:V:156:SER:HB3	2.19	0.42
9:W:5:ALA:HA	9:W:14:ILE:HA	2.01	0.42
13:1:132:HIS:HE1	16:1:1440:HOH:O	2.00	0.42
13:1:161:VAL:O	13:1:164:TYR:HB2	2.19	0.42
3:C:95:GLU:HG3	3:C:95:GLU:O	2.19	0.42
6:F:238:LYS:HZ2	6:F:239:GLU:HG3	1.84	0.42
1:O:210:ILE:HD13	1:O:210:ILE:HA	1.80	0.42
2:P:76:VAL:HG12	2:P:138:TYR:HA	2.00	0.42
3:Q:51:GLU:HA	3:Q:209:ASN:O	2.18	0.42
6:T:184:LEU:CD1	6:T:188:GLU:HB3	2.46	0.42
8:V:95:ILE:O	8:V:97:ALA:N	2.52	0.42
9:W:29:ASN:HD21	9:W:30:LYS:NZ	2.16	0.42
10:X:7:ARG:HA	10:X:12:VAL:HA	2.00	0.42
12:Z:91:ARG:O	12:Z:91:ARG:HG3	2.19	0.42
2:B:53:LYS:HG2	2:B:54:VAL:HG23	2.00	0.42
3:C:41:LYS:HG2	3:C:161:SER:O	2.18	0.42
5:E:74:MET:CE	5:E:109:VAL:HA	2.49	0.42
6:F:198:TYR:O	6:F:202:HIS:HB3	2.19	0.42
7:G:190:VAL:HG11	7:G:232:ARG:HG2	2.01	0.42
9:I:51:ASP:OD2	10:J:90(B):ARG:NH2	2.53	0.42
12:L:15:ALA:HB2	12:L:175:ILE:HG23	2.00	0.42
2:P:230:LYS:O	2:P:234:VAL:HG23	2.19	0.42
6:T:12:ASN:ND2	6:T:131:PRO:HD3	2.34	0.42
12:Z:114:ASP:CB	12:Z:118:SER:HB3	2.48	0.42
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.35	0.42
1:A:180:TRP:HA	1:A:184:LEU:HD11	2.00	0.42
2:B:151:SER:HA	2:B:156:ASN:O	2.18	0.42
6:F:42:CYS:HB2	6:F:184:LEU:O	2.19	0.42
14:N:164:LYS:O	13:1:26:LEU:HD12	2.19	0.42
2:P:176:LEU:HD23	2:P:192:LEU:CD2	2.49	0.42
3:Q:183:PRO:CB	3:Q:189:CYS:HA	2.49	0.42
5:S:47:VAL:HG12	5:S:48:LEU:N	2.34	0.42
10:X:185:ARG:HA	16:X:1258:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:71:LYS:HG3	16:Y:9112:HOH:O	2.18	0.42
14:N:139:ASP:HB2	14:2:165:TRP:HZ2	1.85	0.42
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.73	0.42
6:F:38:ILE:HG22	6:F:164:ALA:HB2	2.00	0.42
8:H:53:GLU:OE2	8:H:57:GLN:HG3	2.18	0.42
12:L:29:ARG:HD2	12:L:193:ARG:NH2	2.34	0.42
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	2.01	0.42
13:1:83:LEU:HA	13:1:83:LEU:HD23	1.84	0.42
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.24	0.42
3:C:55:THR:HB	3:C:56:LEU:HD22	2.02	0.42
4:D:212:LEU:HA	4:D:212:LEU:HD23	1.89	0.42
5:E:74:MET:HE2	5:E:109:VAL:HA	2.00	0.42
4:D:13:SER:HB2	5:E:130:ARG:HB3	2.00	0.42
5:E:220:PRO:O	5:E:222:THR:HG23	2.20	0.42
7:G:179:HIS:HD2	7:G:196:HIS:HE1	1.68	0.42
8:H:211:THR:HG22	8:H:212:ALA:N	2.33	0.42
8:H:87:LEU:HD23	8:H:87:LEU:HA	1.85	0.42
4:R:180(C):HIS:H	4:R:184:LEU:HD11	1.85	0.42
7:U:190:VAL:HG13	7:U:212:VAL:HG11	2.01	0.42
7:U:49:ILE:N	7:U:49:ILE:CD1	2.82	0.42
16:U:2093:HOH:O	8:V:66:HIS:HD2	2.01	0.42
11:Y:174:ASN:HD21	11:Y:189:ASN:HB2	1.85	0.42
12:Z:85:HIS:HD2	16:Z:2097:HOH:O	2.01	0.42
14:2:149:GLU:H	14:2:149:GLU:HG3	1.51	0.42
2:B:82:THR:O	2:B:85:ALA:HB3	2.19	0.42
3:C:72:SER:O	3:C:219:SER:HA	2.20	0.42
4:D:67:ILE:HG21	4:D:213:SER:OG	2.20	0.42
4:D:53:ARG:HG2	4:D:53:ARG:O	2.19	0.42
5:E:107:LEU:HA	16:E:242:HOH:O	2.20	0.42
6:F:203:GLU:HA	6:F:206:LYS:HB3	2.01	0.42
8:H:16:ALA:HA	8:H:159:ILE:HD12	2.01	0.42
9:I:-2:ASN:OD1	9:I:48:LEU:HD12	2.20	0.42
12:L:18:THR:HG21	12:L:30:TYR:HA	1.98	0.42
13:M:112:TYR:OH	13:M:114:ASN:HB3	2.20	0.42
1:O:46:VAL:HG11	1:O:139:ALA:HB1	2.01	0.42
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.54	0.42
3:Q:39:GLY:HA2	3:Q:47:VAL:O	2.20	0.42
5:S:171:GLY:HA3	5:S:199:GLN:O	2.20	0.42
6:T:88:LEU:HD12	6:T:88:LEU:HA	1.76	0.42
10:X:6:ILE:HG23	10:X:13:ILE:HB	2.02	0.42
10:X:52:THR:CG2	10:X:53:VAL:N	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:1495:HOH:O	10:X:69:ARG:HG3	2.19	0.42
13:1:114:ASN:O	13:1:116:LEU:N	2.53	0.42
14:2:44:CYS:HB2	14:2:100:ILE:HB	2.02	0.42
1:A:62:GLU:C	1:A:64:LEU:H	2.22	0.42
7:G:55:PRO:HG2	7:G:56:ASP:H	1.85	0.42
13:M:19:LEU:HD22	13:M:170:SER:HB2	2.02	0.42
1:O:130:ARG:NH1	1:O:130:ARG:HG3	2.32	0.42
2:P:138:TYR:HB2	2:P:149:TYR:HB2	2.01	0.42
5:S:180(C):PHE:CD1	5:S:180(D):ILE:N	2.88	0.42
5:S:40:LEU:HD23	5:S:40:LEU:N	2.34	0.42
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.55	0.42
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.50	0.42
1:A:42:ALA:HB1	1:A:184:LEU:O	2.19	0.42
2:B:194:LEU:HD23	2:B:194:LEU:HA	1.83	0.42
12:L:-2:ASN:HA	12:L:21:ILE:O	2.20	0.42
2:P:181:LYS:O	2:P:184:MET:HG3	2.20	0.42
3:Q:84:ASP:HB3	3:Q:132:PHE:HD2	1.84	0.42
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.55	0.42
5:S:185:ASN:HA	5:S:186:PRO:HD2	1.92	0.42
7:U:179:HIS:NE2	7:U:192:PHE:HE2	2.16	0.42
8:V:162:GLY:O	8:V:166:ASP:HB3	2.19	0.42
9:W:-2:ASN:HA	9:W:21:GLY:O	2.20	0.42
10:X:58:TYR:HE2	10:X:86:GLU:OE1	2.02	0.42
11:Y:83:LEU:HA	11:Y:83:LEU:HD12	1.88	0.42
1:A:58:LEU:HD23	1:A:58:LEU:HA	1.82	0.42
8:H:105:ASP:HB2	8:H:105(A):PRO:CD	2.49	0.42
3:C:101:LEU:HD11	10:J:57:GLU:HB3	2.00	0.42
11:K:112:TYR:O	11:K:119:ARG:HA	2.20	0.42
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.55	0.42
1:O:171:ALA:O	1:O:174:THR:HB	2.19	0.42
2:P:84:ASP:OD1	2:P:132:PHE:HA	2.20	0.42
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.20	0.42
5:S:76:LEU:HA	5:S:137:LEU:O	2.19	0.42
5:S:76:LEU:O	5:S:76:LEU:HD23	2.19	0.42
6:T:62:GLN:HA	6:T:209:GLU:OE2	2.20	0.42
7:U:82:ILE:O	7:U:83:PRO:C	2.59	0.42
8:V:109:HIS:HB3	8:V:111:PHE:CE2	2.54	0.42
10:X:113:ILE:HA	10:X:118:THR:O	2.20	0.42
16:T:1868:HOH:O	13:1:67:ALA:HB3	2.20	0.41
5:E:48:LEU:O	5:E:212:ILE:HA	2.20	0.41
8:H:153:LYS:O	8:H:156:SER:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.35	0.41
1:O:48:ILE:O	1:O:48:ILE:HG13	2.19	0.41
1:O:86:ARG:HD3	16:O:2278:HOH:O	2.19	0.41
2:P:82:THR:O	2:P:85:ALA:HB3	2.20	0.41
4:R:150:HIS:CE1	4:R:152:GLU:HG3	2.54	0.41
4:R:191:LEU:HA	4:R:191:LEU:HD12	1.88	0.41
8:V:173:VAL:HB	8:V:192:LEU:HB2	2.02	0.41
9:W:48:LEU:HD11	10:X:116:LEU:HD13	2.01	0.41
11:Y:76:VAL:CG2	11:Y:103:GLY:HA3	2.50	0.41
13:1:112:TYR:CD2	13:1:120:TYR:CZ	3.08	0.41
14:2:175:MET:SD	14:2:187(B):PHE:HE2	2.43	0.41
2:B:130:ARG:HG3	2:B:130:ARG:NH1	2.35	0.41
2:B:46:ILE:HG21	2:B:148:LEU:HD13	2.02	0.41
1:O:49:ALA:HA	1:O:211:GLU:O	2.20	0.41
3:Q:180(A):ASP:OD1	3:Q:180(C):LYS:HB2	2.19	0.41
3:Q:78:PHE:N	3:Q:78:PHE:CD2	2.88	0.41
5:S:194:VAL:CG1	5:S:207:LEU:HD11	2.50	0.41
5:S:40:LEU:HA	5:S:162:GLY:HA2	2.02	0.41
10:X:189:ASP:O	10:X:193:GLN:HB2	2.21	0.41
12:Z:65:TRP:O	12:Z:68:PHE:HB2	2.21	0.41
3:C:200:VAL:O	3:C:202:GLN:HG2	2.20	0.41
7:G:222:PHE:CD2	7:G:222:PHE:N	2.88	0.41
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.03	0.41
9:I:152:PHE:O	9:I:155:ILE:HG22	2.19	0.41
3:Q:130:ARG:NH1	3:Q:131:PRO:O	2.53	0.41
6:T:208:PHE:H	6:T:208:PHE:HD2	1.67	0.41
6:T:47:VAL:HG12	6:T:48:PHE:N	2.35	0.41
11:Y:15:ALA:HA	11:Y:174:ASN:O	2.20	0.41
1:A:100:TYR:CE1	1:A:107:PRO:HA	2.55	0.41
3:C:163:GLN:CG	3:C:164:THR:N	2.83	0.41
8:H:157:ASP:O	8:H:160:GLN:HB2	2.20	0.41
9:I:55:LEU:HA	9:I:55:LEU:HD23	1.77	0.41
10:J:27:LEU:HA	10:J:27:LEU:HD23	1.75	0.41
13:M:-7:GLN:HG3	13:M:96:TRP:CE3	2.56	0.41
14:N:6:VAL:O	14:N:12:VAL:HG23	2.20	0.41
1:O:15:PHE:H	2:P:23:GLN:NE2	2.18	0.41
2:P:67:LEU:HA	2:P:67:LEU:HD12	1.81	0.41
3:Q:74:VAL:HG22	3:Q:109:VAL:HG22	2.01	0.41
5:S:38:VAL:HG12	5:S:39:GLY:N	2.34	0.41
6:T:167:LYS:C	6:T:169:ARG:H	2.23	0.41
10:X:3:ILE:O	10:X:126:ALA:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:40:ASN:HA	12:Z:40:ASN:HD22	1.72	0.41
13:1:45:ILE:HD12	13:1:52:MET:HG3	2.02	0.41
7:U:94:ALA:HA	14:2:65:LEU:HD11	2.02	0.41
2:B:125:GLN:HG3	3:C:130:ARG:HG2	2.02	0.41
3:C:141:PHE:CE2	3:C:215:VAL:HG22	2.55	0.41
4:D:150:HIS:HB3	4:D:160:TYR:HE1	1.84	0.41
3:C:158:SER:HB2	4:D:59:LEU:HD21	2.02	0.41
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.50	0.41
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.21	0.41
12:L:70:HIS:HE1	16:L:9060:HOH:O	2.03	0.41
4:R:191:LEU:O	4:R:194:LEU:HB2	2.20	0.41
5:S:16:SER:CB	5:S:22:PHE:HE2	2.33	0.41
6:T:70:VAL:O	6:T:71:ASP:HB3	2.21	0.41
7:U:70:ILE:HD12	7:U:92:ALA:HB3	2.02	0.41
9:W:55:LEU:HD21	9:W:95:TYR:CD1	2.54	0.41
10:X:2:ILE:HA	16:X:1314:HOH:O	2.21	0.41
11:Y:205:SER:O	11:Y:206:PHE:HB2	2.20	0.41
11:Y:4:LEU:HG	11:Y:138:LEU:HD21	2.02	0.41
14:2:85:GLU:O	14:2:89:GLU:HB2	2.20	0.41
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.91	0.41
3:C:135:SER:HA	3:C:151:THR:O	2.20	0.41
5:E:76:LEU:C	5:E:76:LEU:HD23	2.41	0.41
12:L:19:ARG:HG2	12:L:21:ILE:HG23	2.02	0.41
13:M:136:PRO:HA	8:V:165:ASN:OD1	2.21	0.41
13:M:38:GLY:HA3	16:M:285:HOH:O	2.21	0.41
2:P:185:LYS:HD3	2:P:186:VAL:N	2.36	0.41
7:U:131:PRO:HB3	16:U:1840:HOH:O	2.21	0.41
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.50	0.41
10:X:115:TYR:CE2	10:X:116:LEU:HG	2.56	0.41
10:X:7:ARG:CB	10:X:12:VAL:HG22	2.51	0.41
1:A:38:LEU:HD12	1:A:38:LEU:C	2.41	0.41
13:M:157:ASN:ND2	13:M:160:ARG:NH1	2.67	0.41
13:M:83:LEU:HA	13:M:83:LEU:HD23	1.66	0.41
7:U:191:GLU:O	7:U:192:PHE:C	2.59	0.41
9:W:16:CYS:SG	9:W:174:VAL:CG1	3.09	0.41
9:W:16:CYS:SG	9:W:174:VAL:HG12	2.61	0.41
9:W:76:PRO:HB3	9:W:109:PHE:CD2	2.56	0.41
10:X:166:MET:HA	10:X:167:PRO:HD3	1.83	0.41
12:Z:33:LYS:HE2	12:Z:33:LYS:HB3	1.66	0.41
14:2:5:ALA:O	14:2:124:TYR:HA	2.20	0.41
1:A:20:LYS:HD2	1:A:25:ASP:OD1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.56	0.41
8:H:114:HIS:HB3	16:H:651:HOH:O	2.20	0.41
8:H:5:GLY:HA2	8:H:14:ILE:HG22	2.02	0.41
8:H:67:SER:O	8:H:71:SER:N	2.54	0.41
11:K:146:LEU:HD23	11:K:151:ALA:HA	2.02	0.41
11:K:1:THR:HG23	11:K:33:LYS:HZ2	1.84	0.41
12:L:86:LEU:HD23	12:L:86:LEU:HA	1.82	0.41
1:O:31:VAL:HG13	1:O:79:SER:O	2.20	0.41
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.89	0.41
4:R:130:ARG:NH1	4:R:130:ARG:CG	2.82	0.41
6:T:212:ILE:HG22	6:T:213:SER:N	2.35	0.41
6:T:35:THR:CG2	6:T:51:GLU:O	2.69	0.41
9:W:166:ASP:OD2	9:W:168:LEU:N	2.54	0.41
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.50	0.41
12:Z:11:PHE:CE1	12:Z:148:VAL:HA	2.56	0.41
12:Z:-5:TYR:OH	12:Z:93:PHE:HD1	2.03	0.41
13:1:-4:ILE:HG21	14:2:115:LEU:HB3	2.03	0.41
14:2:187(A):ILE:O	14:2:187(A):ILE:HG23	2.20	0.41
1:A:171:ALA:O	1:A:174:THR:HB	2.21	0.41
3:C:229:ILE:O	3:C:232:TYR:N	2.53	0.41
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.20	0.41
9:I:109:PHE:CD2	9:I:109:PHE:C	2.94	0.41
14:N:148:LYS:O	14:N:152:VAL:HG23	2.20	0.41
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.02	0.41
3:Q:47:VAL:O	3:Q:48:LEU:HD23	2.21	0.41
5:S:81:LEU:HB2	5:S:133:GLY:O	2.21	0.41
5:S:33:GLN:O	5:S:33:GLN:HG2	2.21	0.41
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.51	0.41
6:T:18:ASP:N	6:T:18:ASP:OD2	2.53	0.41
6:T:192:GLN:O	6:T:196:ILE:HG13	2.21	0.41
7:U:98:GLU:HG2	7:U:102:LYS:HD3	2.02	0.41
7:U:76:MET:SD	7:U:138:PHE:CE2	3.14	0.41
8:V:87:LEU:HA	8:V:87:LEU:HD23	1.74	0.41
10:X:11:SER:HB3	10:X:179:ASP:HB3	2.03	0.41
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	2.03	0.41
16:R:2070:HOH:O	12:Z:70:HIS:CD2	2.74	0.41
2:B:109:VAL:O	2:B:113:VAL:HG23	2.21	0.41
6:F:109:ILE:H	6:F:109:ILE:HG12	1.70	0.41
7:G:107:MET:HA	7:G:108:PRO:HD3	1.80	0.41
9:I:93:GLY:N	9:I:94:PRO:CD	2.84	0.41
12:L:167:ILE:HG13	12:L:168:GLN:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:141:TYR:CD1	2:P:219(E):VAL:HG21	2.56	0.41
3:Q:129:VAL:HG23	3:Q:129:VAL:O	2.20	0.41
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.56	0.41
3:Q:180(B):ARG:NH2	4:R:57:PRO:O	2.53	0.41
5:S:214:ILE:HG12	5:S:215:VAL:N	2.36	0.41
6:T:35:THR:HG21	6:T:51:GLU:O	2.20	0.41
7:U:76:MET:HB2	7:U:138:PHE:CD2	2.56	0.41
7:U:210:LEU:HD23	7:U:210:LEU:HA	1.63	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.83	0.41
10:X:95:TYR:HE1	11:Y:88:TYR:HH	1.68	0.41
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.21	0.41
13:1:95:LEU:HD23	13:1:95:LEU:HA	1.90	0.41
1:A:207:ASN:HA	1:A:233:LEU:CD1	2.50	0.41
2:B:130:ARG:NH1	2:B:131:PRO:O	2.54	0.41
5:E:161:TYR:CE2	6:F:60:VAL:HA	2.56	0.41
5:E:36:VAL:HA	5:E:165:ILE:O	2.21	0.41
6:F:179:LEU:HD11	6:F:192:GLN:HG3	2.03	0.41
7:G:184:ASN:HD22	7:G:184:ASN:C	2.25	0.41
7:G:51:GLN:NE2	7:G:53:LYS:HE3	2.35	0.41
8:H:3:ILE:O	8:H:126:SER:HA	2.20	0.41
8:H:159:ILE:O	8:H:163:ILE:HG13	2.21	0.41
9:I:156:SER:O	9:I:160:LEU:HB2	2.21	0.41
9:I:2:ILE:HA	9:I:128:GLY:HA3	2.03	0.41
10:J:105(B):LYS:HZ2	10:J:105(B):LYS:HB2	1.86	0.41
10:J:52:THR:HG23	10:J:53:VAL:N	2.35	0.41
14:N:105(B):LYS:O	14:N:105(B):LYS:HD3	2.21	0.41
3:Q:39:GLY:HA3	3:Q:48:LEU:HD23	2.04	0.41
4:R:150:HIS:CE1	4:R:152:GLU:CG	3.04	0.41
4:R:212:LEU:HA	4:R:212:LEU:HD23	1.91	0.41
7:U:177:GLU:O	7:U:179(B):LYS:HG3	2.21	0.41
14:2:176:VAL:HG12	14:2:178:LEU:HD13	2.03	0.40
3:C:192:LEU:HA	3:C:192:LEU:HD12	1.84	0.40
6:F:130:ARG:NH1	6:F:130:ARG:CG	2.82	0.40
4:R:225:ASP:O	4:R:226:ASN:C	2.59	0.40
5:S:180(C):PHE:CD1	5:S:180(C):PHE:C	2.95	0.40
2:B:146:TYR:C	2:B:147:GLN:HG3	2.41	0.40
5:E:179:THR:CG2	5:E:180(B):THR:HB	2.51	0.40
5:E:41:ARG:NH1	5:E:42:SER:O	2.54	0.40
7:G:49:ILE:CD1	7:G:193:ALA:HB1	2.50	0.40
7:G:87:ASN:ND2	7:G:87:ASN:C	2.74	0.40
9:I:58:MET:O	9:I:61:TYR:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:93:PHE:N	12:L:94:PRO:CD	2.84	0.40
3:Q:171:THR:O	3:Q:174:GLU:HB2	2.21	0.40
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.51	0.40
6:T:35:THR:CG2	6:T:36:THR:N	2.83	0.40
6:T:67:ILE:HG22	6:T:68:GLN:N	2.37	0.40
1:O:59:ALA:HA	7:U:160:TYR:CD2	2.56	0.40
7:U:194:ILE:HG23	7:U:210:LEU:HD11	2.04	0.40
2:P:101:LYS:HG2	10:X:85:GLN:NE2	2.36	0.40
13:1:40:ASN:HD22	13:1:40:ASN:H	1.68	0.40
13:1:62:LEU:HA	13:1:62:LEU:HD22	1.87	0.40
14:2:106:ASN:O	14:2:107:LYS:HB3	2.21	0.40
2:B:239:THR:OXT	2:B:239:THR:HG22	2.21	0.40
3:Q:55:THR:O	3:Q:56:LEU:HD13	2.21	0.40
4:R:215:ILE:HG22	4:R:221:PHE:CD2	2.51	0.40
6:T:127:ASN:ND2	6:T:127:ASN:C	2.75	0.40
6:T:198:TYR:O	6:T:202:HIS:HB3	2.22	0.40
10:X:90(A):ILE:HD12	10:X:90(A):ILE:HA	1.94	0.40
12:Z:176:LEU:HG	12:Z:186:LYS:HG3	2.03	0.40
2:B:88:LEU:HB3	2:B:116:LEU:HD21	2.03	0.40
6:F:88:LEU:HG	6:F:116:LEU:HD22	2.04	0.40
7:G:37:SER:HA	7:G:50:SER:HA	2.03	0.40
13:M:59:LEU:HA	13:M:59:LEU:HD23	1.94	0.40
2:P:21:LEU:HB2	2:P:24:VAL:HB	2.04	0.40
1:O:17:PRO:HG3	2:P:26:TYR:CE2	2.57	0.40
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.86	0.40
7:U:47:VAL:HG12	7:U:49:ILE:HD12	2.03	0.40
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.56	0.40
5:E:210:LEU:HB3	5:E:229:VAL:HG21	2.04	0.40
8:H:18:THR:HB	8:H:30:ASN:HA	2.03	0.40
9:I:8:SER:O	9:I:6:PRO:HD3	2.21	0.40
9:I:90:ARG:HD2	16:I:9052:HOH:O	2.21	0.40
11:K:104:TYR:HD2	11:K:179:THR:HA	1.86	0.40
11:K:35:ILE:HD11	11:K:45:MET:HE2	2.03	0.40
13:M:156:VAL:O	13:M:159:MET:HB2	2.21	0.40
3:Q:172:VAL:CG2	3:Q:196:SER:HB2	2.51	0.40
5:S:73:HIS:CE1	5:S:107:LEU:O	2.61	0.40
5:S:179:THR:O	5:S:179:THR:HG22	2.21	0.40
2:P:99:TYR:OH	10:X:66:TYR:OH	2.21	0.40
12:Z:97:VAL:HG23	12:Z:99:THR:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	244/250 (98%)	225 (92%)	17 (7%)	2 (1%)	19	29
1	O	244/250 (98%)	225 (92%)	17 (7%)	2 (1%)	19	29
2	B	233/245 (95%)	209 (90%)	18 (8%)	6 (3%)	5	5
2	P	233/245 (95%)	212 (91%)	14 (6%)	7 (3%)	4	3
3	C	236/243 (97%)	210 (89%)	20 (8%)	6 (2%)	5	6
3	Q	236/243 (97%)	211 (89%)	18 (8%)	7 (3%)	4	3
4	D	228/241 (95%)	205 (90%)	21 (9%)	2 (1%)	17	25
4	R	228/241 (95%)	204 (90%)	20 (9%)	4 (2%)	8	10
5	E	228/234 (97%)	208 (91%)	15 (7%)	5 (2%)	6	7
5	S	228/234 (97%)	203 (89%)	20 (9%)	5 (2%)	6	7
6	F	240/248 (97%)	218 (91%)	18 (8%)	4 (2%)	9	11
6	T	240/248 (97%)	214 (89%)	24 (10%)	2 (1%)	19	29
7	G	238/252 (94%)	217 (91%)	20 (8%)	1 (0%)	34	48
7	U	238/252 (94%)	222 (93%)	15 (6%)	1 (0%)	34	48
8	H	220/222 (99%)	203 (92%)	12 (6%)	5 (2%)	6	7
8	V	220/222 (99%)	206 (94%)	10 (4%)	4 (2%)	8	10
9	I	202/205 (98%)	189 (94%)	12 (6%)	1 (0%)	29	41
9	W	202/205 (98%)	190 (94%)	10 (5%)	2 (1%)	15	23
10	J	196/198 (99%)	180 (92%)	14 (7%)	2 (1%)	15	23
10	X	196/198 (99%)	183 (93%)	11 (6%)	2 (1%)	15	23
11	K	210/212 (99%)	195 (93%)	14 (7%)	1 (0%)	29	41
11	Y	210/212 (99%)	198 (94%)	11 (5%)	1 (0%)	29	41
12	L	220/241 (91%)	200 (91%)	18 (8%)	2 (1%)	17	25
12	Z	220/241 (91%)	203 (92%)	16 (7%)	1 (0%)	29	41
13	1	231/266 (87%)	208 (90%)	19 (8%)	4 (2%)	9	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/266 (87%)	210 (91%)	15 (6%)	6 (3%)	5	5
14	2	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
14	N	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6240/6506 (96%)	5718 (92%)	437 (7%)	85 (1%)	11	15

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
2	B	54	VAL
2	B	218(C)	ASP
3	C	58	LEU
4	D	180(E)	SER
6	F	206	LYS
8	H	91	GLN
1	O	167	LYS
2	P	54	VAL
2	P	218(C)	ASP
3	Q	58	LEU
4	R	180(E)	SER
6	T	206	LYS
7	U	55	PRO
8	V	91	GLN
3	C	183	PRO
3	C	203	THR
5	E	202	ARG
10	J	8	VAL
10	J	49	ALA
2	P	182	ASP
2	P	204(A)	SER
3	Q	183	PRO
3	Q	184	ALA
3	Q	203	THR
4	R	122	ALA
5	S	202	ARG
8	V	96	GLY
10	X	8	VAL
13	1	9	ASP
1	A	63	THR
2	B	218(D)	GLY
3	C	72	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	184	ALA
7	G	55	PRO
13	M	2	SER
13	M	9	ASP
13	M	96	TRP
13	M	115	LEU
1	O	63	THR
2	P	218(D)	GLY
5	S	217	LYS
8	V	115	ALA
10	X	49	ALA
13	1	115	LEU
2	B	184	MET
5	E	163	THR
5	E	217	LYS
5	E	231	LYS
6	F	12	ASN
6	F	13	SER
9	I	93	GLY
12	L	70(A)	ASN
13	M	72	ALA
2	P	22	TYR
3	Q	61	THR
4	R	61	SER
8	V	171	SER
13	1	2	SER
2	B	182	ASP
2	B	204(A)	SER
3	C	239	GLU
4	D	180(D)	SER
5	E	170	GLN
8	H	30	ASN
8	H	115	ALA
4	R	180(D)	SER
5	S	163	THR
5	S	227	GLU
6	T	13	SER
9	W	93	GLY
6	F	143	LYS
11	K	39	PRO
12	L	144(Q)	LEU
2	P	35	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	35	THR
3	Q	202	GLN
5	S	170	GLN
9	W	23	GLN
12	Z	94	PRO
8	H	96	GLY
8	H	194	PRO
11	Y	39	PRO
13	1	207	GLY
13	M	207	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/209 (98%)	198 (97%)	7 (3%)	37	56
1	O	205/209 (98%)	195 (95%)	10 (5%)	25	40
2	B	194/204 (95%)	179 (92%)	15 (8%)	13	20
2	P	194/204 (95%)	176 (91%)	18 (9%)	9	13
3	C	210/215 (98%)	196 (93%)	14 (7%)	16	26
3	Q	210/215 (98%)	197 (94%)	13 (6%)	18	29
4	D	186/197 (94%)	178 (96%)	8 (4%)	29	46
4	R	186/197 (94%)	179 (96%)	7 (4%)	33	51
5	E	187/192 (97%)	166 (89%)	21 (11%)	6	8
5	S	187/192 (97%)	168 (90%)	19 (10%)	7	10
6	F	200/205 (98%)	180 (90%)	20 (10%)	7	11
6	T	200/205 (98%)	181 (90%)	19 (10%)	8	12
7	G	205/210 (98%)	190 (93%)	15 (7%)	14	22
7	U	205/210 (98%)	187 (91%)	18 (9%)	10	15
8	H	181/181 (100%)	173 (96%)	8 (4%)	28	45
8	V	181/181 (100%)	173 (96%)	8 (4%)	28	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	172/173 (99%)	166 (96%)	6 (4%)	36	55
9	W	172/173 (99%)	166 (96%)	6 (4%)	36	55
10	J	175/175 (100%)	166 (95%)	9 (5%)	24	39
10	X	175/175 (100%)	167 (95%)	8 (5%)	27	43
11	K	169/169 (100%)	163 (96%)	6 (4%)	35	54
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	42
12	L	185/201 (92%)	179 (97%)	6 (3%)	39	59
12	Z	185/201 (92%)	177 (96%)	8 (4%)	29	46
13	1	199/224 (89%)	190 (96%)	9 (4%)	27	44
13	M	199/224 (89%)	188 (94%)	11 (6%)	21	35
14	2	162/162 (100%)	151 (93%)	11 (7%)	16	25
14	N	162/162 (100%)	154 (95%)	8 (5%)	25	40
All	All	5260/5434 (97%)	4944 (94%)	316 (6%)	19	31

All (316) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	32	LYS
1	A	158	PHE
1	A	170	VAL
1	A	200	SER
1	A	222	ARG
1	A	223	LYS
2	B	58	LEU
2	B	62	ASP
2	B	67	LEU
2	B	71	ASN
2	B	104	ASN
2	B	121	GLN
2	B	126	HIS
2	B	135	SER
2	B	169	THR
2	B	185	LYS
2	B	192	LEU
2	B	203	ASP
2	B	218(C)	ASP
2	B	226	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	233	LEU
3	C	18	ASP
3	C	25	GLU
3	C	53	ARG
3	C	56	LEU
3	C	57	LYS
3	C	61	THR
3	C	75	VAL
3	C	121	GLN
3	C	150	GLN
3	C	174	GLU
3	C	178	LYS
3	C	209	ASN
3	C	215	VAL
3	C	224	LEU
4	D	72	ARG
4	D	110	GLU
4	D	119	LEU
4	D	128	MET
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	238	LYS
5	E	11	ASP
5	E	12	THR
5	E	13	VAL
5	E	18	THR
5	E	57	GLU
5	E	58	LEU
5	E	76	LEU
5	E	78	LEU
5	E	90	ASN
5	E	97	ASN
5	E	105	ARG
5	E	111	ARG
5	E	121	GLN
5	E	178	ARG
5	E	180(C)	PHE
5	E	185	ASN
5	E	189	LEU
5	E	198	SER
5	E	199	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	207	LEU
5	E	231	LYS
6	F	18	ASP
6	F	43	ASN
6	F	56	SER
6	F	73	HIS
6	F	98	SER
6	F	121	GLN
6	F	127	ASN
6	F	129	VAL
6	F	135	SER
6	F	169	ARG
6	F	170	GLN
6	F	171	SER
6	F	176	LEU
6	F	187	ARG
6	F	192	GLN
6	F	203	GLU
6	F	205	ASN
6	F	208	PHE
6	F	214	TRP
6	F	227	ASP
7	G	72	ARG
7	G	87	ASN
7	G	109	CYS
7	G	119	LEU
7	G	121	GLN
7	G	157	TYR
7	G	169	GLN
7	G	174	THR
7	G	184	ASN
7	G	197	MET
7	G	199	ASP
7	G	203	THR
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	18	THR
8	H	30	ASN
8	H	55	VAL
8	H	68	LEU
8	H	84	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	101	VAL
8	H	197	ARG
8	H	221	ILE
9	I	113	PHE
9	I	118	CYS
9	I	131	SER
9	I	160	LEU
9	I	171	TRP
9	I	181	LYS
10	J	6	ILE
10	J	52	THR
10	J	68	ILE
10	J	70	GLU
10	J	77	GLN
10	J	90(B)	ARG
10	J	115	TYR
10	J	122	LEU
10	J	155	LEU
11	K	4	LEU
11	K	9	GLN
11	K	104	TYR
11	K	115	SER
11	K	138	LEU
11	K	146	LEU
12	L	14	LEU
12	L	62	SER
12	L	93	PHE
12	L	99	THR
12	L	138	LEU
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	65	GLU
13	M	71(A)	ASP
13	M	91	ARG
13	M	112	TYR
13	M	136	PRO
13	M	141(C)	ARG
13	M	172	ASN
13	M	181(A)	THR
13	M	204	LYS
14	N	20	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	22	THR
14	N	36	ARG
14	N	65	LEU
14	N	70	TYR
14	N	119	VAL
14	N	132	THR
14	N	149	GLU
1	O	9	SER
1	O	32	LYS
1	O	64	LEU
1	O	83	PRO
1	O	134	VAL
1	O	158	PHE
1	O	170	VAL
1	O	200	SER
1	O	222	ARG
1	O	223	LYS
2	P	58	LEU
2	P	67	LEU
2	P	71	ASN
2	P	91	THR
2	P	116	LEU
2	P	121	GLN
2	P	126	HIS
2	P	135	SER
2	P	150	THR
2	P	153	PRO
2	P	156	ASN
2	P	169	THR
2	P	185	LYS
2	P	203	ASP
2	P	218(C)	ASP
2	P	226	PRO
2	P	232	ILE
2	P	233	LEU
3	Q	18	ASP
3	Q	53	ARG
3	Q	56	LEU
3	Q	57	LYS
3	Q	61	THR
3	Q	75	VAL
3	Q	121	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	156	ILE
3	Q	163	GLN
3	Q	174	GLU
3	Q	178	LYS
3	Q	209	ASN
3	Q	215	VAL
4	R	76	CYS
4	R	110	GLU
4	R	119	LEU
4	R	128	MET
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
5	S	11	ASP
5	S	12	THR
5	S	13	VAL
5	S	58	LEU
5	S	76	LEU
5	S	78	LEU
5	S	90	ASN
5	S	97	ASN
5	S	111	ARG
5	S	117	CYS
5	S	178	ARG
5	S	180(C)	PHE
5	S	185	ASN
5	S	189	LEU
5	S	198	SER
5	S	199	GLN
5	S	207	LEU
5	S	209(C)	VAL
5	S	231	LYS
6	T	18	ASP
6	T	43	ASN
6	T	73	HIS
6	T	98	SER
6	T	121	GLN
6	T	127	ASN
6	T	129	VAL
6	T	135	SER
6	T	169	ARG
6	T	170	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	171	SER
6	T	187	ARG
6	T	192	GLN
6	T	199	LEU
6	T	203	GLU
6	T	205	ASN
6	T	208	PHE
6	T	214	TRP
6	T	227	ASP
7	U	38	LEU
7	U	72	ARG
7	U	76	MET
7	U	87	ASN
7	U	109	CYS
7	U	119	LEU
7	U	121	GLN
7	U	157	TYR
7	U	169	GLN
7	U	171	GLU
7	U	174	THR
7	U	184	ASN
7	U	197	MET
7	U	199	ASP
7	U	204	GLU
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	18	THR
8	V	30	ASN
8	V	38	SER
8	V	55	VAL
8	V	68	LEU
8	V	84	LYS
8	V	197	ARG
8	V	219	VAL
9	W	55	LEU
9	W	113	PHE
9	W	131	SER
9	W	160	LEU
9	W	171	TRP
9	W	181	LYS
10	X	17	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	90	SER
10	X	90(B)	ARG
10	X	108	PRO
10	X	115	TYR
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	104	TYR
11	Y	105(B)	LYS
11	Y	115	SER
11	Y	138	LEU
11	Y	145	ASP
12	Z	14	LEU
12	Z	40	ASN
12	Z	62	SER
12	Z	93	PHE
12	Z	99	THR
12	Z	114	ASP
12	Z	138	LEU
12	Z	145	TYR
13	1	40	ASN
13	1	62	LEU
13	1	71(A)	ASP
13	1	115	LEU
13	1	123	PRO
13	1	141(C)	ARG
13	1	172	ASN
13	1	181(A)	THR
13	1	204	LYS
14	2	20	THR
14	2	22	THR
14	2	36	ARG
14	2	61	TYR
14	2	65	LEU
14	2	105(A)	ASP
14	2	119	VAL
14	2	132	THR
14	2	149	GLU
14	2	177	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	2	187(D)	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (171) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
3	C	82	ASN
3	C	150	GLN
3	C	163	GLN
4	D	23	GLN
4	D	108	ASN
4	D	150	HIS
4	D	199	GLN
4	D	211	GLN
4	D	226	ASN
5	E	73	HIS
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	125	GLN
5	E	185	ASN
5	E	209(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	123	HIS
6	F	127	ASN
6	F	147	HIS
6	F	192	GLN
6	F	221	HIS
7	G	11	HIS
7	G	33	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	121	GLN
7	G	125	GLN
7	G	170	GLN
7	G	178	ASN
7	G	180(C)	HIS
7	G	184	ASN
7	G	196	HIS
7	G	239	GLN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	91	GLN
8	H	116	HIS
8	H	144	GLN
8	H	172	ASN
9	I	29	ASN
9	I	81	GLN
9	I	145	ASN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	186	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
12	L	46	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	85	HIS
12	L	140	ASN
12	L	141	GLN
12	L	144(B)	ASN
12	L	144(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	38	HIS
14	N	157	HIS
14	N	161	GLN
2	P	71	ASN
2	P	95	HIS
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	235	GLN
4	R	23	GLN
4	R	108	ASN
4	R	150	HIS
4	R	199	GLN
4	R	226	ASN
5	S	33	GLN
5	S	73	HIS
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	185	ASN
5	S	209(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	123	HIS
6	T	127	ASN
6	T	192	GLN
6	T	221	HIS
7	U	11	HIS
7	U	33	GLN
7	U	34(A)	ASN
7	U	87	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	170	GLN
7	U	180(C)	HIS
7	U	184	ASN
7	U	239	GLN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	116	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	81	GLN
9	W	145	ASN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	140	HIS
10	X	186	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	189	ASN
11	Y	207	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	70	HIS
12	Z	70(A)	ASN
12	Z	85	HIS
12	Z	123	GLN
12	Z	140	ASN
12	Z	141	GLN
12	Z	144(B)	ASN
12	Z	144(Z)	ASN
12	Z	166	HIS
13	1	10	ASN
13	1	40	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	191	GLN
14	2	38	HIS
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 20 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.