



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:19 am GMT

PDB ID : 4GK7
Title : yeast 20S proteasome in complex with the Syringolin-Glidobactin chimera
Authors : Groll, M.; Stein, M.L.; Bachmann, A.
Deposited on : 2012-08-10
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

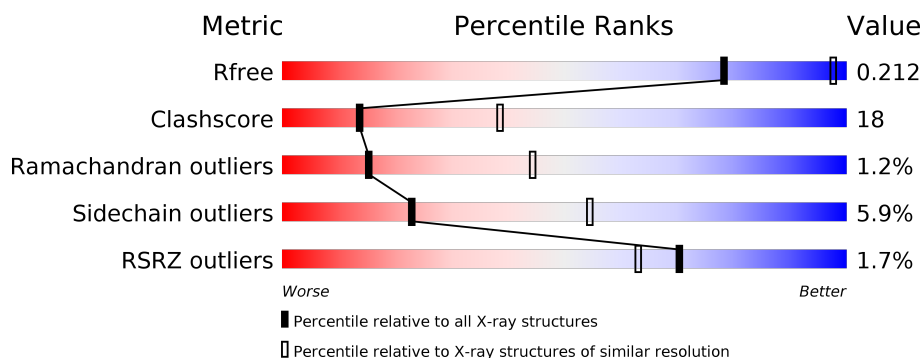
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>0%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>•</div> </div> </div>
1	O	250	<div> <div>0%</div> <div> <div></div> <div>69%</div> <div>29%</div> <div>•</div> </div> </div>
2	B	244	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>7%</div> </div> </div>
2	P	244	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>7%</div> </div> </div>
3	C	241	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>38%</div> <div>•</div> </div> </div>
3	Q	241	<div> <div>5%</div> <div> <div></div> <div>59%</div> <div>38%</div> <div>•</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	
15	1	4	
15	2	4	
15	3	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	4	4	<div><div></div><div>25%</div><div>50%</div><div>25%</div></div>
15	5	4	<div><div></div><div>50%</div><div>50%</div><div></div></div>
15	6	4	<div><div></div><div>75%</div><div>25%</div><div></div></div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51109 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	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	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	a	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	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called SYRINGOLIN-GLIDOBACTIN CHIMERA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	1	4	Total	C	N	O	0	0	0
			38	29	4	5			
15	2	4	Total	C	N	O	0	0	0
			38	29	4	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	4	Total	C	N	O	0	0	0
			38	29	4	5			
15	4	4	Total	C	N	O	0	0	0
			38	29	4	5			
15	5	4	Total	C	N	O	0	0	0
			38	29	4	5			
15	6	4	Total	C	N	O	0	0	0
			38	29	4	5			

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	59	Total	O	0	0
			59	59		
16	B	35	Total	O	0	0
			35	35		
16	C	44	Total	O	0	0
			44	44		
16	D	39	Total	O	0	0
			39	39		
16	E	23	Total	O	0	0
			23	23		
16	F	49	Total	O	0	0
			49	49		
16	G	60	Total	O	0	0
			60	60		
16	H	49	Total	O	0	0
			49	49		
16	I	64	Total	O	0	0
			64	64		
16	J	53	Total	O	0	0
			53	53		
16	K	42	Total	O	0	0
			42	42		
16	L	55	Total	O	0	0
			55	55		
16	M	75	Total	O	0	0
			75	75		
16	N	56	Total	O	0	0
			56	56		
16	O	34	Total	O	0	0
			34	34		

Continued on next page...

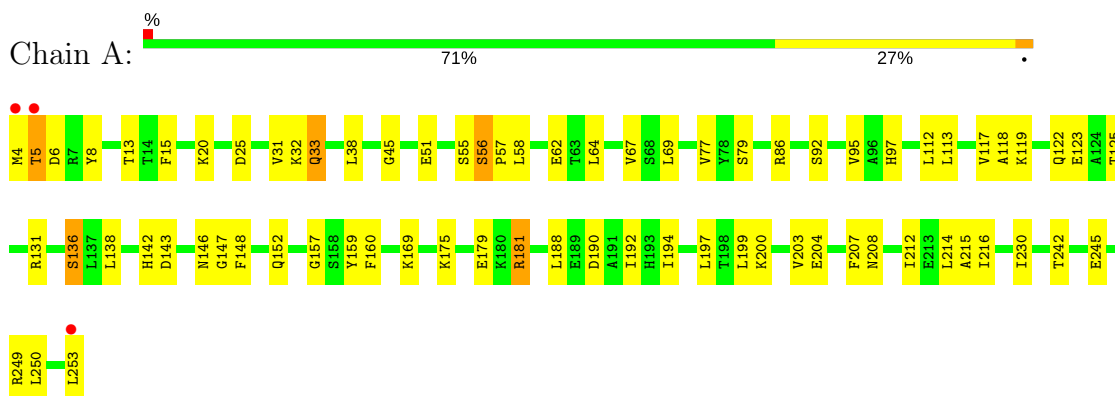
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	P	28	Total 28	O 28	0	0
16	Q	29	Total 29	O 29	0	0
16	R	33	Total 33	O 33	0	0
16	S	21	Total 21	O 21	0	0
16	T	39	Total 39	O 39	0	0
16	U	63	Total 63	O 63	0	0
16	V	47	Total 47	O 47	0	0
16	W	55	Total 55	O 55	0	0
16	X	46	Total 46	O 46	0	0
16	Y	50	Total 50	O 50	0	0
16	Z	51	Total 51	O 51	0	0
16	a	73	Total 73	O 73	0	0
16	b	58	Total 58	O 58	0	0
16	1	1	Total 1	O 1	0	0
16	2	1	Total 1	O 1	0	0
16	3	1	Total 1	O 1	0	0

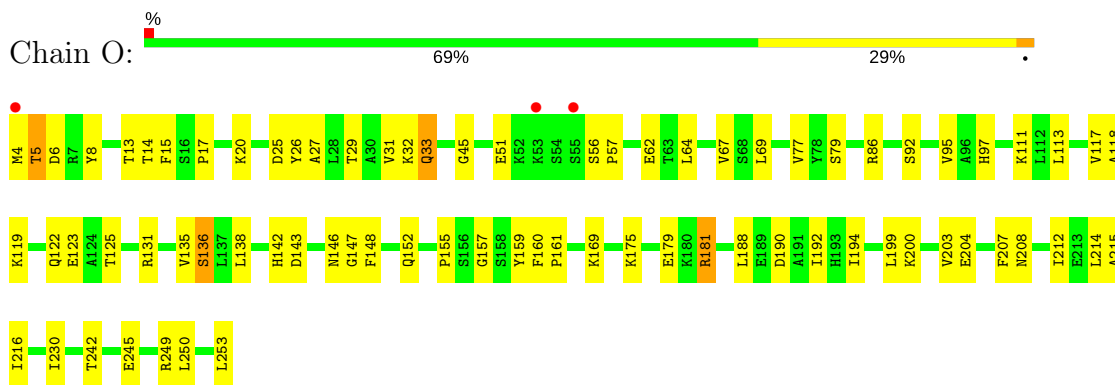
3 Residue-property plots [i](#)

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

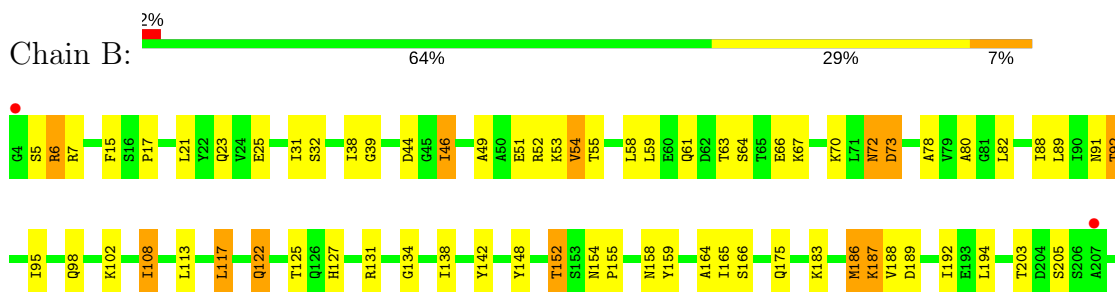
• Molecule 1: Proteasome component Y7



• Molecule 1: Proteasome component Y7

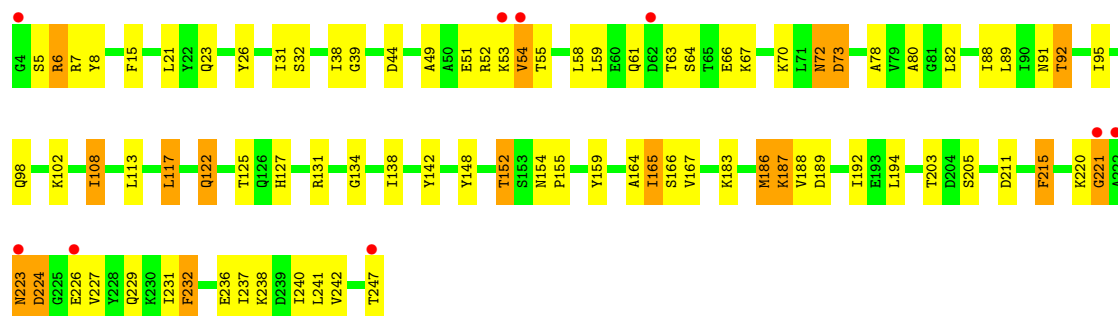


• Molecule 2: Proteasome component Y13

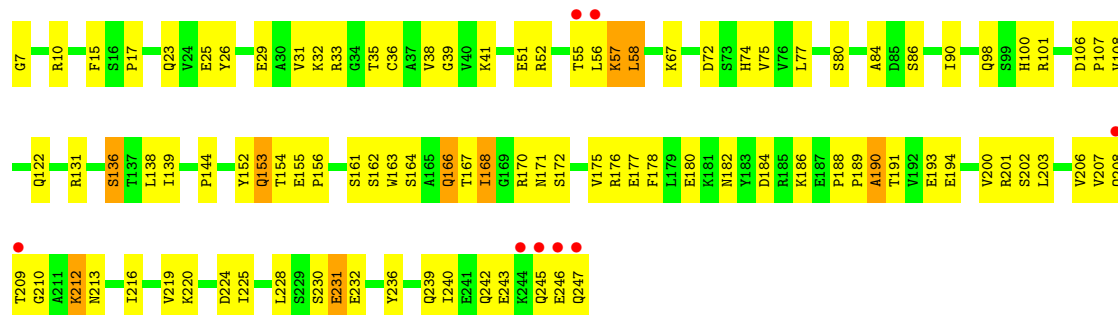




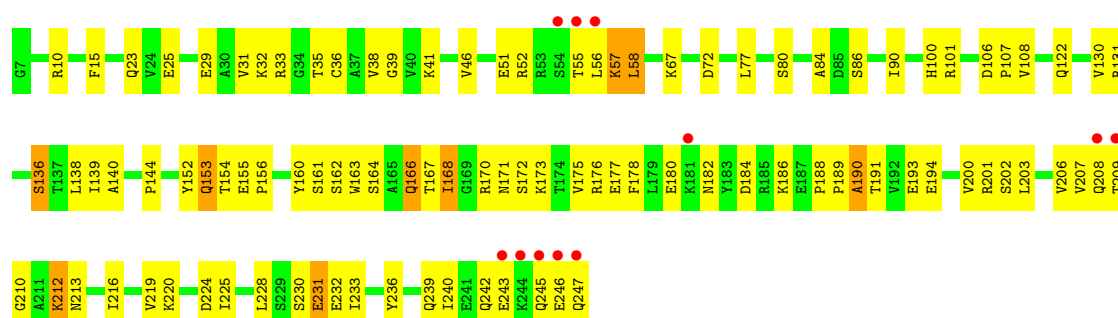
• Molecule 2: Proteasome component Y13



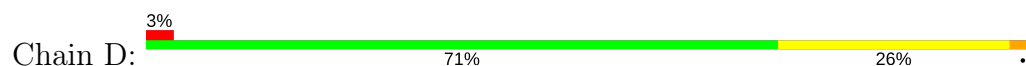
• Molecule 3: Proteasome component PRE6

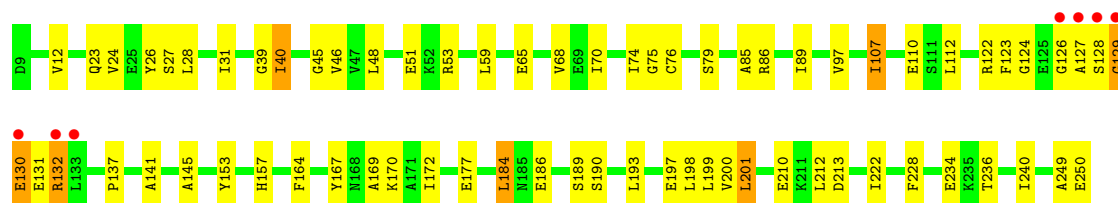


• Molecule 3: Proteasome component PRE6

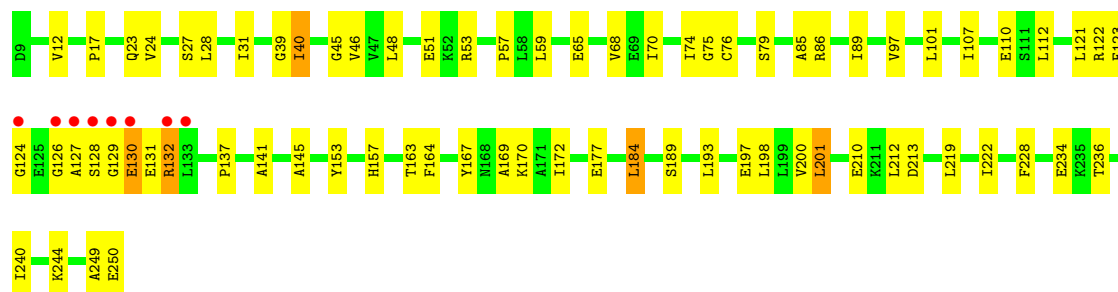


• Molecule 4: Proteasome component PUP2

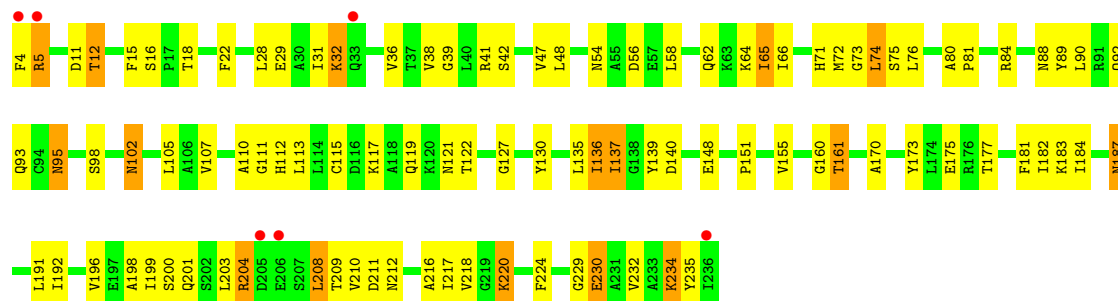




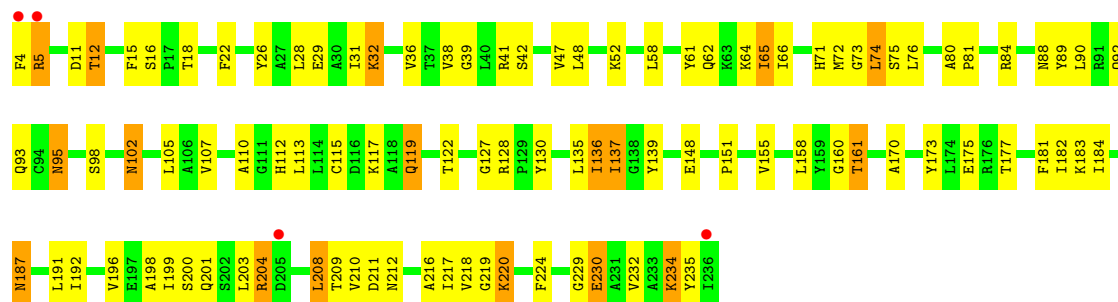
• Molecule 4: Proteasome component PUP2



• Molecule 5: Proteasome component PRE5

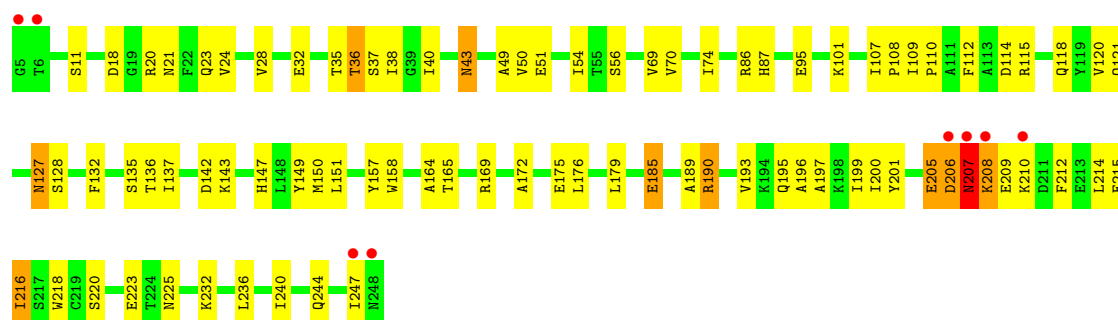


• Molecule 5: Proteasome component PRE5

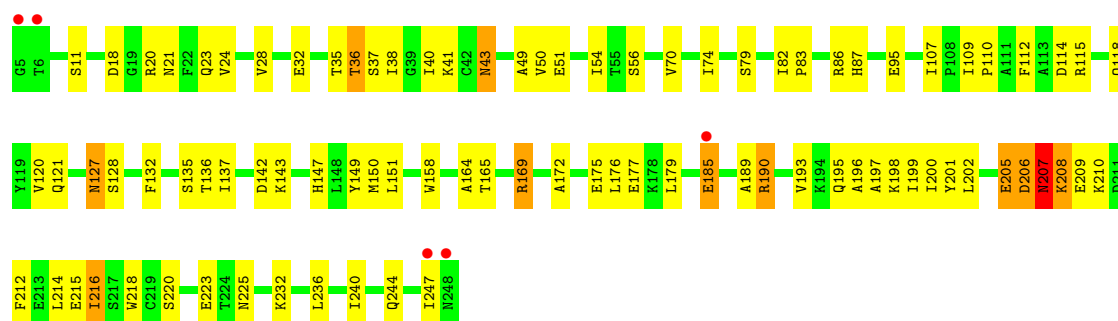


• Molecule 6: Proteasome component C1

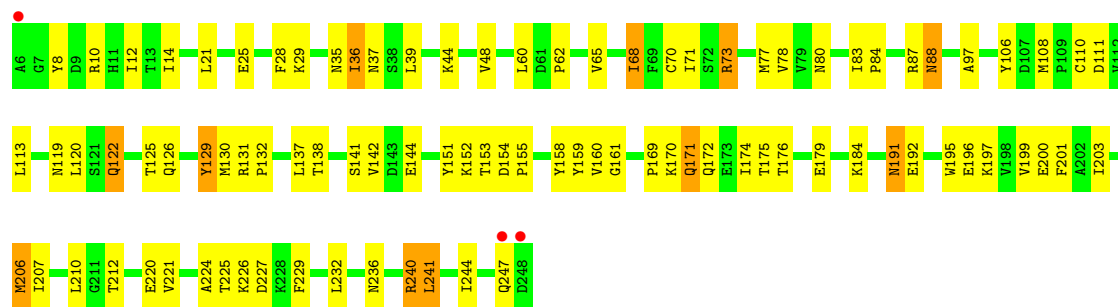




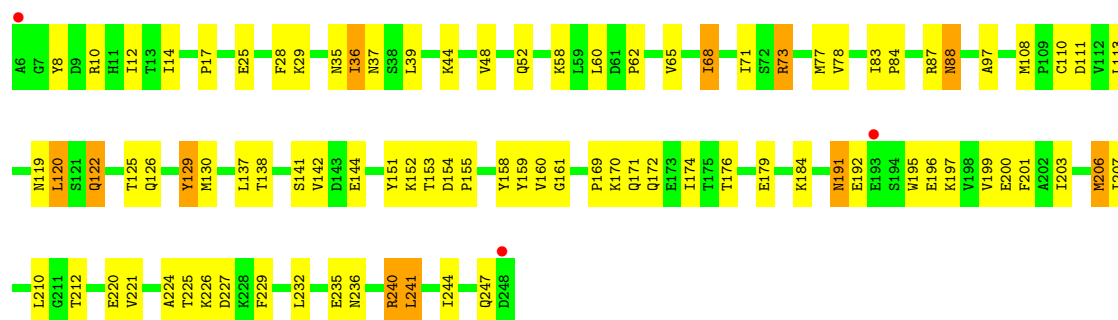
• Molecule 6: Proteasome component C1



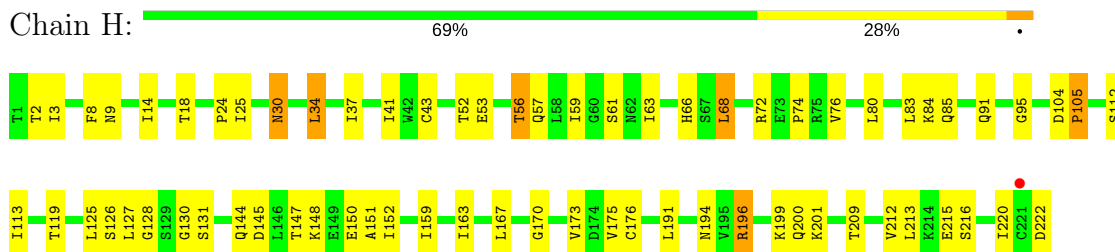
• Molecule 7: Proteasome component C7-alpha



• Molecule 7: Proteasome component C7-alpha



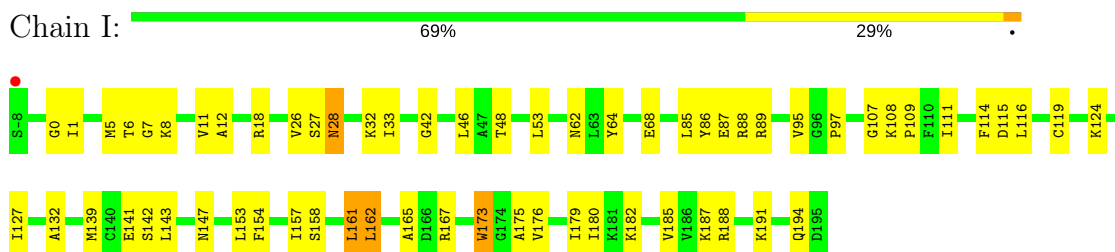
- Molecule 8: Proteasome component PUP1



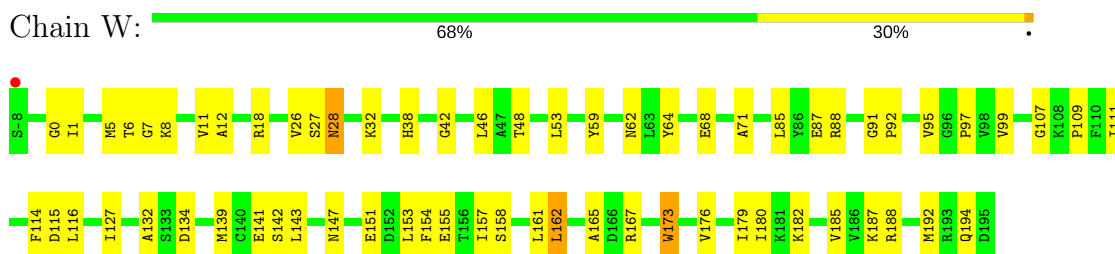
- Molecule 8: Proteasome component PUP1



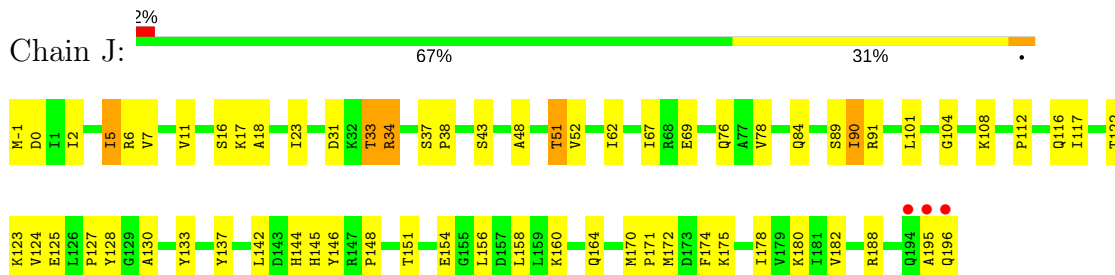
- Molecule 9: Proteasome component PUP3



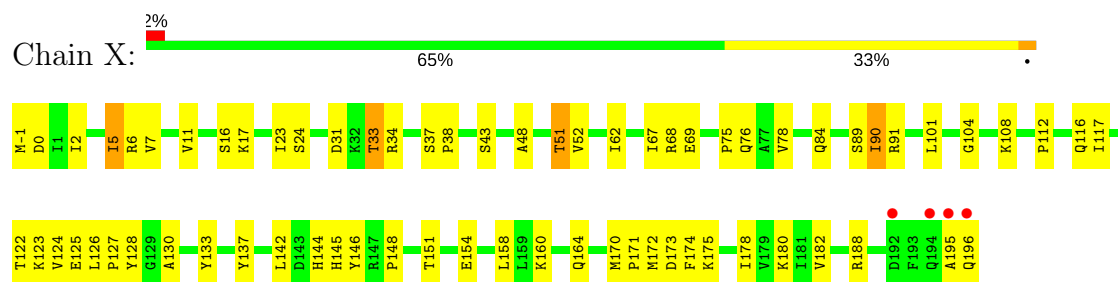
- Molecule 9: Proteasome component PUP3



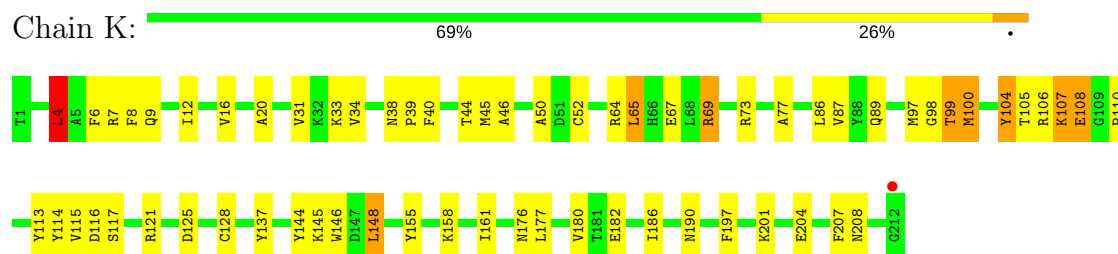
- Molecule 10: Proteasome component C11



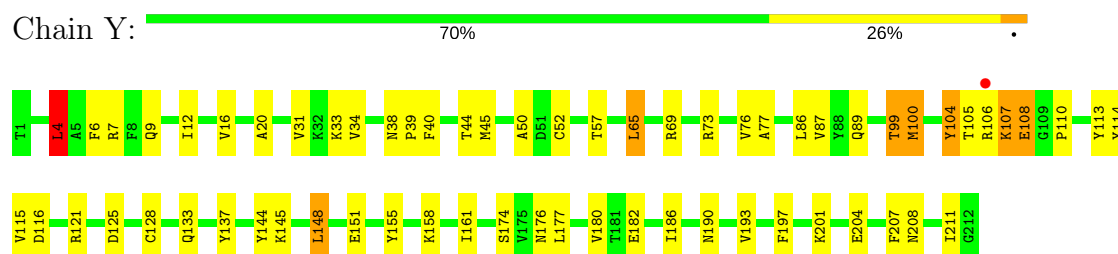
- Molecule 10: Proteasome component C11



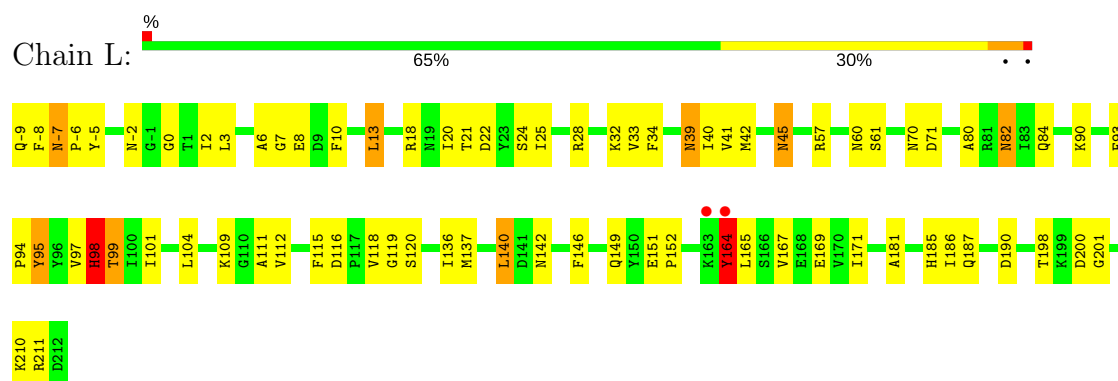
- Molecule 11: Proteasome component PRE2



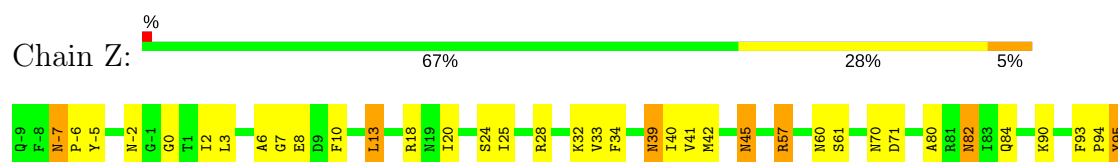
- Molecule 11: Proteasome component PRE2

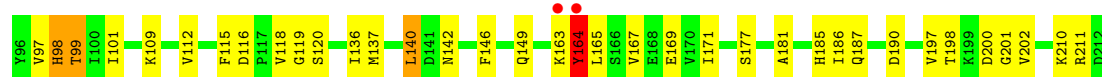


- Molecule 12: Proteasome component C5

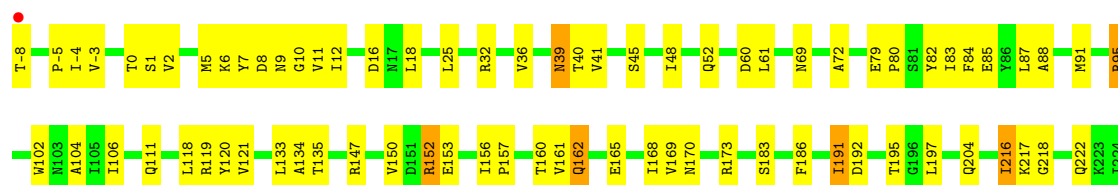


- Molecule 12: Proteasome component C5





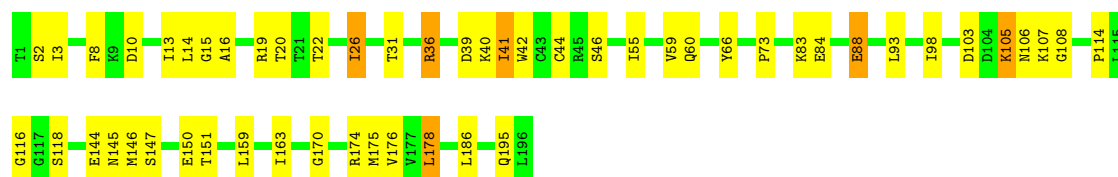
• Molecule 13: Proteasome component PRE4



• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3



• Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA



• Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA



- Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA

Chain 3:  25% 50% 25%



- Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA

Chain 4:  25% 50% 25%



- Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA

Chain 5:  50% 50%



- Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA

Chain 6:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.85Å 298.45Å 145.25Å 90.00° 112.63° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 29.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.80) 97.9 (29.84-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.80Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.241 0.212 , 0.212	Depositor DCC
R_{free} test set	12699 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	51109	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0JT, LYH, MH9

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	0.37	0/1952	0.64	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.38	0/1935	0.64	0/2618
2	P	0.39	0/1935	0.64	0/2618
3	C	0.36	0/1920	0.62	0/2598
3	Q	0.38	0/1920	0.62	0/2598
4	D	0.36	0/1887	0.64	0/2541
4	R	0.36	0/1887	0.64	0/2541
5	E	0.36	0/1823	0.63	0/2463
5	S	0.36	0/1823	0.63	0/2463
6	F	0.39	0/1937	0.62	0/2614
6	T	0.39	0/1937	0.62	0/2614
7	G	0.41	0/1959	0.64	0/2652
7	U	0.39	0/1959	0.63	0/2652
8	H	0.41	0/1716	0.66	0/2326
8	V	0.39	0/1716	0.66	0/2326
9	I	0.39	0/1611	0.67	0/2174
9	W	0.41	0/1611	0.67	0/2174
10	J	0.40	0/1613	0.65	0/2173
10	X	0.40	0/1613	0.65	0/2173
11	K	0.41	0/1681	0.66	1/2274 (0.0%)
11	Y	0.39	0/1681	0.66	1/2274 (0.0%)
12	L	0.40	0/1795	0.69	3/2420 (0.1%)
12	Z	0.39	0/1795	0.69	3/2420 (0.1%)
13	M	0.39	0/1855	0.67	0/2514
13	a	0.38	0/1855	0.67	1/2514 (0.0%)
14	N	0.40	0/1541	0.64	0/2087
14	b	0.39	0/1541	0.64	0/2087
15	1	1.68	0/6	1.40	0/7
15	2	1.23	0/6	1.89	0/7
15	3	1.71	0/6	1.64	0/7
15	4	1.75	0/6	1.44	0/7

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	5	1.31	0/6	1.84	0/7
15	6	1.69	0/6	1.68	0/7
All	All	0.39	0/50486	0.65	9/68234 (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
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	164	TYR	CA-CB-CG	-5.36	103.22	113.40
11	Y	4	LEU	CA-CB-CG	5.32	127.53	115.30
11	K	4	LEU	CA-CB-CG	5.29	127.48	115.30
12	Z	98	HIS	N-CA-C	-5.27	96.77	111.00
12	Z	164	TYR	CA-CB-CG	-5.27	103.39	113.40
12	L	95	TYR	N-CA-C	-5.26	96.80	111.00
12	Z	95	TYR	N-CA-C	-5.21	96.94	111.00
12	L	98	HIS	N-CA-C	-5.08	97.28	111.00
13	a	101	LEU	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	164	TYR	Sidechain
12	Z	164	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	1915	0	1926	66	0
1	O	1915	0	1926	68	0
2	B	1905	0	1901	78	0
2	P	1905	0	1901	84	0
3	C	1891	0	1900	91	0
3	Q	1891	0	1900	88	0
4	D	1862	0	1836	52	0
4	R	1862	0	1836	55	0
5	E	1795	0	1797	95	0
5	S	1795	0	1797	97	0
6	F	1897	0	1886	77	0
6	T	1897	0	1886	79	0
7	G	1921	0	1910	84	0
7	U	1921	0	1910	87	0
8	H	1685	0	1687	57	0
8	V	1685	0	1687	58	0
9	I	1581	0	1574	59	0
9	W	1581	0	1574	59	0
10	J	1585	0	1590	73	0
10	X	1585	0	1590	73	0
11	K	1644	0	1594	55	0
11	Y	1644	0	1594	58	0
12	L	1757	0	1711	64	0
12	Z	1757	0	1711	60	0
13	M	1824	0	1832	60	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	46	0
14	b	1512	0	1480	0	0
15	1	38	0	45	4	0
15	2	38	0	45	1	0
15	3	38	0	45	3	0
15	4	38	0	45	5	0
15	5	38	0	45	2	0
15	6	38	0	45	0	0
16	1	1	0	0	0	0
16	2	1	0	0	0	0
16	3	1	0	0	0	0
16	A	59	0	0	1	0
16	B	35	0	0	0	0
16	C	44	0	0	5	0
16	D	39	0	0	4	0
16	E	23	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	F	49	0	0	2	0
16	G	60	0	0	6	0
16	H	49	0	0	3	0
16	I	64	0	0	2	0
16	J	53	0	0	2	0
16	K	42	0	0	3	0
16	L	55	0	0	4	0
16	M	75	0	0	3	0
16	N	56	0	0	3	0
16	O	34	0	0	1	0
16	P	28	0	0	1	0
16	Q	29	0	0	2	0
16	R	33	0	0	2	0
16	S	21	0	0	0	0
16	T	39	0	0	2	0
16	U	63	0	0	2	0
16	V	47	0	0	5	0
16	W	55	0	0	2	0
16	X	46	0	0	4	0
16	Y	50	0	0	5	0
16	Z	51	0	0	2	0
16	a	73	0	0	0	0
16	b	58	0	0	0	0
All	All	51109	0	49518	1646	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 18.

All (1646) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:203:THR:HG22	2:P:205:SER:H	1.08	1.13
11:K:107:LYS:H	11:K:107:LYS:HD2	1.03	1.11
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.04	1.11
2:B:203:THR:HG22	2:B:205:SER:H	1.11	1.06
2:P:72:ASN:ND2	2:P:73:ASP:H	1.56	1.04
2:B:72:ASN:ND2	2:B:73:ASP:H	1.54	1.03
1:O:131:ARG:HH21	7:U:125:THR:HG22	1.21	1.02
1:A:131:ARG:HH21	7:G:125:THR:HG22	1.23	1.02
11:K:208:ASN:HD21	10:X:148:PRO:HG3	1.21	1.01
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.43	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:97:ALA:HA	7:G:108:MET:HE2	1.44	1.00
10:J:148:PRO:HG3	11:Y:208:ASN:HD21	1.25	1.00
4:R:68:VAL:HG21	4:R:89:ILE:HD12	1.44	0.99
9:W:5:MET:HE3	9:W:157:ILE:HG13	1.44	0.98
13:M:170:ASN:HD22	13:M:173:ARG:HH11	1.04	0.98
13:M:5:MET:HG2	13:M:168:ILE:HD11	1.44	0.98
7:U:97:ALA:HA	7:U:108:MET:HE2	1.44	0.98
4:D:68:VAL:HG21	4:D:89:ILE:HD12	1.45	0.98
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.44	0.98
2:B:125:THR:HG22	3:C:131:ARG:HH21	1.30	0.96
9:I:5:MET:HE3	9:I:157:ILE:HG13	1.46	0.95
3:Q:166:GLN:HE21	3:Q:167:THR:H	1.09	0.94
2:B:15:PHE:H	3:C:23:GLN:HE22	1.09	0.94
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.49	0.94
3:C:166:GLN:HE21	3:C:167:THR:H	1.09	0.94
1:A:125:THR:HG22	2:B:131:ARG:HH21	1.30	0.94
2:P:125:THR:HG22	3:Q:131:ARG:HH21	1.31	0.94
1:O:125:THR:HG22	2:P:131:ARG:HH21	1.31	0.94
10:J:-1:MET:HG2	10:J:0:ASP:H	1.33	0.93
10:X:-1:MET:HG2	10:X:0:ASP:H	1.35	0.92
1:O:15:PHE:H	2:P:23:GLN:HE22	1.14	0.91
5:S:203:LEU:HD11	5:S:208:LEU:HD22	1.52	0.91
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.17	0.91
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.36	0.91
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.51	0.90
5:E:203:LEU:HD11	5:E:208:LEU:HD22	1.53	0.90
2:B:226:GLU:HG2	2:B:227:VAL:H	1.36	0.89
2:P:226:GLU:HG2	2:P:227:VAL:H	1.38	0.88
11:Y:107:LYS:N	11:Y:107:LYS:HD2	1.89	0.88
11:K:107:LYS:N	11:K:107:LYS:HD2	1.88	0.87
2:P:72:ASN:HD22	2:P:73:ASP:H	1.23	0.87
2:B:72:ASN:HD22	2:B:73:ASP:H	1.22	0.86
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.40	0.86
3:C:191:THR:HB	3:C:194:GLU:HG2	1.57	0.85
7:U:71:ILE:HD11	7:U:77:MET:HB3	1.58	0.85
3:Q:191:THR:HB	3:Q:194:GLU:HG2	1.59	0.84
7:G:192:GLU:HG2	7:G:197:LYS:HB2	1.60	0.84
9:W:8:LYS:HD3	9:W:147:ASN:HD22	1.42	0.84
3:Q:201:ARG:HG3	3:Q:240:ILE:HD13	1.58	0.83
3:C:166:GLN:HE22	3:C:176:ARG:HE	1.26	0.83
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.43	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ASN:HD22	2:B:73:ASP:N	1.76	0.83
5:S:209:THR:H	5:S:212:ASN:HD22	1.25	0.83
3:C:101:ARG:NH1	3:C:107:PRO:HB3	1.94	0.83
1:O:86:ARG:HE	7:U:119:ASN:HD21	1.24	0.83
3:Q:236:TYR:O	3:Q:240:ILE:HG13	1.77	0.83
7:U:192:GLU:HG2	7:U:197:LYS:HB2	1.60	0.83
7:G:71:ILE:HD11	7:G:77:MET:HB3	1.61	0.82
8:H:52:THR:O	8:H:56:THR:HB	1.79	0.82
2:B:125:THR:CG2	3:C:131:ARG:HH21	1.92	0.82
9:I:8:LYS:HD3	9:I:147:ASN:HD22	1.45	0.82
12:Z:99:THR:HG23	16:Z:309:HOH:O	1.79	0.82
1:A:15:PHE:H	2:B:23:GLN:HE22	1.26	0.81
5:E:209:THR:H	5:E:212:ASN:HD22	1.26	0.81
2:P:72:ASN:HD22	2:P:73:ASP:N	1.77	0.81
5:S:95:ASN:HD21	12:Z:60:ASN:HD21	1.24	0.81
3:Q:166:GLN:HE22	3:Q:176:ARG:HE	1.25	0.81
3:C:201:ARG:HG3	3:C:240:ILE:HD13	1.61	0.81
3:C:236:TYR:O	3:C:240:ILE:HG13	1.81	0.81
2:P:203:THR:HG22	2:P:205:SER:N	1.92	0.81
3:C:167:THR:HG21	3:C:175:VAL:HG13	1.62	0.80
3:Q:191:THR:HG22	3:Q:193:GLU:H	1.47	0.80
5:E:208:LEU:HD23	5:E:208:LEU:H	1.45	0.80
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.44	0.80
5:S:208:LEU:HD23	5:S:208:LEU:H	1.46	0.80
3:Q:101:ARG:NH1	3:Q:107:PRO:HB3	1.96	0.80
5:E:47:VAL:HG22	5:E:217:ILE:HG13	1.63	0.80
3:C:15:PHE:H	4:D:23:GLN:HE22	1.30	0.79
11:Y:107:LYS:H	11:Y:107:LYS:CD	1.87	0.79
8:V:52:THR:O	8:V:56:THR:HB	1.83	0.79
11:Y:201:LYS:HE2	16:Y:330:HOH:O	1.82	0.79
3:C:166:GLN:NE2	3:C:167:THR:H	1.80	0.79
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.63	0.79
3:C:191:THR:HG22	3:C:193:GLU:H	1.47	0.79
3:Q:167:THR:HG21	3:Q:175:VAL:HG13	1.62	0.79
13:M:152:ARG:HH11	13:M:152:ARG:HG3	1.49	0.78
3:Q:166:GLN:NE2	3:Q:167:THR:H	1.81	0.78
6:T:35:THR:HG21	6:T:51:GLU:O	1.83	0.78
2:P:72:ASN:ND2	2:P:73:ASP:N	2.32	0.78
4:R:169:ALA:HB3	5:S:58:LEU:HD23	1.66	0.78
8:V:34:LEU:HB2	16:V:315:HOH:O	1.82	0.78
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:162:GLN:H	13:M:162:GLN:NE2	1.82	0.77
2:B:72:ASN:ND2	2:B:73:ASP:N	2.30	0.77
5:E:95:ASN:HD21	12:L:60:ASN:HD21	1.27	0.77
11:K:208:ASN:HD21	10:X:148:PRO:CG	1.98	0.77
5:E:181:PHE:HA	5:E:184:ILE:HG12	1.67	0.77
5:E:200:SER:HA	5:E:203:LEU:HG	1.65	0.77
12:L:3:LEU:CD1	12:L:140:LEU:HD21	2.15	0.76
6:F:109:ILE:H	6:F:109:ILE:HD12	1.50	0.76
6:F:35:THR:HG21	6:F:51:GLU:O	1.84	0.76
13:M:39:ASN:H	13:M:39:ASN:HD22	1.33	0.76
5:S:181:PHE:HA	5:S:184:ILE:HG12	1.66	0.76
5:S:200:SER:HA	5:S:203:LEU:HG	1.66	0.76
7:U:122:GLN:O	7:U:125:THR:HB	1.86	0.76
1:A:86:ARG:HE	7:G:119:ASN:HD21	1.31	0.76
1:O:131:ARG:HH21	7:U:125:THR:CG2	1.98	0.76
7:G:122:GLN:O	7:G:125:THR:HB	1.86	0.75
2:B:203:THR:HG22	2:B:205:SER:N	1.95	0.75
2:P:125:THR:CG2	3:Q:131:ARG:HH21	1.98	0.75
12:Z:185:HIS:HD2	12:Z:187:GLN:H	1.35	0.75
14:N:20:THR:HG23	14:N:31:THR:OG1	1.87	0.74
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.35	0.74
12:Z:3:LEU:CD1	12:Z:140:LEU:HD21	2.18	0.74
1:O:125:THR:CG2	2:P:131:ARG:HH21	2.01	0.74
8:H:34:LEU:HB2	16:H:322:HOH:O	1.87	0.73
3:Q:191:THR:HG22	3:Q:193:GLU:N	2.02	0.73
5:S:47:VAL:HG22	5:S:217:ILE:HG13	1.69	0.73
3:C:191:THR:HG22	3:C:193:GLU:N	2.02	0.73
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.69	0.73
1:A:125:THR:CG2	2:B:131:ARG:HH21	1.99	0.73
7:G:60:LEU:O	7:G:62:PRO:HD3	1.88	0.73
10:J:172:MET:HE2	10:X:172:MET:HE2	1.69	0.73
2:B:226:GLU:HG2	2:B:227:VAL:N	2.04	0.73
4:D:45:GLY:HA2	4:D:153:TYR:CE1	2.23	0.73
1:O:181:ARG:HH11	1:O:181:ARG:HB3	1.54	0.72
1:A:181:ARG:HB3	1:A:181:ARG:HH11	1.53	0.72
12:Z:13:LEU:HD13	12:Z:33:VAL:HG13	1.71	0.72
10:J:-1:MET:HG2	10:J:0:ASP:N	2.05	0.72
11:K:105:THR:OG1	11:K:108:GLU:HG3	1.89	0.72
11:Y:211:ILE:HG13	16:Y:339:HOH:O	1.90	0.72
6:T:109:ILE:H	6:T:109:ILE:HD12	1.54	0.72
11:Y:105:THR:OG1	11:Y:108:GLU:HG3	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:185:HIS:HD2	12:L:187:GLN:H	1.36	0.71
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.04	0.71
12:L:13:LEU:HD13	12:L:33:VAL:HG13	1.71	0.71
10:X:137:TYR:CE2	10:X:170:MET:HG3	2.26	0.71
11:K:99:THR:HG22	11:K:115:VAL:HB	1.71	0.71
4:R:45:GLY:HA2	4:R:153:TYR:CE1	2.25	0.71
5:S:72:MET:HE1	5:S:107:VAL:HA	1.71	0.71
11:K:107:LYS:H	11:K:107:LYS:CD	1.87	0.71
3:C:166:GLN:HE21	3:C:167:THR:N	1.87	0.71
10:J:137:TYR:CE2	10:J:170:MET:HG3	2.26	0.71
11:K:201:LYS:HE2	16:K:332:HOH:O	1.90	0.71
13:M:40:THR:OG1	13:M:80:PRO:HG3	1.90	0.71
1:O:181:ARG:NH1	1:O:181:ARG:HB3	2.06	0.71
5:E:73:GLY:HA3	5:E:224:PHE:CE2	2.27	0.70
11:Y:99:THR:HG22	11:Y:115:VAL:O	1.91	0.70
6:F:236:LEU:O	6:F:240:ILE:HG12	1.91	0.70
2:P:226:GLU:HG2	2:P:227:VAL:N	2.06	0.70
1:A:181:ARG:NH1	1:A:181:ARG:HB3	2.06	0.70
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.72	0.70
10:J:148:PRO:CG	11:Y:208:ASN:HD21	2.02	0.70
5:E:208:LEU:CD2	5:E:208:LEU:H	2.05	0.69
5:S:208:LEU:HA	5:S:212:ASN:ND2	2.06	0.69
7:U:60:LEU:O	7:U:62:PRO:HD3	1.92	0.69
10:X:-1:MET:HG2	10:X:0:ASP:N	2.06	0.69
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.92	0.69
4:D:169:ALA:HB3	5:E:58:LEU:HD23	1.74	0.69
11:Y:99:THR:HG22	11:Y:115:VAL:HB	1.73	0.69
1:O:122:GLN:O	1:O:125:THR:HB	1.92	0.69
2:B:78:ALA:HB3	2:B:138:ILE:HB	1.75	0.69
4:D:45:GLY:HA2	4:D:153:TYR:CD1	2.28	0.69
5:E:208:LEU:HA	5:E:212:ASN:ND2	2.08	0.69
5:E:139:TYR:CE2	5:E:220:LYS:HA	2.28	0.69
11:K:99:THR:HG22	11:K:115:VAL:O	1.91	0.69
9:W:116:LEU:HD21	15:4:0:MH9:H3	1.73	0.68
5:S:208:LEU:H	5:S:208:LEU:CD2	2.05	0.68
7:U:226:LYS:HA	7:U:226:LYS:HE3	1.75	0.68
3:Q:57:LYS:O	3:Q:58:LEU:HB2	1.92	0.68
3:C:57:LYS:O	3:C:58:LEU:HB2	1.92	0.68
3:Q:201:ARG:CG	3:Q:240:ILE:HD13	2.23	0.68
8:V:59:ILE:HG12	8:V:83:LEU:HD23	1.74	0.68
1:A:122:GLN:O	1:A:125:THR:HB	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:86:ARG:HE	7:U:119:ASN:ND2	1.90	0.68
2:P:78:ALA:HB3	2:P:138:ILE:HB	1.76	0.68
6:T:236:LEU:O	6:T:240:ILE:HG12	1.94	0.68
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.07	0.68
14:N:103:ASP:HB2	16:N:233:HOH:O	1.94	0.67
10:X:62:ILE:HD11	10:X:78:VAL:HG13	1.74	0.67
4:D:24:VAL:O	4:D:27:SER:HB3	1.94	0.67
16:F:341:HOH:O	7:G:131:ARG:HB2	1.95	0.67
8:H:14:ILE:CD1	8:H:34:LEU:HG	2.25	0.67
14:N:107:LYS:HG2	14:N:108:GLY:N	2.09	0.67
2:P:187:LYS:HD3	2:P:188:VAL:N	2.09	0.67
2:B:187:LYS:HD3	2:B:188:VAL:N	2.10	0.67
7:G:241:LEU:O	7:G:244:ILE:HG13	1.94	0.67
12:L:20:ILE:HG22	12:L:25:ILE:HA	1.77	0.67
13:M:41:VAL:HG23	13:M:191:ILE:HD11	1.76	0.67
4:R:24:VAL:O	4:R:27:SER:HB3	1.94	0.67
3:C:201:ARG:CG	3:C:240:ILE:HD13	2.25	0.67
5:E:72:MET:HE1	5:E:107:VAL:HA	1.74	0.67
8:H:59:ILE:HG12	8:H:83:LEU:HD23	1.77	0.66
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.94	0.66
3:Q:72:ASP:HA	10:X:67:ILE:HD12	1.77	0.66
10:J:51:THR:HG22	10:J:52:VAL:N	2.10	0.66
9:I:116:LEU:HD21	15:I:0:MH9:H3	1.78	0.66
8:H:215:GLU:HG3	9:I:188:ARG:HG2	1.77	0.66
13:M:39:ASN:N	13:M:39:ASN:HD22	1.93	0.66
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.08	0.66
6:F:95:GLU:HG2	6:F:115:ARG:CB	2.23	0.66
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.77	0.66
2:B:122:GLN:O	2:B:125:THR:HB	1.96	0.66
6:T:190:ARG:HG3	6:T:190:ARG:HH11	1.61	0.66
7:G:226:LYS:HE3	7:G:226:LYS:HA	1.77	0.66
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.77	0.66
3:Q:166:GLN:HE21	3:Q:167:THR:N	1.87	0.66
5:S:139:TYR:CE2	5:S:220:LYS:HA	2.31	0.66
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.61	0.66
1:O:242:THR:OG1	1:O:245:GLU:HG3	1.96	0.65
10:J:62:ILE:HD11	10:J:78:VAL:HG13	1.79	0.65
2:P:21:LEU:HD13	2:P:125:THR:HG23	1.78	0.65
5:S:90:LEU:HD11	5:S:110:ALA:HB1	1.78	0.65
7:U:68:ILE:HG13	7:U:220:GLU:HG2	1.79	0.65
1:A:242:THR:OG1	1:A:245:GLU:HG3	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:14:ILE:CD1	8:V:34:LEU:HG	2.26	0.65
10:X:51:THR:HG22	10:X:52:VAL:N	2.11	0.65
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.78	0.65
1:A:131:ARG:HH21	7:G:125:THR:CG2	2.03	0.65
12:L:3:LEU:HD11	12:L:140:LEU:HD21	1.79	0.65
5:S:181:PHE:HA	5:S:184:ILE:CG1	2.26	0.65
5:E:90:LEU:HD11	5:E:110:ALA:HB1	1.79	0.65
2:B:21:LEU:HD13	2:B:125:THR:HG23	1.78	0.65
7:U:241:LEU:O	7:U:244:ILE:HG13	1.96	0.65
9:W:26:VAL:HG13	16:X:223:HOH:O	1.96	0.65
6:F:136:THR:O	6:F:150:MET:HA	1.98	0.64
5:S:73:GLY:HA3	5:S:224:PHE:CE2	2.32	0.64
8:V:215:GLU:HG3	9:W:188:ARG:HG2	1.79	0.64
12:Z:20:ILE:HG22	12:Z:25:ILE:HA	1.78	0.64
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.61	0.64
2:P:247:THR:HG22	2:P:247:THR:OXT	1.98	0.64
4:R:45:GLY:HA2	4:R:153:TYR:CD1	2.31	0.64
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.80	0.64
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.61	0.64
11:K:99:THR:CG2	11:K:115:VAL:HB	2.28	0.64
5:S:84:ARG:HG3	5:S:84:ARG:HH11	1.63	0.64
7:U:235:GLU:HG2	16:U:357:HOH:O	1.98	0.64
5:E:12:THR:HG21	5:E:122:THR:HA	1.80	0.64
6:T:18:ASP:OD1	6:T:20:ARG:HD3	1.98	0.64
6:F:190:ARG:HH11	6:F:190:ARG:HG3	1.63	0.64
2:P:52:ARG:HH22	2:P:64:SER:HB3	1.62	0.64
14:N:36:ARG:HH21	14:N:60:GLN:HE21	1.44	0.64
5:E:175:GLU:OE1	6:F:56:SER:HB2	1.97	0.64
13:M:170:ASN:HD22	13:M:173:ARG:NH1	1.87	0.64
12:L:116:ASP:HB2	12:L:120:SER:HB3	1.80	0.63
12:L:186:ILE:O	8:V:167:LEU:HD22	1.97	0.63
12:Z:116:ASP:HB2	12:Z:120:SER:HB3	1.80	0.63
5:E:182:ILE:O	5:E:182:ILE:HG12	1.97	0.63
2:P:122:GLN:O	2:P:125:THR:HB	1.98	0.63
5:S:203:LEU:HD11	5:S:208:LEU:CD2	2.28	0.63
2:B:125:THR:HG22	3:C:131:ARG:NH2	2.10	0.63
8:H:167:LEU:HD22	12:Z:186:ILE:O	1.97	0.63
10:J:17:LYS:HG2	10:J:178:ILE:HG13	1.80	0.63
1:O:113:LEU:O	1:O:117:VAL:HG23	1.97	0.63
2:P:61:GLN:OE1	2:P:211:ASP:HA	1.98	0.63
12:Z:3:LEU:HD11	12:Z:140:LEU:HD21	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:GLU:OE2	3:C:32:LYS:HE2	1.98	0.63
5:E:181:PHE:HA	5:E:184:ILE:CG1	2.27	0.63
2:B:52:ARG:HH22	2:B:64:SER:HB3	1.63	0.63
5:S:182:ILE:HG12	5:S:182:ILE:O	1.97	0.63
5:S:229:GLY:O	5:S:232:VAL:HG22	1.99	0.63
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.25	0.63
1:A:86:ARG:HE	7:G:119:ASN:ND2	1.96	0.63
2:B:247:THR:HG22	2:B:247:THR:OXT	1.98	0.63
4:D:127:ALA:HA	5:E:127:GLY:HA2	1.81	0.62
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.80	0.62
3:Q:29:GLU:OE2	3:Q:32:LYS:HE2	1.97	0.62
6:T:209:GLU:HG3	6:T:210:LYS:HG3	1.80	0.62
1:O:125:THR:HG22	2:P:131:ARG:NH2	2.11	0.62
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.29	0.62
2:B:61:GLN:OE1	2:B:211:ASP:HA	1.99	0.62
8:V:37:ILE:CD1	8:V:43:CYS:HB2	2.29	0.62
7:G:172:GLN:HE21	7:G:176:THR:HG23	1.64	0.62
5:S:182:ILE:HG23	5:S:183:LYS:HG3	1.81	0.62
3:C:107:PRO:HG2	3:C:144:PRO:HG3	1.81	0.62
5:E:84:ARG:HG3	5:E:84:ARG:HH11	1.64	0.62
2:P:88:ILE:O	2:P:92:THR:HG23	2.00	0.62
11:Y:99:THR:CG2	11:Y:115:VAL:HB	2.30	0.62
12:Z:136:ILE:HD11	12:Z:181:ALA:HB2	1.81	0.62
6:F:209:GLU:HG3	6:F:210:LYS:HG3	1.82	0.62
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.82	0.62
3:Q:107:PRO:HG2	3:Q:144:PRO:HG3	1.82	0.62
12:L:3:LEU:HD13	12:L:140:LEU:HD21	1.82	0.62
14:N:44:CYS:HB2	14:N:98:ILE:HB	1.81	0.62
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.81	0.62
9:W:1:ILE:HG21	9:W:132:ALA:HB3	1.82	0.62
5:S:12:THR:HG21	5:S:122:THR:HA	1.80	0.61
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.82	0.61
13:M:118:LEU:HG	13:M:133:LEU:HD12	1.81	0.61
3:Q:163:TRP:CE2	4:R:59:LEU:HD23	2.35	0.61
5:E:203:LEU:HD11	5:E:208:LEU:CD2	2.29	0.61
5:E:208:LEU:N	5:E:208:LEU:HD23	2.14	0.61
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.82	0.61
5:S:208:LEU:N	5:S:208:LEU:HD23	2.14	0.61
3:C:72:ASP:HA	10:J:67:ILE:HD12	1.83	0.61
4:D:184:LEU:HD22	5:E:58:LEU:HD13	1.83	0.61
4:D:85:ALA:O	4:D:89:ILE:HG12	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:229:GLY:O	5:E:232:VAL:HG22	2.00	0.61
6:F:205:GLU:HG3	6:F:208:LYS:NZ	2.15	0.61
6:T:136:THR:O	6:T:150:MET:HA	2.00	0.61
6:F:69:VAL:HG12	16:F:307:HOH:O	1.99	0.61
4:R:85:ALA:O	4:R:89:ILE:HG12	2.01	0.61
6:T:205:GLU:HG3	6:T:208:LYS:NZ	2.16	0.61
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.83	0.61
13:M:18:LEU:HB2	13:M:183:SER:HB2	1.81	0.61
5:S:95:ASN:ND2	12:Z:60:ASN:HD21	1.98	0.61
1:A:13:THR:O	2:B:131:ARG:HD3	2.01	0.60
13:M:170:ASN:ND2	13:M:173:ARG:HH11	1.88	0.60
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.31	0.60
8:V:18:THR:HB	8:V:30:ASN:HA	1.82	0.60
10:X:17:LYS:HG2	10:X:178:ILE:HG13	1.83	0.60
8:H:37:ILE:CD1	8:H:43:CYS:HB2	2.30	0.60
14:N:107:LYS:HG2	14:N:108:GLY:H	1.65	0.60
3:Q:77:LEU:HD22	3:Q:90:ILE:HD13	1.83	0.60
2:B:232:PHE:HD2	2:B:232:PHE:H	1.50	0.60
5:E:210:VAL:HG13	5:E:211:ASP:N	2.16	0.60
1:A:113:LEU:O	1:A:117:VAL:HG23	2.00	0.60
5:E:182:ILE:HG23	5:E:183:LYS:HG3	1.82	0.60
6:F:18:ASP:OD1	6:F:20:ARG:HD3	2.01	0.60
10:J:137:TYR:HD1	16:Y:323:HOH:O	1.84	0.60
10:X:62:ILE:CD1	10:X:78:VAL:HG13	2.31	0.60
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.10	0.60
9:I:6:THR:CG2	9:I:111:ILE:HG12	2.31	0.60
1:O:86:ARG:HH21	7:U:119:ASN:HD22	1.49	0.60
5:S:210:VAL:HG13	5:S:211:ASP:N	2.17	0.60
11:K:208:ASN:ND2	10:X:148:PRO:HG3	2.06	0.60
10:J:37:SER:HB2	10:J:38:PRO:HD2	1.84	0.60
2:P:187:LYS:HE2	2:P:189:ASP:OD1	2.01	0.60
3:Q:107:PRO:HG2	3:Q:144:PRO:CG	2.31	0.60
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.66	0.60
3:C:57:LYS:HD2	3:C:58:LEU:N	2.16	0.60
9:W:107:GLY:HA2	9:W:182:LYS:HD3	1.83	0.60
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.17	0.59
10:X:37:SER:HB2	10:X:38:PRO:HD2	1.84	0.59
14:N:22:THR:HG22	15:3:1:THR:HA	1.82	0.59
14:N:46:SER:HA	15:3:3:OJT:H33	1.83	0.59
4:R:212:LEU:C	4:R:212:LEU:HD23	2.21	0.59
7:U:172:GLN:HE21	7:U:176:THR:HG23	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LYS:HE2	2:B:189:ASP:OD1	2.02	0.59
3:C:163:TRP:CE2	4:D:59:LEU:HD23	2.37	0.59
2:P:232:PHE:HD2	2:P:232:PHE:H	1.49	0.59
4:R:40:ILE:HG13	4:R:200:VAL:CG2	2.32	0.59
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.83	0.59
3:C:107:PRO:HG2	3:C:144:PRO:CG	2.32	0.59
6:F:114:ASP:O	6:F:118:GLN:HG2	2.02	0.59
1:A:197:LEU:HD23	1:A:197:LEU:C	4.01	0.59
2:B:88:ILE:O	2:B:92:THR:HG23	2.02	0.59
4:D:212:LEU:HD23	4:D:212:LEU:C	2.23	0.59
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.85	0.59
8:H:173:VAL:HB	8:H:191:LEU:HB2	1.84	0.59
8:H:18:THR:HB	8:H:30:ASN:HA	1.83	0.59
6:T:114:ASP:O	6:T:118:GLN:HG2	2.02	0.59
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.85	0.59
10:J:62:ILE:CD1	10:J:78:VAL:HG13	2.33	0.59
12:L:136:ILE:HD11	12:L:181:ALA:HB2	1.85	0.59
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.38	0.59
12:Z:7:GLY:HA3	12:Z:10:PHE:CE2	2.37	0.59
3:Q:171:ASN:HB2	3:Q:206:VAL:HG11	1.84	0.59
6:T:195:GLN:O	6:T:199:ILE:HG12	2.03	0.59
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.85	0.59
9:W:6:THR:CG2	9:W:111:ILE:HG12	2.32	0.59
7:G:68:ILE:HG13	7:G:220:GLU:HG2	1.84	0.59
1:O:249:ARG:HH11	1:O:249:ARG:HG3	1.67	0.59
5:S:192:ILE:O	5:S:196:VAL:HG23	2.02	0.58
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.84	0.58
12:L:-6:PRO:O	13:M:95:ARG:NH1	2.34	0.58
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.84	0.58
5:S:136:ILE:HD13	5:S:136:ILE:N	2.19	0.58
5:S:199:ILE:HG23	5:S:200:SER:N	2.19	0.58
6:T:158:TRP:CZ3	7:U:65:VAL:HA	2.38	0.58
7:G:207:ILE:HG23	7:G:212:THR:O	2.03	0.58
13:M:80:PRO:HD2	13:M:111:GLN:OE1	2.03	0.58
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.19	0.58
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.85	0.58
8:V:173:VAL:HB	8:V:191:LEU:HB2	1.84	0.58
13:M:7:TYR:CE2	13:M:161:VAL:HG22	2.39	0.58
8:V:195:VAL:HG23	16:V:318:HOH:O	2.03	0.58
1:A:249:ARG:HH11	1:A:249:ARG:HG3	1.69	0.58
7:G:87:ARG:HD2	16:G:317:HOH:O	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:192:GLU:HG2	7:U:197:LYS:CB	2.33	0.58
5:E:181:PHE:O	5:E:184:ILE:HG12	2.04	0.58
3:Q:173:LYS:HB2	16:Q:316:HOH:O	2.02	0.58
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.39	0.58
2:P:154:ASN:HB2	2:P:155:PRO:HD2	1.84	0.58
2:B:183:LYS:O	2:B:186:MET:HG3	2.03	0.58
5:E:130:TYR:O	5:E:151:PRO:HB3	2.04	0.58
6:F:205:GLU:O	6:F:208:LYS:HD2	2.04	0.58
3:Q:245:GLN:C	3:Q:247:GLN:H	2.07	0.58
4:R:97:VAL:HG11	11:Y:65:LEU:HD22	1.85	0.58
5:S:181:PHE:O	5:S:184:ILE:HG12	2.03	0.58
9:I:1:ILE:HG21	9:I:132:ALA:HB3	1.84	0.58
11:K:16:VAL:HG21	11:K:34:VAL:HG23	1.84	0.58
6:T:205:GLU:O	6:T:208:LYS:HD2	2.04	0.58
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.86	0.58
7:G:196:GLU:O	7:G:200:GLU:HG3	2.04	0.58
13:M:36:VAL:HG11	13:M:83:ILE:HD13	1.84	0.58
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.85	0.58
7:U:207:ILE:HG23	7:U:212:THR:O	2.04	0.58
6:T:177:GLU:OE2	7:U:58:LYS:HE2	2.03	0.57
9:I:107:GLY:HA2	9:I:182:LYS:HD3	1.86	0.57
11:K:4:LEU:HD11	11:K:161:ILE:HG12	1.86	0.57
5:E:192:ILE:O	5:E:196:VAL:HG23	2.03	0.57
5:E:199:ILE:HG23	5:E:200:SER:N	2.18	0.57
14:N:66:TYR:CD2	14:N:73:PRO:HB3	2.38	0.57
8:V:144:GLN:O	8:V:145:ASP:HB2	2.04	0.57
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.01	0.57
3:C:245:GLN:C	3:C:247:GLN:H	2.07	0.57
10:J:51:THR:HG22	10:J:52:VAL:HG23	1.86	0.57
12:L:111:ALA:HA	16:L:339:HOH:O	2.04	0.57
4:D:40:ILE:HG13	4:D:200:VAL:CG2	2.35	0.57
9:I:139:MET:HE3	9:I:143:LEU:HD11	1.87	0.57
5:S:160:GLY:O	5:S:161:THR:HB	2.04	0.57
5:S:175:GLU:OE1	6:T:56:SER:HB2	2.04	0.57
2:B:142:TYR:CD1	2:B:227:VAL:HG21	2.40	0.57
8:H:144:GLN:O	8:H:145:ASP:HB2	2.04	0.57
10:J:172:MET:CE	10:X:172:MET:HE2	2.34	0.57
12:L:2:ILE:HD13	12:L:45:ASN:HB2	1.85	0.57
3:Q:175:VAL:HG23	3:Q:202:SER:HB2	1.86	0.57
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.50	0.57
5:S:130:TYR:O	5:S:151:PRO:HB3	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PHE:CE1	1:A:212:ILE:HD11	2.39	0.57
6:F:220:SER:HB3	6:F:223:GLU:HB2	1.87	0.57
1:O:13:THR:O	2:P:131:ARG:HD3	2.05	0.57
9:W:139:MET:HE3	9:W:143:LEU:HD11	1.87	0.57
1:A:86:ARG:HH21	7:G:119:ASN:HD22	1.53	0.57
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.86	0.57
12:L:7:GLY:HA3	12:L:10:PHE:CE2	2.39	0.57
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.20	0.57
9:I:26:VAL:HG13	16:J:240:HOH:O	2.05	0.57
10:J:137:TYR:HE1	16:X:232:HOH:O	1.87	0.57
5:E:95:ASN:ND2	12:L:60:ASN:HD21	2.01	0.57
3:C:41:LYS:HG2	3:C:164:SER:O	2.05	0.56
10:J:151:THR:OG1	10:J:154:GLU:HG3	2.05	0.56
3:Q:176:ARG:O	3:Q:180:GLU:HG3	2.05	0.56
3:C:175:VAL:HG23	3:C:202:SER:HB2	1.87	0.56
3:C:77:LEU:HD22	3:C:90:ILE:HD13	1.86	0.56
13:M:162:GLN:H	13:M:162:GLN:HE21	1.52	0.56
2:P:154:ASN:HB2	2:P:155:PRO:CD	2.35	0.56
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.86	0.56
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.86	0.56
3:C:201:ARG:HD3	16:C:336:HOH:O	2.05	0.56
6:F:109:ILE:HD12	6:F:109:ILE:N	2.20	0.56
6:F:195:GLN:O	6:F:199:ILE:HG12	2.04	0.56
2:P:102:LYS:NZ	10:X:84:GLN:NE2	2.54	0.56
7:U:97:ALA:CA	7:U:108:MET:HE2	2.29	0.56
8:V:37:ILE:HD11	8:V:43:CYS:HB2	1.87	0.56
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.03	0.56
3:Q:203:LEU:O	3:Q:207:VAL:HG23	2.06	0.56
3:C:203:LEU:O	3:C:207:VAL:HG23	2.06	0.56
7:G:71:ILE:N	7:G:71:ILE:HD12	2.21	0.56
7:G:80:ASN:HA	16:G:345:HOH:O	2.05	0.56
10:J:51:THR:CG2	10:J:52:VAL:N	2.69	0.56
2:P:91:ASN:O	2:P:95:ILE:HD13	2.05	0.56
4:R:184:LEU:HD22	5:S:58:LEU:HD13	1.87	0.56
6:T:189:ALA:O	6:T:193:VAL:HG23	2.06	0.56
11:Y:4:LEU:HD11	11:Y:161:ILE:HG12	1.86	0.56
4:D:53:ARG:HG2	4:D:53:ARG:O	2.06	0.56
8:H:37:ILE:HD11	8:H:43:CYS:HB2	1.87	0.56
4:R:127:ALA:HB3	4:R:132:ARG:HD3	1.87	0.56
2:B:154:ASN:HB2	2:B:155:PRO:CD	2.36	0.56
2:B:220:LYS:HG3	2:B:226:GLU:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:172:MET:HE3	10:X:172:MET:HE3	1.87	0.56
8:V:84:LYS:HG3	8:V:85:GLN:N	2.20	0.56
2:B:238:LYS:O	2:B:242:VAL:HG23	2.05	0.56
2:B:175:GLN:HG2	3:C:56:LEU:HD12	1.87	0.56
8:H:84:LYS:HG3	8:H:85:GLN:N	2.19	0.56
10:J:23:ILE:HG13	10:X:137:TYR:OH	2.05	0.56
2:P:142:TYR:CD1	2:P:227:VAL:HG21	2.41	0.56
2:B:15:PHE:N	3:C:23:GLN:HE22	1.92	0.56
7:G:192:GLU:HG2	7:G:197:LYS:CB	2.32	0.56
10:X:151:THR:OG1	10:X:154:GLU:HG3	2.05	0.56
12:Z:3:LEU:HD13	12:Z:140:LEU:HD21	1.85	0.56
5:E:72:MET:CE	5:E:107:VAL:HA	2.37	0.55
11:K:6:PHE:HA	11:K:125:ASP:O	2.06	0.55
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.88	0.55
7:U:73:ARG:HB2	7:U:73:ARG:NH1	2.20	0.55
7:G:97:ALA:CA	7:G:108:MET:HE2	2.28	0.55
3:Q:77:LEU:HD22	3:Q:90:ILE:CD1	2.36	0.55
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.88	0.55
12:L:137:MET:CE	9:W:167:ARG:NH2	2.69	0.55
8:H:220:ILE:HD11	9:I:185:VAL:HG21	1.87	0.55
3:Q:41:LYS:HG2	3:Q:164:SER:O	2.06	0.55
12:Z:42:MET:HG3	12:Z:101:ILE:HG22	1.88	0.55
12:Z:136:ILE:HG22	12:Z:140:LEU:HD22	1.88	0.55
7:G:73:ARG:NH1	7:G:73:ARG:HB2	2.21	0.55
6:T:220:SER:HB3	6:T:223:GLU:HB2	1.88	0.55
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.21	0.55
2:B:113:LEU:C	2:B:113:LEU:HD23	2.27	0.55
14:N:19:ARG:HG3	14:N:26:ILE:HG23	1.89	0.55
2:P:113:LEU:C	2:P:113:LEU:HD23	2.27	0.55
5:E:160:GLY:O	5:E:161:THR:HB	2.05	0.55
8:H:25:ILE:N	8:H:25:ILE:HD12	2.22	0.55
12:Z:13:LEU:HD13	12:Z:33:VAL:CG1	2.37	0.55
4:D:97:VAL:HG11	11:K:65:LEU:HD22	1.89	0.55
1:A:131:ARG:NH2	7:G:125:THR:HG22	2.07	0.55
11:K:44:THR:OG1	11:K:100:MET:HB2	2.07	0.55
14:N:105:LYS:HD3	14:N:105:LYS:O	2.07	0.55
2:P:38:ILE:HD13	2:P:166:SER:HB3	1.89	0.55
3:Q:171:ASN:O	3:Q:175:VAL:HG12	2.07	0.55
3:Q:232:GLU:O	3:Q:236:TYR:HD1	1.90	0.55
6:T:87:HIS:HD2	6:T:132:PHE:CE2	2.24	0.55
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ASN:HB2	2:B:155:PRO:HD2	1.86	0.54
3:C:171:ASN:HB2	3:C:206:VAL:HG11	1.88	0.54
8:H:41:ILE:HD12	8:H:76:VAL:HG22	1.89	0.54
12:L:42:MET:HG3	12:L:101:ILE:HG22	1.88	0.54
2:P:183:LYS:O	2:P:186:MET:HG3	2.06	0.54
4:R:212:LEU:HD23	4:R:213:ASP:N	2.22	0.54
1:A:143:ASP:OD1	1:A:146:ASN:HB2	2.08	0.54
13:M:88:ALA:HA	13:M:121:VAL:HG21	1.90	0.54
13:M:197:LEU:HD23	13:M:197:LEU:C	2.26	0.54
10:X:33:THR:HG21	10:X:180:LYS:NZ	2.22	0.54
10:X:51:THR:CG2	10:X:52:VAL:N	2.69	0.54
1:A:199:LEU:HD23	1:A:212:ILE:HD13	1.89	0.54
4:D:212:LEU:HD23	4:D:213:ASP:N	2.22	0.54
5:E:209:THR:OG1	5:E:212:ASN:HB3	2.08	0.54
7:G:172:GLN:NE2	7:G:176:THR:HG23	2.23	0.54
1:O:111:LYS:HG2	16:O:310:HOH:O	2.07	0.54
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.42	0.54
6:T:109:ILE:HD12	6:T:109:ILE:N	2.23	0.54
12:Z:20:ILE:HD12	12:Z:20:ILE:C	2.28	0.54
3:C:155:GLU:HB2	3:C:156:PRO:HD2	1.89	0.54
6:F:189:ALA:O	6:F:193:VAL:HG23	2.08	0.54
7:U:196:GLU:O	7:U:200:GLU:HG3	2.06	0.54
12:Z:2:ILE:HD13	12:Z:45:ASN:HB2	1.88	0.54
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.08	0.54
2:P:232:PHE:CD2	2:P:232:PHE:N	2.76	0.54
3:Q:231:GLU:CD	3:Q:231:GLU:H	2.11	0.54
10:J:137:TYR:OH	10:X:23:ILE:HG13	2.08	0.54
1:A:216:ILE:HD13	1:A:216:ILE:N	4.62	0.54
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.73	0.54
5:E:136:ILE:N	5:E:136:ILE:CD1	2.70	0.54
6:F:74:ILE:CD1	6:F:109:ILE:HG13	2.38	0.54
13:M:84:PHE:CE1	13:M:119:ARG:HD3	2.43	0.54
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.20	0.54
6:T:200:ILE:HG21	6:T:214:LEU:HD13	1.89	0.54
4:D:130:GLU:HG2	4:D:131:GLU:H	1.71	0.54
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.89	0.54
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.90	0.54
5:E:65:ILE:HG21	5:E:216:ALA:HB2	1.90	0.54
2:P:52:ARG:HH22	2:P:64:SER:CB	2.20	0.54
6:T:172:ALA:O	6:T:176:LEU:HD23	2.07	0.54
7:U:39:LEU:HD23	7:U:206:MET:HE3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:5:MET:CE	9:W:157:ILE:HA	2.38	0.54
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.07	0.54
9:I:167:ARG:NH2	12:Z:137:MET:CE	2.70	0.54
10:J:91:ARG:HH11	10:J:91:ARG:HG2	1.73	0.54
1:O:143:ASP:OD1	1:O:146:ASN:HB2	2.08	0.54
2:P:220:LYS:HG3	2:P:226:GLU:O	2.08	0.54
2:P:238:LYS:O	2:P:242:VAL:HG23	2.08	0.54
4:R:121:LEU:HB2	16:R:319:HOH:O	2.07	0.54
5:S:74:LEU:HB2	5:S:136:ILE:HD12	1.89	0.54
10:J:172:MET:CE	10:X:172:MET:CE	2.86	0.54
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.90	0.54
2:B:52:ARG:HH22	2:B:64:SER:CB	2.21	0.53
3:C:106:ASP:OD2	3:C:107:PRO:HD2	2.08	0.53
12:L:13:LEU:HD13	12:L:33:VAL:CG1	2.37	0.53
1:O:207:PHE:CE1	1:O:212:ILE:HD11	2.44	0.53
10:X:43:SER:OG	10:X:101:LEU:HB2	2.08	0.53
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.26	0.53
11:K:145:LYS:HB2	11:K:148:LEU:CD1	2.38	0.53
12:L:136:ILE:HG22	12:L:140:LEU:HD22	1.88	0.53
5:S:65:ILE:HG21	5:S:216:ALA:HB2	1.90	0.53
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.89	0.53
9:I:158:SER:O	9:I:162:LEU:HB2	2.08	0.53
1:A:58:LEU:HD12	7:G:175:THR:HG23	1.90	0.53
11:Y:65:LEU:HB3	11:Y:69:ARG:NH2	2.24	0.53
3:C:232:GLU:O	3:C:236:TYR:HD1	1.92	0.53
4:D:65:GLU:HA	16:D:311:HOH:O	2.08	0.53
12:L:93:PHE:N	12:L:94:PRO:HD3	2.23	0.53
5:S:209:THR:OG1	5:S:212:ASN:HB3	2.09	0.53
6:T:137:ILE:HA	6:T:149:TYR:O	2.09	0.53
3:C:171:ASN:O	3:C:175:VAL:HG12	2.08	0.53
9:I:176:VAL:HG21	9:I:187:LYS:HE3	1.91	0.53
10:J:43:SER:OG	10:J:101:LEU:HB2	2.08	0.53
9:W:115:ASP:OD1	15:4:1:THR:HG23	2.08	0.53
3:C:176:ARG:O	3:C:180:GLU:HG3	2.09	0.53
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.22	0.53
5:E:74:LEU:HB2	5:E:136:ILE:HD12	1.90	0.53
7:G:154:ASP:HB2	7:G:155:PRO:CD	2.39	0.53
9:I:5:MET:CE	9:I:157:ILE:HA	2.39	0.53
14:N:147:SER:OG	14:N:150:GLU:HG3	2.09	0.53
7:U:71:ILE:HD12	7:U:71:ILE:N	2.24	0.53
9:W:176:VAL:HG21	9:W:187:LYS:CE	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.44	0.53
9:I:115:ASP:OD1	15:I:1:THR:HG23	2.09	0.53
7:U:172:GLN:NE2	7:U:176:THR:HG23	2.24	0.53
10:X:33:THR:HG21	10:X:180:LYS:HZ2	1.74	0.53
3:C:231:GLU:H	3:C:231:GLU:CD	2.13	0.52
5:E:137:ILE:HG13	5:E:218:VAL:HG12	1.91	0.52
10:J:33:THR:HG21	10:J:180:LYS:NZ	2.24	0.52
12:L:90:LYS:HE3	12:L:93:PHE:O	2.09	0.52
2:B:232:PHE:N	2:B:232:PHE:HD2	2.07	0.52
11:K:144:TYR:O	11:K:145:LYS:HD2	2.09	0.52
11:K:12:ILE:HB	11:K:180:VAL:HB	1.89	0.52
3:Q:242:GLN:O	3:Q:246:GLU:HG3	2.09	0.52
4:R:130:GLU:HG2	4:R:131:GLU:H	1.72	0.52
6:T:214:LEU:HD21	6:T:216:ILE:HD11	1.91	0.52
9:W:5:MET:HB3	9:W:153:LEU:HD11	1.91	0.52
1:A:119:LYS:HE2	1:A:123:GLU:OE1	2.10	0.52
3:C:242:GLN:O	3:C:246:GLU:HG3	2.09	0.52
8:H:167:LEU:HB3	12:Z:186:ILE:HD13	1.92	0.52
11:K:201:LYS:HE3	11:K:207:PHE:O	2.09	0.52
4:R:53:ARG:HG2	4:R:53:ARG:O	2.10	0.52
6:T:74:ILE:CD1	6:T:109:ILE:HG13	2.39	0.52
8:H:209:THR:CG2	12:Z:149:GLN:HG2	2.39	0.52
12:Z:185:HIS:CD2	12:Z:187:GLN:H	2.22	0.52
1:A:31:VAL:HG11	1:A:136:SER:HB2	1.91	0.52
2:B:91:ASN:O	2:B:95:ILE:HD13	2.09	0.52
5:E:95:ASN:HD21	12:L:60:ASN:ND2	2.04	0.52
6:F:172:ALA:O	6:F:176:LEU:HD23	2.09	0.52
7:G:73:ARG:HH11	7:G:73:ARG:HB2	1.75	0.52
3:Q:152:TYR:CE1	3:Q:162:SER:HB3	2.44	0.52
5:S:64:LYS:O	5:S:75:SER:HA	2.09	0.52
8:V:53:GLU:O	8:V:57:GLN:HG3	2.10	0.52
10:X:91:ARG:HG2	10:X:91:ARG:HH11	1.74	0.52
11:Y:144:TYR:O	11:Y:145:LYS:HD2	2.10	0.52
8:H:24:PRO:HG2	8:H:25:ILE:CD1	2.40	0.52
4:R:31:ILE:HD13	4:R:141:ALA:HB2	1.90	0.52
5:S:48:LEU:HG	5:S:137:ILE:HD13	1.92	0.52
2:B:232:PHE:N	2:B:232:PHE:CD2	2.77	0.52
9:I:111:ILE:HD12	9:I:127:ILE:HG12	1.91	0.52
9:I:176:VAL:HG21	9:I:187:LYS:CE	2.39	0.52
2:P:232:PHE:HD2	2:P:232:PHE:N	2.06	0.52
7:U:154:ASP:HB2	7:U:155:PRO:CD	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:25:ILE:HD12	8:V:25:ILE:N	2.23	0.52
14:N:105:LYS:HD3	14:N:105:LYS:C	2.29	0.52
14:N:40:LYS:C	14:N:41:ILE:HD12	2.30	0.52
8:V:172:ASN:ND2	16:V:331:HOH:O	2.43	0.52
11:Y:145:LYS:HB2	11:Y:148:LEU:CD1	2.39	0.52
3:C:31:VAL:HG11	3:C:136:SER:HB2	1.92	0.52
5:E:187:ASN:HD22	5:E:187:ASN:C	2.13	0.52
5:E:64:LYS:O	5:E:75:SER:HA	2.08	0.52
7:G:236:ASN:N	7:G:236:ASN:HD22	2.08	0.52
1:O:31:VAL:HG11	1:O:136:SER:HB2	1.92	0.52
3:Q:231:GLU:N	3:Q:231:GLU:OE1	2.38	0.52
7:U:97:ALA:HA	7:U:108:MET:CE	2.30	0.52
8:V:41:ILE:HD12	8:V:76:VAL:HG22	1.91	0.52
9:I:167:ARG:NH2	12:Z:137:MET:HE2	2.24	0.52
9:I:28:ASN:HB2	16:I:233:HOH:O	2.09	0.52
13:M:216:ILE:N	13:M:216:ILE:HD13	2.24	0.52
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.40	0.52
1:O:119:LYS:HE2	1:O:123:GLU:OE1	2.09	0.52
4:R:70:ILE:HG13	4:R:74:ILE:HG22	1.91	0.52
5:S:72:MET:CE	5:S:107:VAL:HA	2.39	0.52
7:U:8:TYR:C	7:U:10:ARG:H	2.13	0.52
9:W:5:MET:HE1	9:W:157:ILE:HA	1.92	0.52
9:W:158:SER:O	9:W:162:LEU:HB2	2.10	0.52
2:B:113:LEU:O	2:B:113:LEU:HD23	2.10	0.52
4:D:167:TYR:CE2	4:D:170:LYS:HD3	2.45	0.52
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.45	0.52
13:M:6:LYS:HG3	13:M:156:ILE:HD12	1.92	0.52
7:U:240:ARG:HA	7:U:240:ARG:NE	2.25	0.52
1:A:152:GLN:O	1:A:159:TYR:HA	2.10	0.51
1:A:190:ASP:O	1:A:194:ILE:HG12	2.10	0.51
4:D:24:VAL:O	4:D:28:LEU:HD13	2.11	0.51
1:O:200:LYS:HA	1:O:207:PHE:CE1	2.44	0.51
5:S:136:ILE:CD1	5:S:136:ILE:N	2.73	0.51
5:S:4:PHE:HZ	5:S:18:THR:HG23	1.75	0.51
7:U:73:ARG:HB2	7:U:73:ARG:HH11	1.74	0.51
9:W:176:VAL:HG21	9:W:187:LYS:HE3	1.92	0.51
10:X:51:THR:HG22	10:X:52:VAL:HG23	1.92	0.51
3:C:77:LEU:HD22	3:C:90:ILE:CD1	2.40	0.51
4:D:127:ALA:HB3	4:D:132:ARG:HD3	1.91	0.51
10:J:188:ARG:HH11	10:J:188:ARG:HG2	1.75	0.51
13:M:5:MET:CG	13:M:168:ILE:HD11	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:188:PRO:O	3:Q:190:ALA:N	2.43	0.51
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.75	0.51
5:S:217:ILE:HG12	5:S:218:VAL:N	2.25	0.51
3:C:138:LEU:HG	3:C:168:ILE:HD13	1.91	0.51
14:N:15:GLY:HA2	14:N:174:ARG:O	2.10	0.51
2:B:38:ILE:HD13	2:B:166:SER:HB3	1.92	0.51
4:D:129:GLY:HA3	16:E:315:HOH:O	2.10	0.51
4:D:75:GLY:HA3	4:D:228:PHE:CD2	2.45	0.51
5:E:36:VAL:HG13	5:E:199:ILE:HD11	1.91	0.51
9:I:5:MET:HB3	9:I:153:LEU:HD11	1.93	0.51
9:I:154:PHE:HB2	9:I:179:ILE:HD11	1.92	0.51
4:R:167:TYR:CE2	4:R:170:LYS:HD3	2.45	0.51
6:T:87:HIS:HD2	6:T:132:PHE:HE2	1.58	0.51
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.10	0.51
2:B:192:ILE:HG23	2:B:215:PHE:CE2	2.46	0.51
5:E:111:GLY:HA3	16:E:317:HOH:O	2.10	0.51
7:G:44:LYS:HZ2	7:G:191:ASN:ND2	2.09	0.51
6:F:244:GLN:O	6:F:247:ILE:HG22	2.11	0.51
7:G:83:ILE:N	7:G:84:PRO:HD2	2.25	0.51
2:P:63:THR:HG22	2:P:63:THR:O	2.11	0.51
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.31	0.51
1:A:208:ASN:HA	1:A:250:LEU:CD1	2.41	0.51
1:A:208:ASN:O	1:A:212:ILE:HG13	2.11	0.51
2:B:63:THR:HG22	2:B:63:THR:O	2.11	0.51
4:D:210:GLU:HA	4:D:210:GLU:OE2	2.11	0.51
4:D:70:ILE:HG13	4:D:74:ILE:HG22	1.93	0.51
5:E:48:LEU:HD13	5:E:75:SER:HB3	1.92	0.51
7:G:240:ARG:NE	7:G:240:ARG:HA	2.26	0.51
10:J:127:PRO:HB2	10:J:128:TYR:CD1	2.45	0.51
3:Q:155:GLU:HB2	3:Q:156:PRO:HD2	1.91	0.51
4:R:210:GLU:HA	4:R:210:GLU:OE2	2.11	0.51
10:X:101:LEU:CD2	10:X:116:GLN:HG3	2.40	0.51
3:C:239:GLN:O	3:C:243:GLU:HG2	2.11	0.51
8:H:2:THR:OG1	8:H:130:GLY:HA3	2.11	0.51
5:S:187:ASN:HD22	5:S:187:ASN:C	2.14	0.51
5:S:137:ILE:HG13	5:S:218:VAL:HG12	1.92	0.51
6:T:209:GLU:HG3	6:T:210:LYS:N	2.26	0.51
7:U:83:ILE:N	7:U:84:PRO:HD2	2.25	0.51
7:G:39:LEU:HD23	7:G:206:MET:HE3	1.93	0.51
2:P:192:ILE:HG23	2:P:215:PHE:CE2	2.46	0.51
5:S:74:LEU:CB	5:S:136:ILE:HD12	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.93	0.51
9:W:111:ILE:HD12	9:W:127:ILE:HG12	1.92	0.51
5:E:4:PHE:HZ	5:E:18:THR:HG23	1.75	0.51
7:G:203:ILE:O	7:G:207:ILE:HG13	2.11	0.51
7:G:8:TYR:C	7:G:10:ARG:H	2.13	0.51
3:Q:239:GLN:O	3:Q:243:GLU:HG2	2.10	0.51
6:T:244:GLN:O	6:T:247:ILE:HG22	2.10	0.51
6:T:247:ILE:HG12	6:T:247:ILE:O	2.10	0.51
5:E:136:ILE:HD13	5:E:136:ILE:N	2.26	0.50
10:J:160:LYS:O	10:J:164:GLN:HG3	2.12	0.50
13:M:218:GLY:HA3	13:M:222:GLN:HB3	1.93	0.50
10:X:51:THR:HG22	10:X:52:VAL:H	1.77	0.50
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.56	0.50
1:A:200:LYS:HA	1:A:207:PHE:CE1	2.47	0.50
10:J:128:TYR:CD2	10:J:142:LEU:HD13	2.47	0.50
12:L:6:ALA:HB2	12:L:112:VAL:HG23	1.93	0.50
12:Z:116:ASP:CB	12:Z:120:SER:H	2.23	0.50
3:C:231:GLU:OE1	3:C:231:GLU:N	2.38	0.50
5:E:230:GLU:H	5:E:230:GLU:CD	2.13	0.50
6:F:120:VAL:HG21	6:F:151:LEU:HD21	1.93	0.50
6:F:137:ILE:HA	6:F:149:TYR:O	2.11	0.50
8:H:159:ILE:O	8:H:163:ILE:HG12	2.11	0.50
11:K:86:LEU:HD13	11:K:86:LEU:C	2.32	0.50
14:N:114:PRO:HD2	14:N:118:SER:O	2.12	0.50
2:P:236:GLU:O	2:P:240:ILE:HG22	2.11	0.50
6:T:35:THR:CG2	6:T:36:THR:N	2.74	0.50
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.92	0.50
8:V:220:ILE:HD11	9:W:185:VAL:HG21	1.92	0.50
11:K:33:LYS:HE2	15:2:3:OJT:H37	1.93	0.50
2:B:70:LYS:HE2	2:B:231:ILE:HD11	1.94	0.50
7:G:21:LEU:HA	16:G:304:HOH:O	2.11	0.50
12:L:0:GLY:HA3	12:L:32:LYS:NZ	2.27	0.50
7:U:153:THR:HG22	7:U:159:TYR:HB2	1.94	0.50
1:A:51:GLU:OE1	1:A:203:VAL:HG22	2.11	0.50
3:C:100:HIS:CG	3:C:108:VAL:HG12	2.47	0.50
7:G:153:THR:HG22	7:G:159:TYR:HB2	1.94	0.50
7:G:78:VAL:HG12	7:G:138:THR:HB	1.94	0.50
4:R:24:VAL:O	4:R:28:LEU:HD13	2.12	0.50
5:S:62:GLN:NE2	5:S:80:ALA:HB2	2.27	0.50
9:W:18:ARG:HB2	9:W:173:TRP:HB2	1.94	0.50
5:E:71:HIS:HE1	5:E:105:LEU:O	1.95	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:LEU:C	5:E:76:LEU:HD12	2.31	0.50
9:W:154:PHE:HB2	9:W:179:ILE:HD11	1.94	0.50
6:F:214:LEU:HD21	6:F:216:ILE:HD11	1.93	0.50
7:G:39:LEU:HD12	7:G:39:LEU:C	2.31	0.50
6:F:158:TRP:CZ3	7:G:65:VAL:HA	2.47	0.50
13:M:-4:ILE:HG22	13:M:-3:VAL:N	2.26	0.50
7:U:78:VAL:HG12	7:U:138:THR:HB	1.92	0.50
2:B:220:LYS:O	2:B:221:GLY:C	2.50	0.50
7:G:195:TRP:O	7:G:199:VAL:HG23	2.12	0.50
8:H:196:ARG:NH2	9:I:141:GLU:O	2.45	0.50
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.93	0.50
9:I:33:ILE:HB	16:I:258:HOH:O	2.11	0.50
10:X:127:PRO:HB2	10:X:128:TYR:CD1	2.47	0.50
5:E:181:PHE:CA	5:E:184:ILE:HG12	2.40	0.50
7:G:225:THR:HB	16:G:323:HOH:O	2.11	0.50
3:Q:31:VAL:HG11	3:Q:136:SER:HB2	1.94	0.50
5:S:71:HIS:HE1	5:S:105:LEU:O	1.95	0.50
6:T:200:ILE:HG21	6:T:214:LEU:CD1	2.42	0.50
11:Y:4:LEU:CD1	11:Y:161:ILE:HG12	2.41	0.50
10:J:2:ILE:HG22	10:J:101:LEU:CD1	2.42	0.49
11:K:65:LEU:HB3	11:K:69:ARG:NH2	2.28	0.49
3:Q:106:ASP:OD2	3:Q:107:PRO:HD2	2.12	0.49
5:S:203:LEU:O	5:S:204:ARG:HB2	2.12	0.49
7:U:35:ASN:HD22	7:U:169:PRO:HG2	1.77	0.49
10:J:172:MET:HE1	10:X:171:PRO:CB	2.42	0.49
4:D:31:ILE:HD13	4:D:141:ALA:HB2	1.94	0.49
12:L:-2:ASN:HA	12:L:20:ILE:O	2.11	0.49
3:Q:212:LYS:HD2	3:Q:212:LYS:O	2.12	0.49
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.94	0.49
4:R:112:LEU:HD13	4:R:112:LEU:C	2.33	0.49
12:L:186:ILE:HD13	8:V:167:LEU:HB3	1.94	0.49
10:X:2:ILE:HG22	10:X:101:LEU:CD1	2.41	0.49
2:B:98:GLN:HE22	9:I:62:ASN:HD22	1.59	0.49
1:O:152:GLN:O	1:O:159:TYR:HA	2.11	0.49
2:P:125:THR:HG22	3:Q:131:ARG:NH2	2.12	0.49
3:Q:138:LEU:HG	3:Q:168:ILE:HD13	1.93	0.49
5:S:36:VAL:HG13	5:S:199:ILE:HD11	1.93	0.49
6:T:206:ASP:OD1	6:T:206:ASP:N	2.45	0.49
7:U:170:LYS:O	7:U:174:ILE:HG12	2.13	0.49
10:X:160:LYS:O	10:X:164:GLN:HG3	2.12	0.49
2:B:236:GLU:O	2:B:240:ILE:HG22	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:THR:HB	3:C:51:GLU:HG3	1.93	0.49
8:H:199:LYS:HE3	9:I:142:SER:O	2.12	0.49
11:K:106:ARG:HG2	11:K:106:ARG:HH11	1.77	0.49
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.76	0.49
13:M:152:ARG:CG	13:M:152:ARG:HH11	2.23	0.49
13:M:45:SER:OG	13:M:104:ALA:HB3	2.12	0.49
14:N:14:LEU:O	14:N:175:MET:HA	2.12	0.49
2:P:220:LYS:O	2:P:221:GLY:C	2.50	0.49
3:Q:100:HIS:CG	3:Q:108:VAL:HG12	2.46	0.49
4:R:75:GLY:HA3	4:R:228:PHE:CD2	2.47	0.49
5:S:177:THR:O	5:S:177:THR:HG22	2.12	0.49
9:W:87:GLU:HG2	9:W:88:ARG:HH12	1.77	0.49
11:Y:151:GLU:HB2	16:Y:336:HOH:O	2.13	0.49
5:E:203:LEU:O	5:E:204:ARG:HB2	2.12	0.49
7:G:36:ILE:HG22	7:G:37:ASN:N	2.27	0.49
7:U:36:ILE:HG22	7:U:37:ASN:N	2.27	0.49
9:W:46:LEU:HG	9:W:48:THR:HG22	1.95	0.49
10:X:117:ILE:HG12	10:X:123:LYS:HG3	1.95	0.49
5:E:210:VAL:CG1	5:E:211:ASP:N	2.75	0.49
6:F:40:ILE:HD12	6:F:196:ALA:HB2	1.95	0.49
7:G:78:VAL:CG1	7:G:138:THR:HB	2.43	0.49
12:L:97:VAL:HG23	12:L:99:THR:HG22	1.93	0.49
3:Q:180:GLU:OE2	4:R:57:PRO:HD2	2.11	0.49
6:T:189:ALA:HB3	6:T:223:GLU:HG3	1.94	0.49
3:C:188:PRO:O	3:C:190:ALA:N	2.45	0.49
5:E:62:GLN:NE2	5:E:80:ALA:HB2	2.27	0.49
10:J:84:GLN:HB3	16:J:208:HOH:O	2.13	0.49
1:O:190:ASP:O	1:O:194:ILE:HG12	2.11	0.49
2:P:66:GLU:HG3	2:P:67:LYS:HG3	1.94	0.49
7:U:44:LYS:HZ2	7:U:191:ASN:ND2	2.09	0.49
12:Z:142:ASN:O	12:Z:146:PHE:HA	2.12	0.49
5:E:234:LYS:H	5:E:234:LYS:HD2	1.78	0.49
6:F:200:ILE:HG21	6:F:214:LEU:HD13	1.93	0.49
7:G:170:LYS:O	7:G:174:ILE:HG12	2.13	0.49
10:J:51:THR:HG22	10:J:52:VAL:H	1.75	0.49
11:K:77:ALA:HA	11:K:113:TYR:CE2	2.48	0.49
12:L:116:ASP:CB	12:L:120:SER:H	2.26	0.49
12:L:185:HIS:CD2	12:L:187:GLN:H	2.23	0.49
1:O:208:ASN:HA	1:O:250:LEU:CD1	2.41	0.49
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.78	0.49
5:S:210:VAL:CG1	5:S:211:ASP:N	2.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:44:LYS:NZ	7:U:191:ASN:HD21	2.10	0.49
10:X:5:ILE:HD11	10:X:146:TYR:CD1	2.48	0.49
3:C:212:LYS:HD2	3:C:212:LYS:O	2.13	0.49
1:O:51:GLU:OE1	1:O:203:VAL:HG22	2.13	0.49
2:P:113:LEU:O	2:P:113:LEU:HD23	2.12	0.49
2:P:167:VAL:HA	16:P:315:HOH:O	2.12	0.49
10:X:188:ARG:HG2	10:X:188:ARG:HH11	1.78	0.49
11:Y:77:ALA:HA	11:Y:113:TYR:CE2	2.48	0.49
3:C:152:TYR:CE1	3:C:162:SER:HB3	2.48	0.48
4:D:123:PHE:CZ	4:D:137:PRO:HG3	2.48	0.48
6:F:87:HIS:HD2	6:F:132:PHE:HE2	1.60	0.48
7:G:44:LYS:HB2	7:G:192:GLU:O	2.13	0.48
2:P:223:ASN:O	2:P:224:ASP:HB2	2.13	0.48
6:T:40:ILE:HD12	6:T:196:ALA:HB2	1.95	0.48
2:B:223:ASN:O	2:B:224:ASP:HB2	2.13	0.48
3:C:184:ASP:OD1	3:C:186:LYS:HB2	2.12	0.48
6:F:189:ALA:HB3	6:F:223:GLU:HG3	1.94	0.48
3:Q:171:ASN:CB	3:Q:206:VAL:HG11	2.42	0.48
3:Q:163:TRP:CZ2	4:R:59:LEU:HD23	2.48	0.48
8:V:18:THR:HG21	8:V:30:ASN:ND2	2.28	0.48
6:F:35:THR:CG2	6:F:36:THR:N	2.74	0.48
7:G:35:ASN:HD22	7:G:169:PRO:HG2	1.77	0.48
8:H:148:LYS:O	8:H:152:ILE:HG13	2.13	0.48
9:I:32:LYS:O	9:I:42:GLY:HA2	2.13	0.48
2:P:52:ARG:NH2	2:P:64:SER:HB3	2.28	0.48
5:S:80:ALA:HB3	5:S:81:PRO:HD3	1.94	0.48
7:U:78:VAL:CG1	7:U:138:THR:HB	2.43	0.48
5:E:217:ILE:HG12	5:E:218:VAL:N	2.29	0.48
9:I:6:THR:HG23	9:I:111:ILE:HG12	1.95	0.48
11:K:4:LEU:CD1	11:K:161:ILE:HG12	2.42	0.48
13:M:39:ASN:N	13:M:39:ASN:ND2	2.61	0.48
3:Q:77:LEU:HD12	3:Q:139:ILE:HG12	1.94	0.48
11:Y:201:LYS:HE3	11:Y:207:PHE:O	2.13	0.48
6:F:127:ASN:HD22	6:F:127:ASN:C	2.17	0.48
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.13	0.48
10:J:23:ILE:HD11	10:X:133:TYR:HB3	1.95	0.48
10:J:34:ARG:HD3	10:J:34:ARG:HA	1.61	0.48
12:L:20:ILE:C	12:L:20:ILE:HD12	2.33	0.48
5:S:181:PHE:CA	5:S:184:ILE:HG12	2.39	0.48
9:W:180:ILE:HG23	9:W:185:VAL:HG22	1.95	0.48
10:X:128:TYR:CD2	10:X:142:LEU:HD13	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.78	0.48
5:E:89:TYR:CD1	5:E:117:LYS:HD2	2.48	0.48
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.95	0.48
9:I:46:LEU:HG	9:I:48:THR:HG22	1.94	0.48
2:P:70:LYS:HE2	2:P:231:ILE:HD11	1.95	0.48
4:R:123:PHE:CZ	4:R:137:PRO:HG3	2.48	0.48
5:S:230:GLU:CD	5:S:230:GLU:H	2.17	0.48
12:Z:-2:ASN:HA	12:Z:20:ILE:O	2.13	0.48
5:E:80:ALA:HB3	5:E:81:PRO:HD3	1.95	0.48
9:I:0:GLY:HA3	9:I:32:LYS:HE2	1.96	0.48
5:S:234:LYS:HG2	5:S:235:TYR:CD1	2.49	0.48
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.14	0.48
12:Z:18:ARG:NE	12:Z:190:ASP:OD2	2.46	0.48
6:F:209:GLU:HG3	6:F:210:LYS:N	2.28	0.48
10:J:101:LEU:CD2	10:J:116:GLN:HG3	2.43	0.48
4:R:127:ALA:HA	5:S:127:GLY:HA2	1.96	0.48
5:S:208:LEU:HA	5:S:212:ASN:HD22	1.78	0.48
9:W:0:GLY:HA3	9:W:32:LYS:HE2	1.96	0.48
9:W:71:ALA:HB1	16:W:209:HOH:O	2.14	0.48
9:W:85:LEU:HD11	9:W:97:PRO:HG2	1.95	0.48
10:J:133:TYR:HB3	10:X:23:ILE:HD11	1.96	0.48
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.96	0.48
9:I:87:GLU:HG2	9:I:88:ARG:HH12	1.78	0.48
13:M:165:GLU:O	13:M:169:VAL:HG23	2.14	0.48
2:B:70:LYS:HG3	2:B:229:GLN:OE1	2.14	0.48
5:E:66:ILE:HB	5:E:74:LEU:CD2	2.44	0.48
8:H:200:GLN:O	8:H:201:LYS:HB2	2.13	0.48
9:I:11:VAL:CG1	9:I:109:PRO:HB3	2.44	0.48
12:L:8:GLU:O	12:L:109:LYS:HA	2.13	0.48
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.95	0.48
3:Q:131:ARG:HG3	3:Q:131:ARG:HH11	1.79	0.48
8:V:196:ARG:NH2	9:W:141:GLU:O	2.47	0.48
11:K:208:ASN:ND2	10:X:148:PRO:CG	2.73	0.48
8:H:148:LYS:HD2	16:H:341:HOH:O	2.13	0.47
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.27	0.47
5:S:89:TYR:CD1	5:S:117:LYS:HD2	2.49	0.47
6:T:175:GLU:HB3	6:T:199:ILE:HD12	1.95	0.47
7:U:195:TRP:O	7:U:199:VAL:HG23	2.14	0.47
7:U:236:ASN:HD22	7:U:236:ASN:N	2.12	0.47
10:X:11:VAL:HG23	10:X:112:PRO:HB2	1.97	0.47
8:H:18:THR:HG21	8:H:30:ASN:ND2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:64:ARG:HD2	16:K:328:HOH:O	2.13	0.47
13:M:-3:VAL:HG12	13:M:48:ILE:HG13	1.96	0.47
6:T:197:ALA:O	6:T:201:TYR:HD1	1.98	0.47
2:B:44:ASP:OD2	2:B:188:VAL:HG23	2.13	0.47
2:B:66:GLU:HG3	2:B:67:LYS:HG3	1.97	0.47
3:C:170:ARG:O	3:C:171:ASN:HB2	2.14	0.47
3:C:38:VAL:HG22	3:C:39:GLY:N	2.29	0.47
5:E:234:LYS:HG2	5:E:235:TYR:CD1	2.49	0.47
9:I:18:ARG:HB2	9:I:173:TRP:HB2	1.95	0.47
9:I:5:MET:HE3	9:I:157:ILE:CG1	2.33	0.47
11:K:104:TYR:CE2	11:K:110:PRO:HG3	2.49	0.47
2:P:44:ASP:OD2	2:P:188:VAL:HG23	2.15	0.47
2:P:39:GLY:O	2:P:164:ALA:HA	2.14	0.47
5:S:209:THR:N	5:S:212:ASN:HD22	2.04	0.47
5:S:5:ARG:HG3	5:S:22:PHE:CE1	2.49	0.47
9:W:134:ASP:HB2	16:W:251:HOH:O	2.14	0.47
9:W:12:ALA:HB3	9:W:157:ILE:HD12	1.96	0.47
10:X:90:ILE:HG23	10:X:91:ARG:HG3	1.96	0.47
7:G:160:VAL:HG22	7:G:161:GLY:N	2.29	0.47
7:G:44:LYS:NZ	7:G:191:ASN:HD21	2.13	0.47
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.97	0.47
5:S:48:LEU:HG	5:S:137:ILE:CD1	2.43	0.47
5:S:48:LEU:HD13	5:S:75:SER:HB3	1.94	0.47
1:O:97:HIS:HD2	8:V:61:SER:OG	1.97	0.47
9:W:6:THR:HG23	9:W:111:ILE:HG12	1.96	0.47
3:C:171:ASN:CB	3:C:206:VAL:HG11	2.44	0.47
5:E:177:THR:HG22	5:E:177:THR:O	2.14	0.47
7:G:71:ILE:CD1	7:G:77:MET:HB3	2.40	0.47
9:I:28:ASN:HB3	9:I:173:TRP:CE3	2.49	0.47
9:I:85:LEU:HD11	9:I:97:PRO:HG2	1.95	0.47
14:N:116:GLY:N	16:N:206:HOH:O	2.47	0.47
6:T:43:ASN:HD22	6:T:43:ASN:N	2.12	0.47
11:Y:104:TYR:CE2	11:Y:110:PRO:HG3	2.50	0.47
12:Z:8:GLU:O	12:Z:109:LYS:HA	2.14	0.47
1:A:45:GLY:HA2	1:A:148:PHE:CE2	2.49	0.47
2:B:52:ARG:NH2	2:B:64:SER:HB3	2.28	0.47
6:F:179:LEU:HD11	6:F:195:GLN:HG3	1.97	0.47
12:L:84:GLN:HG3	12:L:119:GLY:O	2.14	0.47
1:O:45:GLY:HA2	1:O:148:PHE:CE2	2.49	0.47
3:Q:172:SER:HA	3:Q:175:VAL:CG1	2.45	0.47
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:66:ILE:HB	5:S:74:LEU:CD2	2.44	0.47
5:S:76:LEU:HD12	5:S:76:LEU:C	2.34	0.47
7:U:184:LYS:HB2	7:U:184:LYS:HE3	1.59	0.47
7:U:39:LEU:HD12	7:U:39:LEU:C	2.35	0.47
10:J:172:MET:HE3	10:X:172:MET:CE	2.44	0.47
12:Z:6:ALA:HB2	12:Z:112:VAL:HG23	1.96	0.47
12:Z:97:VAL:HG23	12:Z:99:THR:HG22	1.96	0.47
1:A:188:LEU:HD21	1:A:216:ILE:HD12	1.97	0.47
1:A:86:ARG:HD3	16:A:316:HOH:O	2.15	0.47
3:C:80:SER:HA	16:C:322:HOH:O	2.13	0.47
5:S:234:LYS:HD2	5:S:234:LYS:H	1.79	0.47
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.96	0.47
7:U:129:TYR:CE2	7:U:130:MET:HG2	2.49	0.47
9:W:11:VAL:CG1	9:W:109:PRO:HB3	2.45	0.47
10:X:116:GLN:NE2	10:X:130:ALA:H	2.11	0.47
11:Y:106:ARG:HH11	11:Y:106:ARG:HG2	1.78	0.47
9:I:194:GLN:HG3	11:Y:197:PHE:CE1	2.49	0.47
11:Y:4:LEU:O	11:Y:4:LEU:HD22	2.15	0.47
4:D:234:GLU:OE2	4:D:234:GLU:N	2.43	0.47
4:D:75:GLY:HA3	4:D:228:PHE:CE2	2.50	0.47
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.97	0.47
6:F:206:ASP:OD1	6:F:206:ASP:N	2.47	0.47
11:K:104:TYR:CE1	11:K:182:GLU:HB2	2.50	0.47
12:L:104:LEU:HB2	16:L:336:HOH:O	2.15	0.47
2:P:70:LYS:HG3	2:P:229:GLN:OE1	2.14	0.47
7:U:44:LYS:NZ	7:U:191:ASN:ND2	2.62	0.47
5:E:48:LEU:HG	5:E:137:ILE:CD1	2.45	0.47
4:R:40:ILE:HG13	4:R:200:VAL:HG23	1.96	0.47
1:O:57:PRO:HG3	7:U:179:GLU:CD	2.36	0.47
3:C:57:LYS:O	3:C:58:LEU:CB	2.62	0.47
5:E:230:GLU:CD	5:E:230:GLU:N	2.68	0.47
6:F:185:GLU:CD	6:F:185:GLU:H	2.17	0.47
6:F:43:ASN:N	6:F:43:ASN:HD22	2.11	0.47
9:I:53:LEU:CD1	9:I:95:VAL:HG21	2.45	0.47
10:J:117:ILE:HG12	10:J:123:LYS:HG3	1.97	0.47
12:L:142:ASN:O	12:L:146:PHE:HA	2.15	0.47
12:L:18:ARG:NE	12:L:190:ASP:OD2	2.47	0.47
13:M:222:GLN:HB2	16:M:355:HOH:O	2.14	0.47
13:M:-5:PRO:C	13:M:-4:ILE:HD12	2.35	0.47
14:N:20:THR:HG23	14:N:31:THR:HG1	1.80	0.47
9:W:32:LYS:O	9:W:42:GLY:HA2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:104:TYR:CE1	11:Y:182:GLU:HB2	2.49	0.47
2:B:82:LEU:HD23	2:B:134:GLY:HA3	1.97	0.47
9:I:27:SER:CB	10:J:124:VAL:HG21	2.45	0.47
11:Y:114:TYR:O	11:Y:121:ARG:HA	2.15	0.47
3:C:36:CYS:H	3:C:51:GLU:HG2	1.79	0.46
5:E:31:ILE:HD11	5:E:151:PRO:CD	2.45	0.46
8:H:53:GLU:O	8:H:57:GLN:HG3	2.13	0.46
11:K:4:LEU:HD22	11:K:4:LEU:O	2.15	0.46
14:N:40:LYS:O	14:N:41:ILE:HD12	2.15	0.46
2:P:237:ILE:O	2:P:241:LEU:HB2	2.15	0.46
5:S:95:ASN:HD21	12:Z:60:ASN:ND2	2.01	0.46
6:T:109:ILE:HB	6:T:110:PRO:HD3	1.96	0.46
6:T:127:ASN:HD22	6:T:127:ASN:C	2.18	0.46
6:T:18:ASP:N	6:T:18:ASP:OD2	2.37	0.46
6:T:79:SER:HA	16:T:333:HOH:O	2.15	0.46
7:U:71:ILE:CD1	7:U:77:MET:HB3	2.38	0.46
11:Y:33:LYS:HE2	15:5:3:OJT:H37	1.97	0.46
11:K:114:TYR:O	11:K:121:ARG:HA	2.16	0.46
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.13	0.46
13:M:6:LYS:HB3	13:M:11:VAL:HG12	1.97	0.46
6:T:28:VAL:O	6:T:32:GLU:HG3	2.15	0.46
6:T:82:ILE:N	6:T:82:ILE:HD13	2.29	0.46
2:B:39:GLY:O	2:B:164:ALA:HA	2.16	0.46
3:C:77:LEU:HD12	3:C:139:ILE:HG12	1.96	0.46
3:C:163:TRP:CZ2	4:D:59:LEU:HD23	2.51	0.46
3:C:161:SER:HB2	4:D:59:LEU:HD21	1.96	0.46
6:F:175:GLU:HB3	6:F:199:ILE:HD12	1.98	0.46
7:G:153:THR:HG22	7:G:159:TYR:CB	2.45	0.46
9:I:7:GLY:HA3	9:I:153:LEU:HD22	1.96	0.46
5:S:12:THR:CG2	5:S:122:THR:HA	2.45	0.46
5:S:38:VAL:HG12	5:S:39:GLY:N	2.29	0.46
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.98	0.46
7:U:87:ARG:HD2	16:U:309:HOH:O	2.14	0.46
9:W:53:LEU:CD1	9:W:95:VAL:HG21	2.44	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.97	0.46
6:F:21:ASN:ND2	6:F:24:VAL:HG23	2.31	0.46
6:F:28:VAL:O	6:F:32:GLU:HG3	2.15	0.46
10:J:196:GLN:OXT	10:J:196:GLN:HG2	2.15	0.46
13:M:120:TYR:HE1	13:M:135:THR:HG22	1.80	0.46
13:M:18:LEU:HD21	13:M:25:LEU:HD22	1.98	0.46
6:T:185:GLU:CD	6:T:185:GLU:H	2.17	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:203:ILE:O	7:U:207:ILE:HG13	2.14	0.46
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.45	0.46
9:W:28:ASN:HB3	9:W:173:TRP:CE3	2.50	0.46
10:X:17:LYS:HD3	10:X:178:ILE:HG12	1.98	0.46
3:C:220:LYS:HB2	3:C:224:ASP:HB3	1.98	0.46
5:E:199:ILE:CG2	5:E:200:SER:N	2.78	0.46
14:N:107:LYS:CG	14:N:108:GLY:H	2.26	0.46
4:R:234:GLU:N	4:R:234:GLU:OE2	2.45	0.46
8:V:159:ILE:O	8:V:163:ILE:HG12	2.15	0.46
11:K:197:PHE:CE1	9:W:194:GLN:HG3	2.50	0.46
9:W:7:GLY:HA3	9:W:153:LEU:HD22	1.97	0.46
12:Z:198:THR:C	12:Z:200:ASP:H	2.19	0.46
12:Z:0:GLY:HA3	12:Z:32:LYS:NZ	2.30	0.46
4:D:112:LEU:C	4:D:112:LEU:HD13	2.36	0.46
6:F:200:ILE:HG21	6:F:214:LEU:CD1	2.45	0.46
12:L:198:THR:C	12:L:200:ASP:H	2.19	0.46
1:O:31:VAL:HG13	1:O:79:SER:O	2.15	0.46
4:R:193:LEU:O	4:R:197:GLU:HG3	2.16	0.46
4:R:75:GLY:HA3	4:R:228:PHE:CE2	2.51	0.46
5:S:199:ILE:CG2	5:S:200:SER:N	2.79	0.46
1:O:131:ARG:NH2	7:U:125:THR:HG22	2.06	0.46
2:B:237:ILE:O	2:B:241:LEU:HB2	2.15	0.46
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.79	0.46
6:F:197:ALA:O	6:F:201:TYR:HD1	1.98	0.46
10:J:16:SER:HB2	10:J:174:PHE:HB2	1.98	0.46
2:P:53:LYS:HG2	2:P:54:VAL:HG23	1.98	0.46
6:T:36:THR:CG2	6:T:51:GLU:OE2	2.64	0.46
8:V:53:GLU:O	8:V:56:THR:HG22	2.15	0.46
10:X:31:ASP:OD2	10:X:33:THR:HG22	2.15	0.46
12:Z:-7:ASN:C	12:Z:-7:ASN:HD22	2.18	0.46
1:A:204:GLU:OE2	1:A:204:GLU:N	2.49	0.46
10:J:148:PRO:HG3	11:Y:208:ASN:ND2	2.10	0.46
1:O:204:GLU:OE2	1:O:204:GLU:N	2.47	0.46
3:Q:184:ASP:OD1	3:Q:186:LYS:HB2	2.15	0.46
3:Q:219:VAL:HG23	3:Q:225:ILE:HG12	1.97	0.46
12:L:137:MET:HE2	9:W:167:ARG:NH2	2.31	0.46
12:Z:116:ASP:HB3	12:Z:120:SER:H	1.80	0.46
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.13	0.46
1:A:118:ALA:HB1	1:A:157:GLY:O	2.16	0.46
2:P:8:TYR:CD2	7:U:12:ILE:HD13	2.51	0.46
7:U:44:LYS:HB2	7:U:192:GLU:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:101:LEU:HD21	10:X:116:GLN:HG3	1.98	0.46
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.28	0.46
5:E:140:ASP:HB2	16:M:353:HOH:O	2.15	0.46
2:P:31:ILE:HD12	2:P:80:ALA:O	2.16	0.46
3:Q:162:SER:HB2	16:Q:324:HOH:O	2.15	0.46
8:V:200:GLN:O	8:V:201:LYS:HB2	2.14	0.46
12:L:149:GLN:HG2	8:V:209:THR:CG2	2.45	0.46
5:E:38:VAL:HG12	5:E:39:GLY:N	2.31	0.45
8:H:72:ARG:NH1	8:H:72:ARG:HG3	2.28	0.45
10:J:11:VAL:HG23	10:J:112:PRO:HB2	1.99	0.45
10:J:31:ASP:OD2	10:J:33:THR:HG22	2.16	0.45
4:R:46:VAL:HG11	4:R:145:ALA:HB1	1.99	0.45
10:X:196:GLN:OXT	10:X:196:GLN:HG2	2.16	0.45
1:A:31:VAL:HG13	1:A:79:SER:O	2.17	0.45
7:G:153:THR:HA	7:G:158:TYR:O	2.16	0.45
10:J:116:GLN:NE2	10:J:130:ALA:H	2.14	0.45
1:O:33:GLN:CA	1:O:33:GLN:NE2	2.77	0.45
2:P:122:GLN:CG	3:Q:84:ALA:HB1	2.46	0.45
5:S:148:GLU:O	5:S:155:VAL:HA	2.16	0.45
7:U:153:THR:HA	7:U:158:TYR:O	2.16	0.45
7:U:71:ILE:HD11	7:U:77:MET:CB	2.40	0.45
7:U:88:ASN:C	7:U:88:ASN:HD22	2.19	0.45
8:V:24:PRO:HG2	8:V:25:ILE:CD1	2.42	0.45
9:I:115:ASP:HB3	15:1:1:THR:HG23	1.97	0.45
2:B:203:THR:CG2	2:B:205:SER:HB2	2.47	0.45
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.98	0.45
12:L:137:MET:HE3	9:W:167:ARG:NH2	2.31	0.45
14:N:20:THR:CG2	14:N:31:THR:OG1	2.60	0.45
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.51	0.45
8:V:212:VAL:HG12	8:V:213:LEU:N	2.32	0.45
10:X:5:ILE:HD11	10:X:146:TYR:HD1	1.80	0.45
8:H:194:ASN:HB3	12:Z:210:LYS:HE3	1.97	0.45
1:A:125:THR:HG22	2:B:131:ARG:NH2	2.13	0.45
7:G:224:ALA:HB2	7:G:229:PHE:HD2	1.81	0.45
11:K:7:ARG:HG2	11:K:110:PRO:HB2	1.99	0.45
4:R:236:THR:O	4:R:240:ILE:HG13	2.17	0.45
7:U:224:ALA:HB2	7:U:229:PHE:HD2	1.81	0.45
4:D:79:SER:HB3	4:D:172:ILE:HD12	1.98	0.45
6:F:247:ILE:O	6:F:247:ILE:HG12	2.16	0.45
6:F:36:THR:HG23	6:F:51:GLU:OE2	2.17	0.45
7:G:108:MET:HE3	7:G:113:LEU:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:16:ASP:HA	13:M:186:PHE:CB	2.46	0.45
2:P:82:LEU:HD23	2:P:134:GLY:HA3	1.98	0.45
8:V:199:LYS:HE3	9:W:142:SER:O	2.17	0.45
11:Y:7:ARG:HG2	11:Y:110:PRO:HB2	1.98	0.45
3:C:172:SER:HA	3:C:175:VAL:CG1	2.46	0.45
3:C:219:VAL:HG23	3:C:225:ILE:HG12	1.98	0.45
6:F:127:ASN:HD22	6:F:128:SER:N	2.15	0.45
11:K:67:GLU:HB2	16:K:328:HOH:O	2.15	0.45
13:M:87:LEU:O	13:M:91:MET:HG2	2.17	0.45
7:U:48:VAL:HG11	7:U:199:VAL:HA	1.99	0.45
2:B:31:ILE:HD12	2:B:80:ALA:O	2.16	0.45
10:J:171:PRO:CB	10:X:172:MET:HE1	2.46	0.45
3:Q:228:LEU:HD12	3:Q:228:LEU:N	2.31	0.45
3:Q:230:SER:HB2	3:Q:231:GLU:OE1	2.17	0.45
5:S:84:ARG:HG3	5:S:84:ARG:NH1	2.31	0.45
9:W:27:SER:CB	10:X:124:VAL:HG21	2.47	0.45
2:B:152:THR:O	2:B:159:TYR:HA	2.17	0.45
3:C:101:ARG:HH11	3:C:107:PRO:HB3	1.77	0.45
3:C:98:GLN:NE2	16:C:301:HOH:O	2.47	0.45
6:F:36:THR:CG2	6:F:51:GLU:OE2	2.64	0.45
9:I:64:TYR:CZ	9:I:68:GLU:HG3	2.52	0.45
10:J:104:GLY:HA2	10:J:182:VAL:HG11	1.98	0.45
13:M:192:ASP:HB3	13:M:195:THR:OG1	2.17	0.45
1:O:118:ALA:HB1	1:O:157:GLY:O	2.16	0.45
1:O:32:LYS:CE	1:O:32:LYS:HA	2.46	0.45
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.51	0.45
3:C:178:PHE:O	3:C:182:ASN:HB2	2.17	0.45
5:E:29:GLU:HA	5:E:32:LYS:HE3	1.99	0.45
8:H:41:ILE:CD1	8:H:76:VAL:HG22	2.46	0.45
10:J:5:ILE:HD11	10:J:146:TYR:HD1	1.82	0.45
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.47	0.45
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.77	0.45
6:T:41:LYS:HD2	16:T:320:HOH:O	2.16	0.45
8:V:148:LYS:O	8:V:152:ILE:HG13	2.17	0.45
16:L:306:HOH:O	9:W:192:MET:HB2	2.16	0.45
1:A:131:ARG:HG2	7:G:126:GLN:HG3	1.98	0.45
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.52	0.45
12:L:39:ASN:HD21	12:L:201:GLY:HA2	1.82	0.45
13:M:8:ASP:OD1	13:M:9:ASN:N	2.50	0.45
14:N:159:LEU:O	14:N:163:ILE:HG13	2.16	0.45
1:O:249:ARG:NH1	1:O:249:ARG:HG3	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:72:ASP:HA	10:X:67:ILE:CD1	2.45	0.45
3:Q:161:SER:HB2	4:R:59:LEU:HD21	1.99	0.45
6:T:206:ASP:O	6:T:207:ASN:HB2	2.17	0.45
7:U:88:ASN:C	7:U:88:ASN:ND2	2.70	0.45
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.47	0.44
9:I:5:MET:HE3	9:I:157:ILE:HA	1.98	0.44
11:K:86:LEU:O	11:K:89:GLN:HB2	2.17	0.44
1:O:86:ARG:HH21	7:U:119:ASN:ND2	2.14	0.44
7:U:25:GLU:O	7:U:28:PHE:HB2	2.17	0.44
5:E:148:GLU:O	5:E:155:VAL:HA	2.17	0.44
5:E:84:ARG:HG3	5:E:84:ARG:NH1	2.32	0.44
7:G:142:VAL:HG21	7:G:225:THR:HA	1.99	0.44
7:G:44:LYS:NZ	7:G:191:ASN:ND2	2.65	0.44
2:P:49:ALA:HB2	2:P:215:PHE:CE1	2.51	0.44
8:V:220:ILE:HG21	9:W:38:HIS:HB3	1.98	0.44
4:D:193:LEU:O	4:D:197:GLU:HG3	2.17	0.44
7:G:201:PHE:CD1	7:G:201:PHE:C	2.90	0.44
14:N:116:GLY:CA	16:N:206:HOH:O	2.65	0.44
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.53	0.44
5:S:31:ILE:HD11	5:S:151:PRO:CD	2.47	0.44
5:S:29:GLU:HA	5:S:32:LYS:HE3	1.99	0.44
6:T:179:LEU:HD11	6:T:195:GLN:HG3	1.99	0.44
10:X:104:GLY:HA2	10:X:182:VAL:HG11	1.99	0.44
2:B:89:LEU:HB3	2:B:117:LEU:HD21	1.99	0.44
5:E:208:LEU:HA	5:E:212:ASN:HD22	1.79	0.44
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.53	0.44
12:L:116:ASP:HB3	12:L:120:SER:H	1.82	0.44
2:P:203:THR:CG2	2:P:205:SER:HB2	2.48	0.44
3:Q:57:LYS:O	3:Q:58:LEU:CB	2.62	0.44
7:U:144:GLU:HA	7:U:226:LYS:NZ	2.33	0.44
8:H:194:ASN:HB3	12:Z:210:LYS:CE	2.47	0.44
12:Z:39:ASN:HD21	12:Z:201:GLY:HA2	1.81	0.44
3:C:230:SER:HB2	3:C:231:GLU:OE1	2.18	0.44
7:G:221:VAL:HB	7:G:232:LEU:HD12	1.99	0.44
14:N:20:THR:HA	15:3:2:LYH:O	2.18	0.44
6:T:36:THR:HG23	6:T:51:GLU:OE2	2.17	0.44
9:W:115:ASP:HB3	15:4:1:THR:HG23	2.00	0.44
1:A:175:LYS:O	1:A:179:GLU:HG3	2.18	0.44
7:G:88:ASN:ND2	7:G:88:ASN:C	2.70	0.44
9:I:115:ASP:HB3	15:1:1:THR:CG2	2.47	0.44
11:K:208:ASN:ND2	10:X:148:PRO:HD3	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:175:LYS:O	1:O:179:GLU:HG3	2.18	0.44
6:T:127:ASN:HD22	6:T:128:SER:N	2.16	0.44
5:S:112:HIS:HB3	6:T:86:ARG:NH2	2.32	0.44
7:U:142:VAL:HG21	7:U:225:THR:HA	1.99	0.44
7:U:174:ILE:HD11	7:U:210:LEU:HD21	2.00	0.44
4:D:177:GLU:OE1	4:D:177:GLU:N	2.49	0.44
5:E:170:ALA:HB2	5:E:198:ALA:O	2.18	0.44
5:E:93:GLN:HG3	5:E:113:LEU:HD13	1.98	0.44
7:G:110:CYS:HB2	7:G:141:SER:OG	2.18	0.44
7:G:129:TYR:CE2	7:G:130:MET:HG2	2.53	0.44
7:G:83:ILE:HG22	7:G:84:PRO:HD3	1.98	0.44
7:G:88:ASN:HD22	7:G:88:ASN:C	2.21	0.44
10:J:145:HIS:HB2	10:J:158:LEU:CD1	2.48	0.44
13:M:48:ILE:O	13:M:52:GLN:HG3	2.17	0.44
13:M:69:ASN:ND2	13:M:72:ALA:HA	2.33	0.44
3:Q:170:ARG:O	3:Q:171:ASN:HB2	2.17	0.44
3:Q:86:SER:O	3:Q:90:ILE:HG12	2.17	0.44
4:R:249:ALA:O	4:R:250:GLU:CB	2.65	0.44
8:V:175:VAL:HG12	8:V:176:CYS:N	2.32	0.44
11:Y:38:ASN:ND2	16:Y:349:HOH:O	2.48	0.44
5:E:102:ASN:HB2	13:M:85:GLU:HG2	1.99	0.44
6:F:74:ILE:HD11	6:F:109:ILE:HG13	1.99	0.44
7:G:174:ILE:HD11	7:G:210:LEU:HD21	2.00	0.44
8:H:68:LEU:HD12	8:H:68:LEU:HA	1.89	0.44
11:K:155:TYR:OH	11:K:204:GLU:OE1	2.34	0.44
1:O:161:PRO:O	2:P:59:LEU:HD12	2.18	0.44
4:R:39:GLY:O	4:R:169:ALA:HA	2.17	0.44
6:T:175:GLU:HB3	6:T:199:ILE:CD1	2.47	0.44
7:U:226:LYS:O	7:U:227:ASP:HB2	2.16	0.44
11:Y:50:ALA:CB	12:Z:118:VAL:HG23	2.48	0.44
12:Z:197:VAL:HG22	12:Z:202:VAL:HG22	1.99	0.44
1:A:188:LEU:O	1:A:192:ILE:HG13	2.17	0.44
6:F:109:ILE:CD1	6:F:109:ILE:H	2.25	0.44
6:F:201:TYR:HE2	6:F:244:GLN:HE21	1.66	0.44
7:G:48:VAL:HG11	7:G:199:VAL:HA	2.00	0.44
7:G:70:CYS:HB3	16:G:342:HOH:O	2.18	0.44
10:J:145:HIS:HB2	10:J:158:LEU:HD11	1.99	0.44
11:K:106:ARG:HG2	11:K:106:ARG:NH1	2.33	0.44
1:O:125:THR:CG2	2:P:131:ARG:NH2	2.78	0.44
4:R:79:SER:HB3	4:R:172:ILE:HD12	1.99	0.44
7:U:201:PHE:CD1	7:U:201:PHE:C	2.90	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:5:ILE:HG13	10:X:6:ARG:N	2.32	0.44
2:B:49:ALA:HB2	2:B:215:PHE:CE1	2.53	0.43
3:C:131:ARG:HH11	3:C:131:ARG:HG3	1.82	0.43
4:D:46:VAL:HG11	4:D:145:ALA:HB1	1.99	0.43
5:E:12:THR:CG2	5:E:122:THR:HA	2.45	0.43
6:F:157:TYR:C	6:F:157:TYR:CD1	2.91	0.43
7:G:25:GLU:O	7:G:28:PHE:HB2	2.18	0.43
10:J:188:ARG:NH1	10:J:188:ARG:HG2	2.33	0.43
10:J:90:ILE:HG23	10:J:91:ARG:HG3	2.00	0.43
12:L:164:TYR:CD1	12:L:165:LEU:N	2.86	0.43
1:O:17:PRO:HA	2:P:26:TYR:CE1	2.53	0.43
2:P:108:ILE:HG12	2:P:113:LEU:HB2	2.00	0.43
4:R:65:GLU:HA	16:R:313:HOH:O	2.17	0.43
5:S:230:GLU:CD	5:S:230:GLU:N	2.70	0.43
6:T:137:ILE:CD1	6:T:165:THR:HG22	2.48	0.43
7:U:153:THR:HG22	7:U:159:TYR:CB	2.48	0.43
8:V:215:GLU:O	8:V:216:SER:HB3	2.18	0.43
13:M:10:GLY:HA3	13:M:191:ILE:O	2.18	0.43
3:Q:178:PHE:O	3:Q:182:ASN:HB2	2.18	0.43
4:R:12:VAL:CG2	4:R:124:GLY:HA2	2.47	0.43
6:T:195:GLN:NE2	6:T:198:LYS:HE3	2.33	0.43
8:V:116:HIS:HB2	16:V:345:HOH:O	2.16	0.43
10:X:170:MET:HA	10:X:171:PRO:HD3	1.76	0.43
3:C:155:GLU:HB2	3:C:156:PRO:CD	2.46	0.43
7:G:226:LYS:O	7:G:227:ASP:HB2	2.18	0.43
10:J:5:ILE:HD11	10:J:146:TYR:CD1	2.52	0.43
1:O:14:THR:HB	2:P:23:GLN:NE2	2.32	0.43
1:O:188:LEU:HD21	1:O:216:ILE:HD12	2.00	0.43
7:U:160:VAL:HG22	7:U:161:GLY:N	2.33	0.43
7:U:36:ILE:HG23	7:U:52:GLN:HB2	2.00	0.43
8:V:72:ARG:NH1	8:V:72:ARG:HG3	2.32	0.43
1:A:97:HIS:HD2	8:H:61:SER:OG	2.02	0.43
2:B:15:PHE:H	3:C:23:GLN:NE2	1.93	0.43
5:E:112:HIS:HB3	6:F:86:ARG:NH2	2.34	0.43
7:G:144:GLU:HA	7:G:226:LYS:NZ	2.32	0.43
9:I:12:ALA:HB3	9:I:157:ILE:HD12	1.99	0.43
10:J:101:LEU:HD21	10:J:116:GLN:HG3	2.01	0.43
12:L:28:ARG:NH1	12:L:211:ARG:HB3	2.32	0.43
3:Q:220:LYS:HB2	3:Q:224:ASP:HB3	2.00	0.43
5:S:170:ALA:HB2	5:S:198:ALA:O	2.18	0.43
12:L:210:LYS:HE3	8:V:194:ASN:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:98:GLN:HB3	9:W:59:TYR:CD2	2.54	0.43
7:G:108:MET:HE3	7:G:113:LEU:HB2	2.01	0.43
13:M:12:ILE:HB	13:M:168:ILE:HD13	2.01	0.43
13:M:-5:PRO:O	13:M:-4:ILE:HD12	2.18	0.43
8:V:46:ALA:HA	15:4:3:OJT:H33	2.01	0.43
12:Z:34:PHE:O	12:Z:41:VAL:HA	2.18	0.43
3:C:200:VAL:HG22	3:C:216:ILE:HD11	2.00	0.43
5:E:137:ILE:HG12	5:E:137:ILE:O	2.18	0.43
8:H:128:GLY:O	8:H:131:SER:HB2	2.18	0.43
8:H:212:VAL:HG12	8:H:213:LEU:N	2.33	0.43
10:J:17:LYS:HD3	10:J:178:ILE:HG12	2.01	0.43
14:N:146:MET:CE	14:N:150:GLU:HB3	2.45	0.43
14:N:163:ILE:CG2	14:N:170:GLY:HA2	2.47	0.43
7:U:44:LYS:HZ3	7:U:191:ASN:HD21	1.64	0.43
10:X:145:HIS:HB2	10:X:158:LEU:HD11	2.00	0.43
1:A:67:VAL:HG11	1:A:215:ALA:HB3	2.01	0.43
4:D:40:ILE:HG13	4:D:200:VAL:HG23	2.00	0.43
7:G:132:PRO:HB3	16:G:303:HOH:O	2.17	0.43
8:H:220:ILE:HD11	9:I:185:VAL:CG2	2.48	0.43
10:J:5:ILE:HG13	10:J:6:ARG:N	2.33	0.43
14:N:55:ILE:O	14:N:59:VAL:HG23	2.18	0.43
1:O:199:LEU:HD23	1:O:212:ILE:HD13	2.01	0.43
3:Q:155:GLU:HB2	3:Q:156:PRO:CD	2.48	0.43
8:V:41:ILE:CD1	8:V:76:VAL:HG22	2.48	0.43
11:Y:105:THR:HG1	11:Y:108:GLU:HG3	1.80	0.43
2:B:148:TYR:OH	2:B:220:LYS:HB2	2.18	0.43
3:C:228:LEU:HD12	3:C:228:LEU:N	2.33	0.43
4:D:39:GLY:O	4:D:169:ALA:HA	2.19	0.43
4:D:201:LEU:HA	4:D:201:LEU:HD12	1.88	0.43
4:D:236:THR:O	4:D:240:ILE:HG13	2.18	0.43
5:E:47:VAL:HG12	5:E:48:LEU:N	2.33	0.43
7:G:111:ASP:HB3	7:G:151:TYR:CZ	2.54	0.43
7:G:184:LYS:HB2	7:G:184:LYS:HE3	1.60	0.43
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.00	0.43
9:I:108:LYS:HA	9:I:109:PRO:HD3	1.92	0.43
10:J:156:LEU:HD13	10:J:196:GLN:HE22	1.83	0.43
12:L:98:HIS:HD2	16:L:305:HOH:O	2.01	0.43
1:O:4:MET:CG	1:O:5:THR:H	2.32	0.43
2:P:165:ILE:HG12	2:P:166:SER:H	1.83	0.43
5:S:137:ILE:HG13	5:S:218:VAL:CG1	2.49	0.43
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:115:ASP:HB3	15:4:1:THR:CG2	2.49	0.43
10:X:90:ILE:HD12	10:X:90:ILE:HA	1.79	0.43
1:A:67:VAL:HG11	1:A:215:ALA:CB	2.49	0.43
3:C:153:GLN:HG2	3:C:154:THR:N	2.34	0.43
4:D:12:VAL:CG2	4:D:124:GLY:HA2	2.48	0.43
9:I:97:PRO:HD2	9:I:114:PHE:HB2	2.00	0.43
10:J:144:HIS:HD2	10:J:145:HIS:CE1	2.37	0.43
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.21	0.43
13:M:204:GLN:HE21	13:M:204:GLN:HB3	1.62	0.43
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.43
1:O:97:HIS:CD2	8:V:61:SER:OG	2.72	0.43
2:P:152:THR:O	2:P:159:TYR:HA	2.18	0.43
2:P:5:SER:O	2:P:7:ARG:N	2.52	0.43
4:R:17:PRO:HA	5:S:26:TYR:CD1	2.53	0.43
6:T:21:ASN:ND2	6:T:24:VAL:HG23	2.34	0.43
7:U:108:MET:HE3	7:U:113:LEU:HD13	2.00	0.43
7:U:174:ILE:HD12	7:U:206:MET:CE	2.49	0.43
2:P:98:GLN:HE22	9:W:62:ASN:HD22	1.67	0.43
10:X:16:SER:HB2	10:X:174:PHE:HB2	2.01	0.43
11:Y:116:ASP:C	11:Y:116:ASP:OD1	2.57	0.43
1:A:92:SER:O	1:A:95:VAL:HG12	2.19	0.43
9:I:5:MET:HE1	9:I:157:ILE:HA	2.00	0.43
11:K:38:ASN:O	11:K:40:PHE:N	2.52	0.43
13:M:41:VAL:CG2	13:M:191:ILE:HD11	2.46	0.43
6:T:190:ARG:CG	6:T:190:ARG:HH11	2.30	0.43
11:Y:76:VAL:N	11:Y:108:GLU:OE2	2.51	0.43
13:M:156:ILE:HB	13:M:157:PRO:CD	2.49	0.42
1:O:188:LEU:O	1:O:192:ILE:HG13	2.19	0.42
5:S:93:GLN:HG3	5:S:113:LEU:HD13	2.00	0.42
6:T:109:ILE:CD1	6:T:142:ASP:HB3	2.49	0.42
10:X:145:HIS:HB2	10:X:158:LEU:CD1	2.49	0.42
12:Z:164:TYR:CD1	12:Z:165:LEU:N	2.87	0.42
1:A:207:PHE:CD1	1:A:212:ILE:HD11	2.55	0.42
3:Q:41:LYS:HD3	3:Q:163:TRP:O	2.20	0.42
5:S:88:ASN:O	5:S:92:GLN:HG3	2.18	0.42
6:T:137:ILE:HD11	6:T:165:THR:HG22	2.01	0.42
10:J:148:PRO:HD3	11:Y:208:ASN:ND2	2.35	0.42
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.53	0.42
3:C:52:ARG:HB2	3:C:213:ASN:HA	2.01	0.42
5:E:73:GLY:HA3	5:E:224:PHE:CZ	2.54	0.42
6:F:18:ASP:OD2	6:F:18:ASP:N	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:97:ALA:HA	7:G:108:MET:CE	2.31	0.42
9:I:86:TYR:CE1	9:I:89:ARG:HD3	2.54	0.42
14:N:107:LYS:CG	14:N:108:GLY:N	2.77	0.42
1:O:77:VAL:HG12	1:O:138:LEU:HB2	2.00	0.42
10:X:173:ASP:OD1	10:X:175:LYS:HD3	2.19	0.42
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.72	0.42
2:B:142:TYR:CD1	2:B:142:TYR:C	2.93	0.42
3:C:86:SER:O	3:C:90:ILE:HG12	2.19	0.42
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.87	0.42
8:H:201:LYS:HE3	12:Z:169:GLU:OE2	2.19	0.42
1:O:142:HIS:HA	1:O:147:GLY:O	2.20	0.42
2:P:127:HIS:HB3	3:Q:130:VAL:HG12	2.00	0.42
12:Z:82:ASN:C	12:Z:82:ASN:HD22	2.23	0.42
12:Z:116:ASP:CG	15:5:1:THR:HG22	2.40	0.42
3:C:161:SER:CB	4:D:59:LEU:HD21	2.50	0.42
5:E:5:ARG:HG3	5:E:22:PHE:CE1	2.54	0.42
6:F:206:ASP:O	6:F:207:ASN:HB2	2.19	0.42
8:H:175:VAL:HG12	8:H:176:CYS:N	2.33	0.42
3:Q:52:ARG:HB2	3:Q:213:ASN:HA	2.00	0.42
13:M:147:ARG:HD2	8:V:165:ASN:HD21	1.84	0.42
12:Z:28:ARG:NH1	12:Z:211:ARG:HB3	2.35	0.42
1:A:230:ILE:HD12	1:A:230:ILE:N	2.34	0.42
5:E:121:ASN:HD22	5:E:121:ASN:N	2.18	0.42
8:H:148:LYS:CD	16:H:341:HOH:O	2.67	0.42
8:H:215:GLU:O	8:H:216:SER:HB3	2.20	0.42
9:I:1:ILE:HD11	9:I:165:ALA:HB2	2.02	0.42
10:J:170:MET:HA	10:J:171:PRO:HD3	1.77	0.42
11:K:8:PHE:HA	11:K:146:TRP:CE3	2.54	0.42
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	2.02	0.42
13:M:79:GLU:O	13:M:83:ILE:HG13	2.20	0.42
1:O:92:SER:O	1:O:95:VAL:HG12	2.19	0.42
6:T:109:ILE:HD12	6:T:142:ASP:HB3	2.01	0.42
6:T:50:VAL:HG22	6:T:51:GLU:N	2.34	0.42
12:L:210:LYS:CE	8:V:194:ASN:HB3	2.50	0.42
9:W:11:VAL:HG13	9:W:109:PRO:HB3	2.01	0.42
9:W:139:MET:CE	9:W:143:LEU:HD11	2.50	0.42
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.87	0.42
1:A:142:HIS:HA	1:A:147:GLY:O	2.20	0.42
1:A:4:MET:CG	1:A:5:THR:H	2.33	0.42
1:A:69:LEU:C	1:A:69:LEU:HD23	2.40	0.42
2:B:5:SER:O	2:B:7:ARG:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.54	0.42
4:D:186:GLU:HG3	4:D:199:LEU:HD11	2.01	0.42
4:D:51:GLU:HG2	4:D:53:ARG:HB2	2.01	0.42
6:F:175:GLU:HB3	6:F:199:ILE:CD1	2.49	0.42
8:H:213:LEU:HG	9:I:191:LYS:HB2	2.02	0.42
14:N:84:GLU:O	14:N:88:GLU:HB2	2.19	0.42
1:O:62:GLU:CD	1:O:62:GLU:H	2.22	0.42
6:T:49:ALA:HA	6:T:215:GLU:O	2.19	0.42
7:U:29:LYS:HD2	7:U:29:LYS:HA	1.84	0.42
1:A:62:GLU:CD	1:A:62:GLU:H	2.23	0.42
1:A:77:VAL:HG12	1:A:138:LEU:HB2	2.00	0.42
3:C:74:HIS:CE1	3:C:75:VAL:HG23	2.54	0.42
5:E:74:LEU:CB	5:E:136:ILE:HD12	2.49	0.42
5:E:196:VAL:O	5:E:199:ILE:HG22	2.20	0.42
8:H:18:THR:HB	8:H:30:ASN:HD22	1.84	0.42
8:H:53:GLU:O	8:H:56:THR:HG22	2.20	0.42
10:J:23:ILE:O	10:X:137:TYR:OH	2.30	0.42
1:O:214:LEU:C	1:O:214:LEU:HD23	2.40	0.42
2:P:148:TYR:OH	2:P:220:LYS:HB2	2.19	0.42
2:P:89:LEU:HB3	2:P:117:LEU:HD21	2.01	0.42
5:S:47:VAL:HG12	5:S:48:LEU:N	2.34	0.42
6:T:127:ASN:C	6:T:127:ASN:ND2	2.73	0.42
7:U:221:VAL:HB	7:U:232:LEU:HD12	2.01	0.42
10:X:91:ARG:HG2	10:X:91:ARG:NH1	2.34	0.42
1:A:214:LEU:C	1:A:214:LEU:HD23	2.40	0.42
2:B:51:GLU:OE2	2:B:203:THR:HG23	2.20	0.42
2:B:21:LEU:O	2:B:25:GLU:HG2	2.19	0.42
4:D:107:ILE:HG22	16:D:322:HOH:O	2.19	0.42
6:F:50:VAL:HG22	6:F:51:GLU:N	2.35	0.42
7:G:106:TYR:OH	8:H:66:HIS:HE1	2.03	0.42
5:S:181:PHE:CD1	5:S:182:ILE:N	2.88	0.42
5:S:5:ARG:HG3	5:S:22:PHE:CD1	2.54	0.42
1:A:181:ARG:CB	1:A:181:ARG:HH11	2.29	0.42
5:E:181:PHE:CD1	5:E:182:ILE:N	2.88	0.42
10:J:117:ILE:HA	10:J:122:THR:O	2.20	0.42
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.19	0.42
3:Q:216:ILE:HG13	3:Q:233:ILE:HD13	2.01	0.42
6:T:74:ILE:HD11	6:T:109:ILE:HG13	2.01	0.42
7:U:120:LEU:HA	7:U:120:LEU:HD12	1.86	0.42
10:X:144:HIS:HD2	10:X:145:HIS:CE1	2.37	0.42
1:A:32:LYS:CE	1:A:32:LYS:HA	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.19	0.41
2:B:108:ILE:HG12	2:B:113:LEU:HB2	2.02	0.41
4:D:249:ALA:O	4:D:250:GLU:CB	2.67	0.41
5:E:173:TYR:CD2	5:E:198:ALA:HA	2.55	0.41
6:F:127:ASN:ND2	6:F:127:ASN:C	2.72	0.41
10:J:23:ILE:HG13	10:J:23:ILE:O	2.20	0.41
1:O:253:LEU:C	1:O:253:LEU:HD13	2.40	0.41
2:P:203:THR:HG21	2:P:205:SER:HB2	2.02	0.41
5:S:158:LEU:HD13	5:S:161:THR:HB	2.02	0.41
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.01	0.41
10:X:75:PRO:HD2	16:X:212:HOH:O	2.20	0.41
11:Y:106:ARG:NH1	11:Y:106:ARG:HG2	2.34	0.41
2:B:127:HIS:HA	16:C:326:HOH:O	2.19	0.41
5:E:98:SER:O	5:E:102:ASN:HA	2.20	0.41
7:G:171:GLN:HB3	7:G:171:GLN:HE21	1.64	0.41
12:L:34:PHE:O	12:L:41:VAL:HA	2.21	0.41
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.54	0.41
3:Q:210:GLY:HA3	3:Q:213:ASN:HB2	2.02	0.41
5:S:52:LYS:HB3	5:S:61:TYR:HB3	2.02	0.41
9:W:97:PRO:HD2	9:W:114:PHE:HB2	2.01	0.41
11:Y:38:ASN:O	11:Y:40:PHE:N	2.53	0.41
12:Z:57:ARG:NH2	16:Z:349:HOH:O	2.53	0.41
10:J:62:ILE:HD13	10:J:78:VAL:HG22	2.02	0.41
13:M:160:THR:HG23	16:M:362:HOH:O	2.19	0.41
4:R:244:LYS:HE2	4:R:244:LYS:HB3	1.89	0.41
6:T:82:ILE:HB	6:T:83:PRO:HD3	2.02	0.41
2:P:102:LYS:HZ1	10:X:84:GLN:NE2	2.17	0.41
11:Y:174:SER:HA	11:Y:193:VAL:HG23	2.03	0.41
12:Z:84:GLN:HG3	12:Z:119:GLY:O	2.20	0.41
2:B:102:LYS:NZ	10:J:84:GLN:NE2	2.68	0.41
2:P:44:ASP:N	2:P:44:ASP:OD2	2.51	0.41
2:P:51:GLU:OE2	2:P:203:THR:HG23	2.20	0.41
2:P:7:ARG:HG2	7:U:8:TYR:CE2	2.56	0.41
5:S:173:TYR:CD2	5:S:198:ALA:HA	2.56	0.41
5:S:41:ARG:NH1	5:S:42:SER:O	2.53	0.41
9:W:99:VAL:O	9:W:111:ILE:HA	2.21	0.41
1:A:249:ARG:NH1	1:A:249:ARG:HG3	2.32	0.41
1:A:57:PRO:HG3	7:G:179:GLU:CD	2.40	0.41
2:B:203:THR:HG21	2:B:205:SER:HB2	2.02	0.41
5:E:15:PHE:H	6:F:23:GLN:HE22	1.66	0.41
5:E:88:ASN:O	5:E:92:GLN:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:205:GLU:HG3	6:F:208:LYS:HZ1	1.86	0.41
7:G:137:LEU:O	7:G:152:LYS:HA	2.19	0.41
7:G:236:ASN:N	7:G:236:ASN:ND2	2.67	0.41
11:K:145:LYS:CB	11:K:148:LEU:HD13	2.50	0.41
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.89	0.41
13:M:156:ILE:HB	13:M:157:PRO:HD3	2.02	0.41
13:M:2:VAL:O	13:M:134:ALA:HA	2.20	0.41
1:O:27:ALA:O	1:O:31:VAL:HG23	2.21	0.41
1:O:69:LEU:HD23	1:O:69:LEU:C	2.41	0.41
4:R:163:THR:HG22	5:S:81:PRO:HD3	2.03	0.41
9:W:64:TYR:CZ	9:W:68:GLU:HG3	2.55	0.41
3:C:206:VAL:O	3:C:206:VAL:HG12	2.20	0.41
9:I:11:VAL:HG13	9:I:109:PRO:HB3	2.02	0.41
10:J:2:ILE:O	10:J:130:ALA:HA	2.20	0.41
11:K:116:ASP:OD1	11:K:116:ASP:C	2.59	0.41
3:Q:131:ARG:HG3	3:Q:131:ARG:NH1	2.36	0.41
3:Q:206:VAL:O	3:Q:206:VAL:HG12	2.20	0.41
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.51	0.41
6:T:175:GLU:OE1	6:T:202:LEU:HD23	2.20	0.41
7:U:110:CYS:HB2	7:U:141:SER:OG	2.20	0.41
7:U:111:ASP:HB3	7:U:151:TYR:CZ	2.55	0.41
7:U:137:LEU:O	7:U:152:LYS:HA	2.20	0.41
9:W:151:GLU:CD	9:W:151:GLU:H	2.23	0.41
5:E:41:ARG:NH1	5:E:42:SER:O	2.53	0.41
6:F:137:ILE:CD1	6:F:165:THR:HG22	2.50	0.41
9:I:11:VAL:HG23	9:I:180:ILE:HB	2.02	0.41
10:J:18:ALA:HB2	10:J:175:LYS:HG2	2.02	0.41
5:S:98:SER:O	5:S:102:ASN:HA	2.21	0.41
6:T:107:ILE:HG23	6:T:107:ILE:O	2.20	0.41
7:U:108:MET:HE3	7:U:113:LEU:HB2	2.03	0.41
7:U:152:LYS:O	7:U:159:TYR:HA	2.21	0.41
12:Z:167:VAL:O	12:Z:171:ILE:HG13	2.20	0.41
2:B:122:GLN:CG	3:C:84:ALA:HB1	2.51	0.41
6:F:54:ILE:HG13	6:F:212:PHE:HA	2.03	0.41
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.01	0.41
12:L:80:ALA:HA	12:L:115:PHE:HZ	1.86	0.41
12:L:169:GLU:OE2	8:V:201:LYS:HE3	2.21	0.41
12:L:82:ASN:C	12:L:82:ASN:HD22	2.22	0.41
3:Q:153:GLN:HG2	3:Q:154:THR:N	2.35	0.41
4:R:157:HIS:O	4:R:164:PHE:HA	2.20	0.41
5:S:119:GLN:C	5:S:119:GLN:NE2	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:196:VAL:HG12	5:S:196:VAL:O	2.21	0.41
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.35	0.41
10:X:33:THR:CG2	10:X:180:LYS:NZ	2.83	0.41
4:D:190:SER:HA	16:D:335:HOH:O	2.21	0.41
4:D:89:ILE:HB	16:D:323:HOH:O	2.20	0.41
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.93	0.41
6:F:109:ILE:CD1	6:F:142:ASP:HB3	2.50	0.41
6:F:70:VAL:HB	6:F:74:ILE:HB	2.03	0.41
9:I:154:PHE:HB2	9:I:179:ILE:CD1	2.51	0.41
9:I:53:LEU:HD12	9:I:95:VAL:HG21	2.02	0.41
14:N:106:ASN:O	14:N:107:LYS:HB3	2.21	0.41
2:P:188:VAL:O	2:P:192:ILE:HG13	2.21	0.41
4:R:86:ARG:HA	4:R:86:ARG:HD3	1.82	0.41
5:S:74:LEU:HA	5:S:135:LEU:O	2.21	0.41
5:S:15:PHE:H	6:T:23:GLN:HE22	1.66	0.41
6:T:54:ILE:HG13	6:T:212:PHE:HA	2.02	0.41
8:V:128:GLY:O	8:V:131:SER:HB2	2.21	0.41
10:X:188:ARG:HG2	10:X:188:ARG:NH1	2.35	0.41
2:P:102:LYS:HZ2	10:X:84:GLN:NE2	2.18	0.41
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.19	0.41
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.21	0.41
12:Z:136:ILE:HD12	12:Z:177:SER:HB3	2.03	0.41
1:A:253:LEU:HD13	1:A:253:LEU:C	2.42	0.41
2:B:46:ILE:HD11	2:B:148:TYR:HB3	2.03	0.41
5:E:196:VAL:O	5:E:196:VAL:HG12	2.21	0.41
6:F:193:VAL:HG13	6:F:216:ILE:HG21	2.02	0.41
9:I:114:PHE:HA	9:I:119:CYS:O	2.21	0.41
10:J:172:MET:HE2	10:X:172:MET:CE	2.43	0.41
10:J:91:ARG:NH1	10:J:91:ARG:HG2	2.34	0.41
13:M:79:GLU:HB2	13:M:82:TYR:CD2	2.56	0.41
2:P:142:TYR:CD1	2:P:142:TYR:C	2.94	0.41
2:P:55:THR:HG22	2:P:59:LEU:HD23	2.03	0.41
3:Q:161:SER:CB	4:R:59:LEU:HD21	2.51	0.41
7:U:8:TYR:C	7:U:10:ARG:N	2.74	0.41
9:W:11:VAL:HG23	9:W:180:ILE:HB	2.03	0.41
9:W:99:VAL:HG23	9:W:114:PHE:HE2	1.86	0.41
3:C:245:GLN:C	3:C:247:GLN:N	2.74	0.41
5:E:74:LEU:HA	5:E:135:LEU:O	2.21	0.41
5:E:54:ASN:ND2	5:E:56:ASP:O	2.53	0.41
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.56	0.41
9:I:161:LEU:HD21	9:I:175:ALA:HB1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:GLN:NE2	9:I:62:ASN:HD22	2.18	0.41
13:M:0:THR:O	13:M:32:ARG:NH1	2.54	0.41
13:M:152:ARG:NH1	13:M:152:ARG:HG3	2.24	0.41
1:O:131:ARG:HG2	7:U:126:GLN:HG3	2.02	0.41
1:O:29:THR:O	1:O:33:GLN:HG2	2.21	0.41
1:O:67:VAL:HG11	1:O:215:ALA:CB	2.51	0.41
3:Q:200:VAL:HG22	3:Q:216:ILE:HD11	2.02	0.41
4:R:212:LEU:C	4:R:212:LEU:CD2	2.89	0.41
7:U:83:ILE:HG22	7:U:84:PRO:HD3	2.02	0.41
8:V:68:LEU:HA	8:V:68:LEU:HD12	1.91	0.41
9:W:87:GLU:HG2	9:W:88:ARG:NH1	2.36	0.41
11:Y:40:PHE:CD1	11:Y:73:ARG:NH1	2.89	0.41
1:A:55:SER:O	1:A:56:SER:HB2	2.21	0.40
4:D:157:HIS:O	4:D:164:PHE:HA	2.20	0.40
5:E:217:ILE:HG12	5:E:218:VAL:H	1.85	0.40
5:E:66:ILE:HB	5:E:74:LEU:HD21	2.03	0.40
8:H:126:SER:O	8:H:127:LEU:HD23	2.21	0.40
9:I:139:MET:CE	9:I:143:LEU:HD11	2.51	0.40
10:J:33:THR:HG21	10:J:180:LYS:HZ2	1.84	0.40
11:K:50:ALA:CB	12:L:118:VAL:HG23	2.51	0.40
14:N:13:ILE:HD12	14:N:151:THR:HG22	2.04	0.40
6:F:101:LYS:NZ	14:N:84:GLU:OE1	2.44	0.40
1:O:135:VAL:O	1:O:155:PRO:HG3	2.21	0.40
4:R:249:ALA:O	4:R:250:GLU:HB2	2.20	0.40
4:R:51:GLU:HG2	4:R:53:ARG:HB2	2.03	0.40
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.56	0.40
7:U:37:ASN:HB2	7:U:52:GLN:OE1	2.21	0.40
9:W:1:ILE:HD11	9:W:165:ALA:HB2	2.03	0.40
10:X:126:LEU:HB3	10:X:127:PRO:CD	2.52	0.40
10:X:68:ARG:HD2	16:X:219:HOH:O	2.21	0.40
11:Y:145:LYS:CB	11:Y:148:LEU:HD13	2.51	0.40
12:Z:80:ALA:HA	12:Z:115:PHE:HZ	1.86	0.40
1:A:86:ARG:HH21	7:G:119:ASN:ND2	2.17	0.40
3:C:166:GLN:HG3	3:C:167:THR:N	2.36	0.40
3:C:7:GLY:N	16:C:332:HOH:O	2.54	0.40
4:D:86:ARG:HD3	4:D:86:ARG:HA	1.82	0.40
10:J:6:ARG:HG2	10:J:6:ARG:HH11	1.87	0.40
12:L:0:GLY:HA3	12:L:32:LYS:HZ2	1.87	0.40
12:L:167:VAL:O	12:L:171:ILE:HG13	2.21	0.40
12:L:21:THR:O	12:L:22:ASP:HB2	2.20	0.40
13:M:152:ARG:NH1	13:M:152:ARG:CG	2.83	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:153:GLU:O	13:M:156:ILE:HG12	2.22	0.40
1:O:67:VAL:HG11	1:O:215:ALA:HB3	2.02	0.40
3:Q:46:VAL:HG11	3:Q:140:ALA:HB1	2.02	0.40
3:Q:80:SER:HB2	3:Q:168:ILE:HG13	2.03	0.40
4:R:201:LEU:HD22	4:R:219:LEU:HD11	2.02	0.40
16:V:339:HOH:O	9:W:155:GLU:HG3	2.21	0.40
10:X:117:ILE:HA	10:X:122:THR:O	2.20	0.40
6:F:49:ALA:HA	6:F:215:GLU:O	2.20	0.40
8:H:3:ILE:O	8:H:126:SER:HA	2.21	0.40
10:J:33:THR:CG2	10:J:180:LYS:NZ	2.85	0.40
11:K:46:ALA:HB3	11:K:98:GLY:O	2.21	0.40
14:N:144:GLU:O	14:N:145:ASN:HB2	2.21	0.40
4:R:177:GLU:N	4:R:177:GLU:OE1	2.50	0.40
1:A:38:LEU:HD12	1:A:38:LEU:C	2.42	0.40
3:C:210:GLY:HA3	3:C:213:ASN:HB2	2.02	0.40
11:K:97:MET:HG2	11:K:117:SER:HB3	2.03	0.40
12:L:151:GLU:O	12:L:152:PRO:C	2.60	0.40
14:N:2:SER:O	14:N:16:ALA:HA	2.20	0.40
14:N:41:ILE:CD1	14:N:41:ILE:N	2.84	0.40
1:O:230:ILE:N	1:O:230:ILE:HD12	2.36	0.40
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.36	0.40
5:S:73:GLY:HA3	5:S:224:PHE:CZ	2.57	0.40
7:U:241:LEU:HA	7:U:241:LEU:HD12	1.90	0.40
8:V:18:THR:HB	8:V:30:ASN:HD22	1.87	0.40
9:W:91:GLY:N	9:W:92:PRO:CD	2.83	0.40
10:X:24:SER:OG	11:Y:133:GLN:NE2	2.54	0.40
2:B:55:THR:HG22	2:B:59:LEU:HD23	2.04	0.40
3:C:41:LYS:HD3	3:C:163:TRP:O	2.21	0.40
6:F:43:ASN:N	6:F:43:ASN:ND2	2.70	0.40
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.15	0.40
7:G:73:ARG:NH2	14:N:39:ASP:OD2	2.55	0.40
3:Q:153:GLN:O	3:Q:160:TYR:HA	2.22	0.40
4:R:121:LEU:HD13	5:S:128:ARG:HH21	1.86	0.40
5:S:219:GLY:O	5:S:220:LYS:C	2.59	0.40
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.03	0.40
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.03	0.40
11:Y:155:TYR:OH	11:Y:204:GLU:OE1	2.36	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	248/250 (99%)	235 (95%)	10 (4%)	3 (1%)	15	44
1	O	248/250 (99%)	236 (95%)	9 (4%)	3 (1%)	15	44
2	B	242/244 (99%)	214 (88%)	22 (9%)	6 (2%)	6	22
2	P	242/244 (99%)	215 (89%)	21 (9%)	6 (2%)	6	22
3	C	239/241 (99%)	220 (92%)	14 (6%)	5 (2%)	8	27
3	Q	239/241 (99%)	221 (92%)	13 (5%)	5 (2%)	8	27
4	D	240/242 (99%)	219 (91%)	16 (7%)	5 (2%)	8	27
4	R	240/242 (99%)	221 (92%)	14 (6%)	5 (2%)	8	27
5	E	231/233 (99%)	207 (90%)	20 (9%)	4 (2%)	11	34
5	S	231/233 (99%)	207 (90%)	20 (9%)	4 (2%)	11	34
6	F	242/244 (99%)	226 (93%)	13 (5%)	3 (1%)	15	44
6	T	242/244 (99%)	226 (93%)	13 (5%)	3 (1%)	15	44
7	G	241/243 (99%)	228 (95%)	12 (5%)	1 (0%)	38	72
7	U	241/243 (99%)	228 (95%)	12 (5%)	1 (0%)	38	72
8	H	220/222 (99%)	206 (94%)	10 (4%)	4 (2%)	10	32
8	V	220/222 (99%)	207 (94%)	9 (4%)	4 (2%)	10	32
9	I	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
9	W	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
10	J	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	12	37
10	X	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	12	37
11	K	210/212 (99%)	199 (95%)	10 (5%)	1 (0%)	32	67
11	Y	210/212 (99%)	199 (95%)	10 (5%)	1 (0%)	32	67
12	L	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	32	67
12	Z	220/222 (99%)	208 (94%)	10 (4%)	2 (1%)	20	52
13	M	231/233 (99%)	215 (93%)	14 (6%)	2 (1%)	20	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/233 (99%)	215 (93%)	14 (6%)	2 (1%)	20	52
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
15	1	1/4 (25%)	0	1 (100%)	0	100	100
15	2	1/4 (25%)	1 (100%)	0	0	100	100
15	3	1/4 (25%)	1 (100%)	0	0	100	100
15	4	1/4 (25%)	0	1 (100%)	0	100	100
15	5	1/4 (25%)	1 (100%)	0	0	100	100
15	6	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6318/6392 (99%)	5894 (93%)	347 (6%)	77 (1%)	15	44

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	169	LYS
2	B	186	MET
2	B	224	ASP
3	C	58	LEU
4	D	130	GLU
4	D	189	SER
6	F	207	ASN
12	L	71	ASP
13	M	1	SER
1	O	5	THR
1	O	169	LYS
2	P	186	MET
2	P	224	ASP
3	Q	58	LEU
4	R	130	GLU
6	T	207	ASN
2	B	6	ARG
2	B	54	VAL
2	B	221	GLY
3	C	189	PRO
3	C	209	THR
4	D	126	GLY
5	E	204	ARG
5	E	220	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	91	GLN
10	J	195	ALA
2	P	6	ARG
2	P	54	VAL
2	P	221	GLY
3	Q	209	THR
4	R	126	GLY
4	R	189	SER
5	S	5	ARG
5	S	204	ARG
5	S	220	LYS
8	V	9	ASN
8	V	91	GLN
10	X	195	ALA
12	Z	71	ASP
13	a	1	SER
3	C	208	GLN
4	D	129	GLY
5	E	5	ARG
6	F	208	LYS
8	H	9	ASN
8	H	95	GLY
10	J	48	ALA
11	K	39	PRO
13	M	102	TRP
3	Q	189	PRO
4	R	129	GLY
6	T	208	LYS
10	X	48	ALA
11	Y	39	PRO
2	B	32	SER
4	D	128	SER
6	F	143	LYS
7	G	247	GLN
2	P	32	SER
3	Q	208	GLN
4	R	128	SER
5	S	161	THR
6	T	143	LYS
7	U	247	GLN
13	a	102	TRP
3	C	190	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	161	THR
3	Q	190	ALA
8	V	95	GLY
12	Z	163	LYS
1	A	56	SER
1	O	56	SER
8	H	105	PRO
8	V	105	PRO
10	J	7	VAL
10	X	7	VAL

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	209/209 (100%)	204 (98%)	5 (2%)	54	85
1	O	209/209 (100%)	204 (98%)	5 (2%)	54	85
2	B	203/203 (100%)	186 (92%)	17 (8%)	13	35
2	P	203/203 (100%)	188 (93%)	15 (7%)	16	42
3	C	213/213 (100%)	201 (94%)	12 (6%)	25	57
3	Q	213/213 (100%)	201 (94%)	12 (6%)	25	57
4	D	198/198 (100%)	188 (95%)	10 (5%)	28	61
4	R	198/198 (100%)	188 (95%)	10 (5%)	28	61
5	E	192/192 (100%)	173 (90%)	19 (10%)	9	26
5	S	192/192 (100%)	173 (90%)	19 (10%)	9	26
6	F	201/201 (100%)	185 (92%)	16 (8%)	14	38
6	T	201/201 (100%)	185 (92%)	16 (8%)	14	38
7	G	207/207 (100%)	195 (94%)	12 (6%)	23	55
7	U	207/207 (100%)	195 (94%)	12 (6%)	23	55
8	H	181/181 (100%)	175 (97%)	6 (3%)	43	77
8	V	181/181 (100%)	175 (97%)	6 (3%)	43	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	172/172 (100%)	167 (97%)	5 (3%)	48	81
9	W	172/172 (100%)	168 (98%)	4 (2%)	56	86
10	J	175/175 (100%)	165 (94%)	10 (6%)	24	56
10	X	175/175 (100%)	165 (94%)	10 (6%)	24	56
11	K	169/169 (100%)	157 (93%)	12 (7%)	17	44
11	Y	169/169 (100%)	158 (94%)	11 (6%)	20	49
12	L	185/185 (100%)	170 (92%)	15 (8%)	14	37
12	Z	185/185 (100%)	171 (92%)	14 (8%)	15	40
13	M	199/199 (100%)	188 (94%)	11 (6%)	25	57
13	a	199/199 (100%)	187 (94%)	12 (6%)	22	54
14	N	162/162 (100%)	154 (95%)	8 (5%)	29	62
14	b	162/162 (100%)	153 (94%)	9 (6%)	25	57
15	1	1/1 (100%)	0	1 (100%)	0	0
15	2	1/1 (100%)	1 (100%)	0	100	100
15	3	1/1 (100%)	0	1 (100%)	0	0
15	4	1/1 (100%)	0	1 (100%)	0	0
15	5	1/1 (100%)	1 (100%)	0	100	100
15	6	1/1 (100%)	0	1 (100%)	0	0
All	All	5338/5338 (100%)	5021 (94%)	317 (6%)	23	54

All (317) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	136	SER
1	A	160	PHE
1	A	181	ARG
2	B	6	ARG
2	B	46	ILE
2	B	58	LEU
2	B	72	ASN
2	B	73	ASP
2	B	92	THR
2	B	108	ILE
2	B	117	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	122	GLN
2	B	152	THR
2	B	158	ASN
2	B	165	ILE
2	B	187	LYS
2	B	194	LEU
2	B	215	PHE
2	B	223	ASN
2	B	232	PHE
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	67	LYS
3	C	122	GLN
3	C	136	SER
3	C	153	GLN
3	C	166	GLN
3	C	168	ILE
3	C	177	GLU
3	C	212	LYS
3	C	231	GLU
4	D	40	ILE
4	D	48	LEU
4	D	76	CYS
4	D	107	ILE
4	D	110	GLU
4	D	132	ARG
4	D	184	LEU
4	D	198	LEU
4	D	201	LEU
4	D	222	ILE
5	E	11	ASP
5	E	12	THR
5	E	16	SER
5	E	28	LEU
5	E	32	LYS
5	E	65	ILE
5	E	74	LEU
5	E	95	ASN
5	E	102	ASN
5	E	115	CYS
5	E	119	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	136	ILE
5	E	137	ILE
5	E	187	ASN
5	E	191	LEU
5	E	201	GLN
5	E	208	LEU
5	E	230	GLU
5	E	234	LYS
6	F	11	SER
6	F	36	THR
6	F	43	ASN
6	F	121	GLN
6	F	127	ASN
6	F	135	SER
6	F	169	ARG
6	F	185	GLU
6	F	190	ARG
6	F	205	GLU
6	F	206	ASP
6	F	207	ASN
6	F	216	ILE
6	F	218	TRP
6	F	225	ASN
6	F	232	LYS
7	G	36	ILE
7	G	68	ILE
7	G	73	ARG
7	G	88	ASN
7	G	120	LEU
7	G	122	GLN
7	G	129	TYR
7	G	171	GLN
7	G	191	ASN
7	G	206	MET
7	G	240	ARG
7	G	241	LEU
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
8	H	222	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	28	ASN
9	I	124	LYS
9	I	161	LEU
9	I	162	LEU
9	I	173	TRP
10	J	5	ILE
10	J	33	THR
10	J	34	ARG
10	J	51	THR
10	J	69	GLU
10	J	76	GLN
10	J	89	SER
10	J	90	ILE
10	J	108	LYS
10	J	125	GLU
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	99	THR
11	K	100	MET
11	K	104	TYR
11	K	107	LYS
11	K	108	GLU
11	K	148	LEU
11	K	186	ILE
12	L	-9	GLN
12	L	-7	ASN
12	L	13	LEU
12	L	24	SER
12	L	39	ASN
12	L	40	ILE
12	L	45	ASN
12	L	57	ARG
12	L	61	SER
12	L	70	ASN
12	L	82	ASN
12	L	98	HIS
12	L	99	THR
12	L	140	LEU
12	L	164	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	39	ASN
13	M	60	ASP
13	M	61	LEU
13	M	95	ARG
13	M	106	ILE
13	M	150	VAL
13	M	152	ARG
13	M	162	GLN
13	M	191	ILE
13	M	216	ILE
13	M	217	LYS
14	N	26	ILE
14	N	36	ARG
14	N	41	ILE
14	N	83	LYS
14	N	88	GLU
14	N	105	LYS
14	N	178	LEU
14	N	195	GLN
1	O	33	GLN
1	O	64	LEU
1	O	136	SER
1	O	160	PHE
1	O	181	ARG
2	P	6	ARG
2	P	58	LEU
2	P	72	ASN
2	P	73	ASP
2	P	92	THR
2	P	108	ILE
2	P	117	LEU
2	P	122	GLN
2	P	152	THR
2	P	165	ILE
2	P	187	LYS
2	P	194	LEU
2	P	215	PHE
2	P	223	ASN
2	P	232	PHE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	67	LYS
3	Q	122	GLN
3	Q	136	SER
3	Q	153	GLN
3	Q	166	GLN
3	Q	168	ILE
3	Q	177	GLU
3	Q	212	LYS
3	Q	231	GLU
4	R	40	ILE
4	R	48	LEU
4	R	76	CYS
4	R	107	ILE
4	R	110	GLU
4	R	132	ARG
4	R	184	LEU
4	R	198	LEU
4	R	201	LEU
4	R	222	ILE
5	S	11	ASP
5	S	12	THR
5	S	16	SER
5	S	28	LEU
5	S	32	LYS
5	S	65	ILE
5	S	74	LEU
5	S	95	ASN
5	S	102	ASN
5	S	115	CYS
5	S	119	GLN
5	S	136	ILE
5	S	137	ILE
5	S	187	ASN
5	S	191	LEU
5	S	201	GLN
5	S	208	LEU
5	S	230	GLU
5	S	234	LYS
6	T	11	SER
6	T	36	THR
6	T	43	ASN
6	T	121	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	127	ASN
6	T	135	SER
6	T	169	ARG
6	T	185	GLU
6	T	190	ARG
6	T	205	GLU
6	T	206	ASP
6	T	207	ASN
6	T	216	ILE
6	T	218	TRP
6	T	225	ASN
6	T	232	LYS
7	U	36	ILE
7	U	68	ILE
7	U	73	ARG
7	U	88	ASN
7	U	120	LEU
7	U	122	GLN
7	U	129	TYR
7	U	171	GLN
7	U	191	ASN
7	U	206	MET
7	U	240	ARG
7	U	241	LEU
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	196	ARG
8	V	222	ASP
9	W	28	ASN
9	W	161	LEU
9	W	162	LEU
9	W	173	TRP
10	X	5	ILE
10	X	33	THR
10	X	34	ARG
10	X	51	THR
10	X	69	GLU
10	X	76	GLN
10	X	89	SER
10	X	90	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	X	108	LYS
10	X	125	GLU
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	87	VAL
11	Y	99	THR
11	Y	100	MET
11	Y	104	TYR
11	Y	107	LYS
11	Y	108	GLU
11	Y	148	LEU
11	Y	186	ILE
12	Z	-7	ASN
12	Z	13	LEU
12	Z	24	SER
12	Z	39	ASN
12	Z	40	ILE
12	Z	45	ASN
12	Z	57	ARG
12	Z	61	SER
12	Z	70	ASN
12	Z	82	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	140	LEU
12	Z	164	TYR
13	a	-4	ILE
13	a	39	ASN
13	a	60	ASP
13	a	61	LEU
13	a	95	ARG
13	a	106	ILE
13	a	150	VAL
13	a	152	ARG
13	a	162	GLN
13	a	191	ILE
13	a	216	ILE
13	a	217	LYS
14	b	26	ILE
14	b	36	ARG
14	b	41	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	b	83	LYS
14	b	88	GLU
14	b	105	LYS
14	b	115	LEU
14	b	178	LEU
14	b	195	GLN
15	1	1	THR
15	3	1	THR
15	4	1	THR
15	6	1	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (202) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	72	ASN
2	B	96	HIS
2	B	98	GLN
2	B	122	GLN
2	B	126	GLN
2	B	158	ASN
2	B	179	GLN
2	B	223	ASN
3	C	23	GLN
3	C	83	ASN
3	C	122	GLN
3	C	126	GLN
3	C	153	GLN
3	C	166	GLN
3	C	242	GLN
3	C	247	GLN
4	D	23	GLN
4	D	99	HIS
4	D	108	ASN
4	D	154	GLN
4	D	168	ASN
4	D	233	ASN
5	E	7	ASN
5	E	33	GLN
5	E	62	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	71	HIS
5	E	102	ASN
5	E	119	GLN
5	E	121	ASN
5	E	123	GLN
5	E	154	ASN
5	E	187	ASN
5	E	201	GLN
5	E	212	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	195	GLN
6	F	244	GLN
7	G	35	ASN
7	G	88	ASN
7	G	119	ASN
7	G	122	GLN
7	G	126	GLN
7	G	171	GLN
7	G	172	GLN
7	G	180	ASN
7	G	191	ASN
7	G	236	ASN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	28	ASN
9	I	147	ASN
10	J	35	GLN
10	J	53	GLN
10	J	76	GLN
10	J	84	GLN
10	J	116	GLN
10	J	145	HIS
10	J	189	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
11	K	188	HIS
11	K	208	ASN
11	K	209	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	39	ASN
12	L	45	ASN
12	L	60	ASN
12	L	70	ASN
12	L	85	HIS
12	L	142	ASN
12	L	143	GLN
12	L	148	ASN
12	L	155	ASN
12	L	185	HIS
13	M	-7	GLN
13	M	9	ASN
13	M	39	ASN
13	M	93	GLN
13	M	99	ASN
13	M	162	GLN
13	M	170	ASN
13	M	204	GLN
14	N	60	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	72	ASN
2	P	96	HIS
2	P	98	GLN
2	P	122	GLN
2	P	126	GLN
2	P	158	ASN
2	P	179	GLN
2	P	223	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	23	GLN
3	Q	83	ASN
3	Q	122	GLN
3	Q	126	GLN
3	Q	153	GLN
3	Q	166	GLN
3	Q	242	GLN
3	Q	247	GLN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	154	GLN
4	R	168	ASN
4	R	218	GLN
4	R	233	ASN
5	S	7	ASN
5	S	33	GLN
5	S	62	GLN
5	S	71	HIS
5	S	102	ASN
5	S	119	GLN
5	S	121	ASN
5	S	123	GLN
5	S	154	ASN
5	S	187	ASN
5	S	201	GLN
5	S	212	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	195	GLN
7	U	35	ASN
7	U	88	ASN
7	U	119	ASN
7	U	122	GLN
7	U	126	GLN
7	U	171	GLN
7	U	172	GLN
7	U	180	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	191	ASN
7	U	236	ASN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	28	ASN
9	W	147	ASN
10	X	35	GLN
10	X	53	GLN
10	X	84	GLN
10	X	116	GLN
10	X	145	HIS
10	X	189	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	188	HIS
11	Y	208	ASN
11	Y	209	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	39	ASN
12	Z	45	ASN
12	Z	60	ASN
12	Z	70	ASN
12	Z	85	HIS
12	Z	142	ASN
12	Z	143	GLN
12	Z	148	ASN
12	Z	155	ASN
12	Z	185	HIS
13	a	9	ASN
13	a	39	ASN
13	a	93	GLN
13	a	99	ASN
13	a	162	GLN
13	a	170	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	a	204	GLN
14	b	60	GLN
14	b	141	ASN
14	b	145	ASN
14	b	157	HIS
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	LYH	1	2	15	5,8,9	1.07	0	6,8,10	1.37	1 (16%)
15	OJT	1	3	8,15	8,8,9	1.36	2 (25%)	8,9,11	1.77	1 (12%)
15	LYH	2	2	15	5,8,9	1.09	0	6,8,10	1.43	1 (16%)
15	OJT	2	3	11,15	8,8,9	1.52	1 (12%)	8,9,11	1.81	2 (25%)
15	LYH	3	2	15	5,8,9	1.10	0	6,8,10	1.67	2 (33%)
15	OJT	3	3	15,14	8,8,9	1.60	2 (25%)	8,9,11	1.67	1 (12%)
15	LYH	4	2	15	5,8,9	1.02	0	6,8,10	1.42	1 (16%)
15	OJT	4	3	8,15	8,8,9	1.34	1 (12%)	8,9,11	1.76	1 (12%)
15	LYH	5	2	15	5,8,9	1.02	0	6,8,10	1.47	1 (16%)
15	OJT	5	3	11,15	8,8,9	1.65	2 (25%)	8,9,11	1.86	2 (25%)
15	LYH	6	2	15	5,8,9	1.09	0	6,8,10	1.75	2 (33%)
15	OJT	6	3	15,14	8,8,9	1.71	2 (25%)	8,9,11	1.68	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LYH	1	2	15	-	0/3/7/9	0/0/0/0
15	OJT	1	3	8,15	-	0/7/8/9	0/0/0/0
15	LYH	2	2	15	-	0/3/7/9	0/0/0/0
15	OJT	2	3	11,15	-	0/7/8/9	0/0/0/0
15	LYH	3	2	15	-	0/3/7/9	0/0/0/0
15	OJT	3	3	15,14	-	0/7/8/9	0/0/0/0
15	LYH	4	2	15	-	0/3/7/9	0/0/0/0
15	OJT	4	3	8,15	-	0/7/8/9	0/0/0/0
15	LYH	5	2	15	-	0/3/7/9	0/0/0/0
15	OJT	5	3	11,15	-	0/7/8/9	0/0/0/0
15	LYH	6	2	15	-	0/3/7/9	0/0/0/0
15	OJT	6	3	15,14	-	0/7/8/9	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	3	OJT	C17-C18	2.08	1.56	1.53
15	3	3	OJT	C17-C18	2.17	1.56	1.53
15	5	3	OJT	C17-C18	2.21	1.56	1.53
15	6	3	OJT	C17-C18	2.31	1.56	1.53
15	1	3	OJT	C19-C18	2.49	1.57	1.53
15	4	3	OJT	C19-C18	2.78	1.57	1.53
15	2	3	OJT	C19-C18	3.31	1.58	1.53
15	3	3	OJT	C19-C18	3.39	1.58	1.53
15	5	3	OJT	C19-C18	3.58	1.58	1.53
15	6	3	OJT	C19-C18	3.67	1.58	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	5	3	OJT	C16-C17-C18	-4.16	107.27	114.01
15	4	3	OJT	C16-C17-C18	-4.07	107.41	114.01
15	1	3	OJT	C16-C17-C18	-4.05	107.44	114.01
15	2	3	OJT	C16-C17-C18	-4.02	107.50	114.01
15	6	3	OJT	C16-C17-C18	-3.79	107.86	114.01
15	3	3	OJT	C16-C17-C18	-3.65	108.08	114.01
15	5	2	LYH	CE-CD-CG	-2.22	107.75	113.08
15	6	2	LYH	CE-CD-CG	-2.20	107.77	113.08
15	3	2	LYH	CE-CD-CG	-2.17	107.85	113.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	2	LYH	CE-CD-CG	-2.08	108.06	113.08
15	2	3	OJT	C17-C16-C14	2.02	117.96	112.29
15	5	3	OJT	C17-C16-C14	2.05	118.02	112.29
15	1	2	LYH	C-CA-N	2.31	114.43	109.86
15	4	2	LYH	C-CA-N	2.44	114.69	109.86
15	3	2	LYH	C-CA-N	2.52	114.85	109.86
15	6	2	LYH	C-CA-N	2.71	115.22	109.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	2	3	OJT	1	0
15	3	2	LYH	1	0
15	3	3	OJT	1	0
15	4	3	OJT	1	0
15	5	3	OJT	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.45	3 (1%) 79 72	35, 55, 84, 105	0
1	O	250/250 (100%)	-0.43	3 (1%) 79 72	36, 55, 84, 105	0
2	B	244/244 (100%)	-0.25	6 (2%) 58 47	39, 56, 94, 118	0
2	P	244/244 (100%)	-0.26	9 (3%) 42 31	39, 57, 95, 118	0
3	C	241/241 (100%)	-0.21	8 (3%) 47 36	40, 59, 110, 129	0
3	Q	241/241 (100%)	-0.21	11 (4%) 33 23	42, 61, 110, 129	0
4	D	242/242 (100%)	-0.24	7 (2%) 52 41	39, 60, 92, 125	0
4	R	242/242 (100%)	-0.19	8 (3%) 47 36	41, 61, 93, 126	0
5	E	233/233 (100%)	-0.30	6 (2%) 56 45	42, 62, 87, 111	0
5	S	233/233 (100%)	-0.27	4 (1%) 70 63	42, 62, 87, 111	0
6	F	244/244 (100%)	-0.35	8 (3%) 47 36	39, 56, 92, 106	0
6	T	244/244 (100%)	-0.26	5 (2%) 65 56	39, 56, 93, 105	0
7	G	243/243 (100%)	-0.47	3 (1%) 79 72	37, 53, 80, 112	0
7	U	243/243 (100%)	-0.43	3 (1%) 79 72	36, 53, 79, 112	0
8	H	222/222 (100%)	-0.55	1 (0%) 90 88	31, 48, 68, 98	0
8	V	222/222 (100%)	-0.50	3 (1%) 75 69	33, 48, 67, 98	0
9	I	204/204 (100%)	-0.56	1 (0%) 90 88	35, 50, 67, 84	0
9	W	204/204 (100%)	-0.52	1 (0%) 90 88	37, 50, 68, 84	0
10	J	198/198 (100%)	-0.45	3 (1%) 74 67	37, 51, 68, 124	0
10	X	198/198 (100%)	-0.45	4 (2%) 65 56	38, 51, 70, 124	0
11	K	212/212 (100%)	-0.46	1 (0%) 90 88	34, 51, 75, 82	0
11	Y	212/212 (100%)	-0.50	1 (0%) 90 88	35, 51, 74, 82	0
12	L	222/222 (100%)	-0.59	2 (0%) 84 79	33, 50, 71, 96	0
12	Z	222/222 (100%)	-0.55	2 (0%) 84 79	33, 50, 71, 95	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.61	1 (0%) 92 90	35, 49, 64, 69	0
13	a	233/233 (100%)	-0.55	1 (0%) 92 90	34, 48, 64, 69	0
14	N	196/196 (100%)	-0.54	0 100 100	33, 45, 67, 77	0
14	b	196/196 (100%)	-0.53	1 (0%) 90 88	33, 46, 68, 77	0
15	1	1/4 (25%)	-0.31	0 100 100	50, 50, 50, 50	0
15	2	1/4 (25%)	-0.20	0 100 100	52, 52, 52, 52	0
15	3	1/4 (25%)	-0.23	0 100 100	57, 57, 57, 57	0
15	4	1/4 (25%)	-0.39	0 100 100	51, 51, 51, 51	0
15	5	1/4 (25%)	0.03	0 100 100	51, 51, 51, 51	0
15	6	1/4 (25%)	0.09	0 100 100	57, 57, 57, 57	0
All	All	6374/6392 (99%)	-0.41	106 (1%) 70 63	31, 53, 84, 129	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	126	GLY	9.9
3	C	55	THR	8.8
4	R	128	SER	8.4
4	D	128	SER	8.4
10	X	196	GLN	7.7
4	D	127	ALA	7.4
4	R	129	GLY	6.7
4	D	129	GLY	6.7
4	R	126	GLY	6.6
7	U	248	ASP	6.4
10	X	195	ALA	6.0
2	B	223	ASN	5.9
2	P	223	ASN	5.7
4	R	127	ALA	5.5
1	A	4	MET	5.5
10	J	196	GLN	5.0
3	C	56	LEU	4.9
3	C	209	THR	4.9
10	J	195	ALA	4.9
5	E	4	PHE	4.9
3	Q	209	THR	4.6
2	B	222	ALA	4.6
10	J	194	GLN	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	S	4	PHE	4.4
5	S	5	ARG	4.4
7	G	248	ASP	4.1
6	F	206	ASP	4.1
7	U	6	ALA	4.0
6	T	247	ILE	3.9
6	T	6	THR	3.9
1	A	5	THR	3.8
6	F	247	ILE	3.8
6	T	5	GLY	3.7
5	E	205	ASP	3.7
10	X	194	GLN	3.7
2	P	222	ALA	3.7
5	S	205	ASP	3.6
4	R	132	ARG	3.5
9	W	-8	SER	3.4
4	D	130	GLU	3.3
3	Q	208	GLN	3.3
6	F	5	GLY	3.3
2	B	247	THR	3.3
3	C	208	GLN	3.2
11	K	212	GLY	3.2
8	H	221	CYS	3.1
10	X	192	ASP	3.1
3	Q	247	GLN	3.1
5	E	206	GLU	3.1
12	L	164	TYR	3.1
5	E	5	ARG	3.1
1	O	4	MET	3.0
3	C	247	GLN	2.9
4	D	133	LEU	2.9
2	P	247	THR	2.9
9	I	-8	SER	2.9
2	P	4	GLY	2.9
2	P	53	LYS	2.9
2	B	4	GLY	2.8
4	D	132	ARG	2.8
13	M	-8	THR	2.8
2	B	221	GLY	2.8
6	F	207	ASN	2.7
7	G	6	ALA	2.7
4	R	124	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	56	LEU	2.6
4	R	133	LEU	2.6
2	P	54	VAL	2.6
13	a	-8	THR	2.6
6	F	210	LYS	2.6
2	P	226	GLU	2.5
3	C	244	LYS	2.5
2	P	221	GLY	2.5
3	Q	245	GLN	2.5
3	Q	244	LYS	2.5
6	F	6	THR	2.5
1	O	55	SER	2.4
6	T	248	ASN	2.4
3	Q	246	GLU	2.4
12	Z	164	TYR	2.4
3	Q	55	THR	2.4
3	Q	54	SER	2.3
7	G	247	GLN	2.3
8	V	221	CYS	2.3
11	Y	106	ARG	2.3
6	F	248	ASN	2.3
6	T	185	GLU	2.3
1	A	253	LEU	2.3
12	L	163	LYS	2.3
12	Z	163	LYS	2.2
5	S	236	ILE	2.2
8	V	222	ASP	2.2
2	B	207	ALA	2.2
14	b	195	GLN	2.1
3	C	245	GLN	2.1
7	U	193	GLU	2.1
6	F	208	LYS	2.1
3	C	246	GLU	2.1
3	Q	243	GLU	2.1
8	V	219	ASN	2.1
5	E	33	GLN	2.0
4	R	130	GLU	2.0
1	O	53	LYS	2.0
2	P	62	ASP	2.0
5	E	236	ILE	2.0
3	Q	181	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	LYH	1	2	9/10	0.88	0.16	-	47,48,50,50	0
15	LYH	6	2	9/10	0.89	0.19	-	46,48,50,50	0
15	LYH	4	2	9/10	0.93	0.20	-	47,48,50,50	0
15	LYH	2	2	9/10	0.94	0.16	-	45,46,47,47	0
15	OJT	6	3	9/10	0.95	0.14	-	38,44,47,50	0
15	LYH	5	2	9/10	0.94	0.18	-	46,47,49,49	0
15	OJT	3	3	9/10	0.96	0.14	-	39,45,50,52	0
15	OJT	2	3	9/10	0.98	0.13	-	39,43,46,46	0
15	OJT	1	3	9/10	0.94	0.14	-	40,45,48,49	0
15	LYH	3	2	9/10	0.92	0.22	-	46,50,52,52	0
15	OJT	5	3	9/10	0.97	0.13	-	42,44,47,47	0
15	OJT	4	3	9/10	0.96	0.17	-	40,43,48,49	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.