



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:09 PM UTC

PDB ID : 8YPK / pdb_00008ypk
EMDB ID : EMD-39482
Title : mouse proteasome 20S subunit in complex with compound 1
Authors : Kashima, A.; Arai, Y.
Deposited on : 2024-03-17
Resolution : 2.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

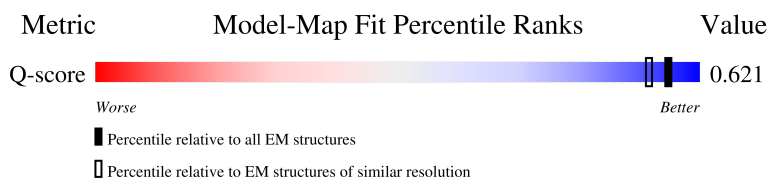
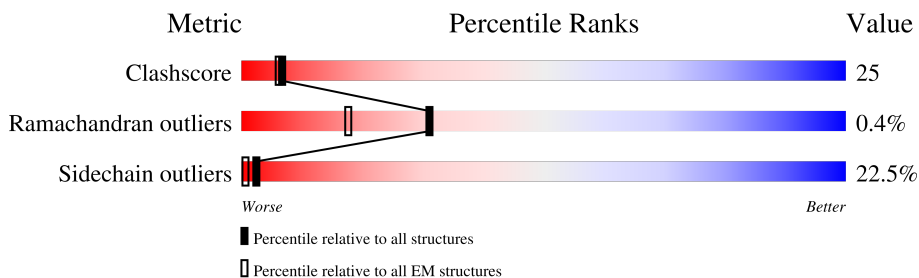
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	205	
1	F	205	
2	P	234	
2	b	234	

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Mol	Chain	Length	Quality of chain
3	I	248	
3	N	248	
4	K	246	
4	R	246	
5	T	201	
5	V	201	
6	S	240	
6	X	240	
7	C	205	
7	D	205	
8	J	255	
8	Q	255	
9	G	263	
9	L	263	
10	H	241	
10	M	241	
11	O	261	
11	Z	261	
12	B	234	
12	E	234	
13	W	264	
13	a	264	
14	U	205	
14	Y	205	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 47992 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	202	Total	C	N	O	S	0	0
			1519	952	259	296	12		
1	F	202	Total	C	N	O	S	0	0
			1519	952	259	296	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	227	Total	C	N	O	S	0	0
			1782	1138	304	334	6		
2	b	227	Total	C	N	O	S	0	0
			1782	1138	304	334	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	232	Total	C	N	O	S	0	0
			1819	1146	322	346	5		
3	I	232	Total	C	N	O	S	0	0
			1819	1146	322	346	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	236	Total	C	N	O	S	0	0
			1831	1163	304	351	13		
4	K	236	Total	C	N	O	S	0	0
			1831	1163	304	351	13		

- Molecule 5 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	196	Total	C	N	O	S	0	0
			1570	1006	267	288	9		
5	V	196	Total	C	N	O	S	0	0
			1570	1006	267	288	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
6	X	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		

- Molecule 7 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	200	Total	C	N	O	S	0	0
			1551	980	270	292	9		
7	C	200	Total	C	N	O	S	0	0
			1551	980	270	292	9		

- Molecule 8 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	235	Total	C	N	O	S	0	0
			1840	1168	315	346	11		
8	Q	235	Total	C	N	O	S	0	0
			1840	1168	315	346	11		

- Molecule 9 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	234	Total	C	N	O	S	0	0
			1836	1150	328	347	11		
9	G	234	Total	C	N	O	S	0	0
			1836	1150	328	347	11		

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	231	Total	C	N	O	S	0	0
			1761	1106	292	352	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	231	Total	C	N	O	S	0	0
			1761	1106	292	352	11		

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	239	Total	C	N	O	S	0	0
			1881	1191	321	359	10		
11	Z	239	Total	C	N	O	S	0	0
			1881	1191	321	359	10		

- Molecule 12 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	220	Total	C	N	O	S	0	0
			1656	1044	282	318	12		
12	E	220	Total	C	N	O	S	0	0
			1656	1044	282	318	12		

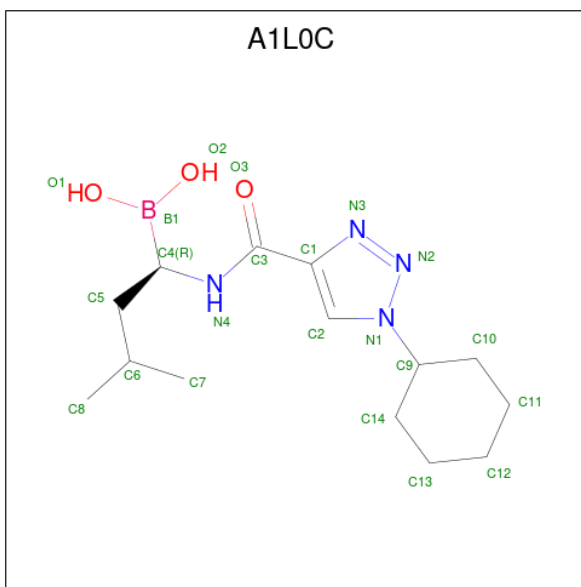
- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	214	Total	C	N	O	S	0	0
			1671	1054	289	316	12		
13	a	214	Total	C	N	O	S	0	0
			1671	1054	289	316	12		

- Molecule 14 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	204	Total	C	N	O	S	0	0
			1592	1013	265	295	19		
14	U	204	Total	C	N	O	S	0	0
			1592	1013	265	295	19		

- Molecule 15 is [(1R)-1-[(1-cyclohexyl-1,2,3-triazol-4-yl)carbonylamino]-3-methyl-butyl]boronic acid (CCD ID: A1L0C) (formula: C₁₄H₂₅BN₄O₃) (labeled as "Ligand of Interest" by depositor).

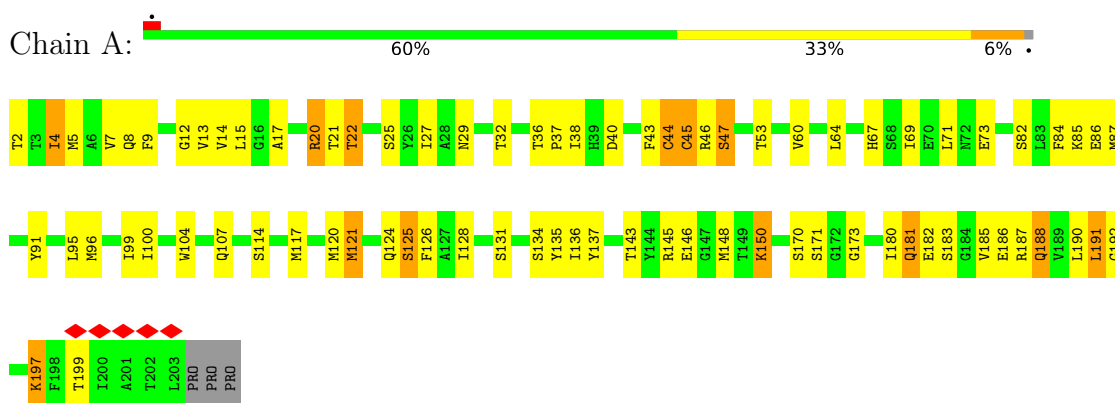


Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	B	C	N	O	0
			22	1	14	4	3	
15	D	1	Total	B	C	N	O	0
			22	1	14	4	3	
15	C	1	Total	B	C	N	O	0
			22	1	14	4	3	
15	F	1	Total	B	C	N	O	0
			22	1	14	4	3	

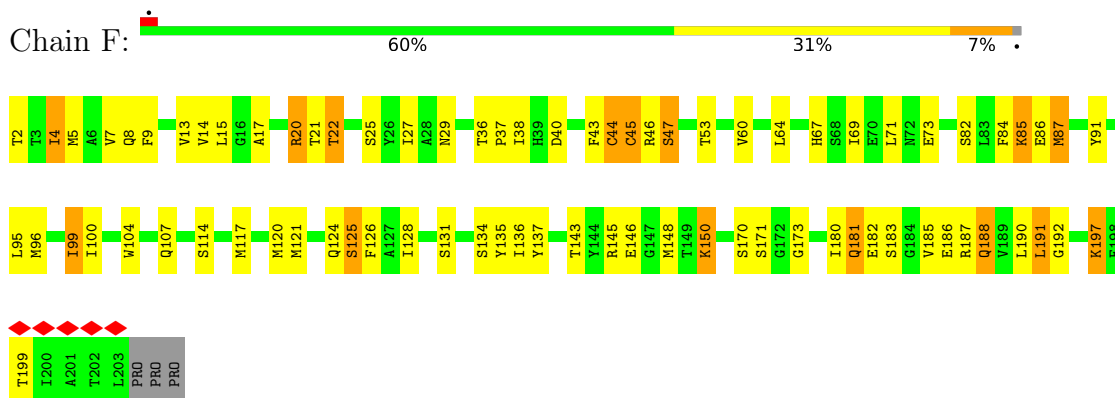
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

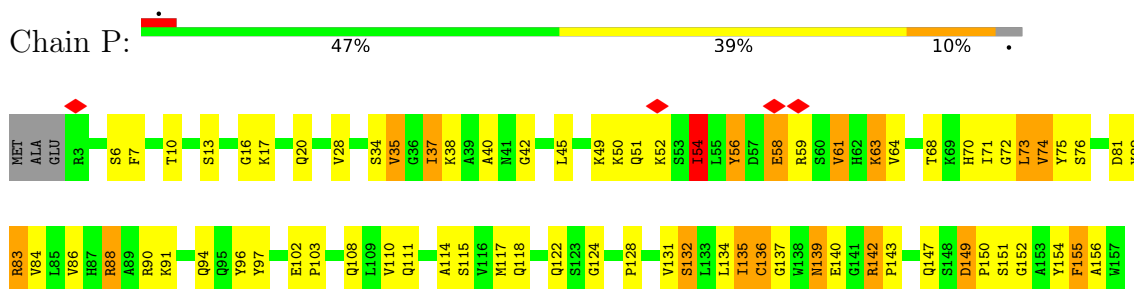
- Molecule 1: Proteasome subunit beta type-6

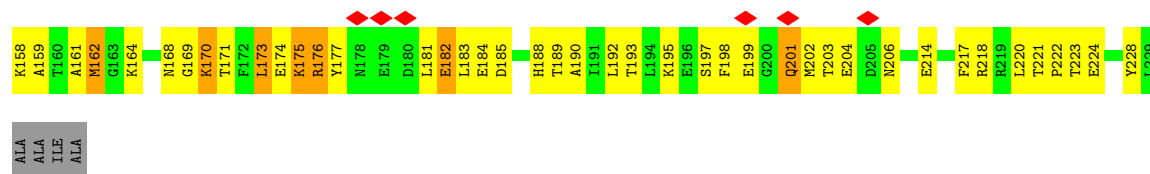


- Molecule 1: Proteasome subunit beta type-6

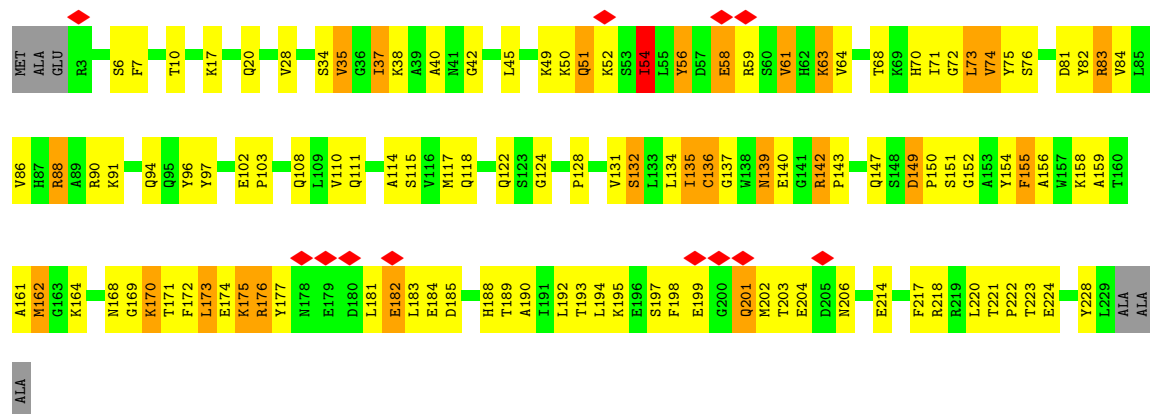


- Molecule 2: Proteasome subunit alpha type-2

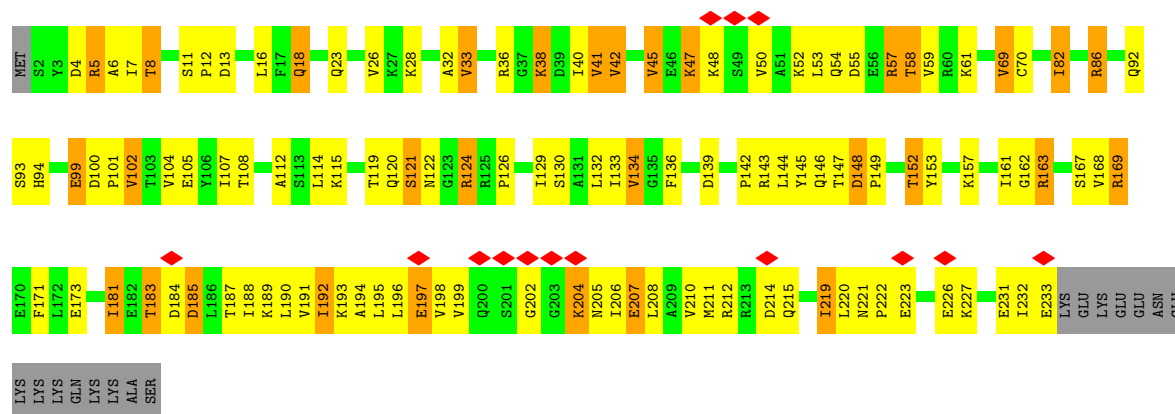




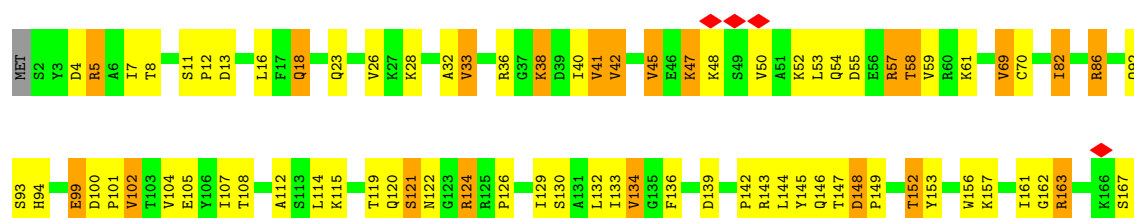
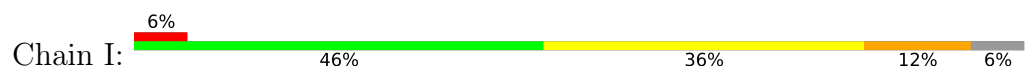
• Molecule 2: Proteasome subunit alpha type-2

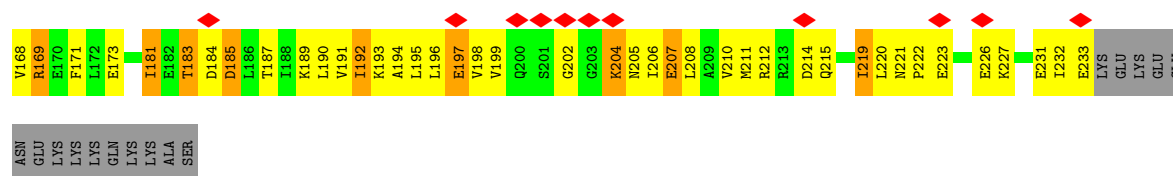


• Molecule 3: Proteasome subunit alpha type-7

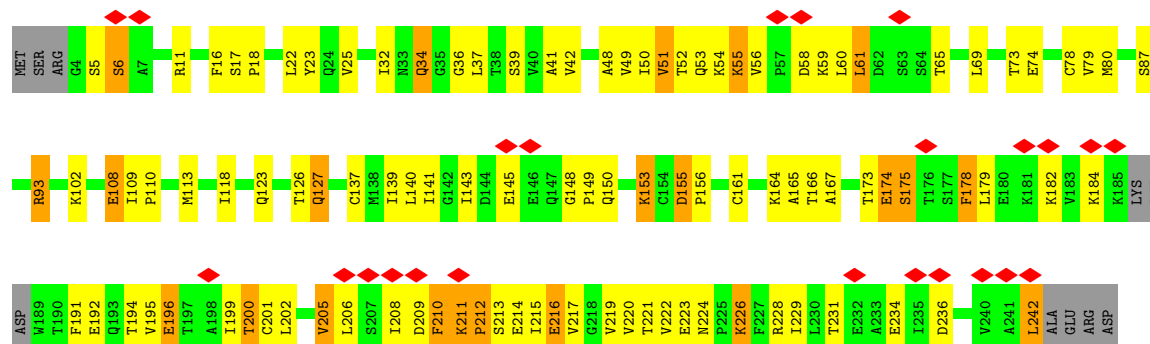


• Molecule 3: Proteasome subunit alpha type-7

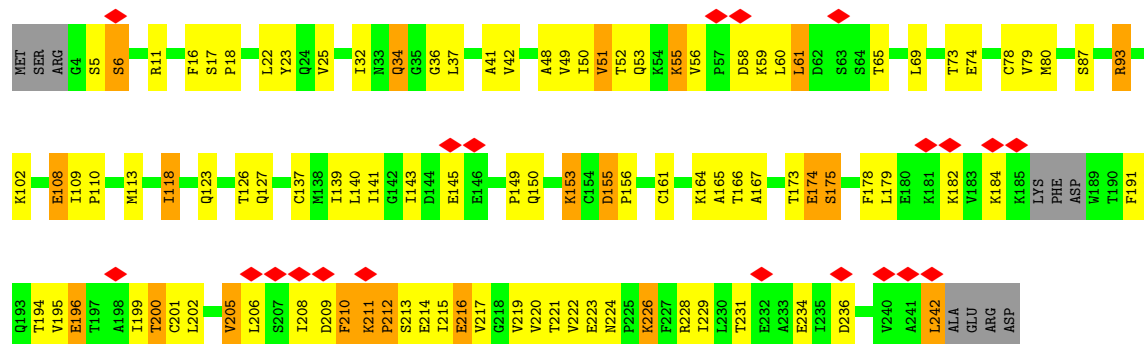




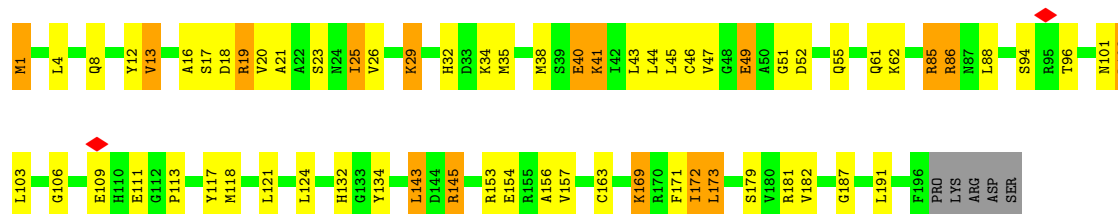
• Molecule 4: Proteasome subunit alpha type-6



• Molecule 4: Proteasome subunit alpha type-6

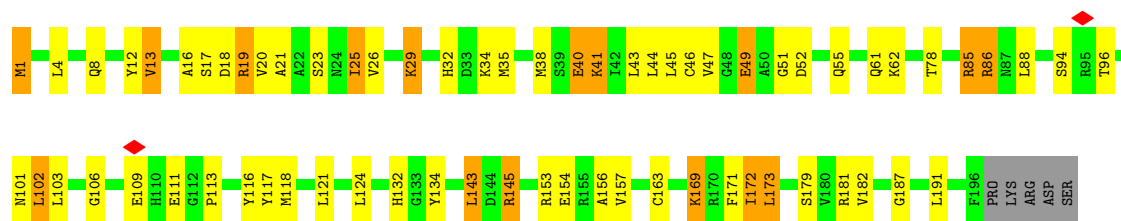


• Molecule 5: Proteasome subunit beta type-2

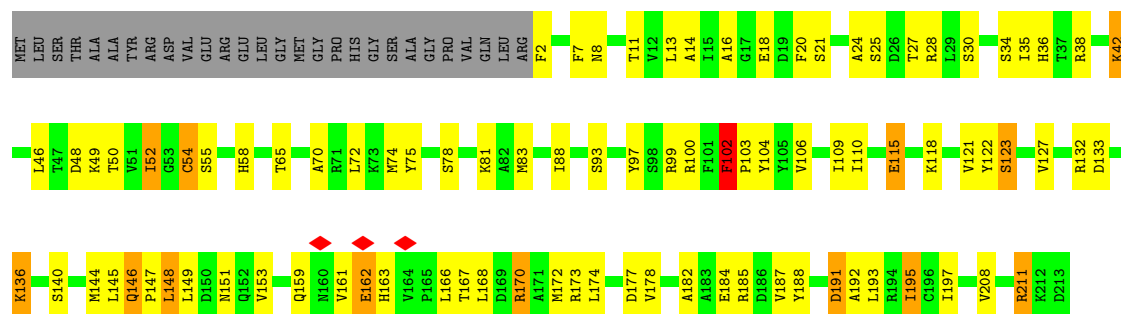


• Molecule 5: Proteasome subunit beta type-2

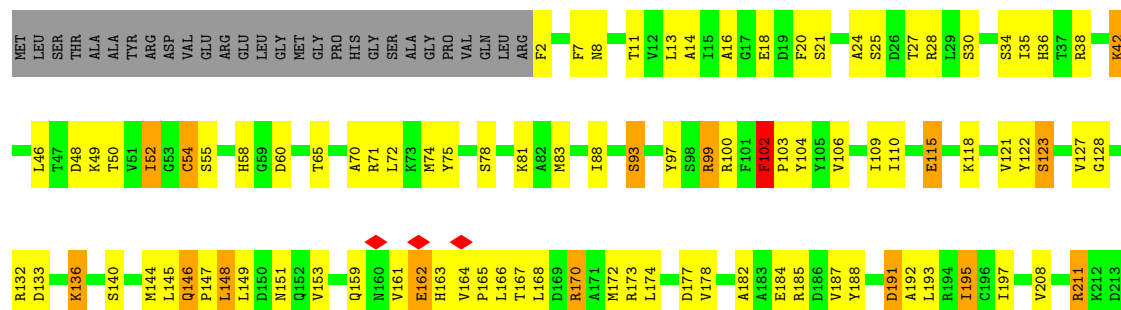




• Molecule 6: Proteasome subunit beta type-1



• Molecule 6: Proteasome subunit beta type-1

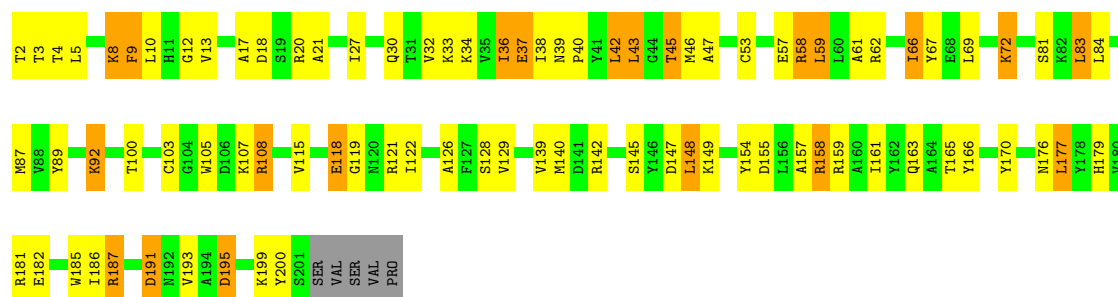


• Molecule 7: Proteasome subunit beta type-5



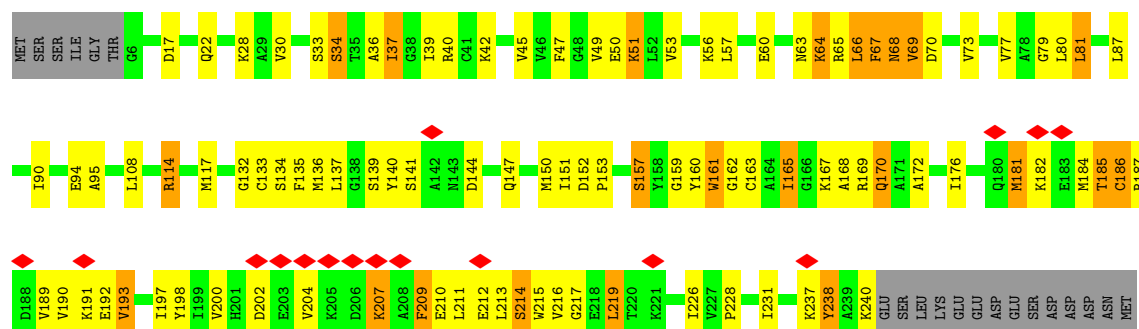
• Molecule 7: Proteasome subunit beta type-5

Chain C: 



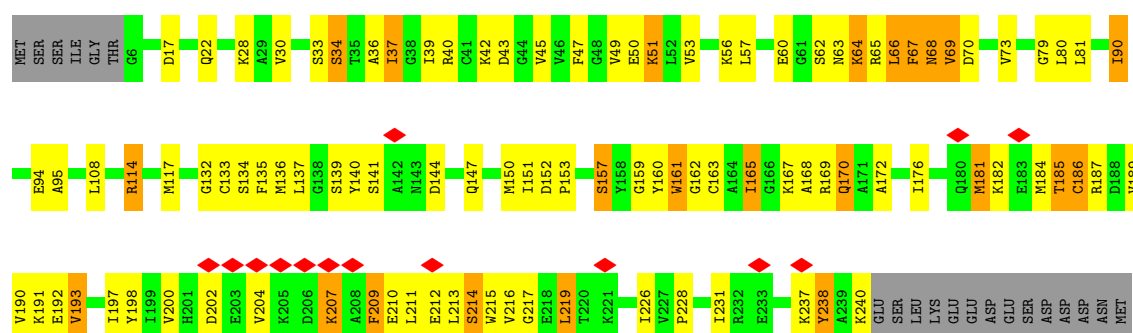
• Molecule 8: Proteasome subunit alpha type-3

Chain J: 



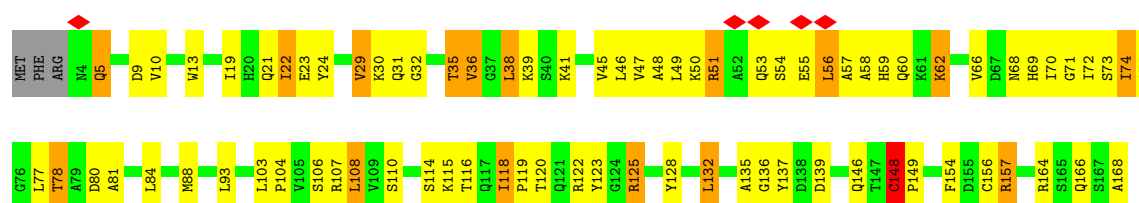
• Molecule 8: Proteasome subunit alpha type-3

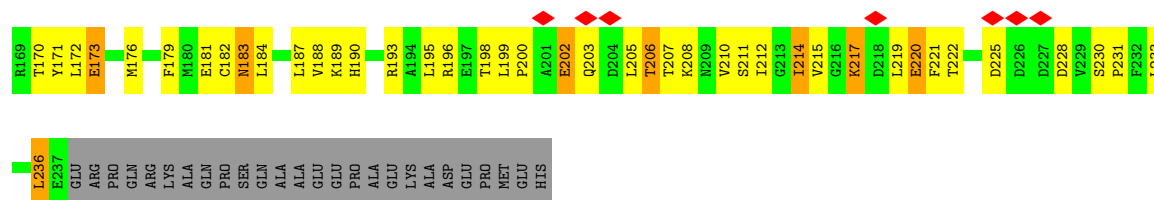
Chain Q: 



• Molecule 9: Proteasome subunit alpha type-1

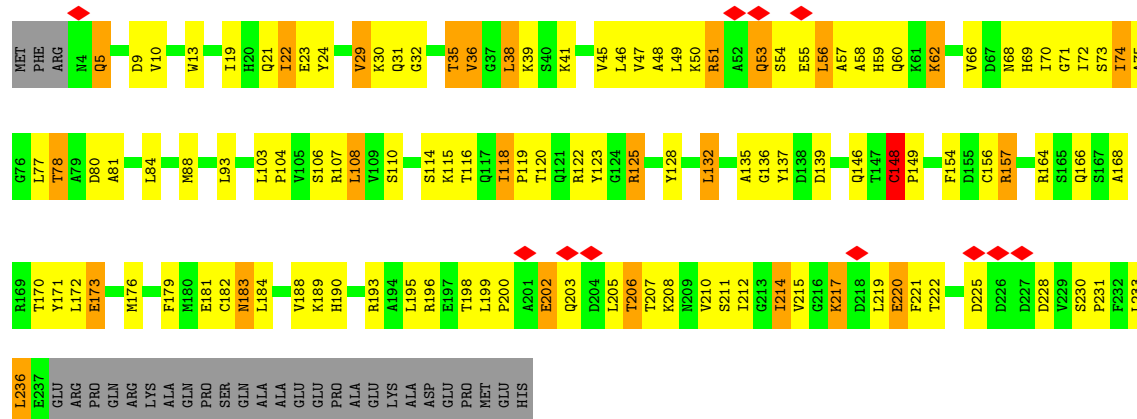
Chain L: 





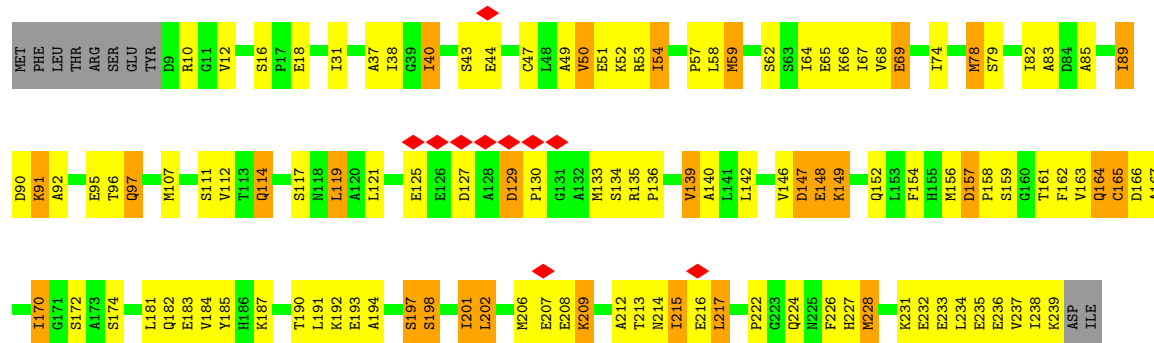
• Molecule 9: Proteasome subunit alpha type-1

Chain G: 43% 36% 10% 11%



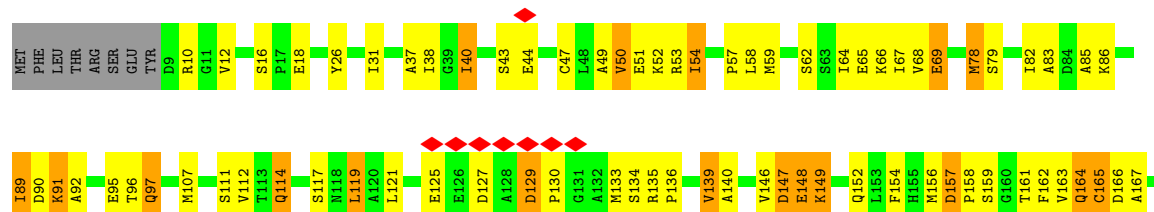
• Molecule 10: Proteasome subunit alpha type-5

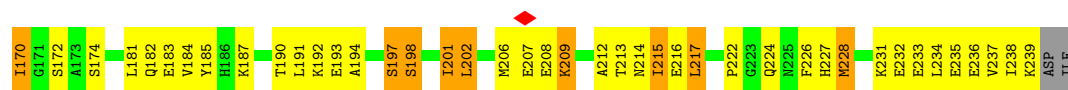
Chain H: 47% 37% 12%



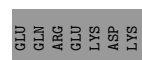
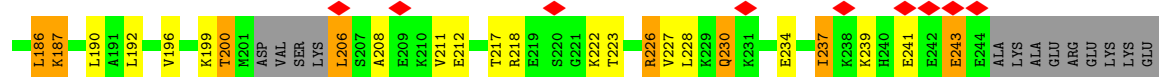
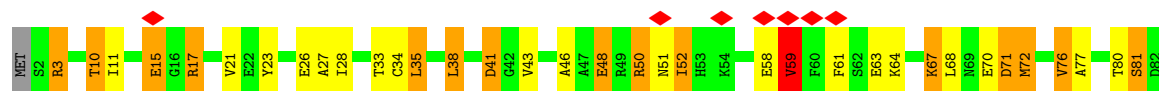
• Molecule 10: Proteasome subunit alpha type-5

Chain M: 47% 37% 11%

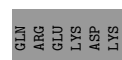
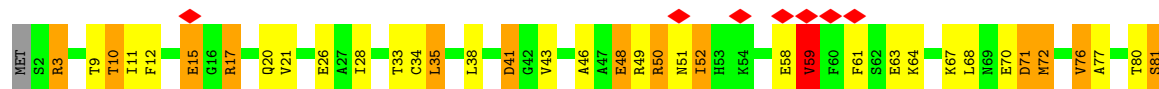




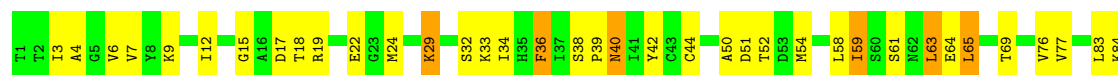
• Molecule 11: Proteasome subunit alpha type-4

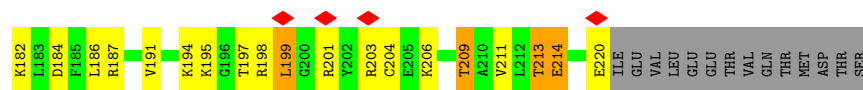


• Molecule 11: Proteasome subunit alpha type-4

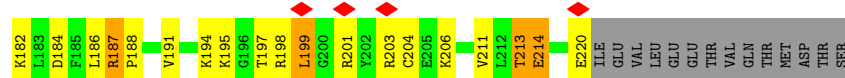
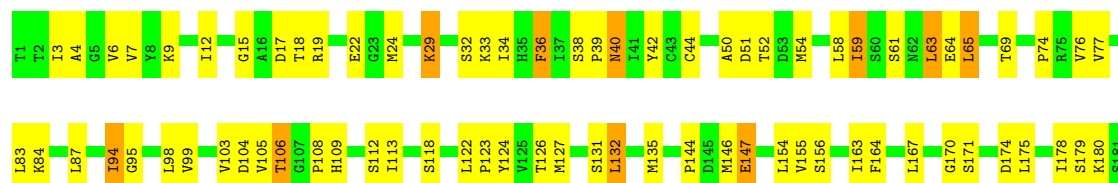


• Molecule 12: Proteasome subunit beta type-7

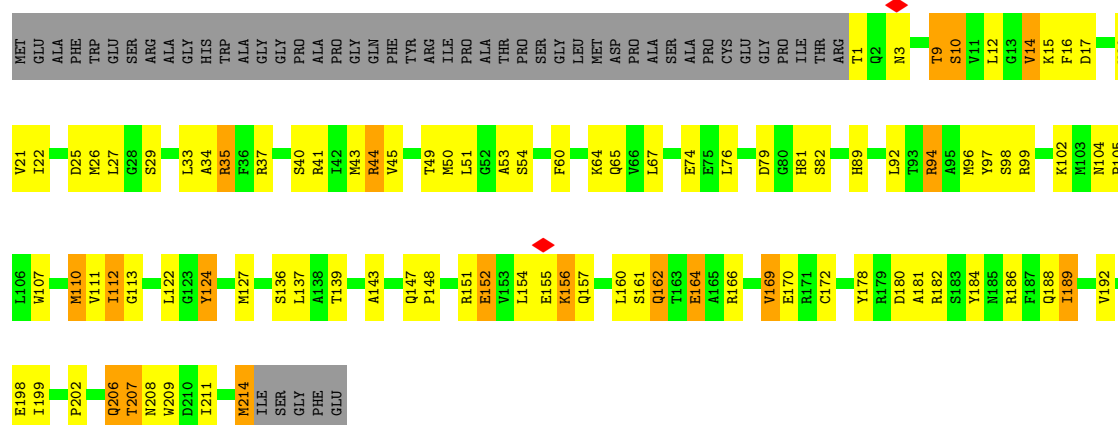




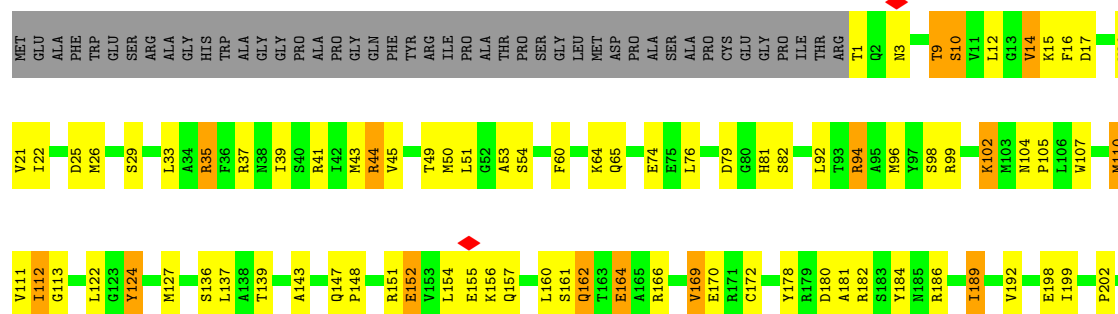
• Molecule 12: Proteasome subunit beta type-7

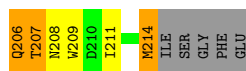


• Molecule 13: Proteasome subunit beta type-4

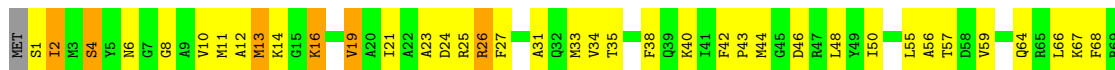


• Molecule 13: Proteasome subunit beta type-4

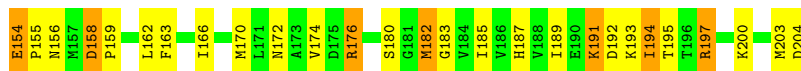




● Molecule 14: Proteasome subunit beta type-3



● Molecule 14: Proteasome subunit beta type-3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.692	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0343	Depositor
Map size (Å)	292.16095, 292.16095, 292.16095	wwPDB
Map dimensions	254, 254, 254	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15024, 1.15024, 1.15024	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1L0C

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	0.40	0/1546	0.75	0/2094
1	F	0.40	0/1546	0.74	0/2094
2	P	0.35	0/1821	0.78	3/2466 (0.1%)
2	b	0.35	0/1821	0.78	3/2466 (0.1%)
3	I	0.35	0/1846	0.76	3/2495 (0.1%)
3	N	0.34	0/1846	0.76	3/2495 (0.1%)
4	K	0.34	0/1863	0.80	6/2518 (0.2%)
4	R	0.33	0/1863	0.80	6/2518 (0.2%)
5	T	0.38	0/1602	0.79	0/2167
5	V	0.38	0/1602	0.79	0/2167
6	S	0.38	0/1674	0.78	2/2257 (0.1%)
6	X	0.38	0/1674	0.78	2/2257 (0.1%)
7	C	0.38	0/1582	0.70	0/2137
7	D	0.38	0/1582	0.70	0/2137
8	J	0.33	0/1875	0.78	2/2524 (0.1%)
8	Q	0.33	0/1875	0.77	1/2524 (0.0%)
9	G	0.35	0/1870	0.80	5/2528 (0.2%)
9	L	0.35	0/1870	0.80	5/2528 (0.2%)
10	H	0.34	0/1788	0.74	2/2415 (0.1%)
10	M	0.34	0/1788	0.74	2/2415 (0.1%)
11	O	0.37	0/1910	0.84	3/2573 (0.1%)
11	Z	0.37	0/1910	0.84	3/2573 (0.1%)
12	B	0.37	0/1683	0.74	0/2276
12	E	0.37	0/1683	0.74	0/2276
13	W	0.38	0/1704	0.74	0/2306
13	a	0.38	0/1704	0.74	0/2306
14	U	0.38	0/1621	0.79	4/2185 (0.2%)
14	Y	0.38	0/1621	0.79	2/2185 (0.1%)
All	All	0.36	0/48770	0.77	57/65882 (0.1%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	102	PHE	CA-C-N	7.83	129.63	119.84
6	S	102	PHE	C-N-CA	7.83	129.63	119.84
6	X	102	PHE	CA-C-N	7.81	129.60	119.84
6	X	102	PHE	C-N-CA	7.81	129.60	119.84
14	Y	100	GLY	CA-C-N	7.37	127.81	119.92
14	Y	100	GLY	C-N-CA	7.37	127.81	119.92
14	U	100	GLY	CA-C-N	7.37	127.81	119.92
14	U	100	GLY	C-N-CA	7.37	127.81	119.92
8	Q	161	TRP	N-CA-C	-6.90	104.86	113.55
8	J	161	TRP	N-CA-C	-6.87	104.90	113.55
4	R	164	LYS	N-CA-C	-6.84	104.94	113.55
4	K	164	LYS	N-CA-C	-6.82	104.96	113.55
9	G	148	CYS	CA-C-N	6.71	126.40	119.56
9	G	148	CYS	C-N-CA	6.71	126.40	119.56
9	L	148	CYS	CA-C-N	6.67	126.37	119.56
9	L	148	CYS	C-N-CA	6.67	126.37	119.56
4	K	224	ASN	CA-C-N	6.53	126.66	119.87
4	K	224	ASN	C-N-CA	6.53	126.66	119.87
4	R	224	ASN	CA-C-N	6.50	126.63	119.87
4	R	224	ASN	C-N-CA	6.50	126.63	119.87
4	R	155	ASP	CA-C-N	6.33	125.96	119.56
4	R	155	ASP	C-N-CA	6.33	125.96	119.56
4	K	155	ASP	CA-C-N	6.32	125.94	119.56
4	K	155	ASP	C-N-CA	6.32	125.94	119.56
11	O	151	ASP	CA-C-N	6.25	126.16	119.28
11	O	151	ASP	C-N-CA	6.25	126.16	119.28
11	Z	151	ASP	CA-C-N	6.22	126.13	119.28
11	Z	151	ASP	C-N-CA	6.22	126.13	119.28
4	K	210	PHE	N-CA-C	6.14	118.95	110.35
4	R	210	PHE	N-CA-C	6.13	118.93	110.35
2	P	149	ASP	CA-C-N	5.76	126.15	119.47
2	P	149	ASP	C-N-CA	5.76	126.15	119.47
2	b	149	ASP	CA-C-N	5.74	126.13	119.47
2	b	149	ASP	C-N-CA	5.74	126.13	119.47
9	G	66	VAL	N-CA-C	-5.70	107.34	112.12
3	N	157	LYS	N-CA-C	-5.68	106.48	113.41
9	L	66	VAL	N-CA-C	-5.65	107.38	112.12
3	I	157	LYS	N-CA-C	-5.64	106.52	113.41
2	b	158	LYS	N-CA-C	-5.50	106.61	113.55
2	P	158	LYS	N-CA-C	-5.49	106.63	113.55
11	Z	160	LYS	N-CA-C	-5.40	106.75	113.55
10	H	157	ASP	CA-C-N	5.38	125.20	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	157	ASP	C-N-CA	5.38	125.20	119.28
11	O	160	LYS	N-CA-C	-5.38	106.77	113.55
10	M	157	ASP	CA-C-N	5.36	125.18	119.28
10	M	157	ASP	C-N-CA	5.36	125.18	119.28
9	L	118	ILE	CA-C-N	5.32	125.14	119.28
9	L	118	ILE	C-N-CA	5.32	125.14	119.28
9	G	118	ILE	CA-C-N	5.29	125.09	119.28
9	G	118	ILE	C-N-CA	5.29	125.09	119.28
3	I	148	ASP	CA-C-N	5.07	125.10	119.32
3	I	148	ASP	C-N-CA	5.07	125.10	119.32
3	N	148	ASP	CA-C-N	5.04	125.06	119.32
3	N	148	ASP	C-N-CA	5.04	125.06	119.32
8	J	77	VAL	N-CA-C	5.01	116.08	108.96
14	U	154	GLU	CA-C-N	5.01	126.10	119.84
14	U	154	GLU	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1519	0	1484	55	0
1	F	1519	0	1484	57	0
2	P	1782	0	1774	102	0
2	b	1782	0	1774	106	0
3	I	1819	0	1845	107	0
3	N	1819	0	1845	106	0
4	K	1831	0	1841	100	0
4	R	1831	0	1841	103	0
5	T	1570	0	1573	55	0
5	V	1570	0	1573	57	0
6	S	1643	0	1638	81	0
6	X	1643	0	1638	88	0
7	C	1551	0	1517	76	0
7	D	1551	0	1517	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	1840	0	1827	102	0
8	Q	1840	0	1827	104	0
9	G	1836	0	1822	119	0
9	L	1836	0	1822	124	0
10	H	1761	0	1749	139	0
10	M	1761	0	1749	136	0
11	O	1881	0	1896	89	0
11	Z	1881	0	1896	86	0
12	B	1656	0	1685	78	0
12	E	1656	0	1685	80	0
13	W	1671	0	1648	92	0
13	a	1671	0	1648	85	0
14	U	1592	0	1612	109	0
14	Y	1592	0	1612	109	0
15	A	22	0	0	1	0
15	C	22	0	0	1	0
15	D	22	0	0	1	0
15	F	22	0	0	1	0
All	All	47992	0	47822	2369	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 25.

All (2369) 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)
8:J:66:LEU:HD22	8:J:214:SER:OG	1.33	1.27
10:M:52:LYS:HB2	10:M:214:ASN:O	1.34	1.25
8:Q:66:LEU:HD22	8:Q:214:SER:OG	1.33	1.22
13:W:178:TYR:CE1	13:W:207:THR:HG22	1.73	1.21
13:a:178:TYR:CE1	13:a:207:THR:HG22	1.73	1.21
10:H:52:LYS:HB2	10:H:214:ASN:O	1.34	1.20
10:H:51:GLU:CG	10:H:206:MET:HE2	1.76	1.15
10:H:51:GLU:HB2	10:H:206:MET:HE3	1.26	1.15
6:S:148:LEU:HD12	6:S:178:VAL:HG12	1.26	1.14
10:H:51:GLU:HG3	10:H:206:MET:HE2	1.15	1.14
10:M:51:GLU:CG	10:M:206:MET:HE2	1.76	1.14
10:M:51:GLU:HG3	10:M:206:MET:HE2	1.15	1.12
14:Y:44:MET:HE2	14:Y:70:LEU:HD23	1.11	1.10
6:X:148:LEU:HD12	6:X:178:VAL:HG12	1.26	1.10
1:A:150:LYS:HE3	1:A:181:GLN:HE22	0.93	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:51:GLU:HB2	10:M:206:MET:HE3	1.26	1.09
4:K:155:ASP:HB2	4:K:156:PRO:HD2	1.10	1.09
1:F:150:LYS:HE3	1:F:181:GLN:HE22	0.93	1.09
6:X:123:SER:HB3	6:X:136:LYS:HG2	1.36	1.07
4:R:34:GLN:HE21	4:R:34:GLN:HA	1.15	1.07
14:U:44:MET:HE2	14:U:70:LEU:HD23	1.11	1.07
9:L:205:LEU:HD22	9:L:210:VAL:CG1	1.84	1.07
9:G:205:LEU:HD22	9:G:210:VAL:CG1	1.84	1.06
4:K:34:GLN:HA	4:K:34:GLN:HE21	1.15	1.05
4:R:155:ASP:HB2	4:R:156:PRO:HD2	1.10	1.05
6:S:123:SER:HB3	6:S:136:LYS:HG2	1.36	1.04
3:I:208:LEU:HD11	3:I:220:LEU:HD12	1.39	1.04
1:F:150:LYS:HE3	1:F:181:GLN:NE2	1.73	1.04
8:J:168:ALA:CB	8:J:200:VAL:CG1	2.36	1.03
14:U:44:MET:CE	14:U:70:LEU:HD23	1.89	1.03
8:J:168:ALA:HB1	8:J:200:VAL:HG13	1.39	1.03
14:Y:44:MET:CE	14:Y:70:LEU:HD23	1.89	1.03
8:Q:168:ALA:CB	8:Q:200:VAL:CG1	2.36	1.03
8:Q:168:ALA:HB1	8:Q:200:VAL:HG13	1.39	1.03
9:G:35:THR:CG2	9:G:62:LYS:HE2	1.89	1.02
3:N:208:LEU:HD11	3:N:220:LEU:HD12	1.39	1.02
1:A:150:LYS:HE3	1:A:181:GLN:NE2	1.73	1.02
10:M:51:GLU:CB	10:M:206:MET:CE	2.38	1.02
10:H:51:GLU:HB2	10:H:206:MET:CE	1.89	1.02
9:L:35:THR:CG2	9:L:62:LYS:HE2	1.89	1.01
10:M:51:GLU:HB2	10:M:206:MET:CE	1.89	1.01
4:K:51:VAL:HG12	4:K:202:LEU:HD22	1.40	1.01
10:H:51:GLU:CB	10:H:206:MET:CE	2.38	1.01
7:C:37:GLU:HG2	7:C:185:TRP:CZ2	1.96	1.01
8:Q:34:SER:HB2	8:Q:65:ARG:HH12	1.24	1.01
7:D:37:GLU:HG2	7:D:185:TRP:CZ2	1.96	1.00
2:b:37:ILE:HD11	2:b:173:LEU:HD21	1.42	1.00
2:P:37:ILE:HD11	2:P:173:LEU:HD21	1.42	1.00
8:Q:42:LYS:HG3	8:Q:182:LYS:O	1.61	1.00
8:J:34:SER:HB2	8:J:65:ARG:HH12	1.24	1.00
4:R:51:VAL:HG12	4:R:202:LEU:HD22	1.39	1.00
4:R:174:GLU:HB3	4:R:205:VAL:HG22	1.42	0.99
8:J:42:LYS:HG3	8:J:182:LYS:O	1.61	0.99
9:L:35:THR:HG23	9:L:62:LYS:HE2	1.45	0.98
4:K:174:GLU:HB3	4:K:205:VAL:HG22	1.42	0.98
9:G:166:GLN:O	9:G:170:THR:HG23	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:107:MET:CE	10:H:112:VAL:HG22	1.94	0.97
9:G:35:THR:HG23	9:G:62:LYS:HE2	1.45	0.97
8:Q:168:ALA:HB1	8:Q:200:VAL:CG1	1.94	0.97
13:a:94:ARG:HH21	13:a:94:ARG:HG3	1.28	0.97
13:W:94:ARG:HH21	13:W:94:ARG:HG3	1.28	0.96
9:L:166:GLN:O	9:L:170:THR:HG23	1.62	0.96
4:R:155:ASP:HB2	4:R:156:PRO:CD	1.95	0.96
10:M:107:MET:CE	10:M:112:VAL:HG22	1.94	0.96
8:Q:117:MET:HE2	8:Q:117:MET:HA	1.46	0.96
4:K:226:LYS:HE2	4:K:226:LYS:N	1.81	0.96
4:K:155:ASP:HB2	4:K:156:PRO:CD	1.95	0.95
4:R:226:LYS:HE2	4:R:226:LYS:N	1.81	0.95
9:G:230:SER:OG	9:G:231:PRO:HD3	1.67	0.95
9:L:199:LEU:HD22	9:L:200:PRO:HD2	1.46	0.95
10:H:54:ILE:H	10:H:54:ILE:HD12	1.32	0.95
9:L:230:SER:OG	9:L:231:PRO:HD3	1.66	0.95
11:O:174:MET:HG2	11:O:196:VAL:HG22	1.48	0.94
2:P:156:ALA:CB	11:O:59:VAL:HG21	1.97	0.94
9:G:199:LEU:HD22	9:G:200:PRO:HD2	1.46	0.94
10:M:51:GLU:CB	10:M:206:MET:HE2	1.97	0.94
11:Z:174:MET:HG2	11:Z:196:VAL:HG22	1.48	0.94
8:J:117:MET:HE2	8:J:117:MET:HA	1.46	0.93
7:D:39:ASN:HB2	7:D:40:PRO:CD	1.99	0.93
8:J:168:ALA:HB1	8:J:200:VAL:CG1	1.94	0.93
2:b:118:GLN:HG3	11:Z:81:SER:HB2	1.49	0.93
11:Z:50:ARG:HG2	11:Z:50:ARG:HH11	1.34	0.93
13:a:178:TYR:CE1	13:a:207:THR:CG2	2.51	0.93
10:H:51:GLU:CB	10:H:206:MET:HE2	1.97	0.93
2:b:156:ALA:CB	11:Z:59:VAL:HG21	1.99	0.92
12:B:112:SER:HB2	12:B:127:MET:CE	1.99	0.92
13:W:44:ARG:HG2	13:W:44:ARG:HH11	1.34	0.92
10:M:54:ILE:H	10:M:54:ILE:HD12	1.32	0.92
13:W:178:TYR:CE1	13:W:207:THR:CG2	2.51	0.92
2:b:73:LEU:HD23	2:b:82:TYR:HE1	1.33	0.92
11:O:50:ARG:HG2	11:O:50:ARG:HH11	1.34	0.92
12:E:112:SER:HB2	12:E:127:MET:CE	1.99	0.92
2:P:73:LEU:HD23	2:P:82:TYR:HE1	1.33	0.92
1:F:145:ARG:HH11	1:F:145:ARG:HG3	1.34	0.92
9:L:56:LEU:HD12	10:M:167:ALA:HB3	1.52	0.92
12:E:40:ASN:HD22	12:E:40:ASN:H	1.14	0.92
6:S:148:LEU:HD12	6:S:178:VAL:CG1	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:39:ASN:HB2	7:C:40:PRO:CD	1.99	0.91
13:a:44:ARG:HG2	13:a:44:ARG:HH11	1.34	0.91
10:H:157:ASP:HB2	10:H:158:PRO:HD2	1.52	0.91
4:R:155:ASP:CB	4:R:156:PRO:HD2	2.00	0.91
8:J:152:ASP:HB2	8:J:153:PRO:CD	2.01	0.91
8:J:187:ARG:HH11	8:J:219:LEU:HD21	1.35	0.91
8:Q:152:ASP:HB2	8:Q:153:PRO:CD	2.01	0.91
8:Q:34:SER:HB2	8:Q:65:ARG:NH1	1.86	0.90
4:R:195:VAL:O	4:R:199:ILE:HD13	1.71	0.90
6:X:148:LEU:HD12	6:X:178:VAL:CG1	2.00	0.90
1:F:150:LYS:CE	1:F:181:GLN:HE22	1.83	0.90
11:Z:230:GLN:HE21	11:Z:230:GLN:HA	1.36	0.90
2:P:10:THR:HG23	2:P:20:GLN:HB2	1.51	0.90
6:S:188:TYR:OH	12:B:24:MET:CE	2.20	0.90
10:H:66:LYS:HB2	10:H:216:GLU:OE2	1.71	0.90
13:a:178:TYR:CZ	13:a:207:THR:HG22	2.06	0.90
12:B:40:ASN:HD22	12:B:40:ASN:H	1.14	0.90
12:E:24:MET:CE	6:X:188:TYR:OH	2.20	0.90
4:K:195:VAL:O	4:K:199:ILE:HD13	1.71	0.90
11:O:230:GLN:HA	11:O:230:GLN:HE21	1.36	0.90
8:J:34:SER:HB2	8:J:65:ARG:NH1	1.86	0.89
12:B:112:SER:HB2	12:B:127:MET:HE2	1.54	0.89
13:W:178:TYR:CZ	13:W:207:THR:HG22	2.06	0.89
2:P:155:PHE:HD2	11:O:51:ASN:HD21	1.18	0.89
4:K:49:VAL:HG22	4:K:219:VAL:HG12	1.55	0.89
10:H:167:ALA:HB3	9:G:56:LEU:HD12	1.54	0.89
10:M:157:ASP:HB2	10:M:158:PRO:HD2	1.52	0.89
10:H:107:MET:HE3	10:H:112:VAL:HG22	1.52	0.89
8:Q:66:LEU:CD2	8:Q:214:SER:OG	2.21	0.89
9:L:68:ASN:HB3	9:L:220:GLU:HG2	1.54	0.89
9:G:199:LEU:CD2	9:G:200:PRO:HD2	2.02	0.89
10:M:107:MET:HE3	10:M:112:VAL:HG22	1.52	0.89
9:G:68:ASN:HB3	9:G:220:GLU:HG2	1.54	0.89
2:b:10:THR:HG23	2:b:20:GLN:HB2	1.51	0.89
14:U:44:MET:HE2	14:U:70:LEU:CD2	2.02	0.89
10:M:66:LYS:HB2	10:M:216:GLU:OE2	1.71	0.89
6:S:188:TYR:OH	12:B:24:MET:HE2	1.71	0.88
2:P:118:GLN:HG3	11:O:81:SER:HB2	1.55	0.88
10:H:206:MET:HE1	10:H:215:ILE:HG22	1.55	0.88
9:L:199:LEU:CD2	9:L:200:PRO:HD2	2.02	0.88
10:M:206:MET:HE1	10:M:215:ILE:HG22	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:HG3	1:A:145:ARG:HH11	1.34	0.88
7:D:176:ASN:HD22	7:D:187:ARG:NH2	1.72	0.88
4:R:49:VAL:HG22	4:R:219:VAL:HG12	1.55	0.88
7:C:159:ARG:HE	7:C:163:GLN:HE21	1.21	0.88
7:C:176:ASN:HD22	7:C:187:ARG:NH2	1.72	0.88
8:Q:187:ARG:HH11	8:Q:219:LEU:HD21	1.35	0.88
10:H:91:LYS:HD2	10:H:119:LEU:HD11	1.57	0.87
12:E:112:SER:HB2	12:E:127:MET:HE2	1.54	0.87
10:M:91:LYS:HD2	10:M:119:LEU:HD11	1.57	0.87
12:E:24:MET:HE2	6:X:188:TYR:OH	1.73	0.87
4:R:174:GLU:HB3	4:R:205:VAL:CG2	2.03	0.87
6:S:188:TYR:CZ	12:B:24:MET:HE3	2.10	0.87
8:J:187:ARG:NH1	8:J:219:LEU:HD21	1.90	0.87
4:K:174:GLU:HB3	4:K:205:VAL:CG2	2.03	0.87
12:E:24:MET:HE3	6:X:188:TYR:CZ	2.10	0.87
1:A:150:LYS:CE	1:A:181:GLN:HE22	1.83	0.86
10:H:157:ASP:HB2	10:H:158:PRO:CD	2.05	0.86
14:Y:44:MET:HE2	14:Y:70:LEU:CD2	2.02	0.86
7:D:159:ARG:HE	7:D:163:GLN:HE21	1.21	0.86
4:K:52:THR:HG23	4:K:216:GLU:HG3	1.58	0.86
8:J:66:LEU:CD2	8:J:214:SER:OG	2.21	0.86
2:b:155:PHE:HD2	11:Z:51:ASN:HD21	1.24	0.86
8:Q:168:ALA:HB3	8:Q:200:VAL:CG1	2.05	0.86
10:M:157:ASP:HB2	10:M:158:PRO:CD	2.05	0.85
8:Q:187:ARG:NH1	8:Q:219:LEU:HD21	1.90	0.85
6:X:13:LEU:HD11	6:X:149:LEU:HD11	1.56	0.85
6:X:72:LEU:HD23	6:X:83:MET:HE3	1.57	0.85
3:N:86:ARG:HG3	3:N:86:ARG:HH21	1.42	0.85
4:K:78:CYS:HB3	4:K:140:LEU:HD23	1.59	0.85
10:H:38:ILE:HD13	10:H:201:ILE:HG22	1.59	0.85
14:U:70:LEU:HD21	14:U:86:LEU:HD13	1.57	0.85
4:R:51:VAL:CG1	4:R:202:LEU:HD22	2.06	0.85
4:R:78:CYS:HB3	4:R:140:LEU:HD23	1.59	0.85
8:J:211:LEU:HD21	8:J:213:LEU:HD11	1.59	0.85
10:M:38:ILE:HD13	10:M:201:ILE:HG22	1.59	0.85
8:Q:211:LEU:HD21	8:Q:213:LEU:HD11	1.59	0.85
7:D:9:PHE:HD1	7:D:9:PHE:H	1.25	0.84
6:S:13:LEU:HD11	6:S:149:LEU:HD11	1.56	0.84
8:J:168:ALA:HB3	8:J:200:VAL:CG1	2.05	0.84
3:I:86:ARG:HH21	3:I:86:ARG:HG3	1.42	0.84
8:Q:66:LEU:HD22	8:Q:214:SER:HG	1.38	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:126:ALA:HB1	7:D:140:MET:HE3	1.60	0.84
8:J:168:ALA:CB	8:J:200:VAL:HG13	2.06	0.84
14:Y:70:LEU:HD21	14:Y:86:LEU:HD13	1.58	0.84
4:R:52:THR:HG23	4:R:216:GLU:HG3	1.58	0.84
4:K:51:VAL:CG1	4:K:202:LEU:HD22	2.06	0.84
6:S:72:LEU:HD23	6:S:83:MET:HE3	1.57	0.84
8:J:152:ASP:HB2	8:J:153:PRO:HD2	1.60	0.84
10:H:146:VAL:HG11	10:H:222:PRO:HA	1.60	0.83
9:L:168:ALA:HB2	9:L:198:THR:CG2	2.08	0.83
9:L:13:TRP:H	8:Q:22:GLN:HE22	1.22	0.83
9:G:205:LEU:HD22	9:G:210:VAL:HG11	1.57	0.83
8:Q:152:ASP:HB2	8:Q:153:PRO:HD2	1.60	0.83
6:X:8:ASN:HD22	6:X:58:HIS:H	1.27	0.83
10:M:38:ILE:CD1	10:M:201:ILE:HG22	2.09	0.83
7:C:126:ALA:HB1	7:C:140:MET:HE3	1.60	0.83
6:S:8:ASN:HD22	6:S:58:HIS:H	1.27	0.82
9:G:168:ALA:HB2	9:G:198:THR:CG2	2.08	0.82
10:H:49:ALA:HB2	10:H:217:LEU:HD12	1.61	0.82
2:P:83:ARG:HG2	2:P:83:ARG:HH11	1.45	0.82
2:b:83:ARG:HG2	2:b:83:ARG:HH11	1.45	0.82
10:H:38:ILE:HD13	10:H:201:ILE:CG2	2.10	0.82
7:C:9:PHE:HD1	7:C:9:PHE:H	1.25	0.82
7:C:39:ASN:HB2	7:C:40:PRO:HD2	1.61	0.82
9:L:205:LEU:HD22	9:L:210:VAL:HG11	1.57	0.82
10:H:51:GLU:HG3	10:H:206:MET:CE	2.05	0.82
10:H:66:LYS:CB	10:H:216:GLU:OE2	2.27	0.82
12:E:76:VAL:HG23	12:E:104:ASP:OD2	1.80	0.82
7:D:39:ASN:HB2	7:D:40:PRO:HD2	1.61	0.81
10:H:38:ILE:CD1	10:H:201:ILE:HG22	2.09	0.81
10:M:146:VAL:HG11	10:M:222:PRO:HA	1.60	0.81
11:Z:77:ALA:HB3	11:Z:164:ILE:HD12	1.61	0.81
6:X:102:PHE:N	6:X:103:PRO:CD	2.43	0.81
11:O:174:MET:HE1	11:O:199:LYS:HG2	1.62	0.81
10:M:66:LYS:CB	10:M:216:GLU:OE2	2.27	0.81
6:S:102:PHE:N	6:S:103:PRO:CD	2.43	0.81
11:O:77:ALA:HB3	11:O:164:ILE:HD12	1.62	0.81
4:R:195:VAL:O	4:R:199:ILE:CD1	2.28	0.81
10:M:38:ILE:HD13	10:M:201:ILE:CG2	2.10	0.81
4:K:195:VAL:O	4:K:199:ILE:CD1	2.28	0.81
2:b:73:LEU:HD23	2:b:82:TYR:CE1	2.15	0.81
10:M:51:GLU:HG3	10:M:206:MET:CE	2.05	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:66:LEU:HD22	8:J:214:SER:HG	1.42	0.80
5:T:88:LEU:HD23	5:T:118:MET:HE3	1.61	0.80
2:P:73:LEU:HD23	2:P:82:TYR:CE1	2.16	0.80
12:B:76:VAL:HG23	12:B:104:ASP:OD2	1.80	0.80
10:M:213:THR:HG22	10:M:231:LYS:HE3	1.64	0.80
5:V:88:LEU:HD23	5:V:118:MET:HE3	1.61	0.80
10:H:51:GLU:CB	10:H:206:MET:HE3	2.05	0.80
10:M:91:LYS:CD	10:M:119:LEU:HD11	2.11	0.80
9:G:183:ASN:H	9:G:183:ASN:HD22	1.29	0.80
8:Q:40:ARG:HD3	8:Q:161:TRP:CE3	2.17	0.80
4:K:139:ILE:HG12	4:K:153:LYS:HG3	1.63	0.80
10:M:49:ALA:HB2	10:M:217:LEU:HD12	1.61	0.80
11:Z:174:MET:HE1	11:Z:199:LYS:HG2	1.62	0.79
8:J:135:PHE:CE2	8:J:151:ILE:HD12	2.17	0.79
13:a:9:THR:O	13:a:54:SER:HB2	1.83	0.79
4:R:178:PHE:CE1	4:R:201:CYS:HB2	2.18	0.79
8:J:40:ARG:HD3	8:J:161:TRP:CE3	2.17	0.79
10:H:213:THR:HG22	10:H:231:LYS:HE3	1.64	0.79
8:Q:135:PHE:CE2	8:Q:151:ILE:HD12	2.17	0.79
4:R:139:ILE:HG12	4:R:153:LYS:HG3	1.63	0.79
10:H:91:LYS:CD	10:H:119:LEU:HD11	2.11	0.79
4:K:178:PHE:CE1	4:K:201:CYS:HB2	2.18	0.79
8:Q:141:SER:HB3	8:Q:144:ASP:HB2	1.65	0.79
8:J:70:ASP:OD2	8:J:95:ALA:HB1	1.83	0.79
4:K:25:VAL:HG21	4:K:126:THR:HG23	1.64	0.79
4:K:34:GLN:HA	4:K:34:GLN:NE2	1.95	0.79
8:J:108:LEU:HD22	8:J:139:SER:HB3	1.65	0.78
10:M:117:SER:OG	10:M:156:MET:HG3	1.83	0.78
2:b:118:GLN:CG	11:Z:81:SER:HB2	2.14	0.78
5:T:153:ARG:O	5:T:157:VAL:HG23	1.84	0.78
13:W:9:THR:O	13:W:54:SER:HB2	1.83	0.78
10:M:202:LEU:HD23	10:M:215:ILE:HG21	1.65	0.78
4:R:25:VAL:HG21	4:R:126:THR:HG23	1.64	0.78
8:J:36:ALA:CB	8:J:49:VAL:HG22	2.14	0.78
6:S:70:ALA:O	6:S:74:MET:HG3	1.84	0.78
7:D:145:SER:HB3	7:D:148:LEU:HD13	1.65	0.78
10:H:92:ALA:O	10:H:96:THR:HG23	1.84	0.78
10:H:181:LEU:HD23	10:H:201:ILE:CD1	2.14	0.78
9:L:183:ASN:H	9:L:183:ASN:HD22	1.29	0.77
10:H:202:LEU:HD23	10:H:215:ILE:HG21	1.65	0.77
8:Q:108:LEU:HD22	8:Q:139:SER:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:50:ARG:HG2	11:O:50:ARG:NH1	1.97	0.77
14:U:100:GLY:N	14:U:101:PRO:CD	2.46	0.77
13:W:92:LEU:HD12	13:W:112:ILE:HD11	1.66	0.77
11:Z:50:ARG:HG2	11:Z:50:ARG:NH1	1.97	0.77
8:Q:36:ALA:CB	8:Q:49:VAL:HG22	2.14	0.77
4:R:34:GLN:HA	4:R:34:GLN:NE2	1.96	0.77
8:Q:70:ASP:OD2	8:Q:95:ALA:HB1	1.83	0.77
8:J:22:GLN:HE22	9:G:13:TRP:H	1.28	0.77
11:O:41:ASP:OD1	11:O:41:ASP:N	2.18	0.77
3:I:41:VAL:HG23	3:I:211:MET:HB3	1.67	0.77
8:J:141:SER:HB3	8:J:144:ASP:HB2	1.65	0.77
13:W:16:PHE:CZ	13:W:162:GLN:HG2	2.20	0.77
13:a:92:LEU:HD12	13:a:112:ILE:HD11	1.66	0.77
5:V:88:LEU:CD2	5:V:118:MET:HE3	2.15	0.77
2:b:94:GLN:OE1	12:B:61:SER:HB2	1.85	0.77
10:H:117:SER:OG	10:H:156:MET:HG3	1.83	0.77
10:M:181:LEU:CD2	10:M:201:ILE:HD13	2.15	0.77
14:Y:100:GLY:N	14:Y:101:PRO:CD	2.46	0.77
2:P:94:GLN:OE1	12:E:61:SER:HB2	1.85	0.76
3:I:148:ASP:HB2	3:I:149:PRO:HD2	1.68	0.76
6:X:70:ALA:O	6:X:74:MET:HG3	1.84	0.76
4:R:102:LYS:HD3	4:R:108:GLU:OE2	1.86	0.76
10:H:181:LEU:CD2	10:H:201:ILE:HD13	2.15	0.76
13:W:152:GLU:O	13:W:152:GLU:HG2	1.85	0.76
8:Q:108:LEU:HD23	8:Q:147:GLN:HB2	1.68	0.76
4:K:102:LYS:HD3	4:K:108:GLU:OE2	1.86	0.76
9:L:168:ALA:HB2	9:L:198:THR:HG23	1.67	0.76
9:L:206:THR:O	9:L:210:VAL:HG22	1.86	0.76
7:C:159:ARG:HE	7:C:163:GLN:NE2	1.84	0.76
9:G:206:THR:O	9:G:210:VAL:HG22	1.86	0.76
11:Z:41:ASP:OD1	11:Z:41:ASP:N	2.17	0.76
10:M:92:ALA:O	10:M:96:THR:HG23	1.84	0.76
11:O:151:ASP:HB2	11:O:152:PRO:HD2	1.66	0.76
10:M:181:LEU:HD23	10:M:201:ILE:CD1	2.14	0.76
7:D:4:THR:HG22	7:D:17:ALA:CB	2.16	0.75
7:C:145:SER:HB3	7:C:148:LEU:HD13	1.65	0.75
6:X:167:THR:HG22	6:X:170:ARG:HB3	1.68	0.75
3:I:86:ARG:HG3	3:I:86:ARG:NH2	1.99	0.75
9:G:168:ALA:HB2	9:G:198:THR:HG23	1.67	0.75
5:T:88:LEU:CD2	5:T:118:MET:HE3	2.15	0.75
6:S:167:THR:HG22	6:S:170:ARG:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:108:LEU:HD23	8:J:147:GLN:HB2	1.68	0.75
11:Z:151:ASP:HB2	11:Z:152:PRO:HD2	1.66	0.75
7:C:4:THR:HG22	7:C:17:ALA:CB	2.16	0.75
3:N:41:VAL:HG23	3:N:211:MET:HB3	1.67	0.75
3:N:148:ASP:HB2	3:N:149:PRO:HD2	1.68	0.75
10:H:51:GLU:HA	10:H:206:MET:CE	2.17	0.75
1:F:191:LEU:N	1:F:191:LEU:HD23	2.01	0.75
10:M:166:ASP:HB3	10:M:185:TYR:CZ	2.21	0.75
2:b:171:THR:O	2:b:175:LYS:HG3	1.86	0.75
13:a:16:PHE:CZ	13:a:162:GLN:HG2	2.20	0.75
13:a:152:GLU:HG2	13:a:152:GLU:O	1.85	0.75
10:M:51:GLU:HA	10:M:206:MET:CE	2.17	0.75
3:N:147:THR:HG22	3:N:153:TYR:HB3	1.69	0.75
1:A:191:LEU:N	1:A:191:LEU:HD23	2.01	0.74
5:V:153:ARG:O	5:V:157:VAL:HG23	1.84	0.74
13:W:94:ARG:HG3	13:W:94:ARG:NH2	1.98	0.74
8:Q:168:ALA:CB	8:Q:200:VAL:HG13	2.06	0.74
2:P:171:THR:O	2:P:175:LYS:HG3	1.86	0.74
10:H:135:ARG:HH21	10:H:135:ARG:HG3	1.53	0.74
8:Q:68:ASN:ND2	13:a:76:LEU:O	2.21	0.74
11:O:95:GLN:HE22	11:O:98:LEU:HD23	1.52	0.74
11:Z:95:GLN:HE22	11:Z:98:LEU:HD23	1.52	0.74
14:U:70:LEU:CD2	14:U:86:LEU:CD1	2.66	0.74
10:M:135:ARG:HH21	10:M:135:ARG:HG3	1.53	0.74
10:H:181:LEU:HD23	10:H:201:ILE:HD13	1.70	0.74
10:M:54:ILE:HD12	10:M:54:ILE:N	2.03	0.74
11:O:151:ASP:HB2	11:O:152:PRO:CD	2.18	0.74
9:L:9:ASP:OD1	11:O:3:ARG:NH1	2.21	0.73
14:Y:70:LEU:CD2	14:Y:86:LEU:CD1	2.66	0.73
3:N:86:ARG:HG3	3:N:86:ARG:NH2	1.99	0.73
3:N:221:ASN:HB2	3:N:222:PRO:HD2	1.71	0.73
7:D:159:ARG:HE	7:D:163:GLN:NE2	1.84	0.73
10:H:166:ASP:HB3	10:H:185:TYR:CZ	2.21	0.73
6:X:8:ASN:ND2	6:X:58:HIS:H	1.86	0.73
10:H:54:ILE:HD12	10:H:54:ILE:N	2.03	0.73
11:O:206:LEU:HD22	11:O:211:VAL:HG11	1.69	0.73
3:I:147:THR:HG22	3:I:153:TYR:HB3	1.69	0.73
3:I:221:ASN:HB2	3:I:222:PRO:HD2	1.70	0.73
6:S:8:ASN:ND2	6:S:58:HIS:H	1.86	0.73
8:J:68:ASN:ND2	13:W:76:LEU:O	2.21	0.73
9:G:19:ILE:HG21	9:G:22:ILE:HD12	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:118:GLN:CG	11:O:81:SER:HB2	2.19	0.73
11:Z:151:ASP:HB2	11:Z:152:PRO:CD	2.18	0.73
5:V:143:LEU:HD13	5:V:163:CYS:SG	2.29	0.73
10:M:37:ALA:HB2	10:M:50:VAL:HG13	1.71	0.73
10:H:44:GLU:OE1	10:H:191:LEU:N	2.20	0.72
13:a:16:PHE:CE1	13:a:162:GLN:CG	2.72	0.72
14:Y:19:VAL:HG23	14:Y:189:ILE:HB	1.71	0.72
4:K:196:GLU:HG2	4:K:242:LEU:HD23	1.71	0.72
3:N:42:VAL:HG13	3:N:210:VAL:HG12	1.72	0.72
4:R:212:PRO:HG3	4:R:236:ASP:OD2	1.89	0.72
10:H:37:ALA:HB2	10:H:50:VAL:HG13	1.71	0.72
11:Z:206:LEU:HD22	11:Z:211:VAL:HG11	1.69	0.72
6:X:145:LEU:HD21	6:X:182:ALA:HB2	1.70	0.72
6:S:145:LEU:HD21	6:S:182:ALA:HB2	1.70	0.72
7:D:10:LEU:HD12	7:D:10:LEU:O	1.90	0.72
5:V:88:LEU:HD22	5:V:118:MET:CE	2.20	0.72
10:M:181:LEU:HD23	10:M:201:ILE:HD13	1.70	0.72
14:U:19:VAL:HG23	14:U:189:ILE:HB	1.71	0.72
4:R:196:GLU:HG2	4:R:242:LEU:HD23	1.71	0.72
4:K:155:ASP:CB	4:K:156:PRO:HD2	2.00	0.72
4:K:212:PRO:HG3	4:K:236:ASP:OD2	1.89	0.72
13:W:16:PHE:CE1	13:W:162:GLN:CG	2.72	0.72
8:Q:185:THR:O	8:Q:189:VAL:HG23	1.89	0.72
7:D:84:LEU:HD21	7:D:100:THR:HG21	1.72	0.72
7:C:10:LEU:O	7:C:10:LEU:HD12	1.90	0.72
10:M:51:GLU:CG	10:M:206:MET:CE	2.61	0.72
1:A:145:ARG:HG3	1:A:145:ARG:NH1	2.04	0.71
3:I:42:VAL:HG13	3:I:210:VAL:HG12	1.72	0.71
3:I:190:LEU:HD12	3:I:190:LEU:O	1.90	0.71
14:Y:158:ASP:OD1	14:Y:158:ASP:N	2.23	0.71
5:V:1:MET:HG2	5:V:134:TYR:H	1.55	0.71
5:V:88:LEU:HD22	5:V:118:MET:HE2	1.72	0.71
2:b:70:HIS:CE1	2:b:103:PRO:HB3	2.25	0.71
1:A:5:MET:HG3	1:A:128:ILE:HG22	1.73	0.71
10:H:107:MET:HE3	10:H:112:VAL:CG2	2.20	0.71
2:P:70:HIS:CE1	2:P:103:PRO:HB3	2.25	0.71
5:T:88:LEU:HD22	5:T:118:MET:CE	2.20	0.71
7:C:84:LEU:HD21	7:C:100:THR:HG21	1.72	0.71
11:O:174:MET:HE1	11:O:199:LYS:CG	2.21	0.71
10:M:38:ILE:CD1	10:M:201:ILE:CG2	2.68	0.71
10:M:38:ILE:HD12	10:M:202:LEU:HD12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:W:151:ARG:NH2	6:X:35:ILE:O	2.23	0.71
1:F:5:MET:HG3	1:F:128:ILE:HG22	1.73	0.71
14:U:70:LEU:HD21	14:U:86:LEU:CD1	2.20	0.71
10:M:44:GLU:HG3	10:M:191:LEU:HB2	1.72	0.71
5:T:143:LEU:HD13	5:T:163:CYS:SG	2.29	0.71
9:L:19:ILE:HG21	9:L:22:ILE:HD12	1.71	0.71
3:I:168:VAL:HA	3:I:197:GLU:OE2	1.91	0.71
14:U:158:ASP:N	14:U:158:ASP:OD1	2.23	0.71
10:H:38:ILE:HD12	10:H:202:LEU:HD12	1.71	0.71
13:a:16:PHE:CE1	13:a:162:GLN:HG3	2.26	0.71
9:G:118:ILE:HB	9:G:119:PRO:HD3	1.72	0.71
8:J:185:THR:O	8:J:189:VAL:HG23	1.89	0.71
10:H:107:MET:HE2	10:H:112:VAL:HG22	1.72	0.71
12:B:213:THR:O	14:Y:197:ARG:HB3	1.91	0.71
2:P:156:ALA:HB2	11:O:59:VAL:HG21	1.72	0.70
9:L:122:ARG:HB2	9:L:125:ARG:HG3	1.72	0.70
9:L:183:ASN:H	9:L:183:ASN:ND2	1.88	0.70
10:H:38:ILE:CD1	10:H:201:ILE:CG2	2.68	0.70
13:W:16:PHE:CE1	13:W:162:GLN:HG3	2.26	0.70
9:G:122:ARG:HB2	9:G:125:ARG:HG3	1.72	0.70
14:U:6:ASN:HD22	14:U:56:ALA:H	1.39	0.70
11:O:35:LEU:C	11:O:35:LEU:HD12	2.16	0.70
11:Z:35:LEU:C	11:Z:35:LEU:HD12	2.16	0.70
3:N:168:VAL:HA	3:N:197:GLU:OE2	1.91	0.70
5:V:18:ASP:OD1	5:V:34:LYS:CE	2.39	0.70
2:b:176:ARG:HG3	2:b:176:ARG:O	1.91	0.70
8:Q:186:CYS:O	8:Q:190:VAL:HG23	1.91	0.70
14:U:98:ARG:O	14:U:98:ARG:HD2	1.92	0.70
5:T:1:MET:HG2	5:T:134:TYR:H	1.55	0.70
8:Q:51:LYS:HG3	8:Q:212:GLU:OE2	1.92	0.70
12:E:213:THR:O	14:U:197:ARG:HB3	1.92	0.70
11:Z:174:MET:HE1	11:Z:199:LYS:CG	2.21	0.70
14:Y:70:LEU:HD21	14:Y:86:LEU:CD1	2.20	0.70
5:T:18:ASP:OD1	5:T:34:LYS:CE	2.39	0.70
8:Q:37:ILE:HD11	8:Q:193:VAL:HG22	1.74	0.70
3:N:190:LEU:HD12	3:N:190:LEU:O	1.90	0.70
8:J:186:CYS:O	8:J:190:VAL:HG23	1.91	0.70
13:W:44:ARG:HG2	13:W:44:ARG:NH1	2.04	0.70
8:J:37:ILE:HD11	8:J:193:VAL:HG22	1.74	0.70
9:L:118:ILE:HB	9:L:119:PRO:HD3	1.72	0.70
12:B:40:ASN:HD22	12:B:40:ASN:N	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:51:LEU:HD21	13:a:110:MET:HG2	1.73	0.70
2:P:122:GLN:O	11:O:127:LYS:HG2	1.92	0.69
2:P:176:ARG:HG3	2:P:176:ARG:O	1.91	0.69
2:b:156:ALA:HB2	11:Z:59:VAL:HG21	1.72	0.69
10:H:44:GLU:HG3	10:H:191:LEU:HB2	1.73	0.69
3:I:40:ILE:HG13	3:I:212:ARG:HG3	1.74	0.69
10:M:206:MET:HE1	10:M:215:ILE:CG2	2.22	0.69
14:Y:6:ASN:HD22	14:Y:56:ALA:H	1.39	0.69
3:N:40:ILE:HG13	3:N:212:ARG:HG3	1.74	0.69
8:J:51:LYS:HG3	8:J:212:GLU:OE2	1.92	0.69
4:K:80:MET:HE2	4:K:87:SER:HA	1.74	0.69
10:H:206:MET:HE1	10:H:215:ILE:CG2	2.22	0.69
13:W:51:LEU:HD21	13:W:110:MET:HG2	1.73	0.69
11:Z:199:LYS:O	11:Z:199:LYS:HG3	1.92	0.69
5:T:88:LEU:HD22	5:T:118:MET:HE2	1.72	0.69
10:M:107:MET:HE2	10:M:112:VAL:HG22	1.72	0.69
8:Q:168:ALA:CB	8:Q:200:VAL:HG11	2.23	0.69
14:Y:98:ARG:HD2	14:Y:98:ARG:O	1.92	0.69
2:P:156:ALA:CB	11:O:59:VAL:CG2	2.70	0.69
9:G:183:ASN:H	9:G:183:ASN:ND2	1.88	0.69
13:a:44:ARG:HG2	13:a:44:ARG:NH1	2.04	0.69
6:S:148:LEU:CD1	6:S:178:VAL:HG12	2.16	0.69
10:M:107:MET:HE3	10:M:112:VAL:CG2	2.20	0.69
8:Q:211:LEU:CD2	8:Q:213:LEU:HD11	2.23	0.69
2:b:156:ALA:CB	11:Z:59:VAL:CG2	2.71	0.69
3:N:11:SER:HB3	3:N:12:PRO:HD2	1.75	0.68
4:R:80:MET:HE2	4:R:87:SER:HA	1.74	0.68
8:J:168:ALA:CB	8:J:200:VAL:HG11	2.23	0.68
10:M:51:GLU:CA	10:M:206:MET:CE	2.71	0.68
9:G:84:LEU:O	9:G:88:MET:HG3	1.94	0.68
4:R:37:LEU:HG	4:R:55:LYS:HZ1	1.58	0.68
9:L:84:LEU:O	9:L:88:MET:HG3	1.94	0.68
11:O:199:LYS:O	11:O:199:LYS:HG3	1.92	0.68
7:C:83:LEU:HD22	7:C:87:MET:HE3	1.76	0.68
10:M:44:GLU:OE1	10:M:191:LEU:N	2.20	0.68
13:a:206:GLN:HA	13:a:206:GLN:HE21	1.58	0.68
8:J:211:LEU:CD2	8:J:213:LEU:HD11	2.23	0.68
14:Y:6:ASN:ND2	14:Y:56:ALA:H	1.92	0.68
7:D:83:LEU:HD22	7:D:87:MET:HE3	1.76	0.68
13:W:206:GLN:HE21	13:W:206:GLN:HA	1.58	0.68
4:R:206:LEU:HD12	4:R:210:PHE:HZ	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:162:GLU:CD	6:S:162:GLU:H	2.02	0.68
5:V:88:LEU:CD2	5:V:118:MET:CE	2.71	0.68
8:Q:50:GLU:O	8:Q:50:GLU:HG3	1.94	0.68
14:U:144:GLN:N	14:U:144:GLN:HE21	1.92	0.68
2:P:72:GLY:HA3	2:P:217:PHE:CE1	2.29	0.68
3:N:183:THR:O	3:N:187:THR:HG23	1.93	0.68
10:H:51:GLU:CA	10:H:206:MET:CE	2.71	0.68
12:B:17:ASP:OD1	12:B:33:LYS:NZ	2.25	0.68
13:W:96:MET:HE3	13:W:127:MET:HA	1.76	0.68
14:Y:144:GLN:N	14:Y:144:GLN:HE21	1.92	0.68
14:U:144:GLN:HE21	14:U:144:GLN:H	1.42	0.68
4:R:178:PHE:CZ	4:R:200:THR:HG22	2.29	0.67
5:T:88:LEU:CD2	5:T:118:MET:CE	2.71	0.67
5:T:121:LEU:O	14:U:57:THR:CB	2.42	0.67
3:I:11:SER:HB3	3:I:12:PRO:HD2	1.75	0.67
3:I:183:THR:O	3:I:187:THR:HG23	1.93	0.67
6:X:148:LEU:CD1	6:X:178:VAL:HG12	2.16	0.67
10:H:215:ILE:HD11	10:H:234:LEU:CD2	2.24	0.67
2:P:28:VAL:HG11	2:P:132:SER:HB2	1.75	0.67
2:P:37:ILE:CD1	2:P:173:LEU:HD21	2.21	0.67
14:U:6:ASN:ND2	14:U:56:ALA:H	1.92	0.67
5:V:1:MET:HA	5:V:1:MET:CE	2.25	0.67
2:b:72:GLY:HA3	2:b:217:PHE:CE1	2.29	0.67
6:X:162:GLU:CD	6:X:162:GLU:H	2.02	0.67
4:K:206:LEU:HD12	4:K:210:PHE:HZ	1.58	0.67
2:b:28:VAL:HG11	2:b:132:SER:HB2	1.75	0.67
2:b:149:ASP:HB2	2:b:150:PRO:HD2	1.77	0.67
9:G:9:ASP:OD1	11:Z:3:ARG:NH1	2.28	0.67
6:X:7:PHE:HE2	6:X:188:TYR:CE2	2.12	0.67
3:N:42:VAL:HB	3:N:191:VAL:HG21	1.75	0.67
5:T:1:MET:CE	5:T:1:MET:HA	2.25	0.67
8:J:36:ALA:HB2	8:J:49:VAL:HG22	1.76	0.67
4:K:178:PHE:CZ	4:K:200:THR:HG22	2.29	0.67
5:T:121:LEU:O	14:U:57:THR:HB	1.94	0.67
2:P:68:THR:HG22	2:P:71:ILE:HB	1.76	0.67
10:M:215:ILE:HD11	10:M:234:LEU:CD2	2.24	0.67
9:G:35:THR:CG2	9:G:62:LYS:CE	2.72	0.67
8:J:42:LYS:CG	8:J:182:LYS:O	2.40	0.66
8:J:50:GLU:HG3	8:J:50:GLU:O	1.94	0.66
10:H:57:PRO:HG2	3:I:173:GLU:HG2	1.77	0.66
12:B:3:ILE:HD11	12:B:127:MET:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:24:MET:HE3	6:X:188:TYR:OH	1.92	0.66
2:P:74:VAL:HG12	2:P:134:LEU:HB2	1.78	0.66
3:N:219:ILE:HD12	3:N:219:ILE:N	2.10	0.66
6:S:7:PHE:HE2	6:S:188:TYR:CE2	2.12	0.66
2:b:37:ILE:CD1	2:b:173:LEU:HD21	2.21	0.66
13:W:178:TYR:HE1	13:W:207:THR:CG2	2.07	0.66
8:Q:42:LYS:CG	8:Q:182:LYS:O	2.40	0.66
3:I:42:VAL:HB	3:I:191:VAL:HG21	1.75	0.66
1:F:150:LYS:CE	1:F:181:GLN:NE2	2.50	0.66
6:X:115:GLU:HA	6:X:115:GLU:OE2	1.94	0.66
2:P:149:ASP:HB2	2:P:150:PRO:HD2	1.77	0.66
14:Y:144:GLN:HE21	14:Y:144:GLN:H	1.42	0.66
14:U:144:GLN:H	14:U:144:GLN:NE2	1.93	0.66
2:b:68:THR:HG22	2:b:71:ILE:HB	1.76	0.66
3:I:219:ILE:HD12	3:I:219:ILE:N	2.10	0.66
12:E:40:ASN:HD22	12:E:40:ASN:N	1.90	0.66
10:H:166:ASP:HB3	10:H:185:TYR:OH	1.96	0.66
12:E:3:ILE:HD11	12:E:127:MET:HB2	1.77	0.66
1:F:145:ARG:HG3	1:F:145:ARG:NH1	2.05	0.66
14:U:176:ARG:NH2	6:X:146:GLN:NE2	2.44	0.66
2:b:74:VAL:HG12	2:b:134:LEU:CB	2.26	0.66
8:Q:36:ALA:HB2	8:Q:49:VAL:HG22	1.76	0.66
13:a:96:MET:HE3	13:a:127:MET:HA	1.76	0.66
14:U:11:MET:HG3	14:U:137:VAL:HG12	1.77	0.66
6:X:123:SER:CB	6:X:136:LYS:HG2	2.22	0.66
5:V:49:GLU:HB3	5:V:52:ASP:HB2	1.79	0.65
2:b:74:VAL:HG12	2:b:134:LEU:HB2	1.78	0.65
9:L:49:LEU:HB2	9:L:195:LEU:HD11	1.78	0.65
8:Q:50:GLU:HB3	8:Q:197:ILE:CG2	2.26	0.65
13:a:178:TYR:HE1	13:a:207:THR:CG2	2.06	0.65
5:T:49:GLU:HB3	5:T:52:ASP:HB2	1.79	0.65
9:L:123:TYR:OH	11:O:3:ARG:HB3	1.96	0.65
10:M:166:ASP:HB3	10:M:185:TYR:OH	1.96	0.65
12:E:50:ALA:HB3	14:U:126:ILE:HD12	1.78	0.65
9:G:206:THR:O	9:G:210:VAL:CG2	2.44	0.65
6:S:115:GLU:HA	6:S:115:GLU:OE2	1.94	0.65
8:J:50:GLU:HB3	8:J:197:ILE:CG2	2.26	0.65
5:V:121:LEU:O	14:Y:57:THR:HB	1.97	0.65
14:Y:144:GLN:H	14:Y:144:GLN:NE2	1.93	0.65
2:P:74:VAL:HG12	2:P:134:LEU:CB	2.26	0.65
7:D:4:THR:HG22	7:D:17:ALA:HB1	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:146:GLN:NE2	14:Y:176:ARG:NH2	2.45	0.65
2:b:122:GLN:O	11:Z:127:LYS:HG2	1.96	0.65
13:a:94:ARG:HG3	13:a:94:ARG:NH2	1.98	0.65
8:J:94:GLU:OE2	8:J:114:ARG:HB3	1.96	0.65
12:B:50:ALA:HB3	14:Y:126:ILE:HD12	1.77	0.65
14:Y:11:MET:HG3	14:Y:137:VAL:HG12	1.77	0.65
2:P:58:GLU:N	2:P:58:GLU:OE2	2.30	0.65
2:P:142:ARG:HG2	2:P:143:PRO:HD2	1.79	0.65
8:Q:50:GLU:HB3	8:Q:197:ILE:HG23	1.79	0.65
5:V:121:LEU:O	14:Y:57:THR:CB	2.45	0.65
1:A:150:LYS:CE	1:A:181:GLN:NE2	2.50	0.64
8:Q:94:GLU:OE2	8:Q:114:ARG:HB3	1.96	0.64
5:V:169:LYS:HG2	5:V:169:LYS:O	1.96	0.64
2:b:58:GLU:N	2:b:58:GLU:OE2	2.30	0.64
9:G:49:LEU:HB2	9:G:195:LEU:HD11	1.78	0.64
4:R:48:ALA:HB3	4:R:220:VAL:CG2	2.28	0.64
4:K:51:VAL:CG1	4:K:202:LEU:CD2	2.75	0.64
3:N:148:ASP:HB2	3:N:149:PRO:CD	2.28	0.64
5:T:169:LYS:HG2	5:T:169:LYS:O	1.96	0.64
9:L:107:ARG:HH22	13:a:74:GLU:CD	2.05	0.64
11:O:212:GLU:HA	11:O:212:GLU:OE2	1.96	0.64
11:Z:230:GLN:HA	11:Z:230:GLN:NE2	2.10	0.64
4:R:51:VAL:CG1	4:R:202:LEU:CD2	2.75	0.64
5:V:18:ASP:O	5:V:34:LYS:HE2	1.98	0.64
8:J:50:GLU:HB3	8:J:197:ILE:HG23	1.78	0.64
4:K:48:ALA:HB3	4:K:220:VAL:CG2	2.27	0.64
9:G:93:LEU:HD11	6:X:74:MET:HG2	1.77	0.64
9:L:206:THR:O	9:L:210:VAL:CG2	2.45	0.64
13:W:160:LEU:HD22	13:W:164:GLU:HB3	1.80	0.64
13:a:160:LEU:HD22	13:a:164:GLU:HB3	1.80	0.64
13:a:178:TYR:OH	13:a:208:ASN:N	2.30	0.64
11:Z:212:GLU:HA	11:Z:212:GLU:OE2	1.96	0.64
1:A:145:ARG:H	1:A:148:MET:HE3	1.63	0.64
4:R:141:ILE:HG13	4:R:141:ILE:O	1.98	0.64
4:K:141:ILE:O	4:K:141:ILE:HG13	1.98	0.64
7:C:4:THR:HB	7:C:45:THR:HG21	1.80	0.64
5:T:154:GLU:H	5:T:154:GLU:CD	2.05	0.63
7:C:36:ILE:CG2	7:C:46:MET:HE2	2.28	0.63
12:E:214:GLU:OE1	14:U:195:THR:CG2	2.47	0.63
9:G:157:ARG:HD2	9:G:176:MET:HE3	1.80	0.63
7:D:4:THR:HB	7:D:45:THR:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:18:ASP:O	5:T:34:LYS:HE2	1.98	0.63
7:D:36:ILE:CG2	7:D:46:MET:HE2	2.28	0.63
4:K:25:VAL:CG2	4:K:126:THR:HG23	2.28	0.63
10:H:213:THR:CG2	10:H:231:LYS:HE3	2.28	0.63
3:I:7:ILE:HG13	3:I:124:ARG:O	1.99	0.63
6:S:35:ILE:O	13:a:151:ARG:NH2	2.31	0.63
5:V:154:GLU:CD	5:V:154:GLU:H	2.05	0.63
9:L:157:ARG:HD2	9:L:176:MET:HE3	1.80	0.63
11:O:226:ARG:O	11:O:226:ARG:HD3	1.99	0.63
12:E:24:MET:HE2	6:X:188:TYR:HH	1.63	0.63
6:X:167:THR:HG23	6:X:170:ARG:H	1.64	0.63
8:J:168:ALA:HB3	8:J:200:VAL:HG11	1.80	0.63
10:M:170:ILE:O	10:M:170:ILE:HG12	1.99	0.63
10:M:213:THR:CG2	10:M:231:LYS:HE3	2.28	0.63
13:W:96:MET:HE2	13:W:110:MET:HE1	1.80	0.63
9:L:139:ASP:HB2	13:a:81:HIS:CE1	2.34	0.63
10:H:147:ASP:N	10:H:147:ASP:OD1	2.31	0.63
3:I:148:ASP:HB2	3:I:149:PRO:CD	2.28	0.63
10:M:66:LYS:CG	10:M:216:GLU:OE2	2.46	0.63
4:K:143:ILE:HD13	4:K:149:PRO:HA	1.81	0.63
7:C:4:THR:HG22	7:C:17:ALA:HB1	1.79	0.63
4:R:25:VAL:CG2	4:R:126:THR:HG23	2.28	0.63
4:R:32:ILE:HD13	4:R:137:CYS:SG	2.39	0.63
10:H:51:GLU:HA	10:H:206:MET:HE1	1.80	0.63
8:Q:184:MET:HE1	8:Q:192:GLU:HG3	1.80	0.63
11:Z:226:ARG:O	11:Z:226:ARG:HD3	1.99	0.63
14:Y:12:ALA:HB3	14:Y:136:VAL:HG23	1.81	0.63
5:V:21:ALA:HB3	5:V:29:LYS:HB2	1.81	0.62
2:b:142:ARG:HG2	2:b:143:PRO:HD2	1.79	0.62
10:M:50:VAL:HG23	10:M:67:ILE:HD11	1.81	0.62
10:M:215:ILE:CD1	10:M:234:LEU:HD21	2.29	0.62
2:P:155:PHE:HD2	11:O:51:ASN:ND2	1.92	0.62
4:K:32:ILE:HD13	4:K:137:CYS:SG	2.39	0.62
10:H:66:LYS:CG	10:H:216:GLU:OE2	2.46	0.62
11:O:208:ALA:O	11:O:230:GLN:NE2	2.29	0.62
13:a:96:MET:HE2	13:a:110:MET:HE1	1.80	0.62
2:P:88:ARG:CG	2:P:88:ARG:HH11	2.13	0.62
10:H:50:VAL:HG23	10:H:67:ILE:HD11	1.80	0.62
10:H:215:ILE:CD1	10:H:234:LEU:HD21	2.29	0.62
3:I:189:LYS:NZ	3:I:231:GLU:OE1	2.33	0.62
10:M:215:ILE:HD11	10:M:234:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:74:MET:HG2	9:L:93:LEU:HD11	1.80	0.62
10:H:215:ILE:HD11	10:H:234:LEU:HD22	1.81	0.62
12:B:214:GLU:OE1	14:Y:195:THR:CG2	2.47	0.62
10:M:68:VAL:HG21	10:M:89:ILE:HG13	1.81	0.62
5:T:21:ALA:HB3	5:T:29:LYS:HB2	1.81	0.62
7:D:166:TYR:CE2	14:Y:33:MET:HE1	2.35	0.62
8:J:184:MET:HE1	8:J:192:GLU:HG3	1.80	0.62
14:U:182:MET:HE3	14:U:203:MET:HE3	1.82	0.62
4:K:141:ILE:HD12	4:K:220:VAL:HG22	1.82	0.62
10:M:216:GLU:HB2	10:M:228:MET:CE	2.30	0.62
10:M:54:ILE:H	10:M:54:ILE:CD1	2.10	0.62
8:Q:152:ASP:CB	8:Q:153:PRO:CD	2.74	0.62
11:Z:21:VAL:HG11	11:Z:153:SER:HB3	1.82	0.62
3:N:7:ILE:HG13	3:N:124:ARG:O	1.99	0.62
6:S:167:THR:HG23	6:S:170:ARG:H	1.64	0.62
3:I:232:ILE:HG22	3:I:232:ILE:O	1.99	0.62
9:G:123:TYR:OH	11:Z:3:ARG:HB3	1.98	0.62
8:Q:117:MET:HA	8:Q:117:MET:CE	2.27	0.62
1:F:145:ARG:H	1:F:148:MET:HE3	1.63	0.62
11:Z:200:THR:O	11:Z:200:THR:HG23	2.00	0.62
6:X:25:SER:HB2	6:X:42:LYS:HG3	1.80	0.62
10:H:216:GLU:HB2	10:H:228:MET:CE	2.30	0.61
3:I:57:ARG:NH2	11:Z:108:GLU:OE1	2.31	0.61
9:G:31:GLN:O	9:G:51:ARG:NH2	2.33	0.61
2:P:54:ILE:HG23	2:P:54:ILE:O	2.00	0.61
3:N:232:ILE:O	3:N:232:ILE:HG22	2.00	0.61
6:S:188:TYR:OH	12:B:24:MET:HE3	1.94	0.61
4:K:37:LEU:HG	4:K:55:LYS:HZ1	1.63	0.61
12:B:22:GLU:O	12:B:22:GLU:HG3	1.99	0.61
10:M:147:ASP:N	10:M:147:ASP:OD1	2.31	0.61
13:W:53:ALA:HB3	13:W:60:PHE:CD1	2.35	0.61
8:Q:168:ALA:HB3	8:Q:200:VAL:HG11	1.80	0.61
14:Y:26:ARG:HG3	14:Y:182:MET:HG3	1.82	0.61
3:N:121:SER:OG	3:N:124:ARG:HD2	2.00	0.61
4:R:143:ILE:HD13	4:R:149:PRO:HA	1.81	0.61
6:S:25:SER:HB2	6:S:42:LYS:HG3	1.80	0.61
9:L:35:THR:CG2	9:L:62:LYS:CE	2.72	0.61
10:H:170:ILE:O	10:H:170:ILE:HG12	1.99	0.61
12:E:17:ASP:OD1	12:E:33:LYS:NZ	2.25	0.61
3:N:189:LYS:NZ	3:N:231:GLU:OE1	2.33	0.61
4:R:141:ILE:HD12	4:R:220:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:45:VAL:HG22	9:L:214:ILE:HG23	1.83	0.61
10:M:51:GLU:HA	10:M:206:MET:HE1	1.80	0.61
13:a:53:ALA:HB3	13:a:60:PHE:CD1	2.35	0.61
11:Z:28:ILE:HD11	11:Z:152:PRO:HG3	1.82	0.61
14:U:12:ALA:HB3	14:U:136:VAL:HG23	1.81	0.61
14:U:26:ARG:HG3	14:U:182:MET:HG3	1.82	0.61
2:b:88:ARG:HH11	2:b:88:ARG:CG	2.13	0.61
11:O:230:GLN:HA	11:O:230:GLN:NE2	2.10	0.61
13:a:169:VAL:HG11	13:a:189:ILE:CD1	2.31	0.61
9:L:200:PRO:HG2	9:L:203:GLN:HG2	1.83	0.61
3:I:86:ARG:HH21	3:I:86:ARG:CG	2.12	0.61
9:G:88:MET:HE3	9:G:108:LEU:HD21	1.83	0.61
4:R:220:VAL:HG23	4:R:220:VAL:O	2.00	0.61
5:V:19:ARG:HB3	5:V:32:HIS:O	2.01	0.61
2:b:149:ASP:HB2	2:b:150:PRO:CD	2.30	0.61
9:L:184:LEU:HD11	9:L:214:ILE:HG21	1.83	0.61
3:I:181:ILE:HA	3:I:187:THR:HG22	1.81	0.61
13:W:169:VAL:HG11	13:W:189:ILE:CD1	2.30	0.61
13:W:178:TYR:OH	13:W:208:ASN:N	2.31	0.61
8:Q:33:SER:CB	8:Q:79:GLY:H	2.13	0.61
8:Q:36:ALA:HB1	8:Q:49:VAL:HG22	1.82	0.61
13:a:178:TYR:OH	13:a:207:THR:HA	2.01	0.61
3:N:33:VAL:HG23	3:N:195:LEU:HD21	1.83	0.61
3:N:57:ARG:CG	3:N:57:ARG:HH11	2.14	0.61
12:E:22:GLU:O	12:E:22:GLU:HG3	1.99	0.61
12:E:191:VAL:O	12:E:191:VAL:HG12	2.01	0.61
14:Y:8:GLY:HA2	14:Y:24:ASP:CG	2.26	0.61
9:G:45:VAL:HG22	9:G:214:ILE:HG23	1.83	0.61
8:J:36:ALA:HB1	8:J:49:VAL:HG22	1.82	0.61
9:L:31:GLN:O	9:L:51:ARG:NH2	2.33	0.61
3:I:57:ARG:HH11	3:I:57:ARG:CG	2.14	0.61
2:P:169:GLY:O	2:P:173:LEU:HB2	2.02	0.60
3:N:8:THR:HG23	3:N:18:GLN:HB2	1.83	0.60
7:D:36:ILE:CG2	7:D:46:MET:CE	2.79	0.60
9:L:58:ALA:N	10:M:164:GLN:O	2.31	0.60
10:H:68:VAL:HG21	10:H:89:ILE:HG13	1.82	0.60
7:C:36:ILE:CG2	7:C:46:MET:CE	2.79	0.60
11:O:28:ILE:HD11	11:O:152:PRO:HG3	1.82	0.60
13:W:16:PHE:CZ	13:W:162:GLN:CG	2.84	0.60
13:W:178:TYR:OH	13:W:207:THR:HA	2.01	0.60
12:E:94:ILE:O	12:E:94:ILE:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:49:LYS:O	2:b:49:LYS:HG2	2.00	0.60
2:b:155:PHE:HD2	11:Z:51:ASN:ND2	1.96	0.60
10:H:96:THR:HG22	10:H:107:MET:HE2	1.83	0.60
11:O:200:THR:O	11:O:200:THR:HG23	2.00	0.60
14:U:8:GLY:HA2	14:U:24:ASP:CG	2.26	0.60
9:L:88:MET:HE3	9:L:108:LEU:HD21	1.83	0.60
11:O:21:VAL:HG11	11:O:153:SER:HB3	1.82	0.60
14:Y:182:MET:HE3	14:Y:203:MET:HE3	1.82	0.60
2:P:149:ASP:HB2	2:P:150:PRO:CD	2.30	0.60
3:N:18:GLN:NE2	3:N:18:GLN:HA	2.16	0.60
5:T:1:MET:H1	5:T:173:LEU:HD11	1.66	0.60
8:J:33:SER:CB	8:J:79:GLY:H	2.13	0.60
3:I:8:THR:HG23	3:I:18:GLN:HB2	1.83	0.60
12:B:94:ILE:HG22	12:B:94:ILE:O	2.01	0.60
13:W:74:GLU:CD	9:G:107:ARG:HH22	2.08	0.60
14:Y:24:ASP:O	14:Y:40:LYS:HE3	2.01	0.60
14:U:24:ASP:O	14:U:40:LYS:HE3	2.01	0.60
14:U:194:ILE:O	14:U:194:ILE:HG22	2.01	0.60
3:N:181:ILE:HA	3:N:187:THR:HG22	1.82	0.60
5:T:1:MET:HA	5:T:1:MET:HE3	1.84	0.60
4:K:220:VAL:HG23	4:K:220:VAL:O	2.00	0.60
10:M:96:THR:HG22	10:M:107:MET:HE2	1.83	0.60
13:W:1:THR:N	13:W:104:ASN:ND2	2.50	0.60
13:W:16:PHE:CE1	13:W:162:GLN:HG2	2.36	0.60
13:a:1:THR:N	13:a:104:ASN:ND2	2.50	0.60
14:Y:8:GLY:HA2	14:Y:24:ASP:OD2	2.01	0.60
13:a:16:PHE:CZ	13:a:162:GLN:CG	2.84	0.60
13:a:16:PHE:CE1	13:a:162:GLN:HG2	2.36	0.60
1:A:134:SER:O	1:F:135:TYR:HA	2.01	0.60
7:C:4:THR:HG22	7:C:17:ALA:HB2	1.82	0.60
3:I:121:SER:OG	3:I:124:ARG:HD2	2.00	0.60
1:A:2:THR:HG21	1:A:47:SER:HB2	1.84	0.60
1:A:135:TYR:HA	1:F:134:SER:O	2.02	0.60
4:K:42:VAL:HG12	4:K:194:THR:HG23	1.84	0.60
2:b:54:ILE:O	2:b:54:ILE:HG23	2.00	0.60
3:I:50:VAL:O	3:I:50:VAL:HG22	2.02	0.60
12:B:191:VAL:O	12:B:191:VAL:HG12	2.01	0.60
14:Y:194:ILE:O	14:Y:194:ILE:HG22	2.01	0.60
14:U:8:GLY:HA2	14:U:24:ASP:OD2	2.01	0.60
2:P:49:LYS:HG2	2:P:49:LYS:O	2.00	0.60
5:T:19:ARG:HB3	5:T:32:HIS:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:117:MET:HA	8:J:117:MET:CE	2.27	0.60
12:E:40:ASN:H	12:E:40:ASN:ND2	1.93	0.60
9:G:184:LEU:HD11	9:G:214:ILE:HG21	1.83	0.60
2:b:169:GLY:O	2:b:173:LEU:HB2	2.01	0.59
3:I:45:VAL:HG21	3:I:61:LYS:HB2	1.84	0.59
13:W:51:LEU:HD21	13:W:110:MET:CG	2.32	0.59
9:G:200:PRO:HG2	9:G:203:GLN:HG2	1.83	0.59
6:X:102:PHE:H	6:X:103:PRO:CD	2.15	0.59
5:V:1:MET:HA	5:V:1:MET:HE3	1.84	0.59
12:E:195:LYS:HE2	6:X:184:GLU:HG3	1.83	0.59
5:T:18:ASP:OD1	5:T:34:LYS:HE2	2.02	0.59
9:L:5:GLN:N	9:L:5:GLN:HE21	2.00	0.59
9:G:5:GLN:N	9:G:5:GLN:HE21	2.00	0.59
9:L:29:VAL:HG13	9:L:75:ALA:O	2.02	0.59
3:I:136:PHE:HE2	3:I:211:MET:O	1.86	0.59
9:G:29:VAL:HG13	9:G:75:ALA:O	2.02	0.59
8:Q:39:ILE:HD12	8:Q:193:VAL:HG23	1.83	0.59
13:a:124:TYR:HB2	13:a:137:LEU:HD13	1.85	0.59
3:N:86:ARG:HH21	3:N:86:ARG:CG	2.12	0.59
4:R:42:VAL:HG12	4:R:194:THR:HG23	1.84	0.59
3:I:33:VAL:HG23	3:I:195:LEU:HD21	1.83	0.59
10:M:31:ILE:HD13	10:M:140:ALA:HB2	1.84	0.59
14:Y:182:MET:CE	14:Y:203:MET:HE3	2.33	0.59
14:U:182:MET:CE	14:U:203:MET:HE3	2.33	0.59
6:X:104:TYR:HB3	6:X:106:VAL:HG23	1.85	0.59
6:S:184:GLU:HG3	12:B:195:LYS:HE2	1.85	0.59
3:I:18:GLN:NE2	3:I:18:GLN:HA	2.16	0.59
3:I:120:GLN:O	3:I:120:GLN:HG2	2.02	0.59
12:E:132:LEU:N	12:E:132:LEU:HD23	2.18	0.59
11:Z:208:ALA:O	11:Z:230:GLN:NE2	2.29	0.59
5:V:4:LEU:HD22	5:V:45:LEU:HB3	1.83	0.59
10:H:125:GLU:OE1	3:I:5:ARG:NH2	2.35	0.59
1:F:2:THR:HG21	1:F:47:SER:HB2	1.84	0.59
6:S:74:MET:HE2	9:L:93:LEU:HD13	1.85	0.59
7:D:4:THR:HG22	7:D:17:ALA:HB2	1.82	0.59
4:K:36:GLY:O	4:K:55:LYS:HE2	2.03	0.59
7:C:37:GLU:HG2	7:C:185:TRP:CE2	2.37	0.59
14:U:107:VAL:O	14:U:107:VAL:HG12	2.02	0.59
2:P:182:GLU:HA	2:P:182:GLU:OE2	2.02	0.59
3:N:59:VAL:O	3:N:59:VAL:HG23	2.02	0.59
6:S:100:ARG:HD2	6:S:100:ARG:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:18:ASP:OD1	5:V:34:LYS:HE2	2.02	0.59
7:C:18:ASP:O	7:C:34:LYS:HD2	2.03	0.59
13:W:124:TYR:HB2	13:W:137:LEU:HD13	1.85	0.59
8:Q:219:LEU:HD13	8:Q:219:LEU:O	2.03	0.59
13:a:51:LEU:HD21	13:a:110:MET:CG	2.32	0.59
14:U:163:PHE:CE1	14:U:197:ARG:HD2	2.37	0.59
5:T:40:GLU:HA	5:T:40:GLU:OE2	2.03	0.58
6:S:46:LEU:HD12	6:S:50:THR:HG22	1.85	0.58
7:C:159:ARG:NE	7:C:163:GLN:HE21	1.96	0.58
12:B:103:VAL:HG22	12:B:108:PRO:HB3	1.85	0.58
13:W:105:PRO:HG3	6:X:2:PHE:CE1	2.38	0.58
14:Y:107:VAL:O	14:Y:107:VAL:HG12	2.02	0.58
6:X:100:ARG:HD2	6:X:100:ARG:O	2.02	0.58
3:N:50:VAL:O	3:N:50:VAL:HG22	2.02	0.58
6:S:72:LEU:HD23	6:S:83:MET:CE	2.33	0.58
10:M:184:VAL:O	10:M:184:VAL:HG12	2.03	0.58
5:T:4:LEU:HD22	5:T:45:LEU:HB3	1.83	0.58
7:D:20:ARG:HH22	14:Y:204:ASP:HB3	1.68	0.58
8:J:39:ILE:HD12	8:J:193:VAL:HG23	1.83	0.58
8:J:57:LEU:CD2	9:G:173:GLU:HG3	2.33	0.58
4:K:178:PHE:HZ	4:K:200:THR:HG22	1.68	0.58
1:F:4:ILE:HD12	1:F:100:ILE:HD12	1.85	0.58
1:F:15:LEU:HD23	1:F:45:CYS:SG	2.44	0.58
2:P:110:VAL:HG22	2:P:135:ILE:HD13	1.85	0.58
3:N:57:ARG:NH2	11:O:108:GLU:OE1	2.33	0.58
3:N:120:GLN:HG2	3:N:120:GLN:O	2.02	0.58
4:R:22:LEU:HD13	4:R:126:THR:CG2	2.33	0.58
6:S:102:PHE:H	6:S:103:PRO:CD	2.15	0.58
10:H:31:ILE:HD13	10:H:140:ALA:HB2	1.84	0.58
10:H:161:THR:HG23	9:G:78:THR:HG21	1.85	0.58
10:H:164:GLN:O	9:G:58:ALA:N	2.32	0.58
7:C:20:ARG:HH22	14:U:204:ASP:HB3	1.68	0.58
7:C:105:TRP:NE1	7:C:182:GLU:HG3	2.19	0.58
12:E:103:VAL:HG22	12:E:108:PRO:HB3	1.85	0.58
4:R:37:LEU:HG	4:R:55:LYS:NZ	2.19	0.58
7:D:159:ARG:NE	7:D:163:GLN:HE21	1.96	0.58
10:M:148:GLU:HG3	10:M:148:GLU:O	2.04	0.58
8:Q:136:MET:HE2	8:Q:165:ILE:HG12	1.86	0.58
13:a:45:VAL:HB	13:a:49:THR:HB	1.85	0.58
14:Y:163:PHE:CE1	14:Y:197:ARG:HD2	2.37	0.58
4:R:36:GLY:O	4:R:55:LYS:HE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:2:PHE:CE1	13:a:105:PRO:HG3	2.39	0.58
9:L:157:ARG:HD2	9:L:176:MET:CE	2.34	0.58
13:a:50:MET:HG2	13:a:113:GLY:O	2.03	0.58
14:Y:26:ARG:HB2	14:Y:182:MET:CG	2.34	0.58
1:A:15:LEU:HD23	1:A:45:CYS:SG	2.44	0.58
1:A:104:TRP:CZ2	1:A:182:GLU:HB2	2.39	0.58
2:P:61:VAL:CG2	4:R:161:CYS:SG	2.92	0.58
3:N:45:VAL:HG21	3:N:61:LYS:HB2	1.84	0.58
7:D:37:GLU:HG2	7:D:185:TRP:CE2	2.37	0.58
10:M:213:THR:HG22	10:M:231:LYS:CE	2.34	0.58
9:G:230:SER:N	9:G:231:PRO:HD2	2.19	0.58
1:F:104:TRP:CZ2	1:F:182:GLU:HB2	2.39	0.58
7:D:105:TRP:NE1	7:D:182:GLU:HG3	2.19	0.58
10:H:148:GLU:HG3	10:H:148:GLU:O	2.04	0.58
3:I:208:LEU:HD11	3:I:220:LEU:CD1	2.26	0.58
8:Q:135:PHE:CZ	8:Q:151:ILE:HD12	2.39	0.58
7:D:18:ASP:O	7:D:34:LYS:HD2	2.03	0.58
9:L:5:GLN:HE21	9:L:5:GLN:H	1.52	0.58
12:B:50:ALA:HB3	14:Y:126:ILE:CD1	2.33	0.58
9:G:157:ARG:HD2	9:G:176:MET:CE	2.34	0.58
3:N:136:PHE:HE2	3:N:211:MET:O	1.86	0.58
2:b:110:VAL:HG22	2:b:135:ILE:HD13	1.85	0.58
10:H:38:ILE:HD12	10:H:202:LEU:CD1	2.34	0.58
12:B:147:GLU:HA	12:B:147:GLU:OE2	2.04	0.58
6:X:46:LEU:HD12	6:X:50:THR:HG22	1.86	0.58
6:S:102:PHE:N	6:S:103:PRO:HD2	2.19	0.57
6:S:104:TYR:HB3	6:S:106:VAL:HG23	1.85	0.57
7:D:66:ILE:HG13	10:M:97:GLN:CG	2.34	0.57
8:J:136:MET:HE2	8:J:165:ILE:HG12	1.86	0.57
9:L:230:SER:N	9:L:231:PRO:HD2	2.19	0.57
3:I:59:VAL:HG23	3:I:59:VAL:O	2.02	0.57
13:W:50:MET:HG2	13:W:113:GLY:O	2.03	0.57
9:G:5:GLN:HE21	9:G:5:GLN:H	1.52	0.57
14:U:100:GLY:N	14:U:101:PRO:HD3	2.19	0.57
4:R:212:PRO:CG	4:R:236:ASP:OD2	2.52	0.57
8:J:135:PHE:CZ	8:J:151:ILE:HD12	2.39	0.57
5:V:40:GLU:HA	5:V:40:GLU:OE2	2.03	0.57
4:R:65:THR:HG21	8:Q:159:GLY:HA3	1.86	0.57
5:V:18:ASP:OD1	5:V:34:LYS:HE3	2.04	0.57
13:W:45:VAL:HB	13:W:49:THR:HB	1.85	0.57
12:E:195:LYS:CE	6:X:184:GLU:HG3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:26:ARG:HB2	14:U:182:MET:CG	2.34	0.57
1:A:4:ILE:HD12	1:A:100:ILE:HD12	1.85	0.57
3:N:5:ARG:NH2	10:M:125:GLU:OE1	2.37	0.57
6:S:123:SER:CB	6:S:136:LYS:HG2	2.22	0.57
4:K:34:GLN:HE21	4:K:34:GLN:CA	2.02	0.57
2:b:182:GLU:HA	2:b:182:GLU:OE2	2.02	0.57
10:H:184:VAL:O	10:H:184:VAL:HG12	2.03	0.57
11:Z:76:VAL:HG11	11:Z:83:ALA:HB1	1.85	0.57
14:Y:13:MET:HB3	14:Y:162:LEU:HD11	1.87	0.57
12:B:132:LEU:N	12:B:132:LEU:HD23	2.18	0.57
2:P:156:ALA:HB3	11:O:59:VAL:CG2	2.35	0.57
3:N:173:GLU:HG2	10:M:57:PRO:HG2	1.87	0.57
6:S:173:ARG:CG	12:B:199:LEU:HD12	2.35	0.57
4:K:22:LEU:HD13	4:K:126:THR:CG2	2.33	0.57
4:K:212:PRO:CG	4:K:236:ASP:OD2	2.52	0.57
4:R:226:LYS:HE2	4:R:226:LYS:CA	2.34	0.57
7:C:166:TYR:CE2	14:U:33:MET:HE1	2.39	0.57
12:B:122:LEU:HB3	12:B:123:PRO:HD2	1.86	0.57
10:M:38:ILE:HD12	10:M:202:LEU:CD1	2.34	0.57
8:J:172:ALA:HB2	8:J:200:VAL:HG21	1.87	0.57
8:J:219:LEU:O	8:J:219:LEU:HD13	2.03	0.57
4:K:123:GLN:NE2	2:b:81:ASP:OD1	2.37	0.57
9:L:78:THR:HG21	10:M:161:THR:HG23	1.85	0.57
11:O:174:MET:CG	11:O:196:VAL:HG22	2.31	0.57
13:W:10:SER:HB3	13:W:139:THR:O	2.05	0.57
9:G:93:LEU:HD13	6:X:74:MET:HE2	1.85	0.57
14:Y:189:ILE:HG13	14:Y:194:ILE:HD13	1.87	0.57
6:S:28:ARG:HB2	6:S:191:ASP:OD2	2.05	0.57
4:K:37:LEU:HG	4:K:55:LYS:NZ	2.19	0.57
9:L:57:ALA:HA	10:M:165:CYS:HB3	1.87	0.57
10:H:97:GLN:CG	7:C:66:ILE:HG13	2.35	0.57
11:O:10:THR:O	11:O:10:THR:OG1	2.22	0.57
12:E:122:LEU:HB3	12:E:123:PRO:HD2	1.86	0.57
11:Z:230:GLN:HE21	11:Z:230:GLN:CA	2.10	0.57
2:P:35:VAL:HG11	2:P:193:THR:HG21	1.86	0.57
9:L:71:GLY:HA3	9:L:221:PHE:CZ	2.40	0.57
2:P:83:ARG:HH11	2:P:83:ARG:CG	2.13	0.56
9:L:230:SER:OG	9:L:231:PRO:CD	2.48	0.56
10:H:213:THR:HG22	10:H:231:LYS:CE	2.34	0.56
7:D:36:ILE:O	7:D:36:ILE:HG13	2.04	0.56
4:K:226:LYS:HE2	4:K:226:LYS:CA	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:157:ARG:CD	9:G:176:MET:HE3	2.35	0.56
13:a:10:SER:HB3	13:a:139:THR:O	2.05	0.56
13:a:122:LEU:HG	13:a:137:LEU:HD12	1.88	0.56
5:T:18:ASP:OD1	5:T:34:LYS:HE3	2.04	0.56
11:O:76:VAL:HG11	11:O:83:ALA:HB1	1.86	0.56
13:W:81:HIS:CE1	9:G:139:ASP:HB2	2.40	0.56
12:E:147:GLU:HA	12:E:147:GLU:OE2	2.04	0.56
13:a:147:GLN:NE2	13:a:147:GLN:HA	2.21	0.56
11:Z:10:THR:O	11:Z:10:THR:OG1	2.22	0.56
11:Z:174:MET:CG	11:Z:196:VAL:HG22	2.31	0.56
14:U:189:ILE:HG13	14:U:194:ILE:HD13	1.87	0.56
6:X:75:TYR:CB	6:X:83:MET:HE2	2.35	0.56
1:A:199:THR:O	1:A:199:THR:HG23	2.05	0.56
9:L:157:ARG:CD	9:L:176:MET:HE3	2.35	0.56
10:M:31:ILE:HD11	10:M:158:PRO:CG	2.35	0.56
13:W:122:LEU:HG	13:W:137:LEU:HD12	1.87	0.56
14:U:13:MET:HB3	14:U:162:LEU:HD11	1.87	0.56
6:X:102:PHE:N	6:X:103:PRO:HD2	2.19	0.56
4:R:178:PHE:HZ	4:R:200:THR:HG22	1.68	0.56
9:G:71:GLY:HA3	9:G:221:PHE:CZ	2.40	0.56
14:U:2:ILE:HG21	14:U:103:TYR:CG	2.40	0.56
6:S:75:TYR:CB	6:S:83:MET:HE2	2.35	0.56
9:G:35:THR:HG23	9:G:62:LYS:CE	2.27	0.56
9:G:119:PRO:HG2	9:G:128:TYR:HE1	1.71	0.56
13:a:22:ILE:CD1	13:a:111:VAL:HG12	2.35	0.56
6:X:28:ARG:HB2	6:X:191:ASP:OD2	2.05	0.56
10:H:31:ILE:HD11	10:H:158:PRO:CG	2.35	0.56
1:F:199:THR:HG23	1:F:199:THR:O	2.05	0.56
4:K:49:VAL:HG21	4:K:195:VAL:HG22	1.88	0.56
3:N:132:LEU:HD22	3:N:144:LEU:HD11	1.88	0.56
4:K:155:ASP:CB	4:K:156:PRO:CD	2.71	0.56
13:W:22:ILE:CD1	13:W:111:VAL:HG12	2.35	0.56
12:E:7:VAL:HG22	12:E:12:ILE:HD13	1.88	0.56
9:G:103:LEU:HD12	9:G:104:PRO:HD2	1.88	0.56
13:a:192:VAL:HG13	13:a:192:VAL:O	2.06	0.56
14:Y:2:ILE:HG21	14:Y:103:TYR:CG	2.41	0.56
2:P:142:ARG:HG2	2:P:143:PRO:CD	2.36	0.56
2:P:190:ALA:O	2:P:193:THR:CG2	2.54	0.56
2:b:83:ARG:HH11	2:b:83:ARG:CG	2.13	0.56
2:b:156:ALA:HB3	11:Z:59:VAL:CG2	2.36	0.56
10:M:79:SER:HB3	10:M:170:ILE:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:35:VAL:HG11	2:b:193:THR:HG21	1.86	0.55
10:H:91:LYS:HD2	10:H:119:LEU:CD1	2.33	0.55
12:E:199:LEU:HD12	6:X:173:ARG:CG	2.35	0.55
8:Q:172:ALA:HB2	8:Q:200:VAL:HG21	1.87	0.55
5:T:171:PHE:CE2	5:T:173:LEU:HB2	2.41	0.55
5:V:145:ARG:HG3	5:V:145:ARG:O	2.04	0.55
9:L:119:PRO:HG2	9:L:128:TYR:HE1	1.71	0.55
7:C:84:LEU:CD2	7:C:100:THR:HG21	2.35	0.55
1:A:173:GLY:HA2	13:a:209:TRP:CH2	2.41	0.55
8:J:176:ILE:O	8:J:181:MET:HE2	2.05	0.55
2:b:142:ARG:HG2	2:b:143:PRO:CD	2.36	0.55
2:b:190:ALA:O	2:b:193:THR:CG2	2.54	0.55
12:E:50:ALA:HB3	14:U:126:ILE:CD1	2.35	0.55
8:J:151:ILE:HG12	8:J:157:SER:HB2	1.89	0.55
9:G:137:TYR:OH	9:G:217:LYS:HB2	2.06	0.55
1:F:8:GLN:HG2	1:F:125:SER:O	2.07	0.55
4:R:48:ALA:HB3	4:R:220:VAL:HG22	1.87	0.55
7:D:69:LEU:HD21	10:M:69:GLU:OE2	2.07	0.55
7:D:84:LEU:CD2	7:D:100:THR:HG21	2.35	0.55
4:K:48:ALA:HB3	4:K:220:VAL:HG22	1.87	0.55
10:H:79:SER:HB3	10:H:170:ILE:HG13	1.88	0.55
3:I:132:LEU:HD22	3:I:144:LEU:HD11	1.88	0.55
10:M:31:ILE:O	10:M:31:ILE:HG22	2.06	0.55
10:M:38:ILE:HD13	10:M:201:ILE:HG21	1.88	0.55
13:W:192:VAL:HG13	13:W:192:VAL:O	2.06	0.55
2:P:218:ARG:HG2	2:P:218:ARG:HH11	1.71	0.55
8:J:185:THR:O	8:J:189:VAL:CG2	2.55	0.55
5:V:171:PHE:CE2	5:V:173:LEU:HB2	2.41	0.55
10:H:78:MET:HE2	10:H:82:ILE:HG23	1.88	0.55
12:B:7:VAL:HG22	12:B:12:ILE:HD13	1.88	0.55
13:W:147:GLN:HA	13:W:147:GLN:NE2	2.21	0.55
2:P:188:HIS:O	2:P:192:LEU:HG	2.07	0.55
6:S:184:GLU:HG3	12:B:195:LYS:CE	2.36	0.55
4:K:192:GLU:OE1	4:K:192:GLU:N	2.34	0.55
2:b:218:ARG:HG2	2:b:218:ARG:HH11	1.71	0.55
9:L:35:THR:HG23	9:L:62:LYS:CE	2.27	0.55
10:H:54:ILE:H	10:H:54:ILE:CD1	2.10	0.55
10:H:165:CYS:HB3	9:G:57:ALA:HA	1.88	0.55
10:M:78:MET:HE2	10:M:82:ILE:HG23	1.88	0.55
8:Q:176:ILE:O	8:Q:181:MET:HE2	2.05	0.55
7:D:39:ASN:CB	7:D:40:PRO:CD	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:159:GLY:HA3	4:K:65:THR:HG21	1.89	0.55
2:b:188:HIS:O	2:b:192:LEU:HG	2.07	0.55
9:L:36:VAL:HG13	9:L:172:LEU:HD11	1.88	0.55
8:J:63:ASN:OD1	9:G:154:PHE:HD2	1.90	0.55
9:L:137:TYR:OH	9:L:217:LYS:HB2	2.06	0.55
3:N:169:ARG:HH11	3:N:169:ARG:HB2	1.72	0.55
8:J:170:GLN:HA	8:J:170:GLN:NE2	2.22	0.55
2:P:139:ASN:C	2:P:139:ASN:HD22	2.16	0.54
2:b:139:ASN:C	2:b:139:ASN:HD22	2.16	0.54
11:O:186:LEU:CD2	11:O:217:THR:HG22	2.37	0.54
3:I:92:GLN:HA	3:I:92:GLN:NE2	2.22	0.54
9:G:36:VAL:HG13	9:G:172:LEU:HD11	1.88	0.54
11:Z:186:LEU:CD2	11:Z:217:THR:HG22	2.37	0.54
14:Y:27:PHE:HB2	14:Y:38:PHE:HB2	1.89	0.54
7:D:67:TYR:CD1	7:D:67:TYR:C	2.85	0.54
9:L:69:HIS:O	9:L:136:GLY:HA2	2.07	0.54
3:I:100:ASP:HB3	3:I:101:PRO:HD2	1.89	0.54
12:B:209:THR:OG1	14:Y:168:GLN:NE2	2.36	0.54
8:Q:185:THR:O	8:Q:189:VAL:CG2	2.55	0.54
6:X:72:LEU:HD23	6:X:83:MET:CE	2.33	0.54
2:P:74:VAL:CG1	2:P:134:LEU:HB2	2.37	0.54
2:P:90:ARG:HB3	12:E:65:LEU:HD21	1.88	0.54
7:D:39:ASN:HB2	7:D:40:PRO:HD3	1.86	0.54
8:J:238:TYR:CD1	8:J:238:TYR:C	2.86	0.54
9:L:173:GLU:HG3	8:Q:57:LEU:CD2	2.37	0.54
7:C:115:VAL:HG22	7:C:121:ARG:HG3	1.89	0.54
11:O:226:ARG:HD3	11:O:226:ARG:C	2.33	0.54
9:G:69:HIS:O	9:G:136:GLY:HA2	2.07	0.54
9:G:171:TYR:CD1	9:G:171:TYR:C	2.86	0.54
4:R:51:VAL:HG12	4:R:202:LEU:CD2	2.26	0.54
6:S:102:PHE:N	6:S:103:PRO:HD3	2.23	0.54
10:H:31:ILE:HG22	10:H:31:ILE:O	2.06	0.54
11:O:160:LYS:HD3	11:O:181:GLU:OE2	2.07	0.54
12:B:58:LEU:HD12	12:B:58:LEU:O	2.07	0.54
13:a:147:GLN:HB3	13:a:148:PRO:HD3	1.89	0.54
6:X:109:ILE:O	6:X:109:ILE:HG22	2.06	0.54
8:J:176:ILE:O	8:J:181:MET:CE	2.56	0.54
7:C:67:TYR:C	7:C:67:TYR:CD1	2.85	0.54
10:M:69:GLU:HG3	10:M:226:PHE:CD2	2.43	0.54
10:M:202:LEU:HD23	10:M:215:ILE:CG2	2.37	0.54
13:W:147:GLN:HB3	13:W:148:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:36:PHE:CD1	12:E:36:PHE:C	2.85	0.54
1:A:8:GLN:HG2	1:A:125:SER:O	2.06	0.54
3:N:100:ASP:HB3	3:N:101:PRO:HD2	1.89	0.54
3:N:221:ASN:HB2	3:N:222:PRO:CD	2.37	0.54
4:R:49:VAL:HG21	4:R:195:VAL:HG22	1.88	0.54
5:T:55:GLN:HG3	7:D:89:TYR:CZ	2.43	0.54
5:T:172:ILE:HG12	5:V:25:ILE:HA	1.89	0.54
8:J:152:ASP:HB2	8:J:153:PRO:HD3	1.89	0.54
2:b:74:VAL:CG1	2:b:134:LEU:HB2	2.37	0.54
10:H:114:GLN:HG3	10:H:162:PHE:CZ	2.43	0.54
14:Y:100:GLY:N	14:Y:101:PRO:HD3	2.19	0.54
2:P:128:PRO:O	4:R:16:PHE:HE2	1.90	0.54
4:R:192:GLU:OE1	4:R:192:GLU:N	2.34	0.54
12:E:3:ILE:CG1	12:E:127:MET:HB2	2.38	0.54
14:Y:16:LYS:HG2	14:Y:156:ASN:HB3	1.89	0.54
4:R:78:CYS:CB	4:R:140:LEU:HD23	2.35	0.54
6:S:109:ILE:O	6:S:109:ILE:HG22	2.06	0.54
4:K:49:VAL:HG21	4:K:195:VAL:CG2	2.37	0.54
9:L:103:LEU:HD12	9:L:104:PRO:HD2	1.88	0.54
12:E:58:LEU:HD12	12:E:58:LEU:O	2.07	0.54
8:Q:151:ILE:HG12	8:Q:157:SER:HB2	1.89	0.54
8:Q:176:ILE:O	8:Q:181:MET:CE	2.56	0.54
14:Y:26:ARG:HB2	14:Y:182:MET:HB2	1.90	0.54
14:U:26:ARG:HB2	14:U:182:MET:HB2	1.90	0.54
1:A:21:THR:OG1	1:A:32:THR:OG1	2.24	0.54
2:P:142:ARG:HH12	11:O:59:VAL:HG12	1.72	0.54
4:R:49:VAL:HG21	4:R:195:VAL:CG2	2.37	0.54
6:S:188:TYR:HH	12:B:24:MET:HE2	1.72	0.54
10:H:134:SER:HB2	3:I:122:ASN:OD1	2.08	0.54
9:G:230:SER:OG	9:G:231:PRO:CD	2.48	0.54
6:X:167:THR:CG2	6:X:170:ARG:HB3	2.37	0.54
5:T:85:ARG:HG3	5:T:124:LEU:HB2	1.89	0.54
7:D:115:VAL:HG22	7:D:121:ARG:HG3	1.89	0.54
8:J:42:LYS:HB2	8:J:184:MET:O	2.08	0.54
12:B:3:ILE:CG1	12:B:127:MET:HB2	2.38	0.54
2:P:63:LYS:HD2	2:P:75:TYR:CE1	2.43	0.53
2:P:159:ALA:HB1	2:P:173:LEU:HD22	1.90	0.53
6:S:167:THR:CG2	6:S:170:ARG:HB3	2.37	0.53
4:K:25:VAL:HG21	4:K:126:THR:CG2	2.37	0.53
4:K:178:PHE:CD1	4:K:178:PHE:C	2.86	0.53
2:b:90:ARG:HB3	12:B:65:LEU:HD21	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:171:TYR:CD1	9:L:171:TYR:C	2.85	0.53
11:O:48:GLU:HG3	11:O:48:GLU:O	2.08	0.53
12:B:36:PHE:CD1	12:B:36:PHE:C	2.85	0.53
10:M:91:LYS:HD2	10:M:119:LEU:CD1	2.33	0.53
13:W:124:TYR:CD1	13:W:124:TYR:C	2.86	0.53
14:U:27:PHE:HB2	14:U:38:PHE:HB2	1.89	0.53
3:N:53:LEU:HD13	11:O:161:ALA:HB3	1.89	0.53
2:b:159:ALA:HB1	2:b:173:LEU:HD22	1.90	0.53
8:Q:42:LYS:HB2	8:Q:184:MET:O	2.08	0.53
13:a:124:TYR:CD1	13:a:124:TYR:C	2.86	0.53
11:Z:160:LYS:HD3	11:Z:181:GLU:OE2	2.07	0.53
11:Z:226:ARG:HD3	11:Z:226:ARG:C	2.33	0.53
14:Y:12:ALA:HB3	14:Y:136:VAL:CG2	2.39	0.53
14:Y:158:ASP:HB2	14:Y:159:PRO:HD2	1.90	0.53
3:N:195:LEU:HD13	3:N:206:ILE:HG23	1.90	0.53
9:L:74:ILE:HG21	9:L:81:ALA:HB1	1.89	0.53
10:H:38:ILE:HD13	10:H:201:ILE:HG21	1.88	0.53
9:G:157:ARG:CD	9:G:176:MET:CE	2.87	0.53
13:a:99:ARG:HB3	13:a:105:PRO:HA	1.90	0.53
9:L:45:VAL:HG11	9:L:188:VAL:HG22	1.91	0.53
9:L:205:LEU:CD2	9:L:210:VAL:CG1	2.74	0.53
10:H:69:GLU:HG3	10:H:226:PHE:CD2	2.42	0.53
11:O:15:GLU:HB2	11:O:17:ARG:HG3	1.91	0.53
13:W:99:ARG:HB3	13:W:105:PRO:HA	1.90	0.53
12:E:163:ILE:HG23	12:E:170:GLY:HA2	1.91	0.53
14:U:16:LYS:HG2	14:U:156:ASN:HB3	1.89	0.53
14:U:158:ASP:HB2	14:U:159:PRO:HD2	1.90	0.53
3:N:208:LEU:HD11	3:N:220:LEU:CD1	2.26	0.53
4:R:178:PHE:CD1	4:R:178:PHE:C	2.86	0.53
6:S:24:ALA:HB1	6:S:193:LEU:HD11	1.91	0.53
7:D:157:ALA:HB3	7:D:177:LEU:HD11	1.90	0.53
13:W:209:TRP:CH2	1:F:173:GLY:HA2	2.43	0.53
5:T:145:ARG:HG3	5:T:145:ARG:O	2.04	0.53
6:S:153:VAL:HG23	6:S:174:LEU:HD21	1.91	0.53
3:I:55:ASP:HB3	3:I:58:THR:HG23	1.90	0.53
3:I:169:ARG:HH11	3:I:169:ARG:HB2	1.72	0.53
9:G:74:ILE:HG21	9:G:81:ALA:HB1	1.89	0.53
1:F:82:SER:O	1:F:86:GLU:HG2	2.08	0.53
3:N:94:HIS:HB3	3:N:102:VAL:HG12	1.91	0.53
4:R:25:VAL:HG21	4:R:126:THR:CG2	2.37	0.53
2:b:63:LYS:HD2	2:b:75:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:216:GLU:HB2	10:H:228:MET:HE3	1.91	0.53
3:I:94:HIS:HB3	3:I:102:VAL:HG12	1.91	0.53
8:Q:170:GLN:NE2	8:Q:170:GLN:HA	2.22	0.53
11:Z:28:ILE:HD11	11:Z:152:PRO:CG	2.39	0.53
11:Z:48:GLU:HG3	11:Z:48:GLU:O	2.08	0.53
3:N:185:ASP:OD1	3:N:185:ASP:N	2.41	0.53
8:J:168:ALA:HB3	8:J:200:VAL:HG12	1.90	0.53
10:H:154:PHE:CZ	10:H:164:GLN:HG3	2.44	0.53
7:C:158:ARG:HD3	7:C:191:ASP:OD2	2.09	0.53
8:Q:238:TYR:CD1	8:Q:238:TYR:C	2.86	0.53
5:V:85:ARG:HG3	5:V:124:LEU:HB2	1.89	0.53
10:H:232:GLU:H	10:H:232:GLU:CD	2.17	0.53
10:M:227:HIS:HE1	10:M:233:GLU:OE1	1.92	0.53
6:X:24:ALA:HB1	6:X:193:LEU:HD11	1.91	0.53
6:S:184:GLU:OE2	6:S:211:ARG:NH1	2.42	0.53
10:H:227:HIS:HE1	10:H:233:GLU:OE1	1.92	0.53
11:O:95:GLN:NE2	14:U:71:ASN:HD22	2.07	0.53
6:X:102:PHE:N	6:X:103:PRO:HD3	2.23	0.53
3:N:54:GLN:HB2	11:O:159:TRP:CZ3	2.44	0.52
7:D:5:LEU:C	7:D:5:LEU:HD12	2.34	0.52
4:K:52:THR:HG22	4:K:69:LEU:HD21	1.91	0.52
7:C:36:ILE:HG13	7:C:36:ILE:O	2.04	0.52
7:C:46:MET:HG2	7:C:53:CYS:HB3	1.91	0.52
10:M:114:GLN:HG3	10:M:162:PHE:CZ	2.43	0.52
10:M:216:GLU:HB2	10:M:228:MET:HE3	1.91	0.52
12:E:3:ILE:CD1	12:E:127:MET:HB2	2.39	0.52
12:E:42:TYR:HB2	12:E:178:ILE:HD11	1.91	0.52
9:G:205:LEU:HD22	9:G:210:VAL:HG12	1.83	0.52
8:Q:216:VAL:O	8:Q:216:VAL:HG13	2.09	0.52
3:N:92:GLN:HA	3:N:92:GLN:NE2	2.22	0.52
4:R:52:THR:HG22	4:R:69:LEU:HD21	1.91	0.52
6:S:27:THR:OG1	6:S:192:ALA:HB3	2.09	0.52
7:D:158:ARG:HD3	7:D:191:ASP:OD2	2.09	0.52
13:W:25:ASP:OD1	13:W:41:ARG:NH1	2.42	0.52
14:U:12:ALA:HB3	14:U:136:VAL:CG2	2.39	0.52
7:D:9:PHE:CD1	7:D:9:PHE:N	2.73	0.52
7:D:12:GLY:HA2	7:D:105:TRP:CZ3	2.44	0.52
7:D:36:ILE:HG22	7:D:46:MET:CE	2.40	0.52
2:b:198:PHE:HZ	2:b:206:ASN:HB3	1.74	0.52
7:C:195:ASP:N	7:C:195:ASP:OD1	2.42	0.52
14:U:26:ARG:CG	14:U:182:MET:HG3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:184:GLU:OE2	6:X:211:ARG:NH1	2.42	0.52
2:b:88:ARG:HG3	2:b:88:ARG:NH1	2.24	0.52
12:E:87:LEU:HD12	12:E:113:ILE:CG2	2.40	0.52
8:Q:228:PRO:HB2	8:Q:231:ILE:HG13	1.91	0.52
13:a:25:ASP:OD1	13:a:41:ARG:NH1	2.42	0.52
4:R:60:LEU:CD2	8:Q:181:MET:HE1	2.40	0.52
4:R:213:SER:O	4:R:213:SER:OG	2.23	0.52
5:T:4:LEU:HD23	5:T:17:SER:HB2	1.92	0.52
7:D:46:MET:HG2	7:D:53:CYS:HB3	1.91	0.52
8:J:30:VAL:HG22	8:J:133:CYS:HA	1.91	0.52
8:J:57:LEU:HD21	9:G:173:GLU:HG3	1.92	0.52
8:J:162:GLY:O	4:K:60:LEU:HD13	2.10	0.52
11:O:77:ALA:CB	11:O:164:ILE:HD12	2.37	0.52
10:M:154:PHE:CZ	10:M:164:GLN:HG3	2.44	0.52
11:Z:15:GLU:HB2	11:Z:17:ARG:HG3	1.91	0.52
14:Y:26:ARG:HB2	14:Y:182:MET:HG3	1.92	0.52
1:A:82:SER:O	1:A:86:GLU:HG2	2.08	0.52
7:D:4:THR:HG21	7:D:45:THR:HG22	1.91	0.52
8:J:228:PRO:HB2	8:J:231:ILE:HG13	1.91	0.52
5:V:4:LEU:HD23	5:V:17:SER:HB2	1.92	0.52
3:I:195:LEU:HD13	3:I:206:ILE:HG23	1.90	0.52
3:I:221:ASN:HB2	3:I:222:PRO:CD	2.37	0.52
12:B:3:ILE:CD1	12:B:127:MET:HB2	2.39	0.52
7:D:66:ILE:HG13	10:M:97:GLN:HG2	1.90	0.52
8:J:152:ASP:CB	8:J:153:PRO:CD	2.74	0.52
2:b:171:THR:O	2:b:175:LYS:CG	2.57	0.52
11:O:28:ILE:HD11	11:O:152:PRO:CG	2.39	0.52
2:P:176:ARG:HH21	2:P:192:LEU:HD13	1.75	0.52
3:N:55:ASP:HB3	3:N:58:THR:HG23	1.90	0.52
3:N:82:ILE:N	3:N:82:ILE:CD1	2.73	0.52
3:N:133:ILE:H	3:N:133:ILE:HD12	1.74	0.52
9:L:19:ILE:CG2	9:L:22:ILE:HD12	2.40	0.52
9:L:157:ARG:CD	9:L:176:MET:CE	2.87	0.52
7:C:4:THR:HG21	7:C:45:THR:HG22	1.91	0.52
12:B:40:ASN:H	12:B:40:ASN:ND2	1.93	0.52
13:a:184:TYR:HD2	13:a:186:ARG:HB3	1.75	0.52
14:U:21:ILE:O	14:U:21:ILE:HG23	2.10	0.52
1:A:43:PHE:CZ	1:A:185:VAL:HG11	2.45	0.52
9:L:50:LYS:HB3	9:L:59:HIS:HB3	1.91	0.52
7:C:5:LEU:C	7:C:5:LEU:HD12	2.34	0.52
7:C:12:GLY:HA2	7:C:105:TRP:CZ3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:42:TYR:HB2	12:B:178:ILE:HD11	1.91	0.52
1:F:43:PHE:CZ	1:F:185:VAL:HG11	2.45	0.52
6:X:102:PHE:H	6:X:103:PRO:HD3	1.74	0.52
5:V:55:GLN:HG3	7:C:89:TYR:CZ	2.45	0.52
9:L:46:LEU:HD11	9:L:135:ALA:CB	2.40	0.52
9:L:196:ARG:O	9:L:196:ARG:HG2	2.10	0.52
10:M:79:SER:O	10:M:139:VAL:HG22	2.09	0.52
13:W:51:LEU:HD11	13:W:92:LEU:HD11	1.91	0.52
9:G:45:VAL:HG11	9:G:188:VAL:HG22	1.91	0.52
8:Q:30:VAL:HG22	8:Q:133:CYS:HA	1.91	0.52
13:a:51:LEU:HD11	13:a:92:LEU:HD11	1.91	0.52
3:N:5:ARG:CZ	10:M:125:GLU:OE1	2.58	0.51
8:J:181:MET:HE1	4:K:60:LEU:CD2	2.40	0.51
9:L:49:LEU:CB	9:L:195:LEU:HD11	2.40	0.51
13:a:9:THR:O	13:a:41:ARG:NH2	2.43	0.51
13:a:20:VAL:CG1	13:a:122:LEU:HD13	2.40	0.51
2:P:198:PHE:HZ	2:P:206:ASN:HB3	1.74	0.51
3:N:163:ARG:HG2	3:N:163:ARG:O	2.11	0.51
8:J:160:TYR:CE2	4:K:61:LEU:HG	2.45	0.51
2:b:88:ARG:CG	2:b:88:ARG:NH1	2.73	0.51
9:L:205:LEU:HD22	9:L:210:VAL:HG12	1.83	0.51
7:C:157:ALA:HB3	7:C:177:LEU:HD11	1.90	0.51
3:I:219:ILE:N	3:I:219:ILE:CD1	2.73	0.51
12:B:87:LEU:HD12	12:B:113:ILE:CG2	2.40	0.51
13:W:9:THR:O	13:W:41:ARG:NH2	2.43	0.51
13:W:181:ALA:HB2	1:F:22:THR:HG21	1.92	0.51
9:G:22:ILE:HD11	9:G:120:THR:HB	1.93	0.51
1:A:100:ILE:O	1:A:100:ILE:HG22	2.11	0.51
6:S:52:ILE:HG13	6:S:110:ILE:HG12	1.92	0.51
7:C:36:ILE:HG22	7:C:46:MET:CE	2.40	0.51
12:B:163:ILE:HG23	12:B:170:GLY:HA2	1.91	0.51
6:X:153:VAL:HG23	6:X:174:LEU:HD21	1.91	0.51
5:T:16:ALA:HA	5:T:179:SER:O	2.11	0.51
4:K:161:CYS:SG	2:b:61:VAL:CG2	2.99	0.51
4:K:221:THR:HG23	4:K:228:ARG:NH1	2.26	0.51
9:L:22:ILE:HD11	9:L:120:THR:HB	1.93	0.51
9:L:77:LEU:HB2	9:L:80:ASP:HB2	1.92	0.51
9:L:118:ILE:CB	9:L:119:PRO:HD3	2.38	0.51
9:L:154:PHE:HD2	8:Q:63:ASN:OD1	1.93	0.51
10:H:79:SER:O	10:H:139:VAL:HG22	2.09	0.51
12:B:15:GLY:HA2	12:B:174:ASP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:203:ARG:HG2	14:Y:154:GLU:OE2	2.11	0.51
9:G:38:LEU:H	9:G:38:LEU:HD23	1.76	0.51
1:F:100:ILE:O	1:F:100:ILE:HG22	2.10	0.51
6:X:20:PHE:CD2	6:X:168:LEU:HD13	2.46	0.51
2:P:88:ARG:NH1	2:P:88:ARG:HG3	2.24	0.51
3:N:219:ILE:N	3:N:219:ILE:CD1	2.73	0.51
7:D:161:ILE:O	7:D:165:THR:HG23	2.10	0.51
8:J:181:MET:HE1	4:K:60:LEU:HD21	1.92	0.51
7:C:161:ILE:O	7:C:165:THR:HG23	2.10	0.51
11:O:206:LEU:HD13	11:O:237:ILE:HD13	1.93	0.51
3:I:50:VAL:HG11	3:I:205:ASN:OD1	2.11	0.51
14:U:26:ARG:HB2	14:U:182:MET:HG3	1.92	0.51
1:A:22:THR:HG21	13:a:181:ALA:HB2	1.91	0.51
6:S:102:PHE:H	6:S:103:PRO:HD3	1.74	0.51
2:b:176:ARG:HH21	2:b:192:LEU:HD13	1.75	0.51
3:I:133:ILE:H	3:I:133:ILE:HD12	1.74	0.51
12:B:87:LEU:HD12	12:B:113:ILE:HG21	1.93	0.51
14:U:83:PRO:HD3	14:U:113:PRO:HD3	1.93	0.51
2:P:81:ASP:OD1	4:R:123:GLN:NE2	2.44	0.51
6:S:38:ARG:NH1	12:B:164:PHE:O	2.43	0.51
8:J:216:VAL:HG13	8:J:216:VAL:O	2.09	0.51
10:M:209:LYS:N	10:M:209:LYS:HD3	2.25	0.51
9:G:50:LYS:HB3	9:G:59:HIS:HB3	1.91	0.51
14:Y:26:ARG:CG	14:Y:182:MET:HG3	2.40	0.51
6:S:20:PHE:CD2	6:S:168:LEU:HD13	2.46	0.51
13:W:184:TYR:HD2	13:W:186:ARG:HB3	1.75	0.51
11:Z:95:GLN:NE2	14:Y:71:ASN:HD22	2.09	0.51
14:Y:21:ILE:HG23	14:Y:21:ILE:O	2.10	0.51
3:N:168:VAL:HG23	3:N:198:VAL:HG11	1.92	0.51
7:D:58:ARG:HH11	7:D:58:ARG:HG3	1.75	0.51
9:L:55:GLU:HG2	10:M:182:GLN:HE21	1.76	0.51
9:L:230:SER:N	9:L:231:PRO:CD	2.74	0.51
3:I:168:VAL:HG23	3:I:198:VAL:HG11	1.92	0.51
12:B:195:LYS:HE3	14:Y:150:GLU:OE1	2.11	0.51
13:W:20:VAL:CG1	13:W:122:LEU:HD13	2.40	0.51
12:E:15:GLY:HA2	12:E:174:ASP:O	2.11	0.51
12:E:199:LEU:HD12	6:X:173:ARG:HG2	1.93	0.51
9:G:205:LEU:CD2	9:G:210:VAL:CG1	2.74	0.51
9:G:230:SER:N	9:G:231:PRO:CD	2.74	0.51
8:Q:51:LYS:NZ	8:Q:62:SER:O	2.39	0.51
14:Y:83:PRO:HD3	14:Y:113:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:122:ASN:OD1	10:M:134:SER:HB2	2.11	0.50
10:H:97:GLN:HG2	7:C:66:ILE:HG13	1.93	0.50
10:H:125:GLU:OE1	3:I:5:ARG:CZ	2.59	0.50
10:H:135:ARG:HG3	10:H:135:ARG:NH2	2.24	0.50
10:H:202:LEU:HD23	10:H:215:ILE:CG2	2.37	0.50
3:I:82:ILE:N	3:I:82:ILE:CD1	2.73	0.50
12:E:167:LEU:HD22	6:X:187:VAL:O	2.11	0.50
9:G:116:THR:O	9:G:116:THR:HG22	2.11	0.50
6:X:75:TYR:C	6:X:75:TYR:CD1	2.89	0.50
6:X:161:VAL:HG12	6:X:163:HIS:H	1.76	0.50
2:P:88:ARG:CG	2:P:88:ARG:NH1	2.73	0.50
3:N:50:VAL:HG11	3:N:205:ASN:OD1	2.11	0.50
3:N:208:LEU:HD12	3:N:208:LEU:C	2.37	0.50
6:S:173:ARG:HG3	12:B:199:LEU:HD12	1.94	0.50
5:V:16:ALA:HA	5:V:179:SER:O	2.10	0.50
2:b:83:ARG:CG	2:b:83:ARG:NH1	2.73	0.50
12:E:87:LEU:HD12	12:E:113:ILE:HG21	1.93	0.50
12:E:199:LEU:HB2	6:X:177:ASP:OD1	2.11	0.50
9:G:77:LEU:HB2	9:G:80:ASP:HB2	1.92	0.50
8:Q:168:ALA:HB3	8:Q:200:VAL:HG12	1.90	0.50
2:P:72:GLY:HA3	2:P:217:PHE:CD1	2.46	0.50
4:R:165:ALA:HB1	4:R:179:LEU:HD13	1.93	0.50
8:Q:49:VAL:HG11	8:Q:65:ARG:HB2	1.94	0.50
6:X:27:THR:OG1	6:X:192:ALA:HB3	2.09	0.50
6:X:52:ILE:HG13	6:X:110:ILE:HG12	1.92	0.50
3:N:208:LEU:CD1	3:N:220:LEU:HD12	2.28	0.50
6:S:173:ARG:HG2	12:B:199:LEU:HD12	1.94	0.50
8:J:49:VAL:HG11	8:J:65:ARG:HB2	1.93	0.50
9:L:116:THR:HG22	9:L:116:THR:O	2.11	0.50
10:H:58:LEU:CD1	3:I:173:GLU:HG3	2.41	0.50
10:H:209:LYS:HD3	10:H:209:LYS:N	2.25	0.50
7:C:176:ASN:HD22	7:C:187:ARG:HH21	1.54	0.50
3:I:208:LEU:CD1	3:I:220:LEU:HD12	2.28	0.50
9:G:46:LEU:HD11	9:G:135:ALA:CB	2.40	0.50
14:Y:13:MET:HB2	14:Y:166:ILE:HD12	1.94	0.50
4:R:113:MET:HE1	12:E:69:THR:HG22	1.93	0.50
12:E:195:LYS:HE3	14:U:150:GLU:OE1	2.11	0.50
13:a:147:GLN:HA	13:a:147:GLN:HE21	1.77	0.50
11:Z:206:LEU:HD13	11:Z:237:ILE:HD13	1.93	0.50
14:Y:125:LEU:HD12	14:Y:125:LEU:N	2.27	0.50
2:P:42:GLY:HA3	2:P:183:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:108:GLN:NE2	14:U:77:GLU:HB3	2.27	0.50
2:P:188:HIS:CE1	2:P:228:TYR:HD1	2.30	0.50
4:R:195:VAL:O	4:R:199:ILE:HD12	2.10	0.50
4:R:221:THR:HG23	4:R:228:ARG:NH1	2.26	0.50
6:S:75:TYR:CD1	6:S:75:TYR:C	2.89	0.50
4:K:195:VAL:O	4:K:199:ILE:HD12	2.10	0.50
2:b:142:ARG:HH12	11:Z:59:VAL:HG12	1.77	0.50
10:M:53:ARG:HG2	10:M:53:ARG:O	2.10	0.50
9:G:196:ARG:O	9:G:196:ARG:HG2	2.11	0.50
8:Q:186:CYS:O	8:Q:190:VAL:CG2	2.59	0.50
14:Y:21:ILE:HG22	14:Y:187:HIS:HB2	1.94	0.50
2:P:149:ASP:CB	2:P:150:PRO:CD	2.89	0.50
4:K:17:SER:HB2	4:K:18:PRO:HD2	1.94	0.50
13:W:136:SER:HB3	13:W:154:LEU:HD11	1.94	0.50
2:P:96:TYR:CD1	2:P:96:TYR:C	2.90	0.50
3:N:92:GLN:HB3	5:T:62:LYS:HG2	1.93	0.50
7:D:176:ASN:HD22	7:D:187:ARG:HH21	1.53	0.50
4:K:78:CYS:CB	4:K:140:LEU:HD23	2.35	0.50
11:O:151:ASP:CB	11:O:152:PRO:CD	2.86	0.50
14:Y:25:ARG:HG3	14:Y:183:GLY:C	2.37	0.50
14:U:25:ARG:HG3	14:U:183:GLY:C	2.37	0.50
2:P:171:THR:O	2:P:175:LYS:CG	2.57	0.50
3:N:108:THR:HG23	3:N:133:ILE:HD13	1.93	0.50
4:R:50:ILE:HG21	4:R:69:LEU:HD22	1.94	0.50
2:b:149:ASP:CB	2:b:150:PRO:CD	2.89	0.50
7:C:39:ASN:HB2	7:C:40:PRO:HD3	1.86	0.50
3:I:163:ARG:HG2	3:I:163:ARG:O	2.11	0.50
10:M:51:GLU:CB	10:M:206:MET:HE3	2.05	0.50
8:Q:108:LEU:HD11	8:Q:137:LEU:HB3	1.94	0.50
11:Z:99:LEU:O	11:Z:99:LEU:HG	2.12	0.50
8:J:63:ASN:ND2	9:G:154:PHE:CD2	2.80	0.49
9:L:154:PHE:CD2	8:Q:63:ASN:ND2	2.79	0.49
12:B:203:ARG:CG	14:Y:154:GLU:OE2	2.60	0.49
12:E:211:VAL:CG1	12:E:213:THR:O	2.60	0.49
9:G:193:ARG:HG3	9:G:236:LEU:CD2	2.42	0.49
1:F:8:GLN:HB3	1:F:13:VAL:HG12	1.94	0.49
11:Z:77:ALA:CB	11:Z:164:ILE:HD12	2.37	0.49
14:U:21:ILE:HG22	14:U:187:HIS:HB2	1.94	0.49
14:U:125:LEU:N	14:U:125:LEU:HD12	2.27	0.49
3:N:54:GLN:HB2	11:O:159:TRP:CE3	2.47	0.49
8:J:108:LEU:HD11	8:J:137:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:188:HIS:CE1	2:b:228:TYR:HD1	2.30	0.49
9:L:38:LEU:HD23	9:L:38:LEU:H	1.76	0.49
9:L:193:ARG:HG3	9:L:236:LEU:CD2	2.42	0.49
10:H:69:GLU:OE2	7:C:69:LEU:HD21	2.12	0.49
10:M:185:TYR:CD1	10:M:185:TYR:C	2.90	0.49
13:W:147:GLN:HA	13:W:147:GLN:HE21	1.77	0.49
13:W:211:ILE:HG22	12:E:123:PRO:HG3	1.94	0.49
8:Q:40:ARG:O	8:Q:181:MET:HB3	2.12	0.49
3:N:5:ARG:NE	10:M:125:GLU:OE1	2.46	0.49
8:J:30:VAL:HG11	8:J:134:SER:HB2	1.93	0.49
12:B:211:VAL:CG1	12:B:213:THR:O	2.60	0.49
6:X:38:ARG:HH21	6:X:38:ARG:HG2	1.77	0.49
9:L:173:GLU:HG3	8:Q:57:LEU:HD21	1.95	0.49
10:H:53:ARG:HG2	10:H:53:ARG:O	2.10	0.49
10:H:157:ASP:CB	10:H:158:PRO:CD	2.79	0.49
3:I:208:LEU:C	3:I:208:LEU:HD12	2.37	0.49
12:E:59:ILE:HG12	12:E:83:LEU:HD23	1.95	0.49
12:E:122:LEU:HD21	1:F:29:ASN:OD1	2.13	0.49
8:Q:30:VAL:HG11	8:Q:134:SER:HB2	1.93	0.49
8:Q:140:TYR:CG	8:Q:217:GLY:HA2	2.47	0.49
14:U:4:SER:O	14:U:4:SER:OG	2.29	0.49
6:S:38:ARG:HH21	6:S:38:ARG:HG2	1.77	0.49
7:D:3:THR:HG22	7:D:161:ILE:HD13	1.94	0.49
8:J:140:TYR:CG	8:J:217:GLY:HA2	2.47	0.49
2:b:114:ALA:HB1	2:b:152:GLY:O	2.12	0.49
7:C:58:ARG:HG3	7:C:58:ARG:HH11	1.75	0.49
3:I:57:ARG:HG2	3:I:57:ARG:NH1	2.28	0.49
8:Q:219:LEU:C	8:Q:219:LEU:CD1	2.85	0.49
2:P:68:THR:HG23	2:P:70:HIS:H	1.78	0.49
3:N:11:SER:HB3	3:N:12:PRO:CD	2.43	0.49
3:N:57:ARG:NH1	3:N:57:ARG:HG2	2.28	0.49
6:S:188:TYR:CZ	12:B:24:MET:CE	2.83	0.49
4:K:50:ILE:HG21	4:K:69:LEU:HD22	1.94	0.49
2:b:96:TYR:C	2:b:96:TYR:CD1	2.90	0.49
7:C:3:THR:HG22	7:C:161:ILE:HD13	1.94	0.49
7:C:176:ASN:HD22	7:C:187:ARG:HH22	1.58	0.49
9:G:47:VAL:HG12	9:G:212:ILE:HG12	1.94	0.49
9:G:74:ILE:HG22	9:G:132:LEU:HD21	1.95	0.49
8:J:40:ARG:O	8:J:181:MET:HB3	2.12	0.49
4:K:165:ALA:HB1	4:K:179:LEU:HD13	1.93	0.49
5:V:41:LYS:HG2	5:V:187:GLY:HA2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:58:LEU:HD11	3:I:173:GLU:HG3	1.95	0.49
10:H:182:GLN:HE21	9:G:55:GLU:HG2	1.77	0.49
13:W:43:MET:O	13:W:43:MET:HG3	2.12	0.49
9:G:93:LEU:CD1	6:X:74:MET:HG2	2.42	0.49
8:Q:152:ASP:HB2	8:Q:153:PRO:HD3	1.89	0.49
1:A:8:GLN:HB3	1:A:13:VAL:HG12	1.94	0.49
6:S:161:VAL:HG12	6:S:163:HIS:H	1.76	0.49
6:S:187:VAL:O	12:B:167:LEU:HD22	2.13	0.49
7:D:195:ASP:OD1	7:D:195:ASP:N	2.42	0.49
2:b:68:THR:HG23	2:b:70:HIS:H	1.78	0.49
9:L:32:GLY:HA2	9:L:51:ARG:HH22	1.78	0.49
12:B:59:ILE:HG12	12:B:83:LEU:HD23	1.95	0.49
2:P:114:ALA:HB1	2:P:152:GLY:O	2.12	0.49
8:J:37:ILE:HD12	8:J:39:ILE:HG13	1.95	0.49
10:H:185:TYR:CD1	10:H:185:TYR:C	2.90	0.49
13:a:43:MET:O	13:a:43:MET:HG3	2.12	0.49
1:F:7:VAL:HG23	1:F:126:PHE:HB3	1.94	0.49
5:T:25:ILE:HA	5:V:172:ILE:HG12	1.93	0.49
9:L:157:ARG:HG3	8:Q:57:LEU:O	2.13	0.49
11:O:91:ARG:HG2	14:U:75:LEU:HD13	1.95	0.49
3:I:53:LEU:HD13	11:Z:161:ALA:HB3	1.95	0.49
3:I:108:THR:HG21	3:I:145:TYR:HB3	1.94	0.49
10:M:135:ARG:HG3	10:M:135:ARG:NH2	2.24	0.49
12:E:99:VAL:HG23	12:E:127:MET:HG3	1.95	0.49
12:E:164:PHE:O	6:X:38:ARG:NH1	2.46	0.49
7:C:154:TYR:OH	7:C:179:HIS:CD2	2.66	0.48
3:I:54:GLN:HB2	11:Z:159:TRP:CZ3	2.48	0.48
3:I:108:THR:HG23	3:I:133:ILE:HD13	1.93	0.48
9:G:199:LEU:HD23	9:G:200:PRO:HD2	1.92	0.48
13:a:136:SER:HB3	13:a:154:LEU:HD11	1.94	0.48
4:R:17:SER:HB2	4:R:18:PRO:HD2	1.94	0.48
7:D:199:LYS:HE2	7:D:200:TYR:CE1	2.48	0.48
8:J:186:CYS:O	8:J:190:VAL:CG2	2.59	0.48
2:b:7:PHE:O	2:b:124:GLY:HA2	2.13	0.48
9:G:19:ILE:CG2	9:G:22:ILE:HD12	2.40	0.48
1:A:38:ILE:HG22	1:A:64:LEU:HD23	1.95	0.48
2:P:84:VAL:HG21	4:R:123:GLN:OE1	2.13	0.48
4:R:60:LEU:HD21	8:Q:181:MET:HE1	1.94	0.48
4:R:61:LEU:HG	8:Q:160:TYR:CE2	2.48	0.48
4:R:139:ILE:HG12	4:R:153:LYS:CG	2.41	0.48
5:V:1:MET:N	5:V:173:LEU:HD11	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:W:22:ILE:HD13	13:W:111:VAL:HG12	1.95	0.48
12:E:199:LEU:HD12	6:X:173:ARG:HG3	1.95	0.48
8:Q:37:ILE:HD12	8:Q:39:ILE:HG13	1.95	0.48
14:Y:137:VAL:HG11	14:Y:145:MET:HB3	1.96	0.48
7:D:142:ARG:NE	7:D:142:ARG:HA	2.27	0.48
5:V:101:ASN:HB3	5:V:132:HIS:CE1	2.49	0.48
2:b:42:GLY:HA3	2:b:183:LEU:HD22	1.93	0.48
2:b:72:GLY:HA3	2:b:217:PHE:CD1	2.46	0.48
10:M:181:LEU:CD2	10:M:201:ILE:CD1	2.83	0.48
13:W:9:THR:HB	13:W:10:SER:H	1.47	0.48
1:A:7:VAL:HG23	1:A:126:PHE:HB3	1.94	0.48
2:P:34:SER:HB2	2:P:162:MET:HE3	1.95	0.48
8:J:219:LEU:CD1	8:J:219:LEU:C	2.86	0.48
9:L:74:ILE:HG22	9:L:132:LEU:HD21	1.95	0.48
9:L:168:ALA:O	9:L:172:LEU:HG	2.14	0.48
9:L:215:VAL:HB	9:L:221:PHE:HD1	1.78	0.48
10:H:232:GLU:OE2	10:H:232:GLU:N	2.30	0.48
11:O:95:GLN:HE22	14:U:71:ASN:HD22	1.61	0.48
12:B:106:THR:HB	12:B:109:HIS:NE2	2.28	0.48
9:G:49:LEU:CB	9:G:195:LEU:HD11	2.41	0.48
9:G:56:LEU:N	9:G:56:LEU:HD23	2.29	0.48
9:G:157:ARG:NE	9:G:176:MET:HE1	2.28	0.48
9:G:168:ALA:O	9:G:172:LEU:HG	2.14	0.48
8:Q:69:VAL:HG23	8:Q:73:VAL:HB	1.96	0.48
11:Z:33:THR:HG23	11:Z:163:CYS:SG	2.53	0.48
14:U:13:MET:HB2	14:U:166:ILE:HD12	1.94	0.48
8:J:69:VAL:HG23	8:J:73:VAL:HB	1.95	0.48
2:b:34:SER:HB2	2:b:162:MET:HE3	1.95	0.48
9:L:47:VAL:HG12	9:L:212:ILE:HG12	1.94	0.48
9:L:157:ARG:NE	9:L:176:MET:HE1	2.28	0.48
9:L:199:LEU:HD23	9:L:200:PRO:HD2	1.92	0.48
7:C:199:LYS:HE2	7:C:200:TYR:CE1	2.48	0.48
3:I:192:ILE:HD11	3:I:208:LEU:HD21	1.95	0.48
13:W:97:TYR:OH	6:X:99:ARG:NH2	2.45	0.48
12:E:106:THR:HB	12:E:109:HIS:NE2	2.28	0.48
1:F:38:ILE:HG22	1:F:64:LEU:HD23	1.95	0.48
6:X:72:LEU:HD21	6:X:88:ILE:HG12	1.96	0.48
3:N:32:ALA:HB3	3:N:161:ILE:HG13	1.96	0.48
4:K:229:ILE:HD12	4:K:229:ILE:N	2.28	0.48
9:L:125:ARG:HD3	10:M:127:ASP:OD2	2.14	0.48
3:I:26:VAL:O	3:I:162:GLY:HA2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:116:THR:HG23	9:G:128:TYR:CD1	2.48	0.48
9:G:196:ARG:HB2	9:G:205:LEU:HD12	1.96	0.48
11:Z:95:GLN:NE2	11:Z:98:LEU:HD23	2.26	0.48
14:U:137:VAL:HG11	14:U:145:MET:HB3	1.96	0.48
1:A:191:LEU:N	1:A:191:LEU:CD2	2.73	0.48
4:R:229:ILE:N	4:R:229:ILE:HD12	2.28	0.48
6:S:72:LEU:HD21	6:S:88:ILE:HG12	1.96	0.48
9:L:116:THR:HG23	9:L:128:TYR:CD1	2.48	0.48
9:L:196:ARG:HB2	9:L:205:LEU:HD12	1.96	0.48
10:H:31:ILE:HD11	10:H:158:PRO:HG3	1.96	0.48
7:C:142:ARG:NE	7:C:142:ARG:HA	2.27	0.48
11:O:99:LEU:O	11:O:99:LEU:HG	2.12	0.48
3:I:32:ALA:HB3	3:I:161:ILE:HG13	1.96	0.48
12:B:99:VAL:HG23	12:B:127:MET:HG3	1.95	0.48
9:G:32:GLY:HA2	9:G:51:ARG:HH22	1.78	0.48
1:F:145:ARG:NH1	1:F:145:ARG:CG	2.73	0.48
14:U:142:SER:HA	14:U:145:MET:HE3	1.96	0.48
14:U:192:ASP:N	14:U:192:ASP:OD1	2.46	0.48
1:A:188:GLN:HE21	1:A:190:LEU:HD21	1.79	0.48
2:P:7:PHE:O	2:P:124:GLY:HA2	2.13	0.48
3:N:26:VAL:O	3:N:162:GLY:HA2	2.14	0.48
3:N:108:THR:HG21	3:N:145:TYR:HB3	1.95	0.48
4:R:143:ILE:HD11	4:R:220:VAL:O	2.14	0.48
7:D:154:TYR:OH	7:D:179:HIS:CD2	2.66	0.48
11:O:68:LEU:HD12	11:O:72:MET:HE2	1.96	0.48
3:I:11:SER:HB3	3:I:12:PRO:CD	2.43	0.48
9:G:137:TYR:CE1	9:G:217:LYS:HA	2.49	0.48
1:F:197:LYS:HD3	1:F:197:LYS:HA	1.57	0.48
11:Z:28:ILE:CD1	11:Z:152:PRO:CG	2.92	0.48
3:N:192:ILE:HD11	3:N:208:LEU:HD21	1.95	0.48
6:S:54:CYS:HB3	6:S:106:VAL:CG1	2.44	0.48
4:K:52:THR:CG2	4:K:69:LEU:HD21	2.44	0.48
2:b:190:ALA:O	2:b:193:THR:HG23	2.14	0.48
9:L:137:TYR:CE1	9:L:217:LYS:HA	2.49	0.48
11:O:33:THR:HG23	11:O:163:CYS:SG	2.53	0.48
12:B:34:ILE:HG12	12:B:44:CYS:SG	2.54	0.48
12:E:38:SER:HB2	12:E:39:PRO:CD	2.44	0.48
11:Z:68:LEU:HD12	11:Z:72:MET:HE2	1.96	0.48
14:U:34:VAL:HG12	14:U:35:THR:HG23	1.96	0.48
6:S:168:LEU:HD12	6:S:168:LEU:O	2.14	0.47
4:K:143:ILE:HD11	4:K:220:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:28:ILE:CD1	11:O:152:PRO:CG	2.92	0.47
11:O:147:LEU:HD21	11:O:162:THR:HG22	1.96	0.47
12:E:63:LEU:HD23	12:E:63:LEU:HA	1.78	0.47
9:G:215:VAL:HB	9:G:221:PHE:HD1	1.78	0.47
5:T:101:ASN:HB3	5:T:132:HIS:CE1	2.48	0.47
4:K:206:LEU:HD12	4:K:210:PHE:CZ	2.45	0.47
9:L:56:LEU:N	9:L:56:LEU:HD23	2.29	0.47
7:C:139:VAL:HG21	7:C:163:GLN:HG3	1.96	0.47
12:E:34:ILE:HG12	12:E:44:CYS:SG	2.54	0.47
12:E:203:ARG:CG	14:U:154:GLU:OE2	2.61	0.47
4:R:52:THR:CG2	4:R:69:LEU:HD21	2.44	0.47
5:T:41:LYS:HG2	5:T:187:GLY:HA2	1.95	0.47
7:C:36:ILE:HG23	7:C:46:MET:HE2	1.96	0.47
11:O:86:LEU:HD22	11:O:114:LEU:HD11	1.96	0.47
8:Q:40:ARG:HD3	8:Q:161:TRP:CZ3	2.49	0.47
6:X:54:CYS:HB3	6:X:106:VAL:CG1	2.44	0.47
1:A:29:ASN:OD1	12:B:122:LEU:HD21	2.13	0.47
9:L:71:GLY:HA3	9:L:221:PHE:CE1	2.49	0.47
7:C:21:ALA:HB2	7:C:32:VAL:HG21	1.96	0.47
11:O:95:GLN:HB3	14:U:68:PHE:CE2	2.49	0.47
3:I:119:THR:HG22	3:I:126:PRO:HB3	1.97	0.47
12:B:38:SER:HB2	12:B:39:PRO:CD	2.44	0.47
12:E:17:ASP:O	12:E:33:LYS:HD2	2.15	0.47
12:E:203:ARG:HG2	14:U:154:GLU:OE2	2.14	0.47
8:Q:150:MET:HG3	8:Q:163:CYS:SG	2.55	0.47
13:a:22:ILE:HD13	13:a:111:VAL:HG12	1.95	0.47
1:F:188:GLN:HE21	1:F:190:LEU:HD21	1.79	0.47
5:T:1:MET:N	5:T:173:LEU:HD11	2.28	0.47
6:S:74:MET:HG2	9:L:93:LEU:CD1	2.45	0.47
4:K:50:ILE:O	4:K:217:VAL:HA	2.14	0.47
2:b:221:THR:HB	2:b:222:PRO:HD2	1.96	0.47
10:H:83:ALA:HB2	3:I:152:THR:HG22	1.96	0.47
12:B:220:GLU:HA	12:B:220:GLU:OE2	2.14	0.47
12:E:24:MET:CE	6:X:188:TYR:CZ	2.85	0.47
14:Y:142:SER:HA	14:Y:145:MET:HE3	1.96	0.47
2:P:190:ALA:O	2:P:193:THR:HG23	2.14	0.47
5:T:44:LEU:HD11	5:T:102:LEU:HD13	1.97	0.47
2:b:139:ASN:C	2:b:139:ASN:ND2	2.73	0.47
9:L:107:ARG:NH2	13:a:74:GLU:OE2	2.27	0.47
7:C:108:ARG:H	7:C:108:ARG:HG3	1.52	0.47
10:M:31:ILE:HD11	10:M:158:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:224:GLN:OE1	10:M:224:GLN:N	2.48	0.47
12:E:220:GLU:HA	12:E:220:GLU:OE2	2.14	0.47
9:G:104:PRO:HB2	9:G:107:ARG:HG3	1.97	0.47
13:a:178:TYR:OH	13:a:207:THR:CA	2.63	0.47
11:Z:95:GLN:HB3	14:Y:68:PHE:CE2	2.50	0.47
3:N:99:GLU:OE1	3:N:99:GLU:N	2.48	0.47
8:J:40:ARG:HD3	8:J:161:TRP:CZ3	2.49	0.47
8:J:150:MET:HG3	8:J:163:CYS:SG	2.55	0.47
4:K:208:ILE:O	4:K:208:ILE:HG22	2.15	0.47
5:V:12:TYR:OH	5:V:156:ALA:HB2	2.14	0.47
10:H:18:GLU:CD	10:H:18:GLU:N	2.73	0.47
12:B:123:PRO:HG3	13:a:211:ILE:HG22	1.96	0.47
14:Y:34:VAL:HG12	14:Y:35:THR:HG23	1.96	0.47
4:R:50:ILE:O	4:R:217:VAL:HA	2.14	0.47
5:T:86:ARG:HH21	14:U:64:GLN:NE2	2.12	0.47
6:S:38:ARG:HH21	6:S:38:ARG:CG	2.27	0.47
7:D:118:GLU:OE1	7:D:118:GLU:HA	2.14	0.47
4:K:51:VAL:HG12	4:K:202:LEU:CD2	2.26	0.47
4:K:113:MET:HE1	12:B:69:THR:HG22	1.96	0.47
2:b:108:GLN:NE2	14:Y:77:GLU:HB3	2.30	0.47
10:H:181:LEU:CD2	10:H:201:ILE:CD1	2.83	0.47
7:C:9:PHE:CD1	7:C:9:PHE:N	2.73	0.47
9:G:118:ILE:CB	9:G:119:PRO:HD3	2.38	0.47
11:Z:97:TYR:CD1	11:Z:97:TYR:C	2.92	0.47
6:X:75:TYR:CG	6:X:83:MET:HE2	2.50	0.47
6:X:168:LEU:HD12	6:X:168:LEU:O	2.15	0.47
2:P:139:ASN:C	2:P:139:ASN:ND2	2.73	0.47
7:D:170:TYR:HE2	14:Y:31:ALA:HB2	1.79	0.47
8:J:50:GLU:HB2	8:J:209:PHE:CD2	2.50	0.47
2:b:83:ARG:HG2	2:b:83:ARG:NH1	2.22	0.47
3:I:181:ILE:CA	3:I:187:THR:HG22	2.45	0.47
6:X:38:ARG:HH21	6:X:38:ARG:CG	2.27	0.47
6:S:197:ILE:N	6:S:197:ILE:HD12	2.30	0.47
4:K:16:PHE:HE2	2:b:128:PRO:O	1.98	0.47
9:L:107:ARG:NH2	13:a:74:GLU:CG	2.78	0.47
10:H:79:SER:O	10:H:139:VAL:CG2	2.63	0.47
13:W:178:TYR:OH	13:W:207:THR:CA	2.63	0.47
9:G:71:GLY:HA3	9:G:221:PHE:CE1	2.49	0.47
11:Z:147:LEU:HD21	11:Z:162:THR:HG22	1.96	0.47
2:P:221:THR:HB	2:P:222:PRO:HD2	1.96	0.46
3:N:40:ILE:HD11	3:N:210:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:208:ILE:O	4:R:208:ILE:HG22	2.15	0.46
5:T:51:GLY:HA3	7:D:119:GLY:HA3	1.97	0.46
6:S:177:ASP:OD1	12:B:199:LEU:HB2	2.15	0.46
7:D:36:ILE:HG22	7:D:46:MET:HE2	1.96	0.46
3:I:40:ILE:HD11	3:I:210:VAL:HB	1.97	0.46
12:E:214:GLU:OE1	14:U:195:THR:HG23	2.13	0.46
13:a:12:LEU:HD11	13:a:172:CYS:HB3	1.97	0.46
11:Z:86:LEU:HD22	11:Z:114:LEU:HD11	1.96	0.46
14:Y:100:GLY:N	14:Y:101:PRO:HD2	2.30	0.46
1:A:91:TYR:HB2	1:A:95:LEU:CD1	2.46	0.46
2:P:28:VAL:CG1	2:P:132:SER:HB2	2.42	0.46
3:N:70:CYS:SG	3:N:134:VAL:HG12	2.56	0.46
3:N:152:THR:HG22	10:M:83:ALA:HB2	1.97	0.46
10:H:40:ILE:HD11	10:H:181:LEU:HD22	1.97	0.46
7:C:118:GLU:OE1	7:C:118:GLU:HA	2.14	0.46
11:O:28:ILE:HG22	11:O:28:ILE:O	2.15	0.46
10:M:232:GLU:OE2	10:M:232:GLU:N	2.30	0.46
9:G:72:ILE:HG21	9:G:88:MET:HE1	1.97	0.46
13:a:43:MET:HG2	13:a:51:LEU:HB3	1.97	0.46
1:F:91:TYR:HB2	1:F:95:LEU:CD1	2.46	0.46
5:V:51:GLY:HA3	7:C:119:GLY:HA3	1.98	0.46
2:b:54:ILE:HD13	2:b:54:ILE:HA	1.80	0.46
2:b:88:ARG:HH11	2:b:88:ARG:HG3	1.81	0.46
10:H:224:GLN:N	10:H:224:GLN:OE1	2.48	0.46
10:M:40:ILE:HD11	10:M:181:LEU:HD22	1.97	0.46
10:M:157:ASP:CB	10:M:158:PRO:CD	2.79	0.46
13:W:44:ARG:NH1	13:W:44:ARG:CG	2.73	0.46
13:W:94:ARG:NH2	13:W:94:ARG:CG	2.73	0.46
12:E:6:VAL:HG22	12:E:155:VAL:HG21	1.98	0.46
11:Z:35:LEU:C	11:Z:35:LEU:CD1	2.88	0.46
14:Y:83:PRO:HD3	14:Y:113:PRO:CD	2.46	0.46
14:Y:120:ILE:HD12	14:Y:136:VAL:HG22	1.97	0.46
6:X:197:ILE:N	6:X:197:ILE:HD12	2.30	0.46
2:P:83:ARG:CG	2:P:83:ARG:NH1	2.73	0.46
3:N:119:THR:HG22	3:N:126:PRO:HB3	1.97	0.46
5:T:12:TYR:OH	5:T:156:ALA:HB2	2.14	0.46
6:S:75:TYR:CG	6:S:83:MET:HE2	2.50	0.46
8:J:136:MET:HE2	8:J:165:ILE:CD1	2.46	0.46
7:C:170:TYR:HE2	14:U:31:ALA:HB2	1.80	0.46
11:O:97:TYR:CD1	11:O:97:TYR:C	2.92	0.46
3:I:99:GLU:N	3:I:99:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:18:GLU:CD	10:M:18:GLU:N	2.73	0.46
13:W:12:LEU:HD11	13:W:172:CYS:HB3	1.97	0.46
13:W:169:VAL:CG1	13:W:189:ILE:HD11	2.46	0.46
8:Q:176:ILE:O	8:Q:176:ILE:HG22	2.14	0.46
2:P:74:VAL:HG12	2:P:134:LEU:HB3	1.98	0.46
6:S:136:LYS:HA	6:S:136:LYS:HD2	1.68	0.46
7:D:139:VAL:HG21	7:D:163:GLN:HG3	1.96	0.46
4:K:213:SER:O	4:K:213:SER:OG	2.23	0.46
3:N:47:LYS:HB2	3:N:47:LYS:HE2	1.57	0.46
12:B:54:MET:HG3	14:Y:95:TYR:CD2	2.50	0.46
13:W:74:GLU:OE2	9:G:107:ARG:NH2	2.28	0.46
8:J:176:ILE:O	8:J:176:ILE:HG22	2.14	0.46
4:K:145:GLU:CD	4:K:145:GLU:N	2.74	0.46
5:V:44:LEU:HD11	5:V:102:LEU:HD13	1.97	0.46
9:L:50:LYS:HE3	9:L:59:HIS:HB2	1.98	0.46
11:O:3:ARG:HG3	11:O:3:ARG:O	2.15	0.46
1:F:2:THR:CB	15:F:301:A1L0C:O2	2.64	0.46
5:T:1:MET:HA	5:T:1:MET:HE2	1.97	0.46
5:V:62:LYS:HG2	3:I:92:GLN:HB3	1.97	0.46
9:L:74:ILE:HG22	9:L:132:LEU:CD2	2.46	0.46
9:L:104:PRO:HB2	9:L:107:ARG:HG3	1.97	0.46
10:H:227:HIS:CE1	10:H:233:GLU:OE1	2.69	0.46
11:O:230:GLN:HE21	11:O:230:GLN:CA	2.10	0.46
10:M:44:GLU:HG3	10:M:191:LEU:CB	2.43	0.46
10:M:194:ALA:O	10:M:198:SER:OG	2.32	0.46
13:W:12:LEU:CD1	13:W:172:CYS:HB3	2.46	0.46
13:W:97:TYR:OH	6:X:60:ASP:OD1	2.28	0.46
2:P:218:ARG:HG2	2:P:218:ARG:NH1	2.31	0.46
2:b:28:VAL:CG1	2:b:132:SER:HB2	2.42	0.46
10:H:127:ASP:OD2	9:G:125:ARG:HD3	2.16	0.46
12:B:17:ASP:O	12:B:33:LYS:HD2	2.15	0.46
10:M:12:VAL:HG22	10:M:125:GLU:HG3	1.98	0.46
12:E:54:MET:HG3	14:U:95:TYR:CD2	2.51	0.46
5:T:13:VAL:HG22	5:T:113:PRO:HB2	1.98	0.46
10:H:194:ALA:O	10:H:198:SER:OG	2.32	0.46
3:I:47:LYS:HE2	3:I:47:LYS:HB2	1.57	0.46
3:I:69:VAL:HG11	3:I:107:ILE:HG21	1.98	0.46
12:B:6:VAL:HG22	12:B:155:VAL:HG21	1.98	0.46
10:M:79:SER:O	10:M:139:VAL:CG2	2.63	0.46
10:M:227:HIS:CE1	10:M:233:GLU:OE1	2.69	0.46
9:G:74:ILE:HG22	9:G:132:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:169:VAL:CG1	13:a:189:ILE:HD11	2.46	0.46
11:Z:28:ILE:HG22	11:Z:28:ILE:O	2.15	0.46
14:U:44:MET:CE	14:U:70:LEU:CD2	2.76	0.46
14:U:83:PRO:HD3	14:U:113:PRO:CD	2.46	0.46
14:U:120:ILE:HD12	14:U:136:VAL:HG22	1.97	0.46
1:A:2:THR:CB	15:A:301:A1L0C:O2	2.64	0.45
4:R:145:GLU:CD	4:R:145:GLU:N	2.74	0.45
6:S:153:VAL:CG2	6:S:174:LEU:CD2	2.94	0.45
7:D:21:ALA:HB2	7:D:32:VAL:HG21	1.96	0.45
13:W:20:VAL:HG11	13:W:122:LEU:HD13	1.99	0.45
13:a:147:GLN:N	13:a:148:PRO:CD	2.79	0.45
6:X:46:LEU:HD12	6:X:50:THR:CG2	2.47	0.45
4:K:109:ILE:HA	4:K:110:PRO:HD3	1.85	0.45
4:K:139:ILE:HG12	4:K:153:LYS:CG	2.41	0.45
5:V:103:LEU:HD23	5:V:117:TYR:HA	1.98	0.45
7:C:27:ILE:O	7:C:27:ILE:HG22	2.16	0.45
10:M:181:LEU:HD21	10:M:201:ILE:HD13	1.97	0.45
13:W:43:MET:HG2	13:W:51:LEU:HB3	1.97	0.45
6:X:153:VAL:CG2	6:X:174:LEU:CD2	2.94	0.45
3:N:204:LYS:HB3	3:N:204:LYS:HE2	1.82	0.45
5:V:172:ILE:H	5:V:172:ILE:HG13	1.64	0.45
2:b:45:LEU:HD11	2:b:136:CYS:HB3	1.99	0.45
10:H:149:LYS:HE3	10:H:149:LYS:HB3	1.49	0.45
3:I:133:ILE:HD12	3:I:133:ILE:N	2.32	0.45
13:W:33:LEU:HD13	1:F:135:TYR:CE1	2.52	0.45
9:G:62:LYS:HE3	9:G:62:LYS:HB3	1.63	0.45
13:a:12:LEU:CD1	13:a:172:CYS:HB3	2.46	0.45
13:a:20:VAL:HG11	13:a:122:LEU:HD13	1.99	0.45
14:Y:21:ILE:CG2	14:Y:187:HIS:HB2	2.47	0.45
14:Y:192:ASP:OD1	14:Y:192:ASP:N	2.46	0.45
3:N:57:ARG:CG	3:N:57:ARG:NH1	2.73	0.45
3:N:69:VAL:HG11	3:N:107:ILE:HG21	1.98	0.45
4:R:37:LEU:CG	4:R:55:LYS:HZ1	2.26	0.45
4:K:123:GLN:OE1	2:b:84:VAL:HG21	2.16	0.45
2:b:197:SER:O	2:b:197:SER:OG	2.31	0.45
9:L:72:ILE:HG21	9:L:88:MET:HE1	1.97	0.45
10:H:38:ILE:HD11	10:H:201:ILE:CG2	2.46	0.45
7:C:36:ILE:HG22	7:C:46:MET:HE2	1.96	0.45
11:O:98:LEU:O	11:O:98:LEU:HG	2.16	0.45
3:I:70:CYS:SG	3:I:134:VAL:HG12	2.56	0.45
13:W:147:GLN:N	13:W:148:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:187:ARG:HA	12:E:188:PRO:HA	1.81	0.45
9:G:108:LEU:O	9:G:108:LEU:HG	2.16	0.45
8:Q:50:GLU:HB2	8:Q:209:PHE:CD2	2.50	0.45
6:X:162:GLU:CD	6:X:162:GLU:N	2.73	0.45
1:A:145:ARG:NH1	1:A:145:ARG:CG	2.73	0.45
4:R:199:ILE:HD12	4:R:199:ILE:N	2.32	0.45
5:T:20:VAL:O	5:T:20:VAL:HG12	2.16	0.45
8:J:51:LYS:O	8:J:210:GLU:N	2.47	0.45
9:L:13:TRP:N	8:Q:22:GLN:HE22	2.00	0.45
12:B:59:ILE:HG12	12:B:83:LEU:CD2	2.47	0.45
8:Q:47:PHE:CB	8:Q:66:LEU:HD21	2.47	0.45
6:X:16:ALA:HB2	6:X:121:VAL:HG23	1.99	0.45
2:P:61:VAL:HG21	4:R:161:CYS:SG	2.56	0.45
7:D:72:LYS:HB3	7:D:72:LYS:HE3	1.61	0.45
10:H:12:VAL:HG22	10:H:125:GLU:HG3	1.98	0.45
3:I:50:VAL:HB	3:I:205:ASN:OD1	2.17	0.45
13:W:14:VAL:HG13	13:W:21:VAL:CG1	2.47	0.45
8:Q:51:LYS:O	8:Q:210:GLU:N	2.47	0.45
2:P:97:TYR:O	2:P:97:TYR:CD1	2.70	0.45
10:H:185:TYR:CD1	9:G:56:LEU:HD13	2.52	0.45
11:O:52:ILE:H	11:O:52:ILE:HG13	1.65	0.45
13:a:22:ILE:HD11	13:a:111:VAL:HG12	1.98	0.45
11:Z:206:LEU:HD12	11:Z:206:LEU:O	2.17	0.45
2:b:56:TYR:CD1	2:b:56:TYR:N	2.85	0.45
2:b:97:TYR:O	2:b:97:TYR:CD1	2.70	0.45
2:b:175:LYS:HE3	2:b:175:LYS:HB2	1.40	0.45
2:b:176:ARG:HH21	2:b:192:LEU:CD1	2.30	0.45
10:H:51:GLU:CG	10:H:206:MET:CE	2.62	0.45
3:I:57:ARG:CG	3:I:57:ARG:NH1	2.73	0.45
13:W:22:ILE:HD11	13:W:111:VAL:HG12	1.98	0.45
9:G:10:VAL:HG12	9:G:21:GLN:HB3	1.98	0.45
8:Q:90:ILE:HD12	8:Q:90:ILE:HA	1.84	0.45
1:F:7:VAL:HG23	1:F:126:PHE:CB	2.47	0.45
1:F:20:ARG:HE	1:F:20:ARG:HB2	1.50	0.45
3:N:40:ILE:O	3:N:40:ILE:HG23	2.16	0.45
3:N:181:ILE:CA	3:N:187:THR:HG22	2.45	0.45
7:D:27:ILE:O	7:D:27:ILE:HG22	2.16	0.45
7:D:38:ILE:HB	7:D:42:LEU:HB3	1.99	0.45
5:V:20:VAL:O	5:V:20:VAL:HG12	2.16	0.45
3:I:134:VAL:HG23	3:I:144:LEU:HD13	1.99	0.45
3:I:148:ASP:CB	3:I:149:PRO:CD	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:215:ILE:HD12	10:M:234:LEU:HD21	1.99	0.45
8:Q:136:MET:HE2	8:Q:165:ILE:CD1	2.46	0.45
1:F:87:MET:HE2	1:F:87:MET:HB3	1.74	0.45
11:Z:3:ARG:HG3	11:Z:3:ARG:O	2.15	0.45
11:Z:95:GLN:HE22	14:Y:71:ASN:HD22	1.64	0.45
11:Z:174:MET:HE2	11:Z:174:MET:HB2	1.76	0.45
14:U:100:GLY:H	14:U:101:PRO:HD3	1.82	0.45
2:P:56:TYR:N	2:P:56:TYR:CD1	2.85	0.45
2:P:111:GLN:HG2	2:P:154:TYR:CZ	2.52	0.45
6:S:97:TYR:O	6:S:97:TYR:CD2	2.70	0.45
8:J:47:PHE:CB	8:J:66:LEU:HD21	2.47	0.45
8:J:198:TYR:HE2	8:J:240:LYS:HE3	1.82	0.45
5:V:1:MET:H2	5:V:173:LEU:CD1	2.29	0.45
9:L:10:VAL:HG12	9:L:21:GLN:HB3	1.98	0.45
9:L:108:LEU:O	9:L:108:LEU:HG	2.16	0.45
10:H:135:ARG:NH2	10:H:135:ARG:CG	2.80	0.45
11:O:107:CYS:O	11:O:111:VAL:HG23	2.17	0.45
10:M:193:GLU:O	10:M:197:SER:OG	2.32	0.45
8:Q:198:TYR:HE2	8:Q:240:LYS:HE3	1.82	0.45
14:U:16:LYS:HB3	14:U:16:LYS:HE3	1.66	0.45
1:A:7:VAL:HG23	1:A:126:PHE:CB	2.47	0.44
2:P:198:PHE:CD2	2:P:198:PHE:O	2.70	0.44
3:N:50:VAL:HB	3:N:205:ASN:OD1	2.17	0.44
3:N:173:GLU:HG3	10:M:58:LEU:CD1	2.47	0.44
5:T:103:LEU:HD23	5:T:117:TYR:HA	1.98	0.44
2:b:74:VAL:HG12	2:b:134:LEU:HB3	1.98	0.44
7:C:83:LEU:HD22	7:C:87:MET:CE	2.47	0.44
12:B:63:LEU:HD23	12:B:63:LEU:HA	1.77	0.44
10:M:149:LYS:HE3	10:M:149:LYS:HB3	1.49	0.44
12:E:59:ILE:HG12	12:E:83:LEU:CD2	2.47	0.44
13:a:1:THR:N	13:a:104:ASN:HD21	2.15	0.44
14:Y:10:VAL:HG12	14:Y:23:ALA:HB2	1.99	0.44
1:A:180:ILE:HG12	1:A:185:VAL:HG13	1.99	0.44
2:P:176:ARG:HH21	2:P:192:LEU:CD1	2.30	0.44
4:K:93:ARG:HH11	4:K:93:ARG:HG2	1.83	0.44
10:H:181:LEU:HD21	10:H:201:ILE:HD13	1.97	0.44
7:C:39:ASN:CB	7:C:40:PRO:CD	2.76	0.44
11:O:95:GLN:NE2	11:O:98:LEU:HD23	2.27	0.44
10:M:135:ARG:HB2	10:M:136:PRO:CD	2.47	0.44
9:G:50:LYS:HE3	9:G:59:HIS:HB2	1.98	0.44
11:Z:91:ARG:HG2	14:Y:75:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:151:ASP:CB	11:Z:152:PRO:CD	2.86	0.44
14:Y:163:PHE:CE1	14:Y:197:ARG:CD	3.00	0.44
14:U:66:LEU:HD13	14:U:90:VAL:HG22	1.99	0.44
8:J:207:LYS:HE3	8:J:207:LYS:HB2	1.54	0.44
4:K:199:ILE:HD12	4:K:199:ILE:N	2.32	0.44
5:V:13:VAL:HG22	5:V:113:PRO:HB2	1.98	0.44
2:b:198:PHE:CD2	2:b:198:PHE:O	2.70	0.44
10:H:167:ALA:CB	9:G:56:LEU:HD12	2.38	0.44
11:O:136:TYR:O	11:O:147:LEU:HA	2.17	0.44
3:I:185:ASP:OD1	3:I:185:ASP:N	2.41	0.44
13:W:110:MET:HE2	13:W:110:MET:HB2	1.73	0.44
13:a:14:VAL:HG13	13:a:21:VAL:CG1	2.47	0.44
13:a:178:TYR:HH	13:a:208:ASN:H	1.64	0.44
2:P:16:GLY:O	11:O:27:ALA:HB2	2.18	0.44
2:P:45:LEU:HD11	2:P:136:CYS:HB3	1.99	0.44
3:N:134:VAL:HG23	3:N:144:LEU:HD13	1.99	0.44
5:T:43:LEU:HD11	5:T:181:ARG:HD3	2.00	0.44
4:K:178:PHE:CE1	4:K:201:CYS:CB	2.97	0.44
4:K:178:PHE:HE1	4:K:201:CYS:HB2	1.79	0.44
5:V:86:ARG:HH21	14:Y:64:GLN:NE2	2.15	0.44
9:L:84:LEU:HD23	9:L:84:LEU:HA	1.83	0.44
10:H:135:ARG:HB2	10:H:136:PRO:CD	2.47	0.44
7:C:72:LYS:HB3	7:C:72:LYS:HE3	1.61	0.44
11:O:206:LEU:HD12	11:O:206:LEU:O	2.17	0.44
3:I:207:GLU:O	3:I:207:GLU:HG2	2.14	0.44
12:E:38:SER:HB2	12:E:39:PRO:HD2	2.00	0.44
14:U:26:ARG:HB2	14:U:182:MET:CB	2.47	0.44
14:U:119:PHE:CD1	14:U:119:PHE:C	2.95	0.44
1:A:121:MET:HE3	1:A:121:MET:HB3	1.79	0.44
3:N:36:ARG:HD2	3:N:142:PRO:O	2.18	0.44
5:V:43:LEU:HD11	5:V:181:ARG:HD3	2.00	0.44
10:H:66:LYS:HG2	10:H:216:GLU:OE2	2.18	0.44
7:C:92:LYS:HD2	7:C:118:GLU:O	2.18	0.44
13:W:1:THR:N	13:W:104:ASN:HD21	2.15	0.44
11:Z:72:MET:SD	11:Z:107:CYS:HA	2.58	0.44
11:Z:107:CYS:O	11:Z:111:VAL:HG23	2.17	0.44
14:Y:125:LEU:HD12	14:Y:125:LEU:H	1.82	0.44
4:R:37:LEU:CD2	4:R:55:LYS:NZ	2.80	0.44
4:R:79:VAL:CG1	4:R:139:ILE:HB	2.48	0.44
6:S:46:LEU:HD12	6:S:50:THR:CG2	2.46	0.44
7:D:20:ARG:NH2	14:Y:204:ASP:HB3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:111:GLN:HG2	2:b:154:TYR:OH	2.17	0.44
9:L:36:VAL:CG1	9:L:172:LEU:HD11	2.48	0.44
3:I:36:ARG:HD2	3:I:142:PRO:O	2.18	0.44
3:I:40:ILE:HG23	3:I:40:ILE:O	2.16	0.44
14:Y:26:ARG:HB2	14:Y:182:MET:CB	2.47	0.44
14:U:125:LEU:HD12	14:U:125:LEU:H	1.82	0.44
2:P:64:VAL:CG1	2:P:217:PHE:HZ	2.31	0.44
6:S:46:LEU:HD11	6:S:52:ILE:HB	2.00	0.44
4:K:37:LEU:CD2	4:K:55:LYS:NZ	2.81	0.44
5:V:1:MET:HA	5:V:1:MET:HE2	1.97	0.44
2:b:111:GLN:HG2	2:b:154:TYR:CZ	2.52	0.44
9:L:148:CYS:CB	9:L:149:PRO:CD	2.96	0.44
7:C:38:ILE:HB	7:C:42:LEU:HB3	1.99	0.44
11:O:115:CYS:SG	11:O:150:SER:OG	2.76	0.44
3:I:54:GLN:HB2	11:Z:159:TRP:CE3	2.52	0.44
12:B:38:SER:HB2	12:B:39:PRO:HD2	2.00	0.44
13:W:1:THR:H2	13:W:104:ASN:ND2	2.16	0.44
14:Y:119:PHE:CD1	14:Y:119:PHE:C	2.95	0.44
14:U:50:ILE:HG23	14:U:50:ILE:O	2.16	0.44
14:U:163:PHE:CE1	14:U:197:ARG:CD	3.00	0.44
1:A:8:GLN:CB	1:A:13:VAL:HG12	2.48	0.44
2:P:181:LEU:HD12	2:P:181:LEU:HA	1.84	0.44
4:R:167:ALA:CB	4:R:175:SER:HB2	2.48	0.44
2:b:134:LEU:HD23	2:b:134:LEU:HA	1.78	0.44
9:G:55:GLU:HA	9:G:55:GLU:OE1	2.18	0.44
11:Z:136:TYR:O	11:Z:147:LEU:HA	2.17	0.44
14:Y:50:ILE:HG23	14:Y:50:ILE:O	2.16	0.44
14:U:182:MET:HE3	14:U:203:MET:CE	2.47	0.44
6:S:16:ALA:HB2	6:S:121:VAL:HG23	1.99	0.44
7:D:36:ILE:HG23	7:D:46:MET:HE2	1.96	0.44
7:D:92:LYS:HD2	7:D:118:GLU:O	2.18	0.44
7:D:106:ASP:OD1	7:D:106:ASP:N	2.47	0.44
7:C:12:GLY:HA2	7:C:105:TRP:HZ3	1.83	0.44
7:C:59:LEU:HD23	7:C:59:LEU:HA	1.81	0.44
11:O:174:MET:HE2	11:O:174:MET:HB2	1.76	0.44
10:M:215:ILE:CD1	10:M:234:LEU:CD2	2.90	0.44
8:Q:64:LYS:H	8:Q:64:LYS:HG2	1.50	0.44
14:Y:44:MET:CE	14:Y:70:LEU:CD2	2.76	0.44
1:A:135:TYR:CE1	13:a:33:LEU:HD13	2.53	0.43
1:A:197:LYS:HA	1:A:197:LYS:HD3	1.57	0.43
4:R:60:LEU:HD13	8:Q:162:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:93:ARG:HA	4:R:93:ARG:HD2	1.68	0.43
7:C:37:GLU:CG	7:C:185:TRP:CZ2	2.86	0.43
12:B:36:PHE:CD1	12:B:36:PHE:O	2.70	0.43
12:B:214:GLU:OE1	14:Y:195:THR:HG23	2.17	0.43
9:G:36:VAL:CG1	9:G:172:LEU:HD11	2.48	0.43
11:Z:98:LEU:O	11:Z:98:LEU:HG	2.16	0.43
14:U:21:ILE:CG2	14:U:187:HIS:HB2	2.47	0.43
14:U:42:PHE:HA	14:U:43:PRO:HD3	1.82	0.43
14:U:176:ARG:NH2	6:X:146:GLN:HE21	2.14	0.43
6:X:97:TYR:CD2	6:X:97:TYR:O	2.70	0.43
6:X:172:MET:HE1	6:X:195:ILE:HG21	2.00	0.43
7:D:83:LEU:HD22	7:D:87:MET:CE	2.47	0.43
8:J:64:LYS:H	8:J:64:LYS:HG2	1.50	0.43
2:b:218:ARG:HG2	2:b:218:ARG:NH1	2.31	0.43
13:W:169:VAL:HG11	13:W:189:ILE:HD11	2.01	0.43
9:G:148:CYS:CB	9:G:149:PRO:CD	2.96	0.43
14:U:91:ALA:HB2	14:U:123:LEU:CD2	2.48	0.43
2:P:88:ARG:HH11	2:P:88:ARG:HG3	1.81	0.43
2:P:111:GLN:HG2	2:P:154:TYR:OH	2.17	0.43
8:J:81:LEU:HD23	8:J:81:LEU:HA	1.78	0.43
4:K:79:VAL:CG1	4:K:139:ILE:HB	2.48	0.43
2:b:195:LYS:HG3	2:b:202:MET:CE	2.49	0.43
9:L:196:ARG:HB2	9:L:205:LEU:CD1	2.49	0.43
1:F:8:GLN:CB	1:F:13:VAL:HG12	2.48	0.43
1:F:126:PHE:CD1	1:F:126:PHE:C	2.96	0.43
14:Y:100:GLY:H	14:Y:101:PRO:HD3	1.82	0.43
14:Y:134:ASP:OD1	14:Y:134:ASP:N	2.51	0.43
14:U:77:GLU:H	14:U:77:GLU:HG2	1.72	0.43
5:T:182:VAL:HG12	5:T:191:LEU:HD13	2.01	0.43
4:K:37:LEU:CG	4:K:55:LYS:HZ1	2.31	0.43
4:K:167:ALA:CB	4:K:175:SER:HB2	2.48	0.43
10:H:78:MET:HE3	10:H:85:ALA:HB3	2.01	0.43
10:H:114:GLN:HG3	10:H:162:PHE:HZ	1.83	0.43
10:H:213:THR:CG2	10:H:231:LYS:CE	2.96	0.43
3:I:204:LYS:HB3	3:I:204:LYS:HE2	1.82	0.43
13:W:17:ASP:N	13:W:160:LEU:O	2.43	0.43
13:W:186:ARG:HG3	13:W:202:PRO:HB2	2.00	0.43
9:G:196:ARG:HB2	9:G:205:LEU:CD1	2.49	0.43
13:a:1:THR:H2	13:a:104:ASN:ND2	2.16	0.43
13:a:17:ASP:N	13:a:160:LEU:O	2.43	0.43
6:X:46:LEU:HD11	6:X:52:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:6:ALA:HB2	10:M:125:GLU:HG2	2.00	0.43
4:R:93:ARG:HG2	4:R:93:ARG:HH11	1.83	0.43
4:R:113:MET:CE	12:E:69:THR:HG22	2.49	0.43
9:L:38:LEU:HD12	9:L:179:PHE:CZ	2.54	0.43
9:L:107:ARG:NH2	13:a:74:GLU:HG2	2.34	0.43
10:H:44:GLU:HG3	10:H:191:LEU:CB	2.43	0.43
11:O:72:MET:SD	11:O:107:CYS:HA	2.58	0.43
3:I:169:ARG:HH11	3:I:169:ARG:CB	2.31	0.43
9:G:188:VAL:HG21	9:G:214:ILE:CD1	2.49	0.43
1:F:46:ARG:HD2	1:F:53:THR:HB	2.01	0.43
1:F:67:HIS:CE1	1:F:71:LEU:HD22	2.54	0.43
1:A:21:THR:HB	1:A:29:ASN:HB3	2.01	0.43
3:N:133:ILE:HD12	3:N:133:ILE:N	2.32	0.43
6:S:14:ALA:CB	6:S:109:ILE:HG21	2.49	0.43
10:H:125:GLU:OE1	3:I:5:ARG:NE	2.51	0.43
10:H:193:GLU:O	10:H:197:SER:OG	2.32	0.43
7:C:20:ARG:NH2	14:U:204:ASP:HB3	2.31	0.43
11:O:71:ASP:HA	11:O:223:THR:HG21	2.00	0.43
3:I:192:ILE:O	3:I:196:LEU:HG	2.18	0.43
9:G:50:LYS:HE3	9:G:59:HIS:CB	2.49	0.43
13:a:186:ARG:HG3	13:a:202:PRO:HB2	2.00	0.43
1:F:36:THR:HA	1:F:37:PRO:HD3	1.87	0.43
11:Z:187:LYS:HB2	11:Z:187:LYS:HE3	1.25	0.43
14:Y:66:LEU:HD13	14:Y:90:VAL:HG22	1.99	0.43
14:U:2:ILE:CG2	14:U:103:TYR:CG	3.02	0.43
14:U:134:ASP:OD1	14:U:134:ASP:N	2.51	0.43
14:U:172:ASN:OD1	6:X:151:ASN:HB2	2.18	0.43
14:U:176:ARG:HA	14:U:176:ARG:HD3	1.65	0.43
6:X:14:ALA:CB	6:X:109:ILE:HG21	2.49	0.43
4:R:6:SER:OG	4:R:23:TYR:CE2	2.72	0.43
4:R:148:GLY:HA3	4:R:149:PRO:HD2	1.87	0.43
4:R:206:LEU:HD12	4:R:210:PHE:CZ	2.45	0.43
6:S:144:MET:SD	6:S:185:ARG:HB2	2.59	0.43
9:L:77:LEU:CB	9:L:80:ASP:HB2	2.48	0.43
10:M:38:ILE:HD11	10:M:201:ILE:CG2	2.46	0.43
13:W:9:THR:HG21	13:W:180:ASP:OD2	2.19	0.43
9:G:77:LEU:CB	9:G:80:ASP:HB2	2.48	0.43
11:Z:115:CYS:SG	11:Z:150:SER:OG	2.76	0.43
14:U:10:VAL:HG12	14:U:23:ALA:HB2	1.99	0.43
3:N:50:VAL:O	3:N:50:VAL:HG13	2.19	0.43
3:N:173:GLU:HG3	10:M:58:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:45:VAL:O	8:J:215:TRP:HA	2.19	0.43
8:J:67:PHE:CD1	8:J:67:PHE:N	2.86	0.43
4:K:93:ARG:HA	4:K:93:ARG:HD2	1.68	0.43
5:V:38:MET:HE1	5:V:61:GLN:HB2	2.01	0.43
2:b:194:LEU:HD23	2:b:194:LEU:HA	1.93	0.43
11:O:72:MET:HE2	11:O:72:MET:HB3	1.73	0.43
3:I:169:ARG:HB2	3:I:169:ARG:NH1	2.34	0.43
10:M:66:LYS:HG2	10:M:216:GLU:OE2	2.18	0.43
13:W:40:SER:HG	13:W:188:GLN:HE22	1.62	0.43
9:G:38:LEU:HD12	9:G:179:PHE:CZ	2.54	0.43
13:a:143:ALA:HA	13:a:147:GLN:HB2	2.01	0.43
1:F:180:ILE:HG12	1:F:185:VAL:HG13	1.99	0.43
11:Z:35:LEU:HG	11:Z:46:ALA:HB3	2.01	0.43
11:Z:71:ASP:HA	11:Z:223:THR:HG21	2.00	0.43
3:N:169:ARG:HH11	3:N:169:ARG:CB	2.31	0.43
3:N:221:ASN:CB	3:N:222:PRO:CD	2.97	0.43
7:D:176:ASN:HD22	7:D:187:ARG:HH22	1.58	0.43
2:b:64:VAL:CG1	2:b:217:PHE:HZ	2.31	0.43
9:L:50:LYS:HE3	9:L:59:HIS:CB	2.49	0.43
9:L:188:VAL:HG21	9:L:214:ILE:CD1	2.49	0.43
10:H:50:VAL:CG2	10:H:67:ILE:HG12	2.49	0.43
10:H:96:THR:HG22	10:H:112:VAL:HG22	2.00	0.43
8:Q:219:LEU:HD13	8:Q:219:LEU:C	2.44	0.43
14:U:91:ALA:HB2	14:U:123:LEU:HD21	2.01	0.43
6:X:144:MET:SD	6:X:185:ARG:HB2	2.59	0.43
1:A:2:THR:CG2	1:A:47:SER:HB2	2.49	0.43
4:R:80:MET:HE3	4:R:80:MET:HB3	1.87	0.43
6:S:148:LEU:CD1	6:S:178:VAL:CG1	2.87	0.43
9:L:55:GLU:OE1	9:L:55:GLU:HA	2.18	0.43
9:L:56:LEU:HD13	10:M:185:TYR:CD1	2.54	0.43
11:O:35:LEU:HG	11:O:46:ALA:HB3	2.01	0.43
10:M:44:GLU:O	10:M:191:LEU:HD22	2.19	0.43
10:M:96:THR:HG22	10:M:112:VAL:HG22	2.00	0.43
12:E:36:PHE:CD1	12:E:36:PHE:O	2.70	0.43
1:A:126:PHE:CD1	1:A:126:PHE:C	2.96	0.42
2:P:201:GLN:CD	2:P:201:GLN:N	2.77	0.42
3:N:53:LEU:O	11:O:159:TRP:HE3	2.02	0.42
6:S:14:ALA:HB2	6:S:109:ILE:HG21	2.01	0.42
6:S:172:MET:HE1	6:S:195:ILE:HG21	2.00	0.42
12:E:4:ALA:HB2	12:E:126:THR:HG22	2.01	0.42
9:G:35:THR:HG22	9:G:48:ALA:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:45:VAL:O	8:Q:215:TRP:HA	2.19	0.42
13:a:9:THR:HG21	13:a:180:ASP:OD2	2.19	0.42
13:a:110:MET:HE2	13:a:110:MET:HB2	1.73	0.42
1:F:60:VAL:HG11	1:F:84:PHE:CE2	2.54	0.42
11:Z:52:ILE:H	11:Z:52:ILE:HG13	1.65	0.42
2:P:195:LYS:HG3	2:P:202:MET:CE	2.48	0.42
3:N:192:ILE:O	3:N:196:LEU:HG	2.18	0.42
4:K:6:SER:OG	4:K:23:TYR:CE2	2.72	0.42
10:H:51:GLU:CA	10:H:206:MET:HE2	2.46	0.42
3:I:50:VAL:O	3:I:50:VAL:HG13	2.19	0.42
3:I:171:PHE:CD1	3:I:171:PHE:C	2.97	0.42
12:E:6:VAL:HG12	12:E:124:TYR:HB3	2.01	0.42
8:Q:67:PHE:CD1	8:Q:67:PHE:N	2.86	0.42
14:Y:55:LEU:O	14:Y:59:VAL:HG23	2.20	0.42
6:X:146:GLN:CB	6:X:147:PRO:HD3	2.49	0.42
1:A:46:ARG:HD2	1:A:53:THR:HB	2.01	0.42
3:N:196:LEU:CD2	3:N:202:GLY:HA3	2.50	0.42
3:N:207:GLU:O	3:N:207:GLU:HG2	2.14	0.42
4:R:49:VAL:HG22	4:R:219:VAL:CG1	2.39	0.42
8:J:132:GLY:HA3	9:G:13:TRP:CZ2	2.54	0.42
5:V:1:MET:H3	5:V:173:LEU:HD11	1.83	0.42
5:V:182:VAL:HG12	5:V:191:LEU:HD13	2.01	0.42
10:H:16:SER:O	9:G:24:TYR:HB3	2.19	0.42
10:H:129:ASP:HB2	10:H:130:PRO:HD2	2.01	0.42
10:H:142:LEU:HD23	10:H:142:LEU:HA	1.87	0.42
10:H:212:ALA:HB2	10:H:235:GLU:HG2	2.01	0.42
3:I:38:LYS:HD3	3:I:38:LYS:HA	1.62	0.42
13:W:74:GLU:CG	9:G:107:ARG:NH2	2.83	0.42
2:P:13:SER:O	11:O:23:TYR:HB3	2.19	0.42
6:S:146:GLN:CB	6:S:147:PRO:HD3	2.49	0.42
7:D:37:GLU:CG	7:D:185:TRP:CZ2	2.85	0.42
8:J:87:LEU:HD23	8:J:87:LEU:HA	1.93	0.42
2:b:35:VAL:HG21	2:b:193:THR:CG2	2.50	0.42
11:O:243:GLU:HA	11:O:243:GLU:OE2	2.20	0.42
3:I:221:ASN:CB	3:I:222:PRO:CD	2.97	0.42
10:M:50:VAL:CG2	10:M:67:ILE:HG12	2.49	0.42
13:a:102:LYS:HE3	13:a:102:LYS:HB2	1.55	0.42
14:Y:191:LYS:NZ	14:Y:191:LYS:HB3	2.34	0.42
6:X:14:ALA:HB2	6:X:109:ILE:HG21	2.01	0.42
1:A:60:VAL:HG11	1:A:84:PHE:CE2	2.54	0.42
1:A:67:HIS:CE1	1:A:71:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:OH	13:W:35:ARG:HD3	2.20	0.42
5:T:38:MET:HE3	5:T:44:LEU:HB3	2.01	0.42
8:J:219:LEU:HD13	8:J:219:LEU:C	2.44	0.42
4:K:126:THR:HG22	4:K:126:THR:O	2.19	0.42
10:H:215:ILE:HD12	10:H:234:LEU:HD21	1.99	0.42
11:O:67:LYS:O	14:U:75:LEU:HD22	2.19	0.42
1:F:2:THR:CG2	1:F:47:SER:HB2	2.49	0.42
14:Y:2:ILE:CG2	14:Y:103:TYR:CG	3.02	0.42
5:T:38:MET:HE1	5:T:61:GLN:HB2	2.01	0.42
2:b:175:LYS:HG3	2:b:175:LYS:H	1.78	0.42
2:b:201:GLN:CD	2:b:201:GLN:N	2.77	0.42
9:L:24:TYR:HB3	10:M:16:SER:O	2.19	0.42
9:L:46:LEU:HD11	9:L:135:ALA:HB3	2.02	0.42
12:B:44:CYS:HB2	12:B:99:VAL:HB	2.01	0.42
12:E:44:CYS:HB2	12:E:99:VAL:HB	2.01	0.42
8:Q:207:LYS:HB2	8:Q:207:LYS:HE3	1.54	0.42
14:Y:42:PHE:HA	14:Y:43:PRO:HD3	1.82	0.42
14:Y:73:TYR:CD1	14:Y:73:TYR:C	2.97	0.42
14:Y:91:ALA:HB2	14:Y:123:LEU:CD2	2.48	0.42
14:U:2:ILE:HG21	14:U:103:TYR:CD2	2.54	0.42
1:A:9:PHE:CE2	1:A:150:LYS:HB2	2.54	0.42
1:A:104:TRP:CE3	1:A:104:TRP:C	2.97	0.42
2:P:34:SER:O	2:P:161:ALA:HA	2.19	0.42
2:P:35:VAL:HG21	2:P:193:THR:CG2	2.50	0.42
3:N:38:LYS:HD3	3:N:38:LYS:HA	1.62	0.42
4:R:109:ILE:HA	4:R:110:PRO:HD3	1.85	0.42
5:T:41:LYS:O	5:T:106:GLY:HA2	2.20	0.42
7:D:108:ARG:H	7:D:108:ARG:HG3	1.52	0.42
4:K:49:VAL:CG2	4:K:195:VAL:HG22	2.50	0.42
5:V:4:LEU:HD11	5:V:47:VAL:HG22	2.01	0.42
3:I:171:PHE:CD2	3:I:197:GLU:OE1	2.72	0.42
12:B:6:VAL:HG12	12:B:124:TYR:HB3	2.01	0.42
12:B:51:ASP:OD1	14:Y:95:TYR:OH	2.35	0.42
10:M:135:ARG:NH2	10:M:135:ARG:CG	2.81	0.42
10:M:212:ALA:HB2	10:M:235:GLU:HG2	2.01	0.42
13:W:43:MET:SD	13:W:64:LYS:HG3	2.60	0.42
12:E:12:ILE:N	12:E:178:ILE:O	2.41	0.42
13:a:43:MET:SD	13:a:64:LYS:HG3	2.60	0.42
11:Z:206:LEU:CD1	11:Z:237:ILE:HD13	2.49	0.42
14:Y:70:LEU:HD13	14:Y:70:LEU:HA	1.86	0.42
6:X:93:SER:OG	6:X:128:GLY:O	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:146:GLN:N	6:X:147:PRO:CD	2.83	0.42
2:P:175:LYS:HE3	2:P:175:LYS:HB2	1.40	0.42
7:D:8:LYS:HB3	7:D:13:VAL:HG22	2.01	0.42
10:H:44:GLU:O	10:H:191:LEU:HD22	2.19	0.42
11:O:164:ILE:HG13	11:O:164:ILE:O	2.19	0.42
13:W:214:MET:HE1	12:E:144:PRO:HB3	2.02	0.42
1:F:21:THR:HB	1:F:29:ASN:HB3	2.01	0.42
11:Z:43:VAL:CG1	11:Z:137:ILE:HB	2.50	0.42
1:A:20:ARG:HD3	1:A:22:THR:HG23	2.02	0.42
3:N:50:VAL:CB	3:N:205:ASN:OD1	2.68	0.42
4:R:126:THR:O	4:R:126:THR:HG22	2.19	0.42
5:T:4:LEU:HD11	5:T:47:VAL:HG22	2.00	0.42
6:S:146:GLN:N	6:S:147:PRO:CD	2.83	0.42
8:J:30:VAL:O	8:J:30:VAL:HG12	2.20	0.42
4:K:41:ALA:O	4:K:165:ALA:HA	2.20	0.42
4:K:118:ILE:HD13	4:K:118:ILE:HA	1.95	0.42
4:K:191:PHE:CD1	4:K:191:PHE:C	2.95	0.42
7:C:185:TRP:CE3	7:C:185:TRP:O	2.73	0.42
12:B:4:ALA:HB2	12:B:126:THR:HG22	2.01	0.42
10:M:114:GLN:HG3	10:M:162:PHE:HZ	1.83	0.42
12:E:18:THR:OG1	12:E:171:SER:HB3	2.20	0.42
9:G:46:LEU:HD11	9:G:135:ALA:HB3	2.02	0.42
13:a:53:ALA:HB2	13:a:110:MET:HG3	2.02	0.42
1:F:9:PHE:CE2	1:F:150:LYS:HB2	2.55	0.42
14:Y:91:ALA:HB2	14:Y:123:LEU:HD21	2.01	0.42
2:P:108:GLN:CD	14:U:77:GLU:HB3	2.45	0.42
2:P:190:ALA:O	2:P:193:THR:HG22	2.20	0.42
4:R:51:VAL:HG22	4:R:217:VAL:HG22	2.01	0.42
8:J:57:LEU:HD23	9:G:173:GLU:HG3	2.01	0.42
4:K:51:VAL:HG22	4:K:217:VAL:HG22	2.02	0.42
7:C:8:LYS:HB3	7:C:13:VAL:HG22	2.01	0.42
7:C:105:TRP:CE2	7:C:182:GLU:HG3	2.55	0.42
13:W:143:ALA:HA	13:W:147:GLN:HB2	2.01	0.42
13:a:136:SER:HB3	13:a:154:LEU:CD1	2.50	0.42
14:U:73:TYR:CD1	14:U:73:TYR:C	2.97	0.42
3:N:169:ARG:HB2	3:N:169:ARG:NH1	2.34	0.41
3:N:171:PHE:CD1	3:N:171:PHE:C	2.97	0.41
7:D:10:LEU:HD12	7:D:10:LEU:C	2.45	0.41
9:L:13:TRP:CZ2	8:Q:132:GLY:HA3	2.55	0.41
9:L:70:ILE:HD13	9:L:108:LEU:HD22	2.02	0.41
10:H:50:VAL:HG23	10:H:67:ILE:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:53:GLN:H	9:G:53:GLN:HG2	1.64	0.41
1:F:104:TRP:C	1:F:104:TRP:CE3	2.97	0.41
14:U:191:LYS:NZ	14:U:191:LYS:HB3	2.34	0.41
2:P:155:PHE:CD1	2:P:155:PHE:N	2.88	0.41
3:N:171:PHE:CD2	3:N:197:GLU:OE1	2.72	0.41
9:L:187:LEU:O	9:L:187:LEU:HG	2.20	0.41
7:C:38:ILE:CG2	7:C:61:ALA:HA	2.49	0.41
3:I:8:THR:HG22	3:I:16:LEU:HD22	2.03	0.41
12:E:51:ASP:OD1	14:U:95:TYR:OH	2.32	0.41
1:F:20:ARG:HD3	1:F:27:ILE:HG12	2.02	0.41
14:Y:2:ILE:HG21	14:Y:103:TYR:CD2	2.55	0.41
14:Y:134:ASP:HB2	14:Y:135:PHE:CD2	2.55	0.41
14:U:134:ASP:HB2	14:U:135:PHE:CD2	2.54	0.41
2:P:134:LEU:HD23	2:P:134:LEU:HA	1.78	0.41
6:S:151:ASN:HB2	14:Y:172:ASN:OD1	2.20	0.41
7:D:2:THR:CB	15:D:301:A1L0C:O2	2.69	0.41
7:D:38:ILE:CG2	7:D:61:ALA:HA	2.49	0.41
5:V:38:MET:HE3	5:V:44:LEU:HB3	2.01	0.41
5:V:41:LYS:O	5:V:106:GLY:HA2	2.20	0.41
2:b:34:SER:O	2:b:161:ALA:HA	2.19	0.41
2:b:181:LEU:HD12	2:b:181:LEU:HA	1.85	0.41
3:I:18:GLN:OE1	11:Z:12:PHE:HB2	2.21	0.41
3:I:104:VAL:HG21	3:I:143:ARG:HB2	2.02	0.41
13:W:15:LYS:HG3	13:W:20:VAL:HG22	2.03	0.41
6:X:75:TYR:HB3	6:X:83:MET:HE2	2.02	0.41
3:N:148:ASP:CB	3:N:149:PRO:CD	2.93	0.41
4:R:178:PHE:HE1	4:R:201:CYS:HB2	1.78	0.41
5:T:35:MET:HG3	5:T:45:LEU:HG	2.03	0.41
5:T:117:TYR:CD1	5:T:117:TYR:C	2.99	0.41
7:D:2:THR:HG21	7:D:47:ALA:HA	2.03	0.41
7:D:185:TRP:C	7:D:185:TRP:CE3	2.99	0.41
7:D:185:TRP:CE3	7:D:185:TRP:O	2.73	0.41
5:V:35:MET:HG3	5:V:45:LEU:HG	2.03	0.41
10:H:74:ILE:CD1	10:H:112:VAL:HG21	2.51	0.41
11:O:187:LYS:HE3	11:O:187:LYS:HB2	1.25	0.41
3:I:108:THR:HG21	3:I:145:TYR:CB	2.50	0.41
3:I:112:ALA:HB2	3:I:147:THR:HG22	2.02	0.41
12:B:144:PRO:HB3	13:a:214:MET:HE1	2.02	0.41
10:M:78:MET:HE3	10:M:85:ALA:HB3	2.01	0.41
13:W:89:HIS:HA	13:W:112:ILE:HD12	2.02	0.41
12:E:132:LEU:N	12:E:132:LEU:CD2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:43:ASP:OD1	8:Q:43:ASP:N	2.54	0.41
1:F:128:ILE:HD11	1:F:137:TYR:CE1	2.56	0.41
11:Z:164:ILE:O	11:Z:164:ILE:HG13	2.19	0.41
14:Y:4:SER:O	14:Y:4:SER:OG	2.29	0.41
14:U:43:PRO:O	14:U:67:LYS:NZ	2.53	0.41
2:P:197:SER:O	2:P:197:SER:OG	2.31	0.41
3:N:11:SER:O	10:M:26:TYR:HB3	2.21	0.41
4:R:39:SER:O	4:R:167:ALA:HA	2.21	0.41
4:R:41:ALA:O	4:R:165:ALA:HA	2.20	0.41
7:D:105:TRP:CE2	7:D:182:GLU:HG3	2.55	0.41
2:b:51:GLN:H	2:b:51:GLN:HG2	1.71	0.41
2:b:177:TYR:CD1	2:b:177:TYR:C	2.99	0.41
10:H:165:CYS:HA	9:G:57:ALA:HA	2.02	0.41
11:O:43:VAL:CG1	11:O:137:ILE:HB	2.50	0.41
11:Z:97:TYR:CE1	11:Z:105:ILE:HA	2.56	0.41
6:S:122:TYR:CE1	6:S:132:ARG:HB2	2.56	0.41
8:J:57:LEU:O	9:G:157:ARG:HG3	2.20	0.41
8:J:168:ALA:CB	8:J:200:VAL:HG12	2.42	0.41
2:b:155:PHE:CD1	2:b:155:PHE:N	2.88	0.41
2:b:172:PHE:O	2:b:172:PHE:CG	2.73	0.41
9:L:35:THR:HG22	9:L:48:ALA:CB	2.50	0.41
9:L:56:LEU:HD12	10:M:167:ALA:CB	2.37	0.41
11:O:86:LEU:HD23	11:O:86:LEU:HA	1.87	0.41
11:O:206:LEU:CD1	11:O:237:ILE:HD13	2.49	0.41
3:I:100:ASP:N	3:I:100:ASP:OD1	2.54	0.41
12:B:3:ILE:HG13	12:B:127:MET:HB2	2.03	0.41
12:B:7:VAL:HG22	12:B:12:ILE:CD1	2.50	0.41
12:B:18:THR:OG1	12:B:171:SER:HB3	2.20	0.41
12:E:6:VAL:HG22	12:E:155:VAL:CG2	2.50	0.41
3:N:100:ASP:OD1	3:N:100:ASP:N	2.54	0.41
3:N:104:VAL:HG21	3:N:143:ARG:HB2	2.02	0.41
4:R:123:GLN:HE22	4:R:127:GLN:NE2	2.19	0.41
8:J:47:PHE:HB3	8:J:66:LEU:HD21	2.03	0.41
2:b:108:GLN:CD	14:Y:77:GLU:HB3	2.46	0.41
2:b:190:ALA:O	2:b:193:THR:HG22	2.20	0.41
7:C:2:THR:HG21	7:C:47:ALA:HA	2.03	0.41
3:I:41:VAL:HG22	3:I:136:PHE:CE2	2.56	0.41
12:E:7:VAL:HG22	12:E:12:ILE:CD1	2.50	0.41
13:a:35:ARG:HD3	1:F:137:TYR:OH	2.21	0.41
14:Y:43:PRO:O	14:Y:67:LYS:NZ	2.53	0.41
14:Y:141:CYS:O	14:Y:141:CYS:SG	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:HD3	1:A:27:ILE:HG12	2.02	0.41
2:P:83:ARG:HG2	2:P:83:ARG:NH1	2.22	0.41
2:P:198:PHE:CD1	2:P:202:MET:HE2	2.55	0.41
9:L:57:ALA:HA	10:M:165:CYS:HA	2.03	0.41
10:H:59:MET:HG3	3:I:156:TRP:CZ2	2.56	0.41
12:B:6:VAL:HG22	12:B:155:VAL:CG2	2.50	0.41
13:W:53:ALA:HB2	13:W:110:MET:HG3	2.02	0.41
13:W:156:LYS:HB2	13:W:156:LYS:HE3	1.77	0.41
12:E:29:LYS:HE3	12:E:29:LYS:HB2	1.46	0.41
13:a:15:LYS:HG3	13:a:20:VAL:HG22	2.03	0.41
14:Y:182:MET:HE3	14:Y:203:MET:CE	2.47	0.41
14:U:153:TRP:CH2	14:U:155:PRO:HA	2.56	0.41
6:X:122:TYR:CE1	6:X:132:ARG:HB2	2.56	0.41
1:A:4:ILE:HG22	1:A:17:ALA:HB2	2.02	0.41
1:A:44:CYS:O	1:A:44:CYS:SG	2.79	0.41
2:P:177:TYR:CD1	2:P:177:TYR:C	2.99	0.41
3:N:8:THR:HG22	3:N:16:LEU:HD22	2.03	0.41
3:N:108:THR:HG21	3:N:145:TYR:CB	2.50	0.41
4:R:17:SER:HB2	4:R:18:PRO:CD	2.51	0.41
4:R:53:GLN:CD	4:R:206:LEU:CD1	2.94	0.41
4:R:150:GLN:HA	4:R:150:GLN:HE21	1.85	0.41
4:R:191:PHE:O	4:R:191:PHE:CD1	2.74	0.41
8:J:136:MET:HE2	8:J:165:ILE:CG1	2.50	0.41
4:K:17:SER:HB2	4:K:18:PRO:CD	2.51	0.41
4:K:53:GLN:CD	4:K:206:LEU:CD1	2.93	0.41
4:K:150:GLN:HA	4:K:150:GLN:HE21	1.85	0.41
4:K:161:CYS:SG	2:b:61:VAL:HG21	2.61	0.41
4:K:211:LYS:CB	4:K:212:PRO:CD	2.99	0.41
5:V:1:MET:N	5:V:173:LEU:CD1	2.84	0.41
7:C:185:TRP:CE3	7:C:185:TRP:C	2.99	0.41
11:O:34:CYS:HB2	11:O:164:ILE:HG13	2.03	0.41
3:I:115:LYS:O	3:I:119:THR:HG23	2.21	0.41
3:I:196:LEU:CD2	3:I:202:GLY:HA3	2.50	0.41
9:G:50:LYS:CB	9:G:59:HIS:HB3	2.51	0.41
8:Q:198:TYR:CE2	8:Q:240:LYS:HE3	2.56	0.41
8:Q:211:LEU:CD2	8:Q:213:LEU:CD1	2.98	0.41
13:a:211:ILE:HA	13:a:214:MET:CG	2.51	0.41
1:F:44:CYS:O	1:F:44:CYS:SG	2.79	0.41
1:F:99:ILE:H	1:F:99:ILE:HG12	1.72	0.41
11:Z:49:ARG:HE	11:Z:212:GLU:HB2	1.86	0.41
11:Z:243:GLU:OE2	11:Z:243:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:100:GLY:H	14:Y:101:PRO:CD	2.28	0.41
14:Y:176:ARG:HA	14:Y:176:ARG:HD3	1.65	0.41
1:A:29:ASN:ND2	12:B:120:ASP:OD1	2.50	0.41
1:A:36:THR:HA	1:A:37:PRO:HD3	1.87	0.41
1:A:182:GLU:O	1:A:182:GLU:HG3	2.21	0.41
3:N:112:ALA:HB2	3:N:147:THR:HG22	2.02	0.41
3:N:188:ILE:CD1	3:N:210:VAL:HG11	2.51	0.41
5:T:1:MET:N	5:T:173:LEU:CD1	2.84	0.41
7:D:69:LEU:CD2	10:M:69:GLU:OE2	2.69	0.41
8:J:198:TYR:CE2	8:J:240:LYS:HE3	2.56	0.41
5:V:117:TYR:CD1	5:V:117:TYR:C	2.99	0.41
2:b:190:ALA:C	2:b:193:THR:HG22	2.46	0.41
10:H:215:ILE:CD1	10:H:234:LEU:CD2	2.90	0.41
11:O:97:TYR:CE1	11:O:105:ILE:HA	2.56	0.41
12:B:29:LYS:HB2	12:B:29:LYS:HE3	1.46	0.41
13:W:136:SER:HB3	13:W:154:LEU:CD1	2.50	0.41
13:a:39:ILE:O	13:a:39:ILE:HG13	2.21	0.41
11:Z:34:CYS:HB2	11:Z:164:ILE:HG13	2.03	0.41
14:U:55:LEU:O	14:U:59:VAL:HG23	2.20	0.41
14:U:86:LEU:HD23	14:U:108:ILE:HD13	2.03	0.41
14:U:97:LYS:HB2	14:U:101:PRO:HA	2.02	0.41
6:X:164:VAL:CG2	6:X:165:PRO:HD2	2.51	0.41
2:P:117:MET:HE2	2:P:150:PRO:HA	2.02	0.40
2:b:70:HIS:O	2:b:137:GLY:HA2	2.21	0.40
9:L:50:LYS:CB	9:L:59:HIS:HB3	2.50	0.40
9:L:137:TYR:CZ	9:L:217:LYS:HB2	2.57	0.40
7:C:43:LEU:HD13	7:C:185:TRP:CD1	2.57	0.40
11:O:38:LEU:O	11:O:179:TYR:OH	2.32	0.40
3:I:168:VAL:HG13	3:I:194:ALA:HB1	2.03	0.40
10:M:129:ASP:HB2	10:M:130:PRO:HD2	2.02	0.40
13:W:67:LEU:HD23	13:W:67:LEU:HA	1.93	0.40
9:G:184:LEU:CD1	9:G:214:ILE:HG21	2.50	0.40
8:Q:30:VAL:O	8:Q:30:VAL:HG12	2.20	0.40
1:F:4:ILE:HG22	1:F:17:ALA:HB2	2.02	0.40
1:F:20:ARG:HD3	1:F:22:THR:HG23	2.02	0.40
1:F:191:LEU:N	1:F:191:LEU:CD2	2.73	0.40
14:Y:55:LEU:HG	14:Y:57:THR:HG22	2.03	0.40
14:Y:97:LYS:HB2	14:Y:101:PRO:HA	2.02	0.40
3:N:115:LYS:O	3:N:119:THR:HG23	2.21	0.40
4:R:49:VAL:CG2	4:R:195:VAL:HG22	2.50	0.40
4:R:191:PHE:CD1	4:R:191:PHE:C	2.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:195:VAL:HG12	4:R:199:ILE:HD13	2.03	0.40
4:R:211:LYS:CB	4:R:212:PRO:CD	2.99	0.40
5:T:154:GLU:CD	5:T:154:GLU:N	2.77	0.40
4:K:195:VAL:HG12	4:K:199:ILE:HD13	2.03	0.40
11:O:33:THR:H	11:O:48:GLU:HG2	1.87	0.40
3:I:50:VAL:CB	3:I:205:ASN:OD1	2.68	0.40
10:M:50:VAL:HG23	10:M:67:ILE:CD1	2.49	0.40
13:W:211:ILE:HA	13:W:214:MET:CG	2.51	0.40
1:F:85:LYS:NZ	1:F:86:GLU:OE2	2.40	0.40
2:P:142:ARG:HA	2:P:143:PRO:HD3	1.90	0.40
5:T:103:LEU:HG	5:T:132:HIS:HD2	1.87	0.40
7:D:43:LEU:HD13	7:D:185:TRP:CD1	2.57	0.40
5:V:153:ARG:HE	5:V:153:ARG:HB2	1.67	0.40
2:b:117:MET:HE2	2:b:150:PRO:HA	2.02	0.40
2:b:188:HIS:CE1	2:b:228:TYR:CD1	3.09	0.40
2:b:198:PHE:CD1	2:b:202:MET:HE2	2.55	0.40
9:L:157:ARG:CG	8:Q:57:LEU:O	2.68	0.40
10:M:51:GLU:CA	10:M:206:MET:HE2	2.46	0.40
10:M:83:ALA:HA	10:M:86:LYS:HE3	2.03	0.40
13:W:27:LEU:HD11	13:W:34:ALA:HB1	2.03	0.40
9:G:70:ILE:HD13	9:G:108:LEU:HD22	2.02	0.40
8:Q:47:PHE:HB3	8:Q:66:LEU:HD21	2.03	0.40
8:Q:136:MET:HE2	8:Q:165:ILE:CG1	2.50	0.40
6:X:136:LYS:HD2	6:X:136:LYS:HA	1.68	0.40
1:A:12:GLY:HA3	1:A:180:ILE:O	2.22	0.40
2:P:70:HIS:O	2:P:137:GLY:HA2	2.21	0.40
4:R:174:GLU:HA	4:R:174:GLU:OE2	2.22	0.40
7:D:12:GLY:HA2	7:D:105:TRP:HZ3	1.83	0.40
7:D:59:LEU:HD23	7:D:59:LEU:HA	1.81	0.40
4:K:191:PHE:CD1	4:K:191:PHE:O	2.74	0.40
5:V:78:THR:HG23	5:V:116:TYR:OH	2.22	0.40
9:L:183:ASN:ND2	9:L:183:ASN:N	2.62	0.40
10:H:91:LYS:CD	10:H:119:LEU:HD21	2.52	0.40
10:H:97:GLN:OE1	10:H:97:GLN:HA	2.17	0.40
7:C:2:THR:CB	15:C:301:A1L0C:O2	2.69	0.40
3:I:50:VAL:CG1	3:I:205:ASN:OD1	2.69	0.40
3:I:196:LEU:HD23	3:I:196:LEU:HA	1.91	0.40
12:E:40:ASN:HD21	12:E:74:PRO:HG2	1.87	0.40
1:F:182:GLU:O	1:F:182:GLU:HG3	2.21	0.40
14:Y:86:LEU:HD23	14:Y:108:ILE:HD13	2.03	0.40
14:Y:153:TRP:CH2	14:Y:155:PRO:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:100:GLY:H	14:U:101:PRO:CD	2.28	0.40
14:U:141:CYS:O	14:U:141:CYS:SG	2.79	0.40
14:U:170:MET:O	14:U:174:VAL:HG22	2.22	0.40
6:X:71:ARG:HA	6:X:71:ARG:HD2	1.92	0.40
2:P:170:LYS:O	2:P:174:GLU:HB3	2.22	0.40
3:N:168:VAL:HG13	3:N:194:ALA:HB1	2.04	0.40
4:R:54:LYS:HB2	4:R:216:GLU:HG2	2.04	0.40
6:S:153:VAL:HG23	6:S:174:LEU:CD2	2.52	0.40
4:K:174:GLU:OE2	4:K:174:GLU:HA	2.22	0.40
2:b:170:LYS:O	2:b:174:GLU:HB3	2.22	0.40
9:L:36:VAL:HB	9:L:47:VAL:CG2	2.52	0.40
9:L:118:ILE:N	9:L:119:PRO:CD	2.85	0.40
1:F:128:ILE:HD11	1:F:137:TYR:CD1	2.57	0.40
11:Z:9:THR:HB	11:Z:20:GLN:HG3	2.03	0.40
11:Z:174:MET:CE	11:Z:199:LYS:HG2	2.43	0.40
14:Y:128:CYS:HA	14:Y:129:PRO:HD2	1.95	0.40
6:X:145:LEU:HD22	6:X:178:VAL:HB	2.03	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 PDB entries followed by that with respect to all EM entries.

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	200/205 (98%)	188 (94%)	11 (6%)	1 (0%)	24	48
1	F	200/205 (98%)	188 (94%)	11 (6%)	1 (0%)	24	48
2	P	225/234 (96%)	206 (92%)	16 (7%)	3 (1%)	9	25
2	b	225/234 (96%)	206 (92%)	16 (7%)	3 (1%)	9	25
3	I	230/248 (93%)	217 (94%)	13 (6%)	0	100	100
3	N	230/248 (93%)	217 (94%)	13 (6%)	0	100	100
4	K	232/246 (94%)	215 (93%)	16 (7%)	1 (0%)	30	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	232/246 (94%)	215 (93%)	16 (7%)	1 (0%)	30	54
5	T	194/201 (96%)	184 (95%)	10 (5%)	0	100	100
5	V	194/201 (96%)	184 (95%)	10 (5%)	0	100	100
6	S	210/240 (88%)	193 (92%)	15 (7%)	2 (1%)	12	32
6	X	210/240 (88%)	193 (92%)	15 (7%)	2 (1%)	12	32
7	C	198/205 (97%)	185 (93%)	13 (7%)	0	100	100
7	D	198/205 (97%)	185 (93%)	13 (7%)	0	100	100
8	J	233/255 (91%)	217 (93%)	16 (7%)	0	100	100
8	Q	233/255 (91%)	218 (94%)	15 (6%)	0	100	100
9	G	232/263 (88%)	215 (93%)	16 (7%)	1 (0%)	30	54
9	L	232/263 (88%)	215 (93%)	16 (7%)	1 (0%)	30	54
10	H	229/241 (95%)	215 (94%)	14 (6%)	0	100	100
10	M	229/241 (95%)	215 (94%)	14 (6%)	0	100	100
11	O	235/261 (90%)	224 (95%)	10 (4%)	1 (0%)	30	54
11	Z	235/261 (90%)	224 (95%)	10 (4%)	1 (0%)	30	54
12	B	218/234 (93%)	206 (94%)	11 (5%)	1 (0%)	24	48
12	E	218/234 (93%)	206 (94%)	11 (5%)	1 (0%)	24	48
13	W	212/264 (80%)	195 (92%)	16 (8%)	1 (0%)	24	48
13	a	212/264 (80%)	195 (92%)	16 (8%)	1 (0%)	24	48
14	U	202/205 (98%)	180 (89%)	20 (10%)	2 (1%)	12	32
14	Y	202/205 (98%)	180 (89%)	20 (10%)	2 (1%)	12	32
All	All	6100/6604 (92%)	5681 (93%)	393 (6%)	26 (0%)	31	54

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	40	ALA
2	b	40	ALA
11	O	59	VAL
11	Z	59	VAL
14	Y	78	GLY
14	U	78	GLY
2	P	199	GLU
6	S	191	ASP
2	b	199	GLU

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Mol	Chain	Res	Type
14	Y	46	ASP
14	U	46	ASP
6	X	191	ASP
4	R	212	PRO
4	K	212	PRO
12	B	95	GLY
13	W	107	TRP
12	E	95	GLY
13	a	107	TRP
2	P	54	ILE
2	b	54	ILE
9	L	202	GLU
9	G	202	GLU
6	S	102	PHE
6	X	102	PHE
1	A	192	GLY
1	F	192	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	159/162 (98%)	123 (77%)	36 (23%)	1	3
1	F	159/162 (98%)	123 (77%)	36 (23%)	1	3
2	P	188/191 (98%)	137 (73%)	51 (27%)	0	1
2	b	188/191 (98%)	137 (73%)	51 (27%)	0	1
3	I	195/211 (92%)	143 (73%)	52 (27%)	0	1
3	N	195/211 (92%)	142 (73%)	53 (27%)	0	1
4	K	201/210 (96%)	164 (82%)	37 (18%)	1	4
4	R	201/210 (96%)	163 (81%)	38 (19%)	1	4
5	T	166/171 (97%)	142 (86%)	24 (14%)	3	8
5	V	166/171 (97%)	142 (86%)	24 (14%)	3	8
6	S	177/198 (89%)	144 (81%)	33 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
6	X	177/198 (89%)	144 (81%)	33 (19%)	1	4	
7	C	156/161 (97%)	119 (76%)	37 (24%)	1	2	
7	D	156/161 (97%)	119 (76%)	37 (24%)	1	2	
8	J	192/211 (91%)	156 (81%)	36 (19%)	1	4	
8	Q	192/211 (91%)	156 (81%)	36 (19%)	1	4	
9	G	200/224 (89%)	149 (74%)	51 (26%)	0	2	
9	L	200/224 (89%)	149 (74%)	51 (26%)	0	2	
10	H	193/203 (95%)	140 (72%)	53 (28%)	0	1	
10	M	193/203 (95%)	140 (72%)	53 (28%)	0	1	
11	O	201/221 (91%)	145 (72%)	56 (28%)	0	1	
11	Z	201/221 (91%)	145 (72%)	56 (28%)	0	1	
12	B	181/195 (93%)	139 (77%)	42 (23%)	1	2	
12	E	181/195 (93%)	140 (77%)	41 (23%)	1	3	
13	W	176/212 (83%)	141 (80%)	35 (20%)	1	4	
13	a	176/212 (83%)	141 (80%)	35 (20%)	1	4	
14	U	174/175 (99%)	142 (82%)	32 (18%)	1	4	
14	Y	174/175 (99%)	141 (81%)	33 (19%)	1	4	
All	All	5118/5490 (93%)	3966 (78%)	1152 (22%)	2	3	

All (1152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	14	VAL
1	A	20	ARG
1	A	22	THR
1	A	25	SER
1	A	40	ASP
1	A	44	CYS
1	A	45	CYS
1	A	47	SER
1	A	69	ILE
1	A	73	GLU
1	A	85	LYS
1	A	87	MET
1	A	96	MET

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Mol	Chain	Res	Type
1	A	99	ILE
1	A	107	GLN
1	A	114	SER
1	A	117	MET
1	A	120	MET
1	A	121	MET
1	A	124	GLN
1	A	125	SER
1	A	131	SER
1	A	136	ILE
1	A	143	THR
1	A	146	GLU
1	A	150	LYS
1	A	170	SER
1	A	171	SER
1	A	181	GLN
1	A	183	SER
1	A	186	GLU
1	A	187	ARG
1	A	188	GLN
1	A	191	LEU
1	A	197	LYS
2	P	6	SER
2	P	17	LYS
2	P	35	VAL
2	P	37	ILE
2	P	38	LYS
2	P	50	LYS
2	P	51	GLN
2	P	52	LYS
2	P	54	ILE
2	P	56	TYR
2	P	58	GLU
2	P	59	ARG
2	P	61	VAL
2	P	63	LYS
2	P	73	LEU
2	P	74	VAL
2	P	76	SER
2	P	83	ARG
2	P	86	VAL
2	P	88	ARG

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Mol	Chain	Res	Type
2	P	91	LYS
2	P	102	GLU
2	P	115	SER
2	P	131	VAL
2	P	132	SER
2	P	135	ILE
2	P	136	CYS
2	P	139	ASN
2	P	140	GLU
2	P	142	ARG
2	P	147	GLN
2	P	151	SER
2	P	155	PHE
2	P	162	MET
2	P	164	LYS
2	P	168	ASN
2	P	170	LYS
2	P	173	LEU
2	P	175	LYS
2	P	176	ARG
2	P	182	GLU
2	P	184	GLU
2	P	185	ASP
2	P	189	THR
2	P	201	GLN
2	P	203	THR
2	P	204	GLU
2	P	214	GLU
2	P	220	LEU
2	P	223	THR
2	P	224	GLU
3	N	4	ASP
3	N	5	ARG
3	N	8	THR
3	N	13	ASP
3	N	18	GLN
3	N	23	GLN
3	N	28	LYS
3	N	33	VAL
3	N	38	LYS
3	N	41	VAL
3	N	42	VAL

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Mol	Chain	Res	Type
3	N	45	VAL
3	N	47	LYS
3	N	48	LYS
3	N	52	LYS
3	N	57	ARG
3	N	58	THR
3	N	69	VAL
3	N	82	ILE
3	N	86	ARG
3	N	93	SER
3	N	99	GLU
3	N	102	VAL
3	N	105	GLU
3	N	114	LEU
3	N	121	SER
3	N	124	ARG
3	N	129	ILE
3	N	130	SER
3	N	134	VAL
3	N	139	ASP
3	N	146	GLN
3	N	152	THR
3	N	163	ARG
3	N	167	SER
3	N	169	ARG
3	N	181	ILE
3	N	183	THR
3	N	184	ASP
3	N	185	ASP
3	N	192	ILE
3	N	193	LYS
3	N	197	GLU
3	N	199	VAL
3	N	204	LYS
3	N	207	GLU
3	N	214	ASP
3	N	215	GLN
3	N	219	ILE
3	N	223	GLU
3	N	226	GLU
3	N	227	LYS
3	N	233	GLU

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Mol	Chain	Res	Type
4	R	5	SER
4	R	6	SER
4	R	11	ARG
4	R	34	GLN
4	R	51	VAL
4	R	55	LYS
4	R	56	VAL
4	R	58	ASP
4	R	59	LYS
4	R	61	LEU
4	R	73	THR
4	R	74	GLU
4	R	93	ARG
4	R	108	GLU
4	R	118	ILE
4	R	127	GLN
4	R	153	LYS
4	R	166	THR
4	R	173	THR
4	R	174	GLU
4	R	175	SER
4	R	178	PHE
4	R	182	LYS
4	R	184	LYS
4	R	196	GLU
4	R	200	THR
4	R	205	VAL
4	R	209	ASP
4	R	211	LYS
4	R	214	GLU
4	R	215	ILE
4	R	216	GLU
4	R	222	VAL
4	R	223	GLU
4	R	226	LYS
4	R	231	THR
4	R	234	GLU
4	R	242	LEU
5	T	1	MET
5	T	8	GLN
5	T	13	VAL
5	T	19	ARG

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Mol	Chain	Res	Type
5	T	23	SER
5	T	25	ILE
5	T	26	VAL
5	T	29	LYS
5	T	40	GLU
5	T	41	LYS
5	T	46	CYS
5	T	49	GLU
5	T	85	ARG
5	T	86	ARG
5	T	94	SER
5	T	96	THR
5	T	102	LEU
5	T	109	GLU
5	T	111	GLU
5	T	143	LEU
5	T	145	ARG
5	T	169	LYS
5	T	172	ILE
5	T	173	LEU
6	S	11	THR
6	S	18	GLU
6	S	21	SER
6	S	30	SER
6	S	34	SER
6	S	36	HIS
6	S	42	LYS
6	S	48	ASP
6	S	49	LYS
6	S	52	ILE
6	S	54	CYS
6	S	55	SER
6	S	65	THR
6	S	78	SER
6	S	81	LYS
6	S	93	SER
6	S	99	ARG
6	S	115	GLU
6	S	118	LYS
6	S	123	SER
6	S	127	VAL
6	S	133	ASP

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Mol	Chain	Res	Type
6	S	136	LYS
6	S	140	SER
6	S	146	GLN
6	S	148	LEU
6	S	159	GLN
6	S	162	GLU
6	S	166	LEU
6	S	170	ARG
6	S	195	ILE
6	S	208	VAL
6	S	211	ARG
7	D	8	LYS
7	D	9	PHE
7	D	30	GLN
7	D	33	LYS
7	D	36	ILE
7	D	37	GLU
7	D	42	LEU
7	D	43	LEU
7	D	45	THR
7	D	57	GLU
7	D	58	ARG
7	D	59	LEU
7	D	62	ARG
7	D	66	ILE
7	D	72	LYS
7	D	81	SER
7	D	83	LEU
7	D	92	LYS
7	D	103	CYS
7	D	107	LYS
7	D	108	ARG
7	D	118	GLU
7	D	122	ILE
7	D	128	SER
7	D	129	VAL
7	D	147	ASP
7	D	148	LEU
7	D	149	LYS
7	D	155	ASP
7	D	158	ARG
7	D	177	LEU

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Mol	Chain	Res	Type
7	D	181	ARG
7	D	186	ILE
7	D	187	ARG
7	D	191	ASP
7	D	193	VAL
7	D	195	ASP
8	J	17	ASP
8	J	28	LYS
8	J	34	SER
8	J	37	ILE
8	J	51	LYS
8	J	53	VAL
8	J	56	LYS
8	J	60	GLU
8	J	64	LYS
8	J	66	LEU
8	J	67	PHE
8	J	68	ASN
8	J	69	VAL
8	J	80	LEU
8	J	81	LEU
8	J	90	ILE
8	J	114	ARG
8	J	157	SER
8	J	165	ILE
8	J	167	LYS
8	J	169	ARG
8	J	170	GLN
8	J	181	MET
8	J	185	THR
8	J	186	CYS
8	J	191	LYS
8	J	193	VAL
8	J	202	ASP
8	J	204	VAL
8	J	207	LYS
8	J	209	PHE
8	J	214	SER
8	J	219	LEU
8	J	226	ILE
8	J	237	LYS
8	J	238	TYR

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Mol	Chain	Res	Type
4	K	5	SER
4	K	6	SER
4	K	11	ARG
4	K	34	GLN
4	K	51	VAL
4	K	55	LYS
4	K	56	VAL
4	K	58	ASP
4	K	59	LYS
4	K	61	LEU
4	K	73	THR
4	K	74	GLU
4	K	93	ARG
4	K	108	GLU
4	K	118	ILE
4	K	127	GLN
4	K	153	LYS
4	K	166	THR
4	K	173	THR
4	K	174	GLU
4	K	175	SER
4	K	182	LYS
4	K	184	LYS
4	K	196	GLU
4	K	200	THR
4	K	205	VAL
4	K	209	ASP
4	K	211	LYS
4	K	214	GLU
4	K	215	ILE
4	K	216	GLU
4	K	222	VAL
4	K	223	GLU
4	K	226	LYS
4	K	231	THR
4	K	234	GLU
4	K	242	LEU
5	V	1	MET
5	V	8	GLN
5	V	13	VAL
5	V	19	ARG
5	V	23	SER

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Mol	Chain	Res	Type
5	V	25	ILE
5	V	26	VAL
5	V	29	LYS
5	V	40	GLU
5	V	41	LYS
5	V	46	CYS
5	V	49	GLU
5	V	85	ARG
5	V	86	ARG
5	V	94	SER
5	V	96	THR
5	V	102	LEU
5	V	109	GLU
5	V	111	GLU
5	V	143	LEU
5	V	145	ARG
5	V	169	LYS
5	V	172	ILE
5	V	173	LEU
2	b	6	SER
2	b	17	LYS
2	b	35	VAL
2	b	37	ILE
2	b	38	LYS
2	b	50	LYS
2	b	51	GLN
2	b	52	LYS
2	b	54	ILE
2	b	56	TYR
2	b	58	GLU
2	b	59	ARG
2	b	61	VAL
2	b	63	LYS
2	b	73	LEU
2	b	74	VAL
2	b	76	SER
2	b	83	ARG
2	b	86	VAL
2	b	88	ARG
2	b	91	LYS
2	b	102	GLU
2	b	115	SER

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Mol	Chain	Res	Type
2	b	131	VAL
2	b	132	SER
2	b	135	ILE
2	b	136	CYS
2	b	139	ASN
2	b	140	GLU
2	b	142	ARG
2	b	147	GLN
2	b	151	SER
2	b	155	PHE
2	b	162	MET
2	b	164	LYS
2	b	168	ASN
2	b	170	LYS
2	b	173	LEU
2	b	175	LYS
2	b	176	ARG
2	b	182	GLU
2	b	184	GLU
2	b	185	ASP
2	b	189	THR
2	b	201	GLN
2	b	203	THR
2	b	204	GLU
2	b	214	GLU
2	b	220	LEU
2	b	223	THR
2	b	224	GLU
9	L	5	GLN
9	L	22	ILE
9	L	23	GLU
9	L	29	VAL
9	L	30	LYS
9	L	35	THR
9	L	36	VAL
9	L	38	LEU
9	L	39	LYS
9	L	41	LYS
9	L	51	ARG
9	L	53	GLN
9	L	54	SER
9	L	56	LEU

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Mol	Chain	Res	Type
9	L	60	GLN
9	L	62	LYS
9	L	73	SER
9	L	74	ILE
9	L	78	THR
9	L	106	SER
9	L	108	LEU
9	L	110	SER
9	L	114	SER
9	L	115	LYS
9	L	125	ARG
9	L	132	LEU
9	L	146	GLN
9	L	148	CYS
9	L	156	CYS
9	L	157	ARG
9	L	164	ARG
9	L	173	GLU
9	L	181	GLU
9	L	182	CYS
9	L	183	ASN
9	L	189	LYS
9	L	190	HIS
9	L	202	GLU
9	L	206	THR
9	L	207	THR
9	L	208	LYS
9	L	211	SER
9	L	214	ILE
9	L	217	LYS
9	L	219	LEU
9	L	220	GLU
9	L	222	THR
9	L	225	ASP
9	L	228	ASP
9	L	233	LEU
9	L	236	LEU
10	H	10	ARG
10	H	40	ILE
10	H	43	SER
10	H	47	CYS
10	H	50	VAL

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Mol	Chain	Res	Type
10	H	54	ILE
10	H	59	MET
10	H	62	SER
10	H	64	ILE
10	H	65	GLU
10	H	69	GLU
10	H	78	MET
10	H	89	ILE
10	H	90	ASP
10	H	91	LYS
10	H	95	GLU
10	H	97	GLN
10	H	111	SER
10	H	114	GLN
10	H	119	LEU
10	H	121	LEU
10	H	129	ASP
10	H	133	MET
10	H	139	VAL
10	H	147	ASP
10	H	148	GLU
10	H	149	LYS
10	H	152	GLN
10	H	159	SER
10	H	163	VAL
10	H	164	GLN
10	H	165	CYS
10	H	170	ILE
10	H	172	SER
10	H	174	SER
10	H	183	GLU
10	H	187	LYS
10	H	190	THR
10	H	192	LYS
10	H	197	SER
10	H	198	SER
10	H	201	ILE
10	H	202	LEU
10	H	207	GLU
10	H	208	GLU
10	H	209	LYS
10	H	215	ILE

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Mol	Chain	Res	Type
10	H	217	LEU
10	H	228	MET
10	H	236	GLU
10	H	237	VAL
10	H	238	ILE
10	H	239	LYS
7	C	8	LYS
7	C	9	PHE
7	C	30	GLN
7	C	33	LYS
7	C	36	ILE
7	C	37	GLU
7	C	42	LEU
7	C	43	LEU
7	C	45	THR
7	C	57	GLU
7	C	58	ARG
7	C	59	LEU
7	C	62	ARG
7	C	66	ILE
7	C	72	LYS
7	C	81	SER
7	C	83	LEU
7	C	92	LYS
7	C	103	CYS
7	C	107	LYS
7	C	108	ARG
7	C	118	GLU
7	C	122	ILE
7	C	128	SER
7	C	129	VAL
7	C	147	ASP
7	C	148	LEU
7	C	149	LYS
7	C	155	ASP
7	C	158	ARG
7	C	177	LEU
7	C	181	ARG
7	C	186	ILE
7	C	187	ARG
7	C	191	ASP
7	C	193	VAL

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Mol	Chain	Res	Type
7	C	195	ASP
11	O	3	ARG
11	O	10	THR
11	O	11	ILE
11	O	15	GLU
11	O	17	ARG
11	O	26	GLU
11	O	35	LEU
11	O	38	LEU
11	O	41	ASP
11	O	48	GLU
11	O	50	ARG
11	O	52	ILE
11	O	58	GLU
11	O	59	VAL
11	O	61	PHE
11	O	63	GLU
11	O	64	LYS
11	O	67	LYS
11	O	70	GLU
11	O	71	ASP
11	O	72	MET
11	O	76	VAL
11	O	80	THR
11	O	81	SER
11	O	95	GLN
11	O	112	THR
11	O	119	GLN
11	O	127	LYS
11	O	132	VAL
11	O	133	SER
11	O	136	TYR
11	O	150	SER
11	O	155	ASN
11	O	160	LYS
11	O	172	VAL
11	O	174	MET
11	O	176	LYS
11	O	180	LYS
11	O	183	GLU
11	O	186	LEU
11	O	187	LYS

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Mol	Chain	Res	Type
11	O	190	LEU
11	O	192	LEU
11	O	200	THR
11	O	206	LEU
11	O	218	ARG
11	O	222	LYS
11	O	226	ARG
11	O	227	VAL
11	O	228	LEU
11	O	230	GLN
11	O	234	GLU
11	O	237	ILE
11	O	239	LYS
11	O	241	GLU
11	O	243	GLU
3	I	4	ASP
3	I	5	ARG
3	I	13	ASP
3	I	18	GLN
3	I	23	GLN
3	I	28	LYS
3	I	33	VAL
3	I	38	LYS
3	I	41	VAL
3	I	42	VAL
3	I	45	VAL
3	I	47	LYS
3	I	48	LYS
3	I	52	LYS
3	I	57	ARG
3	I	58	THR
3	I	69	VAL
3	I	82	ILE
3	I	86	ARG
3	I	93	SER
3	I	99	GLU
3	I	102	VAL
3	I	105	GLU
3	I	114	LEU
3	I	121	SER
3	I	124	ARG
3	I	129	ILE

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Mol	Chain	Res	Type
3	I	130	SER
3	I	134	VAL
3	I	139	ASP
3	I	146	GLN
3	I	152	THR
3	I	163	ARG
3	I	167	SER
3	I	169	ARG
3	I	181	ILE
3	I	183	THR
3	I	184	ASP
3	I	185	ASP
3	I	192	ILE
3	I	193	LYS
3	I	197	GLU
3	I	199	VAL
3	I	204	LYS
3	I	207	GLU
3	I	214	ASP
3	I	215	GLN
3	I	219	ILE
3	I	223	GLU
3	I	226	GLU
3	I	227	LYS
3	I	233	GLU
12	B	9	LYS
12	B	19	ARG
12	B	29	LYS
12	B	32	SER
12	B	36	PHE
12	B	40	ASN
12	B	52	THR
12	B	59	ILE
12	B	63	LEU
12	B	64	GLU
12	B	65	LEU
12	B	77	VAL
12	B	84	LYS
12	B	94	ILE
12	B	98	LEU
12	B	105	VAL
12	B	106	THR

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Mol	Chain	Res	Type
12	B	118	SER
12	B	131	SER
12	B	132	LEU
12	B	135	MET
12	B	146	MET
12	B	147	GLU
12	B	154	LEU
12	B	156	SER
12	B	175	LEU
12	B	179	SER
12	B	180	LYS
12	B	182	LYS
12	B	184	ASP
12	B	186	LEU
12	B	187	ARG
12	B	194	LYS
12	B	197	THR
12	B	198	ARG
12	B	199	LEU
12	B	201	ARG
12	B	204	CYS
12	B	206	LYS
12	B	209	THR
12	B	213	THR
12	B	214	GLU
10	M	10	ARG
10	M	40	ILE
10	M	43	SER
10	M	47	CYS
10	M	50	VAL
10	M	54	ILE
10	M	59	MET
10	M	62	SER
10	M	64	ILE
10	M	65	GLU
10	M	69	GLU
10	M	78	MET
10	M	89	ILE
10	M	90	ASP
10	M	91	LYS
10	M	95	GLU
10	M	97	GLN

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Mol	Chain	Res	Type
10	M	111	SER
10	M	114	GLN
10	M	119	LEU
10	M	121	LEU
10	M	129	ASP
10	M	133	MET
10	M	139	VAL
10	M	147	ASP
10	M	148	GLU
10	M	149	LYS
10	M	152	GLN
10	M	159	SER
10	M	163	VAL
10	M	164	GLN
10	M	165	CYS
10	M	170	ILE
10	M	172	SER
10	M	174	SER
10	M	183	GLU
10	M	187	LYS
10	M	190	THR
10	M	192	LYS
10	M	197	SER
10	M	198	SER
10	M	201	ILE
10	M	202	LEU
10	M	207	GLU
10	M	208	GLU
10	M	209	LYS
10	M	215	ILE
10	M	217	LEU
10	M	228	MET
10	M	236	GLU
10	M	237	VAL
10	M	238	ILE
10	M	239	LYS
13	W	3	ASN
13	W	9	THR
13	W	10	SER
13	W	14	VAL
13	W	26	MET
13	W	29	SER

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Mol	Chain	Res	Type
13	W	35	ARG
13	W	37	ARG
13	W	44	ARG
13	W	65	GLN
13	W	79	ASP
13	W	82	SER
13	W	94	ARG
13	W	98	SER
13	W	102	LYS
13	W	110	MET
13	W	112	ILE
13	W	124	TYR
13	W	152	GLU
13	W	155	GLU
13	W	156	LYS
13	W	157	GLN
13	W	161	SER
13	W	162	GLN
13	W	164	GLU
13	W	166	ARG
13	W	169	VAL
13	W	170	GLU
13	W	182	ARG
13	W	189	ILE
13	W	198	GLU
13	W	199	ILE
13	W	206	GLN
13	W	207	THR
13	W	214	MET
12	E	9	LYS
12	E	19	ARG
12	E	29	LYS
12	E	32	SER
12	E	36	PHE
12	E	40	ASN
12	E	52	THR
12	E	59	ILE
12	E	63	LEU
12	E	64	GLU
12	E	65	LEU
12	E	77	VAL
12	E	84	LYS

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Mol	Chain	Res	Type
12	E	94	ILE
12	E	98	LEU
12	E	105	VAL
12	E	106	THR
12	E	118	SER
12	E	131	SER
12	E	132	LEU
12	E	135	MET
12	E	146	MET
12	E	147	GLU
12	E	154	LEU
12	E	156	SER
12	E	175	LEU
12	E	179	SER
12	E	180	LYS
12	E	182	LYS
12	E	184	ASP
12	E	186	LEU
12	E	187	ARG
12	E	194	LYS
12	E	197	THR
12	E	198	ARG
12	E	199	LEU
12	E	201	ARG
12	E	204	CYS
12	E	206	LYS
12	E	213	THR
12	E	214	GLU
9	G	5	GLN
9	G	22	ILE
9	G	23	GLU
9	G	29	VAL
9	G	30	LYS
9	G	35	THR
9	G	36	VAL
9	G	38	LEU
9	G	39	LYS
9	G	41	LYS
9	G	51	ARG
9	G	53	GLN
9	G	54	SER
9	G	56	LEU

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Mol	Chain	Res	Type
9	G	60	GLN
9	G	62	LYS
9	G	73	SER
9	G	74	ILE
9	G	78	THR
9	G	106	SER
9	G	108	LEU
9	G	110	SER
9	G	114	SER
9	G	115	LYS
9	G	125	ARG
9	G	132	LEU
9	G	146	GLN
9	G	148	CYS
9	G	156	CYS
9	G	157	ARG
9	G	164	ARG
9	G	173	GLU
9	G	181	GLU
9	G	182	CYS
9	G	183	ASN
9	G	189	LYS
9	G	190	HIS
9	G	202	GLU
9	G	206	THR
9	G	207	THR
9	G	208	LYS
9	G	211	SER
9	G	214	ILE
9	G	217	LYS
9	G	219	LEU
9	G	220	GLU
9	G	222	THR
9	G	225	ASP
9	G	228	ASP
9	G	233	LEU
9	G	236	LEU
8	Q	17	ASP
8	Q	28	LYS
8	Q	34	SER
8	Q	37	ILE
8	Q	51	LYS

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Mol	Chain	Res	Type
8	Q	53	VAL
8	Q	56	LYS
8	Q	60	GLU
8	Q	64	LYS
8	Q	66	LEU
8	Q	67	PHE
8	Q	68	ASN
8	Q	69	VAL
8	Q	80	LEU
8	Q	81	LEU
8	Q	90	ILE
8	Q	114	ARG
8	Q	157	SER
8	Q	165	ILE
8	Q	167	LYS
8	Q	169	ARG
8	Q	170	GLN
8	Q	181	MET
8	Q	185	THR
8	Q	186	CYS
8	Q	191	LYS
8	Q	193	VAL
8	Q	202	ASP
8	Q	204	VAL
8	Q	207	LYS
8	Q	209	PHE
8	Q	214	SER
8	Q	219	LEU
8	Q	226	ILE
8	Q	237	LYS
8	Q	238	TYR
13	a	3	ASN
13	a	9	THR
13	a	10	SER
13	a	14	VAL
13	a	26	MET
13	a	29	SER
13	a	35	ARG
13	a	37	ARG
13	a	44	ARG
13	a	65	GLN
13	a	79	ASP

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Mol	Chain	Res	Type
13	a	82	SER
13	a	94	ARG
13	a	98	SER
13	a	102	LYS
13	a	110	MET
13	a	112	ILE
13	a	124	TYR
13	a	152	GLU
13	a	155	GLU
13	a	156	LYS
13	a	157	GLN
13	a	161	SER
13	a	162	GLN
13	a	164	GLU
13	a	166	ARG
13	a	169	VAL
13	a	170	GLU
13	a	182	ARG
13	a	189	ILE
13	a	198	GLU
13	a	199	ILE
13	a	206	GLN
13	a	207	THR
13	a	214	MET
1	F	4	ILE
1	F	14	VAL
1	F	20	ARG
1	F	22	THR
1	F	25	SER
1	F	40	ASP
1	F	44	CYS
1	F	45	CYS
1	F	47	SER
1	F	69	ILE
1	F	73	GLU
1	F	85	LYS
1	F	87	MET
1	F	96	MET
1	F	99	ILE
1	F	107	GLN
1	F	114	SER
1	F	117	MET

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Mol	Chain	Res	Type
1	F	120	MET
1	F	121	MET
1	F	124	GLN
1	F	125	SER
1	F	131	SER
1	F	136	ILE
1	F	143	THR
1	F	146	GLU
1	F	150	LYS
1	F	170	SER
1	F	171	SER
1	F	181	GLN
1	F	183	SER
1	F	186	GLU
1	F	187	ARG
1	F	188	GLN
1	F	191	LEU
1	F	197	LYS
11	Z	3	ARG
11	Z	10	THR
11	Z	11	ILE
11	Z	15	GLU
11	Z	17	ARG
11	Z	26	GLU
11	Z	35	LEU
11	Z	38	LEU
11	Z	41	ASP
11	Z	48	GLU
11	Z	50	ARG
11	Z	52	ILE
11	Z	58	GLU
11	Z	59	VAL
11	Z	61	PHE
11	Z	63	GLU
11	Z	64	LYS
11	Z	67	LYS
11	Z	70	GLU
11	Z	71	ASP
11	Z	72	MET
11	Z	76	VAL
11	Z	80	THR
11	Z	81	SER

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Mol	Chain	Res	Type
11	Z	95	GLN
11	Z	112	THR
11	Z	119	GLN
11	Z	127	LYS
11	Z	132	VAL
11	Z	133	SER
11	Z	136	TYR
11	Z	150	SER
11	Z	155	ASN
11	Z	160	LYS
11	Z	172	VAL
11	Z	174	MET
11	Z	176	LYS
11	Z	180	LYS
11	Z	183	GLU
11	Z	186	LEU
11	Z	187	LYS
11	Z	190	LEU
11	Z	192	LEU
11	Z	200	THR
11	Z	206	LEU
11	Z	218	ARG
11	Z	222	LYS
11	Z	226	ARG
11	Z	227	VAL
11	Z	228	LEU
11	Z	230	GLN
11	Z	234	GLU
11	Z	237	ILE
11	Z	239	LYS
11	Z	241	GLU
11	Z	243	GLU
14	Y	1	SER
14	Y	2	ILE
14	Y	4	SER
14	Y	13	MET
14	Y	14	LYS
14	Y	16	LYS
14	Y	19	VAL
14	Y	26	ARG
14	Y	48	LEU
14	Y	70	LEU

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Mol	Chain	Res	Type
14	Y	76	LYS
14	Y	77	GLU
14	Y	80	GLN
14	Y	107	VAL
14	Y	114	LYS
14	Y	115	THR
14	Y	121	CYS
14	Y	125	LEU
14	Y	136	VAL
14	Y	138	SER
14	Y	142	SER
14	Y	144	GLN
14	Y	151	SER
14	Y	158	ASP
14	Y	176	ARG
14	Y	180	SER
14	Y	182	MET
14	Y	185	ILE
14	Y	191	LYS
14	Y	193	LYS
14	Y	194	ILE
14	Y	197	ARG
14	Y	200	LYS
14	U	1	SER
14	U	2	ILE
14	U	4	SER
14	U	13	MET
14	U	14	LYS
14	U	16	LYS
14	U	19	VAL
14	U	26	ARG
14	U	48	LEU
14	U	70	LEU
14	U	76	LYS
14	U	77	GLU
14	U	80	GLN
14	U	107	VAL
14	U	114	LYS
14	U	121	CYS
14	U	125	LEU
14	U	136	VAL
14	U	138	SER

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Mol	Chain	Res	Type
14	U	142	SER
14	U	144	GLN
14	U	151	SER
14	U	158	ASP
14	U	176	ARG
14	U	180	SER
14	U	182	MET
14	U	185	ILE
14	U	191	LYS
14	U	193	LYS
14	U	194	ILE
14	U	197	ARG
14	U	200	LYS
6	X	11	THR
6	X	18	GLU
6	X	21	SER
6	X	30	SER
6	X	34	SER
6	X	36	HIS
6	X	42	LYS
6	X	48	ASP
6	X	49	LYS
6	X	52	ILE
6	X	54	CYS
6	X	55	SER
6	X	65	THR
6	X	78	SER
6	X	81	LYS
6	X	93	SER
6	X	99	ARG
6	X	115	GLU
6	X	118	LYS
6	X	123	SER
6	X	127	VAL
6	X	133	ASP
6	X	136	LYS
6	X	140	SER
6	X	146	GLN
6	X	148	LEU
6	X	159	GLN
6	X	162	GLU
6	X	166	LEU

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Mol	Chain	Res	Type
6	X	170	ARG
6	X	195	ILE
6	X	208	VAL
6	X	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	181	GLN
1	A	188	GLN
2	P	20	GLN
2	P	108	GLN
2	P	111	GLN
2	P	188	HIS
3	N	15	HIS
3	N	23	GLN
3	N	92	GLN
3	N	146	GLN
3	N	159	ASN
4	R	34	GLN
4	R	127	GLN
4	R	150	GLN
4	R	193	GLN
4	R	224	ASN
5	T	27	GLN
5	T	55	GLN
5	T	61	GLN
5	T	71	ASN
5	T	132	HIS
6	S	8	ASN
6	S	146	GLN
6	S	159	GLN
7	D	11	HIS
7	D	90	GLN
7	D	163	GLN
7	D	176	ASN
7	D	179	HIS
7	D	197	HIS
8	J	22	GLN
8	J	170	GLN
8	J	201	HIS

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Mol	Chain	Res	Type
4	K	34	GLN
4	K	127	GLN
4	K	150	GLN
4	K	172	GLN
4	K	193	GLN
4	K	224	ASN
5	V	8	GLN
5	V	27	GLN
5	V	55	GLN
5	V	61	GLN
5	V	71	ASN
5	V	132	HIS
2	b	20	GLN
2	b	108	GLN
2	b	111	GLN
2	b	139	ASN
2	b	188	HIS
9	L	5	GLN
9	L	20	HIS
9	L	53	GLN
9	L	60	GLN
9	L	146	GLN
9	L	183	ASN
9	L	203	GLN
10	H	99	HIS
10	H	164	GLN
10	H	221	GLN
10	H	227	HIS
7	C	11	HIS
7	C	90	GLN
7	C	163	GLN
7	C	176	ASN
7	C	179	HIS
7	C	197	HIS
11	O	40	ASN
11	O	88	ASN
11	O	95	GLN
11	O	230	GLN
3	I	15	HIS
3	I	23	GLN
3	I	92	GLN
3	I	146	GLN

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Mol	Chain	Res	Type
3	I	159	ASN
12	B	40	ASN
12	B	80	ASN
10	M	99	HIS
10	M	164	GLN
10	M	221	GLN
10	M	227	HIS
13	W	81	HIS
13	W	104	ASN
13	W	147	GLN
13	W	157	GLN
13	W	188	GLN
13	W	206	GLN
12	E	40	ASN
12	E	80	ASN
12	E	193	ASN
9	G	5	GLN
9	G	20	HIS
9	G	53	GLN
9	G	60	GLN
9	G	146	GLN
9	G	183	ASN
9	G	203	GLN
8	Q	22	GLN
13	a	104	ASN
13	a	147	GLN
13	a	157	GLN
13	a	188	GLN
13	a	206	GLN
1	F	78	HIS
1	F	181	GLN
1	F	188	GLN
11	Z	40	ASN
11	Z	95	GLN
11	Z	119	GLN
11	Z	230	GLN
14	Y	6	ASN
14	Y	32	GLN
14	Y	64	GLN
14	Y	144	GLN
14	Y	161	HIS
14	U	6	ASN

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Mol	Chain	Res	Type
14	U	32	GLN
14	U	64	GLN
14	U	144	GLN
14	U	161	HIS
6	X	8	ASN
6	X	146	GLN
6	X	159	GLN
6	X	160	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	A1L0C	C	301	7	19,23,23	0.48	0	25,31,31	0.81	1 (4%)
15	A1L0C	A	301	1	19,23,23	0.48	0	25,31,31	0.77	1 (4%)
15	A1L0C	D	301	7	19,23,23	0.48	0	25,31,31	0.82	1 (4%)
15	A1L0C	F	301	1	19,23,23	0.49	0	25,31,31	0.77	1 (4%)

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	A1L0C	C	301	7	-	4/15/28/28	0/2/2/2
15	A1L0C	A	301	1	-	2/15/28/28	0/2/2/2
15	A1L0C	D	301	7	-	4/15/28/28	0/2/2/2
15	A1L0C	F	301	1	-	2/15/28/28	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	301	A1L0C	C9-N1-N2	-2.28	117.84	120.94
15	C	301	A1L0C	C9-N1-N2	-2.26	117.87	120.94
15	A	301	A1L0C	C9-N1-N2	-2.15	118.03	120.94
15	F	301	A1L0C	C9-N1-N2	-2.12	118.06	120.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	301	A1L0C	O3-C3-N4-C4
15	D	301	A1L0C	C2-C1-C3-N4
15	D	301	A1L0C	C2-C1-C3-O3
15	D	301	A1L0C	N3-C1-C3-N4
15	D	301	A1L0C	N3-C1-C3-O3
15	C	301	A1L0C	C2-C1-C3-N4
15	C	301	A1L0C	C2-C1-C3-O3
15	C	301	A1L0C	N3-C1-C3-N4
15	C	301	A1L0C	N3-C1-C3-O3
15	F	301	A1L0C	O3-C3-N4-C4
15	A	301	A1L0C	C1-C3-N4-C4
15	F	301	A1L0C	C1-C3-N4-C4

There are no ring outliers.

4 monomers are involved in 4 short contacts:

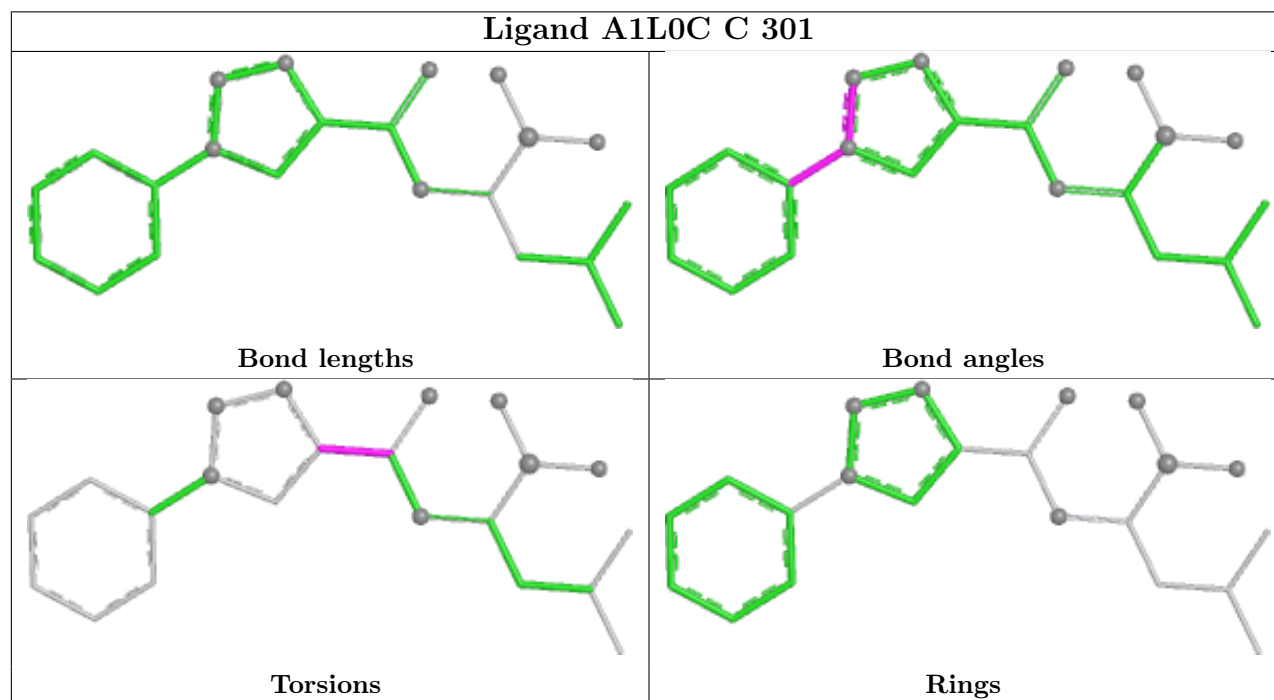
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	301	A1L0C	1	0

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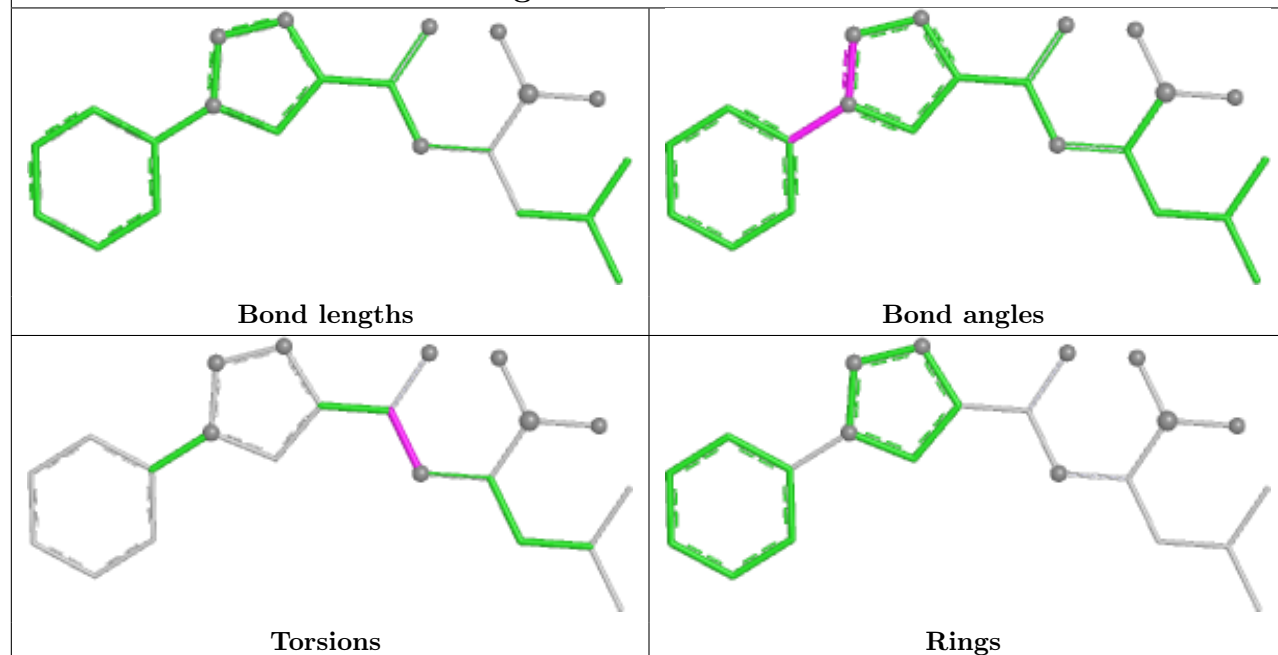
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	301	A1L0C	1	0
15	D	301	A1L0C	1	0
15	F	301	A1L0C	1	0

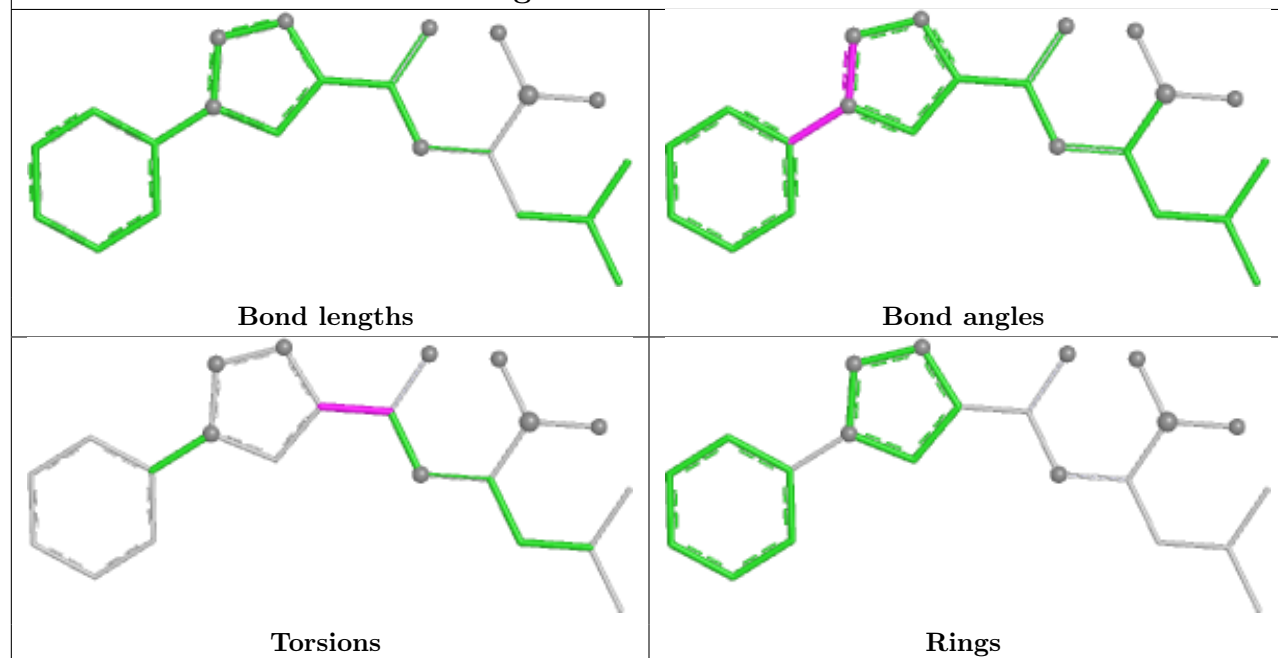
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

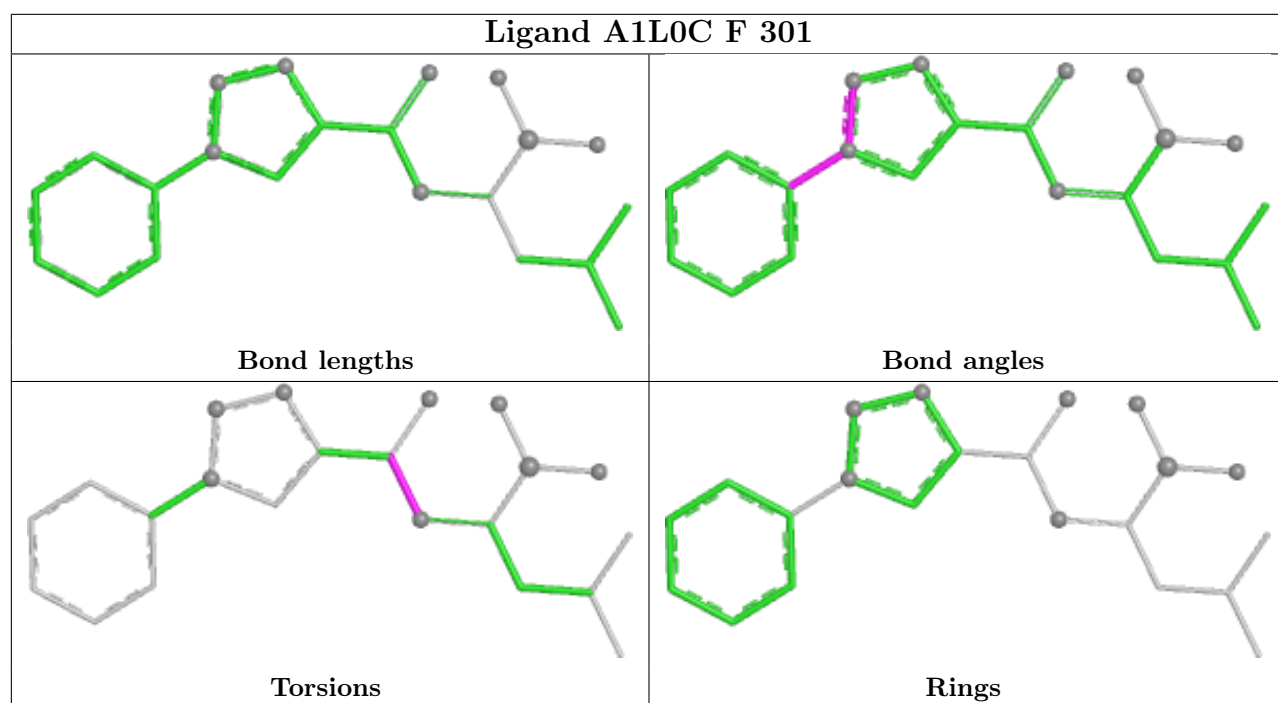


Ligand A1L0C A 301



Ligand A1L0C D 301





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.

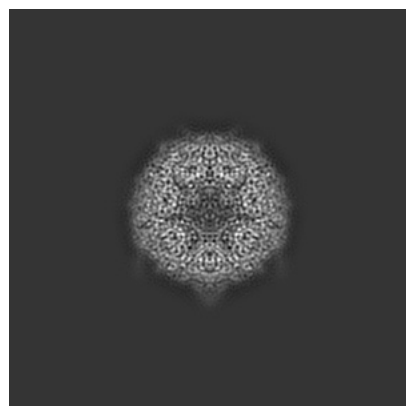
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39482. These allow visual inspection of the internal detail of the map and identification of artifacts.

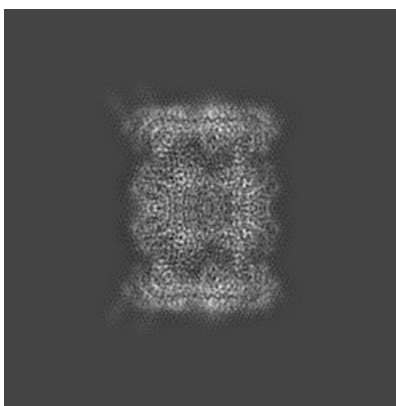
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

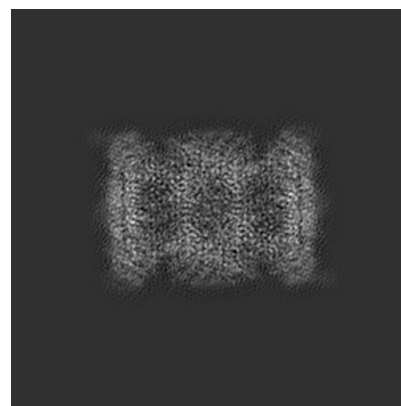
6.1.1 Primary map



X

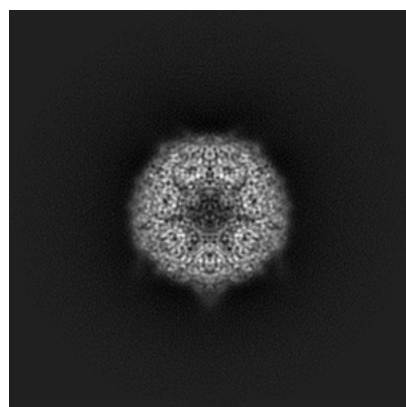


Y

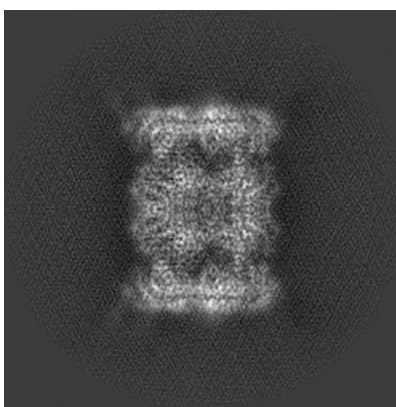


Z

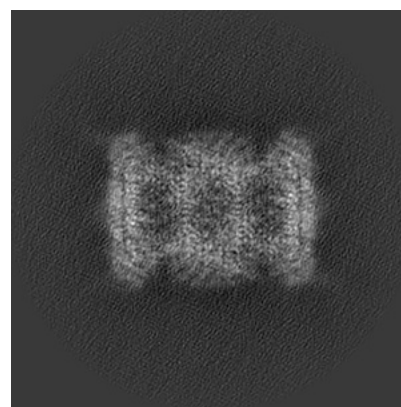
6.1.2 Raw map



X



Y

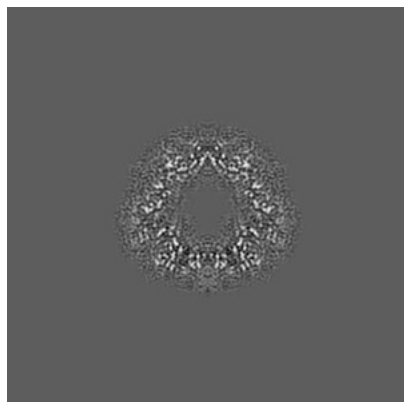


Z

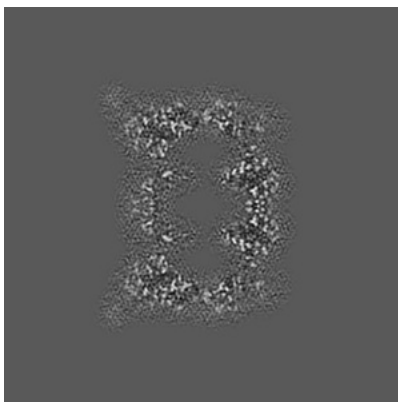
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

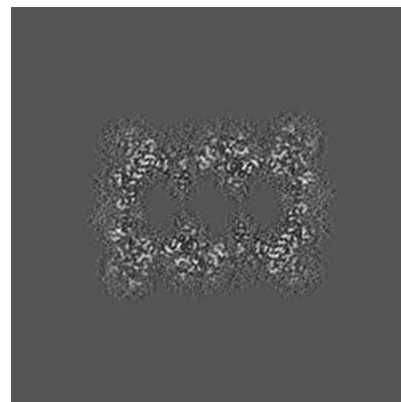
6.2.1 Primary map



X Index: 127

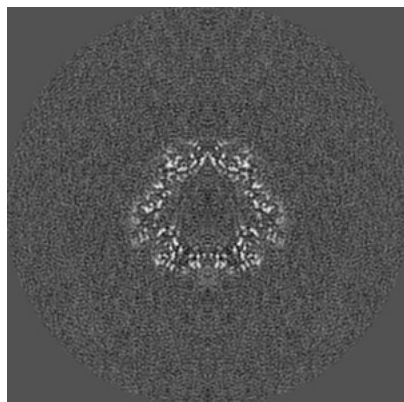


Y Index: 127

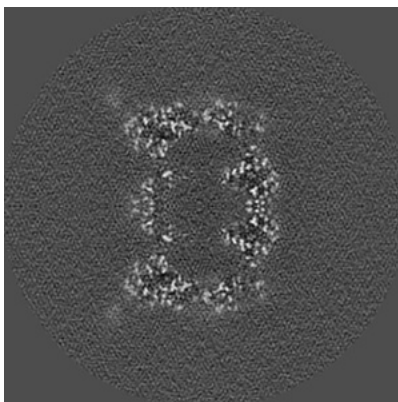


Z Index: 127

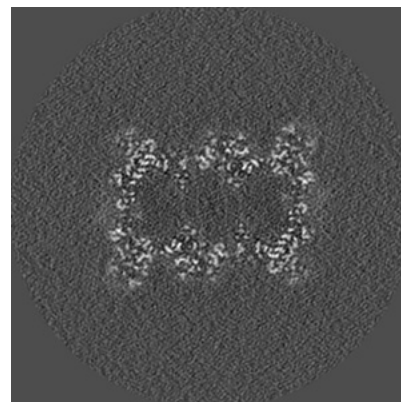
6.2.2 Raw map



X Index: 127



Y Index: 127

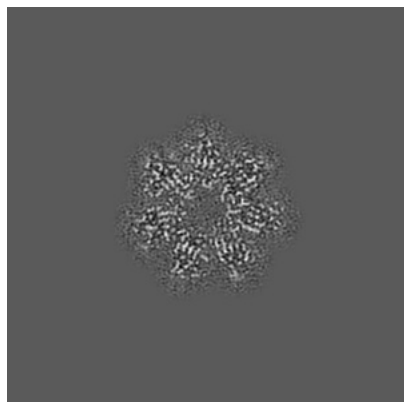


Z Index: 127

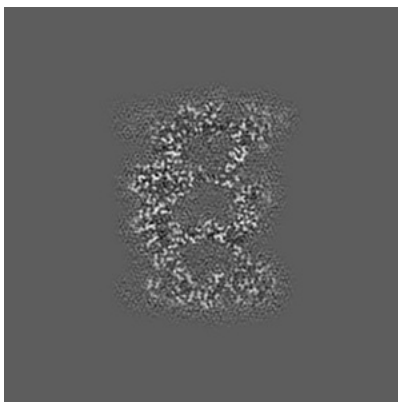
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

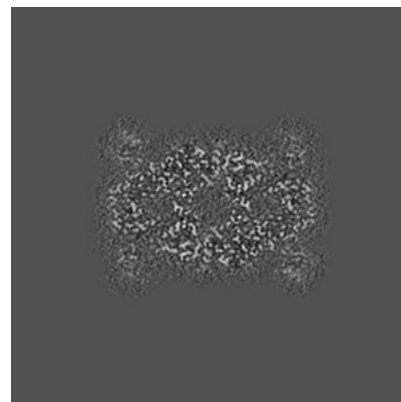
6.3.1 Primary map



X Index: 143

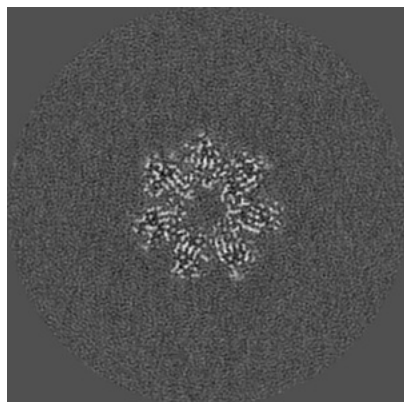


Y Index: 110

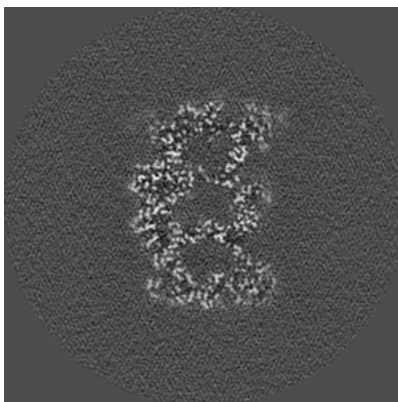


Z Index: 146

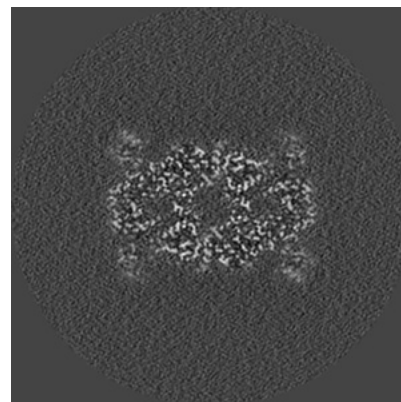
6.3.2 Raw map



X Index: 143



Y Index: 110

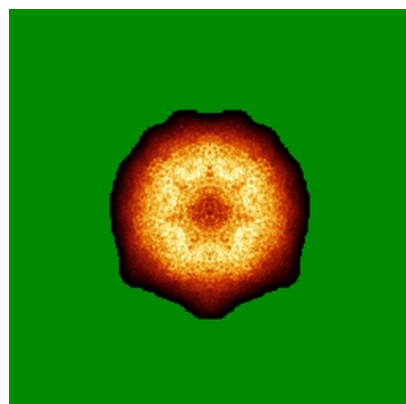


Z Index: 146

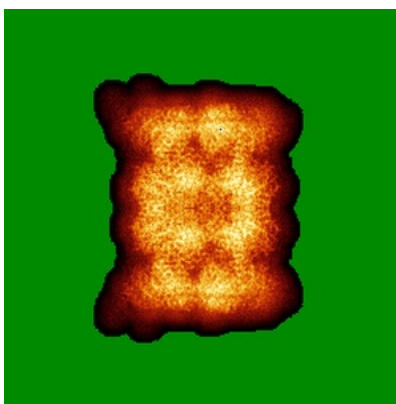
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

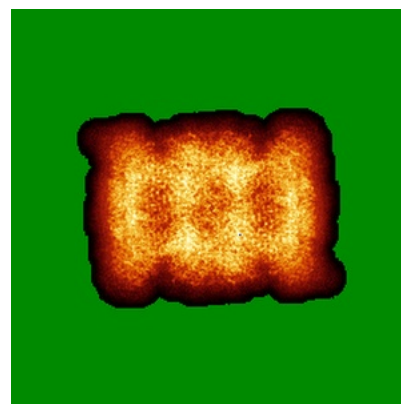
6.4.1 Primary map



X

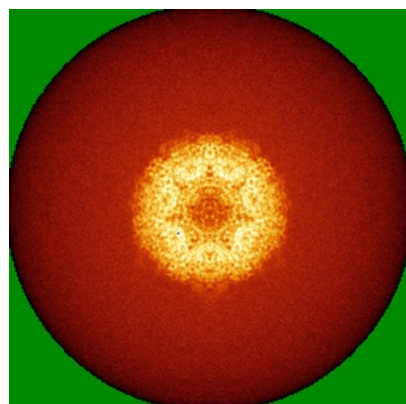


Y

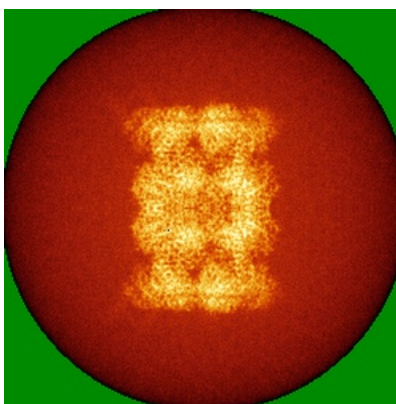


Z

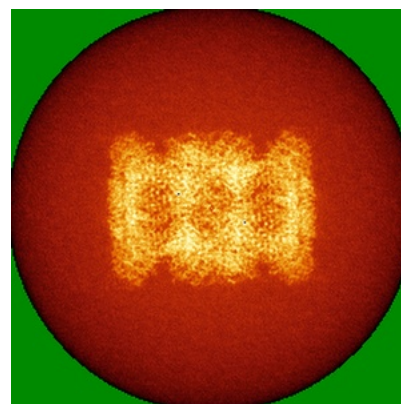
6.4.2 Raw map



X



Y

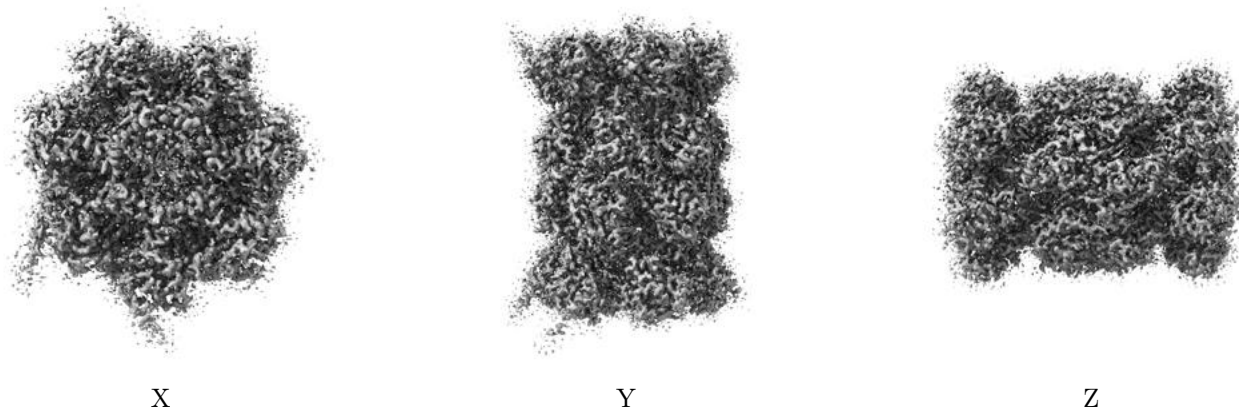


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

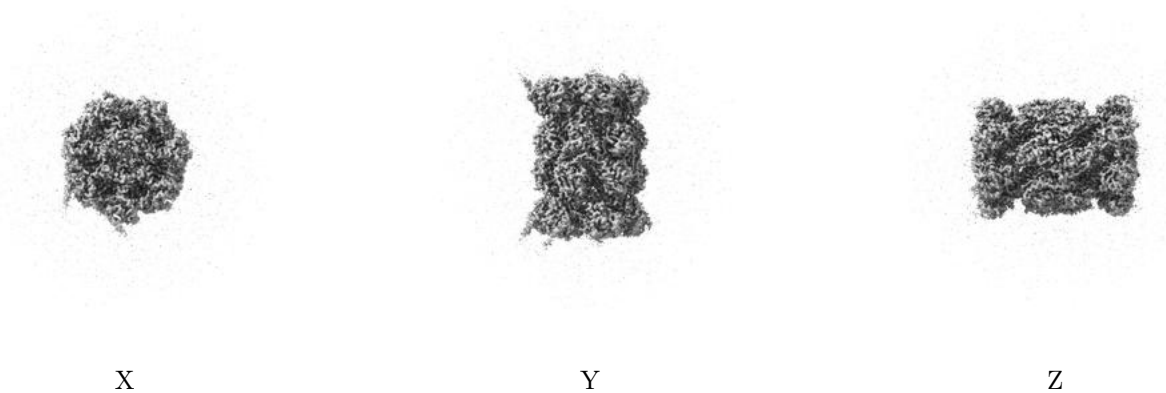
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0343. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

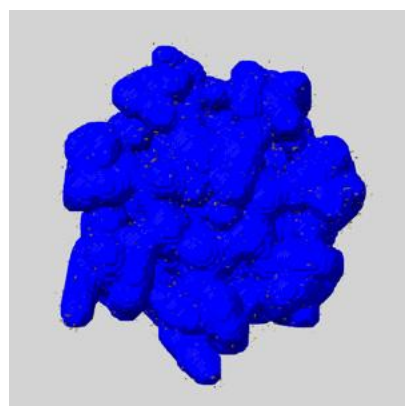
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

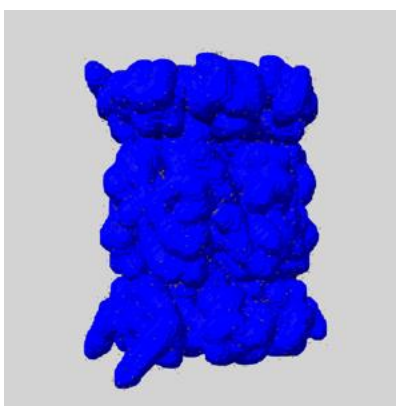
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

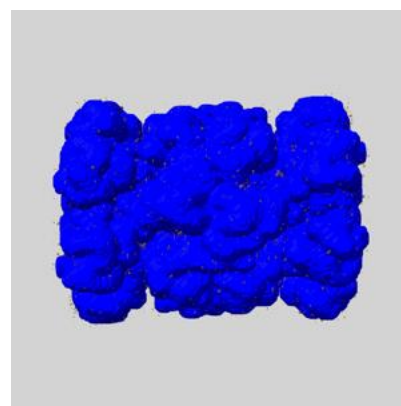
6.6.1 emd_39482_msk_1.map [i](#)



X



Y

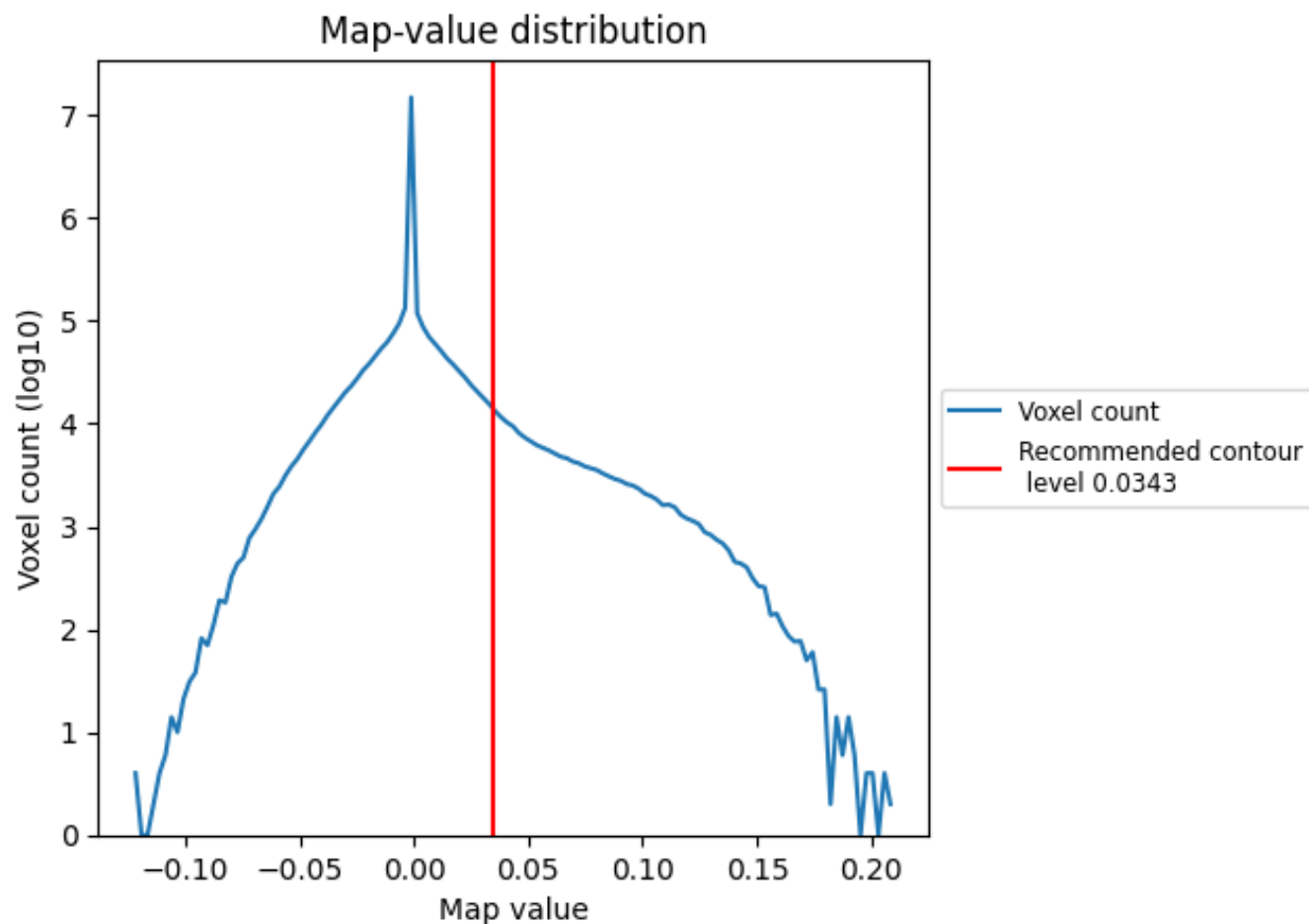


Z

7 Map analysis [i](#)

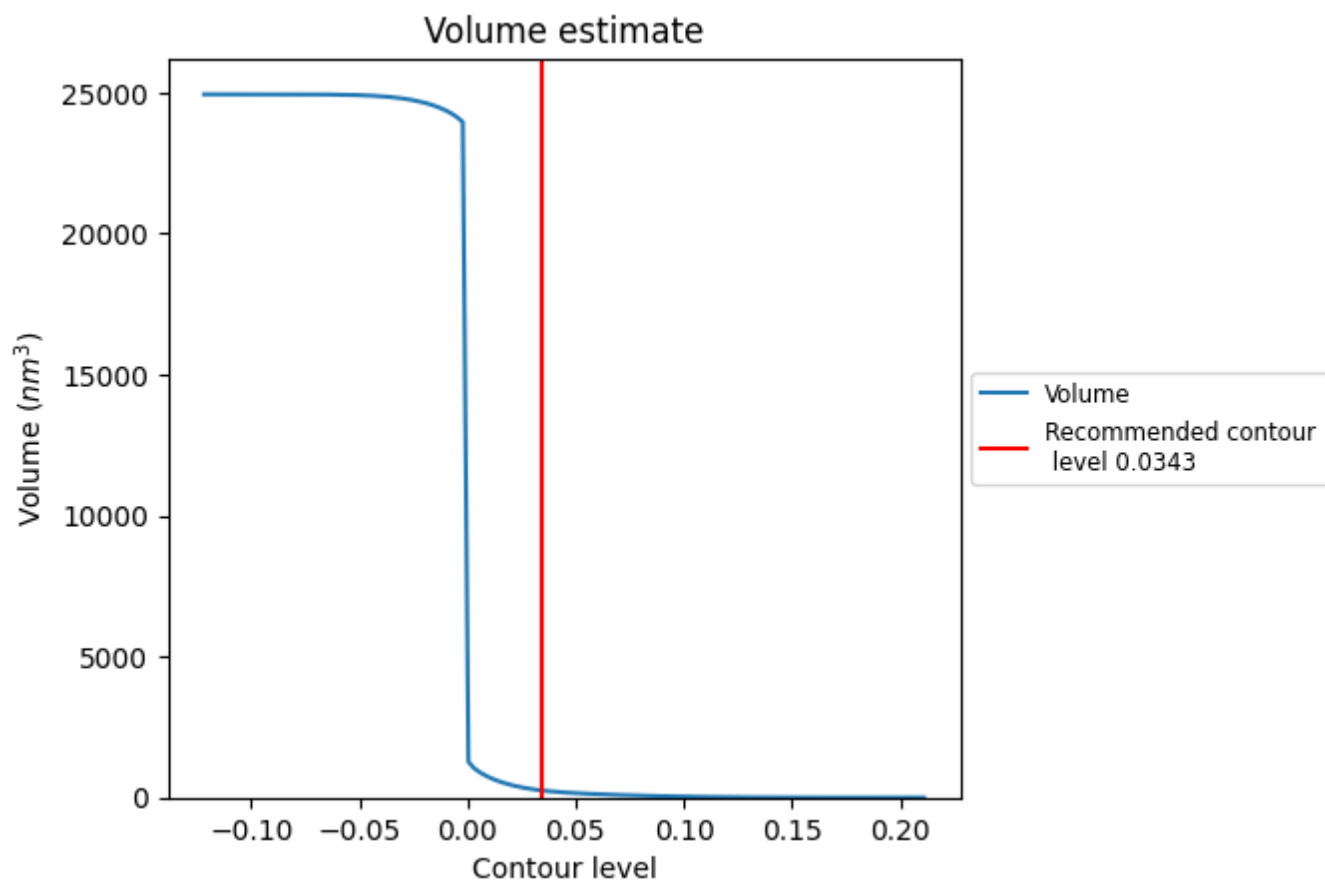
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

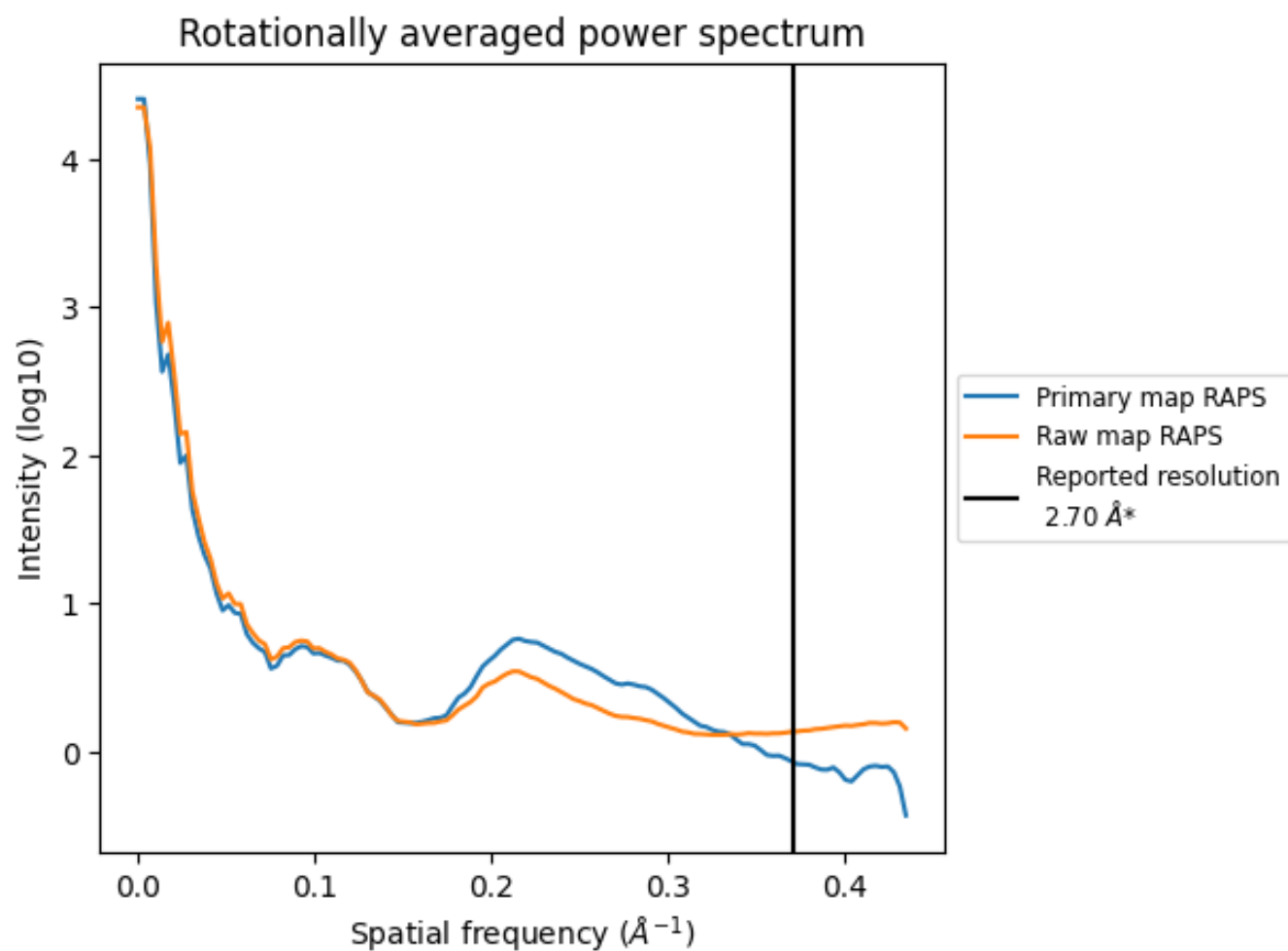
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 254 nm³; this corresponds to an approximate mass of 229 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

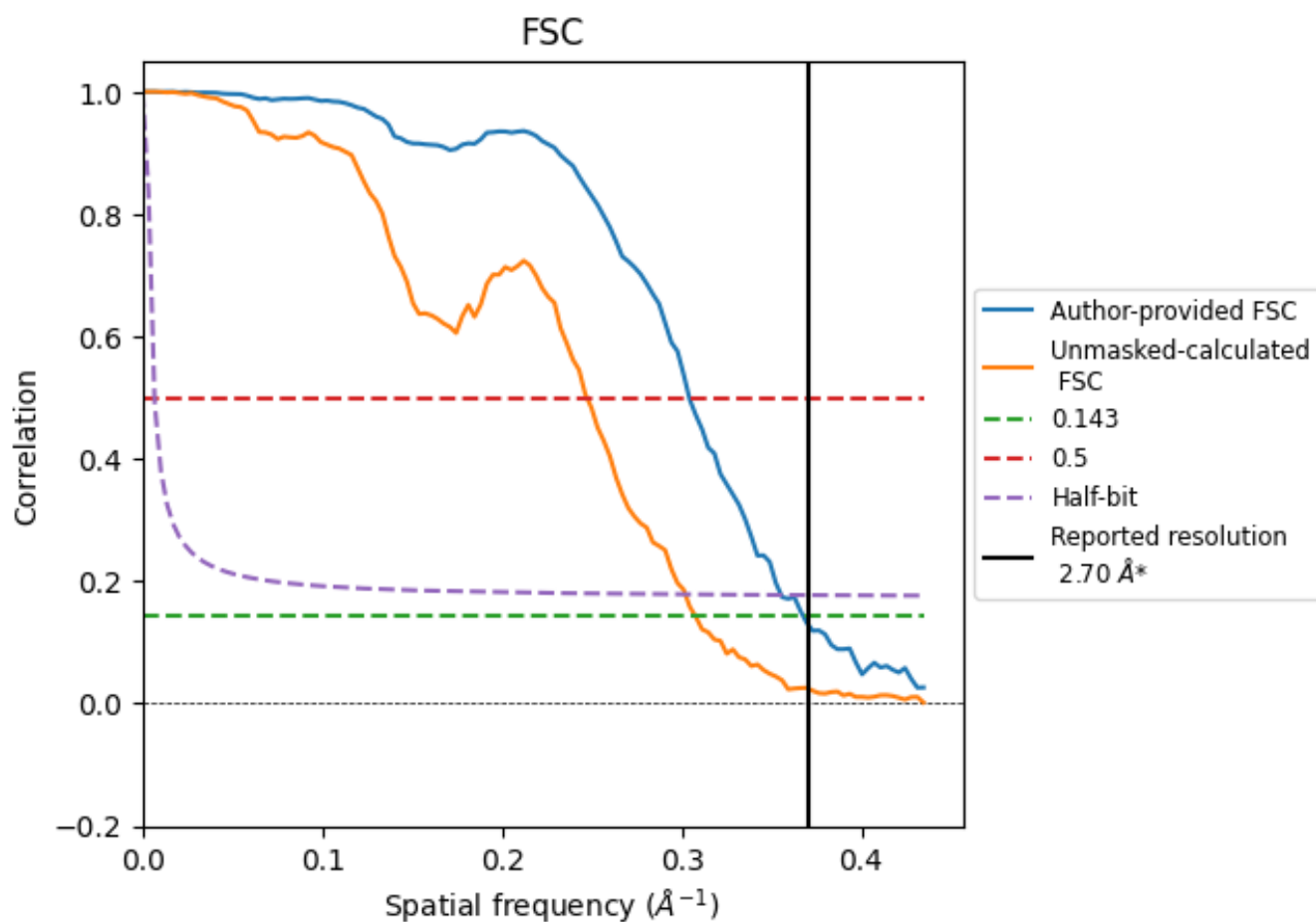


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

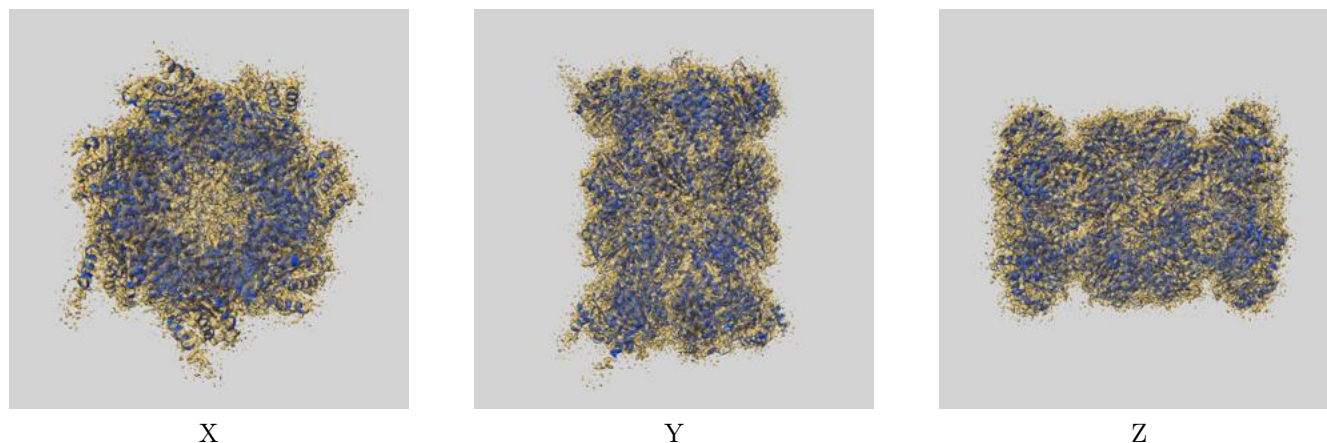
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	3.29	2.81
Unmasked-calculated*	3.25	4.04	3.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

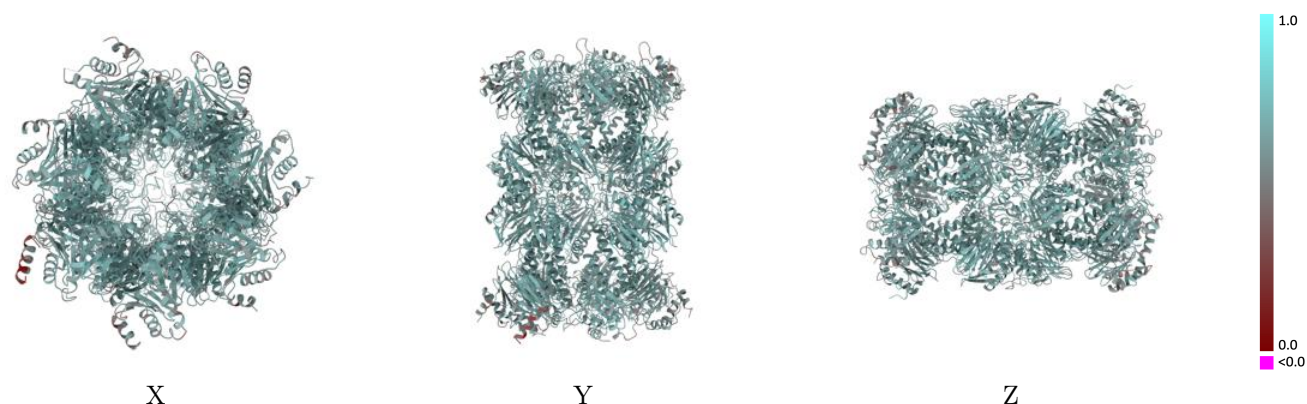
This section contains information regarding the fit between EMDB map EMD-39482 and PDB model 8YPK. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



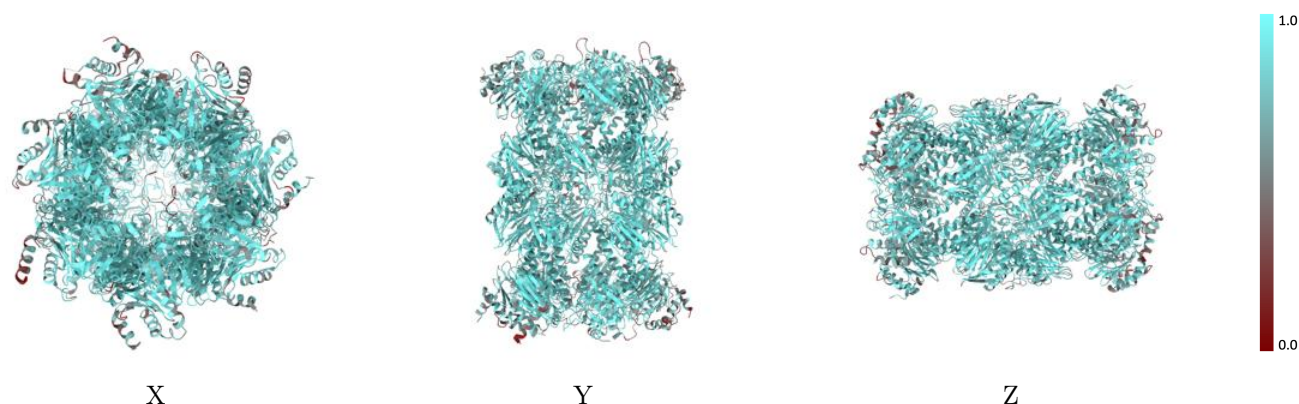
The images above show the 3D surface view of the map at the recommended contour level 0.0343 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



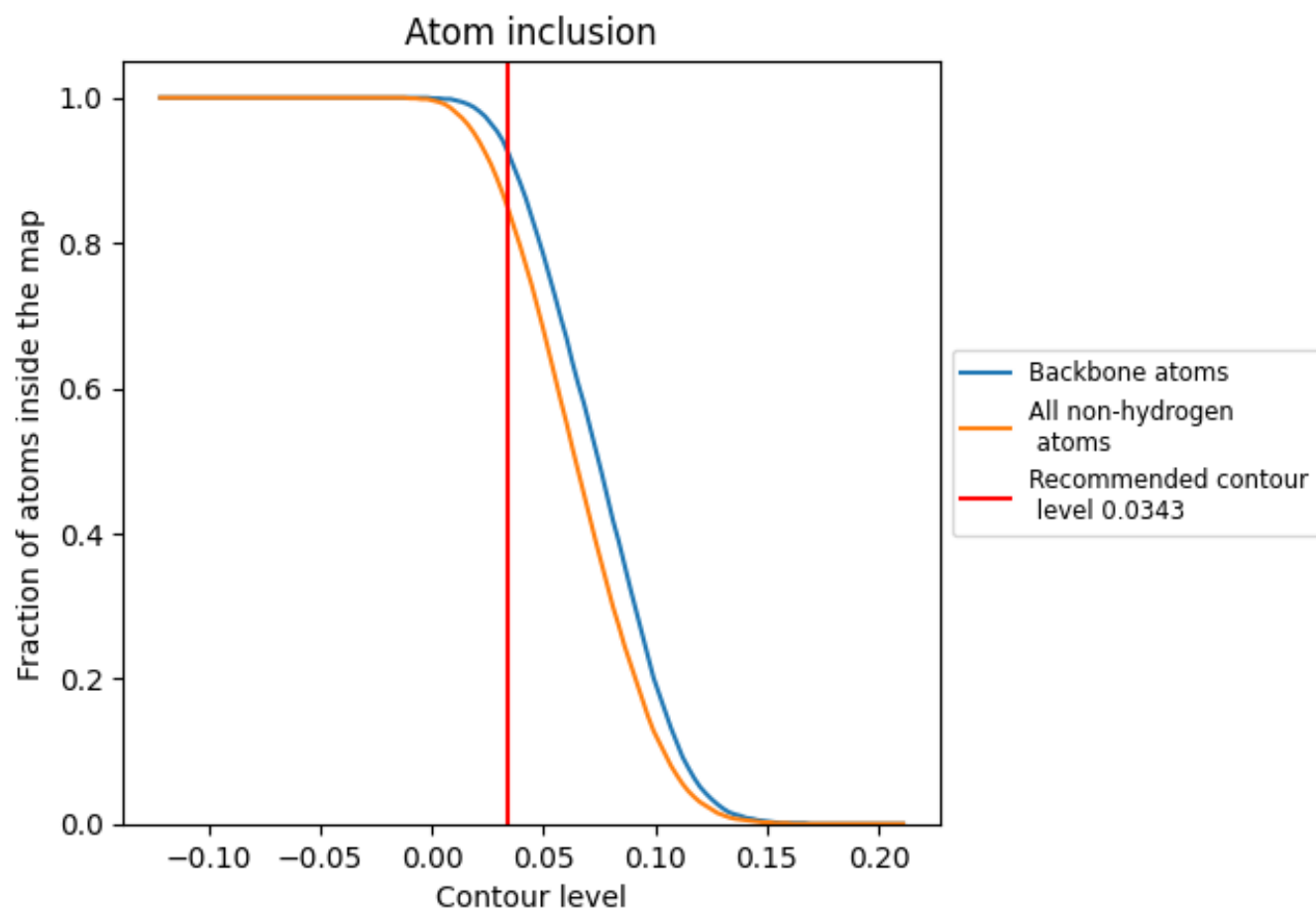
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0343).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0343) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.6210
A	 0.8910	 0.6400
B	 0.8720	 0.6390
C	 0.9050	 0.6460
D	 0.9020	 0.6460
E	 0.8710	 0.6390
F	 0.8910	 0.6400
G	 0.8200	 0.6090
H	 0.8050	 0.6050
I	 0.8080	 0.5970
J	 0.7800	 0.5980
K	 0.7760	 0.6020
L	 0.8210	 0.6110
M	 0.8070	 0.6050
N	 0.8100	 0.5990
O	 0.8000	 0.5930
P	 0.8220	 0.6100
Q	 0.7840	 0.5990
R	 0.7730	 0.6010
S	 0.8770	 0.6350
T	 0.9100	 0.6490
U	 0.9080	 0.6500
V	 0.9090	 0.6480
W	 0.9010	 0.6440
X	 0.8750	 0.6340
Y	 0.9090	 0.6490
Z	 0.8000	 0.5910
a	 0.8980	 0.6440
b	 0.8240	 0.6100

