



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:42 PM UTC

PDB ID : 7LXU / pdb_00007lxu
EMDB ID : EMD-23575
Title : Structure of Plasmodium falciparum 20S proteasome with bound MPI-5
Authors : Metcalfe, R.D.; Morton, C.J.; Xie, S.C.; Liu, B.; Hanssen, E.; Leis, A.P.;
Tilley, L.; Griffin, M.D.W.
Deposited on : 2021-03-05
Resolution : 3.10 Å(reported)

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

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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

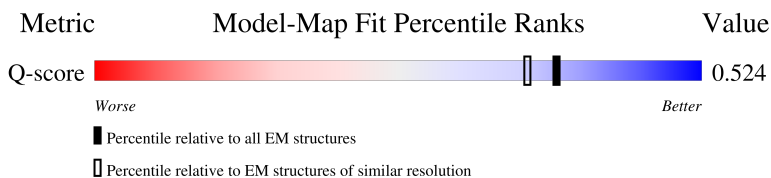
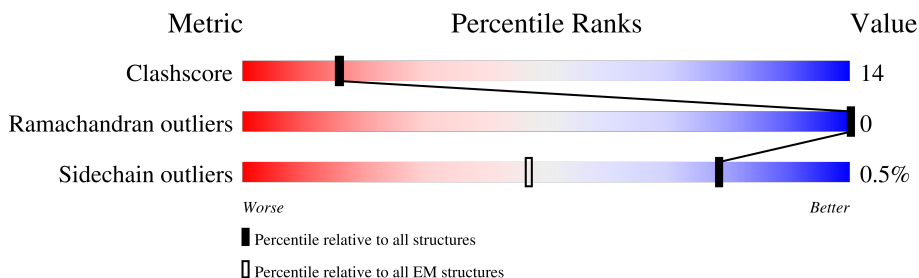
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



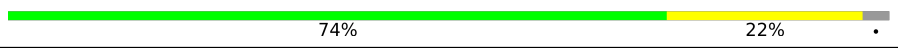
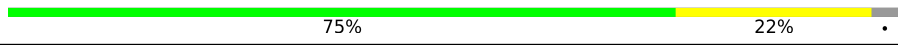
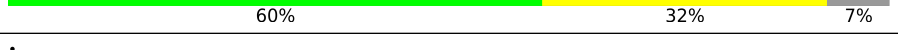
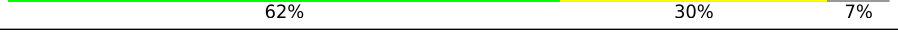
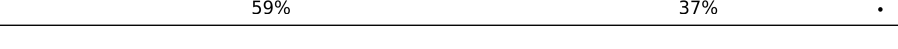
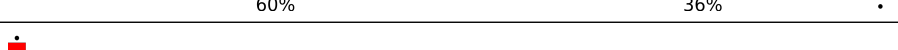
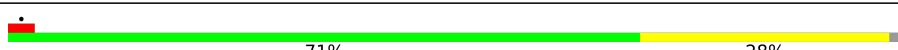
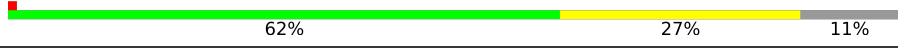
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	260	 67% 30% .
1	O	260	 68% 28% .
2	B	235	 72% 25% .
2	P	235	 72% 25% .

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Mol	Chain	Length	Quality of chain
3	C	246	
3	Q	246	
4	D	241	
4	R	241	
5	E	256	
5	S	256	
6	F	254	
6	T	254	
7	G	252	
7	U	252	
8	H	252	
8	V	252	
9	I	229	
9	W	229	
10	J	218	
10	X	218	
11	K	195	
11	Y	195	
12	L	211	
12	Z	211	
13	M	240	
13	a	240	
14	N	265	
14	b	265	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 50778 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 20S proteasome alpha-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	251	Total	C	N	O	S	0	0
			1986	1248	332	391	15		
1	O	251	Total	C	N	O	S	0	0
			1986	1248	332	391	15		

- Molecule 2 is a protein called 20S proteasome alpha-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1826	1175	298	347	6		
2	P	229	Total	C	N	O	S	0	0
			1826	1175	298	347	6		

- Molecule 3 is a protein called 20S proteasome alpha-3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	242	Total	C	N	O	S	0	0
			1934	1237	315	378	4		
3	Q	242	Total	C	N	O	S	0	0
			1934	1237	315	378	4		

- Molecule 4 is a protein called 20S proteasome alpha-4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	233	Total	C	N	O	S	0	0
			1845	1178	312	347	8		
4	R	233	Total	C	N	O	S	0	0
			1845	1178	312	347	8		

- Molecule 5 is a protein called 20S proteasome alpha-5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	236	Total	C	N	O	S	0	0
			1830	1155	301	363	11		
5	S	236	Total	C	N	O	S	0	0
			1830	1155	301	363	11		

- Molecule 6 is a protein called 20S proteasome alpha-6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	235	Total	C	N	O	S	0	0
			1866	1187	308	360	11		
6	T	235	Total	C	N	O	S	0	0
			1866	1187	308	360	11		

- Molecule 7 is a protein called 20S proteasome alpha-7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	242	Total	C	N	O	S	0	0
			1979	1257	332	377	13		
7	U	242	Total	C	N	O	S	0	0
			1979	1257	332	377	13		

- Molecule 8 is a protein called 20S proteasome beta-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	229	Total	C	N	O	S	0	0
			1846	1170	317	347	12		
8	V	229	Total	C	N	O	S	0	0
			1846	1170	317	347	12		

- Molecule 9 is a protein called 20S proteasome beta-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1676	1058	291	313	14		
9	W	219	Total	C	N	O	S	0	0
			1676	1058	291	313	14		

- Molecule 10 is a protein called 20S proteasome beta-3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	215	Total	C	N	O	S	0	0
			1698	1082	275	327	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	215	Total	C	N	O	S	0	0
			1698	1082	275	327	14		

- Molecule 11 is a protein called 20S proteasome beta-4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	195	Total	C	N	O	S	0	0
			1614	1042	266	298	8		
11	Y	195	Total	C	N	O	S	0	0
			1614	1042	266	298	8		

- Molecule 12 is a protein called 20S proteasome beta-5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	209	Total	C	N	O	S	0	0
			1647	1050	273	317	7		
12	Z	209	Total	C	N	O	S	0	0
			1647	1050	273	317	7		

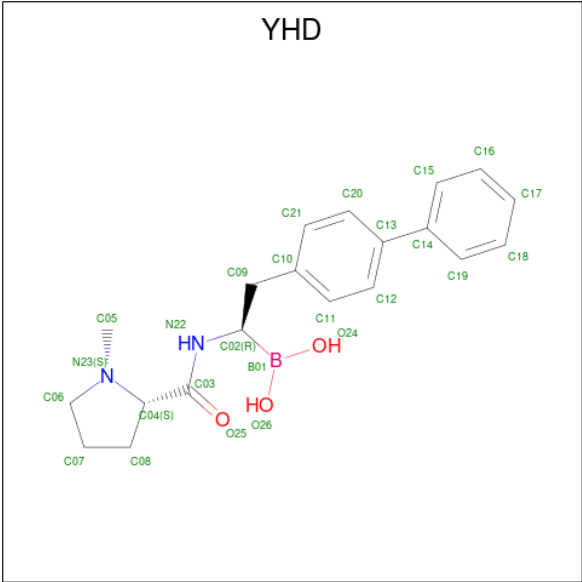
- Molecule 13 is a protein called 20S proteasome beta-6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	213	Total	C	N	O	S	0	0
			1696	1085	283	321	7		
13	a	213	Total	C	N	O	S	0	0
			1696	1085	283	321	7		

- Molecule 14 is a protein called 20S proteasome beta-7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	234	Total	C	N	O	S	0	0
			1920	1225	324	363	8		
14	b	234	Total	C	N	O	S	0	0
			1920	1225	324	363	8		

- Molecule 15 is N-[(1R)-2-([1,1'-biphenyl]-4-yl)-1-boronoethyl]-1-methyl-L-prolinamide (CCD ID: YHD) (formula: C₂₀H₂₅BN₂O₃) (labeled as "Ligand of Interest" by depositor).

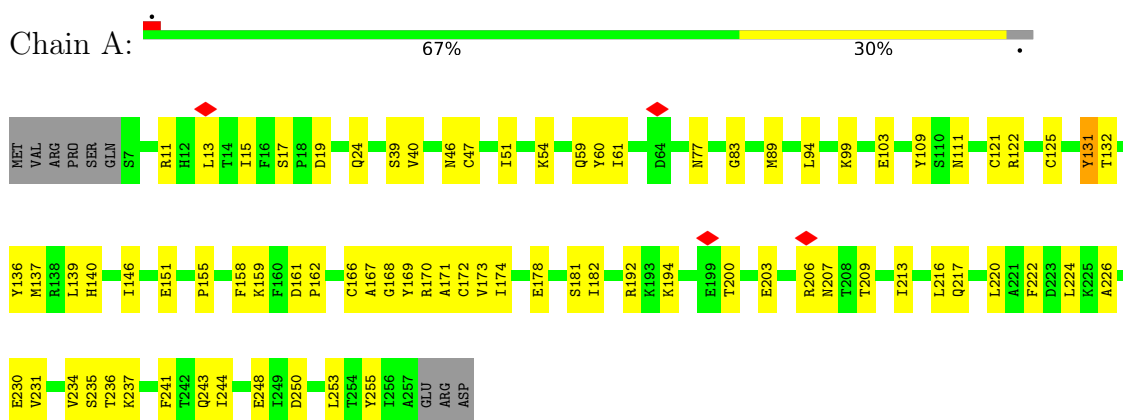


Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	B	C	N	O	0
			26	1	20	2	3	
15	Z	1	Total	B	C	N	O	0
			26	1	20	2	3	

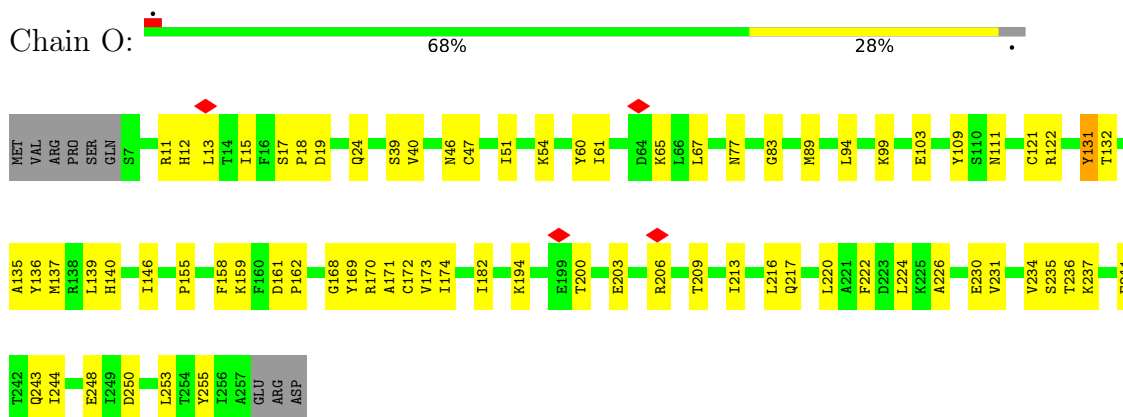
3 Residue-property plots

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

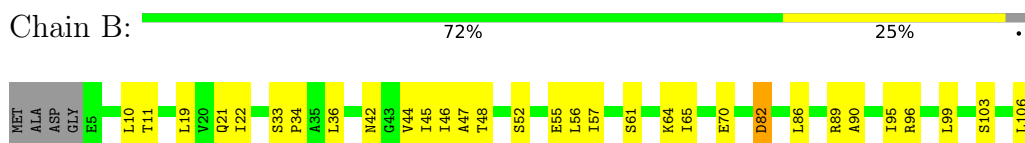
- Molecule 1: 20S proteasome alpha-1 subunit



- Molecule 1: 20S proteasome alpha-1 subunit



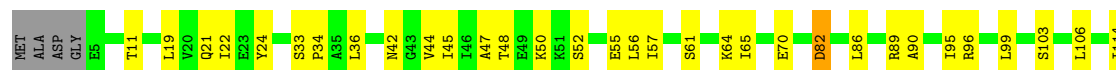
- Molecule 2: 20S proteasome alpha-2 subunit





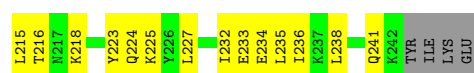
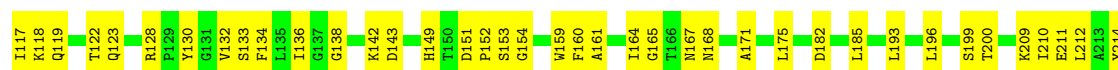
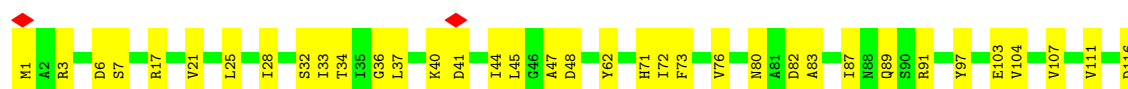
• Molecule 2: 20S proteasome alpha-2 subunit

Chain P: 72% 25% .



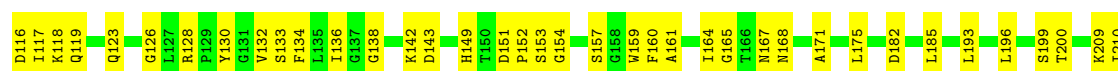
• Molecule 3: 20S proteasome alpha-3 subunit

Chain C: 62% 36% .



• Molecule 3: 20S proteasome alpha-3 subunit

Chain Q: 61% 37% .



• Molecule 4: 20S proteasome alpha-4 subunit

Chain D: 74% 22% .





- Molecule 4: 20S proteasome alpha-4 subunit

Chain R: 75% 22%



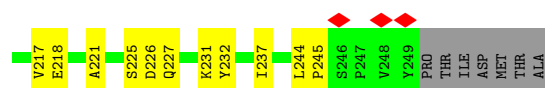
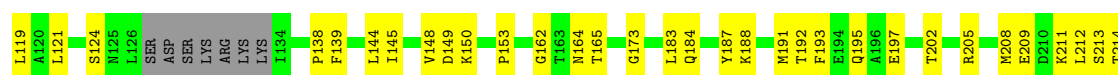
- Molecule 5: 20S proteasome alpha-5 subunit

Chain E: 63% 29% 8%



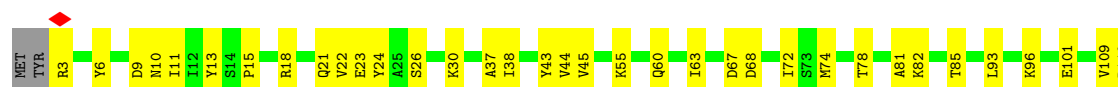
- Molecule 5: 20S proteasome alpha-5 subunit

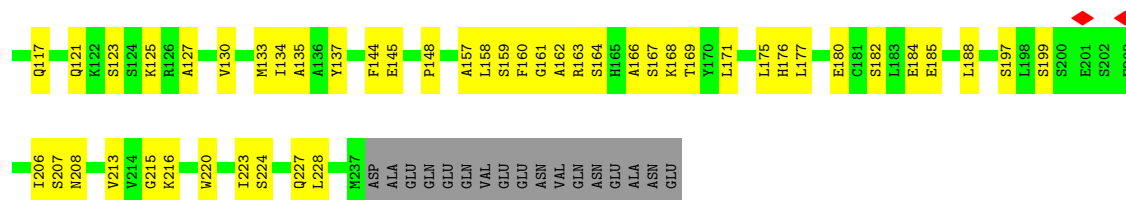
Chain S: 64% 29% 8%

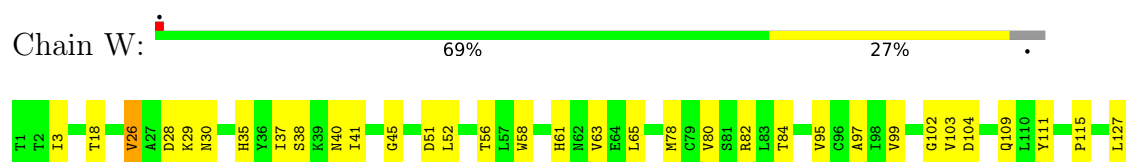


- Molecule 6: 20S proteasome alpha-6 subunit

Chain F: 60% 32% 7%









- Molecule 10: 20S proteasome beta-3 subunit



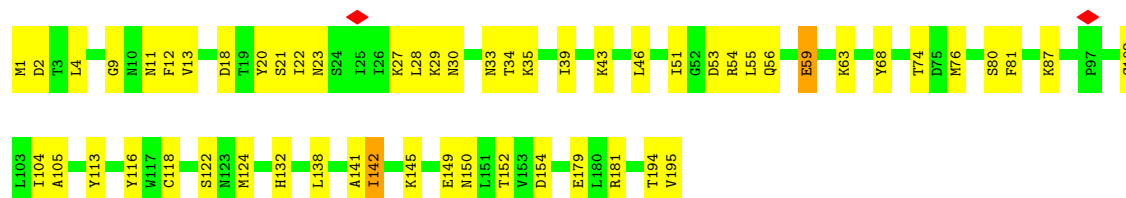
- Molecule 10: 20S proteasome beta-3 subunit



- Molecule 11: 20S proteasome beta-4 subunit



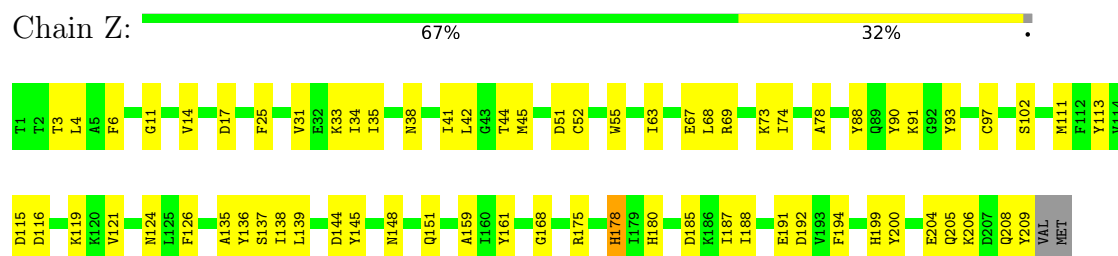
- Molecule 11: 20S proteasome beta-4 subunit



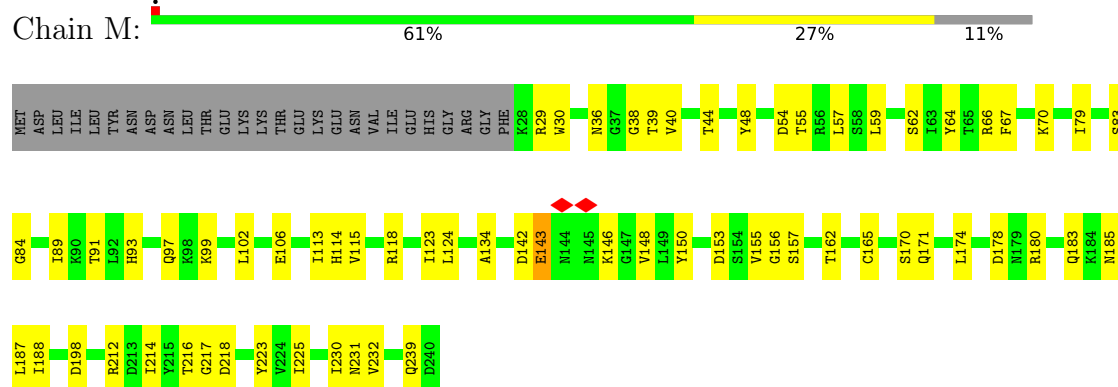
- Molecule 12: 20S proteasome beta-5 subunit



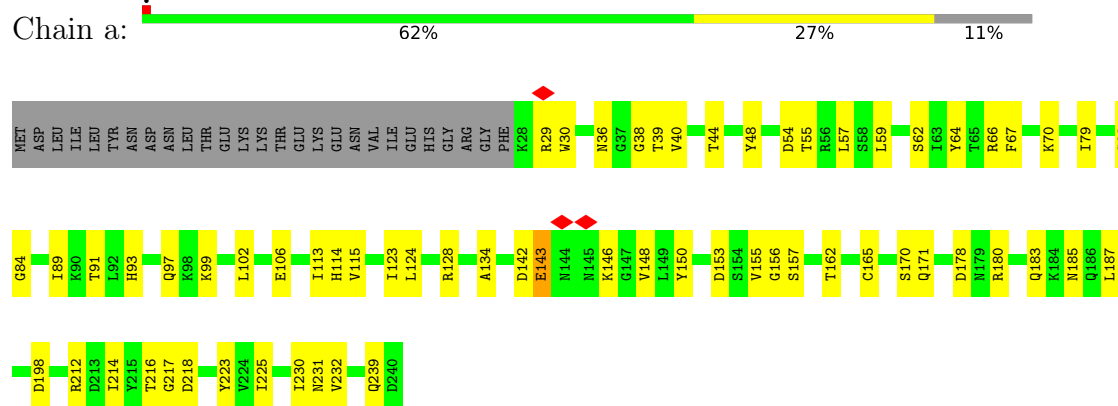
- Molecule 12: 20S proteasome beta-5 subunit



- Molecule 13: 20S proteasome beta-6 subunit

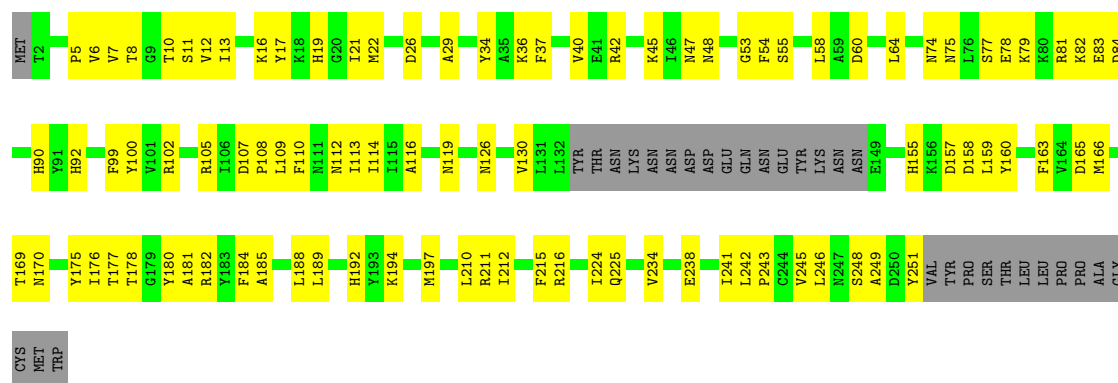


- Molecule 13: 20S proteasome beta-6 subunit



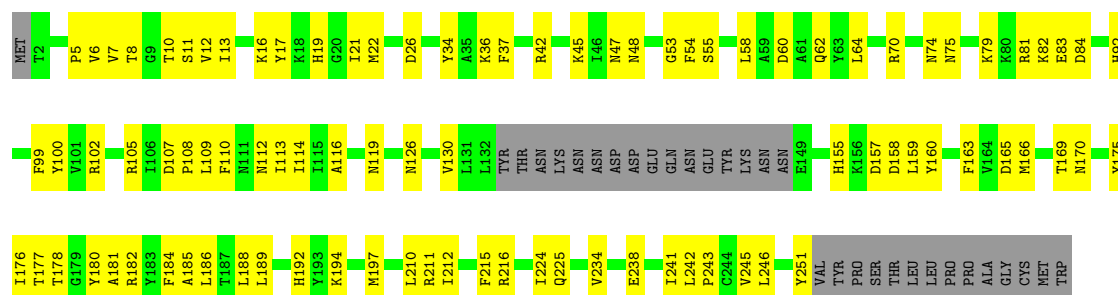
- Molecule 14: 20S proteasome beta-7 subunit

Chain N:  52% 36% 12%



- Molecule 14: 20S proteasome beta-7 subunit

Chain b:  54% 35% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	38738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	45.612	Depositor
Minimum map value	-22.978	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (Å)	524.0, 524.0, 524.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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: YHD

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	0.25	0/2013	0.39	0/2715
1	O	0.25	0/2013	0.39	0/2715
2	B	0.24	0/1860	0.35	0/2512
2	P	0.24	0/1860	0.35	0/2512
3	C	0.24	0/1969	0.37	0/2665
3	Q	0.24	0/1969	0.37	0/2665
4	D	0.23	0/1875	0.41	0/2530
4	R	0.23	0/1875	0.41	0/2530
5	E	0.21	0/1856	0.34	0/2509
5	S	0.21	0/1856	0.34	0/2509
6	F	0.25	0/1900	0.42	0/2558
6	T	0.25	0/1900	0.42	0/2558
7	G	0.25	0/2022	0.38	0/2733
7	U	0.25	0/2022	0.38	0/2733
8	H	0.28	0/1877	0.44	0/2520
8	V	0.28	0/1877	0.44	0/2520
9	I	0.25	0/1712	0.41	0/2328
9	W	0.25	0/1712	0.41	0/2328
10	J	0.25	0/1727	0.38	0/2331
10	X	0.25	0/1727	0.38	0/2331
11	K	0.26	0/1649	0.38	0/2223
11	Y	0.26	0/1649	0.38	0/2223
12	L	0.26	0/1681	0.50	0/2266
12	Z	0.26	0/1681	0.50	0/2266
13	M	0.25	0/1728	0.36	0/2339
13	a	0.25	0/1728	0.36	0/2339
14	N	0.27	0/1959	0.42	0/2645
14	b	0.27	0/1959	0.42	0/2645
All	All	0.25	0/51656	0.40	0/69748

There are no bond length outliers.

There are no bond angle outliers.

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	1986	0	1984	67	0
1	O	1986	0	1984	67	0
2	B	1826	0	1844	51	0
2	P	1826	0	1844	49	0
3	C	1934	0	1935	72	0
3	Q	1934	0	1935	76	0
4	D	1845	0	1878	41	0
4	R	1845	0	1878	40	0
5	E	1830	0	1824	54	0
5	S	1830	0	1824	51	0
6	F	1866	0	1869	60	0
6	T	1866	0	1869	54	0
7	G	1979	0	1923	74	0
7	U	1979	0	1923	71	0
8	H	1846	0	1843	78	0
8	V	1846	0	1843	78	0
9	I	1676	0	1674	56	0
9	W	1676	0	1674	54	0
10	J	1698	0	1685	54	0
10	X	1698	0	1685	60	0
11	K	1614	0	1584	52	0
11	Y	1614	0	1584	48	0
12	L	1647	0	1599	57	0
12	Z	1647	0	1599	59	0
13	M	1696	0	1707	60	0
13	a	1696	0	1707	58	0
14	N	1920	0	1886	79	0
14	b	1920	0	1886	80	0
15	L	26	0	0	0	0
15	Z	26	0	0	0	0
All	All	50778	0	50470	1462	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 14.

All (1462) 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)
13:a:62:SER:OG	14:b:182:ARG:NH2	2.07	0.88
1:O:51:ILE:HG12	1:O:231:VAL:HG12	1.56	0.86
1:A:51:ILE:HG12	1:A:231:VAL:HG12	1.56	0.85
5:E:188:LYS:H	5:E:191:MET:HE3	1.44	0.82
13:M:84:GLY:H	13:M:89:ILE:HD11	1.45	0.82
13:a:84:GLY:H	13:a:89:ILE:HD11	1.45	0.81
13:M:62:SER:OG	14:N:182:ARG:NH2	2.12	0.80
7:G:38:LEU:HB3	7:G:49:CYS:HB3	1.63	0.80
13:M:187:LEU:HD21	9:W:204:ILE:HD11	1.63	0.80
2:P:34:PRO:HA	2:P:164:GLY:HA3	1.64	0.80
3:C:76:VAL:HA	3:C:134:PHE:HB3	1.64	0.79
5:S:188:LYS:H	5:S:191:MET:HE3	1.44	0.79
6:T:67:ASP:OD1	6:T:68:ASP:N	2.15	0.79
8:V:30:CYS:SG	8:V:229:ARG:NH2	2.56	0.79
10:J:121:ASP:HB2	10:J:128:VAL:HG12	1.65	0.79
2:B:34:PRO:HA	2:B:164:GLY:HA3	1.65	0.78
8:H:30:CYS:SG	8:H:229:ARG:NH2	2.56	0.78
14:N:10:THR:HG22	14:N:11:SER:H	1.49	0.78
7:U:38:LEU:HB3	7:U:49:CYS:HB3	1.63	0.78
10:X:121:ASP:HB2	10:X:128:VAL:HG12	1.65	0.78
9:I:173:VAL:HG12	9:I:190:LYS:HB2	1.65	0.78
3:Q:76:VAL:HA	3:Q:134:PHE:HB3	1.64	0.78
1:O:11:ARG:HH21	7:U:7:GLY:HA3	1.49	0.77
11:Y:59:GLU:OE2	11:Y:63:LYS:NZ	2.15	0.77
8:H:167:VAL:HG22	8:H:173:ILE:HG22	1.67	0.77
6:F:67:ASP:OD1	6:F:68:ASP:N	2.15	0.77
11:Y:102:CYS:HB2	11:Y:118:CYS:HB3	1.67	0.77
14:b:10:THR:HG22	14:b:11:SER:H	1.49	0.77
7:G:49:CYS:HA	7:G:218:PHE:HB3	1.67	0.76
7:U:49:CYS:HA	7:U:218:PHE:HB3	1.67	0.76
8:V:167:VAL:HG22	8:V:173:ILE:HG22	1.67	0.76
9:W:173:VAL:HG12	9:W:190:LYS:HB2	1.65	0.76
11:K:59:GLU:OE2	11:K:63:LYS:NZ	2.15	0.76
11:K:102:CYS:HB2	11:K:118:CYS:HB3	1.66	0.75
13:M:38:GLY:HA3	13:M:70:LYS:HE2	1.68	0.75
11:Y:104:ILE:HB	11:Y:116:TYR:HB2	1.69	0.75
13:a:38:GLY:HA3	13:a:70:LYS:HE2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:187:ILE:HG22	12:L:188:ILE:HG13	1.68	0.75
12:Z:187:ILE:HG22	12:Z:188:ILE:HG13	1.68	0.75
1:O:170:ARG:NH1	2:P:55:GLU:O	2.21	0.74
6:T:26:SER:HA	6:T:148:PRO:HG2	1.69	0.74
6:F:26:SER:HA	6:F:148:PRO:HG2	1.68	0.74
13:M:183:GLN:HG3	13:M:188:ILE:HG23	1.70	0.74
1:A:236:THR:O	1:A:237:LYS:HG2	1.88	0.74
1:O:236:THR:O	1:O:237:LYS:HG2	1.88	0.73
8:V:221:ASP:O	8:V:224:SER:OG	2.07	0.73
2:P:95:ILE:HG23	9:W:61:HIS:HB3	1.70	0.73
12:L:38:ASN:ND2	12:L:67:GLU:OE1	2.20	0.73
8:H:221:ASP:O	8:H:224:SER:OG	2.07	0.73
1:A:158:PHE:HA	1:A:168:GLY:HA2	1.71	0.72
11:K:104:ILE:HB	11:K:116:TYR:HB2	1.69	0.72
12:Z:38:ASN:ND2	12:Z:67:GLU:OE1	2.20	0.72
9:I:103:VAL:HG21	9:I:180:LYS:HA	1.72	0.72
9:W:103:VAL:HG21	9:W:180:LYS:HA	1.72	0.72
13:a:183:GLN:HG3	13:a:188:ILE:HG23	1.70	0.72
9:I:41:ILE:HG22	9:I:102:GLY:HA3	1.71	0.72
5:S:148:VAL:HG12	5:S:153:PRO:HB3	1.72	0.71
1:O:158:PHE:HA	1:O:168:GLY:HA2	1.71	0.71
4:D:90:GLU:OE2	4:D:106:TYR:OH	2.08	0.71
4:R:90:GLU:OE2	4:R:106:TYR:OH	2.08	0.71
8:V:140:ILE:HD11	8:V:173:ILE:HG12	1.73	0.71
9:W:41:ILE:HG22	9:W:102:GLY:HA3	1.71	0.70
6:F:45:VAL:HG22	6:F:213:VAL:HG12	1.73	0.70
5:E:148:VAL:HG12	5:E:153:PRO:HB3	1.72	0.70
5:S:14:THR:HG23	6:T:21:GLN:HE22	1.57	0.70
7:G:36:THR:HA	7:G:169:GLY:HA3	1.73	0.70
11:Y:33:ASN:OD1	11:Y:34:THR:N	2.25	0.70
11:K:33:ASN:OD1	11:K:34:THR:N	2.25	0.70
7:U:36:THR:HA	7:U:169:GLY:HA3	1.73	0.70
6:T:163:ARG:HH22	6:T:199:SER:HB3	1.56	0.70
7:U:99:ASN:ND2	14:b:74:ASN:OD1	2.23	0.69
6:F:163:ARG:HH22	6:F:199:SER:HB3	1.56	0.69
8:H:140:ILE:HD11	8:H:173:ILE:HG12	1.73	0.69
9:W:51:ASP:OD1	10:X:101:ARG:NE	2.24	0.69
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.75	0.69
6:T:81:ALA:HB2	6:T:130:VAL:HG21	1.75	0.69
1:A:170:ARG:NH1	2:B:55:GLU:O	2.26	0.69
14:N:81:ARG:NH1	14:N:83:GLU:OE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:204:ILE:HD11	13:a:187:LEU:HD21	1.73	0.69
6:T:45:VAL:HG22	6:T:213:VAL:HG12	1.73	0.68
14:b:81:ARG:NH1	14:b:83:GLU:OE1	2.26	0.68
13:M:153:ASP:OD1	13:M:157:SER:OG	2.11	0.68
5:E:217:VAL:HG23	5:E:237:ILE:HD11	1.76	0.68
11:K:18:ASP:OD1	11:K:35:LYS:NZ	2.27	0.68
1:O:136:TYR:HA	7:U:129:TRP:CE2	2.28	0.68
5:S:217:VAL:HG23	5:S:237:ILE:HD11	1.76	0.68
2:B:65:ILE:HD12	2:B:209:GLU:HG3	1.75	0.68
13:a:153:ASP:OD1	13:a:157:SER:OG	2.11	0.68
11:K:27:LYS:HE3	12:L:136:TYR:CD1	2.28	0.68
2:P:65:ILE:HD12	2:P:209:GLU:HG3	1.75	0.68
13:M:187:LEU:HG	9:W:207:LYS:HZ3	1.59	0.67
4:R:98:MET:HE3	12:Z:78:ALA:HB1	1.77	0.67
8:V:29:LYS:NZ	9:W:139:GLU:OE1	2.27	0.67
1:A:230:GLU:OE1	1:A:243:GLN:NE2	2.28	0.67
7:G:9:ASP:O	7:G:23:GLN:NE2	2.27	0.67
7:U:9:ASP:O	7:U:23:GLN:NE2	2.27	0.67
1:O:230:GLU:OE1	1:O:243:GLN:NE2	2.28	0.67
11:Y:18:ASP:OD1	11:Y:35:LYS:NZ	2.27	0.67
11:Y:152:THR:OG1	11:Y:154:ASP:OD1	2.12	0.67
9:I:45:GLY:HA3	9:I:52:LEU:HD11	1.75	0.67
12:L:4:LEU:HD21	12:L:135:ALA:HB1	1.76	0.67
12:Z:4:LEU:HD21	12:Z:135:ALA:HB1	1.76	0.67
2:B:11:THR:HG22	2:B:19:LEU:HD22	1.76	0.67
7:G:74:ASN:HD22	14:N:130:VAL:HG22	1.60	0.67
9:I:164:PHE:O	13:a:66:ARG:NH2	2.28	0.67
10:J:67:GLU:OE2	10:J:70:ARG:NH2	2.28	0.66
2:P:11:THR:HG22	2:P:19:LEU:HD22	1.76	0.66
8:V:117:PHE:HE1	8:V:239:GLU:HB2	1.61	0.66
9:I:161:ALA:O	9:I:165:ASN:ND2	2.29	0.66
9:W:45:GLY:HA3	9:W:52:LEU:HD11	1.75	0.66
1:O:171:ALA:HB3	2:P:56:LEU:HD22	1.77	0.66
13:a:143:GLU:HB2	13:a:146:LYS:HB2	1.77	0.66
12:L:115:ASP:OD2	12:L:116:ASP:N	2.29	0.66
13:M:143:GLU:HB2	13:M:146:LYS:HB2	1.77	0.66
9:I:207:LYS:HZ3	13:a:187:LEU:HG	1.61	0.66
10:X:67:GLU:OE2	10:X:70:ARG:NH2	2.28	0.66
11:K:145:LYS:HD3	12:Z:138:ILE:HD12	1.77	0.66
8:H:117:PHE:HE1	8:H:239:GLU:HB2	1.61	0.66
6:F:145:GLU:HB2	6:F:158:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:62:LYS:HB3	7:G:65:SER:HB3	1.79	0.65
9:W:161:ALA:O	9:W:165:ASN:ND2	2.29	0.65
12:Z:115:ASP:OD2	12:Z:116:ASP:N	2.29	0.65
13:M:187:LEU:H	9:W:207:LYS:HZ2	1.43	0.65
6:T:117:GLN:NE2	7:U:86:ASP:OD1	2.30	0.65
11:Y:27:LYS:HE3	12:Z:136:TYR:CD1	2.32	0.65
7:G:16:SER:OG	7:G:20:ARG:O	2.14	0.65
7:G:106:HIS:HB2	8:H:137:LYS:HE2	1.77	0.65
1:O:11:ARG:NH2	7:U:6:ALA:O	2.30	0.65
7:U:62:LYS:HB3	7:U:65:SER:HB3	1.79	0.65
14:N:21:ILE:HD11	14:N:159:LEU:HB3	1.78	0.65
2:B:106:LEU:HD11	10:J:80:GLN:NE2	2.12	0.65
6:F:117:GLN:NE2	7:G:86:ASP:OD1	2.30	0.64
7:G:28:TYR:HE1	7:G:156:PRO:HD2	1.62	0.64
3:C:116:ASP:OD1	4:D:81:ARG:NH1	2.30	0.64
3:Q:25:LEU:HD13	3:Q:28:ILE:HD11	1.80	0.64
6:T:145:GLU:HB2	6:T:158:LEU:HD21	1.79	0.64
7:U:28:TYR:HE1	7:U:156:PRO:HD2	1.62	0.64
14:b:21:ILE:HD11	14:b:159:LEU:HB3	1.78	0.64
9:I:136:ALA:HB2	14:b:184:PHE:HD2	1.62	0.64
11:K:152:THR:OG1	11:K:154:ASP:OD1	2.12	0.64
7:U:67:ASN:HA	7:U:217:ASN:HD21	1.63	0.64
7:U:16:SER:OG	7:U:20:ARG:O	2.14	0.64
3:Q:161:ALA:HB1	3:Q:175:LEU:HD13	1.79	0.64
8:H:174:ILE:HD11	14:N:37:PHE:CD1	2.33	0.64
3:C:25:LEU:HD13	3:C:28:ILE:HD11	1.80	0.63
3:C:161:ALA:HB1	3:C:175:LEU:HD13	1.79	0.63
4:D:98:MET:HE3	12:L:78:ALA:HB1	1.80	0.63
4:R:127:PHE:HB3	4:R:129:ILE:HG22	1.81	0.63
10:X:162:MET:HG2	10:X:183:CYS:HA	1.80	0.63
14:b:92:HIS:HD1	14:b:160:TYR:HH	1.43	0.63
3:C:3:ARG:NH1	6:F:9:ASP:OD2	2.29	0.63
6:F:206:ILE:HG23	6:F:208:ASN:H	1.64	0.63
12:Z:115:ASP:HB3	12:Z:119:LYS:HB3	1.79	0.63
7:G:99:ASN:ND2	14:N:74:ASN:OD1	2.30	0.63
5:S:52:ARG:NH1	5:S:61:LYS:O	2.32	0.63
9:W:104:ASP:OD1	9:W:109:GLN:NE2	2.31	0.63
2:B:11:THR:HG23	2:B:21:GLN:HB3	1.80	0.63
3:Q:32:SER:OG	3:Q:48:ASP:O	2.15	0.63
7:G:67:ASN:HA	7:G:217:ASN:HD21	1.63	0.63
7:G:115:VAL:HG12	7:G:140:ILE:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:227:LEU:HD12	8:H:242:THR:HB	1.81	0.62
9:W:95:VAL:HA	9:W:115:PRO:HB3	1.80	0.62
3:C:154:GLY:O	4:D:81:ARG:NH2	2.32	0.62
9:I:140:ALA:HB2	14:b:212:ILE:HD11	1.81	0.62
12:L:115:ASP:HB3	12:L:119:LYS:HB3	1.79	0.62
2:P:11:THR:HG23	2:P:21:GLN:HB3	1.80	0.62
1:O:13:LEU:HD22	1:O:137:MET:O	2.00	0.62
5:E:52:ARG:NH1	5:E:61:LYS:O	2.32	0.62
12:Z:14:VAL:HG11	12:Z:42:LEU:HD11	1.81	0.62
8:H:191:SER:OG	8:V:188:TYR:O	2.10	0.62
9:I:104:ASP:OD1	9:I:109:GLN:NE2	2.31	0.62
3:C:138:GLY:HA2	3:C:215:LEU:HD11	1.82	0.62
6:T:206:ILE:HG23	6:T:208:ASN:H	1.64	0.62
7:U:115:VAL:HG12	7:U:140:ILE:HD12	1.81	0.62
12:Z:161:TYR:OH	12:Z:199:HIS:NE2	2.33	0.62
12:L:161:TYR:OH	12:L:199:HIS:NE2	2.33	0.62
8:V:227:LEU:HD12	8:V:242:THR:HB	1.81	0.62
2:B:95:ILE:HG23	9:I:61:HIS:HB3	1.80	0.61
5:S:46:VAL:HG23	5:S:153:PRO:HB2	1.82	0.61
1:A:131:TYR:CD2	1:A:137:MET:HE2	2.35	0.61
4:D:23:LEU:HD22	4:D:149:PRO:HG2	1.82	0.61
13:a:114:HIS:NE2	13:a:142:ASP:OD2	2.33	0.61
1:A:13:LEU:HD22	1:A:137:MET:O	2.00	0.61
11:K:27:LYS:NZ	11:K:28:LEU:O	2.27	0.61
12:L:14:VAL:HG11	12:L:42:LEU:HD11	1.81	0.61
10:J:162:MET:HG2	10:J:183:CYS:HA	1.80	0.61
1:O:131:TYR:CD2	1:O:137:MET:HE2	2.35	0.61
8:H:218:MET:O	8:H:224:SER:OG	2.19	0.61
2:P:177:ARG:HH22	2:P:193:LEU:HD13	1.66	0.61
1:A:206:ARG:NH1	1:A:255:TYR:OH	2.34	0.61
4:D:36:LYS:NZ	5:E:60:GLU:OE2	2.34	0.61
4:D:127:PHE:HB3	4:D:129:ILE:HG22	1.81	0.61
9:I:95:VAL:HA	9:I:115:PRO:HB3	1.80	0.61
10:J:27:LEU:HD12	12:Z:206:LYS:HE3	1.81	0.61
14:N:105:ARG:NH1	14:N:107:ASP:OD2	2.34	0.61
1:A:131:TYR:HD1	1:A:131:TYR:H	1.48	0.61
9:I:26:VAL:O	13:a:212:ARG:NH1	2.33	0.61
3:Q:3:ARG:NH1	6:T:9:ASP:OD2	2.34	0.61
4:R:23:LEU:HD22	4:R:149:PRO:HG2	1.82	0.61
7:U:74:ASN:HD22	14:b:130:VAL:HG22	1.66	0.61
8:V:218:MET:O	8:V:224:SER:OG	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:ARG:HH22	2:B:193:LEU:HD13	1.66	0.60
4:D:42:VAL:HG21	4:D:186:ILE:HD13	1.83	0.60
7:G:46:ILE:HD11	7:G:149:GLY:HA3	1.83	0.60
6:F:167:SER:HB2	6:F:197:SER:HB2	1.82	0.60
1:O:206:ARG:NH1	1:O:255:TYR:OH	2.34	0.60
6:T:167:SER:HB2	6:T:197:SER:HB2	1.82	0.60
14:b:105:ARG:NH1	14:b:107:ASP:OD2	2.34	0.60
11:K:23:ASN:HB2	11:K:29:LYS:HE3	1.84	0.60
1:O:131:TYR:HD1	1:O:131:TYR:H	1.48	0.60
8:V:38:ASN:ND2	8:V:40:ASN:OD1	2.34	0.60
3:Q:116:ASP:OD1	4:R:81:ARG:NH1	2.34	0.60
5:E:46:VAL:HG23	5:E:153:PRO:HB2	1.82	0.60
3:Q:138:GLY:HA2	3:Q:215:LEU:HD11	1.82	0.60
6:T:3:ARG:NH1	6:T:24:TYR:OH	2.35	0.60
9:W:40:ASN:ND2	9:W:103:VAL:O	2.34	0.60
8:H:38:ASN:ND2	8:H:40:ASN:OD1	2.34	0.60
5:S:214:THR:HG23	5:S:237:ILE:HG21	1.84	0.60
14:b:245:VAL:HG23	14:b:246:LEU:HG	1.84	0.60
3:C:73:PHE:HB3	3:C:223:TYR:HE1	1.66	0.60
8:H:29:LYS:NZ	9:I:139:GLU:OE1	2.35	0.60
1:A:171:ALA:HB3	2:B:56:LEU:HD22	1.84	0.60
9:I:207:LYS:HZ2	13:a:187:LEU:H	1.48	0.60
13:M:124:LEU:HB3	13:M:156:GLY:H	1.67	0.60
14:b:13:ILE:HG23	14:b:177:THR:HG22	1.84	0.60
5:E:214:THR:HG23	5:E:237:ILE:HG21	1.84	0.59
8:H:187:ILE:HD12	8:V:187:ILE:HD12	1.83	0.59
13:M:84:GLY:HA3	13:M:134:ALA:HA	1.84	0.59
1:A:17:SER:OG	1:A:19:ASP:OD1	2.20	0.59
9:I:51:ASP:OD1	10:J:101:ARG:NE	2.31	0.59
10:X:114:PHE:HB3	10:X:130:TYR:HB3	1.84	0.59
13:a:124:LEU:HB3	13:a:156:GLY:H	1.67	0.59
13:a:30:TRP:CZ3	14:b:166:MET:HE2	2.37	0.59
1:A:11:ARG:HH21	7:G:7:GLY:HA3	1.66	0.59
3:C:6:ASP:OD2	4:D:2:SER:OG	2.18	0.59
14:N:13:ILE:HG23	14:N:177:THR:HG22	1.84	0.59
13:a:84:GLY:HA3	13:a:134:ALA:HA	1.85	0.59
6:F:3:ARG:NH1	6:F:24:TYR:OH	2.35	0.59
6:T:182:SER:O	6:T:185:GLU:N	2.34	0.59
13:M:114:HIS:NE2	13:M:142:ASP:OD2	2.33	0.59
4:R:206:VAL:HG13	4:R:217:ILE:HB	1.85	0.59
14:b:11:SER:HB3	14:b:181:ALA:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:44:VAL:HG11	6:F:135:ALA:HB1	1.83	0.59
8:H:18:SER:HB2	8:H:30:CYS:HA	1.85	0.59
5:S:23:GLN:HB3	5:S:138:PRO:HG3	1.85	0.59
14:N:26:ASP:OD1	14:N:42:ARG:NH2	2.36	0.59
6:F:206:ILE:HG12	6:F:207:SER:H	1.68	0.59
7:G:219:SER:HA	7:G:232:ILE:HD12	1.85	0.59
8:H:159:ILE:HG13	8:H:160:LYS:H	1.68	0.59
11:Y:23:ASN:HB2	11:Y:29:LYS:HE3	1.84	0.59
4:D:206:VAL:HG13	4:D:217:ILE:HB	1.85	0.59
14:N:245:VAL:HG23	14:N:246:LEU:HG	1.84	0.59
3:Q:73:PHE:HB3	3:Q:223:TYR:HE1	1.66	0.59
4:R:42:VAL:HG21	4:R:186:ILE:HD13	1.83	0.59
13:M:30:TRP:CZ3	14:N:166:MET:HE2	2.39	0.58
13:M:214:ILE:HG23	9:W:167:LEU:HB3	1.85	0.58
6:T:44:VAL:HG11	6:T:135:ALA:HB1	1.83	0.58
7:U:104:ASN:HB3	8:V:138:LYS:NZ	2.18	0.58
14:b:26:ASP:OD1	14:b:42:ARG:NH2	2.36	0.58
8:V:189:ILE:HD13	8:V:217:ALA:HB2	1.85	0.58
3:C:32:SER:OG	3:C:48:ASP:O	2.15	0.58
5:E:21:LEU:HB2	5:E:24:VAL:HG22	1.85	0.58
1:O:17:SER:OG	1:O:19:ASP:OD1	2.20	0.58
7:U:46:ILE:HD11	7:U:149:GLY:HA3	1.83	0.58
9:I:40:ASN:ND2	9:I:103:VAL:O	2.34	0.58
6:T:159:SER:HB2	6:T:168:LYS:HE3	1.85	0.58
7:U:219:SER:HA	7:U:232:ILE:HD12	1.85	0.58
10:J:114:PHE:HB3	10:J:130:TYR:HB3	1.84	0.58
4:R:36:LYS:NZ	5:S:60:GLU:OE2	2.37	0.58
8:H:189:ILE:HD13	8:H:217:ALA:HB2	1.85	0.58
14:N:11:SER:HB3	14:N:181:ALA:H	1.68	0.58
10:X:136:ALA:HB2	10:X:150:VAL:HB	1.85	0.58
7:G:104:ASN:HB3	8:H:138:LYS:NZ	2.19	0.58
8:V:159:ILE:HG13	8:V:160:LYS:H	1.68	0.58
8:V:174:ILE:HD11	14:b:37:PHE:CD1	2.38	0.58
3:Q:34:THR:HG23	3:Q:47:ALA:HB2	1.85	0.58
5:S:21:LEU:HB2	5:S:24:VAL:HG22	1.85	0.58
13:M:38:GLY:O	13:M:83:SER:OG	2.22	0.58
14:N:53:GLY:N	14:N:114:ILE:O	2.35	0.58
5:S:113:VAL:HG22	5:S:145:ILE:HD12	1.86	0.58
6:T:206:ILE:HG12	6:T:207:SER:H	1.68	0.58
5:E:14:THR:HG23	6:F:21:GLN:HE22	1.69	0.58
5:E:23:GLN:HB3	5:E:138:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:38:GLY:O	13:a:83:SER:OG	2.22	0.58
1:A:167:ALA:O	2:B:61:SER:OG	2.20	0.57
6:F:159:SER:HB2	6:F:168:LYS:HE3	1.85	0.57
8:V:18:SER:HB2	8:V:30:CYS:HA	1.85	0.57
12:Z:17:ASP:OD1	12:Z:33:LYS:NZ	2.27	0.57
14:b:92:HIS:ND1	14:b:160:TYR:OH	2.35	0.57
3:C:34:THR:HG23	3:C:47:ALA:HB2	1.85	0.57
14:N:184:PHE:HD2	9:W:136:ALA:HB2	1.68	0.57
4:D:7:ILE:HD11	4:D:125:ARG:HA	1.85	0.57
12:L:138:ILE:HD12	11:Y:145:LYS:HD3	1.86	0.57
8:V:130:GLU:CD	8:V:130:GLU:H	2.12	0.57
1:A:132:THR:HG22	2:B:128:ARG:HH21	1.69	0.57
10:J:136:ALA:HB2	10:J:150:VAL:HB	1.85	0.57
1:O:132:THR:HG22	2:P:128:ARG:HH21	1.69	0.57
12:Z:191:GLU:OE1	12:Z:191:GLU:N	2.38	0.57
8:H:32:ARG:HG2	14:b:251:TYR:HE1	1.69	0.57
7:U:38:LEU:HD11	7:U:179:ILE:HD11	1.86	0.57
6:F:182:SER:O	6:F:185:GLU:N	2.34	0.57
10:J:63:GLN:NE2	10:J:67:GLU:OE1	2.33	0.57
1:O:161:ASP:OD2	1:O:162:PRO:HD2	2.05	0.57
3:Q:154:GLY:O	4:R:81:ARG:NH2	2.38	0.57
4:R:7:ILE:HD11	4:R:125:ARG:HA	1.86	0.57
12:L:206:LYS:HE2	10:X:197:GLY:HA3	1.86	0.57
10:J:216:ARG:NH1	10:J:218:ASP:OD2	2.37	0.57
9:W:156:CYS:HB2	9:W:189:TYR:HE2	1.70	0.57
14:b:10:THR:HG22	14:b:11:SER:N	2.20	0.57
1:A:161:ASP:OD2	1:A:162:PRO:HD2	2.05	0.57
4:R:219:GLU:O	4:R:223:ASN:ND2	2.38	0.57
10:X:136:ALA:C	10:X:137:TYR:HD1	2.13	0.57
14:b:53:GLY:N	14:b:114:ILE:O	2.35	0.57
5:E:113:VAL:HG22	5:E:145:ILE:HD12	1.86	0.56
8:H:17:ASP:HB2	8:H:225:GLY:HA3	1.87	0.56
12:L:191:GLU:N	12:L:191:GLU:OE1	2.38	0.56
1:O:250:ASP:HA	1:O:253:LEU:HD12	1.87	0.56
8:H:130:GLU:CD	8:H:130:GLU:H	2.13	0.56
9:I:18:THR:HB	9:I:30:ASN:HA	1.87	0.56
1:O:40:VAL:HG22	1:O:173:VAL:HG23	1.86	0.56
1:A:40:VAL:HG22	1:A:173:VAL:HG23	1.86	0.56
5:E:148:VAL:HG23	5:E:227:GLN:HG3	1.86	0.56
14:N:12:VAL:HG23	14:N:114:ILE:HD12	1.88	0.56
7:U:74:ASN:ND2	7:U:228:GLU:OE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:ASN:ND2	7:G:82:GLY:O	2.39	0.56
6:T:157:ALA:HB1	6:T:171:LEU:HD13	1.88	0.56
8:V:17:ASP:HB2	8:V:225:GLY:HA3	1.87	0.56
5:E:38:VAL:HG13	5:E:183:LEU:HD11	1.88	0.56
5:S:148:VAL:HG23	5:S:227:GLN:HG3	1.87	0.56
1:A:250:ASP:HA	1:A:253:LEU:HD12	1.88	0.56
11:K:33:ASN:HD21	11:K:54:ARG:HH22	1.53	0.56
11:Y:13:VAL:HG23	11:Y:113:TYR:HB3	1.88	0.56
2:B:106:LEU:HD11	10:J:80:GLN:HE22	1.70	0.55
9:I:156:CYS:HB2	9:I:189:TYR:HE2	1.70	0.55
10:J:136:ALA:C	10:J:137:TYR:HD1	2.13	0.55
5:S:103:TYR:HB3	13:a:115:VAL:HG13	1.88	0.55
9:W:129:SER:OG	9:W:166:ASP:OD2	2.20	0.55
14:b:12:VAL:HG23	14:b:114:ILE:HD12	1.88	0.55
4:D:219:GLU:O	4:D:223:ASN:ND2	2.38	0.55
11:K:13:VAL:HG23	11:K:113:TYR:HB3	1.88	0.55
13:M:40:VAL:HG23	13:M:83:SER:HB2	1.88	0.55
13:M:212:ARG:NH1	9:W:26:VAL:O	2.40	0.55
2:P:82:ASP:OD2	2:P:82:ASP:N	2.39	0.55
2:P:106:LEU:HD11	10:X:80:GLN:NE2	2.21	0.55
5:S:108:ASN:ND2	5:S:149:ASP:OD2	2.40	0.55
10:X:63:GLN:NE2	10:X:67:GLU:OE1	2.33	0.55
2:B:82:ASP:N	2:B:82:ASP:OD2	2.39	0.55
10:J:196:TRP:HH2	12:Z:168:GLY:HA2	1.70	0.55
14:N:6:VAL:HG23	14:N:7:VAL:HG23	1.89	0.55
4:R:63:ILE:HG21	4:R:84:VAL:HG11	1.88	0.55
3:C:41:ASP:OD2	3:C:185:LEU:N	2.38	0.55
7:G:38:LEU:HD11	7:G:179:ILE:HD11	1.86	0.55
7:G:77:ILE:HG12	7:G:229:PHE:HD1	1.72	0.55
12:L:17:ASP:OD1	12:L:33:LYS:NZ	2.27	0.55
14:N:10:THR:HG22	14:N:11:SER:N	2.20	0.55
1:O:77:ASN:HA	1:O:83:GLY:HA2	1.89	0.55
5:S:38:VAL:HG13	5:S:183:LEU:HD11	1.88	0.55
12:L:35:ILE:HD11	12:L:45:MET:HE3	1.89	0.55
12:L:168:GLY:HA2	10:X:196:TRP:HH2	1.71	0.55
13:M:66:ARG:NH2	9:W:164:PHE:O	2.40	0.55
13:a:40:VAL:HG23	13:a:83:SER:HB2	1.88	0.55
7:G:74:ASN:ND2	7:G:228:GLU:OE2	2.39	0.55
9:W:18:THR:HB	9:W:30:ASN:HA	1.87	0.55
4:D:63:ILE:HG21	4:D:84:VAL:HG11	1.88	0.55
8:H:125:TYR:C	8:H:127:PRO:HD3	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:129:SER:OG	9:I:166:ASP:OD2	2.20	0.55
5:S:184:GLN:OE1	6:T:55:LYS:NZ	2.25	0.55
7:U:150:ASP:HB2	7:U:162:LYS:HE2	1.89	0.55
14:N:251:TYR:HE1	8:V:32:ARG:HG2	1.70	0.55
7:U:34:ASN:ND2	7:U:82:GLY:O	2.39	0.55
11:Y:33:ASN:HD21	11:Y:54:ARG:NH2	2.05	0.55
5:E:108:ASN:ND2	5:E:149:ASP:OD2	2.40	0.55
14:b:6:VAL:HG23	14:b:7:VAL:HG23	1.89	0.55
7:U:45:GLY:HA2	7:U:143:PHE:CD2	2.42	0.54
6:F:13:TYR:N	7:G:23:GLN:OE1	2.27	0.54
13:M:91:THR:HG21	14:N:100:TYR:CZ	2.42	0.54
3:Q:196:LEU:HD13	3:Q:210:ILE:HB	1.89	0.54
14:b:79:LYS:HG2	14:b:84:ASP:HB2	1.90	0.54
2:B:122:THR:HG22	3:C:128:ARG:HH21	1.72	0.54
6:F:157:ALA:HB1	6:F:171:LEU:HD13	1.88	0.54
11:K:4:LEU:HD13	11:K:46:LEU:HG	1.90	0.54
11:K:13:VAL:HG11	11:K:105:ALA:HB1	1.90	0.54
3:Q:44:ILE:HD13	3:Q:214:TYR:HB3	1.88	0.54
3:C:44:ILE:HD13	3:C:214:TYR:HB3	1.88	0.54
4:D:120:HIS:CD2	5:E:135:MET:HB3	2.43	0.54
1:O:15:ILE:HA	2:P:21:GLN:HE22	1.71	0.54
2:P:229:ASP:OD1	2:P:229:ASP:N	2.39	0.54
7:U:77:ILE:HG12	7:U:229:PHE:HD1	1.72	0.54
1:A:77:ASN:HA	1:A:83:GLY:HA2	1.89	0.54
4:D:95:TYR:CD2	11:K:63:LYS:HE3	2.41	0.54
14:N:47:ASN:OD1	14:N:48:ASN:N	2.41	0.54
8:V:125:TYR:C	8:V:127:PRO:HD3	2.32	0.54
11:Y:4:LEU:HD13	11:Y:46:LEU:HG	1.89	0.54
13:a:30:TRP:CE2	14:b:108:PRO:HG3	2.43	0.54
1:O:77:ASN:HB3	1:O:241:PHE:CD2	2.42	0.54
5:S:52:ARG:NH2	5:S:218:GLU:OE2	2.39	0.54
11:Y:33:ASN:HD21	11:Y:54:ARG:HH22	1.52	0.54
11:Y:194:THR:HG22	11:Y:195:VAL:HG23	1.90	0.54
14:N:60:ASP:HB3	14:N:109:LEU:HB2	1.89	0.54
12:Z:35:ILE:HD11	12:Z:45:MET:HE3	1.89	0.54
1:A:77:ASN:HB3	1:A:241:PHE:CD2	2.42	0.54
5:E:52:ARG:NH2	5:E:218:GLU:OE2	2.38	0.54
13:M:218:ASP:HB2	13:M:239:GLN:HG2	1.90	0.54
11:Y:1:MET:HG2	11:Y:22:ILE:HG21	1.90	0.54
14:b:47:ASN:OD1	14:b:48:ASN:N	2.41	0.54
1:A:13:LEU:HD23	1:A:131:TYR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASN:HA	1:A:155:PRO:HD3	1.90	0.54
7:G:45:GLY:HA2	7:G:143:PHE:CD2	2.42	0.54
14:N:34:TYR:HE2	14:N:36:LYS:HD3	1.73	0.54
14:N:242:LEU:HD12	14:N:242:LEU:O	2.08	0.54
5:S:218:GLU:OE1	5:S:231:LYS:NZ	2.40	0.54
6:T:175:LEU:HD23	6:T:175:LEU:H	1.73	0.54
4:D:5:ARG:O	4:D:123:GLY:N	2.37	0.54
7:G:150:ASP:HB2	7:G:162:LYS:HE2	1.89	0.54
11:K:33:ASN:HD21	11:K:54:ARG:NH2	2.05	0.54
12:L:102:SER:HB3	12:L:111:MET:HG3	1.90	0.54
12:L:180:HIS:NE2	12:L:185:ASP:OD2	2.41	0.54
14:N:34:TYR:CE2	14:N:36:LYS:HD3	2.43	0.54
12:Z:180:HIS:NE2	12:Z:185:ASP:OD2	2.41	0.54
3:C:48:ASP:HA	3:C:210:ILE:HG22	1.90	0.53
8:H:122:PHE:CE1	8:H:238:VAL:HG23	2.43	0.53
2:P:44:VAL:H	2:P:213:ALA:HB3	1.73	0.53
14:b:34:TYR:CE2	14:b:36:LYS:HD3	2.43	0.53
8:H:168:ASN:HB2	8:H:172:SER:HB2	1.91	0.53
11:K:194:THR:HG22	11:K:195:VAL:HG23	1.90	0.53
14:b:34:TYR:HE2	14:b:36:LYS:HD3	1.72	0.53
3:Q:48:ASP:HA	3:Q:210:ILE:HG22	1.90	0.53
11:Y:13:VAL:HG11	11:Y:105:ALA:HB1	1.90	0.53
12:Z:102:SER:HB3	12:Z:111:MET:HG3	1.90	0.53
9:W:212:ILE:HG22	10:X:212:LYS:HB2	1.89	0.53
4:D:230:ASP:OD1	4:D:231:GLN:N	2.42	0.53
11:K:116:TYR:HB3	11:K:124:MET:SD	2.49	0.53
2:P:122:THR:HG22	3:Q:128:ARG:HH21	1.73	0.53
4:R:105:ASP:OD1	4:R:106:TYR:N	2.42	0.53
4:R:230:ASP:OD1	4:R:231:GLN:N	2.41	0.53
8:V:121:LYS:HD3	8:V:237:PHE:HB3	1.90	0.53
13:a:218:ASP:HB2	13:a:239:GLN:HG2	1.90	0.53
3:Q:73:PHE:HB3	3:Q:223:TYR:CE1	2.43	0.53
14:b:242:LEU:O	14:b:242:LEU:HD12	2.08	0.53
1:A:231:VAL:HG23	1:A:244:ILE:HB	1.90	0.53
2:B:185:GLU:O	2:B:189:HIS:ND1	2.42	0.53
12:L:26:ILE:O	10:X:190:ARG:NH1	2.39	0.53
10:X:121:ASP:CB	10:X:128:VAL:HG12	2.38	0.53
14:b:60:ASP:HB3	14:b:109:LEU:HB2	1.89	0.53
3:C:133:SER:HB3	3:C:152:PRO:HD3	1.91	0.53
4:D:105:ASP:OD1	4:D:106:TYR:N	2.42	0.53
6:F:38:ILE:HG23	6:F:177:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:79:LYS:HG2	14:N:84:ASP:HB2	1.90	0.53
1:O:39:SER:OG	1:O:51:ILE:O	2.26	0.53
1:O:61:ILE:HD12	7:U:155:GLU:HG3	1.91	0.53
4:R:5:ARG:O	4:R:123:GLY:N	2.37	0.53
1:A:61:ILE:HD12	7:G:155:GLU:HG3	1.91	0.53
3:C:167:ASN:ND2	3:C:199:SER:O	2.38	0.53
8:H:38:ASN:HB3	8:H:41:LEU:HD23	1.91	0.53
2:P:52:SER:OG	2:P:207:ASN:ND2	2.42	0.53
2:B:44:VAL:H	2:B:213:ALA:HB3	1.73	0.53
3:C:73:PHE:HB3	3:C:223:TYR:CE1	2.43	0.53
14:N:212:ILE:HD11	9:W:140:ALA:HB2	1.91	0.53
6:T:38:ILE:HG23	6:T:177:LEU:HD13	1.91	0.53
6:F:117:GLN:NE2	6:F:121:GLN:HE22	2.07	0.52
10:J:121:ASP:CB	10:J:128:VAL:HG12	2.38	0.52
1:O:13:LEU:HD23	1:O:131:TYR:O	2.08	0.52
1:O:46:ASN:HA	1:O:155:PRO:HD3	1.91	0.52
2:P:185:GLU:O	2:P:189:HIS:ND1	2.42	0.52
11:Y:116:TYR:HB3	11:Y:124:MET:SD	2.49	0.52
3:C:196:LEU:HD13	3:C:210:ILE:HB	1.89	0.52
8:V:168:ASN:HB2	8:V:172:SER:HB2	1.91	0.52
9:W:63:VAL:HG22	9:W:78:MET:HE1	1.91	0.52
10:X:216:ARG:NH1	10:X:218:ASP:OD2	2.37	0.52
13:a:93:HIS:O	13:a:97:GLN:HG3	2.10	0.52
11:K:1:MET:HG2	11:K:22:ILE:HG21	1.90	0.52
3:Q:103:GLU:OE1	11:Y:80:SER:OG	2.13	0.52
6:F:175:LEU:H	6:F:175:LEU:HD23	1.73	0.52
1:O:231:VAL:HG23	1:O:244:ILE:HB	1.90	0.52
5:S:110:LYS:O	5:S:114:GLU:HG2	2.10	0.52
7:U:188:ASN:OD1	7:U:189:VAL:N	2.41	0.52
8:V:110:LEU:HD23	8:V:115:LYS:HB3	1.91	0.52
2:B:52:SER:OG	2:B:207:ASN:ND2	2.41	0.52
5:E:110:LYS:O	5:E:114:GLU:HG2	2.10	0.52
2:P:205:GLU:OE2	2:P:224:GLN:NE2	2.43	0.52
8:V:38:ASN:HB3	8:V:41:LEU:HD23	1.91	0.52
8:V:122:PHE:CE1	8:V:238:VAL:HG23	2.43	0.52
11:Y:23:ASN:ND2	11:Y:51:ILE:HD13	2.24	0.52
14:b:225:GLN:NE2	14:b:238:GLU:OE2	2.42	0.52
2:B:48:THR:HG21	2:B:64:LYS:HB2	1.91	0.52
7:G:188:ASN:OD1	7:G:189:VAL:N	2.41	0.52
8:H:110:LEU:HD23	8:H:115:LYS:HB3	1.91	0.52
5:S:121:LEU:HD11	5:S:162:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:208:MET:HG2	5:S:209:GLU:H	1.74	0.52
6:T:117:GLN:NE2	6:T:121:GLN:HE22	2.07	0.52
11:K:23:ASN:ND2	11:K:51:ILE:HD13	2.25	0.52
12:L:31:VAL:O	12:L:175:ARG:NH1	2.38	0.52
13:M:114:HIS:ND1	13:M:150:TYR:OH	2.43	0.52
6:T:133:MET:HB2	6:T:160:PHE:HE2	1.75	0.52
12:Z:6:PHE:HE1	12:Z:139:LEU:HD13	1.74	0.52
14:b:180:TYR:CE2	14:b:184:PHE:HE1	2.28	0.52
2:B:205:GLU:OE2	2:B:224:GLN:NE2	2.42	0.52
2:B:229:ASP:OD1	2:B:229:ASP:N	2.39	0.52
5:E:73:HIS:CE1	5:E:106:ASN:HB3	2.45	0.52
5:E:208:MET:HG2	5:E:209:GLU:H	1.74	0.52
6:F:10:ASN:ND2	6:F:125:LYS:O	2.43	0.52
6:F:133:MET:HB2	6:F:160:PHE:HE2	1.75	0.52
8:H:121:LYS:HD3	8:H:237:PHE:HB3	1.90	0.52
9:I:212:ILE:HG22	10:J:212:LYS:HB2	1.90	0.52
5:S:73:HIS:CE1	5:S:106:ASN:HB3	2.45	0.52
11:Y:27:LYS:NZ	11:Y:28:LEU:O	2.27	0.52
9:I:63:VAL:HG22	9:I:78:MET:HE1	1.91	0.52
12:L:90:TYR:HD1	12:L:93:TYR:HD2	1.58	0.52
13:M:79:ILE:HG12	13:M:225:ILE:HD11	1.92	0.52
14:N:54:PHE:HZ	14:N:58:LEU:HA	1.75	0.52
1:A:89:MET:HE1	7:G:15:PHE:HE1	1.74	0.52
3:C:1:MET:HB2	6:F:123:SER:OG	2.10	0.52
13:M:48:TYR:OH	13:M:198:ASP:OD2	2.26	0.52
12:Z:200:TYR:OH	12:Z:205:GLN:N	2.38	0.52
12:L:200:TYR:OH	12:L:205:GLN:N	2.38	0.51
13:M:143:GLU:HB2	13:M:146:LYS:CB	2.39	0.51
14:N:102:ARG:CZ	14:N:109:LEU:HD23	2.40	0.51
14:N:180:TYR:CE2	14:N:184:PHE:HE1	2.28	0.51
3:Q:6:ASP:OD2	4:R:2:SER:OG	2.24	0.51
3:Q:97:TYR:OH	11:Y:68:TYR:OH	2.24	0.51
3:Q:167:ASN:ND2	3:Q:199:SER:O	2.38	0.51
13:M:185:ASN:HB3	9:W:207:LYS:NZ	2.25	0.51
13:M:212:ARG:CZ	9:W:29:LYS:HZ2	2.23	0.51
14:N:112:ASN:HB3	14:N:178:THR:OG1	2.10	0.51
13:a:113:ILE:HD13	13:a:148:VAL:HG13	1.93	0.51
1:A:15:ILE:HA	2:B:21:GLN:HE22	1.75	0.51
2:B:89:ARG:HG2	2:B:89:ARG:HH11	1.73	0.51
2:P:89:ARG:HH11	2:P:89:ARG:HG2	1.73	0.51
6:T:10:ASN:ND2	6:T:125:LYS:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:91:THR:HG21	14:b:100:TYR:CZ	2.44	0.51
14:b:112:ASN:HB3	14:b:178:THR:OG1	2.10	0.51
6:F:74:MET:HE3	6:F:78:THR:HA	1.93	0.51
13:M:113:ILE:HD13	13:M:148:VAL:HG13	1.93	0.51
3:Q:133:SER:HB3	3:Q:152:PRO:HD3	1.91	0.51
8:V:3:ILE:HG22	8:V:152:ILE:HD12	1.92	0.51
4:D:92:GLN:HG3	11:K:67:LEU:HB2	1.93	0.51
14:N:215:PHE:O	8:V:26:ILE:HD13	2.10	0.51
2:P:48:THR:HG21	2:P:64:LYS:HB2	1.91	0.51
7:G:28:TYR:CE1	7:G:156:PRO:HD2	2.45	0.51
9:I:167:LEU:HB3	13:a:214:ILE:HG23	1.93	0.51
14:N:17:TYR:CE2	14:N:19:HIS:HB2	2.45	0.51
14:N:225:GLN:NE2	14:N:238:GLU:OE2	2.42	0.51
14:b:54:PHE:HZ	14:b:58:LEU:HA	1.75	0.51
13:M:187:LEU:O	9:W:207:LYS:NZ	2.44	0.51
5:S:121:LEU:O	5:S:124:SER:OG	2.27	0.51
10:X:119:TYR:CG	10:X:128:VAL:HG11	2.46	0.51
13:a:143:GLU:HB2	13:a:146:LYS:CB	2.39	0.51
12:L:206:LYS:HE3	10:X:27:LEU:HD12	1.93	0.51
1:O:111:ASN:OD1	9:W:82:ARG:NH2	2.43	0.51
8:V:168:ASN:ND2	8:V:172:SER:O	2.43	0.51
11:Y:21:SER:HB2	11:Y:30:ASN:H	1.76	0.51
1:A:159:LYS:HD3	1:A:172:CYS:SG	2.51	0.51
8:H:19:ARG:NE	8:H:26:ILE:HG12	2.26	0.51
13:M:93:HIS:O	13:M:97:GLN:HG3	2.10	0.51
13:a:30:TRP:NE1	14:b:108:PRO:HG3	2.26	0.51
1:O:159:LYS:HD3	1:O:172:CYS:SG	2.51	0.50
3:Q:130:TYR:HB3	3:Q:132:VAL:HG12	1.93	0.50
7:U:28:TYR:CE1	7:U:156:PRO:HD2	2.45	0.50
7:U:106:HIS:HB2	8:V:137:LYS:HE2	1.92	0.50
5:E:121:LEU:HD11	5:E:162:GLY:HA3	1.92	0.50
5:E:164:ASN:N	5:E:164:ASN:OD1	2.44	0.50
10:J:63:GLN:O	10:J:67:GLU:HG2	2.10	0.50
12:L:6:PHE:HE1	12:L:139:LEU:HD13	1.74	0.50
1:O:51:ILE:HG21	1:O:216:LEU:HD22	1.94	0.50
14:b:17:TYR:CE2	14:b:19:HIS:HB2	2.45	0.50
14:b:102:ARG:CZ	14:b:109:LEU:HD23	2.40	0.50
8:H:246:THR:OG1	8:H:247:GLN:N	2.44	0.50
2:P:119:GLN:NE2	3:Q:82:ASP:HB3	2.27	0.50
3:C:37:LEU:HB2	3:C:44:ILE:HB	1.93	0.50
9:I:3:ILE:HD12	9:I:99:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:42:ASN:HB2	2:P:215:ASP:HB3	1.94	0.50
2:P:103:SER:OG	10:X:88:CYS:SG	2.68	0.50
3:Q:193:LEU:HD11	3:Q:234:GLU:HB3	1.92	0.50
10:X:63:GLN:O	10:X:67:GLU:HG2	2.10	0.50
10:X:67:GLU:HG3	11:Y:87:LYS:NZ	2.26	0.50
13:a:79:ILE:HG12	13:a:225:ILE:HD11	1.92	0.50
2:B:44:VAL:HG11	2:B:137:CYS:HB2	1.94	0.50
8:H:3:ILE:HG22	8:H:152:ILE:HD12	1.92	0.50
13:M:232:VAL:HG12	13:M:232:VAL:O	2.12	0.50
14:N:21:ILE:HG21	14:N:116:ALA:HB1	1.94	0.50
1:O:60:TYR:CG	7:U:28:TYR:HD2	2.30	0.50
6:T:133:MET:HG3	6:T:158:LEU:HD22	1.94	0.50
8:V:19:ARG:NE	8:V:26:ILE:HG12	2.26	0.50
9:W:3:ILE:HD12	9:W:99:VAL:HG22	1.94	0.50
1:A:51:ILE:HG21	1:A:216:LEU:HD22	1.94	0.50
7:G:110:PRO:HG2	7:G:113:ILE:HG12	1.92	0.50
3:Q:1:MET:HB2	6:T:123:SER:OG	2.12	0.50
7:U:99:ASN:OD1	14:b:70:ARG:NH2	2.41	0.50
8:V:19:ARG:HB3	8:V:225:GLY:HA2	1.94	0.50
12:Z:90:TYR:HD1	12:Z:93:TYR:HD2	1.58	0.50
1:A:250:ASP:HA	1:A:253:LEU:HB2	1.94	0.50
3:C:193:LEU:HD11	3:C:234:GLU:HB3	1.92	0.50
5:E:103:TYR:HB3	13:M:115:VAL:HG13	1.92	0.50
5:S:164:ASN:OD1	5:S:164:ASN:N	2.44	0.50
2:B:42:ASN:HB2	2:B:215:ASP:HB3	1.94	0.50
2:B:103:SER:OG	10:J:88:CYS:SG	2.68	0.50
11:K:21:SER:HB2	11:K:30:ASN:H	1.76	0.50
10:X:197:GLY:HA2	10:X:215:ALA:HB3	1.94	0.50
3:C:130:TYR:HB3	3:C:132:VAL:HG12	1.93	0.50
1:O:94:LEU:HG	7:U:120:LEU:HD21	1.94	0.50
2:P:139:VAL:HG22	2:P:144:TYR:HD1	1.77	0.50
13:a:48:TYR:OH	13:a:198:ASP:OD2	2.26	0.50
14:b:21:ILE:HG21	14:b:116:ALA:HB1	1.94	0.50
2:B:139:VAL:HG22	2:B:144:TYR:HD1	1.77	0.49
3:C:97:TYR:OH	11:K:68:TYR:OH	2.27	0.49
4:D:146:GLN:HG3	4:D:159:GLN:HG2	1.94	0.49
9:I:142:TYR:HD2	14:b:246:LEU:HD22	1.76	0.49
9:I:207:LYS:NZ	13:a:187:LEU:O	2.45	0.49
13:M:142:ASP:OD1	13:M:142:ASP:N	2.45	0.49
13:M:165:CYS:SG	13:M:170:SER:HA	2.52	0.49
14:N:82:LYS:HB3	14:N:126:ASN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:250:ASP:HA	1:O:253:LEU:HB2	1.94	0.49
4:R:146:GLN:HG3	4:R:159:GLN:HG2	1.94	0.49
7:U:110:PRO:HG2	7:U:113:ILE:HG12	1.92	0.49
8:V:68:ASN:HA	8:V:71:ARG:HG3	1.94	0.49
13:a:114:HIS:ND1	13:a:150:TYR:OH	2.43	0.49
13:a:165:CYS:SG	13:a:170:SER:HA	2.52	0.49
2:B:99:LEU:HD21	9:I:58:TRP:HA	1.93	0.49
3:C:159:TRP:HA	4:D:54:GLN:HA	1.94	0.49
1:O:12:HIS:NE2	3:Q:5:TYR:CG	2.79	0.49
3:Q:37:LEU:HB2	3:Q:44:ILE:HB	1.93	0.49
3:Q:41:ASP:OD2	3:Q:185:LEU:N	2.38	0.49
6:T:74:MET:HE3	6:T:78:THR:HA	1.93	0.49
13:a:36:ASN:HB3	13:a:57:LEU:HD12	1.94	0.49
2:B:119:GLN:NE2	3:C:82:ASP:HB3	2.27	0.49
4:D:67:GLU:CD	4:D:67:GLU:H	2.20	0.49
10:J:119:TYR:CG	10:J:128:VAL:HG11	2.46	0.49
10:X:47:MET:HE2	10:X:47:MET:HA	1.94	0.49
14:b:54:PHE:CZ	14:b:58:LEU:HA	2.47	0.49
3:C:72:ILE:HG12	3:C:107:VAL:HG22	1.94	0.49
6:F:133:MET:HG3	6:F:158:LEU:HD22	1.94	0.49
7:G:40:LEU:HA	7:G:165:GLY:HA2	1.94	0.49
13:M:30:TRP:NE1	14:N:108:PRO:HG3	2.27	0.49
14:N:108:PRO:HG2	14:N:110:PHE:HE1	1.78	0.49
14:N:249:ALA:HA	8:V:227:LEU:HD13	1.94	0.49
5:S:36:THR:HA	5:S:173:GLY:HA3	1.95	0.49
8:V:130:GLU:OE2	8:V:130:GLU:N	2.40	0.49
14:b:55:SER:HB2	14:b:112:ASN:HB2	1.94	0.49
1:A:39:SER:OG	1:A:51:ILE:O	2.26	0.49
5:E:109:ILE:HD12	5:E:109:ILE:H	1.78	0.49
5:E:218:GLU:OE1	5:E:231:LYS:NZ	2.40	0.49
2:P:22:ILE:HG21	2:P:152:SER:HB3	1.95	0.49
7:U:40:LEU:HA	7:U:165:GLY:HA2	1.94	0.49
12:Z:31:VAL:O	12:Z:175:ARG:NH1	2.38	0.49
3:Q:171:ALA:HB2	3:Q:199:SER:HB3	1.94	0.49
6:T:37:ALA:HB2	6:T:133:MET:SD	2.53	0.49
8:V:246:THR:OG1	8:V:247:GLN:N	2.44	0.49
13:a:232:VAL:O	13:a:232:VAL:HG12	2.12	0.49
14:N:55:SER:HB2	14:N:112:ASN:HB2	1.94	0.49
2:P:33:SER:HB2	2:P:64:LYS:HZ1	1.77	0.49
3:Q:142:LYS:NZ	11:Y:74:THR:HG21	2.27	0.49
7:U:205:ASP:O	7:U:206:HIS:ND1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:32:ARG:O	8:V:45:ARG:NH2	2.46	0.49
10:J:47:MET:HA	10:J:47:MET:HE2	1.94	0.49
10:J:197:GLY:HA2	10:J:215:ALA:HB3	1.94	0.49
11:K:59:GLU:O	11:K:63:LYS:HG2	2.12	0.49
5:S:211:LYS:HG3	5:S:213:SER:HB3	1.95	0.49
8:V:3:ILE:HD12	8:V:46:SER:HB2	1.95	0.49
1:A:13:LEU:HD21	1:A:139:LEU:HD12	1.95	0.49
1:A:122:ARG:NH2	2:B:61:SER:O	2.46	0.49
7:G:18:ASP:OD2	7:G:20:ARG:NH1	2.44	0.49
14:N:54:PHE:CZ	14:N:58:LEU:HA	2.47	0.49
7:G:205:ASP:O	7:G:206:HIS:ND1	2.46	0.49
9:I:166:ASP:OD1	9:I:167:LEU:N	2.46	0.49
11:Y:59:GLU:O	11:Y:63:LYS:HG2	2.12	0.49
12:Z:200:TYR:OH	12:Z:204:GLU:N	2.45	0.49
13:a:54:ASP:HB2	13:a:217:GLY:HA3	1.94	0.49
14:b:82:LYS:HB3	14:b:126:ASN:HB2	1.94	0.49
14:b:108:PRO:HG2	14:b:110:PHE:HE1	1.78	0.49
1:A:13:LEU:HA	1:A:24:GLN:HG3	1.94	0.48
2:B:22:ILE:HG21	2:B:152:SER:HB3	1.95	0.48
10:J:119:TYR:CD2	10:J:128:VAL:HG11	2.48	0.48
12:L:3:THR:CG2	12:L:44:THR:HG21	2.43	0.48
12:L:4:LEU:HD22	12:L:139:LEU:HD11	1.94	0.48
4:R:177:GLN:HB2	4:R:180:MET:HG3	1.95	0.48
6:T:72:ILE:HD11	6:T:85:THR:HG22	1.95	0.48
13:a:84:GLY:N	13:a:89:ILE:HD11	2.21	0.48
5:E:211:LYS:HG3	5:E:213:SER:HB3	1.95	0.48
2:P:44:VAL:HG11	2:P:137:CYS:HB2	1.94	0.48
5:S:205:ARG:HA	5:S:212:LEU:HD21	1.94	0.48
8:V:178:ASP:OD2	8:V:178:ASP:N	2.43	0.48
12:Z:4:LEU:HD22	12:Z:139:LEU:HD11	1.94	0.48
14:b:181:ALA:HB1	14:b:185:ALA:HB3	1.95	0.48
1:A:217:GLN:HG3	1:A:224:LEU:HD22	1.95	0.48
14:N:163:PHE:HB2	14:N:176:ILE:HG21	1.94	0.48
8:V:122:PHE:HE1	8:V:238:VAL:HG23	1.77	0.48
1:A:111:ASN:OD1	9:I:82:ARG:NH2	2.46	0.48
2:B:86:LEU:HD23	2:B:134:LEU:HD11	1.95	0.48
13:M:54:ASP:HB2	13:M:217:GLY:HA3	1.94	0.48
2:P:99:LEU:HD21	9:W:58:TRP:HA	1.94	0.48
3:Q:45:LEU:HD12	3:Q:73:PHE:CE2	2.48	0.48
3:Q:149:HIS:CE1	3:Q:164:ILE:HG21	2.49	0.48
8:V:157:ASP:HB3	8:V:160:LYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:163:PHE:HB2	14:b:176:ILE:HG21	1.94	0.48
6:F:6:TYR:OH	7:G:9:ASP:OD2	2.26	0.48
6:F:37:ALA:HB2	6:F:133:MET:SD	2.53	0.48
8:H:19:ARG:HB3	8:H:225:GLY:HA2	1.94	0.48
8:H:130:GLU:OE2	8:H:130:GLU:N	2.40	0.48
8:H:157:ASP:HB3	8:H:160:LYS:O	2.14	0.48
11:K:129:LYS:NZ	12:Z:209:TYR:HB2	2.28	0.48
1:O:13:LEU:HA	1:O:24:GLN:HG3	1.94	0.48
4:R:67:GLU:CD	4:R:67:GLU:H	2.20	0.48
4:D:177:GLN:HB2	4:D:180:MET:HG3	1.95	0.48
12:L:52:CYS:HB3	12:L:97:CYS:HB2	1.96	0.48
3:Q:72:ILE:HG12	3:Q:107:VAL:HG22	1.95	0.48
5:S:109:ILE:H	5:S:109:ILE:HD12	1.78	0.48
3:C:33:ILE:HA	3:C:165:GLY:HA3	1.96	0.48
8:H:122:PHE:HE1	8:H:238:VAL:HG23	1.77	0.48
14:N:181:ALA:HB1	14:N:185:ALA:HB3	1.95	0.48
2:P:86:LEU:HD23	2:P:134:LEU:HD11	1.95	0.48
7:U:163:TYR:CZ	7:U:166:ILE:HD12	2.49	0.48
10:X:119:TYR:CD2	10:X:128:VAL:HG11	2.48	0.48
11:Y:55:LEU:O	11:Y:59:GLU:HB2	2.14	0.48
13:a:99:LYS:HG3	13:a:123:ILE:HD11	1.96	0.48
12:L:113:TYR:HE1	12:L:119:LYS:HD2	1.79	0.48
12:Z:3:THR:CG2	12:Z:44:THR:HG21	2.43	0.48
3:C:123:GLN:HA	4:D:125:ARG:NH1	2.29	0.48
5:E:36:THR:HA	5:E:173:GLY:HA3	1.95	0.48
7:G:22:TYR:C	7:G:24:VAL:H	2.22	0.48
7:G:125:TYR:CE2	7:G:131:MET:HE2	2.49	0.48
8:H:68:ASN:HA	8:H:71:ARG:HG3	1.94	0.48
10:J:60:THR:HG23	11:K:122:SER:HB2	1.95	0.48
13:M:36:ASN:HB3	13:M:57:LEU:HD12	1.94	0.48
14:N:17:TYR:HB2	14:N:197:MET:O	2.14	0.48
1:O:217:GLN:HG3	1:O:224:LEU:HD22	1.95	0.48
3:Q:17:ARG:NH1	3:Q:17:ARG:HB2	2.29	0.48
3:Q:33:ILE:HA	3:Q:165:GLY:HA3	1.96	0.48
3:Q:232:ILE:O	3:Q:236:ILE:N	2.32	0.48
10:X:103:SER:O	10:X:103:SER:OG	2.31	0.48
12:Z:113:TYR:HE1	12:Z:119:LYS:HD2	1.79	0.48
5:E:193:PHE:HZ	5:E:221:ALA:HB1	1.78	0.48
7:G:163:TYR:CZ	7:G:166:ILE:HD12	2.49	0.48
11:K:76:MET:HE2	11:K:81:PHE:HA	1.96	0.48
3:Q:123:GLN:HA	4:R:125:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:109:LEU:O	14:b:109:LEU:HD12	2.14	0.48
1:A:216:LEU:HB3	1:A:224:LEU:HD21	1.96	0.47
3:C:45:LEU:HD12	3:C:73:PHE:CE2	2.48	0.47
6:F:162:ALA:O	6:F:163:ARG:HD3	2.14	0.47
8:H:3:ILE:HD12	8:H:46:SER:HB2	1.95	0.47
1:O:13:LEU:HD21	1:O:139:LEU:HD12	1.95	0.47
1:O:135:ALA:O	7:U:129:TRP:NE1	2.46	0.47
7:U:125:TYR:CE2	7:U:131:MET:HE2	2.49	0.47
3:C:17:ARG:HB2	3:C:17:ARG:NH1	2.29	0.47
4:D:178:GLU:H	4:D:178:GLU:CD	2.22	0.47
5:E:205:ARG:HA	5:E:212:LEU:HD21	1.95	0.47
10:J:101:ARG:HG3	10:J:101:ARG:HH11	1.79	0.47
13:M:153:ASP:C	13:M:155:VAL:H	2.22	0.47
14:b:92:HIS:CE1	14:b:160:TYR:HH	2.31	0.47
1:A:11:ARG:NH2	7:G:6:ALA:O	2.47	0.47
7:G:167:VAL:HG21	7:G:175:PHE:HB3	1.96	0.47
8:H:211:LEU:HD11	8:H:243:VAL:HG11	1.97	0.47
14:N:109:LEU:HD12	14:N:109:LEU:O	2.14	0.47
5:S:193:PHE:HZ	5:S:221:ALA:HB1	1.78	0.47
9:W:166:ASP:OD1	9:W:167:LEU:N	2.46	0.47
10:X:101:ARG:HG3	10:X:101:ARG:HH11	1.79	0.47
3:C:171:ALA:HB2	3:C:199:SER:HB3	1.95	0.47
7:G:226:SER:O	7:G:226:SER:OG	2.28	0.47
8:H:32:ARG:O	8:H:45:ARG:NH2	2.46	0.47
13:M:171:GLN:HB3	10:X:157:GLU:HG2	1.97	0.47
14:N:64:LEU:HD23	14:N:113:ILE:HG13	1.96	0.47
1:O:226:ALA:HB2	1:O:250:ASP:HB3	1.97	0.47
10:X:11:CYS:SG	10:X:188:LEU:HD21	2.55	0.47
14:b:10:THR:CG2	14:b:11:SER:H	2.25	0.47
10:J:11:CYS:SG	10:J:188:LEU:HD21	2.55	0.47
1:O:89:MET:HE1	7:U:15:PHE:HE1	1.79	0.47
1:O:159:LYS:HD2	1:O:174:ILE:HD13	1.97	0.47
7:U:18:ASP:OD2	7:U:20:ARG:NH1	2.44	0.47
3:C:71:HIS:CE1	3:C:104:VAL:HB	2.50	0.47
11:Y:76:MET:HE2	11:Y:81:PHE:HA	1.97	0.47
1:A:136:TYR:HA	7:G:129:TRP:CE2	2.48	0.47
2:B:96:ARG:HG3	2:B:96:ARG:HH11	1.80	0.47
2:B:203:LEU:O	2:B:205:GLU:N	2.45	0.47
3:C:83:ALA:O	3:C:87:ILE:HG12	2.15	0.47
5:E:91:TYR:CD2	5:E:119:LEU:HD22	2.50	0.47
5:E:121:LEU:O	5:E:124:SER:OG	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:18:ARG:NH2	6:F:23:GLU:OE1	2.48	0.47
8:H:28:ASN:N	8:H:28:ASN:HD22	2.13	0.47
8:H:45:ARG:HB2	8:H:52:SER:HB2	1.96	0.47
2:P:96:ARG:HG3	2:P:96:ARG:HH11	1.80	0.47
3:Q:83:ALA:O	3:Q:87:ILE:HG12	2.15	0.47
5:S:91:TYR:CD2	5:S:119:LEU:HD22	2.50	0.47
8:V:45:ARG:HB2	8:V:52:SER:HB2	1.96	0.47
14:b:17:TYR:HB2	14:b:197:MET:O	2.14	0.47
14:b:64:LEU:HD23	14:b:113:ILE:HG13	1.96	0.47
6:F:72:ILE:HD11	6:F:85:THR:HG22	1.95	0.47
10:J:40:LYS:HD2	12:Z:208:GLN:HE22	1.79	0.47
11:K:55:LEU:O	11:K:59:GLU:HB2	2.14	0.47
13:M:225:ILE:HG12	13:M:230:ILE:HG22	1.97	0.47
8:V:28:ASN:ND2	8:V:28:ASN:O	2.45	0.47
13:a:59:LEU:HD13	13:a:64:TYR:CE2	2.50	0.47
13:a:153:ASP:C	13:a:155:VAL:H	2.22	0.47
14:b:108:PRO:HG2	14:b:110:PHE:CE1	2.50	0.47
8:H:71:ARG:HH21	8:H:128:LEU:HD13	1.80	0.47
12:L:111:MET:HE1	12:L:124:ASN:O	2.15	0.47
13:M:212:ARG:NE	9:W:29:LYS:HZ2	2.13	0.47
4:R:158:ALA:O	5:S:58:LEU:HD13	2.14	0.47
5:S:93:ARG:HG2	12:Z:68:LEU:HD21	1.97	0.47
6:T:81:ALA:O	6:T:85:THR:HG23	2.15	0.47
1:A:60:TYR:CG	7:G:28:TYR:HD2	2.32	0.47
1:A:99:LYS:O	1:A:103:GLU:HG2	2.15	0.47
1:A:159:LYS:HD2	1:A:174:ILE:HD13	1.97	0.47
3:C:149:HIS:CE1	3:C:164:ILE:HG21	2.49	0.47
8:H:178:ASP:OD2	8:H:178:ASP:N	2.43	0.47
10:J:40:LYS:HD2	12:Z:208:GLN:NE2	2.30	0.47
1:O:99:LYS:O	1:O:103:GLU:HG2	2.15	0.47
1:O:216:LEU:HB3	1:O:224:LEU:HD21	1.96	0.47
7:U:167:VAL:HG21	7:U:175:PHE:HB3	1.96	0.47
12:Z:52:CYS:HB3	12:Z:97:CYS:HB2	1.96	0.47
2:B:95:ILE:HG13	9:I:65:LEU:HB2	1.96	0.46
8:H:28:ASN:O	8:H:28:ASN:ND2	2.45	0.46
8:H:168:ASN:ND2	8:H:172:SER:O	2.43	0.46
9:I:187:ARG:HB3	9:I:188:PRO:HD3	1.97	0.46
10:J:43:LYS:HB3	10:J:55:LEU:O	2.15	0.46
12:L:148:ASN:OD1	12:L:151:GLN:HG2	2.15	0.46
13:M:99:LYS:HG3	13:M:123:ILE:HD11	1.96	0.46
6:T:18:ARG:NH2	6:T:23:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:224:SER:O	6:T:228:LEU:N	2.35	0.46
12:Z:51:ASP:O	12:Z:55:TRP:HD1	1.98	0.46
12:Z:111:MET:HE1	12:Z:124:ASN:O	2.15	0.46
1:A:182:ILE:HG13	2:B:56:LEU:HD12	1.96	0.46
5:E:88:LEU:HD21	5:E:139:PHE:CD2	2.50	0.46
2:P:36:LEU:N	2:P:47:ALA:O	2.47	0.46
3:Q:71:HIS:CE1	3:Q:104:VAL:HB	2.50	0.46
3:Q:233:GLU:OE1	3:Q:233:GLU:N	2.40	0.46
8:V:71:ARG:HH21	8:V:128:LEU:HD13	1.80	0.46
13:a:153:ASP:O	13:a:155:VAL:N	2.49	0.46
13:a:225:ILE:HG12	13:a:230:ILE:HG22	1.97	0.46
3:C:232:ILE:O	3:C:236:ILE:N	2.32	0.46
4:D:60:GLU:OE1	4:D:61:LYS:NZ	2.45	0.46
7:G:46:ILE:HD12	7:G:143:PHE:HD2	1.81	0.46
10:J:148:ASP:OD2	10:J:148:ASP:N	2.47	0.46
11:K:20:TYR:HD1	11:K:28:LEU:HD22	1.81	0.46
13:M:102:LEU:O	13:M:106:GLU:HG3	2.16	0.46
14:N:108:PRO:HG2	14:N:110:PHE:CE1	2.50	0.46
1:O:122:ARG:NH2	2:P:61:SER:O	2.48	0.46
2:P:95:ILE:HG13	9:W:65:LEU:HB2	1.97	0.46
6:T:11:ILE:HD12	7:U:132:ARG:HB2	1.96	0.46
13:a:142:ASP:OD1	13:a:142:ASP:N	2.45	0.46
14:b:211:ARG:HH21	14:b:241:ILE:HD11	1.80	0.46
11:K:56:GLN:HG3	12:L:88:TYR:CD2	2.51	0.46
12:L:51:ASP:O	12:L:55:TRP:HD1	1.98	0.46
13:M:59:LEU:HD13	13:M:64:TYR:CE2	2.50	0.46
14:N:211:ARG:HH21	14:N:241:ILE:HD11	1.80	0.46
1:O:131:TYR:CD1	1:O:131:TYR:N	2.83	0.46
1:O:248:GLU:OE2	1:O:248:GLU:N	2.49	0.46
8:V:16:CYS:SG	8:V:33:LYS:HB2	2.55	0.46
8:V:211:LEU:HD11	8:V:243:VAL:HG11	1.97	0.46
12:Z:148:ASN:OD1	12:Z:151:GLN:HG2	2.15	0.46
7:G:35:ASN:HB2	7:G:68:ARG:NH1	2.30	0.46
8:V:9:ASP:OD1	8:V:9:ASP:N	2.46	0.46
8:V:54:LYS:HZ2	9:W:84:THR:CB	2.28	0.46
10:X:69:LEU:HD21	10:X:93:LEU:HD13	1.97	0.46
11:Y:39:ILE:HB	11:Y:43:LYS:HB2	1.98	0.46
1:A:220:LEU:HD12	1:A:222:PHE:CE1	2.51	0.46
2:B:33:SER:HB2	2:B:64:LYS:HZ1	1.80	0.46
2:B:86:LEU:HA	2:B:86:LEU:HD12	1.82	0.46
6:F:81:ALA:O	6:F:85:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:220:LEU:HD12	1:O:222:PHE:CE1	2.51	0.46
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.97	0.46
10:X:43:LYS:HB3	10:X:55:LEU:O	2.15	0.46
14:b:165:ASP:OD1	14:b:166:MET:N	2.48	0.46
7:G:87:ALA:O	7:G:91:ILE:HG12	2.16	0.46
8:H:16:CYS:SG	8:H:33:LYS:HB2	2.55	0.46
12:L:137:SER:OG	11:Y:138:LEU:O	2.22	0.46
12:L:200:TYR:OH	12:L:204:GLU:N	2.45	0.46
2:B:36:LEU:N	2:B:47:ALA:O	2.47	0.46
3:C:233:GLU:OE1	3:C:233:GLU:N	2.40	0.46
7:G:190:ARG:HD2	7:G:190:ARG:HA	1.81	0.46
8:H:26:ILE:HD13	14:b:215:PHE:O	2.16	0.46
6:T:162:ALA:O	6:T:163:ARG:HD3	2.15	0.46
8:V:139:ILE:HG21	8:V:167:VAL:HG11	1.98	0.46
13:a:102:LEU:O	13:a:106:GLU:HG3	2.16	0.46
9:I:37:ILE:HB	9:I:41:ILE:HG13	1.98	0.46
10:J:69:LEU:HD21	10:J:93:LEU:HD13	1.97	0.46
12:Z:3:THR:O	12:Z:4:LEU:HD23	2.16	0.46
1:A:226:ALA:HB2	1:A:250:ASP:HB3	1.97	0.46
1:A:248:GLU:OE2	1:A:248:GLU:N	2.48	0.46
5:E:184:GLN:OE1	6:F:55:LYS:NZ	2.35	0.46
8:H:9:ASP:OD1	8:H:9:ASP:N	2.46	0.46
9:I:215:GLU:OE1	10:J:209:ILE:HG13	2.16	0.46
13:M:223:TYR:HA	13:M:231:ASN:O	2.16	0.46
3:Q:160:PHE:CZ	4:R:55:ASN:HB3	2.50	0.46
4:R:178:GLU:CD	4:R:178:GLU:H	2.22	0.46
5:S:51:GLU:CD	5:S:208:MET:HG3	2.41	0.46
7:U:35:ASN:HB2	7:U:68:ARG:NH1	2.30	0.46
7:U:87:ALA:O	7:U:91:ILE:HG12	2.16	0.46
14:b:119:ASN:N	14:b:158:ASP:O	2.41	0.46
1:A:131:TYR:CD1	1:A:131:TYR:N	2.83	0.45
8:H:161:LYS:HA	8:H:161:LYS:HD3	1.70	0.45
10:J:121:ASP:HB3	10:J:125:GLU:HB3	1.98	0.45
1:O:12:HIS:CE1	3:Q:5:TYR:HB3	2.51	0.45
7:U:46:ILE:HD12	7:U:143:PHE:HD2	1.80	0.45
6:F:110:ARG:NH2	14:N:78:GLU:HB3	2.32	0.45
10:J:114:PHE:HA	10:J:131:GLU:O	2.17	0.45
13:M:180:ARG:NH2	13:M:198:ASP:OD1	2.31	0.45
14:N:5:PRO:HD3	14:N:110:PHE:CD2	2.52	0.45
14:N:248:SER:HB3	8:V:30:CYS:SG	2.57	0.45
3:Q:159:TRP:HA	4:R:54:GLN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:88:LEU:HD21	5:S:139:PHE:CD2	2.50	0.45
9:W:80:VAL:HG21	9:W:111:TYR:CG	2.51	0.45
14:b:11:SER:HB3	14:b:180:TYR:H	1.81	0.45
5:E:51:GLU:CD	5:E:208:MET:HG3	2.41	0.45
9:I:136:ALA:HB2	14:b:184:PHE:CD2	2.47	0.45
14:N:194:LYS:O	14:N:197:MET:HG3	2.16	0.45
7:U:22:TYR:C	7:U:24:VAL:H	2.22	0.45
10:X:76:TYR:O	10:X:80:GLN:HB2	2.16	0.45
2:B:168:GLN:OE1	2:B:168:GLN:HA	2.17	0.45
3:C:6:ASP:OD1	3:C:7:SER:N	2.48	0.45
6:F:15:PRO:O	7:G:29:LYS:NZ	2.35	0.45
14:N:11:SER:HB3	14:N:180:TYR:H	1.82	0.45
14:N:92:HIS:ND1	14:N:160:TYR:OH	2.35	0.45
3:Q:6:ASP:OD1	3:Q:7:SER:N	2.49	0.45
7:U:190:ARG:HA	7:U:190:ARG:HD2	1.81	0.45
8:V:28:ASN:N	8:V:28:ASN:HD22	2.13	0.45
12:Z:34:ILE:HG23	12:Z:42:LEU:HD13	1.98	0.45
14:b:5:PRO:HD3	14:b:110:PHE:CD2	2.52	0.45
2:B:139:VAL:HG22	2:B:144:TYR:CD1	2.52	0.45
8:H:190:GLN:OE1	8:H:190:GLN:HA	2.16	0.45
11:K:166:GLU:OE1	12:Z:137:SER:HA	2.16	0.45
13:M:178:ASP:OD2	10:X:190:ARG:NE	2.48	0.45
9:W:37:ILE:HB	9:W:41:ILE:HG13	1.98	0.45
7:G:238:THR:OG1	7:G:239:PRO:HD3	2.17	0.45
8:H:18:SER:OG	8:H:227:LEU:O	2.32	0.45
11:K:39:ILE:HB	11:K:43:LYS:HB2	1.98	0.45
10:X:114:PHE:HA	10:X:131:GLU:O	2.16	0.45
1:A:60:TYR:CD1	7:G:28:TYR:HD2	2.35	0.45
7:G:236:ILE:C	7:G:239:PRO:HD2	2.42	0.45
8:H:138:LYS:HE2	8:H:138:LYS:HA	1.99	0.45
10:J:216:ARG:HH12	12:Z:192:ASP:HB3	1.82	0.45
13:M:30:TRP:CE2	14:N:108:PRO:HG3	2.52	0.45
14:N:165:ASP:OD1	14:N:166:MET:N	2.48	0.45
2:P:168:GLN:HA	2:P:168:GLN:OE1	2.17	0.45
9:W:137:VAL:CG1	9:W:158:ALA:HA	2.47	0.45
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.99	0.45
11:Y:20:TYR:HD1	11:Y:28:LEU:HD22	1.81	0.45
14:b:12:VAL:HG22	14:b:178:THR:HG22	1.99	0.45
12:L:208:GLN:NE2	10:X:40:LYS:HD2	2.32	0.45
2:P:203:LEU:O	2:P:205:GLU:N	2.45	0.45
3:Q:142:LYS:HZ3	11:Y:74:THR:HG21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:238:THR:OG1	7:U:239:PRO:HD3	2.17	0.45
9:W:178:ILE:HG22	9:W:178:ILE:O	2.17	0.45
10:X:115:LYS:HB3	10:X:131:GLU:HB2	1.99	0.45
10:X:148:ASP:OD2	10:X:148:ASP:N	2.47	0.45
10:X:172:ASP:OD1	10:X:172:ASP:N	2.48	0.45
11:Y:87:LYS:HB2	11:Y:87:LYS:HE2	1.68	0.45
12:Z:11:GLY:HA3	12:Z:178:HIS:HE1	1.82	0.45
13:a:223:TYR:HA	13:a:231:ASN:O	2.16	0.45
14:b:102:ARG:HB3	14:b:107:ASP:O	2.17	0.45
3:C:89:GLN:HG2	3:C:117:ILE:HD13	1.99	0.45
4:D:103:PRO:HB2	4:D:105:ASP:OD1	2.17	0.45
10:J:76:TYR:O	10:J:80:GLN:HB2	2.17	0.45
12:L:3:THR:O	12:L:4:LEU:HD23	2.16	0.45
12:L:34:ILE:HG23	12:L:42:LEU:HD13	1.99	0.45
14:N:5:PRO:HB2	14:N:8:THR:HG22	1.99	0.45
1:O:169:TYR:CD1	2:P:57:ILE:HG13	2.52	0.45
3:Q:89:GLN:HG2	3:Q:117:ILE:HD13	1.99	0.45
3:Q:227:LEU:HD23	3:Q:227:LEU:H	1.82	0.45
5:S:148:VAL:HG21	5:S:227:GLN:HA	1.99	0.45
8:V:38:ASN:HD21	8:V:129:VAL:HB	1.82	0.45
10:X:121:ASP:HB3	10:X:125:GLU:HB3	1.98	0.45
12:Z:63:ILE:HG12	12:Z:74:ILE:HD13	1.99	0.45
12:Z:88:TYR:CZ	12:Z:91:LYS:HD2	2.52	0.45
4:D:79:ASP:HB3	4:D:127:PHE:HD1	1.82	0.45
5:E:41:CYS:O	5:E:187:TYR:OH	2.31	0.45
8:H:139:ILE:HG21	8:H:167:VAL:HG11	1.98	0.45
9:I:80:VAL:HG21	9:I:111:TYR:CG	2.51	0.45
12:L:88:TYR:CZ	12:L:91:LYS:HD2	2.52	0.45
14:N:119:ASN:N	14:N:158:ASP:O	2.41	0.45
4:R:45:VAL:HG11	4:R:61:LYS:HB3	1.98	0.45
10:X:169:LYS:HD2	10:X:169:LYS:HA	1.75	0.45
11:Y:53:ASP:OD1	12:Z:91:LYS:NZ	2.50	0.45
4:D:45:VAL:HG11	4:D:61:LYS:HB3	1.98	0.44
12:L:11:GLY:HA3	12:L:178:HIS:HE1	1.82	0.44
13:M:39:THR:HG22	13:M:216:THR:HG23	2.00	0.44
7:U:104:ASN:HB3	8:V:138:LYS:HZ1	1.81	0.44
7:U:197:TYR:OH	7:U:237:LEU:HD12	2.17	0.44
8:V:138:LYS:HE2	8:V:138:LYS:HA	1.99	0.44
14:b:165:ASP:HB3	14:b:169:THR:HB	1.99	0.44
1:A:47:CYS:HA	1:A:235:SER:HA	1.99	0.44
5:E:148:VAL:HG21	5:E:227:GLN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:137:TYR:CE2	6:F:216:LYS:HA	2.52	0.44
9:I:137:VAL:CG1	9:I:158:ALA:HA	2.47	0.44
9:I:204:ILE:O	9:I:207:LYS:HG2	2.18	0.44
14:N:241:ILE:O	14:N:243:PRO:HD2	2.17	0.44
3:Q:40:LYS:HD2	3:Q:182:ASP:OD1	2.17	0.44
8:V:161:LYS:HA	8:V:161:LYS:HD3	1.70	0.44
8:V:190:GLN:OE1	8:V:190:GLN:HA	2.16	0.44
14:b:194:LYS:O	14:b:197:MET:HG3	2.16	0.44
3:C:40:LYS:HD2	3:C:182:ASP:OD1	2.17	0.44
9:I:19:ARG:O	9:I:33:LYS:NZ	2.50	0.44
10:J:47:MET:HG3	10:J:89:PHE:CZ	2.52	0.44
11:K:11:ASN:OD1	11:K:11:ASN:N	2.51	0.44
11:K:179:GLU:OE2	11:K:181:ARG:NH2	2.51	0.44
6:T:137:TYR:CE2	6:T:216:LYS:HA	2.52	0.44
8:V:110:LEU:H	8:V:115:LYS:NZ	2.15	0.44
10:X:162:MET:HB2	10:X:162:MET:HE2	1.75	0.44
11:Y:53:ASP:OD1	12:Z:88:TYR:OH	2.22	0.44
11:Y:56:GLN:HG3	12:Z:88:TYR:CD2	2.53	0.44
1:A:94:LEU:HG	7:G:120:LEU:HD21	2.00	0.44
3:C:21:VAL:HG11	3:C:153:SER:HB3	2.00	0.44
3:C:80:ASN:O	3:C:80:ASN:ND2	2.50	0.44
7:G:221:ILE:HG23	7:G:221:ILE:O	2.18	0.44
11:K:87:LYS:HB2	11:K:87:LYS:HE2	1.68	0.44
13:M:153:ASP:O	13:M:155:VAL:N	2.48	0.44
1:A:109:TYR:HB2	8:H:61:HIS:HB2	1.99	0.44
3:C:227:LEU:HD23	3:C:227:LEU:H	1.82	0.44
6:F:30:LYS:HA	6:F:161:GLY:HA2	2.00	0.44
6:F:133:MET:HE3	6:F:160:PHE:CE2	2.53	0.44
8:H:110:LEU:H	8:H:115:LYS:NZ	2.15	0.44
10:J:169:LYS:HD2	10:J:169:LYS:HA	1.74	0.44
12:L:63:ILE:HG12	12:L:74:ILE:HD13	1.99	0.44
14:N:10:THR:CG2	14:N:11:SER:H	2.25	0.44
6:T:133:MET:HE3	6:T:160:PHE:CE2	2.53	0.44
9:W:204:ILE:O	9:W:207:LYS:HG2	2.18	0.44
10:X:47:MET:HG3	10:X:89:PHE:CZ	2.52	0.44
10:X:115:LYS:HE2	10:X:133:TYR:HD2	1.83	0.44
10:X:151:VAL:HG11	10:X:159:LEU:HB3	1.99	0.44
4:D:45:VAL:HG21	4:D:61:LYS:HB2	2.00	0.44
6:F:22:VAL:HG12	6:F:127:ALA:HB2	1.99	0.44
6:F:121:GLN:HG2	7:G:125:TYR:HE2	1.82	0.44
8:H:38:ASN:HD21	8:H:129:VAL:HB	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:113:TYR:CE1	12:L:115:ASP:HB2	2.53	0.44
5:S:41:CYS:O	5:S:187:TYR:OH	2.31	0.44
7:U:77:ILE:HG12	7:U:229:PHE:CD1	2.53	0.44
7:U:236:ILE:C	7:U:239:PRO:HD2	2.42	0.44
7:G:197:TYR:OH	7:G:237:LEU:HD12	2.17	0.44
14:N:12:VAL:HG22	14:N:178:THR:HG22	1.99	0.44
14:N:99:PHE:CD2	14:N:166:MET:HA	2.53	0.44
5:S:202:THR:HG21	5:S:245:PRO:HG2	2.00	0.44
10:X:60:THR:HG23	11:Y:122:SER:HB2	2.00	0.44
11:Y:179:GLU:OE2	11:Y:181:ARG:NH2	2.51	0.44
12:Z:113:TYR:CE1	12:Z:115:ASP:HB2	2.53	0.44
14:b:5:PRO:HB2	14:b:8:THR:HG22	1.99	0.44
14:b:241:ILE:O	14:b:243:PRO:HD2	2.17	0.44
3:C:73:PHE:HE1	3:C:215:LEU:HG	1.83	0.44
5:E:42:VAL:HG23	5:E:44:ASP:H	1.83	0.44
7:G:187:ILE:HG22	7:G:188:ASN:O	2.18	0.44
10:J:151:VAL:HG11	10:J:159:LEU:HB3	1.99	0.44
12:L:137:SER:O	11:Y:142:ILE:HD11	2.18	0.44
13:M:84:GLY:N	13:M:89:ILE:HD11	2.21	0.44
4:R:95:TYR:CD2	11:Y:63:LYS:HE3	2.53	0.44
5:S:90:ASP:OD1	12:Z:69:ARG:HD3	2.17	0.44
2:B:90:ALA:HA	2:B:114:ILE:HD11	2.00	0.44
10:J:30:GLY:HA2	10:J:36:THR:HA	2.00	0.44
10:J:115:LYS:HB3	10:J:131:GLU:HB2	1.99	0.44
8:V:218:MET:HE3	8:V:225:GLY:N	2.33	0.44
9:W:38:SER:OG	9:W:41:ILE:HG12	2.18	0.44
2:B:188:ILE:O	2:B:192:ILE:HG12	2.18	0.43
6:F:224:SER:O	6:F:228:LEU:N	2.35	0.43
9:I:38:SER:OG	9:I:41:ILE:HG12	2.18	0.43
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.99	0.43
14:N:102:ARG:HB3	14:N:107:ASP:O	2.17	0.43
14:N:165:ASP:HB3	14:N:169:THR:HB	1.99	0.43
1:O:47:CYS:HA	1:O:235:SER:HA	1.99	0.43
4:R:79:ASP:HB3	4:R:127:PHE:HD1	1.82	0.43
4:R:228:LEU:O	4:R:231:GLN:NE2	2.44	0.43
7:U:139:ILE:HD11	7:U:168:ILE:HG12	2.00	0.43
11:Y:11:ASN:N	11:Y:11:ASN:OD1	2.50	0.43
11:Y:154:ASP:OD1	11:Y:154:ASP:N	2.51	0.43
13:a:39:THR:HG22	13:a:216:THR:HG23	1.99	0.43
14:b:99:PHE:CD2	14:b:166:MET:HA	2.53	0.43
8:H:20:THR:HB	8:H:28:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:178:ILE:HG22	9:I:178:ILE:O	2.17	0.43
10:J:172:ASP:OD1	10:J:172:ASP:N	2.48	0.43
13:M:29:ARG:HA	13:M:29:ARG:HD2	1.78	0.43
5:S:42:VAL:HG23	5:S:44:ASP:H	1.83	0.43
6:T:30:LYS:HA	6:T:161:GLY:HA2	2.00	0.43
8:V:20:THR:HB	8:V:28:ASN:HD21	1.83	0.43
12:Z:67:GLU:HG2	12:Z:73:LYS:HA	2.00	0.43
1:A:54:LYS:HG3	1:A:230:GLU:HG2	2.01	0.43
2:B:33:SER:HB2	2:B:64:LYS:NZ	2.33	0.43
10:J:162:MET:HE2	10:J:162:MET:HB2	1.75	0.43
2:P:139:VAL:HG22	2:P:144:TYR:CD1	2.52	0.43
3:Q:21:VAL:HG11	3:Q:153:SER:HB3	2.00	0.43
4:R:103:PRO:HB2	4:R:105:ASP:OD1	2.17	0.43
8:V:40:ASN:ND2	8:V:156:TYR:O	2.51	0.43
8:V:52:SER:O	8:V:56:ILE:HG12	2.19	0.43
3:C:224:GLN:HG2	3:C:225:LYS:N	2.32	0.43
7:G:32:ASN:HD21	7:G:172:LYS:HE3	1.84	0.43
2:P:188:ILE:O	2:P:192:ILE:HG12	2.18	0.43
6:T:134:ILE:HB	6:T:144:PHE:HB2	2.00	0.43
9:W:3:ILE:HD11	9:W:127:LEU:HD12	2.01	0.43
2:B:134:LEU:C	2:B:135:LEU:HD12	2.43	0.43
7:G:139:ILE:HD11	7:G:168:ILE:HG12	2.00	0.43
9:I:102:GLY:HA2	9:I:178:ILE:HG21	2.01	0.43
10:J:115:LYS:HE2	10:J:133:TYR:HD2	1.83	0.43
14:N:216:ARG:HA	14:N:216:ARG:HD3	1.76	0.43
2:P:90:ALA:HA	2:P:114:ILE:HD11	2.00	0.43
13:a:180:ARG:NH2	13:a:198:ASP:OD1	2.31	0.43
1:A:216:LEU:O	1:A:220:LEU:HD23	2.19	0.43
3:C:143:ASP:OD1	3:C:143:ASP:N	2.51	0.43
5:E:225:SER:OG	5:E:226:ASP:N	2.52	0.43
6:F:121:GLN:HB3	7:G:131:MET:CE	2.49	0.43
6:F:134:ILE:HB	6:F:144:PHE:HB2	2.00	0.43
7:G:36:THR:O	7:G:68:ARG:NH2	2.50	0.43
2:P:33:SER:HB2	2:P:64:LYS:NZ	2.32	0.43
3:Q:193:LEU:HD13	3:Q:235:LEU:HD23	2.01	0.43
3:Q:209:LYS:HD2	3:Q:209:LYS:HA	1.78	0.43
3:Q:224:GLN:HG2	3:Q:225:LYS:N	2.33	0.43
4:R:45:VAL:HG21	4:R:61:LYS:HB2	2.00	0.43
3:C:175:LEU:HA	3:C:175:LEU:HD23	1.86	0.43
6:F:121:GLN:HB3	7:G:131:MET:HE1	2.00	0.43
3:Q:41:ASP:O	3:Q:216:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:143:ASP:OD1	3:Q:143:ASP:N	2.51	0.43
3:Q:215:LEU:HD23	3:Q:223:TYR:HD1	1.84	0.43
3:Q:238:LEU:HD12	3:Q:241:GLN:NE2	2.34	0.43
6:T:22:VAL:HG12	6:T:127:ALA:HB2	1.99	0.43
7:U:187:ILE:HG22	7:U:188:ASN:O	2.18	0.43
7:U:221:ILE:HG23	7:U:221:ILE:O	2.18	0.43
8:V:115:LYS:HB3	8:V:115:LYS:HE2	1.92	0.43
10:X:55:LEU:HD11	10:X:65:LEU:HD23	2.01	0.43
14:b:175:TYR:HB2	14:b:189:LEU:HD13	2.01	0.43
14:b:216:ARG:HA	14:b:216:ARG:HD3	1.76	0.43
3:C:118:LYS:HD2	3:C:151:ASP:O	2.19	0.43
6:F:43:TYR:CD1	6:F:215:GLY:HA3	2.53	0.43
2:P:70:GLU:CD	2:P:70:GLU:H	2.26	0.43
2:P:134:LEU:C	2:P:135:LEU:HD12	2.43	0.43
3:Q:37:LEU:HD23	3:Q:37:LEU:HA	1.91	0.43
4:R:201:SER:HB2	4:R:222:ILE:HG22	2.01	0.43
6:T:43:TYR:CD1	6:T:215:GLY:HA3	2.53	0.43
10:X:67:GLU:HG3	11:Y:87:LYS:HZ2	1.84	0.43
12:Z:90:TYR:HD1	12:Z:93:TYR:CD2	2.37	0.43
12:Z:192:ASP:HA	12:Z:194:PHE:CE1	2.54	0.43
1:A:194:LYS:HA	1:A:194:LYS:HD3	1.78	0.43
3:C:107:VAL:HG21	3:C:138:GLY:HA3	2.01	0.43
4:D:201:SER:HB2	4:D:222:ILE:HG22	2.01	0.43
6:F:63:ILE:HG23	6:F:220:TRP:HZ2	1.84	0.43
12:L:192:ASP:HA	12:L:194:PHE:CE1	2.54	0.43
5:S:149:ASP:OD1	5:S:149:ASP:N	2.52	0.43
7:U:32:ASN:HD21	7:U:172:LYS:HE3	1.84	0.43
8:V:140:ILE:O	8:V:144:ASN:HB2	2.19	0.43
8:V:159:ILE:HG13	8:V:160:LYS:N	2.33	0.43
10:X:30:GLY:HA2	10:X:36:THR:HA	2.00	0.43
5:E:192:THR:HG23	5:E:195:GLN:H	1.84	0.43
5:E:202:THR:HG21	5:E:245:PRO:HG2	2.00	0.43
6:F:82:LYS:HE2	6:F:82:LYS:HB2	1.89	0.43
8:H:52:SER:O	8:H:56:ILE:HG12	2.19	0.43
8:H:218:MET:HE3	8:H:225:GLY:N	2.33	0.43
7:U:36:THR:O	7:U:68:ARG:NH2	2.50	0.43
7:U:193:ILE:HD11	7:U:220:TRP:HZ3	1.84	0.43
9:W:182:SER:OG	9:W:183:TYR:N	2.52	0.43
7:G:131:MET:HE3	7:G:131:MET:HA	2.01	0.42
7:G:200:ILE:O	7:G:204:ASP:HB3	2.19	0.42
8:H:193:LEU:HD13	8:H:213:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:194:LYS:HA	1:O:194:LYS:HD3	1.78	0.42
3:Q:73:PHE:HE1	3:Q:215:LEU:HG	1.83	0.42
5:S:13:ASN:HB3	6:T:126:ARG:HB3	1.99	0.42
10:X:29:LEU:O	10:X:37:VAL:HG22	2.19	0.42
14:b:170:ASN:OD1	14:b:170:ASN:N	2.52	0.42
1:A:121:CYS:HB3	1:A:146:ILE:HD12	2.00	0.42
2:B:70:GLU:CD	2:B:70:GLU:H	2.26	0.42
3:C:196:LEU:O	3:C:200:THR:HG22	2.19	0.42
3:C:238:LEU:HD12	3:C:241:GLN:NE2	2.34	0.42
6:F:11:ILE:HD12	7:G:132:ARG:HB2	2.00	0.42
6:F:93:LEU:HD12	13:M:102:LEU:HD13	2.00	0.42
8:H:140:ILE:O	8:H:144:ASN:HB2	2.19	0.42
9:I:28:ASP:OD1	9:I:28:ASP:N	2.50	0.42
14:N:16:LYS:HB3	14:N:21:ILE:HD13	2.01	0.42
14:N:75:ASN:C	14:N:75:ASN:HD22	2.27	0.42
1:O:216:LEU:O	1:O:220:LEU:HD23	2.19	0.42
2:P:42:ASN:OD1	2:P:42:ASN:N	2.52	0.42
3:Q:111:VAL:HG22	3:Q:136:ILE:HD12	2.02	0.42
3:Q:196:LEU:O	3:Q:200:THR:HG22	2.19	0.42
8:V:38:ASN:HD21	8:V:129:VAL:CG1	2.32	0.42
10:X:188:LEU:HD13	10:X:195:GLY:HA2	2.00	0.42
1:A:200:THR:HB	1:A:203:GLU:HB2	2.01	0.42
3:C:41:ASP:O	3:C:216:THR:HA	2.18	0.42
8:H:3:ILE:HD13	8:H:44:CYS:HB3	2.01	0.42
10:J:188:LEU:HD13	10:J:195:GLY:HA2	2.00	0.42
1:O:200:THR:HB	1:O:203:GLU:HB2	2.01	0.42
2:P:45:ILE:HD11	2:P:184:ILE:HG13	2.01	0.42
5:S:225:SER:OG	5:S:226:ASP:N	2.52	0.42
6:T:159:SER:HB3	6:T:164:SER:HB2	2.02	0.42
5:E:205:ARG:NH1	5:E:244:LEU:HD12	2.35	0.42
7:G:193:ILE:HD11	7:G:220:TRP:HZ3	1.85	0.42
9:I:3:ILE:HD11	9:I:127:LEU:HD12	2.01	0.42
10:J:29:LEU:O	10:J:37:VAL:HG22	2.19	0.42
14:N:170:ASN:OD1	14:N:170:ASN:N	2.52	0.42
14:N:210:LEU:HD13	14:N:224:ILE:HG13	2.02	0.42
1:O:54:LYS:HG3	1:O:230:GLU:HG2	2.01	0.42
3:Q:80:ASN:O	3:Q:80:ASN:ND2	2.50	0.42
5:S:197:GLU:OE2	5:S:232:TYR:OH	2.23	0.42
6:T:117:GLN:HE21	6:T:121:GLN:HE22	1.68	0.42
7:U:131:MET:HE3	7:U:131:MET:HA	2.01	0.42
8:V:199:LYS:HD2	8:V:199:LYS:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:102:GLY:HA2	9:W:178:ILE:HG21	2.01	0.42
14:b:75:ASN:C	14:b:75:ASN:HD22	2.27	0.42
3:C:111:VAL:HG22	3:C:136:ILE:HD12	2.01	0.42
7:G:111:LEU:HD22	7:G:142:SER:HB3	2.01	0.42
11:K:53:ASP:OD1	12:L:91:LYS:NZ	2.52	0.42
11:K:154:ASP:OD1	11:K:154:ASP:N	2.51	0.42
1:O:234:VAL:HG12	1:O:234:VAL:O	2.20	0.42
3:Q:118:LYS:HD2	3:Q:151:ASP:O	2.19	0.42
5:S:205:ARG:NH1	5:S:244:LEU:HD12	2.35	0.42
7:U:111:LEU:HD22	7:U:142:SER:HB3	2.01	0.42
9:W:137:VAL:HG11	9:W:158:ALA:HA	2.01	0.42
1:A:209:THR:O	1:A:213:ILE:HG13	2.19	0.42
3:C:142:LYS:HZ3	11:K:74:THR:HG21	1.85	0.42
9:I:207:LYS:NZ	13:a:185:ASN:HB3	2.34	0.42
11:K:4:LEU:HB2	11:K:132:HIS:HB2	2.01	0.42
11:K:141:ALA:HB3	12:Z:137:SER:HB3	2.02	0.42
14:N:45:LYS:HG3	14:N:234:VAL:HG21	2.02	0.42
7:U:220:TRP:NE1	7:U:222:CYS:SG	2.93	0.42
8:V:3:ILE:HD13	8:V:44:CYS:HB3	2.01	0.42
10:X:24:ALA:HB1	10:X:184:LEU:HD22	2.02	0.42
3:C:87:ILE:O	3:C:91:ARG:HG3	2.20	0.42
3:C:193:LEU:HD13	3:C:235:LEU:HD23	2.01	0.42
5:E:113:VAL:HG12	5:E:164:ASN:HD22	1.84	0.42
8:H:38:ASN:HB2	8:H:63:CYS:SG	2.60	0.42
9:I:137:VAL:HG11	9:I:158:ALA:HA	2.01	0.42
10:J:24:ALA:HB1	10:J:184:LEU:HD22	2.02	0.42
11:K:128:ASN:HB2	12:Z:209:TYR:HA	2.02	0.42
3:Q:216:THR:O	3:Q:218:LYS:HG3	2.20	0.42
9:W:28:ASP:OD1	9:W:28:ASP:N	2.50	0.42
12:Z:38:ASN:HB3	12:Z:41:ILE:H	1.85	0.42
1:A:178:GLU:OE1	1:A:178:GLU:N	2.46	0.42
6:F:101:GLU:OE2	14:N:90:HIS:HB2	2.20	0.42
8:H:159:ILE:HG13	8:H:160:LYS:N	2.33	0.42
9:I:27:ALA:O	13:a:212:ARG:NH1	2.40	0.42
10:J:55:LEU:HD11	10:J:65:LEU:HD23	2.01	0.42
11:K:56:GLN:HG3	12:L:88:TYR:CE2	2.55	0.42
14:N:175:TYR:HB2	14:N:189:LEU:HD13	2.01	0.42
3:Q:37:LEU:HD21	3:Q:175:LEU:HD22	2.02	0.42
6:T:121:GLN:NE2	7:U:86:ASP:OD1	2.53	0.42
6:T:176:HIS:O	6:T:180:GLU:HG2	2.20	0.42
11:Y:4:LEU:HB2	11:Y:132:HIS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:17:TYR:CE1	14:b:22:MET:HB2	2.55	0.42
1:A:234:VAL:HG12	1:A:234:VAL:O	2.20	0.42
3:C:103:GLU:OE1	11:K:80:SER:OG	2.26	0.42
3:C:119:GLN:HG3	4:D:78:ALA:HB1	2.02	0.42
3:C:168:ASN:OD1	3:C:168:ASN:N	2.53	0.42
3:C:215:LEU:HD23	3:C:223:TYR:HD1	1.84	0.42
4:D:223:ASN:O	4:D:227:GLU:HG2	2.19	0.42
6:F:96:LYS:HB2	6:F:96:LYS:HE3	1.89	0.42
9:I:152:LYS:HB2	9:I:152:LYS:HE3	1.89	0.42
10:J:10:GLY:HA3	10:J:43:LYS:HE3	2.01	0.42
10:J:22:ALA:HA	10:J:202:VAL:HA	2.02	0.42
12:L:67:GLU:HG2	12:L:73:LYS:HA	2.00	0.42
12:L:137:SER:HB3	11:Y:141:ALA:HB3	2.02	0.42
5:S:16:SER:OG	5:S:20:ARG:O	2.29	0.42
6:T:63:ILE:HG23	6:T:220:TRP:HZ2	1.84	0.42
9:W:138:LEU:HD23	9:W:138:LEU:HA	1.91	0.42
9:W:173:VAL:HG13	9:W:189:TYR:HB3	2.01	0.42
11:Y:9:GLY:HA3	11:Y:12:PHE:CE2	2.55	0.42
12:Z:25:PHE:CD2	13:a:171:GLN:NE2	2.88	0.42
13:a:30:TRP:CD1	14:b:108:PRO:HG3	2.55	0.42
1:A:15:ILE:HD11	2:B:10:LEU:HD13	2.02	0.42
3:C:62:TYR:OH	3:C:225:LYS:HB3	2.20	0.42
3:C:161:ALA:HB3	4:D:53:LEU:HD22	2.02	0.42
3:C:211:GLU:C	3:C:212:LEU:HD12	2.45	0.42
5:E:88:LEU:HD21	5:E:139:PHE:CE2	2.55	0.42
8:H:21:SER:HA	8:H:26:ILE:HA	2.02	0.42
8:H:80:GLU:HG3	8:H:82:ILE:HG13	2.01	0.42
1:O:65:LYS:HD2	1:O:65:LYS:HA	1.80	0.42
1:O:109:TYR:HB2	8:V:61:HIS:HB2	2.01	0.42
1:O:209:THR:O	1:O:213:ILE:HG13	2.20	0.42
3:Q:168:ASN:OD1	3:Q:168:ASN:N	2.53	0.42
3:Q:211:GLU:C	3:Q:212:LEU:HD12	2.45	0.42
4:R:223:ASN:O	4:R:227:GLU:HG2	2.20	0.42
7:U:72:VAL:HG12	7:U:95:ARG:HG3	2.02	0.42
13:a:223:TYR:CE2	13:a:232:VAL:HG22	2.55	0.42
3:C:37:LEU:HD21	3:C:175:LEU:HD22	2.02	0.41
3:C:160:PHE:CZ	4:D:55:ASN:HB3	2.55	0.41
7:G:72:VAL:HG12	7:G:95:ARG:HG3	2.02	0.41
8:H:38:ASN:HD21	8:H:129:VAL:CG1	2.32	0.41
11:K:138:LEU:O	12:Z:137:SER:OG	2.28	0.41
12:L:57:LYS:HE2	13:M:118:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:174:LEU:HD23	13:M:174:LEU:HA	1.81	0.41
14:N:17:TYR:CE1	14:N:22:MET:HB2	2.55	0.41
14:N:188:LEU:O	14:N:192:HIS:HB2	2.20	0.41
1:O:121:CYS:HB3	1:O:146:ILE:HD12	2.00	0.41
3:C:216:THR:O	3:C:218:LYS:HG3	2.20	0.41
4:D:16:LEU:HD21	5:E:137:ARG:CZ	2.50	0.41
8:H:153:PHE:HB2	8:H:165:TYR:HB2	2.02	0.41
10:J:197:GLY:HA3	12:Z:206:LYS:HE2	2.01	0.41
2:P:50:LYS:HB3	2:P:50:LYS:HE2	1.85	0.41
3:Q:157:SER:OG	3:Q:159:TRP:NE1	2.51	0.41
4:R:60:GLU:OE1	4:R:61:LYS:NZ	2.45	0.41
6:T:223:ILE:HG23	6:T:227:GLN:HG3	2.02	0.41
7:U:200:ILE:O	7:U:204:ASP:HB3	2.19	0.41
10:X:109:PRO:HG2	10:X:137:TYR:HB2	2.02	0.41
12:Z:4:LEU:HD11	12:Z:159:ALA:HB3	2.01	0.41
14:b:16:LYS:HB3	14:b:21:ILE:HD13	2.01	0.41
3:C:122:THR:O	4:D:125:ARG:NH1	2.53	0.41
5:E:210:ASP:OD1	5:E:210:ASP:N	2.53	0.41
6:F:166:ALA:O	6:F:169:THR:OG1	2.39	0.41
7:G:71:HIS:NE2	14:N:77:SER:HA	2.35	0.41
10:J:75:LEU:HD12	10:J:75:LEU:HA	1.80	0.41
12:L:4:LEU:HD11	12:L:159:ALA:HB3	2.01	0.41
12:L:38:ASN:HB3	12:L:41:ILE:H	1.85	0.41
5:S:88:LEU:HD21	5:S:139:PHE:CE2	2.55	0.41
6:T:93:LEU:HD12	13:a:102:LEU:HD13	2.03	0.41
10:X:22:ALA:HA	10:X:202:VAL:HA	2.02	0.41
10:X:70:ARG:HE	10:X:70:ARG:HB3	1.60	0.41
11:Y:43:LYS:NZ	11:Y:76:MET:O	2.46	0.41
13:a:29:ARG:O	13:a:29:ARG:NH1	2.53	0.41
3:C:36:GLY:HA2	3:C:45:LEU:HD23	2.03	0.41
3:C:209:LYS:HA	3:C:209:LYS:HD2	1.78	0.41
6:F:117:GLN:HE21	6:F:121:GLN:HE22	1.68	0.41
8:H:40:ASN:ND2	8:H:156:TYR:O	2.51	0.41
9:I:173:VAL:HG13	9:I:189:TYR:HB3	2.01	0.41
12:L:144:ASP:O	12:L:145:TYR:HB3	2.21	0.41
12:L:192:ASP:HB3	10:X:216:ARG:HH12	1.83	0.41
2:P:106:LEU:HD11	10:X:80:GLN:HE22	1.85	0.41
5:S:113:VAL:HG12	5:S:164:ASN:HD22	1.84	0.41
10:X:90:ALA:O	10:X:137:TYR:OH	2.33	0.41
5:E:211:LYS:HA	5:E:211:LYS:HD3	1.81	0.41
7:G:27:ILE:HD11	7:G:133:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:106:HIS:HB2	8:H:137:LYS:CE	2.48	0.41
7:G:220:TRP:NE1	7:G:222:CYS:SG	2.93	0.41
1:O:182:ILE:HG13	2:P:56:LEU:HD12	2.02	0.41
3:Q:107:VAL:HG21	3:Q:138:GLY:HA3	2.01	0.41
7:U:10:LEU:HD23	7:U:10:LEU:HA	1.89	0.41
8:V:37:ILE:HD11	8:V:56:ILE:HG23	2.02	0.41
8:V:80:GLU:HG3	8:V:82:ILE:HG13	2.01	0.41
9:W:97:ALA:HB1	9:W:127:LEU:HD13	2.03	0.41
9:W:211:PRO:HD3	10:X:214:LYS:HB2	2.02	0.41
12:Z:144:ASP:O	12:Z:145:TYR:HB3	2.21	0.41
13:a:124:LEU:HD23	13:a:124:LEU:HA	1.94	0.41
5:E:149:ASP:OD1	5:E:149:ASP:N	2.52	0.41
6:F:159:SER:HB3	6:F:164:SER:HB2	2.02	0.41
7:G:46:ILE:HD12	7:G:46:ILE:H	1.86	0.41
7:G:65:SER:OG	7:G:66:TYR:N	2.53	0.41
8:H:1:THR:OG1	8:H:2:THR:N	2.54	0.41
11:K:9:GLY:HA3	11:K:12:PHE:CE2	2.55	0.41
11:K:29:LYS:NZ	12:L:121:VAL:HG11	2.36	0.41
4:R:110:TYR:CD1	4:R:110:TYR:C	2.99	0.41
6:T:84:LEU:HD23	6:T:84:LEU:HA	1.90	0.41
6:T:166:ALA:O	6:T:169:THR:OG1	2.39	0.41
10:X:10:GLY:HA3	10:X:43:LYS:HE3	2.01	0.41
14:b:188:LEU:O	14:b:192:HIS:HB2	2.20	0.41
1:A:192:ARG:HH11	1:A:207:ASN:HB3	1.86	0.41
1:A:250:ASP:OD1	1:A:250:ASP:N	2.52	0.41
2:B:45:ILE:HD11	2:B:184:ILE:HG13	2.01	0.41
5:E:78:MET:HB2	5:E:82:MET:HE1	2.03	0.41
3:Q:36:GLY:HA2	3:Q:45:LEU:HD23	2.03	0.41
4:R:146:GLN:HE22	4:R:148:GLU:HG3	1.86	0.41
7:U:65:SER:OG	7:U:66:TYR:N	2.53	0.41
7:U:84:ASP:OD1	7:U:84:ASP:N	2.54	0.41
8:V:193:LEU:HD13	8:V:213:CYS:SG	2.59	0.41
12:Z:51:ASP:OD1	13:a:128:ARG:NE	2.41	0.41
14:b:210:LEU:HD13	14:b:224:ILE:HG13	2.02	0.41
1:A:125:CYS:SG	1:A:166:CYS:HB2	2.61	0.41
5:E:223:LYS:HB2	5:E:226:ASP:OD1	2.21	0.41
6:F:176:HIS:O	6:F:180:GLU:HG2	2.20	0.41
8:H:4:ILE:HD11	8:H:189:ILE:HD11	2.03	0.41
8:H:28:ASN:N	8:H:28:ASN:ND2	2.69	0.41
8:H:37:ILE:HD11	8:H:56:ILE:HG23	2.02	0.41
8:H:220:ASN:ND2	8:V:190:GLN:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:29:ARG:O	13:M:29:ARG:NH1	2.53	0.41
13:M:44:THR:HG22	13:M:162:THR:O	2.21	0.41
1:O:83:GLY:HA3	1:O:241:PHE:CE1	2.55	0.41
3:Q:62:TYR:OH	3:Q:225:LYS:HB3	2.20	0.41
3:Q:87:ILE:O	3:Q:91:ARG:HG3	2.20	0.41
8:V:22:SER:O	8:V:22:SER:OG	2.36	0.41
1:A:59:GLN:HG3	1:A:61:ILE:HG22	2.03	0.41
1:A:131:TYR:HE2	1:A:140:HIS:CE1	2.39	0.41
1:A:169:TYR:CD1	2:B:57:ILE:HG13	2.56	0.41
2:B:42:ASN:OD1	2:B:42:ASN:N	2.52	0.41
6:F:109:VAL:HG21	6:F:144:PHE:CG	2.56	0.41
7:G:50:CYS:HB3	7:G:68:ARG:HH21	1.86	0.41
8:H:54:LYS:HZ2	9:I:84:THR:CB	2.34	0.41
10:J:109:PRO:HG2	10:J:137:TYR:HB2	2.02	0.41
11:K:142:ILE:HD11	12:Z:137:SER:O	2.21	0.41
12:L:196:LEU:HD22	10:X:214:LYS:HD2	2.02	0.41
1:O:60:TYR:HB3	7:U:28:TYR:CE2	2.56	0.41
1:O:131:TYR:HE2	1:O:140:HIS:CE1	2.39	0.41
3:Q:238:LEU:HA	3:Q:241:GLN:HE21	1.86	0.41
5:S:144:LEU:HD12	5:S:144:LEU:HA	1.90	0.41
6:T:184:GLU:O	6:T:188:LEU:HD23	2.21	0.41
8:V:38:ASN:HB2	8:V:63:CYS:SG	2.60	0.41
10:X:28:ARG:NH1	10:X:30:GLY:HA3	2.36	0.41
11:Y:2:ASP:HB2	11:Y:35:LYS:NZ	2.36	0.41
13:a:55:THR:HB	13:a:67:PHE:HA	2.03	0.41
14:b:58:LEU:HD11	14:b:62:GLN:HE21	1.86	0.41
5:E:149:ASP:CG	5:E:150:LYS:H	2.29	0.41
9:I:182:SER:OG	9:I:183:TYR:N	2.52	0.41
10:J:190:ARG:NE	13:a:178:ASP:OD2	2.54	0.41
12:L:3:THR:HG23	12:L:44:THR:HG21	2.02	0.41
14:N:10:THR:H	14:N:42:ARG:NH1	2.19	0.41
1:O:18:PRO:HA	2:P:24:TYR:CD1	2.56	0.41
3:Q:126:GLY:HA3	4:R:2:SER:HA	2.03	0.41
5:S:149:ASP:CG	5:S:150:LYS:H	2.29	0.41
8:V:4:ILE:HD11	8:V:189:ILE:HD11	2.03	0.41
9:W:99:VAL:HG13	9:W:127:LEU:CD1	2.51	0.41
13:a:44:THR:HG22	13:a:162:THR:O	2.21	0.41
14:b:45:LYS:HG3	14:b:234:VAL:HG21	2.02	0.41
1:A:151:GLU:HG2	9:I:75:ARG:NH1	2.36	0.40
1:A:173:VAL:HG11	1:A:181:SER:HB2	2.03	0.40
2:B:46:ILE:HD11	2:B:219:PHE:HZ	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:184:GLU:O	6:F:188:LEU:HD23	2.21	0.40
7:G:77:ILE:HG12	7:G:229:PHE:CD1	2.53	0.40
8:H:176:LYS:HE2	8:H:176:LYS:HB3	1.86	0.40
12:L:25:PHE:CG	13:M:171:GLN:NE2	2.83	0.40
5:S:165:THR:HG22	6:T:60:GLN:NE2	2.36	0.40
6:T:43:TYR:CG	6:T:183:LEU:HD21	2.57	0.40
2:B:174:LEU:HD23	2:B:174:LEU:HA	1.92	0.40
4:D:171:PHE:O	4:D:174:LYS:HG3	2.21	0.40
4:D:228:LEU:O	4:D:231:GLN:NE2	2.44	0.40
5:E:50:SER:HB2	5:E:67:LEU:HD21	2.03	0.40
10:J:13:LEU:HD13	10:J:151:VAL:HG12	2.03	0.40
12:L:6:PHE:O	12:L:143:TYR:OH	2.28	0.40
3:Q:1:MET:HG2	6:T:9:ASP:OD1	2.21	0.40
3:Q:160:PHE:CE2	4:R:55:ASN:HB3	2.57	0.40
4:R:171:PHE:O	4:R:174:LYS:HG3	2.21	0.40
6:T:223:ILE:HG22	6:T:228:LEU:HB2	2.04	0.40
9:W:35:HIS:HD2	9:W:56:THR:HG21	1.86	0.40
9:W:207:LYS:HA	9:W:207:LYS:HD2	1.91	0.40
10:X:69:LEU:HD11	10:X:93:LEU:HD13	2.02	0.40
11:Y:149:GLU:HG3	11:Y:150:ASN:N	2.37	0.40
13:a:153:ASP:OD1	13:a:153:ASP:N	2.54	0.40
14:b:186:LEU:HD12	14:b:186:LEU:HA	1.92	0.40
3:C:76:VAL:HG21	3:C:83:ALA:CB	2.52	0.40
5:E:165:THR:HG22	6:F:60:GLN:NE2	2.36	0.40
6:F:223:ILE:HG22	6:F:228:LEU:HB2	2.04	0.40
7:G:219:SER:HB2	7:G:230:GLN:O	2.22	0.40
9:I:43:CYS:HA	9:I:100:LEU:HA	2.04	0.40
9:I:97:ALA:HB1	9:I:127:LEU:HD13	2.03	0.40
13:M:153:ASP:OD1	13:M:153:ASP:N	2.54	0.40
14:N:155:HIS:C	14:N:157:ASP:H	2.30	0.40
1:O:250:ASP:OD1	1:O:250:ASP:N	2.52	0.40
3:Q:119:GLN:HB2	3:Q:154:GLY:HA3	2.03	0.40
4:R:94:TYR:CE2	4:R:98:MET:HG3	2.57	0.40
7:U:27:ILE:HD11	7:U:133:PRO:HG2	2.02	0.40
8:V:153:PHE:HB2	8:V:165:TYR:HB2	2.02	0.40
14:b:155:HIS:C	14:b:157:ASP:H	2.30	0.40
3:C:142:LYS:NZ	11:K:74:THR:HG21	2.36	0.40
3:C:211:GLU:OE1	3:C:211:GLU:N	2.54	0.40
4:D:146:GLN:HE22	4:D:148:GLU:HG3	1.86	0.40
5:E:16:SER:OG	5:E:20:ARG:O	2.29	0.40
5:E:233:ASN:OD1	5:E:233:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:195:ASP:OD1	8:V:192:TYR:HE1	2.04	0.40
11:K:2:ASP:HB2	11:K:35:LYS:NZ	2.36	0.40
11:K:50:SER:O	11:K:54:ARG:HG3	2.21	0.40
12:L:90:TYR:HD1	12:L:93:TYR:CD2	2.37	0.40
13:M:55:THR:HB	13:M:67:PHE:HA	2.03	0.40
13:M:223:TYR:CE2	13:M:232:VAL:HG22	2.55	0.40
14:N:29:ALA:HB2	14:N:40:VAL:HG11	2.04	0.40
14:N:155:HIS:O	14:N:155:HIS:CG	2.74	0.40
1:O:60:TYR:CD1	7:U:28:TYR:HD2	2.39	0.40
2:P:226:GLU:N	2:P:226:GLU:OE1	2.55	0.40
5:S:192:THR:HG23	5:S:195:GLN:H	1.84	0.40
7:U:90:ILE:O	7:U:94:ALA:N	2.45	0.40
1:A:83:GLY:HA3	1:A:241:PHE:CE1	2.55	0.40
4:D:94:TYR:CE2	4:D:98:MET:HG3	2.57	0.40
5:E:148:VAL:HA	5:E:153:PRO:HA	2.02	0.40
6:F:223:ILE:HG23	6:F:227:GLN:HG3	2.02	0.40
8:H:13:MET:HE3	8:H:232:ASN:HB2	2.04	0.40
8:H:115:LYS:HB3	8:H:115:LYS:HE2	1.92	0.40
9:I:99:VAL:HG13	9:I:127:LEU:HD11	2.04	0.40
10:J:69:LEU:HD11	10:J:93:LEU:HD13	2.02	0.40
11:K:24:SER:O	11:K:26:ILE:N	2.55	0.40
11:K:51:ILE:HD12	11:K:51:ILE:H	1.87	0.40
1:O:67:LEU:HD12	1:O:67:LEU:H	1.87	0.40
1:O:216:LEU:HG	1:O:220:LEU:HD21	2.03	0.40
3:Q:175:LEU:HD23	3:Q:175:LEU:HA	1.86	0.40
4:R:194:PHE:HA	4:R:197:VAL:H	1.87	0.40
7:U:91:ILE:HG12	7:U:91:ILE:H	1.74	0.40
8:V:13:MET:HE3	8:V:232:ASN:HB2	2.04	0.40
8:V:21:SER:HA	8:V:26:ILE:HA	2.02	0.40
12:Z:121:VAL:HG13	12:Z:126:PHE:CZ	2.56	0.40
14:b:82:LYS:H	14:b:82:LYS:HG2	1.72	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	249/260 (96%)	224 (90%)	25 (10%)	0	100	100
1	O	249/260 (96%)	224 (90%)	25 (10%)	0	100	100
2	B	227/235 (97%)	214 (94%)	13 (6%)	0	100	100
2	P	227/235 (97%)	213 (94%)	14 (6%)	0	100	100
3	C	240/246 (98%)	224 (93%)	16 (7%)	0	100	100
3	Q	240/246 (98%)	224 (93%)	16 (7%)	0	100	100
4	D	231/241 (96%)	216 (94%)	15 (6%)	0	100	100
4	R	231/241 (96%)	216 (94%)	15 (6%)	0	100	100
5	E	232/256 (91%)	221 (95%)	11 (5%)	0	100	100
5	S	232/256 (91%)	221 (95%)	11 (5%)	0	100	100
6	F	233/254 (92%)	214 (92%)	19 (8%)	0	100	100
6	T	233/254 (92%)	214 (92%)	19 (8%)	0	100	100
7	G	240/252 (95%)	224 (93%)	16 (7%)	0	100	100
7	U	240/252 (95%)	224 (93%)	16 (7%)	0	100	100
8	H	225/252 (89%)	211 (94%)	14 (6%)	0	100	100
8	V	225/252 (89%)	211 (94%)	14 (6%)	0	100	100
9	I	217/229 (95%)	194 (89%)	23 (11%)	0	100	100
9	W	217/229 (95%)	194 (89%)	23 (11%)	0	100	100
10	J	213/218 (98%)	191 (90%)	22 (10%)	0	100	100
10	X	213/218 (98%)	191 (90%)	22 (10%)	0	100	100
11	K	193/195 (99%)	181 (94%)	12 (6%)	0	100	100
11	Y	193/195 (99%)	181 (94%)	12 (6%)	0	100	100
12	L	207/211 (98%)	186 (90%)	21 (10%)	0	100	100
12	Z	207/211 (98%)	186 (90%)	21 (10%)	0	100	100
13	M	211/240 (88%)	194 (92%)	17 (8%)	0	100	100
13	a	211/240 (88%)	194 (92%)	17 (8%)	0	100	100
14	N	230/265 (87%)	208 (90%)	22 (10%)	0	100	100
14	b	230/265 (87%)	208 (90%)	22 (10%)	0	100	100
All	All	6296/6708 (94%)	5803 (92%)	493 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	222/231 (96%)	221 (100%)	1 (0%)	81	85
1	O	222/231 (96%)	221 (100%)	1 (0%)	81	85
2	B	201/205 (98%)	200 (100%)	1 (0%)	81	85
2	P	201/205 (98%)	200 (100%)	1 (0%)	81	85
3	C	209/213 (98%)	209 (100%)	0	100	100
3	Q	209/213 (98%)	209 (100%)	0	100	100
4	D	199/207 (96%)	197 (99%)	2 (1%)	68	79
4	R	199/207 (96%)	197 (99%)	2 (1%)	68	79
5	E	204/223 (92%)	204 (100%)	0	100	100
5	S	204/223 (92%)	204 (100%)	0	100	100
6	F	210/227 (92%)	210 (100%)	0	100	100
6	T	210/227 (92%)	210 (100%)	0	100	100
7	G	221/229 (96%)	220 (100%)	1 (0%)	81	85
7	U	221/229 (96%)	220 (100%)	1 (0%)	81	85
8	H	208/231 (90%)	207 (100%)	1 (0%)	81	85
8	V	208/231 (90%)	207 (100%)	1 (0%)	81	85
9	I	185/194 (95%)	183 (99%)	2 (1%)	65	78
9	W	185/194 (95%)	183 (99%)	2 (1%)	65	78
10	J	189/191 (99%)	188 (100%)	1 (0%)	81	85
10	X	189/191 (99%)	188 (100%)	1 (0%)	81	85
11	K	174/174 (100%)	172 (99%)	2 (1%)	65	78
11	Y	174/174 (100%)	172 (99%)	2 (1%)	65	78
12	L	174/176 (99%)	173 (99%)	1 (1%)	78	83
12	Z	174/176 (99%)	173 (99%)	1 (1%)	78	83
13	M	191/216 (88%)	190 (100%)	1 (0%)	81	85
13	a	191/216 (88%)	190 (100%)	1 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	210/239 (88%)	210 (100%)	0	100	100
14	b	210/239 (88%)	210 (100%)	0	100	100
All	All	5594/5912 (95%)	5568 (100%)	26 (0%)	78	85

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	TYR
2	B	82	ASP
4	D	183	LYS
4	D	232	GLU
7	G	20	ARG
8	H	28	ASN
9	I	26	VAL
9	I	144	ASP
10	J	137	TYR
11	K	59	GLU
11	K	142	ILE
12	L	178	HIS
13	M	143	GLU
1	O	131	TYR
2	P	82	ASP
4	R	183	LYS
4	R	232	GLU
7	U	20	ARG
8	V	28	ASN
9	W	26	VAL
9	W	144	ASP
10	X	137	TYR
11	Y	59	GLU
11	Y	142	ILE
12	Z	178	HIS
13	a	143	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	63	GLN
1	A	197	GLN

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Mol	Chain	Res	Type
1	A	243	GLN
2	B	67	GLN
2	B	179	ASN
3	C	109	GLN
3	C	149	HIS
5	E	108	ASN
6	F	21	GLN
6	F	31	GLN
6	F	121	GLN
6	F	138	HIS
7	G	52	ASN
7	G	74	ASN
7	G	233	HIS
8	H	38	ASN
9	I	30	ASN
9	I	145	ASN
10	J	50	ASN
10	J	80	GLN
11	K	69	GLN
11	K	101	ASN
11	K	114	GLN
14	N	62	GLN
14	N	89	GLN
1	O	63	GLN
1	O	197	GLN
1	O	243	GLN
2	P	179	ASN
3	Q	109	GLN
3	Q	149	HIS
6	T	21	GLN
6	T	31	GLN
6	T	121	GLN
6	T	138	HIS
7	U	52	ASN
7	U	74	ASN
7	U	104	ASN
7	U	233	HIS
8	V	28	ASN
8	V	38	ASN
9	W	145	ASN
10	X	6	ASN
10	X	50	ASN

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Mol	Chain	Res	Type
10	X	80	GLN
11	Y	69	GLN
11	Y	101	ASN
11	Y	114	GLN
14	b	62	GLN
14	b	89	GLN
14	b	112	ASN
14	b	225	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	YHD	Z	301	12	24,28,28	1.96	6 (25%)	33,38,38	3.14	19 (57%)
15	YHD	L	301	12	24,28,28	1.96	6 (25%)	33,38,38	3.15	20 (60%)

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	YHD	Z	301	12	-	8/15/30/30	0/3/3/3
15	YHD	L	301	12	-	8/15/30/30	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	301	YHD	C14-C13	5.76	1.62	1.49
15	Z	301	YHD	C14-C13	5.76	1.62	1.49
15	Z	301	YHD	C12-C11	2.54	1.42	1.38
15	L	301	YHD	C12-C11	2.50	1.42	1.38
15	Z	301	YHD	C20-C21	2.47	1.42	1.38
15	L	301	YHD	C20-C21	2.44	1.42	1.38
15	Z	301	YHD	O25-C03	2.40	1.28	1.23
15	L	301	YHD	O25-C03	2.39	1.28	1.23
15	L	301	YHD	C04-N23	2.37	1.52	1.46
15	Z	301	YHD	C04-N23	2.37	1.52	1.46
15	L	301	YHD	C09-C10	2.25	1.56	1.51
15	Z	301	YHD	C09-C10	2.23	1.56	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	301	YHD	C21-C10-C11	-6.22	108.99	118.23
15	Z	301	YHD	C21-C10-C11	-6.21	109.01	118.23
15	L	301	YHD	C20-C13-C12	-6.01	106.93	117.68
15	Z	301	YHD	C20-C13-C12	-5.99	106.95	117.68
15	L	301	YHD	C18-C19-C14	5.05	126.29	120.54
15	Z	301	YHD	C18-C19-C14	5.04	126.28	120.54
15	Z	301	YHD	C15-C14-C19	-4.88	108.95	117.68
15	L	301	YHD	C15-C14-C19	-4.87	108.96	117.68
15	L	301	YHD	C16-C15-C14	4.84	126.04	120.54
15	Z	301	YHD	C16-C15-C14	4.82	126.02	120.54
15	Z	301	YHD	C09-C02-N22	4.43	116.11	110.39
15	L	301	YHD	C09-C02-N22	4.43	116.11	110.39
15	Z	301	YHD	C11-C12-C13	4.35	126.71	121.12
15	L	301	YHD	C21-C20-C13	4.33	126.67	121.12
15	L	301	YHD	C11-C12-C13	4.31	126.66	121.12
15	Z	301	YHD	C21-C20-C13	4.27	126.61	121.12
15	L	301	YHD	C04-C03-N22	3.84	124.94	116.52
15	L	301	YHD	C19-C14-C13	3.84	127.87	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	301	YHD	C19-C14-C13	3.83	127.87	121.25
15	Z	301	YHD	C04-C03-N22	3.82	124.91	116.52
15	Z	301	YHD	C12-C13-C14	3.54	127.36	121.25
15	L	301	YHD	C12-C13-C14	3.51	127.31	121.25
15	Z	301	YHD	C20-C21-C10	3.38	125.44	121.00
15	L	301	YHD	C20-C21-C10	3.37	125.43	121.00
15	L	301	YHD	C12-C11-C10	3.29	125.32	121.00
15	Z	301	YHD	C12-C11-C10	3.26	125.28	121.00
15	L	301	YHD	C18-C17-C16	-3.06	115.68	119.87
15	Z	301	YHD	C18-C17-C16	-3.05	115.69	119.87
15	L	301	YHD	C09-C10-C11	2.70	125.92	120.90
15	Z	301	YHD	C09-C10-C11	2.69	125.91	120.90
15	Z	301	YHD	O25-C03-N22	-2.69	118.15	122.96
15	L	301	YHD	O25-C03-N22	-2.67	118.17	122.96
15	L	301	YHD	C20-C13-C14	2.61	125.76	121.25
15	L	301	YHD	C10-C09-C02	2.57	119.25	113.76
15	Z	301	YHD	C20-C13-C14	2.56	125.68	121.25
15	Z	301	YHD	C10-C09-C02	2.56	119.25	113.76
15	L	301	YHD	C09-C10-C21	2.25	125.09	120.90
15	Z	301	YHD	C09-C10-C21	2.24	125.07	120.90
15	L	301	YHD	C07-C08-C04	2.03	108.37	104.14

There are no chirality outliers.

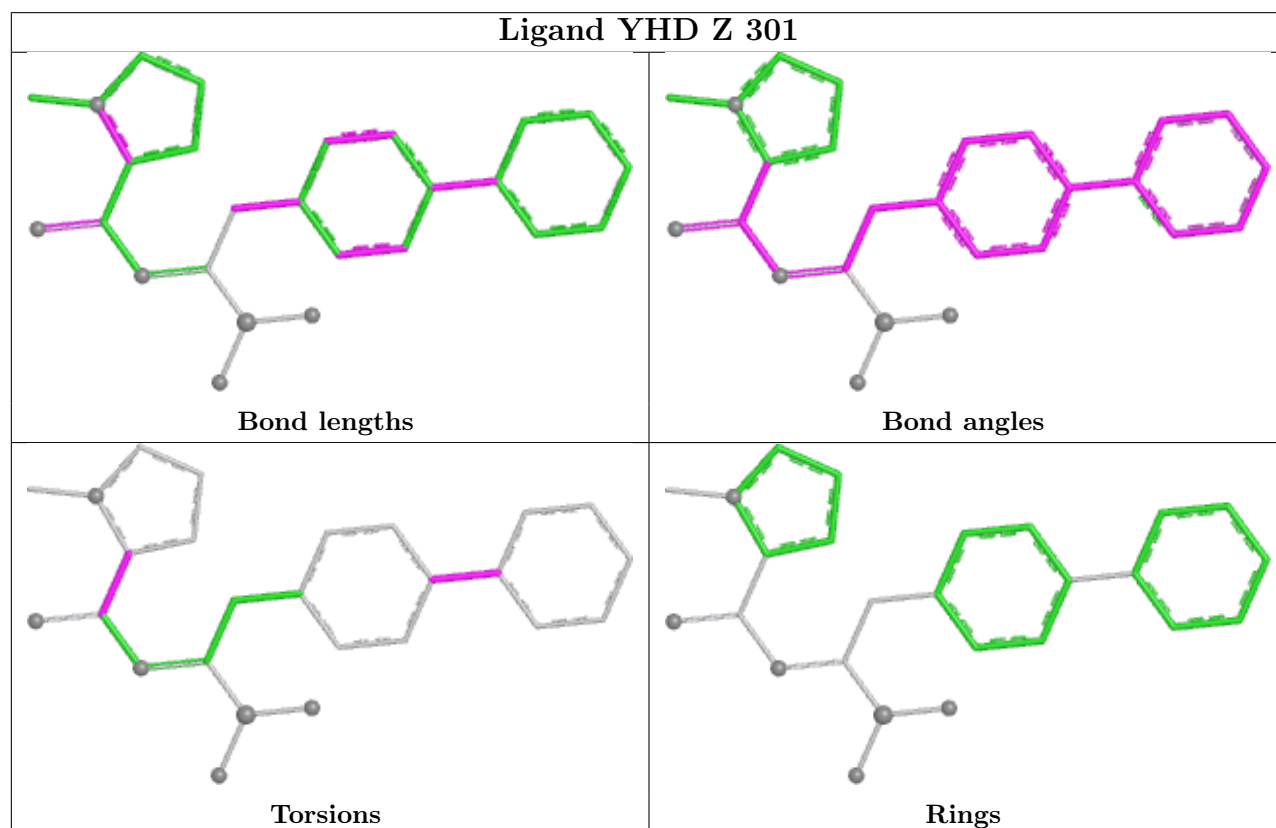
All (16) torsion outliers are listed below:

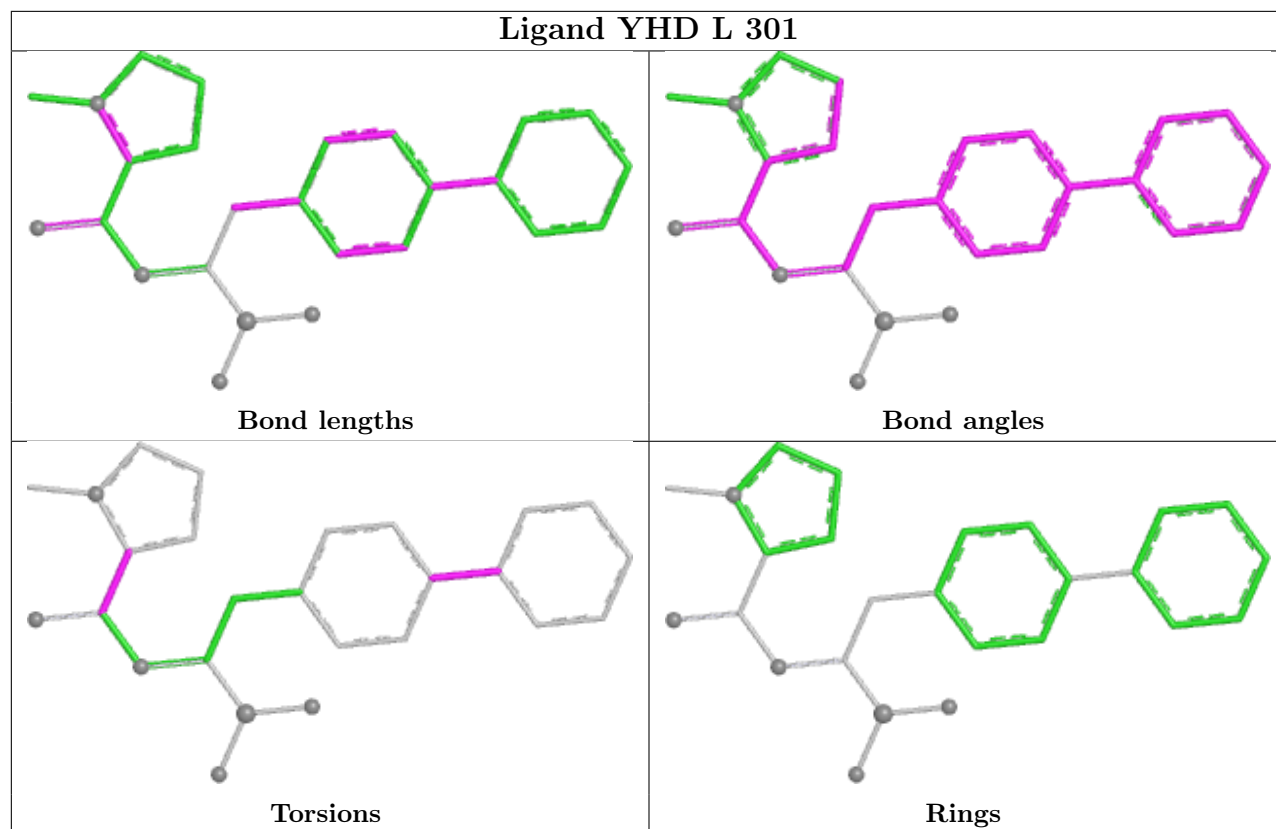
Mol	Chain	Res	Type	Atoms
15	L	301	YHD	C12-C13-C14-C19
15	L	301	YHD	C12-C13-C14-C15
15	L	301	YHD	C20-C13-C14-C15
15	Z	301	YHD	C12-C13-C14-C19
15	Z	301	YHD	C12-C13-C14-C15
15	Z	301	YHD	C20-C13-C14-C15
15	L	301	YHD	C20-C13-C14-C19
15	Z	301	YHD	C20-C13-C14-C19
15	L	301	YHD	O25-C03-C04-N23
15	Z	301	YHD	O25-C03-C04-N23
15	L	301	YHD	N22-C03-C04-N23
15	Z	301	YHD	N22-C03-C04-N23
15	L	301	YHD	O25-C03-C04-C08
15	Z	301	YHD	O25-C03-C04-C08
15	L	301	YHD	N22-C03-C04-C08
15	Z	301	YHD	N22-C03-C04-C08

There are no ring outliers.

No monomer is involved in short contacts.

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.





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.

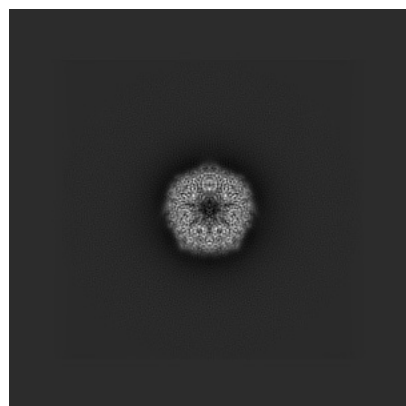
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23575. These allow visual inspection of the internal detail of the map and identification of artifacts.

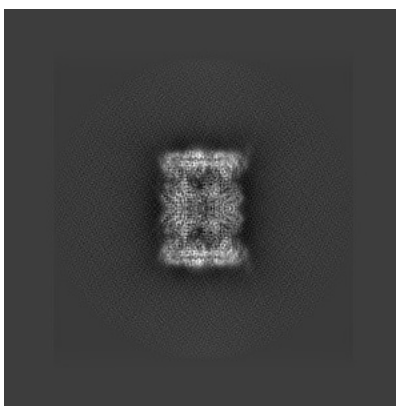
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

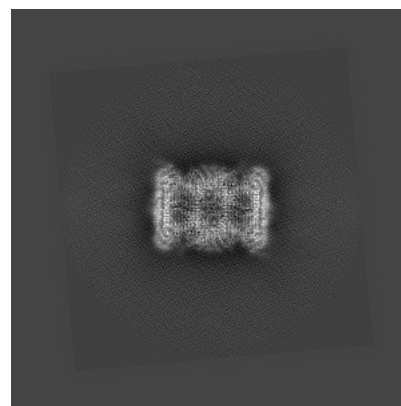
6.1.1 Primary map



X

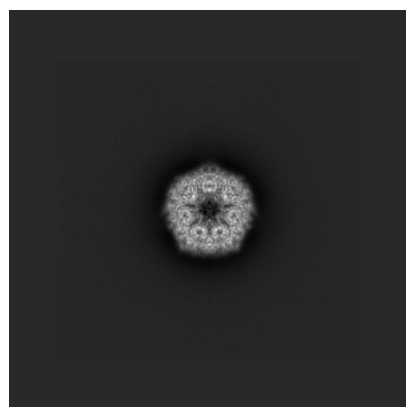


Y

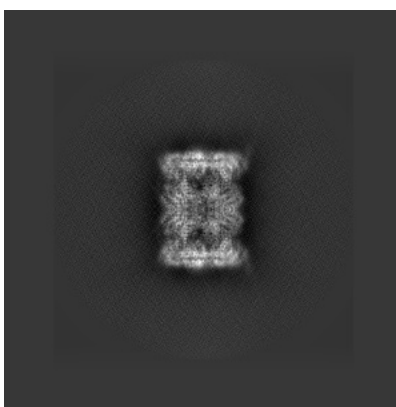


Z

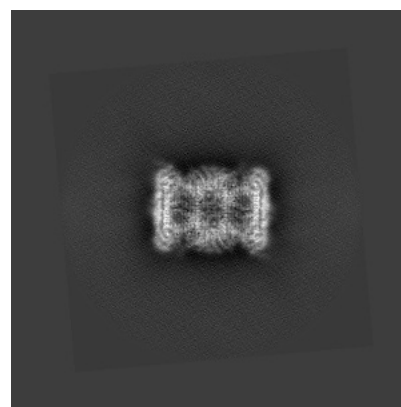
6.1.2 Raw map



X



Y

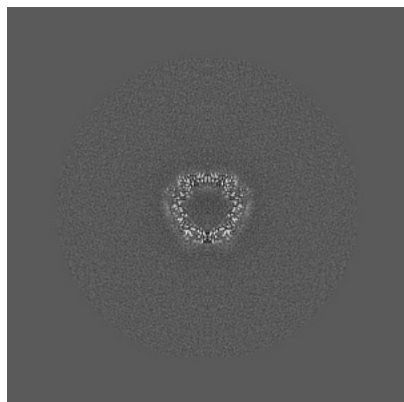


Z

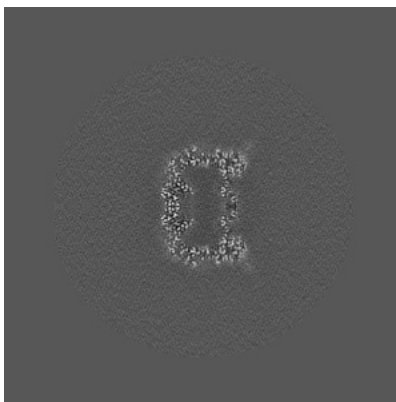
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

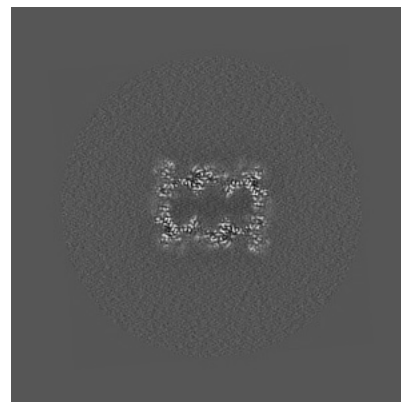
6.2.1 Primary map



X Index: 200

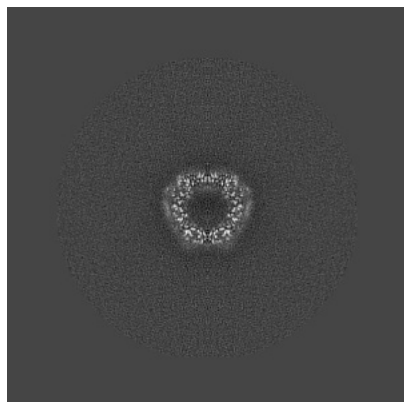


Y Index: 200

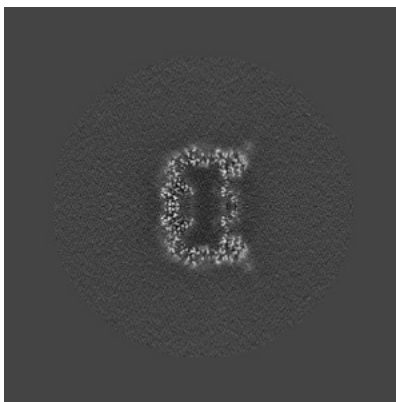


Z Index: 200

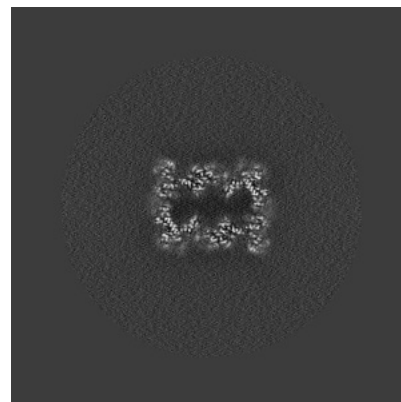
6.2.2 Raw map



X Index: 200



Y Index: 200

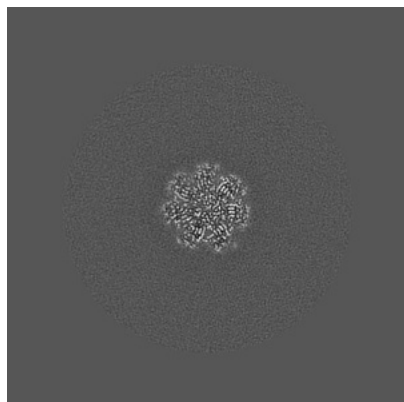


Z Index: 200

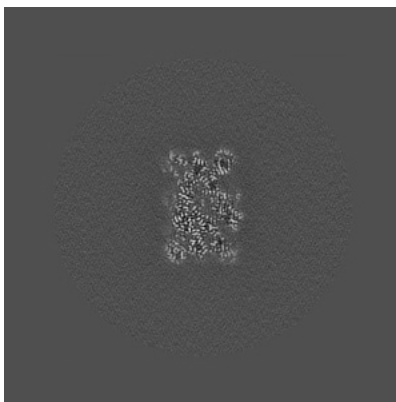
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

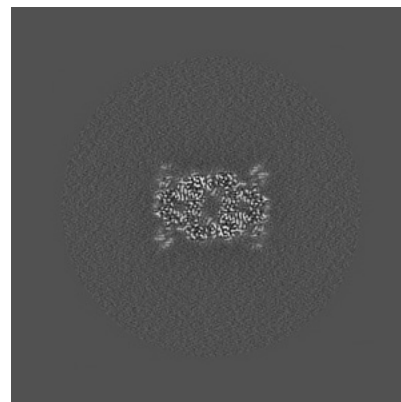
6.3.1 Primary map



X Index: 244

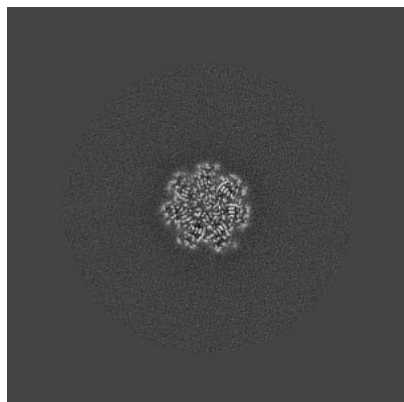


Y Index: 222

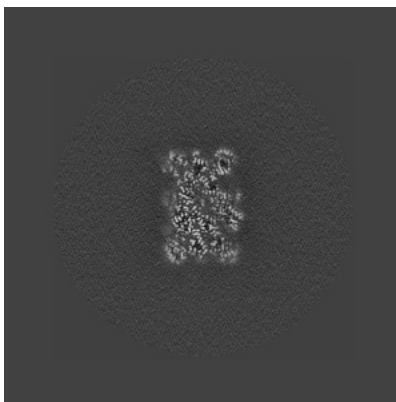


Z Index: 181

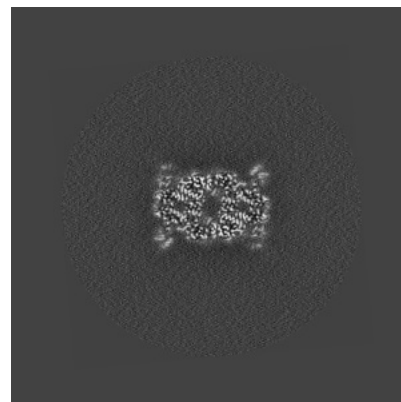
6.3.2 Raw map



X Index: 244



Y Index: 222

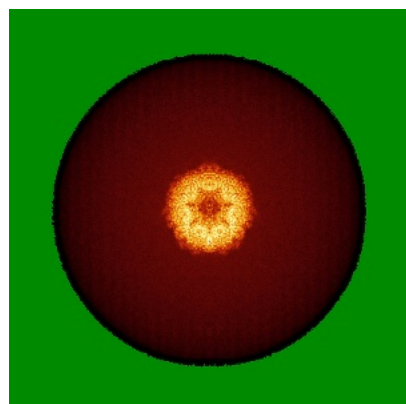


Z Index: 181

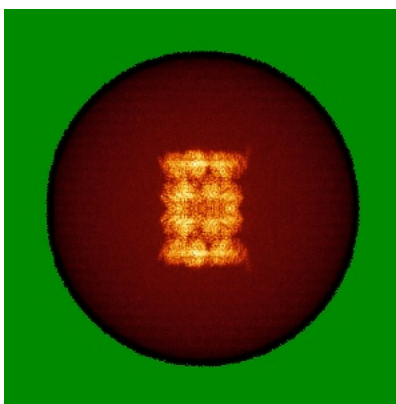
The images above show the largest variance slices of the map in three orthogonal directions.

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

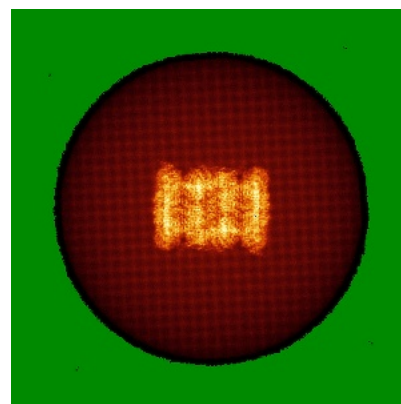
6.4.1 Primary map



X

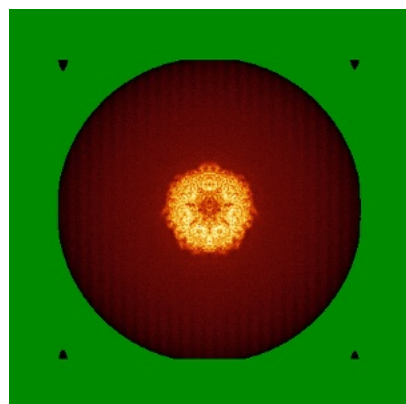


Y

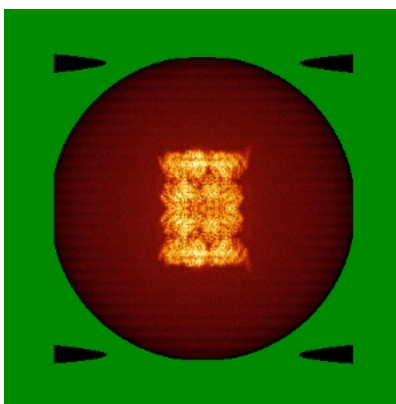


Z

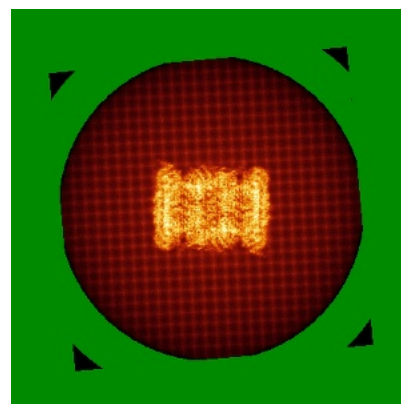
6.4.2 Raw map



X



Y

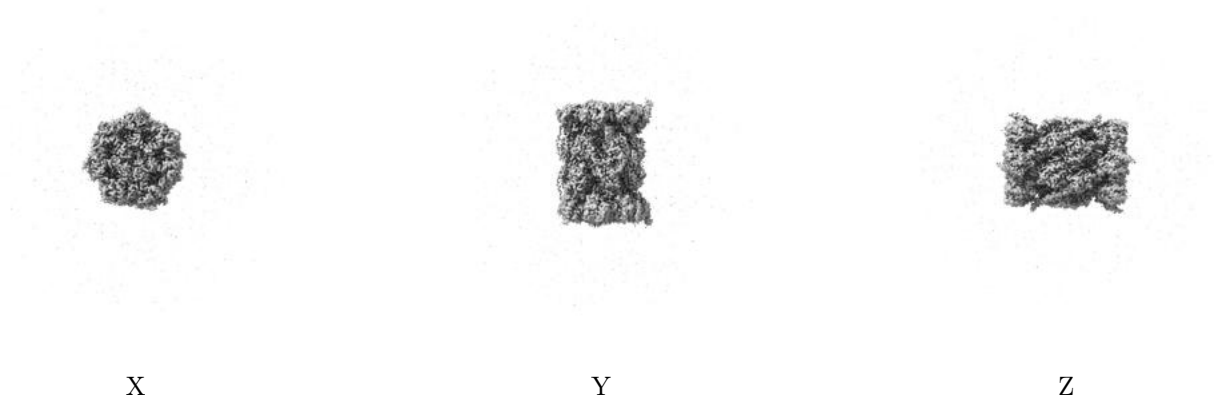


Z

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 5.0. 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.

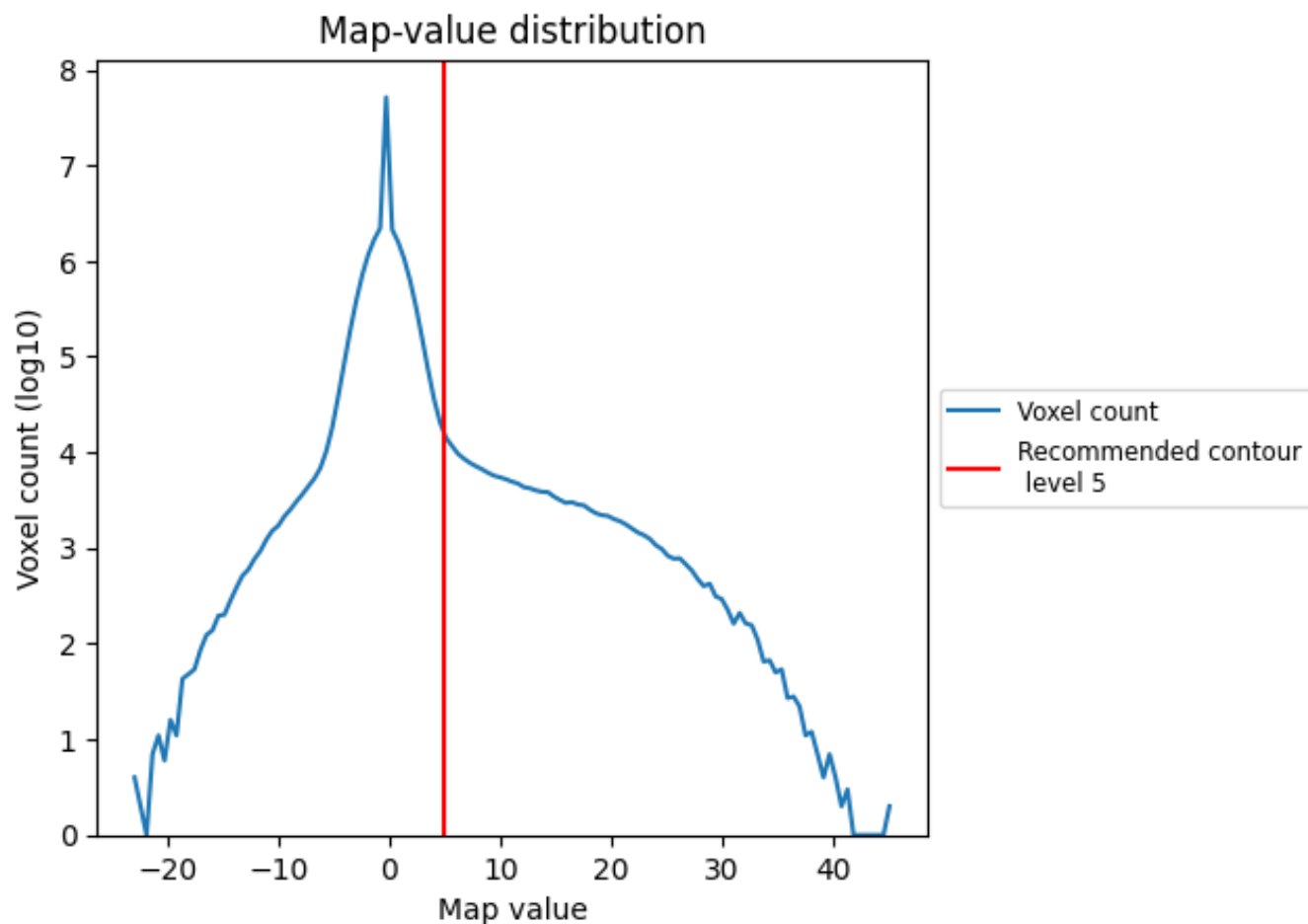
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

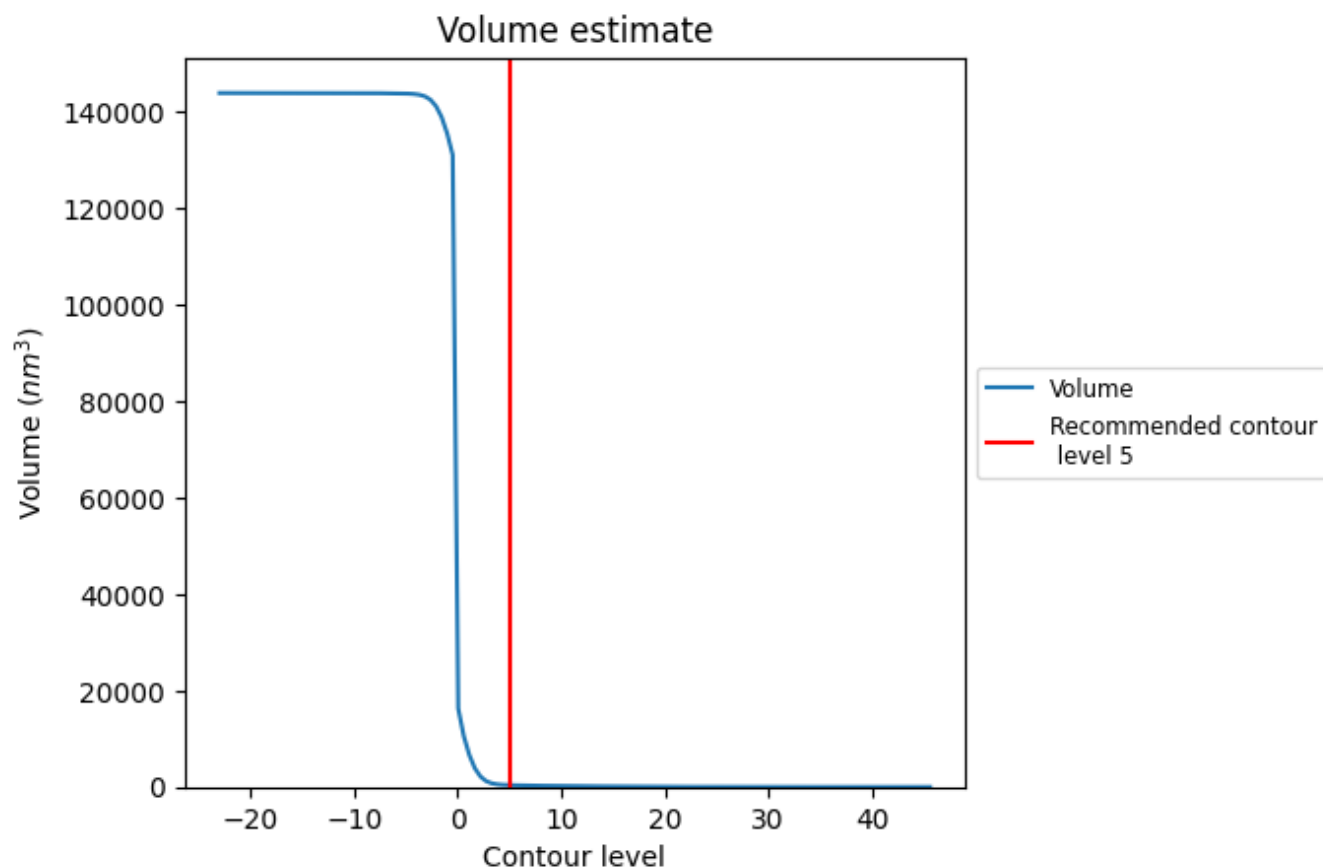
This section contains the results of statistical analysis of the map.

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.

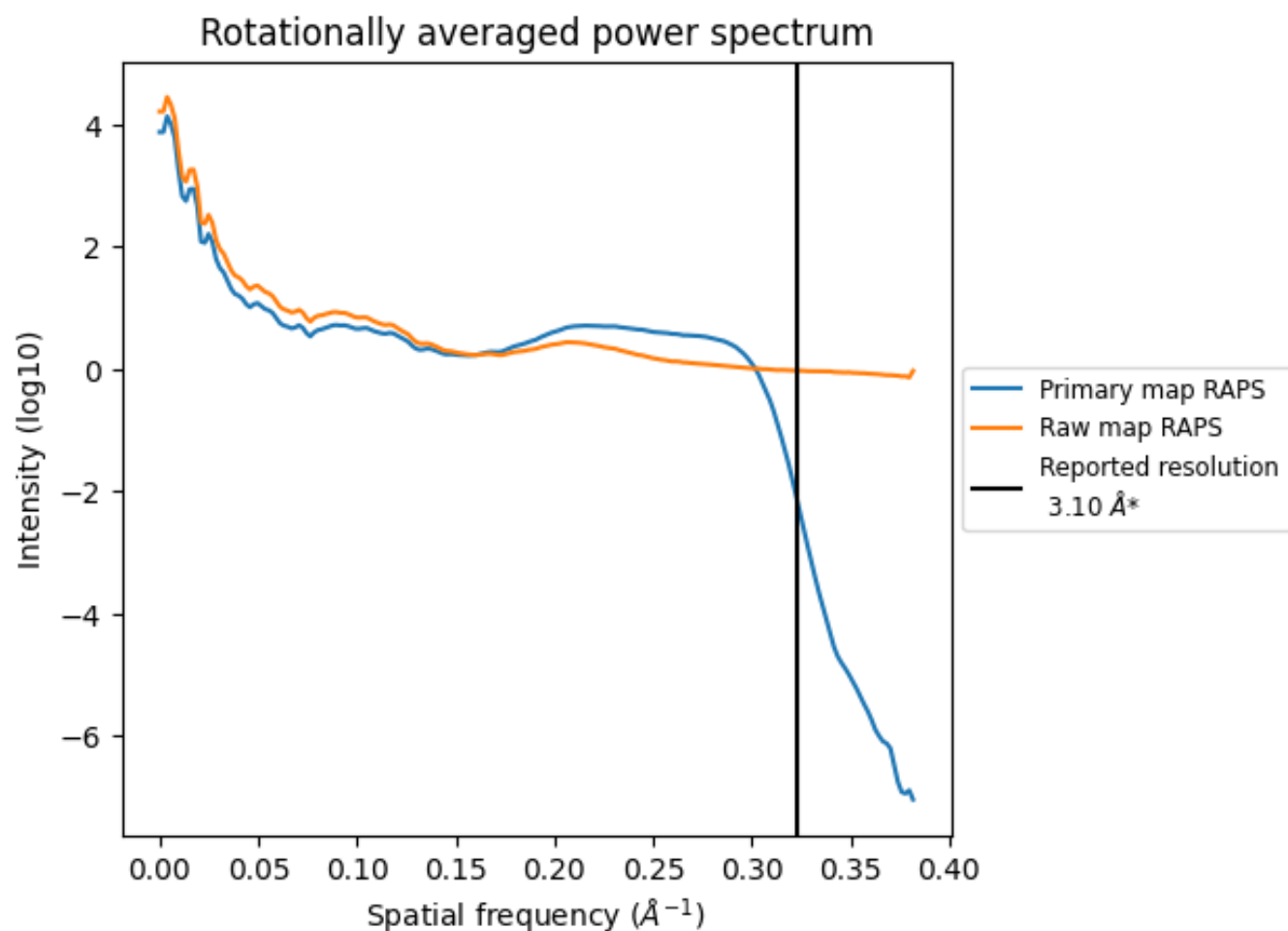
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 381 nm^3 ; this corresponds to an approximate mass of 344 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 ⓘ

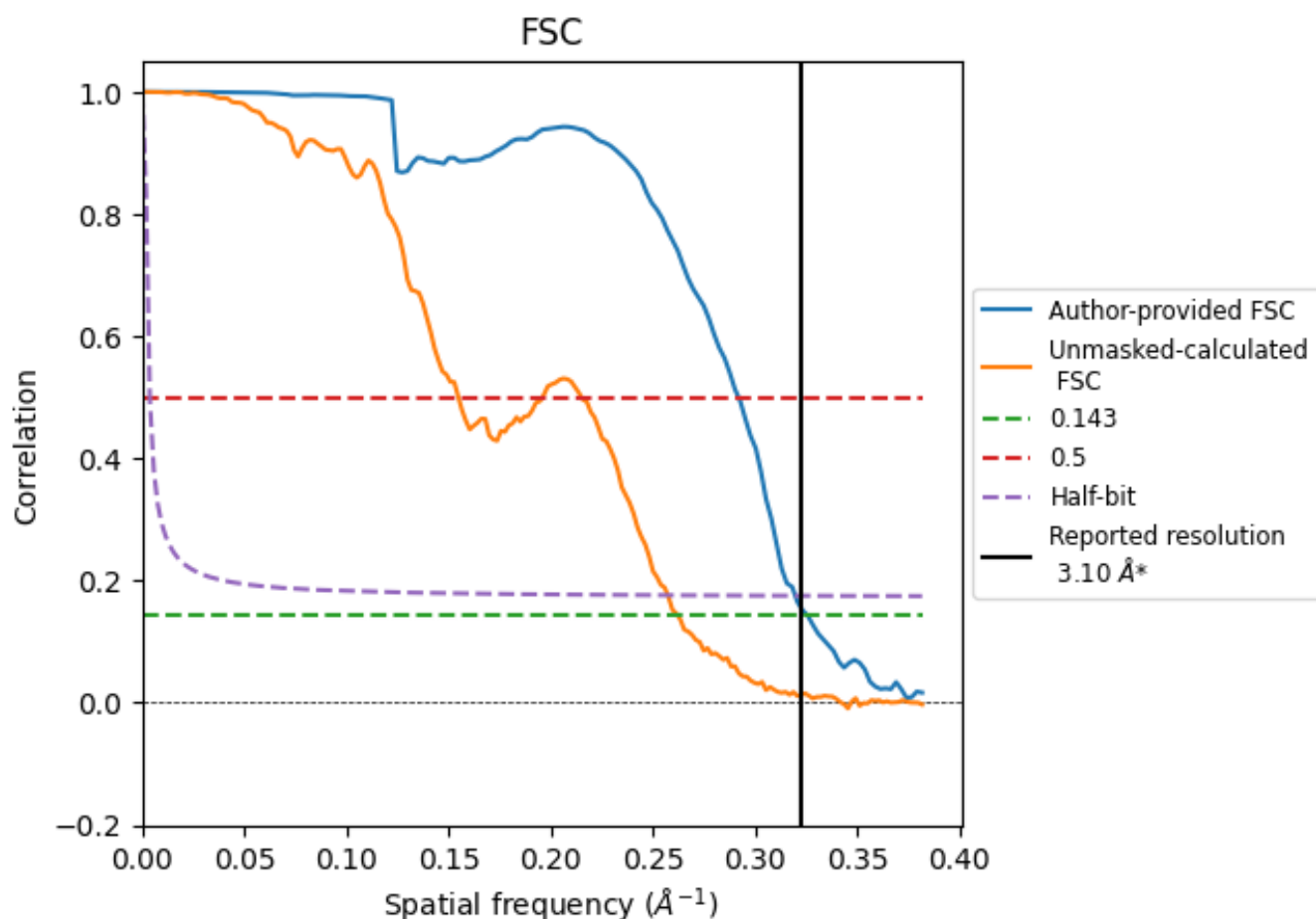


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

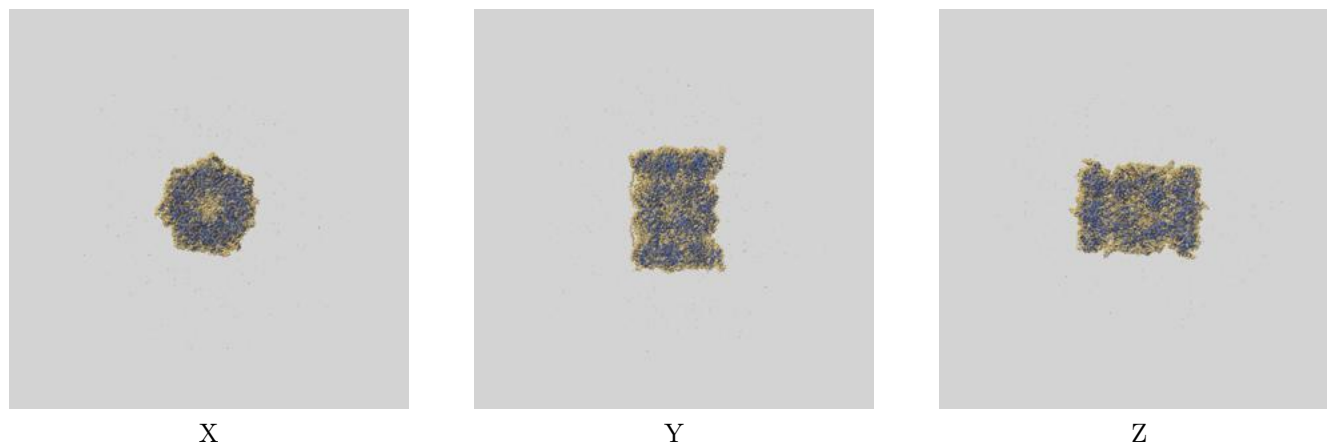
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.43	3.13
Unmasked-calculated*	3.82	6.46	3.89

*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 3.82 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

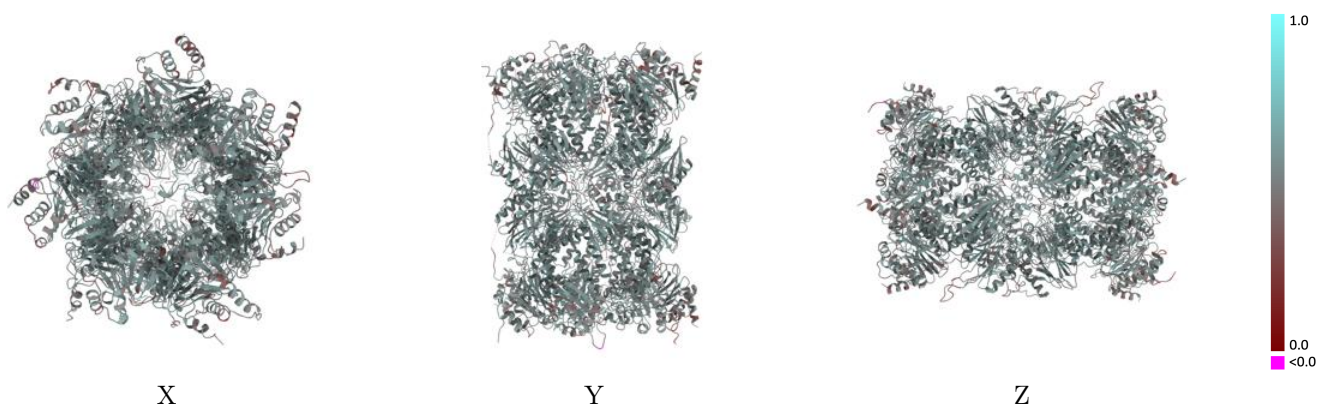
This section contains information regarding the fit between EMDB map EMD-23575 and PDB model 7LXU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



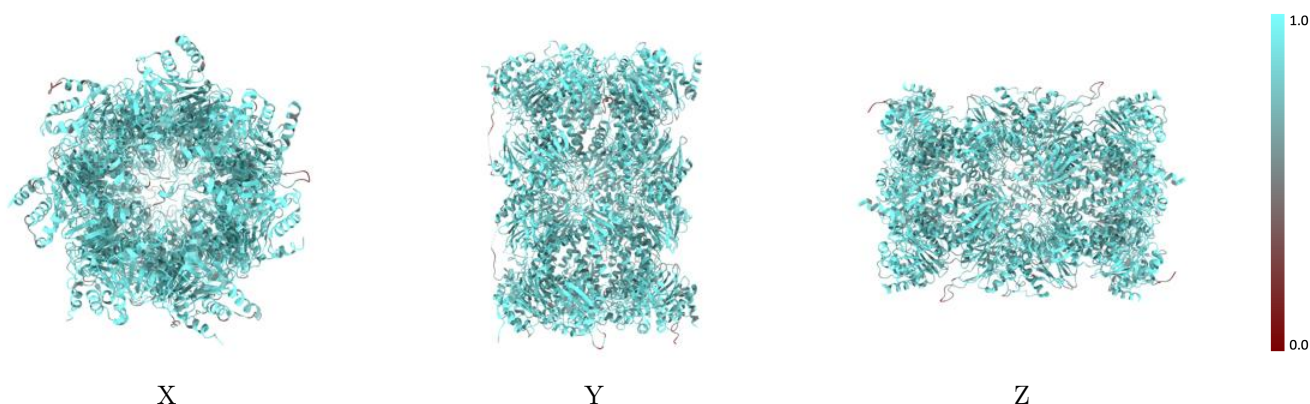
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



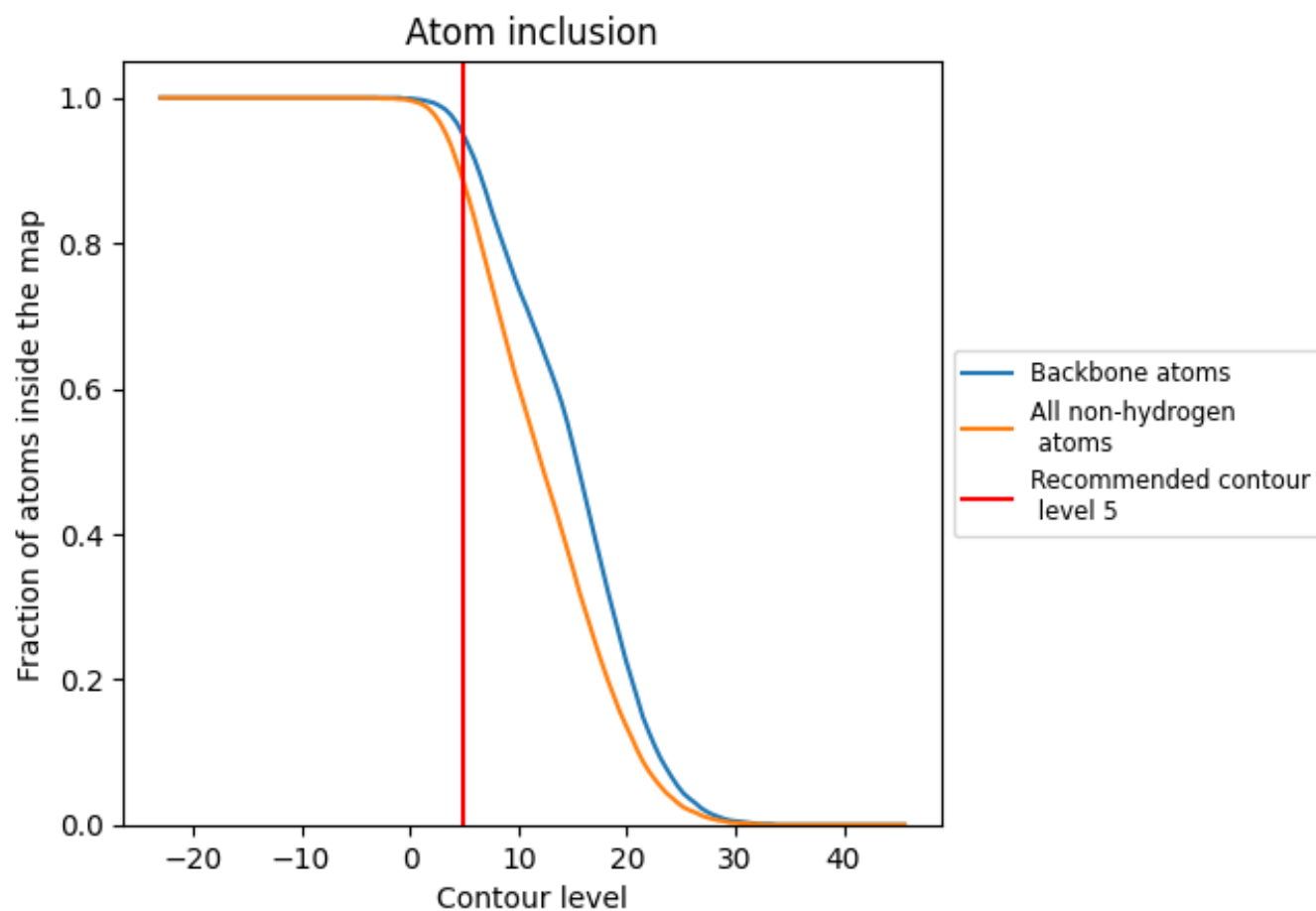
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.5240
A	 0.8660	 0.5140
B	 0.9080	 0.5300
C	 0.8880	 0.5130
D	 0.8730	 0.5090
E	 0.8590	 0.5060
F	 0.8720	 0.5180
G	 0.9030	 0.5270
H	 0.8860	 0.5320
I	 0.8760	 0.5150
J	 0.8570	 0.5260
K	 0.8660	 0.5370
L	 0.8770	 0.5320
M	 0.8920	 0.5380
N	 0.9140	 0.5400
O	 0.8650	 0.5150
P	 0.9060	 0.5300
Q	 0.8910	 0.5150
R	 0.8720	 0.5070
S	 0.8610	 0.5050
T	 0.8710	 0.5170
U	 0.9050	 0.5270
V	 0.8880	 0.5320
W	 0.8820	 0.5150
X	 0.8640	 0.5240
Y	 0.8690	 0.5350
Z	 0.8730	 0.5340
a	 0.8910	 0.5370
b	 0.9140	 0.5390

