



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 09:12 AM UTC

PDB ID : 7LXV / pdb_00007lxv
EMDB ID : EMD-23576
Title : Structure of human 20S proteasome with bound MPI-5
Authors : Metcalfe, R.D.; Morton, C.J.; Liu, B.; Xie, S.C.; Hanssen, E.; Leis, A.P.;
Tilley, L.; Griffin, M.D.W.
Deposited on : 2021-03-05
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

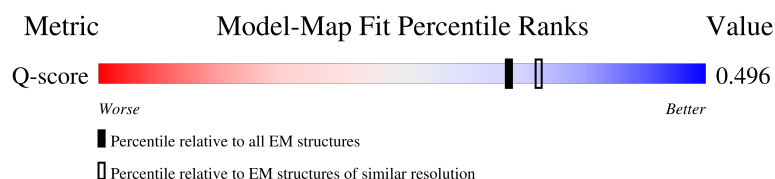
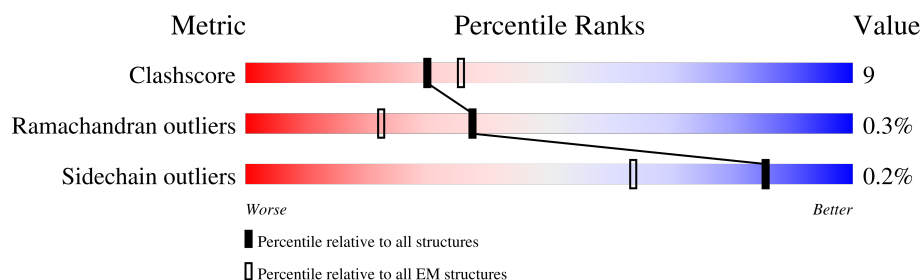
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	234	
1	O	234	
2	B	261	
2	P	261	

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Mol	Chain	Length	Quality of chain
3	C	248	
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	205	
14	b	205	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 48314 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	229	Total	C	N	O	S	0	0
			1787	1144	301	336	6		
1	O	229	Total	C	N	O	S	0	0
			1787	1144	301	336	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	239	Total	C	N	O	S	0	0
			1884	1193	322	359	10		
2	P	239	Total	C	N	O	S	0	0
			1884	1193	322	359	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	235	Total	C	N	O	S	0	0
			1852	1164	329	354	5		
3	Q	235	Total	C	N	O	S	0	0
			1852	1164	329	354	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	236	Total	C	N	O	S	0	0
			1804	1133	297	363	11		
4	R	236	Total	C	N	O	S	0	0
			1804	1133	297	363	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	236	Total	C	N	O	S	0	0
			1857	1162	334	350	11		
5	S	236	Total	C	N	O	S	0	0
			1857	1162	334	350	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	239	Total	C	N	O	S	0	0
			1874	1189	320	354	11		
6	T	239	Total	C	N	O	S	0	0
			1874	1189	320	354	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	242	Total	C	N	O	S	0	0
			1884	1193	318	360	13		
7	U	242	Total	C	N	O	S	0	0
			1884	1193	318	360	13		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
8	V	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
9	W	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	199	Total	C	N	O	S	0	0
			1543	974	269	291	9		
11	Y	199	Total	C	N	O	S	0	0
			1543	974	269	291	9		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		
12	Z	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

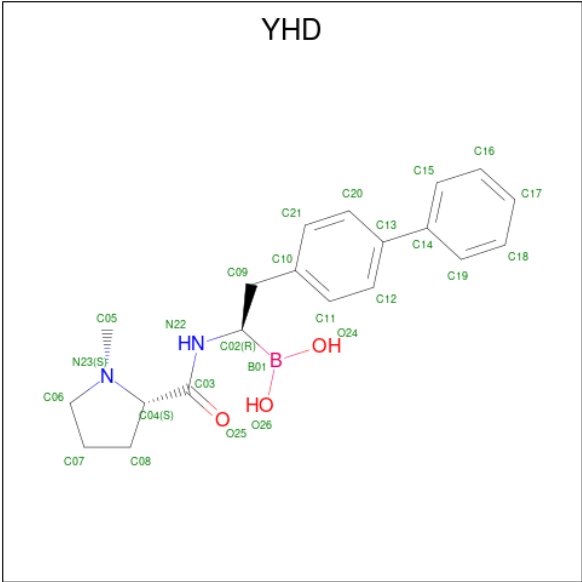
- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1657	1048	285	312	12		
13	a	212	Total	C	N	O	S	0	0
			1657	1048	285	312	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
14	b	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		

- 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).

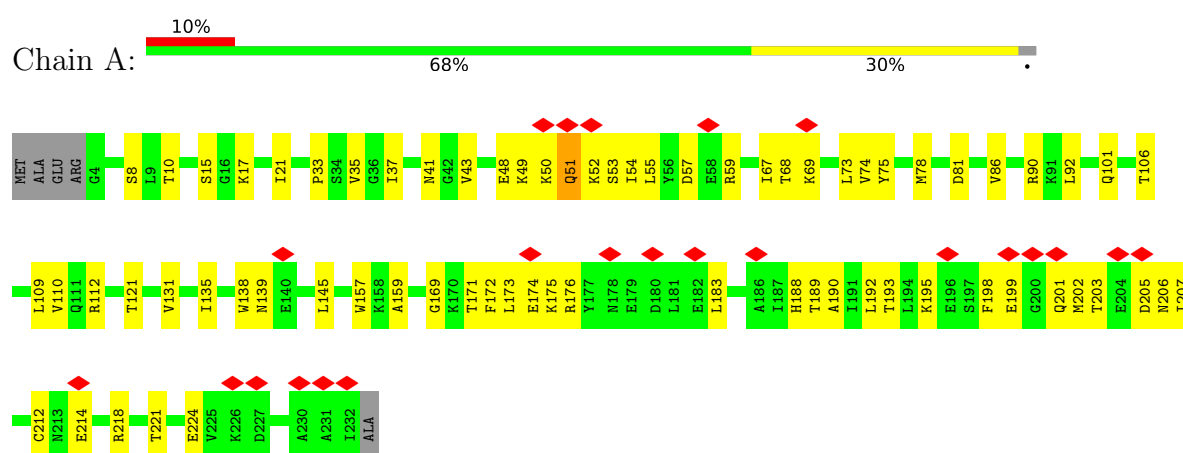


Mol	Chain	Residues	Atoms					AltConf
15	K	1	Total	B	C	N	O	0
			26	1	20	2	3	
15	Y	1	Total	B	C	N	O	0
			26	1	20	2	3	

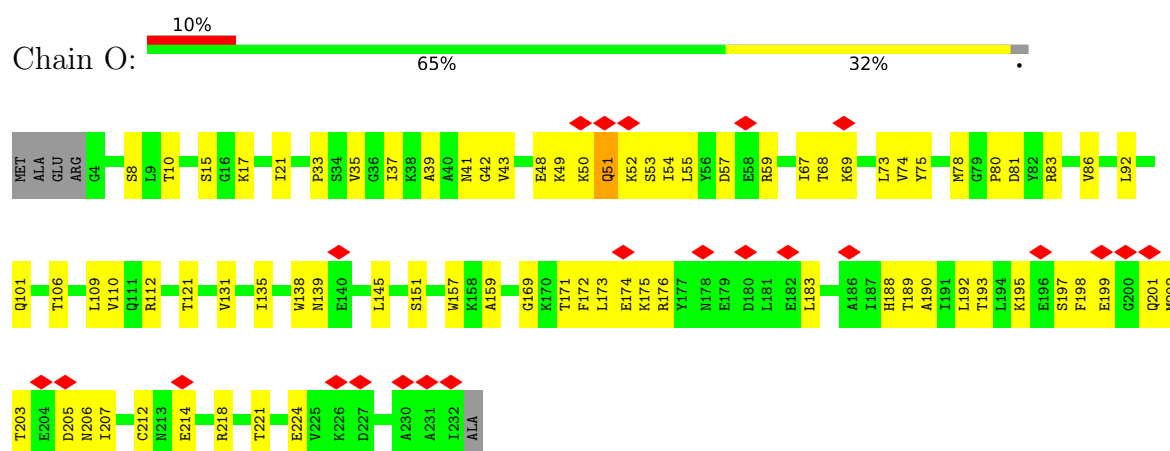
3 Residue-property plots

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.

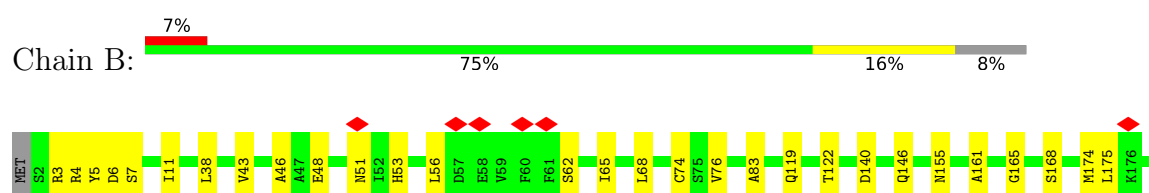
• Molecule 1: Proteasome subunit alpha type-2

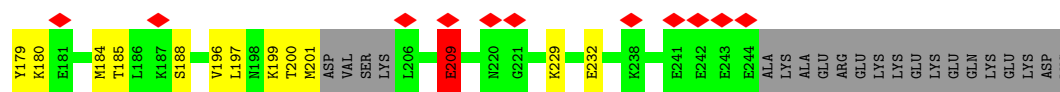


• Molecule 1: Proteasome subunit alpha type-2

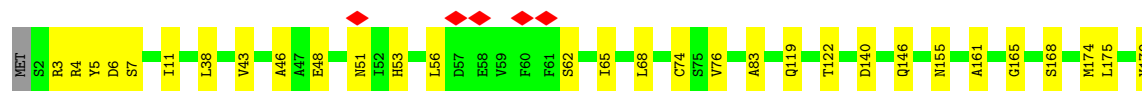
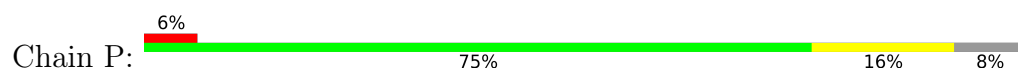


• Molecule 2: Proteasome subunit alpha type-4

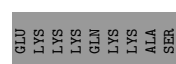
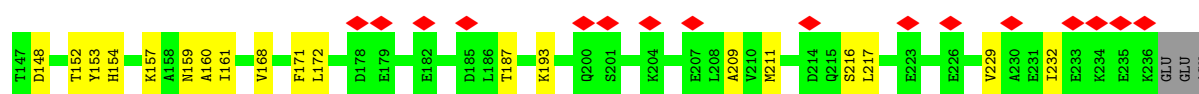
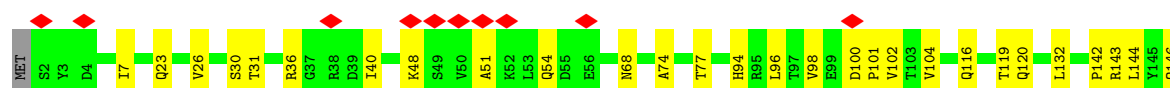
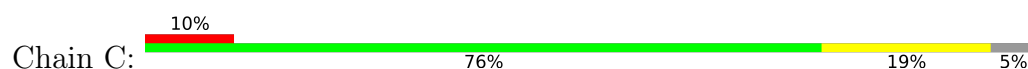




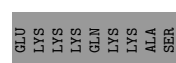
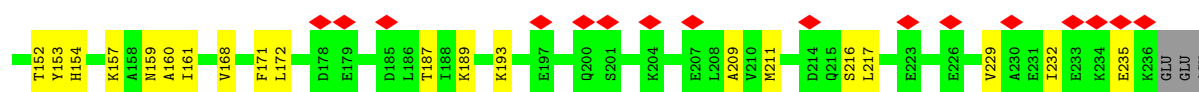
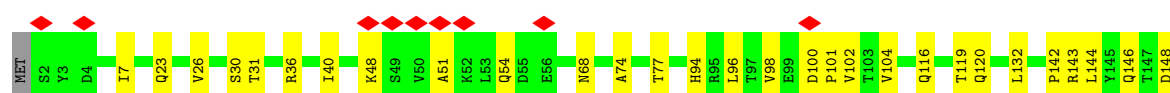
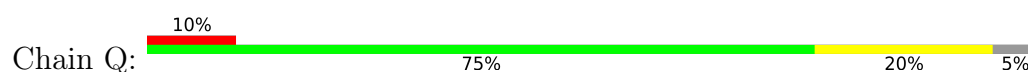
- Molecule 2: Proteasome subunit alpha type-4



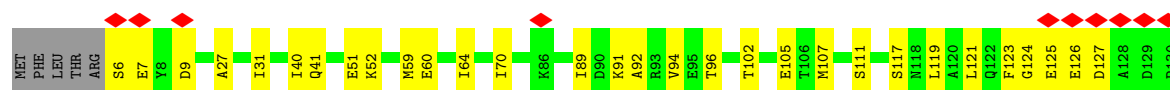
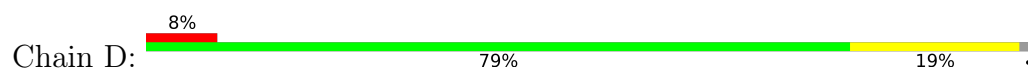
- Molecule 3: Proteasome subunit alpha type-7



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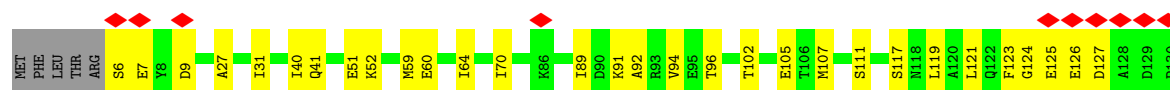
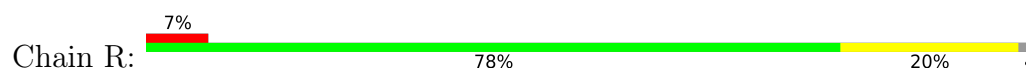


- Molecule 4: Proteasome subunit alpha type-5

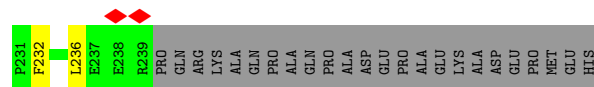
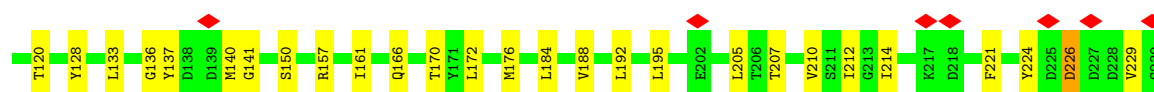
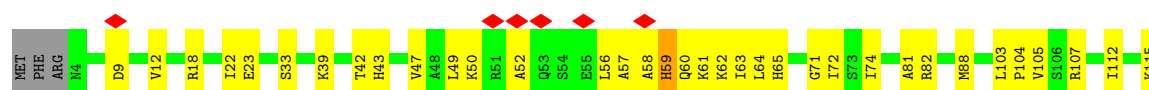




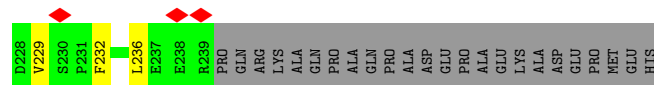
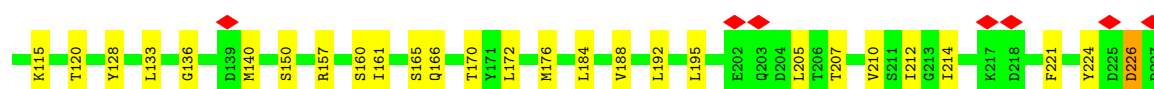
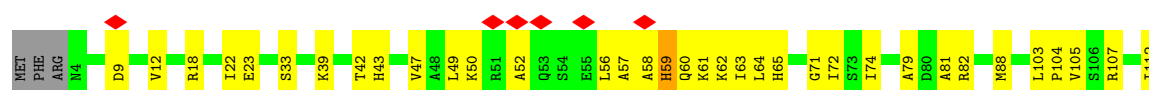
• Molecule 4: Proteasome subunit alpha type-5



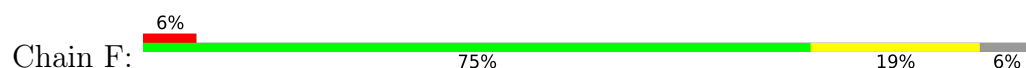
• Molecule 5: Proteasome subunit alpha type-1

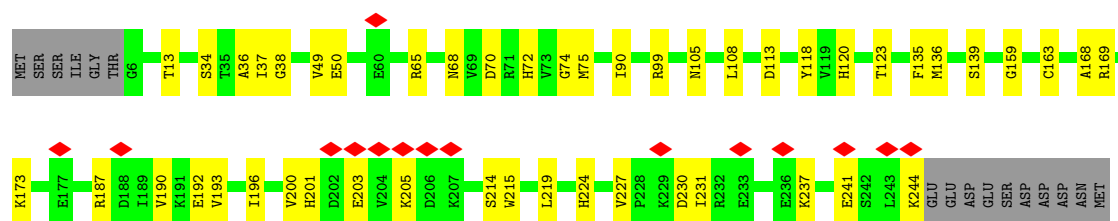


• Molecule 5: Proteasome subunit alpha type-1

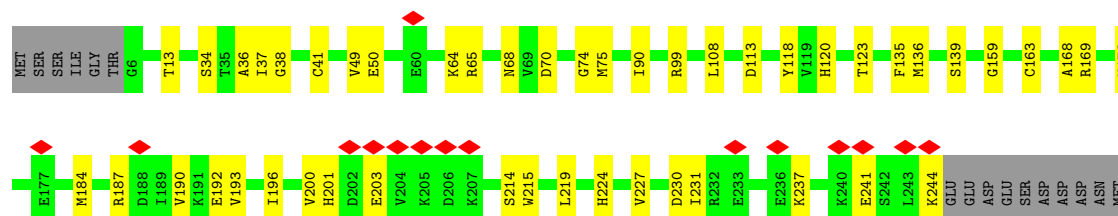
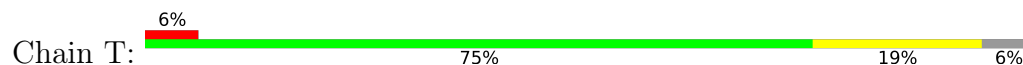


• Molecule 6: Proteasome subunit alpha type-3

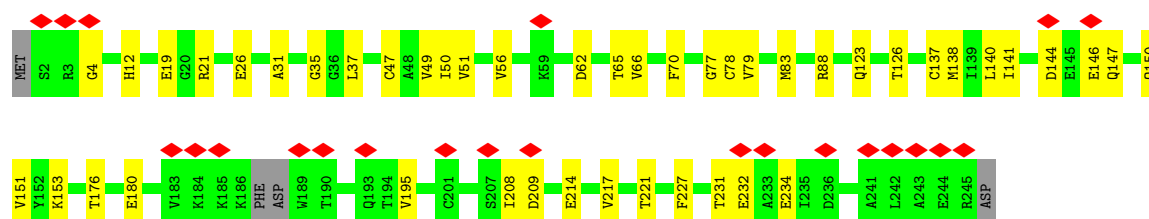
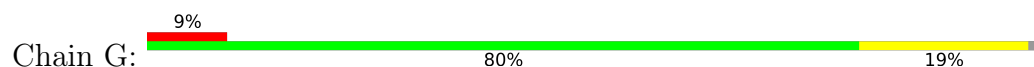




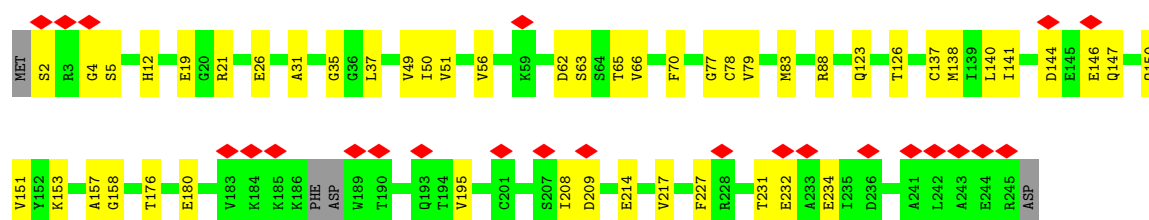
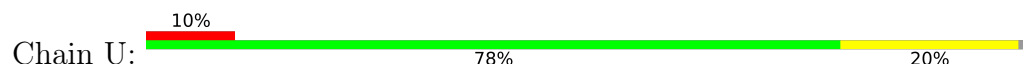
• Molecule 6: Proteasome subunit alpha type-3



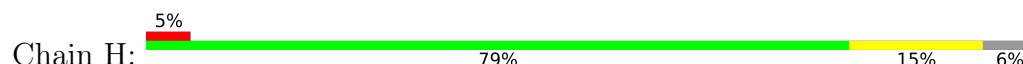
• Molecule 7: Proteasome subunit alpha type-6

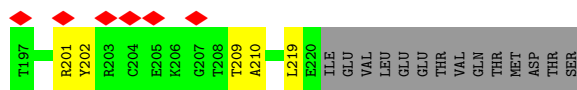


• Molecule 7: Proteasome subunit alpha type-6

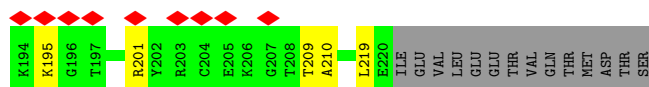
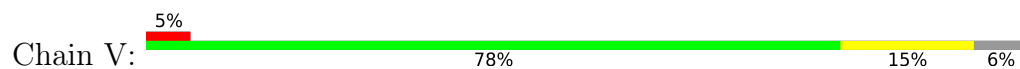


• Molecule 8: Proteasome subunit beta type-7

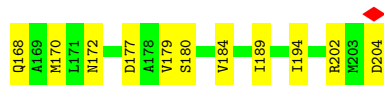
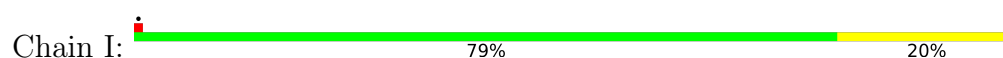




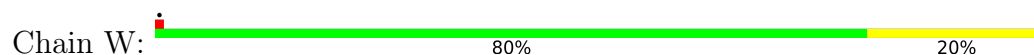
- Molecule 8: Proteasome subunit beta type-7



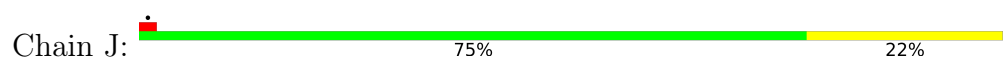
- Molecule 9: Proteasome subunit beta type-3



- Molecule 9: Proteasome subunit beta type-3

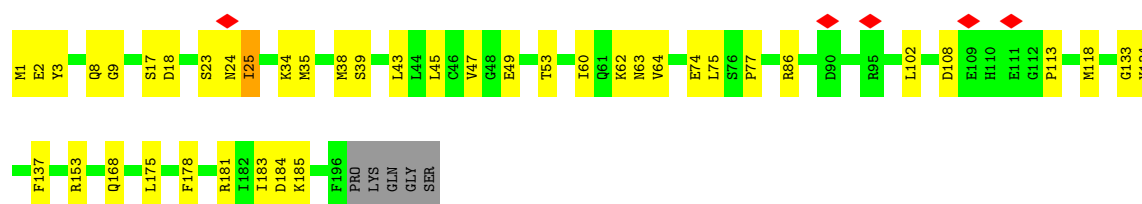


- Molecule 10: Proteasome subunit beta type-2



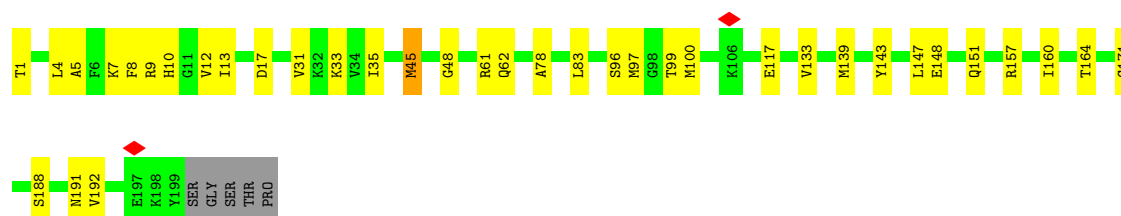
- Molecule 10: Proteasome subunit beta type-2

Chain X:  77% 20%



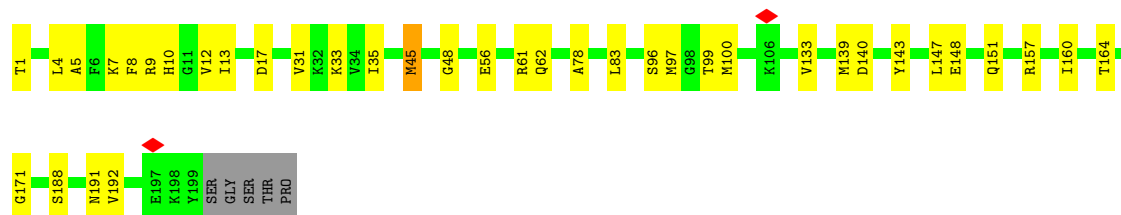
- Molecule 11: Proteasome subunit beta type-5

Chain K:  79% 18%



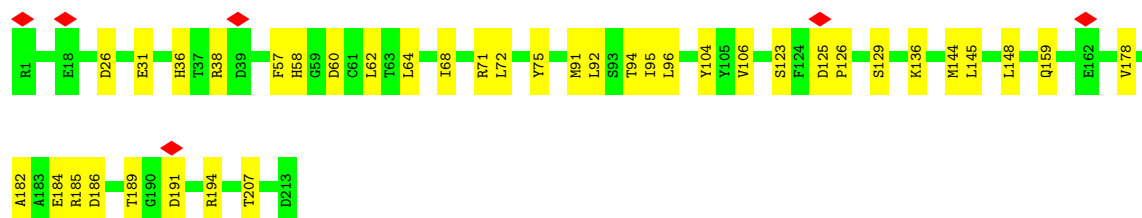
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  79% 18%



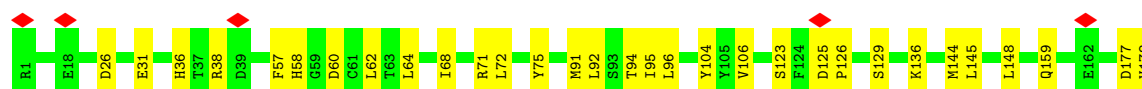
- Molecule 12: Proteasome subunit beta type-1

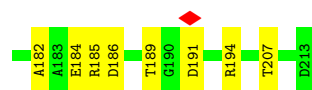
Chain L:  82% 18%



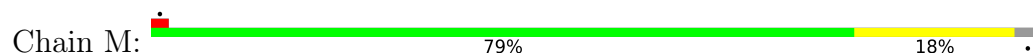
- Molecule 12: Proteasome subunit beta type-1

Chain Z:  82% 18%

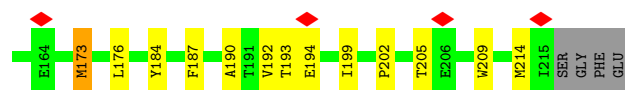
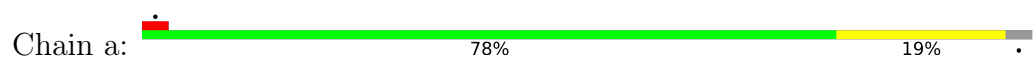




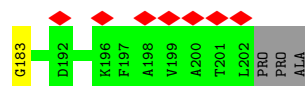
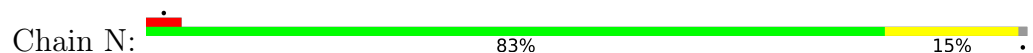
• Molecule 13: Proteasome subunit beta type-4



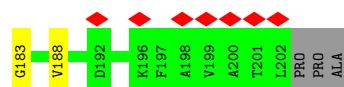
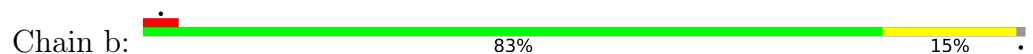
• Molecule 13: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-6



• Molecule 14: Proteasome subunit beta type-6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192367	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	28.628	Depositor
Minimum map value	-20.277	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (Å)	392.99997, 392.99997, 392.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

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	0.24	0/1826	0.56	0/2474
1	O	0.24	0/1826	0.56	0/2474
2	B	0.24	0/1913	0.55	2/2577 (0.1%)
2	P	0.24	0/1913	0.55	2/2577 (0.1%)
3	C	0.25	0/1878	0.55	0/2534
3	Q	0.25	0/1878	0.55	0/2534
4	D	0.23	0/1832	0.54	2/2475 (0.1%)
4	R	0.23	0/1832	0.54	2/2475 (0.1%)
5	E	0.25	0/1891	0.59	0/2555
5	S	0.25	0/1891	0.59	0/2555
6	F	0.24	0/1909	0.52	0/2570
6	T	0.24	0/1909	0.52	0/2570
7	G	0.23	0/1916	0.50	0/2587
7	U	0.22	0/1916	0.50	0/2587
8	H	0.24	0/1686	0.54	2/2282 (0.1%)
8	V	0.24	0/1686	0.54	2/2282 (0.1%)
9	I	0.27	0/1620	0.58	1/2184 (0.0%)
9	W	0.27	0/1620	0.58	1/2184 (0.0%)
10	J	0.28	0/1603	0.55	2/2168 (0.1%)
10	X	0.28	0/1603	0.55	2/2168 (0.1%)
11	K	0.26	0/1574	0.50	1/2127 (0.0%)
11	Y	0.26	0/1574	0.50	1/2127 (0.0%)
12	L	0.26	0/1684	0.51	0/2268
12	Z	0.26	0/1684	0.51	0/2268
13	M	0.26	0/1690	0.52	0/2286
13	a	0.26	0/1690	0.52	0/2286
14	N	0.25	0/1540	0.46	0/2085
14	b	0.25	0/1540	0.46	0/2085
All	All	0.25	0/49124	0.54	20/66344 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	209	GLU	CA-CB-CG	7.33	128.75	114.10
2	B	209	GLU	CA-CB-CG	7.32	128.74	114.10
8	H	170	GLY	CA-C-N	6.18	133.34	121.54
8	H	170	GLY	C-N-CA	6.18	133.34	121.54
8	V	170	GLY	CA-C-N	6.17	133.33	121.54
8	V	170	GLY	C-N-CA	6.17	133.33	121.54
9	W	29	ILE	N-CA-C	-5.73	98.16	107.28
9	I	29	ILE	N-CA-C	-5.71	98.19	107.28
4	D	124	GLY	CA-C-N	-5.53	113.81	122.49
4	D	124	GLY	C-N-CA	-5.53	113.81	122.49
4	R	124	GLY	CA-C-N	-5.53	113.82	122.49
4	R	124	GLY	C-N-CA	-5.53	113.82	122.49
2	B	209	GLU	CB-CG-CD	5.50	121.95	112.60
2	P	209	GLU	CB-CG-CD	5.48	121.91	112.60
10	X	23	SER	CA-C-N	5.32	131.70	121.54
10	X	23	SER	C-N-CA	5.32	131.70	121.54
10	J	23	SER	CA-C-N	5.30	131.67	121.54
10	J	23	SER	C-N-CA	5.30	131.67	121.54
11	K	45	MET	CA-CB-CG	5.14	124.38	114.10
11	Y	45	MET	CA-CB-CG	5.13	124.35	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1787	0	1782	48	0
1	O	1787	0	1782	54	0
2	B	1884	0	1899	28	0
2	P	1884	0	1899	28	0
3	C	1852	0	1881	34	0
3	Q	1852	0	1881	36	0
4	D	1804	0	1784	32	0
4	R	1804	0	1784	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1857	0	1845	46	0
5	S	1857	0	1845	45	0
6	F	1874	0	1861	38	0
6	T	1874	0	1861	39	0
7	G	1884	0	1897	34	0
7	U	1884	0	1897	37	0
8	H	1659	0	1681	34	0
8	V	1659	0	1681	33	0
9	I	1591	0	1612	37	0
9	W	1591	0	1612	36	0
10	J	1571	0	1573	33	0
10	X	1571	0	1573	33	0
11	K	1543	0	1503	33	0
11	Y	1543	0	1503	32	0
12	L	1654	0	1656	28	0
12	Z	1654	0	1656	30	0
13	M	1657	0	1638	34	0
13	a	1657	0	1638	33	0
14	N	1514	0	1487	25	0
14	b	1514	0	1487	25	0
15	K	26	0	0	4	0
15	Y	26	0	0	4	0
All	All	48314	0	48198	877	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 9.

All (877) 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)
6:T:159:GLY:H	7:U:65:THR:HG21	1.37	0.90
6:F:159:GLY:H	7:G:65:THR:HG21	1.35	0.90
2:P:155:ASN:OD1	3:Q:77:THR:OG1	1.90	0.89
10:J:18:ASP:O	10:J:34:LYS:NZ	2.08	0.86
10:X:18:ASP:O	10:X:34:LYS:NZ	2.08	0.86
5:S:49:LEU:HG	5:S:195:LEU:HD21	1.58	0.86
5:E:74:ILE:HD13	5:E:81:ALA:HB1	1.58	0.86
5:E:49:LEU:HG	5:E:195:LEU:HD21	1.58	0.85
3:Q:100:ASP:OD1	3:Q:101:PRO:HD2	1.78	0.84
5:S:74:ILE:HD13	5:S:81:ALA:HB1	1.58	0.84
2:B:155:ASN:OD1	3:C:77:THR:OG1	1.98	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:209:THR:HG22	9:W:168:GLN:HE21	1.44	0.82
3:C:100:ASP:OD1	3:C:101:PRO:HD2	1.78	0.81
8:H:171:SER:O	8:H:172:ASN:ND2	2.13	0.81
8:V:171:SER:O	8:V:172:ASN:ND2	2.13	0.80
10:J:35:MET:SD	10:J:181:ARG:NH1	2.54	0.80
8:H:209:THR:HG22	9:I:168:GLN:HE21	1.44	0.80
10:X:35:MET:SD	10:X:181:ARG:NH1	2.54	0.79
5:E:47:VAL:HG12	5:E:195:LEU:HD13	1.64	0.79
10:J:38:MET:HE1	10:J:60:ILE:HG22	1.64	0.79
4:R:206:MET:HE1	4:R:215:ILE:HG22	1.65	0.78
5:S:47:VAL:HG12	5:S:195:LEU:HD13	1.64	0.78
3:C:104:VAL:HG11	3:C:143:ARG:HB2	1.64	0.78
4:D:206:MET:HE1	4:D:215:ILE:HG22	1.65	0.77
3:Q:104:VAL:HG11	3:Q:143:ARG:HB2	1.64	0.77
10:X:38:MET:HE1	10:X:60:ILE:HG22	1.64	0.77
3:Q:96:LEU:HD22	10:X:62:LYS:HD2	1.69	0.75
12:L:144:MET:HE1	12:L:186:ASP:HB2	1.67	0.75
3:C:159:ASN:OD1	3:C:160:ALA:N	2.20	0.75
7:U:138:MET:HE2	7:U:140:LEU:HD21	1.69	0.75
6:T:50:GLU:OE2	6:T:201:HIS:ND1	2.19	0.75
3:Q:159:ASN:OD1	3:Q:160:ALA:N	2.20	0.75
7:G:138:MET:HE2	7:G:140:LEU:HD21	1.69	0.74
6:F:50:GLU:OE2	6:F:201:HIS:ND1	2.19	0.74
12:Z:144:MET:HE1	12:Z:186:ASP:HB2	1.67	0.74
1:A:106:THR:H	1:A:139:ASN:HD21	1.36	0.73
1:O:106:THR:H	1:O:139:ASN:HD21	1.36	0.73
3:C:157:LYS:NZ	4:D:60:GLU:OE2	2.22	0.73
1:O:221:THR:HG22	1:O:224:GLU:OE1	1.89	0.72
3:Q:157:LYS:NZ	4:R:60:GLU:OE2	2.22	0.72
1:A:221:THR:HG22	1:A:224:GLU:OE1	1.89	0.72
7:G:144:ASP:HB2	7:G:150:GLN:HE21	1.55	0.72
14:N:40:ARG:HH12	14:N:183:GLY:HA2	1.54	0.72
14:b:40:ARG:HH12	14:b:183:GLY:HA2	1.55	0.71
3:Q:68:ASN:HA	3:Q:211:MET:HE1	1.73	0.71
3:C:68:ASN:HA	3:C:211:MET:HE1	1.73	0.71
13:M:135:PRO:HB2	13:M:154:LEU:HD23	1.72	0.70
13:a:135:PRO:HB2	13:a:154:LEU:HD23	1.72	0.70
3:Q:146:GLN:OE1	3:Q:159:ASN:ND2	2.24	0.70
7:U:144:ASP:HB2	7:U:150:GLN:HE21	1.55	0.70
3:C:146:GLN:OE1	3:C:159:ASN:ND2	2.24	0.70
5:S:33:SER:OG	5:S:62:LYS:NZ	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:123:GLN:O	7:G:126:THR:HG22	1.93	0.69
5:E:33:SER:OG	5:E:62:LYS:NZ	2.26	0.69
7:U:123:GLN:O	7:U:126:THR:HG22	1.93	0.68
7:U:141:ILE:HG22	7:U:151:VAL:HG22	1.76	0.68
1:A:172:PHE:HA	1:A:175:LYS:HE3	1.76	0.67
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.75	0.67
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.76	0.67
11:Y:8:PHE:HE1	11:Y:13:ILE:HG12	1.60	0.67
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.75	0.66
3:C:209:ALA:HB1	3:C:217:LEU:HD11	1.78	0.66
4:R:52:LYS:HD2	4:R:64:ILE:HB	1.78	0.66
1:A:159:ALA:HB1	1:A:173:LEU:HD23	1.77	0.66
5:E:42:THR:HG23	5:E:43:HIS:ND1	2.11	0.66
13:M:26:MET:HE1	13:M:202:PRO:HB3	1.78	0.66
4:R:117:SER:OG	5:S:82:ARG:NH2	2.28	0.66
1:O:172:PHE:HA	1:O:175:LYS:HE3	1.77	0.66
2:P:62:SER:OG	2:P:65:ILE:O	2.13	0.66
10:X:8:GLN:HE21	10:X:113:PRO:HG2	1.61	0.65
3:Q:209:ALA:HB1	3:Q:217:LEU:HD11	1.78	0.65
11:K:8:PHE:HE1	11:K:13:ILE:HG12	1.60	0.65
14:N:165:GLU:OE2	13:a:37:ARG:NH1	2.28	0.65
13:a:26:MET:HE1	13:a:202:PRO:HB3	1.78	0.65
4:D:52:LYS:HD2	4:D:64:ILE:HB	1.78	0.65
8:H:166:ASP:OD1	8:H:168:GLY:N	2.26	0.65
9:W:157:MET:HE1	9:W:165:THR:OG1	1.97	0.65
2:B:51:ASN:HB3	2:B:56:LEU:HD22	1.78	0.65
13:M:37:ARG:NH1	14:b:165:GLU:OE2	2.29	0.65
3:C:51:ALA:HB3	3:C:54:GLN:HB2	1.78	0.65
1:O:159:ALA:HB1	1:O:173:LEU:HD23	1.77	0.65
3:Q:51:ALA:HB3	3:Q:54:GLN:HB2	1.78	0.65
5:S:42:THR:HG23	5:S:43:HIS:ND1	2.11	0.65
10:J:8:GLN:HE21	10:J:113:PRO:HG2	1.61	0.65
14:N:141:ALA:HB2	14:b:162:LEU:HD21	1.78	0.65
9:I:157:MET:HE1	9:I:165:THR:OG1	1.97	0.64
6:T:215:TRP:CE3	6:T:227:VAL:HG22	2.32	0.64
12:Z:148:LEU:HD23	12:Z:178:VAL:HG12	1.79	0.64
4:D:117:SER:OG	5:E:82:ARG:NH2	2.31	0.64
3:C:96:LEU:HD22	10:J:62:LYS:HD2	1.79	0.64
9:W:3:MET:SD	9:W:103:TYR:HB3	2.38	0.64
6:F:192:GLU:O	6:F:196:ILE:HD12	1.98	0.64
2:P:51:ASN:HB3	2:P:56:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:102:LEU:HD12	10:X:118:MET:HE2	1.79	0.64
9:I:3:MET:SD	9:I:103:TYR:HB3	2.38	0.63
6:F:215:TRP:CE3	6:F:227:VAL:HG22	2.32	0.63
12:L:148:LEU:HD23	12:L:178:VAL:HG12	1.79	0.63
2:B:62:SER:OG	2:B:65:ILE:O	2.13	0.63
10:J:102:LEU:HD12	10:J:118:MET:HE2	1.79	0.63
13:M:173:MET:HE2	13:M:173:MET:HA	1.81	0.63
13:a:173:MET:HE2	13:a:173:MET:HA	1.81	0.63
4:R:162:PHE:O	5:S:60:GLN:NE2	2.24	0.63
2:B:119:GLN:O	2:B:122:THR:HG22	1.99	0.62
6:T:192:GLU:O	6:T:196:ILE:HD12	1.98	0.62
8:V:166:ASP:OD1	8:V:168:GLY:N	2.26	0.62
6:T:159:GLY:N	7:U:65:THR:HG21	2.12	0.62
4:D:162:PHE:O	5:E:60:GLN:NE2	2.27	0.62
6:F:187:ARG:HH11	6:F:187:ARG:HA	1.65	0.62
14:N:37:ILE:HD11	14:N:43:CYS:HB3	1.82	0.62
2:P:11:ILE:HG22	3:Q:7:ILE:HD11	1.81	0.62
14:b:37:ILE:HD11	14:b:43:CYS:HB3	1.82	0.62
2:P:119:GLN:O	2:P:122:THR:HG22	1.99	0.62
4:D:125:GLU:N	4:D:125:GLU:OE1	2.33	0.61
7:U:2:SER:N	7:U:5:SER:HG	1.96	0.61
14:N:162:LEU:HD21	14:b:141:ALA:HB2	1.81	0.61
9:I:202:ARG:HH12	11:Y:191:ASN:HD21	1.48	0.61
4:R:125:GLU:OE1	4:R:125:GLU:N	2.33	0.61
7:U:4:GLY:N	7:U:19:GLU:OE2	2.33	0.61
4:R:41:GLN:NE2	4:R:151:PRO:O	2.33	0.61
6:T:187:ARG:HA	6:T:187:ARG:HH11	1.65	0.61
5:E:157:ARG:HD2	5:E:176:MET:CG	2.31	0.60
7:G:4:GLY:N	7:G:19:GLU:OE2	2.33	0.60
11:K:192:VAL:HG11	9:W:204:ASP:HB3	1.82	0.60
5:S:192:LEU:HD12	5:S:205:LEU:HD13	1.82	0.60
6:F:169:ARG:HH12	6:F:173:LYS:HZ1	1.48	0.60
5:E:192:LEU:HD12	5:E:205:LEU:HD13	1.82	0.60
13:M:51:LEU:HD21	13:M:110:MET:HE3	1.83	0.60
4:D:41:GLN:NE2	4:D:151:PRO:O	2.33	0.60
1:A:171:THR:O	1:A:174:GLU:HG3	2.01	0.60
5:S:157:ARG:HD2	5:S:176:MET:CG	2.31	0.60
1:O:171:THR:O	1:O:174:GLU:HG3	2.01	0.60
5:S:184:LEU:HD11	5:S:214:ILE:HD13	1.84	0.60
5:E:140:MET:HE3	13:M:80:GLY:HA3	1.84	0.60
3:C:104:VAL:HG11	3:C:143:ARG:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:184:LEU:HD11	5:E:214:ILE:HD13	1.84	0.60
12:L:145:LEU:HD21	12:L:182:ALA:HB2	1.84	0.60
12:Z:145:LEU:HD21	12:Z:182:ALA:HB2	1.84	0.59
2:B:11:ILE:HG22	3:C:7:ILE:HD11	1.83	0.59
8:H:106:THR:OG1	8:H:109:HIS:NE2	2.28	0.59
3:Q:132:LEU:HD12	3:Q:144:LEU:HD11	1.84	0.59
6:F:159:GLY:N	7:G:65:THR:HG21	2.12	0.59
3:Q:104:VAL:HG11	3:Q:143:ARG:CB	2.31	0.59
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.85	0.59
3:C:132:LEU:HD12	3:C:144:LEU:HD11	1.84	0.59
9:I:204:ASP:HB3	11:Y:192:VAL:HG11	1.85	0.59
13:a:51:LEU:HD21	13:a:110:MET:HE3	1.83	0.59
8:H:63:LEU:HD11	8:H:79:ALA:HB2	1.83	0.59
13:a:67:LEU:HD11	13:a:88:ILE:HD12	1.83	0.59
5:S:18:ARG:NE	5:S:23:GLU:OE2	2.32	0.59
5:S:115:LYS:NZ	5:S:128:TYR:OH	2.36	0.59
13:M:67:LEU:HD11	13:M:88:ILE:HD12	1.83	0.59
9:I:44:MET:HE3	9:I:66:LEU:HD22	1.85	0.58
11:K:191:ASN:HD21	9:W:202:ARG:HH12	1.49	0.58
6:T:75:MET:HE3	6:T:135:PHE:CD2	2.39	0.58
12:Z:31:GLU:OE1	12:Z:36:HIS:NE2	2.30	0.58
6:F:34:SER:OG	6:F:65:ARG:NH1	2.36	0.58
8:V:63:LEU:HD11	8:V:79:ALA:HB2	1.83	0.58
8:H:210:ALA:HB2	12:Z:159:GLN:HG3	1.85	0.58
5:E:18:ARG:NE	5:E:23:GLU:OE2	2.32	0.58
8:V:106:THR:OG1	8:V:109:HIS:NE2	2.28	0.58
5:E:88:MET:HG3	5:E:112:ILE:HD11	1.85	0.58
5:E:115:LYS:NZ	5:E:128:TYR:OH	2.36	0.58
5:E:133:LEU:HD11	5:E:161:ILE:HG12	1.86	0.58
6:F:75:MET:HE3	6:F:135:PHE:CD2	2.39	0.58
7:U:214:GLU:N	7:U:214:GLU:OE1	2.37	0.58
12:L:31:GLU:OE1	12:L:36:HIS:NE2	2.30	0.58
7:U:49:VAL:HG21	7:U:195:VAL:HG22	1.86	0.57
4:D:6:SER:OG	4:D:7:GLU:N	2.37	0.57
5:S:133:LEU:HD11	5:S:161:ILE:HG12	1.86	0.57
6:F:68:ASN:OD1	6:F:224:HIS:ND1	2.30	0.57
7:G:214:GLU:OE1	7:G:214:GLU:N	2.37	0.57
10:J:25:ILE:HD11	11:K:133:VAL:HG11	1.85	0.57
4:R:105:GLU:OE2	12:Z:75:TYR:OH	2.19	0.57
6:T:34:SER:OG	6:T:65:ARG:NH1	2.36	0.57
13:M:70:MET:HE1	13:M:91:TRP:NE1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:34:LYS:HD2	10:J:47:VAL:HG12	1.87	0.57
13:M:86:ARG:NH2	13:M:119:GLU:OE1	2.36	0.57
13:a:70:MET:HE1	13:a:91:TRP:NE1	2.20	0.57
1:A:145:LEU:HD22	1:A:157:TRP:HB2	1.87	0.57
9:I:10:VAL:HG23	9:I:53:ALA:HB2	1.87	0.57
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.85	0.57
8:V:219:LEU:HD11	9:W:194:ILE:HG13	1.86	0.57
11:Y:17:ASP:OD1	11:Y:33:LYS:NZ	2.36	0.57
9:W:44:MET:HE3	9:W:66:LEU:HD22	1.85	0.57
10:X:34:LYS:HD2	10:X:47:VAL:HG12	1.87	0.57
7:G:49:VAL:HG21	7:G:195:VAL:HG22	1.86	0.57
6:T:136:MET:HE2	6:T:163:CYS:HB3	1.87	0.57
1:A:74:VAL:HG22	1:A:75:TYR:H	1.70	0.56
8:V:40:ASN:OD1	8:V:41:ILE:HG13	2.05	0.56
1:O:74:VAL:HG22	1:O:75:TYR:H	1.70	0.56
1:O:145:LEU:HD22	1:O:157:TRP:HB2	1.87	0.56
6:T:68:ASN:OD1	6:T:224:HIS:ND1	2.30	0.56
6:F:136:MET:HE2	6:F:163:CYS:HB3	1.87	0.56
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.88	0.56
5:S:88:MET:HG3	5:S:112:ILE:HD11	1.86	0.56
2:B:165:GLY:O	2:B:168:SER:OG	2.15	0.56
9:W:10:VAL:HG23	9:W:53:ALA:HB2	1.87	0.56
5:E:105:VAL:HG21	5:E:136:GLY:HA3	1.88	0.55
4:R:178:GLN:O	4:R:182:GLN:HG3	2.06	0.55
12:Z:91:MET:O	12:Z:94:THR:HG22	2.06	0.55
4:D:178:GLN:O	4:D:182:GLN:HG3	2.06	0.55
1:A:37:ILE:HD13	1:A:159:ALA:HB1	1.89	0.55
4:D:105:GLU:OE2	12:L:75:TYR:OH	2.19	0.55
5:S:9:ASP:O	5:S:12:VAL:HG12	2.07	0.55
1:A:138:TRP:HE1	1:A:214:GLU:HG3	1.72	0.55
1:A:190:ALA:O	1:A:193:THR:HG22	2.07	0.55
3:C:23:GLN:O	3:C:26:VAL:HG12	2.07	0.55
6:F:120:HIS:O	6:F:123:THR:OG1	2.23	0.55
1:O:67:ILE:HD11	1:O:73:LEU:HD13	1.88	0.55
5:E:9:ASP:O	5:E:12:VAL:HG12	2.07	0.55
1:O:138:TRP:HE1	1:O:214:GLU:HG3	1.72	0.55
8:H:40:ASN:OD1	8:H:41:ILE:HG13	2.05	0.55
13:M:5:MET:HE2	13:M:5:MET:HA	1.89	0.55
7:U:62:ASP:O	7:U:65:THR:HG22	2.07	0.55
10:J:39:SER:OG	10:J:74:GLU:OE2	2.25	0.55
3:Q:116:GLN:O	3:Q:119:THR:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:140:MET:HE3	13:a:80:GLY:HA3	1.89	0.55
6:T:120:HIS:O	6:T:123:THR:OG1	2.23	0.55
1:A:68:THR:HG22	1:A:69:LYS:H	1.73	0.54
3:Q:23:GLN:O	3:Q:26:VAL:HG12	2.07	0.54
13:M:193:THR:HG22	13:M:194:GLU:H	1.72	0.54
10:X:25:ILE:HD11	11:Y:133:VAL:HG11	1.89	0.54
13:a:5:MET:HE2	13:a:5:MET:HA	1.89	0.54
1:A:67:ILE:HD11	1:A:73:LEU:HD13	1.88	0.54
12:L:91:MET:O	12:L:94:THR:HG22	2.06	0.54
3:C:116:GLN:O	3:C:119:THR:HG22	2.07	0.54
1:O:190:ALA:O	1:O:193:THR:HG22	2.07	0.54
4:R:59:MET:SD	4:R:64:ILE:HD11	2.48	0.54
5:S:105:VAL:HG21	5:S:136:GLY:HA3	1.88	0.54
7:G:62:ASP:O	7:G:65:THR:HG22	2.07	0.54
11:Y:8:PHE:CE2	11:Y:10:HIS:HB2	2.43	0.54
10:X:35:MET:HG2	10:X:45:LEU:HG	1.90	0.54
1:O:68:THR:HG22	1:O:69:LYS:H	1.72	0.54
3:Q:153:TYR:C	3:Q:154:HIS:HD2	2.16	0.54
1:O:37:ILE:HD13	1:O:159:ALA:HB1	1.89	0.54
14:b:14:LEU:HD23	14:b:44:CYS:SG	2.48	0.54
4:D:59:MET:SD	4:D:64:ILE:HD11	2.48	0.54
6:F:230:ASP:OD1	6:F:231:ILE:N	2.40	0.54
13:a:86:ARG:NH2	13:a:119:GLU:OE1	2.36	0.54
9:W:14:LYS:HG3	9:W:118:PRO:HB2	1.90	0.53
3:C:148:ASP:OD1	3:C:152:THR:OG1	2.25	0.53
3:C:229:VAL:O	3:C:232:ILE:HG22	2.08	0.53
11:K:8:PHE:CE2	11:K:10:HIS:HB2	2.43	0.53
1:O:15:SER:HB3	1:O:17:LYS:HE2	1.89	0.53
1:O:203:THR:HG22	1:O:205:ASP:H	1.74	0.53
3:Q:229:VAL:O	3:Q:232:ILE:HG22	2.08	0.53
6:T:230:ASP:OD1	6:T:231:ILE:N	2.40	0.53
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.90	0.53
11:Y:61:ARG:NH1	11:Y:62:GLN:OE1	2.42	0.53
12:L:194:ARG:HE	12:L:207:THR:HG22	1.74	0.53
3:Q:148:ASP:OD1	3:Q:152:THR:OG1	2.25	0.53
10:X:2:GLU:OE2	10:X:3:TYR:N	2.39	0.53
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.48	0.53
2:P:165:GLY:O	2:P:168:SER:OG	2.15	0.53
1:A:15:SER:HB3	1:A:17:LYS:HE2	1.89	0.53
9:I:14:LYS:HG3	9:I:118:PRO:HB2	1.90	0.53
10:J:8:GLN:NE2	10:J:9:GLY:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:35:MET:HG2	10:J:45:LEU:HG	1.90	0.53
5:E:22:ILE:HD11	5:E:120:THR:HG23	1.91	0.53
5:E:71:GLY:HA3	5:E:221:PHE:CZ	2.44	0.53
2:P:185:THR:HG23	2:P:188:SER:H	1.74	0.53
5:S:71:GLY:HA3	5:S:221:PHE:CZ	2.44	0.53
6:T:214:SER:HA	6:T:227:VAL:HG23	1.91	0.53
3:C:153:TYR:C	3:C:154:HIS:HD2	2.16	0.53
1:O:67:ILE:HG21	1:O:109:LEU:HD11	1.90	0.53
6:T:215:TRP:CD1	6:T:219:LEU:HD21	2.44	0.53
11:Y:48:GLY:N	11:Y:96:SER:O	2.37	0.53
6:F:215:TRP:CD1	6:F:219:LEU:HD21	2.44	0.52
13:a:193:THR:HG22	13:a:194:GLU:H	1.73	0.52
1:A:67:ILE:HG21	1:A:109:LEU:HD11	1.90	0.52
12:L:159:GLN:HG3	8:V:210:ALA:HB2	1.92	0.52
1:O:176:ARG:HH21	1:O:189:THR:HG22	1.74	0.52
5:S:157:ARG:HD2	5:S:176:MET:SD	2.50	0.52
11:Y:157:ARG:NH1	11:Y:188:SER:OG	2.43	0.52
10:X:39:SER:OG	10:X:74:GLU:OE2	2.25	0.52
2:B:185:THR:HG23	2:B:188:SER:H	1.74	0.52
5:E:192:LEU:HD11	5:E:210:VAL:HG11	1.91	0.52
8:H:164:PHE:O	12:Z:38:ARG:NH2	2.39	0.52
11:K:48:GLY:N	11:K:96:SER:O	2.37	0.52
8:H:78:THR:HG22	8:H:82:MET:HE2	1.92	0.52
11:K:17:ASP:OD1	11:K:33:LYS:NZ	2.36	0.52
11:K:157:ARG:NH1	11:K:188:SER:OG	2.43	0.52
3:Q:96:LEU:HD22	10:X:62:LYS:CD	2.38	0.52
6:F:214:SER:HA	6:F:227:VAL:HG23	1.91	0.52
1:A:176:ARG:HH21	1:A:189:THR:HG22	1.74	0.52
2:B:180:LYS:H	2:B:184:MET:HE2	1.75	0.52
11:K:160:ILE:O	11:K:164:THR:HG23	2.10	0.52
1:O:101:GLN:HE22	8:V:57:GLN:HG3	1.75	0.52
5:S:22:ILE:HD11	5:S:120:THR:HG23	1.91	0.52
11:K:61:ARG:NH1	11:K:62:GLN:OE1	2.42	0.52
12:L:71:ARG:NH1	12:L:95:ILE:HD11	2.25	0.52
2:P:197:LEU:HA	2:P:200:THR:HG22	1.91	0.52
9:W:134:ASP:OD1	9:W:135:PHE:N	2.40	0.52
3:C:36:ARG:HD2	3:C:142:PRO:O	2.09	0.52
5:E:157:ARG:HD2	5:E:176:MET:SD	2.50	0.52
8:H:30:ASN:OD1	8:H:187:ARG:NH1	2.42	0.52
8:V:30:ASN:OD1	8:V:187:ARG:NH1	2.42	0.52
10:X:18:ASP:HB3	10:X:175:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:14:LEU:HD21	14:b:101:ALA:HB3	1.91	0.52
10:J:18:ASP:HB3	10:J:175:LEU:HD23	1.91	0.52
10:X:153:ARG:NH2	10:X:184:ASP:OD2	2.42	0.52
5:E:58:ALA:O	5:E:59:HIS:HB2	2.10	0.51
10:J:153:ARG:NH2	10:J:184:ASP:OD2	2.42	0.51
14:N:127:ILE:HD11	14:N:136:TYR:CD1	2.46	0.51
5:S:58:ALA:O	5:S:59:HIS:HB2	2.10	0.51
7:U:234:GLU:N	7:U:234:GLU:OE1	2.42	0.51
1:A:203:THR:HG22	1:A:205:ASP:H	1.74	0.51
2:B:197:LEU:HA	2:B:200:THR:HG22	1.91	0.51
1:A:51:GLN:HG3	1:A:53:SER:O	2.10	0.51
14:N:40:ARG:NH1	14:N:183:GLY:HA2	2.23	0.51
1:O:51:GLN:HG3	1:O:53:SER:O	2.10	0.51
8:V:78:THR:HG22	8:V:82:MET:HE2	1.92	0.51
10:X:8:GLN:NE2	10:X:9:GLY:O	2.42	0.51
11:Y:160:ILE:O	11:Y:164:THR:HG23	2.10	0.51
12:Z:194:ARG:HE	12:Z:207:THR:HG22	1.74	0.51
14:b:127:ILE:HD11	14:b:136:TYR:CD1	2.46	0.51
7:G:147:GLN:OE1	7:G:147:GLN:N	2.43	0.51
9:W:29:ILE:O	9:W:32:GLN:N	2.43	0.51
8:H:195:LYS:HG3	12:Z:184:GLU:OE1	2.10	0.51
14:N:14:LEU:HD21	14:N:101:ALA:HB3	1.91	0.51
3:Q:36:ARG:HD2	3:Q:142:PRO:O	2.09	0.51
4:R:182:GLN:HG2	5:S:56:LEU:HD11	1.93	0.51
12:Z:71:ARG:NH1	12:Z:95:ILE:HD11	2.25	0.51
7:U:147:GLN:N	7:U:147:GLN:OE1	2.43	0.51
1:A:78:MET:HE2	1:A:81:ASP:OD1	2.11	0.51
7:G:35:GLY:O	7:G:37:LEU:HD12	2.11	0.51
7:G:234:GLU:N	7:G:234:GLU:OE1	2.42	0.51
12:L:38:ARG:NH2	8:V:164:PHE:O	2.39	0.51
5:S:192:LEU:HD11	5:S:210:VAL:HG11	1.91	0.51
14:b:40:ARG:NH1	14:b:183:GLY:HA2	2.23	0.51
8:H:219:LEU:HD11	9:I:194:ILE:HG13	1.92	0.51
7:U:35:GLY:O	7:U:37:LEU:HD12	2.11	0.51
13:M:190:ALA:HB2	13:M:199:ILE:HD13	1.93	0.51
2:P:180:LYS:H	2:P:184:MET:HE2	1.75	0.51
8:V:209:THR:HG21	9:W:167:SER:HB2	1.93	0.51
8:V:209:THR:HG22	9:W:168:GLN:NE2	2.21	0.51
12:L:57:PHE:HD2	12:L:60:ASP:OD1	1.95	0.50
7:G:31:ALA:HB1	7:G:83:MET:HE2	1.94	0.50
1:O:169:GLY:O	1:O:173:LEU:HD13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLY:O	1:A:173:LEU:HD13	2.12	0.50
1:O:68:THR:HG22	1:O:69:LYS:N	2.26	0.50
10:X:63:ASN:C	10:X:63:ASN:HD22	2.17	0.50
12:Z:57:PHE:HD2	12:Z:60:ASP:OD1	1.95	0.50
1:A:68:THR:HG22	1:A:69:LYS:N	2.26	0.50
5:S:157:ARG:HD2	5:S:176:MET:HG3	1.93	0.50
13:a:190:ALA:HB2	13:a:199:ILE:HD13	1.93	0.50
7:U:31:ALA:HB1	7:U:83:MET:HE2	1.94	0.50
13:a:25:ASP:HA	13:a:187:PHE:HA	1.94	0.50
5:E:172:LEU:O	5:E:176:MET:HB2	2.12	0.50
13:M:50:MET:HE2	13:M:192:VAL:HB	1.94	0.50
9:I:29:ILE:O	9:I:32:GLN:N	2.43	0.50
1:O:78:MET:HE2	1:O:81:ASP:OD1	2.11	0.50
10:X:1:MET:HE2	10:X:133:GLY:HA2	1.93	0.50
11:K:133:VAL:HG21	10:X:137:PHE:HB3	1.94	0.50
6:T:90:ILE:HG13	6:T:118:TYR:CE1	2.47	0.50
6:T:169:ARG:HH12	6:T:173:LYS:HZ1	1.60	0.50
6:T:190:VAL:HG11	6:T:215:TRP:CZ3	2.46	0.50
10:X:1:MET:HG2	10:X:134:TYR:CD2	2.47	0.50
5:E:157:ARG:HD2	5:E:176:MET:HG3	1.93	0.49
6:F:90:ILE:HG13	6:F:118:TYR:CE1	2.47	0.49
10:J:1:MET:HG2	10:J:134:TYR:CD2	2.47	0.49
6:T:68:ASN:C	13:a:76:LEU:HD12	2.37	0.49
5:E:192:LEU:HB3	5:E:236:LEU:HD21	1.94	0.49
5:S:192:LEU:HB3	5:S:236:LEU:HD21	1.94	0.49
9:W:140:THR:HG21	9:W:179:VAL:HG23	1.94	0.49
1:A:54:ILE:HG22	7:G:180:GLU:HG2	1.95	0.49
6:F:190:VAL:HG11	6:F:215:TRP:CZ3	2.46	0.49
9:I:140:THR:HG21	9:I:179:VAL:HG23	1.94	0.49
6:T:38:GLY:N	6:T:136:MET:HE1	2.27	0.49
12:Z:68:ILE:HD11	12:Z:92:LEU:HD13	1.94	0.49
5:S:172:LEU:O	5:S:176:MET:HB2	2.12	0.49
10:J:1:MET:HE2	10:J:133:GLY:HA2	1.93	0.49
6:T:70:ASP:CG	6:T:99:ARG:HH22	2.21	0.49
10:X:77:PRO:HD2	10:X:108:ASP:HB2	1.95	0.49
10:J:2:GLU:OE2	10:J:3:TYR:N	2.39	0.49
14:N:52:THR:HA	14:N:55:VAL:HG12	1.95	0.49
9:W:177:ASP:OD1	9:W:180:SER:N	2.46	0.49
13:a:50:MET:HE2	13:a:192:VAL:HB	1.94	0.49
4:D:92:ALA:O	4:D:96:THR:HG23	2.12	0.49
4:R:92:ALA:O	4:R:96:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:MET:SD	2:B:196:VAL:HG22	2.52	0.49
3:C:23:GLN:HA	3:C:26:VAL:HG12	1.95	0.49
1:O:92:LEU:HD13	1:O:112:ARG:HB3	1.95	0.49
6:T:90:ILE:HG21	6:T:118:TYR:CD1	2.48	0.49
3:C:30:SER:HB3	3:C:48:LYS:NZ	2.28	0.49
6:F:38:GLY:N	6:F:136:MET:HE1	2.27	0.49
2:P:174:MET:SD	2:P:196:VAL:HG22	2.52	0.49
3:Q:30:SER:HB3	3:Q:48:LYS:NZ	2.28	0.49
5:S:107:ARG:NH2	13:a:81:HIS:HB2	2.28	0.49
6:F:70:ASP:CG	6:F:99:ARG:HH22	2.21	0.48
13:M:25:ASP:HA	13:M:187:PHE:HA	1.94	0.48
14:b:52:THR:HA	14:b:55:VAL:HG12	1.95	0.48
1:A:92:LEU:HD13	1:A:112:ARG:HB3	1.95	0.48
5:E:50:LYS:HB3	5:E:59:HIS:HB3	1.94	0.48
3:Q:23:GLN:HA	3:Q:26:VAL:HG12	1.95	0.48
10:X:17:SER:HB2	10:X:34:LYS:HE2	1.94	0.48
12:L:68:ILE:HD11	12:L:92:LEU:HD13	1.94	0.48
13:a:187:PHE:HE1	13:a:205:THR:HG23	1.78	0.48
6:F:70:ASP:CA	13:M:76:LEU:HD11	2.44	0.48
10:J:63:ASN:C	10:J:63:ASN:HD22	2.17	0.48
1:O:138:TRP:NE1	1:O:214:GLU:HG3	2.28	0.48
1:O:197:SER:O	1:O:197:SER:OG	2.29	0.48
4:R:40:ILE:HD11	4:R:181:LEU:HD22	1.95	0.48
2:B:174:MET:HE1	2:B:199:LYS:HD2	1.95	0.48
4:D:40:ILE:HD11	4:D:181:LEU:HD22	1.95	0.48
8:H:209:THR:HG21	9:I:167:SER:HB2	1.96	0.48
9:I:177:ASP:OD1	9:I:180:SER:N	2.46	0.48
10:J:17:SER:HB2	10:J:34:LYS:HE2	1.94	0.48
12:L:184:GLU:OE1	8:V:195:LYS:HG3	2.12	0.48
13:M:187:PHE:HE1	13:M:205:THR:HG23	1.78	0.48
4:R:91:LYS:HG2	4:R:119:LEU:HD11	1.95	0.48
1:A:138:TRP:NE1	1:A:214:GLU:HG3	2.28	0.48
10:J:137:PHE:HB3	11:Y:133:VAL:HG21	1.96	0.48
2:P:174:MET:HE1	2:P:199:LYS:HD2	1.95	0.48
4:R:125:GLU:HG2	4:R:126:GLU:OE1	2.14	0.48
5:E:107:ARG:NH2	13:M:81:HIS:HB2	2.29	0.48
6:F:90:ILE:HG21	6:F:118:TYR:CD1	2.48	0.48
9:I:134:ASP:OD1	9:I:135:PHE:N	2.40	0.48
10:J:168:GLN:NE2	10:J:178:PHE:HE1	2.12	0.48
11:K:4:LEU:HD13	11:K:139:MET:HE2	1.95	0.48
12:L:64:LEU:HD22	12:L:106:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:57:TYR:CD2	14:N:119:MET:HE3	2.49	0.48
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.94	0.48
10:X:168:GLN:NE2	10:X:178:PHE:HE1	2.12	0.48
1:A:101:GLN:HE22	8:H:57:GLN:HG3	1.79	0.48
1:O:35:VAL:HG11	1:O:193:THR:HG21	1.96	0.48
1:O:55:LEU:HD12	7:U:176:THR:HG23	1.96	0.48
6:T:203:GLU:OE1	6:T:203:GLU:N	2.44	0.48
8:V:29:LYS:NZ	9:W:150:GLU:OE2	2.38	0.48
3:C:153:TYR:C	3:C:154:HIS:CD2	2.92	0.48
10:J:77:PRO:HD2	10:J:108:ASP:HB2	1.95	0.48
1:A:35:VAL:HG11	1:A:193:THR:HG21	1.96	0.47
2:B:46:ALA:HB1	2:B:197:LEU:HD11	1.95	0.47
4:D:102:THR:HG23	12:L:94:THR:HG21	1.96	0.47
8:H:123:PRO:HB3	13:a:214:MET:SD	2.54	0.47
8:H:144:PRO:HB3	13:a:214:MET:HE1	1.95	0.47
4:D:91:LYS:HG2	4:D:119:LEU:HD11	1.95	0.47
4:D:125:GLU:HG2	4:D:126:GLU:OE1	2.14	0.47
6:F:37:ILE:HD11	6:F:193:VAL:HG13	1.96	0.47
12:Z:64:LEU:HD22	12:Z:106:VAL:HG21	1.95	0.47
14:b:134:TYR:N	14:b:134:TYR:CD2	2.81	0.47
3:C:168:VAL:O	3:C:172:LEU:HD23	2.14	0.47
6:F:68:ASN:C	13:M:76:LEU:HD12	2.39	0.47
12:L:38:ARG:NH1	12:L:191:ASP:OD1	2.45	0.47
1:O:54:ILE:HG22	7:U:180:GLU:HG2	1.96	0.47
14:N:134:TYR:N	14:N:134:TYR:CD2	2.81	0.47
2:P:140:ASP:OD1	2:P:146:GLN:NE2	2.46	0.47
3:Q:168:VAL:O	3:Q:172:LEU:HD23	2.14	0.47
5:S:72:ILE:HG21	5:S:88:MET:HE1	1.96	0.47
7:U:51:VAL:HG22	7:U:217:VAL:HG22	1.96	0.47
4:D:182:GLN:HG2	5:E:56:LEU:HD11	1.97	0.47
2:P:46:ALA:HB1	2:P:197:LEU:HD11	1.95	0.47
3:Q:40:ILE:HG21	3:Q:187:THR:HG21	1.96	0.47
11:Y:4:LEU:HD13	11:Y:139:MET:HE2	1.95	0.47
2:B:140:ASP:OD1	2:B:146:GLN:NE2	2.46	0.47
12:Z:96:LEU:HD23	12:Z:126:PRO:O	2.15	0.47
1:A:21:ILE:HD11	1:A:121:THR:HG21	1.97	0.47
1:A:57:ASP:OD1	1:A:59:ARG:HG2	2.14	0.47
3:C:40:ILE:HG21	3:C:187:THR:HG21	1.96	0.47
5:E:72:ILE:HG21	5:E:88:MET:HE1	1.96	0.47
6:F:75:MET:HE3	6:F:135:PHE:CG	2.50	0.47
7:G:137:CYS:SG	7:G:153:LYS:HD2	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:9:ARG:HG3	11:K:9:ARG:HH11	1.79	0.47
13:M:214:MET:SD	8:V:123:PRO:HB3	2.55	0.47
1:O:57:ASP:OD1	1:O:59:ARG:HG2	2.14	0.47
2:P:51:ASN:HB3	2:P:56:LEU:CD2	2.44	0.47
2:P:174:MET:CE	2:P:199:LYS:HD2	2.45	0.47
6:T:37:ILE:HD11	6:T:193:VAL:HG13	1.96	0.47
13:a:57:TYR:CD2	14:b:119:MET:HE3	2.49	0.47
1:O:35:VAL:HG21	1:O:193:THR:HG23	1.97	0.47
10:X:64:VAL:HG13	10:X:75:LEU:HD12	1.97	0.47
7:G:231:THR:HG22	7:G:232:GLU:N	2.30	0.47
7:U:231:THR:HG22	7:U:232:GLU:N	2.30	0.47
7:G:51:VAL:HG22	7:G:217:VAL:HG22	1.96	0.46
9:W:141:CYS:SG	9:W:145:MET:HE2	2.55	0.46
13:M:193:THR:HG22	13:M:194:GLU:N	2.31	0.46
3:Q:153:TYR:C	3:Q:154:HIS:CD2	2.92	0.46
6:T:75:MET:HE3	6:T:135:PHE:CG	2.50	0.46
7:U:146:GLU:HB2	7:U:147:GLN:OE1	2.15	0.46
3:C:193:LYS:HG3	3:C:232:ILE:HD11	1.97	0.46
5:E:64:LEU:HD13	5:E:74:ILE:HD12	1.96	0.46
11:K:8:PHE:CE1	11:K:13:ILE:HG12	2.46	0.46
7:U:137:CYS:SG	7:U:153:LYS:HD2	2.55	0.46
6:F:13:THR:HG22	7:G:12:HIS:O	2.16	0.46
12:L:123:SER:HB3	12:L:136:LYS:HG2	1.96	0.46
1:O:49:LYS:O	1:O:206:ASN:HB2	2.16	0.46
1:A:49:LYS:O	1:A:206:ASN:HB2	2.16	0.46
10:J:63:ASN:O	10:J:63:ASN:ND2	2.45	0.46
10:J:64:VAL:HG13	10:J:75:LEU:HD12	1.97	0.46
11:K:83:LEU:HD11	11:K:97:MET:HE1	1.97	0.46
12:L:96:LEU:HD23	12:L:126:PRO:O	2.15	0.46
14:N:70:LEU:O	14:N:72:GLU:HG3	2.15	0.46
5:S:64:LEU:HD13	5:S:74:ILE:HD12	1.96	0.46
6:T:215:TRP:CZ3	6:T:227:VAL:HG22	2.51	0.46
1:A:218:ARG:HG2	1:A:218:ARG:HH11	1.81	0.46
2:B:174:MET:CE	2:B:199:LYS:HD2	2.45	0.46
13:M:171:ARG:NH2	8:V:140:ASP:OD2	2.41	0.46
1:O:21:ILE:HD11	1:O:121:THR:HG21	1.97	0.46
11:Y:9:ARG:HG3	11:Y:9:ARG:HH11	1.79	0.46
9:I:141:CYS:SG	9:I:145:MET:HE2	2.55	0.46
4:R:195:ILE:O	4:R:199:LEU:HD23	2.16	0.46
10:X:63:ASN:O	10:X:63:ASN:ND2	2.45	0.46
11:Y:83:LEU:HD11	11:Y:97:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:123:SER:HB3	12:Z:136:LYS:HG2	1.96	0.46
12:Z:123:SER:CB	12:Z:136:LYS:HG2	2.46	0.46
9:I:150:GLU:HG3	12:Z:185:ARG:CG	2.46	0.46
1:O:43:VAL:HB	1:O:212:CYS:SG	2.56	0.46
2:B:51:ASN:HB3	2:B:56:LEU:CD2	2.44	0.46
6:F:203:GLU:OE1	6:F:203:GLU:N	2.44	0.46
7:G:146:GLU:HB2	7:G:147:GLN:OE1	2.15	0.46
1:A:43:VAL:HB	1:A:212:CYS:SG	2.56	0.46
9:I:66:LEU:HD11	9:I:90:VAL:HG22	1.98	0.46
9:I:66:LEU:CD1	9:I:90:VAL:HG22	2.46	0.46
1:O:101:GLN:OE1	8:V:57:GLN:NE2	2.48	0.46
6:T:70:ASP:CA	13:a:76:LEU:HD11	2.46	0.46
9:W:66:LEU:CD1	9:W:90:VAL:HG22	2.46	0.46
13:a:193:THR:HG22	13:a:194:GLU:N	2.31	0.46
4:D:51:GLU:HB2	4:D:206:MET:HE2	1.99	0.45
12:L:36:HIS:HB3	13:M:132:TYR:CZ	2.51	0.45
13:M:214:MET:HE1	8:V:144:PRO:HB3	1.98	0.45
3:Q:193:LYS:HG3	3:Q:232:ILE:HD11	1.97	0.45
6:T:13:THR:HG22	7:U:12:HIS:O	2.16	0.45
6:T:108:LEU:HD22	6:T:139:SER:HB3	1.98	0.45
6:F:108:LEU:HD22	6:F:139:SER:HB3	1.98	0.45
6:F:237:LYS:HG3	6:F:241:GLU:OE2	2.16	0.45
6:T:237:LYS:HG3	6:T:241:GLU:OE2	2.16	0.45
1:A:55:LEU:HD12	7:G:176:THR:HG23	1.98	0.45
4:D:117:SER:OG	4:D:160:GLY:O	2.33	0.45
4:D:195:ILE:O	4:D:199:LEU:HD23	2.16	0.45
2:P:229:LYS:HB2	2:P:232:GLU:OE1	2.17	0.45
9:W:11:MET:HE3	9:W:149:CYS:SG	2.57	0.45
9:W:46:ASP:O	9:W:194:ILE:HD11	2.16	0.45
14:b:70:LEU:O	14:b:72:GLU:HG3	2.16	0.45
1:A:35:VAL:HG21	1:A:193:THR:HG23	1.97	0.45
12:L:123:SER:CB	12:L:136:LYS:HG2	2.46	0.45
1:O:218:ARG:HG2	1:O:218:ARG:HH11	1.81	0.45
4:R:52:LYS:HE3	4:R:52:LYS:HB2	1.81	0.45
9:W:66:LEU:HD11	9:W:90:VAL:HG22	1.98	0.45
12:Z:58:HIS:NE2	12:Z:62:LEU:HD11	2.31	0.45
2:B:229:LYS:HB2	2:B:232:GLU:OE1	2.17	0.45
5:E:166:GLN:O	5:E:170:THR:HG23	2.17	0.45
6:F:215:TRP:CZ3	6:F:227:VAL:HG22	2.51	0.45
8:H:201:ARG:HD2	8:H:201:ARG:HA	1.75	0.45
12:L:58:HIS:NE2	12:L:62:LEU:HD11	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:188:VAL:O	5:S:192:LEU:HD23	2.17	0.45
5:E:88:MET:CG	5:E:112:ILE:HD11	2.47	0.45
6:F:241:GLU:O	6:F:244:LYS:HB2	2.17	0.45
8:H:139:GLU:OE2	8:H:139:GLU:HA	2.17	0.45
9:I:46:ASP:O	9:I:194:ILE:HD11	2.16	0.45
2:P:53:HIS:HB3	2:P:56:LEU:CD1	2.47	0.45
4:R:102:THR:HG23	12:Z:94:THR:HG21	1.99	0.45
10:X:185:LYS:HB3	10:X:185:LYS:HE3	1.82	0.45
4:D:121:LEU:HA	4:D:123:PHE:CE2	2.53	0.44
7:G:66:VAL:O	7:G:66:VAL:HG13	2.17	0.44
9:I:11:MET:HE3	9:I:149:CYS:SG	2.57	0.44
2:P:209:GLU:OE1	2:P:209:GLU:O	2.35	0.44
6:T:241:GLU:O	6:T:244:LYS:HB2	2.17	0.44
7:U:21:ARG:HH21	7:U:26:GLU:CD	2.24	0.44
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.17	0.44
11:Y:8:PHE:CE1	11:Y:13:ILE:HG12	2.46	0.44
2:B:53:HIS:HB3	2:B:56:LEU:CD1	2.48	0.44
4:D:202:LEU:HB3	4:D:206:MET:HE3	2.00	0.44
4:R:51:GLU:HB2	4:R:206:MET:HE2	1.99	0.44
5:S:166:GLN:O	5:S:170:THR:HG23	2.17	0.44
13:a:43:MET:HE3	13:a:45:VAL:HG22	2.00	0.44
5:E:212:ILE:HD12	5:E:229:VAL:HG23	1.99	0.44
8:H:209:THR:HG22	9:I:168:GLN:NE2	2.23	0.44
2:B:6:ASP:OD2	2:B:7:SER:N	2.51	0.44
4:D:70:ILE:HD11	4:D:89:ILE:HD12	2.00	0.44
7:G:144:ASP:CB	7:G:150:GLN:HE21	2.26	0.44
9:W:3:MET:HE1	9:W:105:GLU:OE1	2.18	0.44
12:Z:125:ASP:OD2	12:Z:129:SER:N	2.51	0.44
3:C:98:VAL:HG13	11:K:78:ALA:HB2	1.99	0.44
5:E:62:LYS:HA	5:E:62:LYS:HD2	1.80	0.44
7:G:21:ARG:HH21	7:G:26:GLU:CD	2.24	0.44
8:H:209:THR:HG23	9:I:164:GLU:OE1	2.18	0.44
12:L:125:ASP:OD2	12:L:129:SER:N	2.51	0.44
4:R:202:LEU:HD22	4:R:206:MET:HE3	2.00	0.44
4:D:107:MET:HE2	4:D:111:SER:C	2.43	0.44
5:E:224:TYR:HD2	5:E:232:PHE:HE2	1.65	0.44
12:L:68:ILE:O	12:L:72:LEU:HD13	2.18	0.44
12:L:148:LEU:HD13	9:W:151:SER:HB2	2.00	0.44
10:X:86:ARG:HE	10:X:86:ARG:HA	1.83	0.44
10:J:88:LEU:HD12	10:J:88:LEU:HA	1.81	0.44
4:R:70:ILE:HD11	4:R:89:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:TYR:HA	2:B:184:MET:HE3	1.99	0.44
3:C:171:PHE:HZ	3:C:193:LYS:HD2	1.83	0.44
14:N:12:VAL:HG21	14:N:101:ALA:HB1	2.00	0.44
4:R:6:SER:OG	4:R:7:GLU:N	2.37	0.44
12:Z:38:ARG:NH1	12:Z:191:ASP:OD1	2.45	0.44
13:a:96:MET:HE3	13:a:127:MET:HA	2.00	0.44
1:A:75:TYR:HB2	1:A:131:VAL:HG13	2.00	0.43
2:B:76:VAL:HG11	2:B:83:ALA:HB1	2.00	0.43
5:E:188:VAL:O	5:E:192:LEU:HD23	2.17	0.43
6:F:38:GLY:H	6:F:136:MET:HE1	1.83	0.43
6:F:169:ARG:NH1	6:F:173:LYS:HZ1	2.14	0.43
2:P:6:ASP:OD2	2:P:7:SER:N	2.51	0.43
4:R:121:LEU:HD12	5:S:79:ALA:HB3	2.00	0.43
1:A:73:LEU:HD21	1:A:86:VAL:HG22	2.00	0.43
3:C:68:ASN:CA	3:C:211:MET:HE1	2.46	0.43
13:M:63:LEU:HD13	13:M:110:MET:SD	2.58	0.43
5:S:52:ALA:HB1	5:S:57:ALA:HB3	2.00	0.43
5:S:212:ILE:HD12	5:S:229:VAL:HG23	1.99	0.43
14:b:107:GLU:HB2	14:b:110:GLN:NE2	2.33	0.43
6:F:168:ALA:HB1	6:F:200:VAL:HG22	2.00	0.43
7:G:88:ARG:HD2	7:G:88:ARG:HA	1.84	0.43
12:L:26:ASP:OD1	12:L:189:THR:HA	2.18	0.43
13:M:96:MET:HE3	13:M:127:MET:HA	2.00	0.43
4:R:121:LEU:HA	4:R:123:PHE:CE2	2.53	0.43
4:R:235:GLU:O	4:R:239:LYS:HG2	2.19	0.43
6:T:38:GLY:H	6:T:136:MET:HE1	1.83	0.43
12:Z:36:HIS:HB3	13:a:132:TYR:CZ	2.53	0.43
2:B:209:GLU:O	2:B:209:GLU:OE1	2.35	0.43
5:E:52:ALA:HB1	5:E:57:ALA:HB3	2.00	0.43
9:I:151:SER:HB2	12:Z:148:LEU:HD13	2.00	0.43
13:M:187:PHE:CE1	13:M:205:THR:HG23	2.54	0.43
13:M:209:TRP:CH2	14:b:172:GLY:HA2	2.54	0.43
14:N:107:GLU:HB2	14:N:110:GLN:NE2	2.33	0.43
3:Q:171:PHE:HZ	3:Q:193:LYS:HD2	1.83	0.43
7:U:208:ILE:O	7:U:209:ASP:HB2	2.19	0.43
2:B:161:ALA:HB1	2:B:175:LEU:HD13	2.00	0.43
13:M:6:VAL:HA	13:M:29:SER:O	2.18	0.43
7:U:66:VAL:O	7:U:66:VAL:HG13	2.17	0.43
1:A:202:MET:CE	1:A:207:ILE:HG21	2.48	0.43
8:H:29:LYS:NZ	9:I:150:GLU:OE2	2.40	0.43
13:M:43:MET:HE3	13:M:45:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:202:LEU:HB3	4:R:206:MET:HE3	2.00	0.43
5:S:224:TYR:HD2	5:S:232:PHE:HE2	1.65	0.43
8:V:201:ARG:HD2	8:V:201:ARG:HA	1.75	0.43
1:A:121:THR:O	1:A:121:THR:HG22	2.19	0.43
1:A:138:TRP:CD1	1:A:214:GLU:HA	2.53	0.43
9:I:13:MET:HB3	9:I:162:LEU:HD11	2.01	0.43
14:N:8:PHE:HB3	14:N:152:CYS:SG	2.59	0.43
1:O:33:PRO:HD2	1:O:48:GLU:HG2	2.01	0.43
2:P:76:VAL:HG11	2:P:83:ALA:HB1	1.99	0.43
4:R:107:MET:HE2	4:R:111:SER:C	2.43	0.43
11:Y:45:MET:HB3	15:Y:301:YHD:C11	2.48	0.43
1:A:188:HIS:O	1:A:192:LEU:HD23	2.19	0.43
4:D:165:CYS:CB	4:D:168:ARG:HG3	2.48	0.43
12:L:185:ARG:CG	9:W:150:GLU:HG3	2.49	0.43
1:O:73:LEU:HD21	1:O:86:VAL:HG22	2.00	0.43
6:T:113:ASP:CG	7:U:88:ARG:HH21	2.26	0.43
4:D:235:GLU:O	4:D:239:LYS:HG2	2.19	0.43
9:I:3:MET:HE1	9:I:105:GLU:OE1	2.18	0.43
10:J:86:ARG:HE	10:J:86:ARG:HA	1.83	0.43
1:O:138:TRP:CD1	1:O:214:GLU:HA	2.53	0.43
10:X:43:LEU:HD12	10:X:183:ILE:HD11	2.01	0.43
12:Z:68:ILE:O	12:Z:72:LEU:HD13	2.18	0.43
13:a:63:LEU:HD13	13:a:110:MET:SD	2.58	0.43
14:b:8:PHE:HB3	14:b:152:CYS:SG	2.59	0.43
5:E:192:LEU:HD21	5:E:212:ILE:HD11	1.99	0.43
9:I:11:MET:SD	9:I:145:MET:HG2	2.59	0.43
1:O:202:MET:CE	1:O:207:ILE:HG21	2.48	0.43
2:P:161:ALA:HB1	2:P:175:LEU:HD13	2.00	0.43
5:S:88:MET:CG	5:S:112:ILE:HD11	2.47	0.43
5:S:192:LEU:HD21	5:S:212:ILE:HD11	1.99	0.43
6:T:168:ALA:HB1	6:T:200:VAL:HG22	2.00	0.43
9:W:13:MET:HB3	9:W:162:LEU:HD11	2.01	0.43
13:a:6:VAL:HA	13:a:29:SER:O	2.18	0.43
13:a:214:MET:O	13:a:214:MET:HG2	2.19	0.43
4:D:202:LEU:HD22	4:D:206:MET:HE3	2.00	0.42
5:E:63:ILE:C	5:E:64:LEU:HD12	2.44	0.42
8:H:78:THR:HG22	8:H:82:MET:CE	2.49	0.42
11:K:45:MET:HB3	15:K:301:YHD:C11	2.48	0.42
13:M:214:MET:O	13:M:214:MET:HG2	2.19	0.42
14:N:161:ALA:HA	14:N:164:MET:HE3	2.01	0.42
4:R:117:SER:OG	4:R:160:GLY:O	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:165:CYS:CB	4:R:168:ARG:HG3	2.48	0.42
9:W:11:MET:SD	9:W:145:MET:HG2	2.59	0.42
11:Y:5:ALA:N	11:Y:100:MET:HE1	2.34	0.42
14:b:133:SER:HA	14:b:136:TYR:CD2	2.54	0.42
2:P:179:TYR:HA	2:P:184:MET:HE3	2.00	0.42
8:V:78:THR:HG22	8:V:82:MET:CE	2.49	0.42
9:W:141:CYS:HB3	9:W:177:ASP:OD2	2.19	0.42
14:b:12:VAL:HG21	14:b:101:ALA:HB1	2.00	0.42
1:A:41:ASN:OD1	1:A:183:LEU:HB2	2.19	0.42
9:I:150:GLU:HG3	12:Z:185:ARG:HG2	2.01	0.42
3:Q:26:VAL:HG23	3:Q:74:ALA:O	2.19	0.42
8:V:59:ILE:HG13	8:V:83:LEU:CD2	2.49	0.42
12:Z:26:ASP:OD1	12:Z:189:THR:HA	2.18	0.42
13:a:187:PHE:CE1	13:a:205:THR:HG23	2.54	0.42
7:G:208:ILE:O	7:G:209:ASP:HB2	2.19	0.42
10:J:185:LYS:HE3	10:J:185:LYS:HB3	1.82	0.42
1:O:195:LYS:HA	1:O:198:PHE:HB2	2.02	0.42
4:D:202:LEU:HD23	4:D:202:LEU:HA	1.87	0.42
9:I:202:ARG:NH2	9:I:204:ASP:OD2	2.43	0.42
11:K:5:ALA:N	11:K:100:MET:HE1	2.34	0.42
14:N:1:THR:OG1	14:N:33:LYS:NZ	2.46	0.42
3:Q:94:HIS:CG	3:Q:102:VAL:HG12	2.54	0.42
6:T:64:LYS:HE3	6:T:64:LYS:HB2	1.79	0.42
7:U:56:VAL:HG12	7:U:66:VAL:HG11	2.01	0.42
8:V:63:LEU:CD2	8:V:82:MET:HE1	2.50	0.42
11:Y:83:LEU:HD21	11:Y:99:THR:HG21	2.02	0.42
3:C:26:VAL:HG23	3:C:74:ALA:O	2.19	0.42
4:D:51:GLU:HA	4:D:206:MET:HE2	2.01	0.42
9:I:141:CYS:HB3	9:I:177:ASP:OD2	2.19	0.42
10:J:170:ARG:HH21	11:Y:140:ASP:CG	2.26	0.42
14:N:133:SER:HA	14:N:136:TYR:CD2	2.54	0.42
1:O:75:TYR:HB2	1:O:131:VAL:HG13	2.00	0.42
9:W:137:VAL:HG11	9:W:145:MET:HB3	2.02	0.42
10:X:38:MET:HE3	10:X:38:MET:HB3	1.90	0.42
11:Y:139:MET:O	11:Y:143:TYR:N	2.52	0.42
1:A:90:ARG:HB3	8:H:65:LEU:HD21	2.00	0.42
1:A:172:PHE:O	1:A:175:LYS:HG2	2.20	0.42
2:B:4:ARG:HD2	2:B:5:TYR:CZ	2.55	0.42
3:C:94:HIS:CG	3:C:102:VAL:HG12	2.54	0.42
8:H:159:ILE:O	8:H:163:ILE:HG13	2.20	0.42
11:K:1:THR:OG1	15:K:301:YHD:C09	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:139:MET:O	11:K:143:TYR:N	2.52	0.42
1:O:83:ARG:NH2	7:U:158:GLY:O	2.45	0.42
1:O:121:THR:O	1:O:121:THR:HG22	2.19	0.42
2:P:68:LEU:HD11	2:P:74:CYS:HB3	2.01	0.42
14:b:161:ALA:HA	14:b:164:MET:HE3	2.01	0.42
1:A:195:LYS:HA	1:A:198:PHE:HB2	2.02	0.42
3:C:40:ILE:CG2	3:C:187:THR:HG21	2.50	0.42
10:J:63:ASN:C	10:J:63:ASN:ND2	2.78	0.42
11:K:83:LEU:HD21	11:K:99:THR:HG21	2.02	0.42
1:A:8:SER:OG	1:A:10:THR:O	2.38	0.42
8:H:63:LEU:CD2	8:H:82:MET:HE1	2.50	0.42
9:I:137:VAL:HG11	9:I:145:MET:HB3	2.02	0.42
3:Q:68:ASN:CA	3:Q:211:MET:HE1	2.46	0.42
4:R:91:LYS:HA	4:R:94:VAL:HG12	2.01	0.42
5:S:63:ILE:C	5:S:64:LEU:HD12	2.44	0.42
6:T:136:MET:CE	6:T:163:CYS:HB3	2.50	0.42
11:Y:35:ILE:HD11	11:Y:45:MET:HE1	2.02	0.42
2:B:38:LEU:HD12	2:B:43:VAL:HG22	2.02	0.42
8:H:113:ILE:HG12	8:H:119:THR:HG22	2.02	0.42
14:N:133:SER:HA	14:N:136:TYR:HD2	1.84	0.42
2:P:4:ARG:HD2	2:P:5:TYR:CZ	2.55	0.42
7:U:144:ASP:CB	7:U:150:GLN:HE21	2.26	0.42
2:B:68:LEU:HD11	2:B:74:CYS:HB3	2.01	0.41
3:C:31:THR:HA	3:C:161:ILE:O	2.20	0.41
5:E:39:LYS:HE2	5:E:157:ARG:HA	2.02	0.41
8:H:59:ILE:HD12	8:H:82:MET:HB3	2.02	0.41
9:I:204:ASP:HB2	11:Y:171:GLY:HA3	2.02	0.41
10:J:34:LYS:HE2	10:J:34:LYS:HB2	1.87	0.41
2:P:48:GLU:HG3	2:P:201:MET:HE2	2.01	0.41
5:S:103:LEU:HD12	5:S:104:PRO:HD2	2.02	0.41
8:V:59:ILE:HD12	8:V:82:MET:HB3	2.02	0.41
8:V:187:ARG:HA	8:V:188:PRO:HA	1.87	0.41
11:Y:35:ILE:HD11	11:Y:45:MET:CE	2.50	0.41
6:F:36:ALA:CB	6:F:49:VAL:HG12	2.50	0.41
7:G:231:THR:HB	7:G:234:GLU:OE1	2.20	0.41
8:H:187:ARG:HA	8:H:188:PRO:HA	1.87	0.41
10:J:43:LEU:HD12	10:J:183:ILE:HD11	2.01	0.41
12:L:104:TYR:HB3	12:L:106:VAL:HG22	2.02	0.41
14:N:172:GLY:HA2	13:a:209:TRP:CH2	2.54	0.41
1:O:80:PRO:HG2	7:U:157:ALA:O	2.20	0.41
2:P:38:LEU:HD12	2:P:43:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:39:LYS:HE2	5:S:157:ARG:HA	2.02	0.41
5:S:160:SER:C	5:S:165:SER:HG	2.27	0.41
11:Y:33:LYS:HA	11:Y:45:MET:HG2	2.02	0.41
2:B:3:ARG:HH12	4:D:9:ASP:C	2.28	0.41
7:G:56:VAL:HG12	7:G:66:VAL:HG11	2.01	0.41
8:H:59:ILE:HG13	8:H:83:LEU:CD2	2.49	0.41
1:O:41:ASN:OD1	1:O:183:LEU:HB2	2.19	0.41
4:R:51:GLU:HA	4:R:206:MET:HE2	2.01	0.41
8:V:159:ILE:O	8:V:163:ILE:HG13	2.20	0.41
1:A:198:PHE:O	1:A:199:GLU:HB2	2.20	0.41
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.56	0.41
6:F:205:LYS:HZ2	6:F:205:LYS:HG2	1.73	0.41
7:G:56:VAL:HG23	7:G:56:VAL:O	2.21	0.41
7:G:70:PHE:HB2	7:G:78:CYS:SG	2.60	0.41
1:O:50:LYS:H	1:O:50:LYS:HG2	1.69	0.41
4:R:27:ALA:O	4:R:31:ILE:HG12	2.20	0.41
7:U:50:ILE:HD12	7:U:79:VAL:HB	2.02	0.41
10:X:63:ASN:C	10:X:63:ASN:ND2	2.78	0.41
11:Y:45:MET:HE3	15:Y:301:YHD:C19	2.51	0.41
3:C:116:GLN:NE2	3:C:120:GLN:OE1	2.46	0.41
6:F:72:HIS:CE1	6:F:105:ASN:HB3	2.56	0.41
10:J:38:MET:HE3	10:J:38:MET:HB3	1.90	0.41
14:N:158:ASN:O	14:N:162:LEU:HD13	2.21	0.41
1:O:39:ALA:N	1:O:42:GLY:O	2.47	0.41
1:O:188:HIS:O	1:O:192:LEU:HD23	2.19	0.41
3:Q:40:ILE:CG2	3:Q:187:THR:HG21	2.50	0.41
6:T:169:ARG:HH22	6:T:173:LYS:HZ3	1.68	0.41
7:U:56:VAL:HG23	7:U:56:VAL:O	2.21	0.41
11:Y:147:LEU:HD22	11:Y:151:GLN:HB3	2.03	0.41
11:Y:148:GLU:HB2	11:Y:151:GLN:HG3	2.02	0.41
1:A:33:PRO:HD2	1:A:48:GLU:HG2	2.01	0.41
4:D:27:ALA:O	4:D:31:ILE:HG12	2.20	0.41
4:D:91:LYS:HA	4:D:94:VAL:HG12	2.01	0.41
11:K:7:LYS:HG2	11:K:12:VAL:HG22	2.03	0.41
11:K:33:LYS:HA	11:K:45:MET:HG2	2.02	0.41
11:K:35:ILE:HD11	11:K:45:MET:HE1	2.01	0.41
14:N:37:ILE:HD13	14:N:83:PHE:HE2	1.86	0.41
1:O:49:LYS:N	1:O:206:ASN:O	2.49	0.41
2:P:179:TYR:HA	2:P:184:MET:CE	2.51	0.41
3:Q:31:THR:HA	3:Q:161:ILE:O	2.20	0.41
7:U:77:GLY:HA3	7:U:227:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:35:ILE:HD12	11:Y:56:GLU:OE1	2.21	0.41
12:Z:104:TYR:HB3	12:Z:106:VAL:HG22	2.02	0.41
5:E:61:LYS:HB3	5:E:61:LYS:HE2	1.73	0.41
7:G:77:GLY:HA3	7:G:227:PHE:CD1	2.55	0.41
9:I:168:GLN:O	9:I:172:ASN:ND2	2.52	0.41
1:O:21:ILE:HG21	1:O:151:SER:HB2	2.02	0.41
2:P:3:ARG:HH12	4:R:9:ASP:C	2.27	0.41
7:U:231:THR:HB	7:U:234:GLU:OE1	2.20	0.41
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.02	0.41
14:b:158:ASN:O	14:b:162:LEU:HD13	2.21	0.41
5:E:207:THR:OG1	5:E:226:ASP:O	2.39	0.41
11:K:147:LEU:HD22	11:K:151:GLN:HB3	2.03	0.41
14:N:59:VAL:HG11	14:N:83:PHE:CE2	2.56	0.41
1:O:8:SER:OG	1:O:10:THR:O	2.38	0.41
3:Q:189:LYS:NZ	3:Q:235:GLU:OE1	2.40	0.41
4:R:187:LYS:H	4:R:187:LYS:HG2	1.72	0.41
6:T:36:ALA:CB	6:T:49:VAL:HG12	2.50	0.41
8:V:63:LEU:HD21	8:V:82:MET:HE1	2.03	0.41
9:W:19:VAL:HG12	9:W:189:ILE:HB	2.02	0.41
9:W:170:MET:HE3	9:W:184:VAL:HG13	2.03	0.41
14:b:133:SER:HA	14:b:136:TYR:HD2	1.85	0.41
1:A:50:LYS:H	1:A:50:LYS:HG2	1.69	0.41
1:A:101:GLN:OE1	8:H:57:GLN:NE2	2.53	0.41
5:E:103:LEU:HD12	5:E:104:PRO:HD2	2.02	0.41
7:G:47:CYS:SG	7:G:221:THR:HG22	2.61	0.41
8:H:202:TYR:HE2	12:Z:177:ASP:OD2	2.04	0.41
11:K:35:ILE:HD11	11:K:45:MET:CE	2.50	0.41
11:K:45:MET:HE3	15:K:301:YHD:C19	2.51	0.41
1:O:17:LYS:HE3	1:O:17:LYS:HB2	1.92	0.41
1:O:172:PHE:O	1:O:175:LYS:HG2	2.20	0.41
3:Q:98:VAL:HG13	11:Y:78:ALA:HB2	2.03	0.41
3:Q:116:GLN:NE2	3:Q:120:GLN:OE1	2.46	0.41
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.56	0.41
9:W:11:MET:SD	9:W:170:MET:HG2	2.61	0.41
11:Y:1:THR:OG1	15:Y:301:YHD:C09	2.67	0.41
14:b:37:ILE:HD13	14:b:83:PHE:HE2	1.86	0.41
14:b:59:VAL:HG11	14:b:83:PHE:CE2	2.56	0.41
2:B:48:GLU:HG3	2:B:201:MET:HE2	2.01	0.41
2:B:179:TYR:HA	2:B:184:MET:CE	2.51	0.41
10:J:49:GLU:O	10:J:53:THR:HG23	2.21	0.41
11:K:117:GLU:OE1	11:K:117:GLU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:164:THR:HB	11:K:171:GLY:HA2	2.03	0.41
11:K:191:ASN:ND2	9:W:202:ARG:HH12	2.17	0.41
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.50	0.41
13:M:22:ILE:HG12	13:M:50:MET:SD	2.61	0.41
3:Q:116:GLN:HA	3:Q:119:THR:HG22	2.03	0.41
7:U:70:PHE:HB2	7:U:78:CYS:SG	2.61	0.41
9:W:202:ARG:NH2	9:W:204:ASP:OD2	2.43	0.41
10:X:34:LYS:HE2	10:X:34:LYS:HB2	1.87	0.41
3:C:116:GLN:HA	3:C:119:THR:HG22	2.03	0.40
9:I:19:VAL:HG12	9:I:189:ILE:HB	2.02	0.40
9:I:170:MET:HE3	9:I:184:VAL:HG13	2.03	0.40
14:N:134:TYR:N	14:N:134:TYR:HD2	2.20	0.40
4:R:149:LYS:HB2	4:R:152:GLN:OE1	2.21	0.40
11:Y:31:VAL:HG11	15:Y:301:YHD:C20	2.51	0.40
13:a:22:ILE:HG12	13:a:50:MET:SD	2.61	0.40
13:a:27:LEU:HD22	13:a:184:TYR:HB2	2.03	0.40
10:J:59:TYR:O	10:J:62:LYS:HG2	2.21	0.40
11:K:148:GLU:HB2	11:K:151:GLN:HG3	2.02	0.40
5:S:207:THR:OG1	5:S:226:ASP:O	2.39	0.40
6:T:41:CYS:HB2	6:T:184:MET:O	2.21	0.40
10:X:8:GLN:NE2	10:X:113:PRO:HG2	2.31	0.40
10:X:49:GLU:O	10:X:53:THR:HG23	2.21	0.40
13:a:176:LEU:HA	13:a:176:LEU:HD23	1.91	0.40
14:b:134:TYR:N	14:b:134:TYR:HD2	2.20	0.40
5:E:137:TYR:CE1	5:E:141:GLY:HA2	2.56	0.40
6:F:113:ASP:CG	7:G:88:ARG:HH21	2.30	0.40
7:U:63:SER:HA	7:U:66:VAL:HG12	2.04	0.40
7:U:78:CYS:HB3	7:U:140:LEU:HD23	2.03	0.40
10:X:18:ASP:OD1	10:X:18:ASP:C	2.64	0.40
5:E:50:LYS:CB	5:E:59:HIS:HB3	2.52	0.40
7:G:50:ILE:HD12	7:G:79:VAL:HB	2.02	0.40
8:H:63:LEU:HD21	8:H:82:MET:HE1	2.03	0.40
9:I:11:MET:SD	9:I:170:MET:HG2	2.61	0.40
11:K:31:VAL:HG11	15:K:301:YHD:C20	2.51	0.40
11:K:171:GLY:HA3	9:W:204:ASP:HB2	2.04	0.40
1:O:198:PHE:O	1:O:199:GLU:HB2	2.20	0.40
5:S:61:LYS:HB3	5:S:61:LYS:HE2	1.73	0.40
8:V:97:ALA:HB1	8:V:127:MET:SD	2.62	0.40
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.50	0.40
14:b:175:ARG:HG2	14:b:188:VAL:HG12	2.04	0.40
5:E:22:ILE:HD12	5:E:150:SER:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:70:MET:HE1	13:M:91:TRP:CE2	2.57	0.40
13:M:70:MET:HE3	13:M:70:MET:HB2	1.94	0.40
5:S:22:ILE:HD12	5:S:150:SER:HA	2.04	0.40
9:W:135:PHE:CD2	9:W:149:CYS:HB3	2.56	0.40
11:Y:7:LYS:HG2	11:Y:12:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	227/234 (97%)	217 (96%)	7 (3%)	3 (1%)	9	33
1	O	227/234 (97%)	217 (96%)	7 (3%)	3 (1%)	9	33
2	B	235/261 (90%)	230 (98%)	5 (2%)	0	100	100
2	P	235/261 (90%)	230 (98%)	5 (2%)	0	100	100
3	C	233/248 (94%)	227 (97%)	5 (2%)	1 (0%)	30	59
3	Q	233/248 (94%)	227 (97%)	5 (2%)	1 (0%)	30	59
4	D	234/241 (97%)	226 (97%)	7 (3%)	1 (0%)	30	59
4	R	234/241 (97%)	226 (97%)	7 (3%)	1 (0%)	30	59
5	E	234/263 (89%)	227 (97%)	5 (2%)	2 (1%)	14	42
5	S	234/263 (89%)	227 (97%)	5 (2%)	2 (1%)	14	42
6	F	237/255 (93%)	234 (99%)	3 (1%)	0	100	100
6	T	237/255 (93%)	234 (99%)	3 (1%)	0	100	100
7	G	238/246 (97%)	234 (98%)	4 (2%)	0	100	100
7	U	238/246 (97%)	234 (98%)	4 (2%)	0	100	100
8	H	218/234 (93%)	213 (98%)	5 (2%)	0	100	100
8	V	218/234 (93%)	213 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	197 (98%)	4 (2%)	1 (0%)	24	54
9	W	202/205 (98%)	197 (98%)	4 (2%)	1 (0%)	24	54
10	J	194/201 (96%)	191 (98%)	1 (0%)	2 (1%)	12	40
10	X	194/201 (96%)	191 (98%)	1 (0%)	2 (1%)	12	40
11	K	197/204 (97%)	194 (98%)	3 (2%)	0	100	100
11	Y	197/204 (97%)	194 (98%)	3 (2%)	0	100	100
12	L	211/213 (99%)	209 (99%)	2 (1%)	0	100	100
12	Z	211/213 (99%)	209 (99%)	2 (1%)	0	100	100
13	M	210/219 (96%)	205 (98%)	5 (2%)	0	100	100
13	a	210/219 (96%)	205 (98%)	5 (2%)	0	100	100
14	N	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
14	b	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
All	All	6140/6458 (95%)	6002 (98%)	118 (2%)	20 (0%)	37	65

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	226	ASP
9	I	30	GLN
5	S	226	ASP
9	W	30	GLN
3	C	216	SER
10	J	25	ILE
3	Q	216	SER
10	X	25	ILE
1	A	51	GLN
5	E	59	HIS
1	O	51	GLN
5	S	59	HIS
1	A	201	GLN
4	D	127	ASP
10	J	24	ASN
1	O	201	GLN
4	R	127	ASP
10	X	24	ASN
1	A	52	LYS
1	O	52	LYS

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	188/191 (98%)	188 (100%)	0	100	100
1	O	188/191 (98%)	188 (100%)	0	100	100
2	B	201/221 (91%)	200 (100%)	1 (0%)	81	81
2	P	201/221 (91%)	200 (100%)	1 (0%)	81	81
3	C	199/211 (94%)	199 (100%)	0	100	100
3	Q	199/211 (94%)	199 (100%)	0	100	100
4	D	198/203 (98%)	198 (100%)	0	100	100
4	R	198/203 (98%)	198 (100%)	0	100	100
5	E	202/224 (90%)	201 (100%)	1 (0%)	81	81
5	S	202/224 (90%)	201 (100%)	1 (0%)	81	81
6	F	197/212 (93%)	197 (100%)	0	100	100
6	T	197/212 (93%)	197 (100%)	0	100	100
7	G	206/210 (98%)	206 (100%)	0	100	100
7	U	206/210 (98%)	206 (100%)	0	100	100
8	H	181/195 (93%)	181 (100%)	0	100	100
8	V	181/195 (93%)	181 (100%)	0	100	100
9	I	173/174 (99%)	173 (100%)	0	100	100
9	W	173/174 (99%)	173 (100%)	0	100	100
10	J	167/171 (98%)	167 (100%)	0	100	100
10	X	167/171 (98%)	167 (100%)	0	100	100
11	K	154/159 (97%)	154 (100%)	0	100	100
11	Y	154/159 (97%)	154 (100%)	0	100	100
12	L	178/178 (100%)	178 (100%)	0	100	100
12	Z	178/178 (100%)	178 (100%)	0	100	100
13	M	175/181 (97%)	174 (99%)	1 (1%)	78	80
13	a	175/181 (97%)	174 (99%)	1 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	157/159 (99%)	156 (99%)	1 (1%)	78	80
14	b	157/159 (99%)	156 (99%)	1 (1%)	78	80
All	All	5152/5378 (96%)	5144 (100%)	8 (0%)	85	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	209	GLU
5	E	65	HIS
13	M	173	MET
14	N	134	TYR
2	P	209	GLU
5	S	65	HIS
13	a	173	MET
14	b	134	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	139	ASN
2	B	102	GLN
2	B	146	GLN
4	D	97	GLN
4	D	224	GLN
5	E	175	HIS
6	F	110	HIS
7	G	12	HIS
7	G	100	ASN
7	G	150	GLN
8	H	57	GLN
8	H	80	ASN
8	H	172	ASN
9	I	168	GLN
10	J	8	GLN
10	J	65	GLN
10	J	71	ASN
10	J	132	HIS
12	L	77	HIS
12	L	151	ASN

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Mol	Chain	Res	Type
12	L	152	GLN
14	N	77	HIS
14	N	110	GLN
1	O	101	GLN
1	O	139	ASN
2	P	142	HIS
2	P	146	GLN
4	R	224	GLN
6	T	110	HIS
7	U	100	ASN
7	U	150	GLN
8	V	57	GLN
8	V	80	ASN
8	V	172	ASN
9	W	168	GLN
10	X	8	GLN
10	X	65	GLN
10	X	71	ASN
10	X	132	HIS
12	Z	77	HIS
12	Z	151	ASN
12	Z	152	GLN
14	b	77	HIS
14	b	110	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	K	301	11	24,28,28	1.83	6 (25%)	33,38,38	3.10	19 (57%)
15	YHD	Y	301	11	24,28,28	1.83	6 (25%)	33,38,38	3.11	19 (57%)

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	K	301	11	-	8/15/30/30	0/3/3/3
15	YHD	Y	301	11	-	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	K	301	YHD	C14-C13	4.94	1.60	1.49
15	Y	301	YHD	C14-C13	4.94	1.60	1.49
15	Y	301	YHD	C20-C21	2.62	1.43	1.38
15	K	301	YHD	C20-C21	2.61	1.43	1.38
15	K	301	YHD	O25-C03	2.42	1.28	1.23
15	Y	301	YHD	O25-C03	2.42	1.28	1.23
15	K	301	YHD	C04-N23	2.39	1.52	1.46
15	Y	301	YHD	C04-N23	2.39	1.52	1.46
15	K	301	YHD	C12-C11	2.11	1.42	1.38
15	Y	301	YHD	C09-C10	2.11	1.56	1.51
15	K	301	YHD	C09-C10	2.08	1.56	1.51
15	Y	301	YHD	C12-C11	2.07	1.42	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	301	YHD	C21-C10-C11	-6.21	109.00	118.23
15	K	301	YHD	C21-C10-C11	-6.21	109.00	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	301	YHD	C20-C13-C12	-5.95	107.03	117.68
15	K	301	YHD	C20-C13-C12	-5.90	107.12	117.68
15	K	301	YHD	C18-C19-C14	5.12	126.36	120.54
15	Y	301	YHD	C18-C19-C14	5.09	126.33	120.54
15	K	301	YHD	C15-C14-C19	-4.67	109.32	117.68
15	Y	301	YHD	C15-C14-C19	-4.64	109.38	117.68
15	K	301	YHD	C16-C15-C14	4.41	125.56	120.54
15	Y	301	YHD	C16-C15-C14	4.36	125.50	120.54
15	Y	301	YHD	C11-C12-C13	4.34	126.69	121.12
15	K	301	YHD	C11-C12-C13	4.29	126.63	121.12
15	Y	301	YHD	C21-C20-C13	4.20	126.52	121.12
15	K	301	YHD	C21-C20-C13	4.16	126.46	121.12
15	Y	301	YHD	C09-C02-N22	3.93	115.46	110.39
15	K	301	YHD	C09-C02-N22	3.92	115.45	110.39
15	Y	301	YHD	C20-C13-C14	3.87	127.93	121.25
15	K	301	YHD	C20-C13-C14	3.86	127.91	121.25
15	Y	301	YHD	C12-C11-C10	3.64	125.78	121.00
15	Y	301	YHD	C04-C03-N22	3.63	124.50	116.52
15	K	301	YHD	C12-C11-C10	3.62	125.76	121.00
15	Y	301	YHD	C10-C09-C02	3.61	121.48	113.76
15	K	301	YHD	C04-C03-N22	3.61	124.43	116.52
15	K	301	YHD	C10-C09-C02	3.60	121.48	113.76
15	K	301	YHD	C09-C10-C21	3.36	127.15	120.90
15	Y	301	YHD	C09-C10-C21	3.33	127.11	120.90
15	K	301	YHD	C19-C14-C13	3.24	126.85	121.25
15	Y	301	YHD	C19-C14-C13	3.22	126.81	121.25
15	K	301	YHD	C20-C21-C10	3.07	125.03	121.00
15	Y	301	YHD	C20-C21-C10	3.03	124.98	121.00
15	Y	301	YHD	C18-C17-C16	-2.92	115.88	119.87
15	K	301	YHD	C18-C17-C16	-2.90	115.90	119.87
15	K	301	YHD	O25-C03-N22	-2.65	118.21	122.96
15	Y	301	YHD	O25-C03-N22	-2.65	118.22	122.96
15	Y	301	YHD	C12-C13-C14	2.19	125.04	121.25
15	K	301	YHD	C12-C13-C14	2.15	124.97	121.25
15	K	301	YHD	C07-C08-C04	2.06	108.43	104.14
15	Y	301	YHD	C07-C08-C04	2.05	108.42	104.14

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	K	301	YHD	C02-C09-C10-C11

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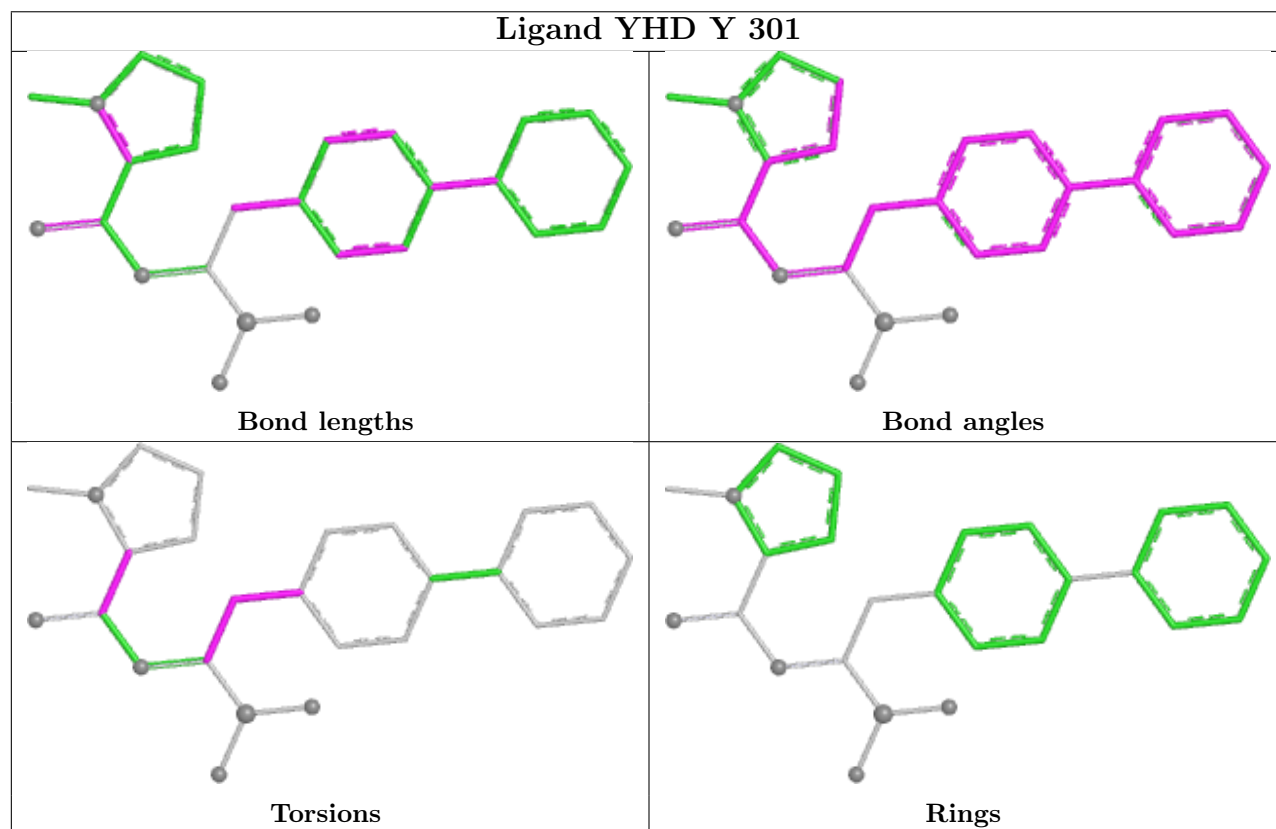
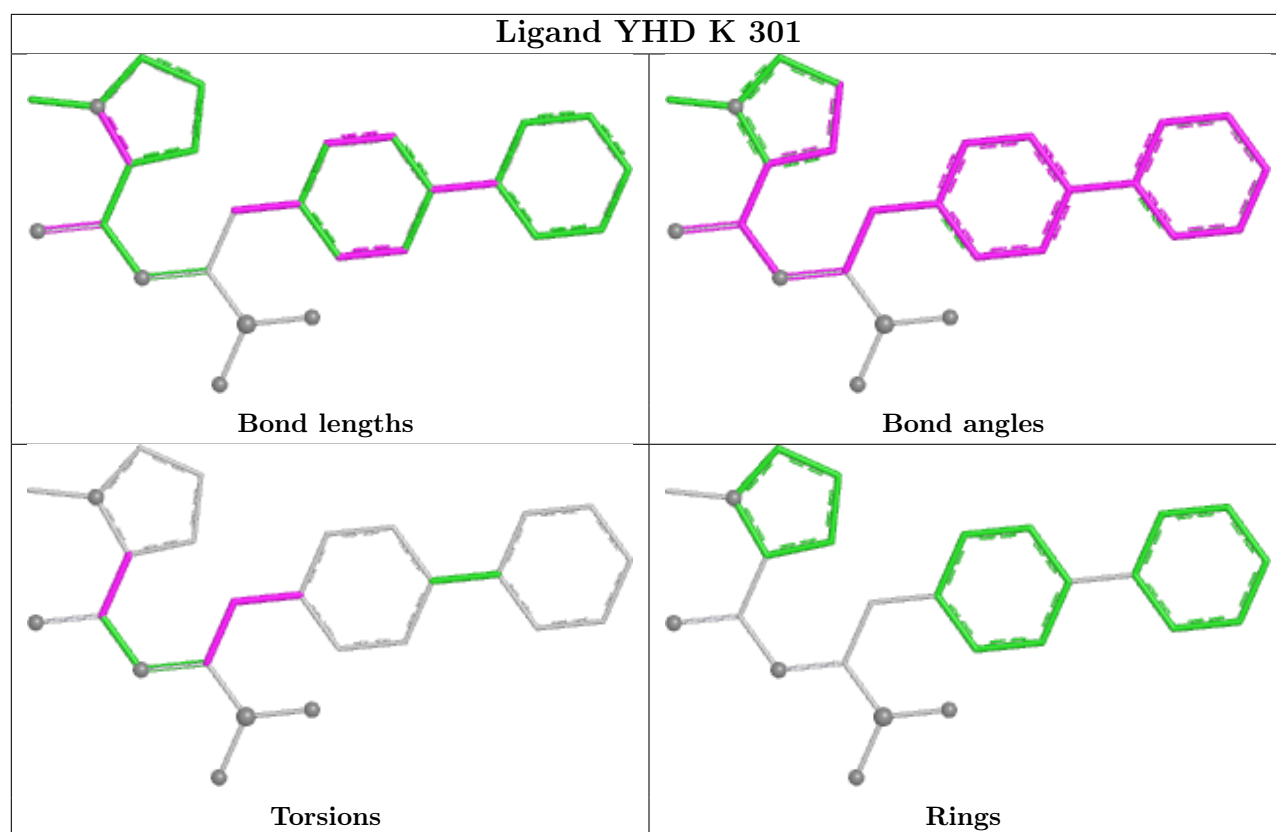
Mol	Chain	Res	Type	Atoms
15	K	301	YHD	C02-C09-C10-C21
15	K	301	YHD	B01-C02-C09-C10
15	Y	301	YHD	C02-C09-C10-C11
15	Y	301	YHD	C02-C09-C10-C21
15	Y	301	YHD	B01-C02-C09-C10
15	K	301	YHD	O25-C03-C04-N23
15	Y	301	YHD	O25-C03-C04-N23
15	K	301	YHD	N22-C03-C04-N23
15	Y	301	YHD	N22-C03-C04-N23
15	K	301	YHD	N22-C03-C04-C08
15	Y	301	YHD	N22-C03-C04-C08
15	K	301	YHD	O25-C03-C04-C08
15	Y	301	YHD	O25-C03-C04-C08
15	K	301	YHD	N22-C02-C09-C10
15	Y	301	YHD	N22-C02-C09-C10

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	301	YHD	4	0
15	Y	301	YHD	4	0

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

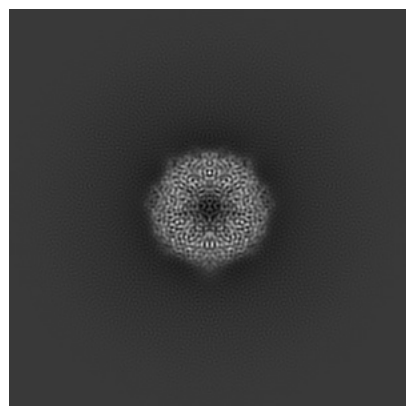
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23576. These allow visual inspection of the internal detail of the map and identification of artifacts.

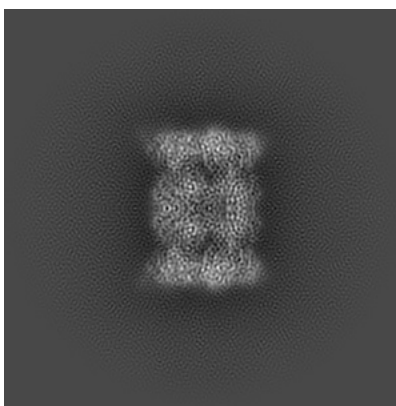
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

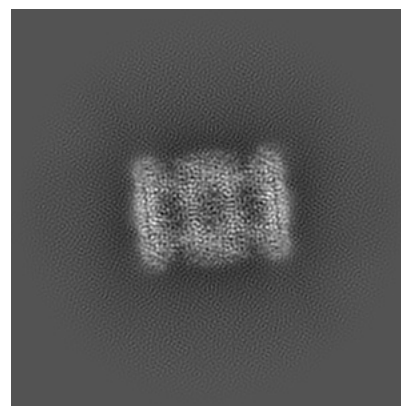
6.1.1 Primary map



X

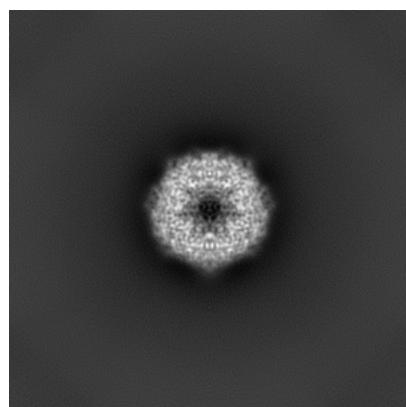


Y

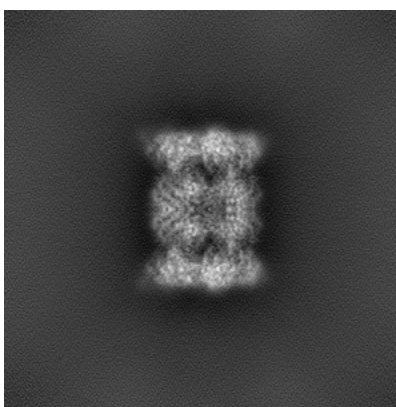


Z

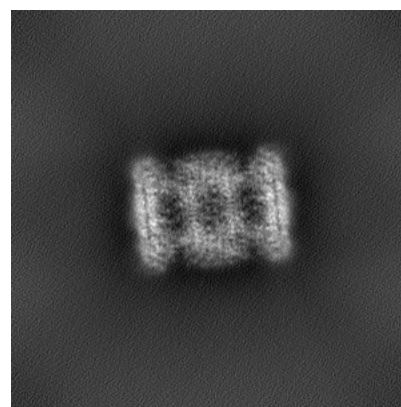
6.1.2 Raw map



X



Y

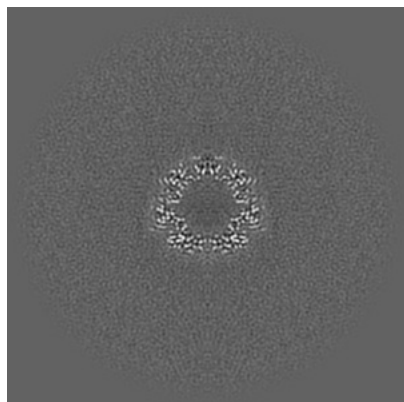


Z

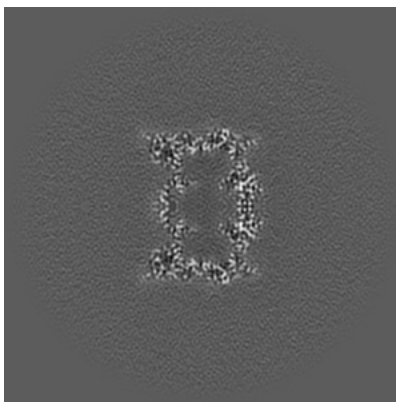
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

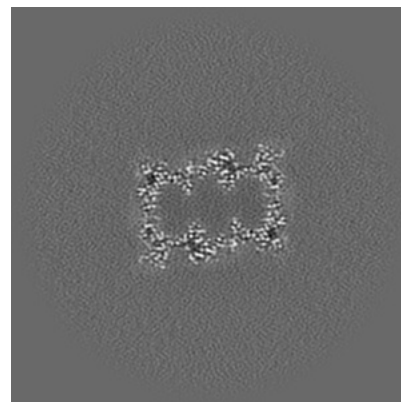
6.2.1 Primary map



X Index: 150

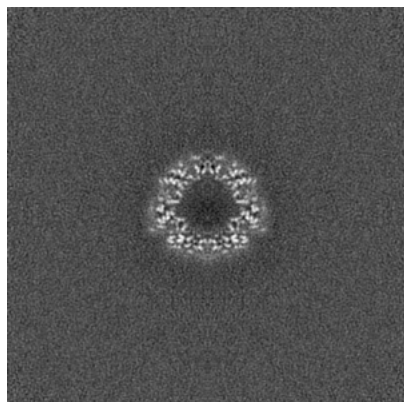


Y Index: 150

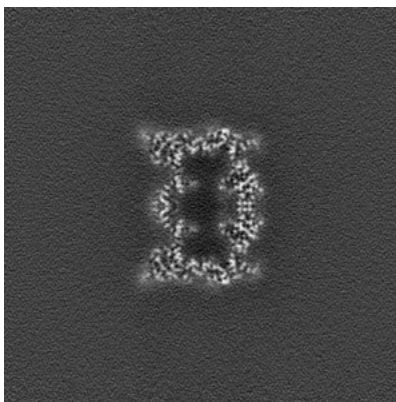


Z Index: 150

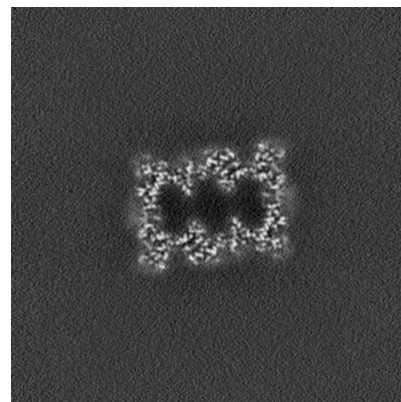
6.2.2 Raw map



X Index: 150



Y Index: 150

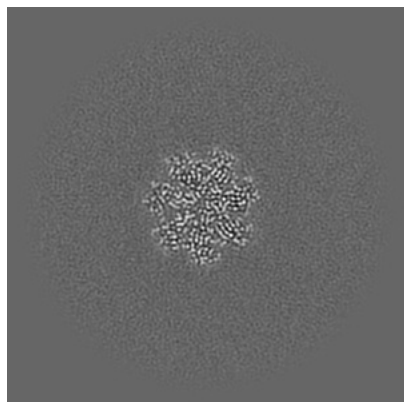


Z Index: 150

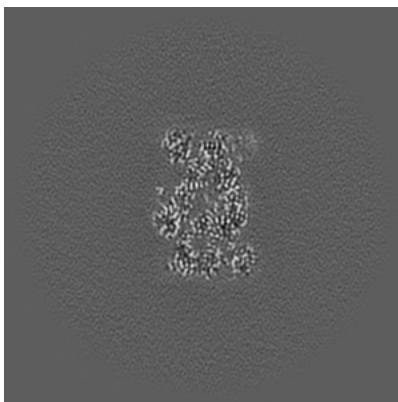
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

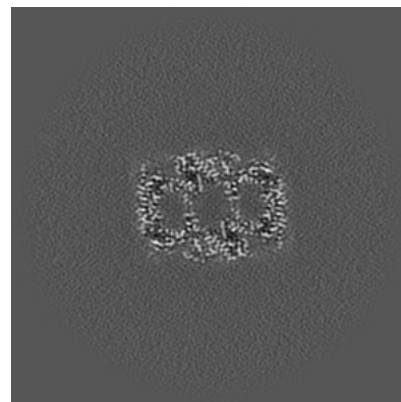
6.3.1 Primary map



X Index: 106

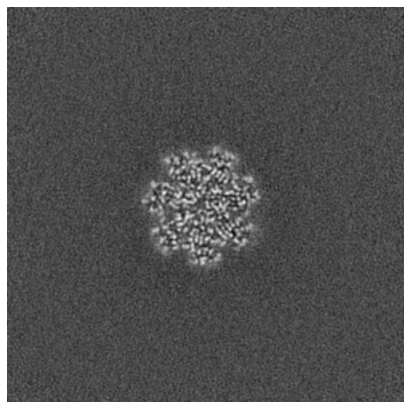


Y Index: 129

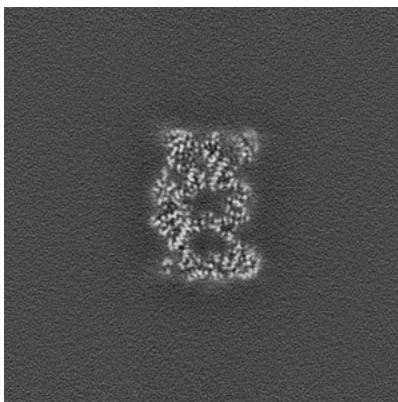


Z Index: 138

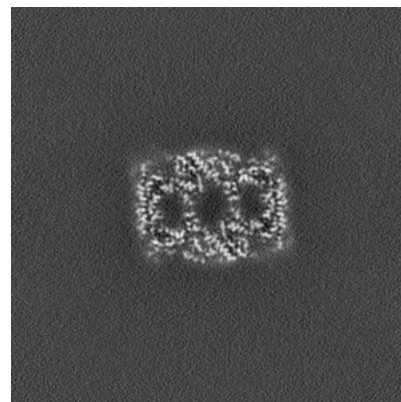
6.3.2 Raw map



X Index: 106



Y Index: 133

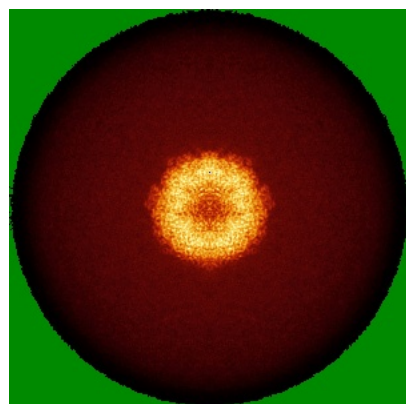


Z Index: 138

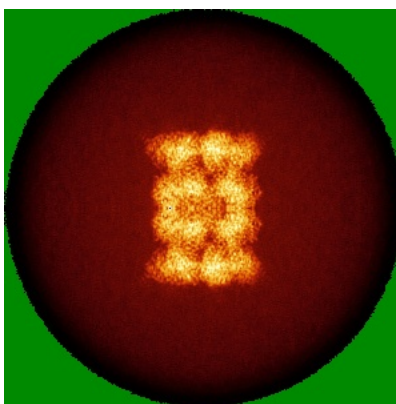
The images above show the largest variance slices of the map in three orthogonal directions.

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

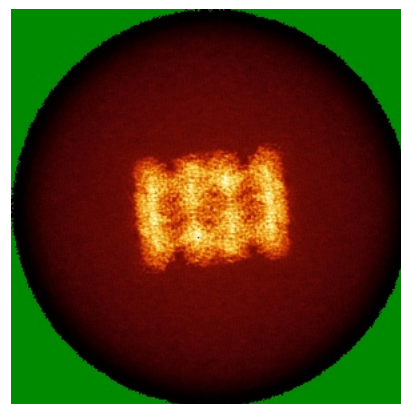
6.4.1 Primary map



X

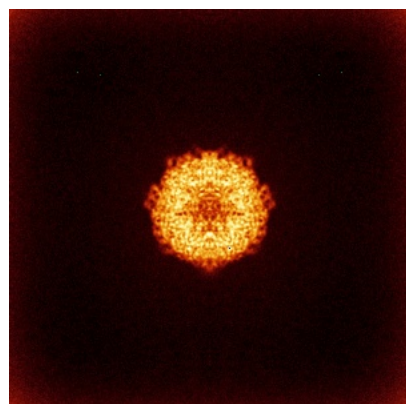


Y

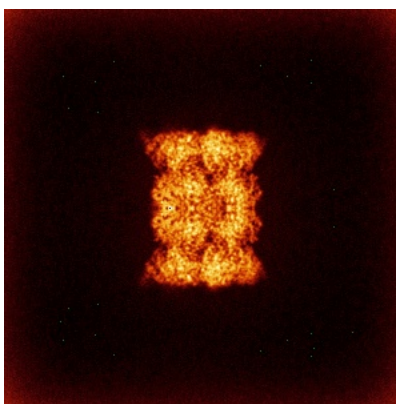


Z

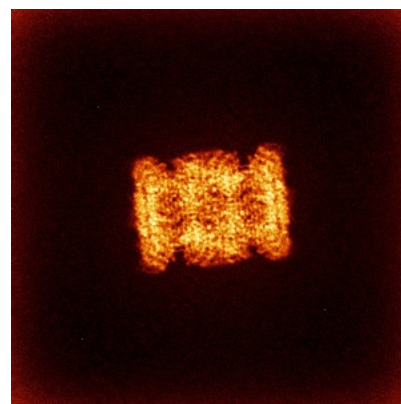
6.4.2 Raw map



X



Y

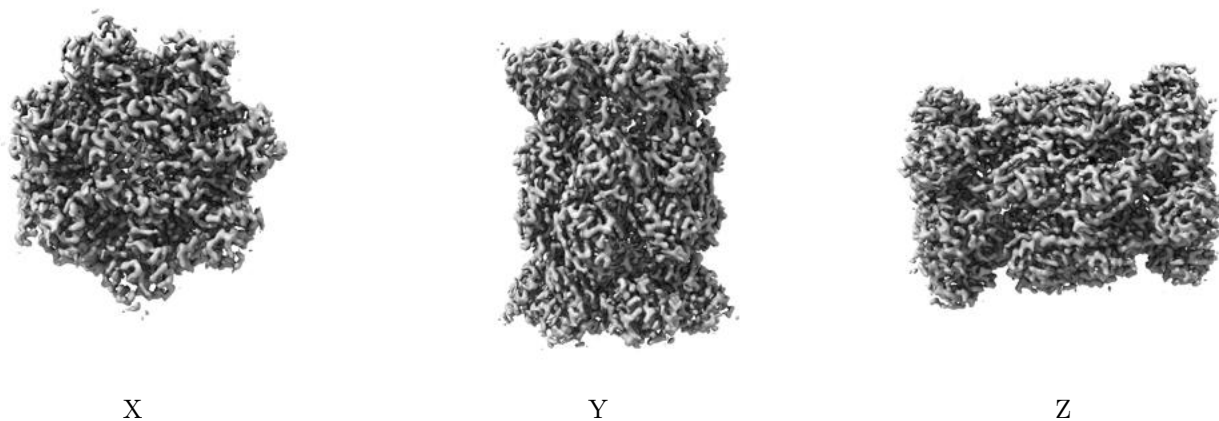


Z

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.

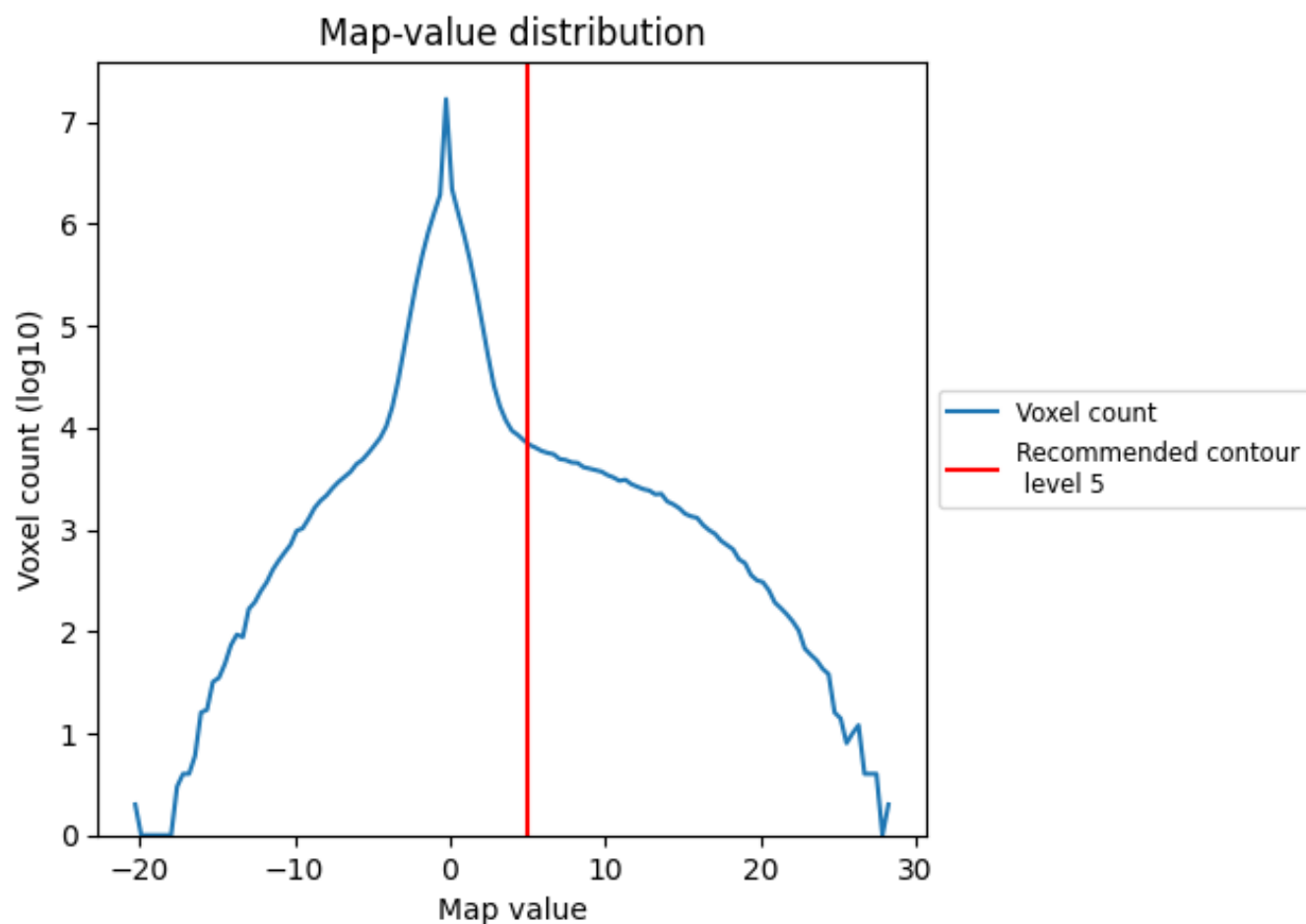
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

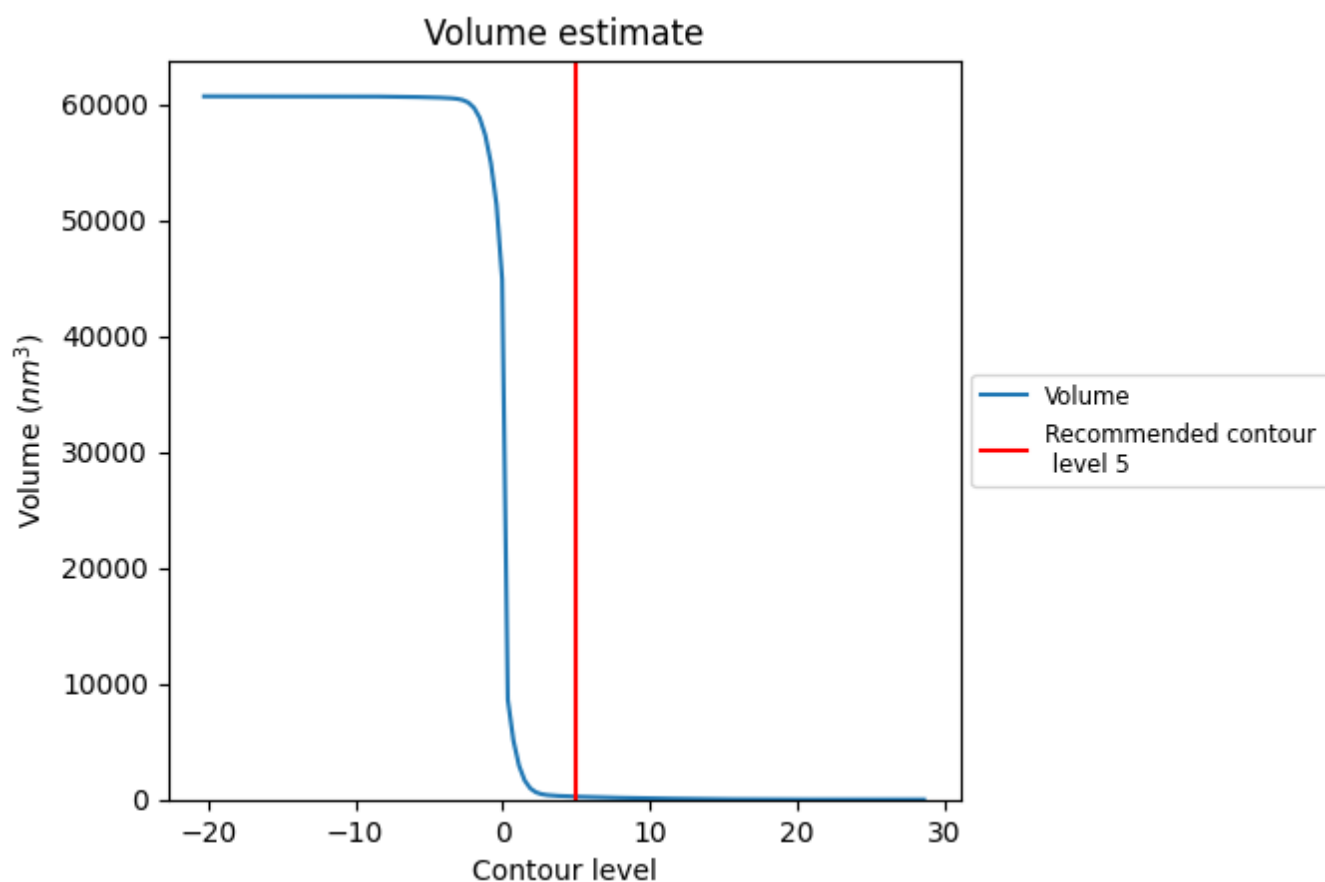
This section contains the results of statistical analysis of the map.

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.

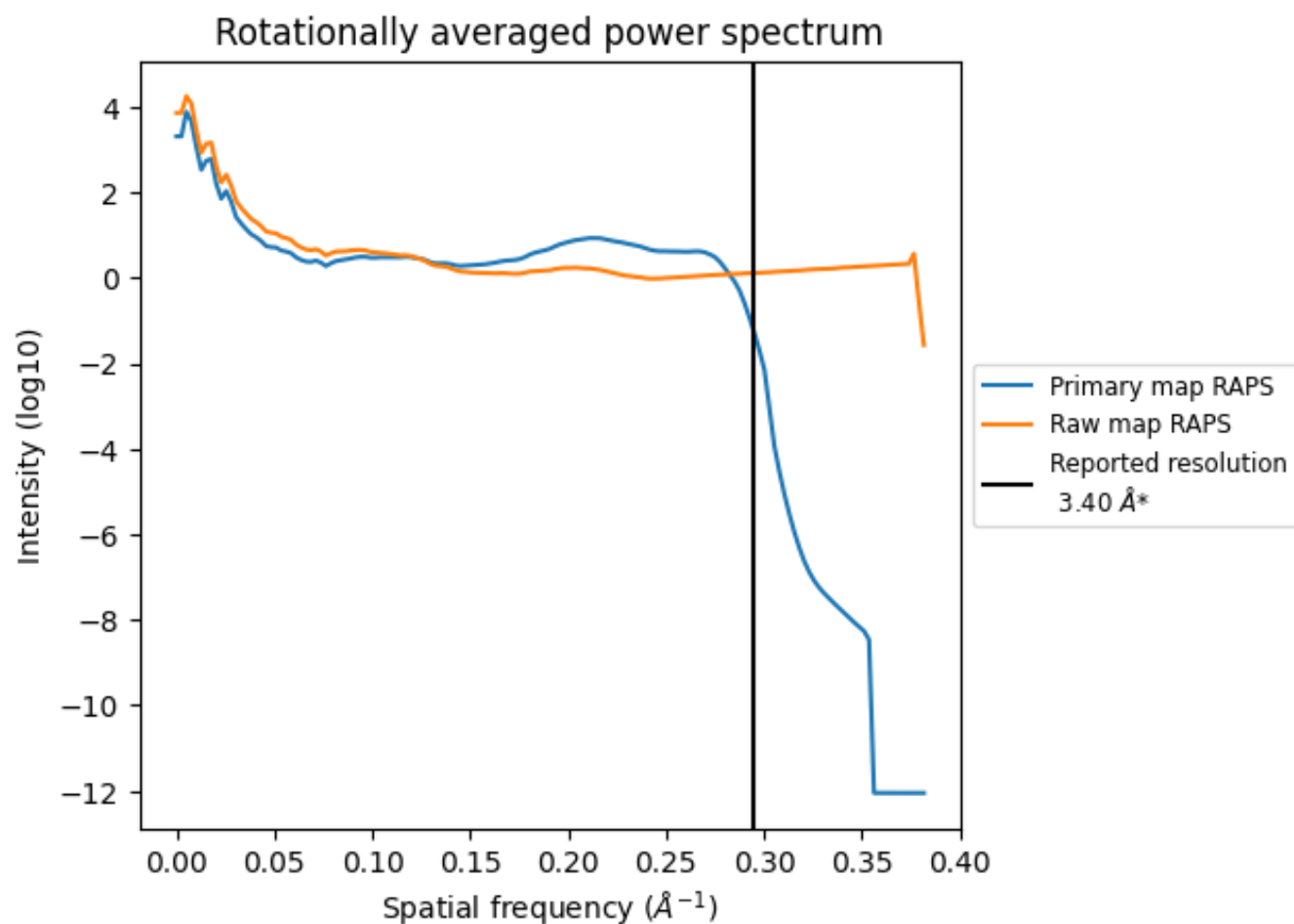
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm³; this corresponds to an approximate mass of 228 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 ⓘ

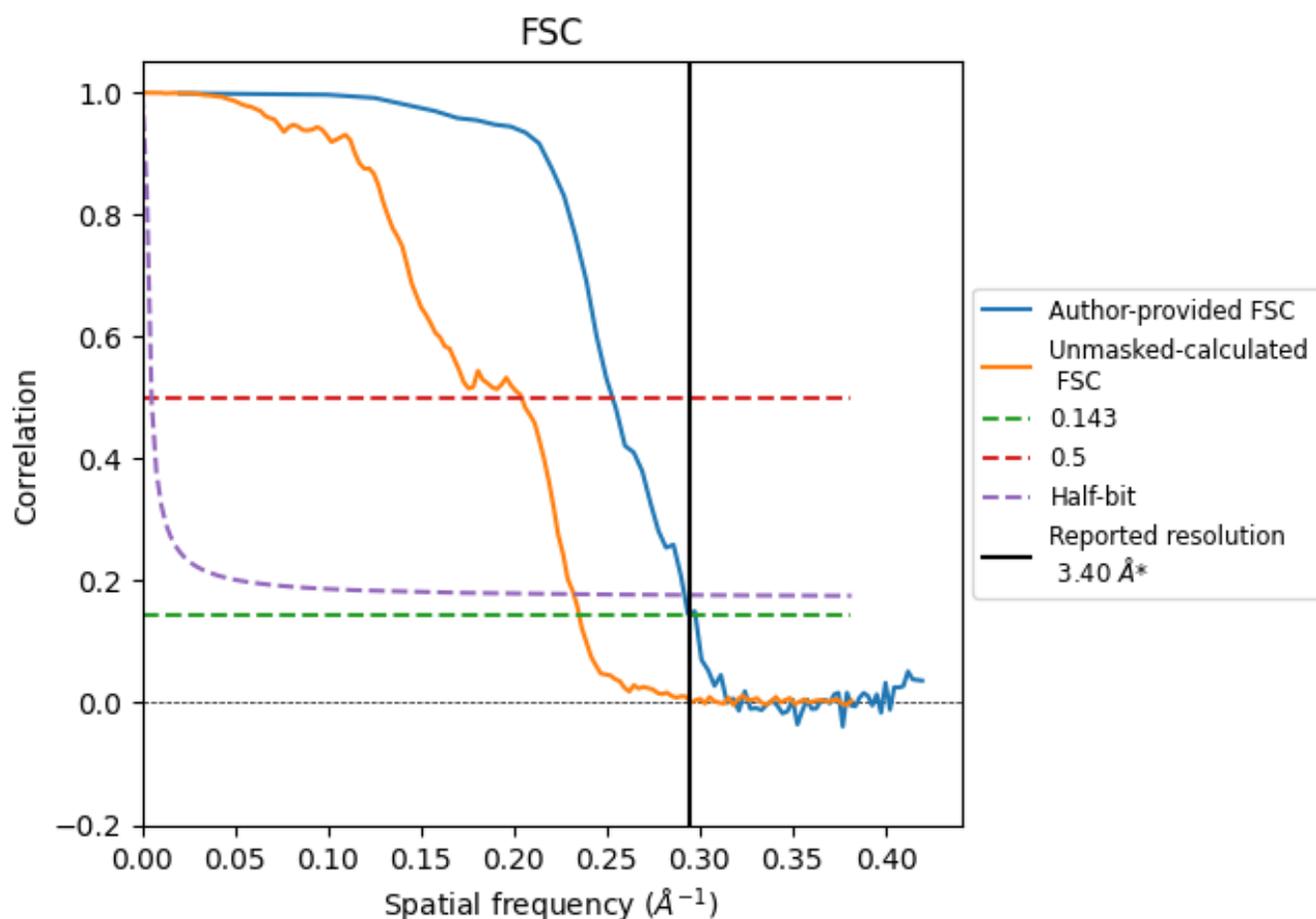


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

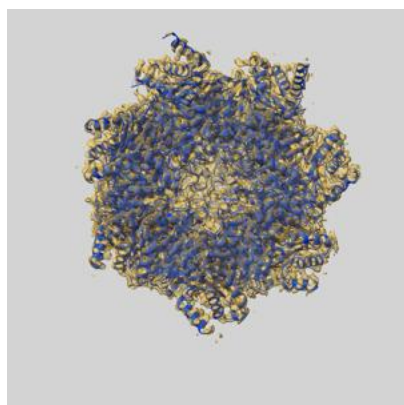
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.36	3.95	3.44
Unmasked-calculated*	4.25	4.90	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.25 differs from the reported value 3.4 by more than 10 %

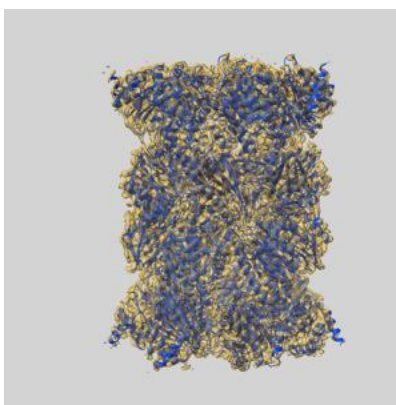
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23576 and PDB model 7LXV. Per-residue inclusion information can be found in section [3](#) on page [8](#).

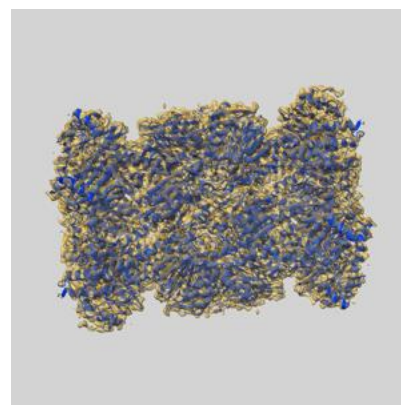
9.1 Map-model overlay [i](#)



X



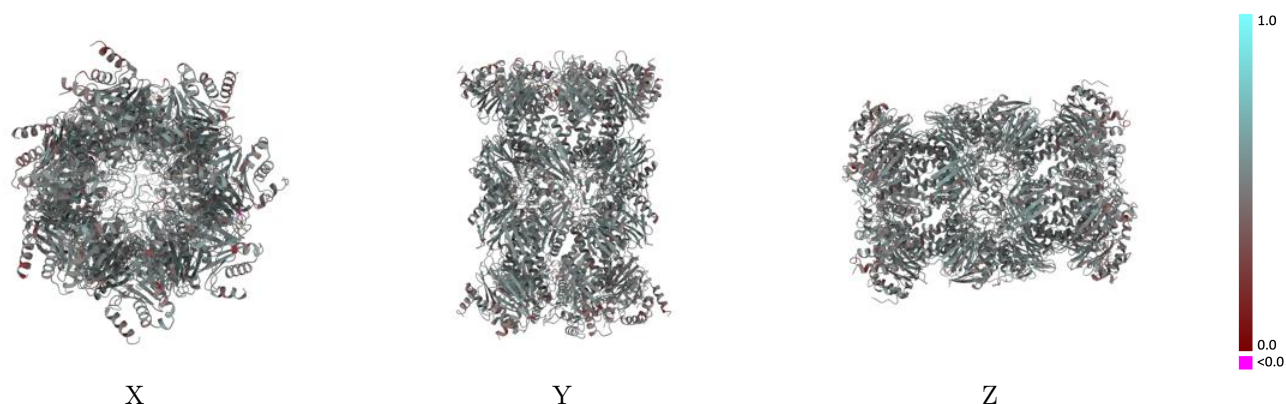
Y



Z

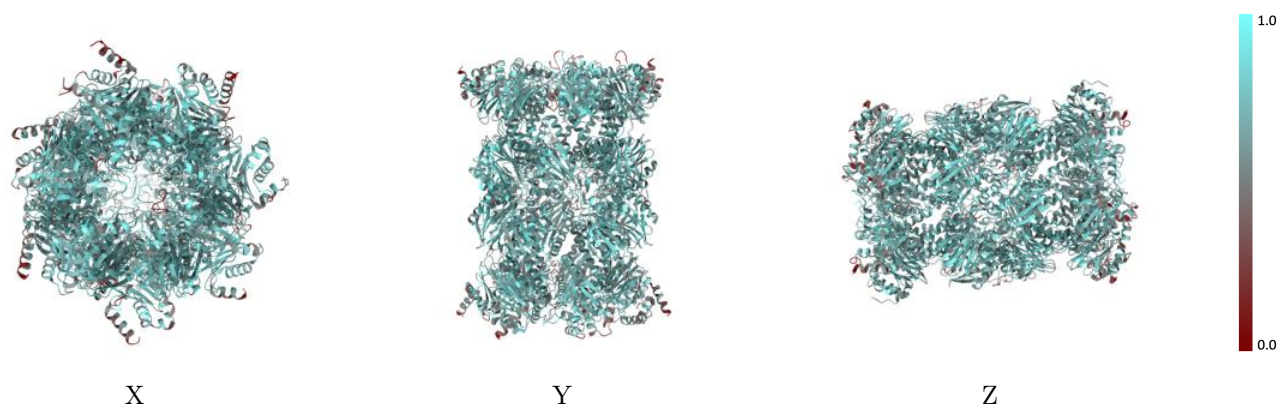
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



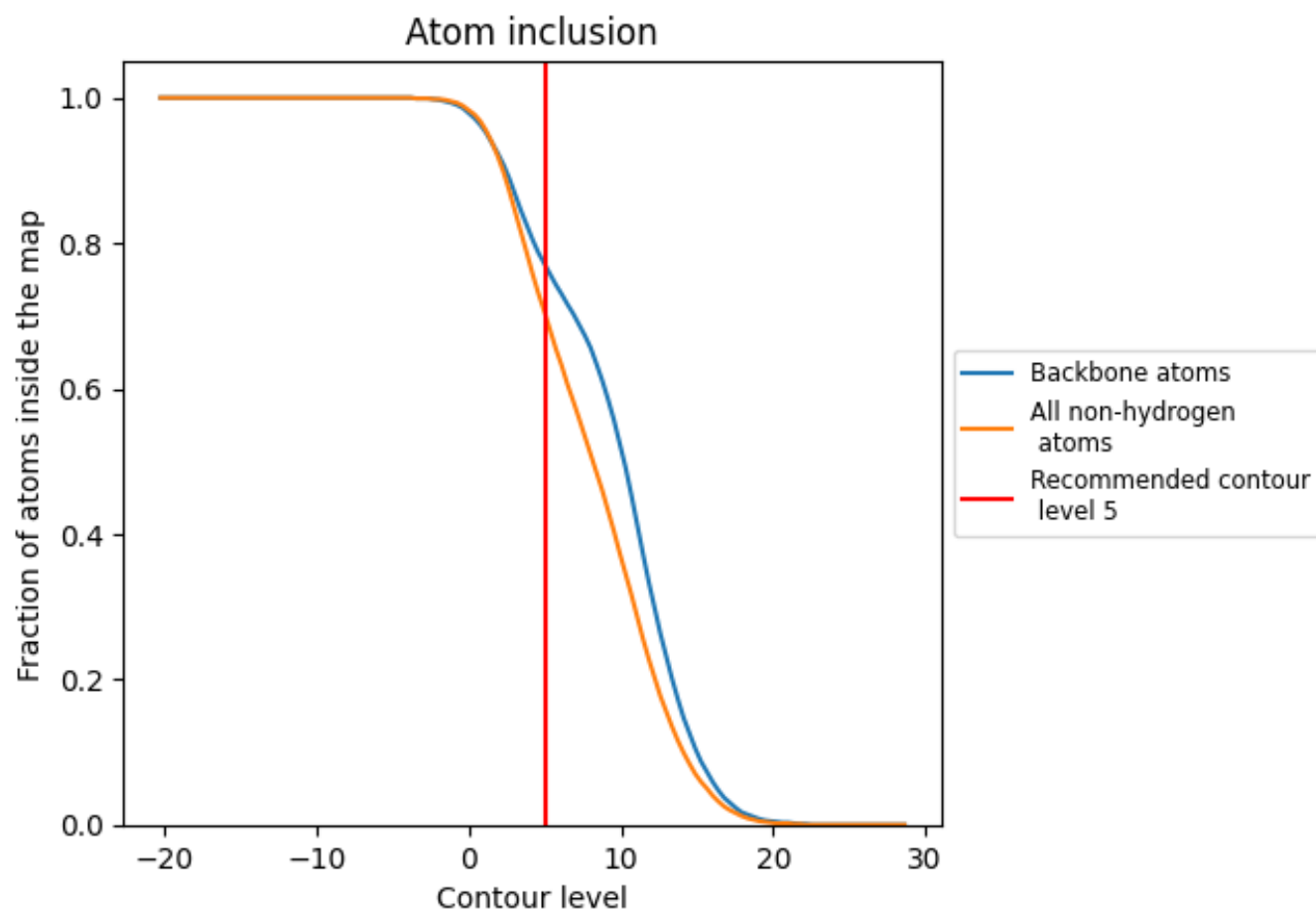
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 77% of all backbone atoms, 70% 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	 0.7030	 0.4960
A	 0.6920	 0.4810
B	 0.6820	 0.4880
C	 0.6840	 0.4890
D	 0.6700	 0.4920
E	 0.6900	 0.4840
F	 0.6820	 0.4900
G	 0.6490	 0.4780
H	 0.6930	 0.5020
I	 0.7340	 0.5130
J	 0.7390	 0.5110
K	 0.7570	 0.5130
L	 0.7160	 0.4980
M	 0.7470	 0.5050
N	 0.7320	 0.5100
O	 0.6910	 0.4810
P	 0.6830	 0.4870
Q	 0.6890	 0.4870
R	 0.6690	 0.4910
S	 0.6910	 0.4850
T	 0.6810	 0.4890
U	 0.6490	 0.4770
V	 0.6940	 0.5010
W	 0.7340	 0.5140
X	 0.7390	 0.5130
Y	 0.7590	 0.5110
Z	 0.7150	 0.5000
a	 0.7470	 0.5050
b	 0.7310	 0.5100

