



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 10:20 PM EST

PDB ID : 6MUW
EMDB ID : EMD-9258
Title : The structure of the Plasmodium falciparum 20S proteasome.
Authors : Metcalfe, R.D.; Xie, S.C.; Hanssen, E.; Gillett, D.L.; Leis, A.P.; Tilley, L.; Griffin, M.D.W.
Deposited on : 2018-10-23
Resolution : 3.60 Å(reported)
Based on initial model : 5FMG

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

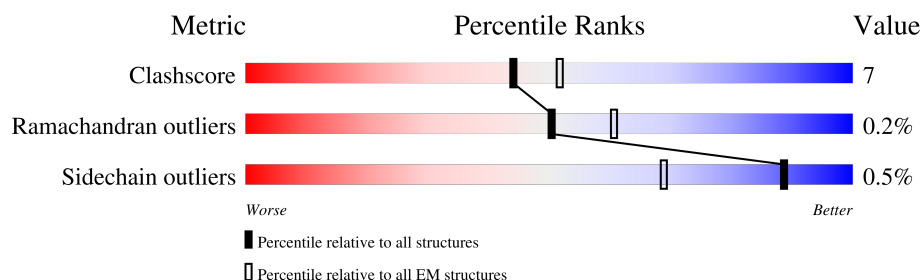
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	O	260	
2	B	235	
2	P	235	
3	C	246	
3	Q	246	
4	D	241	
4	R	241	

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Mol	Chain	Length	Quality of chain
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 14 unique types of molecules in this entry. The entry contains 49798 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	241	Total	C	N	O	S	0	0
			1926	1232	314	377	3		
3	Q	241	Total	C	N	O	S	0	0
			1926	1232	314	377	3		

- 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	243	Total	C	N	O	S	0	0
			1888	1189	314	374	11		
5	S	243	Total	C	N	O	S	0	0
			1888	1189	314	374	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	236	Total	C	N	O	S	0	0
			1878	1196	309	362	11		
6	T	236	Total	C	N	O	S	0	0
			1878	1196	309	362	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	234	Total	C	N	O	S	0	0
			1912	1218	320	362	12		
7	U	234	Total	C	N	O	S	0	0
			1912	1218	320	362	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	196	Total	C	N	O	S	0	0
			1569	992	268	297	12		
8	V	196	Total	C	N	O	S	0	0
			1569	992	268	297	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	222	Total	C	N	O	S	0	0
			1702	1076	296	316	14		
9	W	222	Total	C	N	O	S	0	0
			1702	1076	296	316	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	205	Total	C	N	O	S	0	0
			1612	1029	261	308	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	205	Total	C	N	O	S	0	0
			1612	1029	261	308	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	204	Total	C	N	O	S	0	0
			1600	1021	265	307	7		
12	Z	204	Total	C	N	O	S	0	0
			1600	1021	265	307	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		

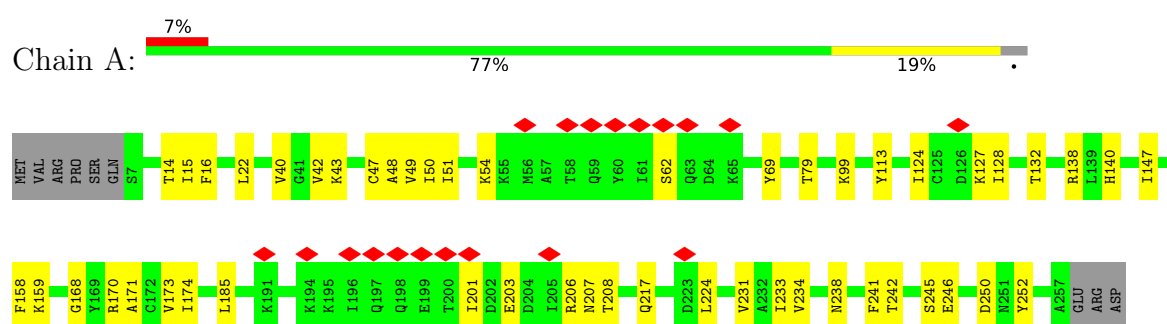
- Molecule 14 is a protein called 20S proteasome beta-7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	224	Total	C	N	O	S	0	0
			1845	1177	313	348	7		
14	b	224	Total	C	N	O	S	0	0
			1845	1177	313	348	7		

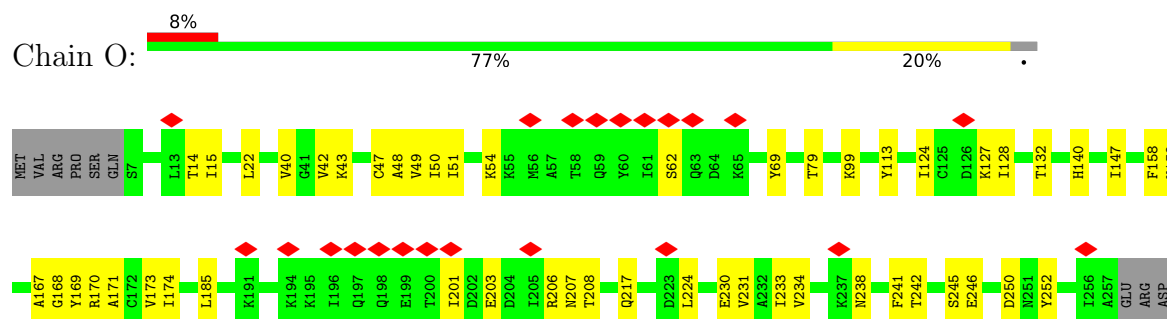
3 Residue-property plots

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.

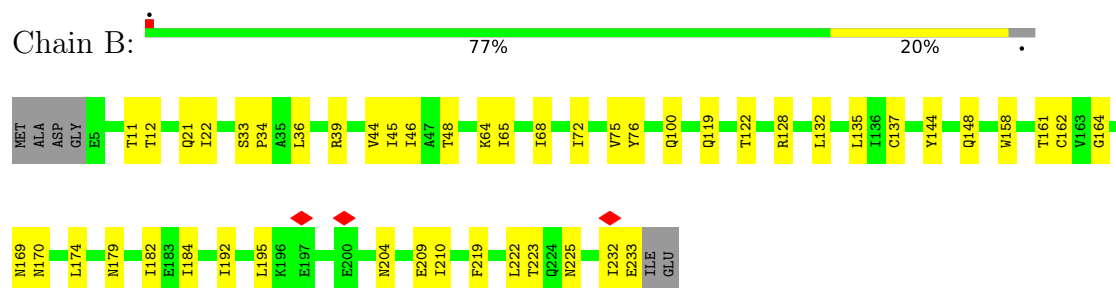
- Molecule 1: 20S proteasome alpha-1 subunit



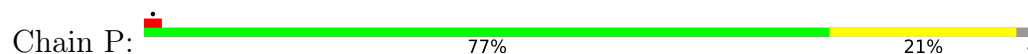
- Molecule 1: 20S proteasome alpha-1 subunit

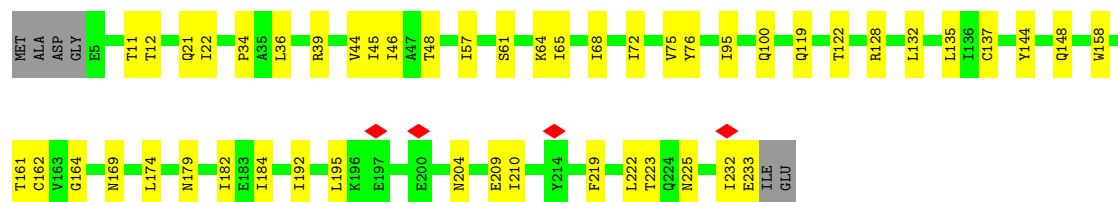


- Molecule 2: 20S proteasome alpha-2 subunit

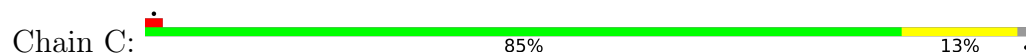


- Molecule 2: 20S proteasome alpha-2 subunit

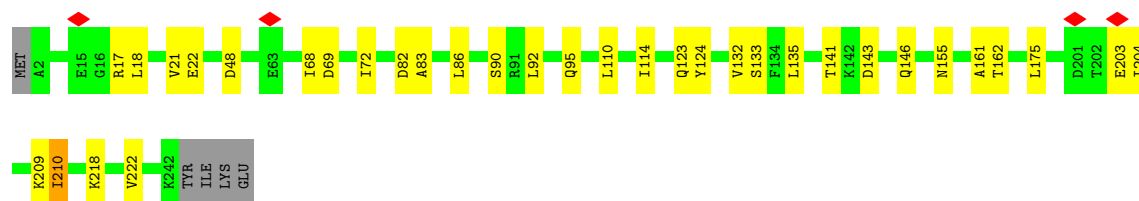
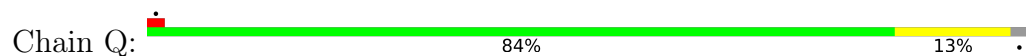




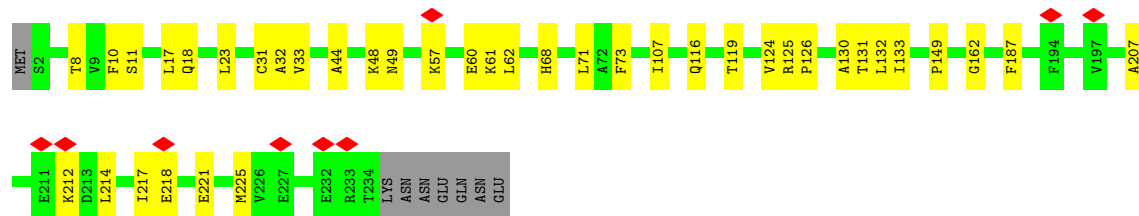
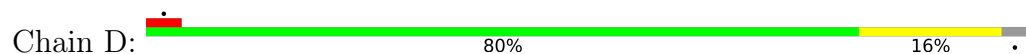
- Molecule 3: 20S proteasome alpha-3 subunit



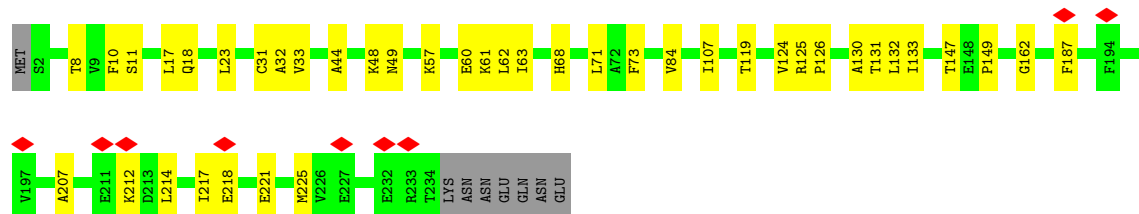
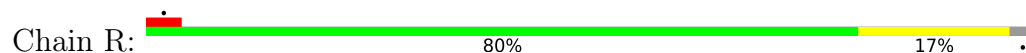
- Molecule 3: 20S proteasome alpha-3 subunit



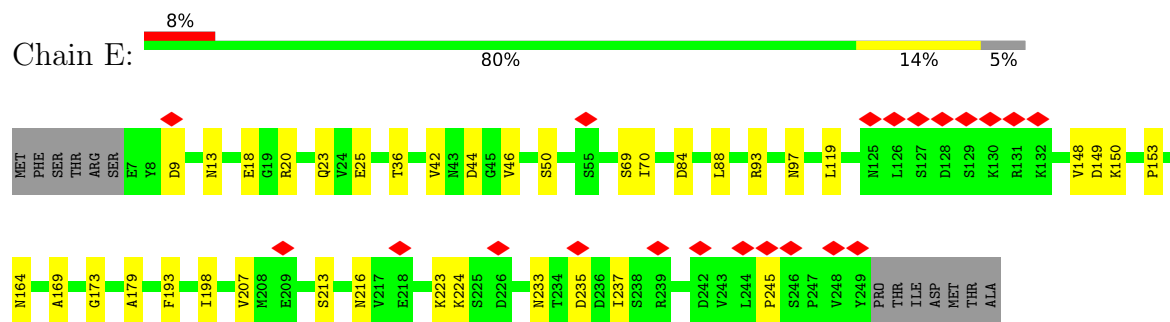
- Molecule 4: 20S proteasome alpha-4 subunit



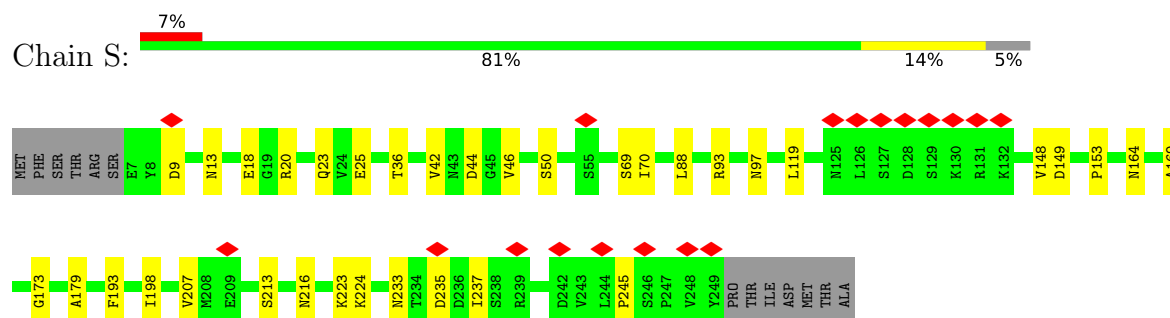
- Molecule 4: 20S proteasome alpha-4 subunit



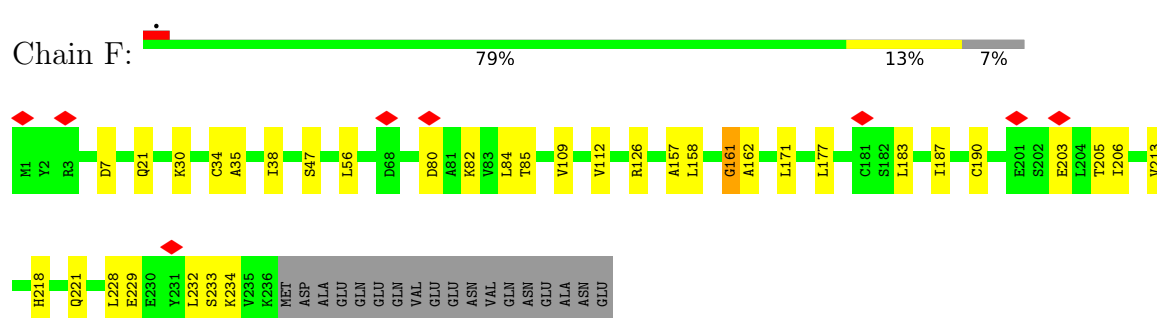
- Molecule 5: 20S proteasome alpha-5 subunit



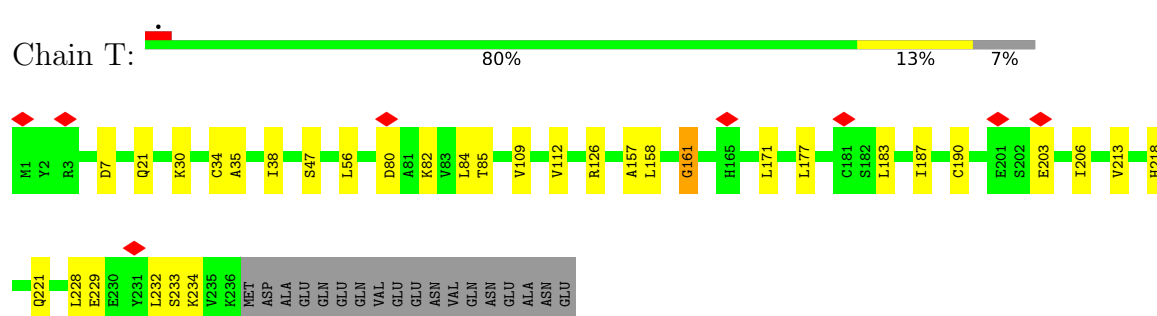
- Molecule 5: 20S proteasome alpha-5 subunit



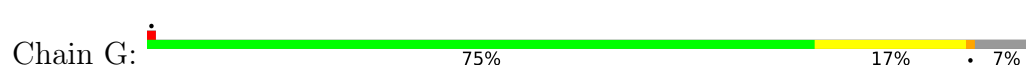
- Molecule 6: 20S proteasome alpha-6 subunit

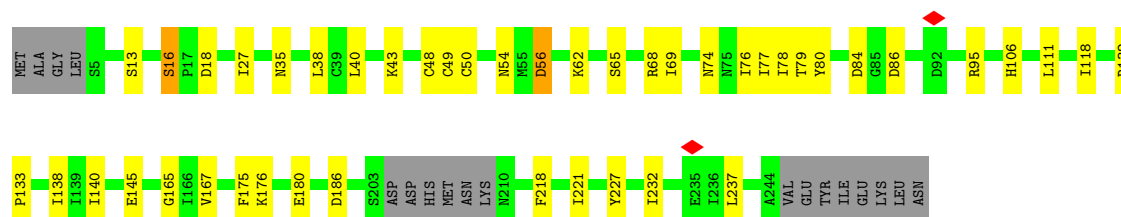


- Molecule 6: 20S proteasome alpha-6 subunit



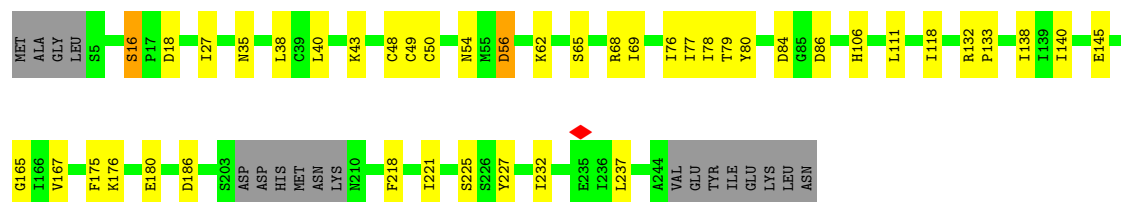
- Molecule 7: 20S proteasome alpha-7 subunit





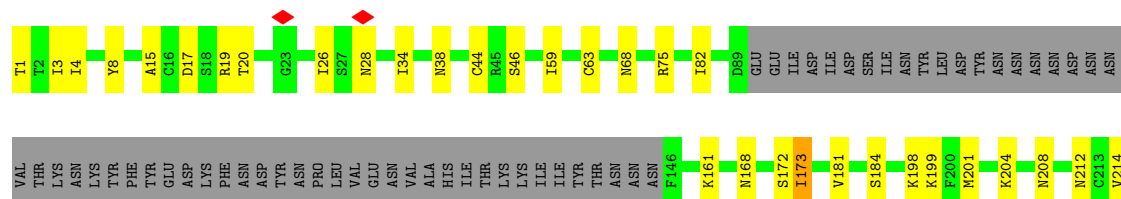
• Molecule 7: 20S proteasome alpha-7 subunit

Chain U: 76% 16% 7%



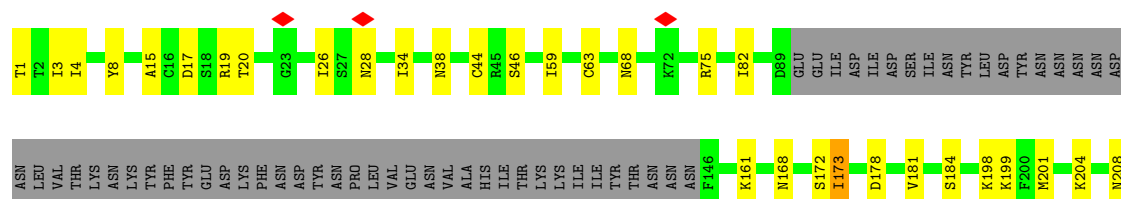
• Molecule 8: 20S proteasome beta-1 subunit

Chain H: 63% 14% 22%



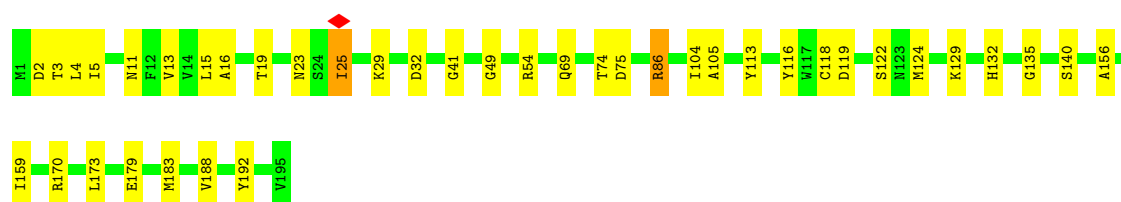
• Molecule 8: 20S proteasome beta-1 subunit

Chain V: 62% 15% 22%

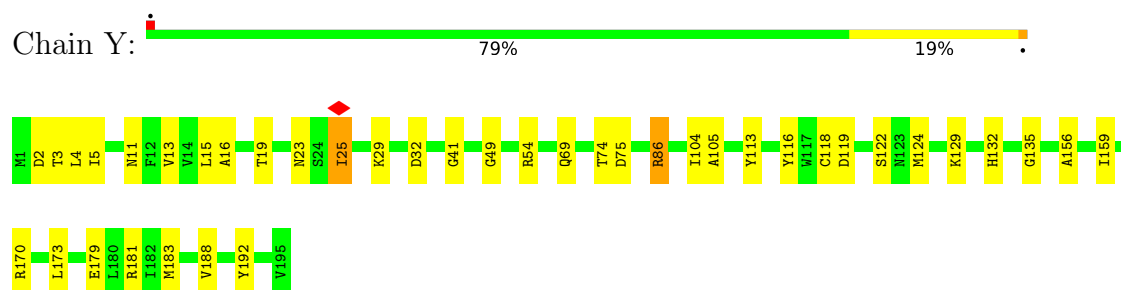


• Molecule 9: 20S proteasome beta-2 subunit

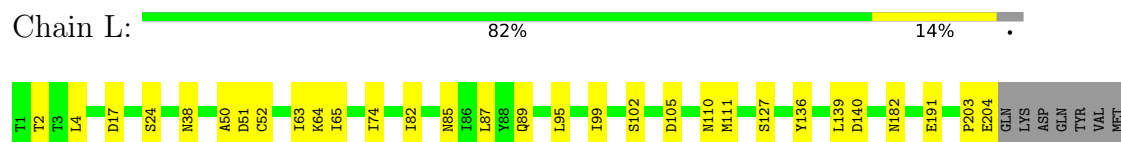
Chain I: 80% 16% 0%



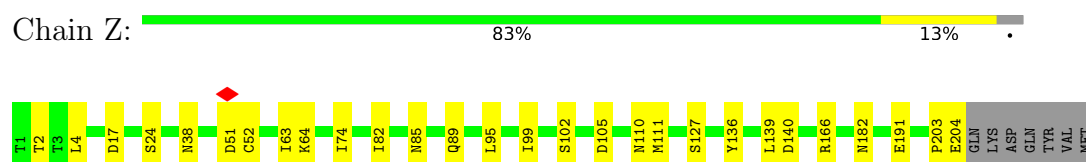
- Molecule 11: 20S proteasome beta-4 subunit



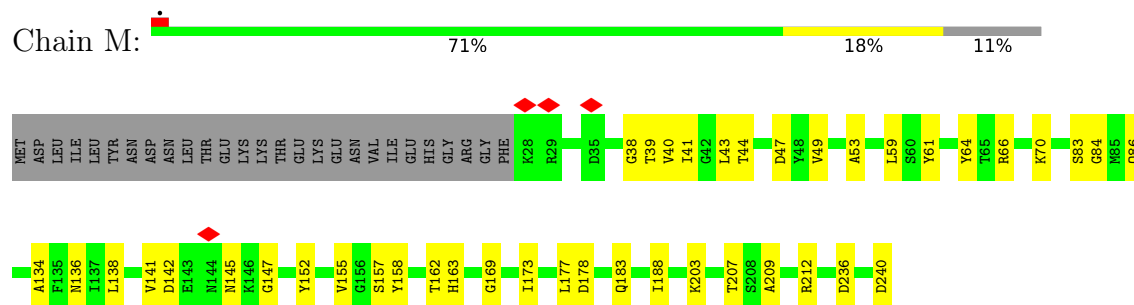
- Molecule 12: 20S proteasome beta-5 subunit



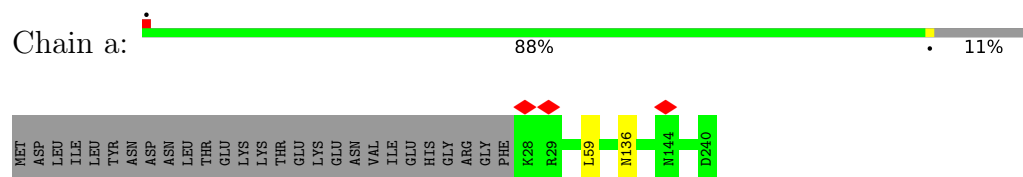
- Molecule 12: 20S proteasome beta-5 subunit



- Molecule 13: 20S proteasome beta-6 subunit

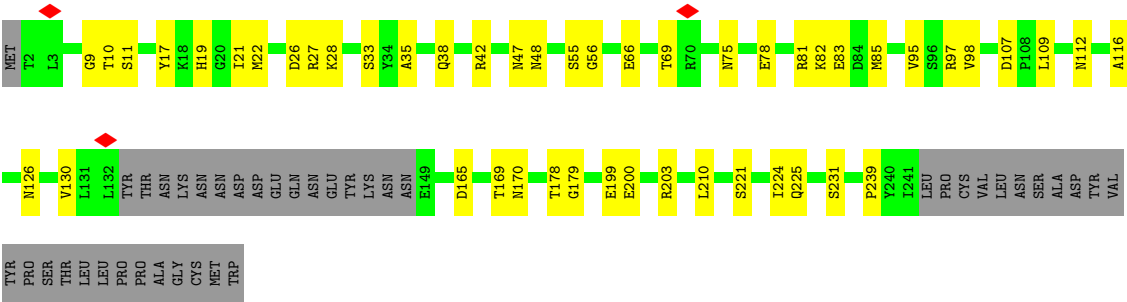


- Molecule 13: 20S proteasome beta-6 subunit

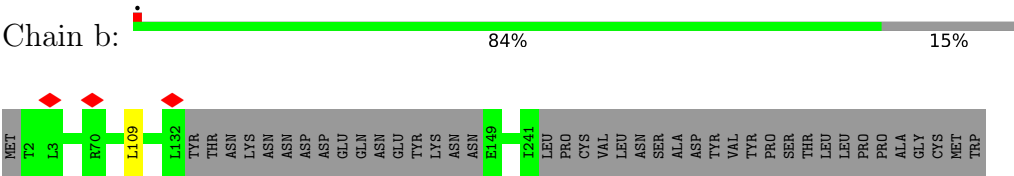


- Molecule 14: 20S proteasome beta-7 subunit





● Molecule 14: 20S proteasome beta-7 subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	36211	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	32.031	Depositor
Minimum map value	-18.409	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.0	Depositor
Map size (\AA)	450.63998, 450.63998, 450.63998	wwPDB
Map dimensions	344, 344, 344	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

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	0.34	0/2013	0.60	0/2715
1	O	0.34	0/2013	0.60	0/2715
2	B	0.36	0/1860	0.55	0/2512
2	P	0.36	0/1860	0.55	0/2512
3	C	0.37	0/1961	0.58	0/2655
3	Q	0.37	0/1961	0.58	0/2655
4	D	0.35	0/1875	0.57	1/2530 (0.0%)
4	R	0.35	0/1875	0.57	1/2530 (0.0%)
5	E	0.34	0/1915	0.57	0/2586
5	S	0.34	0/1915	0.57	0/2586
6	F	0.37	0/1913	0.59	1/2576 (0.0%)
6	T	0.37	0/1913	0.59	1/2576 (0.0%)
7	G	0.39	0/1953	0.63	1/2639 (0.0%)
7	U	0.39	0/1953	0.63	1/2639 (0.0%)
8	H	0.40	0/1594	0.61	0/2135
8	V	0.40	0/1594	0.61	0/2135
9	I	0.36	0/1738	0.58	0/2361
9	W	0.36	0/1738	0.58	0/2361
10	J	0.42	0/1638	0.58	0/2211
10	X	0.42	0/1638	0.58	0/2211
11	K	0.42	0/1649	0.59	1/2223 (0.0%)
11	Y	0.42	0/1649	0.59	1/2223 (0.0%)
12	L	0.40	0/1633	0.60	0/2202
12	Z	0.40	0/1633	0.60	0/2202
13	M	0.40	0/1728	0.64	1/2339 (0.0%)
13	a	0.40	0/1728	0.64	1/2339 (0.0%)
14	N	0.38	0/1882	0.62	1/2538 (0.0%)
14	b	0.38	0/1882	0.62	1/2538 (0.0%)
All	All	0.38	0/50704	0.59	12/68444 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	109	LEU	CA-CB-CG	9.94	138.16	115.30
14	b	109	LEU	CA-CB-CG	9.93	138.15	115.30
13	a	59	LEU	CA-CB-CG	6.38	129.98	115.30
13	M	59	LEU	CA-CB-CG	6.38	129.98	115.30
7	U	56	ASP	CB-CG-OD2	5.89	123.60	118.30
7	G	56	ASP	CB-CG-OD2	5.87	123.59	118.30
11	Y	173	LEU	CA-CB-CG	5.86	128.77	115.30
11	K	173	LEU	CA-CB-CG	5.85	128.75	115.30
6	T	158	LEU	CA-CB-CG	5.71	128.43	115.30
6	F	158	LEU	CA-CB-CG	5.70	128.41	115.30
4	R	132	LEU	CA-CB-CG	5.06	126.93	115.30
4	D	132	LEU	CA-CB-CG	5.05	126.92	115.30

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	35	0
1	O	1986	0	1984	35	0
2	B	1826	0	1844	32	0
2	P	1826	0	1844	33	0
3	C	1926	0	1923	20	0
3	Q	1926	0	1923	21	0
4	D	1845	0	1878	24	0
4	R	1845	0	1878	25	0
5	E	1888	0	1891	24	0
5	S	1888	0	1891	21	0
6	F	1878	0	1881	24	0
6	T	1878	0	1881	22	0
7	G	1912	0	1864	31	0
7	U	1912	0	1864	29	0
8	H	1569	0	1566	24	0
8	V	1569	0	1566	27	0
9	I	1702	0	1711	24	0
9	W	1702	0	1711	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1612	0	1608	30	0
10	X	1612	0	1608	32	0
11	K	1614	0	1584	25	0
11	Y	1614	0	1584	25	0
12	L	1600	0	1558	21	0
12	Z	1600	0	1558	19	0
13	M	1696	0	1707	29	0
13	a	1696	0	1707	0	0
14	N	1845	0	1814	33	0
14	b	1845	0	1814	0	0
All	All	49798	0	49626	626	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 7.

All (626) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:48:CYS:SG	7:U:49:CYS:N	2.64	0.71
7:G:48:CYS:SG	7:G:49:CYS:N	2.64	0.71
3:Q:203:GLU:HG2	3:Q:204:ILE:HG12	1.77	0.67
3:C:203:GLU:HG2	3:C:204:ILE:HG12	1.77	0.67
5:E:97:ASN:HD21	12:L:64:LYS:HB3	1.61	0.66
8:H:19:ARG:HD2	8:H:26:ILE:HD12	1.76	0.65
8:V:19:ARG:HD2	8:V:26:ILE:HD12	1.76	0.65
5:S:97:ASN:HD21	12:Z:64:LYS:HB3	1.62	0.64
8:H:38:ASN:ND2	8:H:63:CYS:SG	2.71	0.64
8:V:38:ASN:ND2	8:V:63:CYS:SG	2.71	0.64
7:G:78:ILE:HG12	7:G:140:ILE:HG12	1.80	0.63
7:U:78:ILE:HG12	7:U:140:ILE:HG12	1.81	0.63
5:E:13:ASN:HB3	6:F:126:ARG:HB3	1.80	0.63
7:G:68:ARG:HD3	7:G:80:TYR:HB2	1.81	0.63
7:U:68:ARG:HD3	7:U:80:TYR:HB2	1.81	0.63
5:S:23:GLN:HE22	4:R:10:PHE:HB2	1.64	0.63
9:I:214:SER:HB3	10:J:210:LYS:HB3	1.82	0.62
1:A:158:PHE:HA	1:A:168:GLY:HA2	1.81	0.62
1:O:158:PHE:HA	1:O:168:GLY:HA2	1.81	0.62
5:E:148:VAL:HG21	5:E:224:LYS:HA	1.82	0.62
5:S:148:VAL:HG21	5:S:224:LYS:HA	1.82	0.62
4:R:62:LEU:HD21	4:R:207:ALA:HB2	1.82	0.62
7:G:50:CYS:SG	7:G:68:ARG:NH1	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:50:CYS:SG	7:U:68:ARG:NH1	2.73	0.61
4:D:62:LEU:HD21	4:D:207:ALA:HB2	1.81	0.61
4:R:207:ALA:HB1	4:R:214:LEU:HD11	1.83	0.61
2:P:34:PRO:HA	2:P:164:GLY:HA3	1.81	0.61
4:D:207:ALA:HB1	4:D:214:LEU:HD11	1.83	0.61
2:B:34:PRO:HA	2:B:164:GLY:HA3	1.81	0.61
9:I:103:VAL:HG21	9:I:180:LYS:HA	1.83	0.60
6:T:7:ASP:O	6:T:21:GLN:NE2	2.34	0.60
6:F:7:ASP:O	6:F:21:GLN:NE2	2.34	0.60
13:M:38:GLY:HA3	13:M:70:LYS:HE3	1.82	0.60
9:W:103:VAL:HG21	9:W:180:LYS:HA	1.83	0.60
7:U:86:ASP:OD2	7:U:132:ARG:NH1	2.33	0.60
7:G:86:ASP:OD2	7:G:132:ARG:NH1	2.33	0.60
6:F:157:ALA:HB1	6:F:171:LEU:HD13	1.84	0.59
9:I:81:SER:O	9:I:85:GLN:NE2	2.36	0.59
9:W:81:SER:O	9:W:85:GLN:NE2	2.36	0.59
13:M:41:ILE:HD12	13:M:173:ILE:HG21	1.84	0.59
6:T:157:ALA:HB1	6:T:171:LEU:HD13	1.84	0.59
13:M:240:ASP:HB3	9:W:19:ARG:HH12	1.68	0.59
11:Y:156:ALA:HA	11:Y:159:ILE:HD12	1.83	0.59
11:K:156:ALA:HA	11:K:159:ILE:HD12	1.83	0.59
5:E:164:ASN:OD1	6:F:82:LYS:NZ	2.35	0.58
10:J:28:ARG:NH2	10:J:35:THR:O	2.36	0.58
11:K:86:ARG:HG3	11:K:124:MET:HB2	1.84	0.58
10:X:28:ARG:NH2	10:X:35:THR:O	2.36	0.58
7:G:16:SER:OG	7:G:18:ASP:OD1	2.21	0.58
11:K:104:ILE:HB	11:K:116:TYR:HB2	1.85	0.58
11:Y:104:ILE:HB	11:Y:116:TYR:HB2	1.85	0.58
7:U:16:SER:OG	7:U:18:ASP:OD1	2.21	0.58
11:Y:86:ARG:HG3	11:Y:124:MET:HB2	1.84	0.58
14:N:26:ASP:O	14:N:42:ARG:NH1	2.37	0.58
1:A:99:LYS:HD3	1:A:127:LYS:HD2	1.85	0.58
1:O:99:LYS:HD3	1:O:127:LYS:HD2	1.85	0.57
4:R:119:THR:HG22	4:R:126:PRO:HB3	1.86	0.57
4:D:119:THR:HG22	4:D:126:PRO:HB3	1.86	0.57
10:X:198:ALA:HB3	10:X:213:LEU:HB2	1.85	0.57
5:E:36:THR:HA	5:E:173:GLY:HA3	1.85	0.57
10:J:55:LEU:HB3	10:J:62:ILE:HG12	1.87	0.57
5:S:36:THR:HA	5:S:173:GLY:HA3	1.85	0.57
10:X:55:LEU:HB3	10:X:62:ILE:HG12	1.87	0.57
10:X:137:TYR:O	10:X:152:ASN:ND2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:137:TYR:O	10:J:152:ASN:ND2	2.36	0.57
10:J:198:ALA:HB3	10:J:213:LEU:HB2	1.86	0.57
1:O:14:THR:HB	2:P:128:ARG:HB3	1.86	0.57
12:L:38:ASN:HD21	12:L:63:ILE:HG21	1.70	0.57
1:O:47:CYS:SG	1:O:48:ALA:N	2.78	0.57
1:A:47:CYS:SG	1:A:48:ALA:N	2.78	0.57
10:X:210:LYS:HB3	9:W:214:SER:HB3	1.85	0.57
12:Z:38:ASN:HD21	12:Z:63:ILE:HG21	1.70	0.57
7:G:106:HIS:HB2	8:H:82:ILE:HG21	1.86	0.56
8:V:168:ASN:ND2	8:V:172:SER:OG	2.38	0.56
8:H:168:ASN:ND2	8:H:172:SER:OG	2.39	0.56
6:T:30:LYS:HA	6:T:161:GLY:HA3	1.87	0.56
2:B:119:GLN:NE2	3:C:82:ASP:OD1	2.38	0.56
6:F:30:LYS:HA	6:F:161:GLY:HA3	1.87	0.56
14:N:75:ASN:HD21	14:N:85:MET:HA	1.69	0.56
7:U:77:ILE:HG23	7:U:221:ILE:HD13	1.88	0.56
7:G:77:ILE:HG23	7:G:221:ILE:HD13	1.88	0.56
4:D:48:LYS:NZ	4:D:49:ASN:O	2.39	0.56
7:U:49:CYS:HA	7:U:218:PHE:HB3	1.87	0.56
1:A:14:THR:HB	2:B:128:ARG:HB3	1.87	0.56
7:G:49:CYS:HA	7:G:218:PHE:HB3	1.88	0.56
4:R:48:LYS:NZ	4:R:49:ASN:O	2.39	0.56
3:C:90:SER:HB2	3:C:114:ILE:HD12	1.88	0.56
3:Q:90:SER:HB2	3:Q:114:ILE:HD12	1.88	0.56
14:N:17:TYR:HE2	14:N:22:MET:HB2	1.70	0.56
14:N:55:SER:HB2	14:N:112:ASN:HB2	1.87	0.56
1:A:238:ASN:ND2	1:A:242:THR:OG1	2.39	0.55
4:R:31:CYS:HA	4:R:162:GLY:HA3	1.87	0.55
1:O:238:ASN:ND2	1:O:242:THR:OG1	2.39	0.55
4:D:31:CYS:HA	4:D:162:GLY:HA3	1.87	0.55
8:H:4:ILE:HD13	8:H:214:VAL:HG22	1.88	0.55
8:V:4:ILE:HD13	8:V:214:VAL:HG22	1.89	0.55
1:A:15:ILE:HA	2:B:21:GLN:HE22	1.69	0.55
5:E:149:ASP:N	5:E:149:ASP:OD1	2.39	0.55
7:U:176:LYS:NZ	7:U:180:GLU:OE2	2.38	0.55
14:N:82:LYS:HB3	14:N:126:ASN:HB3	1.88	0.55
9:W:182:SER:OG	9:W:183:TYR:N	2.39	0.55
7:G:176:LYS:NZ	7:G:180:GLU:OE2	2.38	0.55
9:I:182:SER:OG	9:I:183:TYR:N	2.39	0.55
5:S:149:ASP:OD1	5:S:149:ASP:N	2.39	0.55
1:A:206:ARG:HH21	1:A:252:TYR:HE1	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:34:ILE:HG13	8:V:44:CYS:HB3	1.89	0.54
8:H:34:ILE:HG13	8:H:44:CYS:HB3	1.89	0.54
13:M:183:GLN:HG3	13:M:188:ILE:HG23	1.89	0.54
5:S:13:ASN:HB3	6:T:126:ARG:HB3	1.88	0.54
1:O:206:ARG:HH21	1:O:252:TYR:HE1	1.55	0.54
10:J:216:ARG:HH12	12:Z:191:GLU:HG2	1.72	0.54
13:M:61:TYR:HH	9:W:129:SER:HG	1.53	0.54
10:X:4:ILE:HB	10:X:108:ASN:HD21	1.72	0.54
10:J:4:ILE:HB	10:J:108:ASN:HD21	1.72	0.54
5:S:164:ASN:OD1	6:T:82:LYS:NZ	2.39	0.54
1:A:203:GLU:O	1:A:207:ASN:N	2.41	0.54
11:K:13:VAL:HG11	11:K:105:ALA:HB1	1.89	0.54
13:M:47:ASP:OD1	13:M:47:ASP:N	2.40	0.54
11:Y:13:VAL:HG11	11:Y:105:ALA:HB1	1.89	0.54
1:O:203:GLU:O	1:O:207:ASN:N	2.41	0.54
8:H:4:ILE:HG13	8:H:181:VAL:HG23	1.89	0.54
5:S:20:ARG:NH1	5:S:25:GLU:OE1	2.41	0.54
8:V:4:ILE:HG13	8:V:181:VAL:HG23	1.88	0.54
2:B:232:ILE:HG23	2:B:233:GLU:HG3	1.89	0.54
5:E:20:ARG:NH1	5:E:25:GLU:OE1	2.41	0.53
7:G:38:LEU:HB3	7:G:49:CYS:HB2	1.90	0.53
2:P:232:ILE:HG23	2:P:233:GLU:HG3	1.89	0.53
7:U:38:LEU:HB3	7:U:49:CYS:HB2	1.90	0.53
6:F:229:GLU:HA	6:F:233:SER:HB3	1.89	0.53
11:Y:49:GLY:O	11:Y:54:ARG:NH2	2.40	0.53
6:T:229:GLU:HA	6:T:233:SER:HB3	1.89	0.53
3:C:69:ASP:OD1	3:C:95:GLN:NE2	2.41	0.53
11:K:49:GLY:O	11:K:54:ARG:NH2	2.40	0.53
1:O:167:ALA:O	2:P:61:SER:OG	2.21	0.53
3:Q:69:ASP:OD1	3:Q:95:GLN:NE2	2.41	0.53
7:G:74:ASN:HD22	14:N:130:VAL:HB	1.74	0.53
2:P:45:ILE:HD11	2:P:184:ILE:HG13	1.89	0.53
3:C:48:ASP:HA	3:C:210:ILE:HG22	1.89	0.53
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.89	0.53
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.89	0.53
2:B:45:ILE:HD11	2:B:184:ILE:HG13	1.89	0.53
1:A:54:LYS:NZ	1:A:69:TYR:O	2.40	0.53
11:K:129:LYS:NZ	12:Z:204:GLU:O	2.41	0.53
4:R:31:CYS:SG	4:R:32:ALA:N	2.82	0.53
1:O:54:LYS:NZ	1:O:69:TYR:O	2.39	0.53
3:C:218:LYS:HE3	3:C:222:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:CYS:SG	4:D:32:ALA:N	2.82	0.52
3:Q:48:ASP:HA	3:Q:210:ILE:HG22	1.89	0.52
5:E:46:VAL:HG23	5:E:153:PRO:HB2	1.91	0.52
3:Q:218:LYS:HE3	3:Q:222:VAL:HG21	1.91	0.52
5:S:46:VAL:HG23	5:S:153:PRO:HB2	1.91	0.52
9:W:17:ASP:O	9:W:33:LYS:NZ	2.39	0.52
2:B:100:GLN:OE1	10:J:72:ARG:NH1	2.42	0.52
9:I:17:ASP:O	9:I:33:LYS:NZ	2.39	0.52
13:M:178:ASP:OD2	10:X:190:ARG:NH2	2.37	0.52
4:D:187:PHE:HE1	4:D:225:MET:HG2	1.75	0.52
9:I:67:ARG:HG3	9:I:74:PRO:HD3	1.92	0.52
9:W:67:ARG:HG3	9:W:74:PRO:HD3	1.92	0.52
1:O:79:THR:HA	8:V:68:ASN:HD21	1.75	0.52
10:J:39:THR:OG1	12:Z:203:PRO:O	2.26	0.52
8:V:82:ILE:HG21	7:U:106:HIS:HB2	1.91	0.52
4:D:60:GLU:OE2	4:D:61:LYS:NZ	2.38	0.52
8:H:19:ARG:HB2	8:H:225:GLY:HA2	1.91	0.52
9:I:28:ASP:OD1	9:I:28:ASP:N	2.42	0.52
9:W:28:ASP:OD1	9:W:28:ASP:N	2.42	0.52
8:V:19:ARG:HB2	8:V:225:GLY:HA2	1.91	0.52
9:I:211:PRO:HG3	10:J:214:LYS:HB2	1.91	0.52
14:N:21:ILE:HG21	14:N:116:ALA:HB1	1.92	0.52
4:R:60:GLU:OE2	4:R:61:LYS:NZ	2.38	0.52
4:R:187:PHE:HE1	4:R:225:MET:HG2	1.75	0.52
2:B:11:THR:HG22	2:B:21:GLN:HG2	1.92	0.52
2:P:11:THR:HG22	2:P:21:GLN:HG2	1.92	0.52
2:B:36:LEU:HD11	2:B:174:LEU:HD11	1.91	0.51
2:B:48:THR:HG21	2:B:64:LYS:HD2	1.93	0.51
5:E:169:ALA:HB3	6:F:56:LEU:HD13	1.92	0.51
13:M:44:THR:HG22	13:M:49:VAL:HG12	1.91	0.51
10:X:85:ASP:N	10:X:85:ASP:OD1	2.39	0.51
2:P:48:THR:HG21	2:P:64:LYS:HD2	1.93	0.51
10:J:85:ASP:OD1	10:J:85:ASP:N	2.39	0.51
11:K:170:ARG:NH1	12:Z:140:ASP:OD2	2.43	0.51
2:P:36:LEU:HD11	2:P:174:LEU:HD11	1.91	0.51
3:C:124:TYR:HB3	4:D:124:VAL:HG12	1.92	0.51
1:O:50:ILE:HG13	1:O:147:ILE:HD12	1.92	0.51
2:P:179:ASN:H	2:P:182:ILE:HD11	1.74	0.51
2:B:179:ASN:H	2:B:182:ILE:HD11	1.74	0.51
11:K:13:VAL:HG23	11:K:113:TYR:HB3	1.92	0.51
11:Y:13:VAL:HG23	11:Y:113:TYR:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG13	1:A:147:ILE:HD12	1.92	0.51
14:N:9:GLY:N	14:N:56:GLY:O	2.42	0.51
6:F:47:SER:OG	6:F:190:CYS:SG	2.67	0.51
14:N:199:GLU:OE2	14:N:203:ARG:NH2	2.44	0.51
12:Z:127:SER:HB3	12:Z:136:TYR:HD1	1.76	0.51
5:E:198:ILE:HB	5:E:245:PRO:HG3	1.93	0.51
12:L:127:SER:HB3	12:L:136:TYR:HD1	1.76	0.51
14:N:17:TYR:HD1	14:N:19:HIS:H	1.59	0.51
14:N:27:ARG:NH1	14:N:225:GLN:OE1	2.43	0.51
9:I:3:ILE:O	9:I:127:LEU:N	2.44	0.50
5:S:198:ILE:HB	5:S:245:PRO:HG3	1.93	0.50
6:T:47:SER:OG	6:T:190:CYS:SG	2.67	0.50
14:N:28:LYS:HD2	14:N:221:SER:HB3	1.93	0.50
9:W:3:ILE:O	9:W:127:LEU:N	2.44	0.50
7:U:35:ASN:HD21	7:U:54:ASN:H	1.59	0.50
5:E:42:VAL:HG23	5:E:44:ASP:H	1.77	0.50
4:R:124:VAL:HG12	3:Q:124:TYR:HB3	1.93	0.50
1:O:51:ILE:HG23	1:O:231:VAL:HG12	1.93	0.50
1:A:51:ILE:HG23	1:A:231:VAL:HG12	1.93	0.50
13:M:83:SER:OG	13:M:83:SER:O	2.30	0.50
5:S:42:VAL:HG23	5:S:44:ASP:H	1.77	0.50
3:C:161:ALA:HB1	3:C:175:LEU:HD13	1.94	0.50
13:M:152:TYR:HB3	13:M:158:TYR:HA	1.94	0.50
14:N:28:LYS:HE3	14:N:35:ALA:HB2	1.93	0.50
3:Q:161:ALA:HB1	3:Q:175:LEU:HD13	1.94	0.50
7:G:35:ASN:HD21	7:G:54:ASN:H	1.59	0.50
14:N:210:LEU:HD13	14:N:224:ILE:HD12	1.93	0.50
7:G:95:ARG:NH1	14:N:78:GLU:OE2	2.44	0.50
7:G:167:VAL:HG11	7:G:175:PHE:HB2	1.94	0.50
13:M:64:TYR:OH	14:N:165:ASP:OD2	2.25	0.50
14:N:200:GLU:OE2	14:N:203:ARG:NH1	2.45	0.50
2:P:119:GLN:NE2	3:Q:82:ASP:OD1	2.45	0.50
7:U:167:VAL:HG11	7:U:175:PHE:HB2	1.94	0.50
1:O:15:ILE:HA	2:P:21:GLN:HE22	1.75	0.49
2:P:68:ILE:HB	2:P:72:ILE:HB	1.93	0.49
2:B:68:ILE:HB	2:B:72:ILE:HB	1.93	0.49
14:N:224:ILE:HB	14:N:239:PRO:HG2	1.94	0.49
10:X:172:ASP:N	10:X:172:ASP:OD1	2.40	0.49
11:K:5:ILE:HB	11:K:16:ALA:HB3	1.94	0.49
10:J:172:ASP:N	10:J:172:ASP:OD1	2.40	0.49
11:Y:5:ILE:HB	11:Y:16:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:LEU:HD11	3:C:162:THR:HB	1.95	0.49
14:N:178:THR:OG1	14:N:179:GLY:N	2.45	0.49
3:Q:135:LEU:HD11	3:Q:162:THR:HB	1.95	0.49
10:X:29:LEU:HB3	10:X:38:SER:HB3	1.93	0.49
6:T:109:VAL:HA	6:T:112:VAL:HG12	1.94	0.49
8:V:208:ASN:O	8:V:212:ASN:ND2	2.45	0.49
5:E:18:GLU:OE2	5:E:20:ARG:NH1	2.46	0.49
6:F:109:VAL:HA	6:F:112:VAL:HG12	1.94	0.49
8:H:208:ASN:O	8:H:212:ASN:ND2	2.45	0.49
10:J:29:LEU:HB3	10:J:38:SER:HB3	1.93	0.49
5:S:18:GLU:OE2	5:S:20:ARG:NH1	2.46	0.49
5:S:213:SER:OG	5:S:216:ASN:OD1	2.29	0.49
11:K:140:SER:OG	12:Z:166:ARG:NH2	2.44	0.49
12:L:24:SER:O	12:L:24:SER:OG	2.30	0.49
5:S:169:ALA:HB3	6:T:56:LEU:HD13	1.95	0.49
5:E:213:SER:OG	5:E:216:ASN:OD1	2.29	0.49
12:Z:24:SER:O	12:Z:24:SER:OG	2.30	0.49
7:U:50:CYS:HB2	7:U:69:ILE:HD11	1.94	0.49
7:G:50:CYS:HB2	7:G:69:ILE:HD11	1.94	0.48
10:J:110:ILE:HD11	10:J:150:VAL:HG13	1.95	0.48
10:X:110:ILE:HD11	10:X:150:VAL:HG13	1.95	0.48
11:Y:2:ASP:OD1	11:Y:2:ASP:N	2.46	0.48
2:P:148:GLN:OE1	2:P:158:TRP:NE1	2.46	0.48
2:B:148:GLN:OE1	2:B:158:TRP:NE1	2.46	0.48
11:K:2:ASP:OD1	11:K:2:ASP:N	2.46	0.48
9:W:174:ASP:HB3	9:W:187:ARG:HG3	1.94	0.48
7:U:62:LYS:HB2	7:U:65:SER:HB2	1.94	0.48
9:I:174:ASP:HB3	9:I:187:ARG:HG3	1.94	0.48
10:J:48:ASN:ND2	10:J:84:MET:O	2.46	0.48
12:L:50:ALA:HB3	13:M:155:VAL:HG13	1.94	0.48
10:X:48:ASN:ND2	10:X:84:MET:O	2.46	0.48
9:W:61:HIS:HB3	2:P:95:ILE:HG23	1.95	0.48
2:B:65:ILE:HG12	2:B:75:VAL:HG22	1.96	0.48
7:G:62:LYS:HB2	7:G:65:SER:HB2	1.94	0.48
11:K:86:ARG:HG2	11:K:122:SER:HB3	1.93	0.48
11:Y:86:ARG:HG2	11:Y:122:SER:HB3	1.93	0.48
2:P:65:ILE:HG12	2:P:75:VAL:HG22	1.96	0.48
1:A:113:TYR:OH	9:I:106:ASN:ND2	2.47	0.48
7:G:84:ASP:OD1	7:G:84:ASP:N	2.45	0.48
9:I:104:ASP:OD2	9:I:109:GLN:NE2	2.46	0.48
13:M:86:GLN:HB3	14:N:169:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:203:LYS:O	13:M:207:THR:OG1	2.28	0.48
14:N:38:GLN:OE1	8:V:219:HIS:NE2	2.47	0.48
5:S:69:SER:O	5:S:93:ARG:NE	2.46	0.48
11:K:3:THR:HG22	11:K:135:GLY:HA3	1.95	0.48
11:Y:3:THR:HG22	11:Y:135:GLY:HA3	1.95	0.48
9:W:104:ASP:OD2	9:W:109:GLN:NE2	2.46	0.48
5:E:69:SER:O	5:E:93:ARG:NE	2.46	0.48
1:A:250:ASP:OD1	1:A:250:ASP:N	2.47	0.48
10:X:10:GLY:HA3	10:X:43:LYS:HE3	1.95	0.48
7:U:84:ASP:OD1	7:U:84:ASP:N	2.45	0.48
10:J:10:GLY:HA3	10:J:43:LYS:HE3	1.95	0.48
3:Q:209:LYS:HB3	3:Q:210:ILE:H	1.48	0.48
11:K:4:LEU:HB2	11:K:132:HIS:HB2	1.96	0.48
11:Y:4:LEU:HB2	11:Y:132:HIS:HB2	1.96	0.48
1:O:250:ASP:OD1	1:O:250:ASP:N	2.47	0.48
1:A:245:SER:OG	1:A:246:GLU:N	2.47	0.47
8:H:198:LYS:H	8:H:201:MET:HE3	1.79	0.47
1:O:245:SER:OG	1:O:246:GLU:N	2.47	0.47
13:M:141:VAL:HG12	13:M:147:GLY:HA2	1.95	0.47
10:X:75:LEU:HD11	3:Q:92:LEU:HD22	1.95	0.47
1:O:173:VAL:HG23	1:O:185:LEU:HD22	1.95	0.47
1:A:173:VAL:HG23	1:A:185:LEU:HD22	1.95	0.47
2:B:65:ILE:HD12	2:B:209:GLU:HG2	1.96	0.47
1:A:79:THR:HA	8:H:68:ASN:HD21	1.80	0.47
6:F:233:SER:O	6:F:233:SER:OG	2.32	0.47
13:M:142:ASP:OD1	13:M:142:ASP:N	2.46	0.47
6:T:233:SER:O	6:T:233:SER:OG	2.32	0.47
2:P:65:ILE:HD12	2:P:209:GLU:HG2	1.96	0.47
3:Q:83:ALA:HB2	3:Q:132:VAL:HG21	1.97	0.47
8:H:15:ALA:HB2	8:H:230:ILE:HG23	1.96	0.47
3:C:83:ALA:HB2	3:C:132:VAL:HG21	1.97	0.47
11:K:183:MET:HG2	11:K:188:VAL:HG22	1.96	0.47
12:L:182:ASN:OD1	12:L:182:ASN:N	2.48	0.47
14:N:107:ASP:OD1	14:N:107:ASP:N	2.46	0.47
12:Z:182:ASN:OD1	12:Z:182:ASN:N	2.47	0.47
8:V:15:ALA:HB2	8:V:230:ILE:HG23	1.96	0.47
8:H:3:ILE:HD12	8:H:46:SER:HB3	1.97	0.46
13:M:173:ILE:HD11	13:M:209:ALA:HB2	1.96	0.46
4:R:11:SER:HB3	4:R:17:LEU:HG	1.97	0.46
4:R:57:LYS:HD2	4:R:60:GLU:H	1.81	0.46
4:D:57:LYS:HD2	4:D:60:GLU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:179:GLU:HG3	11:K:192:TYR:HB3	1.97	0.46
11:Y:183:MET:HG2	11:Y:188:VAL:HG22	1.96	0.46
4:D:11:SER:HB3	4:D:17:LEU:HG	1.97	0.46
2:P:11:THR:OG1	2:P:122:THR:O	2.31	0.46
8:V:3:ILE:HD12	8:V:46:SER:HB3	1.97	0.46
2:B:169:ASN:N	2:B:169:ASN:OD1	2.48	0.46
3:C:143:ASP:OD2	3:C:146:GLN:NE2	2.48	0.46
11:Y:179:GLU:HG3	11:Y:192:TYR:HB3	1.97	0.46
2:P:169:ASN:OD1	2:P:169:ASN:N	2.48	0.46
8:V:198:LYS:H	8:V:201:MET:HE3	1.80	0.46
1:A:234:VAL:HG22	1:A:241:PHE:HD1	1.81	0.46
2:B:11:THR:OG1	2:B:122:THR:O	2.31	0.46
3:C:18:LEU:HD22	3:C:21:VAL:HG23	1.98	0.46
5:E:88:LEU:HD23	5:E:119:LEU:HD23	1.96	0.46
13:M:39:THR:HG22	13:M:169:GLY:H	1.80	0.46
5:S:88:LEU:HD23	5:S:119:LEU:HD23	1.96	0.46
1:O:234:VAL:HG22	1:O:241:PHE:HD1	1.81	0.46
8:H:1:THR:O	8:H:184:SER:N	2.43	0.46
13:M:84:GLY:HA3	13:M:134:ALA:HA	1.97	0.46
14:N:81:ARG:NE	14:N:83:GLU:OE1	2.48	0.46
14:N:170:ASN:OD1	14:N:170:ASN:N	2.49	0.46
3:Q:143:ASP:OD2	3:Q:146:GLN:NE2	2.48	0.46
5:E:97:ASN:HD22	12:L:65:ILE:HG13	1.80	0.46
10:J:61:ASP:OD2	10:J:106:PHE:N	2.42	0.46
3:Q:18:LEU:HD22	3:Q:21:VAL:HG23	1.98	0.46
11:K:19:THR:HB	11:K:32:ASP:HA	1.97	0.46
1:O:159:LYS:HZ2	1:O:174:ILE:HD13	1.80	0.46
4:D:71:LEU:HD12	4:D:133:ILE:HG12	1.98	0.45
5:E:233:ASN:HD21	5:E:235:ASP:HB2	1.81	0.45
10:J:51:VAL:HG22	10:J:86:VAL:HG22	1.98	0.45
13:M:236:ASP:OD1	13:M:236:ASP:N	2.44	0.45
10:X:61:ASP:OD2	10:X:106:PHE:N	2.42	0.45
4:R:8:THR:HG23	4:R:18:GLN:HB3	1.98	0.45
4:R:71:LEU:HD12	4:R:133:ILE:HG12	1.98	0.45
6:F:228:LEU:O	6:F:233:SER:N	2.48	0.45
5:S:233:ASN:HD21	5:S:235:ASP:HB2	1.82	0.45
10:X:51:VAL:HG22	10:X:86:VAL:HG22	1.98	0.45
10:X:72:ARG:NH1	2:P:100:GLN:OE1	2.46	0.45
11:Y:19:THR:HB	11:Y:32:ASP:HA	1.97	0.45
6:T:228:LEU:O	6:T:233:SER:N	2.48	0.45
4:D:8:THR:HG23	4:D:18:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ILE:HB	2:B:222:LEU:HD12	1.98	0.45
3:Q:86:LEU:HD23	3:Q:86:LEU:HA	1.84	0.45
1:A:113:TYR:HB2	9:I:75:ARG:NE	2.32	0.45
9:I:59:LEU:HD21	9:I:79:CYS:HB2	1.99	0.45
10:J:56:SER:OG	10:J:108:ASN:O	2.32	0.45
9:W:59:LEU:HD21	9:W:79:CYS:HB2	1.99	0.45
9:W:61:HIS:HB3	2:P:95:ILE:HD12	1.98	0.45
9:W:174:ASP:OD1	9:W:174:ASP:N	2.48	0.45
2:P:210:ILE:HB	2:P:222:LEU:HD12	1.98	0.45
2:B:39:ARG:NH2	2:B:144:TYR:O	2.49	0.45
2:B:170:ASN:OD1	2:B:170:ASN:N	4.17	0.45
9:I:174:ASP:OD1	9:I:174:ASP:N	2.48	0.45
8:V:1:THR:O	8:V:184:SER:N	2.43	0.45
2:B:192:ILE:HD11	2:B:210:ILE:HD11	1.98	0.45
4:D:10:PHE:HB2	5:E:23:GLN:HE22	1.82	0.45
10:J:18:SER:OG	10:J:19:ASN:N	2.49	0.45
10:X:18:SER:OG	10:X:19:ASN:N	2.49	0.45
10:X:56:SER:OG	10:X:108:ASN:O	2.32	0.45
2:P:39:ARG:NH2	2:P:144:TYR:O	2.49	0.45
2:P:76:TYR:HB2	2:P:132:LEU:HD12	1.98	0.45
3:C:155:ASN:N	3:C:155:ASN:OD1	2.48	0.45
12:L:4:LEU:HD22	12:L:139:LEU:HD11	1.98	0.45
2:P:192:ILE:HD11	2:P:210:ILE:HD11	1.98	0.45
12:Z:4:LEU:HD22	12:Z:139:LEU:HD11	1.98	0.45
2:B:76:TYR:HB2	2:B:132:LEU:HD12	1.99	0.45
3:C:86:LEU:HD23	3:C:86:LEU:HA	1.84	0.45
4:D:73:PHE:HA	4:D:131:THR:HA	1.99	0.45
13:M:44:THR:OG1	13:M:162:THR:O	2.29	0.45
4:R:73:PHE:HA	4:R:131:THR:HA	1.99	0.45
1:A:159:LYS:HZ2	1:A:174:ILE:HD13	1.81	0.45
3:C:209:LYS:HB3	3:C:210:ILE:H	1.48	0.45
6:F:34:CYS:SG	6:F:35:ALA:N	2.90	0.45
8:H:8:TYR:OH	8:H:232:ASN:ND2	2.50	0.45
14:N:97:ARG:HA	14:N:97:ARG:HD2	1.84	0.45
5:S:179:ALA:HB2	5:S:207:VAL:HG21	1.99	0.45
6:T:34:CYS:SG	6:T:35:ALA:N	2.90	0.45
10:X:214:LYS:HB2	9:W:211:PRO:HG3	1.99	0.44
3:Q:155:ASN:OD1	3:Q:155:ASN:N	2.48	0.44
5:E:179:ALA:HB2	5:E:207:VAL:HG21	1.99	0.44
14:N:17:TYR:HE1	14:N:19:HIS:HB2	1.83	0.44
8:V:8:TYR:OH	8:V:232:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:76:ILE:HG12	7:U:111:LEU:HD13	1.99	0.44
7:U:111:LEU:HA	7:U:111:LEU:HD12	1.72	0.44
1:A:40:VAL:HG22	1:A:173:VAL:HG22	1.98	0.44
3:C:123:GLN:NE2	4:D:125:ARG:O	2.51	0.44
7:G:76:ILE:HG12	7:G:111:LEU:HD13	1.99	0.44
12:L:105:ASP:OD1	12:L:110:ASN:ND2	2.45	0.44
4:R:107:ILE:HG22	4:R:133:ILE:HD13	2.00	0.44
12:Z:105:ASP:OD1	12:Z:110:ASN:ND2	2.45	0.44
1:A:16:PHE:H	2:B:21:GLN:NE2	2.16	0.44
3:C:68:ILE:HG21	3:C:110:LEU:HD21	1.99	0.44
4:D:107:ILE:HG22	4:D:133:ILE:HD13	2.00	0.44
12:L:102:SER:HB2	12:L:111:MET:HG3	1.98	0.44
13:M:157:SER:O	13:M:157:SER:OG	2.33	0.44
1:O:169:TYR:CE2	2:P:57:ILE:HG12	2.53	0.44
10:J:69:LEU:HD11	10:J:93:LEU:HD21	1.99	0.44
4:R:23:LEU:HD13	4:R:149:PRO:HD2	1.99	0.44
1:O:40:VAL:HG22	1:O:173:VAL:HG22	1.98	0.44
8:V:161:LYS:HD3	8:V:161:LYS:HA	1.75	0.44
3:Q:68:ILE:HG21	3:Q:110:LEU:HD21	1.99	0.44
4:D:23:LEU:HD13	4:D:149:PRO:HD2	1.99	0.44
1:O:62:SER:O	1:O:62:SER:OG	2.35	0.44
1:A:62:SER:O	1:A:62:SER:OG	2.35	0.44
10:X:69:LEU:HD11	10:X:93:LEU:HD21	1.99	0.44
1:A:132:THR:HG22	2:B:128:ARG:HH21	1.82	0.44
9:W:106:ASN:ND2	1:O:113:TYR:OH	2.50	0.44
12:Z:102:SER:HB2	12:Z:111:MET:HG3	1.98	0.44
13:M:43:LEU:HD23	13:M:43:LEU:HA	1.79	0.43
6:T:82:LYS:HA	6:T:85:THR:HG22	1.99	0.43
6:F:82:LYS:HA	6:F:85:THR:HG22	2.00	0.43
6:F:234:LYS:HA	6:F:234:LYS:HD2	1.81	0.43
7:G:111:LEU:HD12	7:G:111:LEU:HA	1.72	0.43
12:L:85:ASN:O	12:L:89:GLN:NE2	2.51	0.43
6:T:234:LYS:HA	6:T:234:LYS:HD2	1.81	0.43
12:Z:85:ASN:O	12:Z:89:GLN:NE2	2.51	0.43
7:G:40:LEU:HA	7:G:165:GLY:HA2	1.99	0.43
8:H:59:ILE:HD13	8:H:59:ILE:HA	1.88	0.43
12:L:51:ASP:HB3	12:L:95:LEU:HD22	1.99	0.43
11:Y:23:ASN:HB3	11:Y:29:LYS:HG3	1.99	0.43
11:K:23:ASN:HB3	11:K:29:LYS:HG3	1.99	0.43
14:N:47:ASN:OD1	14:N:48:ASN:N	2.50	0.43
7:U:40:LEU:HA	7:U:165:GLY:HA2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:204:GLU:O	11:Y:129:LYS:NZ	2.51	0.43
13:M:145:ASN:OD1	13:M:145:ASN:N	2.52	0.43
2:P:135:LEU:HD23	2:P:135:LEU:HA	1.88	0.43
12:Z:2:THR:N	12:Z:17:ASP:OD2	2.51	0.43
3:Q:72:ILE:HG21	3:Q:110:LEU:HD23	2.00	0.43
2:B:161:THR:OG1	2:B:162:CYS:N	2.51	0.43
3:C:72:ILE:HG21	3:C:110:LEU:HD23	2.00	0.43
4:D:218:GLU:N	4:D:221:GLU:OE2	2.48	0.43
12:L:2:THR:N	12:L:17:ASP:OD2	2.51	0.43
2:P:161:THR:OG1	2:P:162:CYS:N	2.51	0.43
12:Z:51:ASP:HB3	12:Z:95:LEU:HD22	1.99	0.43
4:D:116:GLN:NE2	5:E:84:ASP:OD1	2.48	0.43
6:F:80:ASP:OD2	6:F:126:ARG:NH1	2.43	0.43
10:J:159:LEU:HD23	10:J:159:LEU:HA	1.85	0.43
10:X:65:LEU:HD22	10:X:107:VAL:HG21	2.00	0.43
10:X:159:LEU:HD23	10:X:159:LEU:HA	1.85	0.43
6:T:80:ASP:OD2	6:T:126:ARG:NH1	2.43	0.43
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.88	0.43
8:H:161:LYS:HD3	8:H:161:LYS:HA	1.75	0.43
10:J:65:LEU:HD22	10:J:107:VAL:HG21	2.00	0.43
6:F:187:ILE:HD12	6:F:232:LEU:HD13	2.01	0.43
10:J:28:ARG:HD2	10:J:196:TRP:CE3	2.54	0.43
10:X:28:ARG:HD2	10:X:196:TRP:CE3	2.54	0.43
6:T:187:ILE:HD12	6:T:232:LEU:HD13	2.01	0.43
2:P:195:LEU:O	2:P:204:ASN:ND2	2.52	0.43
1:A:15:ILE:HA	1:A:15:ILE:HD13	1.90	0.43
1:O:132:THR:HG22	2:P:128:ARG:HH21	1.82	0.43
2:B:195:LEU:O	2:B:204:ASN:ND2	2.52	0.42
10:J:55:LEU:HD13	10:J:109:PRO:HB3	2.01	0.42
10:X:55:LEU:HD13	10:X:109:PRO:HB3	2.01	0.42
4:R:218:GLU:N	4:R:221:GLU:OE2	2.48	0.42
1:O:15:ILE:HA	1:O:15:ILE:HD13	1.90	0.42
9:I:133:ASN:ND2	9:I:165:ASN:O	2.52	0.42
8:V:59:ILE:HD13	8:V:59:ILE:HA	1.88	0.42
8:V:204:LYS:HD3	8:V:204:LYS:HA	1.80	0.42
9:I:5:GLY:HA3	9:I:14:LEU:HD23	1.99	0.42
10:J:188:LEU:HD23	10:J:188:LEU:HA	1.89	0.42
13:M:66:ARG:NH2	9:W:164:PHE:O	2.53	0.42
9:W:5:GLY:HA3	9:W:14:LEU:HD23	2.00	0.42
9:W:133:ASN:ND2	9:W:165:ASN:O	2.52	0.42
3:Q:17:ARG:NH1	3:Q:22:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ARG:NH1	3:C:22:GLU:OE2	2.52	0.42
8:H:19:ARG:HH11	8:H:26:ILE:HG21	1.83	0.42
11:K:118:CYS:O	11:K:132:HIS:NE2	2.46	0.42
10:X:188:LEU:HD23	10:X:188:LEU:HA	1.89	0.42
4:R:125:ARG:O	3:Q:123:GLN:NE2	2.53	0.42
6:T:84:LEU:HD23	6:T:84:LEU:HA	1.87	0.42
1:A:43:LYS:HE2	1:A:170:ARG:HA	2.00	0.42
13:M:163:HIS:HD2	13:M:177:LEU:HB2	1.83	0.42
6:F:84:LEU:HD23	6:F:84:LEU:HA	1.87	0.42
11:K:74:THR:OG1	11:K:75:ASP:N	2.52	0.42
11:Y:74:THR:OG1	11:Y:75:ASP:N	2.52	0.42
11:Y:118:CYS:O	11:Y:132:HIS:NE2	2.46	0.42
1:O:43:LYS:HE2	1:O:170:ARG:HA	2.00	0.42
5:E:70:ILE:HA	5:E:93:ARG:HG2	2.01	0.42
7:G:145:GLU:HG2	7:G:227:TYR:HD2	1.84	0.42
12:L:203:PRO:O	10:X:39:THR:OG1	2.33	0.42
14:N:10:THR:HG22	14:N:11:SER:H	1.85	0.42
5:S:70:ILE:HA	5:S:93:ARG:HG2	2.01	0.42
7:U:27:ILE:HD11	7:U:133:PRO:HG2	2.02	0.42
7:G:27:ILE:HD11	7:G:133:PRO:HG2	2.02	0.42
12:L:191:GLU:HG2	10:X:216:ARG:HH12	1.85	0.42
14:N:66:GLU:HA	14:N:69:THR:HG22	2.02	0.42
14:N:231:SER:O	14:N:231:SER:OG	2.37	0.42
11:Y:41:GLY:HA3	11:Y:69:GLN:HE22	1.83	0.42
2:P:46:ILE:HD11	2:P:219:PHE:HZ	1.85	0.42
8:V:19:ARG:HH11	8:V:26:ILE:HG21	1.83	0.42
2:B:46:ILE:HD11	2:B:219:PHE:HZ	1.84	0.42
14:N:26:ASP:N	14:N:26:ASP:OD1	2.38	0.42
6:F:228:LEU:HA	6:F:232:LEU:HD12	2.02	0.41
10:J:154:VAL:HG11	10:J:193:ILE:HD11	2.01	0.41
11:K:41:GLY:HA3	11:K:69:GLN:HE22	1.83	0.41
6:T:183:LEU:HD11	6:T:213:VAL:HG11	2.01	0.41
6:T:228:LEU:HA	6:T:232:LEU:HD12	2.02	0.41
7:U:145:GLU:HG2	7:U:227:TYR:HD2	1.84	0.41
1:A:128:ILE:HD11	1:A:140:HIS:HB2	2.02	0.41
6:F:183:LEU:HD11	6:F:213:VAL:HG11	2.01	0.41
7:G:232:ILE:HB	7:G:237:LEU:HD11	2.02	0.41
11:K:11:ASN:OD1	11:K:11:ASN:N	2.54	0.41
12:L:63:ILE:HD12	12:L:74:ILE:HD13	2.02	0.41
13:M:40:VAL:HG12	13:M:53:ALA:HB2	2.02	0.41
13:M:138:LEU:HD23	13:M:138:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:154:VAL:HG11	10:X:193:ILE:HD11	2.01	0.41
11:Y:11:ASN:OD1	11:Y:11:ASN:N	2.54	0.41
9:W:17:ASP:OD1	9:W:17:ASP:N	2.49	0.41
1:O:128:ILE:HD11	1:O:140:HIS:HB2	2.02	0.41
12:Z:63:ILE:HD12	12:Z:74:ILE:HD13	2.02	0.41
1:A:174:ILE:HD12	1:A:174:ILE:HA	1.93	0.41
5:E:150:LYS:HE3	5:E:150:LYS:HB2	1.88	0.41
6:F:205:THR:O	6:F:205:THR:OG1	2.37	0.41
12:L:87:LEU:HD23	12:L:87:LEU:HA	1.90	0.41
7:U:232:ILE:HB	7:U:237:LEU:HD11	2.02	0.41
8:H:204:LYS:HD3	8:H:204:LYS:HA	1.80	0.41
9:I:167:LEU:HD23	9:I:167:LEU:HA	1.93	0.41
4:D:217:ILE:HD13	4:D:217:ILE:HA	1.97	0.41
8:H:17:ASP:HB2	8:H:225:GLY:HA3	2.03	0.41
9:I:17:ASP:OD1	9:I:17:ASP:N	2.49	0.41
11:K:118:CYS:SG	11:K:119:ASP:N	2.91	0.41
11:Y:118:CYS:SG	11:Y:119:ASP:N	2.91	0.41
3:C:143:ASP:OD1	3:C:143:ASP:N	2.53	0.41
4:D:68:HIS:HB3	4:D:212:LYS:HA	2.02	0.41
6:F:38:ILE:HG23	6:F:177:LEU:HD13	2.02	0.41
7:G:118:ILE:HD13	7:G:118:ILE:HA	1.87	0.41
6:T:38:ILE:HG23	6:T:177:LEU:HD13	2.02	0.41
7:U:78:ILE:HG23	7:U:138:ILE:HG23	2.03	0.41
1:A:49:VAL:HB	1:A:233:ILE:HG22	2.03	0.41
1:A:138:ARG:HD3	7:G:13:SER:HA	2.02	0.41
2:B:22:ILE:HD13	2:B:22:ILE:HA	1.87	0.41
6:F:218:HIS:CD2	6:F:221:GLN:HE22	2.38	0.41
7:G:78:ILE:HG23	7:G:138:ILE:HG23	2.03	0.41
6:T:218:HIS:CD2	6:T:221:GLN:HE22	2.38	0.41
8:V:17:ASP:HB2	8:V:225:GLY:HA3	2.03	0.41
8:V:178:ASP:N	8:V:178:ASP:OD1	2.42	0.41
8:V:199:LYS:HA	8:V:199:LYS:HD2	1.74	0.41
3:Q:143:ASP:N	3:Q:143:ASP:OD1	2.53	0.41
7:U:18:ASP:OD1	7:U:18:ASP:N	2.40	0.41
2:B:33:SER:O	2:B:33:SER:OG	2.84	0.41
4:D:130:ALA:HB2	4:D:149:PRO:HD3	2.03	0.41
11:Y:25:ILE:H	11:Y:25:ILE:HG12	1.54	0.41
4:R:68:HIS:HB3	4:R:212:LYS:HA	2.02	0.41
1:O:49:VAL:HB	1:O:233:ILE:HG22	2.03	0.41
1:O:174:ILE:HD12	1:O:174:ILE:HA	1.93	0.41
1:O:201:ILE:N	1:O:203:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:22:ILE:HD13	2:P:22:ILE:HA	1.87	0.41
1:A:201:ILE:N	1:A:203:GLU:OE1	2.54	0.41
5:E:237:ILE:HD12	5:E:237:ILE:HA	1.90	0.41
7:G:35:ASN:OD1	7:G:68:ARG:NH2	2.54	0.41
7:G:43:LYS:HB3	7:G:186:ASP:HA	2.03	0.41
12:L:52:CYS:HB2	12:L:99:ILE:HD11	2.02	0.41
12:L:140:ASP:OD2	11:Y:170:ARG:NH1	2.54	0.41
4:R:130:ALA:HB2	4:R:149:PRO:HD3	2.03	0.41
4:R:217:ILE:HD13	4:R:217:ILE:HA	1.97	0.41
9:W:167:LEU:HD23	9:W:167:LEU:HA	1.93	0.41
1:O:22:LEU:HD23	1:O:22:LEU:HA	1.80	0.41
2:P:44:VAL:HG11	2:P:137:CYS:HB2	2.02	0.41
7:U:35:ASN:OD1	7:U:68:ARG:NH2	2.54	0.41
7:U:43:LYS:HB3	7:U:186:ASP:HA	2.03	0.41
7:U:118:ILE:HD13	7:U:118:ILE:HA	1.87	0.41
7:U:225:SER:O	7:U:225:SER:OG	2.38	0.41
2:B:44:VAL:HG11	2:B:137:CYS:HB2	2.02	0.41
6:F:203:GLU:HG3	6:F:206:ILE:HG12	2.03	0.41
7:G:18:ASP:OD1	7:G:18:ASP:N	2.40	0.41
8:H:82:ILE:HD13	8:H:173:ILE:HG21	2.02	0.41
14:N:33:SER:O	14:N:33:SER:OG	2.32	0.41
11:Y:15:LEU:HD11	11:Y:105:ALA:HB3	2.02	0.41
1:O:170:ARG:HE	1:O:170:ARG:HB3	1.71	0.41
12:Z:52:CYS:HB2	12:Z:99:ILE:HD11	2.02	0.41
1:A:124:ILE:HD13	1:A:124:ILE:HA	1.86	0.40
9:I:4:CYS:HA	9:I:126:ALA:HA	2.03	0.40
11:K:15:LEU:HD11	11:K:105:ALA:HB3	2.02	0.40
5:S:193:PHE:CZ	5:S:223:LYS:HG3	2.56	0.40
5:S:237:ILE:HD12	5:S:237:ILE:HA	1.91	0.40
6:T:203:GLU:HG3	6:T:206:ILE:HG12	2.03	0.40
1:O:217:GLN:HA	1:O:224:LEU:HD11	2.03	0.40
8:V:20:THR:HG23	8:V:28:ASN:HB2	2.03	0.40
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.80	0.40
1:A:42:VAL:HA	1:A:171:ALA:HA	2.03	0.40
1:A:217:GLN:HA	1:A:224:LEU:HD11	2.03	0.40
5:E:193:PHE:CZ	5:E:223:LYS:HG3	2.56	0.40
9:I:138:LEU:HD12	9:I:138:LEU:HA	1.92	0.40
13:M:212:ARG:HA	13:M:212:ARG:HD3	1.88	0.40
14:N:95:VAL:HA	14:N:98:VAL:HG12	2.03	0.40
4:R:33:VAL:HG13	4:R:44:ALA:HB3	2.02	0.40
4:R:131:THR:HG1	4:R:147:THR:HG1	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:223:THR:OG1	2:P:225:ASN:OD1	2.36	0.40
8:V:82:ILE:HD13	8:V:173:ILE:HG21	2.02	0.40
8:H:20:THR:HG23	8:H:28:ASN:HB2	2.03	0.40
8:H:199:LYS:HD3	8:V:252:TYR:CG	2.57	0.40
9:I:57:LEU:HD23	9:I:57:LEU:HA	1.90	0.40
10:J:22:ALA:HA	10:J:202:VAL:HA	2.03	0.40
10:J:23:ILE:HB	10:J:112:VAL:HG21	2.04	0.40
11:K:25:ILE:H	11:K:25:ILE:HG12	1.54	0.40
12:L:82:ILE:HD13	12:L:82:ILE:HA	1.89	0.40
4:D:33:VAL:HG13	4:D:44:ALA:HB3	2.02	0.40
9:I:62:ASN:HB3	9:I:82:ARG:HH11	1.87	0.40
10:X:22:ALA:HA	10:X:202:VAL:HA	2.03	0.40
10:X:23:ILE:HB	10:X:112:VAL:HG21	2.04	0.40
10:X:188:LEU:HD13	10:X:195:GLY:HA2	2.04	0.40
1:O:42:VAL:HA	1:O:171:ALA:HA	2.03	0.40
1:O:54:LYS:HE3	1:O:230:GLU:HG3	2.02	0.40
7:U:48:CYS:SG	7:U:79:THR:HG21	2.61	0.40
1:A:170:ARG:HE	1:A:170:ARG:HB3	1.71	0.40
2:B:223:THR:OG1	2:B:225:ASN:OD1	2.36	0.40
6:F:34:CYS:HB2	6:F:162:ALA:HB3	2.03	0.40
7:G:48:CYS:SG	7:G:79:THR:HG21	2.61	0.40
8:H:218:MET:HG2	8:H:224:SER:HA	2.02	0.40
10:J:188:LEU:HD13	10:J:195:GLY:HA2	2.04	0.40
11:Y:181:ARG:HA	11:Y:181:ARG:HD3	1.78	0.40
4:R:63:ILE:HG21	4:R:84:VAL:HG11	2.04	0.40
9:W:4:CYS:HA	9:W:126:ALA:HA	2.03	0.40
1:O:124:ILE:HA	1:O:124:ILE:HD13	1.86	0.40
12:Z:82:ILE:HD13	12:Z:82:ILE:HA	1.89	0.40
8:V:218:MET:HG2	8:V:224:SER:HA	2.02	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%)	225 (90%)	24 (10%)	0	100	100
1	O	249/260 (96%)	224 (90%)	25 (10%)	0	100	100
2	B	227/235 (97%)	216 (95%)	11 (5%)	0	100	100
2	P	227/235 (97%)	216 (95%)	11 (5%)	0	100	100
3	C	239/246 (97%)	222 (93%)	16 (7%)	1 (0%)	34	71
3	Q	239/246 (97%)	222 (93%)	16 (7%)	1 (0%)	34	71
4	D	231/241 (96%)	207 (90%)	24 (10%)	0	100	100
4	R	231/241 (96%)	207 (90%)	24 (10%)	0	100	100
5	E	241/256 (94%)	217 (90%)	23 (10%)	1 (0%)	34	71
5	S	241/256 (94%)	219 (91%)	21 (9%)	1 (0%)	34	71
6	F	234/254 (92%)	213 (91%)	20 (8%)	1 (0%)	34	71
6	T	234/254 (92%)	213 (91%)	20 (8%)	1 (0%)	34	71
7	G	230/252 (91%)	209 (91%)	21 (9%)	0	100	100
7	U	230/252 (91%)	209 (91%)	21 (9%)	0	100	100
8	H	192/252 (76%)	168 (88%)	24 (12%)	0	100	100
8	V	192/252 (76%)	168 (88%)	24 (12%)	0	100	100
9	I	220/229 (96%)	200 (91%)	19 (9%)	1 (0%)	29	68
9	W	220/229 (96%)	200 (91%)	19 (9%)	1 (0%)	29	68
10	J	201/218 (92%)	179 (89%)	22 (11%)	0	100	100
10	X	201/218 (92%)	179 (89%)	22 (11%)	0	100	100
11	K	193/195 (99%)	172 (89%)	20 (10%)	1 (0%)	29	68
11	Y	193/195 (99%)	172 (89%)	20 (10%)	1 (0%)	29	68
12	L	202/211 (96%)	174 (86%)	28 (14%)	0	100	100
12	Z	202/211 (96%)	174 (86%)	28 (14%)	0	100	100
13	M	211/240 (88%)	188 (89%)	23 (11%)	0	100	100
13	a	211/240 (88%)	187 (89%)	24 (11%)	0	100	100
14	N	220/265 (83%)	197 (90%)	23 (10%)	0	100	100
14	b	220/265 (83%)	197 (90%)	23 (10%)	0	100	100
All	All	6180/6708 (92%)	5574 (90%)	596 (10%)	10 (0%)	50	79

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	25	ILE
11	Y	25	ILE
6	F	161	GLY
6	T	161	GLY
5	E	9	ASP
5	S	9	ASP
3	C	210	ILE
3	Q	210	ILE
9	I	24	PRO
9	W	24	PRO

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%)	88	95
1	O	222/231 (96%)	221 (100%)	1 (0%)	88	95
2	B	201/205 (98%)	200 (100%)	1 (0%)	88	95
2	P	201/205 (98%)	200 (100%)	1 (0%)	88	95
3	C	208/213 (98%)	206 (99%)	2 (1%)	76	88
3	Q	208/213 (98%)	206 (99%)	2 (1%)	76	88
4	D	199/207 (96%)	199 (100%)	0	100	100
4	R	199/207 (96%)	199 (100%)	0	100	100
5	E	211/223 (95%)	210 (100%)	1 (0%)	88	95
5	S	211/223 (95%)	210 (100%)	1 (0%)	88	95
6	F	211/227 (93%)	211 (100%)	0	100	100
6	T	211/227 (93%)	211 (100%)	0	100	100
7	G	213/229 (93%)	211 (99%)	2 (1%)	78	90
7	U	213/229 (93%)	211 (99%)	2 (1%)	78	90
8	H	176/231 (76%)	174 (99%)	2 (1%)	73	88
8	V	176/231 (76%)	174 (99%)	2 (1%)	73	88
9	I	188/194 (97%)	186 (99%)	2 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	188/194 (97%)	186 (99%)	2 (1%)	73	88
10	J	180/191 (94%)	179 (99%)	1 (1%)	86	94
10	X	180/191 (94%)	179 (99%)	1 (1%)	86	94
11	K	174/174 (100%)	173 (99%)	1 (1%)	86	94
11	Y	174/174 (100%)	173 (99%)	1 (1%)	86	94
12	L	169/176 (96%)	169 (100%)	0	100	100
12	Z	169/176 (96%)	169 (100%)	0	100	100
13	M	191/216 (88%)	190 (100%)	1 (0%)	88	95
13	a	191/216 (88%)	190 (100%)	1 (0%)	88	95
14	N	201/239 (84%)	201 (100%)	0	100	100
14	b	201/239 (84%)	201 (100%)	0	100	100
All	All	5488/5912 (93%)	5460 (100%)	28 (0%)	89	95

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	THR
2	B	12	THR
3	C	133	SER
3	C	141	THR
5	E	50	SER
7	G	16	SER
7	G	56	ASP
8	H	75	ARG
8	H	173	ILE
9	I	67	ARG
9	I	218	GLU
10	J	204	THR
11	K	86	ARG
13	M	136	ASN
5	S	50	SER
10	X	204	THR
11	Y	86	ARG
9	W	67	ARG
9	W	218	GLU
1	O	208	THR
2	P	12	THR
13	a	136	ASN

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Mol	Chain	Res	Type
8	V	75	ARG
8	V	173	ILE
3	Q	133	SER
3	Q	141	THR
7	U	16	SER
7	U	56	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	152	ASN
1	A	238	ASN
2	B	21	GLN
2	B	157	ASN
2	B	170	ASN
4	D	18	GLN
5	E	23	GLN
5	E	97	ASN
6	F	218	HIS
7	G	104	ASN
7	G	108	ASN
8	H	168	ASN
8	H	212	ASN
9	I	71	ASN
9	I	85	GLN
9	I	106	ASN
10	J	8	ASN
10	J	80	GLN
10	J	108	ASN
11	K	23	ASN
11	K	56	GLN
11	K	88	ASN
11	K	101	ASN
12	L	38	ASN
12	L	180	HIS
13	M	144	ASN
13	M	183	GLN
14	N	38	GLN
14	N	75	ASN
14	N	167	HIS
5	S	23	GLN

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Mol	Chain	Res	Type
5	S	97	ASN
10	X	8	ASN
10	X	80	GLN
10	X	108	ASN
10	X	182	GLN
11	Y	23	ASN
11	Y	56	GLN
11	Y	88	ASN
11	Y	101	ASN
14	b	75	ASN
4	R	18	GLN
6	T	218	HIS
9	W	71	ASN
9	W	85	GLN
9	W	106	ASN
9	W	201	HIS
1	O	74	ASN
1	O	152	ASN
1	O	238	ASN
2	P	21	GLN
2	P	157	ASN
2	P	170	ASN
12	Z	38	ASN
12	Z	180	HIS
13	a	144	ASN
13	a	183	GLN
13	a	185	ASN
8	V	162	GLN
8	V	168	ASN
8	V	212	ASN
7	U	104	ASN
7	U	108	ASN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

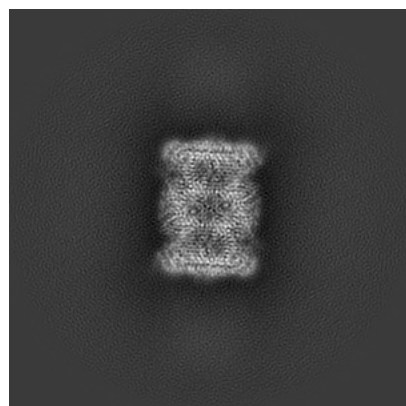
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9258. These allow visual inspection of the internal detail of the map and identification of artifacts.

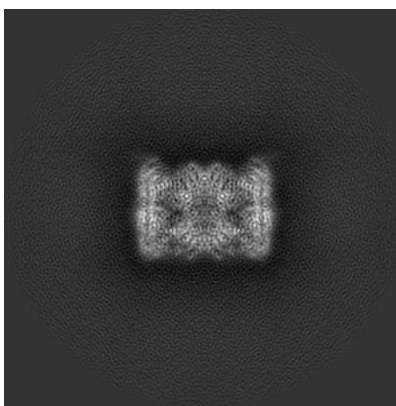
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

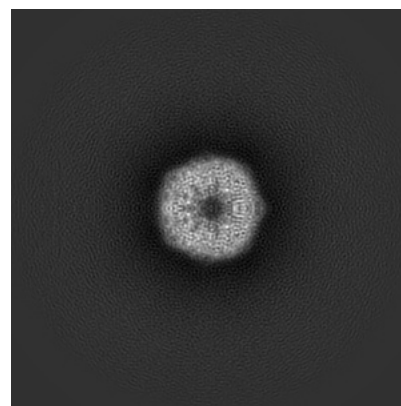
6.1.1 Primary map



X

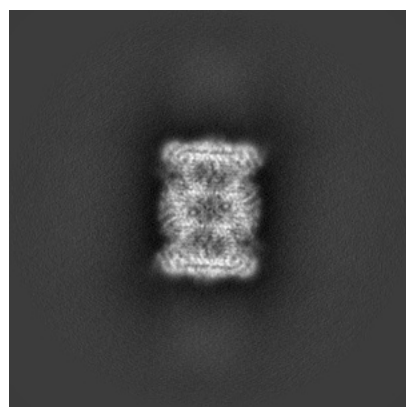


Y

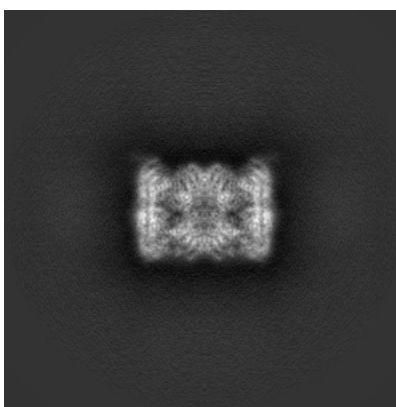


Z

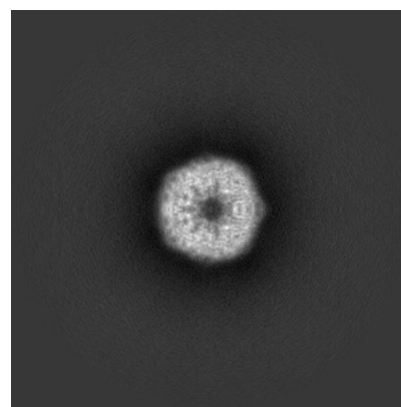
6.1.2 Raw map



X



Y

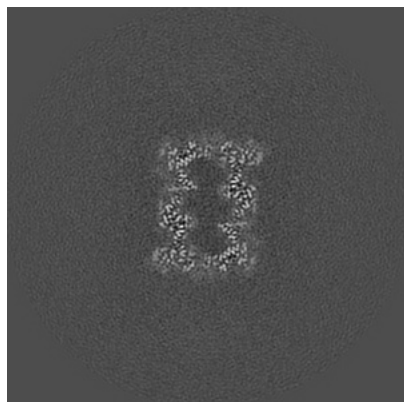


Z

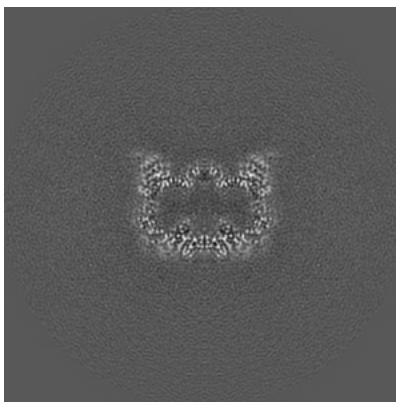
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

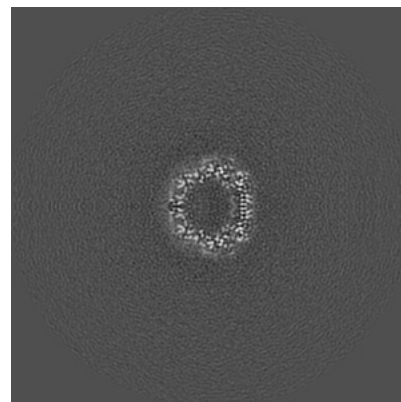
6.2.1 Primary map



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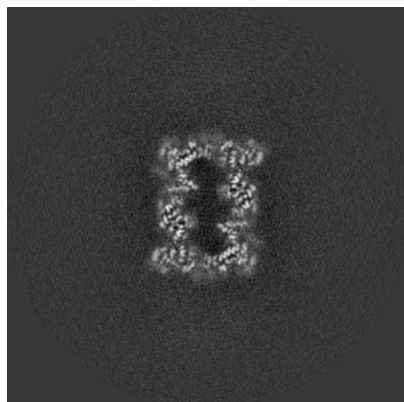


Y Index: 172

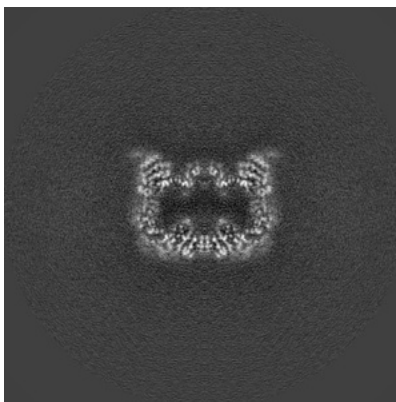


Z Index: 172

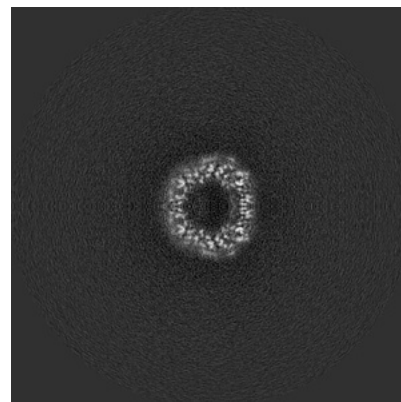
6.2.2 Raw map



X Index: 172



Y Index: 172

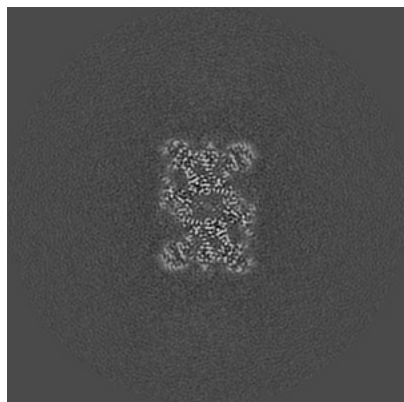


Z Index: 172

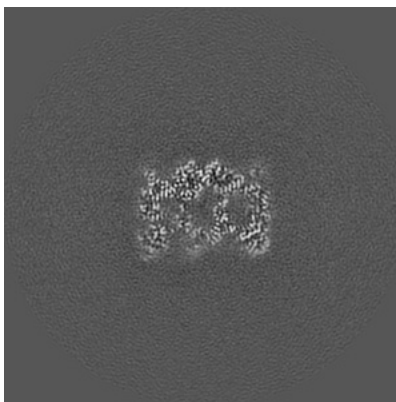
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

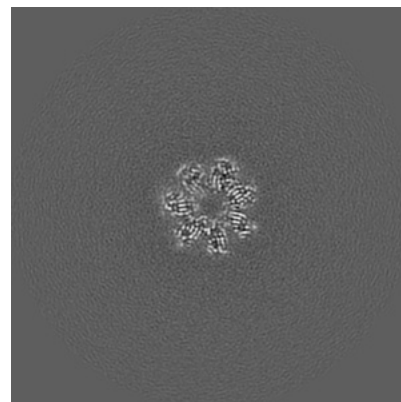
6.3.1 Primary map



X Index: 191

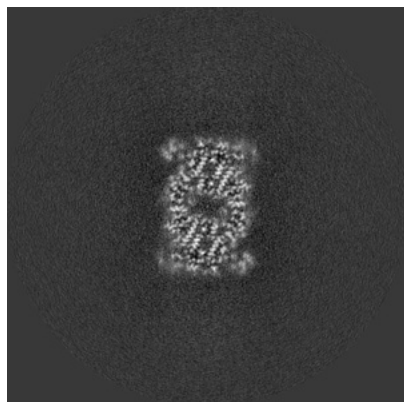


Y Index: 187

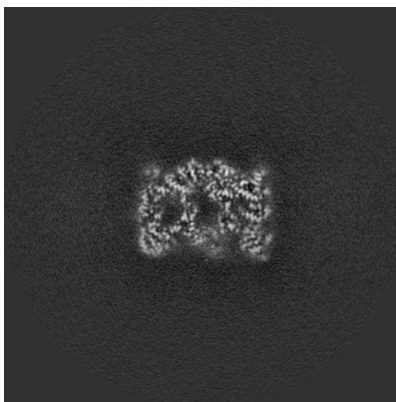


Z Index: 158

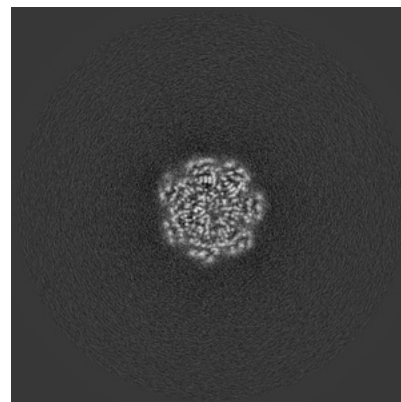
6.3.2 Raw map



X Index: 153



Y Index: 156

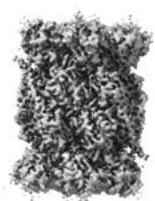


Z Index: 127

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

6.4 Orthogonal surface views [i](#)

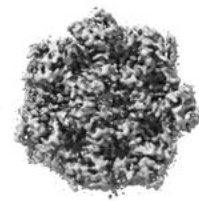
6.4.1 Primary map



X



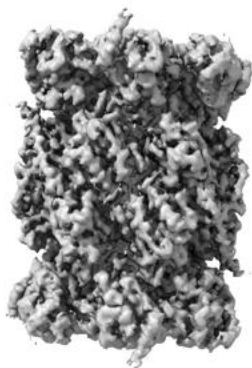
Y



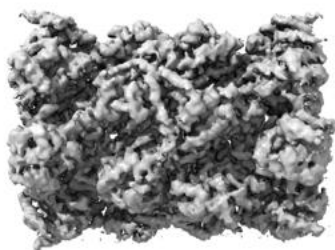
Z

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.

6.4.2 Raw map



X



Y



Z

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.

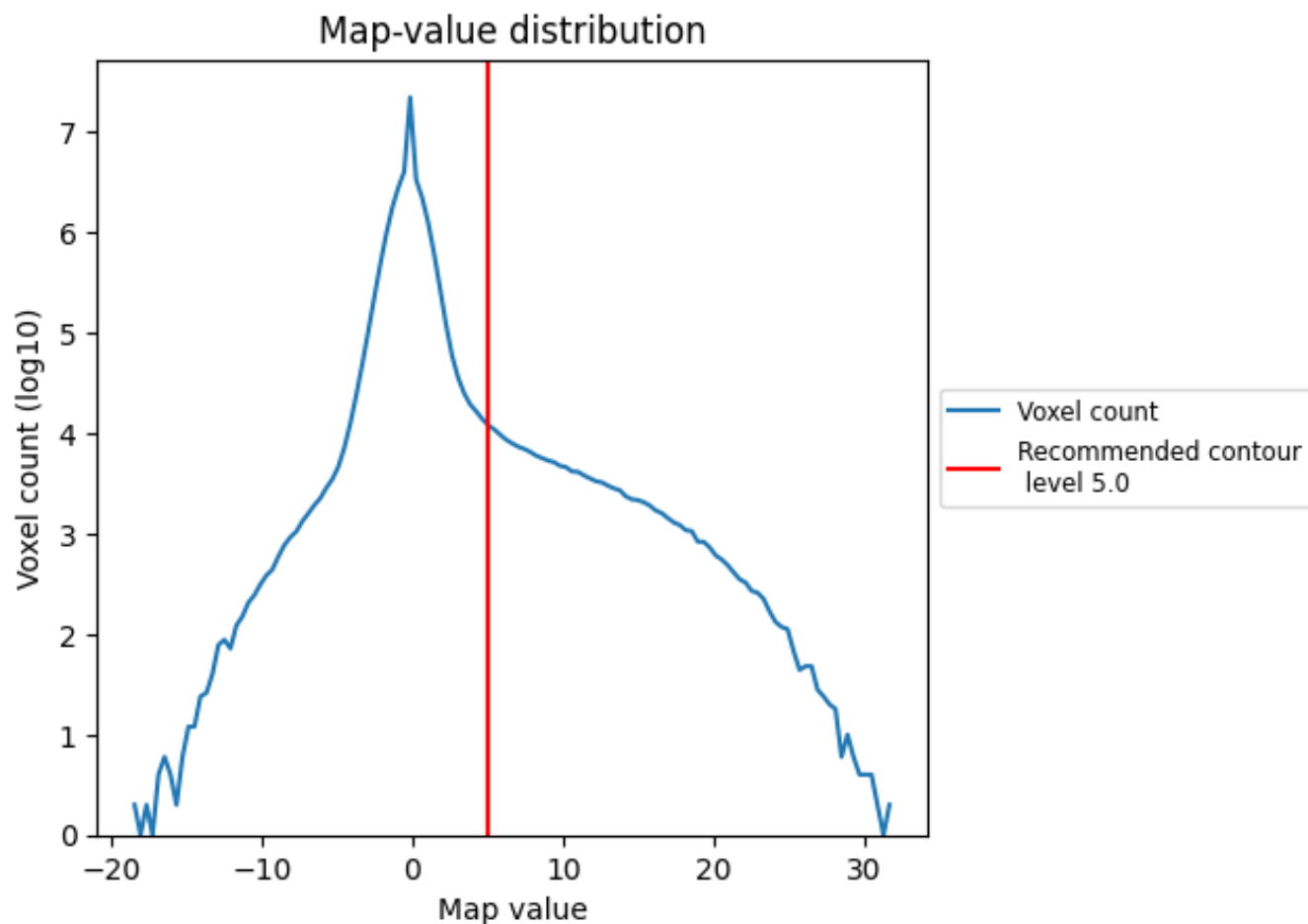
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

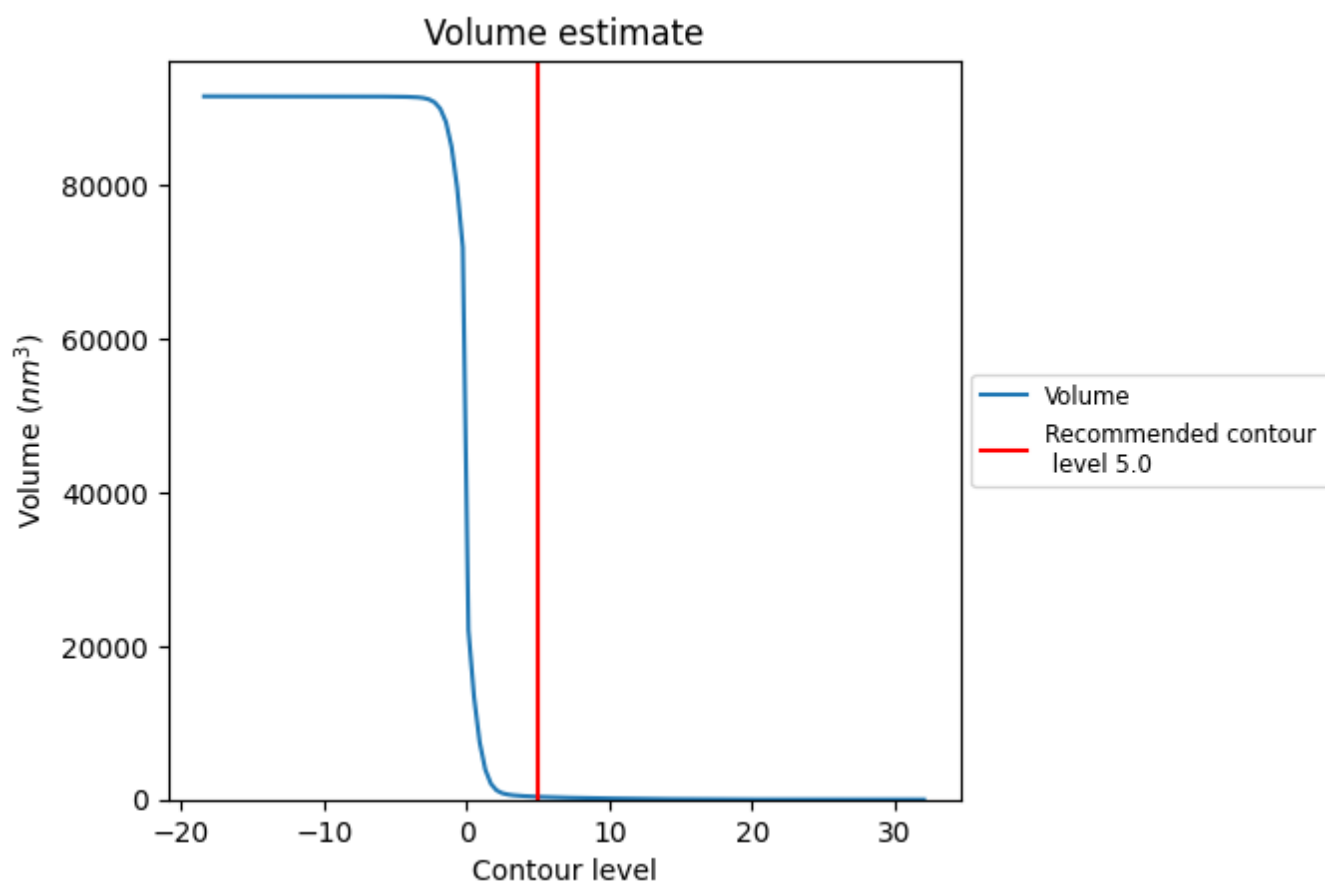
This section contains the results of statistical analysis of the map.

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.

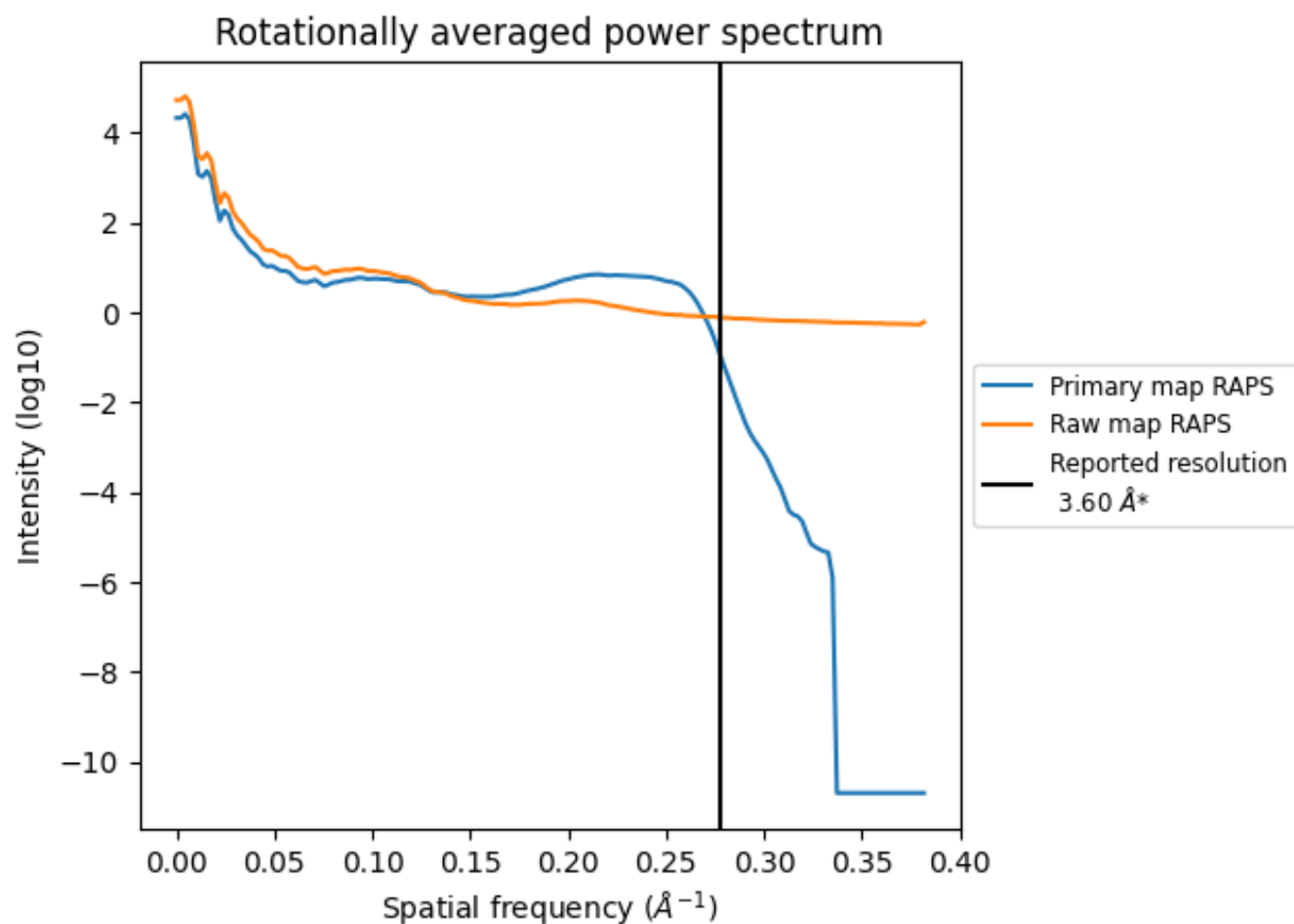
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 361 nm³; this corresponds to an approximate mass of 326 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 ⓘ

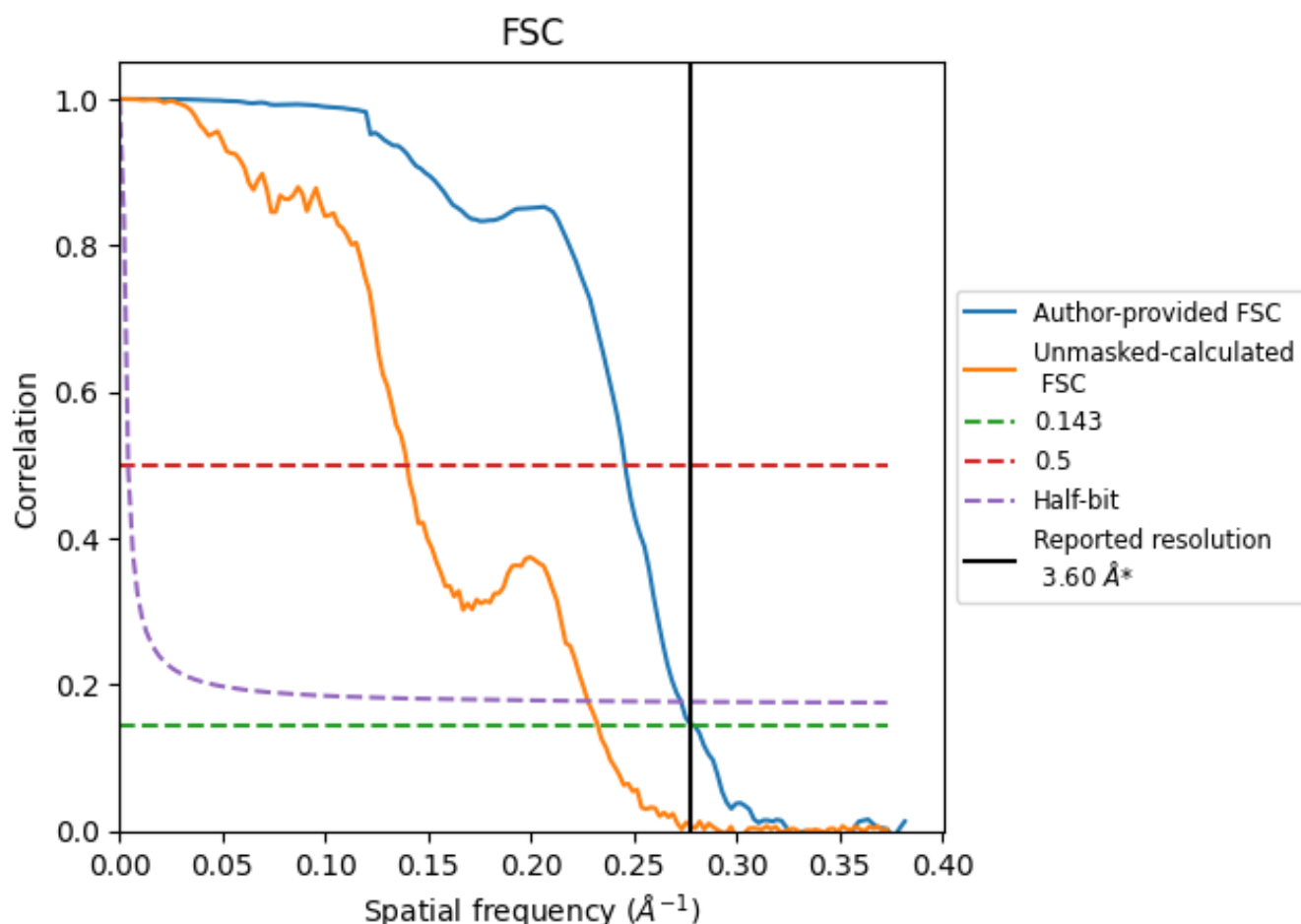


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

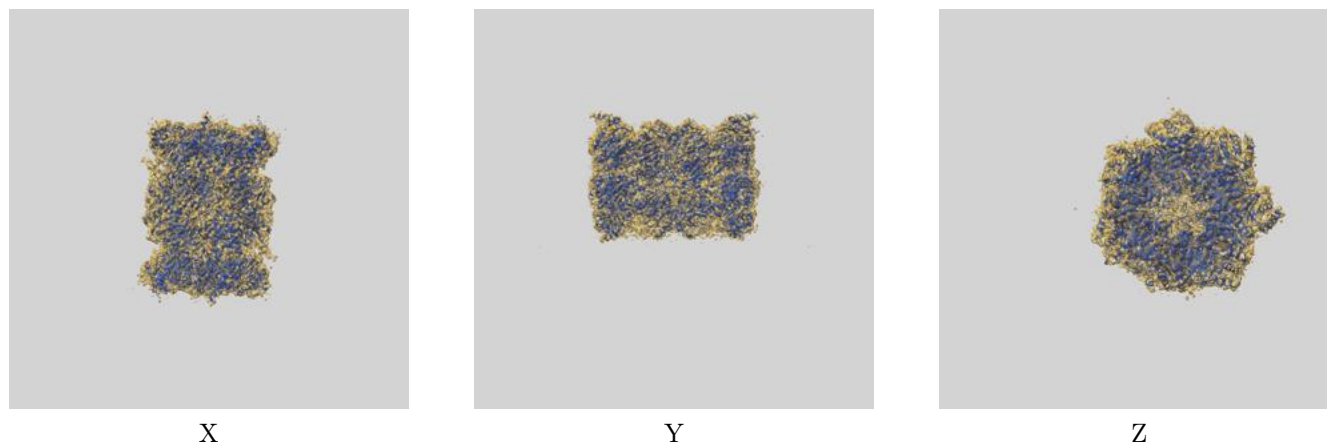
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.07	3.66
Unmasked-calculated*	4.30	7.15	4.39

*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 4.30 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

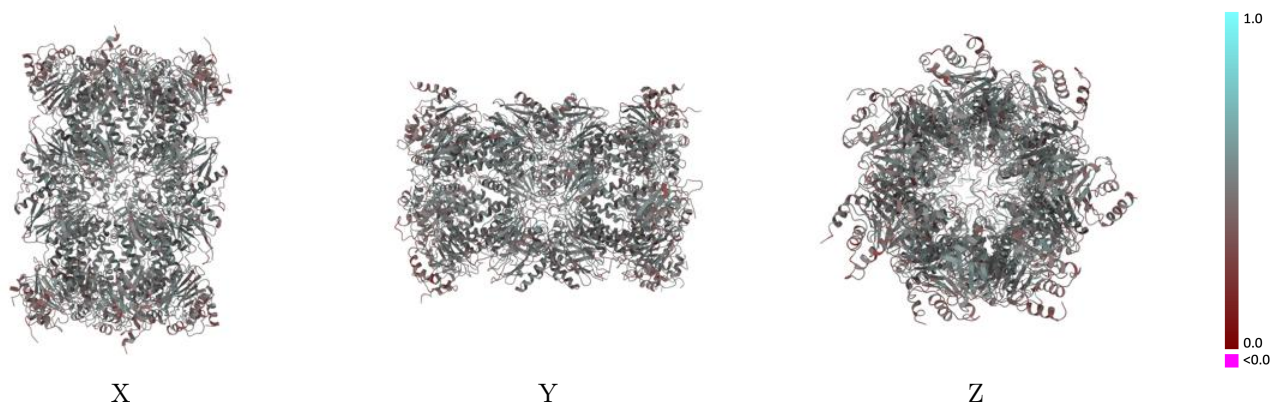
This section contains information regarding the fit between EMDB map EMD-9258 and PDB model 6MUW. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



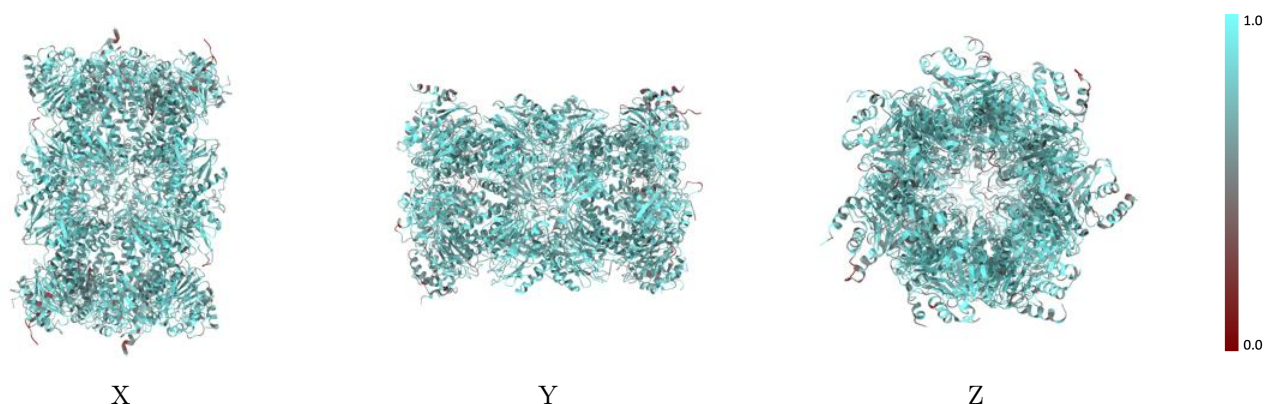
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



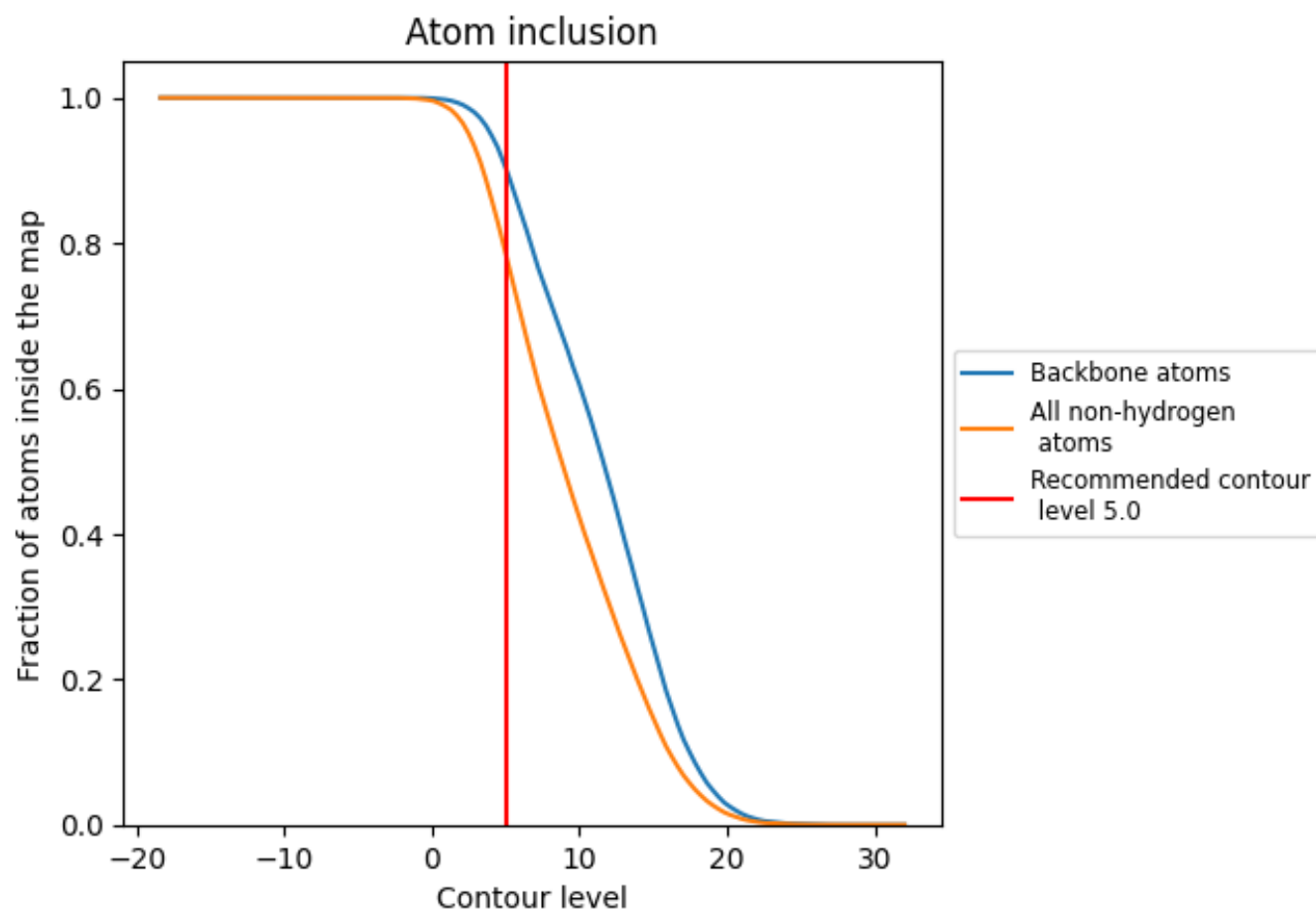
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.0).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 79% 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 (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7856	 0.4610
A	 0.7129	 0.4300
B	 0.7777	 0.4580
C	 0.7984	 0.4550
D	 0.7514	 0.4550
E	 0.7100	 0.4420
F	 0.7807	 0.4590
G	 0.7973	 0.4610
H	 0.7933	 0.4490
I	 0.7959	 0.4560
J	 0.8351	 0.4910
K	 0.8272	 0.4800
L	 0.8205	 0.4730
M	 0.8222	 0.4790
N	 0.8092	 0.4720
O	 0.7083	 0.4320
P	 0.7805	 0.4590
Q	 0.7931	 0.4570
R	 0.7442	 0.4560
S	 0.7186	 0.4420
T	 0.7817	 0.4560
U	 0.7968	 0.4620
V	 0.7946	 0.4480
W	 0.7918	 0.4550
X	 0.8383	 0.4920
Y	 0.8285	 0.4820
Z	 0.8160	 0.4720
a	 0.8192	 0.4780
b	 0.8081	 0.4710

