



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 03:01 PM EST

PDB ID : 7LS5
EMDB ID : EMD-23502
Title : Cryo-EM structure of the Pre3-1 20S proteasome core particle
Authors : Schnell, H.M.; Walsh Jr, R.M.; Rawson, S.; Hanna, J.W.
Deposited on : 2021-02-17
Resolution : 2.74 Å(reported)
Based on initial model : 4G4S

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

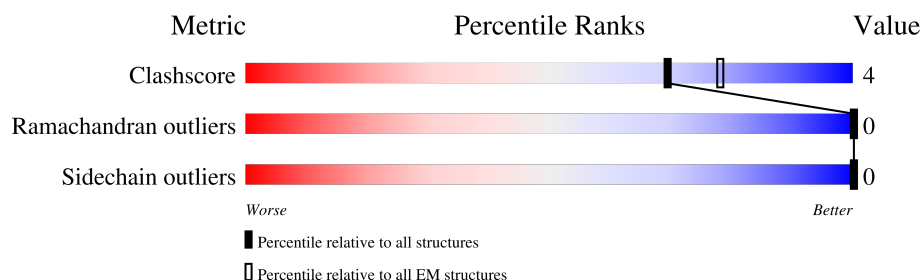
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 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	252	
1	O	252	
2	B	250	
2	P	250	
3	C	258	
3	Q	258	
4	D	254	
4	R	254	

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Mol	Chain	Length	Quality of chain
5	E	260	
5	S	260	
6	F	234	
6	T	234	
7	G	288	
7	U	288	
8	H	215	
8	V	215	
9	I	261	
9	W	261	
10	J	205	
10	X	205	
11	K	212	
11	Y	212	
12	L	287	
12	Z	287	
13	1	241	
13	M	241	
14	2	266	
14	N	266	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 98042 atoms, of which 48895 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-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	243	Total	C	H	N	O	S	0	0
			3832	1221	1912	322	369	8		
1	O	240	Total	C	H	N	O	S	0	0
			3793	1209	1895	318	363	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	250	Total	C	H	N	O	S	0	0
			3845	1219	1930	315	377	4		
2	P	246	Total	C	H	N	O	S	0	0
			3776	1200	1895	308	370	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	239	Total	C	H	N	O	S	0	0
			3754	1186	1878	315	372	3		
3	Q	244	Total	C	H	N	O	S	0	0
			3806	1201	1902	321	379	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	237	Total	C	H	N	O	S	0	0
			3735	1165	1874	326	366	4		
4	R	235	Total	C	H	N	O	S	0	0
			3694	1153	1850	323	364	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	235	Total	C	H	N	O	S	0	0
			3609	1136	1796	304	366	7		
5	S	236	Total	C	H	N	O	S	0	0
			3616	1138	1799	305	367	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	231	Total	C	H	N	O	S	0	0
			3551	1114	1778	307	348	4		
6	T	231	Total	C	H	N	O	S	0	0
			3551	1114	1778	307	348	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	244	Total	C	H	N	O	S	0	0
			3784	1205	1888	330	357	4		
7	U	243	Total	C	H	N	O	S	0	0
			3777	1203	1885	329	356	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	196	Total	C	H	N	O	S	0	0
			2996	957	1480	250	302	7		
8	V	196	Total	C	H	N	O	S	0	0
			2996	957	1480	250	302	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	15	ASP	GLY	engineered mutation	UNP P38624
V	15	ASP	GLY	variant	UNP P38624

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	220	Total	C	H	N	O	S	0	0
			3347	1054	1677	291	319	6		
9	W	220	Total	C	H	N	O	S	0	0
			3347	1054	1677	291	319	6		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	204	Total	C	H	N	O	S	0	0
			3153	1010	1572	258	305	8		
10	X	203	Total	C	H	N	O	S	0	0
			3142	1007	1567	257	303	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	194	Total	C	H	N	O	S	0	0
			3111	987	1558	263	298	5		
11	Y	194	Total	C	H	N	O	S	0	0
			3112	987	1559	263	298	5		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	198	ARG	-	expression tag	UNP P22141
K	199	THR	-	expression tag	UNP P22141
K	200	LEU	-	expression tag	UNP P22141
K	201	GLN	-	expression tag	UNP P22141
K	202	VAL	-	expression tag	UNP P22141
K	203	ASP	-	expression tag	UNP P22141
K	204	GLY	-	expression tag	UNP P22141
K	205	SER	-	expression tag	UNP P22141
K	206	GLU	-	expression tag	UNP P22141
K	207	ASN	-	expression tag	UNP P22141
K	208	LEU	-	expression tag	UNP P22141
K	209	TYR	-	expression tag	UNP P22141
K	210	PHE	-	expression tag	UNP P22141
K	211	GLN	-	expression tag	UNP P22141
Y	198	ARG	-	expression tag	UNP P22141
Y	199	THR	-	expression tag	UNP P22141
Y	200	LEU	-	expression tag	UNP P22141
Y	201	GLN	-	expression tag	UNP P22141
Y	202	VAL	-	expression tag	UNP P22141
Y	203	ASP	-	expression tag	UNP P22141
Y	204	GLY	-	expression tag	UNP P22141
Y	205	SER	-	expression tag	UNP P22141
Y	206	GLU	-	expression tag	UNP P22141
Y	207	ASN	-	expression tag	UNP P22141
Y	208	LEU	-	expression tag	UNP P22141

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	209	TYR	-	expression tag	UNP P22141
Y	210	PHE	-	expression tag	UNP P22141
Y	211	GLN	-	expression tag	UNP P22141

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	212	Total	C	H	N	O	S	0	0
			3237	1045	1593	280	312	7		
12	Z	212	Total	C	H	N	O	S	0	0
			3237	1045	1593	280	312	7		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	222	Total	C	H	N	O	S	0	0
			3467	1115	1710	303	335	4		
13	1	222	Total	C	H	N	O	S	0	0
			3466	1115	1709	303	335	4		

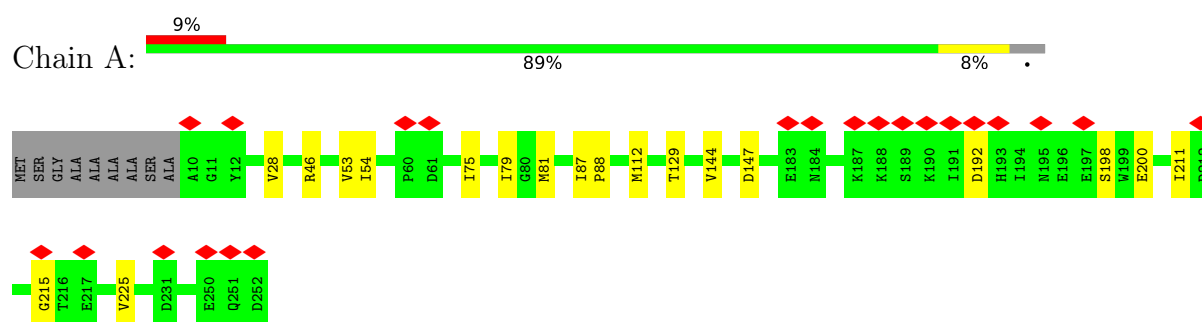
- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	233	Total	C	H	N	O	S	0	0
			3654	1154	1830	312	351	7		
14	2	233	Total	C	H	N	O	S	0	0
			3654	1154	1830	312	351	7		

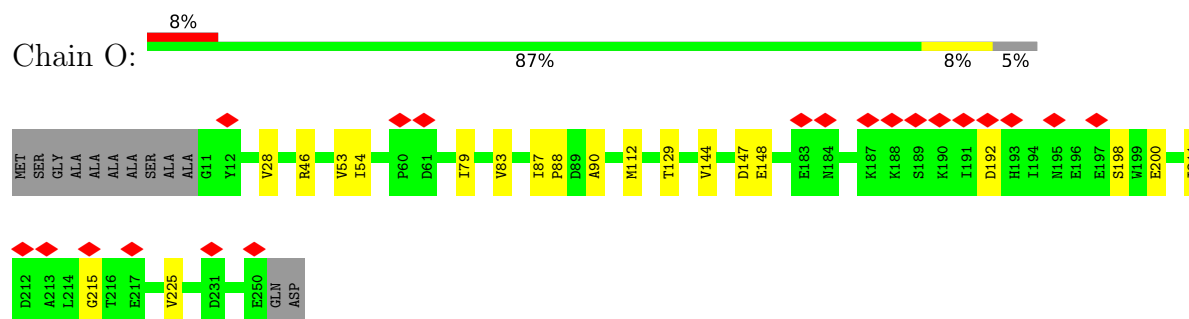
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

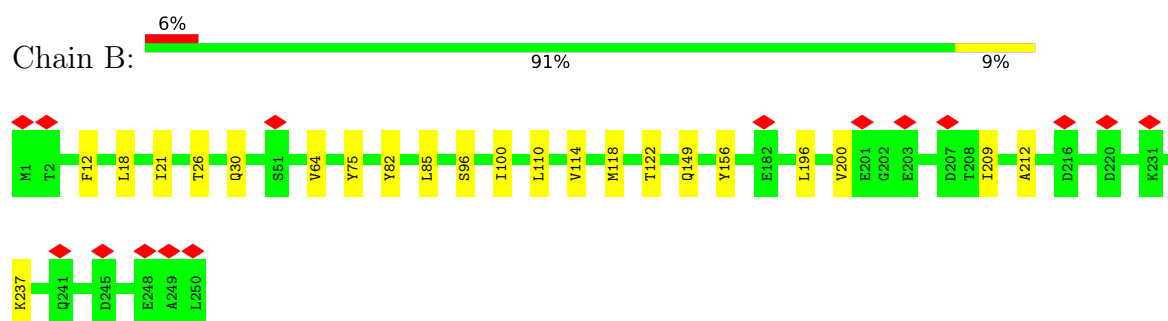
- Molecule 1: Proteasome subunit alpha type-1



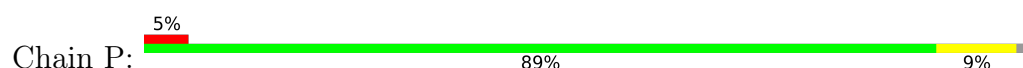
- Molecule 1: Proteasome subunit alpha type-1

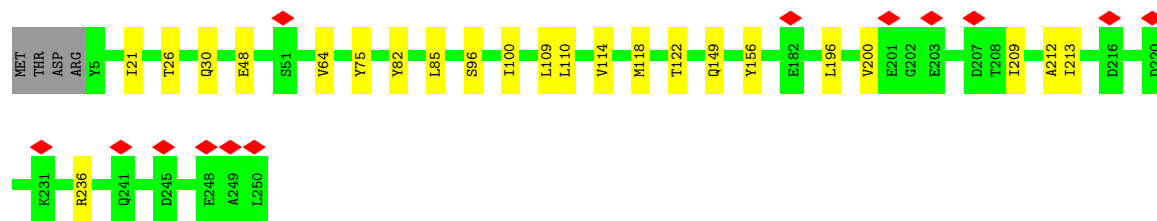


- Molecule 2: Proteasome subunit alpha type-2

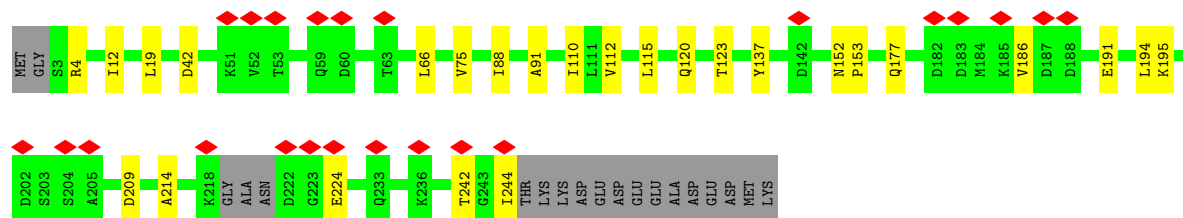
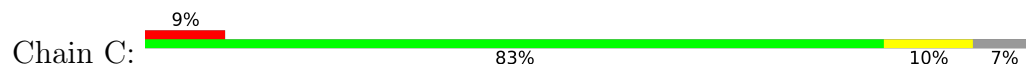


- Molecule 2: Proteasome subunit alpha type-2

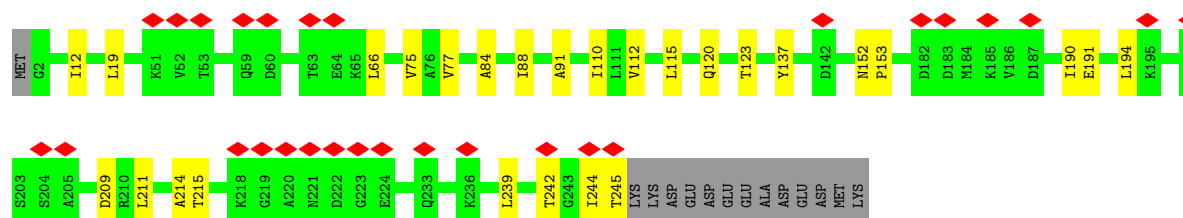
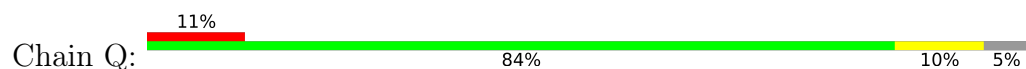




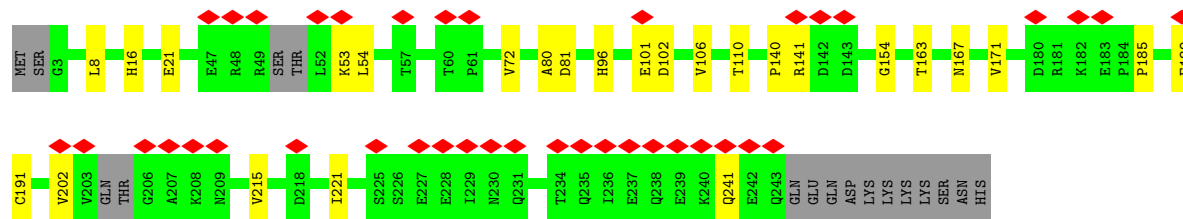
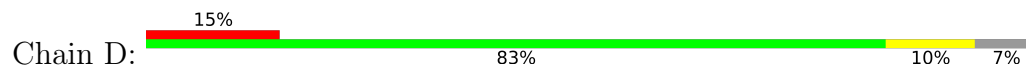
• Molecule 3: Proteasome subunit alpha type-3



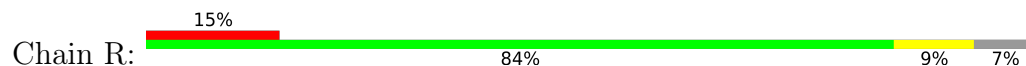
• Molecule 3: Proteasome subunit alpha type-3

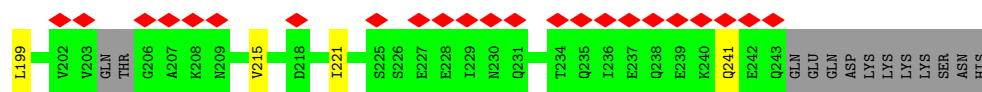


• Molecule 4: Proteasome subunit alpha type-4

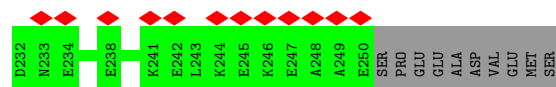
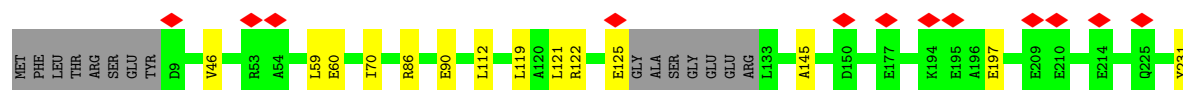
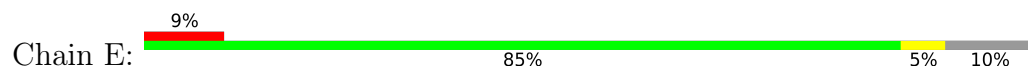


• Molecule 4: Proteasome subunit alpha type-4

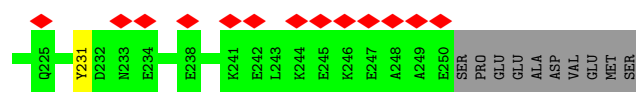
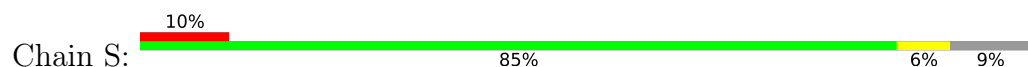




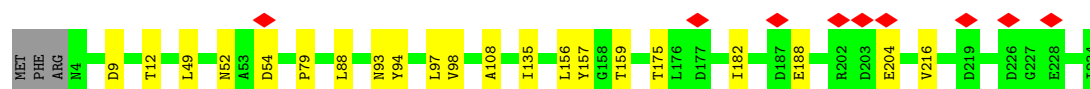
• Molecule 5: Proteasome subunit alpha type-5



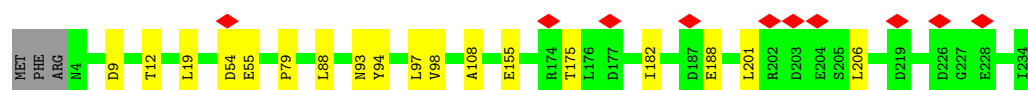
• Molecule 5: Proteasome subunit alpha type-5



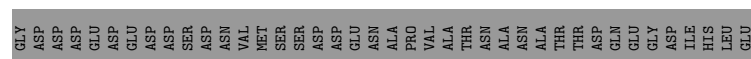
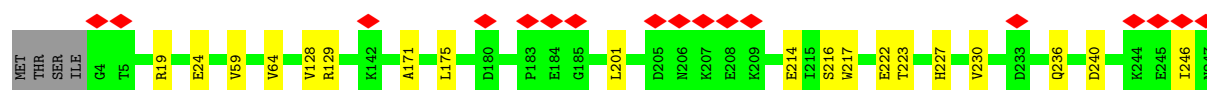
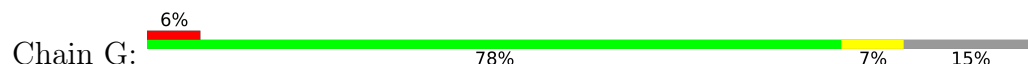
• Molecule 6: Proteasome subunit alpha type-6



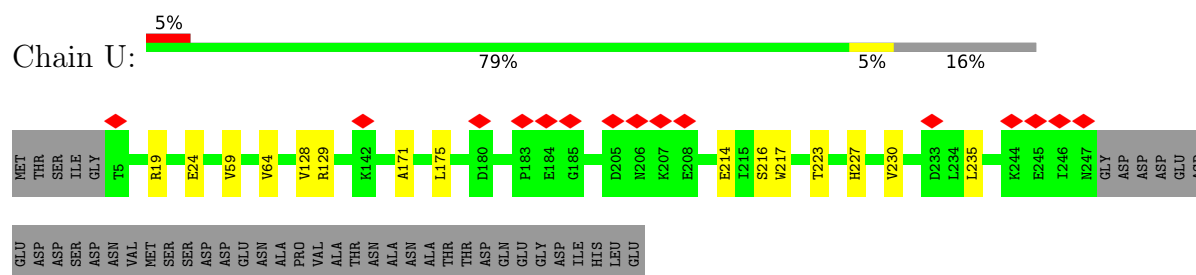
• Molecule 6: Proteasome subunit alpha type-6



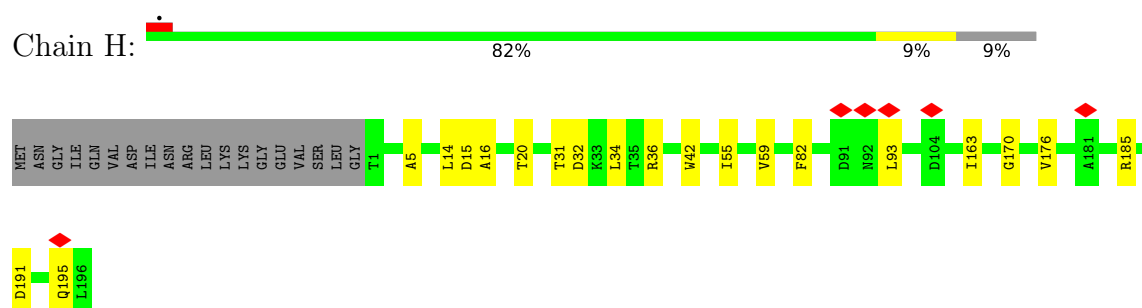
• Molecule 7: Proteasome subunit alpha type-7



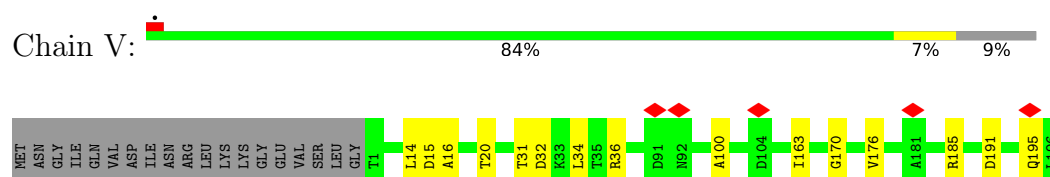
- Molecule 7: Proteasome subunit alpha type-7



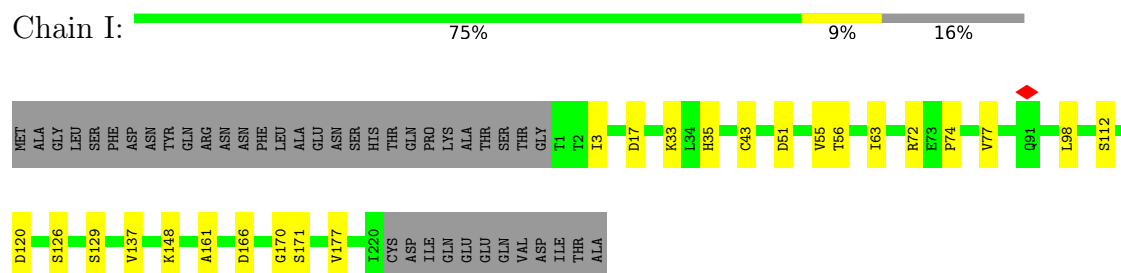
- Molecule 8: Proteasome subunit beta type-1



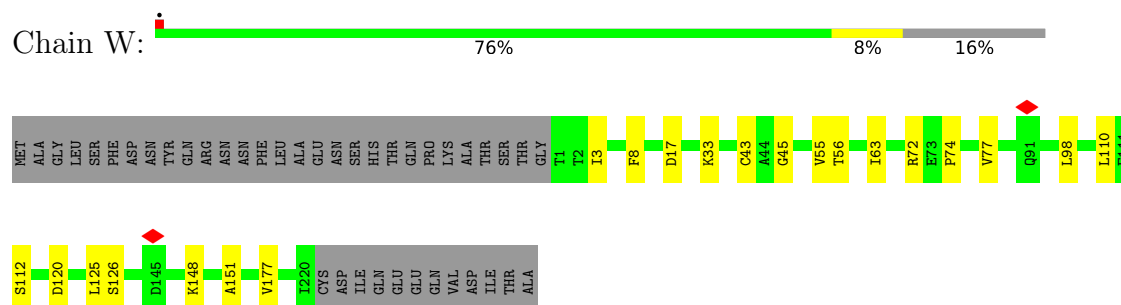
- Molecule 8: Proteasome subunit beta type-1



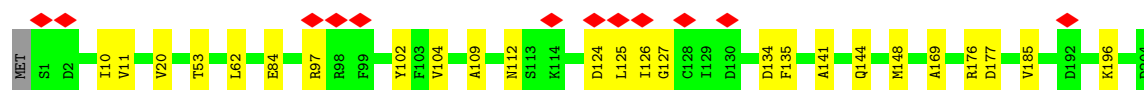
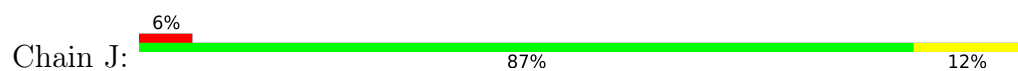
- Molecule 9: Proteasome subunit beta type-2



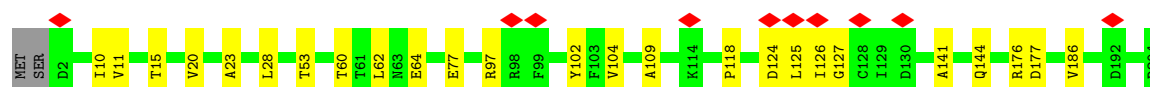
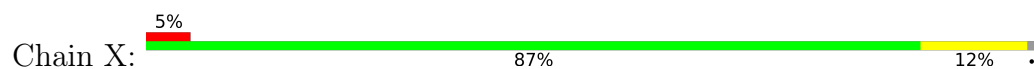
- Molecule 9: Proteasome subunit beta type-2



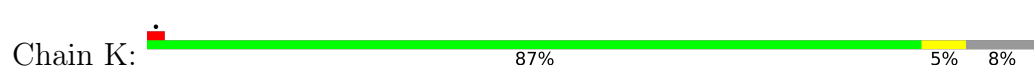
- Molecule 10: Proteasome subunit beta type-3



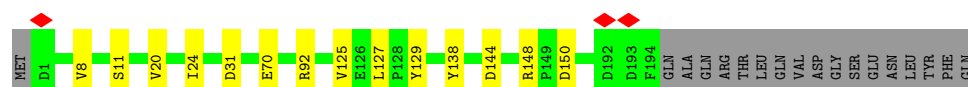
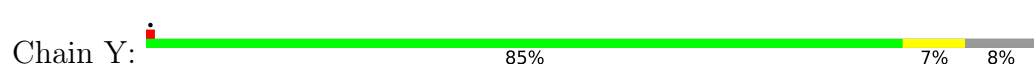
- Molecule 10: Proteasome subunit beta type-3



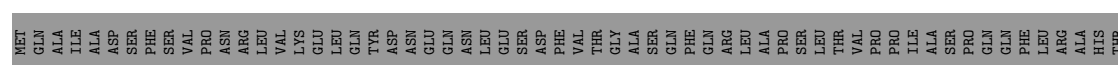
- Molecule 11: Proteasome subunit beta type-4



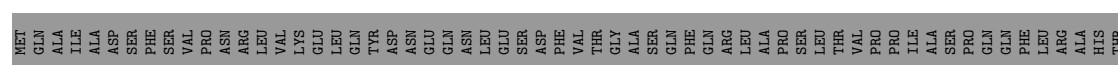
- Molecule 11: Proteasome subunit beta type-4

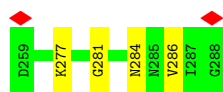


- Molecule 12: Proteasome subunit beta type-5



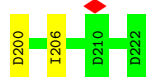
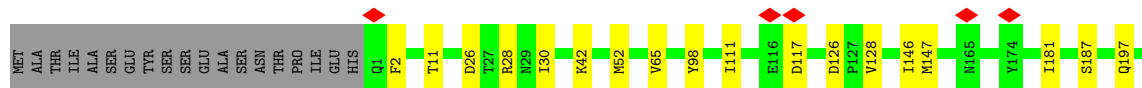
- Molecule 12: Proteasome subunit beta type-5





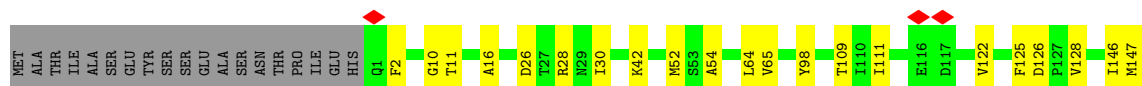
• Molecule 13: Proteasome subunit beta type-6

Chain M: 84% 8% 8%



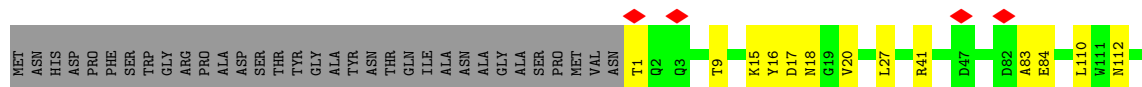
• Molecule 13: Proteasome subunit beta type-6

Chain 1: 81% 11% 8%



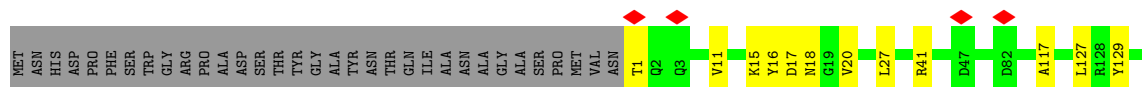
• Molecule 14: Proteasome subunit beta type-7

Chain N: 78% 10% 12%



• Molecule 14: Proteasome subunit beta type-7

Chain 2: 79% 9% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	216361	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.94	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.419	Depositor
Minimum map value	-1.469	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/1958	0.48	0/2652
1	O	0.30	0/1936	0.50	0/2622
2	B	0.30	0/1952	0.48	0/2642
2	P	0.30	0/1918	0.48	0/2597
3	C	0.29	0/1905	0.49	0/2577
3	Q	0.29	0/1934	0.50	0/2618
4	D	0.29	0/1888	0.51	0/2552
4	R	0.29	0/1871	0.51	0/2530
5	E	0.27	0/1837	0.47	0/2475
5	S	0.27	0/1841	0.47	0/2480
6	F	0.28	0/1800	0.49	0/2433
6	T	0.28	0/1800	0.49	0/2433
7	G	0.32	0/1936	0.49	0/2614
7	U	0.31	0/1932	0.49	0/2609
8	H	0.31	0/1545	0.50	0/2093
8	V	0.31	0/1545	0.49	0/2093
9	I	0.29	0/1701	0.51	0/2307
9	W	0.28	0/1701	0.48	0/2307
10	J	0.31	0/1611	0.48	0/2174
10	X	0.31	0/1605	0.48	0/2166
11	K	0.30	0/1581	0.50	0/2132
11	Y	0.30	0/1581	0.50	0/2132
12	L	0.30	0/1681	0.49	0/2274
12	Z	0.30	0/1681	0.49	0/2274
13	1	0.30	0/1795	0.49	0/2420
13	M	0.30	0/1795	0.51	0/2420
14	2	0.30	0/1855	0.51	0/2514
14	N	0.30	0/1855	0.51	0/2514
All	All	0.30	0/50040	0.49	0/67654

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1920	1912	1910	12	0
1	O	1898	1895	1893	13	0
2	B	1915	1930	1929	17	0
2	P	1881	1895	1893	19	0
3	C	1876	1878	1876	21	0
3	Q	1904	1902	1901	19	0
4	D	1861	1874	1871	20	0
4	R	1844	1850	1847	16	0
5	E	1813	1796	1794	9	0
5	S	1817	1799	1797	9	0
6	F	1773	1778	1775	13	0
6	T	1773	1778	1775	11	0
7	G	1896	1888	1886	14	0
7	U	1892	1885	1883	14	0
8	H	1516	1480	1482	12	0
8	V	1516	1480	1482	11	0
9	I	1670	1677	1679	15	0
9	W	1670	1677	1679	12	0
10	J	1581	1572	1574	16	0
10	X	1575	1567	1566	18	0
11	K	1553	1558	1560	9	0
11	Y	1553	1559	1560	11	0
12	L	1644	1593	1592	12	0
12	Z	1644	1593	1592	18	0
13	1	1757	1709	1711	19	0
13	M	1757	1710	1711	16	0
14	2	1824	1830	1832	17	0
14	N	1824	1830	1832	16	0
All	All	49147	48895	48882	359	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 4.

All (359) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:28:ARG:NE	13:M:200:ASP:OD2	2.01	0.93
12:Z:83:ARG:NH1	12:Z:201:ASP:OD1	2.01	0.93
12:L:83:ARG:NH1	12:L:201:ASP:OD1	2.01	0.93
4:D:101:GLU:OE2	12:L:197:ARG:NH2	2.03	0.92
13:1:28:ARG:NE	13:1:200:ASP:OD2	2.01	0.92
4:R:101:GLU:OE2	12:Z:197:ARG:NH2	2.04	0.88
8:V:14:LEU:HD11	8:V:100:ALA:HB3	1.62	0.81
1:O:198:SER:OG	1:O:200:GLU:OE1	2.02	0.77
9:I:43:CYS:SG	9:I:98:LEU:HD22	2.26	0.76
1:A:198:SER:OG	1:A:200:GLU:OE1	2.02	0.74
10:X:62:LEU:CD1	10:X:104:VAL:HG21	2.21	0.70
7:G:217:TRP:CZ3	7:G:223:THR:HG23	2.27	0.69
10:J:62:LEU:CD1	10:J:104:VAL:HG21	2.22	0.69
6:T:54:ASP:OD1	6:T:55:GLU:N	2.25	0.69
11:K:129:TYR:OH	11:K:144:ASP:OD1	2.11	0.68
4:R:163:THR:HG21	4:R:171:VAL:HG13	1.76	0.67
4:D:163:THR:HG21	4:D:171:VAL:HG13	1.75	0.67
13:M:26:ASP:OD1	13:M:42:LYS:NZ	2.27	0.67
13:1:26:ASP:OD1	13:1:42:LYS:NZ	2.28	0.67
11:Y:129:TYR:OH	11:Y:144:ASP:OD1	2.11	0.66
1:A:147:ASP:OD2	9:I:72:ARG:NH2	2.29	0.65
7:G:216:SER:OG	7:G:227:HIS:NE2	2.29	0.65
5:E:46:VAL:HG11	5:E:145:ALA:HB1	1.79	0.64
7:U:216:SER:OG	7:U:227:HIS:NE2	2.29	0.64
3:C:12:ILE:HG22	4:D:8:LEU:HD12	1.79	0.64
1:O:147:ASP:OD2	9:W:72:ARG:NH2	2.30	0.64
5:S:46:VAL:HG11	5:S:145:ALA:HB1	1.79	0.64
2:P:21:ILE:HD11	2:P:122:THR:HG21	1.80	0.63
9:W:17:ASP:OD1	9:W:33:LYS:NZ	2.31	0.63
5:S:197:GLU:OE2	5:S:231:TYR:OH	2.10	0.63
8:V:15:ASP:OD1	8:V:16:ALA:N	2.32	0.63
10:J:124:ASP:OD1	10:J:127:GLY:N	2.32	0.62
7:G:19:ARG:NH2	7:G:24:GLU:OE1	2.32	0.62
13:1:126:ASP:OD2	13:1:128:VAL:HG22	1.98	0.62
3:Q:12:ILE:HG22	4:R:8:LEU:HD12	1.81	0.62
8:H:15:ASP:OD1	8:H:16:ALA:N	2.33	0.62
11:K:125:VAL:HG23	11:K:127:LEU:CD1	2.30	0.62
13:M:126:ASP:OD2	13:M:128:VAL:HG22	1.99	0.62
9:W:112:SER:OG	9:W:120:ASP:OD1	2.16	0.62
4:R:215:VAL:HG23	4:R:221:ILE:HG12	1.81	0.61
10:J:84:GLU:OE1	10:J:112:ASN:ND2	2.32	0.61
4:D:53:LYS:HD3	4:D:54:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:281:GLY:O	12:Z:284:ASN:ND2	2.34	0.61
8:V:191:ASP:O	8:V:195:GLN:NE2	2.32	0.61
8:H:191:ASP:O	8:H:195:GLN:NE2	2.32	0.61
10:X:10:ILE:HG21	10:X:141:ALA:HB3	1.83	0.60
13:1:52:MET:HG3	13:1:111:ILE:HG22	1.82	0.60
10:X:124:ASP:OD1	10:X:127:GLY:N	2.34	0.60
12:Z:102:VAL:HG11	12:Z:105:GLN:OE1	2.01	0.60
10:J:10:ILE:HG21	10:J:141:ALA:HB3	1.83	0.60
5:E:197:GLU:OE2	5:E:231:TYR:OH	2.10	0.60
12:L:281:GLY:O	12:L:284:ASN:ND2	2.34	0.60
4:D:215:VAL:HG23	4:D:221:ILE:HG12	1.82	0.59
3:Q:91:ALA:HB2	3:Q:115:LEU:HD11	1.83	0.59
13:M:52:MET:HG3	13:M:111:ILE:HG22	1.82	0.59
7:G:201:LEU:HD12	7:G:246:ILE:HD11	1.85	0.59
9:I:17:ASP:OD1	9:I:33:LYS:NZ	2.32	0.59
2:B:21:ILE:HD11	2:B:122:THR:HG21	1.84	0.59
7:G:217:TRP:CH2	7:G:223:THR:HG23	2.38	0.59
11:Y:125:VAL:HG23	11:Y:127:LEU:CD1	2.33	0.59
10:X:97:ARG:HH22	11:Y:92:ARG:HD3	1.68	0.58
14:2:17:ASP:OD1	14:2:18:ASN:N	2.36	0.58
12:L:102:VAL:HG11	12:L:105:GLN:OE1	2.03	0.58
4:R:154:GLY:O	5:S:86:ARG:NH2	2.37	0.58
11:K:138:TYR:OH	11:Y:24:ILE:O	2.22	0.58
14:N:17:ASP:OD1	14:N:18:ASN:N	2.37	0.58
2:P:96:SER:O	2:P:100:ILE:HD12	2.04	0.58
5:S:90:GLU:OE2	12:Z:145:ARG:NH1	2.37	0.58
3:C:91:ALA:HB2	3:C:115:LEU:HD11	1.84	0.57
2:B:96:SER:O	2:B:100:ILE:HD12	2.05	0.57
5:S:119:LEU:HD23	5:S:122:ARG:HH21	1.70	0.57
3:C:12:ILE:CG2	4:D:8:LEU:HD12	2.34	0.57
10:J:97:ARG:HH22	11:K:92:ARG:HD3	1.69	0.57
4:D:154:GLY:O	5:E:86:ARG:NH2	2.37	0.57
12:Z:126:ALA:CB	13:1:128:VAL:HG23	2.35	0.57
3:Q:12:ILE:CG2	4:R:8:LEU:HD12	2.34	0.56
9:I:112:SER:OG	9:I:120:ASP:OD1	2.16	0.56
5:E:90:GLU:OE2	12:L:145:ARG:NH1	2.38	0.56
11:K:24:ILE:O	11:Y:138:TYR:OH	2.22	0.56
6:F:93:ASN:OD1	6:F:97:LEU:HD23	2.06	0.56
12:Z:96:ALA:HB2	12:Z:107:VAL:HG21	1.86	0.56
12:L:96:ALA:HB2	12:L:107:VAL:HG21	1.87	0.56
14:2:129:TYR:HE1	14:2:144:THR:HG22	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:148:LYS:HE3	9:I:177:VAL:HG11	1.88	0.55
6:T:93:ASN:OD1	6:T:97:LEU:HD23	2.06	0.55
8:H:20:THR:HG23	8:H:31:THR:HG21	1.88	0.55
7:U:217:TRP:CZ3	7:U:223:THR:HG23	2.41	0.55
10:X:62:LEU:HD11	10:X:104:VAL:HG21	1.88	0.55
3:C:195:LYS:HD3	3:C:244:ILE:HD11	1.87	0.55
3:C:120:GLN:NE2	4:D:81:ASP:OD1	2.39	0.55
9:I:170:GLY:O	9:I:171:SER:OG	2.18	0.55
1:A:79:ILE:HD11	1:A:112:MET:O	2.06	0.54
10:J:62:LEU:HD11	10:J:104:VAL:HG21	1.89	0.54
13:M:147:MET:HE2	10:X:176:ARG:NH2	2.21	0.54
1:O:79:ILE:HD11	1:O:112:MET:O	2.07	0.54
1:A:75:ILE:HD11	1:A:81:MET:HE2	1.90	0.54
2:P:64:VAL:HG11	2:P:212:ALA:CB	2.37	0.54
14:2:16:TYR:CE2	14:2:170:VAL:HG22	2.43	0.54
5:E:119:LEU:HD23	5:E:122:ARG:HH21	1.73	0.54
14:N:15:LYS:HB3	14:N:20:VAL:HG12	1.89	0.54
11:Y:148:ARG:NH1	11:Y:150:ASP:OD1	2.41	0.54
2:P:200:VAL:HG21	2:P:209:ILE:HD11	1.90	0.53
14:N:16:TYR:CE2	14:N:170:VAL:HG22	2.44	0.53
2:B:200:VAL:HG21	2:B:209:ILE:HD11	1.89	0.53
12:L:126:ALA:CB	13:M:128:VAL:HG23	2.38	0.53
3:Q:120:GLN:NE2	4:R:81:ASP:OD1	2.38	0.53
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.91	0.53
14:2:127:LEU:HG	14:2:142:LEU:HD12	1.90	0.52
6:F:88:LEU:HD11	6:F:108:ALA:HB1	1.92	0.52
11:K:148:ARG:NH1	11:K:150:ASP:OD1	2.42	0.52
7:G:236:GLN:NE2	7:G:240:ASP:OD1	2.40	0.52
6:T:88:LEU:HD11	6:T:108:ALA:HB1	1.92	0.52
14:2:129:TYR:CE1	14:2:144:THR:HG22	2.45	0.52
2:B:21:ILE:HD11	2:B:122:THR:CG2	2.40	0.52
4:R:96:HIS:ND1	4:R:102:ASP:O	2.43	0.52
8:H:32:ASP:OD1	8:H:185:ARG:NH2	2.41	0.52
10:J:134:ASP:OD1	10:J:135:PHE:N	2.41	0.52
2:P:21:ILE:HD11	2:P:122:THR:CG2	2.40	0.52
1:A:28:VAL:HG21	1:A:129:THR:HG23	1.92	0.52
9:W:148:LYS:HE3	9:W:177:VAL:HG11	1.91	0.51
13:1:54:ALA:CB	13:1:109:THR:HG22	2.40	0.51
2:B:12:PHE:CE1	2:B:18:LEU:HD11	2.45	0.51
8:H:20:THR:CG2	8:H:31:THR:HG21	2.40	0.51
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:LEU:HD23	2:B:209:ILE:HD12	1.93	0.51
6:F:49:LEU:HD21	6:F:204:GLU:OE2	2.09	0.51
3:Q:191:GLU:HG2	3:Q:242:THR:HG22	1.92	0.51
14:N:159:VAL:HG23	14:N:159:VAL:O	2.11	0.51
7:U:19:ARG:NH2	7:U:24:GLU:OE1	2.41	0.51
12:Z:180:TYR:CD2	12:Z:258:GLU:HA	2.45	0.51
7:G:64:VAL:HG13	7:G:214:GLU:OE1	2.10	0.50
8:H:5:ALA:HB2	8:H:14:LEU:HD23	1.93	0.50
7:U:64:VAL:HG13	7:U:214:GLU:OE1	2.10	0.50
8:H:36:ARG:HD2	14:2:233:ILE:HD11	1.93	0.50
1:O:28:VAL:HG21	1:O:129:THR:HG23	1.93	0.50
14:N:127:LEU:HG	14:N:142:LEU:HD12	1.94	0.50
8:H:55:ILE:HD11	8:H:93:LEU:HD13	1.94	0.50
12:L:180:TYR:CD2	12:L:258:GLU:HA	2.45	0.50
5:S:31:ILE:HD13	5:S:141:ALA:HB2	1.93	0.50
6:F:157:TYR:CE1	7:G:59:VAL:HG12	2.47	0.50
14:N:233:ILE:HD11	8:V:36:ARG:HD2	1.94	0.49
2:P:196:LEU:HD23	2:P:209:ILE:HD12	1.94	0.49
14:2:159:VAL:HG23	14:2:159:VAL:O	2.12	0.49
3:C:4:ARG:NH1	5:E:125:GLU:OE2	2.46	0.49
10:X:125:LEU:HG	10:X:126:ILE:HG23	1.95	0.49
7:G:216:SER:HG	7:G:227:HIS:CE1	2.27	0.49
10:J:185:VAL:HG21	10:J:196:LYS:HE3	1.92	0.49
13:1:30:ILE:HD13	13:1:197:GLN:HG2	1.94	0.49
8:V:20:THR:HG23	8:V:31:THR:HG21	1.94	0.49
12:Z:111:ILE:HD12	12:Z:132:GLU:OE1	2.12	0.49
2:P:64:VAL:HG11	2:P:212:ALA:HB3	1.95	0.48
8:V:20:THR:CG2	8:V:31:THR:HG21	2.43	0.48
10:J:125:LEU:HG	10:J:126:ILE:HG23	1.95	0.48
7:U:217:TRP:HE1	7:U:230:VAL:HG22	1.79	0.48
8:H:14:LEU:CD1	8:H:42:TRP:HB2	2.44	0.48
3:Q:19:LEU:HD13	3:Q:123:THR:CG2	2.44	0.48
2:P:213:ILE:HD11	2:P:236:ARG:NH1	2.29	0.48
13:1:64:LEU:HD23	13:1:109:THR:HG21	1.96	0.48
3:Q:194:LEU:HD12	3:Q:242:THR:HG21	1.96	0.48
12:Z:79:THR:HB	12:Z:92:VAL:HG12	1.96	0.47
7:U:217:TRP:NE1	7:U:230:VAL:HG22	2.30	0.47
6:F:157:TYR:CD1	7:G:59:VAL:HG12	2.49	0.47
3:C:191:GLU:HG2	3:C:242:THR:HG22	1.95	0.47
2:B:85:LEU:HD21	2:B:118:MET:CE	2.44	0.47
3:C:19:LEU:HD13	3:C:123:THR:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:LYS:CD	4:D:54:LEU:HD12	2.42	0.47
4:R:68:ASP:OD1	4:R:69:SER:N	2.41	0.47
8:V:32:ASP:OD1	8:V:185:ARG:NH2	2.42	0.47
6:F:9:ASP:OD1	6:F:12:THR:OG1	2.18	0.47
12:L:277:LYS:NZ	12:L:286:VAL:O	2.32	0.47
1:O:87:ILE:N	1:O:88:PRO:HD2	2.30	0.47
14:2:174:GLU:OE2	14:2:209:LYS:NZ	2.45	0.47
1:A:87:ILE:N	1:A:88:PRO:HD2	2.30	0.46
4:R:111:ARG:NH2	12:Z:146:GLU:OE1	2.48	0.46
6:T:182:ILE:HD13	6:T:188:GLU:HG3	1.96	0.46
13:1:52:MET:SD	13:1:65:VAL:HG22	2.55	0.46
10:X:28:LEU:CD2	11:Y:125:VAL:HG11	2.45	0.46
4:D:96:HIS:ND1	4:D:102:ASP:O	2.44	0.46
13:M:146:ILE:HG23	13:M:187:SER:HB3	1.97	0.46
2:P:48:GLU:OE1	2:P:48:GLU:N	2.46	0.46
6:T:175:THR:HG22	6:T:175:THR:O	2.16	0.46
2:P:85:LEU:HD21	2:P:118:MET:CE	2.44	0.46
12:Z:277:LYS:NZ	12:Z:286:VAL:O	2.34	0.46
2:B:85:LEU:HD21	2:B:118:MET:HE3	1.98	0.46
4:D:16:HIS:ND1	4:D:21:GLU:OE2	2.49	0.46
13:M:52:MET:SD	13:M:65:VAL:HG22	2.56	0.46
4:R:16:HIS:ND1	4:R:21:GLU:OE1	2.48	0.46
13:1:11:THR:HG21	13:1:146:ILE:HD12	1.98	0.46
9:I:77:VAL:CG1	14:2:230:THR:HG22	2.45	0.46
6:T:94:TYR:CE1	6:T:98:VAL:HG21	2.51	0.46
10:X:20:VAL:HG11	10:X:109:ALA:HB1	1.97	0.46
10:X:141:ALA:HB2	10:X:177:ASP:HB2	1.98	0.46
14:N:230:THR:HG22	9:W:77:VAL:CG1	2.46	0.45
4:D:140:PRO:O	4:D:141:ARG:HG2	2.16	0.45
5:S:59:LEU:HD23	5:S:60:GLU:N	2.32	0.45
13:1:146:ILE:HG23	13:1:187:SER:HB3	1.97	0.45
10:J:97:ARG:NH1	10:J:102:TYR:CZ	2.84	0.45
6:F:175:THR:O	6:F:175:THR:HG22	2.17	0.45
1:O:192:ASP:OD1	1:O:192:ASP:O	2.34	0.45
5:S:70:ILE:HG21	5:S:112:LEU:HD11	1.98	0.45
11:K:148:ARG:NH1	11:K:148:ARG:HB2	2.32	0.45
10:X:97:ARG:NH1	10:X:102:TYR:CZ	2.85	0.45
1:A:46:ARG:NH2	1:A:192:ASP:OD1	2.49	0.45
2:B:110:LEU:O	2:B:114:VAL:HG23	2.17	0.45
4:R:241:GLN:O	4:R:241:GLN:NE2	2.46	0.45
4:D:189:GLU:CD	4:D:189:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:217:TRP:CZ3	7:G:222:GLU:HB2	2.51	0.45
10:J:141:ALA:HB2	10:J:177:ASP:HB2	1.99	0.45
3:Q:244:ILE:O	3:Q:245:THR:HG22	2.16	0.45
12:Z:131:TRP:HE1	13:1:98:TYR:HH	1.65	0.45
12:L:131:TRP:HE1	13:M:98:TYR:HH	1.63	0.45
10:X:60:THR:O	10:X:64:GLU:OE2	2.35	0.45
5:E:121:LEU:HD12	6:F:79:PRO:HB2	1.98	0.45
3:Q:75:VAL:HG21	3:Q:88:ILE:CD1	2.47	0.45
12:Z:202:ILE:HD11	12:Z:220:TYR:CD2	2.52	0.44
13:M:30:ILE:HD13	13:M:197:GLN:HG2	1.99	0.44
5:S:121:LEU:HD12	6:T:79:PRO:HB2	1.98	0.44
9:W:45:GLY:HA2	9:W:98:LEU:HD23	1.99	0.44
14:2:15:LYS:HB3	14:2:20:VAL:HG12	1.99	0.44
6:F:182:ILE:HD13	6:F:188:GLU:HG3	1.98	0.44
9:I:129:SER:OG	9:I:166:ASP:OD2	2.23	0.44
13:M:11:THR:HG21	13:M:146:ILE:HD12	1.99	0.44
12:L:202:ILE:HD11	12:L:220:TYR:CD2	2.52	0.44
14:N:193:ARG:NH1	14:N:217:MET:SD	2.90	0.44
3:Q:110:ILE:HD11	11:Y:70:GLU:HG2	2.00	0.44
7:U:230:VAL:HG12	7:U:235:LEU:HB2	2.00	0.44
10:J:20:VAL:HG11	10:J:109:ALA:HB1	1.98	0.44
14:N:83:ALA:O	14:N:84:GLU:HB2	2.17	0.44
7:U:217:TRP:CD1	7:U:230:VAL:HG22	2.53	0.44
6:T:201:LEU:HD11	6:T:206:LEU:HG	2.00	0.44
5:E:59:LEU:HD23	5:E:60:GLU:N	2.32	0.44
6:T:9:ASP:OD1	6:T:12:THR:OG1	2.19	0.44
11:Y:148:ARG:NH1	11:Y:148:ARG:HB2	2.32	0.44
9:I:51:ASP:O	9:I:55:VAL:HG12	2.17	0.44
4:R:34:VAL:HG11	4:R:199:LEU:HG	1.99	0.44
2:P:110:LEU:O	2:P:114:VAL:HG23	2.18	0.44
13:1:16:ALA:HB2	13:1:122:VAL:HG23	1.99	0.44
5:E:70:ILE:HG21	5:E:112:LEU:HD11	1.98	0.43
11:K:125:VAL:HG23	11:K:127:LEU:HD11	2.00	0.43
13:1:109:THR:OG1	13:1:125:PHE:HB2	2.17	0.43
14:2:193:ARG:NH1	14:2:217:MET:SD	2.91	0.43
2:P:196:LEU:CD2	2:P:209:ILE:HD12	2.48	0.43
14:2:27:LEU:HB2	14:2:192:SER:HB2	2.00	0.43
3:C:177:GLN:HG2	4:D:54:LEU:CD1	2.47	0.43
4:R:189:GLU:H	4:R:189:GLU:CD	2.21	0.43
3:C:75:VAL:HG21	3:C:88:ILE:CD1	2.48	0.43
4:D:241:GLN:O	4:D:241:GLN:NE2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:TYR:HB3	2:B:82:TYR:CD1	2.54	0.43
14:N:129:TYR:HE1	14:N:144:THR:HG22	1.83	0.43
1:O:54:ILE:HD12	1:O:225:VAL:HG22	2.00	0.43
12:Z:126:ALA:HB2	13:1:128:VAL:HG23	1.99	0.43
4:D:72:VAL:HG13	4:D:221:ILE:HD13	2.01	0.43
9:I:63:ILE:HG23	9:I:74:PRO:HB3	2.01	0.43
7:U:171:ALA:O	7:U:175:LEU:HD23	2.19	0.43
2:B:196:LEU:CD2	2:B:209:ILE:HD12	2.47	0.43
6:F:135:ILE:HD12	6:F:216:VAL:HG12	2.01	0.43
2:P:75:TYR:HB3	2:P:82:TYR:CD1	2.54	0.43
3:C:112:VAL:HG22	3:C:137:TYR:CG	2.54	0.43
3:C:209:ASP:OD1	3:C:209:ASP:N	2.52	0.43
8:V:34:LEU:CD1	8:V:176:VAL:HG23	2.49	0.43
1:A:192:ASP:OD1	1:A:192:ASP:O	2.37	0.42
8:H:34:LEU:CD1	8:H:176:VAL:HG23	2.48	0.42
3:Q:112:VAL:HG22	3:Q:137:TYR:CG	2.54	0.42
9:W:43:CYS:SG	9:W:98:LEU:HD22	2.59	0.42
3:C:194:LEU:HD12	3:C:242:THR:HG21	2.02	0.42
3:C:224:GLU:OE1	3:C:224:GLU:HA	2.19	0.42
14:N:174:GLU:OE1	14:N:209:LYS:NZ	2.48	0.42
1:O:129:THR:HG22	1:O:129:THR:O	2.18	0.42
8:V:14:LEU:CD1	8:V:100:ALA:HB3	2.42	0.42
4:D:106:VAL:O	4:D:110:THR:HG22	2.20	0.42
4:D:185:PRO:HB2	4:D:191:CYS:SG	2.60	0.42
13:1:181:ILE:HD11	13:1:206:ILE:CD1	2.49	0.42
3:C:110:ILE:HD11	11:K:70:GLU:HG2	2.01	0.42
10:J:11:VAL:HG23	10:J:53:THR:CG2	2.49	0.42
14:N:27:LEU:HB2	14:N:192:SER:HB2	2.00	0.42
1:O:46:ARG:NH2	1:O:192:ASP:OD1	2.52	0.42
3:Q:120:GLN:HG3	4:R:80:ALA:HB1	2.00	0.42
9:W:63:ILE:HG23	9:W:74:PRO:HB3	2.01	0.42
10:X:11:VAL:HG23	10:X:53:THR:CG2	2.49	0.42
12:Z:79:THR:CB	12:Z:92:VAL:HG12	2.50	0.42
2:B:212:ALA:HB2	2:B:237:LYS:HD2	2.02	0.42
1:O:83:VAL:HG11	1:O:90:ALA:CB	2.49	0.42
1:O:147:ASP:OD1	1:O:148:GLU:N	2.53	0.42
2:P:149:GLN:O	2:P:156:TYR:HA	2.20	0.42
3:C:123:THR:O	3:C:123:THR:HG22	2.19	0.42
12:L:126:ALA:HB2	13:M:128:VAL:HG23	2.01	0.42
13:M:117:ASP:C	13:M:117:ASP:OD1	2.58	0.42
3:Q:123:THR:HG22	3:Q:123:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:190:ILE:HD11	3:Q:215:THR:HG21	2.01	0.42
3:Q:209:ASP:OD1	3:Q:209:ASP:N	2.52	0.42
2:B:149:GLN:O	2:B:156:TYR:HA	2.20	0.42
9:W:3:ILE:O	9:W:126:SER:HA	2.20	0.42
7:G:171:ALA:O	7:G:175:LEU:HD23	2.19	0.42
1:A:129:THR:O	1:A:129:THR:HG22	2.19	0.41
2:B:64:VAL:HG11	2:B:212:ALA:CB	2.50	0.41
9:I:3:ILE:O	9:I:126:SER:HA	2.20	0.41
3:Q:152:ASN:HB2	3:Q:153:PRO:CD	2.50	0.41
13:1:2:PHE:HB3	14:2:1:THR:HG23	2.02	0.41
1:A:53:VAL:CG1	1:A:144:VAL:HG11	2.51	0.41
3:C:120:GLN:HG3	4:D:80:ALA:HB1	2.02	0.41
13:M:2:PHE:HB3	14:N:1:THR:HG23	2.01	0.41
2:B:18:LEU:HD22	2:B:21:ILE:HD12	2.02	0.41
4:D:167:ASN:OD1	4:D:202:VAL:HG13	2.21	0.41
9:I:137:VAL:HG21	9:I:161:ALA:HB2	2.02	0.41
1:O:53:VAL:CG1	1:O:144:VAL:HG11	2.50	0.41
14:2:11:VAL:HG23	14:2:41:ARG:HH12	1.85	0.41
14:2:20:VAL:HG21	14:2:117:ALA:HB1	2.03	0.41
1:A:211:ILE:O	1:A:215:GLY:N	2.54	0.41
7:G:128:VAL:HG22	7:G:129:ARG:N	2.36	0.41
4:R:185:PRO:HB2	4:R:191:CYS:SG	2.61	0.41
6:T:19:LEU:HD21	7:U:129:ARG:HD2	2.02	0.41
7:U:217:TRP:CH2	7:U:223:THR:HG23	2.55	0.41
3:C:152:ASN:HB2	3:C:153:PRO:CD	2.51	0.41
9:I:77:VAL:HG11	14:2:230:THR:HG22	2.02	0.41
9:I:137:VAL:HG22	14:2:157:LYS:NZ	2.36	0.41
10:J:144:GLN:OE1	10:J:144:GLN:N	2.51	0.41
14:N:9:THR:O	14:N:41:ARG:NH1	2.53	0.41
10:X:15:THR:HG23	10:X:118:PRO:HB2	2.03	0.41
3:C:42:ASP:N	3:C:42:ASP:OD1	2.53	0.41
3:C:42:ASP:OD1	3:C:186:VAL:HG23	2.20	0.41
9:I:35:HIS:HB2	9:I:56:THR:HG21	2.02	0.41
2:P:122:THR:HG22	2:P:122:THR:O	2.21	0.41
11:Y:8:VAL:HG22	11:Y:11:SER:O	2.21	0.41
11:Y:20:VAL:HG23	11:Y:31:ASP:HB2	2.02	0.41
10:J:176:ARG:NH2	13:1:147:MET:HE3	2.35	0.41
10:X:23:ALA:CB	10:X:186:VAL:HG22	2.51	0.41
2:B:26:THR:O	2:B:30:GLN:OE1	2.39	0.41
3:C:66:LEU:HD23	3:C:214:ALA:HB2	2.03	0.41
6:F:52:ASN:ND2	6:F:54:ASP:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:59:VAL:HG11	8:H:82:PHE:CE2	2.56	0.41
2:P:26:THR:O	2:P:30:GLN:OE1	2.39	0.41
2:P:85:LEU:HD21	2:P:118:MET:HE3	2.02	0.41
3:Q:77:VAL:HG11	3:Q:84:ALA:CB	2.51	0.41
9:W:8:PHE:HB3	9:W:151:ALA:HB2	2.03	0.41
10:X:144:GLN:OE1	10:X:144:GLN:N	2.51	0.41
6:F:94:TYR:CE1	6:F:98:VAL:HG21	2.55	0.41
6:F:156:LEU:HD13	6:F:159:THR:HB	2.02	0.40
13:M:181:ILE:HD11	13:M:206:ILE:CD1	2.51	0.40
2:P:109:LEU:HD22	10:X:77:GLU:OE2	2.21	0.40
13:M:2:PHE:CB	14:N:1:THR:HG23	2.52	0.40
3:Q:211:LEU:CD1	3:Q:239:LEU:HD21	2.51	0.40
9:W:55:VAL:HG13	9:W:56:THR:N	2.37	0.40
9:W:110:LEU:HG	9:W:125:LEU:HD12	2.04	0.40
13:1:10:GLY:HA3	13:1:42:LYS:NZ	2.37	0.40
2:B:18:LEU:HD12	2:B:18:LEU:N	2.36	0.40
7:G:217:TRP:NE1	7:G:230:VAL:HG22	2.37	0.40
3:Q:66:LEU:HD23	3:Q:214:ALA:HB2	2.03	0.40
10:X:23:ALA:HB2	10:X:186:VAL:HG22	2.02	0.40
1:A:54:ILE:HD13	1:A:225:VAL:HG13	2.03	0.40
10:J:148:MET:HG2	10:J:169:ALA:HA	2.04	0.40
6:T:155:GLU:HG2	7:U:59:VAL:HG11	2.04	0.40
12:Z:111:ILE:HD11	12:Z:121:MET:CG	2.51	0.40
12:Z:191:VAL:HG22	12:Z:197:ARG:HG3	2.02	0.40
14:N:110:LEU:O	14:N:112:ASN:N	2.55	0.40
1:O:211:ILE:O	1:O:215:GLY:N	2.52	0.40
2:P:64:VAL:HG11	2:P:212:ALA:HB2	2.03	0.40
7:U:128:VAL:HG22	7:U:129:ARG:N	2.36	0.40
7:U:217:TRP:CD1	7:U:230:VAL:CG2	3.04	0.40
8:V:14:LEU:HD11	8:V:100:ALA:CB	2.43	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	241/252 (96%)	239 (99%)	2 (1%)	0	100	100
1	O	238/252 (94%)	237 (100%)	1 (0%)	0	100	100
2	B	248/250 (99%)	248 (100%)	0	0	100	100
2	P	244/250 (98%)	244 (100%)	0	0	100	100
3	C	235/258 (91%)	232 (99%)	3 (1%)	0	100	100
3	Q	242/258 (94%)	239 (99%)	3 (1%)	0	100	100
4	D	231/254 (91%)	230 (100%)	1 (0%)	0	100	100
4	R	229/254 (90%)	229 (100%)	0	0	100	100
5	E	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	S	232/260 (89%)	229 (99%)	3 (1%)	0	100	100
6	F	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
6	T	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
7	G	242/288 (84%)	240 (99%)	2 (1%)	0	100	100
7	U	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
8	H	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
8	V	194/215 (90%)	188 (97%)	6 (3%)	0	100	100
9	I	218/261 (84%)	215 (99%)	3 (1%)	0	100	100
9	W	218/261 (84%)	215 (99%)	3 (1%)	0	100	100
10	J	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
10	X	201/205 (98%)	192 (96%)	9 (4%)	0	100	100
11	K	192/212 (91%)	188 (98%)	4 (2%)	0	100	100
11	Y	192/212 (91%)	188 (98%)	4 (2%)	0	100	100
12	L	210/287 (73%)	207 (99%)	3 (1%)	0	100	100
12	Z	210/287 (73%)	208 (99%)	2 (1%)	0	100	100
13	1	220/241 (91%)	217 (99%)	3 (1%)	0	100	100
13	M	220/241 (91%)	216 (98%)	4 (2%)	0	100	100
14	2	231/266 (87%)	220 (95%)	11 (5%)	0	100	100
14	N	231/266 (87%)	220 (95%)	11 (5%)	0	100	100
All	All	6245/6966 (90%)	6138 (98%)	107 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/210 (99%)	207 (100%)	0	100	100
1	O	205/210 (98%)	205 (100%)	0	100	100
2	B	209/209 (100%)	209 (100%)	0	100	100
2	P	205/209 (98%)	205 (100%)	0	100	100
3	C	201/216 (93%)	201 (100%)	0	100	100
3	Q	203/216 (94%)	203 (100%)	0	100	100
4	D	209/226 (92%)	209 (100%)	0	100	100
4	R	207/226 (92%)	207 (100%)	0	100	100
5	E	194/215 (90%)	194 (100%)	0	100	100
5	S	194/215 (90%)	194 (100%)	0	100	100
6	F	190/193 (98%)	190 (100%)	0	100	100
6	T	190/193 (98%)	190 (100%)	0	100	100
7	G	201/239 (84%)	201 (100%)	0	100	100
7	U	201/239 (84%)	201 (100%)	0	100	100
8	H	163/179 (91%)	163 (100%)	0	100	100
8	V	163/179 (91%)	163 (100%)	0	100	100
9	I	179/214 (84%)	179 (100%)	0	100	100
9	W	179/214 (84%)	179 (100%)	0	100	100
10	J	172/173 (99%)	172 (100%)	0	100	100
10	X	171/173 (99%)	171 (100%)	0	100	100
11	K	172/188 (92%)	172 (100%)	0	100	100
11	Y	172/188 (92%)	172 (100%)	0	100	100
12	L	169/235 (72%)	169 (100%)	0	100	100
12	Z	169/235 (72%)	169 (100%)	0	100	100
13	1	185/201 (92%)	185 (100%)	0	100	100
13	M	185/201 (92%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2	199/224 (89%)	199 (100%)	0	100	100
14	N	199/224 (89%)	199 (100%)	0	100	100
All	All	5293/5844 (91%)	5293 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	94	HIS
5	E	73	HIS
9	I	144	GLN
12	L	284	ASN
2	P	94	HIS
5	S	73	HIS
7	U	143	ASN
7	U	146	HIS
9	W	144	GLN
12	Z	284	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

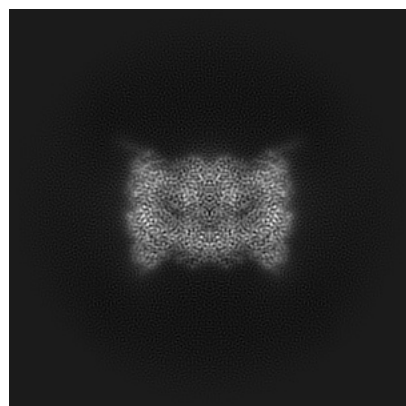
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23502. These allow visual inspection of the internal detail of the map and identification of artifacts.

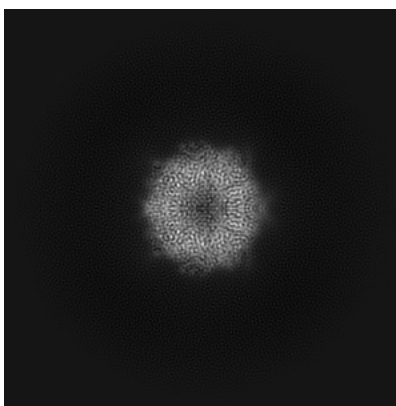
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

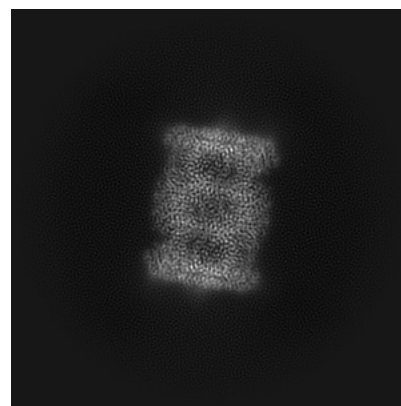
6.1.1 Primary map



X

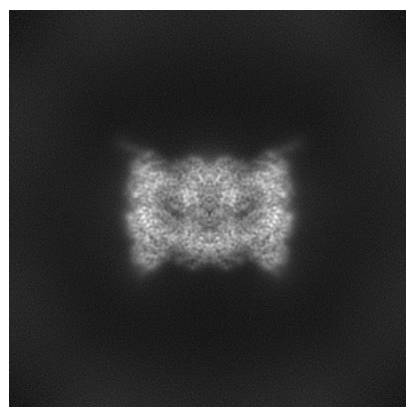


Y

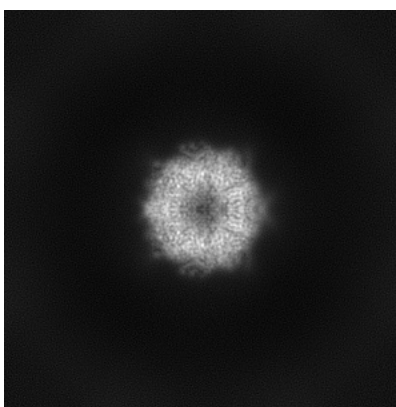


Z

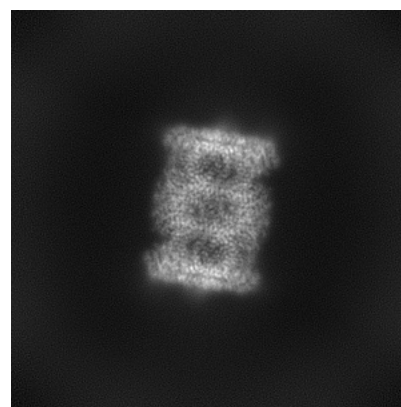
6.1.2 Raw map



X



Y

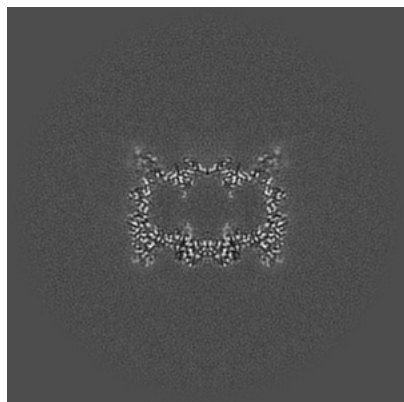


Z

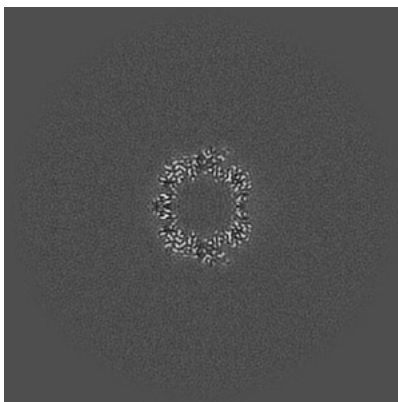
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

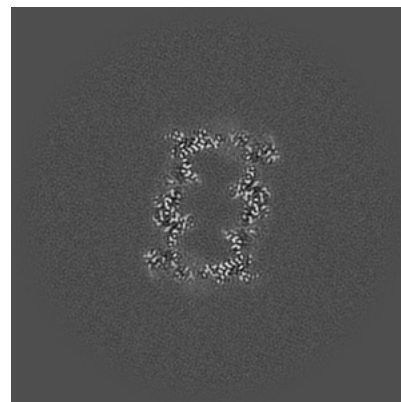
6.2.1 Primary map



X Index: 180

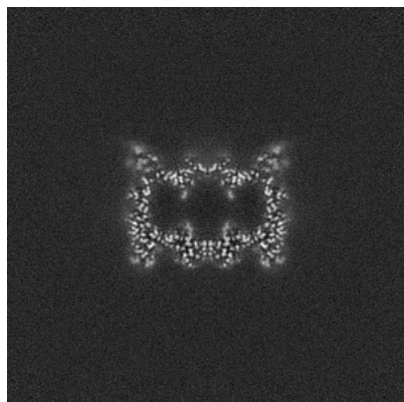


Y Index: 180

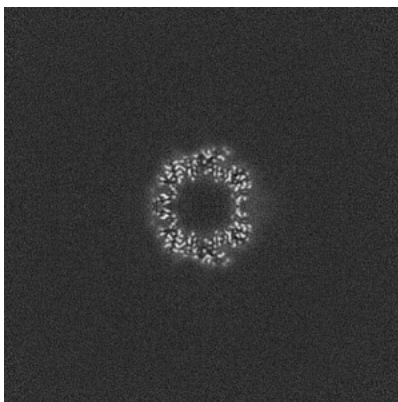


Z Index: 180

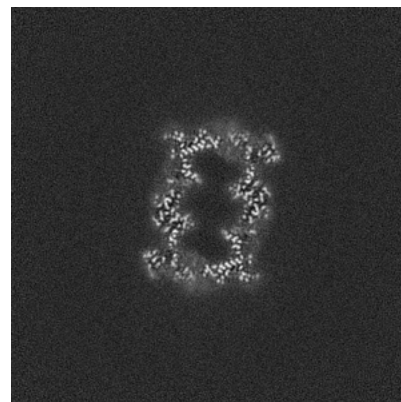
6.2.2 Raw map



X Index: 180



Y Index: 180

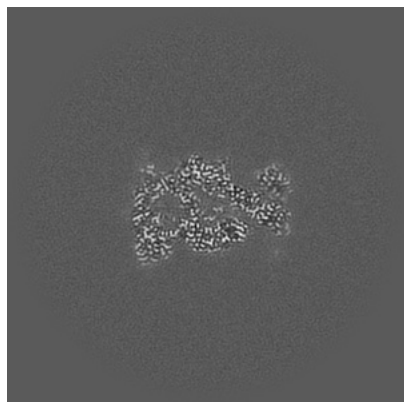


Z Index: 180

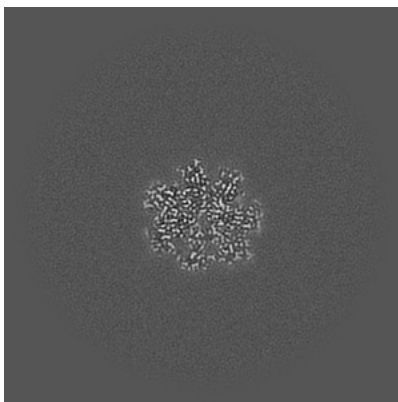
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

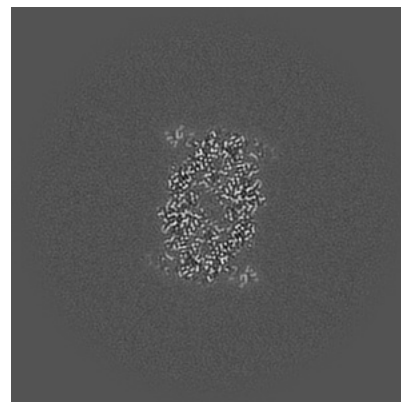
6.3.1 Primary map



X Index: 154

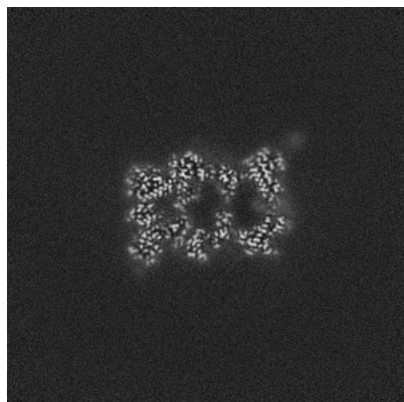


Y Index: 126

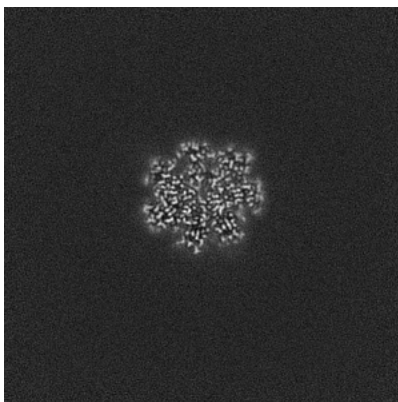


Z Index: 155

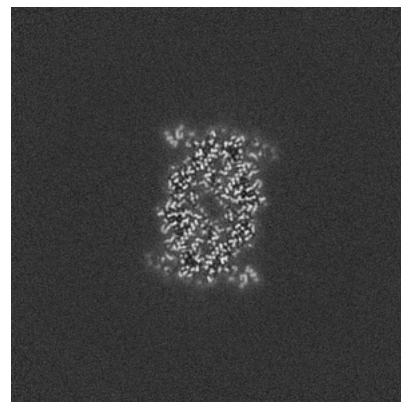
6.3.2 Raw map



X Index: 194



Y Index: 234

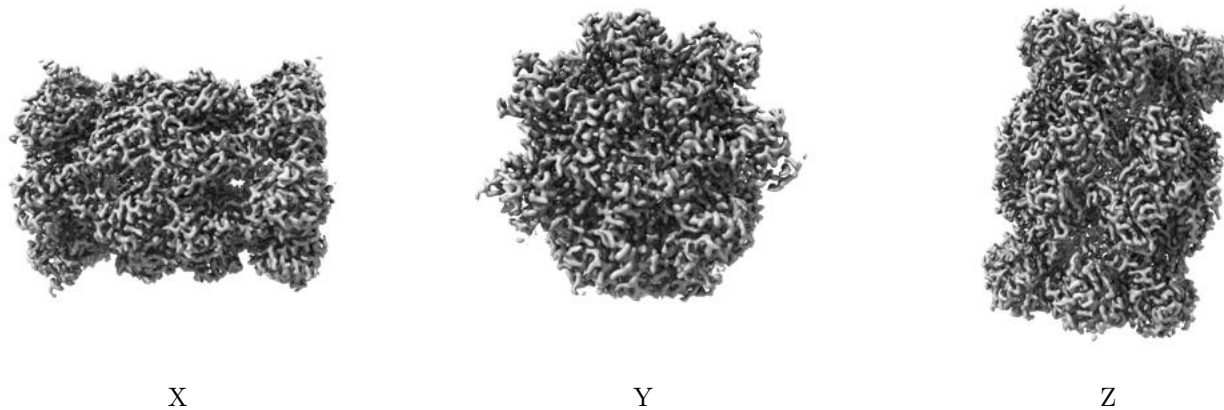


Z Index: 155

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

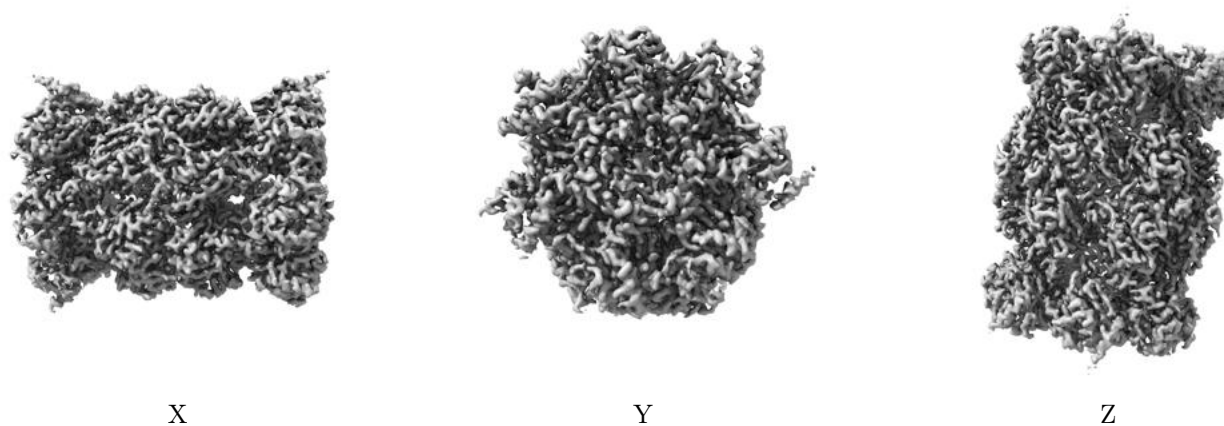
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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



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.

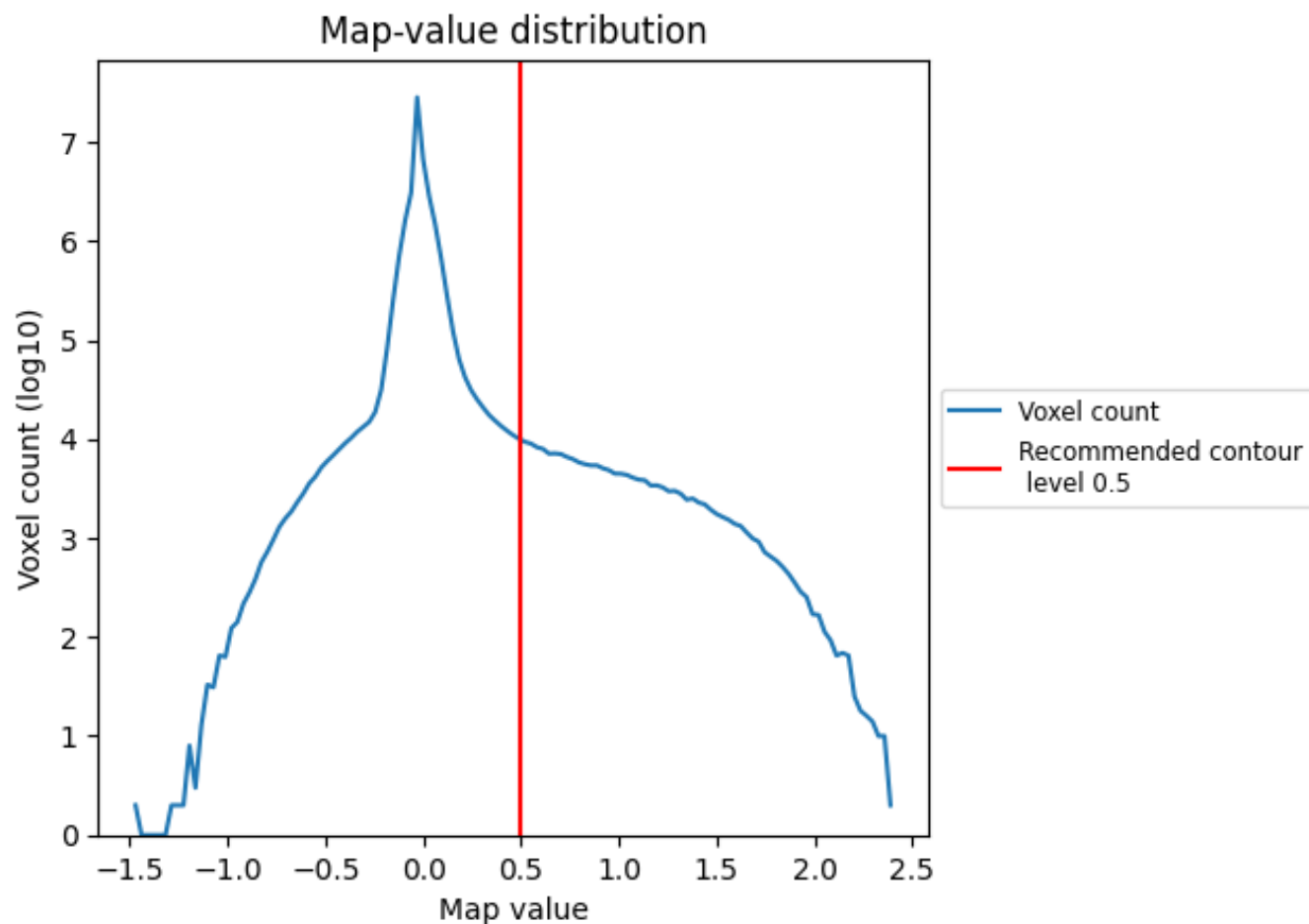
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

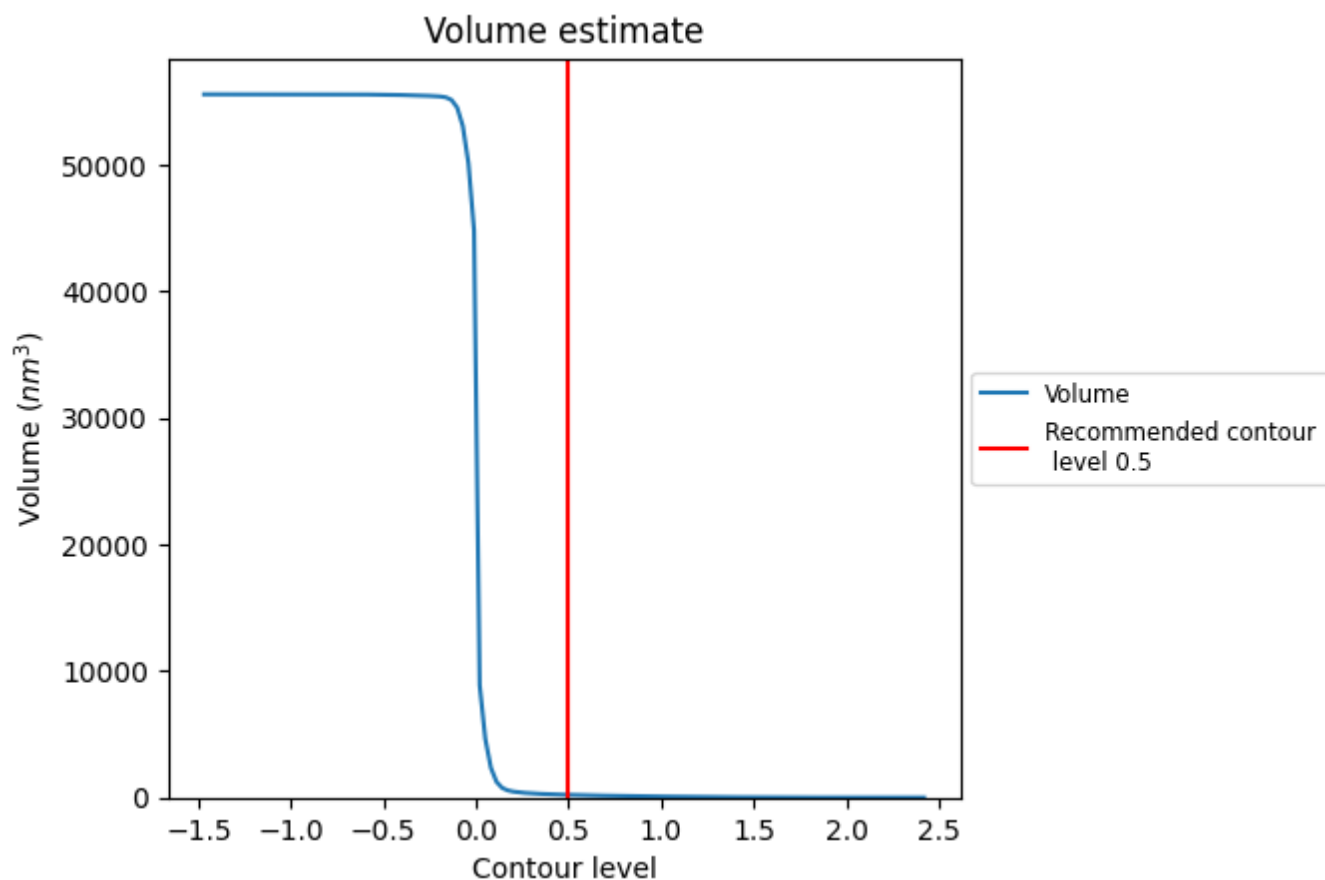
This section contains the results of statistical analysis of the map.

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.

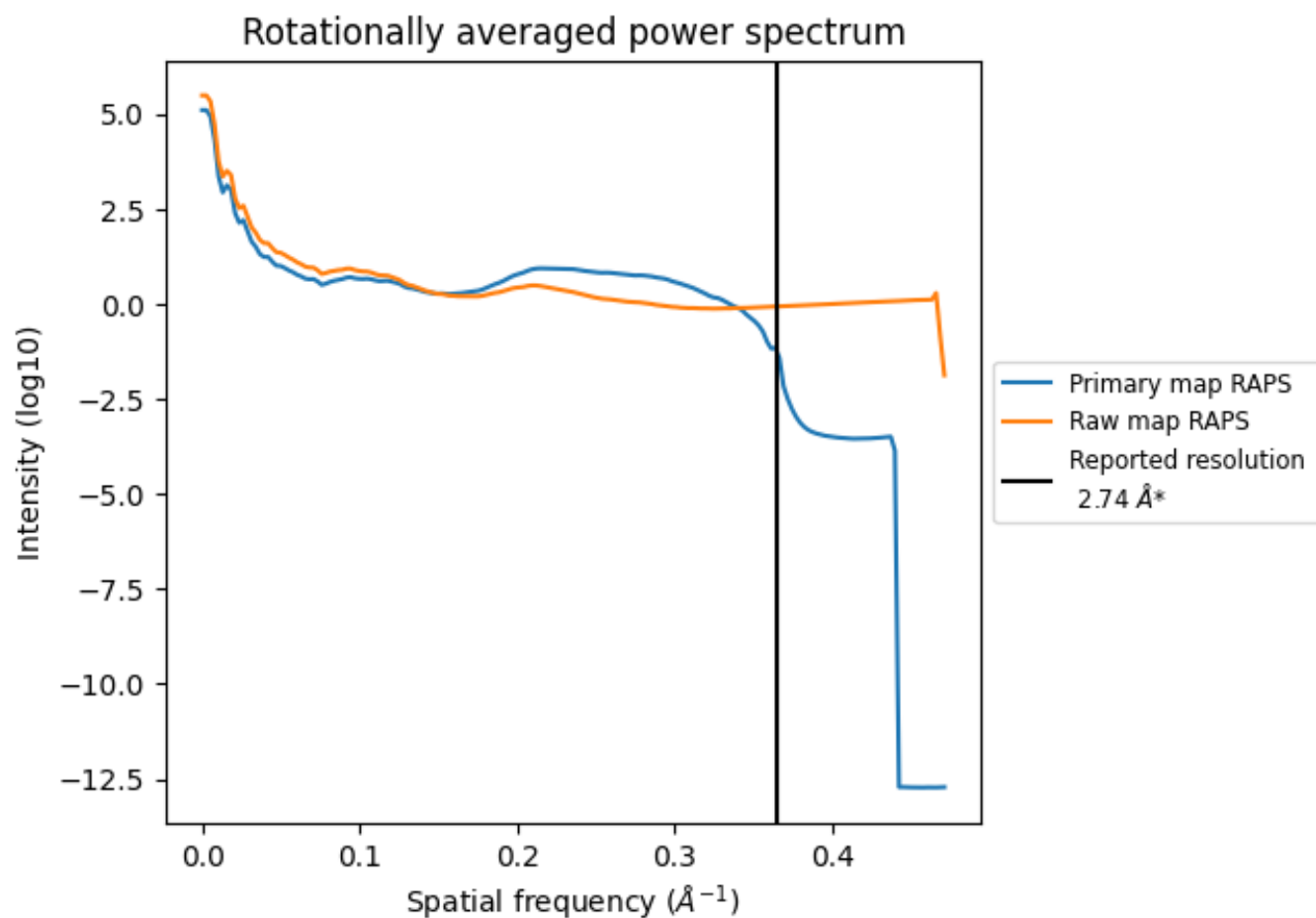
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm³; this corresponds to an approximate mass of 192 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 ⓘ

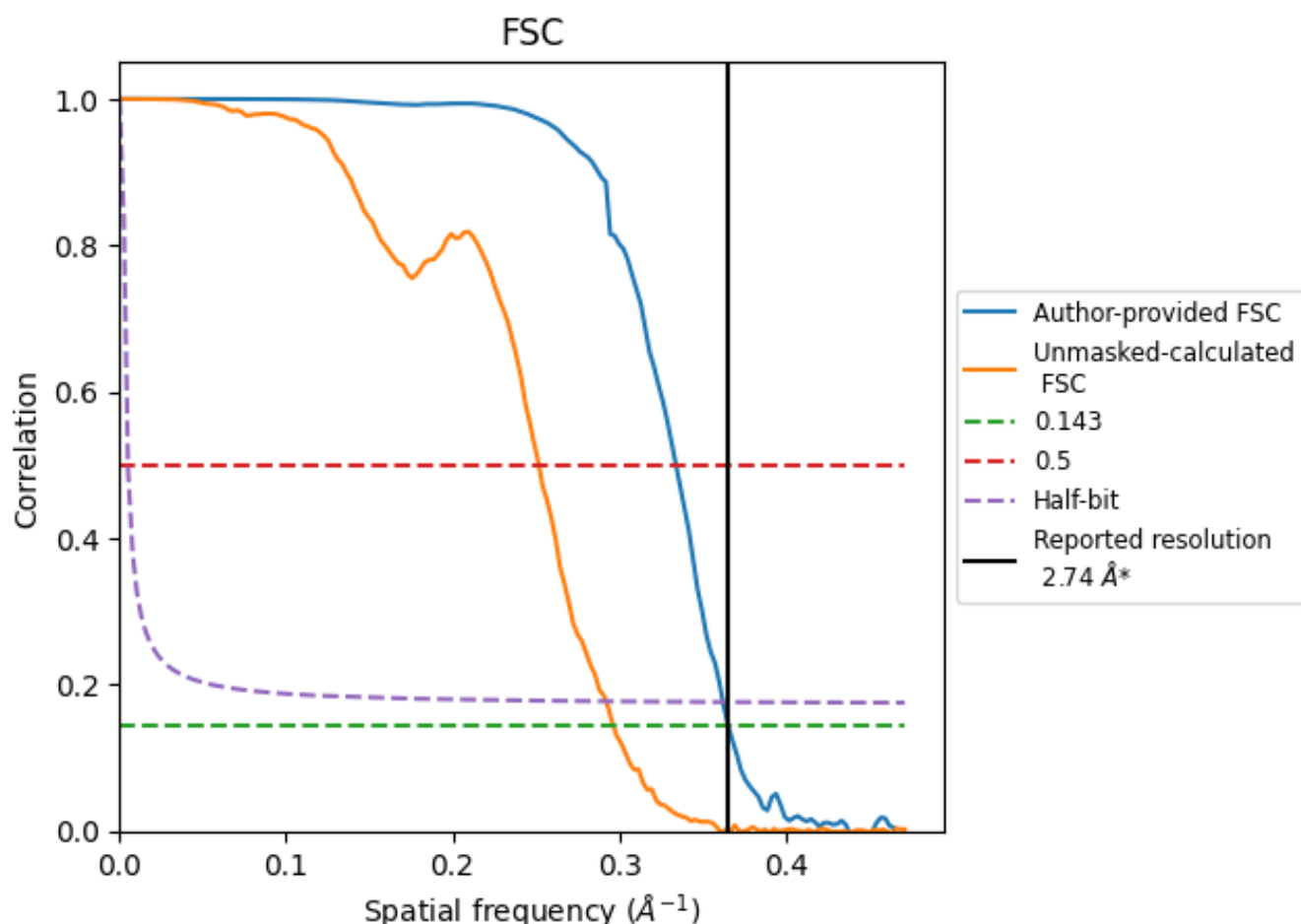


*Reported resolution corresponds to spatial frequency of 0.365 \AA^{-1}

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 0.365 \AA^{-1}

8.2 Resolution estimates

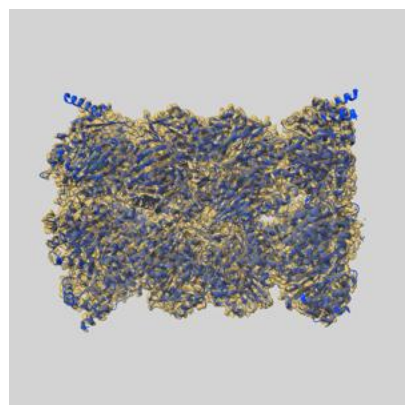
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.74	2.99	2.76
Unmasked-calculated*	3.37	3.97	3.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.37 differs from the reported value 2.74 by more than 10 %

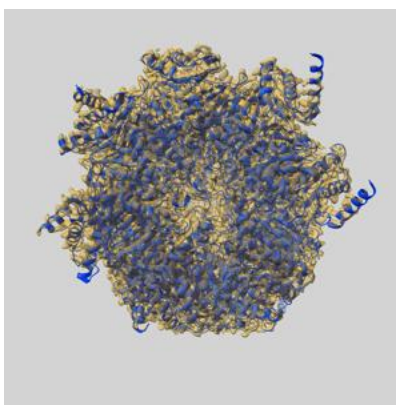
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23502 and PDB model 7LS5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

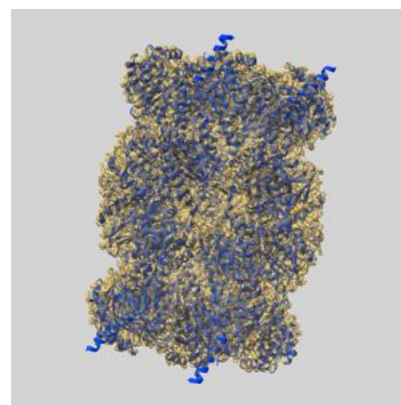
9.1 Map-model overlay [i](#)



X



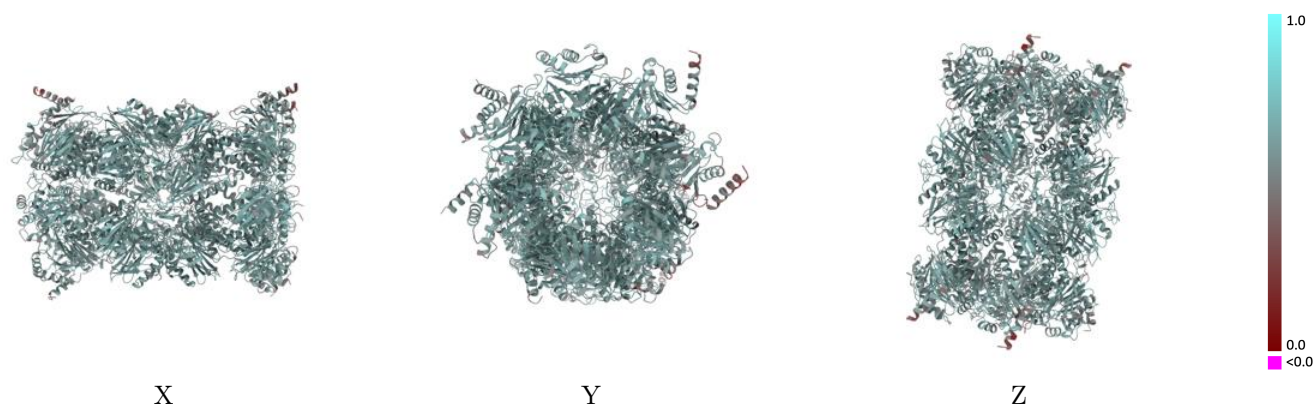
Y



Z

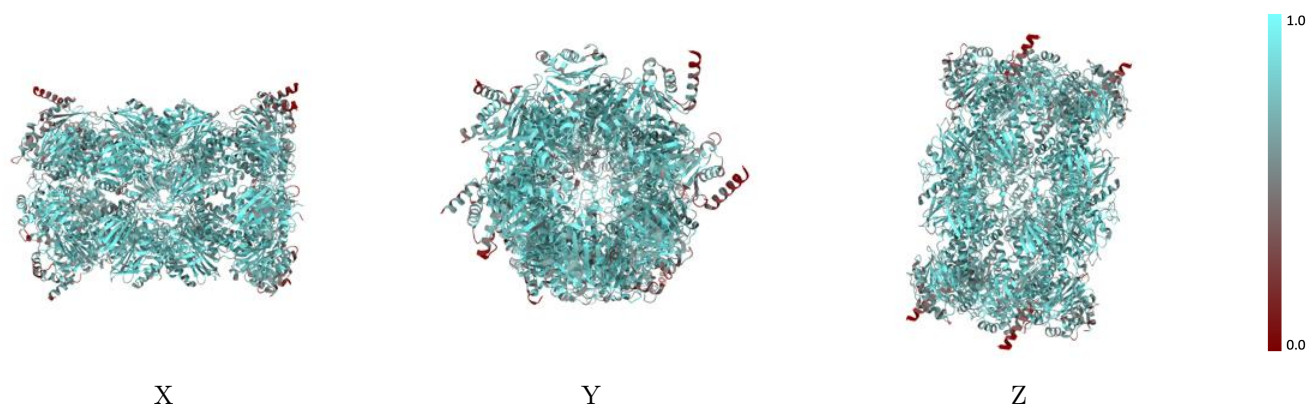
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



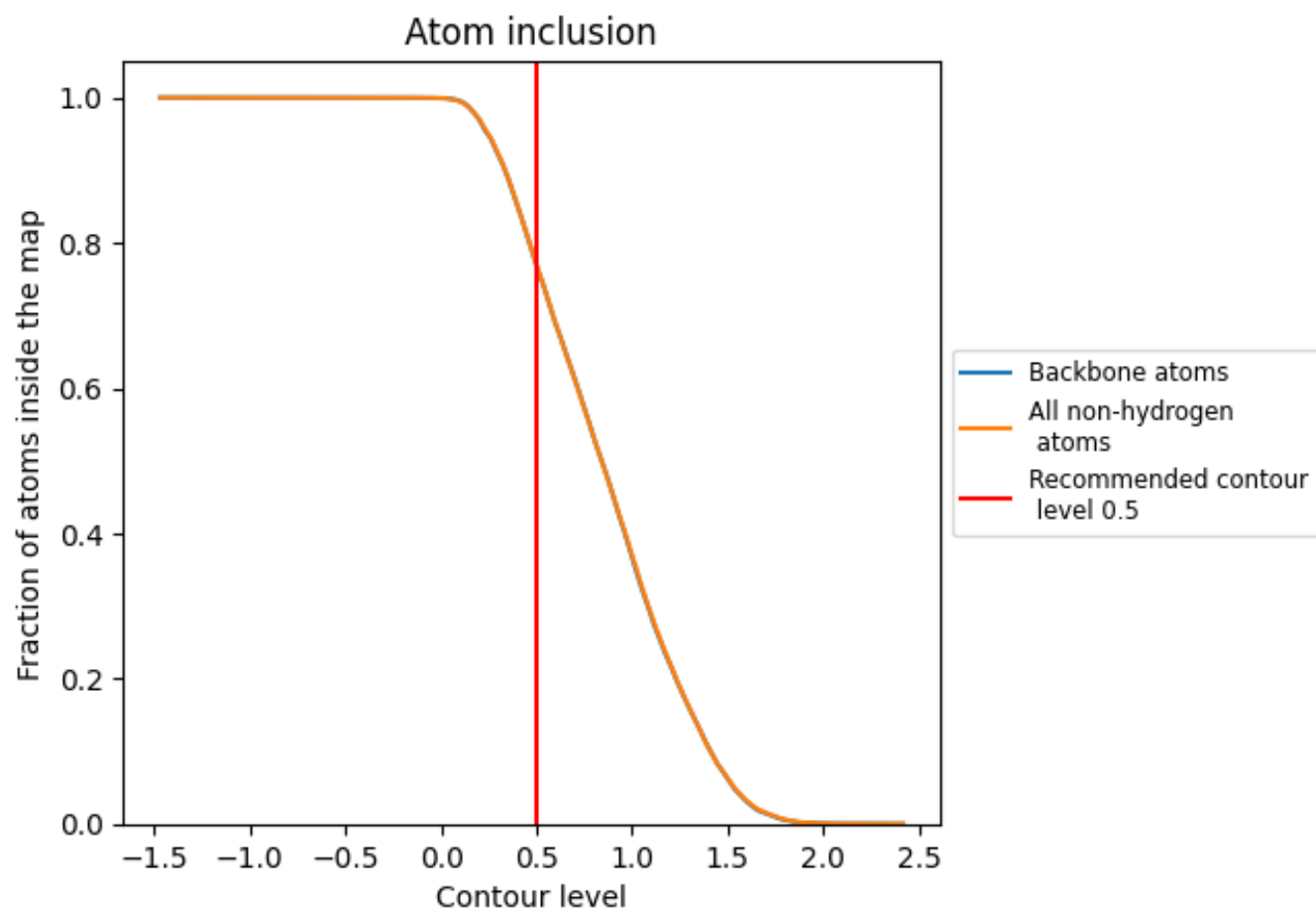
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7700	 0.5980
1	 0.8002	 0.6050
2	 0.8237	 0.6140
A	 0.7574	 0.5940
B	 0.7618	 0.5950
C	 0.7351	 0.5870
D	 0.6745	 0.5600
E	 0.6933	 0.5810
F	 0.7700	 0.6010
G	 0.7674	 0.5970
H	 0.8340	 0.6090
I	 0.8049	 0.6100
J	 0.8239	 0.6130
K	 0.8151	 0.6090
L	 0.8328	 0.6090
M	 0.7973	 0.6030
N	 0.8243	 0.6140
O	 0.7642	 0.5980
P	 0.7706	 0.5960
Q	 0.7284	 0.5880
R	 0.6770	 0.5590
S	 0.6901	 0.5840
T	 0.7677	 0.6000
U	 0.7669	 0.5960
V	 0.8367	 0.6080
W	 0.8018	 0.6090
X	 0.8271	 0.6110
Y	 0.8158	 0.6100
Z	 0.8334	 0.6060

