



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:45 AM UTC

PDB ID : 6XMJ / pdb_00006xmj
EMDB ID : EMD-22259
Title : Human 20S proteasome bound to an engineered 11S (PA26) activator
Authors : de la Pena, A.H.; Opoku-Nsiah, K.A.; Williams, S.K.; Chopra, N.; Sali, A.;
Gestwicki, J.E.; Lander, G.C.
Deposited on : 2020-06-30
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

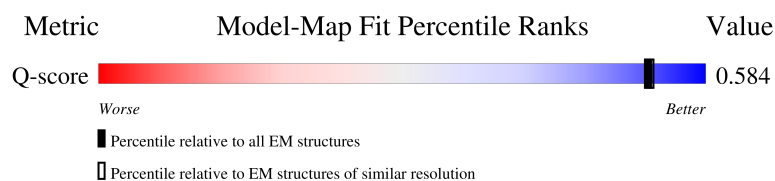
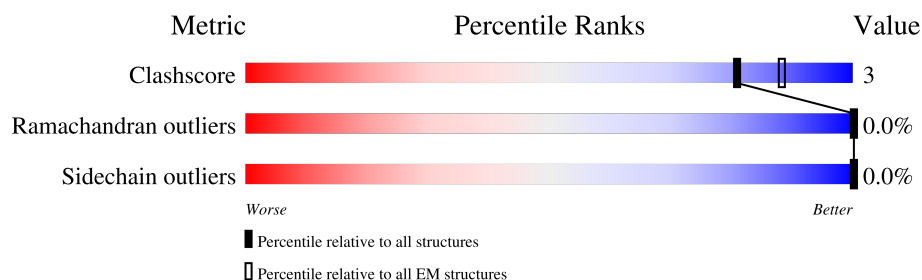
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	244	8% 91% 6% .
2	B	233	5% 92% 5% .
3	C	250	17% 94% . .
4	D	243	21% 95% .

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Mol	Chain	Length	Quality of chain
5	E	234	
6	F	238	
7	G	245	
8	H	202	
9	I	220	
10	J	204	
11	K	199	
12	L	201	
13	M	213	
14	N	217	
15	O	228	
15	P	228	
15	Q	228	
15	R	228	
15	S	228	
15	T	228	
15	U	228	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 34917 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	237	Total	C	N	O	S	0	0
			1810	1152	302	343	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	227	Total	C	N	O	S	0	0
			1666	1056	281	324	5		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	244	Total	C	N	O	S	0	0
			1854	1171	317	358	8		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	242	Total	C	N	O	S	0	0
			1724	1068	314	337	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	225	Total	C	N	O	S	0	0
			1707	1075	281	340	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1854	1177	314	352	11		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	213	Total	C	N	O	S	0	0
			1637	1033	281	313	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	217	Total	C	N	O	S	0	0
			1676	1057	287	320	12		

- Molecule 15 is a protein called Proteasome activator protein PA26.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	207	Total	C	N	O	S	0	0
			1615	1020	282	308	5		
15	P	207	Total	C	N	O	S	0	0
			1618	1021	283	309	5		
15	Q	204	Total	C	N	O	S	0	0
			1579	995	279	300	5		
15	R	207	Total	C	N	O	S	0	0
			1618	1021	283	309	5		
15	S	207	Total	C	N	O	S	0	0
			1618	1021	283	309	5		
15	T	207	Total	C	N	O	S	0	0
			1618	1021	283	309	5		
15	U	207	Total	C	N	O	S	0	0
			1618	1021	283	309	5		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	49	VAL	THR	engineered mutation	UNP Q9U8G2
O	102	ALA	GLU	engineered mutation	UNP Q9U8G2
O	226	ASN	SER	engineered mutation	UNP Q9U8G2
O	227	LEU	-	expression tag	UNP Q9U8G2
O	228	SER	-	expression tag	UNP Q9U8G2
O	229	TYR	-	expression tag	UNP Q9U8G2
O	230	TYR	-	expression tag	UNP Q9U8G2
O	231	THR	-	expression tag	UNP Q9U8G2
P	49	VAL	THR	engineered mutation	UNP Q9U8G2
P	102	ALA	GLU	engineered mutation	UNP Q9U8G2
P	226	ASN	SER	engineered mutation	UNP Q9U8G2
P	227	LEU	-	expression tag	UNP Q9U8G2
P	228	SER	-	expression tag	UNP Q9U8G2
P	229	TYR	-	expression tag	UNP Q9U8G2
P	230	TYR	-	expression tag	UNP Q9U8G2
P	231	THR	-	expression tag	UNP Q9U8G2
Q	49	VAL	THR	engineered mutation	UNP Q9U8G2
Q	102	ALA	GLU	engineered mutation	UNP Q9U8G2
Q	226	ASN	SER	engineered mutation	UNP Q9U8G2

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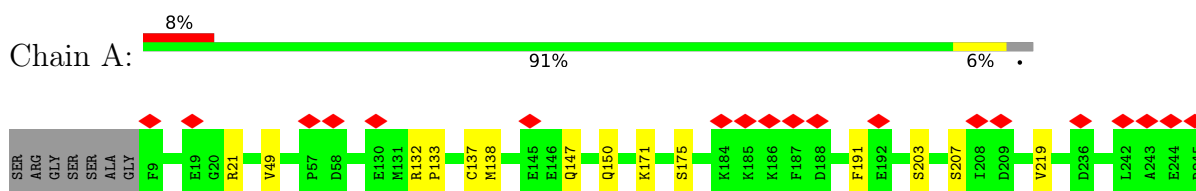
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Chain	Residue	Modelled	Actual	Comment	Reference
Q	227	LEU	-	expression tag	UNP Q9U8G2
Q	228	SER	-	expression tag	UNP Q9U8G2
Q	229	TYR	-	expression tag	UNP Q9U8G2
Q	230	TYR	-	expression tag	UNP Q9U8G2
Q	231	THR	-	expression tag	UNP Q9U8G2
R	49	VAL	THR	engineered mutation	UNP Q9U8G2
R	102	ALA	GLU	engineered mutation	UNP Q9U8G2
R	226	ASN	SER	engineered mutation	UNP Q9U8G2
R	227	LEU	-	expression tag	UNP Q9U8G2
R	228	SER	-	expression tag	UNP Q9U8G2
R	229	TYR	-	expression tag	UNP Q9U8G2
R	230	TYR	-	expression tag	UNP Q9U8G2
R	231	THR	-	expression tag	UNP Q9U8G2
S	49	VAL	THR	engineered mutation	UNP Q9U8G2
S	102	ALA	GLU	engineered mutation	UNP Q9U8G2
S	226	ASN	SER	engineered mutation	UNP Q9U8G2
S	227	LEU	-	expression tag	UNP Q9U8G2
S	228	SER	-	expression tag	UNP Q9U8G2
S	229	TYR	-	expression tag	UNP Q9U8G2
S	230	TYR	-	expression tag	UNP Q9U8G2
S	231	THR	-	expression tag	UNP Q9U8G2
T	49	VAL	THR	engineered mutation	UNP Q9U8G2
T	102	ALA	GLU	engineered mutation	UNP Q9U8G2
T	226	ASN	SER	engineered mutation	UNP Q9U8G2
T	227	LEU	-	expression tag	UNP Q9U8G2
T	228	SER	-	expression tag	UNP Q9U8G2
T	229	TYR	-	expression tag	UNP Q9U8G2
T	230	TYR	-	expression tag	UNP Q9U8G2
T	231	THR	-	expression tag	UNP Q9U8G2
U	49	VAL	THR	engineered mutation	UNP Q9U8G2
U	102	ALA	GLU	engineered mutation	UNP Q9U8G2
U	226	ASN	SER	engineered mutation	UNP Q9U8G2
U	227	LEU	-	expression tag	UNP Q9U8G2
U	228	SER	-	expression tag	UNP Q9U8G2
U	229	TYR	-	expression tag	UNP Q9U8G2
U	230	TYR	-	expression tag	UNP Q9U8G2
U	231	THR	-	expression tag	UNP Q9U8G2

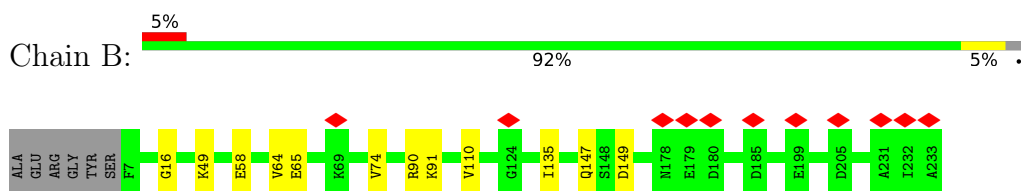
3 Residue-property plots

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

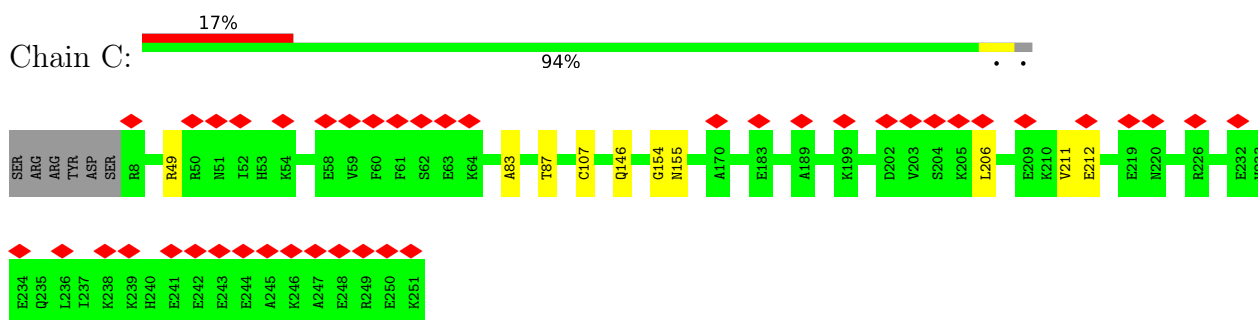
- Molecule 1: Proteasome subunit alpha type-6



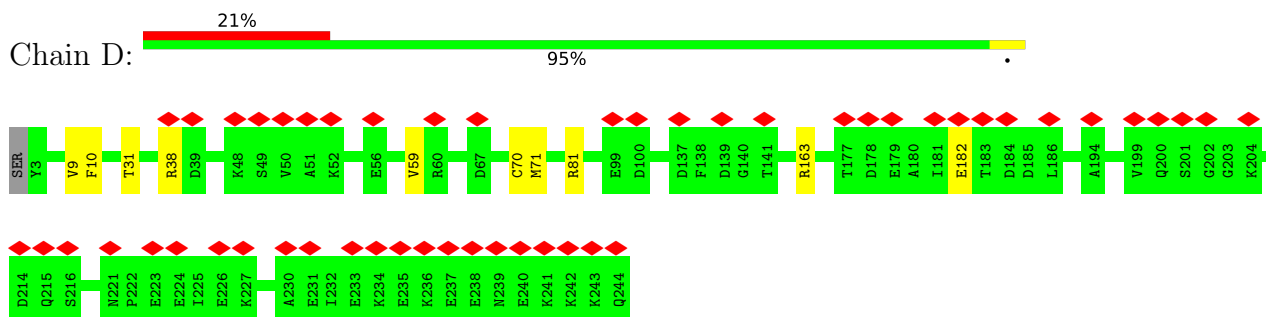
- Molecule 2: Proteasome subunit alpha type-2



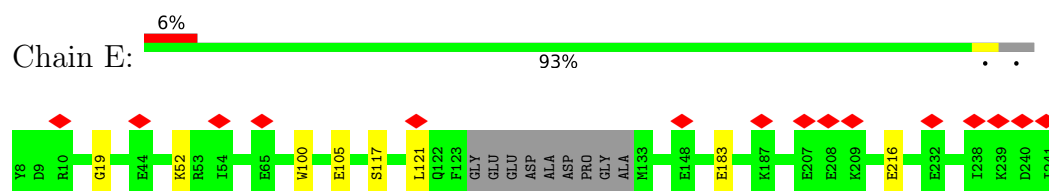
- Molecule 3: Proteasome subunit alpha type-4



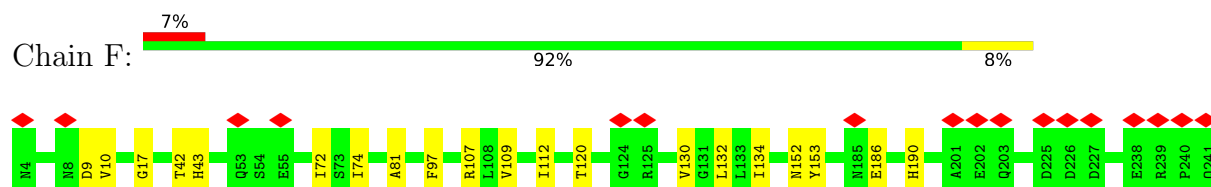
- Molecule 4: Proteasome subunit alpha type-7



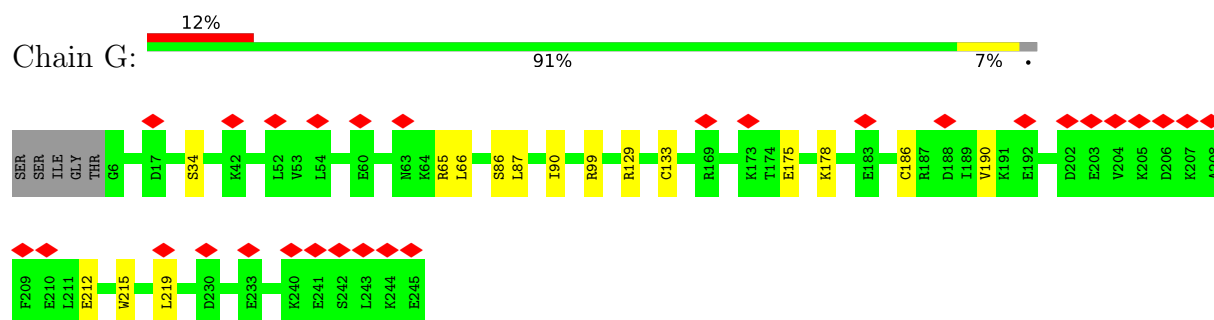
- Molecule 5: Proteasome subunit alpha type-5



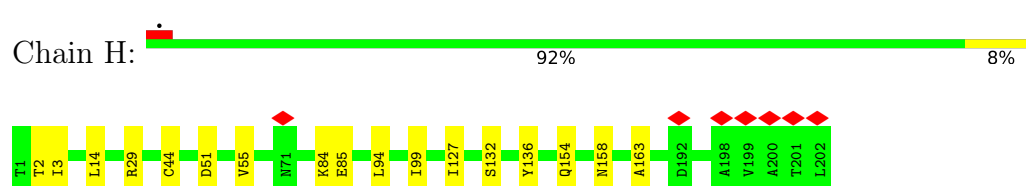
- Molecule 6: Proteasome subunit alpha type-1



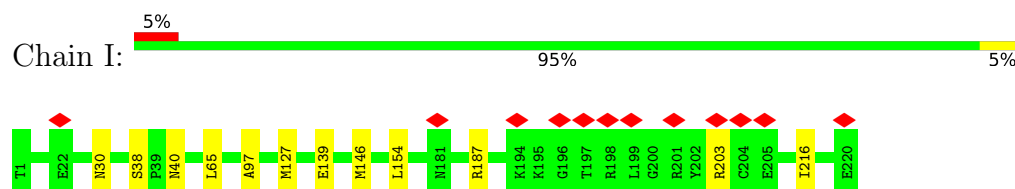
- Molecule 7: Proteasome subunit alpha type-3



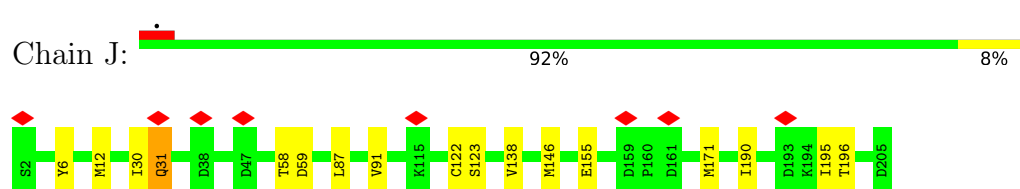
- Molecule 8: Proteasome subunit beta type-6



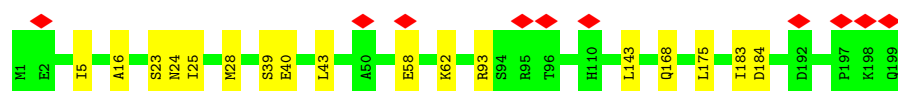
- Molecule 9: Proteasome subunit beta type-7



- Molecule 10: Proteasome subunit beta type-3



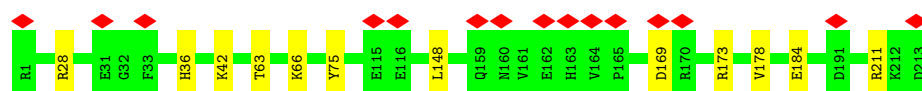
- Molecule 11: Proteasome subunit beta type-2



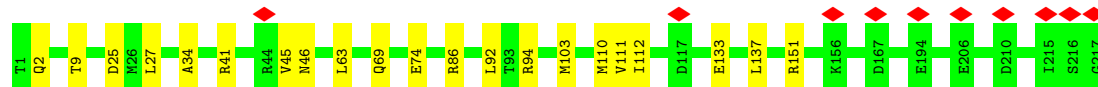
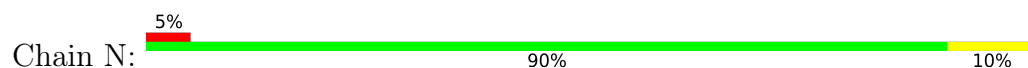
- Molecule 12: Proteasome subunit beta type-5



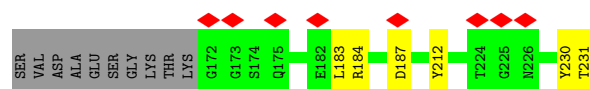
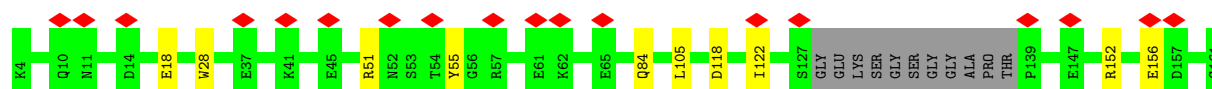
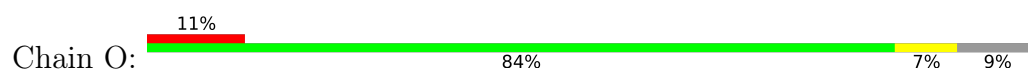
- Molecule 13: Proteasome subunit beta type-1



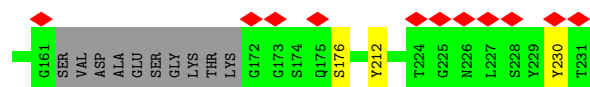
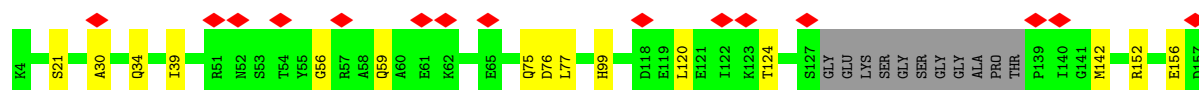
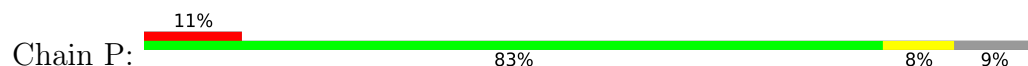
- Molecule 14: Proteasome subunit beta type-4



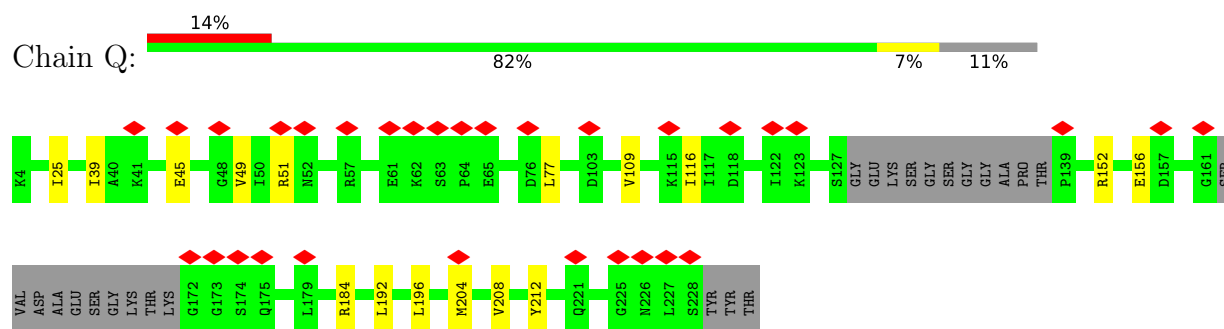
- Molecule 15: Proteasome activator protein PA26



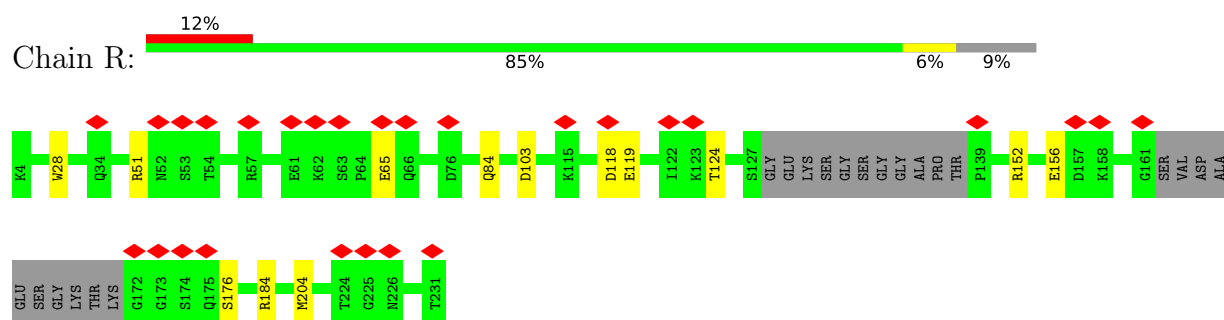
- Molecule 15: Proteasome activator protein PA26



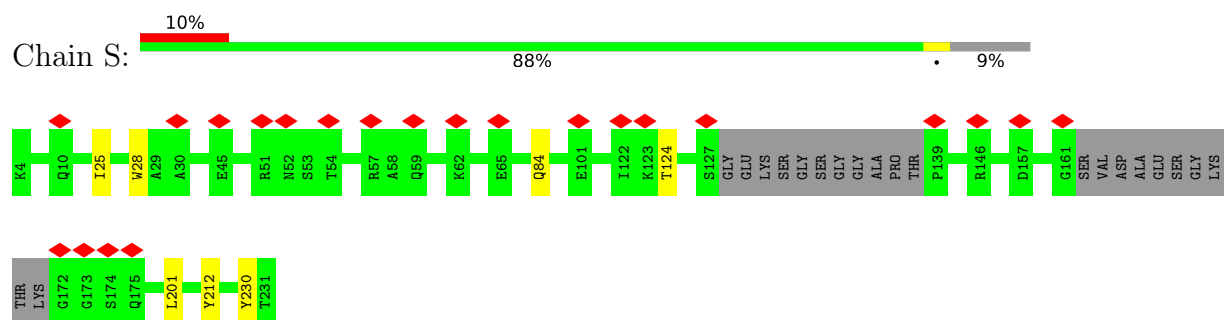
- Molecule 15: Proteasome activator protein PA26



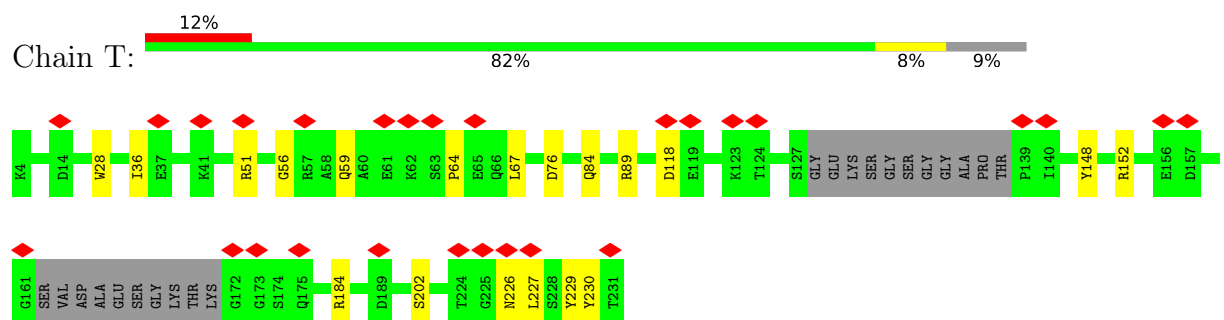
- Molecule 15: Proteasome activator protein PA26



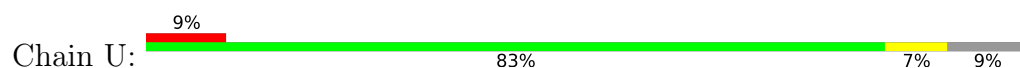
- Molecule 15: Proteasome activator protein PA26

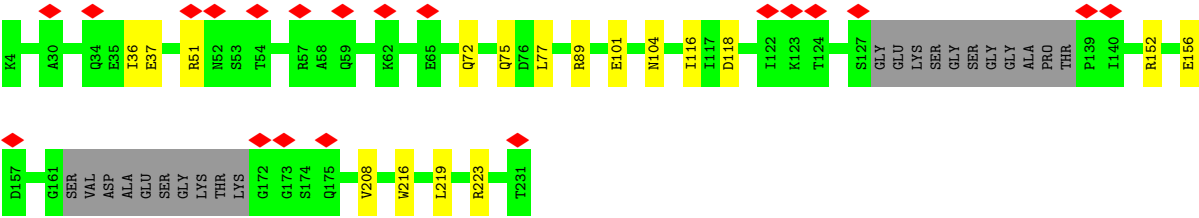


- Molecule 15: Proteasome activator protein PA26



- Molecule 15: Proteasome activator protein PA26





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	234960	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed by Relion during reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.379	Depositor
Minimum map value	-0.218	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	263.68, 263.68, 263.68	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.03, 1.03, 1.03	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	0.19	0/1843	0.42	0/2502
2	B	0.19	0/1700	0.40	0/2315
3	C	0.23	0/1883	0.45	0/2550
4	D	0.22	0/1748	0.47	0/2385
5	E	0.24	0/1733	0.46	0/2345
6	F	0.21	0/1885	0.42	0/2552
7	G	0.21	0/1889	0.42	0/2549
8	H	0.22	0/1535	0.43	0/2078
9	I	0.21	0/1670	0.45	0/2265
10	J	0.26	0/1614	0.50	0/2177
11	K	0.21	0/1603	0.43	0/2174
12	L	0.22	0/1579	0.45	0/2134
13	M	0.19	0/1667	0.39	0/2249
14	N	0.21	0/1709	0.45	0/2317
15	O	0.19	0/1637	0.40	0/2212
15	P	0.20	0/1640	0.43	0/2216
15	Q	0.19	0/1599	0.43	0/2161
15	R	0.19	0/1640	0.43	0/2216
15	S	0.20	0/1640	0.43	0/2216
15	T	0.23	0/1640	0.44	0/2216
15	U	0.20	0/1640	0.43	0/2216
All	All	0.21	0/35494	0.43	0/48045

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	1810	0	1780	9	0
2	B	1666	0	1558	8	0
3	C	1854	0	1798	6	0
4	D	1724	0	1531	6	0
5	E	1707	0	1670	9	0
6	F	1850	0	1822	14	0
7	G	1854	0	1811	10	0
8	H	1509	0	1473	12	0
9	I	1643	0	1644	8	0
10	J	1585	0	1598	12	0
11	K	1570	0	1547	10	0
12	L	1548	0	1499	8	0
13	M	1637	0	1607	8	0
14	N	1676	0	1633	14	0
15	O	1615	0	1643	10	0
15	P	1618	0	1647	13	0
15	Q	1579	0	1606	13	0
15	R	1618	0	1647	8	0
15	S	1618	0	1647	7	0
15	T	1618	0	1647	12	0
15	U	1618	0	1647	10	0
All	All	34917	0	34455	178	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 3.

All (178) 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)
5:E:117:SER:O	5:E:121:LEU:HD13	1.77	0.85
15:P:30:ALA:O	15:P:34:GLN:NE2	2.20	0.74
15:Q:152:ARG:NH1	15:Q:156:GLU:OE2	2.21	0.74
15:P:152:ARG:NH1	15:P:156:GLU:OE2	2.21	0.73
12:L:61:ARG:NH1	12:L:62:GLN:OE1	2.22	0.72
9:I:203:ARG:NH1	10:J:155:GLU:OE1	2.22	0.72
11:K:58:GLU:OE1	11:K:62:LYS:NZ	2.24	0.71
6:F:120:THR:O	7:G:129:ARG:NH1	2.26	0.69
4:D:38:ARG:NH2	4:D:182:GLU:O	2.25	0.69
12:L:36:GLU:OE2	12:L:186:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:152:ARG:NH1	15:R:156:GLU:OE2	2.28	0.67
14:N:9:THR:O	14:N:41:ARG:NH2	2.29	0.65
12:L:9:ARG:NH2	12:L:146:ASP:OD1	2.29	0.65
9:I:30:ASN:O	9:I:187:ARG:NH2	2.30	0.65
6:F:97:PHE:O	13:M:66:LYS:NZ	2.24	0.64
14:N:25:ASP:OD1	14:N:41:ARG:NH1	2.31	0.64
11:K:168:GLN:NE2	11:K:175:LEU:O	2.31	0.64
7:G:34:SER:OG	7:G:65:ARG:NH1	2.31	0.63
3:C:154:GLY:O	4:D:81:ARG:NH2	2.30	0.63
7:G:186:CYS:O	7:G:190:VAL:HG23	1.99	0.63
3:C:49:ARG:NH2	3:C:212:GLU:OE1	2.31	0.62
8:H:3:ILE:HD12	8:H:99:ILE:HD12	1.79	0.62
1:A:147:GLN:OE1	1:A:150:GLN:NE2	2.31	0.62
15:U:152:ARG:NH1	15:U:156:GLU:OE2	2.34	0.61
5:E:52:LYS:NZ	5:E:216:GLU:OE2	2.33	0.61
10:J:6:TYR:CE1	10:J:31:GLN:HG3	2.36	0.60
10:J:87:LEU:O	10:J:91:VAL:HG23	2.02	0.60
3:C:107:CYS:HB2	3:C:146:GLN:NE2	2.18	0.59
11:K:5:ILE:CG2	11:K:16:ALA:HB3	2.31	0.59
1:A:49:VAL:HG22	1:A:219:VAL:HG23	1.86	0.58
15:P:56:GLY:N	15:P:59:GLN:OE1	2.36	0.58
8:H:84:LYS:NZ	8:H:85:GLU:OE2	2.37	0.58
14:N:2:GLN:NE2	14:N:103:MET:O	2.37	0.58
15:T:148:TYR:OH	15:T:152:ARG:NH1	2.36	0.58
13:M:28:ARG:O	13:M:42:LYS:NZ	2.36	0.58
15:U:116:ILE:HG22	15:U:208:VAL:HG22	1.85	0.57
5:E:121:LEU:HD12	5:E:121:LEU:N	2.19	0.57
10:J:58:THR:HG23	10:J:59:ASP:N	2.18	0.57
1:A:132:ARG:NH1	1:A:133:PRO:O	2.37	0.57
11:K:5:ILE:HD11	11:K:143:LEU:HD11	1.87	0.57
4:D:9:VAL:HG23	4:D:10:PHE:H	1.70	0.57
10:J:30:ILE:O	10:J:31:GLN:C	2.47	0.57
10:J:122:CYS:SG	10:J:123:SER:N	2.78	0.57
13:M:169:ASP:OD2	13:M:173:ARG:NH1	2.36	0.57
15:U:36:ILE:HG12	15:U:77:LEU:HD21	1.86	0.57
15:U:37:GLU:N	15:U:37:GLU:OE1	2.37	0.56
2:B:64:VAL:HG22	2:B:74:VAL:HG12	1.86	0.56
4:D:70:CYS:SG	4:D:71:MET:N	2.79	0.56
5:E:105:GLU:OE2	13:M:75:TYR:OH	2.22	0.55
2:B:16:GLY:O	15:S:230:TYR:OH	2.23	0.55
15:T:51:ARG:O	15:T:184:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:25:ILE:HG13	15:Q:212:TYR:CD2	2.41	0.55
15:Q:116:ILE:HG22	15:Q:208:VAL:HG22	1.88	0.55
6:F:109:VAL:HA	6:F:112:ILE:HD12	1.89	0.55
15:O:152:ARG:NH1	15:O:187:ASP:OD2	2.40	0.55
15:T:229:TYR:CE1	15:T:230:TYR:CE2	2.94	0.55
5:E:117:SER:O	5:E:121:LEU:CD1	2.53	0.54
5:E:183:GLU:N	5:E:183:GLU:OE1	2.39	0.54
15:S:124:THR:HG21	15:S:201:LEU:CD1	2.38	0.54
3:C:155:ASN:ND2	15:T:229:TYR:HA	2.23	0.54
6:F:74:ILE:HG22	6:F:132:LEU:HD22	1.89	0.54
15:T:56:GLY:N	15:T:59:GLN:OE1	2.38	0.53
15:T:89:ARG:NH2	15:T:118:ASP:OD1	2.41	0.53
5:E:121:LEU:N	5:E:121:LEU:CD1	2.73	0.52
15:T:76:ASP:OD2	15:U:51:ARG:NH2	2.42	0.52
13:M:184:GLU:OE2	13:M:211:ARG:NH1	2.40	0.52
15:P:142:MET:SD	15:Q:192:LEU:HD21	2.50	0.52
13:M:148:LEU:HD23	13:M:178:VAL:HG12	1.92	0.52
14:N:63:LEU:HD13	14:N:110:MET:HE1	1.92	0.52
15:O:28:TRP:NE1	15:O:84:GLN:OE1	2.41	0.52
2:B:65:GLU:OE1	2:B:90:ARG:NH2	2.41	0.52
11:K:24:ASN:OD1	11:K:25:ILE:N	2.42	0.52
15:O:156:GLU:OE1	15:P:176:SER:OG	2.27	0.52
9:I:216:ILE:HD13	10:J:196:THR:HG23	1.91	0.51
15:Q:51:ARG:O	15:Q:184:ARG:NH2	2.44	0.51
15:T:28:TRP:NE1	15:T:84:GLN:OE1	2.43	0.51
5:E:100:TRP:O	12:L:57:ARG:NH2	2.41	0.51
8:H:127:ILE:HD11	8:H:136:TYR:CD1	2.46	0.51
12:L:130:SER:OG	12:L:167:ASP:OD2	2.28	0.51
7:G:99:ARG:NH1	14:N:69:GLN:OE1	2.44	0.51
11:K:43:LEU:HD12	11:K:183:ILE:HD11	1.93	0.51
1:A:191:PHE:HE1	1:A:219:VAL:HG21	1.76	0.50
6:F:107:ARG:NH1	14:N:74:GLU:OE2	2.43	0.50
13:M:36:HIS:O	14:N:151:ARG:NH2	2.45	0.50
5:E:19:GLY:O	15:O:230:TYR:OH	2.24	0.50
15:O:118:ASP:OD2	15:O:122:ILE:HD12	2.12	0.50
6:F:74:ILE:HD12	15:O:231:THR:HG21	1.92	0.50
15:U:104:ASN:OD1	15:U:223:ARG:NH2	2.43	0.50
15:R:65:GLU:OE1	15:R:65:GLU:N	2.44	0.49
7:G:86:SER:O	7:G:90:ILE:HD12	2.12	0.49
15:U:89:ARG:NH1	15:U:118:ASP:OD1	2.45	0.49
15:R:124:THR:HG21	15:R:204:MET:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:VAL:HG22	2:B:74:VAL:CG1	2.43	0.49
2:B:110:VAL:HG22	2:B:135:ILE:HD13	1.93	0.49
3:C:83:ALA:O	3:C:87:THR:HG23	2.12	0.49
9:I:38:SER:OG	9:I:40:ASN:OD1	2.25	0.49
15:R:28:TRP:NE1	15:R:84:GLN:OE1	2.46	0.49
8:H:2:THR:HG21	8:H:163:ALA:CB	2.44	0.48
7:G:66:LEU:HD12	7:G:212:GLU:HG2	1.95	0.48
15:P:142:MET:SD	15:Q:196:LEU:HD11	2.53	0.48
15:S:124:THR:CG2	15:S:201:LEU:HD13	2.43	0.48
15:T:64:PRO:HG2	15:T:67:LEU:HD12	1.96	0.48
15:R:118:ASP:OD1	15:R:119:GLU:N	2.47	0.48
6:F:17:GLY:O	15:P:230:TYR:OH	2.28	0.47
14:N:86:ARG:NH1	14:N:133:GLU:OE2	2.47	0.47
14:N:111:VAL:HG13	14:N:137:LEU:HD12	1.96	0.47
15:Q:156:GLU:OE1	15:R:176:SER:OG	2.31	0.47
13:M:63:THR:HG23	14:N:94:ARG:HH12	1.78	0.47
14:N:45:VAL:HG12	14:N:46:ASN:H	1.78	0.47
2:B:147:GLN:NE2	2:B:149:ASP:OD2	2.45	0.47
4:D:31:THR:OG1	4:D:163:ARG:O	2.32	0.47
6:F:186:GLU:O	6:F:190:HIS:ND1	2.44	0.47
15:U:216:TRP:HA	15:U:219:LEU:HD12	1.95	0.47
11:K:39:SER:OG	11:K:40:GLU:N	2.48	0.47
10:J:138:VAL:HB	10:J:146:MET:HE3	1.96	0.47
11:K:184:ASP:N	11:K:184:ASP:OD1	2.47	0.47
14:N:27:LEU:HD11	14:N:34:ALA:HB1	1.97	0.47
15:P:21:SER:OG	15:P:212:TYR:OH	2.30	0.47
9:I:146:MET:HE1	9:I:154:LEU:HD22	1.97	0.46
15:S:124:THR:HG21	15:S:201:LEU:HD12	1.96	0.46
2:B:91:LYS:HG2	9:I:65:LEU:HD21	1.98	0.46
15:O:18:GLU:OE2	15:O:212:TYR:OH	2.31	0.46
6:F:9:ASP:OD1	6:F:10:VAL:N	2.48	0.46
10:J:12:MET:HE3	10:J:171:MET:SD	2.56	0.46
10:J:58:THR:CG2	10:J:59:ASP:N	2.77	0.46
11:K:23:SER:OG	11:K:28:MET:SD	2.73	0.46
14:N:92:LEU:CD1	14:N:112:ILE:HD11	2.46	0.46
15:Q:45:GLU:O	15:Q:49:VAL:HG23	2.15	0.45
6:F:42:THR:OG1	6:F:43:HIS:ND1	2.45	0.45
12:L:51:ASP:OD2	12:L:51:ASP:N	2.49	0.45
15:P:39:ILE:HD12	15:P:77:LEU:HD13	1.98	0.45
15:U:72:GLN:OE1	15:U:75:GLN:NE2	2.49	0.45
8:H:51:ASP:HB3	8:H:94:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:74:ILE:HG22	6:F:132:LEU:CD2	2.47	0.45
15:S:28:TRP:NE1	15:S:84:GLN:OE1	2.48	0.45
15:P:99:HIS:HB3	15:Q:109:VAL:HG22	1.98	0.45
15:P:120:LEU:O	15:P:124:THR:OG1	2.35	0.45
14:N:92:LEU:HD12	14:N:112:ILE:HD11	2.00	0.44
10:J:59:ASP:OD1	11:K:93:ARG:NH2	2.50	0.44
15:O:55:TYR:HD2	15:O:183:LEU:HD23	1.83	0.44
15:Q:39:ILE:HD12	15:Q:77:LEU:HD22	2.00	0.44
6:F:72:ILE:HG22	6:F:134:ILE:HG12	1.98	0.44
6:F:152:ASN:OD1	6:F:153:TYR:N	2.50	0.44
9:I:97:ALA:HB1	9:I:127:MET:SD	2.58	0.43
8:H:14:LEU:HD23	8:H:44:CYS:SG	2.58	0.43
15:P:75:GLN:HE21	15:Q:192:LEU:HD22	1.82	0.43
15:S:25:ILE:HG13	15:S:212:TYR:CD2	2.54	0.43
1:A:171:LYS:O	1:A:175:SER:OG	2.27	0.43
7:G:87:LEU:HD12	7:G:133:CYS:SG	2.59	0.43
8:H:154:GLN:HG3	8:H:158:ASN:HD21	1.84	0.43
8:H:127:ILE:HD12	8:H:132:SER:HB2	2.01	0.42
15:S:124:THR:HG21	15:S:201:LEU:HD13	2.01	0.42
15:R:51:ARG:O	15:R:184:ARG:NH2	2.52	0.42
3:C:206:LEU:HD21	3:C:211:VAL:HG11	2.01	0.42
2:B:49:LYS:NZ	2:B:58:GLU:O	2.44	0.42
7:G:215:TRP:CZ3	7:G:219:LEU:HD11	2.55	0.42
8:H:2:THR:HG21	8:H:163:ALA:HB3	2.02	0.42
1:A:191:PHE:CE1	1:A:219:VAL:HG21	2.54	0.42
12:L:160:ILE:HG21	12:L:174:VAL:HG13	2.02	0.41
7:G:175:GLU:OE2	7:G:178:LYS:NZ	2.52	0.41
15:P:76:ASP:OD1	15:Q:51:ARG:NH2	2.53	0.41
15:T:36:ILE:HG21	15:T:202:SER:OG	2.21	0.41
15:T:36:ILE:HG21	15:T:202:SER:HG	1.86	0.41
8:H:29:ARG:NH2	9:I:139:GLU:OE1	2.54	0.41
15:O:105:LEU:HD22	15:U:101:GLU:HG3	2.02	0.41
15:T:226:ASN:C	15:T:227:LEU:HD23	2.45	0.41
4:D:59:VAL:HG12	4:D:59:VAL:O	2.21	0.41
1:A:203:SER:O	1:A:207:SER:N	2.48	0.41
6:F:81:ALA:HB2	6:F:130:VAL:HG21	2.02	0.41
10:J:190:ILE:HG22	10:J:195:ILE:HG12	2.03	0.41
15:Q:204:MET:O	15:Q:208:VAL:HG23	2.21	0.41
1:A:137:CYS:SG	1:A:138:MET:N	2.94	0.41
8:H:51:ASP:O	8:H:55:VAL:HG23	2.20	0.41
12:L:137:GLY:O	12:L:141:ARG:NE	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:190:VAL:HG21	7:G:215:TRP:CZ2	2.56	0.40
15:O:51:ARG:O	15:O:184:ARG:NH2	2.54	0.40
1:A:21:ARG:NH1	15:R:103:ASP:OD2	2.54	0.40
8:H:127:ILE:HD11	8:H:136:TYR:CE1	2.56	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	235/244 (96%)	230 (98%)	5 (2%)	0	100	100
2	B	225/233 (97%)	221 (98%)	4 (2%)	0	100	100
3	C	242/250 (97%)	233 (96%)	9 (4%)	0	100	100
4	D	240/243 (99%)	223 (93%)	17 (7%)	0	100	100
5	E	221/234 (94%)	214 (97%)	7 (3%)	0	100	100
6	F	236/238 (99%)	228 (97%)	8 (3%)	0	100	100
7	G	238/245 (97%)	235 (99%)	3 (1%)	0	100	100
8	H	200/202 (99%)	195 (98%)	5 (2%)	0	100	100
9	I	218/220 (99%)	215 (99%)	3 (1%)	0	100	100
10	J	202/204 (99%)	191 (95%)	10 (5%)	1 (0%)	24	60
11	K	197/199 (99%)	189 (96%)	8 (4%)	0	100	100
12	L	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
13	M	211/213 (99%)	209 (99%)	2 (1%)	0	100	100
14	N	215/217 (99%)	204 (95%)	11 (5%)	0	100	100
15	O	201/228 (88%)	195 (97%)	6 (3%)	0	100	100
15	P	201/228 (88%)	195 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	Q	198/228 (87%)	195 (98%)	3 (2%)	0	100	100
15	R	201/228 (88%)	190 (94%)	11 (6%)	0	100	100
15	S	201/228 (88%)	193 (96%)	8 (4%)	0	100	100
15	T	201/228 (88%)	190 (94%)	11 (6%)	0	100	100
15	U	201/228 (88%)	195 (97%)	6 (3%)	0	100	100
All	All	4483/4739 (95%)	4336 (97%)	146 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	31	GLN

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	191/208 (92%)	191 (100%)	0	100	100
2	B	160/190 (84%)	160 (100%)	0	100	100
3	C	186/210 (89%)	186 (100%)	0	100	100
4	D	152/207 (73%)	152 (100%)	0	100	100
5	E	185/196 (94%)	185 (100%)	0	100	100
6	F	198/204 (97%)	198 (100%)	0	100	100
7	G	191/202 (95%)	191 (100%)	0	100	100
8	H	155/157 (99%)	155 (100%)	0	100	100
9	I	177/181 (98%)	177 (100%)	0	100	100
10	J	172/173 (99%)	172 (100%)	0	100	100
11	K	164/170 (96%)	164 (100%)	0	100	100
12	L	153/156 (98%)	152 (99%)	1 (1%)	76	86
13	M	173/178 (97%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	175/179 (98%)	175 (100%)	0	100	100
15	O	171/186 (92%)	171 (100%)	0	100	100
15	P	172/186 (92%)	172 (100%)	0	100	100
15	Q	166/186 (89%)	166 (100%)	0	100	100
15	R	172/186 (92%)	172 (100%)	0	100	100
15	S	172/186 (92%)	172 (100%)	0	100	100
15	T	172/186 (92%)	172 (100%)	0	100	100
15	U	172/186 (92%)	172 (100%)	0	100	100
All	All	3629/3913 (93%)	3628 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	51	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	150	GLN
3	C	146	GLN
5	E	97	GLN
5	E	182	GLN
5	E	224	GLN
5	E	227	HIS
6	F	53	GLN
6	F	86	ASN
7	G	180	GLN
7	G	221	ASN
8	H	77	HIS
8	H	158	ASN
10	J	145	GLN
10	J	169	GLN
11	K	63	ASN
11	K	189	HIS
13	M	77	HIS
14	N	81	HIS
14	N	157	GLN

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Mol	Chain	Res	Type
15	O	10	GLN
15	P	75	GLN
15	P	200	HIS
15	Q	111	HIS
15	R	47	HIS
15	R	52	ASN
15	S	72	GLN
15	T	221	GLN
15	U	75	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

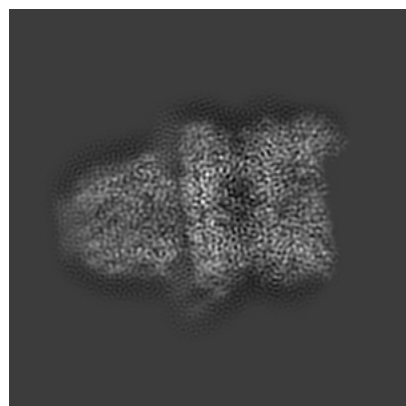
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22259. These allow visual inspection of the internal detail of the map and identification of artifacts.

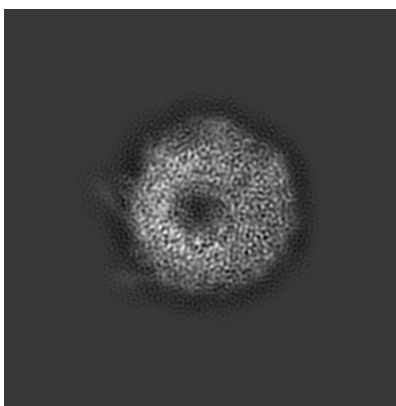
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

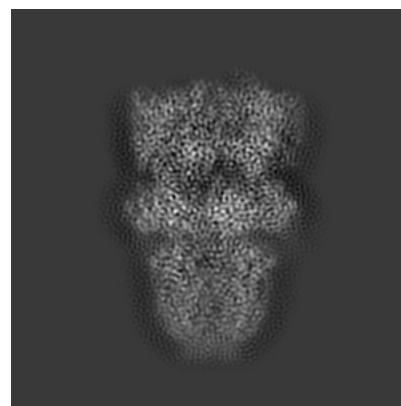
6.1.1 Primary map



X

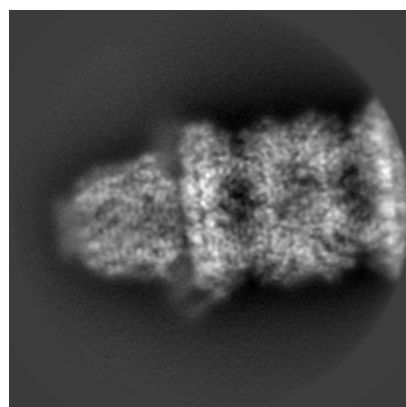


Y

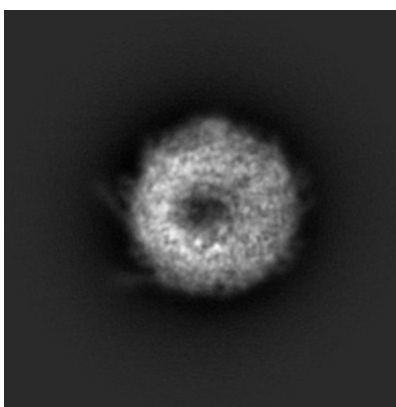


Z

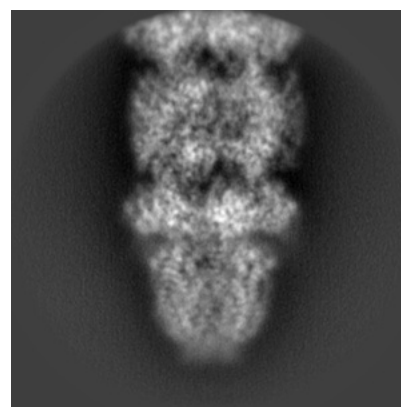
6.1.2 Raw map



X



Y

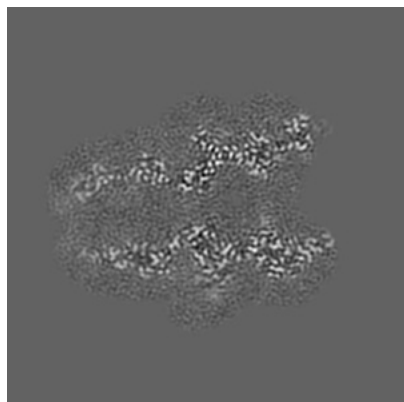


Z

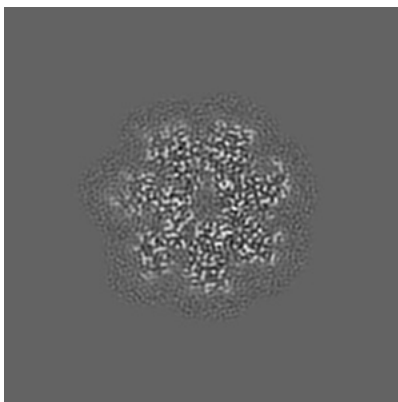
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

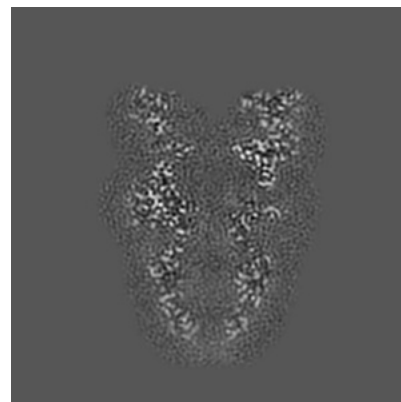
6.2.1 Primary map



X Index: 128

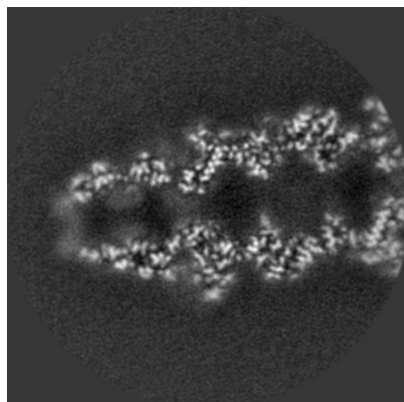


Y Index: 128

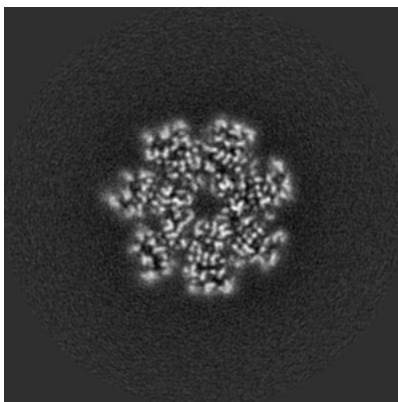


Z Index: 128

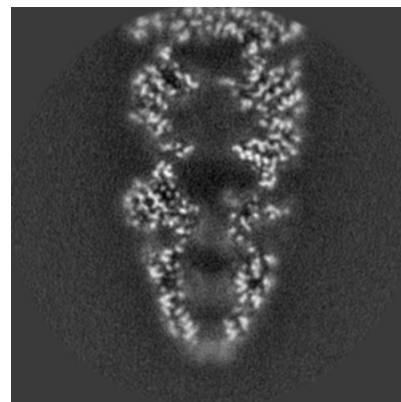
6.2.2 Raw map



X Index: 128



Y Index: 128

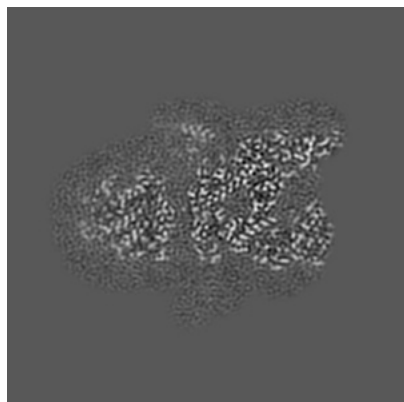


Z Index: 128

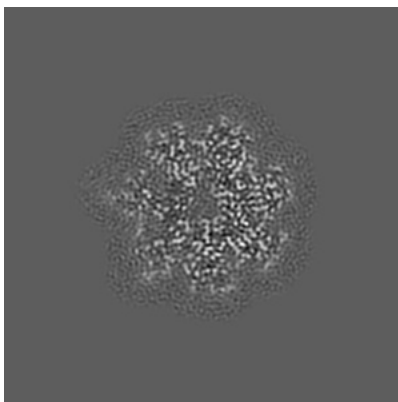
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

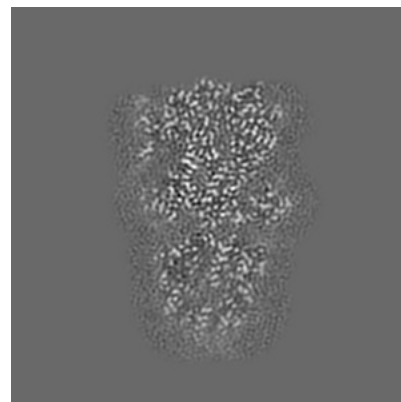
6.3.1 Primary map



X Index: 153

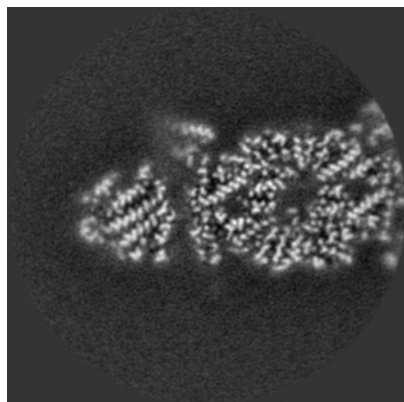


Y Index: 126

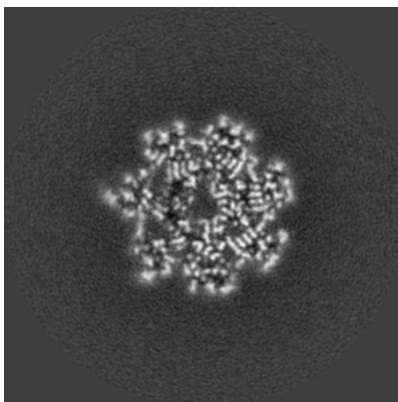


Z Index: 103

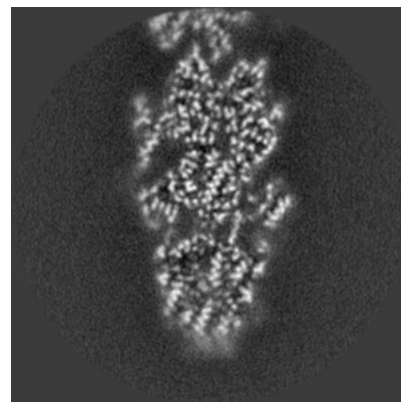
6.3.2 Raw map



X Index: 154



Y Index: 126

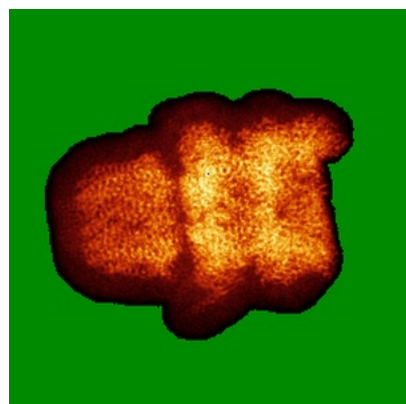


Z Index: 102

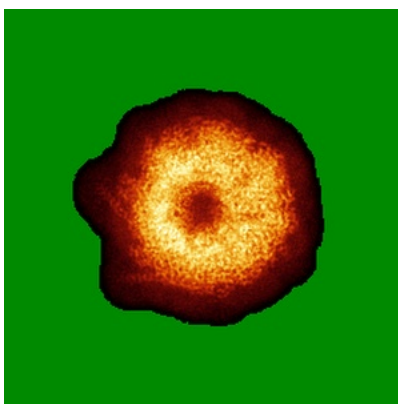
The images above show the largest variance slices of the map in three orthogonal directions.

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

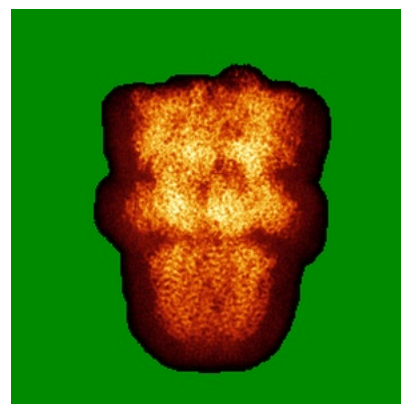
6.4.1 Primary map



X

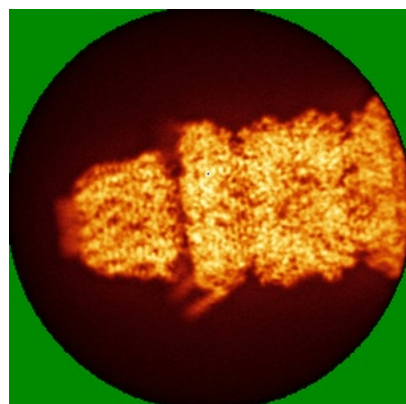


Y

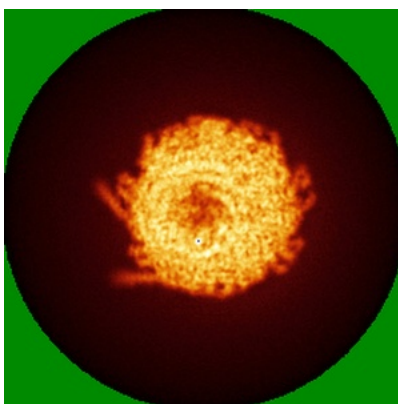


Z

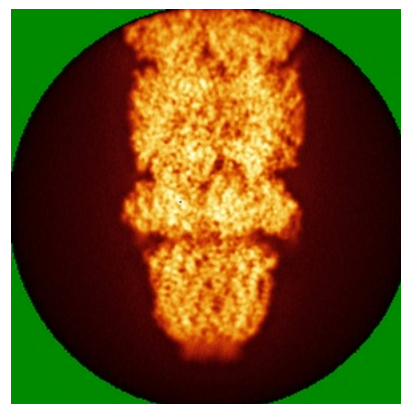
6.4.2 Raw map



X



Y

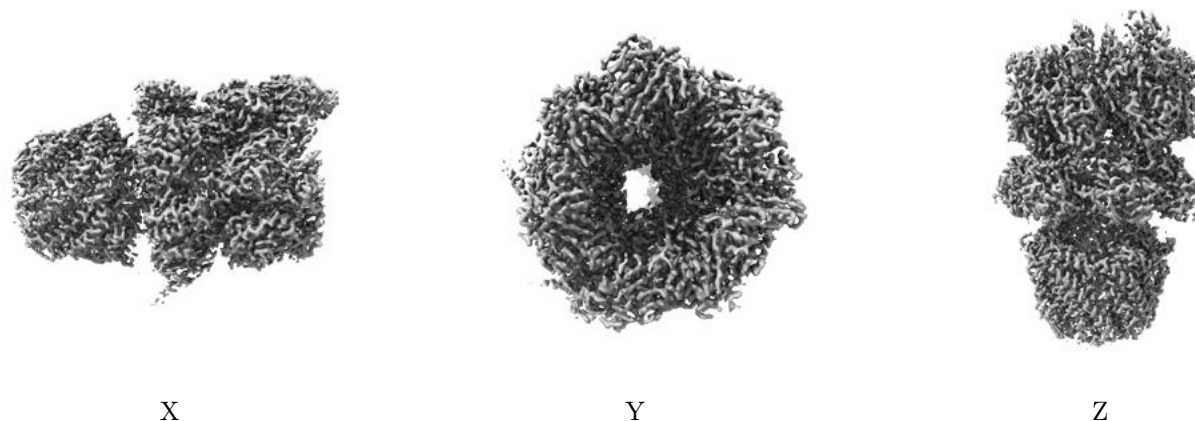


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

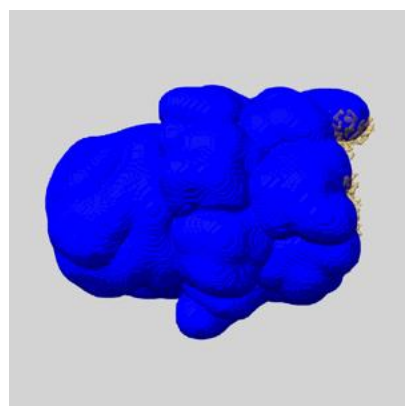
6.6 Mask visualisation [i](#)

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

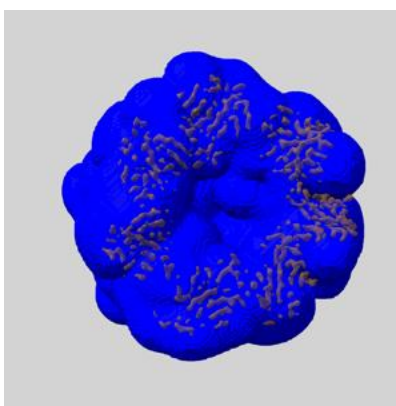
A mask typically either:

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

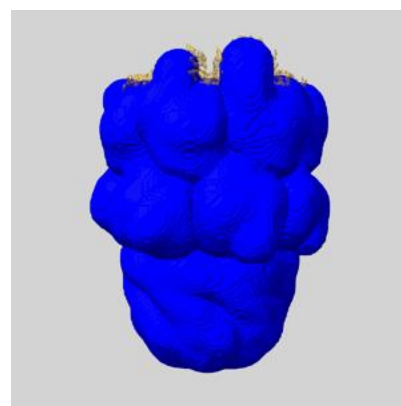
6.6.1 emd_22259_msk_1.map [i](#)



X



Y

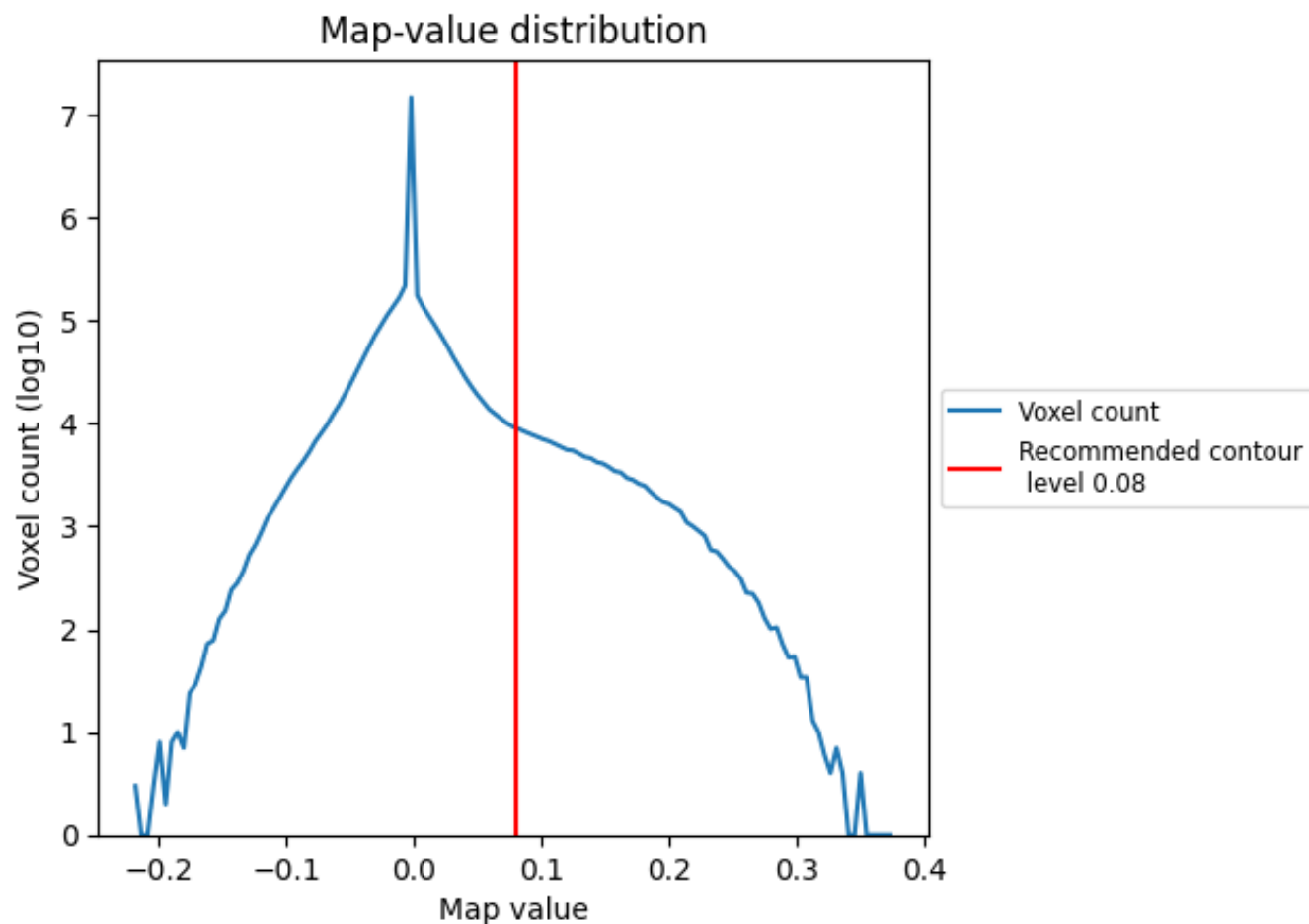


Z

7 Map analysis [i](#)

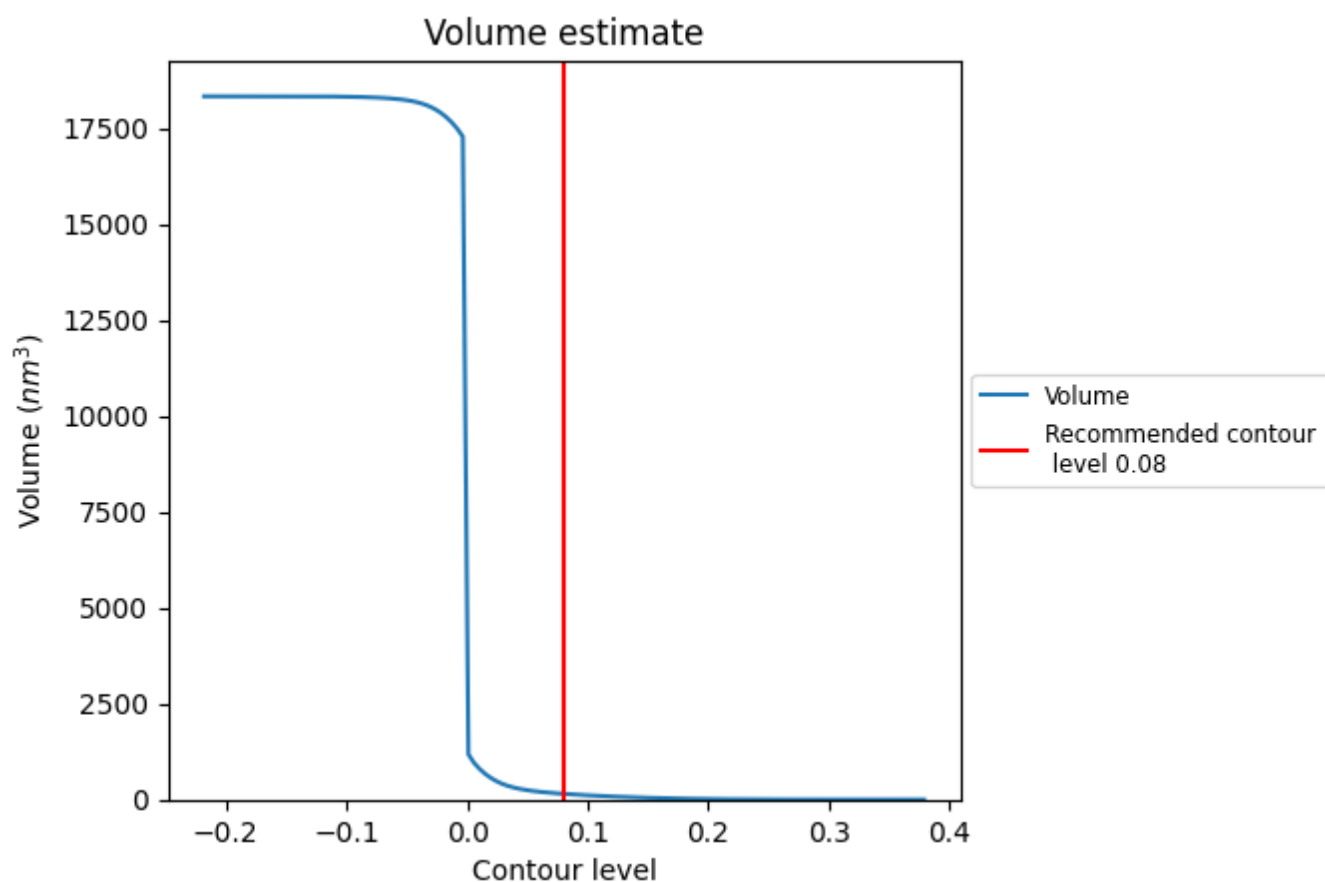
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

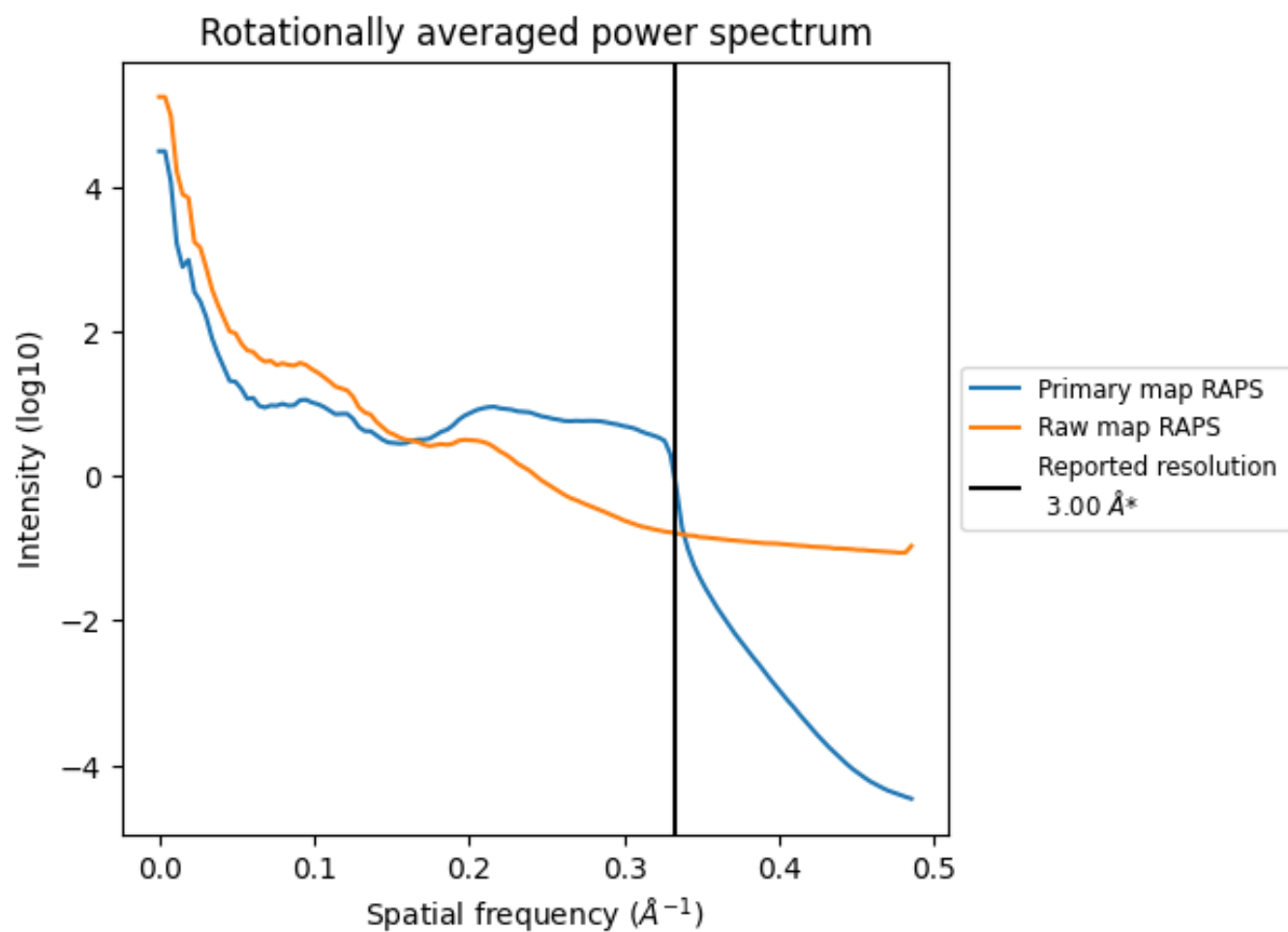
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm³; this corresponds to an approximate mass of 135 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 ⓘ

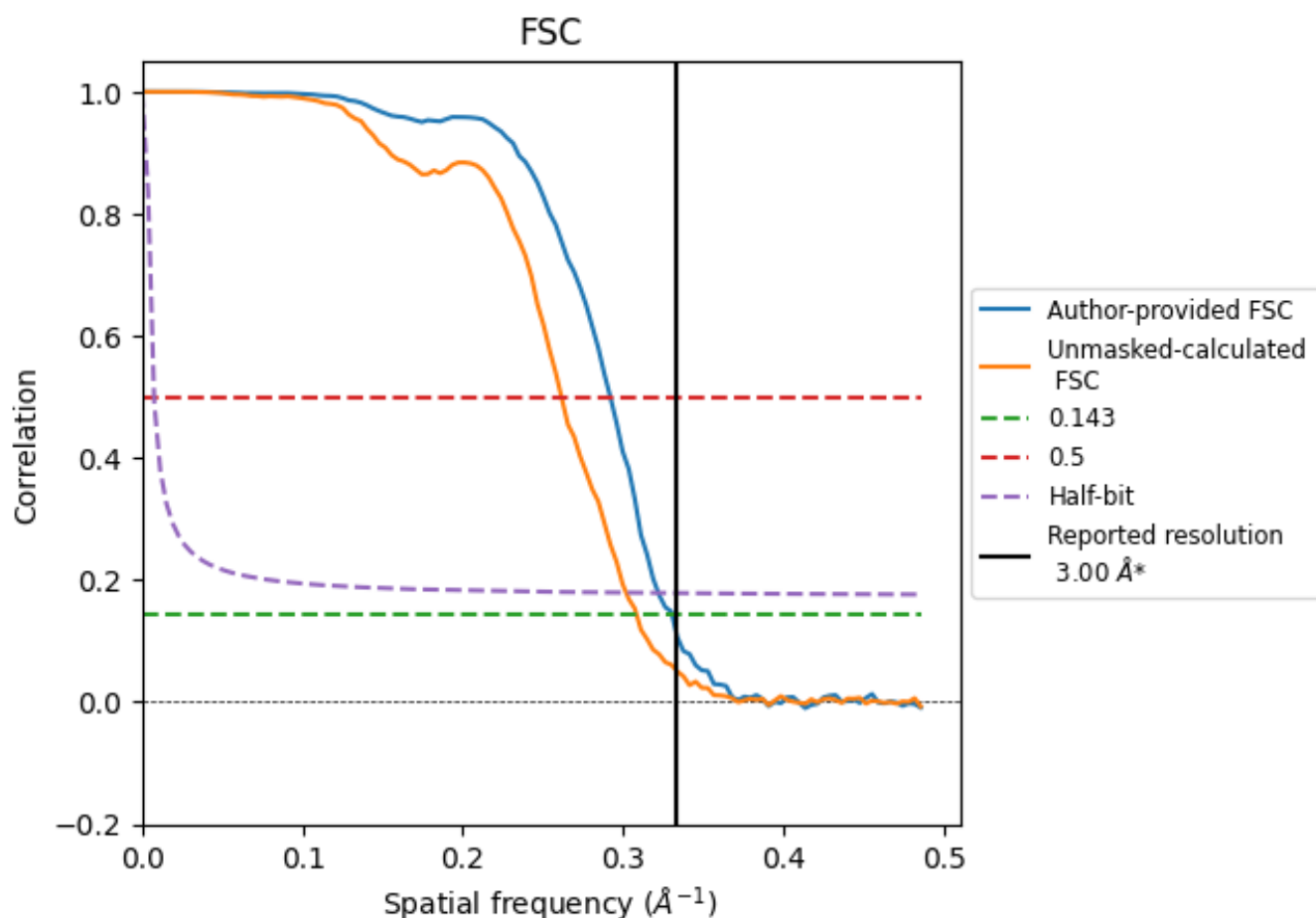


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

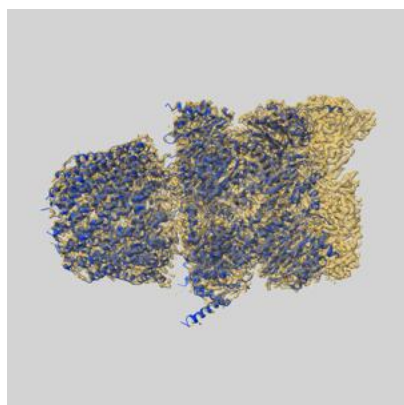
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.43	3.11
Unmasked-calculated*	3.24	3.83	3.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

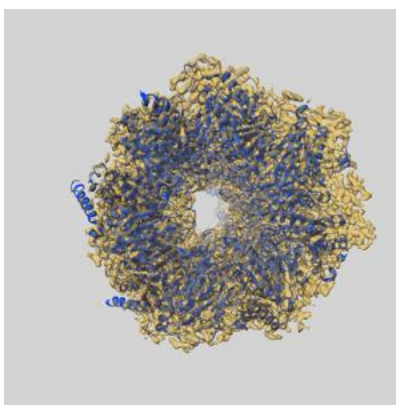
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22259 and PDB model 6XMJ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

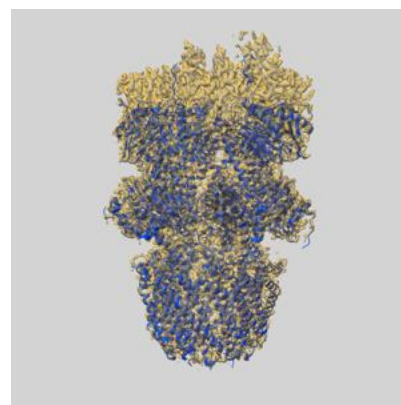
9.1 Map-model overlay [i](#)



X



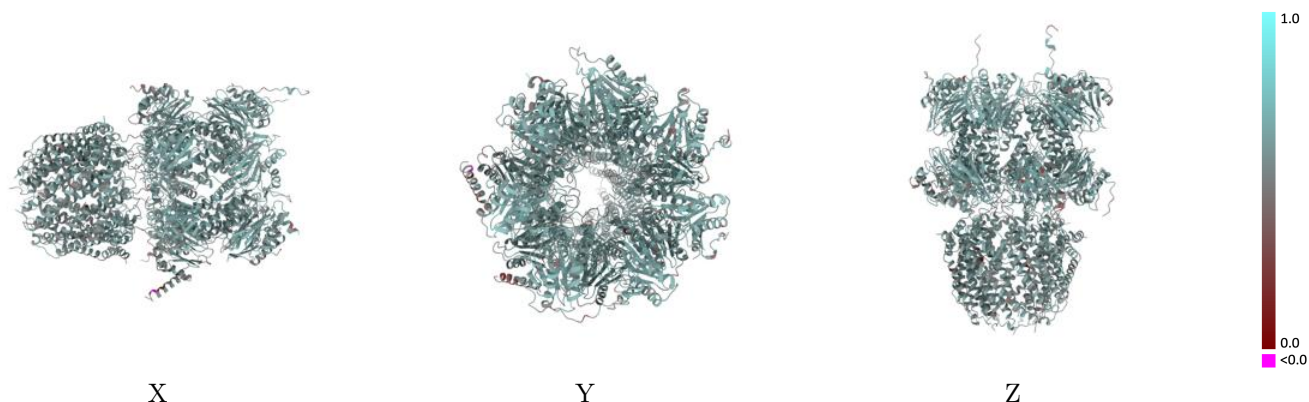
Y



Z

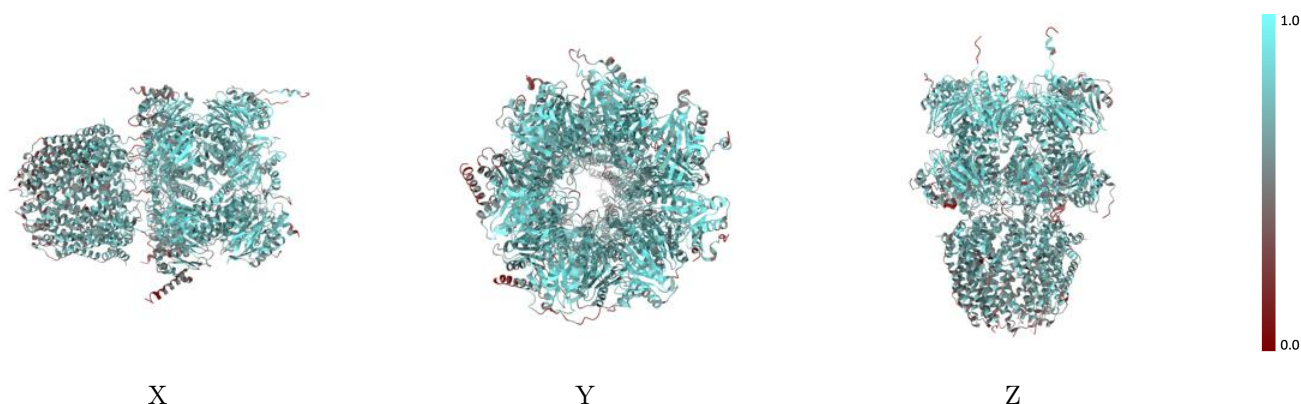
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



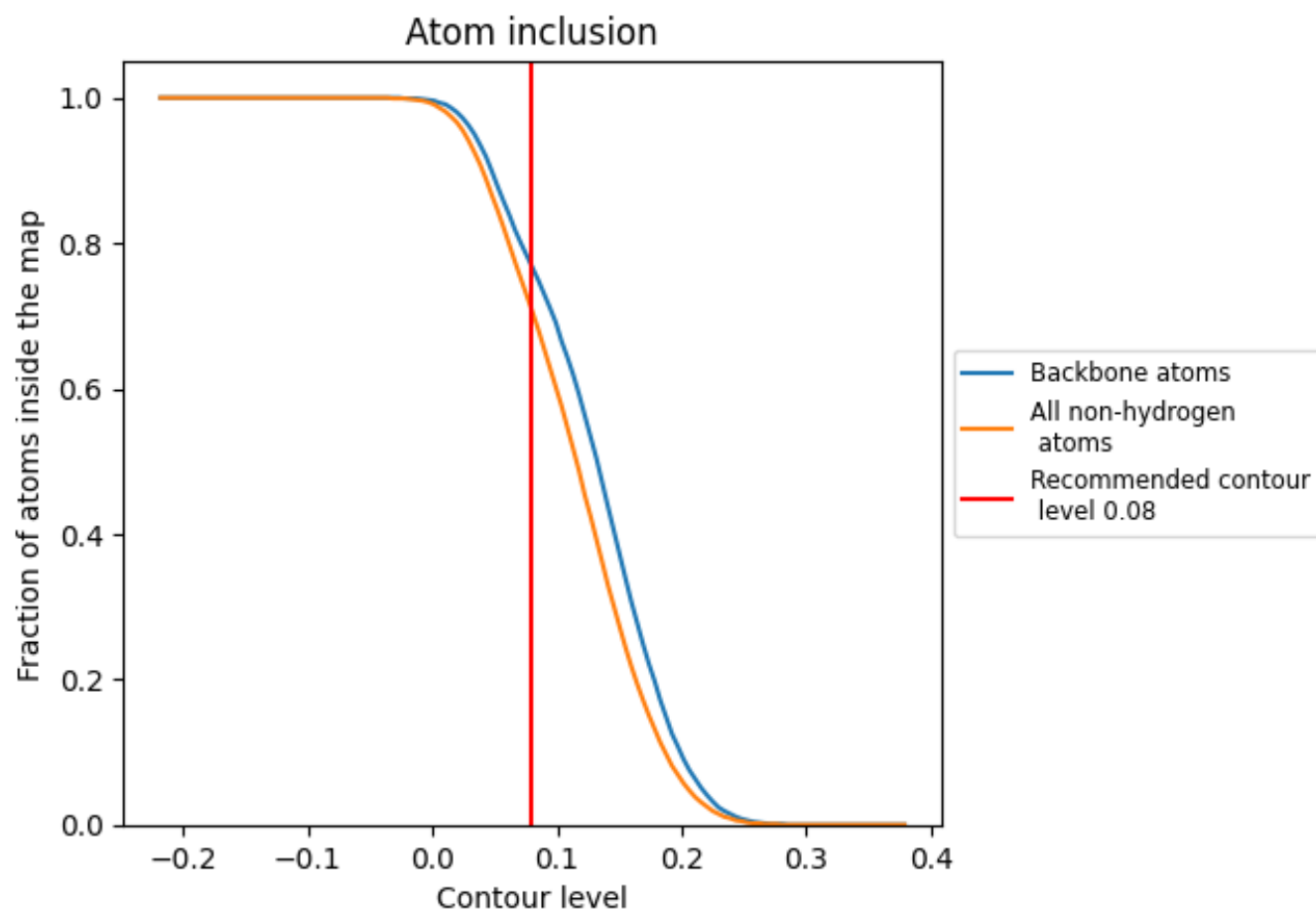
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 71% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7070	 0.5840
A	 0.7230	 0.5930
B	 0.7510	 0.5970
C	 0.6720	 0.5650
D	 0.6580	 0.5610
E	 0.7200	 0.5900
F	 0.7520	 0.6010
G	 0.7090	 0.5860
H	 0.7800	 0.6070
I	 0.7600	 0.5970
J	 0.7700	 0.6020
K	 0.7650	 0.5980
L	 0.7760	 0.6020
M	 0.7380	 0.6020
N	 0.7740	 0.6020
O	 0.6530	 0.5650
P	 0.6390	 0.5660
Q	 0.6290	 0.5620
R	 0.6300	 0.5700
S	 0.6500	 0.5660
T	 0.6490	 0.5640
U	 0.6500	 0.5690

