



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 03:02 AM EST

PDB ID : 7TEJ
EMDB ID : EMD-25847
Title : Cryo-EM structure of the 20S Alpha 3 Deletion proteasome core particle
Authors : Walsh Jr., R.M.; Rawson, S.; Schnell, H.M.; Hanna, J.
Deposited on : 2022-01-05
Resolution : 2.74 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.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) : 2.31.3

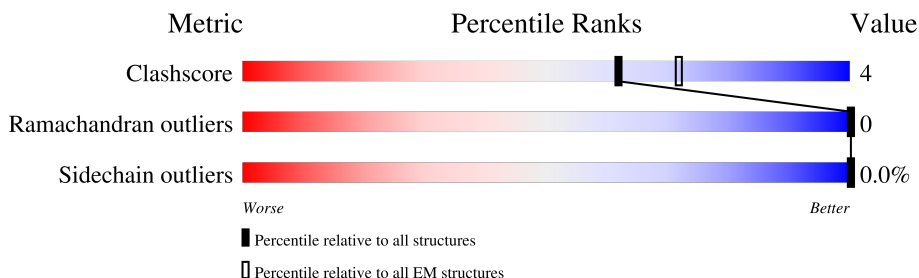
1 Overall quality at a glance

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	1	241	
1	M	241	
2	2	266	
2	N	266	
3	A	252	
3	O	252	
4	B	250	
4	P	250	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	254	
5	D	254	
5	Q	254	
5	R	254	
6	E	260	
6	S	260	
7	F	234	
7	T	234	
8	G	288	
8	U	288	
9	H	215	
9	V	215	
10	I	261	
10	W	261	
11	J	205	
11	X	205	
12	K	198	
12	Y	198	
13	L	287	
13	Z	287	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 91490 atoms, of which 45742 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 beta type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	202	Total	C	H	N	O	S	0	0
			3163	1009	1568	276	306	4		
1	M	202	Total	C	H	N	O	S	0	0
			3163	1009	1568	276	306	4		

- Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	218	Total	C	H	N	O	S	0	0
			3412	1081	1706	291	328	6		
2	N	218	Total	C	H	N	O	S	0	0
			3412	1081	1706	291	328	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	236	Total	C	H	N	O	S	0	0
			3732	1191	1863	313	357	8		
3	O	236	Total	C	H	N	O	S	0	0
			3732	1191	1863	313	357	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B	244	Total	C	H	N	O	S	0	0
			3743	1188	1880	306	366	3		
4	P	244	Total	C	H	N	O	S	0	0
			3743	1188	1880	306	366	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	C	225	Total	C	H	N	O	S	0	0
			3547	1108	1781	306	348	4		
5	D	197	Total	C	H	N	O	S	0	0
			3132	979	1579	268	302	4		
5	Q	228	Total	C	H	N	O	S	0	0
			3596	1121	1806	312	353	4		
5	R	197	Total	C	H	N	O	S	0	0
			3132	979	1579	268	302	4		

- Molecule 6 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	171	Total	C	H	N	O	S	0	0
			2656	839	1330	222	261	4		
6	S	171	Total	C	H	N	O	S	0	0
			2656	839	1330	222	261	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	223	Total	C	H	N	O	S	0	0
			3438	1079	1728	297	330	4		
7	T	223	Total	C	H	N	O	S	0	0
			3438	1079	1728	297	330	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	232	Total	C	H	N	O	S	0	0
			3608	1151	1804	314	335	4		
8	U	232	Total	C	H	N	O	S	0	0
			3607	1151	1803	314	335	4		

- Molecule 9 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	181	Total	C	H	N	O	S	0	0
			2786	891	1383	232	273	7		
9	V	181	Total	C	H	N	O	S	0	0
			2786	891	1383	232	273	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	203	Total	C	H	N	O	S	0	0
			3131	988	1574	270	293	6		
10	W	203	Total	C	H	N	O	S	0	0
			3131	988	1574	270	293	6		

- Molecule 11 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	203	Total	C	H	N	O	S	0	0
			3142	1007	1567	257	303	8		
11	X	203	Total	C	H	N	O	S	0	0
			3142	1007	1567	257	303	8		

- Molecule 12 is a protein called Proteasome subunit beta type-4.

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

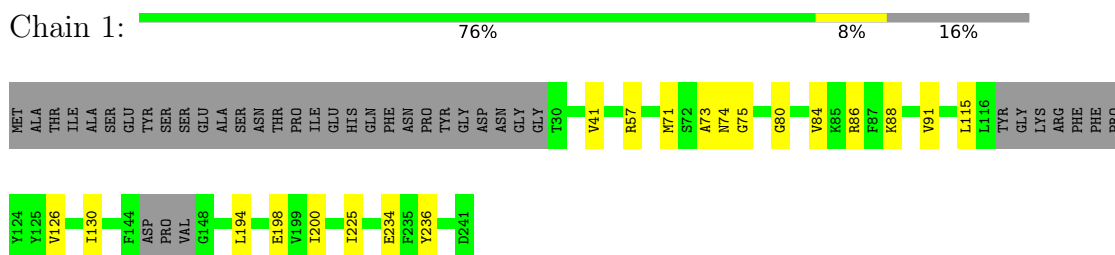
- Molecule 13 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	201	Total	C	H	N	O	S	0	0
			3120	1010	1538	268	298	6		
13	Z	201	Total	C	H	N	O	S	0	0
			3120	1010	1538	268	298	6		

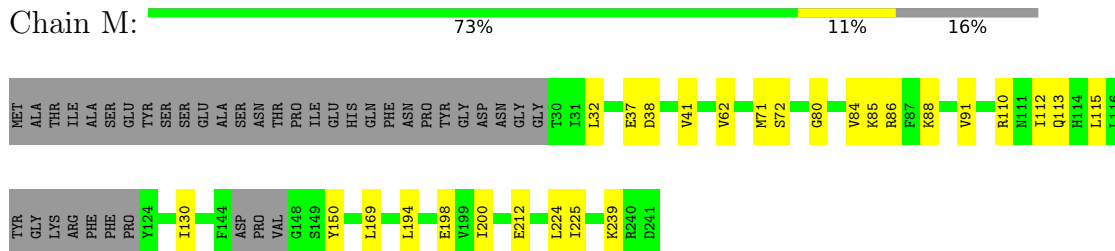
3 Residue-property plots

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.

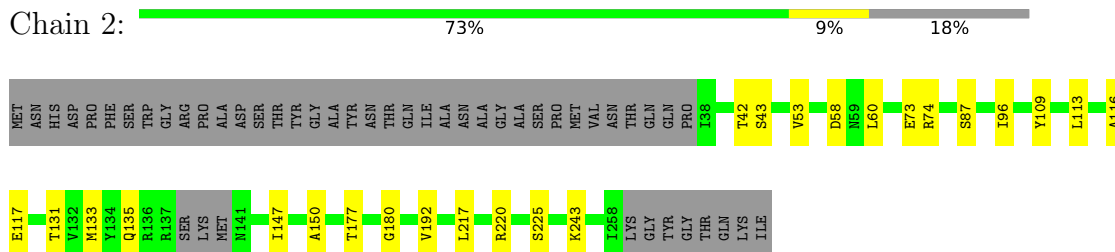
• Molecule 1: Proteasome subunit beta type-6



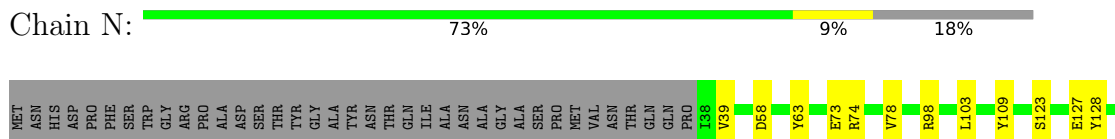
• Molecule 1: Proteasome subunit beta type-6



• Molecule 2: Proteasome subunit beta type-7

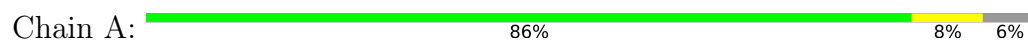


• Molecule 2: Proteasome subunit beta type-7

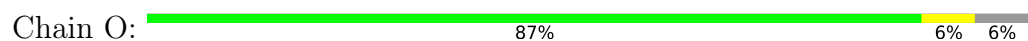




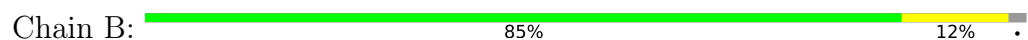
- Molecule 3: Proteasome subunit alpha type-1



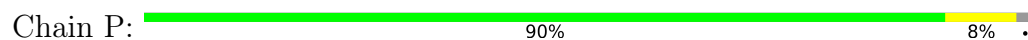
- Molecule 3: Proteasome subunit alpha type-1



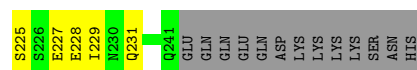
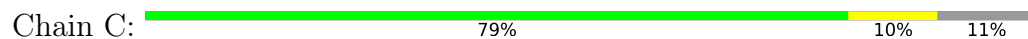
- Molecule 4: Proteasome subunit alpha type-2



- Molecule 4: Proteasome subunit alpha type-2

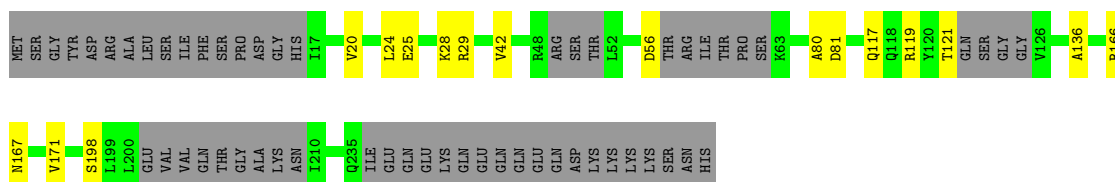


- Molecule 5: Proteasome subunit alpha type-4

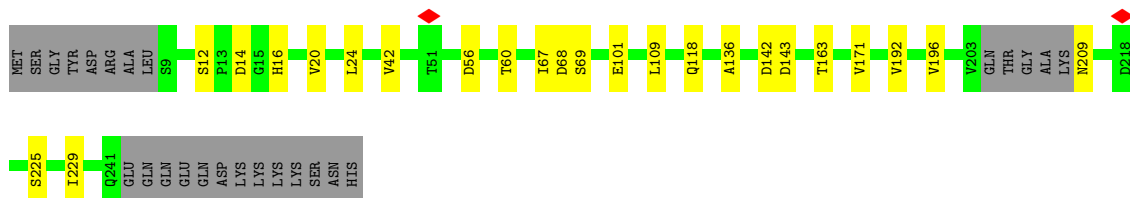
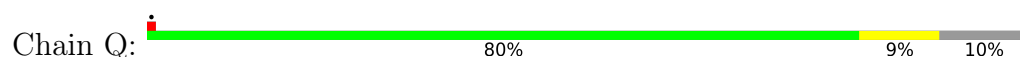


- Molecule 5: Proteasome subunit alpha type-4

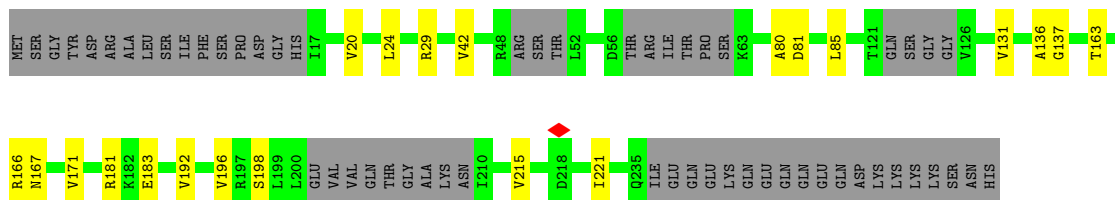




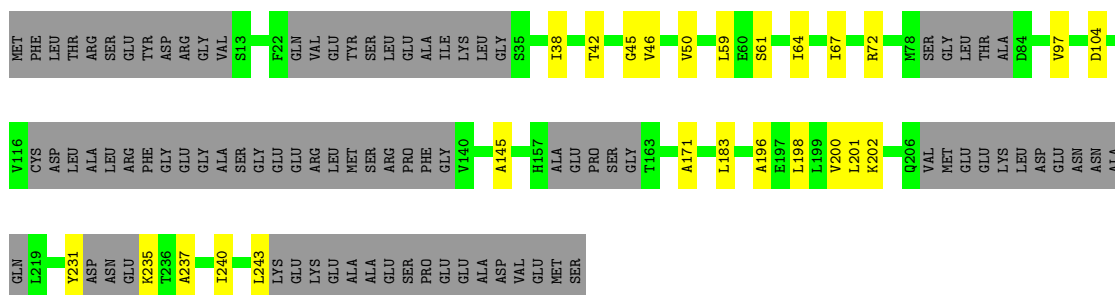
- Molecule 5: Proteasome subunit alpha type-4



- Molecule 5: Proteasome subunit alpha type-4

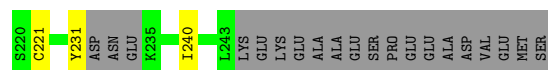
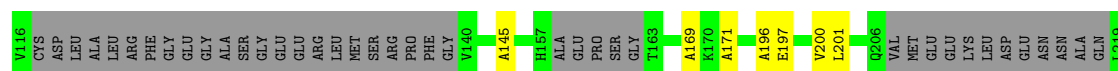


- Molecule 6: Proteasome subunit alpha type-5



- Molecule 6: Proteasome subunit alpha type-5





• Molecule 7: Proteasome subunit alpha type-6

Chain F: 82% 13% 5%



• Molecule 7: Proteasome subunit alpha type-6

Chain T: 83% 12% 5%



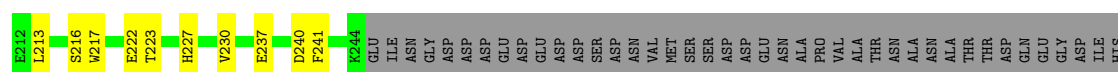
• Molecule 8: Proteasome subunit alpha type-7

Chain G: 70% 10% 19%



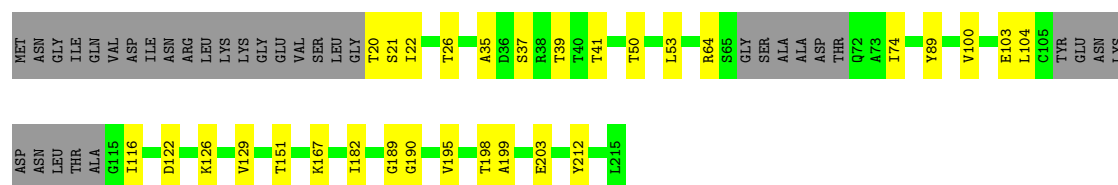
• Molecule 8: Proteasome subunit alpha type-7

Chain U: 69% 11% 19%



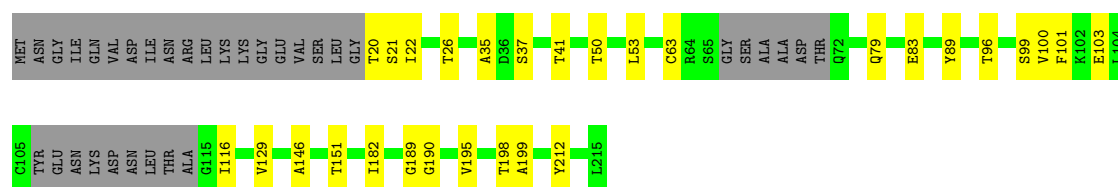
• Molecule 9: Proteasome subunit beta type-1

Chain H:  70% 14% 16%



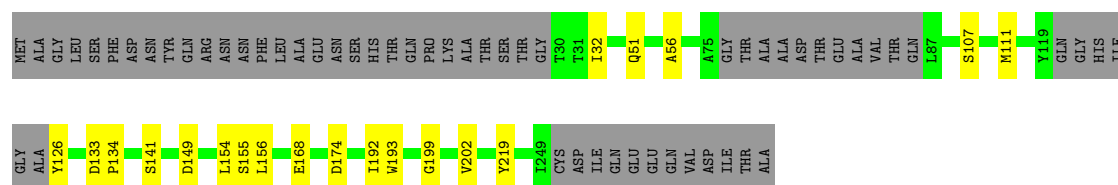
• Molecule 9: Proteasome subunit beta type-1

Chain V:  71% 13% 16%



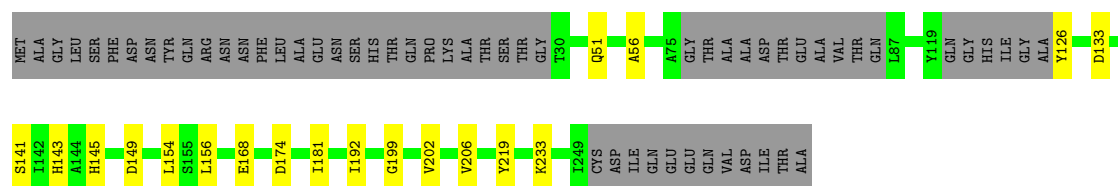
• Molecule 10: Proteasome subunit beta type-2

Chain I:  70% 8% 22%




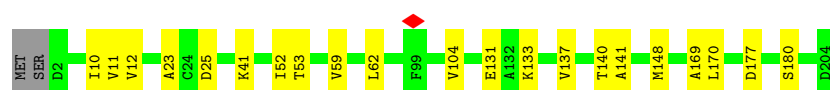
• Molecule 10: Proteasome subunit beta type-2

Chain W:  70% 7% 22%




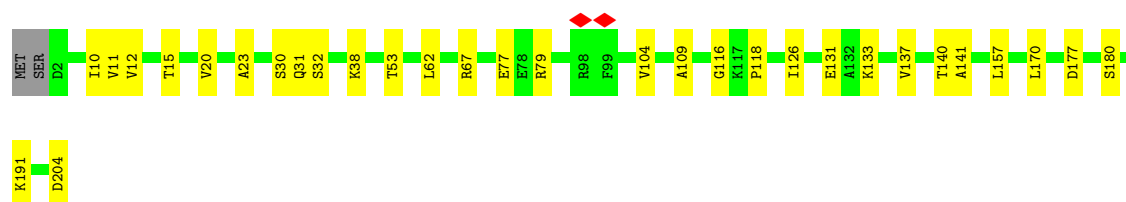
• Molecule 11: Proteasome subunit beta type-3

Chain J:  89% 10% .



• Molecule 11: Proteasome subunit beta type-3

Chain X:  84% 15% .



- Molecule 12: Proteasome subunit beta type-4

Chain K: 89% 9%



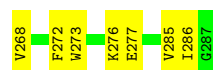
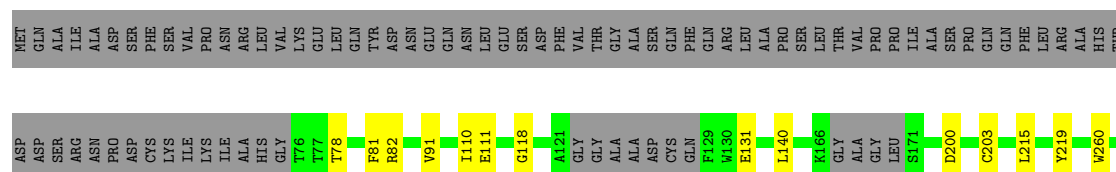
- Molecule 12: Proteasome subunit beta type-4

Chain Y: 91% 7%



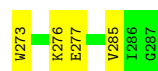
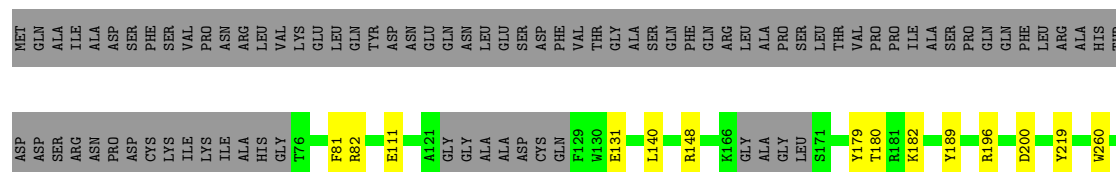
- Molecule 13: Proteasome subunit beta type-5

Chain L: 63% 7% 30%



- Molecule 13: Proteasome subunit beta type-5

Chain Z: 64% 6% 30%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	150227	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 ($e^-/\text{\AA}^2$)	53.85	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.451	Depositor
Minimum map value	-2.835	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.148	Depositor
Recommended contour level	0.385	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	1	0.29	0/1623	0.50	0/2183
1	M	0.30	0/1623	0.52	0/2183
2	2	0.28	0/1734	0.53	0/2353
2	N	0.28	0/1734	0.53	0/2353
3	A	0.30	0/1906	0.49	0/2581
3	O	0.30	0/1906	0.49	0/2581
4	B	0.30	0/1899	0.50	0/2571
4	P	0.31	0/1899	0.49	0/2571
5	C	0.28	0/1792	0.52	0/2425
5	D	0.29	0/1573	0.53	0/2125
5	Q	0.28	0/1817	0.52	0/2460
5	R	0.28	0/1573	0.51	0/2125
6	E	0.26	0/1340	0.49	0/1800
6	S	0.25	0/1340	0.49	0/1800
7	F	0.27	0/1735	0.50	0/2341
7	T	0.26	0/1735	0.50	0/2341
8	G	0.31	0/1841	0.50	0/2484
8	U	0.30	0/1841	0.48	0/2484
9	H	0.29	0/1429	0.51	0/1931
9	V	0.29	0/1429	0.50	0/1931
10	I	0.29	0/1585	0.51	0/2145
10	W	0.29	0/1585	0.51	0/2145
11	J	0.32	0/1605	0.50	0/2166
11	X	0.32	0/1605	0.50	0/2166
12	K	0.31	0/1581	0.52	0/2132
12	Y	0.31	0/1581	0.53	0/2132
13	L	0.32	0/1617	0.52	0/2185
13	Z	0.31	0/1617	0.51	0/2185
All	All	0.29	0/46545	0.51	0/62879

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	1	1595	1568	1565	12	0
1	M	1595	1568	1565	17	0
2	2	1706	1706	1704	16	0
2	N	1706	1706	1704	16	0
3	A	1869	1863	1861	11	0
3	O	1869	1863	1861	10	0
4	B	1863	1880	1879	19	0
4	P	1863	1880	1879	12	0
5	C	1766	1781	1778	19	0
5	D	1553	1579	1574	12	0
5	Q	1790	1806	1804	18	0
5	R	1553	1579	1574	15	0
6	E	1326	1330	1323	19	0
6	S	1326	1330	1323	19	0
7	F	1710	1728	1725	20	0
7	T	1710	1728	1725	20	0
8	G	1804	1804	1800	23	0
8	U	1804	1803	1800	22	0
9	H	1403	1383	1380	20	0
9	V	1403	1383	1380	22	0
10	I	1557	1574	1571	13	0
10	W	1557	1574	1571	13	0
11	J	1575	1567	1566	12	0
11	X	1575	1567	1566	21	0
12	K	1553	1558	1560	11	0
12	Y	1553	1558	1560	10	0
13	L	1582	1538	1535	14	0
13	Z	1582	1538	1535	11	0
All	All	45748	45742	45668	411	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 (411) 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:Z:82:ARG:NH1	13:Z:200:ASP:OD1	1.96	0.98
5:Q:14:ASP:O	5:R:29:ARG:NH1	2.06	0.88
6:S:197:GLU:OE2	6:S:231:TYR:OH	1.92	0.86
10:W:141:SER:OG	10:W:149:ASP:OD1	1.95	0.83
5:R:163:THR:HG21	5:R:171:VAL:HG13	1.59	0.83
3:O:131:ARG:NH1	3:O:134:MET:SD	2.53	0.82
7:F:164:ARG:NH1	7:F:200:SER:O	2.12	0.82
5:C:14:ASP:O	5:D:29:ARG:NH1	2.13	0.81
10:I:141:SER:OG	10:I:149:ASP:OD1	1.99	0.80
5:Q:68:ASP:OD1	5:Q:69:SER:N	2.16	0.79
2:2:96:ILE:HD13	2:2:147:ILE:HD11	1.64	0.79
13:L:82:ARG:NH1	13:L:200:ASP:OD1	2.16	0.79
9:H:190:GLY:O	9:H:212:TYR:OH	2.02	0.78
9:H:64:ARG:NH2	9:H:74:ILE:HD11	1.99	0.78
9:V:190:GLY:O	9:V:212:TYR:OH	2.02	0.77
2:N:58:ASP:OD1	2:N:74:ARG:NH2	2.18	0.76
11:X:116:GLY:O	11:X:191:LYS:NZ	2.19	0.76
5:Q:101:GLU:OE1	11:X:67:ARG:NH2	2.18	0.76
7:F:86:ASN:OD1	7:F:89:ARG:NH2	2.18	0.76
5:C:12:SER:OG	5:C:14:ASP:OD1	2.02	0.76
4:B:26:THR:O	4:B:30:GLN:NE2	2.19	0.76
5:C:68:ASP:OD1	5:C:69:SER:N	2.17	0.76
13:Z:276:LYS:NZ	13:Z:285:VAL:O	2.21	0.74
5:R:85:LEU:HD12	5:R:131:VAL:HG21	1.70	0.73
4:B:26:THR:HG22	4:B:30:GLN:HE22	1.53	0.71
6:E:38:ILE:CD1	6:E:171:ALA:HB2	2.21	0.70
8:U:19:ARG:NH2	8:U:24:GLU:OE1	2.24	0.70
8:G:217:TRP:CZ3	8:G:223:THR:HG23	2.25	0.70
4:B:21:ILE:HD11	4:B:122:THR:HG23	1.73	0.69
11:X:77:GLU:OE1	11:X:79:ARG:NH1	2.25	0.69
7:F:107:ARG:NH2	2:N:109:TYR:O	2.26	0.68
2:2:73:GLU:OE1	2:2:243:LYS:NZ	2.26	0.68
13:L:273:TRP:O	13:L:277:GLU:OE1	2.12	0.68
9:H:22:ILE:HG22	9:H:35:ALA:HB2	1.76	0.67
8:U:240:ASP:OD1	8:U:241:PHE:N	2.27	0.67
3:O:24:ARG:NH2	3:O:29:GLU:OE1	2.28	0.67
6:E:97:VAL:HG11	13:L:140:LEU:HD21	1.77	0.66
8:U:217:TRP:CZ3	8:U:223:THR:HG23	2.31	0.66
11:X:131:GLU:OE1	11:X:133:LYS:NZ	2.26	0.66
9:H:39:THR:HG23	9:H:50:THR:HG21	1.76	0.66
9:H:53:LEU:HD12	9:H:195:VAL:HG23	1.78	0.66
2:N:73:GLU:OE1	2:N:243:LYS:NZ	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:167:LYS:NZ	9:H:203:GLU:OE1	2.30	0.64
1:M:71:MET:HG3	1:M:130:ILE:HG22	1.79	0.64
11:X:10:ILE:HG21	11:X:141:ALA:HB3	1.79	0.64
2:2:109:TYR:O	7:T:107:ARG:NH2	2.30	0.64
8:U:217:TRP:CH2	8:U:223:THR:HG23	2.33	0.64
2:2:133:MET:HE3	2:2:147:ILE:HD12	1.79	0.63
2:2:58:ASP:OD1	2:2:74:ARG:NH2	2.31	0.63
8:G:240:ASP:OD1	8:G:241:PHE:N	2.32	0.62
8:G:171:ALA:O	8:G:175:LEU:HD23	1.98	0.62
11:J:62:LEU:CD1	11:J:104:VAL:HG21	2.30	0.62
5:Q:163:THR:HG21	5:Q:171:VAL:HG13	1.82	0.62
9:V:41:THR:HG23	9:V:41:THR:O	2.00	0.61
9:V:79:GLN:NE2	9:V:83:GLU:OE2	2.34	0.61
9:H:41:THR:O	9:H:41:THR:HG23	2.01	0.61
5:C:227:GLU:O	5:C:231:GLN:NE2	2.33	0.61
5:Q:118:GLN:HG3	5:R:80:ALA:HB1	1.83	0.60
12:K:24:ILE:O	12:Y:138:TYR:OH	2.18	0.60
2:N:78:VAL:HG12	2:N:78:VAL:O	2.00	0.60
2:2:133:MET:CE	2:2:147:ILE:HD12	2.32	0.60
6:S:46:VAL:HG11	6:S:145:ALA:HB1	1.82	0.60
7:F:68:GLU:N	7:F:68:GLU:OE1	2.35	0.60
1:1:86:ARG:HG2	1:1:115:LEU:HD22	1.85	0.59
1:M:200:ILE:HD11	1:M:225:ILE:HD11	1.84	0.59
6:E:42:THR:OG1	6:E:45:GLY:O	2.11	0.59
6:E:196:ALA:O	6:E:200:VAL:HG23	2.03	0.59
9:V:22:ILE:HG22	9:V:35:ALA:HB2	1.85	0.59
11:J:10:ILE:HG21	11:J:141:ALA:HB3	1.83	0.59
7:F:97:LEU:HD12	1:M:85:LYS:HD3	1.86	0.58
6:E:38:ILE:HG23	6:E:200:VAL:HG13	1.84	0.58
5:C:118:GLN:HG3	5:D:80:ALA:HB1	1.85	0.58
6:E:38:ILE:HD13	6:E:171:ALA:HB2	1.85	0.58
1:M:37:GLU:O	1:M:38:ASP:OD1	2.21	0.58
6:E:38:ILE:HD12	6:E:171:ALA:HB2	1.85	0.57
11:J:177:ASP:OD2	11:J:180:SER:OG	2.13	0.57
4:P:21:ILE:HD11	4:P:122:THR:HG23	1.84	0.57
4:P:64:VAL:HG11	4:P:212:ALA:HB3	1.86	0.57
6:S:38:ILE:HG23	6:S:200:VAL:HG13	1.84	0.57
5:Q:142:ASP:OD1	5:Q:143:ASP:N	2.38	0.57
6:S:97:VAL:HG11	13:Z:140:LEU:HD21	1.86	0.57
13:L:276:LYS:NZ	13:L:285:VAL:O	2.34	0.57
8:U:171:ALA:O	8:U:175:LEU:HD23	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:131:GLU:OE1	11:J:133:LYS:NZ	2.34	0.57
6:S:42:THR:OG1	6:S:45:GLY:O	2.17	0.56
11:J:140:THR:OG1	11:J:177:ASP:OD2	2.22	0.56
4:P:21:ILE:O	4:P:25:LEU:HD23	2.05	0.56
3:A:131:ARG:NH1	3:A:134:MET:SD	2.79	0.56
5:C:224:LEU:HB2	5:C:229:ILE:HD11	1.88	0.56
2:N:192:VAL:HG23	2:N:192:VAL:O	2.06	0.56
12:K:138:TYR:OH	12:Y:24:ILE:O	2.24	0.55
2:2:42:THR:HG23	2:2:43:SER:N	2.20	0.55
5:D:42:VAL:HG11	5:D:136:ALA:HB1	1.88	0.55
5:C:142:ASP:OD1	5:C:143:ASP:N	2.38	0.55
7:T:68:GLU:N	7:T:68:GLU:OE1	2.37	0.55
2:2:131:THR:HG23	2:2:135:GLN:HE22	1.72	0.55
4:B:64:VAL:HG11	4:B:212:ALA:HB3	1.89	0.55
13:Z:273:TRP:O	13:Z:277:GLU:OE1	2.26	0.54
7:F:88:LEU:HD11	7:F:108:ALA:HB1	1.89	0.54
9:H:53:LEU:CD1	9:H:195:VAL:HG23	2.37	0.54
11:J:62:LEU:HD11	11:J:104:VAL:HG21	1.88	0.54
11:X:62:LEU:CD1	11:X:104:VAL:HG21	2.37	0.54
8:G:216:SER:OG	8:G:227:HIS:NE2	2.37	0.54
6:E:201:LEU:HB3	6:E:243:LEU:HD22	1.90	0.53
6:E:104:ASP:OD1	1:M:110:ARG:NH1	2.42	0.53
5:Q:20:VAL:O	5:Q:24:LEU:HD23	2.08	0.53
1:1:200:ILE:HD11	1:1:225:ILE:HD11	1.90	0.53
13:Z:131:GLU:N	13:Z:131:GLU:OE1	2.42	0.53
9:H:22:ILE:HG22	9:H:35:ALA:CB	2.39	0.53
4:B:115:ALA:HB1	4:B:154:GLY:O	2.09	0.53
10:W:141:SER:HB3	10:W:154:LEU:HD13	1.91	0.53
4:P:115:ALA:HB1	4:P:154:GLY:O	2.08	0.53
11:X:62:LEU:HD11	11:X:104:VAL:HG21	1.91	0.53
5:C:42:VAL:HG11	5:C:136:ALA:HB1	1.91	0.52
11:X:31:GLN:HG3	11:X:32:SER:H	1.73	0.52
3:O:53:VAL:CG2	3:O:144:VAL:HG11	2.39	0.52
1:1:80:GLY:O	1:1:84:VAL:HG23	2.10	0.52
10:I:141:SER:HB3	10:I:154:LEU:HD13	1.92	0.52
9:V:198:THR:HG22	9:V:199:ALA:N	2.25	0.52
7:F:80:ASP:OD2	7:F:129:GLY:N	2.38	0.51
8:G:235:LEU:O	8:G:239:ILE:HG12	2.10	0.51
8:U:150:LEU:HD23	8:U:156:TYR:HB3	1.92	0.51
2:2:53:VAL:HG21	2:2:150:ALA:HB1	1.91	0.51
3:O:176:GLN:O	3:O:176:GLN:NE2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:38:ILE:CD1	6:S:171:ALA:HB2	2.40	0.51
6:S:50:VAL:HG23	6:S:67:ILE:HD11	1.92	0.51
10:W:133:ASP:OD1	10:W:133:ASP:N	2.44	0.51
1:M:41:VAL:HG12	1:M:225:ILE:HD12	1.92	0.51
9:V:99:SER:O	9:V:103:GLU:HG2	2.10	0.51
2:2:220:ARG:NH1	10:I:168:GLU:OE2	2.42	0.50
8:G:217:TRP:CH2	8:G:223:THR:HG23	2.45	0.50
6:E:38:ILE:HD11	6:E:183:LEU:HD11	1.92	0.50
10:I:107:SER:O	10:I:111:MET:HG3	2.11	0.50
5:C:20:VAL:O	5:C:24:LEU:HD23	2.11	0.50
9:V:22:ILE:HG22	9:V:35:ALA:CB	2.41	0.50
6:S:38:ILE:HD13	6:S:171:ALA:HB2	1.93	0.50
9:V:182:ILE:HG23	9:V:189:GLY:HA2	1.94	0.50
7:F:79:PRO:O	7:F:82:ARG:HG2	2.11	0.50
7:T:156:LEU:HD13	7:T:159:THR:HB	1.92	0.50
4:B:48:GLU:HG2	4:B:200:VAL:HG22	1.94	0.50
8:U:108:ILE:HG21	8:U:146:HIS:HB2	1.92	0.50
2:2:192:VAL:HG23	2:2:192:VAL:O	2.12	0.50
5:C:225:SER:OG	5:C:228:GLU:OE2	2.30	0.50
1:1:71:MET:HG3	1:1:130:ILE:HG22	1.94	0.49
4:B:15:SER:O	5:C:29:ARG:NE	2.45	0.49
9:H:64:ARG:HH12	9:H:116:ILE:HD11	1.77	0.49
10:I:202:VAL:O	10:I:219:TYR:N	2.45	0.49
4:P:201:GLU:OE1	4:P:201:GLU:N	2.39	0.49
5:Q:56:ASP:O	5:Q:60:THR:OG1	2.27	0.49
1:M:194:LEU:HD23	1:M:198:GLU:HG3	1.92	0.49
4:B:32:VAL:HG13	4:B:48:GLU:OE2	2.12	0.49
12:K:81:SER:O	12:K:85:GLN:HG2	2.12	0.49
8:G:103:LYS:HZ2	2:N:98:ARG:NE	2.10	0.49
13:L:268:VAL:HG11	11:X:204:ASP:HB3	1.94	0.49
5:Q:209:ASN:OD1	5:Q:209:ASN:O	2.30	0.49
9:V:26:THR:HG23	9:V:129:VAL:HG23	1.95	0.49
8:G:20:ASN:ND2	8:G:23:VAL:HG23	2.28	0.49
9:H:182:ILE:HG23	9:H:189:GLY:HA2	1.93	0.49
1:1:234:GLU:OE1	1:1:236:TYR:OH	2.25	0.49
11:J:23:ALA:HB1	11:J:170:LEU:HD22	1.95	0.49
5:Q:67:ILE:HG21	5:Q:109:LEU:HD21	1.94	0.49
5:R:20:VAL:O	5:R:24:LEU:HD23	2.13	0.49
1:1:194:LEU:HD23	1:1:198:GLU:HG3	1.95	0.48
5:R:137:GLY:HA2	5:R:215:VAL:HG11	1.94	0.48
7:F:227:GLY:O	7:F:230:VAL:HG22	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:129:TYR:OH	12:K:144:ASP:OD1	2.26	0.48
13:Z:148:ARG:NH2	13:Z:179:TYR:O	2.43	0.48
5:C:118:GLN:NE2	5:D:81:ASP:OD1	2.46	0.48
5:R:181:ARG:NH1	6:S:60:GLU:OE2	2.42	0.48
12:K:3:ILE:HG13	12:K:46:ALA:HB2	1.94	0.48
6:S:42:THR:HG21	6:S:196:ALA:HB2	1.95	0.48
2:N:239:LEU:HD21	2:N:241:PHE:HB2	1.96	0.48
7:T:65:LYS:O	7:T:89:ARG:NH2	2.43	0.48
5:D:166:ARG:O	5:D:167:ASN:OD1	2.32	0.48
4:P:75:TYR:HB3	4:P:82:TYR:CD1	2.49	0.48
5:R:166:ARG:O	5:R:167:ASN:OD1	2.32	0.48
7:T:66:CYS:HA	7:T:89:ARG:HE	1.79	0.48
6:S:38:ILE:CG2	6:S:200:VAL:HG13	2.43	0.48
12:Y:6:ILE:HD11	12:Y:143:LEU:HD21	1.95	0.48
5:Q:12:SER:N	5:Q:16:HIS:O	2.35	0.47
6:S:40:ILE:HD13	6:S:169:ALA:HB1	1.96	0.47
3:O:129:THR:HG22	3:O:129:THR:O	2.14	0.47
4:B:213:ILE:HD11	4:B:236:ARG:NH2	2.30	0.47
5:C:225:SER:O	5:C:229:ILE:HD12	2.15	0.47
2:N:123:SER:O	2:N:127:GLU:OE1	2.31	0.47
9:V:22:ILE:HD11	9:V:146:ALA:HB3	1.95	0.47
9:V:53:LEU:HD23	9:V:63:CYS:SG	2.53	0.47
8:G:103:LYS:HD2	2:N:98:ARG:HD3	1.95	0.47
4:B:63:LYS:N	4:B:210:GLU:OE1	2.46	0.47
5:D:25:GLU:OE2	5:D:28:LYS:NZ	2.43	0.47
2:N:220:ARG:NH1	10:W:168:GLU:OE2	2.44	0.47
9:V:37:SER:O	9:V:50:THR:HG22	2.14	0.47
5:Q:225:SER:O	5:Q:229:ILE:HD12	2.15	0.47
6:S:36:THR:O	6:S:36:THR:HG23	2.15	0.47
6:S:201:LEU:HD22	6:S:240:ILE:CD1	2.44	0.47
5:D:20:VAL:O	5:D:24:LEU:HD23	2.15	0.47
1:M:80:GLY:O	1:M:84:VAL:HG23	2.15	0.47
4:B:106:PRO:HG2	4:B:109:LEU:HD13	1.97	0.47
9:H:198:THR:HG22	9:H:199:ALA:N	2.29	0.47
5:Q:42:VAL:HG11	5:Q:136:ALA:HB1	1.97	0.47
6:S:201:LEU:HD13	6:S:240:ILE:HD13	1.97	0.46
10:W:51:GLN:HG2	10:W:56:ALA:HB2	1.97	0.46
3:A:28:VAL:HG21	3:A:129:THR:HG23	1.97	0.46
4:B:227:ILE:HG21	4:B:230:ASP:OD2	2.14	0.46
8:U:237:GLU:O	8:U:240:ASP:OD1	2.33	0.46
9:V:53:LEU:HD13	9:V:195:VAL:HG23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:202:VAL:O	10:W:219:TYR:N	2.45	0.46
4:B:122:THR:O	4:B:122:THR:HG22	2.15	0.46
6:E:61:SER:HA	6:E:64:ILE:HD12	1.98	0.46
4:P:169:VAL:HG23	4:P:170:ALA:N	2.30	0.46
8:U:210:ASP:OD1	8:U:211:PHE:N	2.48	0.46
12:Y:81:SER:O	12:Y:85:GLN:HG2	2.14	0.46
6:E:72:ARG:N	6:E:72:ARG:HD3	2.31	0.46
8:U:217:TRP:CZ3	8:U:222:GLU:HB2	2.51	0.46
7:F:81:ALA:HB2	7:F:130:VAL:HG21	1.97	0.46
4:P:64:VAL:HG11	4:P:212:ALA:CB	2.46	0.46
5:R:42:VAL:HG11	5:R:136:ALA:HB1	1.97	0.46
8:U:216:SER:OG	8:U:227:HIS:NE2	2.41	0.46
5:C:181:ARG:NH2	5:D:56:ASP:OD1	2.48	0.46
9:H:26:THR:HG23	9:H:129:VAL:HG23	1.96	0.46
13:L:203:CYS:SG	13:L:215:LEU:HD12	2.56	0.46
11:X:23:ALA:HB1	11:X:170:LEU:HD22	1.97	0.46
3:A:87:ILE:N	3:A:88:PRO:HD2	2.30	0.46
10:W:126:TYR:HB3	10:W:156:LEU:HD13	1.98	0.46
6:E:231:TYR:HA	6:E:235:LYS:HE2	1.99	0.45
2:N:146:ALA:HB3	2:N:177:THR:HG21	1.98	0.45
3:O:87:ILE:N	3:O:88:PRO:HD2	2.31	0.45
4:P:92:VAL:HG22	4:P:96:SER:OG	2.16	0.45
5:R:215:VAL:HG22	5:R:221:ILE:HG12	1.98	0.45
3:A:53:VAL:CG2	3:A:144:VAL:HG11	2.46	0.45
5:D:117:GLN:O	5:D:121:THR:HG23	2.17	0.45
8:G:170:SER:O	8:G:174:GLU:OE1	2.35	0.45
9:V:53:LEU:CD1	9:V:195:VAL:HG23	2.46	0.45
7:F:29:ILE:HD11	7:F:149:PRO:HD3	1.99	0.45
9:V:101:PHE:CD1	9:V:116:ILE:HD13	2.51	0.45
4:B:21:ILE:HG21	4:B:153:SER:HB3	1.98	0.45
7:F:156:LEU:HD23	8:G:58:LEU:HA	1.98	0.45
11:X:141:ALA:HB2	11:X:177:ASP:HB2	1.99	0.45
12:Y:35:ARG:NE	12:Y:57:GLU:OE2	2.36	0.45
9:H:151:THR:HG22	9:V:151:THR:HG22	1.99	0.45
11:J:12:VAL:HG23	11:J:137:VAL:HG12	1.98	0.45
13:L:110:ILE:HG22	13:L:118:GLY:O	2.17	0.45
13:L:110:ILE:HG21	13:L:131:GLU:HG3	1.97	0.45
11:X:11:VAL:HG23	11:X:53:THR:HG22	1.99	0.45
2:N:226:ARG:NH2	2:N:248:GLU:OE2	2.50	0.45
5:Q:229:ILE:HD12	5:Q:229:ILE:H	1.82	0.45
2:2:60:LEU:HB2	2:2:225:SER:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:237:ALA:HA	6:E:240:ILE:HG22	1.98	0.44
8:G:8:ASP:OD2	8:G:25:TYR:OH	2.29	0.44
8:G:103:LYS:NZ	9:H:103:GLU:OE2	2.30	0.44
12:K:107:ASP:O	12:K:111:ASN:N	2.50	0.44
13:L:111:GLU:HG2	13:L:260:TRP:CZ2	2.52	0.44
3:O:28:VAL:HG21	3:O:129:THR:HG23	1.99	0.44
8:U:217:TRP:CD1	8:U:230:VAL:CG2	3.00	0.44
9:H:37:SER:O	9:H:50:THR:HG22	2.18	0.44
9:H:122:ASP:O	9:H:126:LYS:N	2.49	0.44
2:N:146:ALA:HB3	2:N:177:THR:CG2	2.48	0.44
8:U:102:TYR:CD1	9:V:96:THR:HG23	2.53	0.44
12:Y:129:TYR:OH	12:Y:144:ASP:OD1	2.25	0.44
7:T:182:ILE:HD13	7:T:188:GLU:HG3	2.00	0.44
11:X:126:ILE:O	11:X:126:ILE:HG22	2.16	0.44
13:Z:111:GLU:HG2	13:Z:260:TRP:CZ2	2.53	0.44
4:B:92:VAL:HG22	4:B:96:SER:OG	2.18	0.44
10:I:155:SER:O	10:I:156:LEU:HD23	2.18	0.44
2:N:103:LEU:HD11	2:N:128:TYR:CD2	2.53	0.44
5:R:192:VAL:O	5:R:196:VAL:HG23	2.18	0.44
11:X:177:ASP:OD2	11:X:180:SER:OG	2.09	0.44
3:A:112:MET:SD	3:A:117:LEU:HB2	2.58	0.44
5:C:169:LYS:O	5:C:173:GLU:HG3	2.18	0.43
10:I:51:GLN:HG2	10:I:56:ALA:HB2	2.00	0.43
11:J:25:ASP:OD1	11:J:41:LYS:NZ	2.51	0.43
12:Y:38:SER:OG	12:Y:73:GLU:OE2	2.33	0.43
7:F:164:ARG:NH1	7:F:202:ARG:HG2	2.32	0.43
5:R:85:LEU:CD1	5:R:131:VAL:HG21	2.46	0.43
6:S:47:VAL:HG23	6:S:200:VAL:HG21	1.99	0.43
1:1:74:ASN:OD1	1:1:75:GLY:N	2.49	0.43
5:D:171:VAL:CG2	5:D:198:SER:OG	2.67	0.43
8:G:217:TRP:CZ3	8:G:222:GLU:HB2	2.53	0.43
8:G:233:ASP:OD1	8:G:234:LEU:N	2.50	0.43
12:K:38:SER:OG	12:K:73:GLU:OE2	2.27	0.43
5:R:171:VAL:CG2	5:R:198:SER:OG	2.66	0.43
7:T:74:LEU:HD13	7:T:81:ALA:CB	2.49	0.43
12:Y:161:LYS:O	12:Y:165:GLN:HG3	2.17	0.43
13:Z:81:PHE:HA	13:Z:200:ASP:O	2.18	0.43
1:1:41:VAL:HG12	1:1:225:ILE:HD12	1.99	0.43
10:I:192:ILE:HG23	10:I:199:GLY:HA2	2.00	0.43
1:M:88:LYS:HA	1:M:91:VAL:HG12	1.99	0.43
4:B:91:LYS:O	4:B:95:THR:HG22	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:50:LYS:O	7:T:210:ASN:OD1	2.36	0.43
9:V:96:THR:O	9:V:100:VAL:HG23	2.18	0.43
11:X:140:THR:OG1	11:X:177:ASP:OD2	2.33	0.43
6:E:198:LEU:O	6:E:202:LYS:HG3	2.19	0.43
8:G:237:GLU:O	8:G:240:ASP:OD1	2.37	0.43
12:K:3:ILE:HG22	12:K:102:LEU:HD12	2.01	0.43
3:O:164:VAL:HG13	3:O:166:TYR:CE1	2.53	0.43
10:W:233:LYS:HE2	11:X:157:LEU:CD2	2.49	0.43
1:M:212:GLU:OE2	1:M:239:LYS:NZ	2.46	0.43
7:T:7:ASP:O	7:T:21:GLN:NE2	2.44	0.43
8:U:136:ILE:HD11	8:U:164:THR:HG22	2.00	0.43
11:J:52:ILE:HG22	11:J:59:VAL:HG22	2.01	0.43
2:N:253:ASP:O	2:N:256:LYS:HG2	2.19	0.43
8:U:111:PHE:CZ	8:U:115:LEU:HD11	2.53	0.43
13:L:78:THR:HG22	13:L:91:VAL:HG12	2.00	0.43
13:L:81:PHE:HA	13:L:200:ASP:O	2.19	0.43
2:2:116:ALA:HB3	2:2:117:GLU:OE1	2.18	0.43
3:A:32:PHE:CE1	3:A:159:PRO:HD2	2.54	0.43
4:B:74:VAL:HG22	4:B:75:TYR:H	1.83	0.43
10:I:174:ASP:OD1	10:I:174:ASP:O	2.36	0.43
5:Q:12:SER:OG	5:Q:14:ASP:OD1	2.31	0.43
5:R:183:GLU:O	5:R:183:GLU:HG3	2.18	0.43
7:T:175:THR:HG22	7:T:175:THR:O	2.19	0.43
10:W:143:HIS:O	10:W:145:HIS:N	2.52	0.43
11:X:12:VAL:HG23	11:X:137:VAL:HG12	2.01	0.43
2:2:87:SER:OG	2:2:177:THR:HG21	2.19	0.42
3:A:104:PHE:HB2	3:A:112:MET:CE	2.49	0.42
8:U:199:ILE:HG21	8:U:213:LEU:HD13	2.00	0.42
7:F:156:LEU:HD13	7:F:159:THR:HB	2.00	0.42
13:Z:82:ARG:O	13:Z:219:TYR:OH	2.28	0.42
1:M:112:ILE:CD1	1:M:130:ILE:HG21	2.49	0.42
3:O:112:MET:SD	3:O:117:LEU:HB2	2.59	0.42
6:S:46:VAL:O	6:S:221:CYS:HA	2.20	0.42
7:T:81:ALA:HB2	7:T:130:VAL:HG21	1.99	0.42
13:L:82:ARG:O	13:L:219:TYR:OH	2.32	0.42
6:S:201:LEU:HD22	6:S:240:ILE:HD11	2.02	0.42
7:T:227:GLY:O	7:T:230:VAL:HG22	2.19	0.42
9:V:22:ILE:HG21	9:V:63:CYS:HB3	2.01	0.42
11:X:30:SER:O	11:X:31:GLN:HG2	2.19	0.42
5:Q:101:GLU:HG2	12:Y:81:SER:HB3	2.02	0.42
6:S:110:GLU:O	6:S:113:THR:OG1	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:180:THR:HG22	13:Z:182:LYS:H	1.85	0.42
4:B:182:GLU:OE1	4:B:182:GLU:N	2.52	0.42
7:F:171:TYR:HD2	7:F:174:ARG:NH2	2.18	0.42
12:K:24:ILE:HG12	12:Y:138:TYR:OH	2.19	0.42
1:M:41:VAL:HG12	1:M:225:ILE:CD1	2.50	0.42
8:U:110:ALA:HB1	9:V:89:TYR:CD1	2.54	0.42
1:M:62:VAL:HG23	1:M:224:LEU:HD13	2.00	0.42
2:N:39:VAL:HG22	2:N:63:TYR:HD1	1.84	0.42
7:T:156:LEU:HD23	8:U:58:LEU:HA	2.01	0.42
1:1:73:ALA:HB1	1:1:126:VAL:HG21	2.01	0.42
5:C:67:ILE:HG21	5:C:109:LEU:HD21	2.00	0.42
5:C:118:GLN:CG	5:D:80:ALA:HB1	2.50	0.42
6:E:237:ALA:O	6:E:240:ILE:HG22	2.19	0.42
8:G:150:LEU:HD23	8:G:156:TYR:HB3	2.01	0.42
10:I:133:ASP:HB2	10:I:134:PRO:CD	2.50	0.42
5:C:107:GLU:OE1	5:C:148:TYR:OH	2.33	0.42
6:E:50:VAL:HG23	6:E:67:ILE:HD11	2.01	0.42
7:F:182:ILE:HD13	7:F:188:GLU:HG3	2.02	0.42
1:1:57:ARG:NH2	10:I:193:TRP:O	2.45	0.42
2:2:113:LEU:HD22	2:2:117:GLU:OE1	2.19	0.42
12:K:151:MET:HB3	12:K:155:GLU:HB2	2.01	0.42
13:L:272:PHE:HZ	13:L:285:VAL:HG21	1.85	0.42
10:W:126:TYR:CB	10:W:156:LEU:HD13	2.50	0.42
5:Q:192:VAL:O	5:Q:196:VAL:HG23	2.20	0.41
6:E:59:LEU:HD22	6:E:64:ILE:HD11	2.02	0.41
9:H:100:VAL:O	9:H:104:LEU:HD23	2.20	0.41
7:T:74:LEU:HD23	7:T:74:LEU:H	1.84	0.41
7:T:88:LEU:HD11	7:T:108:ALA:HB1	2.02	0.41
8:U:136:ILE:CD1	8:U:164:THR:HG22	2.51	0.41
6:E:46:VAL:HG21	6:E:145:ALA:HB1	2.02	0.41
8:G:217:TRP:CD1	8:G:230:VAL:CG2	3.03	0.41
11:J:11:VAL:HG23	11:J:53:THR:CG2	2.51	0.41
3:A:115:ASP:HB3	3:A:155:TYR:CZ	2.56	0.41
4:B:194:LEU:O	4:B:198:GLU:OE1	2.39	0.41
8:G:217:TRP:HZ3	8:G:222:GLU:HB2	1.85	0.41
11:J:148:MET:HG2	11:J:169:ALA:HA	2.03	0.41
1:M:113:GLN:NE2	1:M:150:TYR:CE1	2.88	0.41
10:W:181:ILE:HD11	10:W:206:VAL:HG21	2.03	0.41
12:K:8:VAL:HG22	12:K:11:SER:O	2.21	0.41
5:C:143:ASP:OD1	5:C:143:ASP:O	2.38	0.41
5:D:119:ARG:NE	5:D:119:ARG:HA	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:110:ALA:HB1	9:H:89:TYR:CD1	2.56	0.41
9:H:20:THR:HG22	9:H:21:SER:N	2.36	0.41
8:U:99:LYS:HA	8:U:102:TYR:O	2.19	0.41
11:X:20:VAL:HG11	11:X:109:ALA:HB1	2.02	0.41
2:2:180:GLY:HA2	2:2:217:LEU:HD21	2.03	0.41
3:A:176:GLN:O	3:A:180:THR:HG23	2.21	0.41
7:F:74:LEU:HD22	7:F:81:ALA:CB	2.50	0.41
7:F:201:LEU:HD11	7:F:206:LEU:HG	2.02	0.41
4:P:110:LEU:O	4:P:114:VAL:HG23	2.21	0.41
1:1:41:VAL:HG12	1:1:225:ILE:CD1	2.50	0.41
7:T:128:TYR:O	7:T:149:PRO:HB3	2.21	0.41
8:U:61:GLN:CD	8:U:61:GLN:O	2.59	0.41
7:T:49:LEU:HB2	7:T:197:ILE:HD11	2.02	0.41
9:V:20:THR:HG22	9:V:21:SER:N	2.36	0.41
9:V:26:THR:CG2	9:V:129:VAL:HG23	2.51	0.41
7:F:79:PRO:HA	7:F:82:ARG:HG2	2.03	0.41
8:G:136:ILE:HD11	8:G:164:THR:HG22	2.03	0.41
10:W:174:ASP:OD1	10:W:174:ASP:O	2.38	0.41
10:W:192:ILE:HG23	10:W:199:GLY:HA2	2.03	0.41
7:F:173:GLU:OE1	7:F:174:ARG:N	2.54	0.40
8:G:216:SER:OG	8:G:227:HIS:CE1	2.75	0.40
7:T:29:ILE:HD11	7:T:149:PRO:HD3	2.03	0.40
8:U:113:ASP:O	8:U:117:GLN:HG2	2.21	0.40
11:X:15:THR:HG23	11:X:118:PRO:CB	2.51	0.40
8:G:113:ASP:O	8:G:117:GLN:HG2	2.20	0.40
1:M:62:VAL:HG12	1:M:72:SER:HB3	2.03	0.40
4:P:196:LEU:CD2	4:P:209:ILE:HD12	2.51	0.40
5:Q:118:GLN:NE2	5:R:81:ASP:OD1	2.54	0.40
7:T:207:THR:OG1	7:T:210:ASN:HB2	2.22	0.40
1:1:88:LYS:HA	1:1:91:VAL:HG12	2.02	0.40
3:A:164:VAL:HG13	3:A:166:TYR:CE1	2.56	0.40
13:L:286:ILE:HD11	11:X:38:LYS:NZ	2.36	0.40
3:O:104:PHE:HB2	3:O:112:MET:CE	2.51	0.40
3:A:129:THR:O	3:A:129:THR:HG22	2.21	0.40
10:I:32:ILE:O	10:I:155:SER:HA	2.21	0.40
10:I:126:TYR:HB2	10:I:156:LEU:HD13	2.03	0.40
1:M:32:LEU:HD11	1:M:169:LEU:CD1	2.51	0.40
1:M:86:ARG:HG2	1:M:115:LEU:HD22	2.04	0.40
4:P:40:THR:HG21	4:P:182:GLU:HA	2.04	0.40
7:T:116:ALA:HB2	7:T:147:PHE:HZ	1.85	0.40
13:Z:189:TYR:O	13:Z:196:ARG:HA	2.22	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	1	196/241 (81%)	192 (98%)	4 (2%)	0	100	100
1	M	196/241 (81%)	192 (98%)	4 (2%)	0	100	100
2	2	214/266 (80%)	209 (98%)	5 (2%)	0	100	100
2	N	214/266 (80%)	209 (98%)	5 (2%)	0	100	100
3	A	232/252 (92%)	230 (99%)	2 (1%)	0	100	100
3	O	232/252 (92%)	230 (99%)	2 (1%)	0	100	100
4	B	242/250 (97%)	242 (100%)	0	0	100	100
4	P	242/250 (97%)	239 (99%)	3 (1%)	0	100	100
5	C	219/254 (86%)	216 (99%)	3 (1%)	0	100	100
5	D	187/254 (74%)	186 (100%)	1 (0%)	0	100	100
5	Q	224/254 (88%)	221 (99%)	3 (1%)	0	100	100
5	R	187/254 (74%)	185 (99%)	2 (1%)	0	100	100
6	E	157/260 (60%)	157 (100%)	0	0	100	100
6	S	157/260 (60%)	157 (100%)	0	0	100	100
7	F	217/234 (93%)	213 (98%)	4 (2%)	0	100	100
7	T	217/234 (93%)	216 (100%)	1 (0%)	0	100	100
8	G	226/288 (78%)	224 (99%)	2 (1%)	0	100	100
8	U	226/288 (78%)	223 (99%)	3 (1%)	0	100	100
9	H	175/215 (81%)	171 (98%)	4 (2%)	0	100	100
9	V	175/215 (81%)	172 (98%)	3 (2%)	0	100	100
10	I	197/261 (76%)	193 (98%)	4 (2%)	0	100	100
10	W	197/261 (76%)	194 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	201/205 (98%)	197 (98%)	4 (2%)	0	100	100
11	X	201/205 (98%)	196 (98%)	5 (2%)	0	100	100
12	K	192/198 (97%)	187 (97%)	5 (3%)	0	100	100
12	Y	192/198 (97%)	186 (97%)	6 (3%)	0	100	100
13	L	195/287 (68%)	194 (100%)	1 (0%)	0	100	100
13	Z	195/287 (68%)	194 (100%)	1 (0%)	0	100	100
All	All	5705/6930 (82%)	5625 (99%)	80 (1%)	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	1	169/201 (84%)	169 (100%)	0	100	100
1	M	169/201 (84%)	169 (100%)	0	100	100
2	2	186/224 (83%)	186 (100%)	0	100	100
2	N	186/224 (83%)	185 (100%)	1 (0%)	88	92
3	A	202/210 (96%)	202 (100%)	0	100	100
3	O	202/210 (96%)	202 (100%)	0	100	100
4	B	203/209 (97%)	202 (100%)	1 (0%)	88	92
4	P	203/209 (97%)	203 (100%)	0	100	100
5	C	201/226 (89%)	201 (100%)	0	100	100
5	D	176/226 (78%)	176 (100%)	0	100	100
5	Q	204/226 (90%)	204 (100%)	0	100	100
5	R	176/226 (78%)	176 (100%)	0	100	100
6	E	143/215 (66%)	143 (100%)	0	100	100
6	S	143/215 (66%)	143 (100%)	0	100	100
7	F	183/193 (95%)	183 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	183/193 (95%)	183 (100%)	0	100	100
8	G	191/239 (80%)	191 (100%)	0	100	100
8	U	191/239 (80%)	191 (100%)	0	100	100
9	H	151/178 (85%)	151 (100%)	0	100	100
9	V	151/178 (85%)	151 (100%)	0	100	100
10	I	169/214 (79%)	169 (100%)	0	100	100
10	W	169/214 (79%)	169 (100%)	0	100	100
11	J	171/173 (99%)	171 (100%)	0	100	100
11	X	171/173 (99%)	171 (100%)	0	100	100
12	K	172/175 (98%)	172 (100%)	0	100	100
12	Y	172/175 (98%)	172 (100%)	0	100	100
13	L	165/235 (70%)	165 (100%)	0	100	100
13	Z	165/235 (70%)	165 (100%)	0	100	100
All	All	4967/5836 (85%)	4965 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	50	LYS
2	N	137	ARG

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

Mol	Chain	Res	Type
1	1	114	HIS
4	B	30	GLN
5	C	231	GLN
6	E	99	HIS
10	I	201	ASN
10	I	218	ASN
12	K	98	GLN
13	L	141	HIS
1	M	114	HIS
6	S	188	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

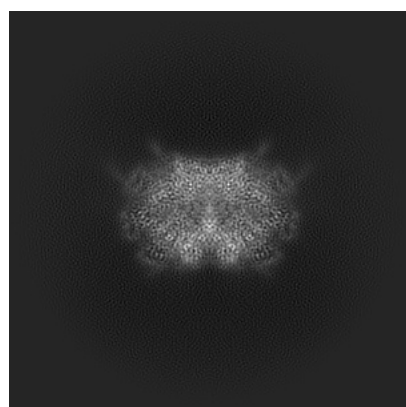
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25847. These allow visual inspection of the internal detail of the map and identification of artifacts.

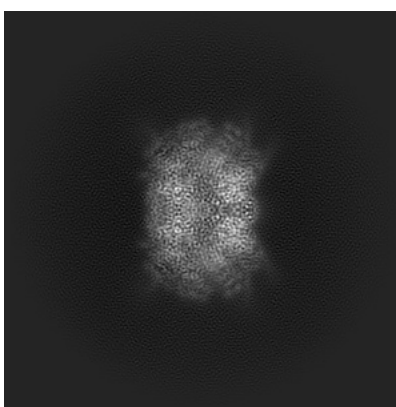
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

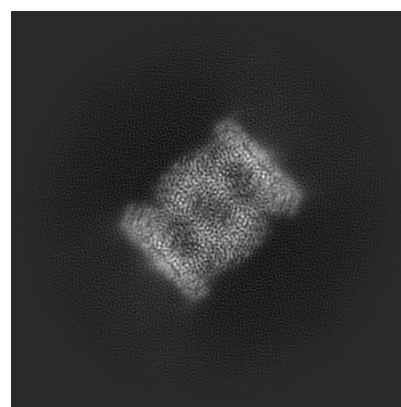
6.1.1 Primary map



X



Y

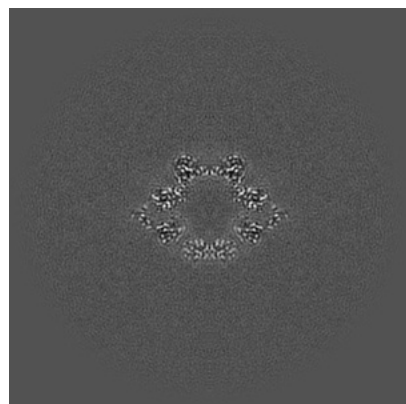


Z

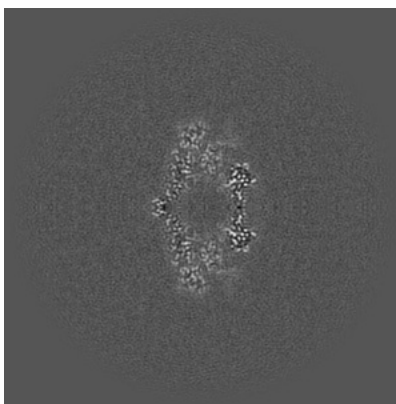
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

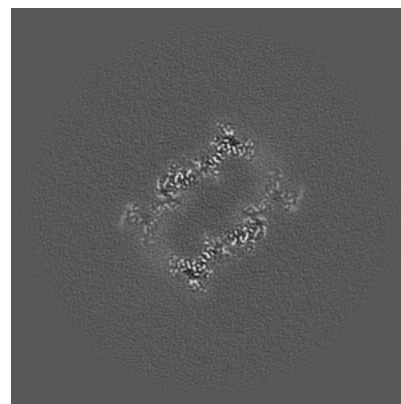
6.2.1 Primary map



X Index: 180



Y Index: 180

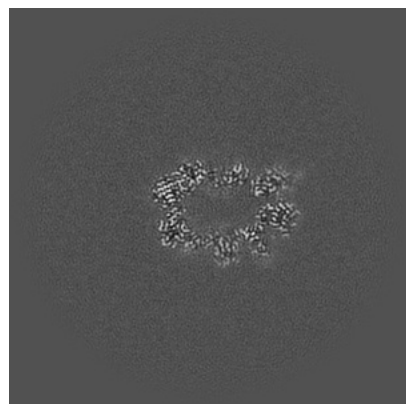


Z Index: 180

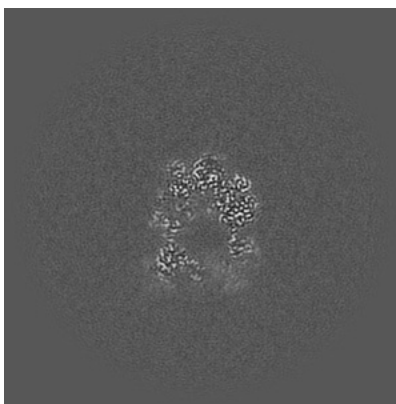
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

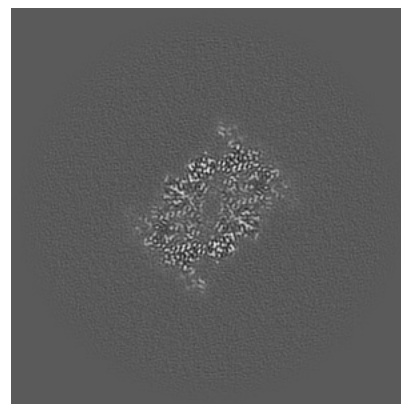
6.3.1 Primary map



X Index: 195



Y Index: 155

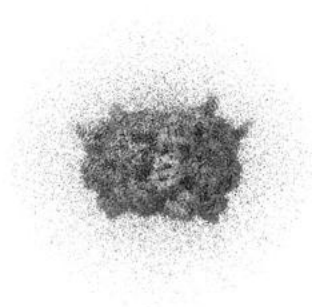


Z Index: 154

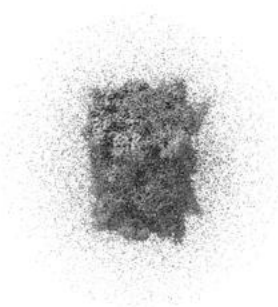
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

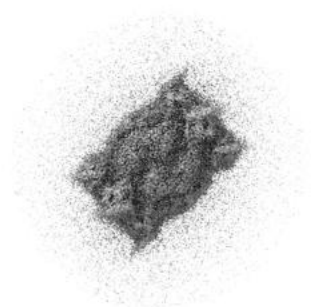
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.385. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

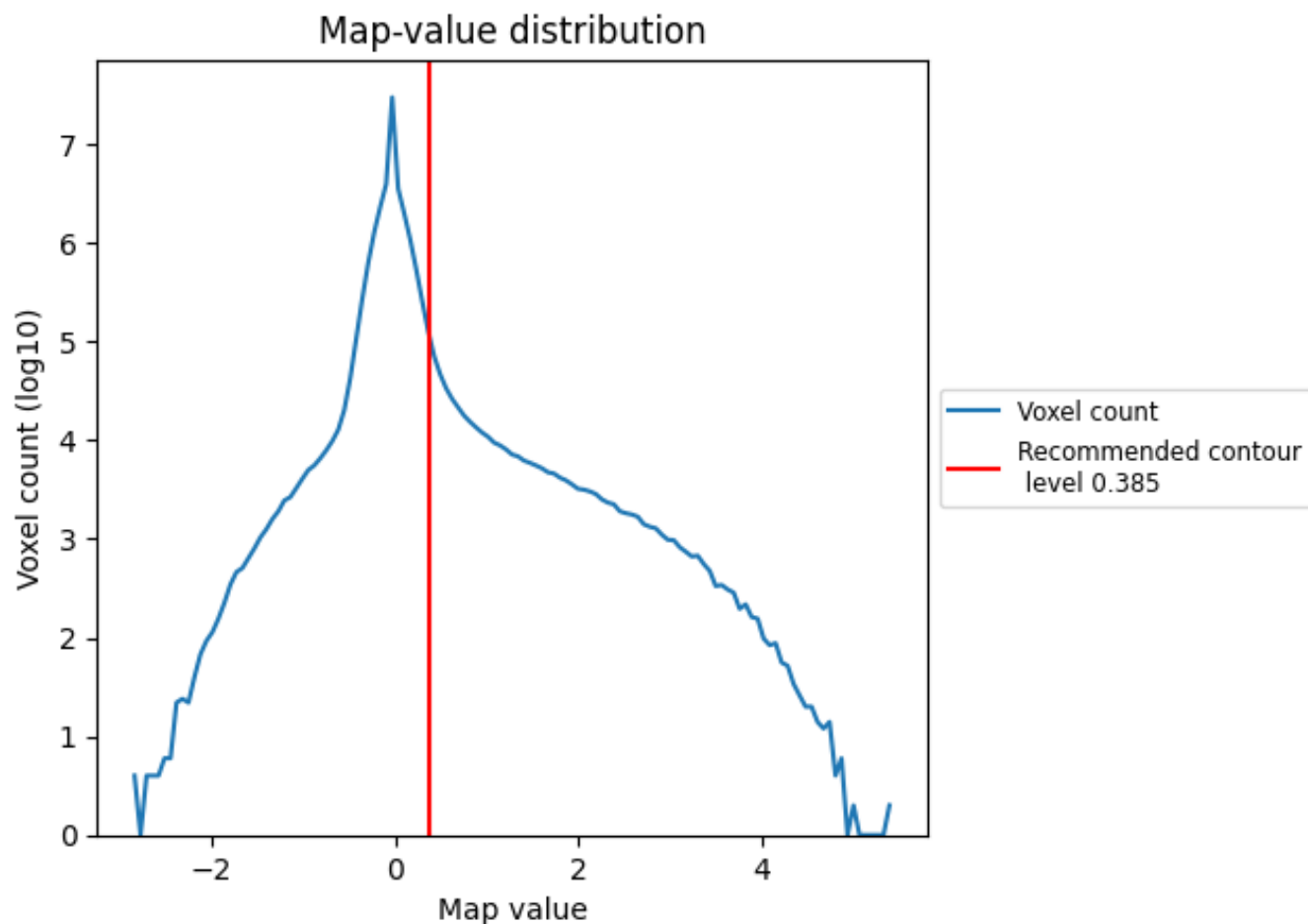
6.5 Mask visualisation

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

7 Map analysis [i](#)

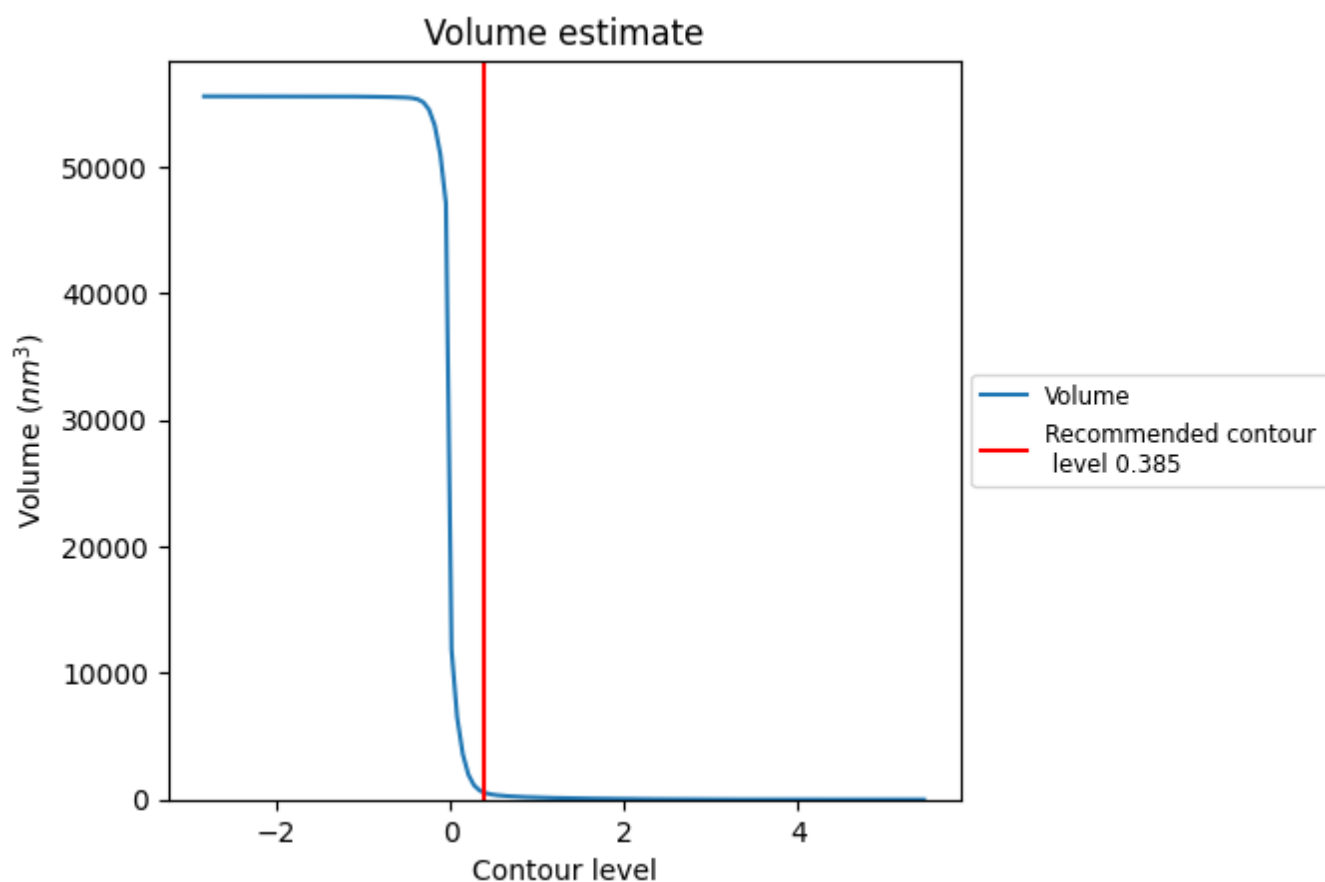
This section contains the results of statistical analysis of the map.

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.

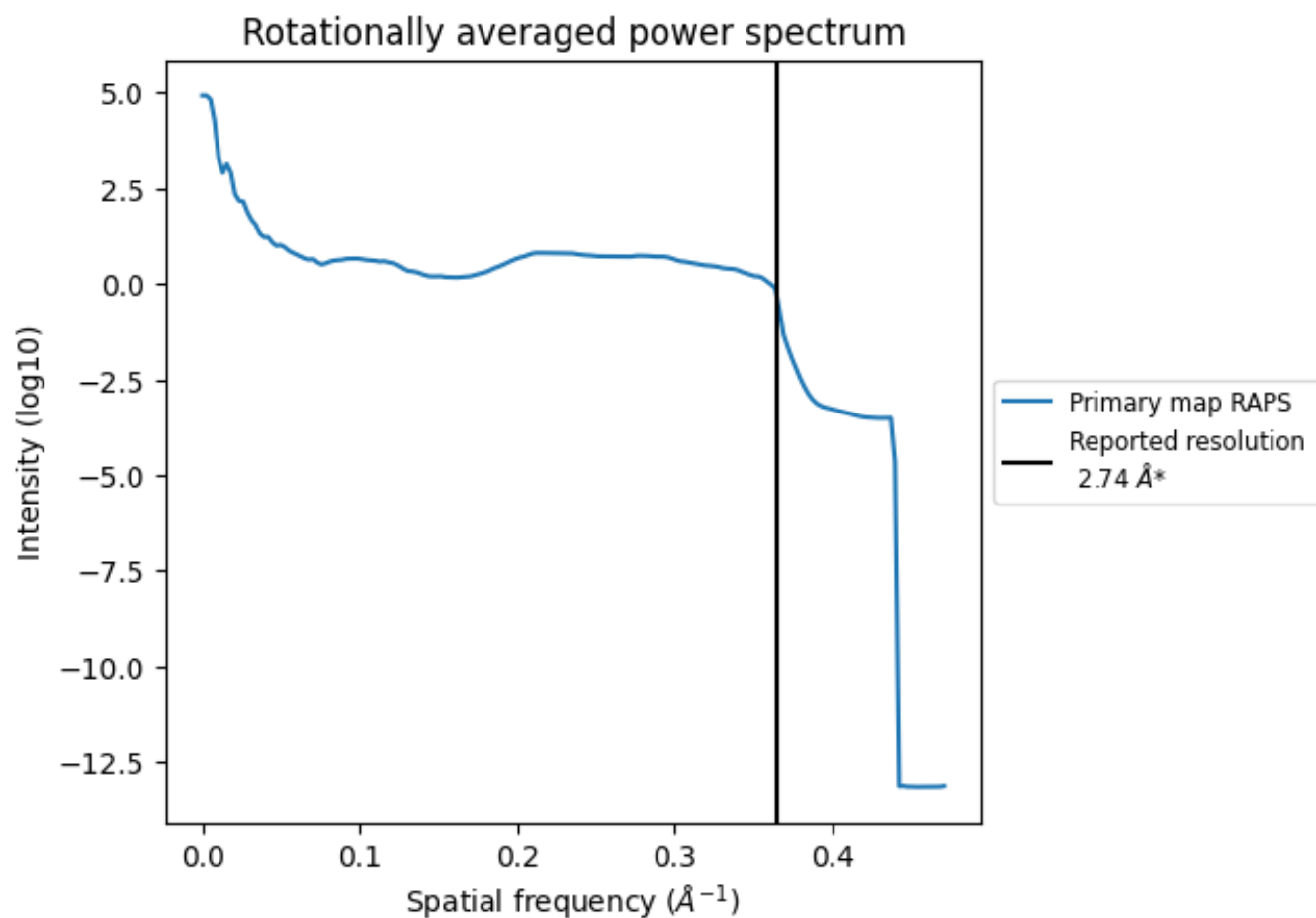
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 569 nm³; this corresponds to an approximate mass of 514 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 Å⁻¹

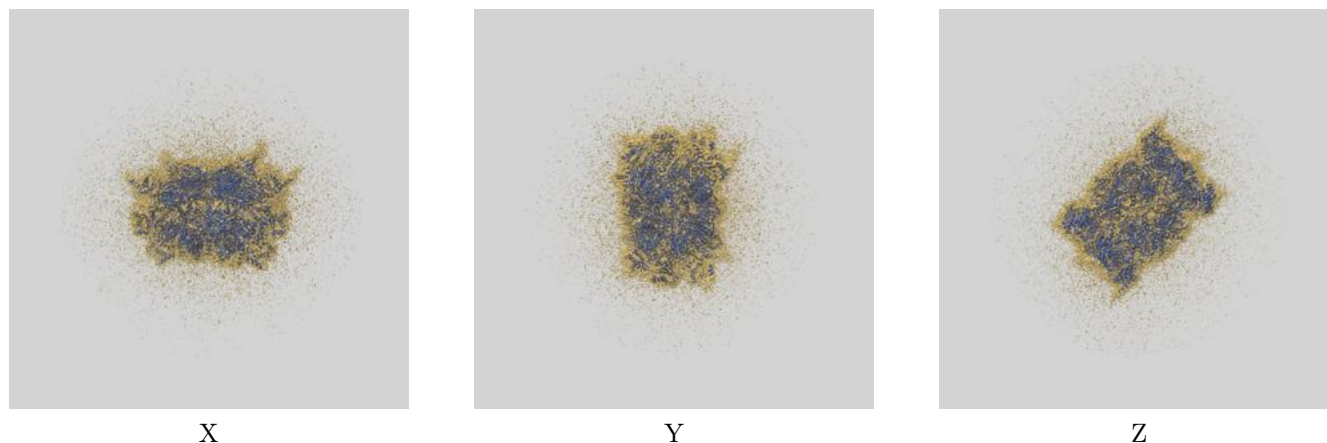
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

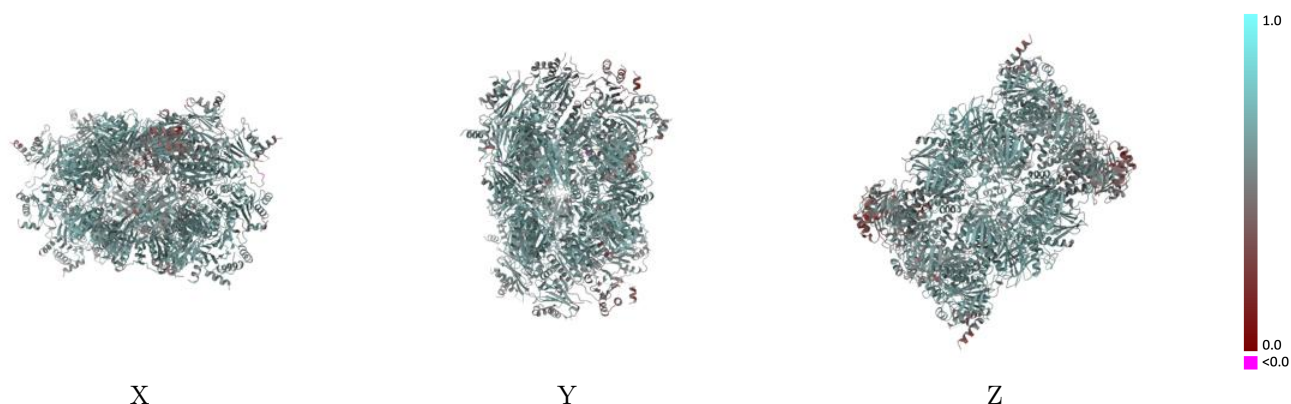
This section contains information regarding the fit between EMDB map EMD-25847 and PDB model 7TEJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



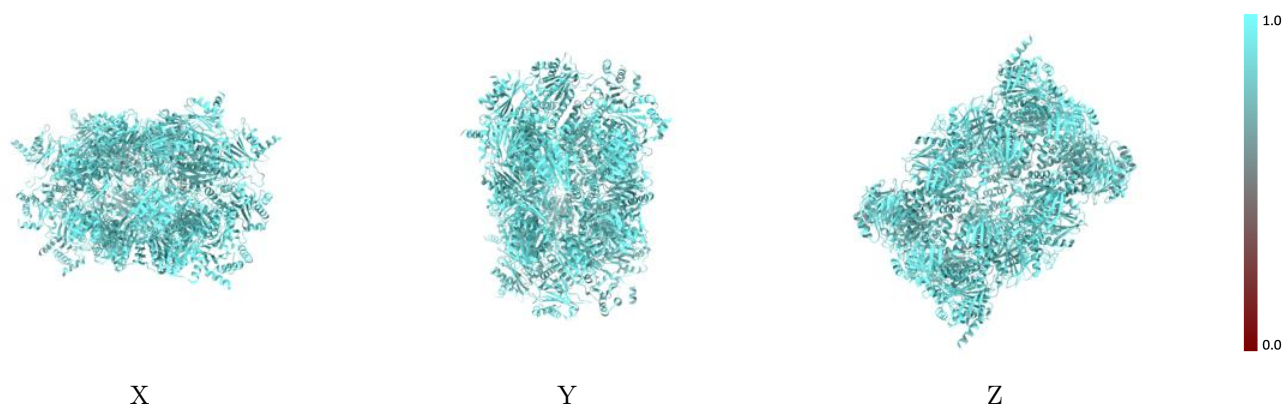
The images above show the 3D surface view of the map at the recommended contour level 0.385 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



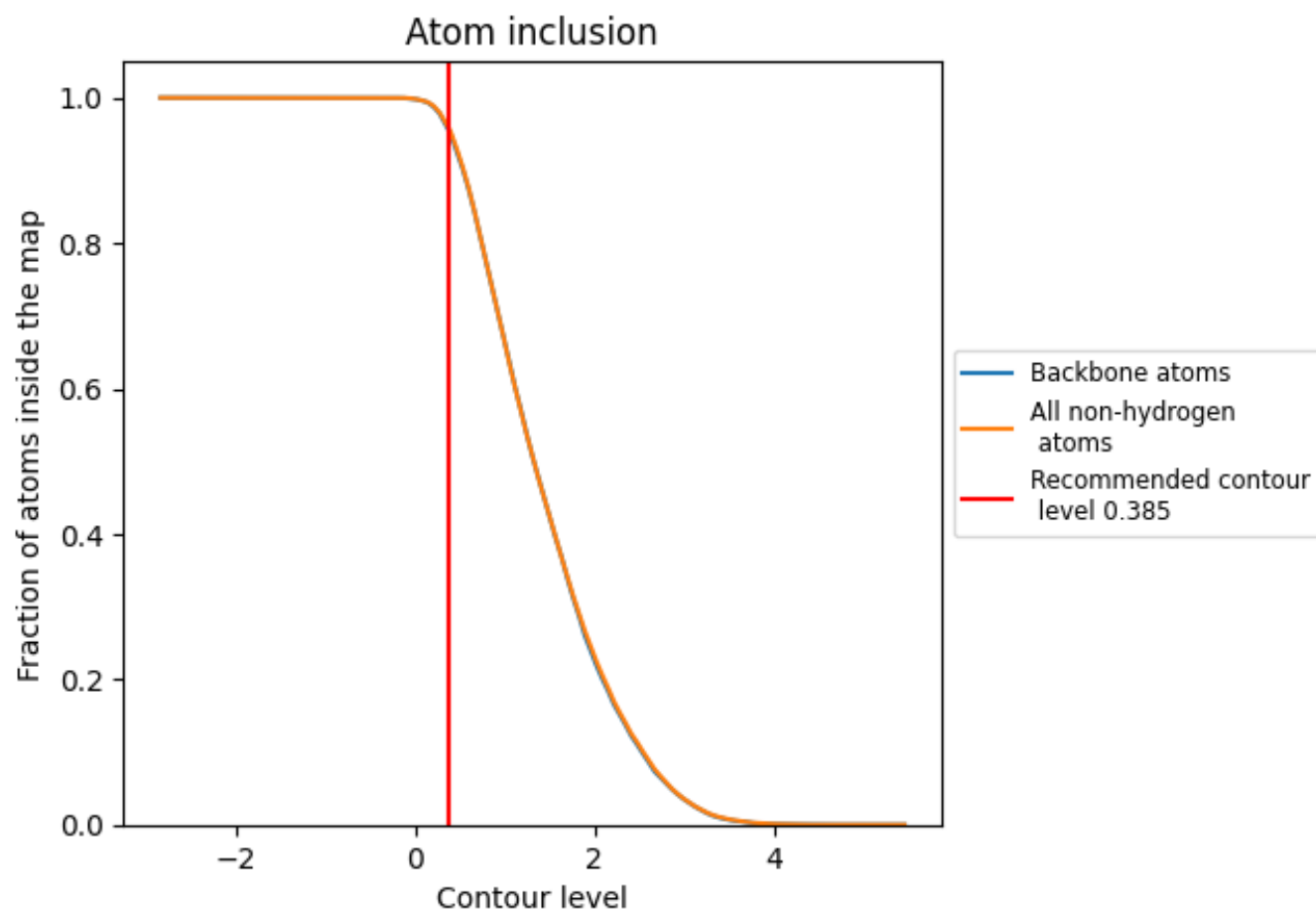
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.385).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.385) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9561	 0.5730
1	 0.9495	 0.5720
2	 0.9719	 0.5940
A	 0.9558	 0.5780
B	 0.9592	 0.5880
C	 0.9503	 0.5590
D	 0.9493	 0.5400
E	 0.8738	 0.4490
F	 0.9487	 0.5420
G	 0.9566	 0.5770
H	 0.9688	 0.5920
I	 0.9798	 0.6080
J	 0.9697	 0.6160
K	 0.9717	 0.6050
L	 0.9619	 0.5900
M	 0.9495	 0.5720
N	 0.9737	 0.5930
O	 0.9580	 0.5800
P	 0.9630	 0.5860
Q	 0.9475	 0.5500
R	 0.9460	 0.5410
S	 0.8653	 0.4450
T	 0.9409	 0.5370
U	 0.9572	 0.5740
V	 0.9724	 0.5920
W	 0.9778	 0.6090
X	 0.9716	 0.6120
Y	 0.9743	 0.6100
Z	 0.9599	 0.5880

