



Full wwPDB EM Validation Report ⓘ

Jul 27, 2026 – 04:43 PM EDT

PDB ID : 10OG / pdb_000010og
EMDB ID : EMD-75334
Title : 20S Alpha 3 Deletion proteasome core particle in complex with Fub1 and Blm10
Authors : Walsh Jr, R.M.; Rawson, S.; Fermin Perez, E.; Venclovaite, U.; Hanna, J.
Deposited on : 2026-01-29
Resolution : 4.10 Å(reported)
Based on initial model : .

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.dev133
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) : 2.50

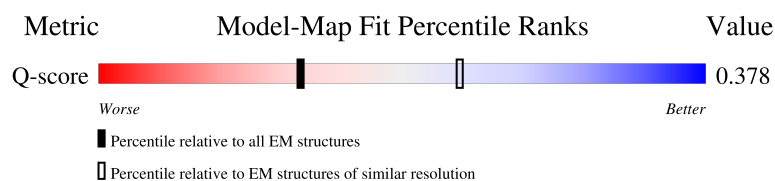
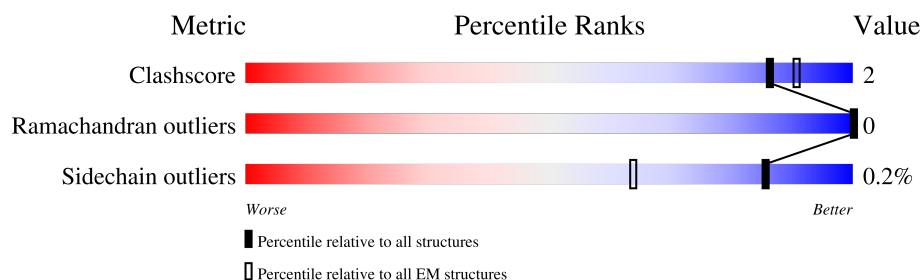
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.



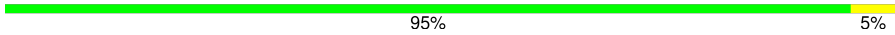
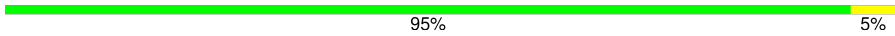
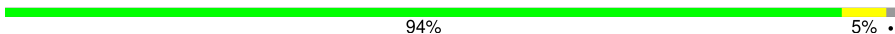
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	252	 91% • 6%
1	O	252	 91% • 6%
2	B	250	 88% • 7%
2	P	250	 89% • 7%

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Mol	Chain	Length	Quality of chain
3	F	234	
3	T	234	
4	G	288	
4	U	288	
5	H	215	
5	V	215	
6	I	261	
6	W	261	
7	J	205	
7	X	205	
8	K	198	
8	Y	198	
9	L	287	
9	Z	287	
10	1	241	
10	M	241	
11	2	266	
11	N	266	
12	C	254	
12	D	254	
12	Q	254	
12	R	254	
13	CA	2167	
13	DA	2167	
14	E	260	

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Mol	Chain	Length	Quality of chain
14	S	260	84% 7% 8%
15	a	250	31% 68%
15	b	250	29% 68%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 157179 atoms, of which 78487 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	238	Total	C	H	N	O	S	0	0
			3764	1198	1882	316	360	8		
1	O	238	Total	C	H	N	O	S	0	0
			3764	1198	1882	316	360	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	232	Total	C	H	N	O	S	0	0
			3562	1128	1789	293	349	3		
2	P	232	Total	C	H	N	O	S	0	0
			3562	1128	1789	293	349	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	234	Total	C	H	N	O	S	0	0
			3615	1134	1812	313	351	5		
3	T	234	Total	C	H	N	O	S	0	0
			3615	1134	1812	313	351	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	241	Total	C	H	N	O	S	0	0
			3756	1197	1875	327	353	4		
4	U	241	Total	C	H	N	O	S	0	0
			3756	1197	1875	327	353	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	196	Total	C	H	N	O	S	0	0
			2992	955	1480	250	300	7		
5	V	196	Total	C	H	N	O	S	0	0
			2992	955	1480	250	300	7		

- Molecule 6 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	220	Total	C	H	N	O	S	0	0
			3349	1054	1679	291	319	6		
6	W	220	Total	C	H	N	O	S	0	0
			3349	1054	1679	291	319	6		

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

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

- Molecule 8 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	K	195	Total	C	H	N	O	S	0	0
			3130	992	1569	264	299	6		
8	Y	195	Total	C	H	N	O	S	0	0
			3130	992	1569	264	299	6		

- Molecule 9 is a protein called Proteasome subunit beta type-5.

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

- Molecule 10 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	M	221	Total	C	H	N	O	S	0	0
			3449	1110	1701	301	333	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	1	221	Total	C	H	N	O	S	0	0
			3449	1110	1701	301	333	4		

- Molecule 11 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	N	230	Total	C	H	N	O	S	0	0
			3595	1137	1798	307	346	7		
11	2	230	Total	C	H	N	O	S	0	0
			3595	1137	1798	307	346	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	C	165	Total	C	H	N	O	S	0	0
			2616	812	1327	219	255	3		
12	D	188	Total	C	H	N	O	S	0	0
			2952	915	1483	253	297	4		
12	Q	165	Total	C	H	N	O	S	0	0
			2616	812	1327	219	255	3		
12	R	188	Total	C	H	N	O	S	0	0
			2952	915	1483	253	297	4		

- Molecule 13 is a protein called Proteasome activator BLM10.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	CA	1878	Total	C	H	N	O	S	0	0
			30567	9844	15290	2532	2832	69		
13	DA	1878	Total	C	H	N	O	S	0	0
			30567	9844	15290	2532	2832	69		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	-23	MET	-	initiating methionine	UNP P43583
CA	-22	HIS	-	expression tag	UNP P43583
CA	-21	HIS	-	expression tag	UNP P43583
CA	-20	HIS	-	expression tag	UNP P43583
CA	-19	HIS	-	expression tag	UNP P43583
CA	-18	HIS	-	expression tag	UNP P43583
CA	-17	HIS	-	expression tag	UNP P43583
CA	-16	HIS	-	expression tag	UNP P43583

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Chain	Residue	Modelled	Actual	Comment	Reference
CA	-15	HIS	-	expression tag	UNP P43583
CA	-14	HIS	-	expression tag	UNP P43583
CA	-13	HIS	-	expression tag	UNP P43583
CA	-12	HIS	-	expression tag	UNP P43583
CA	-11	HIS	-	expression tag	UNP P43583
CA	-10	THR	-	expression tag	UNP P43583
CA	-9	ALA	-	expression tag	UNP P43583
CA	-8	ASN	-	expression tag	UNP P43583
CA	-7	ASN	-	expression tag	UNP P43583
CA	-6	ASP	-	expression tag	UNP P43583
CA	-5	ASP	-	expression tag	UNP P43583
CA	-4	ASP	-	expression tag	UNP P43583
CA	-3	ILE	-	expression tag	UNP P43583
CA	-2	LYS	-	expression tag	UNP P43583
CA	-1	SER	-	expression tag	UNP P43583
CA	0	PRO	-	expression tag	UNP P43583
DA	-23	MET	-	initiating methionine	UNP P43583
DA	-22	HIS	-	expression tag	UNP P43583
DA	-21	HIS	-	expression tag	UNP P43583
DA	-20	HIS	-	expression tag	UNP P43583
DA	-19	HIS	-	expression tag	UNP P43583
DA	-18	HIS	-	expression tag	UNP P43583
DA	-17	HIS	-	expression tag	UNP P43583
DA	-16	HIS	-	expression tag	UNP P43583
DA	-15	HIS	-	expression tag	UNP P43583
DA	-14	HIS	-	expression tag	UNP P43583
DA	-13	HIS	-	expression tag	UNP P43583
DA	-12	HIS	-	expression tag	UNP P43583
DA	-11	HIS	-	expression tag	UNP P43583
DA	-10	THR	-	expression tag	UNP P43583
DA	-9	ALA	-	expression tag	UNP P43583
DA	-8	ASN	-	expression tag	UNP P43583
DA	-7	ASN	-	expression tag	UNP P43583
DA	-6	ASP	-	expression tag	UNP P43583
DA	-5	ASP	-	expression tag	UNP P43583
DA	-4	ASP	-	expression tag	UNP P43583
DA	-3	ILE	-	expression tag	UNP P43583
DA	-2	LYS	-	expression tag	UNP P43583
DA	-1	SER	-	expression tag	UNP P43583
DA	0	PRO	-	expression tag	UNP P43583

- Molecule 14 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	E	238	Total	C	H	N	O	S	0	0
			3686	1159	1839	310	370	8		
14	S	238	Total	C	H	N	O	S	0	0
			3686	1159	1839	310	370	8		

- Molecule 15 is a protein called Silencing boundary-establishment protein FUB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	a	81	Total	C	H	N	O	S	0	0
			1177	393	559	101	121	3		
15	b	81	Total	C	H	N	O	S	0	0
			1178	393	560	101	121	3		

3 Residue-property plots [i](#)

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

- Molecule 1: Proteasome subunit alpha type-1

Chain A:  91% 6%



- Molecule 1: Proteasome subunit alpha type-1

Chain O:  91% 6%



- Molecule 2: Proteasome subunit alpha type-2

Chain B:  88% 7%

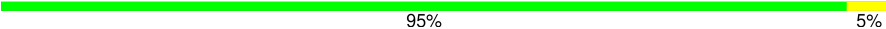


- Molecule 2: Proteasome subunit alpha type-2

Chain P:  89% 7%



- Molecule 3: Proteasome subunit alpha type-6

Chain F:  95% 5%



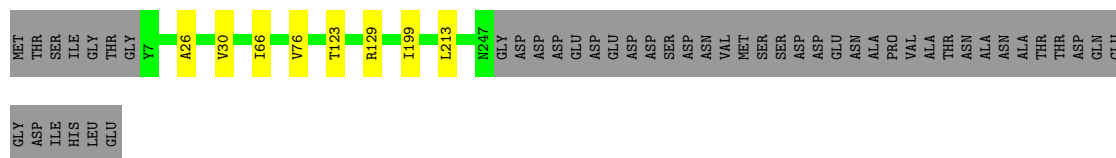
- Molecule 3: Proteasome subunit alpha type-6

Chain T:  95% 5%



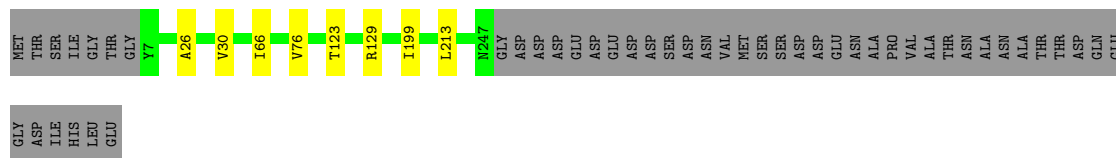
- Molecule 4: Proteasome subunit alpha type-7

Chain G:  81% 16%



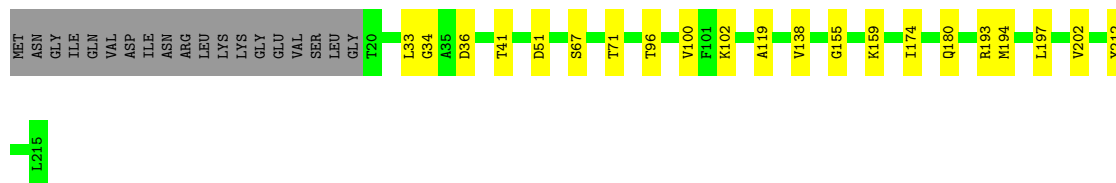
- Molecule 4: Proteasome subunit alpha type-7

Chain U:  81% 16%



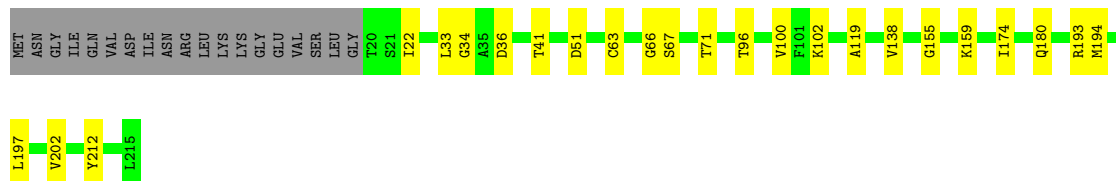
- Molecule 5: Proteasome subunit beta type-1

Chain H:  81% 10% 9%



- Molecule 5: Proteasome subunit beta type-1

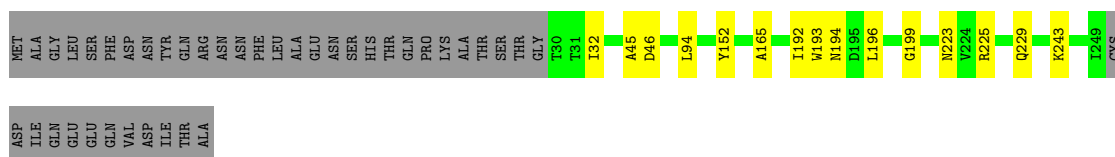
Chain V:  80% 11% 9%



- Molecule 6: Proteasome subunit beta type-2

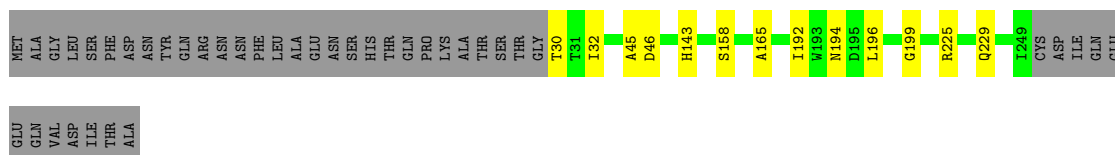
Chain I:  79% 6% 16%





• Molecule 6: Proteasome subunit beta type-2

Chain W: 79% 5% 16%



• Molecule 7: Proteasome subunit beta type-3

Chain J: 94% 5%



• Molecule 7: Proteasome subunit beta type-3

Chain X: 92% 7%



• Molecule 8: Proteasome subunit beta type-4

Chain K: 94% 5%



• Molecule 8: Proteasome subunit beta type-4

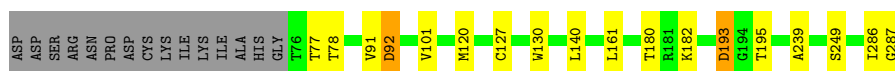
Chain Y: 94% 5%



• Molecule 9: Proteasome subunit beta type-5

Chain L: 68% 6% 26%

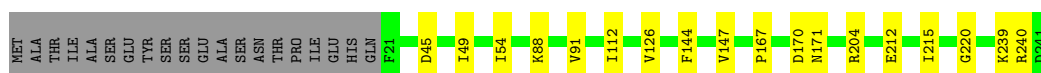




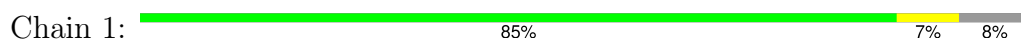
- Molecule 9: Proteasome subunit beta type-5



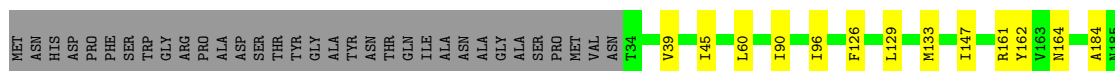
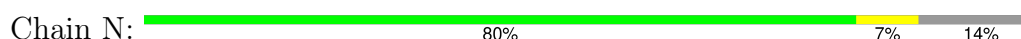
- Molecule 10: Proteasome subunit beta type-6



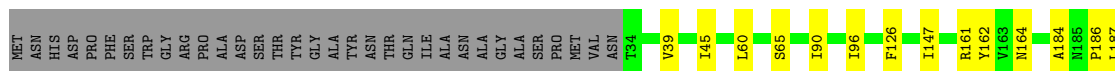
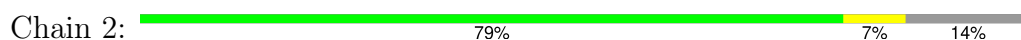
- Molecule 10: Proteasome subunit beta type-6



- Molecule 11: Proteasome subunit beta type-7



- Molecule 11: Proteasome subunit beta type-7



- Molecule 12: Proteasome subunit alpha type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13428	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.253	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00265	Depositor
Map size (Å)	571.2, 571.2, 571.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	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	0.13	0/1919	0.35	0/2599
1	O	0.13	0/1919	0.35	0/2599
2	B	0.14	0/1806	0.36	0/2445
2	P	0.13	0/1806	0.34	0/2445
3	F	0.12	0/1831	0.33	0/2473
3	T	0.13	0/1831	0.34	0/2473
4	G	0.12	0/1921	0.32	0/2594
4	U	0.12	0/1921	0.32	0/2594
5	H	0.14	0/1541	0.34	0/2087
5	V	0.14	0/1541	0.33	0/2087
6	I	0.14	0/1701	0.40	0/2307
6	W	0.13	0/1701	0.41	0/2307
7	J	0.15	0/1605	0.37	0/2166
7	X	0.15	0/1605	0.37	0/2166
8	K	0.12	0/1589	0.33	0/2142
8	Y	0.13	0/1589	0.34	0/2142
9	L	0.14	0/1681	0.36	0/2274
9	Z	0.15	0/1681	0.36	0/2274
10	1	0.14	0/1786	0.39	0/2408
10	M	0.14	0/1786	0.38	0/2408
11	2	0.13	0/1828	0.37	0/2480
11	N	0.13	0/1828	0.37	0/2480
12	C	0.14	0/1299	0.41	0/1751
12	D	0.13	0/1486	0.38	0/2010
12	Q	0.12	0/1299	0.36	0/1751
12	R	0.13	0/1486	0.41	0/2010
13	CA	0.12	0/15622	0.34	0/21165
13	DA	0.12	0/15622	0.35	0/21165
14	E	0.13	0/1872	0.35	0/2522
14	S	0.13	0/1872	0.35	0/2522
15	a	0.14	0/641	0.38	0/873
15	b	0.13	0/641	0.35	0/873
All	All	0.13	0/80256	0.35	0/108592

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	1
4	U	0	1
12	Q	0	1
13	CA	0	1
13	DA	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	CA	1518	ASP	Peptide
13	DA	1518	ASP	Peptide
4	G	129	ARG	Sidechain
12	Q	76	SER	Peptide
4	U	129	ARG	Sidechain

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	1882	1882	1881	7	0
1	O	1882	1882	1881	6	0
2	B	1773	1789	1787	6	0
2	P	1773	1789	1787	6	0
3	F	1803	1812	1809	7	0
3	T	1803	1812	1809	7	0
4	G	1881	1875	1873	4	0
4	U	1881	1875	1873	4	0
5	H	1512	1480	1478	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	1512	1480	1478	18	0
6	I	1670	1679	1676	13	0
6	W	1670	1679	1676	11	0
7	J	1575	1567	1566	12	0
7	X	1575	1567	1566	11	0
8	K	1561	1569	1569	8	0
8	Y	1561	1569	1569	8	0
9	L	1644	1593	1592	12	0
9	Z	1644	1593	1592	19	0
10	1	1748	1701	1700	15	0
10	M	1748	1701	1700	15	0
11	2	1797	1798	1797	15	0
11	N	1797	1798	1797	11	0
12	C	1289	1327	1320	6	0
12	D	1469	1483	1479	7	0
12	Q	1289	1327	1320	0	0
12	R	1469	1483	1479	8	0
13	CA	15277	15290	15281	61	0
13	DA	15277	15290	15281	49	0
14	E	1847	1839	1837	8	0
14	S	1847	1839	1837	11	0
15	a	618	559	556	4	0
15	b	618	560	556	7	0
All	All	78692	78487	78402	333	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 2.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:177:ARG:HD3	9:Z:101:VAL:HG11	1.82	0.62
1:A:129:THR:HG22	1:A:129:THR:O	2.00	0.61
1:O:129:THR:HG22	1:O:129:THR:O	2.00	0.61
9:L:101:VAL:HG11	7:X:177:ARG:HD3	1.83	0.60
11:2:65:SER:HA	15:a:129:PHE:CE1	2.37	0.59
13:DA:1781:VAL:HG12	13:DA:1781:VAL:O	2.03	0.59
13:CA:1781:VAL:HG12	13:CA:1781:VAL:O	2.03	0.58
5:H:33:LEU:HD21	5:H:119:ALA:HB3	1.85	0.58
12:D:42:VAL:HG11	12:D:136:ALA:HB1	1.86	0.58
11:2:192:VAL:HG13	11:2:192:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:189:ILE:HD11	2:P:213:ILE:HD11	1.86	0.57
11:N:192:VAL:O	11:N:192:VAL:HG13	2.04	0.57
13:DA:617:ASP:HA	13:DA:724:ILE:HD11	1.86	0.57
9:Z:77:THR:HG21	9:Z:239:ALA:HB1	1.86	0.57
13:DA:2076:PHE:HB3	13:DA:2077:PRO:HD3	1.88	0.56
13:CA:1510:CYS:SG	13:CA:1638:LEU:HD13	2.46	0.56
13:CA:2076:PHE:HB3	13:CA:2077:PRO:HD3	1.87	0.55
11:2:45:ILE:HD12	11:2:184:ALA:HB1	1.88	0.55
7:J:142:ALA:HB2	7:J:178:ASP:HB2	1.89	0.55
11:N:45:ILE:HD12	11:N:184:ALA:HB1	1.89	0.55
5:V:41:THR:HG23	5:V:41:THR:O	2.08	0.54
12:C:106:VAL:O	12:C:110:THR:HG23	2.08	0.54
5:H:41:THR:O	5:H:41:THR:HG23	2.08	0.54
13:DA:1510:CYS:SG	13:DA:1638:LEU:HD13	2.48	0.53
11:N:96:ILE:HD13	11:N:147:ILE:HD11	1.90	0.53
3:F:74:LEU:HD22	3:F:81:ALA:HB1	1.89	0.53
2:B:189:ILE:HD11	2:B:213:ILE:HD11	1.92	0.52
6:W:30:THR:N	6:W:158:SER:HG	2.08	0.52
7:J:177:ARG:CD	9:Z:101:VAL:HG11	2.39	0.52
9:L:130:TRP:CD2	9:L:161:LEU:HD21	2.45	0.52
9:Z:130:TRP:CD2	9:Z:161:LEU:HD21	2.45	0.52
9:L:77:THR:HG21	9:L:239:ALA:HB1	1.91	0.51
3:T:74:LEU:HD22	3:T:81:ALA:HB1	1.92	0.51
5:V:33:LEU:HD21	5:V:119:ALA:HB3	1.90	0.51
9:L:193:ASP:C	9:L:193:ASP:OD1	2.54	0.51
11:2:96:ILE:HD13	11:2:147:ILE:HD11	1.92	0.51
13:CA:1018:VAL:O	13:CA:1022:THR:HG23	2.10	0.51
13:DA:1018:VAL:O	13:DA:1022:THR:HG23	2.11	0.51
13:DA:1386:LEU:HA	13:DA:1389:ILE:HG22	1.93	0.51
5:H:174:ILE:HG22	5:H:194:MET:HE2	1.93	0.50
3:F:144:LEU:C	3:F:144:LEU:HD23	2.37	0.50
13:CA:1386:LEU:HA	13:CA:1389:ILE:HG22	1.93	0.50
9:L:101:VAL:HG11	7:X:177:ARG:CD	2.40	0.50
13:CA:662:ILE:HG21	13:CA:695:ILE:CD1	2.42	0.50
9:Z:193:ASP:OD1	9:Z:193:ASP:C	2.54	0.50
4:G:123:THR:HG22	4:G:123:THR:O	2.12	0.50
4:U:123:THR:HG22	4:U:123:THR:O	2.12	0.50
14:E:236:THR:O	14:E:240:ILE:HG12	2.12	0.50
3:T:144:LEU:C	3:T:144:LEU:HD23	2.36	0.49
7:J:149:MET:HG2	7:J:170:ALA:HA	1.94	0.49
13:DA:2079:PRO:HD2	13:DA:2082:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:GLU:O	2:B:117:ILE:HG12	2.12	0.49
11:N:187:LEU:HD21	6:W:165:ALA:O	2.12	0.49
1:A:28:VAL:HG21	1:A:129:THR:HG23	1.95	0.49
4:G:66:ILE:HG12	4:G:76:VAL:HG12	1.93	0.49
10:M:167:PRO:C	7:X:149:MET:HE1	2.38	0.49
12:D:175:LEU:O	12:D:179:TYR:O	2.30	0.49
4:U:66:ILE:HG12	4:U:76:VAL:HG12	1.94	0.49
6:I:196:LEU:HD22	10:1:215:ILE:O	2.12	0.49
7:J:173:ASN:ND2	10:1:171:ASN:OD1	2.46	0.49
7:X:101:GLY:HA2	15:b:151:GLY:HA3	1.94	0.49
13:CA:326:TYR:CG	13:CA:327:PRO:HD2	2.48	0.49
8:K:2:ASP:HB2	8:K:47:ALA:HB1	1.95	0.49
5:H:193:ARG:HH22	11:2:258:ILE:HB	1.77	0.49
3:T:126:ARG:HG2	3:T:126:ARG:HH11	1.78	0.49
13:DA:829:VAL:HG21	13:DA:881:VAL:HG13	1.94	0.48
13:CA:1376:LEU:O	13:CA:1377:GLU:HG2	2.13	0.48
9:L:286:ILE:HG23	9:L:287:GLY:N	2.28	0.48
13:CA:1322:ILE:HB	13:CA:1323:PRO:HD3	1.95	0.48
13:DA:1376:LEU:O	13:DA:1377:GLU:HG2	2.13	0.48
5:H:51:ASP:HB3	11:2:260:GLY:HA2	1.95	0.48
6:I:165:ALA:O	11:2:187:LEU:HD21	2.14	0.48
5:V:174:ILE:HG22	5:V:194:MET:HE2	1.95	0.48
7:X:149:MET:HG2	7:X:170:ALA:HA	1.95	0.48
12:R:175:LEU:O	12:R:179:TYR:O	2.31	0.48
9:Z:171:SER:OG	15:b:167:ALA:HB3	2.14	0.48
12:R:42:VAL:HG11	12:R:136:ALA:HB1	1.94	0.48
14:S:236:THR:O	14:S:240:ILE:HG12	2.12	0.48
3:F:126:ARG:HG2	3:F:126:ARG:HH11	1.78	0.48
13:CA:811:PHE:CE1	13:CA:873:LEU:HD13	2.49	0.48
13:DA:1322:ILE:HB	13:DA:1323:PRO:HD3	1.95	0.48
4:G:199:ILE:HG21	4:G:213:LEU:HD13	1.96	0.47
9:Z:78:THR:HG22	9:Z:91:VAL:HG12	1.96	0.47
9:Z:286:ILE:HG23	9:Z:287:GLY:N	2.28	0.47
10:1:126:VAL:HG13	10:1:126:VAL:O	2.13	0.47
9:Z:102:ALA:HB1	15:a:199:ILE:HD12	1.96	0.47
13:CA:1806:THR:HG21	13:CA:1889:GLU:HG2	1.94	0.47
13:CA:1957:VAL:HG23	13:CA:1959:LEU:HG	1.95	0.47
7:J:149:MET:HE1	10:1:167:PRO:C	2.38	0.47
10:M:171:ASN:OD1	7:X:173:ASN:ND2	2.47	0.47
6:W:143:HIS:CE1	15:b:133:TYR:CE2	3.02	0.47
12:C:174:PHE:O	12:C:177:LYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:174:MET:SD	8:Y:174:MET:SD	3.13	0.47
13:CA:410:PHE:CE1	13:CA:414:ILE:HD11	2.49	0.47
12:C:169:LYS:O	12:C:172:ARG:HB3	2.15	0.47
12:C:212:ILE:HG13	12:C:229:ILE:HD12	1.97	0.47
9:L:78:THR:HG22	9:L:91:VAL:HG12	1.97	0.47
11:2:39:VAL:O	11:2:90:ILE:HG12	2.14	0.47
11:2:60:LEU:HD23	11:2:223:ARG:O	2.14	0.46
13:CA:619:ILE:CD1	13:CA:648:VAL:HG21	2.45	0.46
13:CA:829:VAL:HG21	13:CA:881:VAL:HG13	1.97	0.46
14:E:46:VAL:HG11	14:E:145:ALA:HB1	1.98	0.46
13:DA:619:ILE:CD1	13:DA:648:VAL:HG21	2.45	0.46
13:DA:662:ILE:HG21	13:DA:695:ILE:CD1	2.45	0.46
13:DA:1806:THR:HG21	13:DA:1889:GLU:HG2	1.97	0.46
13:DA:1510:CYS:SG	13:DA:1638:LEU:HD22	2.56	0.46
13:DA:1851:LYS:O	13:DA:1855:ILE:HG12	2.15	0.46
7:J:177:ARG:NE	10:1:170:ASP:OD2	2.47	0.46
10:M:126:VAL:O	10:M:126:VAL:HG13	2.14	0.46
13:DA:605:LEU:CD1	13:DA:648:VAL:HG13	2.46	0.46
13:DA:326:TYR:CG	13:DA:327:PRO:HD2	2.50	0.46
3:T:185:ASN:HB2	3:T:186:PRO:HA	1.97	0.46
9:Z:112:ILE:HG23	9:Z:135:GLY:HA2	1.97	0.46
13:DA:410:PHE:CZ	13:DA:414:ILE:HD11	2.51	0.46
13:CA:756:LYS:HA	13:CA:800:LEU:HD21	1.98	0.46
13:CA:2020:ASN:HD21	14:E:1:MET:HE1	1.81	0.46
5:V:66:GLY:O	15:b:132:GLU:HG2	2.16	0.46
12:D:167:ASN:O	12:D:168:SER:C	2.58	0.46
10:M:54:ILE:HD12	10:M:54:ILE:N	2.31	0.46
5:V:67:SER:O	5:V:71:THR:HG23	2.16	0.46
13:CA:1851:LYS:O	13:CA:1855:ILE:HG12	2.16	0.46
13:DA:410:PHE:CE1	13:DA:414:ILE:HD11	2.51	0.46
13:DA:662:ILE:HG21	13:DA:695:ILE:HD11	1.96	0.46
12:C:68:ASP:HB3	12:C:71:VAL:HG12	1.97	0.46
13:DA:756:LYS:HA	13:DA:800:LEU:HD21	1.97	0.46
5:H:180:GLN:HE21	5:V:159:LYS:HE2	1.81	0.45
13:CA:847:ILE:HG21	13:CA:899:PHE:HZ	1.81	0.45
2:B:75:TYR:HB3	2:B:82:TYR:CD1	2.51	0.45
5:V:102:LYS:HB2	5:V:138:VAL:CG2	2.46	0.45
13:CA:1915:VAL:HG21	13:CA:1966:LEU:CD2	2.47	0.45
13:DA:649:ILE:HG21	13:DA:690:SER:HB3	1.98	0.45
8:K:173:PRO:HD3	8:Y:25:ILE:O	2.17	0.45
12:C:171:VAL:O	12:C:172:ARG:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:200:PHE:CD1	15:b:202:PRO:HD2	2.51	0.45
11:N:126:PHE:CZ	11:N:161:ARG:HB3	2.50	0.45
7:X:142:ALA:HB2	7:X:178:ASP:HB2	1.98	0.45
13:CA:439:VAL:HG11	13:CA:462:ILE:HD11	1.98	0.45
13:DA:2082:ILE:HB	13:DA:2083:PRO:HD3	1.97	0.45
6:I:225:ARG:HG3	10:1:212:GLU:OE2	2.17	0.45
12:R:167:ASN:O	12:R:168:SER:C	2.58	0.45
13:CA:662:ILE:HG21	13:CA:695:ILE:HD11	1.99	0.45
13:CA:2079:PRO:HD2	13:CA:2082:ILE:HD12	1.98	0.45
13:DA:811:PHE:CE1	13:DA:873:LEU:HD13	2.51	0.45
13:DA:1792:HIS:CD2	13:DA:1797:VAL:HG11	2.52	0.45
11:2:65:SER:H	15:a:127:PRO:HB2	1.80	0.45
13:DA:1472:GLN:O	13:DA:1512:LYS:HD2	2.17	0.45
5:H:102:LYS:HB2	5:H:138:VAL:CG2	2.47	0.45
10:M:212:GLU:OE2	6:W:225:ARG:HG3	2.17	0.45
10:M:215:ILE:O	6:W:196:LEU:HD22	2.16	0.45
9:Z:77:THR:HG21	9:Z:239:ALA:CB	2.46	0.45
13:CA:2082:ILE:HB	13:CA:2083:PRO:HD3	1.98	0.44
1:O:28:VAL:HG21	1:O:129:THR:HG23	1.99	0.44
13:CA:1792:HIS:CD2	13:CA:1797:VAL:HG11	2.52	0.44
3:F:185:ASN:HB2	3:F:186:PRO:HA	1.97	0.44
6:I:196:LEU:HD11	10:1:49:ILE:HD12	1.98	0.44
5:V:34:GLY:HA2	5:V:193:ARG:O	2.16	0.44
13:CA:617:ASP:HA	13:CA:724:ILE:HD11	1.99	0.44
12:R:179:TYR:HB2	12:R:194:LEU:HD11	1.99	0.44
8:K:25:ILE:O	8:Y:173:PRO:HD3	2.18	0.44
10:1:112:ILE:HG21	10:1:144:PHE:CE2	2.52	0.44
13:CA:665:VAL:O	13:CA:669:LEU:HG	2.18	0.44
10:M:239:LYS:O	10:M:240:ARG:HG2	2.18	0.44
7:X:159:GLU:HG3	7:X:160:PRO:HD2	2.00	0.44
13:CA:291:VAL:O	13:CA:291:VAL:CG1	2.66	0.44
13:DA:2020:ASN:HD21	14:S:1:MET:HE1	1.83	0.44
7:X:11:ILE:CG2	7:X:146:LEU:HD11	2.48	0.44
6:I:192:ILE:HG23	6:I:199:GLY:HA2	1.99	0.44
13:CA:266:VAL:HG21	13:CA:1410:LEU:HG	1.99	0.44
12:D:175:LEU:HA	12:D:179:TYR:HB3	1.99	0.44
5:H:67:SER:O	5:H:71:THR:HG23	2.18	0.44
10:1:49:ILE:HD13	10:1:54:ILE:HA	2.00	0.44
13:CA:912:LEU:O	13:CA:916:THR:HG23	2.18	0.44
3:F:34:VAL:HG13	3:F:197:ILE:HD11	2.00	0.43
8:Y:2:ASP:HB2	8:Y:47:ALA:HB1	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:PHE:CE2	2:B:247:LEU:HD22	2.53	0.43
6:W:30:THR:HB	15:b:224:ASP:OD2	2.18	0.43
13:CA:410:PHE:CZ	13:CA:414:ILE:HD11	2.52	0.43
13:DA:780:GLN:OE1	13:DA:1229:ILE:HA	2.18	0.43
10:1:54:ILE:N	10:1:54:ILE:HD12	2.32	0.43
5:H:34:GLY:HA2	5:H:193:ARG:O	2.18	0.43
5:H:197:LEU:HD22	5:H:202:VAL:HG12	2.01	0.43
10:M:112:ILE:HG21	10:M:144:PHE:CE2	2.53	0.43
2:P:75:TYR:HB3	2:P:82:TYR:CD1	2.53	0.43
1:A:83:VAL:HG11	1:A:90:ALA:CB	2.48	0.43
1:O:129:THR:O	1:O:129:THR:CG2	2.67	0.43
13:DA:291:VAL:O	13:DA:291:VAL:CG1	2.66	0.43
13:DA:685:ILE:O	13:DA:689:VAL:HG23	2.18	0.43
13:DA:912:LEU:O	13:DA:916:THR:HG23	2.18	0.43
5:H:96:THR:O	5:H:100:VAL:HG23	2.19	0.43
10:1:200:ILE:HD11	10:1:225:ILE:HD11	2.01	0.43
7:X:12:VAL:HG23	7:X:54:THR:HG23	2.00	0.43
13:DA:1957:VAL:HG23	13:DA:1959:LEU:HG	2.00	0.43
12:R:157:SER:HA	14:S:63:SER:HB2	2.01	0.43
9:Z:193:ASP:OD1	9:Z:195:THR:HG23	2.18	0.43
13:CA:605:LEU:CD1	13:CA:648:VAL:HG13	2.49	0.43
5:H:159:LYS:HE2	5:V:180:GLN:HE21	1.84	0.43
10:M:170:ASP:OD2	7:X:177:ARG:NE	2.50	0.42
13:DA:2011:ALA:HB2	13:DA:2063:LEU:HB3	2.00	0.42
2:B:64:VAL:HG11	2:B:212:ALA:HB2	2.01	0.42
9:L:92:ASP:HA	9:L:249:SER:O	2.19	0.42
11:N:39:VAL:O	11:N:90:ILE:HG12	2.19	0.42
11:2:126:PHE:CZ	11:2:161:ARG:HB3	2.53	0.42
13:CA:685:ILE:O	13:CA:689:VAL:HG23	2.18	0.42
11:N:186:PRO:HA	6:W:194:ASN:OD1	2.19	0.42
1:O:216:THR:HG22	1:O:217:GLU:N	2.35	0.42
12:D:179:TYR:HB2	12:D:194:LEU:HD11	2.00	0.42
13:DA:665:VAL:O	13:DA:669:LEU:HG	2.18	0.42
8:K:146:HIS:CE1	9:Z:218:ASN:HD21	2.37	0.42
5:V:51:ASP:HA	5:V:193:ARG:HH11	1.85	0.42
13:CA:1750:PHE:CE2	13:CA:1784:LEU:HD11	2.54	0.42
1:O:83:VAL:HG11	1:O:90:ALA:CB	2.49	0.42
14:E:64:ILE:HG22	14:E:66:LYS:H	1.84	0.42
12:R:226:SER:HA	12:R:229:ILE:HG12	2.02	0.42
13:DA:105:TYR:CE1	13:DA:117:ARG:HA	2.54	0.42
13:DA:1872:ILE:O	13:DA:1873:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:194:ASN:OD1	11:2:186:PRO:HA	2.20	0.42
9:L:180:THR:HG22	9:L:182:LYS:H	1.84	0.42
13:CA:324:LEU:HG	13:CA:325:PRO:HD2	2.00	0.42
13:CA:1023:LEU:HD21	13:CA:1179:ILE:HD13	2.01	0.42
3:F:78:ALA:N	3:F:79:PRO:HD2	2.35	0.42
13:CA:923:ALA:O	13:CA:926:THR:HG22	2.20	0.42
14:S:225:GLN:HG2	14:S:226:ASP:OD1	2.20	0.42
6:I:32:ILE:HG12	6:I:45:ALA:HB2	2.01	0.42
13:CA:1856:ILE:HD12	13:CA:1883:ILE:HG13	2.02	0.42
12:D:44:LEU:O	12:D:212:ILE:HA	2.20	0.42
13:DA:1559:ASN:N	13:DA:1560:PRO:CD	2.83	0.42
12:R:175:LEU:O	12:R:179:TYR:HB3	2.19	0.42
5:H:155:GLY:HA2	5:V:180:GLN:OE1	2.19	0.41
7:J:142:ALA:HB2	7:J:178:ASP:CB	2.50	0.41
9:L:120:MET:HA	9:L:127:CYS:SG	2.60	0.41
13:CA:782:THR:HG21	13:CA:824:PRO:HB3	2.02	0.41
13:CA:826:ALA:HB2	13:CA:880:ASP:HB3	2.02	0.41
14:E:163:THR:HG22	14:E:164:PHE:N	2.34	0.41
7:J:11:ILE:CG2	7:J:146:LEU:HD11	2.50	0.41
10:M:49:ILE:HD12	6:W:196:LEU:HD11	2.01	0.41
4:U:199:ILE:HG21	4:U:213:LEU:HD13	2.00	0.41
13:CA:1293:PRO:HA	13:CA:1296:TYR:CE2	2.55	0.41
11:N:60:LEU:HD23	11:N:223:ARG:O	2.19	0.41
8:Y:66:LEU:HB2	12:R:94:GLN:HG3	2.02	0.41
9:Z:180:THR:HG22	9:Z:182:LYS:H	1.85	0.41
13:CA:1240:LEU:HD23	13:CA:1243:VAL:HG21	2.01	0.41
13:CA:1959:LEU:HB3	13:CA:1963:GLN:HB2	2.02	0.41
14:S:46:VAL:HG11	14:S:145:ALA:HB1	2.02	0.41
14:S:83:ALA:O	14:S:86:ARG:HG2	2.19	0.41
1:A:83:VAL:HG11	1:A:90:ALA:HB2	2.02	0.41
6:I:193:TRP:HZ3	10:1:241:ASP:OXT	2.03	0.41
11:N:258:ILE:HB	5:V:193:ARG:HH22	1.86	0.41
11:2:65:SER:HA	15:a:129:PHE:CZ	2.56	0.41
2:P:189:ILE:CD1	2:P:213:ILE:HD11	2.51	0.41
9:Z:140:LEU:HD21	14:S:97:VAL:HG11	2.02	0.41
13:CA:1172:VAL:HA	13:CA:1175:VAL:HG12	2.03	0.41
13:CA:1429:LYS:O	13:CA:1433:GLU:HG2	2.21	0.41
13:DA:331:TYR:CZ	13:DA:1533:PRO:HG3	2.54	0.41
14:S:12:VAL:HG13	14:S:13:SER:N	2.35	0.41
14:S:163:THR:HG22	14:S:164:PHE:N	2.34	0.41
5:H:180:GLN:OE1	5:V:155:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:159:GLU:HG3	7:J:160:PRO:HD2	2.01	0.41
8:K:27:VAL:HG12	8:Y:171:ARG:O	2.21	0.41
11:2:162:TYR:CE1	11:2:164:ASN:HB3	2.56	0.41
6:W:32:ILE:HG12	6:W:45:ALA:HB2	2.03	0.41
9:Z:92:ASP:HA	9:Z:249:SER:O	2.20	0.41
12:D:41:CYS:SG	12:D:214:VAL:HG13	2.60	0.41
14:E:12:VAL:HG13	14:E:13:SER:N	2.35	0.41
14:E:225:GLN:HG2	14:E:226:ASP:OD1	2.20	0.41
7:J:11:ILE:HG12	7:J:142:ALA:HB3	2.02	0.41
13:CA:1012:ILE:O	13:CA:1016:VAL:HG23	2.21	0.41
13:CA:2066:GLY:HA2	13:CA:2106:THR:HG21	2.03	0.41
13:DA:1750:PHE:CE2	13:DA:1784:LEU:HD11	2.56	0.41
6:I:152:TYR:CD1	11:2:258:ILE:HD11	2.55	0.41
5:V:197:LEU:HD22	5:V:202:VAL:HG12	2.03	0.41
8:K:139:TYR:OH	8:Y:25:ILE:O	2.37	0.41
9:L:193:ASP:OD1	9:L:195:THR:HG23	2.21	0.41
2:P:113:GLU:O	2:P:117:ILE:HG12	2.21	0.41
2:P:204:PHE:CE2	2:P:247:LEU:HD22	2.56	0.41
6:W:192:ILE:HG23	6:W:199:GLY:HA2	2.03	0.41
13:CA:709:PHE:CD2	13:CA:747:SER:HA	2.56	0.41
13:CA:1169:TYR:O	13:CA:1172:VAL:HG22	2.21	0.41
13:DA:1023:LEU:HD21	13:DA:1179:ILE:HD13	2.02	0.41
13:DA:1749:MET:HE2	13:DA:1763:LYS:HB3	2.03	0.41
6:I:223:ASN:HB3	10:1:239:LYS:HE2	2.02	0.41
8:K:171:ARG:O	8:Y:27:VAL:HG12	2.20	0.41
10:M:204:ARG:HH12	6:W:229:GLN:NE2	2.19	0.41
10:1:239:LYS:O	10:1:240:ARG:HG2	2.21	0.41
1:O:192:ASP:O	1:O:193:HIS:ND1	2.54	0.41
5:V:96:THR:O	5:V:100:VAL:HG23	2.21	0.41
13:CA:327:PRO:HG3	13:CA:1580:TYR:HB3	2.02	0.41
13:CA:1510:CYS:SG	13:CA:1638:LEU:HD22	2.61	0.41
13:DA:823:ILE:HB	13:DA:824:PRO:HD3	2.02	0.41
10:M:45:ASP:HA	10:M:220:GLY:O	2.21	0.41
13:CA:408:PHE:CZ	13:CA:435:ILE:HG21	2.56	0.41
13:CA:1872:ILE:O	13:CA:1873:LYS:HB2	2.21	0.41
13:DA:1429:LYS:O	13:DA:1433:GLU:HG2	2.21	0.41
13:DA:1856:ILE:HD12	13:DA:1883:ILE:HG13	2.03	0.41
1:A:129:THR:O	1:A:129:THR:CG2	2.68	0.40
9:Z:76:THR:N	15:b:170:ASP:OD1	2.54	0.40
13:CA:394:VAL:HG12	13:CA:404:ILE:HD12	2.02	0.40
13:CA:605:LEU:HD21	13:CA:615:ILE:HB	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:CA:2137:LEU:HG	13:CA:2139:ARG:HG2	2.03	0.40
13:DA:293:LEU:O	13:DA:299:ASN:HA	2.21	0.40
14:S:64:ILE:HG22	14:S:66:LYS:H	1.86	0.40
1:A:216:THR:HG22	1:A:217:GLU:N	2.36	0.40
4:G:26:ALA:O	4:G:30:VAL:HG23	2.21	0.40
10:M:49:ILE:HD13	10:M:54:ILE:HA	2.03	0.40
11:N:162:TYR:CE1	11:N:164:ASN:HB3	2.56	0.40
3:T:72:LEU:HD12	3:T:72:LEU:C	2.47	0.40
5:V:212:TYR:CD1	5:V:212:TYR:C	2.99	0.40
13:DA:1819:ASP:CG	13:DA:1820:PRO:HD2	2.46	0.40
13:DA:2004:VAL:HG22	13:DA:2007:ARG:NH2	2.35	0.40
1:A:59:VAL:HG13	1:A:59:VAL:O	2.21	0.40
6:I:243:LYS:HZ1	9:Z:286:ILE:HD11	1.86	0.40
7:J:177:ARG:HA	9:Z:101:VAL:HG11	2.03	0.40
5:V:22:ILE:HD12	5:V:63:CYS:HB2	2.03	0.40
5:V:33:LEU:O	5:V:194:MET:HA	2.21	0.40
13:CA:387:MET:N	13:CA:388:PRO:HD2	2.36	0.40
13:CA:1332:HIS:CE1	13:CA:1334:TYR:HH	2.39	0.40
13:CA:1781:VAL:O	13:CA:1781:VAL:CG1	2.69	0.40
14:S:52:LYS:HE3	14:S:218:GLN:HB2	2.03	0.40
3:F:176:LEU:HA	3:F:179:PHE:CE2	2.56	0.40
6:I:229:GLN:NE2	10:1:204:ARG:HH12	2.19	0.40
9:L:140:LEU:HD21	14:E:97:VAL:HG11	2.03	0.40
10:M:147:VAL:O	10:M:147:VAL:HG12	2.21	0.40
11:N:129:LEU:O	11:N:133:MET:HG2	2.21	0.40
2:P:82:TYR:CZ	2:P:86:VAL:HG21	2.56	0.40
3:T:78:ALA:N	3:T:79:PRO:HD2	2.36	0.40
4:U:26:ALA:O	4:U:30:VAL:HG23	2.21	0.40
13:CA:823:ILE:HB	13:CA:824:PRO:HD3	2.04	0.40
13:DA:1332:HIS:CE1	13:DA:1334:TYR:HH	2.39	0.40
13:DA:2066:GLY:HA2	13:DA:2106:THR:HG21	2.03	0.40
2:B:94:HIS:ND1	6:I:94:LEU:HD21	2.37	0.40
5:H:212:TYR:CD1	5:H:212:TYR:C	2.99	0.40
10:M:88:LYS:HA	10:M:91:VAL:HG12	2.02	0.40
3:T:176:LEU:HA	3:T:179:PHE:CE2	2.56	0.40
13:CA:531:THR:HG21	13:CA:588:ASN:HD21	1.86	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	236/252 (94%)	232 (98%)	4 (2%)	0	100	100
1	O	236/252 (94%)	231 (98%)	5 (2%)	0	100	100
2	B	230/250 (92%)	227 (99%)	3 (1%)	0	100	100
2	P	230/250 (92%)	227 (99%)	3 (1%)	0	100	100
3	F	232/234 (99%)	229 (99%)	3 (1%)	0	100	100
3	T	232/234 (99%)	228 (98%)	4 (2%)	0	100	100
4	G	239/288 (83%)	236 (99%)	3 (1%)	0	100	100
4	U	239/288 (83%)	236 (99%)	3 (1%)	0	100	100
5	H	194/215 (90%)	188 (97%)	6 (3%)	0	100	100
5	V	194/215 (90%)	188 (97%)	6 (3%)	0	100	100
6	I	218/261 (84%)	211 (97%)	7 (3%)	0	100	100
6	W	218/261 (84%)	211 (97%)	7 (3%)	0	100	100
7	J	201/205 (98%)	196 (98%)	5 (2%)	0	100	100
7	X	201/205 (98%)	196 (98%)	5 (2%)	0	100	100
8	K	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
8	Y	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
9	L	210/287 (73%)	206 (98%)	4 (2%)	0	100	100
9	Z	210/287 (73%)	206 (98%)	4 (2%)	0	100	100
10	1	219/241 (91%)	212 (97%)	7 (3%)	0	100	100
10	M	219/241 (91%)	211 (96%)	8 (4%)	0	100	100
11	2	228/266 (86%)	220 (96%)	8 (4%)	0	100	100
11	N	228/266 (86%)	220 (96%)	8 (4%)	0	100	100
12	C	151/254 (59%)	151 (100%)	0	0	100	100
12	D	182/254 (72%)	176 (97%)	6 (3%)	0	100	100
12	Q	151/254 (59%)	151 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	R	182/254 (72%)	175 (96%)	7 (4%)	0	100	100
13	CA	1872/2167 (86%)	1815 (97%)	57 (3%)	0	100	100
13	DA	1872/2167 (86%)	1812 (97%)	60 (3%)	0	100	100
14	E	234/260 (90%)	228 (97%)	6 (3%)	0	100	100
14	S	234/260 (90%)	228 (97%)	6 (3%)	0	100	100
15	a	73/250 (29%)	70 (96%)	3 (4%)	0	100	100
15	b	73/250 (29%)	71 (97%)	2 (3%)	0	100	100
All	All	9824/11764 (84%)	9570 (97%)	254 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/210 (97%)	203 (100%)	1 (0%)	81	82
1	O	204/210 (97%)	203 (100%)	1 (0%)	81	82
2	B	192/209 (92%)	192 (100%)	0	100	100
2	P	192/209 (92%)	191 (100%)	1 (0%)	81	82
3	F	193/193 (100%)	193 (100%)	0	100	100
3	T	193/193 (100%)	193 (100%)	0	100	100
4	G	200/239 (84%)	200 (100%)	0	100	100
4	U	200/239 (84%)	200 (100%)	0	100	100
5	H	162/178 (91%)	161 (99%)	1 (1%)	78	80
5	V	162/178 (91%)	161 (99%)	1 (1%)	78	80
6	I	179/214 (84%)	178 (99%)	1 (1%)	78	80
6	W	179/214 (84%)	178 (99%)	1 (1%)	78	80
7	J	171/173 (99%)	170 (99%)	1 (1%)	78	80
7	X	171/173 (99%)	170 (99%)	1 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	173/175 (99%)	173 (100%)	0	100	100
8	Y	173/175 (99%)	173 (100%)	0	100	100
9	L	169/235 (72%)	167 (99%)	2 (1%)	63	73
9	Z	169/235 (72%)	167 (99%)	2 (1%)	63	73
10	1	184/201 (92%)	184 (100%)	0	100	100
10	M	184/201 (92%)	184 (100%)	0	100	100
11	2	196/224 (88%)	195 (100%)	1 (0%)	81	82
11	N	196/224 (88%)	196 (100%)	0	100	100
12	C	150/226 (66%)	150 (100%)	0	100	100
12	D	169/226 (75%)	169 (100%)	0	100	100
12	Q	150/226 (66%)	149 (99%)	1 (1%)	76	79
12	R	169/226 (75%)	169 (100%)	0	100	100
13	CA	1731/1986 (87%)	1729 (100%)	2 (0%)	88	89
13	DA	1731/1986 (87%)	1729 (100%)	2 (0%)	88	89
14	E	199/215 (93%)	199 (100%)	0	100	100
14	S	199/215 (93%)	199 (100%)	0	100	100
15	a	64/207 (31%)	64 (100%)	0	100	100
15	b	64/207 (31%)	63 (98%)	1 (2%)	55	69
All	All	8672/10222 (85%)	8652 (100%)	20 (0%)	85	87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
5	H	36	ASP
6	I	46	ASP
7	J	144	ASP
9	L	92	ASP
9	L	193	ASP
11	2	257	ASP
1	O	32	PHE
2	P	130	PHE
5	V	36	ASP
6	W	46	ASP
7	X	144	ASP
9	Z	92	ASP

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Mol	Chain	Res	Type
9	Z	193	ASP
13	CA	1524	THR
13	CA	1791	ASP
15	b	127	PRO
12	Q	78	LEU
13	DA	1524	THR
13	DA	1791	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	176	GLN
3	F	21	GLN
3	F	93	ASN
3	F	110	HIS
4	G	169	GLN
4	G	206	ASN
5	H	79	GLN
6	I	170	HIS
6	I	201	ASN
6	I	218	ASN
7	J	64	ASN
7	J	169	GLN
7	J	173	ASN
8	K	37	GLN
8	K	146	HIS
9	L	263	HIS
9	L	266	HIS
9	L	283	ASN
10	M	216	GLN
11	N	35	GLN
11	N	51	ASN
11	N	59	ASN
11	N	95	HIS
11	2	35	GLN
1	O	41	ASN
1	O	176	GLN
2	P	190	HIS
3	T	21	GLN
3	T	93	ASN
3	T	110	HIS

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Mol	Chain	Res	Type
3	T	166	GLN
4	U	169	GLN
4	U	182	HIS
6	W	145	HIS
6	W	170	HIS
7	X	169	GLN
7	X	173	ASN
8	Y	37	GLN
8	Y	146	HIS
9	Z	241	HIS
9	Z	263	HIS
12	C	96	HIS
12	C	162	GLN
13	CA	87	GLN
13	CA	100	HIS
13	CA	146	ASN
13	CA	283	HIS
13	CA	353	HIS
13	CA	354	ASN
13	CA	372	ASN
13	CA	427	HIS
13	CA	633	ASN
13	CA	723	HIS
13	CA	846	HIS
13	CA	865	GLN
13	CA	886	HIS
13	CA	964	HIS
13	CA	1004	HIS
13	CA	1153	ASN
13	CA	1470	GLN
13	CA	1532	ASN
13	CA	1714	HIS
13	CA	1742	HIS
13	CA	1759	HIS
12	D	178	ASN
12	D	204	GLN
14	E	91	HIS
14	E	188	HIS
15	a	178	HIS
15	a	195	GLN
15	b	161	ASN
12	Q	96	HIS

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Mol	Chain	Res	Type
12	Q	162	GLN
13	DA	146	ASN
13	DA	313	HIS
13	DA	353	HIS
13	DA	372	ASN
13	DA	399	HIS
13	DA	427	HIS
13	DA	633	ASN
13	DA	636	HIS
13	DA	723	HIS
13	DA	808	ASN
13	DA	886	HIS
13	DA	963	GLN
13	DA	964	HIS
13	DA	1004	HIS
13	DA	1196	ASN
13	DA	1405	GLN
13	DA	1742	HIS
13	DA	1745	ASN
13	DA	1814	ASN
13	DA	1962	ASN
12	R	178	ASN
14	S	91	HIS
14	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 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.

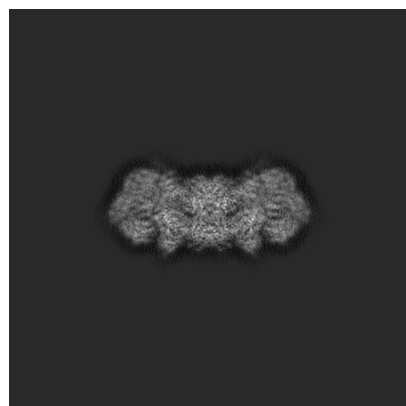
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75334. These allow visual inspection of the internal detail of the map and identification of artifacts.

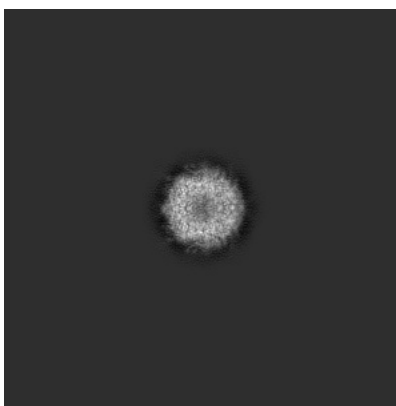
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

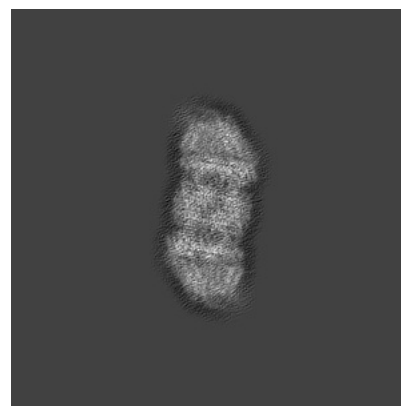
6.1.1 Primary map



X

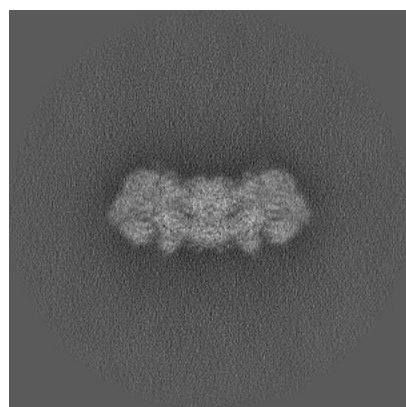


Y

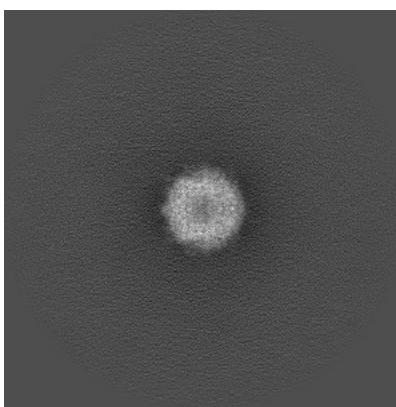


Z

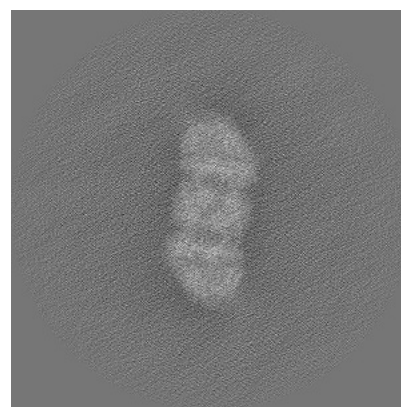
6.1.2 Raw map



X



Y

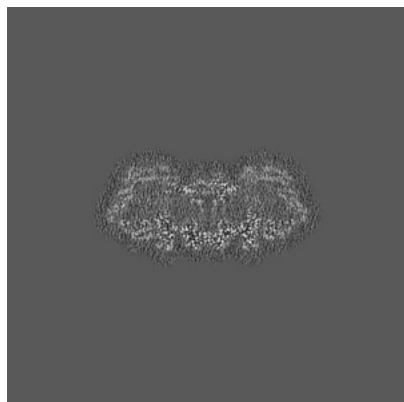


Z

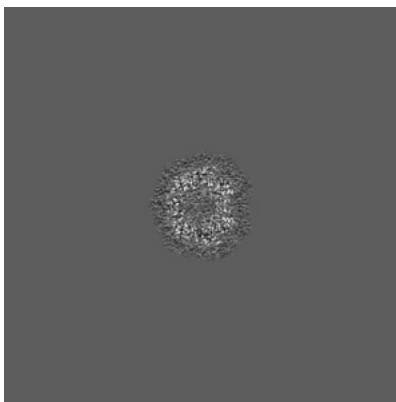
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

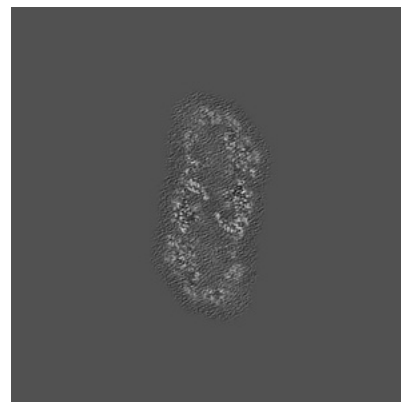
6.2.1 Primary map



X Index: 240

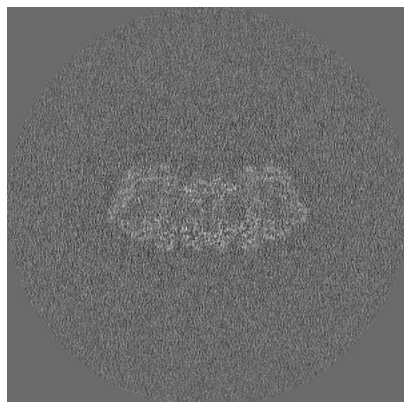


Y Index: 240

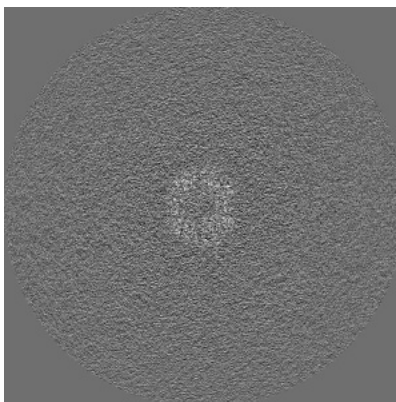


Z Index: 240

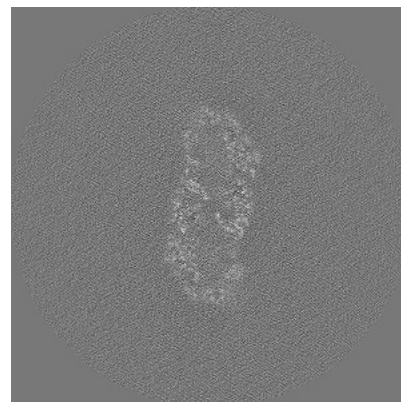
6.2.2 Raw map



X Index: 240



Y Index: 240

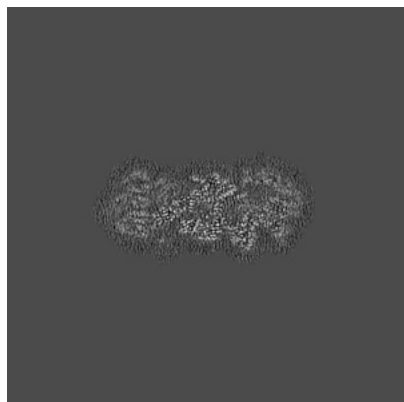


Z Index: 240

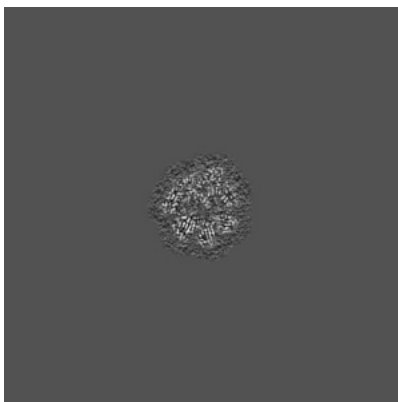
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

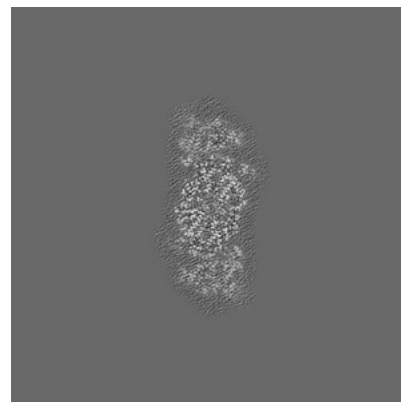
6.3.1 Primary map



X Index: 262

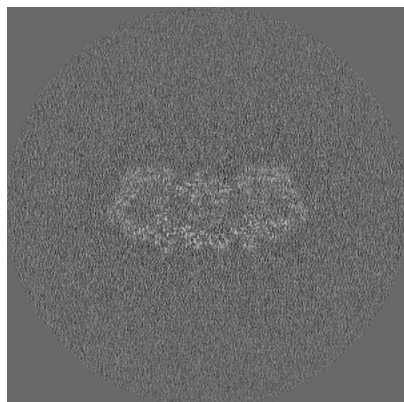


Y Index: 229

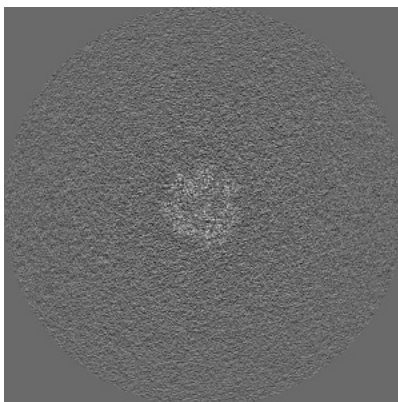


Z Index: 215

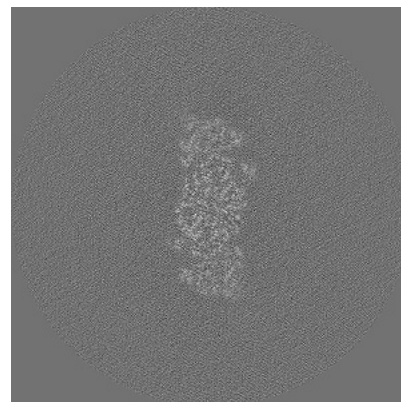
6.3.2 Raw map



X Index: 242



Y Index: 250

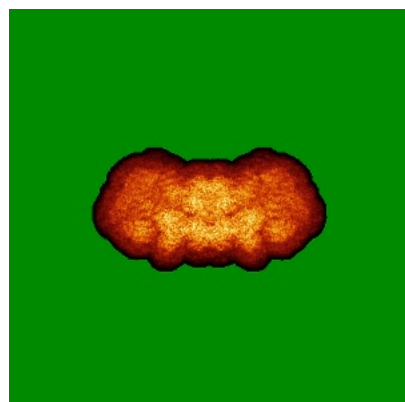


Z Index: 216

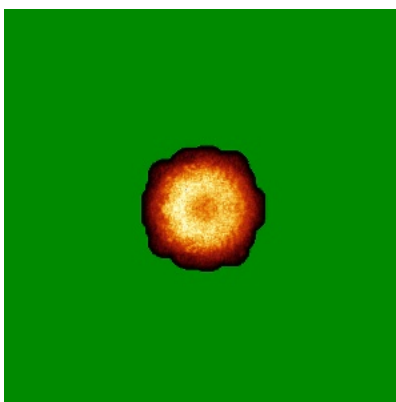
The images above show the largest variance slices of the map in three orthogonal directions.

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

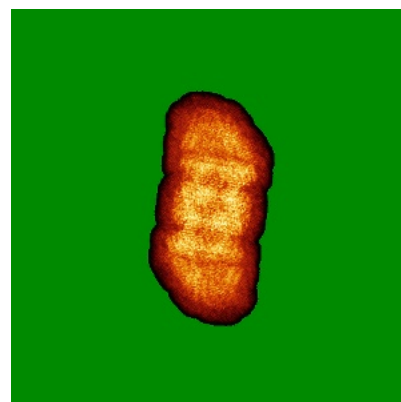
6.4.1 Primary map



X

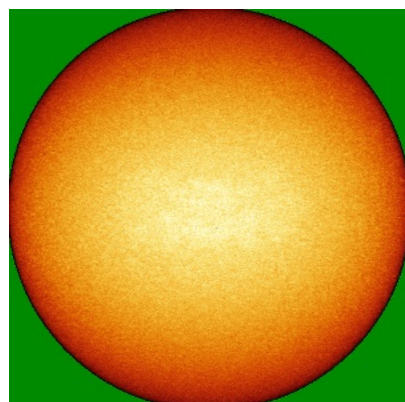


Y

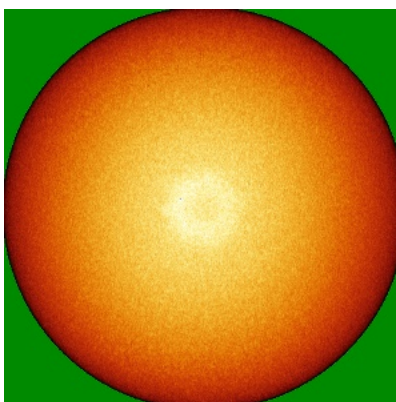


Z

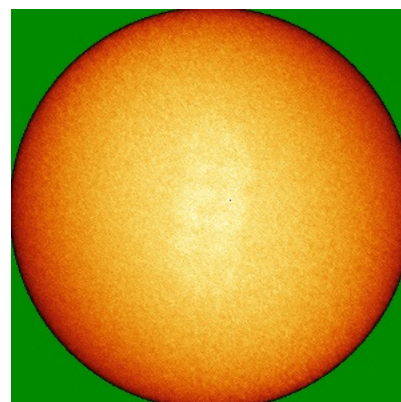
6.4.2 Raw map



X



Y

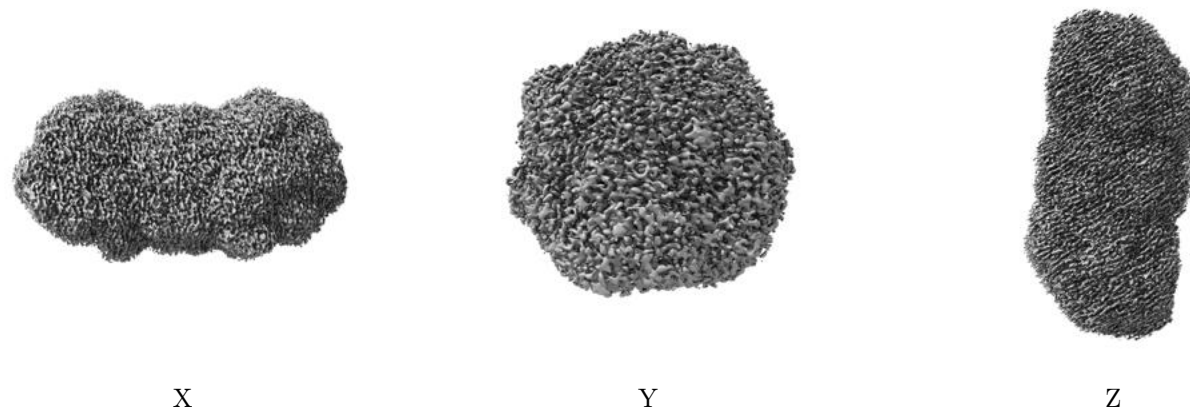


Z

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.

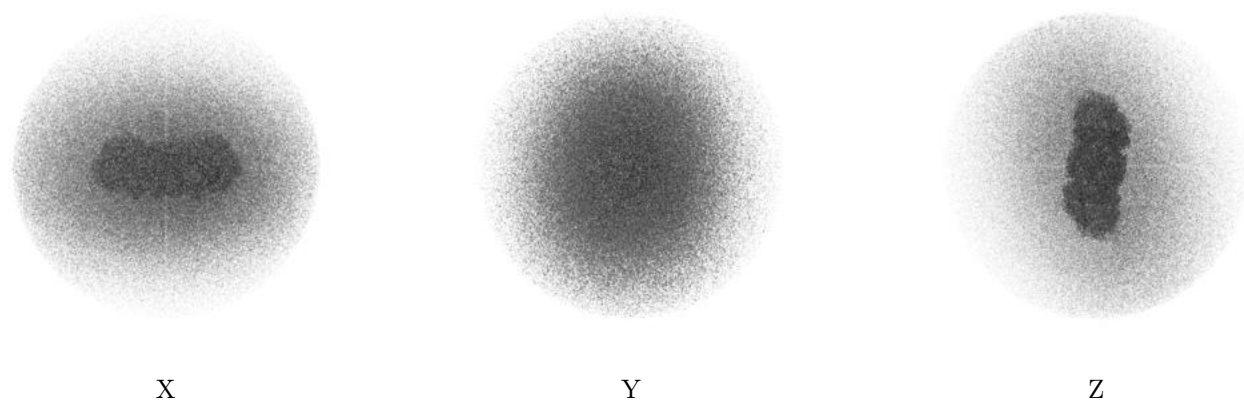
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00265. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

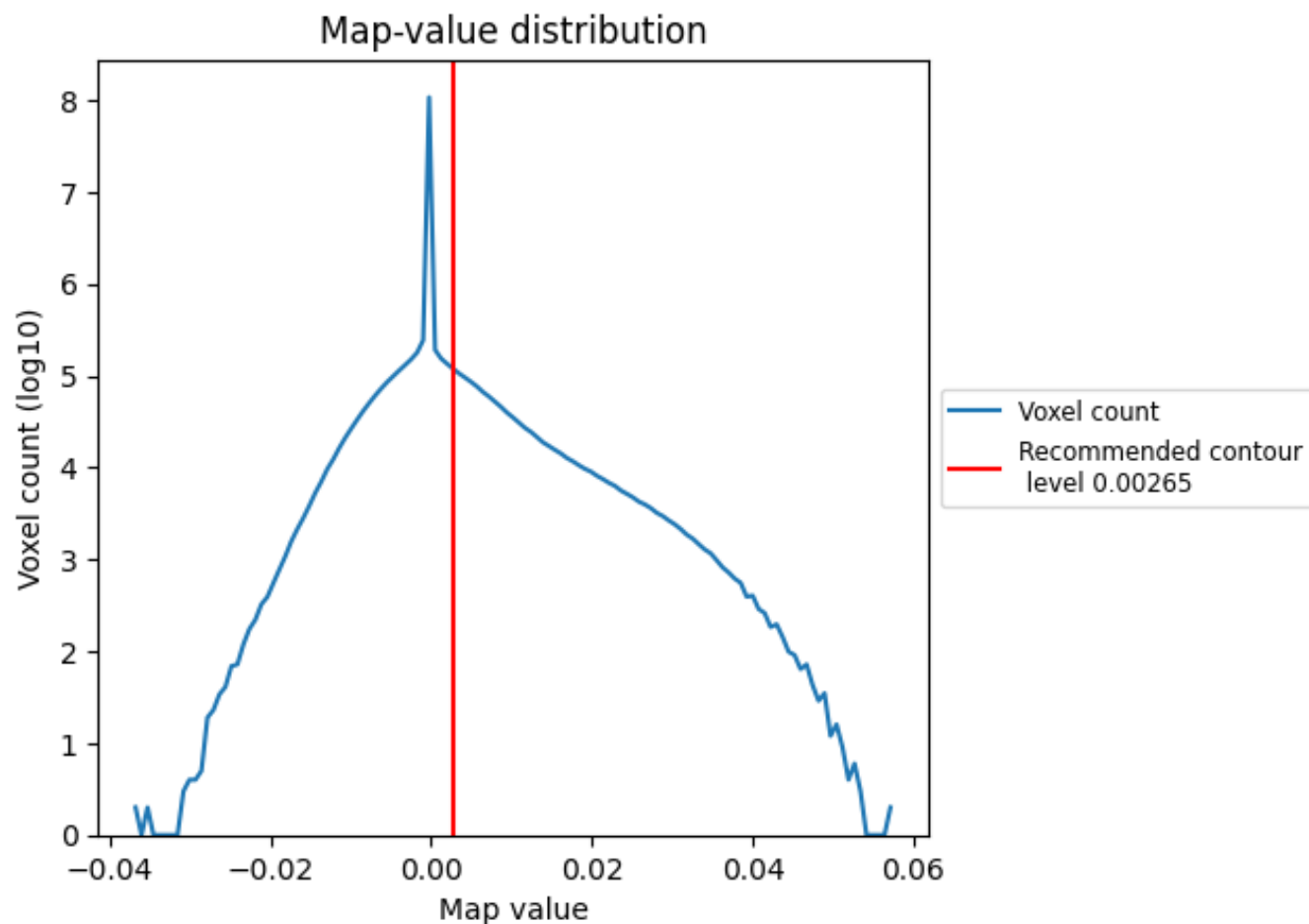
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

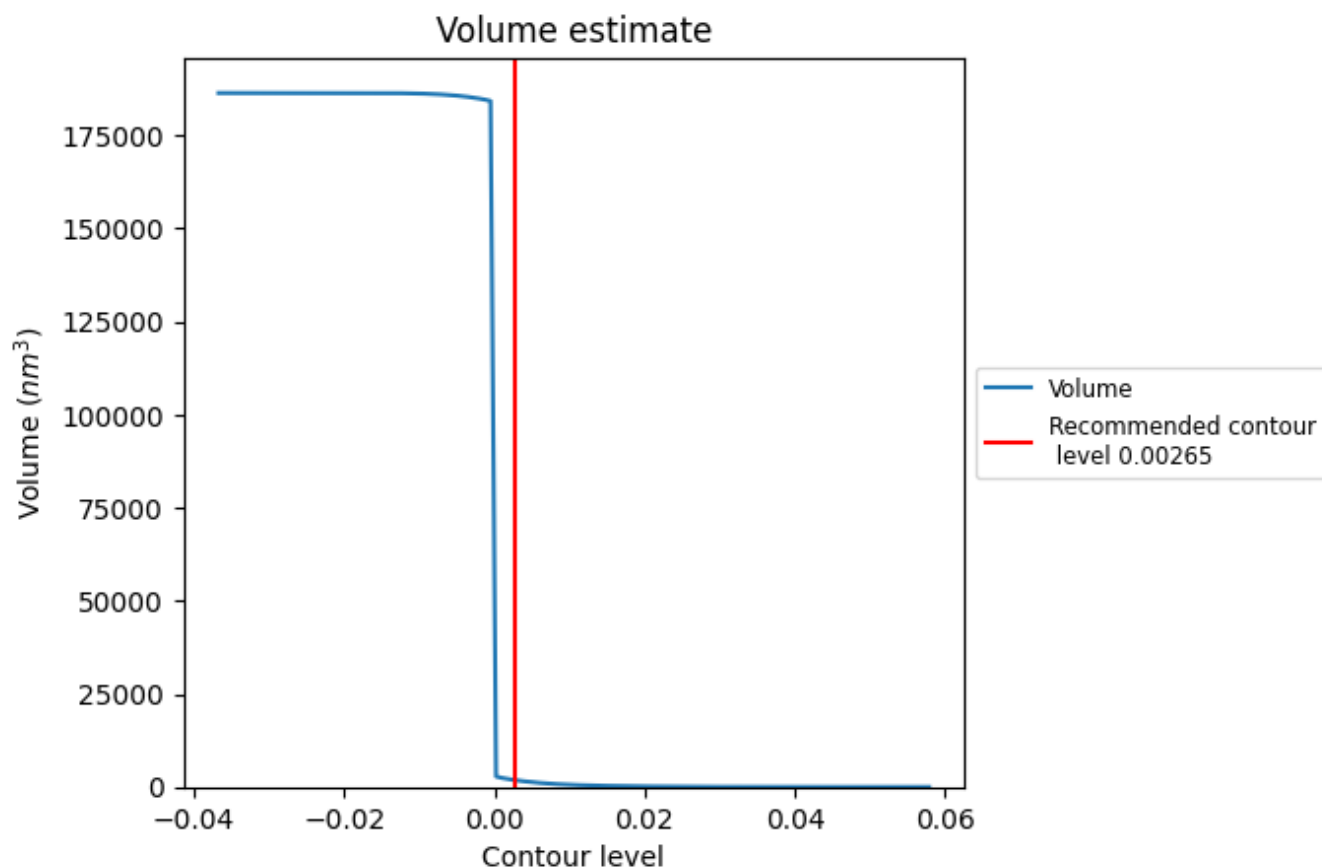
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

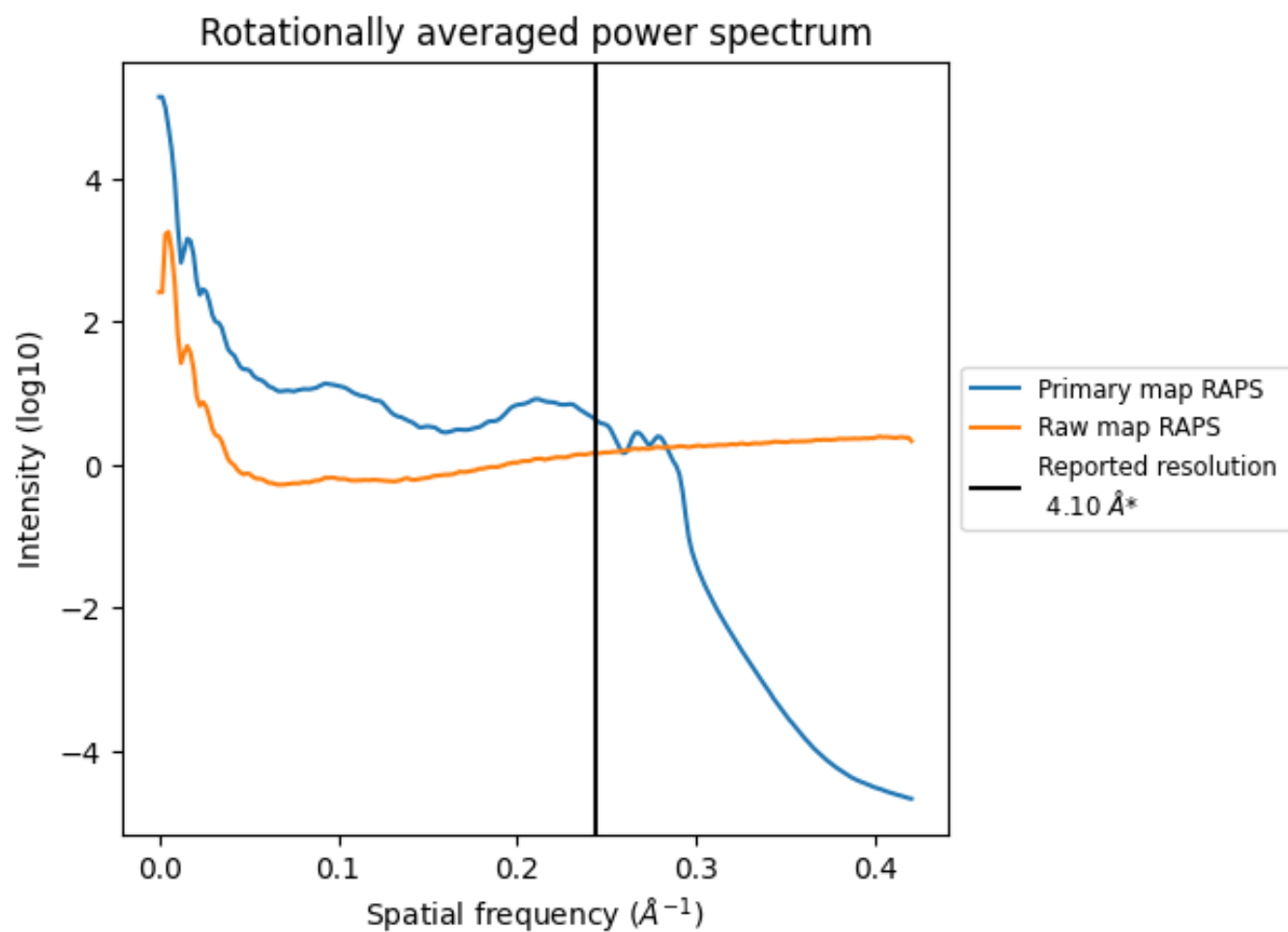
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1865 nm^3 ; this corresponds to an approximate mass of 1685 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 ⓘ

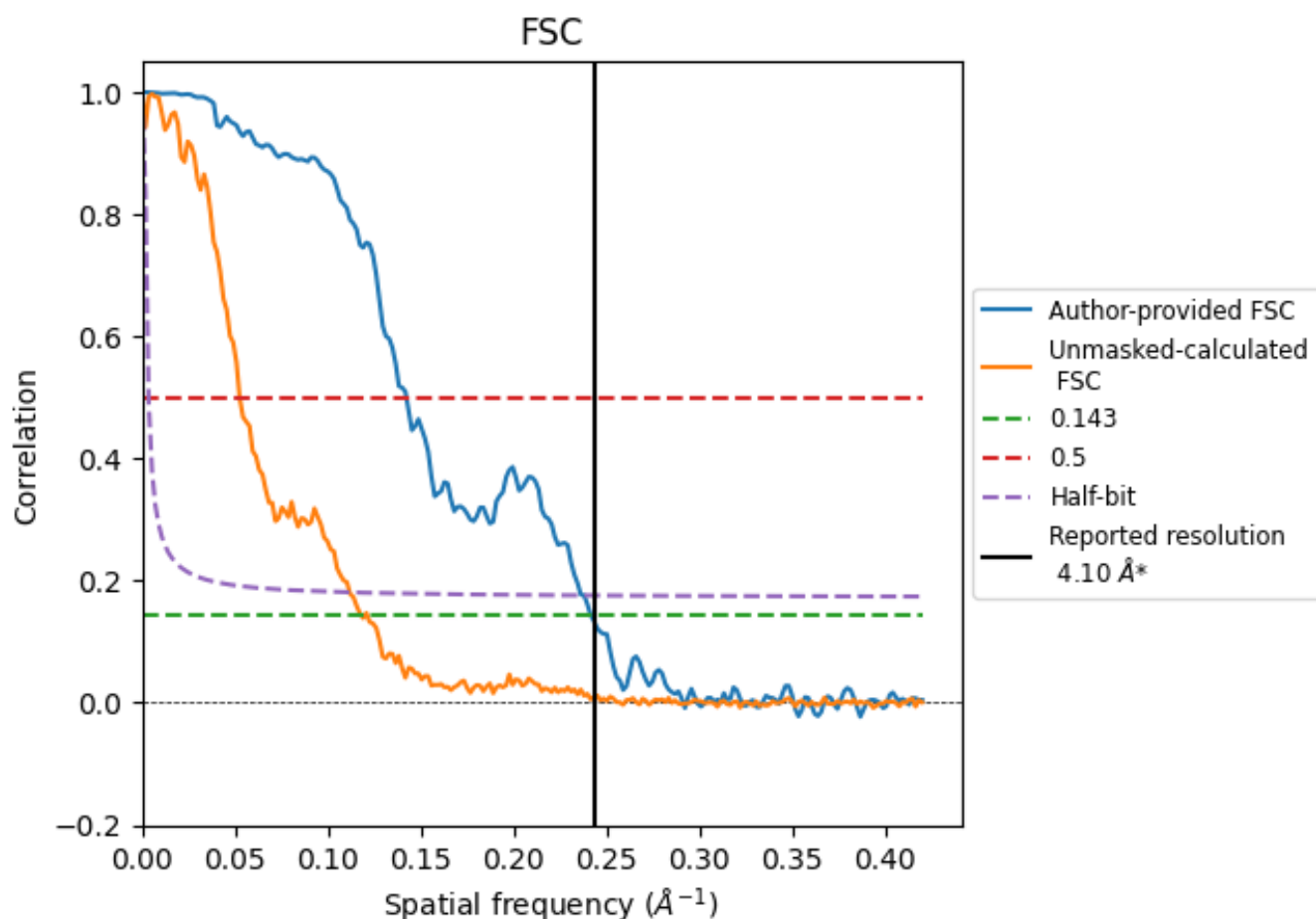


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

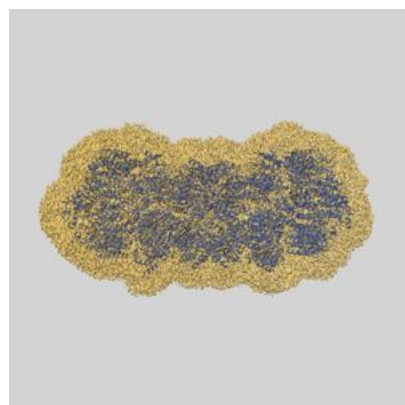
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	7.03	4.20
Unmasked-calculated*	8.47	19.05	8.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.47 differs from the reported value 4.1 by more than 10 %

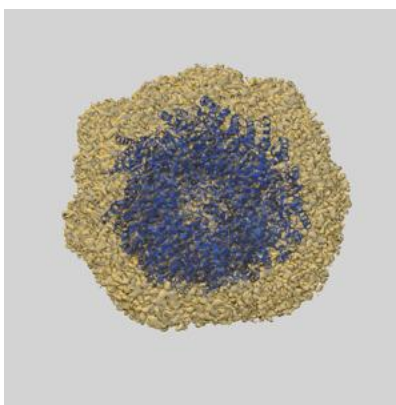
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75334 and PDB model 10OG. Per-residue inclusion information can be found in section 3 on page 10.

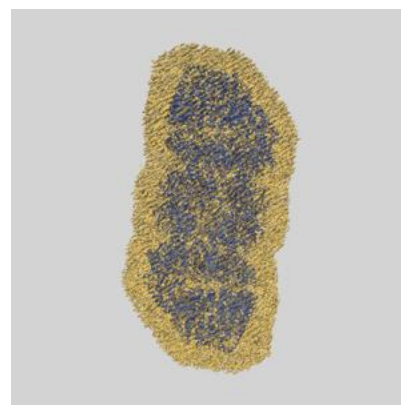
9.1 Map-model overlay [i](#)



X



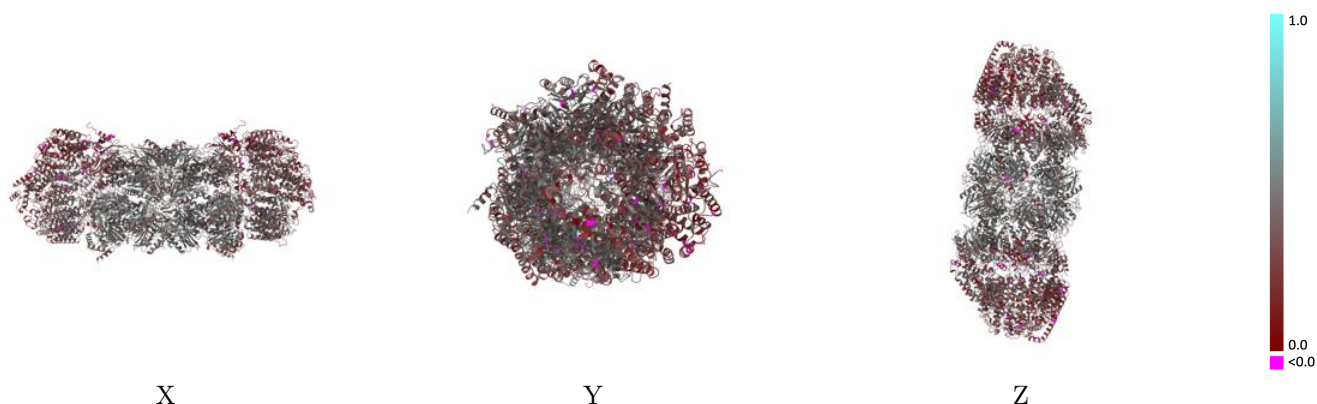
Y



Z

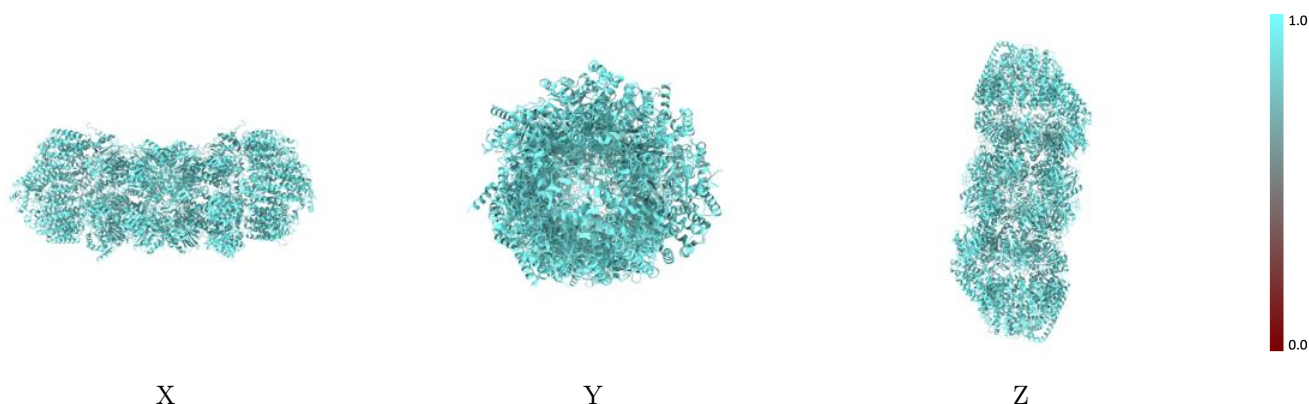
The images above show the 3D surface view of the map at the recommended contour level 0.00265 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



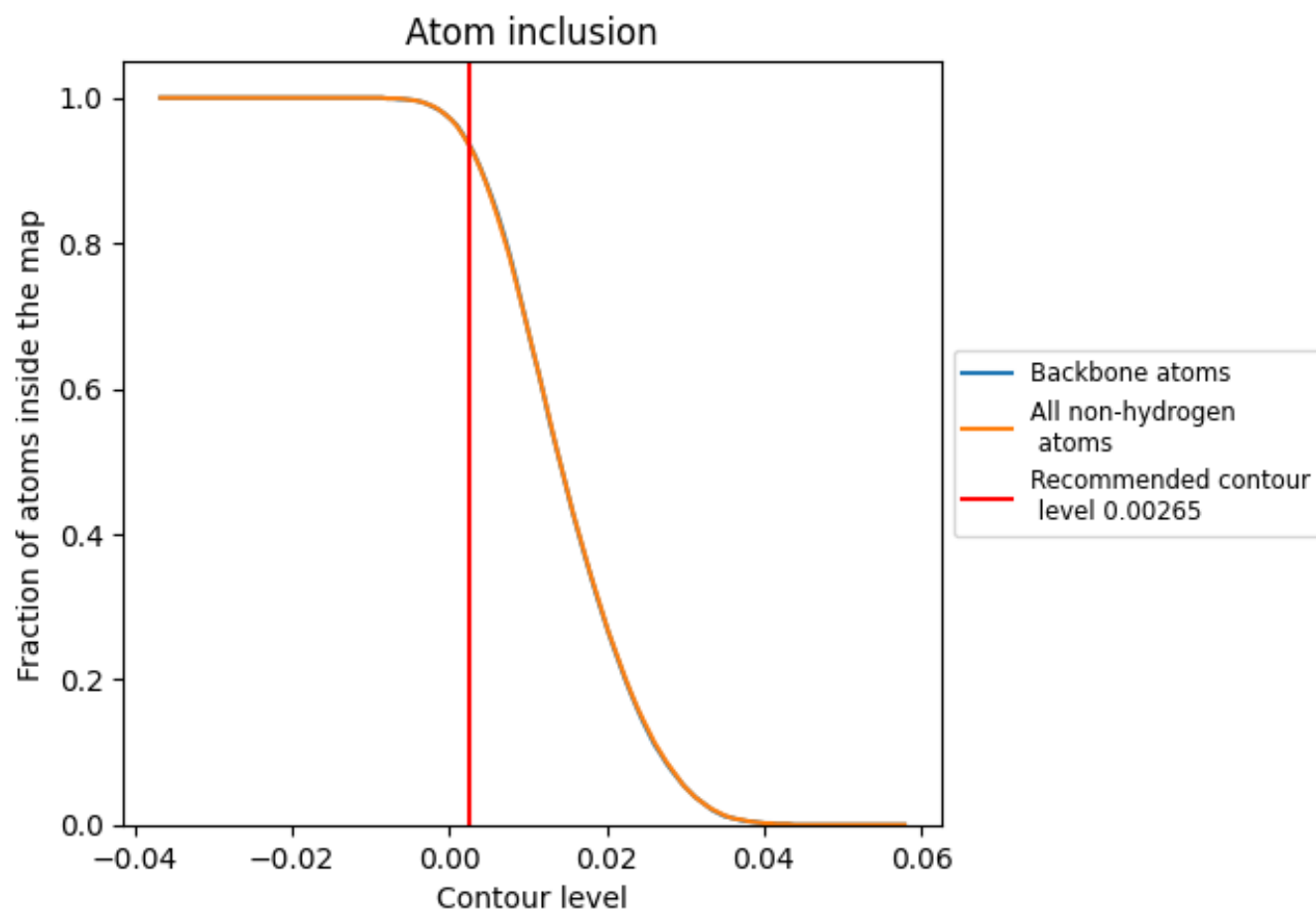
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00265).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.00265) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.3780
1	 0.9510	 0.4390
2	 0.9610	 0.4520
A	 0.9560	 0.4320
B	 0.9480	 0.4330
C	 0.8890	 0.2910
CA	 0.9190	 0.3210
D	 0.8900	 0.2540
DA	 0.9230	 0.3240
E	 0.9280	 0.3780
F	 0.9540	 0.4310
G	 0.9560	 0.4350
H	 0.9490	 0.4520
I	 0.9610	 0.4510
J	 0.9570	 0.4510
K	 0.9470	 0.4260
L	 0.9540	 0.4410
M	 0.9620	 0.4370
N	 0.9510	 0.4430
O	 0.9450	 0.4220
P	 0.9390	 0.4200
Q	 0.9110	 0.3000
R	 0.8810	 0.2600
S	 0.9290	 0.3820
T	 0.9470	 0.4280
U	 0.9530	 0.4300
V	 0.9500	 0.4500
W	 0.9540	 0.4410
X	 0.9390	 0.4370
Y	 0.9360	 0.4150
Z	 0.9580	 0.4440
a	 0.9420	 0.4020
b	 0.9370	 0.3970

