



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:26 AM UTC

PDB ID : 9LU1 / pdb_00009lu1
EMDB ID : EMD-63386
Title : protein structure of DDB1-DDA1-DET1-Ube2e2 bound to COP1 dimer
Authors : Su, M.-Y.; Wang, S.; Teng, F.
Deposited on : 2025-02-07
Resolution : 3.62 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

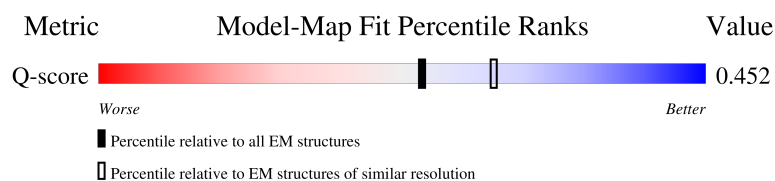
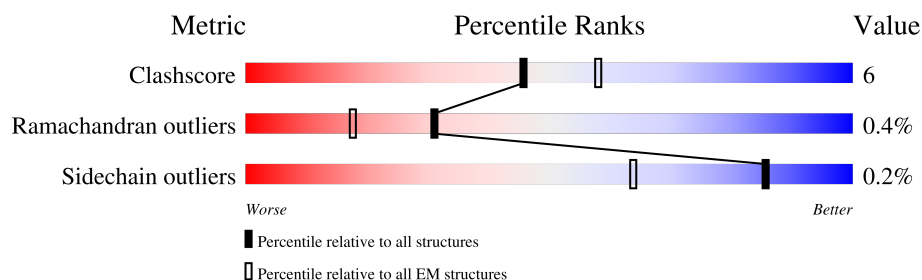
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.62 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	11773 (3.12 - 4.12)

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	731	
1	E	731	
2	B	102	
3	C	201	

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Mol	Chain	Length	Quality of chain
4	R	550	 77%19%•
5	S	1140	 83%13%•

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17116 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called E3 ubiquitin-protein ligase COP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	389	Total	C	N	O	S	0	0
			2049	1255	393	400	1		
1	E	373	Total	C	N	O	S	0	0
			2278	1443	404	423	8		

- Molecule 2 is a protein called DET1- and DDB1-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	55	Total	C	N	O	0	0
			404	268	66	70		

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	150	Total	C	N	O	S	0	0
			1054	678	188	187	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	76	GLY	SER	engineered mutation	UNP Q96LR5
C	139	SER	CYS	engineered mutation	UNP Q96LR5

- Molecule 4 is a protein called DET1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	526	Total	C	N	O	S	0	0
			4037	2599	713	709	16		

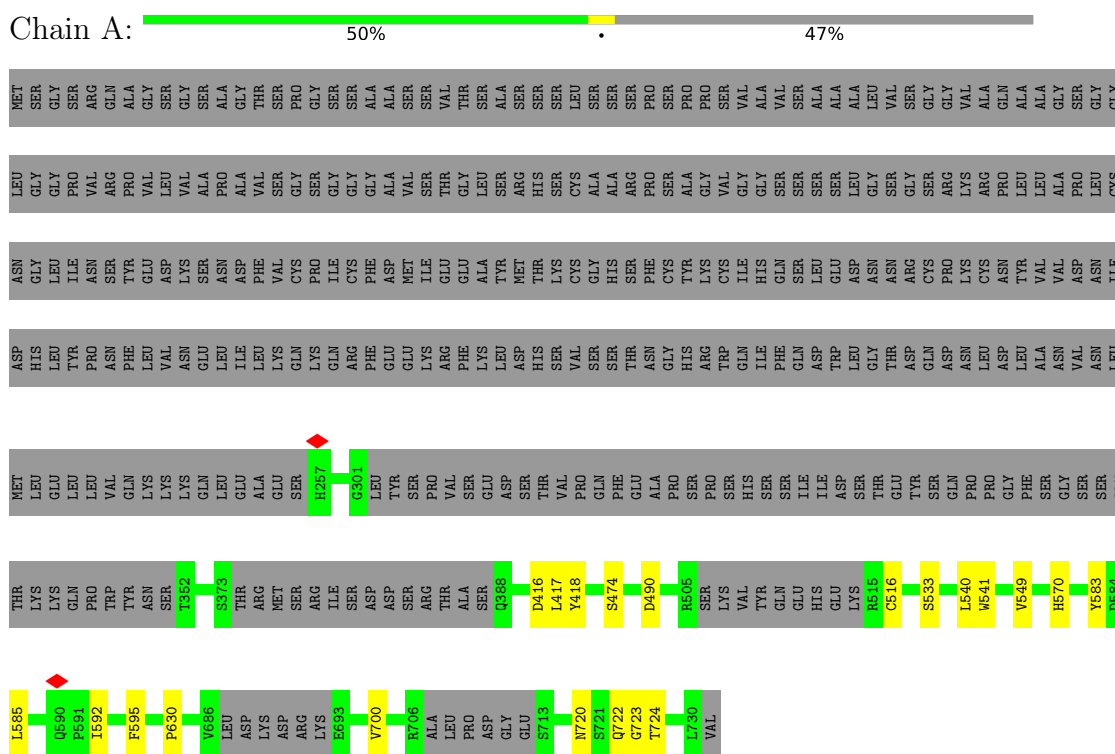
- Molecule 5 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	1096	7294	4626	1297	1339	32	0	0

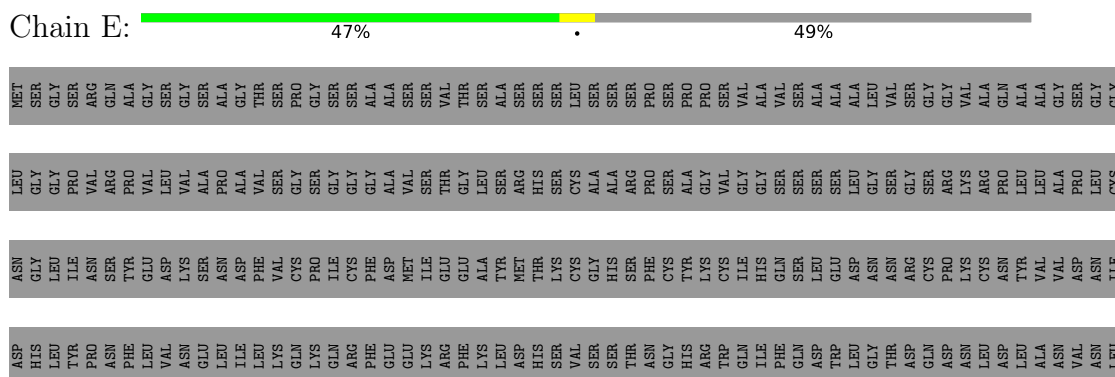
3 Residue-property plots

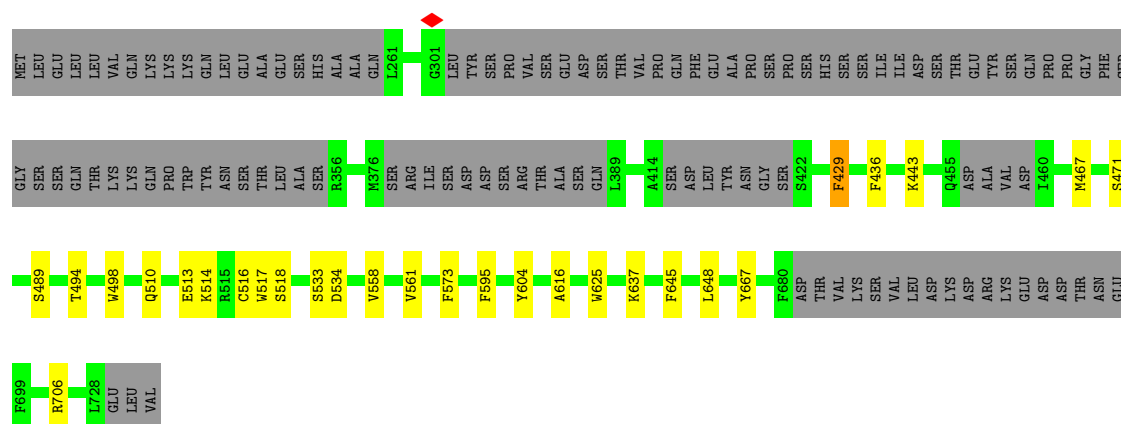
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: E3 ubiquitin-protein ligase COP1



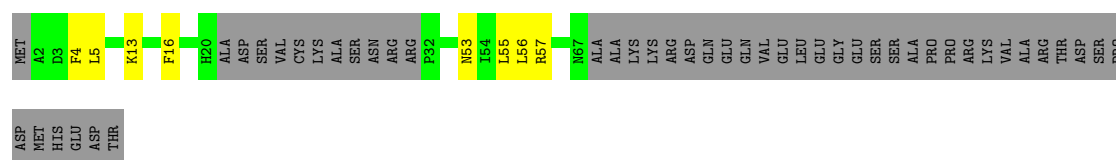
• Molecule 1: E3 ubiquitin-protein ligase COP1





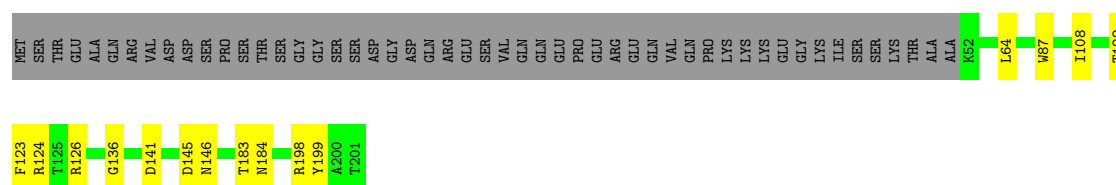
- Molecule 2: DET1- and DDB1-associated protein 1

Chain B: 46% 8% 46%



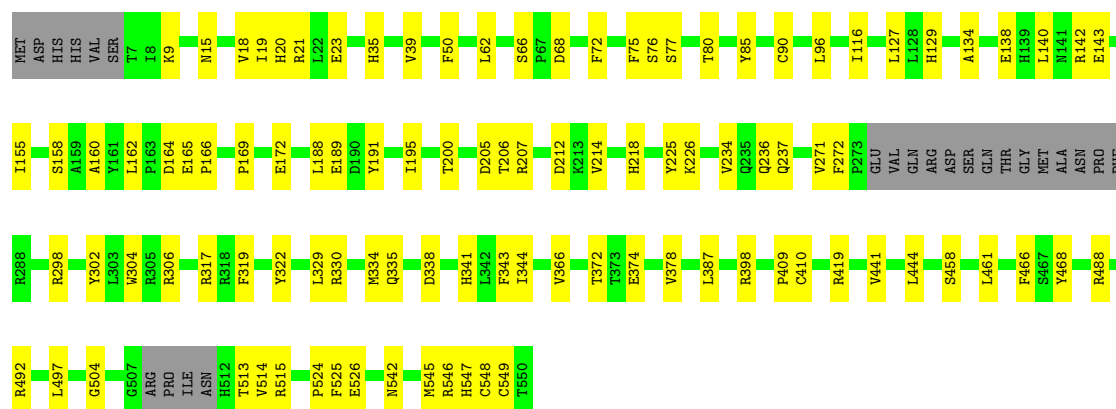
- Molecule 3: Ubiquitin-conjugating enzyme E2 E2

Chain C: 67% 7% 25%



- Molecule 4: DET1 homolog

Chain R: 77% 19% .



- Molecule 5: DNA damage-binding protein 1

P1023	N885	L606	M362	K191	H1
T1024	N889	S653	V364	T192	V6
Q1025	R889	D654	L367	Q209	F23
F1030	T894	A694	Q374	E210	T24
G1031	T895	M695	V376	R211	N30
T1032	E896	T698	L699	E213	L31
M1036	L899	L699	S386	E216	L32
L1037	N904	K723	L387	A217	N36
G1038	I909	S730	R388	R218	I41
L1039	T1041	C731	I389	T232	G48
S1042	D925	C732	R391	Q233	P69
Y1043	L926	L736	D423	Q234	M57
D1053	M927	R739	I424	T237	T68
M1054	R928	R739	M437	T248	G59
R1057	L931	Q743	L438	T257	F67
W1073	M938	ASP	V443	P250	R68
H1077	N941	THR	D454	T258	P69
I1089	R947	GLY	G748	D261	D75
R1102	P951	S755	Q456	R262	L76
P1103	M954	A756	R514	N262	I79
K1104	F972	S757	M534	S269	N107
M1105	N973	S766	E537	R270	V108
A1110	C977	L770	V538	Y271	R114
D1115	D980	PHE	A539	L273	R114
GLY	GLY	SER	L546	G274	I124
GLY	ALA	THR	SER	D275	I131
GLY	ALA	ALA	ASP	R279	L139
MET	THR	PRO	SER	M282	I143
LYS	T985	HIS	ASN	L283	N156
R1122	L992	GLU	G551	K287	N156
L1129	Q993	THR	L555	GLU	L159
H1140	E994	S781	W561	GLN	E160
	E1002	F799	S665	MET	E161
	V1006	H805	ALA	ASP	I165
	Q1015	L821	R567	GLY	D166
ASN	ASN	D824	K570	THR	V167
LEU	LEU	R828	K579	GLU	I181
GLU	GLU	F829	G583	THR	Y182
THR	THR	I830	P588	V321	Q183
SER	SER	V850		R361	R188
THR	THR			V190	H189

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42109	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.89	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.289	Depositor
Minimum map value	-0.525	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.186	Depositor
Map size ($\text{\AA}$)	510.0, 510.0, 510.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.09	0/2059	0.27	0/2862
1	E	0.11	0/2316	0.30	0/3190
2	B	0.14	0/415	0.39	0/569
3	C	0.12	0/1083	0.24	0/1496
4	R	0.14	0/4140	0.32	0/5638
5	S	0.14	0/7410	0.30	0/10145
All	All	0.13	0/17423	0.30	0/23900

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	R	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	R	165	GLU	Peptide

5.2 Too-close contacts [i](#)

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	2049	0	1088	13	0
1	E	2278	0	1597	20	0
2	B	404	0	358	7	0
3	C	1054	0	929	9	0
4	R	4037	0	3759	62	0
5	S	7294	0	6214	95	0
All	All	17116	0	13945	193	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 6.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:209:GLN:OE1	5:S:210:GLU:N	2.16	0.76
1:E:513:GLU:OE2	1:E:513:GLU:N	2.20	0.69
5:S:248:ILE:HG22	5:S:250:PRO:HD3	1.75	0.68
4:R:466:PHE:O	4:R:492:ARG:NH1	2.27	0.67
5:S:824:ASP:OD2	5:S:828:TYR:OH	2.12	0.67
1:E:517:TRP:NE1	1:E:534:ASP:OD2	2.29	0.66
4:R:338:ASP:OD2	4:R:341:HIS:ND1	2.29	0.66
5:S:821:LEU:HD11	5:S:830:ILE:HD11	1.77	0.65
4:R:419:ARG:NH1	5:S:160:GLU:OE2	2.30	0.65
5:S:188:ARG:NH1	5:S:216:ALA:O	2.30	0.65
5:S:361:ASP:OD1	5:S:362:MET:N	2.30	0.65
5:S:424:THR:HA	5:S:437:MET:HA	1.77	0.65
3:C:87:TRP:HB2	3:C:108:ILE:HB	1.78	0.64
4:R:546:ARG:NH2	4:R:548:CYS:SG	2.69	0.63
4:R:140:LEU:HD23	4:R:158:SER:HB3	1.81	0.63
5:S:258:ILE:HG21	5:S:273:LEU:HD23	1.80	0.63
4:R:387:LEU:HD22	4:R:441:VAL:HG13	1.82	0.61
1:A:570:HIS:HA	1:A:585:LEU:H	1.66	0.60
5:S:212:VAL:HG12	5:S:213:GLU:H	1.66	0.60
1:E:513:GLU:H	1:E:513:GLU:CD	2.09	0.60
4:R:96:LEU:HD13	4:R:116:ILE:HD13	1.84	0.59
4:R:504:GLY:O	4:R:542:ASN:ND2	2.34	0.59
5:S:24:THR:HG23	5:S:30:ASN:HD21	1.67	0.58
1:E:637:LYS:O	1:E:667:TYR:OH	2.21	0.58
4:R:547:HIS:NE2	4:R:549:CYS:SG	2.72	0.58
5:S:938:MET:SD	5:S:938:MET:N	2.64	0.57
5:S:1057:ARG:NH1	5:S:1110:ALA:O	2.37	0.57
5:S:755:SER:OG	5:S:756:ALA:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:409:PRO:HD2	5:S:114:ARG:HG3	1.87	0.56
4:R:302:TYR:HE2	4:R:378:VAL:HG22	1.69	0.56
5:S:739:ARG:NH1	5:S:757:SER:OG	2.39	0.56
1:A:541:TRP:HA	1:A:549:VAL:H	1.71	0.56
2:B:16:PHE:HD2	5:S:321:VAL:HG11	1.71	0.56
5:S:218:MET:HE1	5:S:261:HIS:HB3	1.87	0.56
1:A:700:VAL:HA	1:A:720:ASN:HA	1.88	0.55
5:S:107:ASN:OD1	5:S:108:VAL:N	2.39	0.55
5:S:232:ILE:HG12	5:S:237:ILE:HD12	1.88	0.55
5:S:234:GLN:HG3	5:S:257:THR:HG22	1.88	0.55
5:S:6:VAL:HG22	5:S:1040:VAL:HG22	1.88	0.55
5:S:374:GLN:OE1	5:S:391:ARG:NH1	2.36	0.55
1:E:561:VAL:HG23	1:E:573:PHE:HB3	1.88	0.54
4:R:545:MET:SD	4:R:545:MET:N	2.81	0.54
4:R:85:TYR:HD1	4:R:127:LEU:HA	1.72	0.54
1:E:533:SER:OG	1:E:534:ASP:N	2.41	0.54
5:S:588:PRO:HA	5:S:606:LEU:HA	1.89	0.53
5:S:931:LEU:HD13	5:S:947:ARG:HG3	1.89	0.53
4:R:212:ASP:OD1	4:R:236:GLN:NE2	2.41	0.53
4:R:18:VAL:HA	4:R:21:ARG:HG3	1.90	0.52
3:C:141:ASP:N	3:C:141:ASP:OD1	2.40	0.52
5:S:161:GLU:HG2	5:S:182:TYR:CG	2.44	0.52
5:S:271:TYR:HB2	5:S:283:LEU:HB3	1.91	0.52
5:S:166:ASP:OD1	5:S:167:VAL:N	2.42	0.52
4:R:15:ASN:HD22	4:R:20:HIS:HB2	1.74	0.52
4:R:66:SER:OG	4:R:68:ASP:OD1	2.24	0.52
4:R:80:THR:HA	4:R:134:ALA:HB2	1.92	0.52
5:S:275:ASP:OD2	5:S:279:ARG:HB2	2.10	0.52
1:E:489:SER:HB2	1:E:516:CYS:SG	2.50	0.52
1:E:429:PHE:O	1:E:706:ARG:NH2	2.44	0.51
5:S:1025:GLN:O	5:S:1042:SER:OG	2.28	0.51
4:R:62:LEU:HD22	4:R:62:LEU:H	1.75	0.51
5:S:565:SER:O	5:S:567:ARG:N	2.44	0.51
5:S:830:ILE:HG12	5:S:850:VAL:HG12	1.92	0.51
1:A:720:ASN:CG	1:A:724:THR:HG22	2.36	0.51
5:S:539:ALA:HB2	5:S:561:TRP:HA	1.94	0.50
4:R:35:HIS:O	4:R:39:VAL:HG12	2.11	0.50
5:S:1048:TYR:HD1	5:S:1089:ILE:HD11	1.77	0.50
4:R:302:TYR:OH	4:R:306:ARG:NH2	2.42	0.50
4:R:513:THR:C	4:R:515:ARG:H	2.20	0.50
5:S:1030:PHE:CZ	5:S:1038:GLY:HA3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:372:THR:OG1	4:R:374:GLU:OE2	2.20	0.49
4:R:143:GLU:HB3	4:R:218:HIS:H	1.77	0.49
5:S:653:SER:OG	5:S:654:ASP:N	2.44	0.49
5:S:695:ASN:N	5:S:698:THR:O	2.45	0.49
5:S:131:ILE:HD11	5:S:143:ILE:HD12	1.94	0.49
3:C:145:ASP:OD2	3:C:146:ASN:N	2.45	0.49
5:S:889:ARG:HG3	5:S:904:ASN:HB3	1.95	0.49
4:R:62:LEU:HD12	4:R:72:PHE:HE2	1.78	0.49
4:R:461:LEU:O	4:R:468:TYR:OH	2.25	0.49
5:S:367:LEU:HD12	5:S:374:GLN:HE21	1.78	0.49
2:B:16:PHE:CE2	5:S:321:VAL:HG21	2.48	0.48
4:R:525:PHE:CE2	5:S:951:PRO:HG3	2.48	0.48
5:S:972:PHE:HB3	5:S:1002:GLU:H	1.78	0.48
1:A:540:LEU:O	1:A:549:VAL:N	2.45	0.48
4:R:344:ILE:HG13	4:R:366:VAL:HB	1.96	0.48
1:A:416:ASP:O	4:R:322:TYR:OH	2.21	0.48
5:S:386:SER:OG	5:S:387:LEU:N	2.46	0.48
5:S:904:ASN:N	5:S:904:ASN:OD1	2.46	0.48
4:R:164:ASP:O	4:R:166:PRO:HD2	2.14	0.48
1:E:467:MET:HE1	1:E:498:TRP:CE3	2.48	0.48
4:R:138:GLU:HA	4:R:160:ALA:HB2	1.96	0.48
5:S:59:GLY:HA2	5:S:1073:TRP:CZ3	2.49	0.48
5:S:212:VAL:HG12	5:S:213:GLU:N	2.28	0.48
5:S:1054:MET:HE1	5:S:1129:LEU:HD22	1.96	0.47
5:S:941:ASN:OD1	5:S:941:ASN:N	2.48	0.47
5:S:723:LYS:HB2	5:S:736:LEU:HD12	1.95	0.47
1:E:429:PHE:HB3	1:E:436:PHE:HA	1.96	0.47
1:E:494:THR:HG22	1:E:510:GLN:HB3	1.97	0.47
4:R:234:VAL:O	4:R:237:GLN:NE2	2.45	0.47
5:S:973:ASN:ND2	5:S:1077:HIS:O	2.43	0.47
5:S:423:ASP:O	5:S:438:LEU:N	2.47	0.47
5:S:894:THR:HG23	5:S:896:GLU:H	1.79	0.47
5:S:376:VAL:HG12	5:S:389:ILE:HG12	1.97	0.47
5:S:114:ARG:HE	5:S:114:ARG:HB3	1.53	0.46
5:S:75:ASP:OD1	5:S:75:ASP:N	2.49	0.46
2:B:53:ASN:HD21	2:B:56:LEU:HD12	1.80	0.46
4:R:191:TYR:HE2	4:R:214:VAL:HB	1.81	0.46
4:R:207:ARG:HD3	4:R:207:ARG:HA	1.80	0.46
5:S:567:ARG:HA	5:S:579:LYS:HA	1.97	0.46
3:C:122:THR:OG1	3:C:124:ARG:NH2	2.48	0.46
2:B:4:PHE:CD2	2:B:5:LEU:HG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:69:PRO:HG2	5:S:76:LEU:HD12	1.98	0.46
4:R:488:ARG:HB2	4:R:497:LEU:HD11	1.96	0.46
5:S:139:LEU:HD23	5:S:156:ASN:HB3	1.97	0.46
5:S:389:ILE:HD11	5:S:799:PHE:CZ	2.52	0.45
2:B:55:LEU:C	2:B:57:ARG:H	2.23	0.45
4:R:50:PHE:HB2	4:R:547:HIS:HB3	1.97	0.45
5:S:32:LEU:HD22	5:S:41:ILE:HG12	1.99	0.45
5:S:555:LEU:HA	5:S:570:LYS:HA	1.98	0.45
2:B:16:PHE:CE1	5:S:48:GLY:HA2	2.52	0.45
3:C:64:LEU:HD21	4:R:317:ARG:HH12	1.82	0.45
5:S:766:SER:HB2	5:S:805:HIS:NE2	2.32	0.45
5:S:67:PHE:HB3	5:S:124:ILE:HG21	1.99	0.45
5:S:514:ARG:O	5:S:534:MET:N	2.49	0.45
4:R:317:ARG:HE	4:R:317:ARG:HB3	1.55	0.45
5:S:694:ALA:HA	5:S:699:LEU:HA	1.99	0.45
1:A:516:CYS:HA	1:A:533:SER:HA	1.98	0.44
1:E:595:PHE:HB3	1:E:625:TRP:CZ3	2.52	0.44
1:E:616:ALA:HB2	1:E:648:LEU:HD11	1.98	0.44
5:S:537:GLU:O	5:S:561:TRP:N	2.35	0.44
4:R:302:TYR:CE2	4:R:378:VAL:HG22	2.52	0.44
1:A:583:TYR:HA	1:A:592:ILE:H	1.82	0.44
1:A:474:SER:H	1:A:490:ASP:HA	1.82	0.44
5:S:1032:THR:OG1	5:S:1036:MET:HG3	2.18	0.44
5:S:730:SER:HB2	5:S:732:CYS:SG	2.58	0.44
5:S:994:GLU:N	5:S:994:GLU:OE1	2.51	0.44
4:R:19:ILE:O	4:R:23:GLU:HG2	2.17	0.44
4:R:162:LEU:HD23	4:R:188:LEU:C	2.42	0.44
1:E:518:SER:OG	1:E:561:VAL:HG12	2.18	0.43
5:S:57:MET:HE1	5:S:79:ILE:HG21	2.01	0.43
5:S:182:TYR:CZ	5:S:189:HIS:HB2	2.53	0.43
5:S:191:LYS:HE3	5:S:193:TYR:CZ	2.53	0.43
5:S:282:MET:HB2	5:S:305:LEU:HD11	2.00	0.43
3:C:183:THR:OG1	3:C:184:ASN:N	2.49	0.43
4:R:75:PHE:CE2	4:R:142:ARG:HA	2.53	0.43
5:S:165:ILE:HB	5:S:181:VAL:HG23	2.00	0.43
5:S:159:LEU:HD12	5:S:159:LEU:HA	1.84	0.43
4:R:526:GLU:OE2	5:S:928:ARG:NH1	2.52	0.43
5:S:954:MET:HE3	5:S:954:MET:HB3	1.83	0.43
1:A:722:GLN:HG2	1:A:723:GLY:H	1.84	0.43
1:E:443:LYS:HE2	1:E:471:SER:HA	2.01	0.42
4:R:96:LEU:HD23	4:R:96:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:PHE:O	5:S:270:ARG:NH1	2.53	0.42
1:E:516:CYS:HA	1:E:533:SER:HB2	2.01	0.42
4:R:205:ASP:OD1	4:R:206:THR:N	2.53	0.42
5:S:23:PHE:HB3	5:S:30:ASN:ND2	2.34	0.42
3:C:123:PHE:HB2	3:C:136:GLY:O	2.19	0.42
4:R:525:PHE:HE2	5:S:951:PRO:HG3	1.84	0.42
5:S:269:SER:O	5:S:269:SER:OG	2.36	0.42
5:S:367:LEU:HD23	5:S:367:LEU:HA	1.78	0.42
5:S:899:LEU:HD23	5:S:899:LEU:HA	1.92	0.42
4:R:335:GLN:HG2	4:R:343:PHE:HB3	2.02	0.42
5:S:925:ASP:OD1	5:S:926:LEU:N	2.40	0.42
4:R:304:TRP:HB2	4:R:319:PHE:HE2	1.84	0.42
5:S:1102:ARG:HA	5:S:1105:MET:HG3	2.01	0.42
4:R:458:SER:HA	4:R:524:PRO:O	2.20	0.42
5:S:183:GLN:OE1	5:S:188:ARG:NE	2.52	0.42
5:S:977:CYS:SG	5:S:992:LEU:HB3	2.60	0.42
4:R:169:PRO:HG2	4:R:172:GLU:CD	2.45	0.41
4:R:90:CYS:SG	5:S:909:ILE:HD11	2.61	0.41
1:A:417:LEU:HG	1:A:418:TYR:CD1	2.56	0.41
1:A:595:PHE:HA	1:A:630:PRO:O	2.20	0.41
4:R:155:ILE:HG12	4:R:195:ILE:HG12	2.02	0.41
4:R:334:MET:C	4:R:334:MET:SD	3.04	0.41
3:C:198:ARG:O	4:R:298:ARG:NH2	2.53	0.41
4:R:398:ARG:NH2	4:R:410:CYS:O	2.53	0.41
4:R:444:LEU:HA	4:R:444:LEU:HD23	1.79	0.41
1:E:533:SER:O	1:E:558:VAL:HG22	2.20	0.41
5:S:1053:ASP:O	5:S:1057:ARG:HG3	2.21	0.41
4:R:85:TYR:CD1	4:R:127:LEU:HA	2.52	0.41
1:E:604:TYR:OH	1:E:645:PHE:HB3	2.20	0.41
4:R:225:TYR:CD2	4:R:226:LYS:HG3	2.56	0.41
5:S:364:VAL:HG23	5:S:375:LEU:HB3	2.03	0.41
1:A:417:LEU:HG	1:A:418:TYR:HD1	1.86	0.40
4:R:189:GLU:HB2	4:R:191:TYR:HE1	1.87	0.40
1:E:443:LYS:HG2	1:E:471:SER:C	2.46	0.40
4:R:129:HIS:NE2	4:R:200:THR:O	2.54	0.40
5:S:262:ASN:ND2	5:S:316:TYR:H	2.20	0.40
1:E:514:LYS:H	1:E:514:LYS:HG2	1.76	0.40
5:S:1104:LYS:HA	5:S:1104:LYS:HD2	1.94	0.40
3:C:126:ARG:HD2	3:C:199:TYR:CD2	2.57	0.40
4:R:76:SER:OG	4:R:77:SER:N	2.55	0.40
4:R:329:LEU:C	4:R:330:ARG:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:992:LEU:HD23	5:S:992:LEU:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	377/731 (52%)	354 (94%)	23 (6%)	0	100	100
1	E	361/731 (49%)	342 (95%)	18 (5%)	1 (0%)	36	64
2	B	51/102 (50%)	44 (86%)	6 (12%)	1 (2%)	6	29
3	C	148/201 (74%)	141 (95%)	7 (5%)	0	100	100
4	R	520/550 (94%)	477 (92%)	39 (8%)	4 (1%)	16	46
5	S	1076/1140 (94%)	1015 (94%)	58 (5%)	3 (0%)	36	64
All	All	2533/3455 (73%)	2373 (94%)	151 (6%)	9 (0%)	31	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	13	LYS
4	R	272	PHE
4	R	514	VAL
5	S	885	ASN
5	S	36	ASN
1	E	429	PHE
4	R	271	VAL
4	R	9	LYS
5	S	443	VAL

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	34/634 (5%)	34 (100%)	0	100	100
1	E	121/634 (19%)	121 (100%)	0	100	100
2	B	37/93 (40%)	37 (100%)	0	100	100
3	C	89/176 (51%)	89 (100%)	0	100	100
4	R	400/499 (80%)	400 (100%)	0	100	100
5	S	575/999 (58%)	573 (100%)	2 (0%)	86	81
All	All	1256/3035 (41%)	1254 (100%)	2 (0%)	85	84

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

Mol	Chain	Res	Type
5	S	209	GLN
5	S	1006	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
4	R	15	ASN
4	R	20	HIS
4	R	37	HIS
4	R	43	HIS
4	R	98	GLN
4	R	335	GLN
5	S	262	ASN
5	S	826	ASN

5.3.3 RNA ⓘ

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.

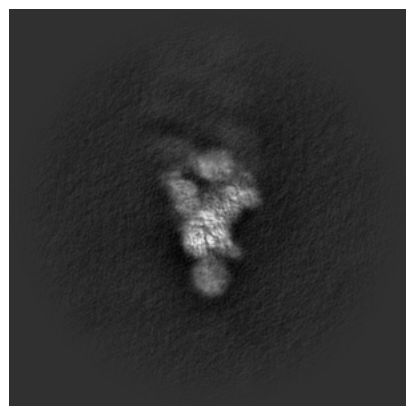
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63386. These allow visual inspection of the internal detail of the map and identification of artifacts.

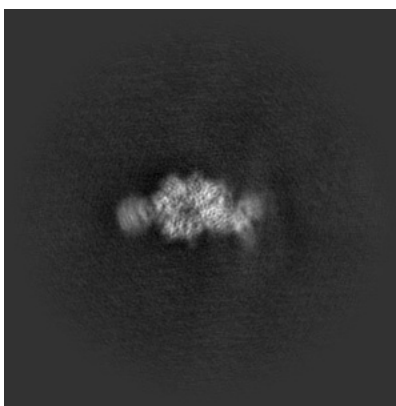
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

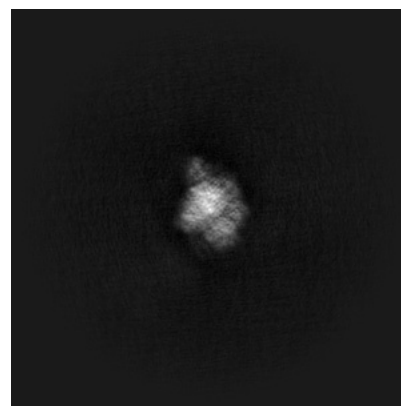
6.1.1 Primary map



X

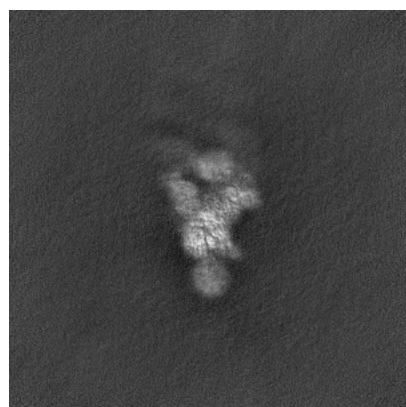


Y

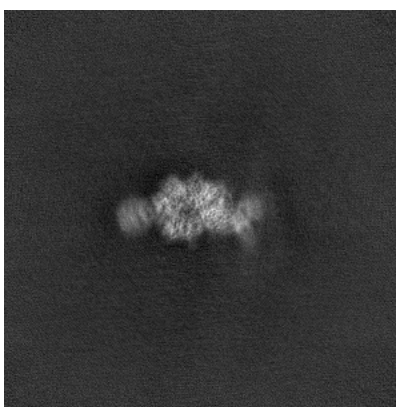


Z

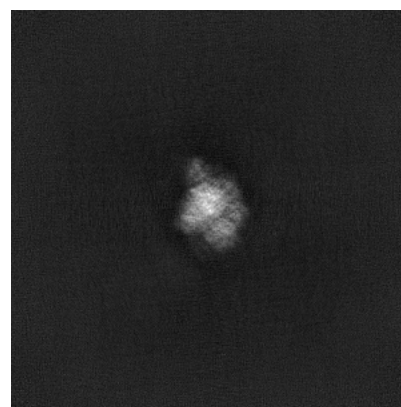
6.1.2 Raw map



X



Y



Z

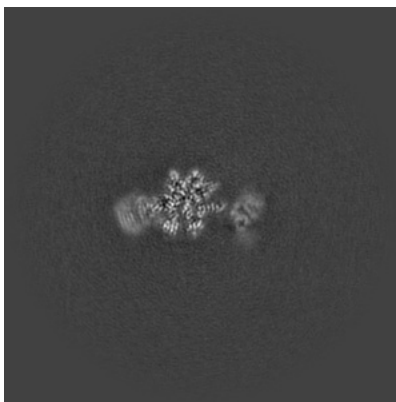
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

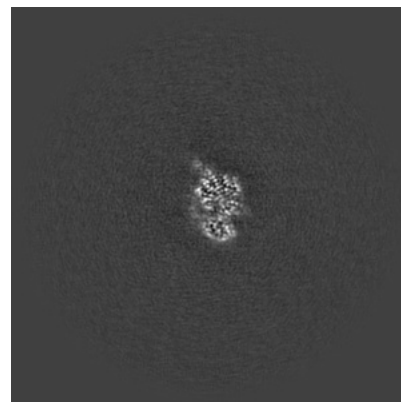
6.2.1 Primary map



X Index: 300

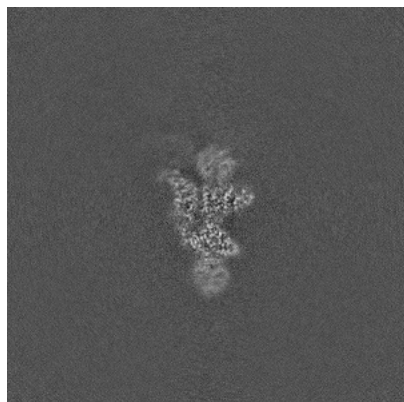


Y Index: 300

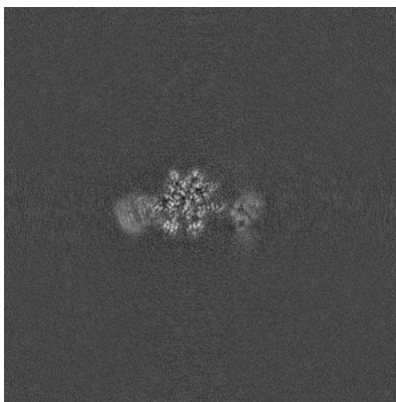


Z Index: 300

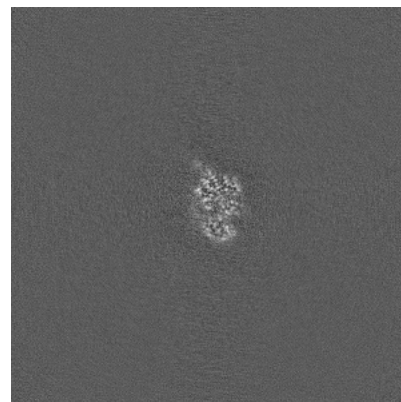
6.2.2 Raw map



X Index: 300



Y Index: 300

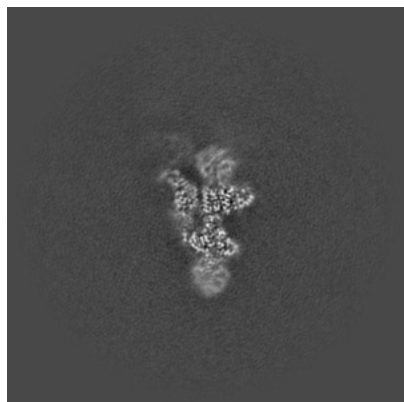


Z Index: 300

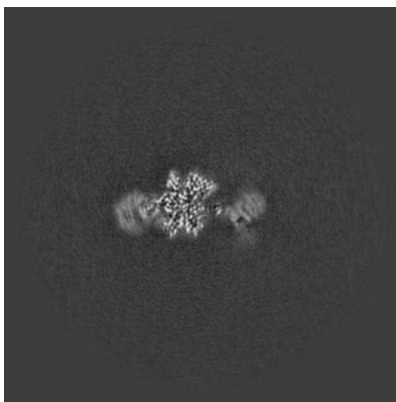
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

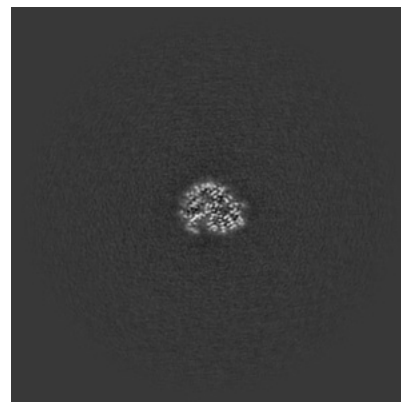
6.3.1 Primary map



X Index: 298



Y Index: 304

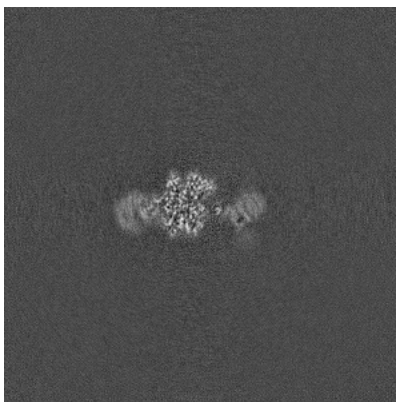


Z Index: 248

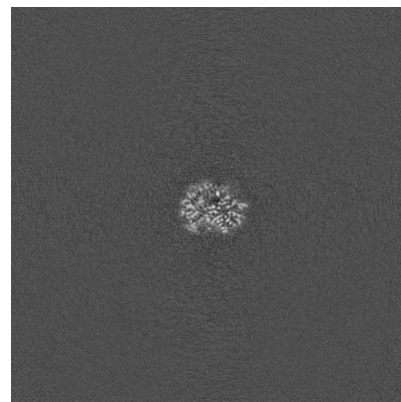
6.3.2 Raw map



X Index: 298



Y Index: 305

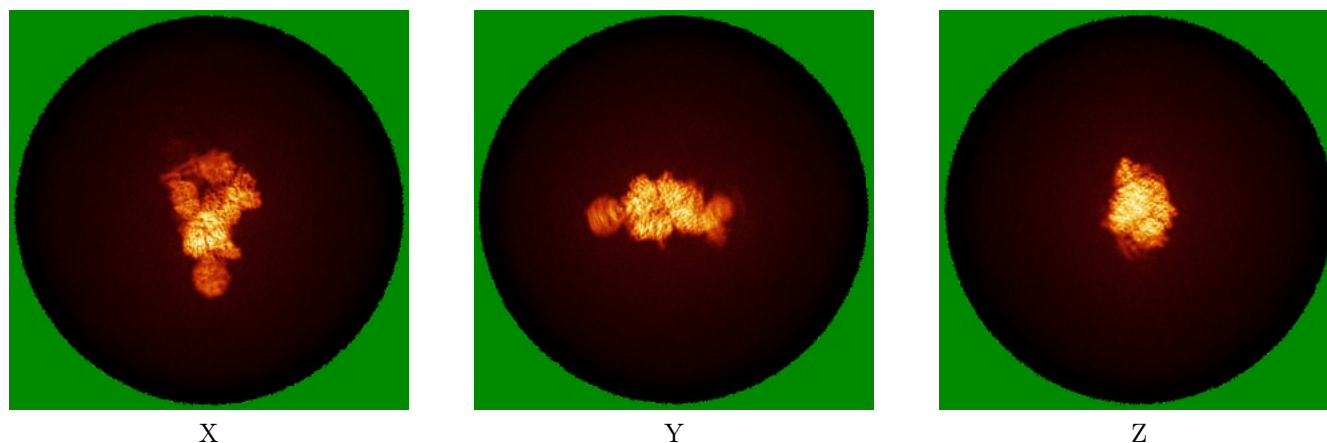


Z Index: 252

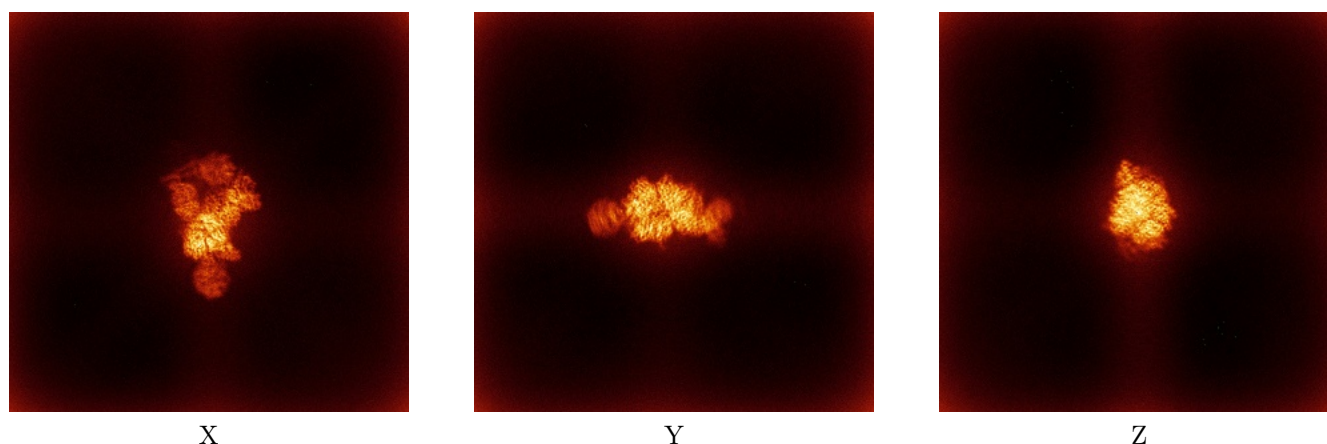
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

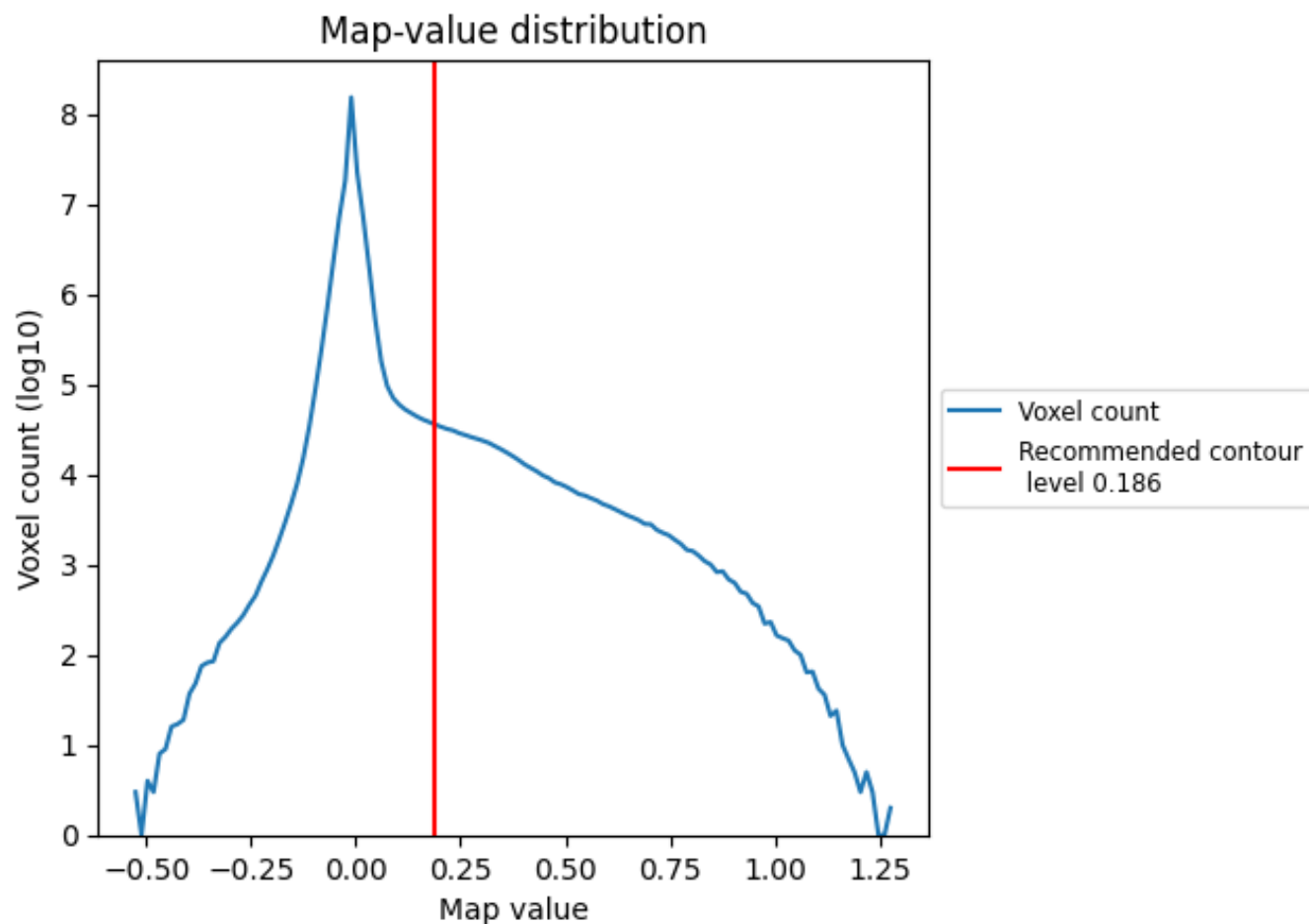
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

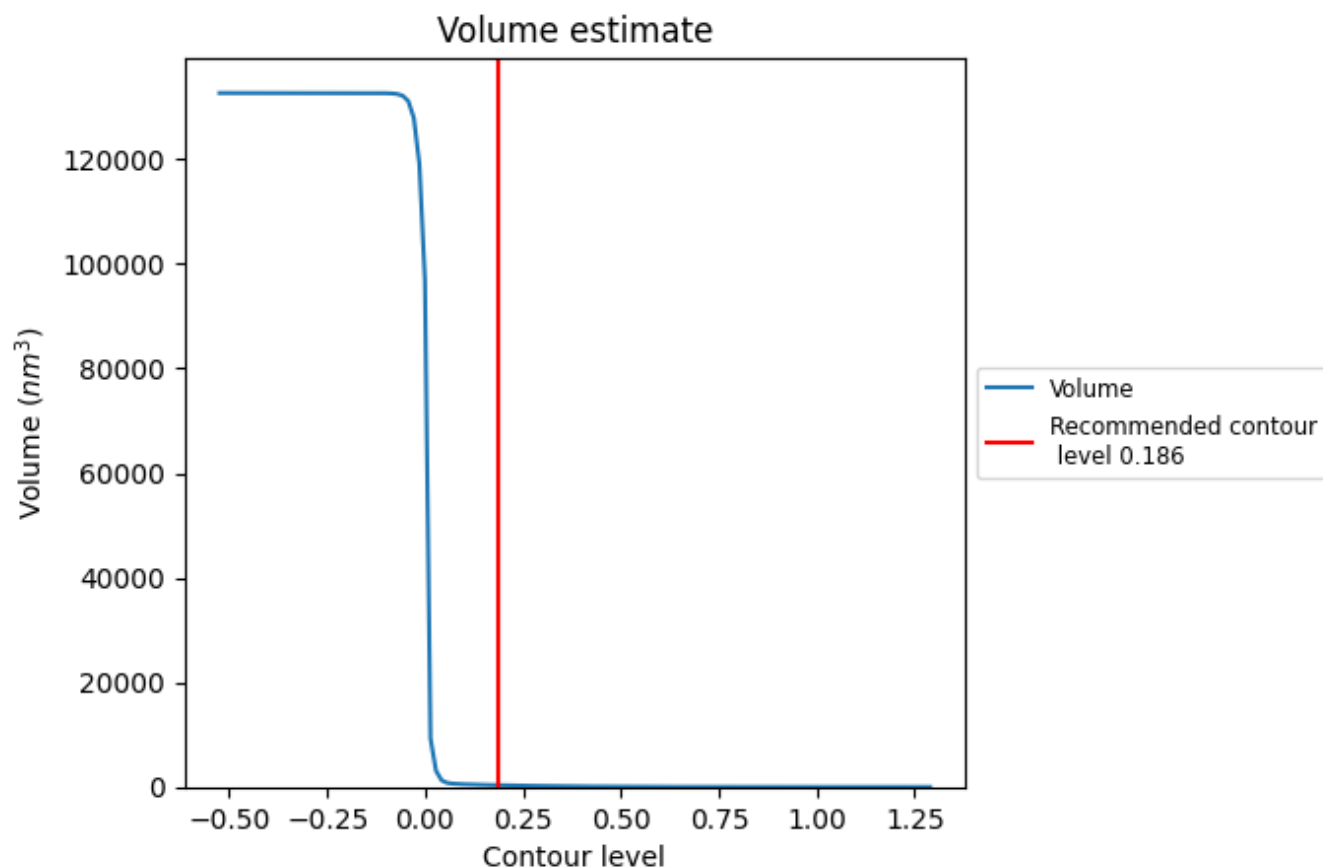
This section contains the results of statistical analysis of the map.

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.

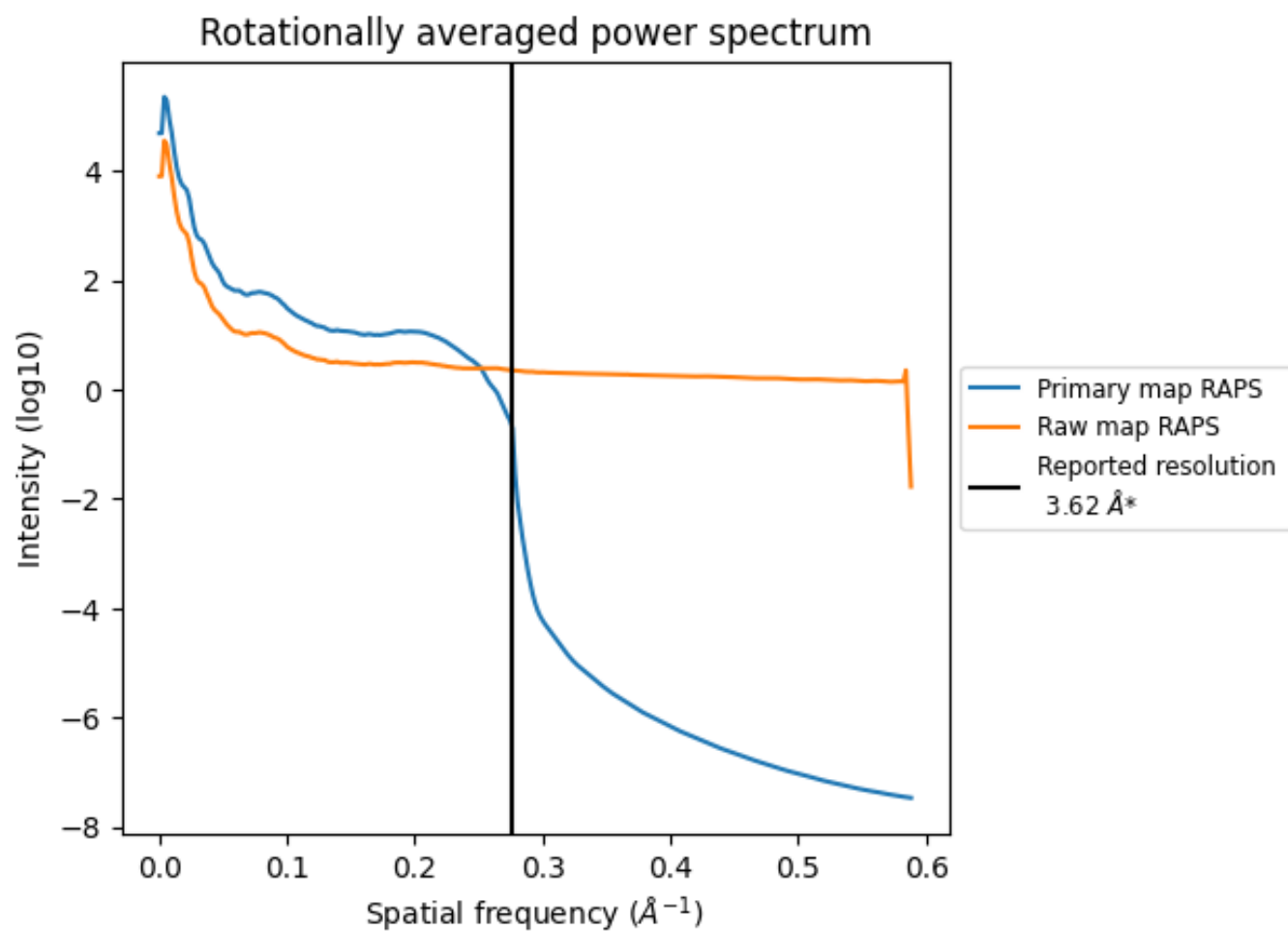
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 335 nm^3 ; this corresponds to an approximate mass of 303 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 ⓘ

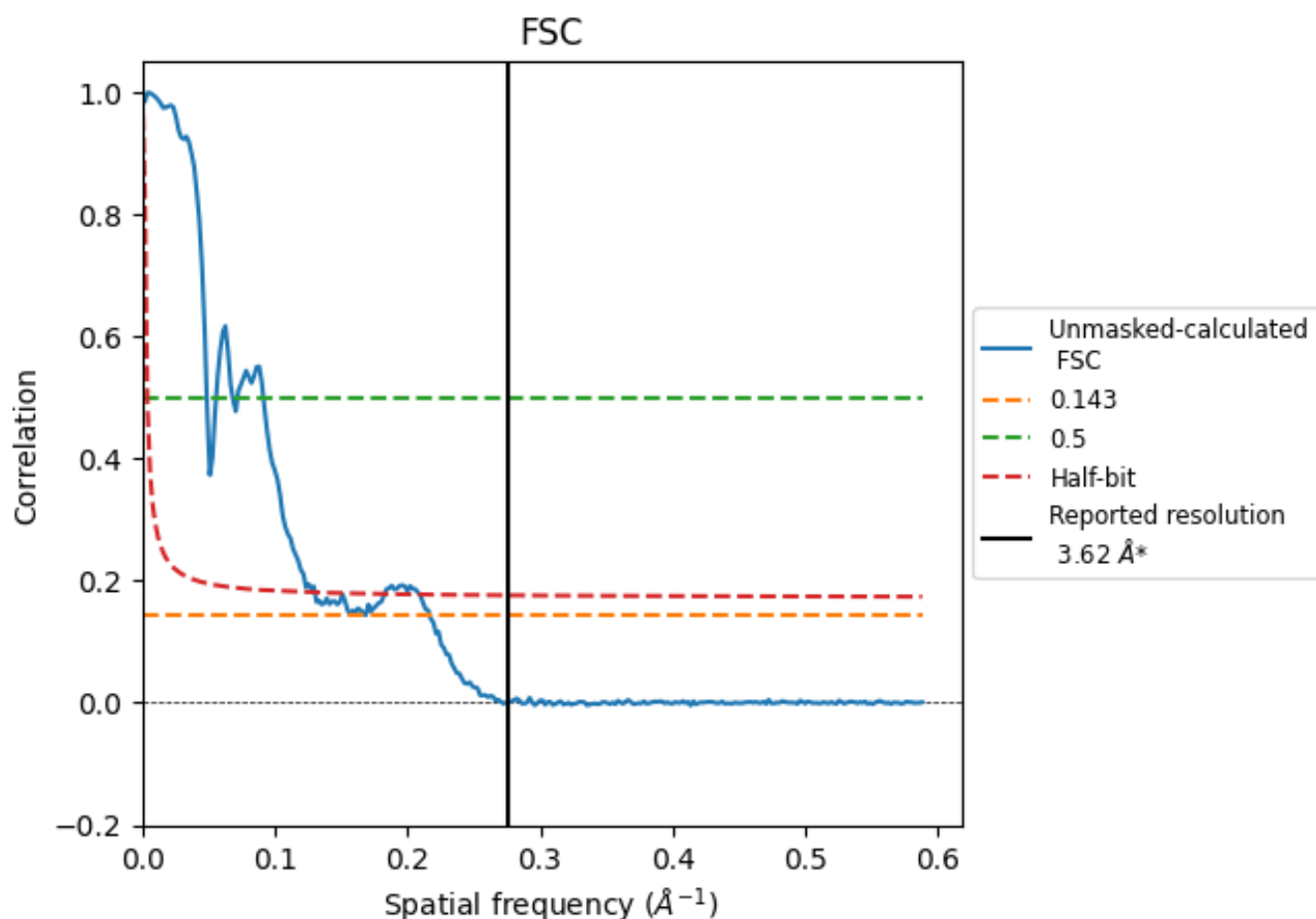


*Reported resolution corresponds to spatial frequency of 0.276 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.276 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

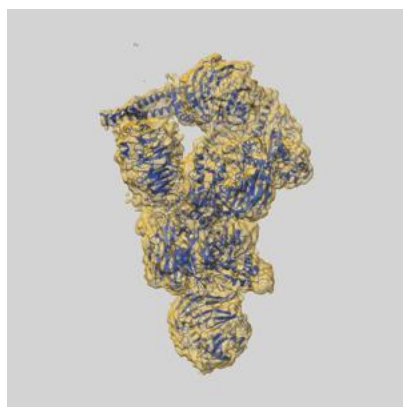
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.93	20.53	7.68

*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 5.93 differs from the reported value 3.62 by more than 10 %

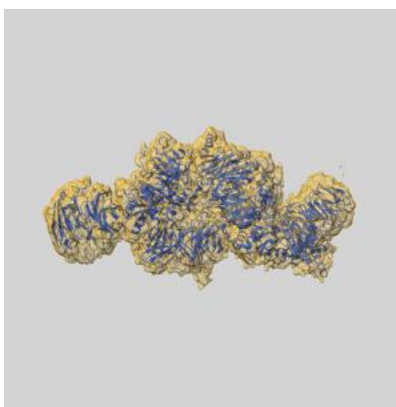
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63386 and PDB model 9LU1. Per-residue inclusion information can be found in section [3](#) on page [6](#).

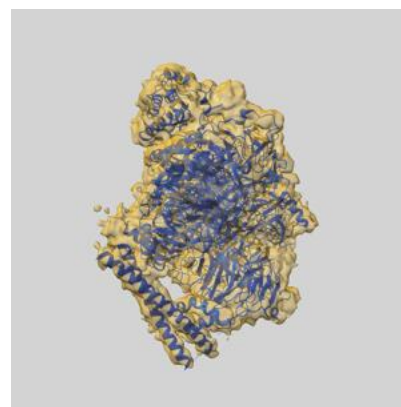
9.1 Map-model overlay [i](#)



X



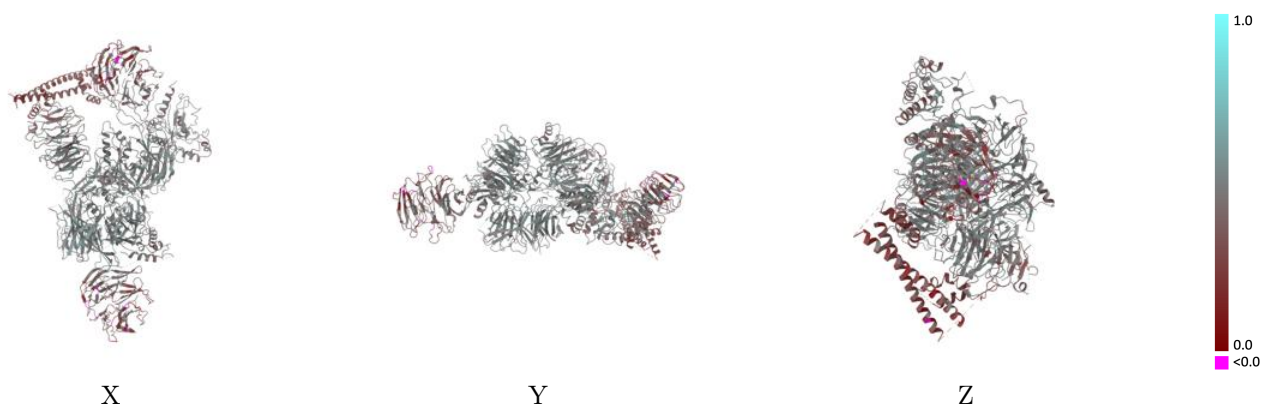
Y



Z

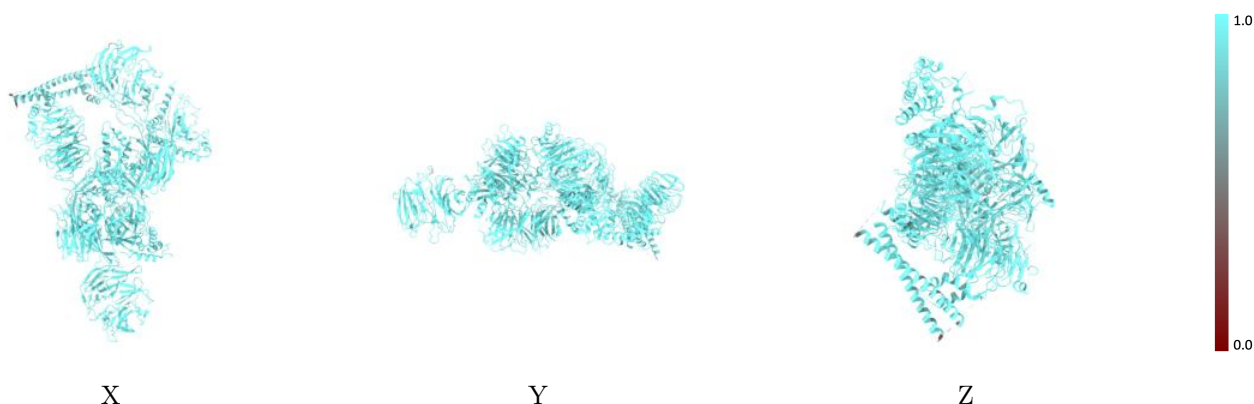
The images above show the 3D surface view of the map at the recommended contour level 0.186 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



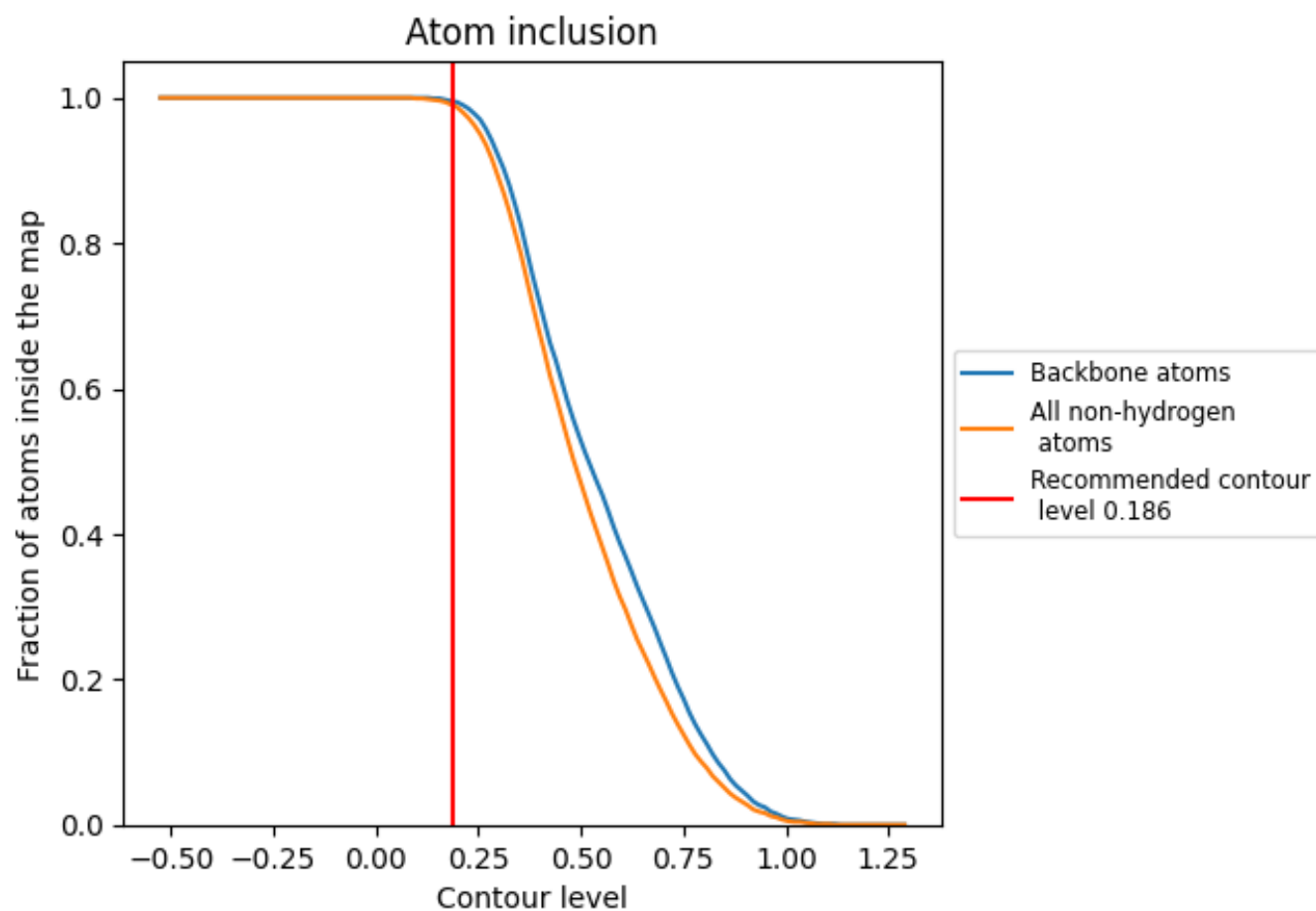
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.186).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.186) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9900	0.4520
A	0.9730	0.3520
B	1.0000	0.4760
C	0.9970	0.4600
E	0.9840	0.4250
R	0.9910	0.4900
S	0.9950	0.4660

1.0

0.0

<0.0