



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:24 PM UTC

PDB ID : 7AI7 / pdb_00007ai7
EMDB ID : EMD-11793
Title : MutS in Intermediate state
Authors : Fernandez-Leiro, R.; Bhairosing-Kok, D.; Sixma, T.K.; Lamers, M.H.
Deposited on : 2020-09-26
Resolution : 3.90 Å(reported)
Based on initial model : 1E3M

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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

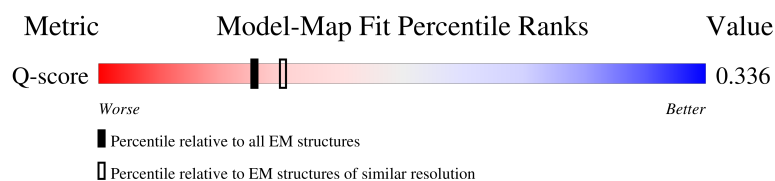
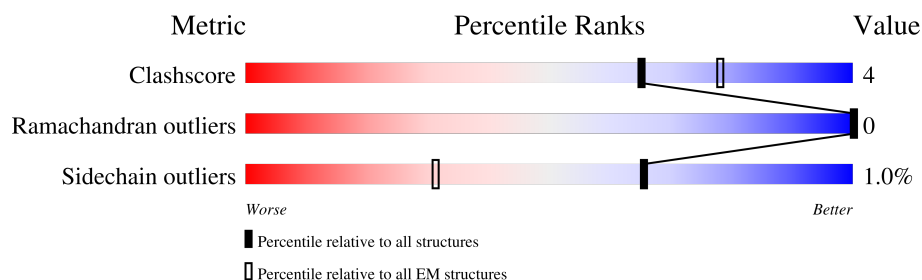
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	853	
1	B	853	
2	C	14	
3	D	14	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12085 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 DNA mismatch repair protein MutS.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	791	Total	C	N	O	S	0	0
			6218	3907	1108	1174	29		
1	B	669	Total	C	N	O	S	0	0
			5261	3301	943	993	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	835	ARG	ASP	conflict	UNP P23909
B	835	ARG	ASP	conflict	UNP P23909

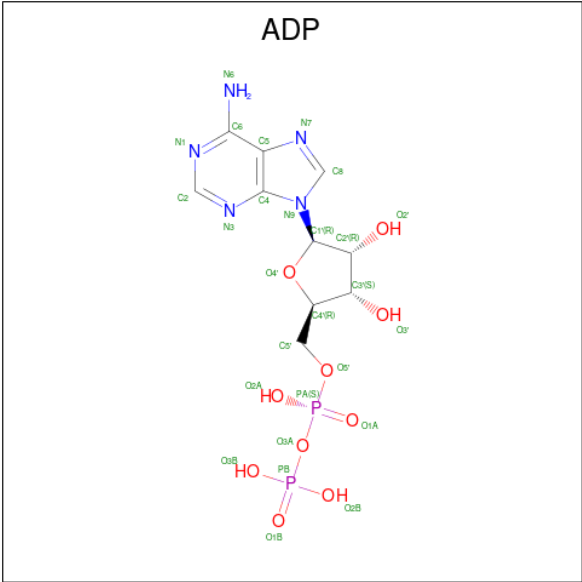
- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*AP*TP*CP*CP*TP*AP*AP*CP*TP*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	13	Total	C	N	O	P	0	0
			266	127	50	76	13		

- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*TP*TP*AP*GP*CP*TP*TP*AP*GP*GP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	14	Total	C	N	O	P	0	0
			286	137	49	86	14		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

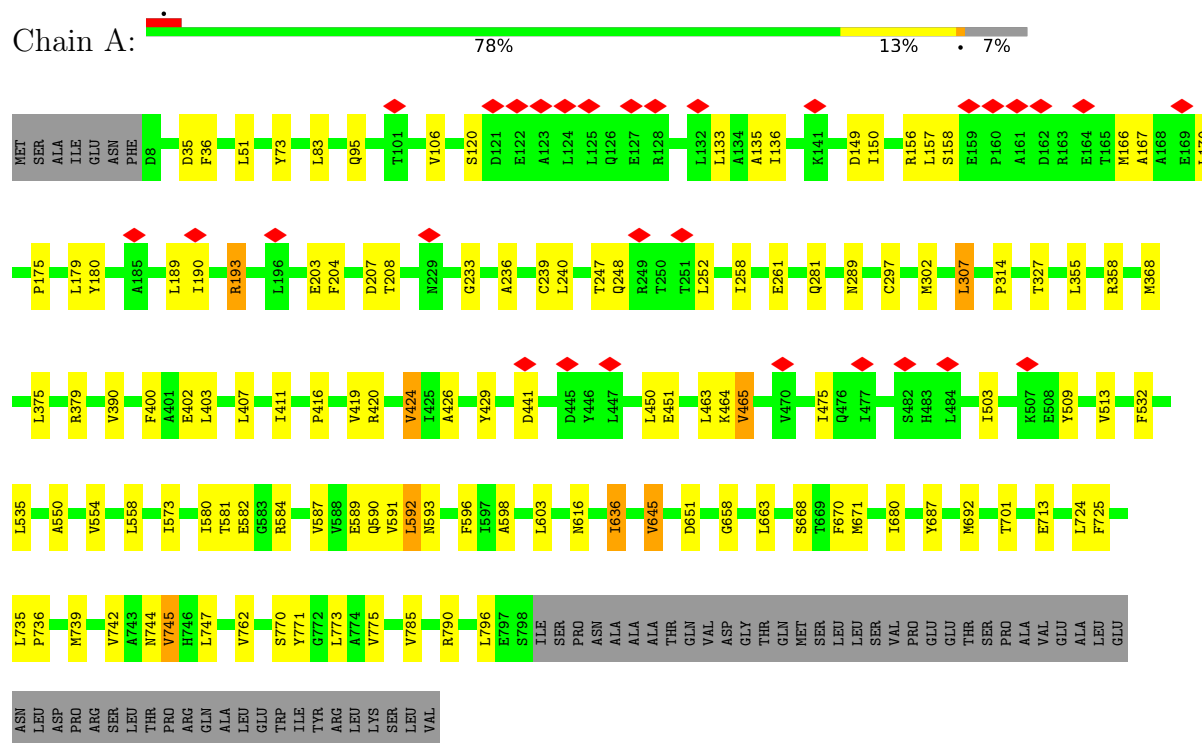


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

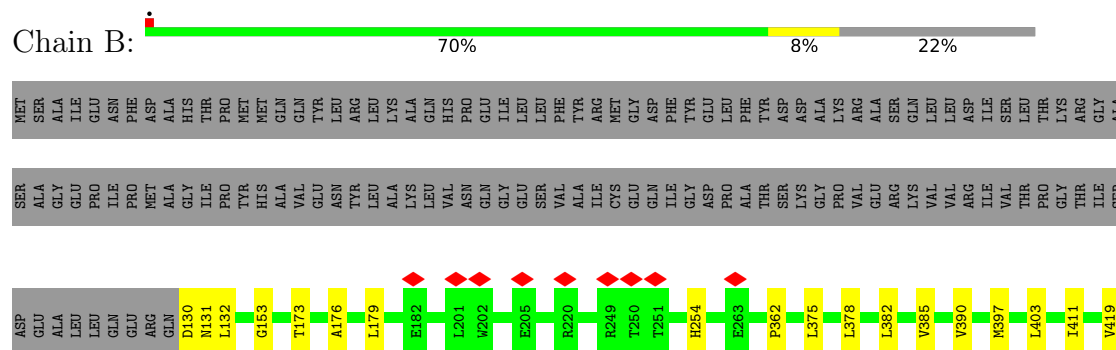
3 Residue-property plots

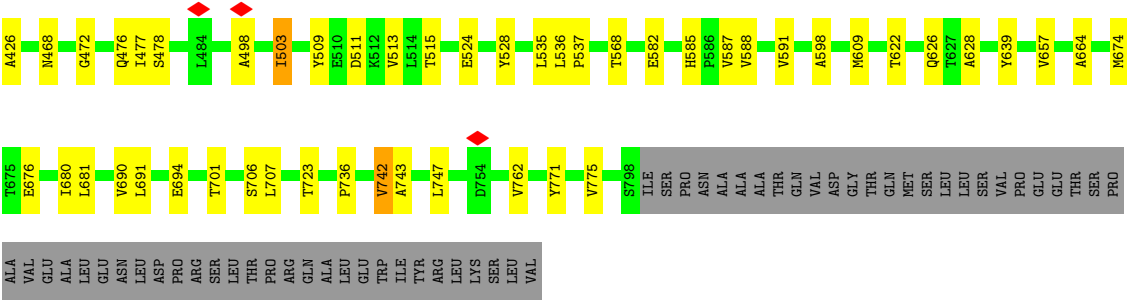
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

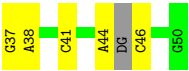


• Molecule 1: DNA mismatch repair protein MutS

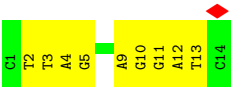




● Molecule 2: DNA (5'-D(P*GP*AP*TP*CP*CP*TP*AP*AP*CP*TP*AP*AP*G)-3')



● Molecule 3: DNA (5'-D(P*CP*TP*TP*AP*GP*CP*TP*TP*AP*GP*GP*AP*TP*C)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67679	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.657	Depositor
Minimum map value	-0.276	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	262.08, 262.08, 262.08	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.17, 1.17, 1.17	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	1.22	10/6324 (0.2%)	1.66	27/8562 (0.3%)
1	B	1.06	1/5347 (0.0%)	1.59	6/7238 (0.1%)
2	C	0.34	0/297	0.60	0/453
3	D	0.32	0/319	0.69	0/490
All	All	1.12	11/12287 (0.1%)	1.59	33/16743 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	PRO	C-O	-7.04	1.14	1.24
1	A	745	VAL	C-O	6.86	1.30	1.23
1	A	307	LEU	C-O	-6.37	1.15	1.24
1	A	464	LYS	C-O	-6.09	1.17	1.24
1	A	770	SER	C-O	6.08	1.31	1.24
1	B	568	THR	C-O	-6.07	1.16	1.23
1	A	281	GLN	C-O	5.83	1.30	1.24
1	A	463	LEU	C-O	5.82	1.30	1.24
1	A	744	ASN	C-O	5.56	1.30	1.23
1	A	193	ARG	C-O	5.55	1.30	1.23
1	A	581	THR	C-O	5.03	1.29	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	636	ILE	N-CA-C	-7.74	105.02	112.29
1	A	451	GLU	N-CA-C	-6.42	104.14	112.23
1	B	478	SER	CA-C-O	-6.37	114.62	121.56
1	A	297	CYS	N-CA-C	-6.30	105.17	112.92
1	A	658	GLY	CA-C-O	-6.30	117.19	122.29
1	A	592	LEU	CA-C-N	6.17	128.86	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	LEU	C-N-CA	6.17	128.86	120.54
1	A	180	TYR	CA-C-O	-6.15	113.80	121.55
1	A	429	TYR	N-CA-C	-6.14	104.66	111.36
1	A	36	PHE	CB-CA-C	-5.97	100.51	110.19
1	A	532	PHE	CA-C-O	-5.84	114.36	120.55
1	B	639	TYR	CA-C-O	-5.82	115.12	121.87
1	A	247	THR	CA-C-O	-5.77	114.76	120.70
1	B	179	LEU	CA-C-O	-5.67	114.51	120.80
1	A	36	PHE	N-CA-C	5.64	117.92	108.73
1	A	771	TYR	CA-C-N	5.61	126.05	119.94
1	A	771	TYR	C-N-CA	5.61	126.05	119.94
1	A	670	PHE	CB-CA-C	-5.42	102.34	110.90
1	A	149	ASP	CA-C-O	-5.38	115.17	120.98
1	B	477	ILE	CA-C-O	-5.36	115.65	121.92
1	A	441	ASP	CA-C-N	5.29	126.80	120.13
1	A	441	ASP	C-N-CA	5.29	126.80	120.13
1	A	651	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	743	ALA	CA-C-O	-5.20	115.53	121.40
1	A	573	ILE	N-CA-C	-5.15	105.52	110.72
1	A	593	ASN	CA-C-O	-5.14	115.40	120.90
1	B	639	TYR	N-CA-C	-5.11	103.78	110.53
1	A	379	ARG	CA-C-O	-5.09	115.47	120.82
1	A	465	VAL	CA-C-N	5.02	126.53	121.35
1	A	465	VAL	C-N-CA	5.02	126.53	121.35
1	A	358	ARG	N-CA-CB	-5.02	104.67	112.30
1	A	725	PHE	CA-C-N	5.02	127.98	120.95
1	A	725	PHE	C-N-CA	5.02	127.98	120.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6218	0	6262	59	0
1	B	5261	0	5304	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	266	0	148	3	0
3	D	286	0	160	6	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
All	All	12085	0	11898	96	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 (96) 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)
1:A:713:GLU:HA	1:A:739:MET:HE1	1.72	0.71
3:D:4:DA:H2'	3:D:5:DG:C8	2.27	0.68
1:A:307:LEU:HD13	1:A:554:VAL:HB	1.81	0.62
1:A:248:GLN:HG2	1:A:252:LEU:HD11	1.82	0.61
1:A:509:TYR:O	1:A:513:VAL:HG23	2.02	0.60
3:D:9:DA:H2'	3:D:10:DG:C8	2.41	0.56
1:B:362:PRO:HB3	1:B:424:VAL:HG13	1.88	0.55
1:A:95:GLN:HE21	1:A:106:VAL:HG21	1.72	0.54
1:B:509:TYR:O	1:B:513:VAL:HG23	2.07	0.54
1:A:747:LEU:HD21	1:A:762:VAL:HG22	1.90	0.53
1:A:736:PRO:HA	1:A:742:VAL:HB	1.89	0.53
1:A:170:LEU:HB3	1:A:193:ARG:HD2	1.91	0.53
1:A:133:LEU:HG	1:A:240:LEU:HD11	1.91	0.53
1:A:166:MET:HE3	1:A:166:MET:HA	1.89	0.52
1:B:582:GLU:HA	1:B:598:ALA:HB1	1.92	0.52
1:A:416:PRO:HG2	1:A:424:VAL:HG12	1.92	0.52
1:A:400:PHE:HB3	1:A:403:LEU:HD13	1.93	0.51
1:A:207:ASP:OD1	1:A:208:THR:N	2.43	0.51
1:A:120:SER:HB2	1:A:687:TYR:CG	2.44	0.51
1:A:587:VAL:O	1:A:591:VAL:HG23	2.11	0.51
1:A:327:THR:HG23	1:A:390:VAL:HG22	1.92	0.50
1:B:385:VAL:HB	1:B:390:VAL:HG11	1.93	0.50
1:A:616:ASN:HB2	1:A:775:VAL:HG11	1.92	0.50
1:A:135:ALA:HA	1:A:179:LEU:O	2.11	0.49
1:A:450:LEU:HD11	1:A:465:VAL:HG11	1.93	0.49
1:A:289:ASN:HB3	1:B:664:ALA:CB	2.42	0.49
1:B:747:LEU:HD21	1:B:762:VAL:HG22	1.95	0.49
1:A:156:ARG:HB3	1:A:261:GLU:HB2	1.95	0.49
3:D:2:DT:H2''	3:D:3:DT:C5	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:VAL:HG21	1:B:528:TYR:CD2	2.48	0.48
1:A:167:ALA:HB2	1:A:189:LEU:HD22	1.95	0.48
1:A:133:LEU:HG	1:A:240:LEU:CD1	2.44	0.48
1:A:603:LEU:HD11	1:A:724:LEU:CD1	2.43	0.48
1:A:450:LEU:HD12	1:A:450:LEU:C	2.39	0.48
1:A:402:GLU:HG2	1:A:403:LEU:HD12	1.96	0.47
1:A:302:MET:HG2	1:A:550:ALA:HB2	1.96	0.47
1:A:580:ILE:HG12	1:A:645:VAL:HG22	1.96	0.47
1:A:175:PRO:HD2	1:A:193:ARG:HD3	1.97	0.47
1:A:773:LEU:HD13	1:A:790:ARG:HG2	1.95	0.47
1:A:582:GLU:HA	1:A:598:ALA:HB1	1.96	0.47
1:A:475:ILE:HD11	1:A:503:ILE:HG12	1.97	0.46
1:B:403:LEU:HD22	1:B:535:LEU:HD23	1.98	0.46
1:A:745:VAL:CG1	1:A:762:VAL:HG13	2.45	0.46
1:B:609:MET:HB3	1:B:742:VAL:HG23	1.96	0.46
1:A:302:MET:CG	1:A:550:ALA:HB2	2.45	0.46
1:A:407:LEU:HD21	1:A:535:LEU:HD11	1.98	0.46
1:B:468:ASN:O	1:B:472:GLY:N	2.48	0.46
1:A:419:VAL:HA	1:A:424:VAL:HG11	1.97	0.45
1:A:203:GLU:HB3	1:A:239:CYS:HA	1.97	0.45
1:B:736:PRO:HA	1:B:742:VAL:HG13	1.97	0.45
1:A:589:GLU:HG3	1:A:590:GLN:N	2.32	0.45
1:B:511:ASP:O	1:B:515:THR:HG22	2.17	0.45
1:B:674:MET:SD	1:B:707:LEU:HD21	2.57	0.45
1:B:676:GLU:O	1:B:680:ILE:HD13	2.17	0.45
2:C:41:DC:H42	3:D:10:DG:H1	1.65	0.45
1:B:131:ASN:OD1	1:B:132:LEU:HD12	2.17	0.45
1:B:476:GLN:HE21	1:B:498:ALA:HB3	1.81	0.44
1:A:51:LEU:HD21	1:A:83:LEU:HG	1.99	0.44
1:A:796:LEU:HD12	1:B:706:SER:HB3	2.00	0.44
1:A:592:LEU:HD23	1:A:592:LEU:HA	1.90	0.44
1:B:587:VAL:O	1:B:591:VAL:HG22	2.18	0.43
1:B:628:ALA:HB2	1:B:691:LEU:HD11	2.00	0.43
1:A:157:LEU:HD11	1:A:233:GLY:C	2.43	0.43
1:B:375:LEU:HA	1:B:378:LEU:HD12	1.98	0.43
1:A:680:ILE:HG21	1:A:692:MET:HE3	2.01	0.43
2:C:37:DG:H1'	2:C:38:DA:C8	2.54	0.43
1:A:136:ILE:HG21	1:A:190:ILE:HG21	2.00	0.43
1:A:668:SER:H	1:A:671:MET:HB3	1.84	0.43
1:A:355:LEU:HD13	1:A:368:MET:HE1	2.00	0.43
1:B:153:GLY:HA3	1:B:254:HIS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:11:DG:H2''	3:D:12:DA:C8	2.53	0.43
1:A:35:ASP:O	1:A:73:TYR:HB3	2.19	0.42
1:A:157:LEU:HD11	1:A:233:GLY:O	2.19	0.42
1:A:735:LEU:N	1:A:736:PRO:CD	2.82	0.42
1:B:585:HIS:HB2	1:B:626:GLN:HB3	2.00	0.42
1:B:132:LEU:HD22	1:B:173:THR:O	2.19	0.42
1:B:585:HIS:HB3	1:B:588:VAL:HG12	2.02	0.42
1:A:157:LEU:HD13	1:A:258:ILE:HD11	2.02	0.41
1:A:663:LEU:HD21	1:B:622:THR:HA	2.01	0.41
1:B:130:ASP:C	1:B:176:ALA:HB2	2.45	0.41
1:A:589:GLU:HB3	1:A:596:PHE:HB2	2.02	0.41
1:A:785:VAL:HG21	1:B:681:LEU:HD13	2.02	0.41
1:A:158:SER:HB3	1:A:261:GLU:HB3	2.02	0.41
1:A:307:LEU:HD11	1:A:558:LEU:HD11	2.02	0.41
1:B:411:ILE:C	1:B:426:ALA:HB2	2.45	0.41
1:A:701:THR:HG21	1:B:701:THR:HG21	2.01	0.41
1:B:382:LEU:HD12	1:B:397:MET:HE1	2.03	0.41
1:A:591:VAL:HG12	1:A:591:VAL:O	2.21	0.41
1:A:204:PHE:CE2	1:A:236:ALA:HA	2.56	0.41
3:D:12:DA:H2''	3:D:13:DT:C2	2.56	0.41
1:B:503:ILE:H	1:B:503:ILE:HG13	1.54	0.40
1:A:411:ILE:C	1:A:426:ALA:HB2	2.46	0.40
1:B:690:VAL:O	1:B:723:THR:HA	2.21	0.40
1:B:771:TYR:O	1:B:775:VAL:HG23	2.20	0.40
2:C:44:DA:H2'	2:C:46:DC:O4'	2.22	0.40
1:B:536:LEU:N	1:B:537:PRO:CD	2.85	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	789/853 (92%)	757 (96%)	32 (4%)	0	100	100
1	B	667/853 (78%)	641 (96%)	26 (4%)	0	100	100
All	All	1456/1706 (85%)	1398 (96%)	58 (4%)	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	656/710 (92%)	649 (99%)	7 (1%)	65	74
1	B	554/710 (78%)	549 (99%)	5 (1%)	70	75
All	All	1210/1420 (85%)	1198 (99%)	12 (1%)	65	75

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ILE
1	A	375	LEU
1	A	420	ARG
1	A	424	VAL
1	A	584	ARG
1	A	636	ILE
1	A	645	VAL
1	B	503	ILE
1	B	524	GLU
1	B	657	VAL
1	B	694	GLU
1	B	742	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	95	GLN
1	A	242	GLN
1	A	483	HIS
1	B	216	GLN
1	B	312	HIS
1	B	476	GLN
1	B	557	ASN
1	B	590	GLN
1	B	643	GLN
1	B	744	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADP	B	1801	-	28,29,29	0.62	1 (3%)	43,45,45	0.59	0
4	ADP	A	1801	-	28,29,29	0.57	0	43,45,45	0.69	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	B	1801	-	-	3/16/32/32	0/3/3/3
4	ADP	A	1801	-	-	4/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1801	ADP	PB-O3B	-2.28	1.46	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	ADP	C3'-C2'-C1'	2.10	105.43	101.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

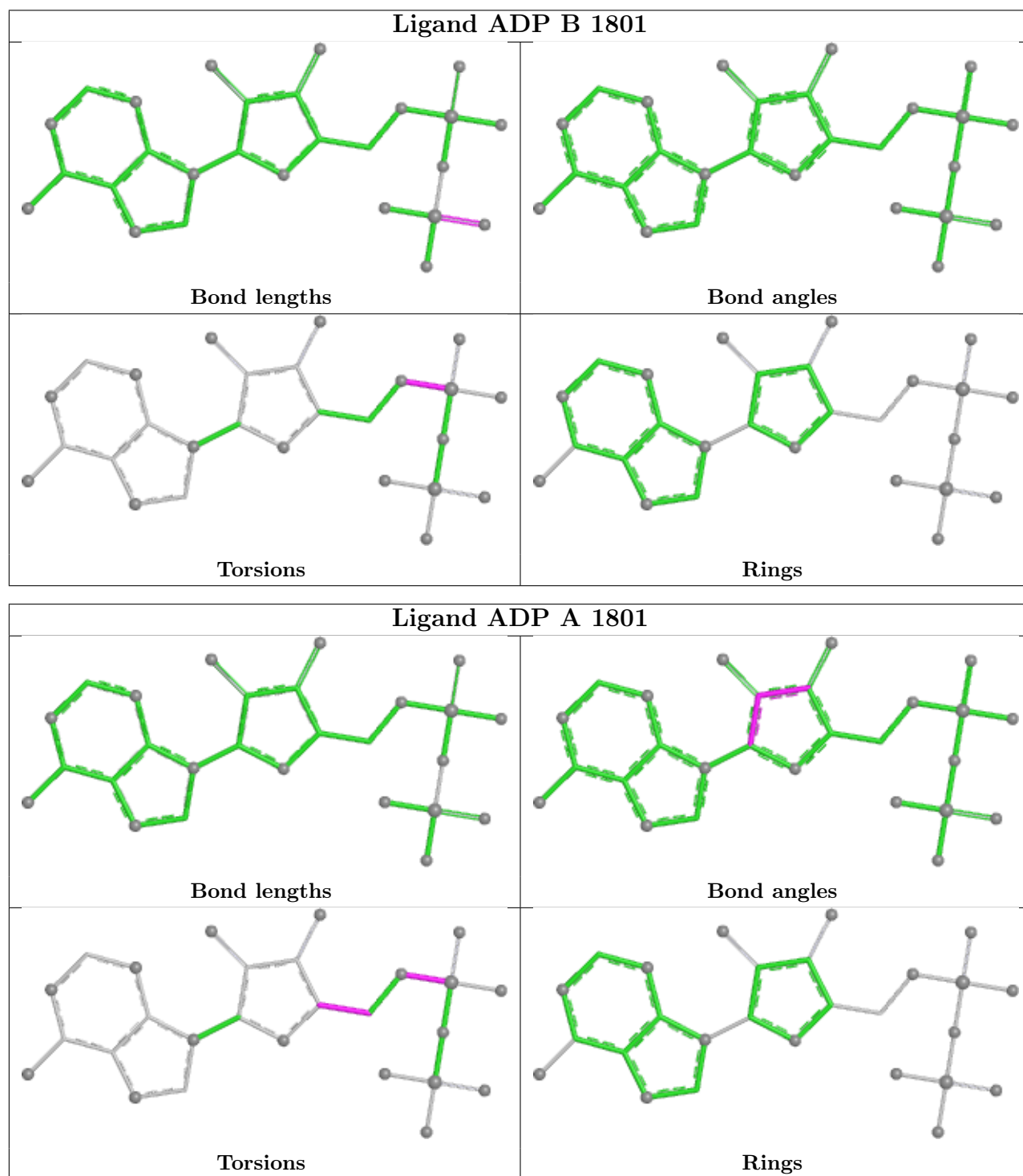
Mol	Chain	Res	Type	Atoms
4	A	1801	ADP	C5'-O5'-PA-O3A
4	B	1801	ADP	C5'-O5'-PA-O1A
4	B	1801	ADP	C5'-O5'-PA-O2A
4	B	1801	ADP	C5'-O5'-PA-O3A
4	A	1801	ADP	O4'-C4'-C5'-O5'
4	A	1801	ADP	C3'-C4'-C5'-O5'
4	A	1801	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

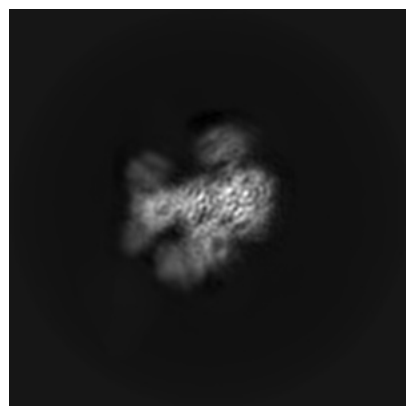
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11793. These allow visual inspection of the internal detail of the map and identification of artifacts.

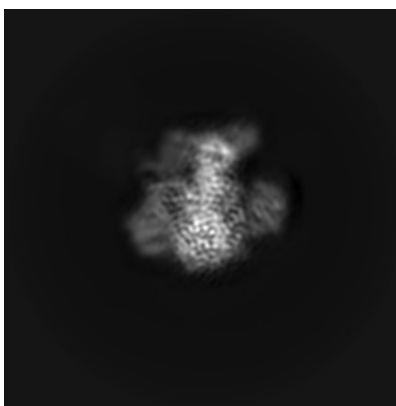
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

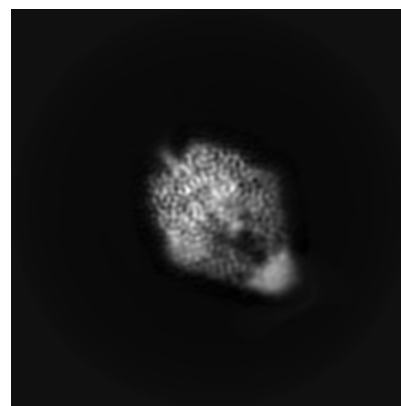
6.1.1 Primary map



X

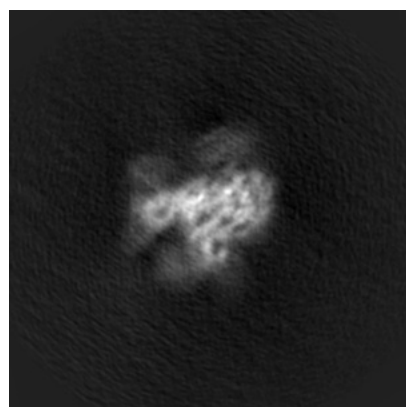


Y

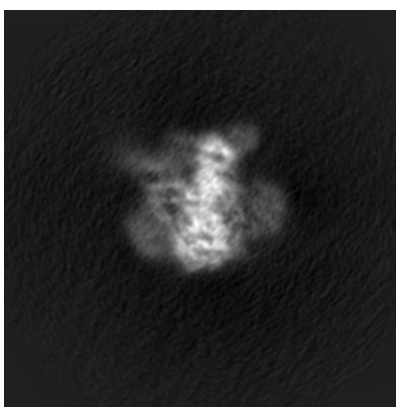


Z

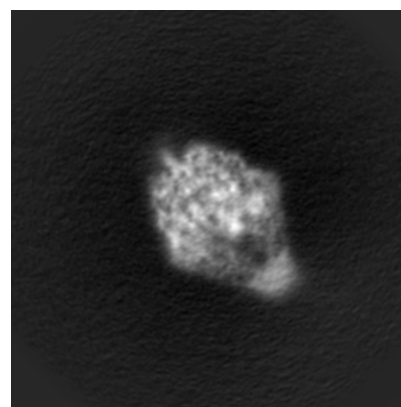
6.1.2 Raw map



X



Y

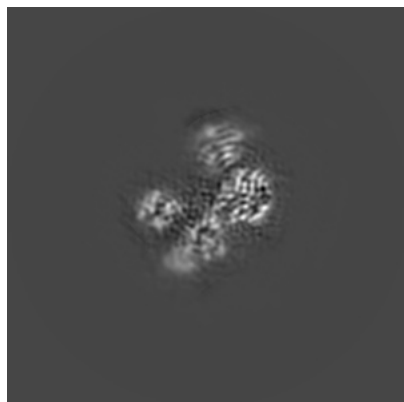


Z

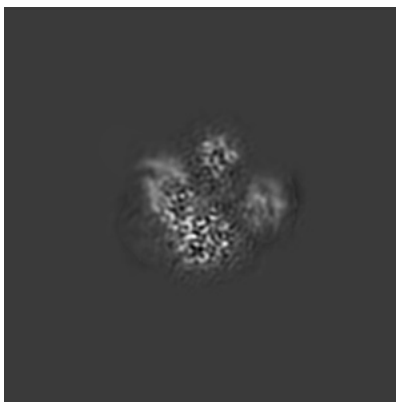
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

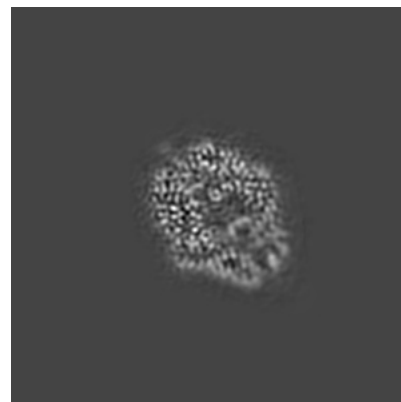
6.2.1 Primary map



X Index: 112

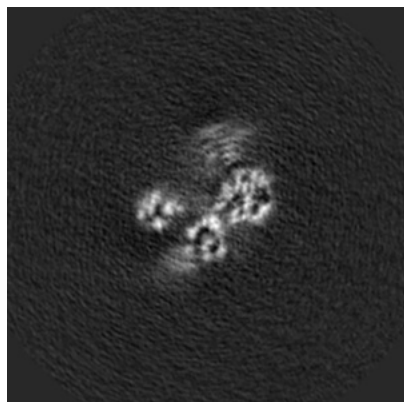


Y Index: 112

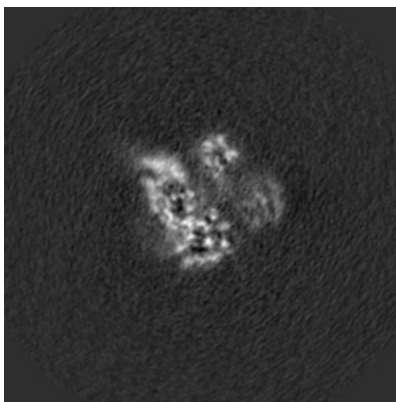


Z Index: 112

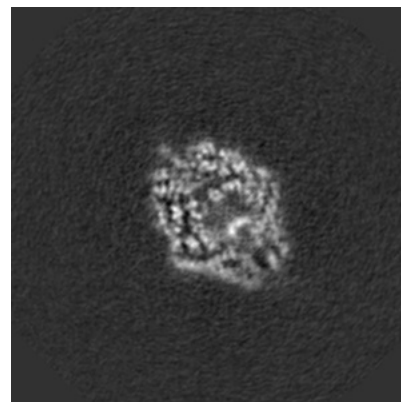
6.2.2 Raw map



X Index: 112



Y Index: 112

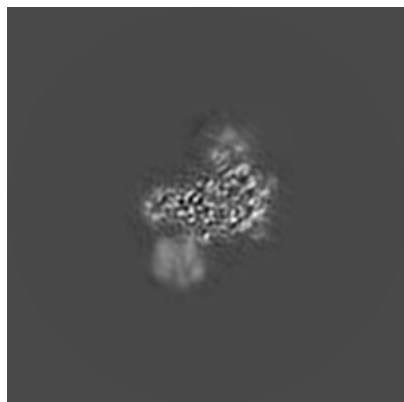


Z Index: 112

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

6.3 Largest variance slices [i](#)

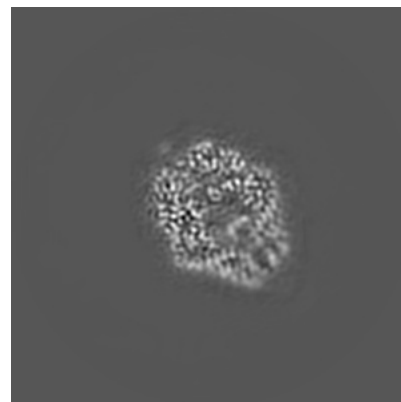
6.3.1 Primary map



X Index: 100

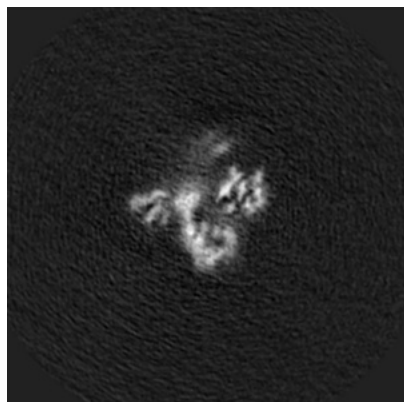


Y Index: 121

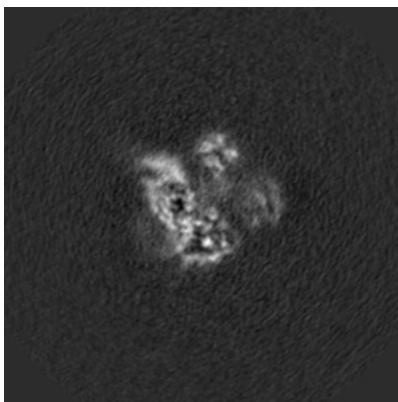


Z Index: 113

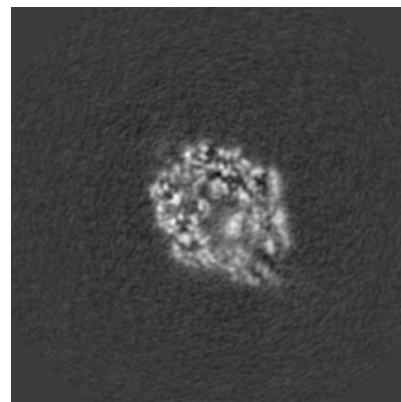
6.3.2 Raw map



X Index: 125



Y Index: 111

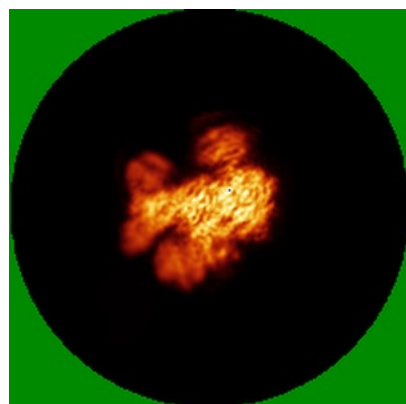


Z Index: 117

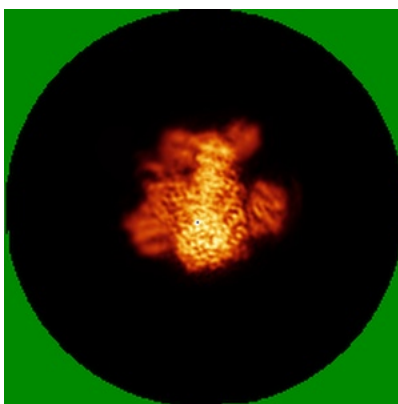
The images above show the largest variance slices of the map in three orthogonal directions.

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

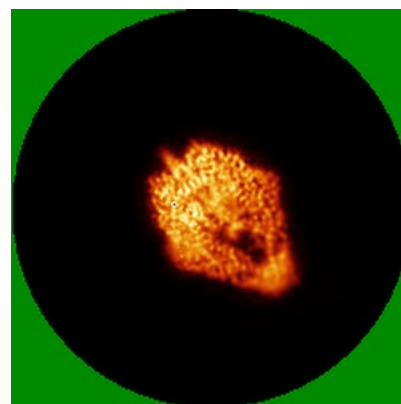
6.4.1 Primary map



X

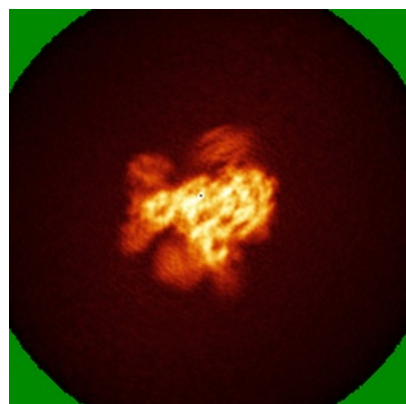


Y

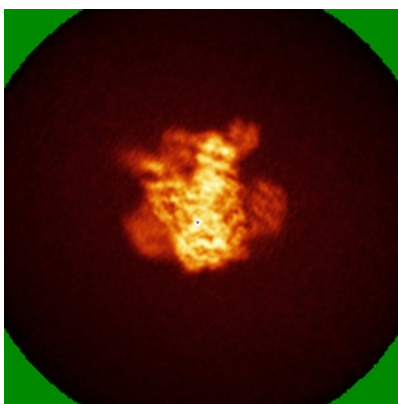


Z

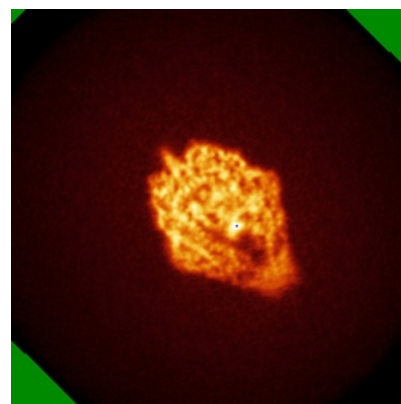
6.4.2 Raw map



X



Y

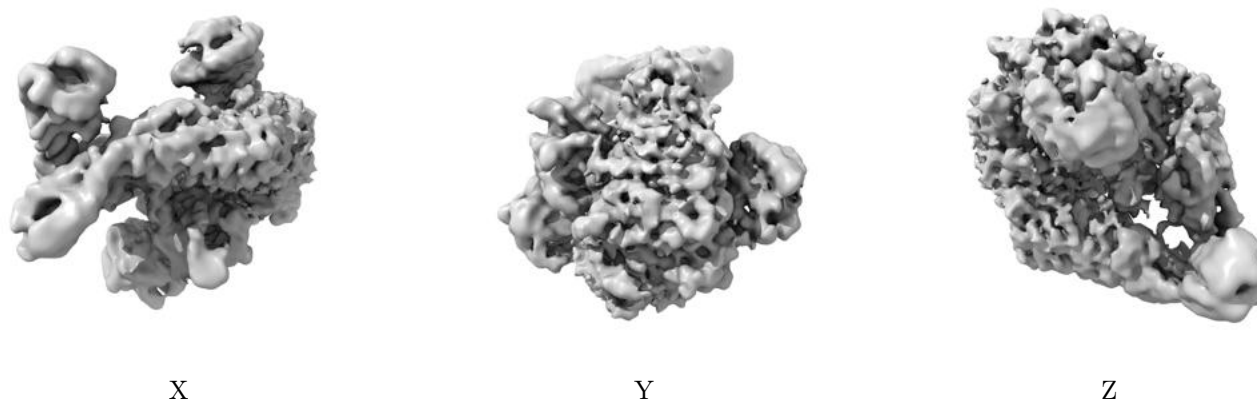


Z

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.

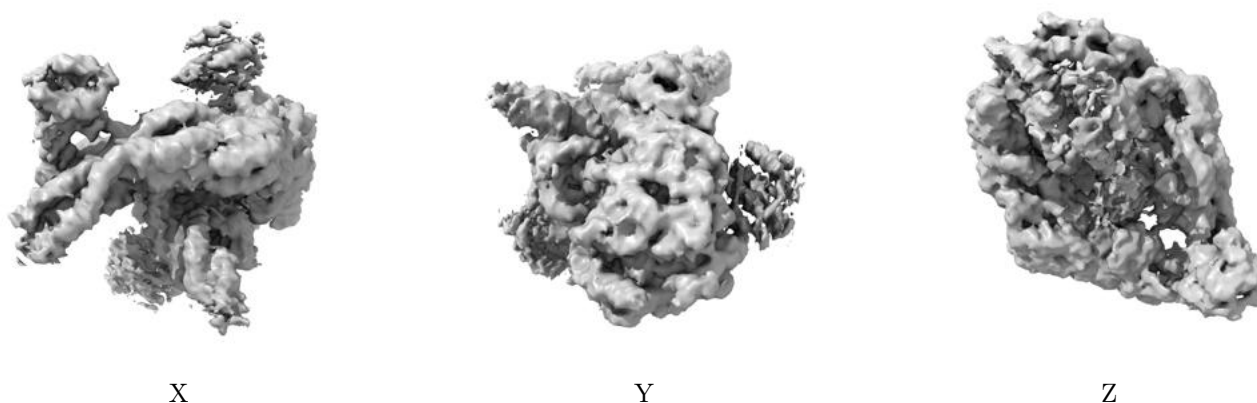
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

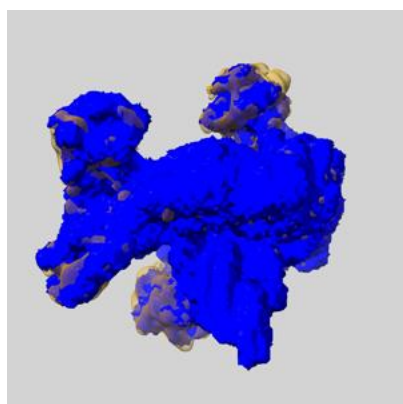
6.6 Mask visualisation [i](#)

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

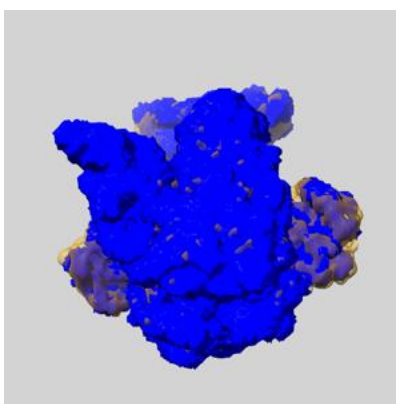
A mask typically either:

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

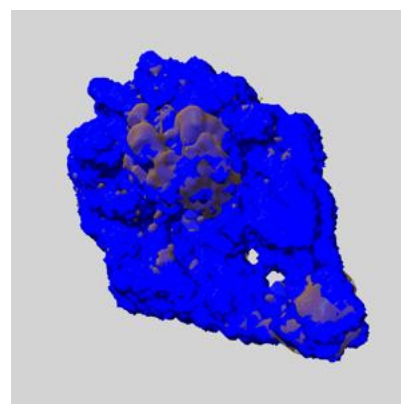
6.6.1 emd_11793_msk_1.map [i](#)



X



Y

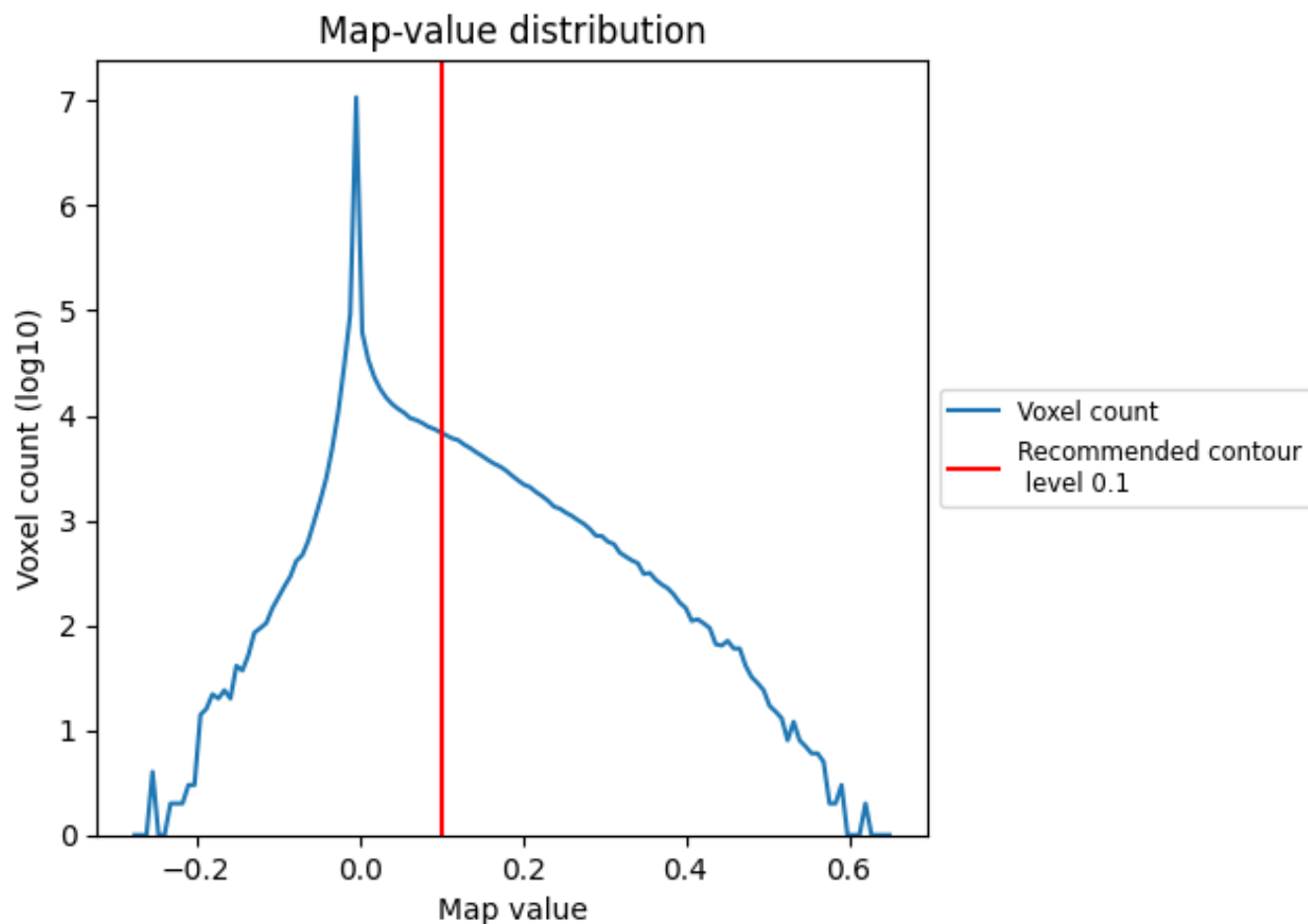


Z

7 Map analysis [i](#)

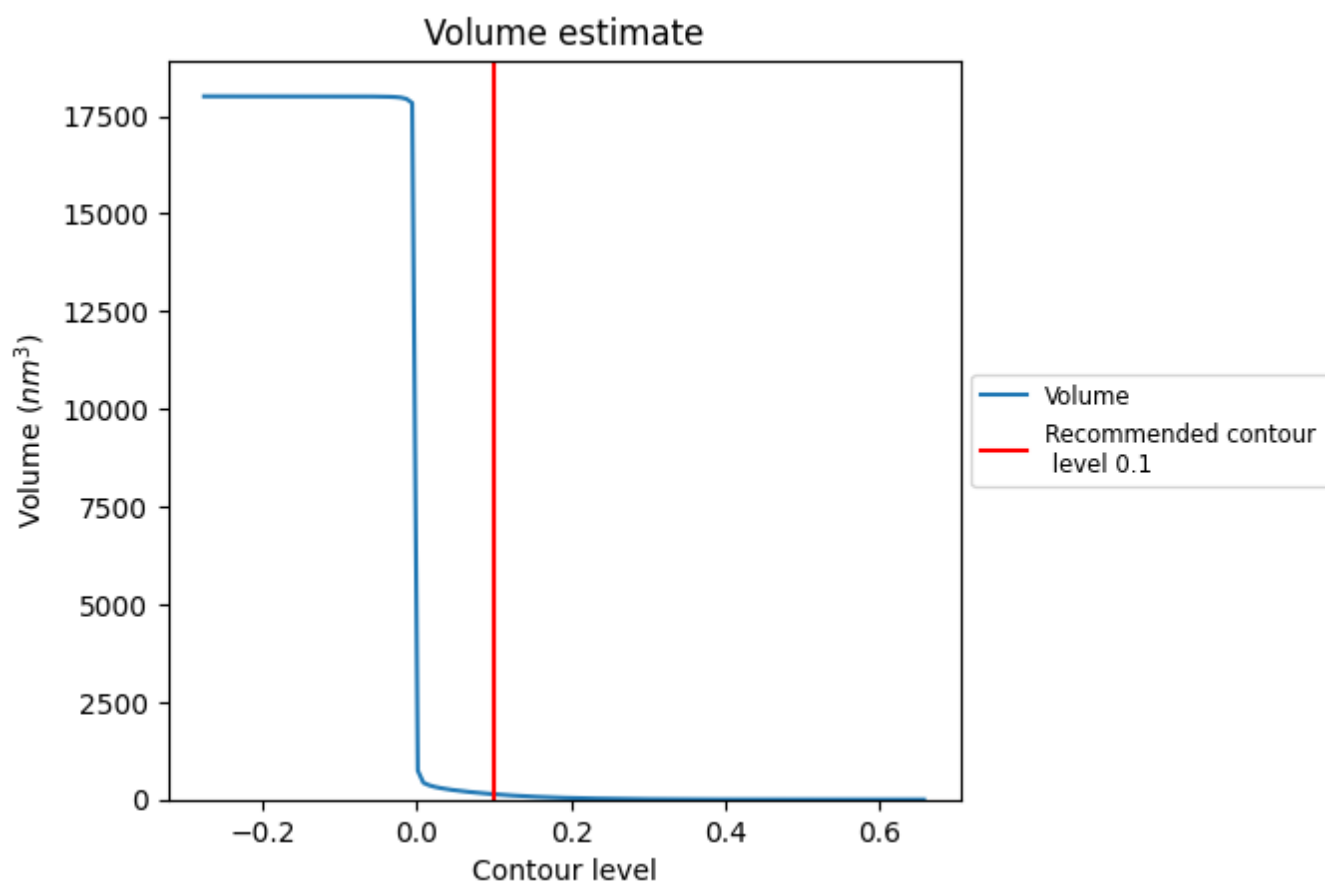
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

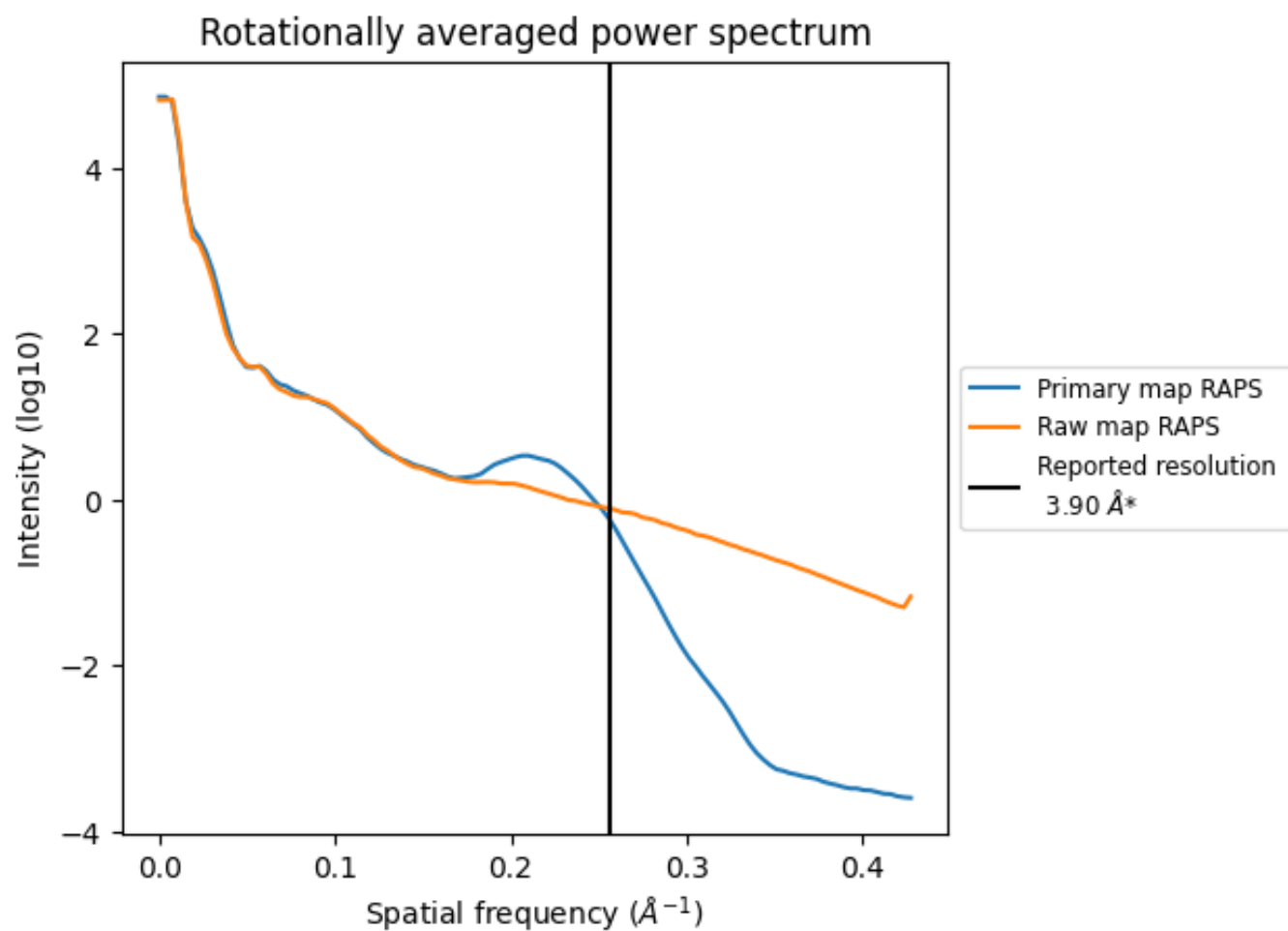
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm^3 ; this corresponds to an approximate mass of 124 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 ⓘ

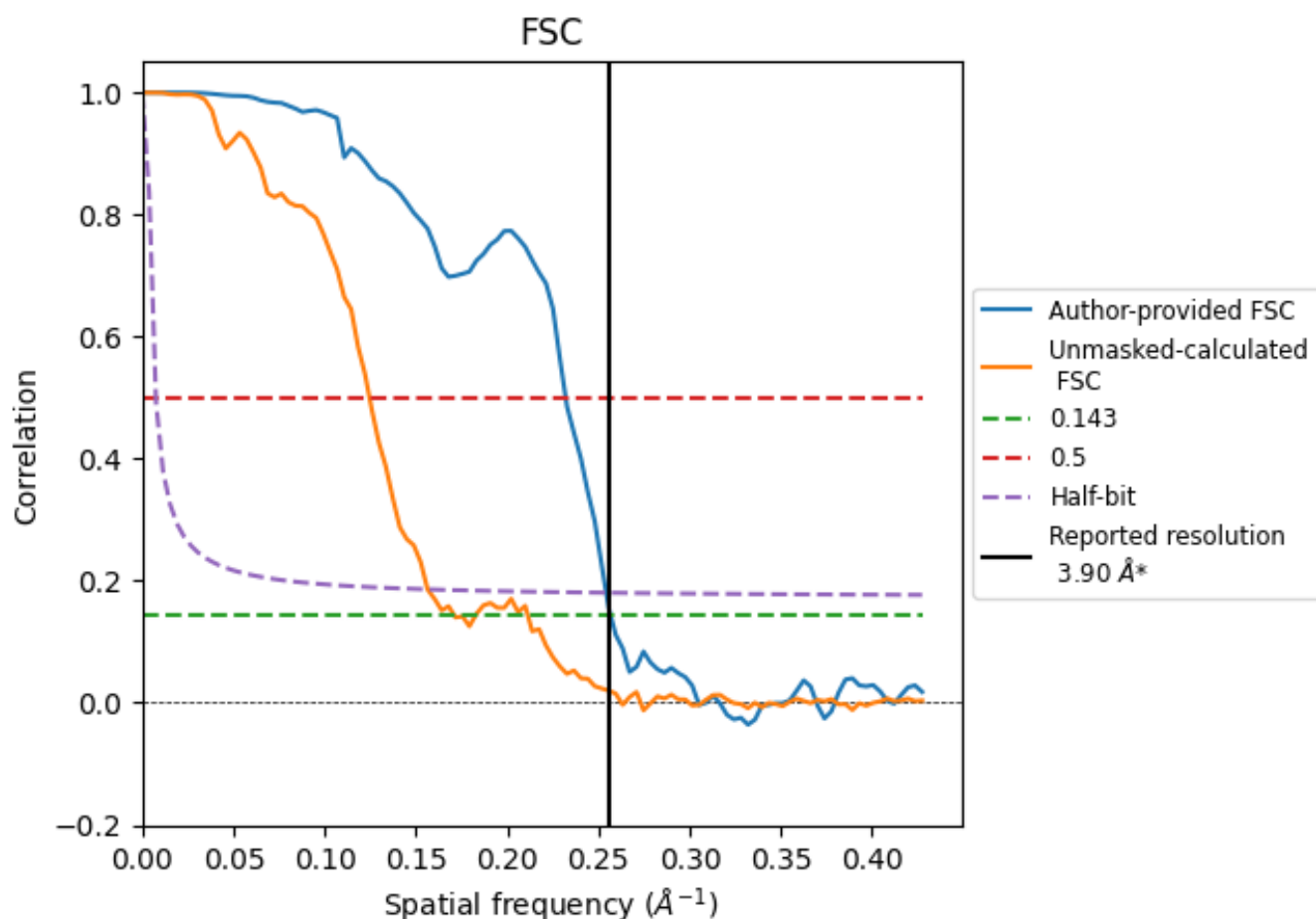


*Reported resolution corresponds to spatial frequency of $0.256 \text{ \AA}^{-1}$

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

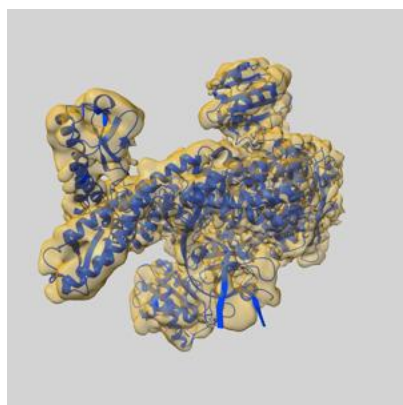
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.90	4.31	3.93
Unmasked-calculated*	5.84	8.03	6.39

*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 5.84 differs from the reported value 3.9 by more than 10 %

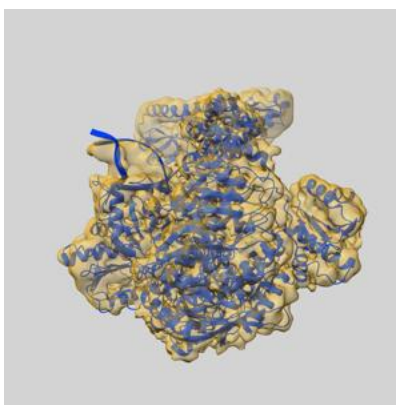
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11793 and PDB model 7AI7. Per-residue inclusion information can be found in section 3 on page 5.

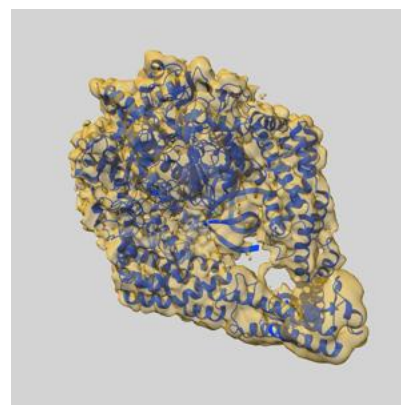
9.1 Map-model overlay [i](#)



X



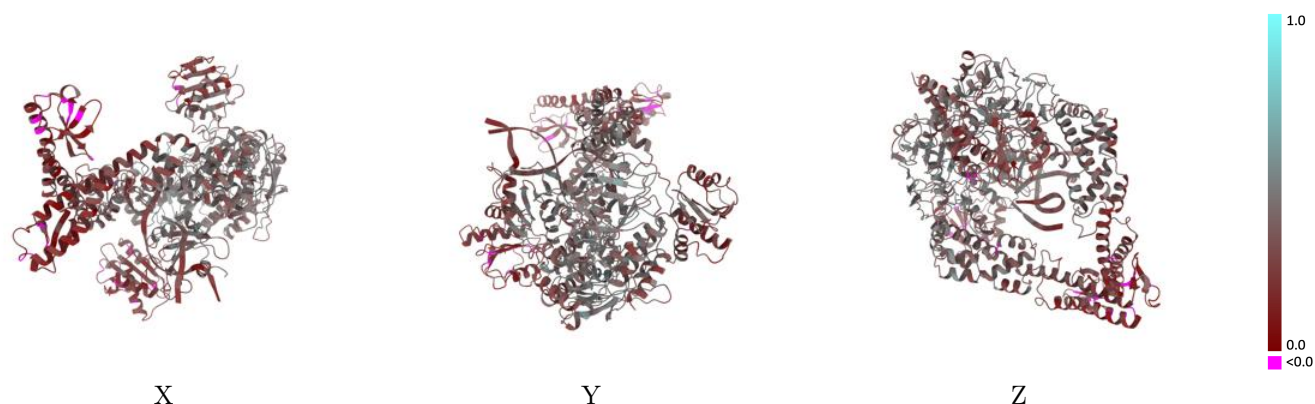
Y



Z

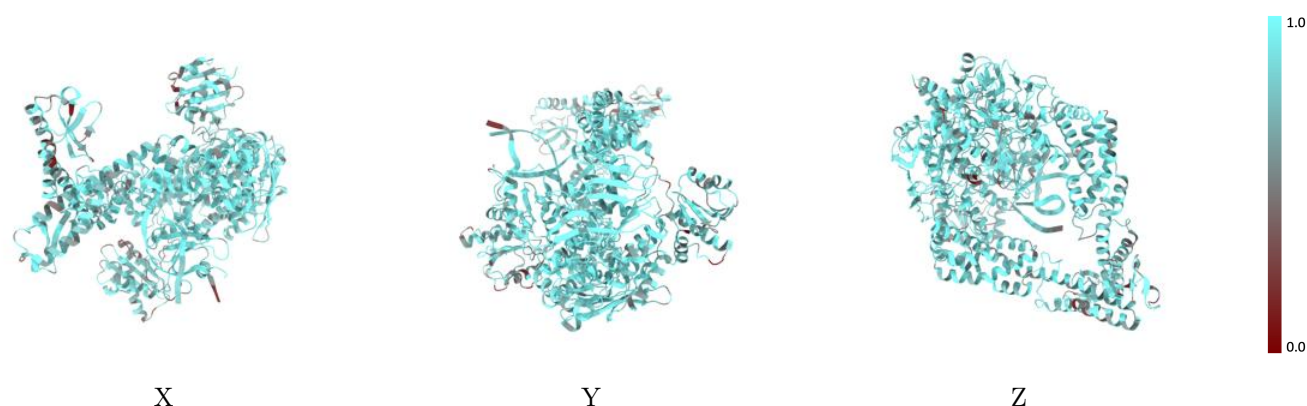
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



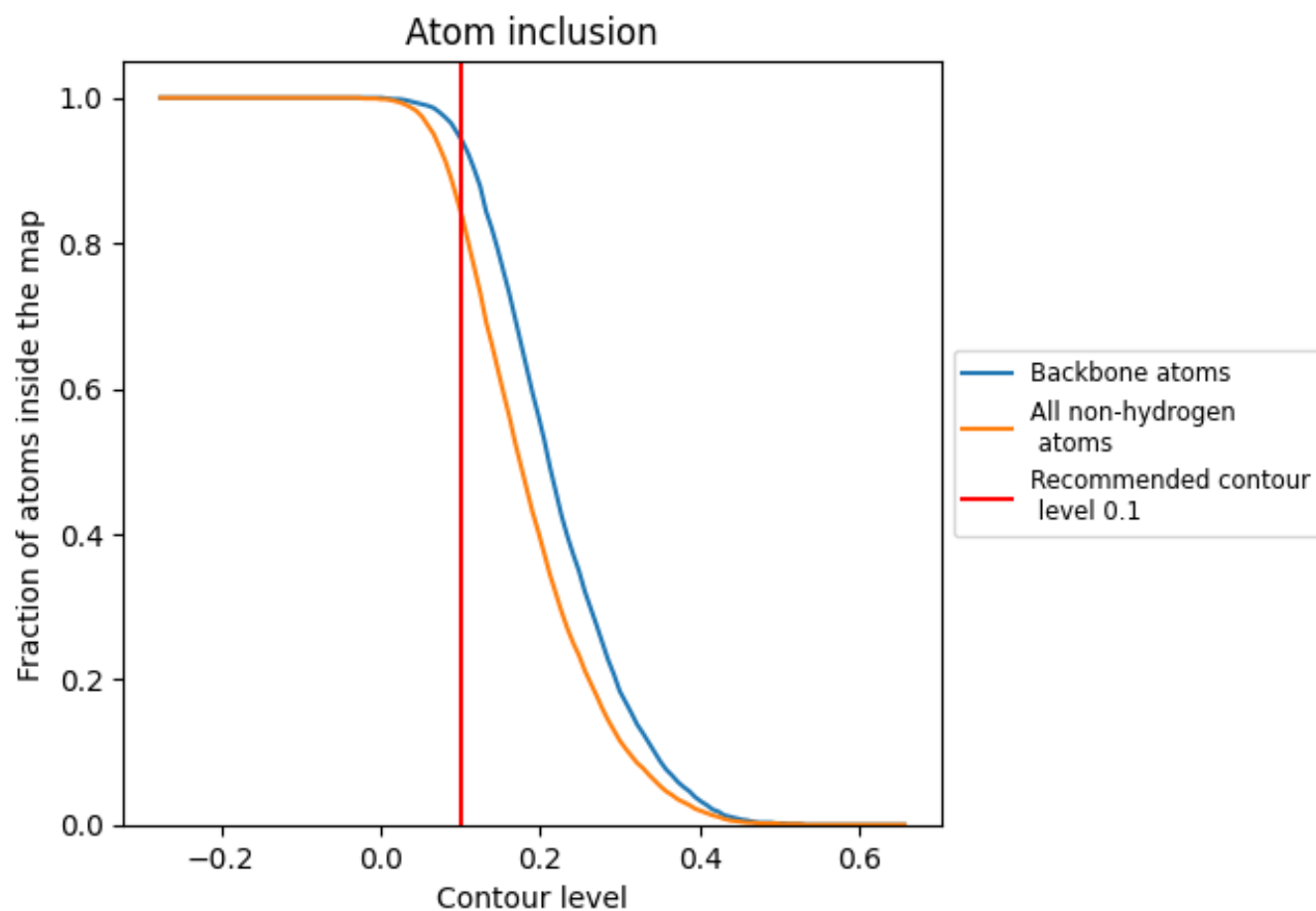
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8460	0.3360
A	0.8490	0.3290
B	0.8440	0.3470
C	0.8120	0.3240
D	0.8570	0.2720

