



Full wwPDB EM Validation Report ⓘ

Oct 14, 2025 – 08:21 AM JST

PDB ID : 9JU6 / pdb_00009ju6
EMDB ID : EMD-61821
Title : Tribolium castaneum ABCH-9C in complex with NBD-ceramide(d36:1)
Authors : Chen, J.; Duan, Y.; Zhou, Y.; Yang, Q.
Deposited on : 2024-10-07
Resolution : 3.02 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

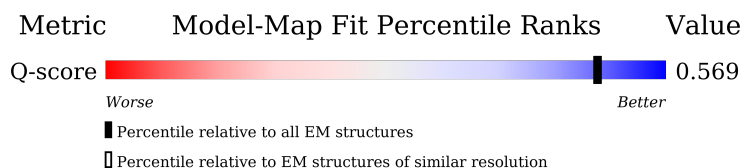
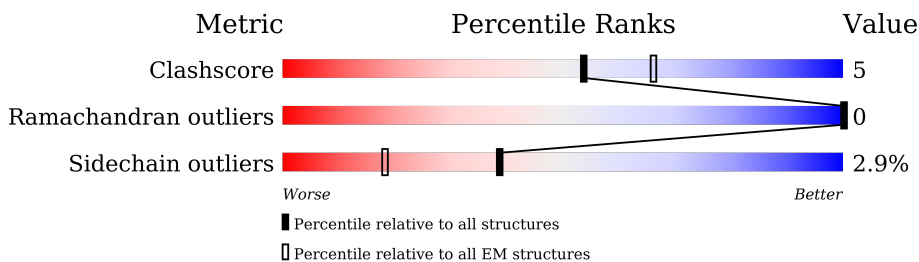
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13913 (2.52 - 3.52)

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	792	
1	B	792	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10225 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.

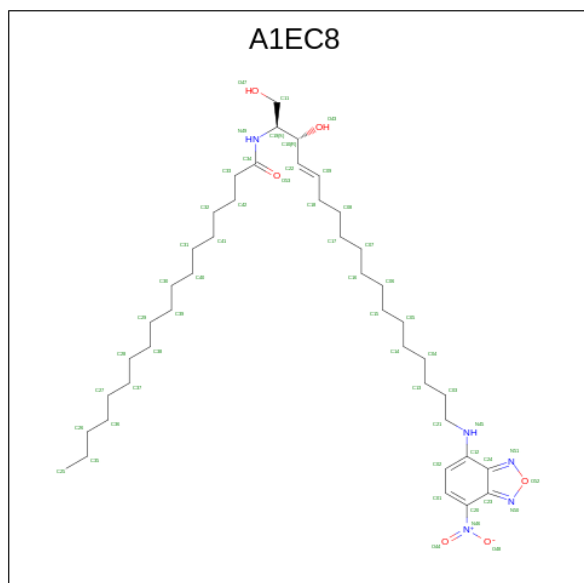
- Molecule 1 is a protein called ABC transporter G family member 23-like Protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	642	Total	C	N	O	S	0	0
			5034	3268	835	897	34		
1	B	642	Total	C	N	O	S	0	0
			5034	3268	835	897	34		

There are 6 discrepancies between the modelled and reference sequences:

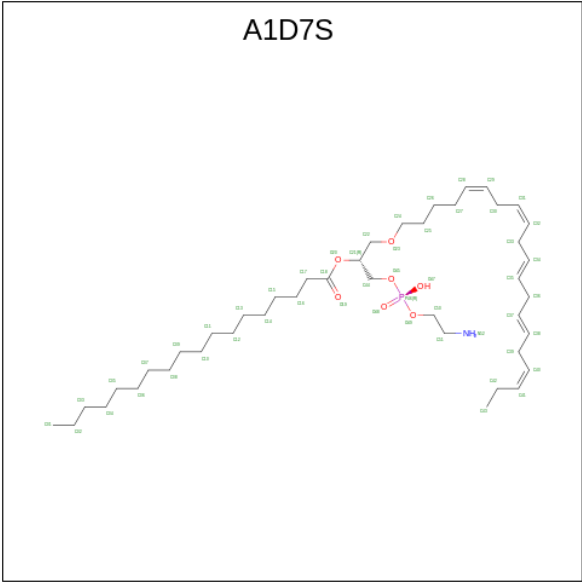
Chain	Residue	Modelled	Actual	Comment	Reference
A	363	LEU	-	insertion	UNP A0A139WBS7
A	364	ASN	-	insertion	UNP A0A139WBS7
A	365	GLY	GLN	conflict	UNP A0A139WBS7
B	363	LEU	-	insertion	UNP A0A139WBS7
B	364	ASN	-	insertion	UNP A0A139WBS7
B	365	GLY	GLN	conflict	UNP A0A139WBS7

- Molecule 2 is {N}-[({E},2 {S},3 {R})]-18-[(4-nitro-2,1,3-benzoxadiazol-7-yl)amino]-1,3-bis(oxidanyl)octadec-4-en-2-yl]octadecanamide (CCD ID: A1EC8) (formula: C₄₂H₇₃N₅O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			53	42	5	6	

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-[(5 {Z},8 {Z},11 {E},14 {E},17 {Z})-icosa-5,8,11,14,17-pentaenoxy]propan-2-yl] octadecanoate (CCD ID: A1D7S) (formula: C₄₃H₇₈NO₇P) (labeled as "Ligand of Interest" by depositor).

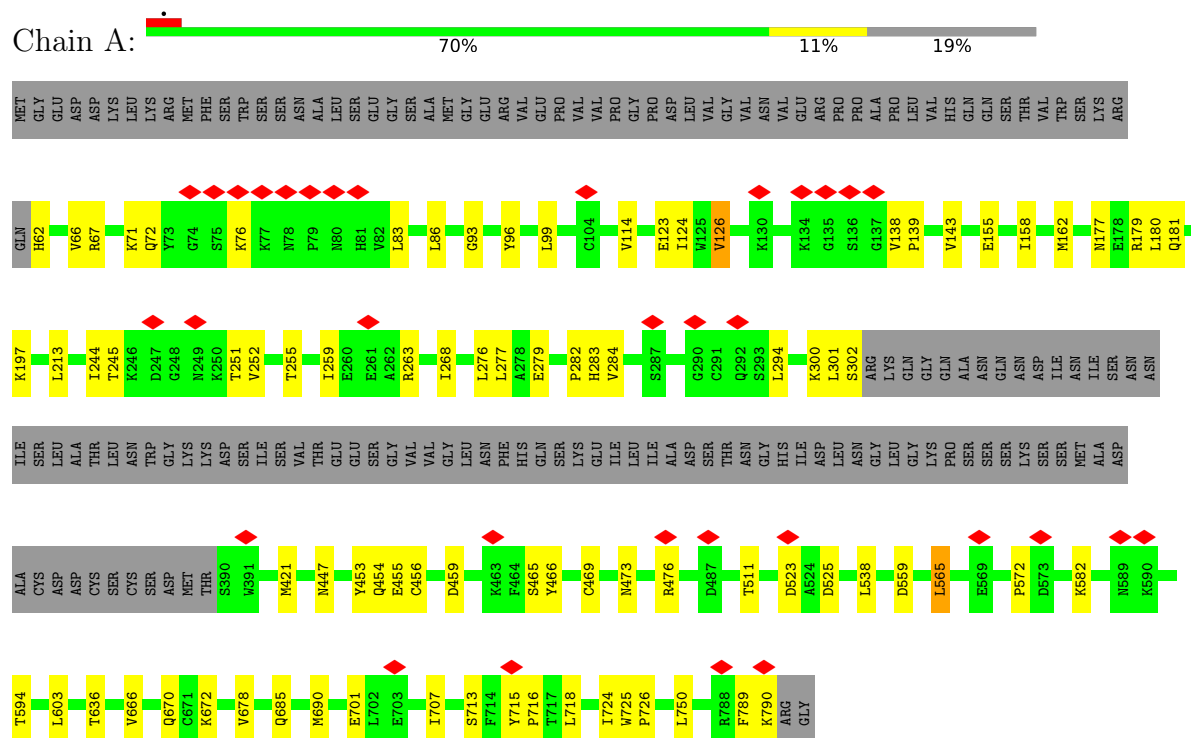


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	43	1	7	1	
3	B	1	Total	C	N	O	P	0
			52	43	1	7	1	

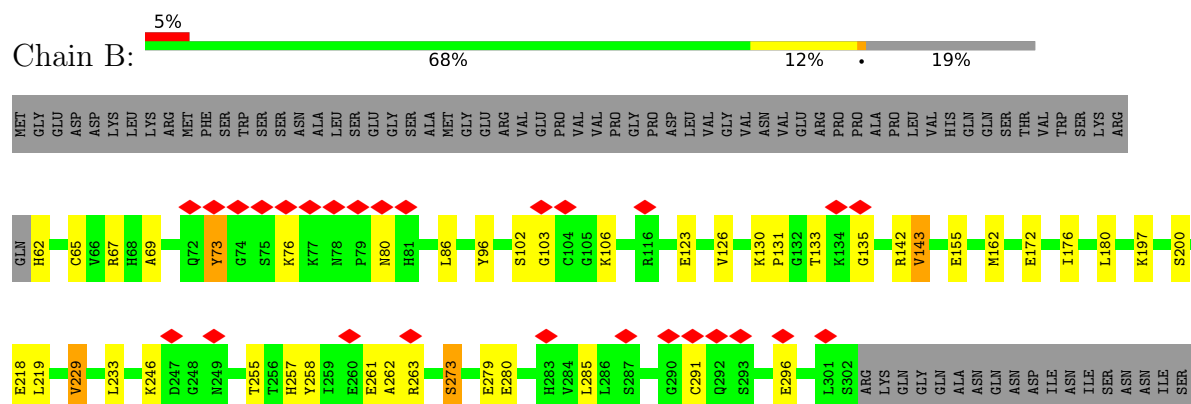
3 Residue-property plots

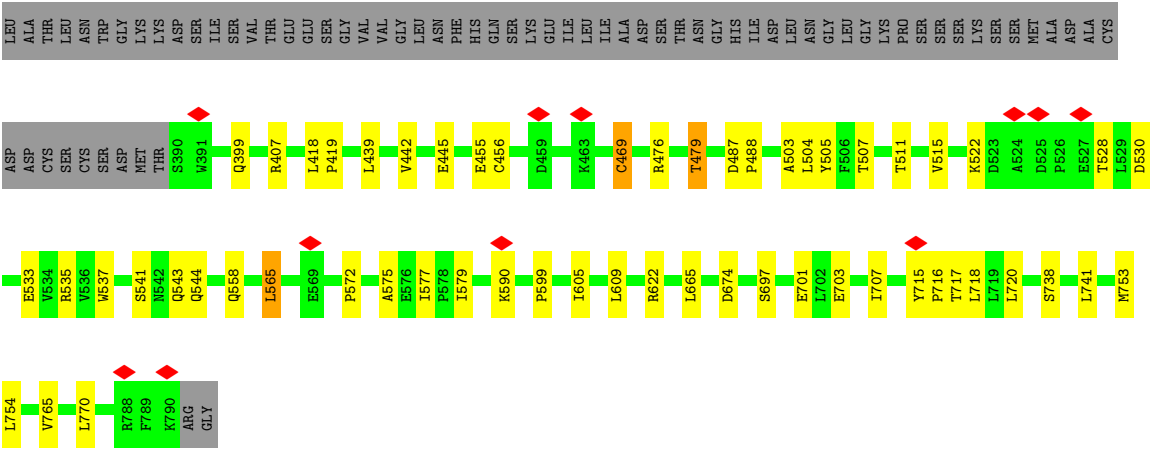
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ABC transporter G family member 23-like Protein



• Molecule 1: ABC transporter G family member 23-like Protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	241308	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.256	Depositor
Minimum map value	-1.539	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.33	Depositor
Map size (\AA)	322.2, 322.2, 322.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.074, 1.074, 1.074	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1D7S, A1EC8

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	0.18	0/5146	0.31	0/6980
1	B	0.18	0/5146	0.32	0/6980
All	All	0.18	0/10292	0.31	0/13960

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5034	0	5132	48	0
1	B	5034	0	5132	59	0
2	A	53	0	0	0	0
3	A	52	0	0	0	0
3	B	52	0	0	0	0
All	All	10225	0	10264	103	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 5.

All (103) 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:B:102:SER:OG	1:B:103:GLY:N	2.31	0.62
1:B:62:HIS:ND1	1:B:65:CYS:SG	2.66	0.62
1:B:258:TYR:HB3	1:B:261:GLU:HG2	1.82	0.61
1:B:622:ARG:NH2	1:B:697:SER:O	2.32	0.59
1:A:456:CYS:HB2	1:A:469:CYS:HB3	1.83	0.59
1:A:447:ASN:O	1:A:454:GLN:NE2	2.36	0.59
1:A:283:HIS:CE1	1:A:284:VAL:HG23	2.38	0.58
1:B:273:SER:O	1:B:273:SER:OG	2.19	0.58
1:A:582:LYS:NZ	1:B:533:GLU:OE2	2.37	0.57
1:A:454:GLN:O	1:A:455:GLU:HG3	2.04	0.57
1:B:130:LYS:HG2	1:B:131:PRO:HD2	1.87	0.57
1:A:268:ILE:HD12	1:A:282:PRO:HG3	1.87	0.57
1:B:155:GLU:O	1:B:407:ARG:NH1	2.37	0.57
1:A:99:LEU:HB3	1:A:259:ILE:HD12	1.88	0.56
1:A:244:ILE:HG13	1:A:245:THR:HG23	1.88	0.55
1:A:525:ASP:OD1	1:A:525:ASP:N	2.34	0.55
1:A:301:LEU:HD12	1:A:301:LEU:H	1.73	0.54
1:A:603:LEU:HD22	1:A:685:GLN:HG3	1.90	0.54
1:A:96:TYR:OH	1:A:279:GLU:OE2	2.25	0.54
1:A:565:LEU:HD13	1:A:572:PRO:HA	1.89	0.54
1:A:126:VAL:HG13	1:A:138:VAL:HG21	1.90	0.53
1:A:162:MET:HG3	1:A:180:LEU:HD13	1.89	0.52
1:B:96:TYR:OH	1:B:279:GLU:OE2	2.27	0.52
1:B:280:GLU:HB2	1:B:285:LEU:HG	1.92	0.52
1:A:707:ILE:HD13	1:B:707:ILE:HG21	1.91	0.51
1:B:543:GLN:OE1	1:B:544:GLN:NE2	2.44	0.51
1:A:177:ASN:O	1:A:181:GLN:HG2	2.11	0.51
1:B:577:ILE:HG22	1:B:579:ILE:H	1.75	0.51
1:A:523:ASP:OD1	1:A:523:ASP:N	2.44	0.50
1:B:73:TYR:HB2	1:B:80:ASN:HB3	1.95	0.49
1:B:229:VAL:HG13	1:B:233:LEU:HB3	1.94	0.49
1:B:455:GLU:O	1:B:455:GLU:HG3	2.12	0.49
1:A:263:ARG:HD3	1:A:294:LEU:HD12	1.95	0.48
1:B:133:THR:HG23	1:B:135:GLY:H	1.77	0.48
1:B:558:GLN:NE2	1:B:575:ALA:O	2.45	0.48
1:B:162:MET:HG3	1:B:180:LEU:HD13	1.96	0.48
1:A:67:ARG:HB2	1:A:123:GLU:HG2	1.96	0.48
1:B:565:LEU:HD13	1:B:572:PRO:HA	1.96	0.47
1:A:66:VAL:HG22	1:A:124:ILE:HD13	1.96	0.47
1:B:445:GLU:OE2	1:B:511:THR:OG1	2.32	0.47
1:B:456:CYS:HB3	1:B:469:CYS:HB3	1.97	0.46
1:A:476:ARG:NH2	1:A:559:ASP:OD2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:LYS:HB3	1:A:790:LYS:HE3	1.72	0.46
1:B:530:ASP:O	1:B:535:ARG:NH2	2.49	0.46
1:B:258:TYR:CB	1:B:261:GLU:HG2	2.44	0.46
1:B:442:VAL:HB	1:B:505:TYR:HA	1.98	0.46
1:B:717:THR:HG22	1:B:741:LEU:HD13	1.98	0.46
1:A:93:GLY:H	1:A:251:THR:HG22	1.81	0.45
1:B:476:ARG:HD3	1:B:479:THR:HG22	1.99	0.45
1:A:71:LYS:HB3	1:A:83:LEU:HB2	1.97	0.45
1:B:102:SER:O	1:B:257:HIS:HE1	1.99	0.45
1:B:197:LYS:HB2	1:B:197:LYS:HE3	1.83	0.45
1:A:245:THR:HG21	1:A:252:VAL:HG23	1.98	0.45
1:A:725:TRP:CD2	1:A:726:PRO:HD2	2.52	0.45
1:A:670:GLN:NE2	1:A:672:LYS:HE3	2.32	0.45
1:B:263:ARG:HB3	1:B:263:ARG:CZ	2.46	0.45
1:A:83:LEU:HD22	1:A:86:LEU:HD22	1.98	0.45
1:A:179:ARG:HA	1:A:179:ARG:HD2	1.79	0.44
1:A:162:MET:HE3	1:A:162:MET:HB3	1.80	0.44
1:A:789:PHE:CD1	1:A:789:PHE:C	2.96	0.44
1:A:466:TYR:O	1:A:511:THR:OG1	2.27	0.44
1:B:172:GLU:O	1:B:176:ILE:HG13	2.18	0.44
1:A:158:ILE:O	1:A:162:MET:HG2	2.18	0.43
1:B:142:ARG:NH1	1:B:218:GLU:OE2	2.43	0.43
1:B:487:ASP:OD1	1:B:488:PRO:HD2	2.18	0.43
1:B:599:PRO:HG3	1:B:754:LEU:HD12	2.00	0.43
1:B:106:LYS:HD2	1:B:255:THR:HG23	2.01	0.43
1:B:507:THR:OG1	1:B:535:ARG:NH1	2.50	0.43
1:B:718:LEU:HD23	1:B:718:LEU:HA	1.85	0.43
1:B:76:LYS:HE2	1:B:76:LYS:HB2	1.79	0.43
1:A:76:LYS:HD2	1:A:76:LYS:HA	1.80	0.43
1:B:665:LEU:HD23	1:B:665:LEU:HA	1.85	0.43
1:A:453:TYR:CE2	1:A:455:GLU:HB3	2.54	0.42
1:A:678:VAL:HG13	1:A:750:LEU:HD11	2.01	0.42
1:B:439:LEU:HD23	1:B:504:LEU:HD13	2.00	0.42
1:A:459:ASP:OD1	1:A:465:SER:HB2	2.19	0.42
1:B:246:LYS:O	1:B:246:LYS:HG3	2.19	0.42
1:B:503:ALA:HB3	1:B:537:TRP:HE3	1.84	0.42
1:B:511:THR:O	1:B:515:VAL:HG23	2.20	0.42
1:B:399:GLN:HE21	1:B:399:GLN:HB3	1.66	0.42
1:B:715:TYR:HB2	1:B:716:PRO:HD3	2.01	0.42
1:A:277:LEU:HD23	1:A:300:LYS:HD2	2.02	0.42
1:A:582:LYS:HE2	1:B:535:ARG:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD23	1:A:279:GLU:HB2	2.01	0.42
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.90	0.42
1:B:69:ALA:HB3	1:B:86:LEU:HB3	2.00	0.42
1:A:582:LYS:HB2	1:B:537:TRP:CD1	2.54	0.41
1:B:291:CYS:HB3	1:B:296:GLU:HB2	2.03	0.41
1:B:720:LEU:O	1:B:738:SER:HB2	2.20	0.41
1:B:67:ARG:HB2	1:B:123:GLU:HG2	2.02	0.41
1:A:72:GLN:OE1	1:A:72:GLN:C	2.63	0.41
1:A:155:GLU:H	1:A:197:LYS:HG2	1.86	0.41
1:B:261:GLU:HG3	1:B:262:ALA:N	2.36	0.41
1:B:753:MET:HE3	1:B:765:VAL:HG13	2.03	0.41
1:B:703:GLU:O	1:B:707:ILE:HG23	2.21	0.41
1:A:718:LEU:HD12	1:A:718:LEU:HA	1.96	0.40
1:A:138:VAL:HB	1:A:139:PRO:HD3	2.03	0.40
1:B:418:LEU:HB3	1:B:419:PRO:HD3	2.03	0.40
1:B:590:LYS:HZ2	1:B:590:LYS:HG2	1.80	0.40
1:B:605:ILE:O	1:B:609:LEU:HB2	2.20	0.40
1:A:538:LEU:HD23	1:A:538:LEU:HA	1.94	0.40
1:A:715:TYR:HB2	1:A:716:PRO:HD3	2.04	0.40
1:B:143:VAL:HG23	1:B:219:LEU:HD23	2.03	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	638/792 (81%)	611 (96%)	27 (4%)	0	100	100
1	B	638/792 (81%)	611 (96%)	27 (4%)	0	100	100
All	All	1276/1584 (81%)	1222 (96%)	54 (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	550/679 (81%)	533 (97%)	17 (3%)	35	67
1	B	550/679 (81%)	535 (97%)	15 (3%)	40	70
All	All	1100/1358 (81%)	1068 (97%)	32 (3%)	39	69

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	114	VAL
1	A	126	VAL
1	A	143	VAL
1	A	213	LEU
1	A	255	THR
1	A	302	SER
1	A	421	MET
1	A	473	ASN
1	A	565	LEU
1	A	594	THR
1	A	636	THR
1	A	666	VAL
1	A	690	MET
1	A	701	GLU
1	A	713	SER
1	A	724	ILE
1	B	73	TYR
1	B	126	VAL
1	B	143	VAL
1	B	200	SER
1	B	229	VAL
1	B	273	SER
1	B	469	CYS
1	B	479	THR
1	B	522	LYS
1	B	528	THR

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Mol	Chain	Res	Type
1	B	541	SER
1	B	565	LEU
1	B	674	ASP
1	B	701	GLU
1	B	770	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	185	ASN
1	A	239	ASN
1	A	240	HIS
1	A	283	HIS
1	A	408	ASN
1	A	422	GLN
1	A	443	ASN
1	A	444	HIS
1	A	454	GLN
1	A	550	GLN
1	A	554	GLN
1	A	571	ASN
1	A	705	ASN
1	B	203	GLN
1	B	240	HIS
1	B	257	HIS
1	B	399	GLN
1	B	443	ASN
1	B	444	HIS
1	B	451	GLN
1	B	497	GLN
1	B	544	GLN
1	B	550	GLN
1	B	570	GLN
1	B	571	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](#)

3 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
3	A1D7S	A	802	-	51,51,51	1.03	3 (5%)	52,55,55	1.36	6 (11%)
2	A1EC8	A	801	-	50,54,54	2.06	4 (8%)	50,63,63	1.50	4 (8%)
3	A1D7S	B	801	-	51,51,51	1.03	3 (5%)	52,55,55	1.35	6 (11%)

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
3	A1D7S	A	802	-	-	26/54/54/54	-
2	A1EC8	A	801	-	-	25/48/50/50	0/2/2/2
3	A1D7S	B	801	-	-	29/54/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1EC8	O44-N46	10.37	1.40	1.22
2	A	801	A1EC8	C34-N49	6.58	1.48	1.34
2	A	801	A1EC8	C12-N45	4.45	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	A1D7S	O20-C18	2.84	1.42	1.34
3	A	802	A1D7S	O20-C18	2.82	1.42	1.34
3	A	802	A1D7S	O20-C21	-2.57	1.40	1.46
3	B	801	A1D7S	O20-C21	-2.55	1.40	1.46
2	A	801	A1EC8	C33-C34	2.42	1.56	1.51
3	B	801	A1D7S	P46-O45	2.05	1.67	1.59
3	A	802	A1D7S	P46-O45	2.01	1.67	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	A1EC8	C18-C09-C22	6.00	152.22	125.39
2	A	801	A1EC8	C10-C22-C09	-5.47	112.60	124.79
3	A	802	A1D7S	C36-C35-C34	-4.54	85.23	123.57
3	B	801	A1D7S	C36-C35-C34	-4.40	86.41	123.57
2	A	801	A1EC8	C01-C20-N46	4.10	120.85	116.47
3	B	801	A1D7S	O20-C18-C17	3.89	119.89	111.50
3	A	802	A1D7S	O20-C18-C17	3.88	119.87	111.50
3	A	802	A1D7S	C30-C29-C28	3.47	152.83	123.57
3	A	802	A1D7S	C33-C32-C31	3.46	152.74	123.57
3	B	801	A1D7S	C33-C32-C31	3.45	152.70	123.57
3	B	801	A1D7S	C39-C38-C37	3.44	152.62	123.57
3	A	802	A1D7S	C39-C38-C37	3.43	152.51	123.57
3	B	801	A1D7S	C30-C29-C28	3.40	152.26	123.57
2	A	801	A1EC8	C33-C34-N49	2.48	120.13	115.83
3	A	802	A1D7S	O47-P46-O48	-2.26	101.04	112.24
3	B	801	A1D7S	O47-P46-O48	-2.23	101.21	112.24

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	A1EC8	O47-C11-C19-N49
2	A	801	A1EC8	C02-C12-N45-C21
2	A	801	A1EC8	C24-C12-N45-C21
2	A	801	A1EC8	C01-C20-N46-O44
2	A	801	A1EC8	C23-C20-N46-O44
3	A	802	A1D7S	C44-O45-P46-O48
3	A	802	A1D7S	C44-O45-P46-O49
3	B	801	A1D7S	C37-C38-C39-C40
3	B	801	A1D7S	C40-C41-C42-C43
3	B	801	A1D7S	C44-O45-P46-O47

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Mol	Chain	Res	Type	Atoms
3	B	801	A1D7S	C44-O45-P46-O49
3	B	801	A1D7S	C50-O49-P46-O45
3	B	801	A1D7S	C50-O49-P46-O47
3	B	801	A1D7S	C50-O49-P46-O48
2	A	801	A1EC8	C34-C33-C42-C32
2	A	801	A1EC8	C41-C31-C40-C30
3	A	802	A1D7S	C15-C16-C17-C18
3	A	802	A1D7S	O23-C24-C25-C26
2	A	801	A1EC8	C42-C32-C41-C31
2	A	801	A1EC8	C14-C04-C13-C03
3	A	802	A1D7S	C03-C04-C05-C06
2	A	801	A1EC8	C39-C30-C40-C31
2	A	801	A1EC8	C18-C08-C17-C07
3	B	801	A1D7S	C03-C04-C05-C06
3	A	802	A1D7S	O49-C50-C51-N52
2	A	801	A1EC8	O47-C11-C19-C10
3	B	801	A1D7S	O23-C24-C25-C26
2	A	801	A1EC8	C36-C26-C35-C25
3	A	802	A1D7S	C06-C07-C08-C09
2	A	801	A1EC8	C40-C30-C39-C29
3	B	801	A1D7S	C07-C08-C09-C10
3	A	802	A1D7S	C21-C22-O23-C24
3	A	802	A1D7S	C24-C25-C26-C27
3	B	801	A1D7S	C15-C16-C17-C18
3	A	802	A1D7S	O20-C21-C22-O23
3	B	801	A1D7S	O20-C21-C22-O23
2	A	801	A1EC8	C14-C05-C15-C06
3	B	801	A1D7S	C21-C22-O23-C24
3	B	801	A1D7S	C08-C09-C10-C11
3	B	801	A1D7S	C24-C25-C26-C27
3	B	801	A1D7S	O49-C50-C51-N52
3	A	802	A1D7S	C12-C13-C14-C15
3	A	802	A1D7S	C29-C30-C31-C32
3	B	801	A1D7S	C28-C29-C30-C31
3	B	801	A1D7S	C29-C30-C31-C32
3	B	801	A1D7S	C32-C33-C34-C35
3	B	801	A1D7S	C12-C13-C14-C15
2	A	801	A1EC8	C21-C03-C13-C04
2	A	801	A1EC8	C15-C06-C16-C07
2	A	801	A1EC8	C41-C32-C42-C33
3	A	802	A1D7S	C40-C41-C42-C43
2	A	801	A1EC8	C38-C28-C37-C27

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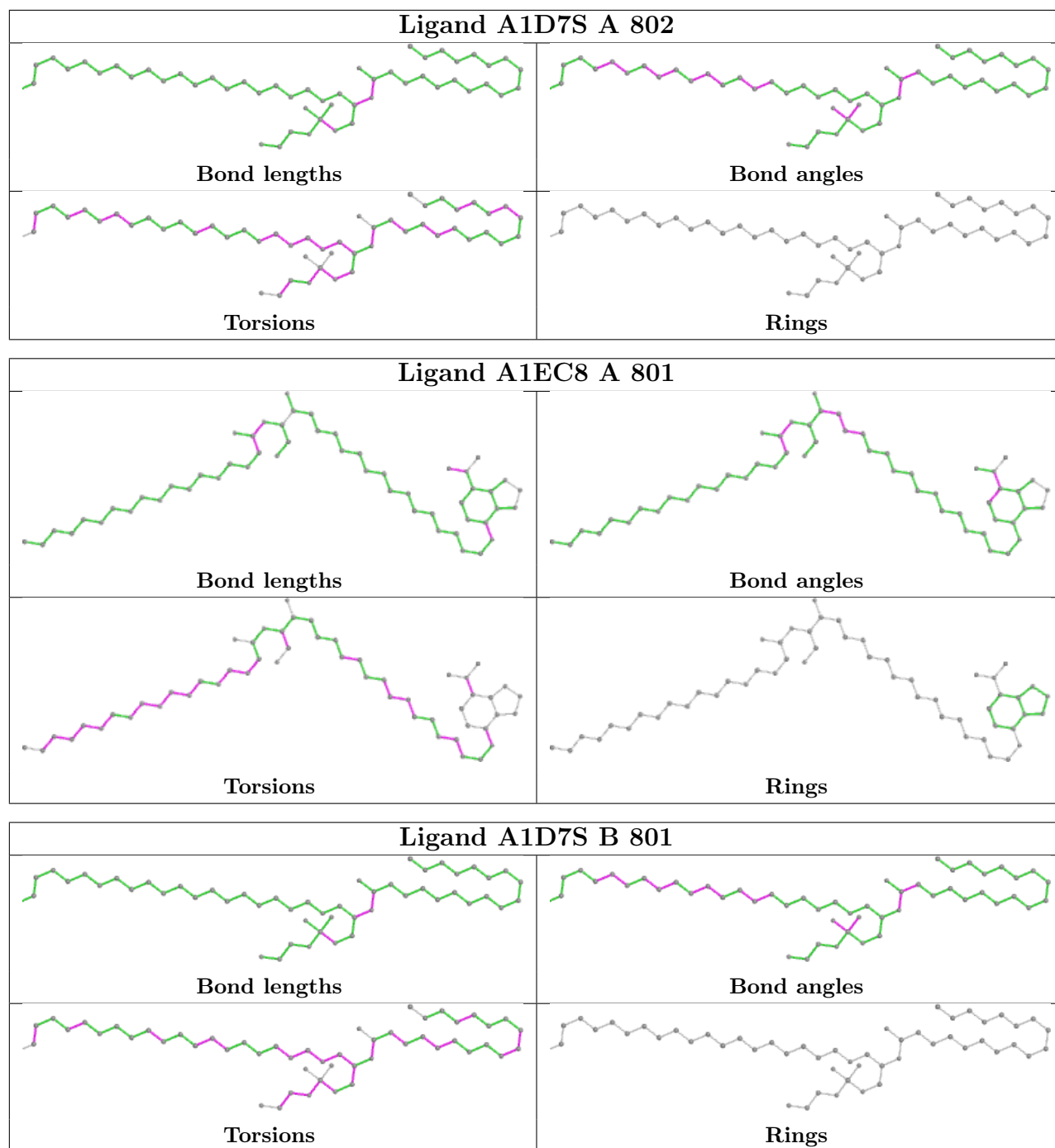
Mol	Chain	Res	Type	Atoms
2	A	801	A1EC8	C35-C26-C36-C27
3	A	802	A1D7S	C25-C26-C27-C28
2	A	801	A1EC8	C37-C27-C36-C26
2	A	801	A1EC8	C38-C29-C39-C30
3	B	801	A1D7S	C13-C14-C15-C16
3	A	802	A1D7S	C21-C44-O45-P46
3	A	802	A1D7S	C50-O49-P46-O47
3	B	801	A1D7S	C44-O45-P46-O48
3	B	801	A1D7S	C51-C50-O49-P46
3	B	801	A1D7S	O20-C21-C44-O45
3	A	802	A1D7S	C13-C14-C15-C16
3	B	801	A1D7S	O19-C18-O20-C21
3	B	801	A1D7S	C17-C18-O20-C21
3	B	801	A1D7S	C25-C24-O23-C22
3	A	802	A1D7S	C25-C24-O23-C22
3	A	802	A1D7S	C44-C21-C22-O23
3	B	801	A1D7S	C44-C21-C22-O23
2	A	801	A1EC8	C39-C29-C38-C28
3	A	802	A1D7S	C05-C06-C07-C08
3	A	802	A1D7S	C34-C35-C36-C37
3	A	802	A1D7S	C35-C36-C37-C38
3	A	802	A1D7S	C37-C38-C39-C40
2	A	801	A1EC8	C16-C06-C15-C05
3	A	802	A1D7S	O19-C18-O20-C21
3	B	801	A1D7S	C22-C21-C44-O45
3	A	802	A1D7S	C50-O49-P46-O45
2	A	801	A1EC8	C36-C27-C37-C28
3	A	802	A1D7S	C17-C18-O20-C21

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

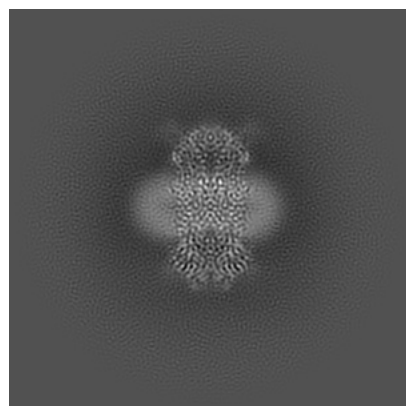
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61821. These allow visual inspection of the internal detail of the map and identification of artifacts.

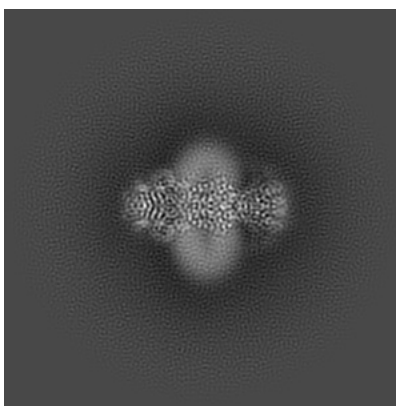
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

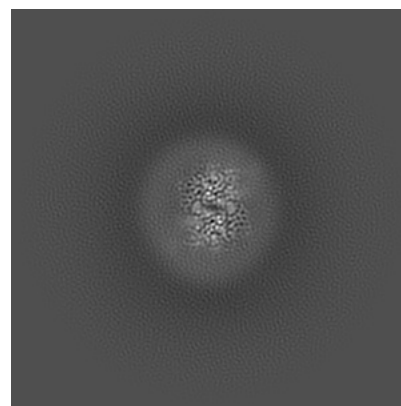
6.1.1 Primary map



X

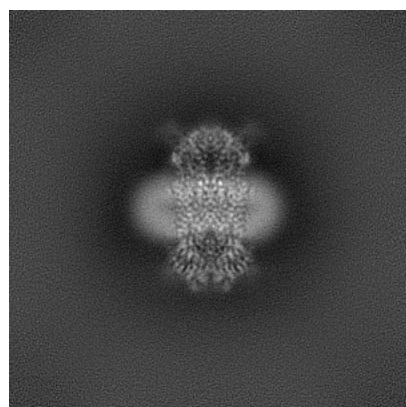


Y

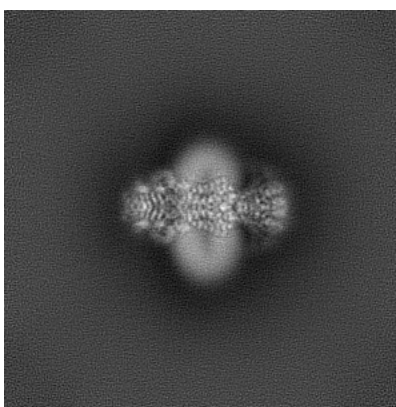


Z

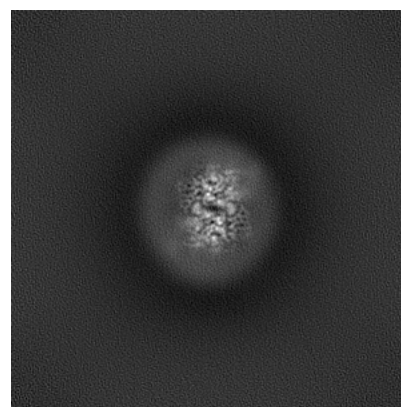
6.1.2 Raw map



X



Y

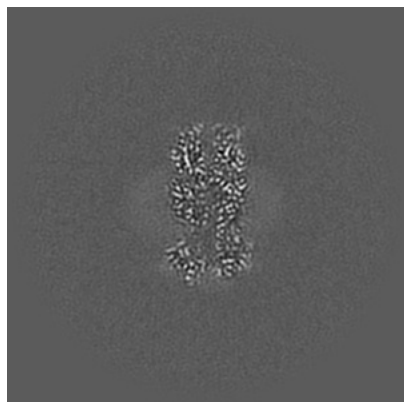


Z

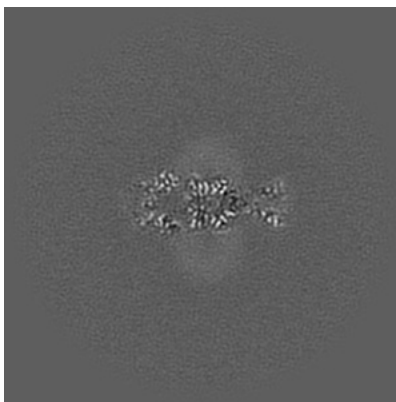
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

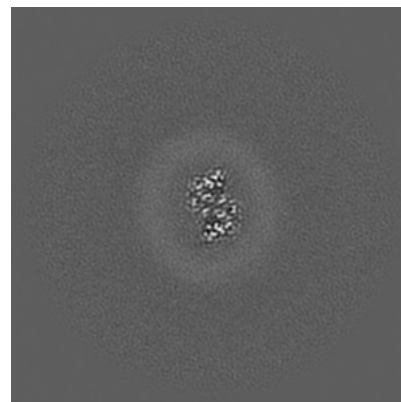
6.2.1 Primary map



X Index: 150

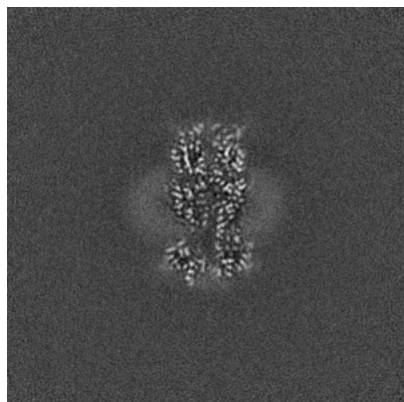


Y Index: 150

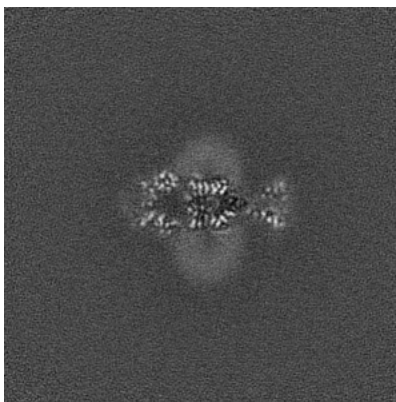


Z Index: 150

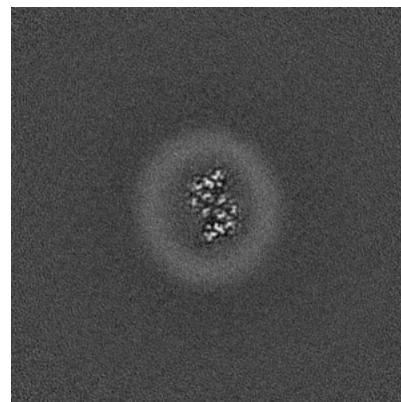
6.2.2 Raw map



X Index: 150



Y Index: 150

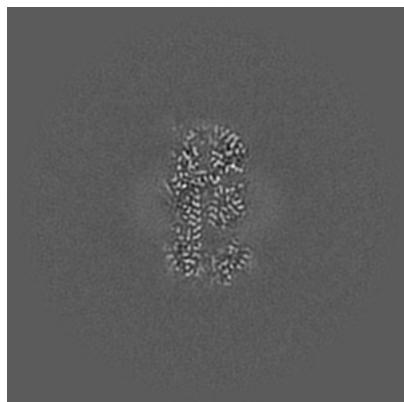


Z Index: 150

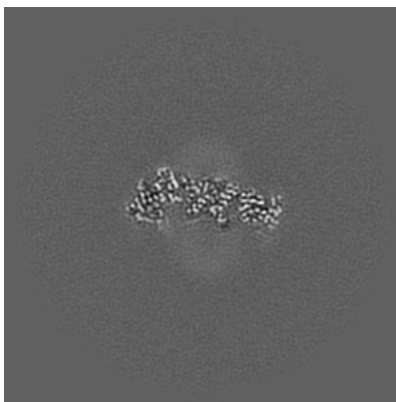
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

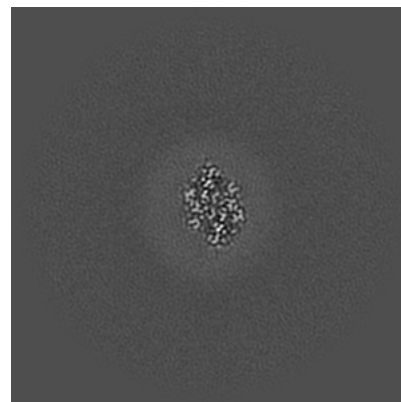
6.3.1 Primary map



X Index: 155

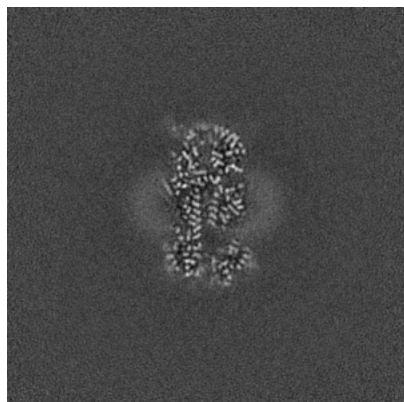


Y Index: 136

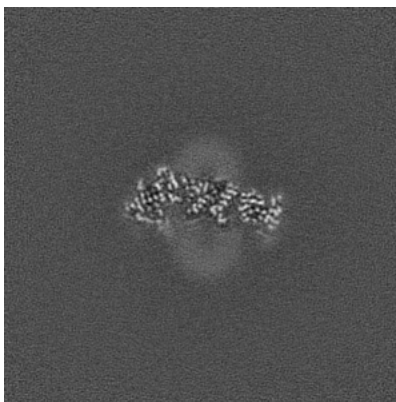


Z Index: 165

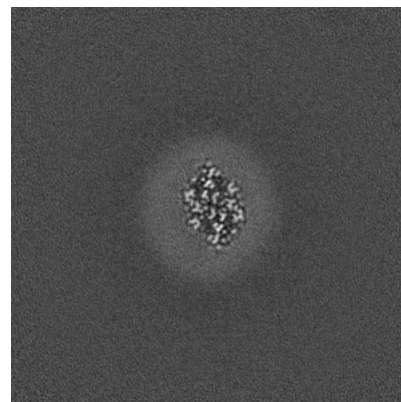
6.3.2 Raw map



X Index: 155



Y Index: 136

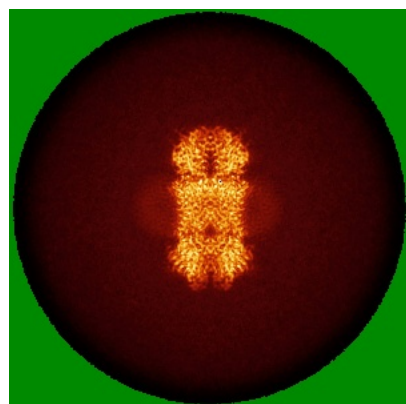


Z Index: 165

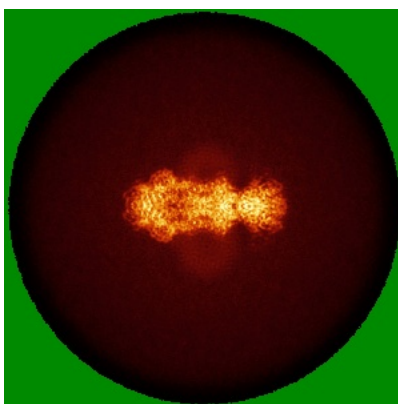
The images above show the largest variance slices of the map in three orthogonal directions.

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

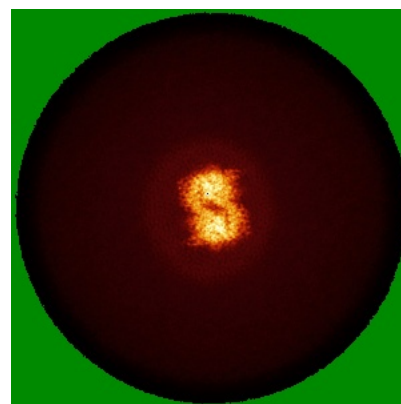
6.4.1 Primary map



X

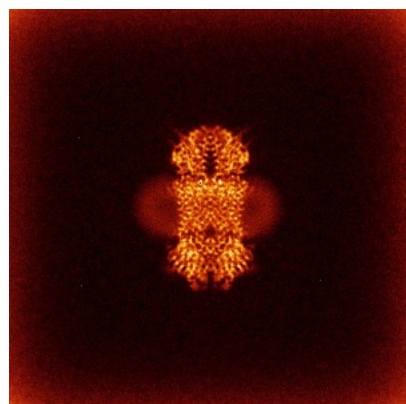


Y

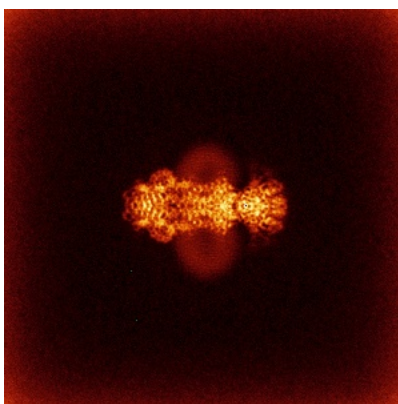


Z

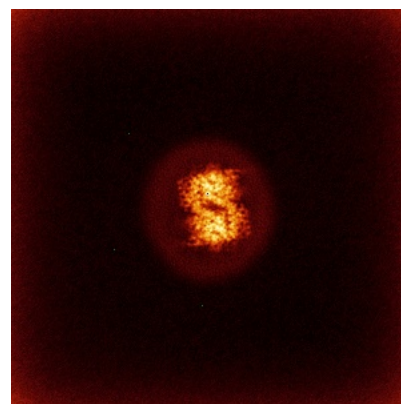
6.4.2 Raw map



X



Y

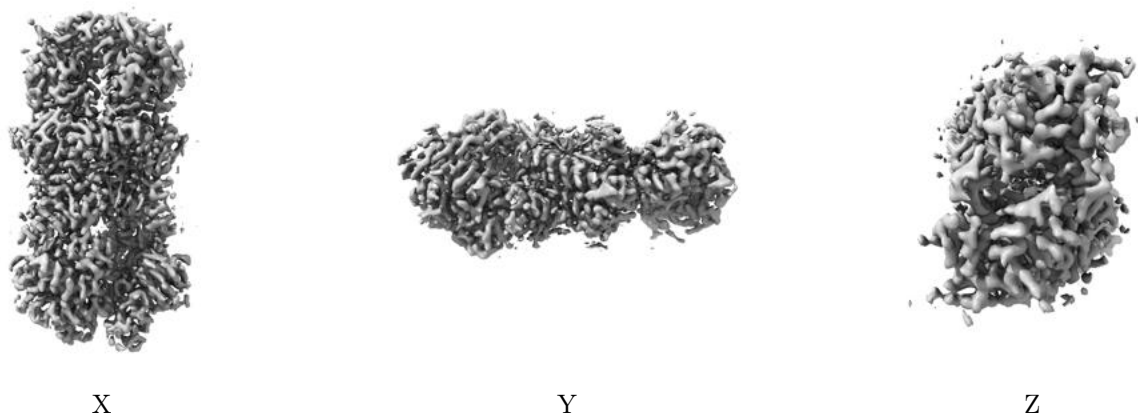


Z

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.

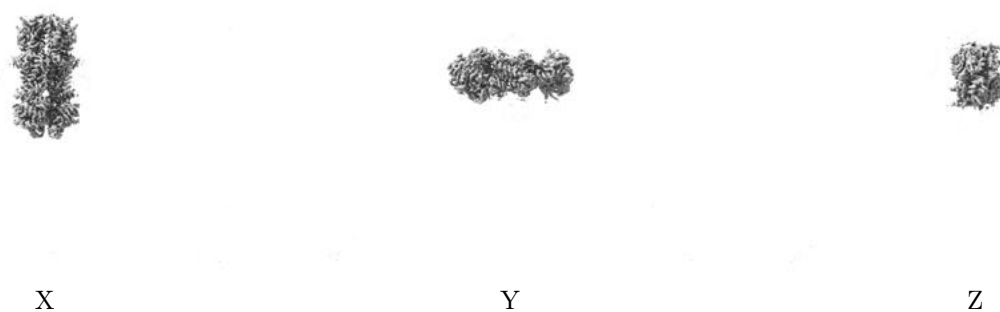
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.33. 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.

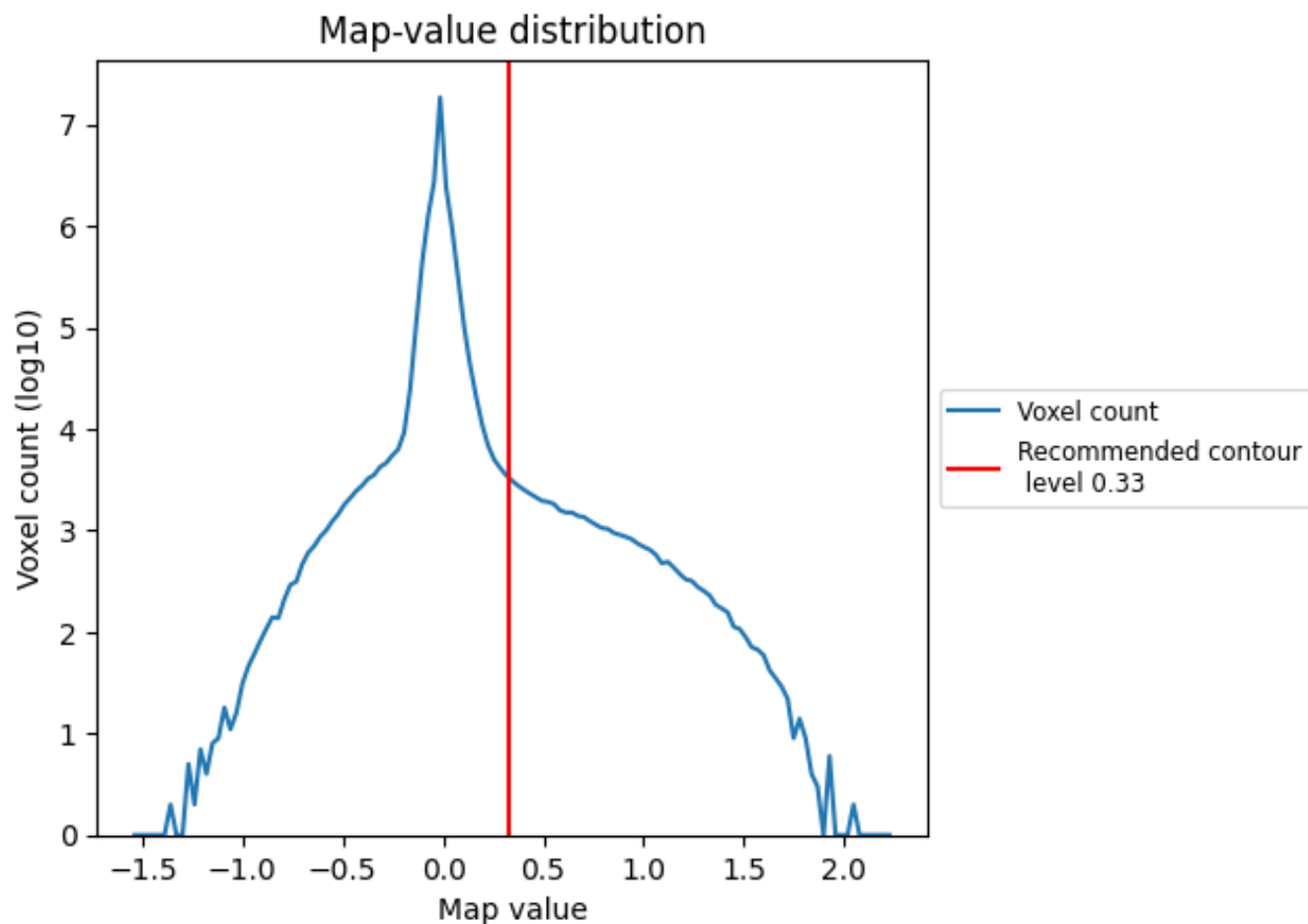
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

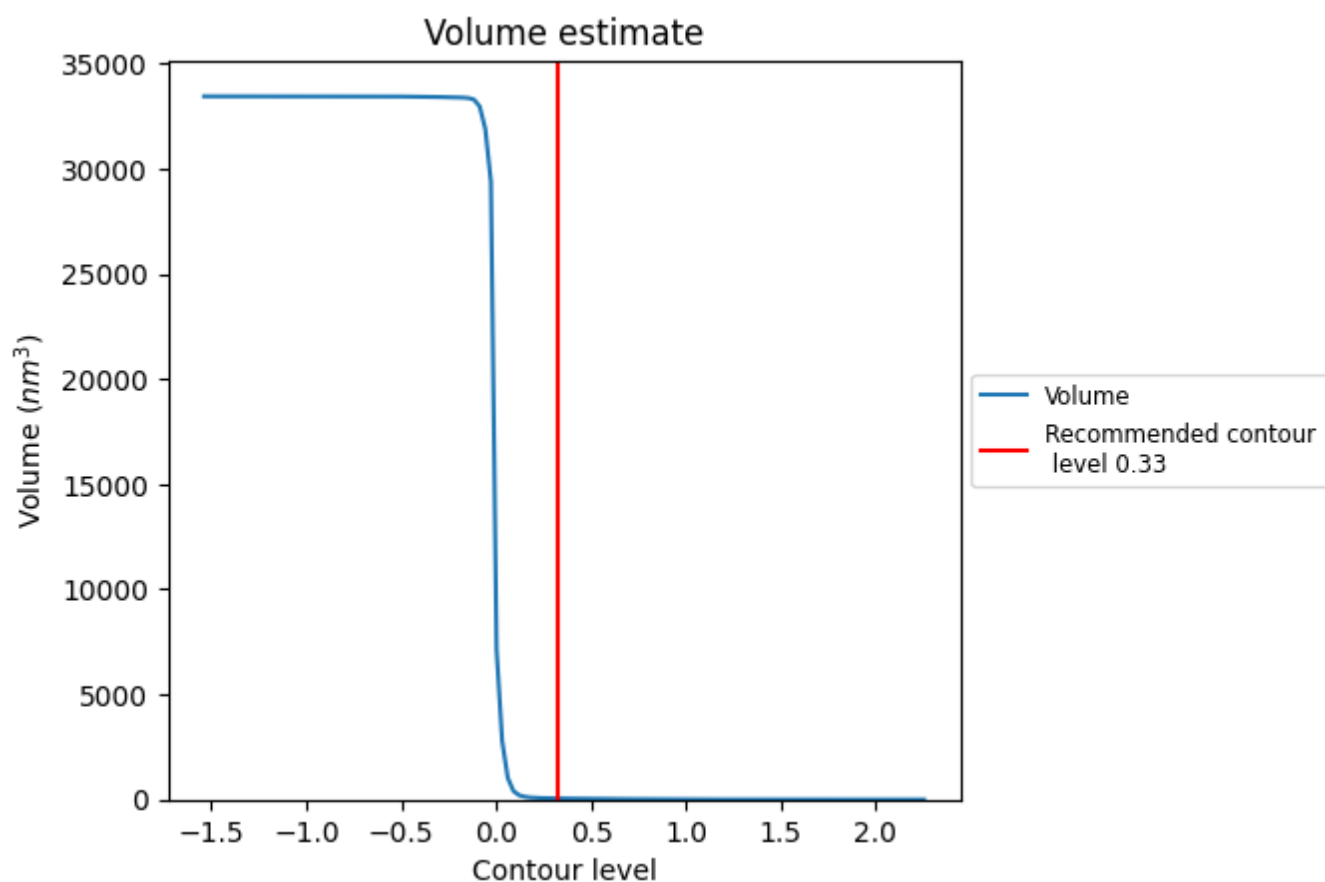
This section contains the results of statistical analysis of the map.

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.

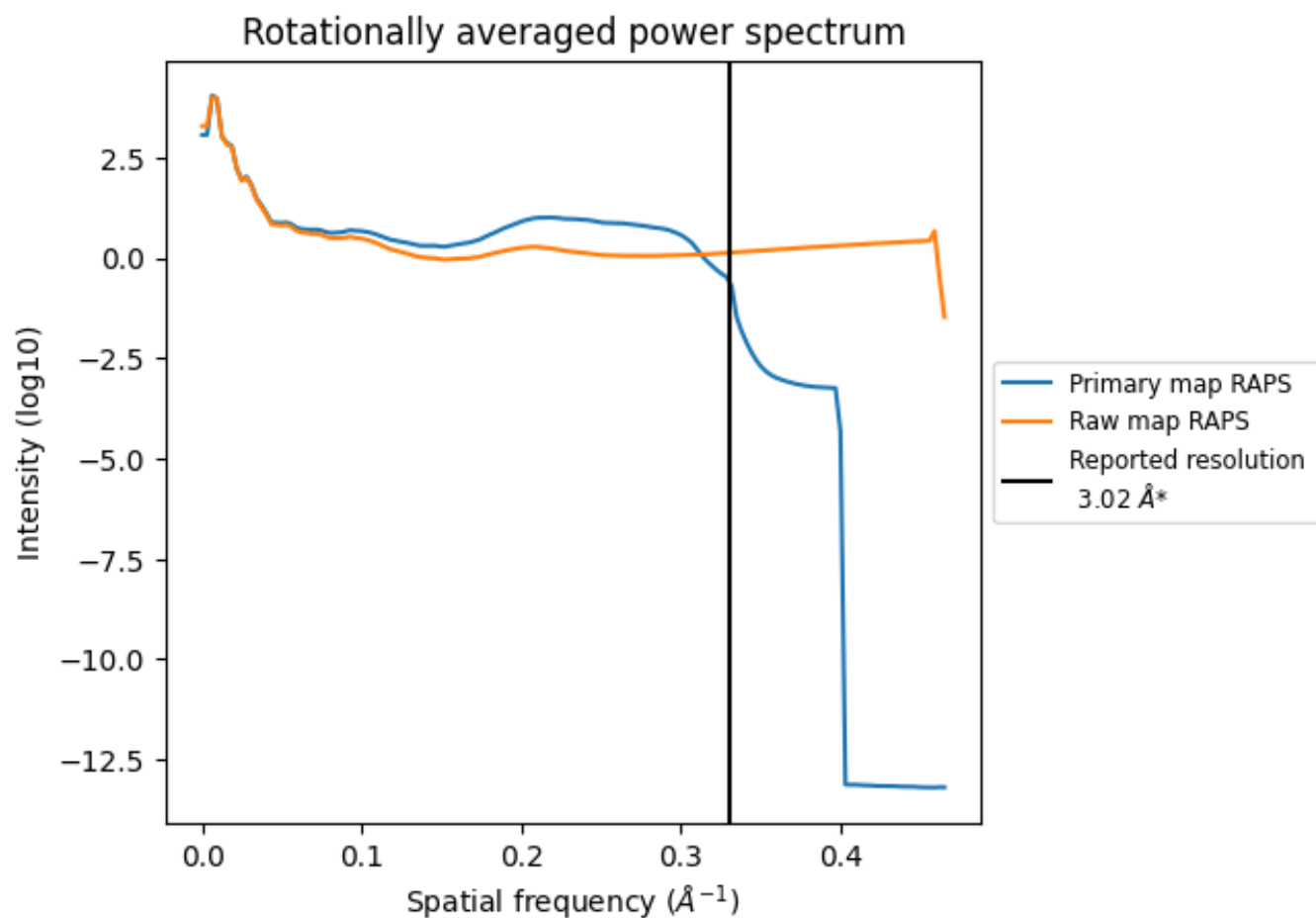
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 53 nm³; this corresponds to an approximate mass of 47 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 ⓘ

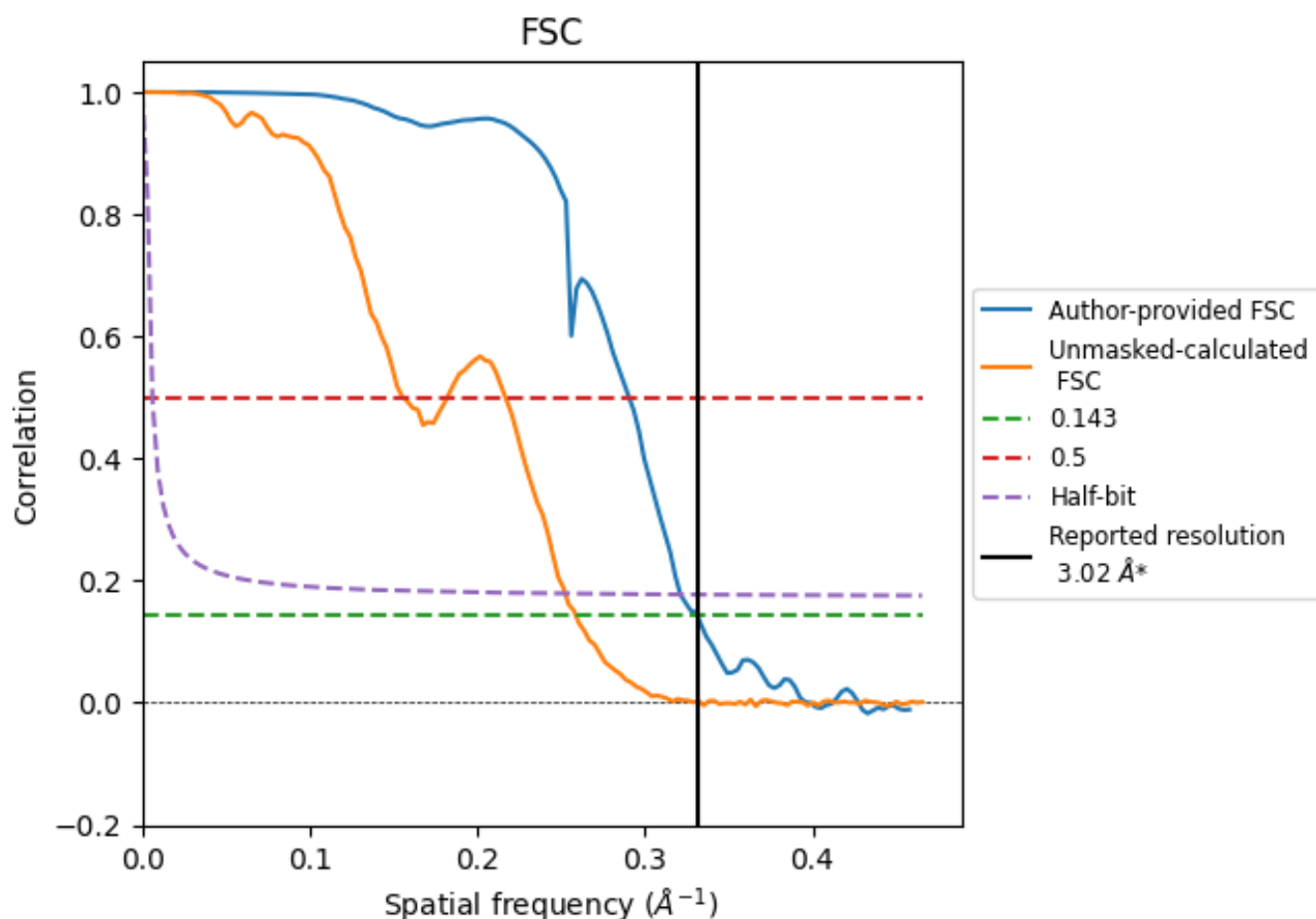


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

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 0.331 \AA^{-1}

8.2 Resolution estimates [i](#)

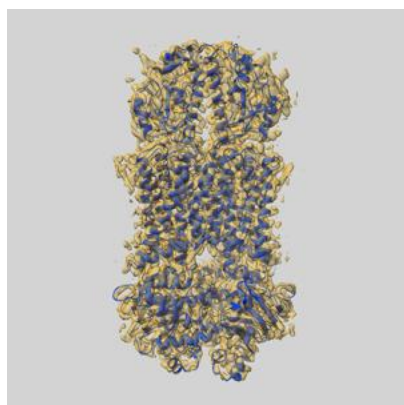
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.44	3.11
Unmasked-calculated*	3.86	6.42	3.96

*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 3.86 differs from the reported value 3.02 by more than 10 %

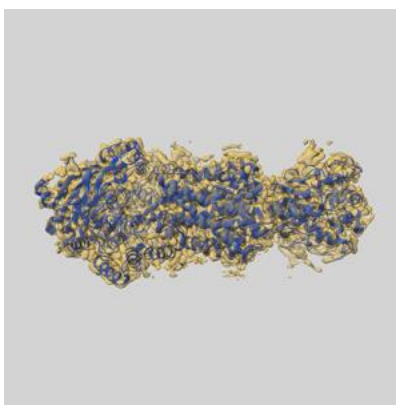
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61821 and PDB model 9JU6. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

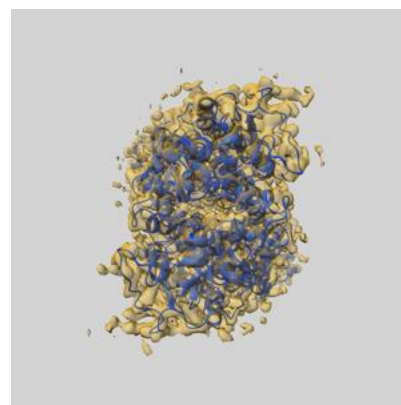
9.1 Map-model overlay [i](#)



X



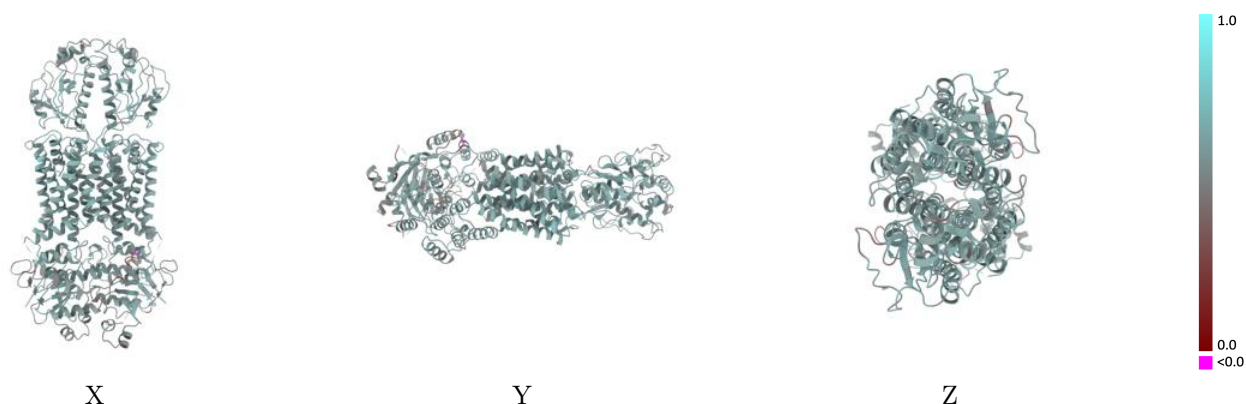
Y



Z

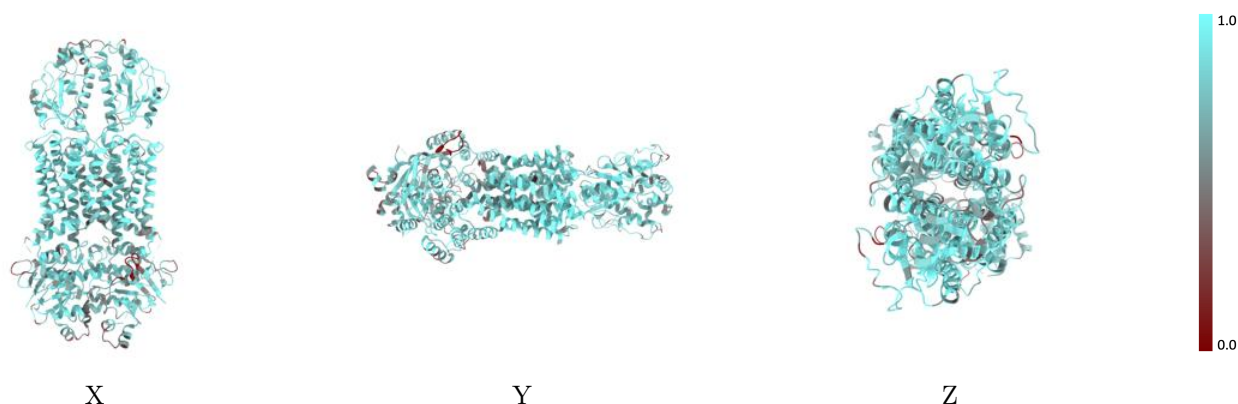
The images above show the 3D surface view of the map at the recommended contour level 0.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



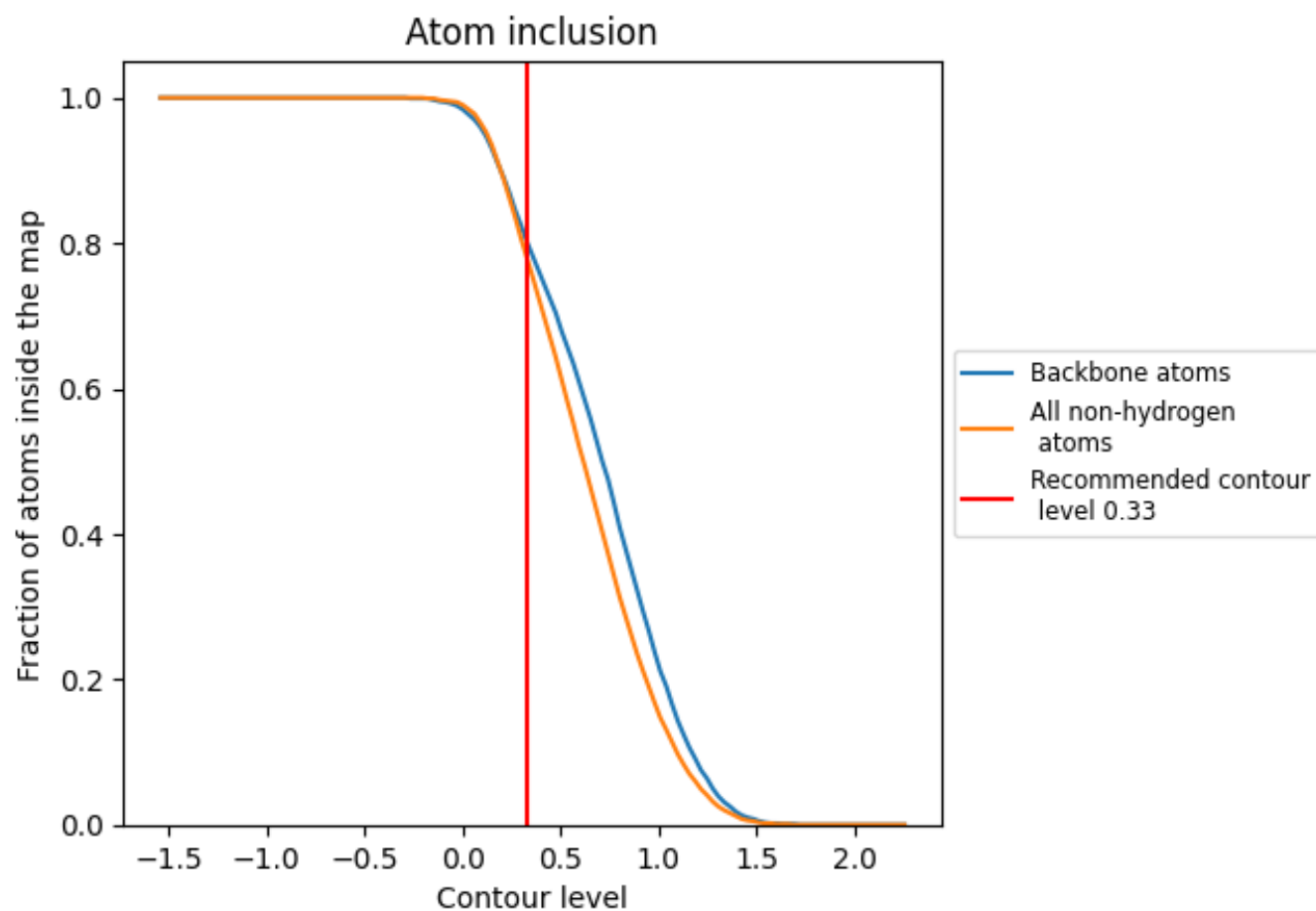
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.33).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 78% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7800	<div></div> 0.5690
A	<div></div> 0.7790	<div></div> 0.5710
B	<div></div> 0.7820	<div></div> 0.5660

