Full wwPDB EM Validation Report

Nov 12, 2026 – 03:38 pm GMT

PDB ID	:	33ZH / pdb_000033zh
EMDB ID	:	EMD-59685
Title	:	E. coli bifunctional acetaldehyde-CoA/alcohol dehydrogenase (AdhE) after reconstitution by acetone extract of E. coli cells, the map focused on the ADH domain.
Authors	:	Opatowsky, Y.; Isupov, M.N.; Das, S.
Deposited on	:	2026-09-01
Resolution	:	2.56 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:

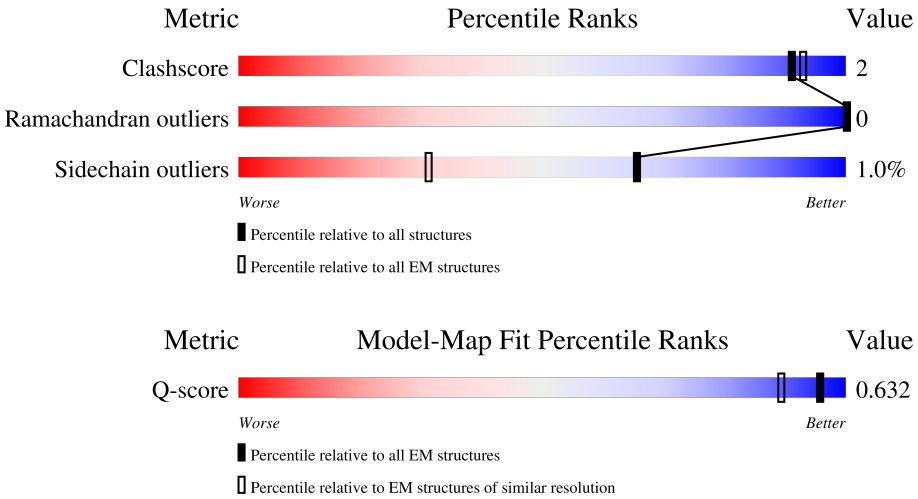
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.56 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	7558 (2.06 - 3.06)

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 <=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	C	897	46% · 52%
1	D	897	46% · 52%
1	E	897	46% · 52%
1	F	897	46% · 52%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13816 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 Bifunctional aldehyde-alcohol dehydrogenase AdhE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	427	Total	C	N	O	S	0	0
			3182	2014	544	610	14		
1	C	432	Total	C	N	O	S	0	0
			3346	2132	573	625	16		
1	F	427	Total	C	N	O	S	0	0
			3182	2014	544	610	14		
1	E	432	Total	C	N	O	S	0	0
			3346	2132	573	625	16		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	889	ILE	-	expression tag	UNP P0A9Q7
D	890	ILE	-	expression tag	UNP P0A9Q7
D	891	ALA	-	expression tag	UNP P0A9Q7
D	892	ALA	-	expression tag	UNP P0A9Q7
D	893	ASN	-	expression tag	UNP P0A9Q7
D	894	SER	-	expression tag	UNP P0A9Q7
D	895	SER	-	expression tag	UNP P0A9Q7
D	896	ASN	-	expression tag	UNP P0A9Q7
D	897	THR	-	expression tag	UNP P0A9Q7
C	889	ILE	-	expression tag	UNP P0A9Q7
C	890	ILE	-	expression tag	UNP P0A9Q7
C	891	ALA	-	expression tag	UNP P0A9Q7
C	892	ALA	-	expression tag	UNP P0A9Q7
C	893	ASN	-	expression tag	UNP P0A9Q7
C	894	SER	-	expression tag	UNP P0A9Q7
C	895	SER	-	expression tag	UNP P0A9Q7
C	896	ASN	-	expression tag	UNP P0A9Q7
C	897	THR	-	expression tag	UNP P0A9Q7
F	889	ILE	-	expression tag	UNP P0A9Q7
F	890	ILE	-	expression tag	UNP P0A9Q7
F	891	ALA	-	expression tag	UNP P0A9Q7
F	892	ALA	-	expression tag	UNP P0A9Q7

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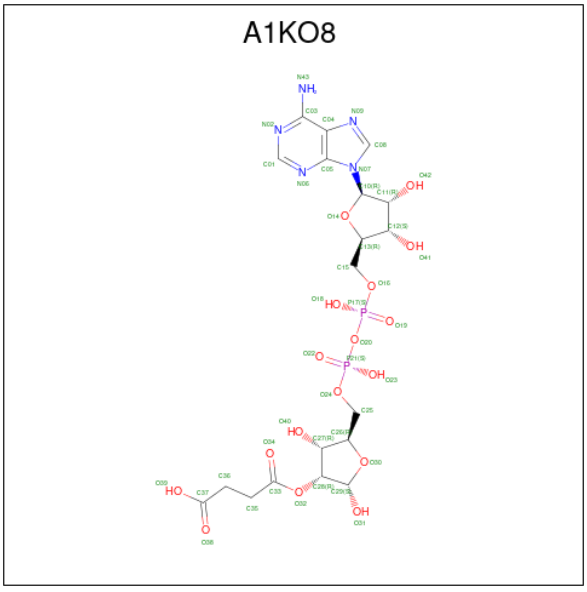
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Chain	Residue	Modelled	Actual	Comment	Reference
F	893	ASN	-	expression tag	UNP P0A9Q7
F	894	SER	-	expression tag	UNP P0A9Q7
F	895	SER	-	expression tag	UNP P0A9Q7
F	896	ASN	-	expression tag	UNP P0A9Q7
F	897	THR	-	expression tag	UNP P0A9Q7
E	889	ILE	-	expression tag	UNP P0A9Q7
E	890	ILE	-	expression tag	UNP P0A9Q7
E	891	ALA	-	expression tag	UNP P0A9Q7
E	892	ALA	-	expression tag	UNP P0A9Q7
E	893	ASN	-	expression tag	UNP P0A9Q7
E	894	SER	-	expression tag	UNP P0A9Q7
E	895	SER	-	expression tag	UNP P0A9Q7
E	896	ASN	-	expression tag	UNP P0A9Q7
E	897	THR	-	expression tag	UNP P0A9Q7

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	C	1	Total Fe 1 1	0
2	E	1	Total Fe 1 1	0

- Molecule 3 is 2''-o-succinyl-ADP-D-ribose (CCD ID: A1KO8) (formula: $C_{19}H_{27}N_5O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			43	19	5	17	2	
3	E	1	Total	C	N	O	P	0
			43	19	5	17	2	

- Molecule 4 is water.

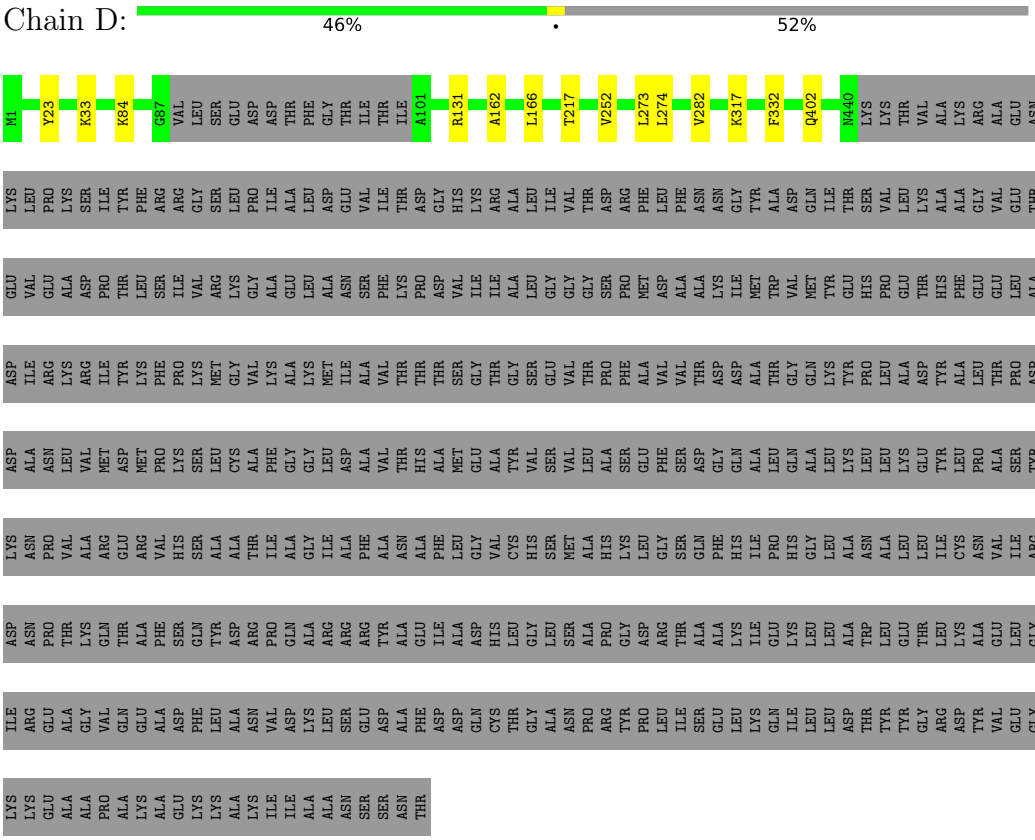
Mol	Chain	Residues	Atoms		AltConf
4	D	103	Total	O	0
			103	103	
4	C	233	Total	O	0
			233	233	
4	F	103	Total	O	0
			103	103	
4	E	233	Total	O	0
			233	233	

3 Residue-property plots (i)

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

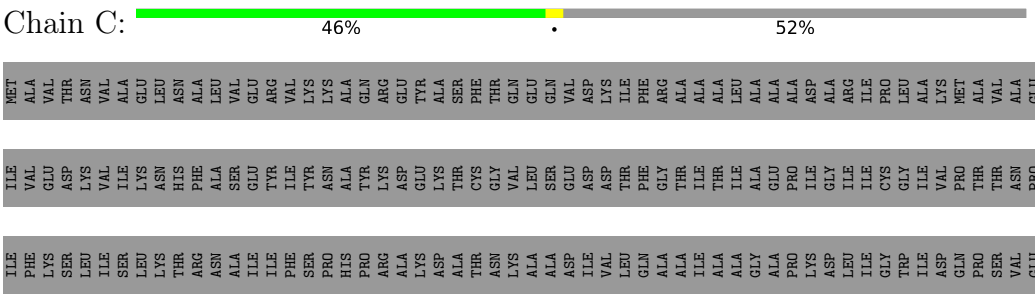
• Molecule 1: Bifunctional aldehyde-alcohol dehydrogenase AdhE

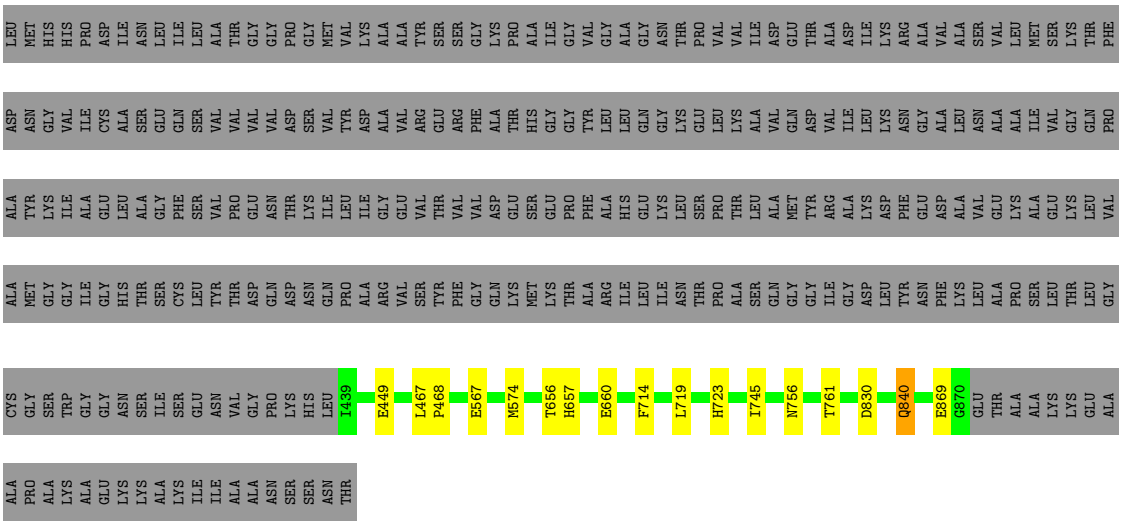
Chain D:



• Molecule 1: Bifunctional aldehyde-alcohol dehydrogenase AdhE

Chain C:





• Molecule 1: Bifunctional aldehyde-alcohol dehydrogenase AdhE

Chain F:

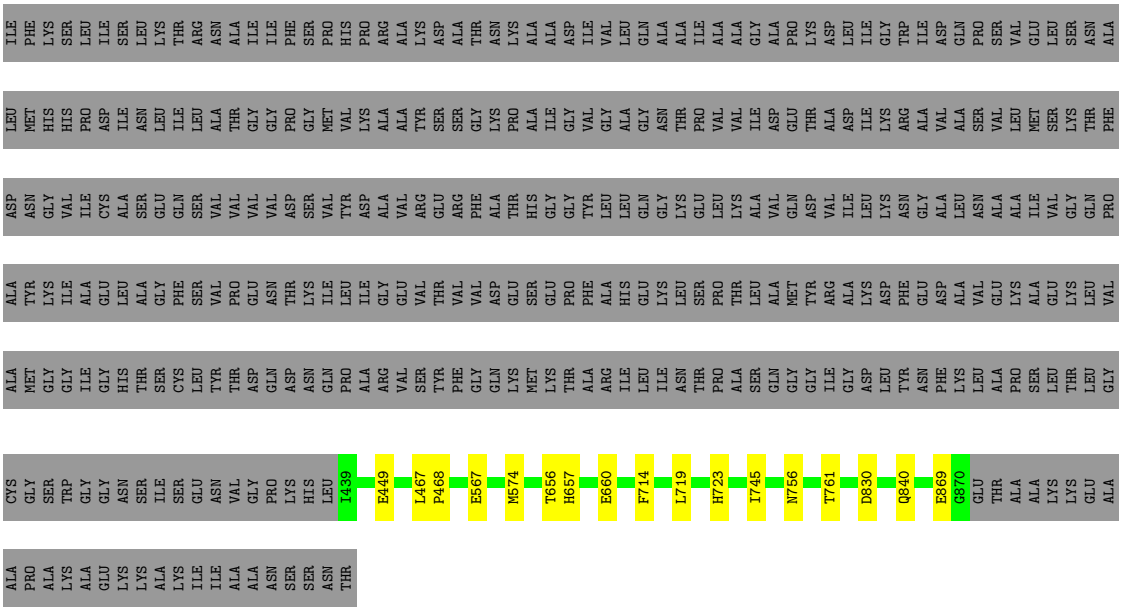




• Molecule 1: Bifunctional aldehyde-alcohol dehydrogenase AdhE

Chain E:




ILE PHE LYS SER LEU ILE SER LEU LYS THR ARG ASN ALA ILE ILE PHE SER PRO HIS PRO ARG ALA LYS ASP ALA THR ASN LYS ALA ALA ASP ILE VAL LEU GLN GLN ALA ALA ILE ALA ALA GLY ALA PRO LYS ASP LEU ILE GLY TRP ILE ASP GLN PRO SER VAL GLU LEU SER ASN ALA
LEU MET HIS HIS PRO ASP ILE ASN LEU ILE LEU LEU ALA THR GLY GLY PRO GLY MET VAL LYS ALA ALA TYR SER SER GLY LYS PRO ALA ILE GLY VAL GLY ALA GLY ASN THR PRO VAL VAL ILE ASP GLU THR ALA ASP ILE LYS ARG ALA VAL ALA ILE VAL GLN ASP VAL ILE LEU LYS ASN GLY ALA LEU ASN ALA ALA ILE VAL GLY GLN PRO
ASP ASN GLY VAL ILE CYS ALA SER GLU GLN SER VAL VAL VAL ASP SER VAL TYR ASP ALA VAL GLU ARG PHE ALA THR HIS GLY GLY TYR LEU LEU GLN GLY LYS GLU LEU LYS ALA VAL GLN ASP VAL ILE LEU LYS ASN GLY ALA LEU ASN ALA ALA ILE VAL GLY PRO
ALA TYR LYS ILE ALA GLU LEU ALA GLY PHE SER VAL PRO GLU ASN THR LYS ILE LEU ILE GLY GLU VAL THR VAL ASP VAL THR ALA MET TYR ARG ALA LYS ASP PHE GLU GLY LEU ALA VAL GLU LYS ALA LEU ASN VAL GLU LYS ALA GLU LEU VAL
ALA MET GLY GLY ILE GLY HIS THR SER CYS LEU TYR THR ASP GLN ASP ASN GLN PRO ALA ARG VAL SER TYR PHE GLY GLN LYS MET LYS THR ALA ARG ILE LEU ILE ASN THR PRO ALA SER GLN GLY GLY ILE GLY ASP LEU TYR ASN PHE LYS LEU ALA PRO SER LEU THR LEU GLY
CYS GLY SER TRP GLY GLY ASN SER ILE SER GLU ASN VAL GLY PRO LYS HIS LEU I439 E449 L467 P468 E567 M574 T656 H657 E660 F714 L719 H723 I745 N756 T761 D830 Q840 E869 G870 GLU THR ALA ALA LYS LYS GLU ALA
ALA PRO ALA LYS ALA GLU LYS LYS ALA LYS ILE ILE ALA ALA ASN SER SER ASN THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	351318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.356	Depositor
Minimum map value	-2.047	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.229	Depositor
Map size (Å)	335.6, 335.6, 335.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.839, 0.839, 0.839	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, A1KO8

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	C	0.49	0/3417	1.09	0/4630
1	D	0.50	0/3236	1.09	0/4389
1	E	0.49	0/3417	1.09	0/4630
1	F	0.50	0/3236	1.09	0/4389
All	All	0.50	0/13306	1.09	0/18038

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	C	3346	0	3349	11	0
1	D	3182	0	3232	10	0
1	E	3346	0	3349	10	0
1	F	3182	0	3232	10	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	C	43	0	0	0	0
3	E	43	0	0	0	0
4	C	233	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	103	0	0	7	0
4	E	233	0	0	5	0
4	F	103	0	0	7	0
All	All	13816	0	13162	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (41) 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:C:756:ASN:HA	4:C:1017:HOH:O	1.96	0.64
1:E:756:ASN:HA	4:E:1018:HOH:O	1.96	0.64
1:C:449:GLU:HB3	4:C:1135:HOH:O	1.99	0.62
1:E:449:GLU:HB3	4:E:1135:HOH:O	1.99	0.60
1:D:162:ALA:HB1	1:D:166:LEU:HD12	1.85	0.58
1:F:162:ALA:HB1	1:F:166:LEU:HD12	1.86	0.57
1:E:656:THR:HG23	1:E:745:ILE:HD13	1.88	0.55
1:C:656:THR:HG23	1:C:745:ILE:HD13	1.88	0.55
1:F:217:THR:HB	4:F:910:HOH:O	2.09	0.53
1:D:217:THR:HB	4:D:910:HOH:O	2.09	0.52
1:C:657:HIS:CD2	1:C:723:HIS:CE1	3.01	0.49
1:E:657:HIS:CD2	1:E:723:HIS:CE1	3.01	0.49
1:D:23:TYR:CE2	1:D:131:ARG:HA	2.48	0.49
1:F:23:TYR:CE2	1:F:131:ARG:HA	2.48	0.47
1:F:84:LYS:HG3	4:F:906:HOH:O	2.15	0.47
1:D:84:LYS:HG3	4:D:906:HOH:O	2.15	0.46
1:D:402:GLN:HB2	4:D:955:HOH:O	2.14	0.46
1:D:274:LEU:HD13	1:D:282:VAL:HG21	1.98	0.46
1:F:402:GLN:HB2	4:F:954:HOH:O	2.14	0.46
1:E:761:THR:HG22	4:E:1218:HOH:O	2.16	0.45
1:D:402:GLN:CB	4:D:955:HOH:O	2.65	0.45
1:C:567:GLU:HG2	4:C:1071:HOH:O	2.17	0.45
1:F:274:LEU:HD13	1:F:282:VAL:HG21	1.98	0.44
1:C:761:THR:HG22	4:C:1218:HOH:O	2.16	0.44
1:F:402:GLN:CB	4:F:954:HOH:O	2.65	0.44
1:C:657:HIS:HD2	1:C:723:HIS:CE1	2.35	0.44
1:E:567:GLU:HG2	4:E:1071:HOH:O	2.17	0.43
1:E:467:LEU:HB3	1:E:468:PRO:HD3	2.00	0.42
1:C:840:GLN:H	1:C:840:GLN:HG3	1.54	0.42
1:D:33:LYS:HD2	4:D:927:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:869:GLU:HB2	4:C:1202:HOH:O	2.18	0.42
1:E:657:HIS:HD2	1:E:723:HIS:CE1	2.35	0.42
1:E:869:GLU:HB2	4:E:1202:HOH:O	2.18	0.42
1:C:467:LEU:HB3	1:C:468:PRO:HD3	2.00	0.42
1:F:84:LYS:HB2	4:F:916:HOH:O	2.20	0.41
1:F:317:LYS:HE2	4:F:989:HOH:O	2.20	0.41
1:D:84:LYS:HB2	4:D:917:HOH:O	2.20	0.41
1:D:317:LYS:HE2	4:D:989:HOH:O	2.20	0.41
1:F:33:LYS:HD2	4:F:927:HOH:O	2.20	0.41
1:E:660:GLU:HG2	1:E:719:LEU:HA	2.03	0.41
1:C:660:GLU:HG2	1:C:719:LEU:HA	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	C	430/897 (48%)	423 (98%)	7 (2%)	0	100	100
1	D	423/897 (47%)	411 (97%)	12 (3%)	0	100	100
1	E	430/897 (48%)	423 (98%)	7 (2%)	0	100	100
1	F	423/897 (47%)	411 (97%)	12 (3%)	0	100	100
All	All	1706/3588 (48%)	1668 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	C	350/713 (49%)	346 (99%)	4 (1%)	65	77
1	D	335/713 (47%)	332 (99%)	3 (1%)	70	80
1	E	350/713 (49%)	346 (99%)	4 (1%)	65	77
1	F	335/713 (47%)	332 (99%)	3 (1%)	70	80
All	All	1370/2852 (48%)	1356 (99%)	14 (1%)	65	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	252	VAL
1	D	273	LEU
1	D	332	PHE
1	C	574	MET
1	C	714	PHE
1	C	830	ASP
1	C	840	GLN
1	F	252	VAL
1	F	273	LEU
1	F	332	PHE
1	E	574	MET
1	E	714	PHE
1	E	830	ASP
1	E	840	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	78	ASN
1	D	283	GLN
1	D	397	ASN
1	C	704	HIS
1	C	732	GLN
1	F	78	ASN
1	F	397	ASN
1	E	704	HIS
1	E	732	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	A1KO8	E	902	-	43,46,46	1.31	4 (9%)	60,69,69	1.82	12 (20%)
3	A1KO8	C	902	-	43,46,46	1.31	4 (9%)	60,69,69	1.82	12 (20%)

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	A1KO8	E	902	-	-	16/31/63/63	0/4/4/4
3	A1KO8	C	902	-	-	16/31/63/63	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	A1KO8	C04-C05	4.95	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	902	A1KO8	C04-C05	4.95	1.48	1.39
3	C	902	A1KO8	O32-C33	4.33	1.46	1.34
3	E	902	A1KO8	O32-C33	4.33	1.46	1.34
3	C	902	A1KO8	C08-N09	2.44	1.36	1.31
3	E	902	A1KO8	C08-N09	2.43	1.36	1.31
3	C	902	A1KO8	C04-N09	-2.01	1.35	1.39
3	E	902	A1KO8	C04-N09	-2.01	1.35	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	902	A1KO8	C04-C05-N06	-5.89	119.07	126.75
3	E	902	A1KO8	C04-C05-N06	-5.89	119.07	126.75
3	C	902	A1KO8	N02-C01-N06	-4.42	121.69	128.60
3	C	902	A1KO8	N06-C05-N07	4.42	134.36	127.08
3	E	902	A1KO8	N06-C05-N07	4.41	134.35	127.08
3	E	902	A1KO8	N02-C01-N06	-4.40	121.72	128.60
3	C	902	A1KO8	O32-C33-C35	4.20	120.56	111.50
3	E	902	A1KO8	O32-C33-C35	4.20	120.56	111.50
3	C	902	A1KO8	C01-N06-C05	3.64	120.36	111.75
3	E	902	A1KO8	C01-N06-C05	3.64	120.36	111.75
3	C	902	A1KO8	C05-C04-N09	-3.62	106.21	110.62
3	E	902	A1KO8	C05-C04-N09	-3.62	106.21	110.62
3	C	902	A1KO8	P17-O20-P21	-3.17	121.95	132.83
3	E	902	A1KO8	P17-O20-P21	-3.17	121.95	132.83
3	C	902	A1KO8	C28-O32-C33	-3.12	112.33	117.53
3	E	902	A1KO8	C28-O32-C33	-3.12	112.33	117.53
3	C	902	A1KO8	C04-N09-C08	2.89	107.62	103.51
3	E	902	A1KO8	C04-N09-C08	2.88	107.60	103.51
3	C	902	A1KO8	C05-N07-C08	2.46	108.39	105.73
3	E	902	A1KO8	C05-N07-C08	2.45	108.38	105.73
3	E	902	A1KO8	C03-C04-N09	2.42	136.52	132.02
3	C	902	A1KO8	C03-C04-N09	2.40	136.49	132.02
3	C	902	A1KO8	C01-N02-C03	2.02	122.23	118.77
3	E	902	A1KO8	C01-N02-C03	2.00	122.21	118.77

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	902	A1KO8	O24-C25-C26-C27
3	C	902	A1KO8	C25-O24-P21-O22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	902	A1KO8	C25-O24-P21-O23
3	C	902	A1KO8	C15-O16-P17-O20
3	E	902	A1KO8	O24-C25-C26-C27
3	E	902	A1KO8	C25-O24-P21-O22
3	E	902	A1KO8	C25-O24-P21-O23
3	E	902	A1KO8	C15-O16-P17-O20
3	C	902	A1KO8	O24-C25-C26-O30
3	C	902	A1KO8	O14-C13-C15-O16
3	E	902	A1KO8	O24-C25-C26-O30
3	E	902	A1KO8	O14-C13-C15-O16
3	C	902	A1KO8	O34-C33-O32-C28
3	E	902	A1KO8	O34-C33-O32-C28
3	C	902	A1KO8	C35-C33-O32-C28
3	E	902	A1KO8	C35-C33-O32-C28
3	C	902	A1KO8	C12-C13-C15-O16
3	E	902	A1KO8	C12-C13-C15-O16
3	C	902	A1KO8	C15-O16-P17-O19
3	E	902	A1KO8	C15-O16-P17-O19
3	C	902	A1KO8	C29-C28-O32-C33
3	E	902	A1KO8	C29-C28-O32-C33
3	C	902	A1KO8	O32-C33-C35-C36
3	E	902	A1KO8	O32-C33-C35-C36
3	C	902	A1KO8	C35-C36-C37-O39
3	E	902	A1KO8	C35-C36-C37-O39
3	C	902	A1KO8	C35-C36-C37-O38
3	E	902	A1KO8	C35-C36-C37-O38
3	C	902	A1KO8	C25-O24-P21-O20
3	E	902	A1KO8	C25-O24-P21-O20
3	C	902	A1KO8	C15-O16-P17-O18
3	E	902	A1KO8	C15-O16-P17-O18

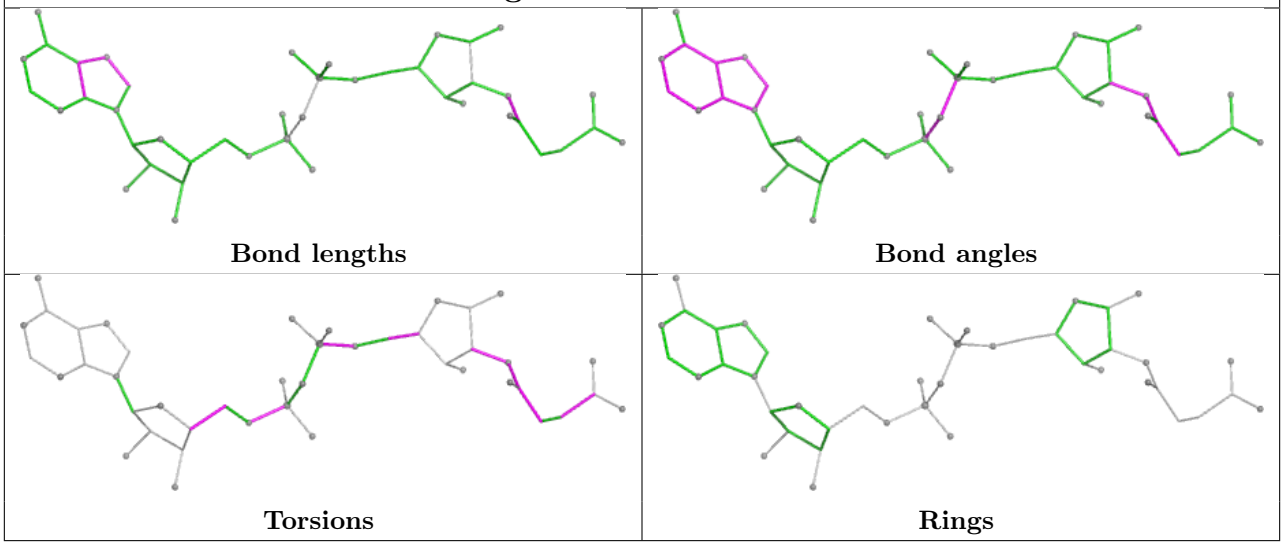
There are no ring outliers.

No monomer is involved in short contacts.

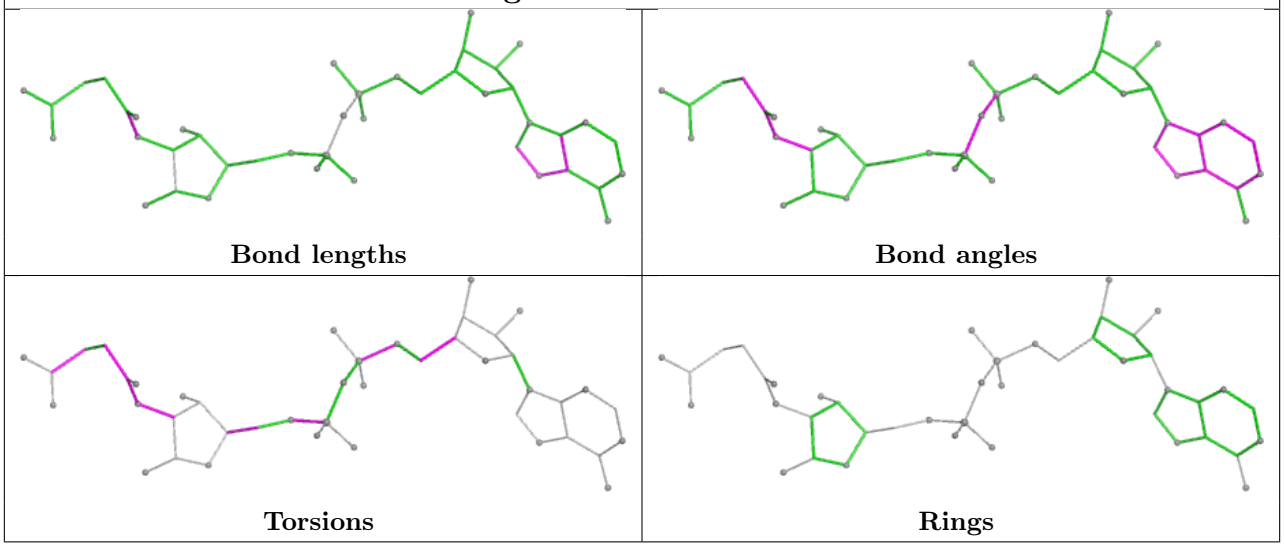
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand A1KO8 E 902



Ligand A1KO8 C 902



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.

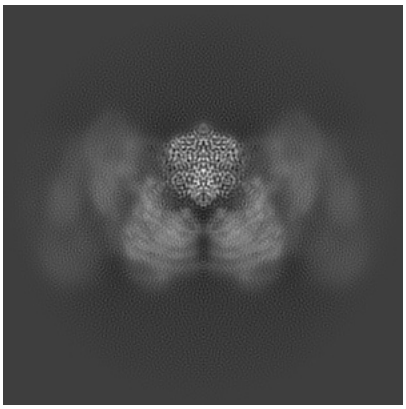
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-59685. These allow visual inspection of the internal detail of the map and identification of artifacts.

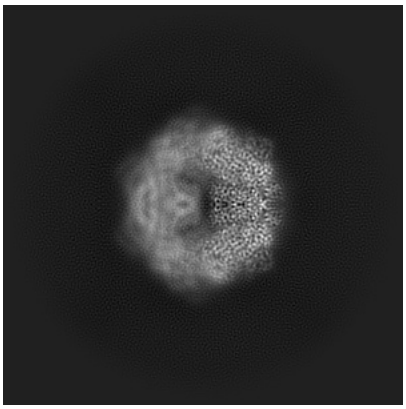
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

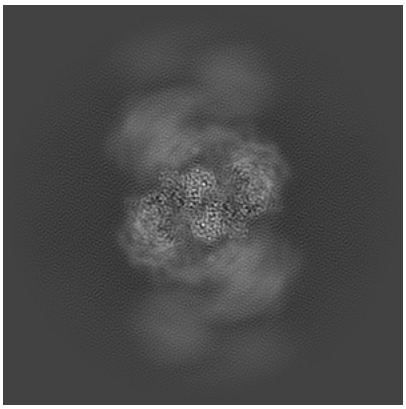
6.1.1 Primary map



X

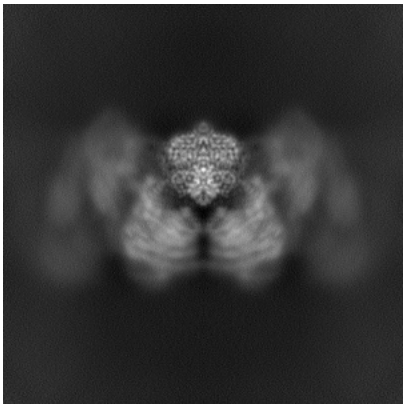


Y

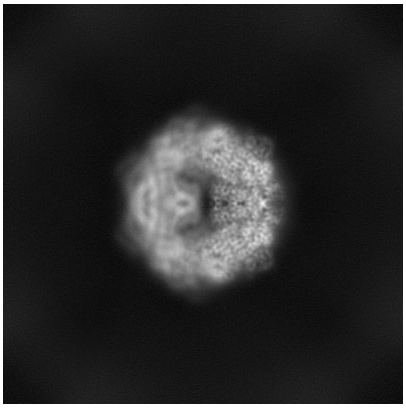


Z

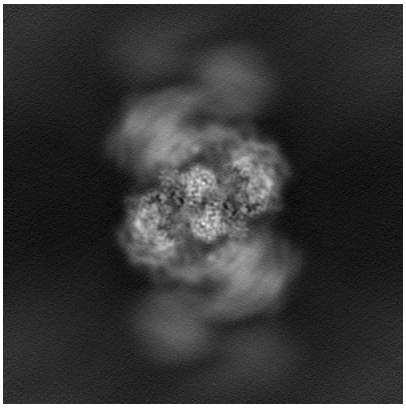
6.1.2 Raw map



X



Y

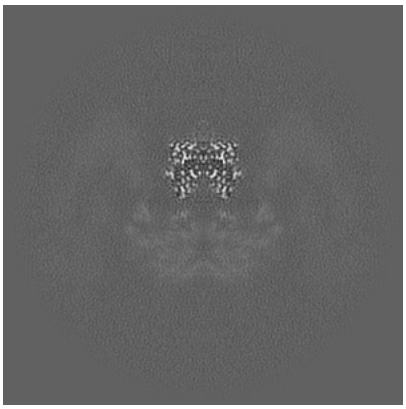


Z

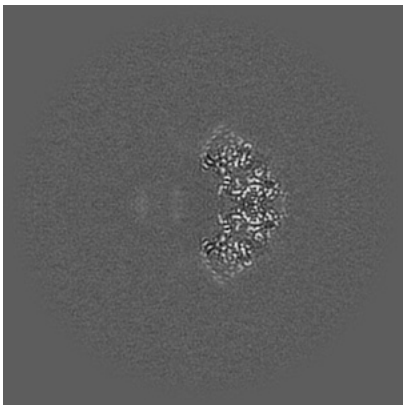
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

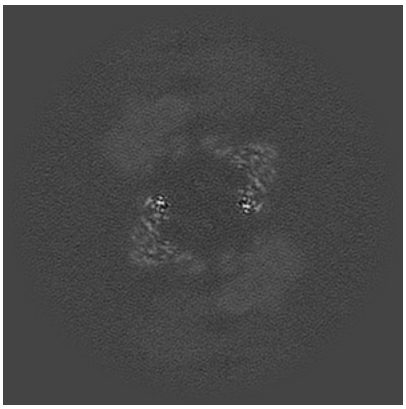
6.2.1 Primary map



X Index: 200

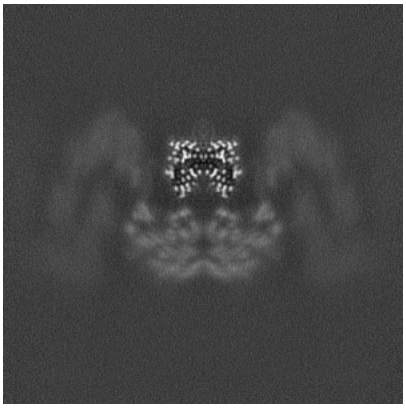


Y Index: 200

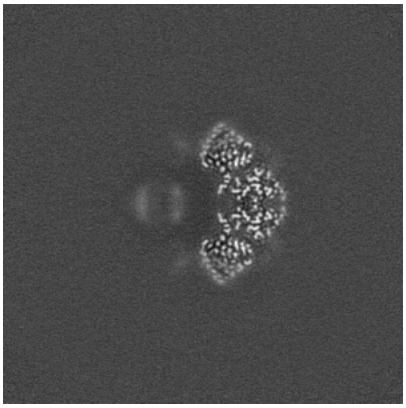


Z Index: 200

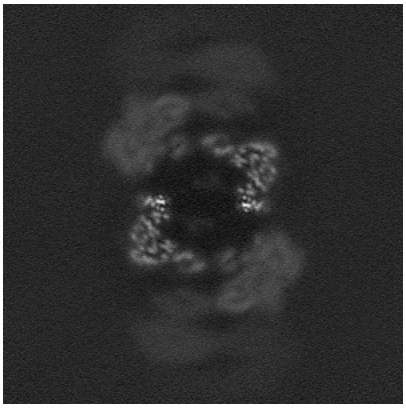
6.2.2 Raw map



X Index: 200



Y Index: 200

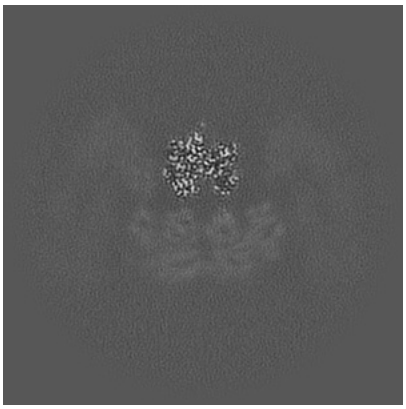


Z Index: 200

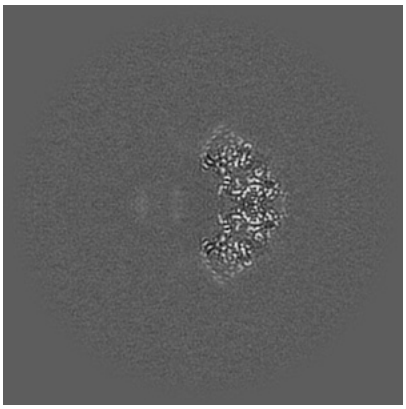
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

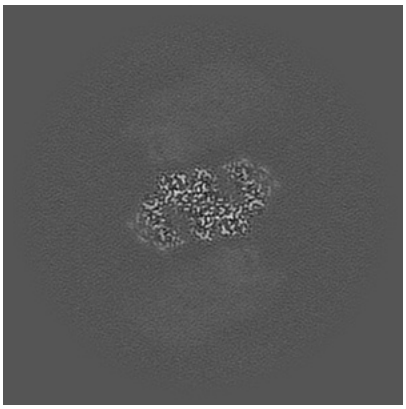
6.3.1 Primary map



X Index: 204

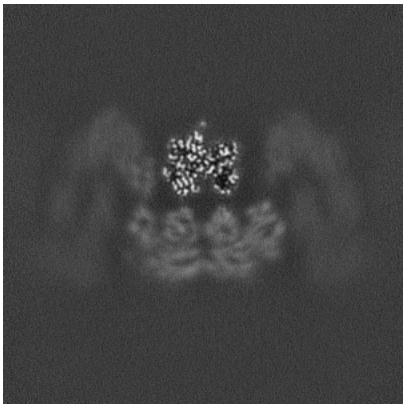


Y Index: 200

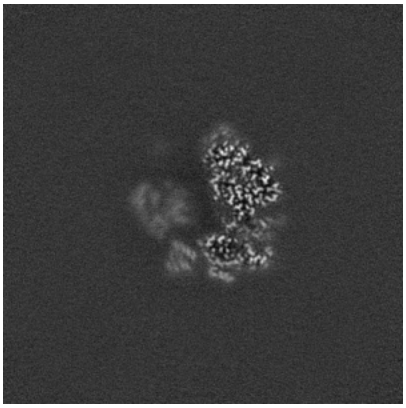


Z Index: 246

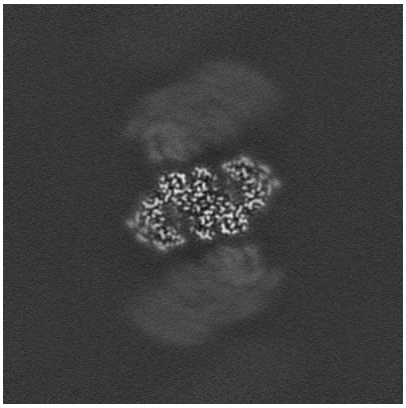
6.3.2 Raw map



X Index: 204



Y Index: 192

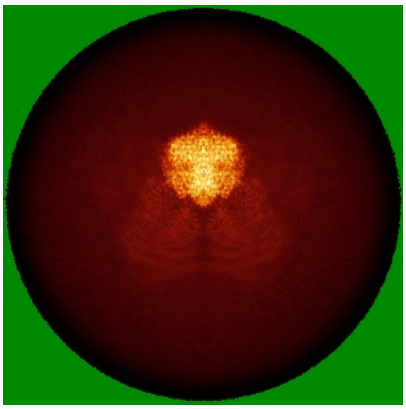


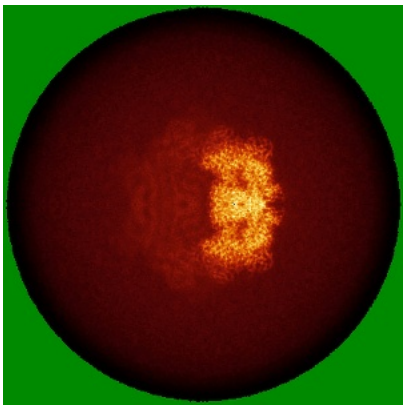
Z Index: 246

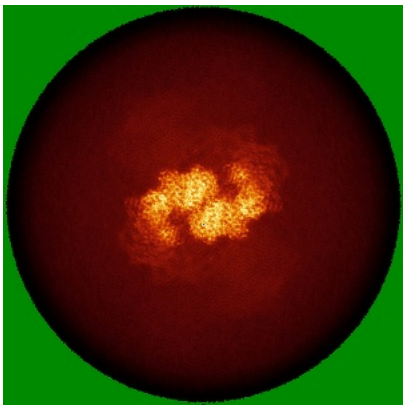
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

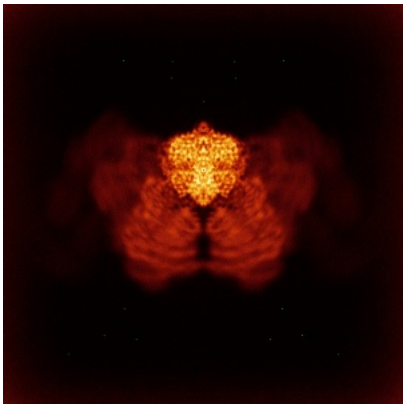
6.4.1 Primary map

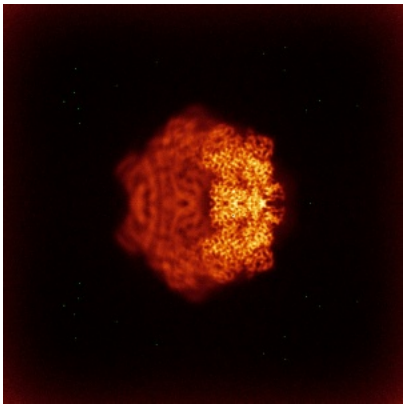

X

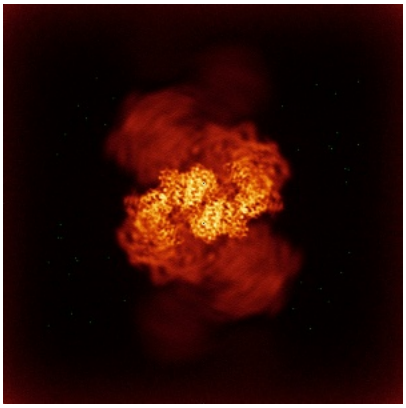

Y


Z

6.4.2 Raw map


X

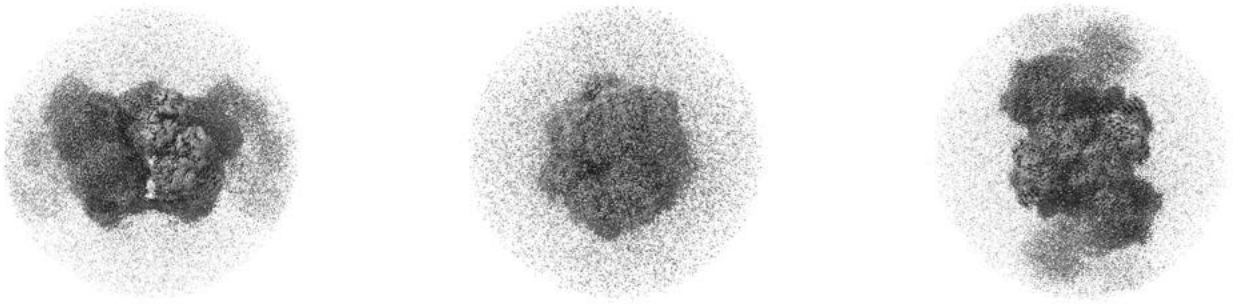

Y


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)

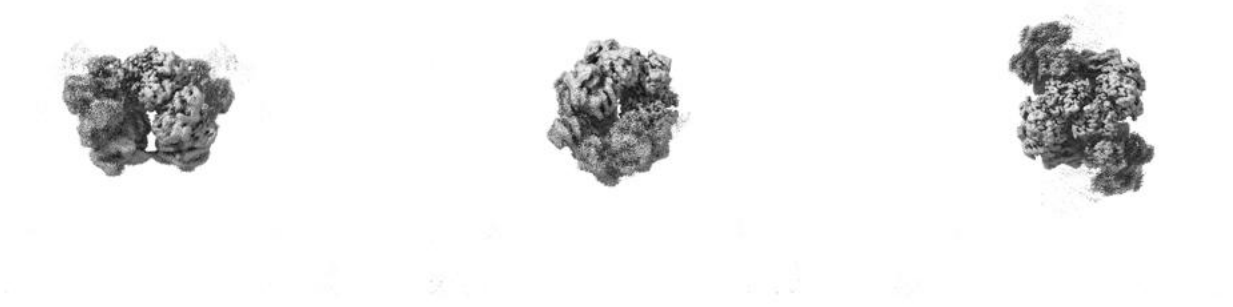
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.229. 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



X Y Z

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.

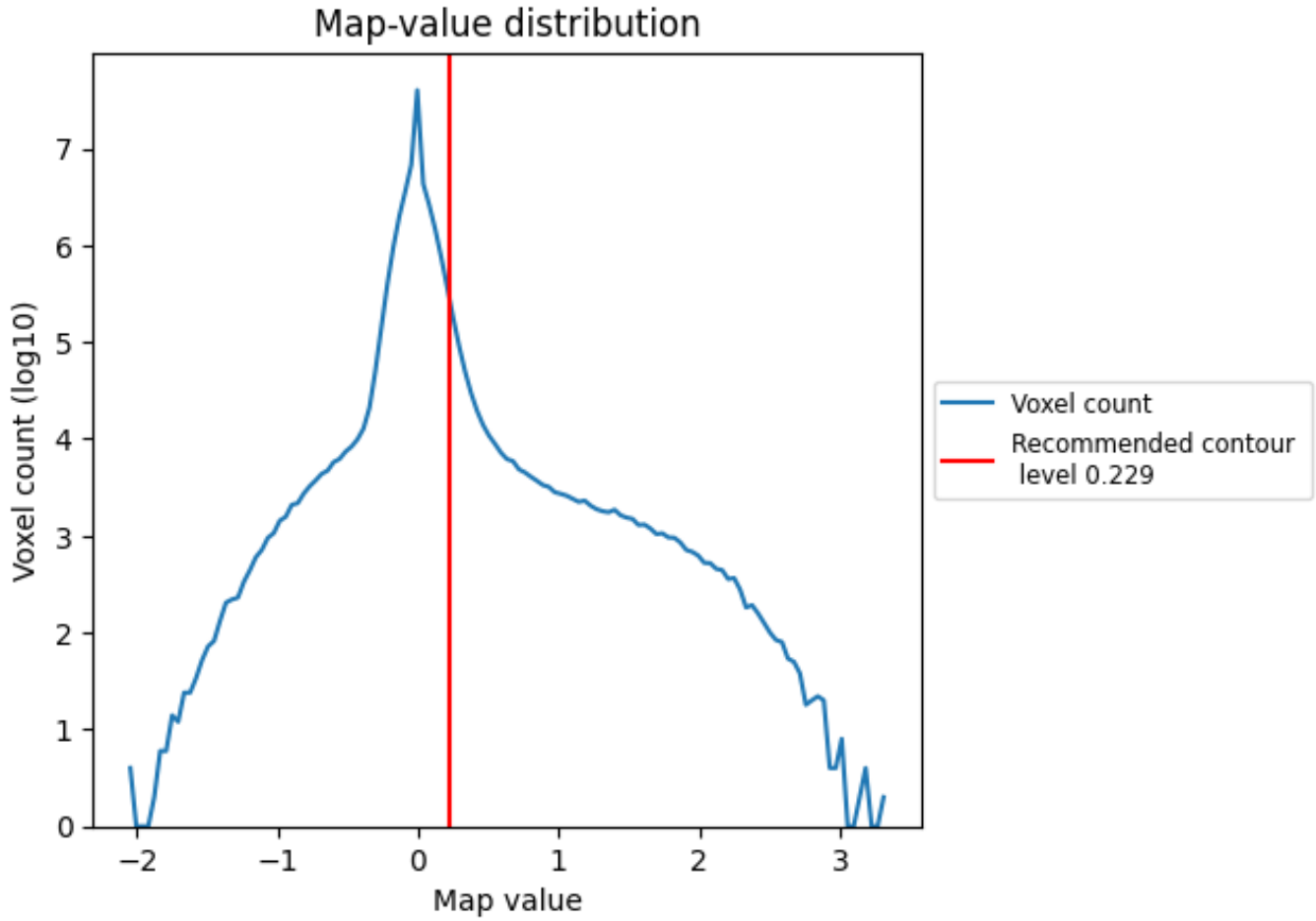
6.6 Mask visualisation (i)

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

7 Map analysis

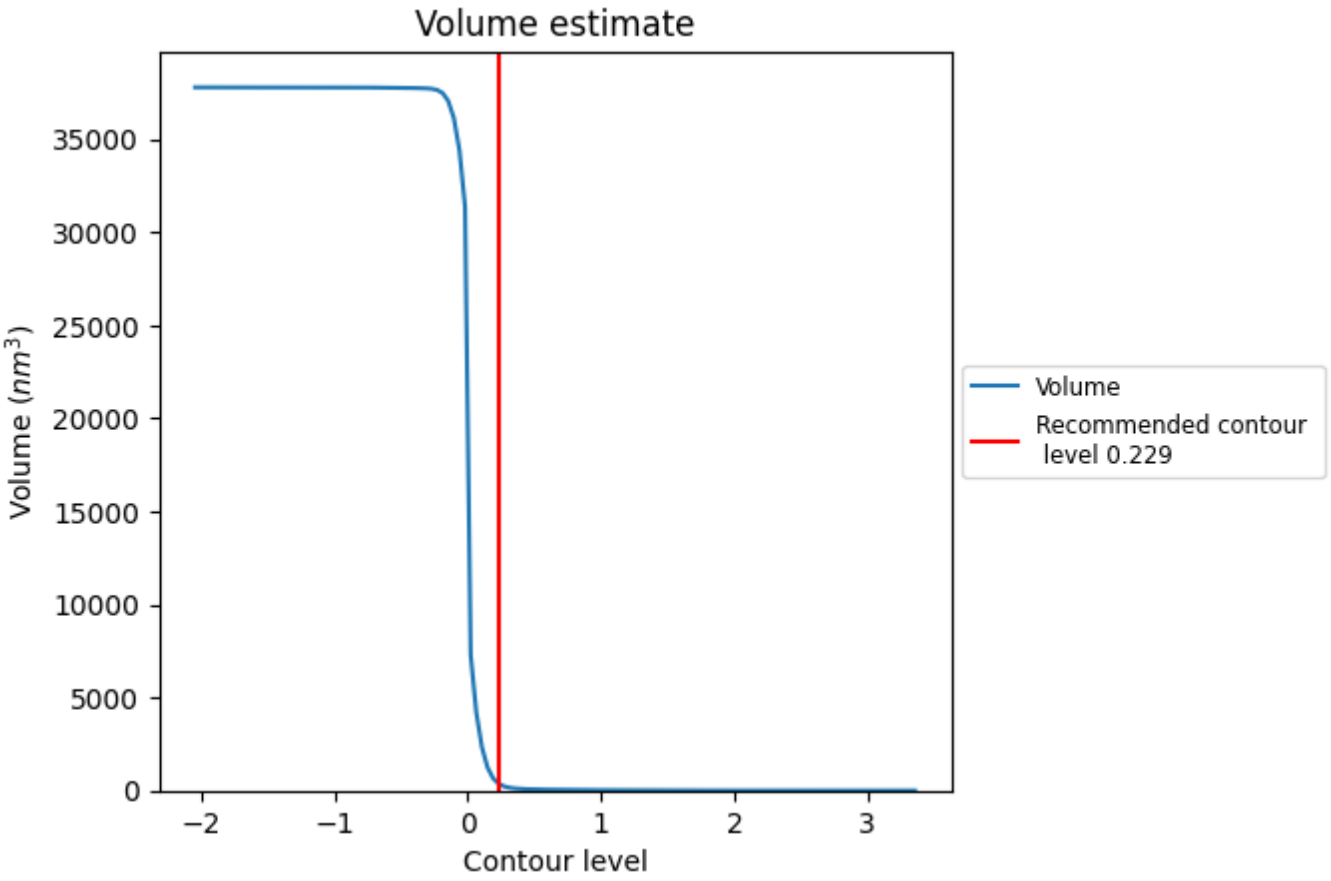
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

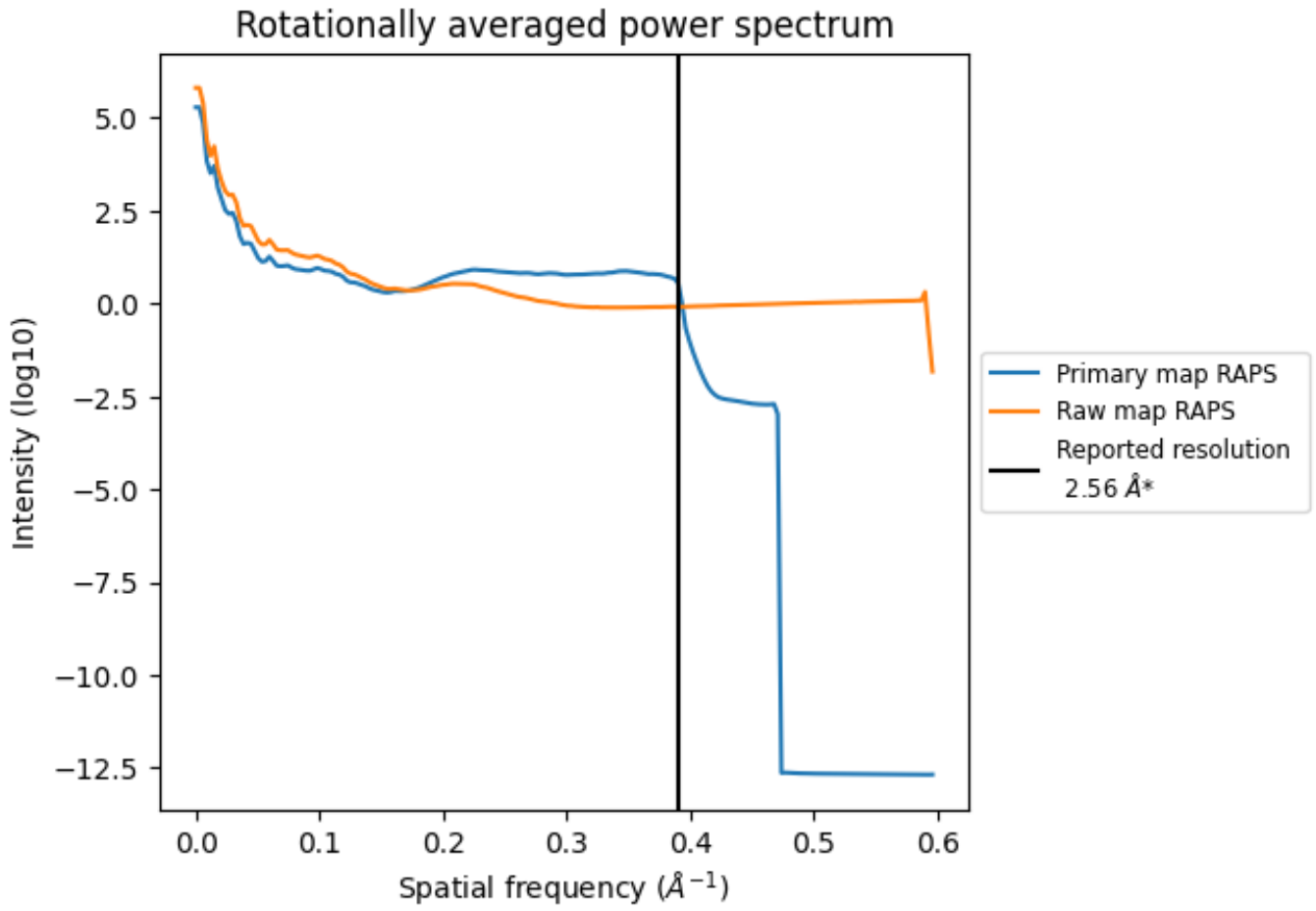
7.2 Volume estimate



The volume at the recommended contour level is 383 nm^3; this corresponds to an approximate mass of 346 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 (i)

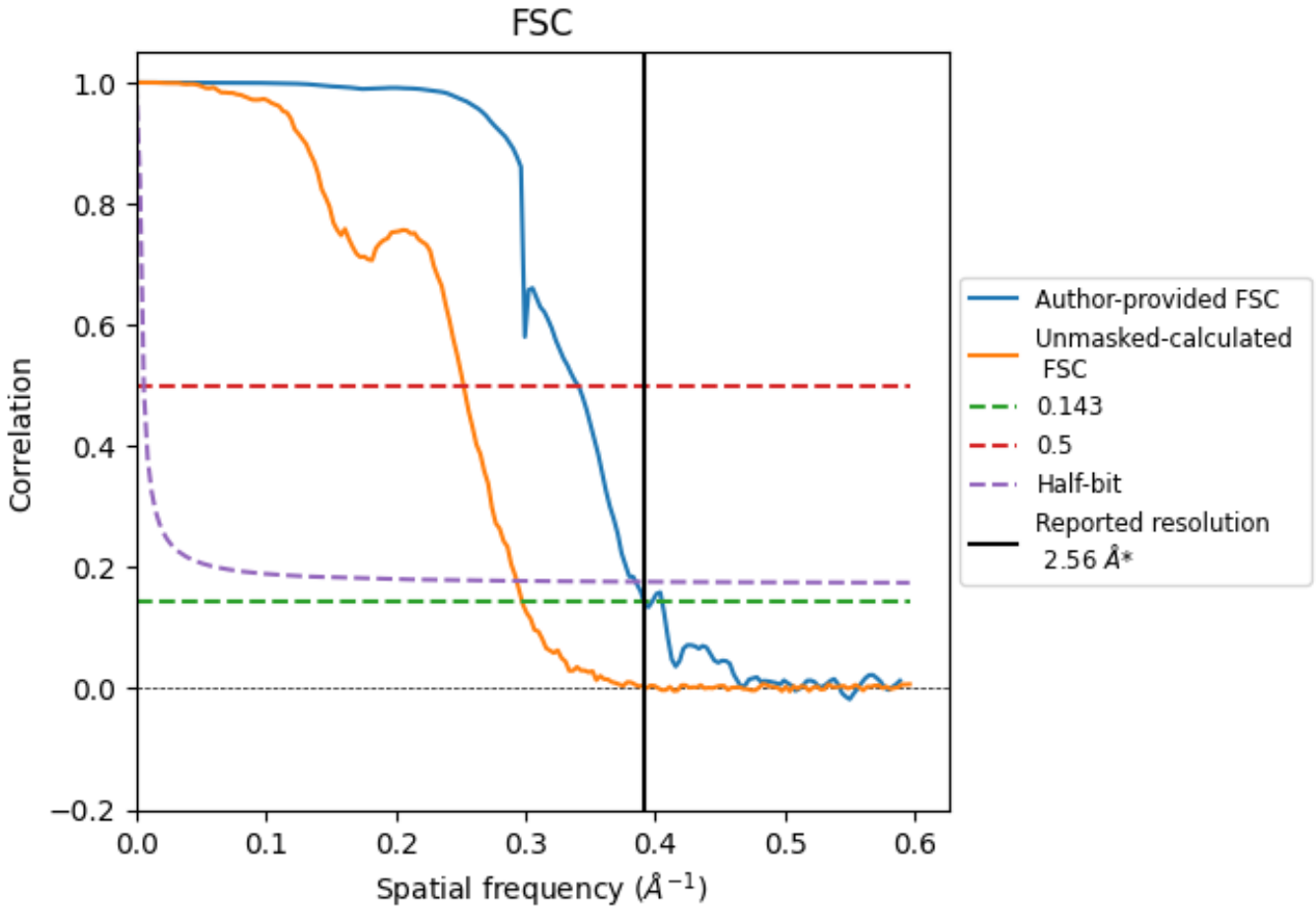


*Reported resolution corresponds to spatial frequency of 0.391 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.391 $Å^{-1}$

8.2 Resolution estimates (i)

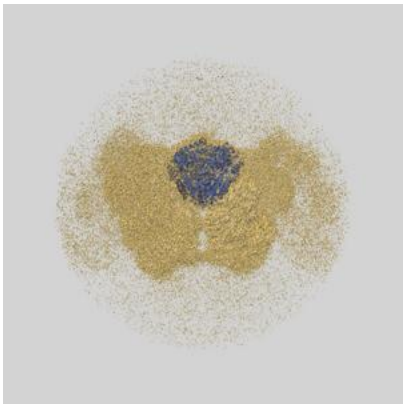
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	2.56	2.94	2.60
Unmasked-calculated*	3.36	3.97	3.41

*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 3.36 differs from the reported value 2.56 by more than 10 %

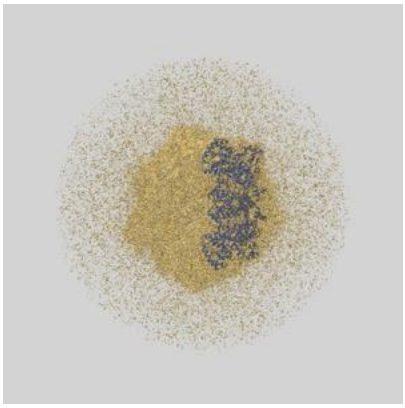
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-59685 and PDB model 33ZH. Per-residue inclusion information can be found in section 3 on page 6.

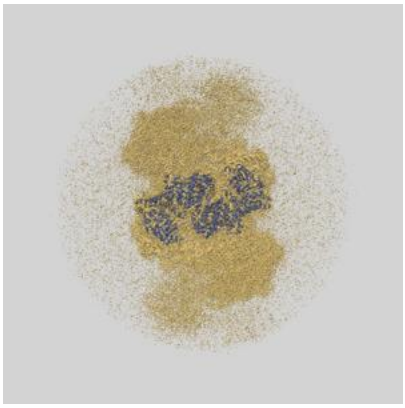
9.1 Map-model overlay



X



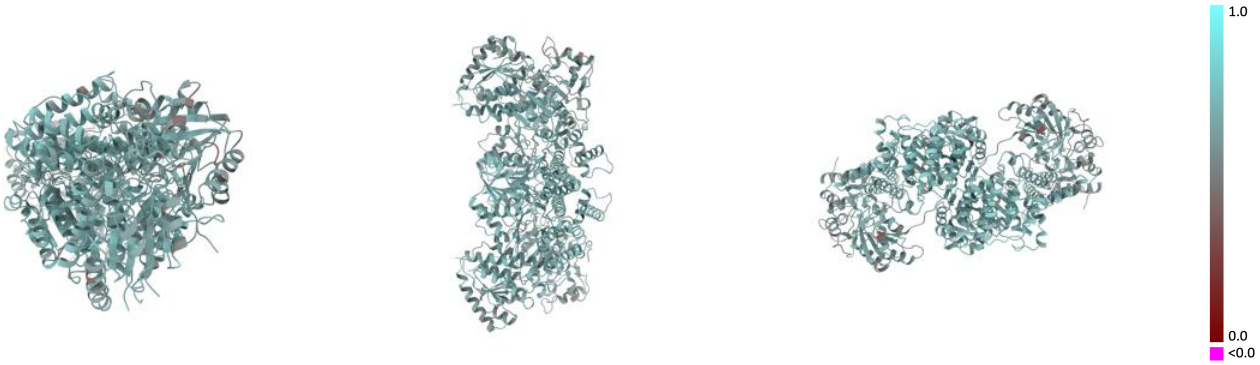
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.229 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.

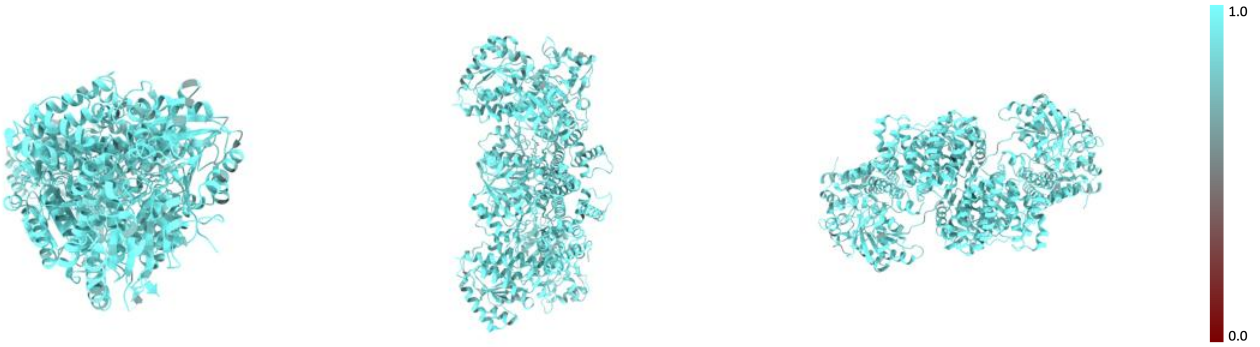
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

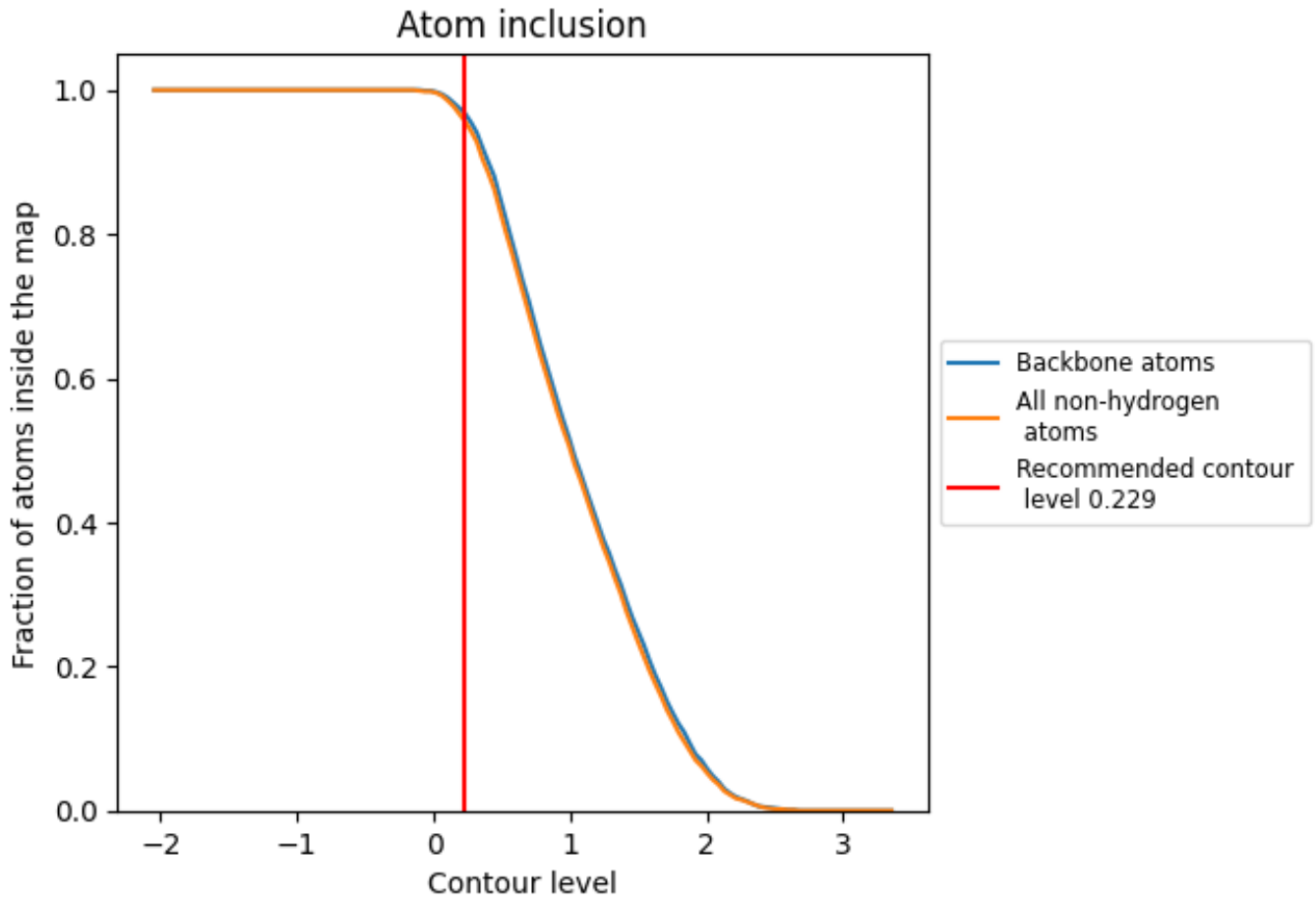
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.229).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.229) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9570	0.6320
C	0.9790	0.6580
D	0.9370	0.6050
E	0.9790	0.6580
F	0.9370	0.6040