



Full wwPDB EM Validation Report ⓘ

May 20, 2026 – 02:12 PM JST

PDB ID : 9W63 / pdb_00009w63
EMDB ID : EMD-65675
Title : Cryo-EM structure of C20:5-CoA bound state human ABCD3 in inward-facing conformation
Authors : Aiba, S.; Okamoto, H.H.; Kusakizako, T.; Nureki, O.
Deposited on : 2025-08-03
Resolution : 3.29 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

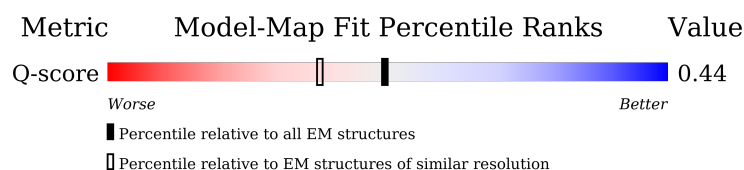
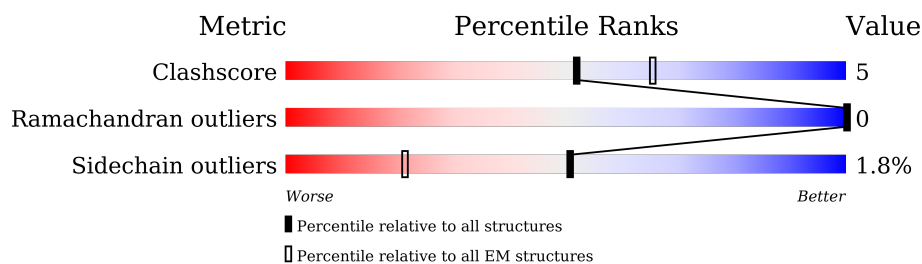
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.29 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	14466 (2.79 - 3.79)

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	914	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4868 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 Isoform 1 of ATP-binding cassette sub-family D member 3, Green fluorescent protein.

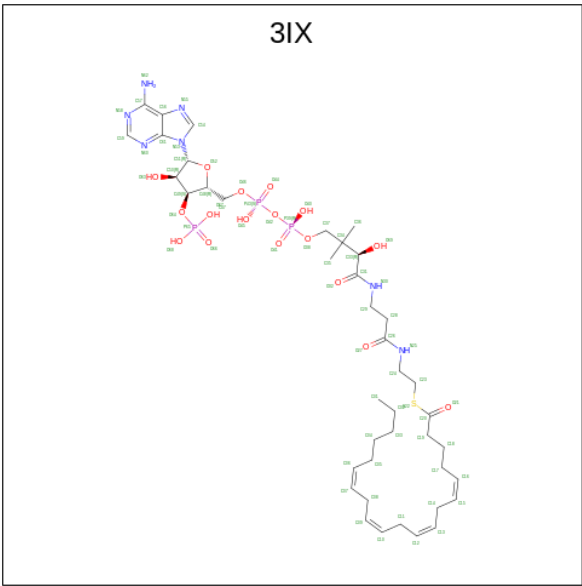
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	573	4659	3005	807	821	26	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	660	LEU	-	linker	UNP P28288
A	661	GLU	-	linker	UNP P28288
A	662	VAL	-	linker	UNP P28288
A	663	LEU	-	linker	UNP P28288
A	664	PHE	-	linker	UNP P28288
A	665	GLN	-	linker	UNP P28288
A	666	GLY	-	linker	UNP P28288
A	667	PRO	-	linker	UNP P28288
A	668	ALA	-	linker	UNP P28288
A	669	VAL	MET	conflict	UNP P42212
A	732	LEU	PHE	conflict	UNP P42212
A	733	THR	SER	conflict	UNP P42212
A	874	LYS	ALA	conflict	UNP P42212
A	899	LEU	HIS	conflict	UNP P42212
A	907	HIS	-	expression tag	UNP P42212
A	908	HIS	-	expression tag	UNP P42212
A	909	HIS	-	expression tag	UNP P42212
A	910	HIS	-	expression tag	UNP P42212
A	911	HIS	-	expression tag	UNP P42212
A	912	HIS	-	expression tag	UNP P42212
A	913	HIS	-	expression tag	UNP P42212
A	914	HIS	-	expression tag	UNP P42212

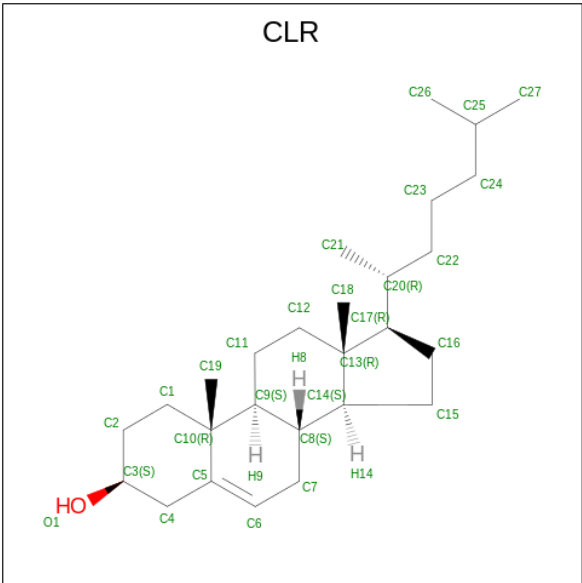
- Molecule 2 is S-[2-[3-[[[(2R)-4-[[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonoxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethyl] (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenethioate (CCD ID: 3IX) (formula: C₄₁H₆₆N₇O₁₇P₃S) (labeled as "Ligand of Interest" by

depositor).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			69	41	7	17	3	1	

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	A	1	28	27	1	0
3	A	1	28	27	1	0

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Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	

VAL	GLU	VAL	GLU
LYS	ASP	LYS	ASP
PHE	GLY	PHE	GLY
GLU	SER	GLU	SER
GLY	VAL	GLY	VAL
ASP	GLN	ASP	GLN
THR	LEU	THR	LEU
LEU	ALA	LEU	ALA
VAL	ASP	VAL	ASP
ASN	HIS	ASN	HIS
ARG	TYR	ARG	TYR
ILE	GLN	ILE	GLN
GLU	GLN	GLU	GLN
LEU	ASN	LEU	ASN
LYS	THR	LYS	THR
GLY	PRO	GLY	PRO
ILE	ILE	ILE	ILE
ASP	GLY	ASP	GLY
PHE	ASP	PHE	ASP
LYS	GLY	LYS	GLY
GLU	PRO	GLU	PRO
VAL	VAL	VAL	VAL
ASP	LEU	ASP	LEU
GLY	LEU	GLY	LEU
ASN	PRO	ASN	PRO
ILE	ASP	ILE	ASP
LEU	ASN	LEU	ASN
GLY	HIS	GLY	HIS
HIS	TYR	HIS	TYR
LYS	LEU	LYS	LEU
GLU	SER	GLU	SER
TYR	THR	TYR	THR
ASN	GLN	ASN	GLN
TYR	SER	TYR	SER
ASN	LYS	ASN	LYS
SER	LEU	SER	LEU
HIS	SER	HIS	SER
ASN	LYS	ASN	LYS
VAL	ASP	VAL	ASP
TYR	PRO	TYR	PRO
ILE	ASN	ILE	ASN
MET	GLU	MET	GLU
ALA	LYS	ALA	LYS
ASP	ARG	ASP	ARG
LYS	ASP	LYS	ASP
GLN	HIS	GLN	HIS
LYS	MET	LYS	MET
ASN	VAL	ASN	VAL
GLY	LEU	GLY	LEU
ILE	LEU	ILE	LEU
LYS	GLU	LYS	GLU
VAL	PHE	VAL	PHE
ASN	THR	ASN	THR
PHE	ALA	PHE	ALA
LYS	ALA	LYS	ALA
ILE	GLY	ILE	GLY
ARG	ILE	ARG	ILE
HIS	THR	HIS	THR
ASN	LEU	ASN	LEU
ILE		ILE	

GLY
MET
ASP
GLU
LEU
TYR
LYS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	119378	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.487	Depositor
Minimum map value	-10.718	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.567	Depositor
Recommended contour level	2.2	Depositor
Map size (Å)	157.14671, 143.86671, 157.14671	wwPDB
Map dimensions	142, 130, 142	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.106667, 1.106667, 1.106667	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: 3IX, CLR

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	0.73	0/4759	1.38	14/6418 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	PHE	CA-CB-CG	6.66	120.45	113.80
1	A	219	PHE	CA-CB-CG	6.44	120.24	113.80
1	A	359	GLN	CB-CA-C	5.89	120.07	110.95
1	A	333	VAL	CB-CA-C	-5.81	104.42	112.04
1	A	359	GLN	CA-C-O	-5.79	114.93	120.90
1	A	110	ILE	N-CA-C	-5.71	104.80	110.62
1	A	251	ILE	N-CA-CB	5.62	117.49	110.47
1	A	317	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	359	GLN	N-CA-C	-5.49	104.93	111.03
1	A	83	THR	N-CA-CB	5.25	117.83	110.12
1	A	164	GLU	CB-CG-CD	5.17	121.40	112.60
1	A	310	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	357	TYR	CA-C-O	-5.11	115.43	120.90
1	A	511	ARG	CB-CA-C	5.03	114.97	110.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4659	0	4740	52	0
2	A	69	0	0	1	0
3	A	140	0	230	8	0
All	All	4868	0	4970	53	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 (53) 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:85:TYR:CZ	1:A:149:GLU:HG2	2.25	0.70
1:A:220:LYS:CB	1:A:363:MET:HE1	2.26	0.65
1:A:220:LYS:HB2	1:A:363:MET:HE1	1.80	0.64
1:A:109:LEU:HD13	1:A:125:TYR:CE1	2.35	0.61
1:A:436:ALA:O	1:A:500:PRO:HA	2.01	0.60
1:A:93:LEU:HD22	1:A:209:LYS:HB2	1.85	0.58
1:A:219:PHE:HB2	3:A:1004:CLR:H151	1.88	0.56
1:A:521:ASP:O	1:A:525:TYR:N	2.38	0.55
1:A:518:THR:O	1:A:522:GLN:HG2	2.07	0.55
1:A:610:TYR:HB3	1:A:632:HIS:CE1	2.45	0.52
1:A:131:ALA:O	1:A:134:PRO:HD2	2.11	0.51
1:A:545:TYR:O	1:A:549:VAL:HG23	2.10	0.51
1:A:218:ILE:HG22	3:A:1004:CLR:H152	1.94	0.50
1:A:408:ARG:HD3	1:A:451:ASN:HD21	1.78	0.49
1:A:293:HIS:NE2	1:A:297:ARG:HD2	2.28	0.49
1:A:527:ASP:HB2	1:A:531:ASP:HB2	1.95	0.48
1:A:221:LEU:HG	1:A:363:MET:HE2	1.94	0.48
1:A:268:VAL:HG21	1:A:295:VAL:HG21	1.96	0.47
1:A:67:LEU:O	1:A:71:LEU:HG	2.15	0.47
1:A:215:VAL:HG13	3:A:1004:CLR:H161	1.96	0.47
1:A:307:ILE:HG12	1:A:310:ARG:HH12	1.80	0.46
1:A:220:LYS:HB2	1:A:363:MET:CE	2.44	0.46
1:A:222:THR:HG23	1:A:227:ALA:HA	1.96	0.46
1:A:220:LYS:HB3	1:A:363:MET:HE1	1.97	0.46
1:A:231:ALA:HB2	3:A:1003:CLR:H191	1.97	0.46
1:A:219:PHE:HA	3:A:1004:CLR:H72	1.97	0.46
1:A:319:ILE:O	1:A:324:LEU:HB2	2.16	0.46
1:A:333:VAL:O	1:A:336:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HG11	3:A:1006:CLR:H213	1.98	0.45
1:A:518:THR:HG22	1:A:564:VAL:HG22	1.99	0.45
1:A:524:ILE:HB	1:A:527:ASP:OD1	2.16	0.45
1:A:390:ARG:O	1:A:393:GLU:HG2	2.17	0.44
1:A:500:PRO:HD2	1:A:505:LEU:HD11	1.99	0.44
1:A:175:MET:HE1	1:A:394:LEU:HD12	1.99	0.44
1:A:238:VAL:HG11	3:A:1003:CLR:H232	1.99	0.44
1:A:527:ASP:OD2	1:A:587:HIS:NE2	2.51	0.44
1:A:483:PHE:O	1:A:486:LEU:HB2	2.18	0.44
1:A:329:GLY:HA3	2:A:1001:3IX:C19	2.48	0.43
1:A:127:LEU:O	1:A:128:ASN:C	2.60	0.43
1:A:82:GLU:OE2	1:A:157:ARG:NE	2.48	0.42
1:A:520:ARG:O	1:A:524:ILE:HG12	2.19	0.42
3:A:1006:CLR:H183	3:A:1006:CLR:H20	1.88	0.42
1:A:76:PRO:HD2	1:A:82:GLU:OE1	2.20	0.42
1:A:636:TYR:HB3	1:A:650:ILE:HD11	2.01	0.42
1:A:121:ASP:O	1:A:125:TYR:HD2	2.03	0.42
1:A:175:MET:HE2	1:A:182:ILE:HG21	2.01	0.42
1:A:444:HIS:H	1:A:460:ASN:ND2	2.18	0.41
1:A:108:THR:OG1	1:A:362:ARG:NH2	2.53	0.41
1:A:120:LYS:NZ	1:A:121:ASP:OD1	2.50	0.41
1:A:519:LEU:O	1:A:522:GLN:HB2	2.20	0.41
1:A:483:PHE:O	1:A:486:LEU:N	2.53	0.41
1:A:248:ARG:HG3	1:A:251:ILE:HD13	2.03	0.41
1:A:581:MET:HG3	1:A:609:ILE:HD13	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	569/914 (62%)	542 (95%)	27 (5%)	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	508/801 (63%)	499 (98%)	9 (2%)	51 70

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	A	91	VAL
1	A	324	LEU
1	A	332	VAL
1	A	374	ILE
1	A	375	VAL
1	A	405	LYS
1	A	519	LEU
1	A	525	TYR

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

Mol	Chain	Res	Type
1	A	106	ASN
1	A	177	ASN
1	A	184	ASN
1	A	342	HIS
1	A	359	GLN
1	A	451	ASN
1	A	460	ASN
1	A	632	HIS

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](#)

6 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
2	3IX	A	1001	-	66,71,71	0.76	2 (3%)	87,97,97	1.04	7 (8%)
3	CLR	A	1002	-	31,31,31	0.74	0	48,48,48	1.25	3 (6%)
3	CLR	A	1005	-	31,31,31	0.77	1 (3%)	48,48,48	1.05	2 (4%)
3	CLR	A	1006	-	31,31,31	0.66	1 (3%)	48,48,48	1.38	8 (16%)
3	CLR	A	1003	-	31,31,31	0.80	1 (3%)	48,48,48	1.09	4 (8%)
3	CLR	A	1004	-	31,31,31	0.72	0	48,48,48	1.06	3 (6%)

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
2	3IX	A	1001	-	-	22/70/86/86	0/3/3/3
3	CLR	A	1002	-	-	3/10/68/68	0/4/4/4
3	CLR	A	1005	-	-	0/10/68/68	0/4/4/4
3	CLR	A	1006	-	-	7/10/68/68	0/4/4/4
3	CLR	A	1003	-	-	1/10/68/68	0/4/4/4
3	CLR	A	1004	-	-	5/10/68/68	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	3IX	C04-C03	-3.51	1.31	1.51
3	A	1005	CLR	C18-C13	2.19	1.58	1.54
3	A	1006	CLR	C18-C13	2.16	1.58	1.54
2	A	1001	3IX	P65-O64	2.14	1.63	1.59
3	A	1003	CLR	C18-C13	2.09	1.58	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	CLR	C21-C20-C17	3.97	119.01	112.92
2	A	1001	3IX	C03-C04-C05	3.47	128.90	113.79
3	A	1002	CLR	C13-C17-C20	3.33	124.71	119.49
3	A	1006	CLR	C16-C17-C20	3.24	117.16	112.15
2	A	1001	3IX	C36-C34-C33	2.98	113.98	108.82
3	A	1004	CLR	C16-C17-C20	2.81	116.49	112.15
3	A	1002	CLR	C1-C2-C3	2.76	114.01	110.47
3	A	1006	CLR	C9-C10-C5	-2.73	105.37	109.65
2	A	1001	3IX	O64-C49-C50	-2.71	101.87	111.68
3	A	1006	CLR	C14-C8-C9	2.68	112.68	109.09
3	A	1003	CLR	C11-C9-C8	2.62	115.52	111.75
3	A	1005	CLR	C12-C11-C9	2.61	117.64	113.11
3	A	1006	CLR	C11-C9-C8	2.40	115.22	111.75
3	A	1006	CLR	C22-C20-C17	2.37	115.19	110.28
3	A	1006	CLR	C19-C10-C9	2.37	114.51	111.68
2	A	1001	3IX	C19-C18-C17	-2.33	109.07	113.23
3	A	1006	CLR	C13-C17-C20	-2.32	115.85	119.49
3	A	1006	CLR	C7-C8-C9	-2.23	107.01	109.71
3	A	1004	CLR	C11-C9-C10	2.23	116.01	113.08
2	A	1001	3IX	C35-C34-C37	2.12	111.68	108.23
2	A	1001	3IX	C24-N25-C26	2.11	126.75	122.84
3	A	1003	CLR	C16-C17-C20	2.11	115.41	112.15
3	A	1003	CLR	C14-C8-C9	2.09	111.89	109.09
3	A	1003	CLR	C12-C11-C9	2.08	116.71	113.11
2	A	1001	3IX	C28-C26-N25	-2.05	112.97	116.42
3	A	1005	CLR	C11-C12-C13	2.03	116.27	112.78
3	A	1004	CLR	C22-C20-C17	2.02	114.47	110.28

There are no chirality outliers.

All (38) torsion outliers are listed below:

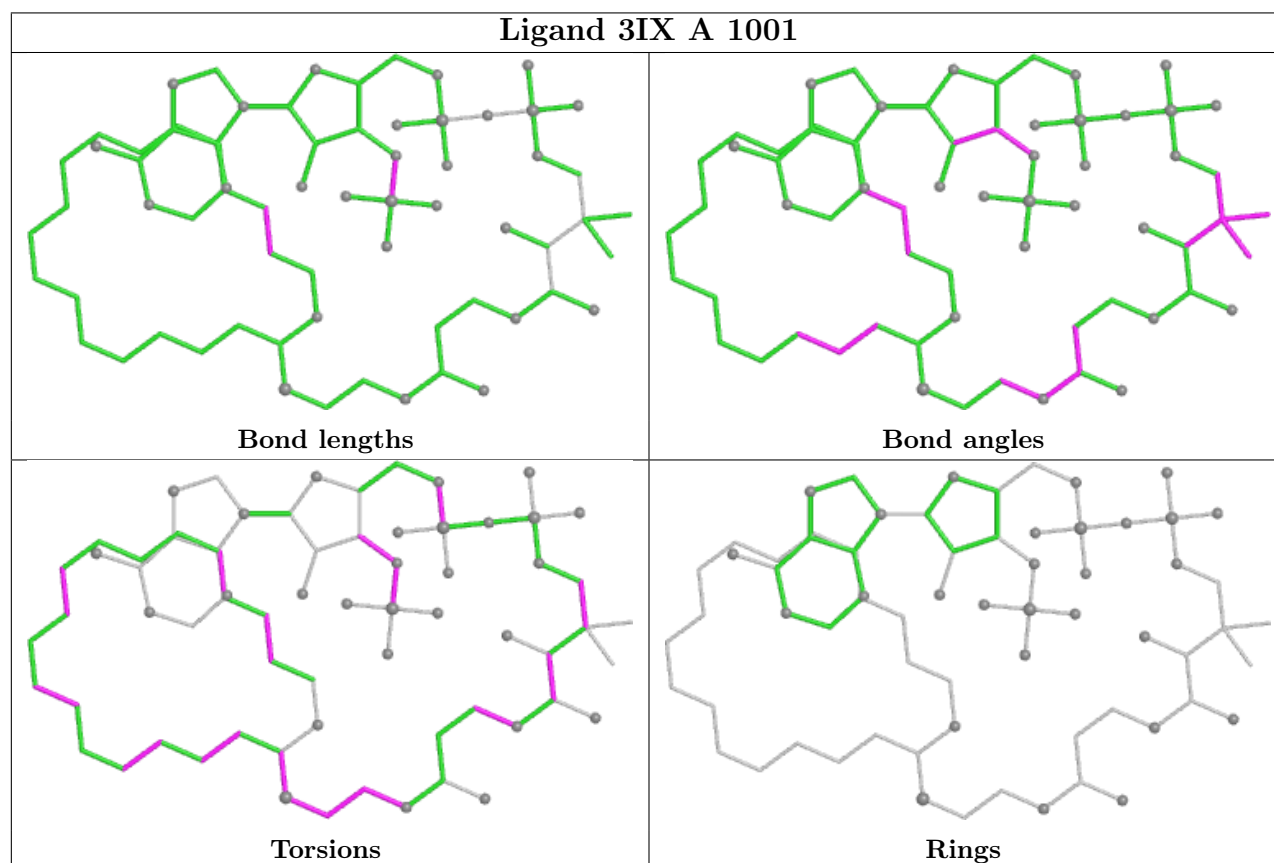
Mol	Chain	Res	Type	Atoms
2	A	1001	3IX	C09-C10-C11-C12
2	A	1001	3IX	C17-C18-C19-C20
2	A	1001	3IX	C19-C20-S22-C23
2	A	1001	3IX	O21-C20-S22-C23
2	A	1001	3IX	C23-C24-N25-C26
2	A	1001	3IX	N30-C31-C33-C34
2	A	1001	3IX	O32-C31-C33-C34
2	A	1001	3IX	C49-O64-P65-O66
3	A	1004	CLR	C16-C17-C20-C21
3	A	1004	CLR	C13-C17-C20-C21
3	A	1006	CLR	C13-C17-C20-C21
3	A	1006	CLR	C16-C17-C20-C21
3	A	1006	CLR	C16-C17-C20-C22
3	A	1004	CLR	C13-C17-C20-C22
3	A	1006	CLR	C13-C17-C20-C22
2	A	1001	3IX	C02-C03-C04-C05
3	A	1004	CLR	C16-C17-C20-C22
2	A	1001	3IX	C28-C29-N30-C31
3	A	1006	CLR	C21-C20-C22-C23
3	A	1006	CLR	C17-C20-C22-C23
3	A	1002	CLR	C13-C17-C20-C22
3	A	1002	CLR	C16-C17-C20-C22
2	A	1001	3IX	C48-C49-O64-P65
2	A	1001	3IX	C50-C49-O64-P65
3	A	1006	CLR	C22-C23-C24-C25
3	A	1002	CLR	C16-C17-C20-C21
2	A	1001	3IX	S22-C23-C24-N25
2	A	1001	3IX	N30-C31-C33-O69
2	A	1001	3IX	C47-O46-P43-O42
3	A	1004	CLR	C17-C20-C22-C23
3	A	1003	CLR	C22-C23-C24-C25
2	A	1001	3IX	C04-C05-C06-C07
2	A	1001	3IX	C15-C16-C17-C18
2	A	1001	3IX	C12-C13-C14-C15
2	A	1001	3IX	C24-C23-S22-C20
2	A	1001	3IX	C49-O64-P65-O67
2	A	1001	3IX	C47-O46-P43-O44
2	A	1001	3IX	C35-C34-C37-O38

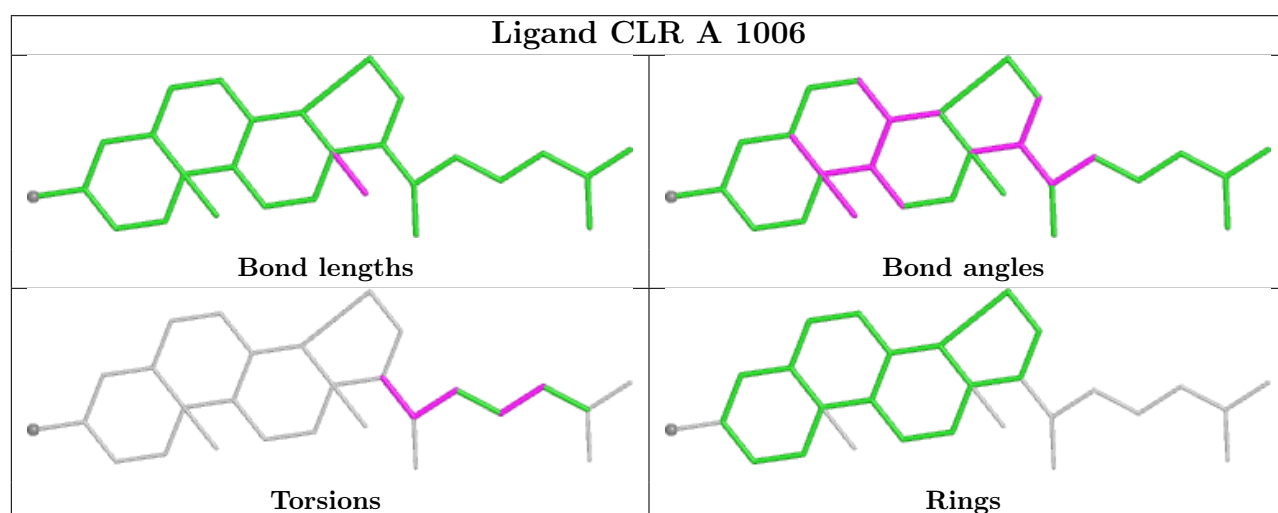
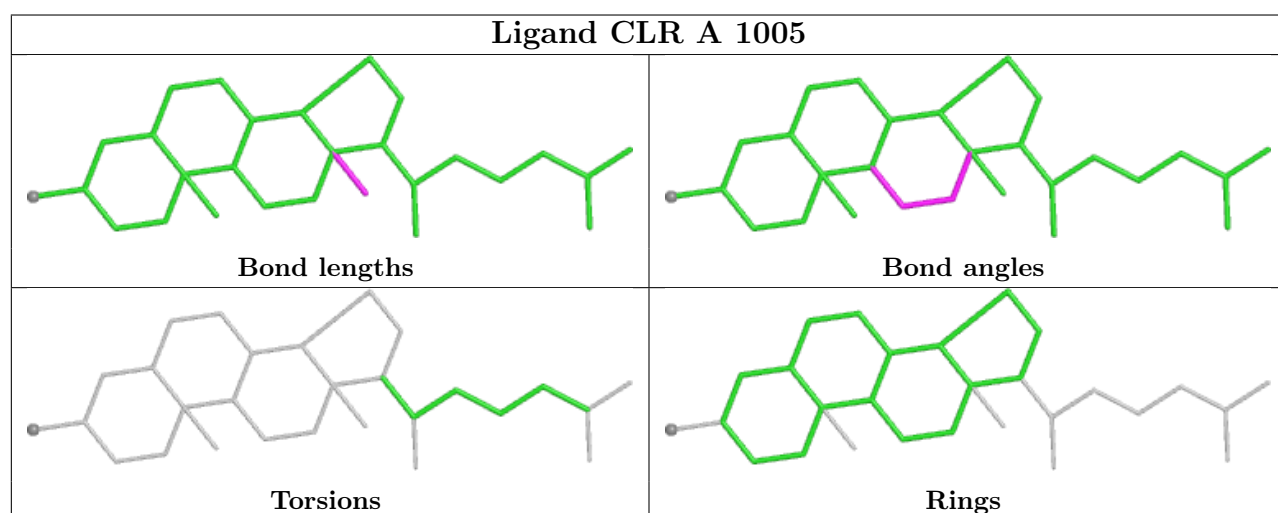
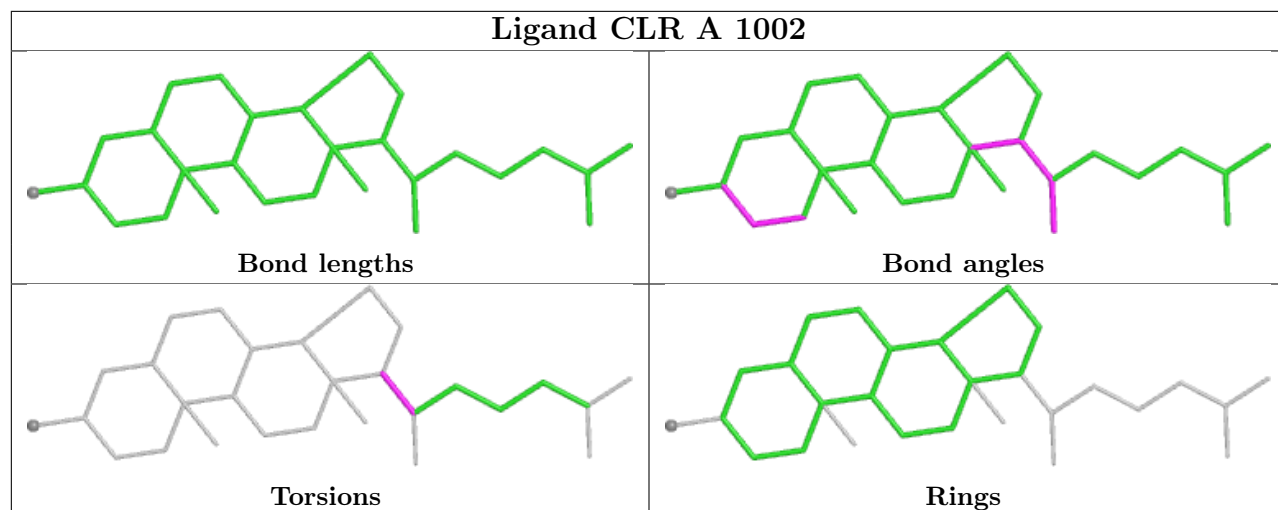
There are no ring outliers.

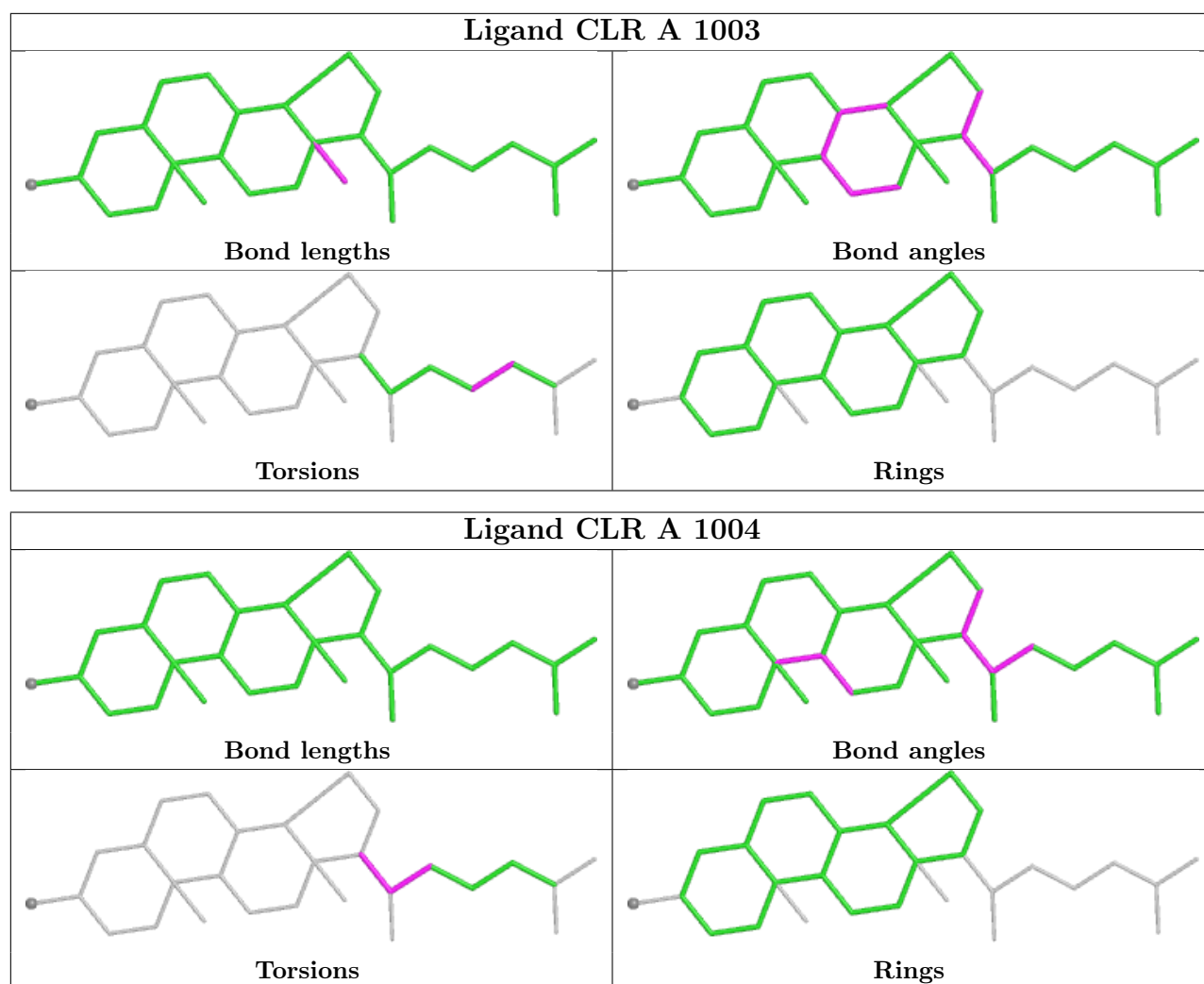
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	3IX	1	0
3	A	1006	CLR	2	0
3	A	1003	CLR	2	0
3	A	1004	CLR	4	0

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.

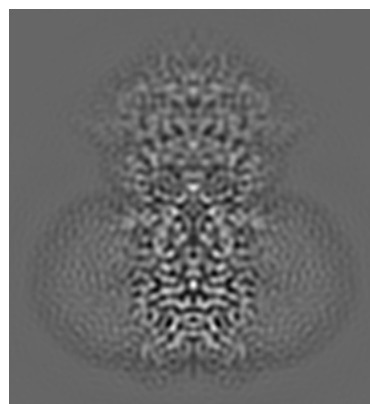
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65675. These allow visual inspection of the internal detail of the map and identification of artifacts.

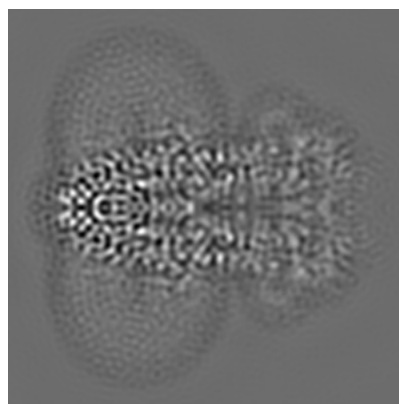
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

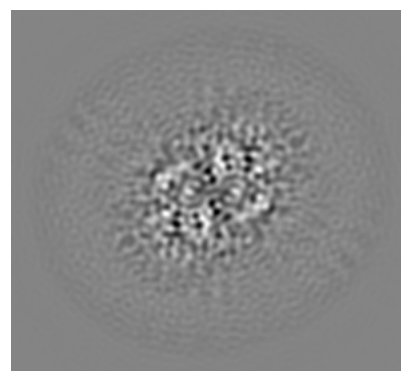
6.1.1 Primary map



X

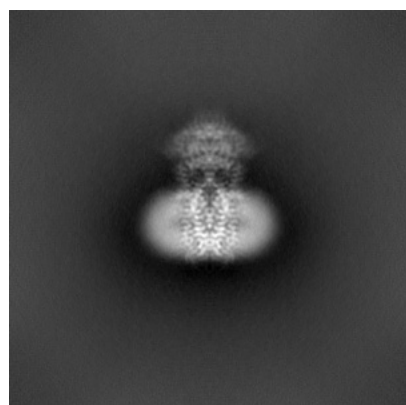


Y

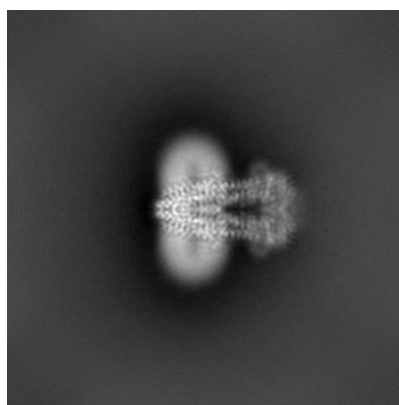


Z

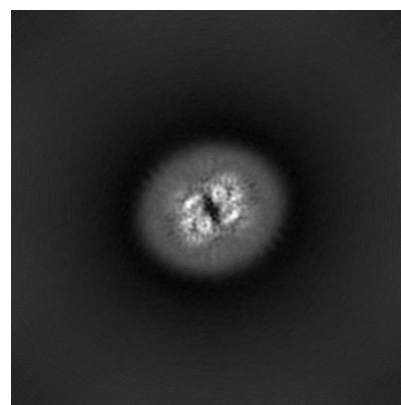
6.1.2 Raw map



X



Y

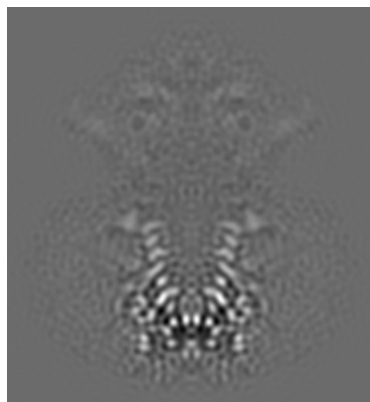


Z

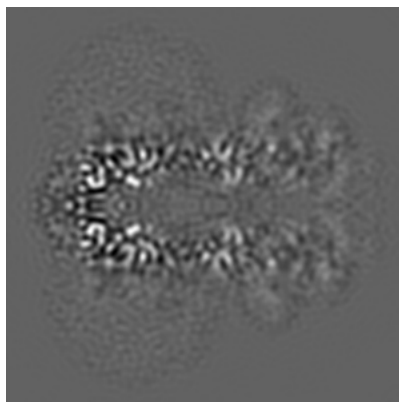
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

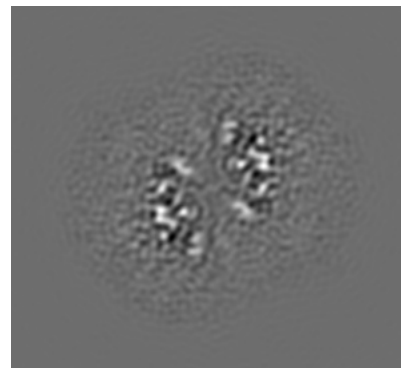
6.2.1 Primary map



X Index: 71

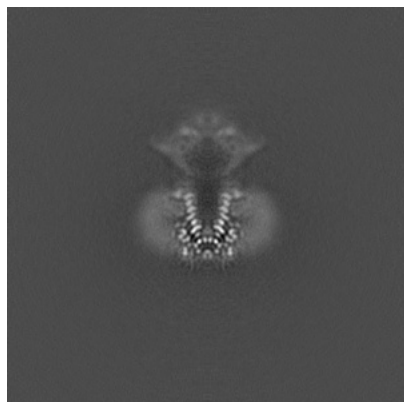


Y Index: 65

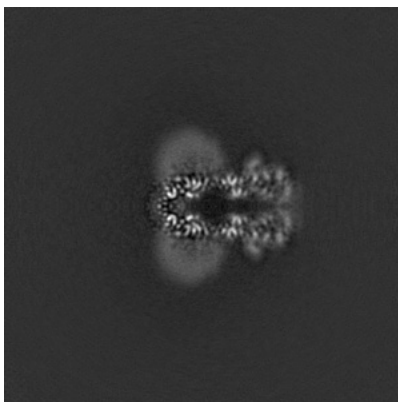


Z Index: 71

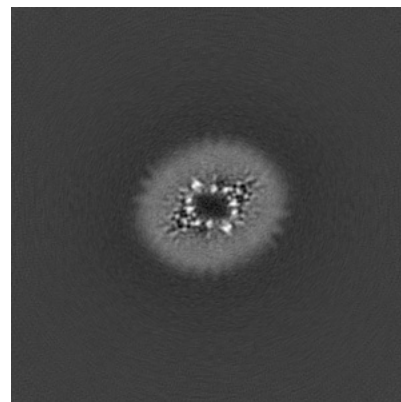
6.2.2 Raw map



X Index: 150



Y Index: 150

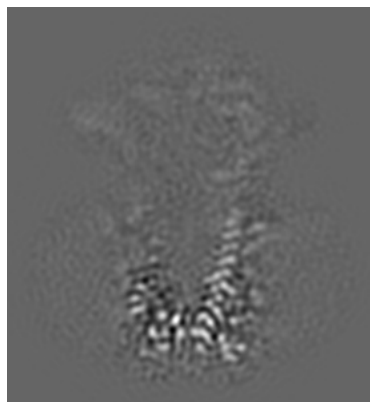


Z Index: 150

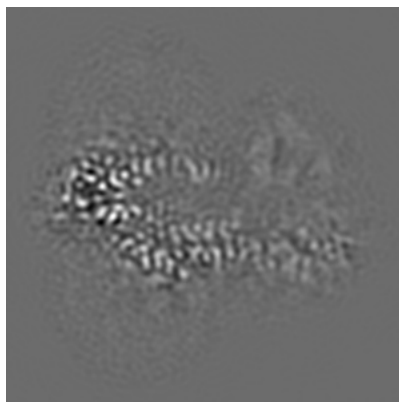
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

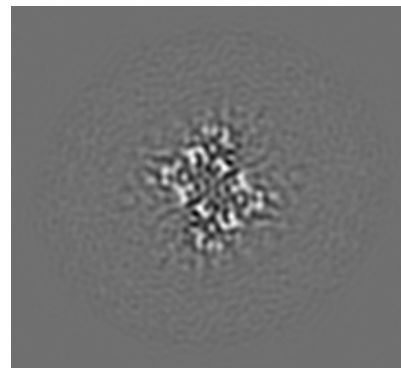
6.3.1 Primary map



X Index: 73

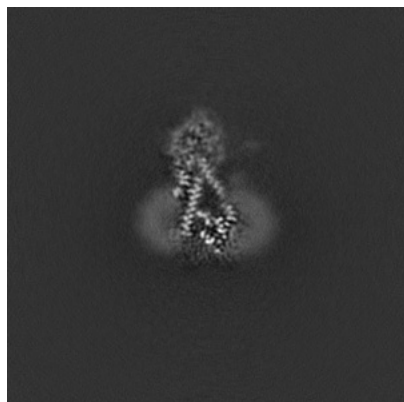


Y Index: 56

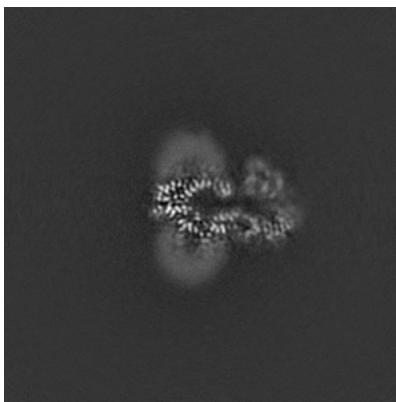


Z Index: 33

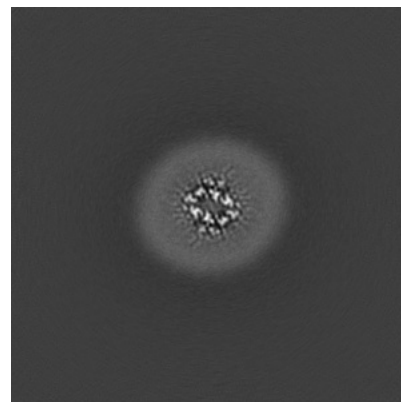
6.3.2 Raw map



X Index: 141



Y Index: 143

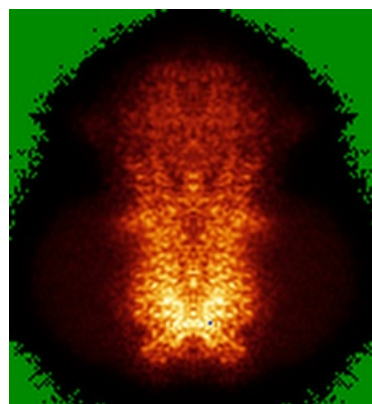


Z Index: 131

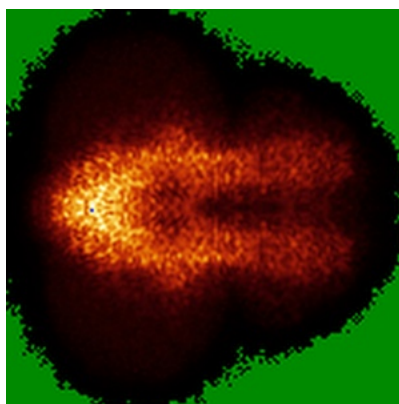
The images above show the largest variance slices of the map in three orthogonal directions.

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

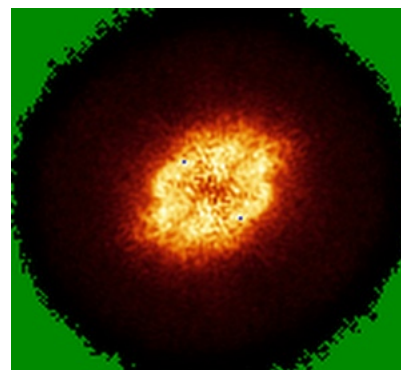
6.4.1 Primary map



X

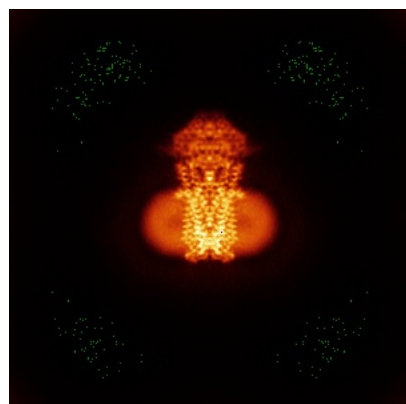


Y

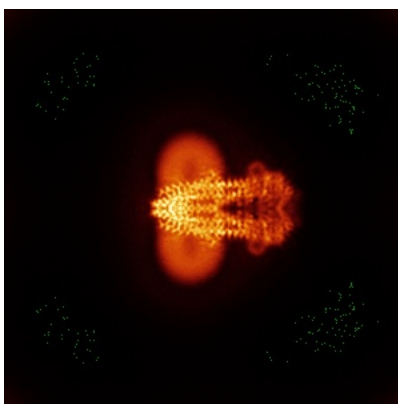


Z

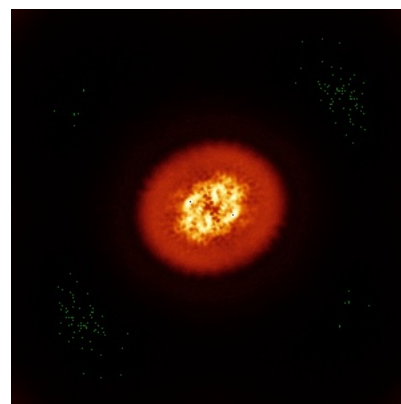
6.4.2 Raw map



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](#)

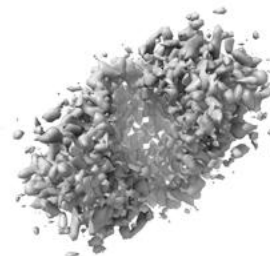
6.5.1 Primary map



X



Y



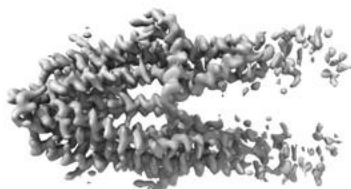
Z

The images above show the 3D surface view of the map at the recommended contour level 2.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

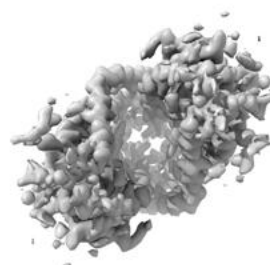
6.5.2 Raw map



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.

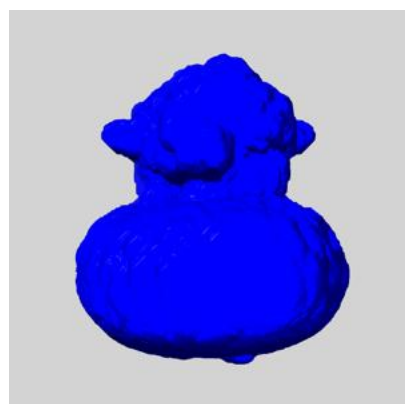
6.6 Mask visualisation [i](#)

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

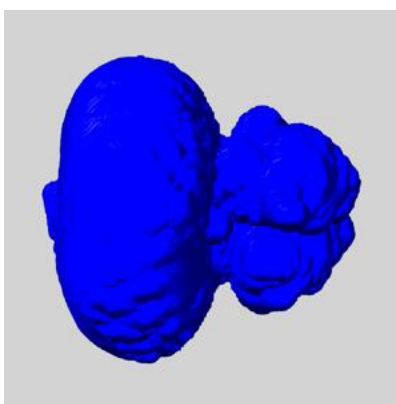
A mask typically either:

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

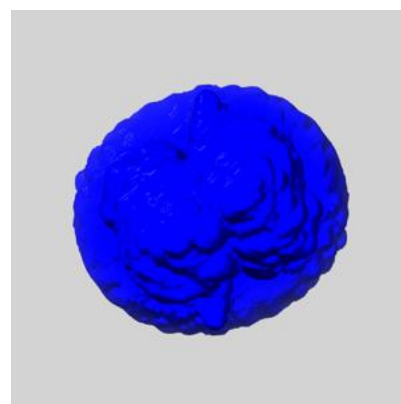
6.6.1 emd_65675_msk_1.map [i](#)



X



Y

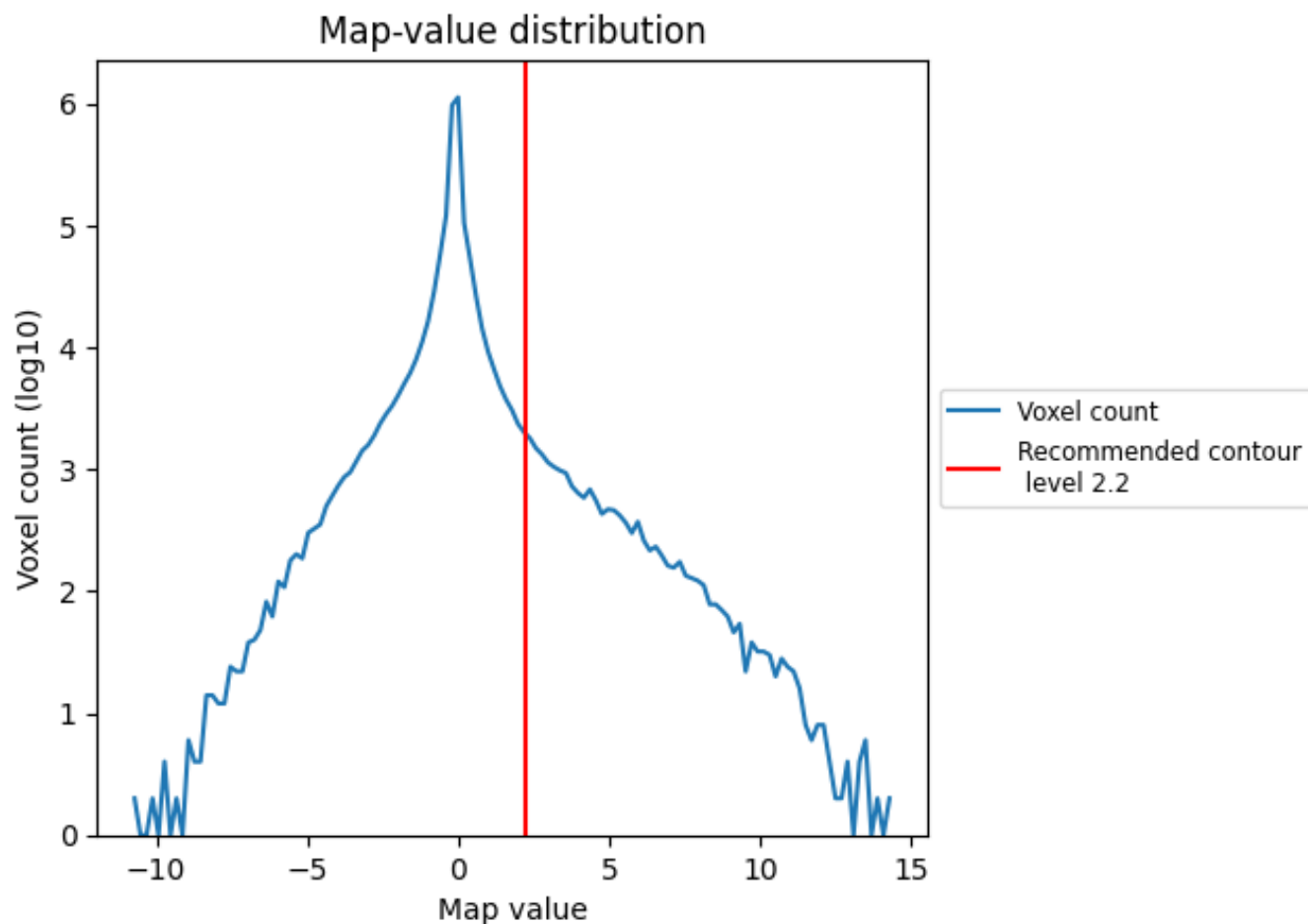


Z

7 Map analysis [i](#)

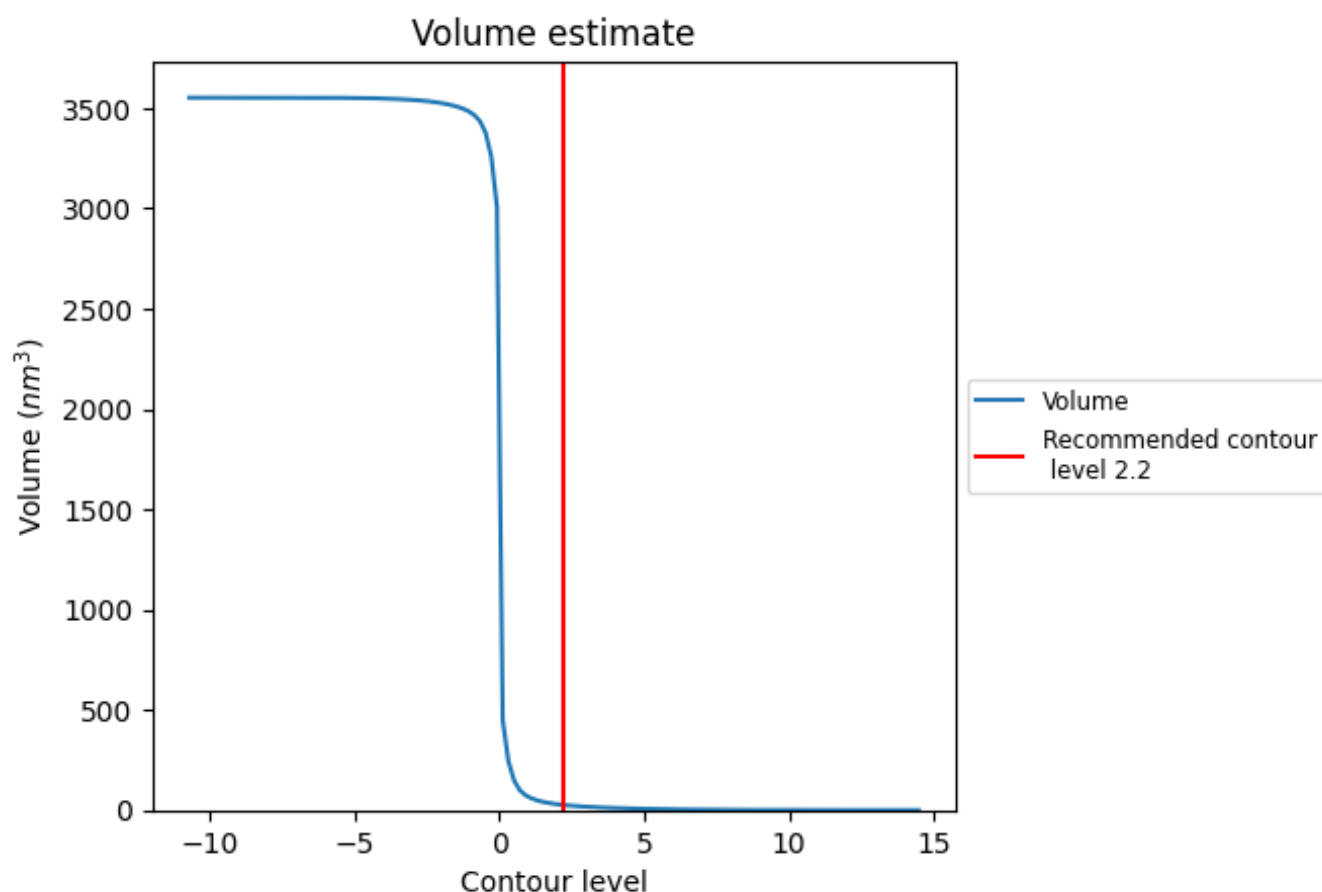
This section contains the results of statistical analysis of the map.

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 26 nm³; this corresponds to an approximate mass of 23 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.

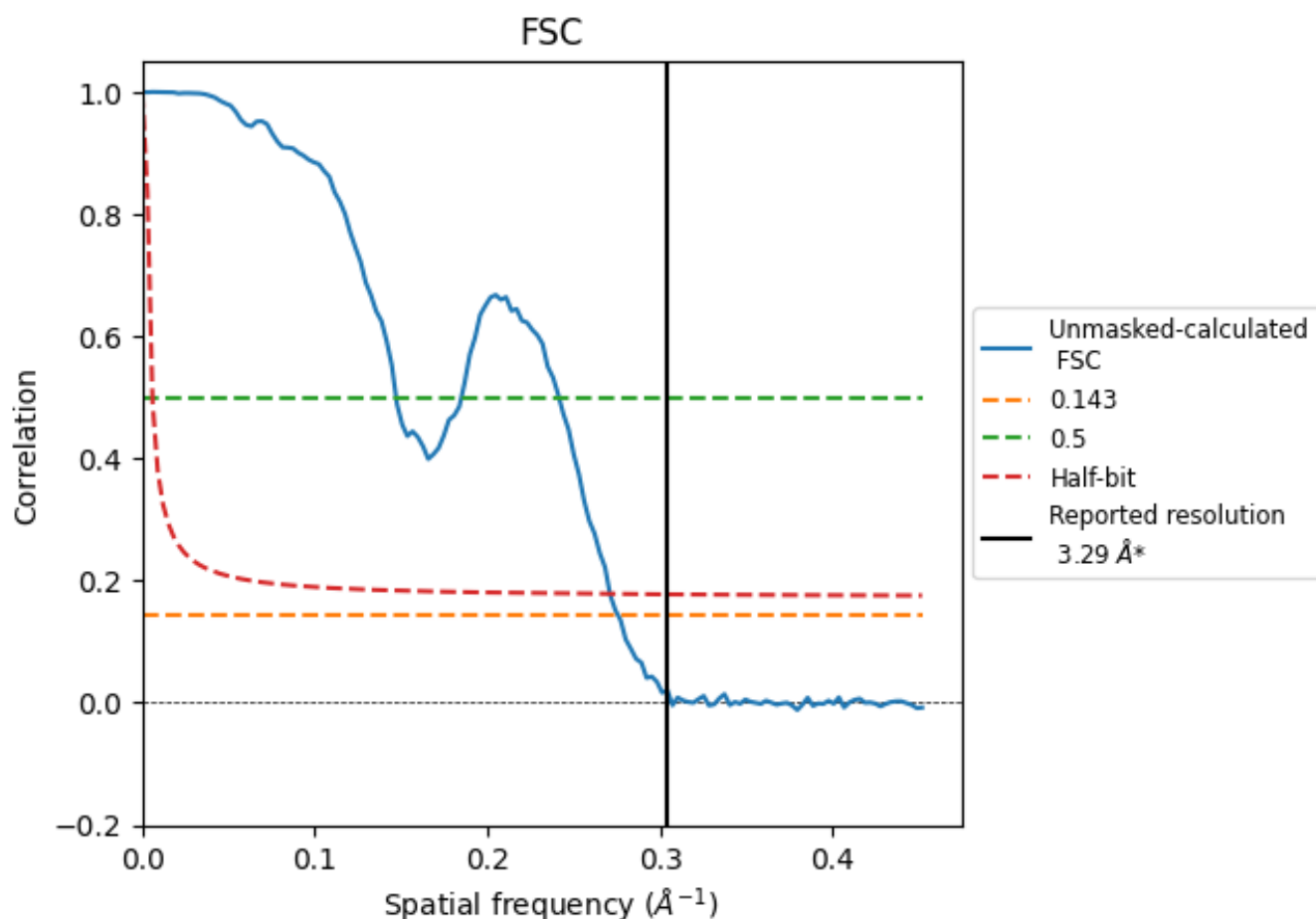
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.304 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.63	6.80	3.69

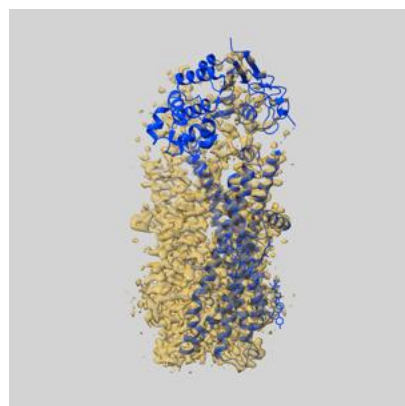
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.63 differs from the reported value 3.29 by more than 10 %

9 Map-model fit [i](#)

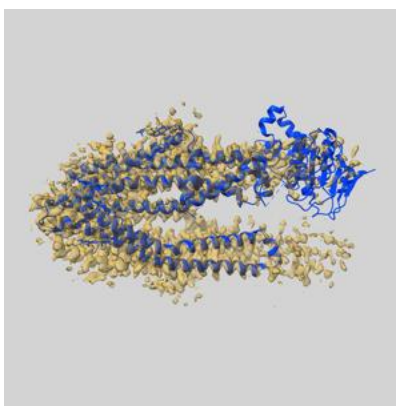
This section contains information regarding the fit between EMDB map EMD-65675 and PDB model 9W63. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

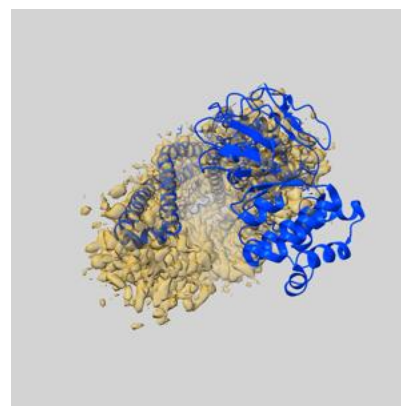
9.1.1 Map-model overlay [i](#)



X

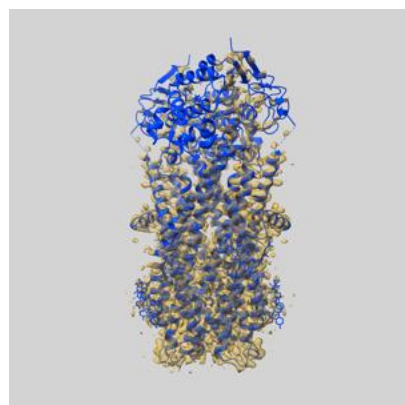


Y

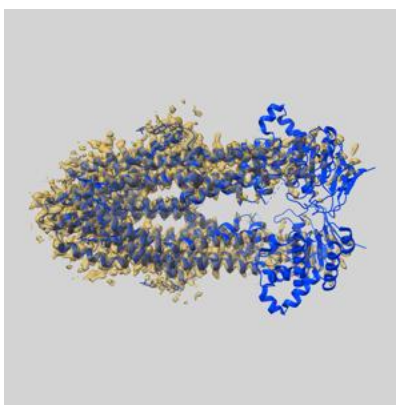


Z

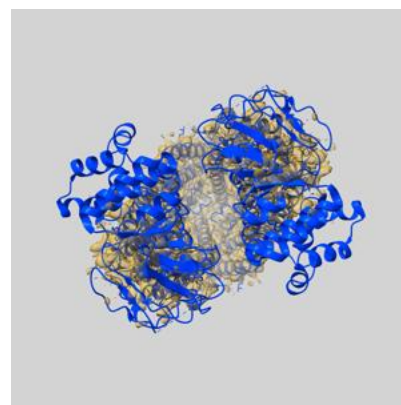
9.1.2 Map-model assembly overlay [i](#)



X



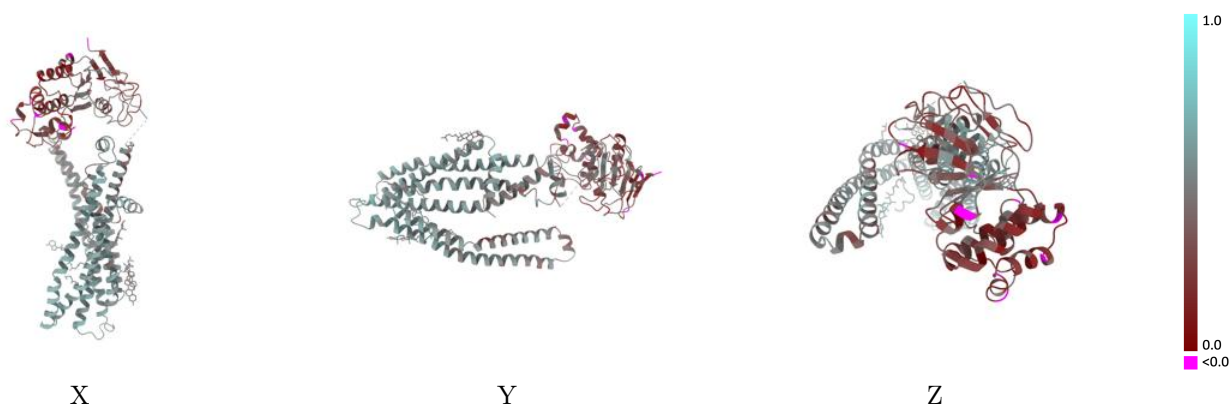
Y



Z

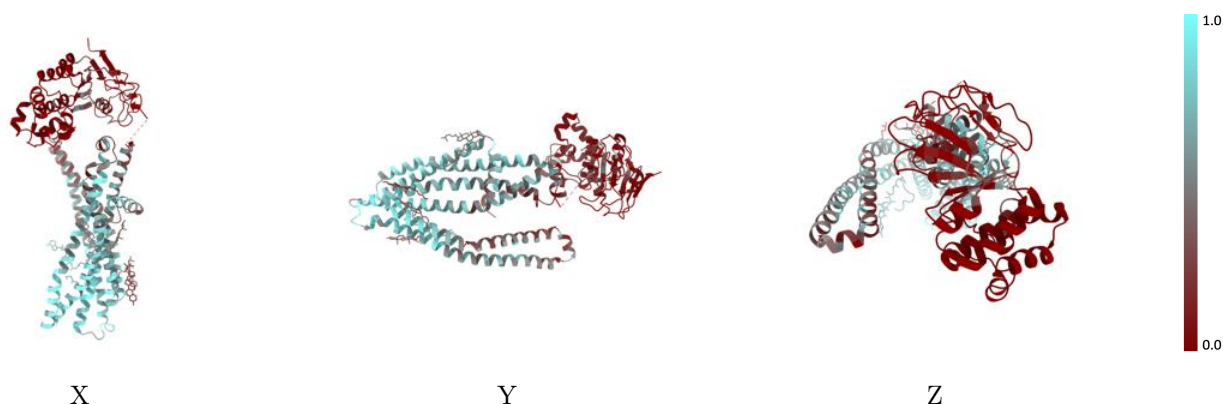
The images above show the 3D surface view of the map at the recommended contour level 2.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



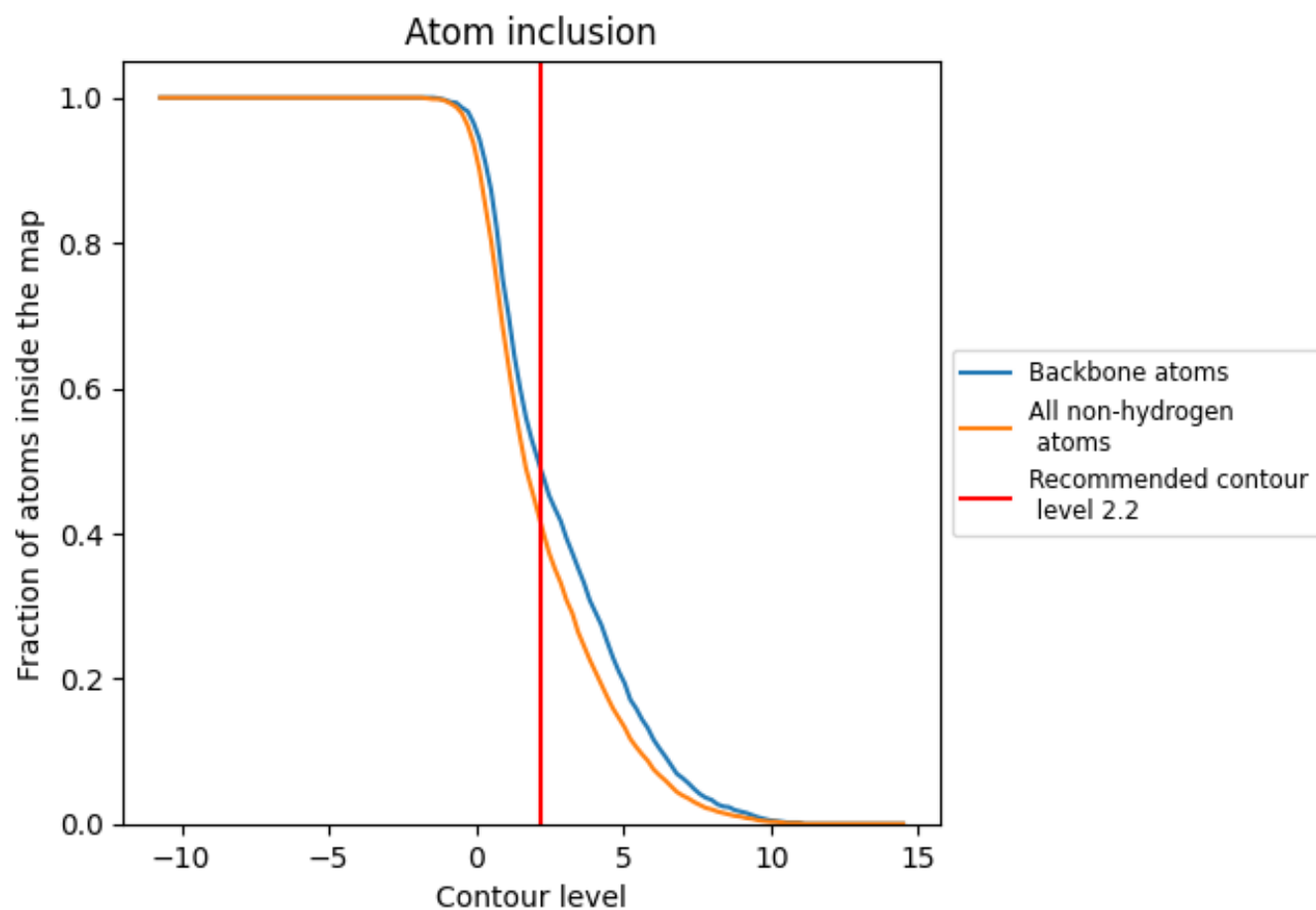
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 41% 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 (2.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4130	<div></div> 0.4400
A	<div></div> 0.4130	<div></div> 0.4400

