



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 08:00 AM UTC

PDB ID : 7TDG / pdb_00007tdg
EMDB ID : EMD-25828
Title : Rabbit RyR1 with AMP-PCP and high Ca²⁺ embedded in nanodisc in inactivated conformation (Dataset-A)
Authors : Nayak, A.R.; Samso, M.
Deposited on : 2021-12-31
Resolution : 3.80 Å(reported)

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

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A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

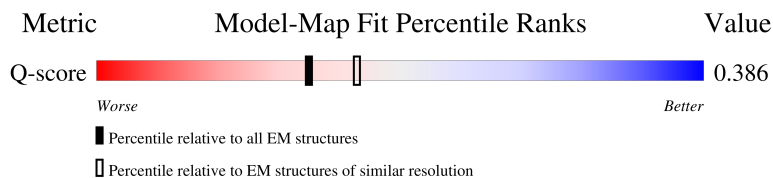
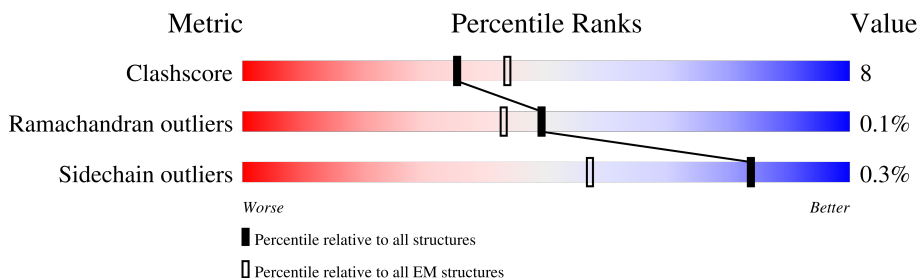
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	5037	
1	B	5037	
1	C	5037	
1	D	5037	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 117345 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 Ryanodine receptor 1, RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4134	Total	C	N	O	S	0	0
			29247	18513	5182	5395	157		
1	C	4134	Total	C	N	O	S	0	0
			29244	18513	5179	5395	157		
1	D	4134	Total	C	N	O	S	0	0
			29228	18502	5176	5393	157		
1	B	4134	Total	C	N	O	S	0	0
			29246	18514	5182	5393	157		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

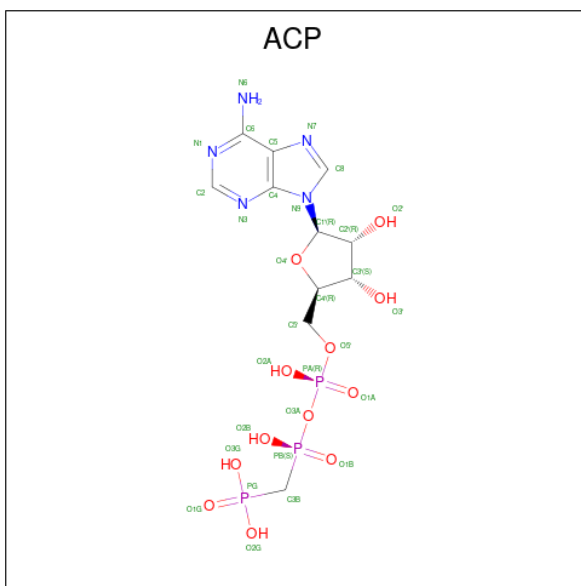
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	
3	C	2	Total	Ca	0
			2	2	
3	D	2	Total	Ca	0
			2	2	
3	B	2	Total	Ca	0
			2	2	

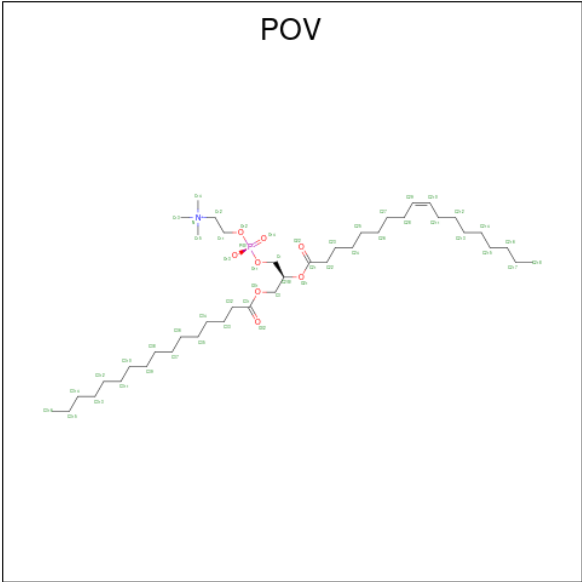
- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID:

ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



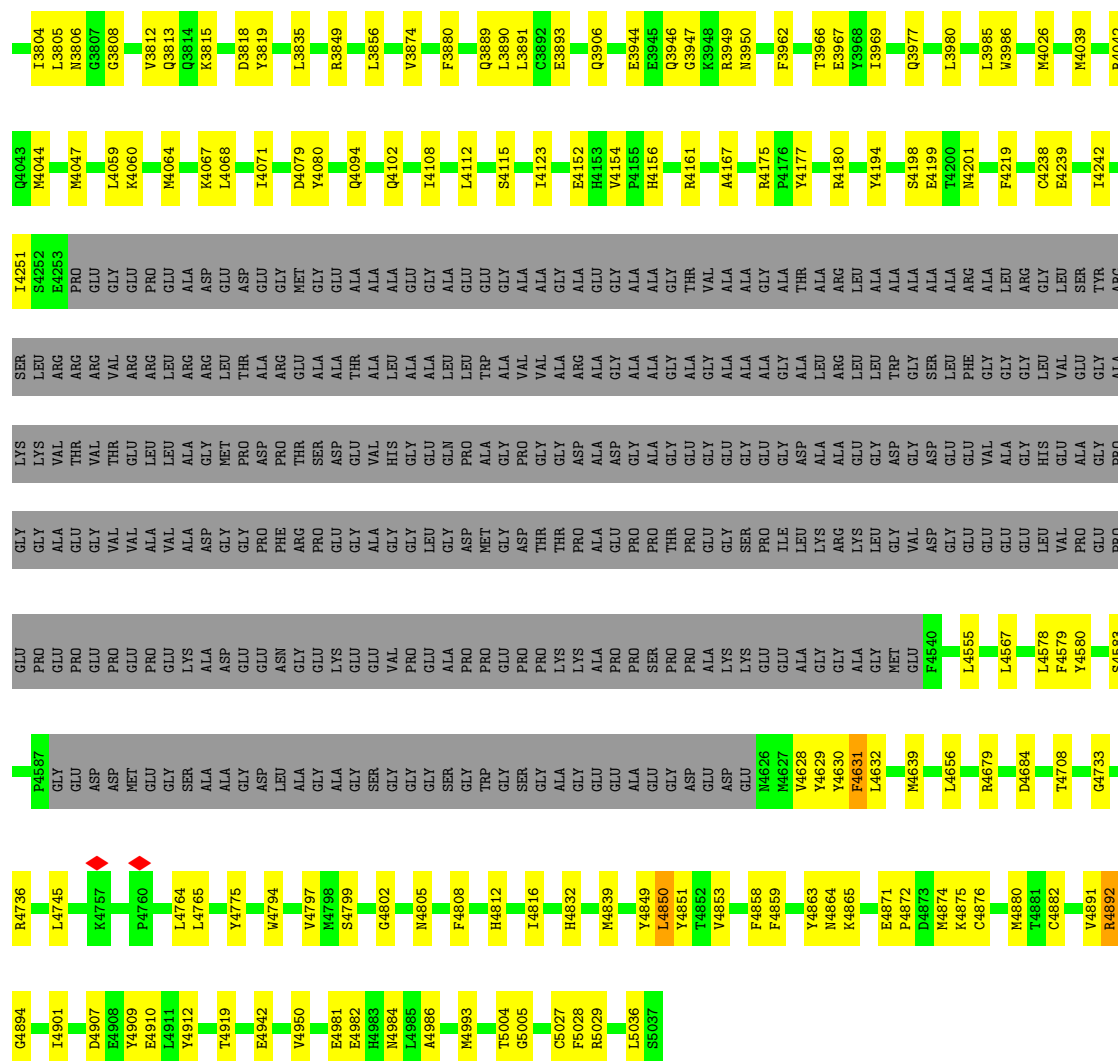
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 11	N 5	O 12	P 3	0
4	C	1	Total 31	C 11	N 5	O 12	P 3	0
4	D	1	Total 31	C 11	N 5	O 12	P 3	0
4	B	1	Total 31	C 11	N 5	O 12	P 3	0

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).

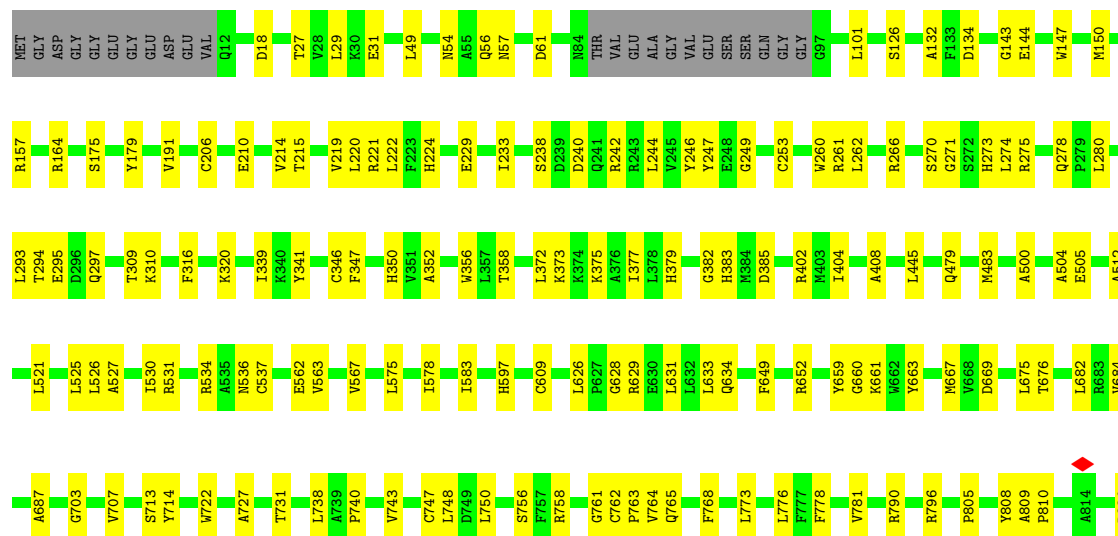


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C				0
			16	16				
5	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
5	C	1	Total	C				0
			16	16				
5	C	1	Total	C	N	O	P	0
			45	35	1	8	1	
5	C	1	Total	C				0
			16	16				
5	D	1	Total	C	N	O	P	0
			45	35	1	8	1	
5	B	1	Total	C				0
			16	16				
5	B	1	Total	C	N	O	P	0
			45	35	1	8	1	





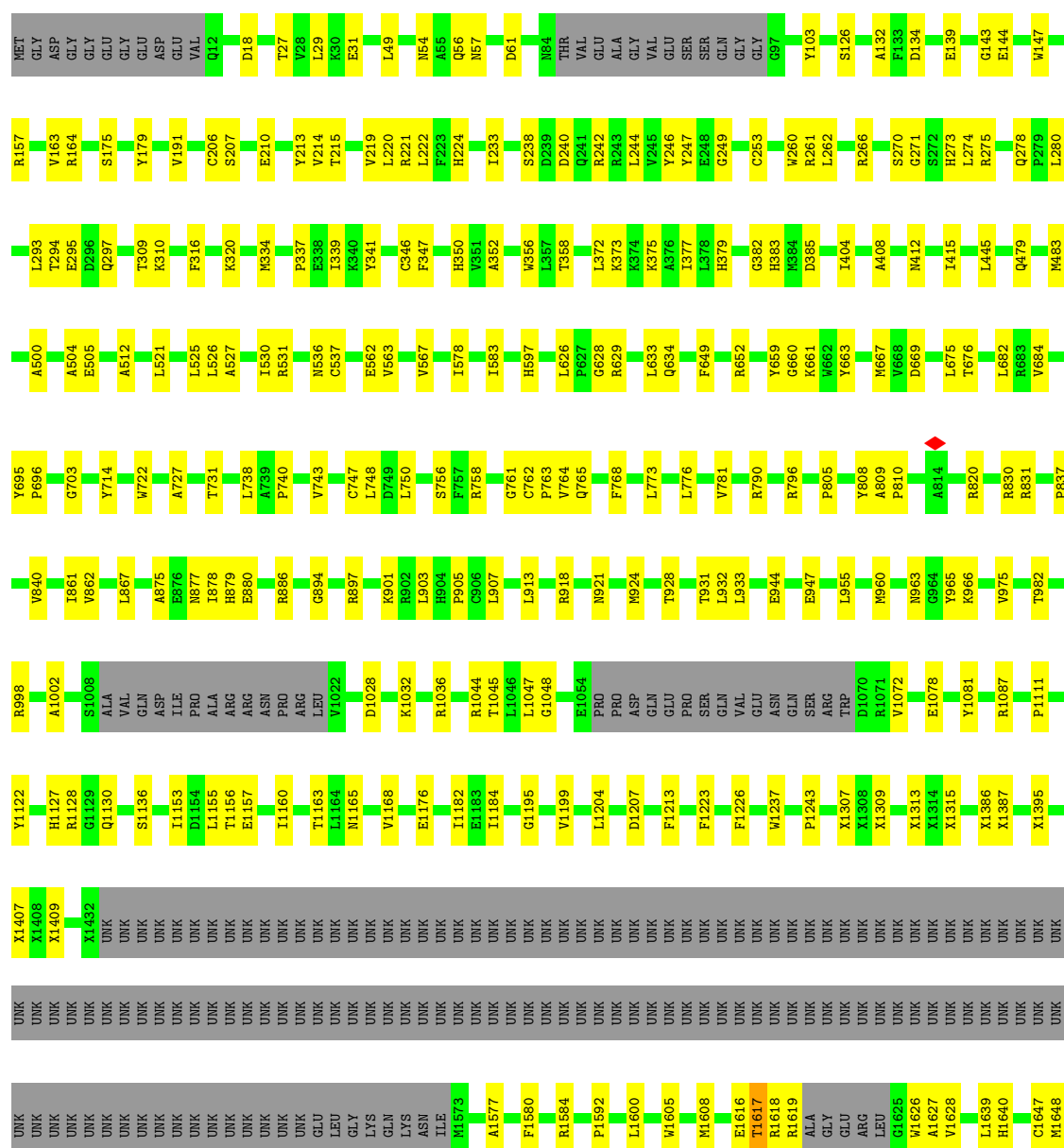
● Molecule 1: Ryanodine receptor 1, RyR1













M4874	V4628	ALA	LEU	ASP	ALA	THR	R4175
K4875	Y4629	GLY	LYS	ALA	ALA	ALA	F4176
C4876	Y4630	GLY	ARG	ALA	ARG	ARG	Y4177
	F4631	ALA	LYS	GLY	LEU	LEU	
M4880	L4632	GLY	LEU	GLY	LEU	ALA	R4180
T4881	L4639	MET	GLY	ASP	TRP	ALA	Y4194
C4882	M4639	GLY	VAL	ASP	GLY	ALA	
			ASP	ASP	GLY	ALA	
V4891	L4656		GLY	GLY	LEU	ALA	S4198
R4892			GLY	GLY	LEU	ALA	E4199
A4893	R4679		GLY	VAL	PHE	ARG	T4200
C4894			GLY	GLY	GLY	ALA	N4201
	D4684		GLY	GLY	GLY	ARG	
D4907			LEU	HIS	LEU	GLY	C4238
E4908	T4708		VAL	GLY	VAL	LEU	E4239
Y4909			PRO	ALA	GLY	SER	
E4910	G4733		GLY	GLY	GLY	TYR	I4242
L4911			PRO	PRO	ALA	ARG	
Y4912	R4736		GLY	GLY	LYS	SER	I4251
R4913			PRO	GLY	LYS	LEU	S4282
	E4739		GLY	VAL	VAL	ARG	E4283
F4916			PRO	GLY	THR	ARG	PRO
E4942	L4745		GLY	ASP	VAL	GLY	GLY
			MET	ASP	GLY	GLY	GLY
D4953	K4757		GLY	GLY	LEU	PRO	
			GLY	GLY	LEU	ARG	
T4956	P4760		SER	ALA	ALA	GLY	GLY
			ALA	ALA	ASP	ASP	GLY
H4978	L4764		ALA	ASP	GLY	LEU	GLY
	L4765		GLY	GLY	PRO	THR	ASP
E4981			ASP	GLY	ASP	ALA	GLY
E4982	Y4775		LEU	ASN	PHE	GLY	GLY
H4983			ALA	GLY	ARG	THR	MET
N4984	G4793		GLY	GLY	PRO	ALA	GLY
L4985			ALA	LYS	SER	ALA	GLY
A4986	V4797		GLY	GLY	ASP	THR	GLY
			SER	GLY	VAL	ALA	ALA
M4993	F4808		GLY	VAL	HIS	LEU	ALA
Y4994	I4816		GLY	PRO	GLY	GLY	GLY
L4995			SER	ALA	GLY	LEU	ALA
	H4832		GLY	ALA	PRO	LEU	ALA
D4999			TRP	PRO	ALA	TRP	GLY
	M4839		GLY	GLY	GLY	ALA	GLY
E5002			SER	PRO	ASP	VAL	ALA
H5003	Y4849		GLY	PRO	THR	VAL	ALA
T5004	L4850		ALA	LYS	GLY	VAL	ALA
G5005	Y4851		GLY	LYS	THR	ARG	ALA
	T4852		GLY	ALA	ASP	ALA	ALA
Y5009	V4853		GLY	PRO	GLY	GLY	GLY
			ALA	PRO	ASP	ALA	GLY
M5013			ALA	PRO	PRO	GLY	GLY
	F4858		ALA	SER	PRO	ALA	ALA
	F4859		GLY	GLY	THR	GLY	ALA
C5027			ASP	GLY	PRO	GLY	GLY
F5028	N4864		GLY	ALA	PRO	THR	ALA
R5029	K4865		ASP	ALA	GLY	GLY	VAL
			ASP	GLY	GLY	ALA	ALA
L5036	E4871		GLY	GLY	PRO	GLY	ALA
S5037	P4872		M4526	LYS	GLY	ALA	ALA
			M4527	GLY	PRO	GLY	ALA
	D4873			ILE	GLY	GLY	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	90530	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.283	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	477.36002, 477.36002, 477.36002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.105, 1.105, 1.105	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: CA, ACP, ZN, POV

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	0.16	0/25300	0.39	0/34345
1	B	0.16	0/25299	0.39	1/34344 (0.0%)
1	C	0.17	0/25297	0.40	1/34342 (0.0%)
1	D	0.17	0/25281	0.41	5/34322 (0.0%)
All	All	0.16	0/101177	0.40	7/137353 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1618	ARG	O-C-N	-19.86	100.89	123.33
1	D	4895	GLY	CA-C-N	-7.34	111.09	122.69
1	D	4895	GLY	C-N-CA	-7.34	111.09	122.69
1	C	1618	ARG	O-C-N	-6.81	113.53	122.59
1	D	821	LEU	CA-C-N	6.55	130.44	120.82

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1617	THR	Mainchain
1	C	1618	ARG	Mainchain
1	D	1618	ARG	Mainchain

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	29247	0	24751	425	0
1	B	29246	0	24757	448	0
1	C	29244	0	24747	412	0
1	D	29228	0	24714	434	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	31	0	14	1	0
4	B	31	0	14	1	0
4	C	31	0	14	2	0
4	D	31	0	14	1	0
5	A	61	0	85	18	0
5	B	61	0	85	19	0
5	C	77	0	105	17	0
5	D	45	0	65	16	0
All	All	117345	0	99365	1711	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 8.

The worst 5 of 1711 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:4858:PHE:CE2	5:A:5106:POV:H33A	1.60	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4858:PHE:CE2	5:B:5106:POV:H33A	1.60	1.36
1:D:4858:PHE:CE2	5:D:5105:POV:H33A	1.59	1.36
1:D:1618:ARG:O	1:D:1626:TRP:HA	1.12	1.29
1:D:1618:ARG:O	1:D:1626:TRP:CA	1.91	1.17

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	3203/5037 (64%)	2993 (93%)	207 (6%)	3 (0%)	48	79
1	B	3203/5037 (64%)	2988 (93%)	215 (7%)	0	100	100
1	C	3203/5037 (64%)	2989 (93%)	212 (7%)	2 (0%)	48	79
1	D	3203/5037 (64%)	2994 (94%)	207 (6%)	2 (0%)	48	79
All	All	12812/20148 (64%)	11964 (93%)	841 (7%)	7 (0%)	49	79

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1797	ARG
1	A	2868	SER
1	C	1796	ALA
1	D	2868	SER
1	C	1797	ARG

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	A	2512/3264 (77%)	2505 (100%)	7 (0%)	86	84
1	B	2512/3264 (77%)	2505 (100%)	7 (0%)	86	84
1	C	2512/3264 (77%)	2504 (100%)	8 (0%)	86	84
1	D	2508/3264 (77%)	2502 (100%)	6 (0%)	87	87
All	All	10044/13056 (77%)	10016 (100%)	28 (0%)	84	84

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4861	LYS
1	B	4891	VAL
1	D	4632	LEU
1	B	4631	PHE
1	D	4631	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4558	ASN
1	B	3813	GLN
1	D	921	ASN
1	B	3806	ASN
1	B	4714	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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
4	ACP	D	5104	-	31,33,33	1.60	10 (32%)	47,52,52	1.96	14 (29%)
5	POV	B	5106	-	44,44,51	0.94	0	50,52,59	0.77	2 (4%)
5	POV	C	5107	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
5	POV	C	5105	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
5	POV	A	5105	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
4	ACP	C	5104	-	31,33,33	1.64	10 (32%)	47,52,52	1.98	14 (29%)
5	POV	A	5106	-	44,44,51	0.94	0	50,52,59	0.78	2 (4%)
5	POV	D	5105	-	44,44,51	0.94	0	50,52,59	0.78	2 (4%)
4	ACP	B	5104	-	31,33,33	1.64	10 (32%)	47,52,52	1.99	14 (29%)
5	POV	B	5105	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
5	POV	C	5106	-	44,44,51	0.94	0	50,52,59	0.77	2 (4%)
4	ACP	A	5104	-	31,33,33	1.64	10 (32%)	47,52,52	1.99	14 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACP	D	5104	-	-	6/19/38/38	0/3/3/3
5	POV	B	5106	-	-	20/48/48/55	-
5	POV	C	5107	-	-	2/11/11/55	-
5	POV	C	5105	-	-	2/11/11/55	-
5	POV	A	5105	-	-	2/11/11/55	-
4	ACP	C	5104	-	-	6/19/38/38	0/3/3/3
5	POV	A	5106	-	-	20/48/48/55	-
5	POV	D	5105	-	-	20/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACP	B	5104	-	-	6/19/38/38	0/3/3/3
5	POV	B	5105	-	-	2/11/11/55	-
5	POV	C	5106	-	-	20/48/48/55	-
4	ACP	A	5104	-	-	6/19/38/38	0/3/3/3

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5105	POV	C314-C313	208.78	16.36	1.50
5	C	5107	POV	C314-C313	208.78	16.36	1.50
5	C	5105	POV	C314-C313	208.77	16.36	1.50
5	B	5105	POV	C314-C313	208.77	16.36	1.50
5	A	5105	POV	C32-C33	-4.09	1.26	1.51

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5105	POV	C314-C313-C312	-13.41	22.80	113.36
5	B	5105	POV	C314-C313-C312	-13.41	22.82	113.36
5	C	5107	POV	C314-C313-C312	-13.41	22.84	113.36
5	A	5105	POV	C314-C313-C312	-13.41	22.85	113.36
4	A	5104	ACP	C5-C4-N3	-5.00	119.84	126.72

There are no chirality outliers.

5 of 112 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5104	ACP	PB-C3B-PG-O1G
4	A	5104	ACP	PB-C3B-PG-O2G
4	A	5104	ACP	PB-C3B-PG-O3G
4	A	5104	ACP	PG-C3B-PB-O1B
4	A	5104	ACP	PG-C3B-PB-O3A

There are no ring outliers.

12 monomers are involved in 75 short contacts:

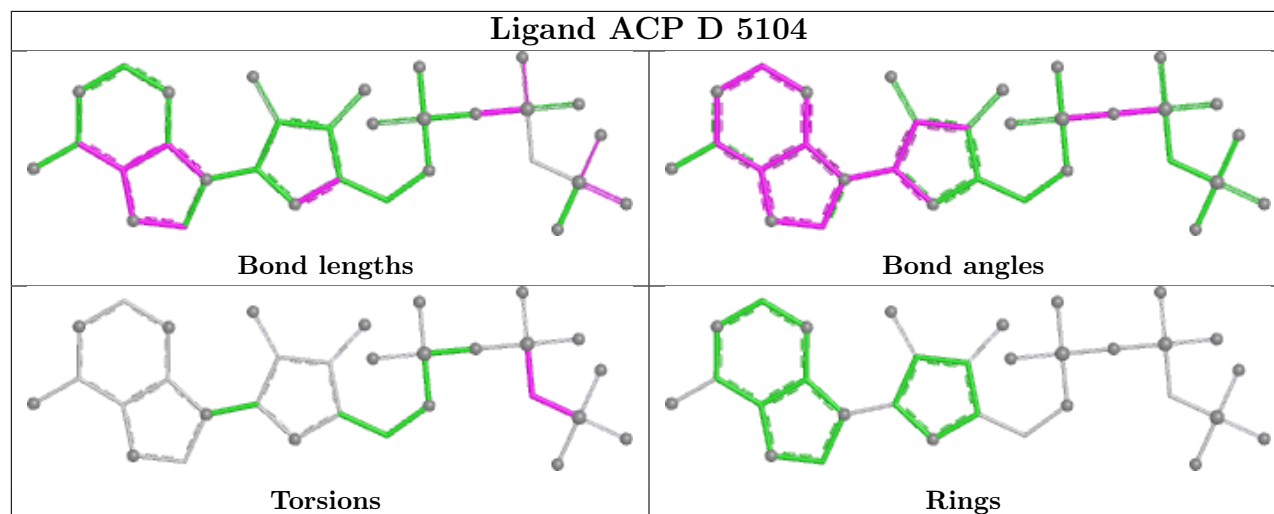
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5104	ACP	1	0
5	B	5106	POV	17	0
5	C	5107	POV	4	0

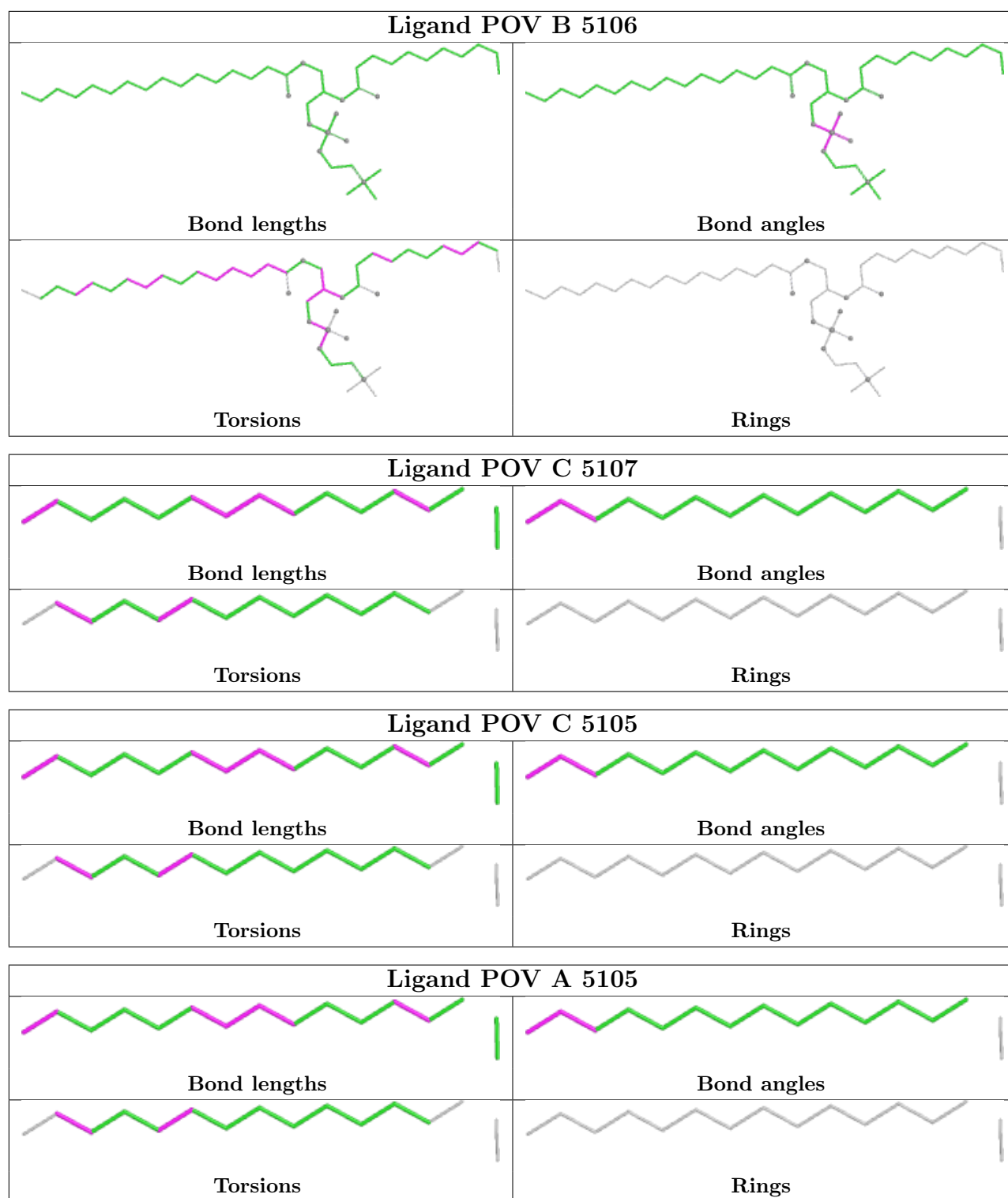
Continued on next page...

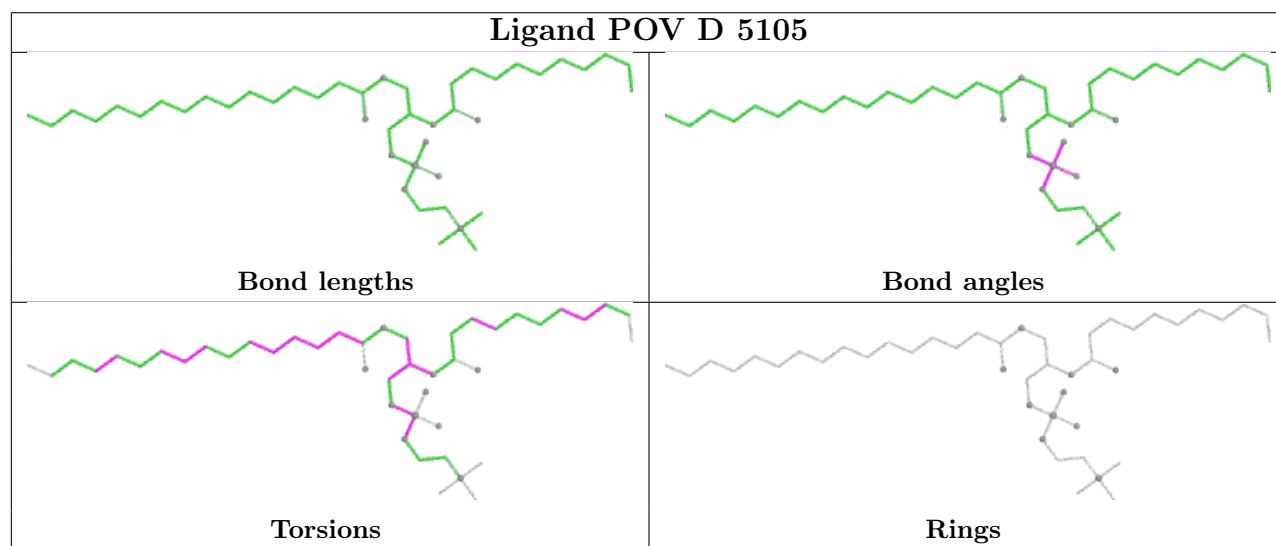
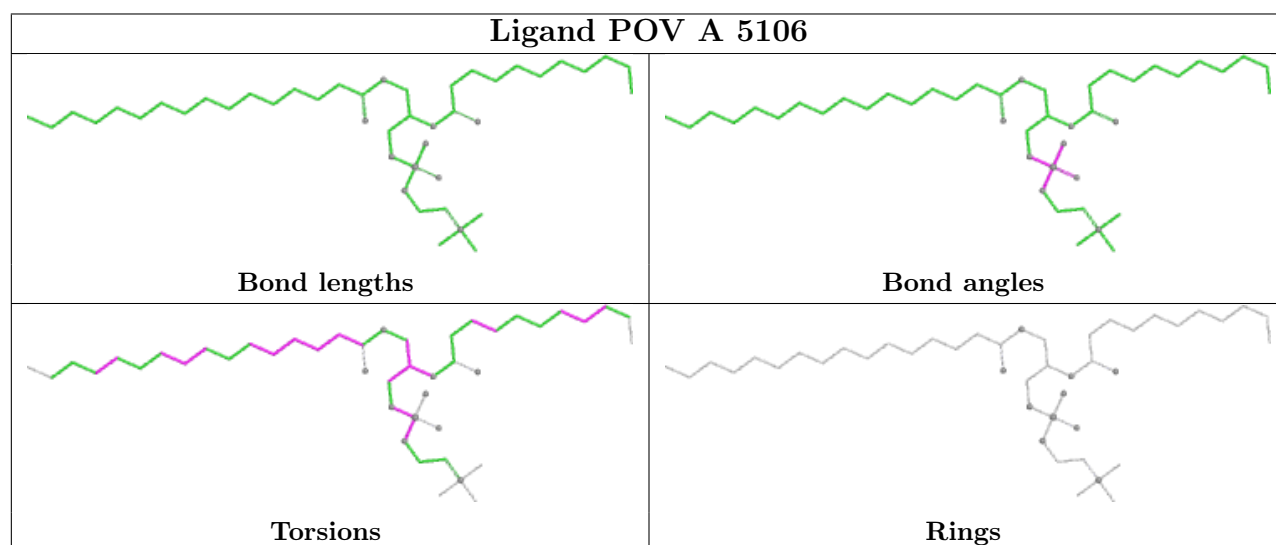
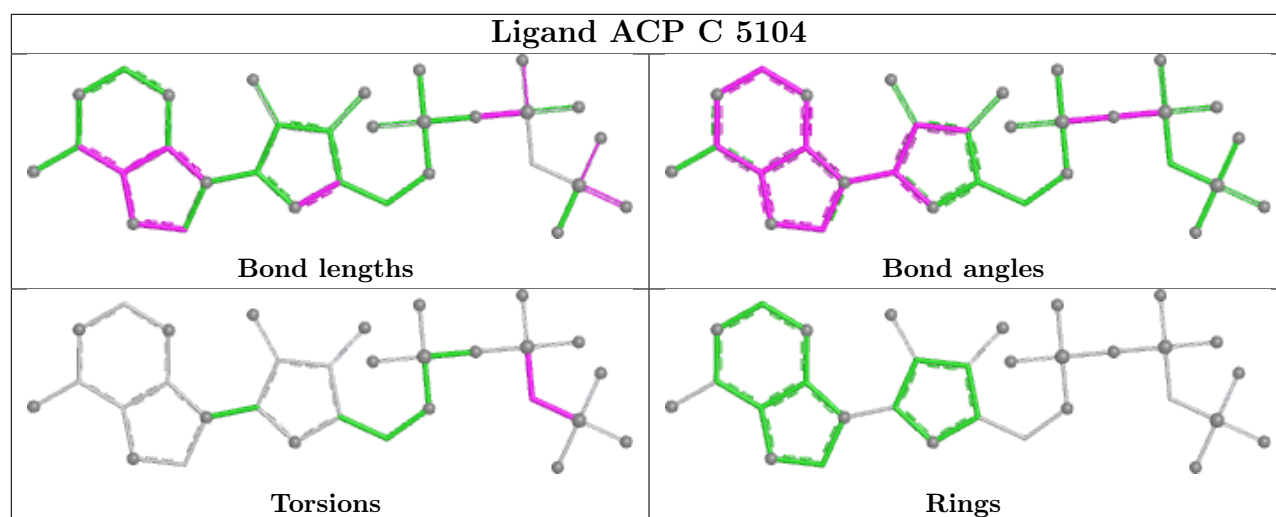
Continued from previous page...

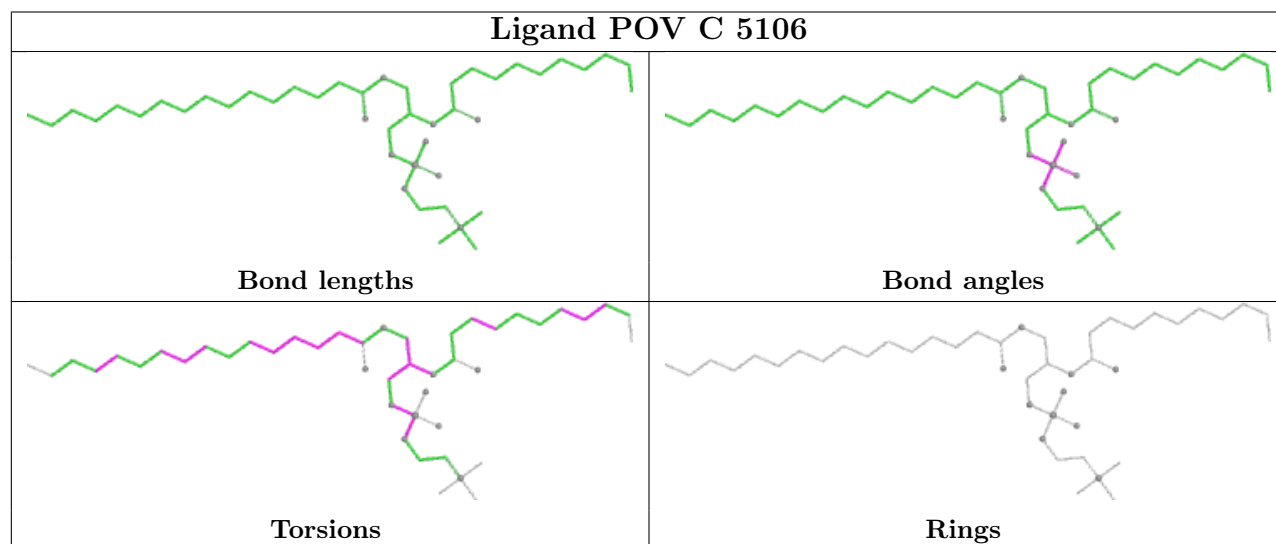
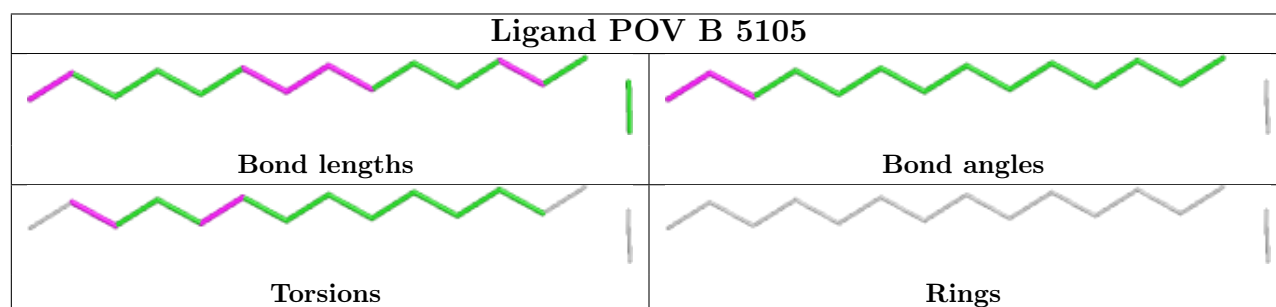
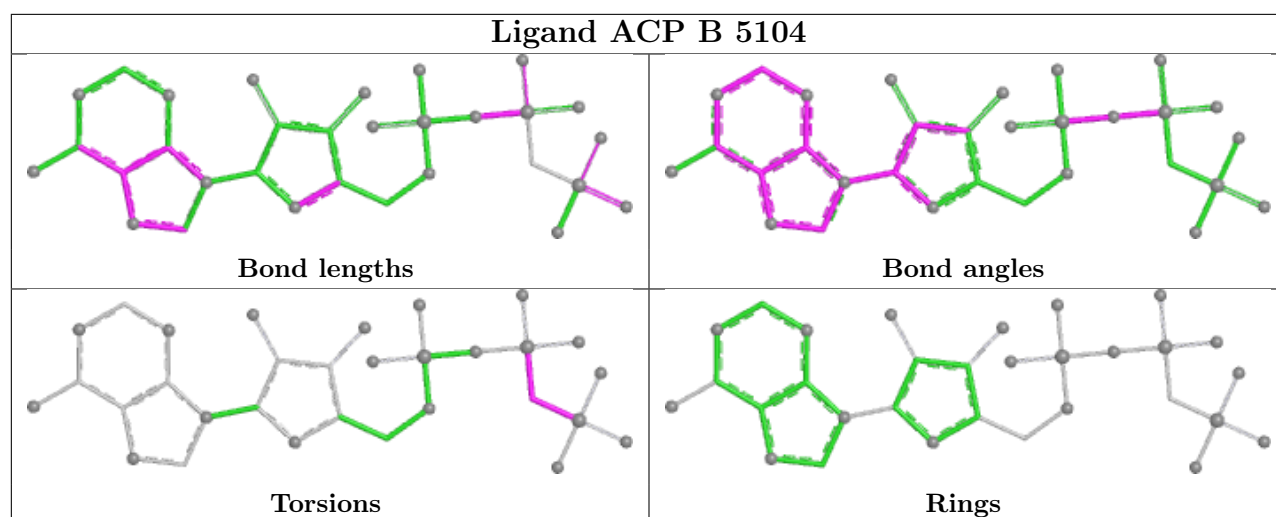
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5105	POV	2	0
5	A	5105	POV	2	0
4	C	5104	ACP	2	0
5	A	5106	POV	16	0
5	D	5105	POV	16	0
4	B	5104	ACP	1	0
5	B	5105	POV	2	0
5	C	5106	POV	11	0
4	A	5104	ACP	1	0

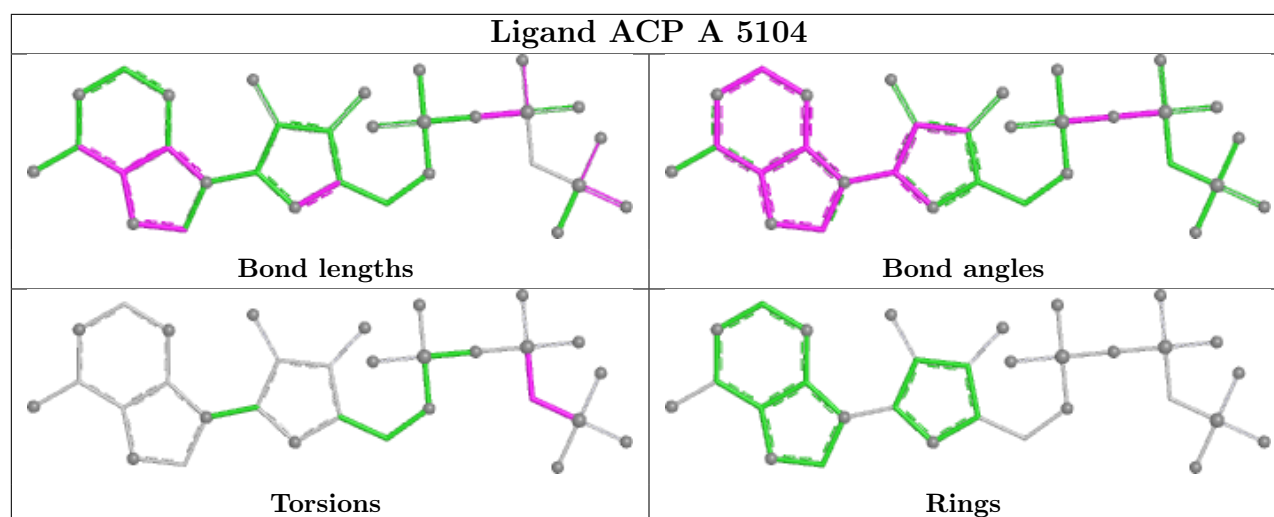
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	7
1	D	7
1	B	7
1	A	7

The worst 5 of 28 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3122:UNK	C	3123:UNK	N	14.33
1	D	3122:UNK	C	3123:UNK	N	14.33
1	B	3122:UNK	C	3123:UNK	N	14.33
1	A	3122:UNK	C	3123:UNK	N	14.32
1	A	3221:UNK	C	3222:UNK	N	13.70

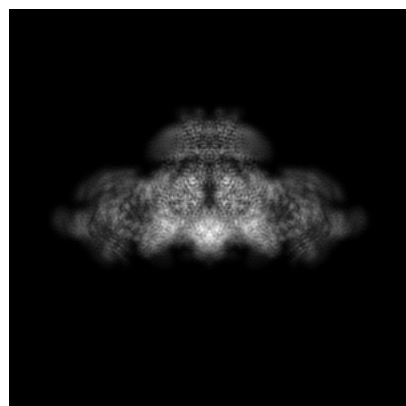
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25828. These allow visual inspection of the internal detail of the map and identification of artifacts.

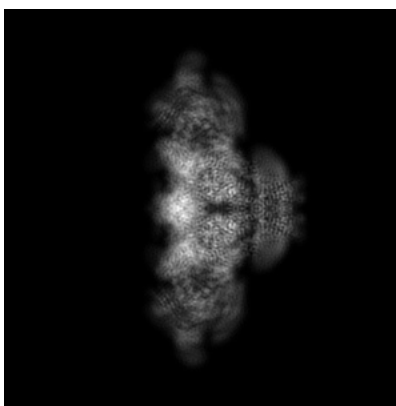
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

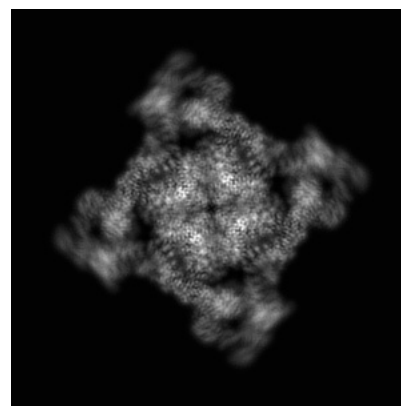
6.1.1 Primary map



X

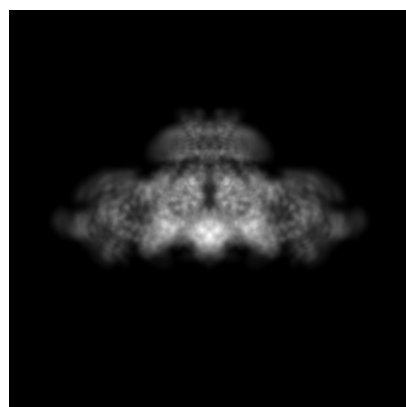


Y

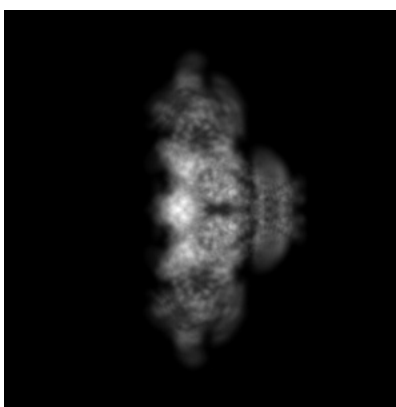


Z

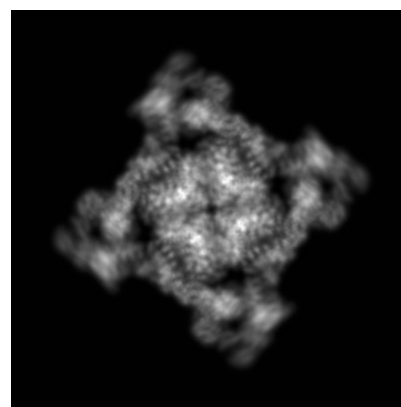
6.1.2 Raw map



X



Y

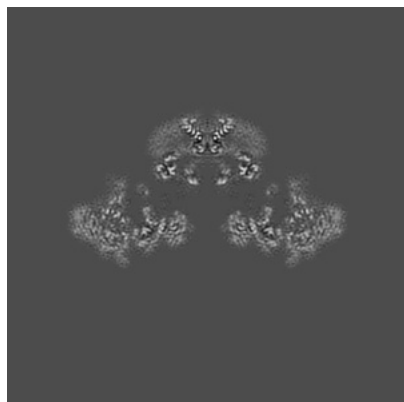


Z

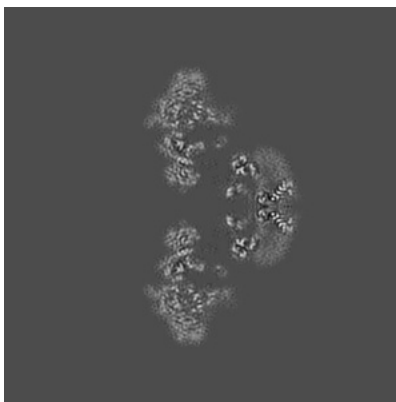
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

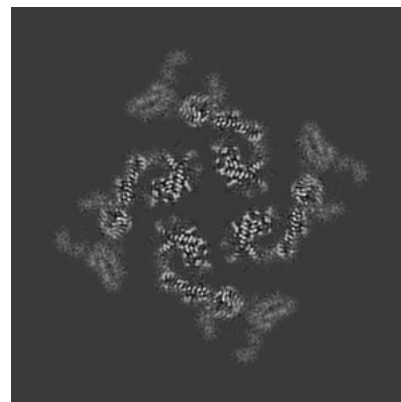
6.2.1 Primary map



X Index: 216

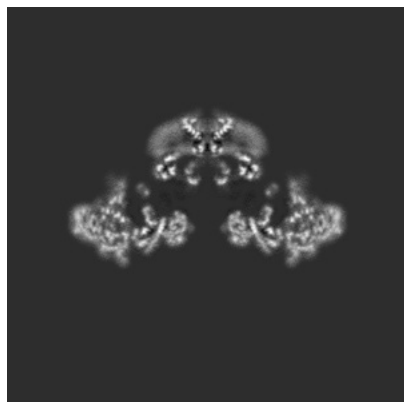


Y Index: 216

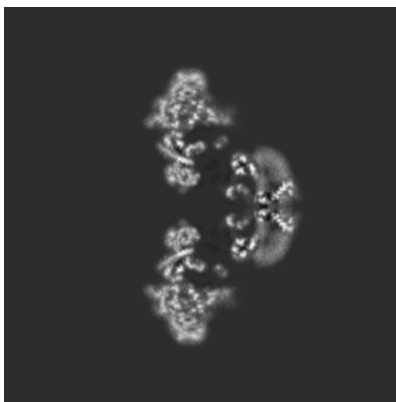


Z Index: 216

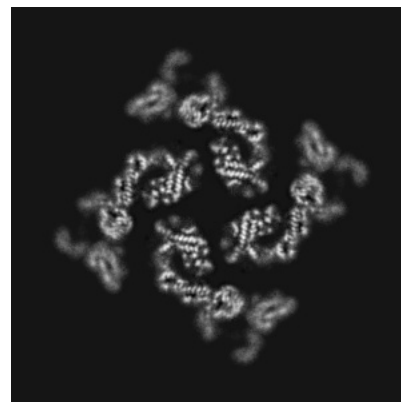
6.2.2 Raw map



X Index: 216



Y Index: 216

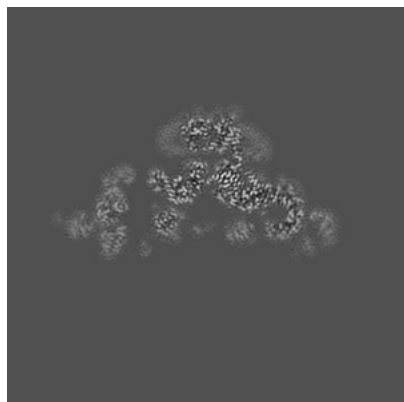


Z Index: 216

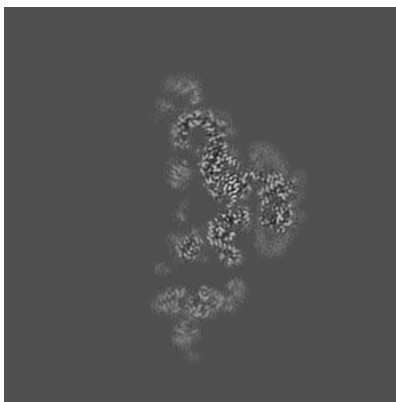
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

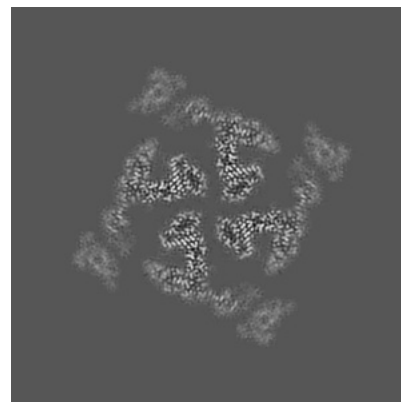
6.3.1 Primary map



X Index: 233

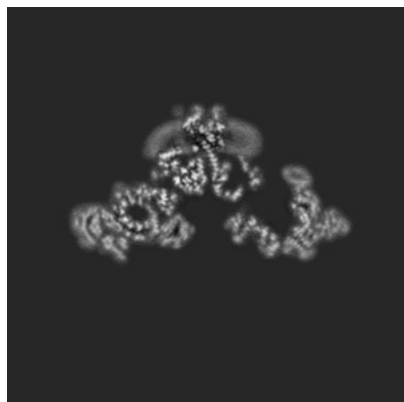


Y Index: 199

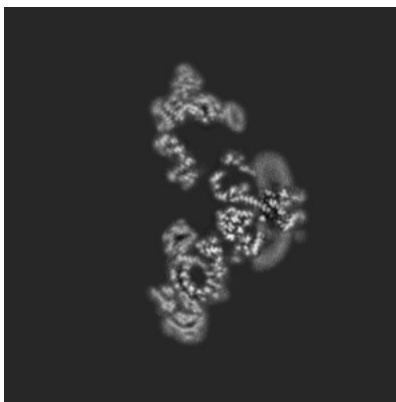


Z Index: 228

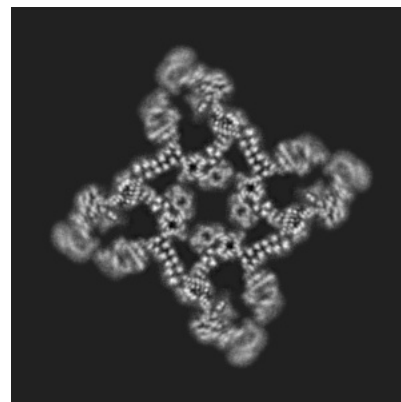
6.3.2 Raw map



X Index: 207



Y Index: 225

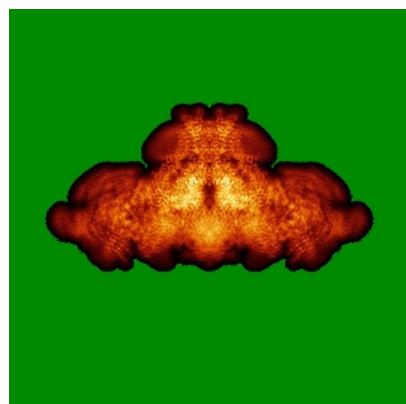


Z Index: 198

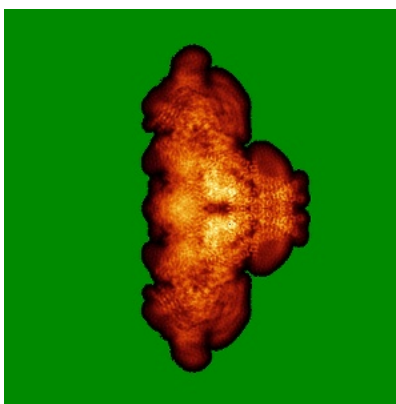
The images above show the largest variance slices of the map in three orthogonal directions.

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

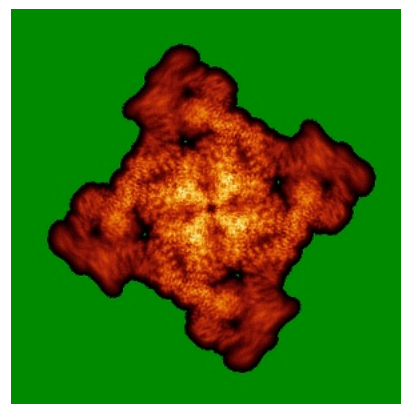
6.4.1 Primary map



X

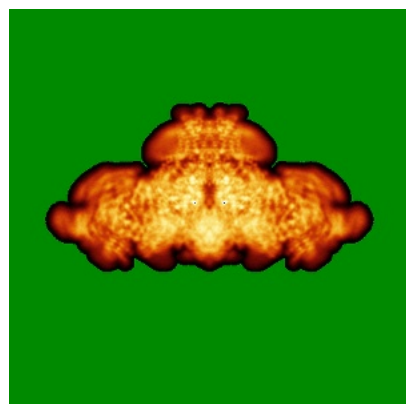


Y

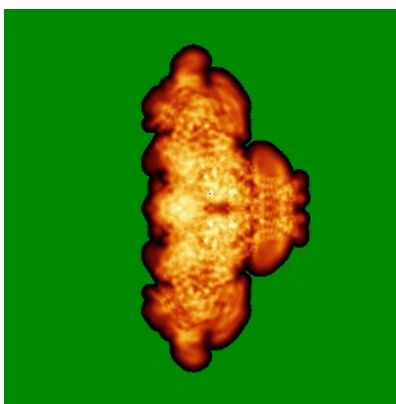


Z

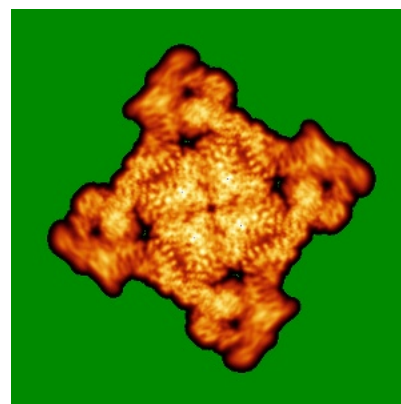
6.4.2 Raw map



X



Y

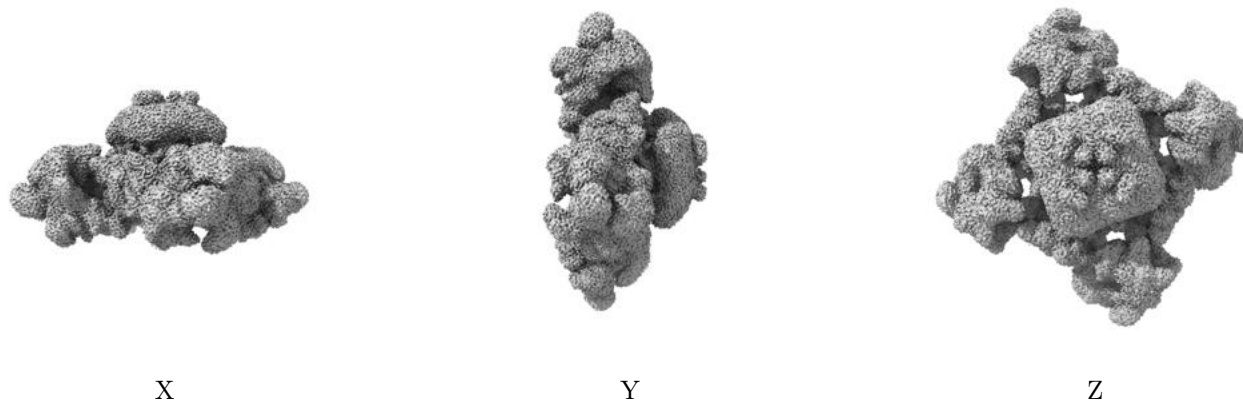


Z

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.

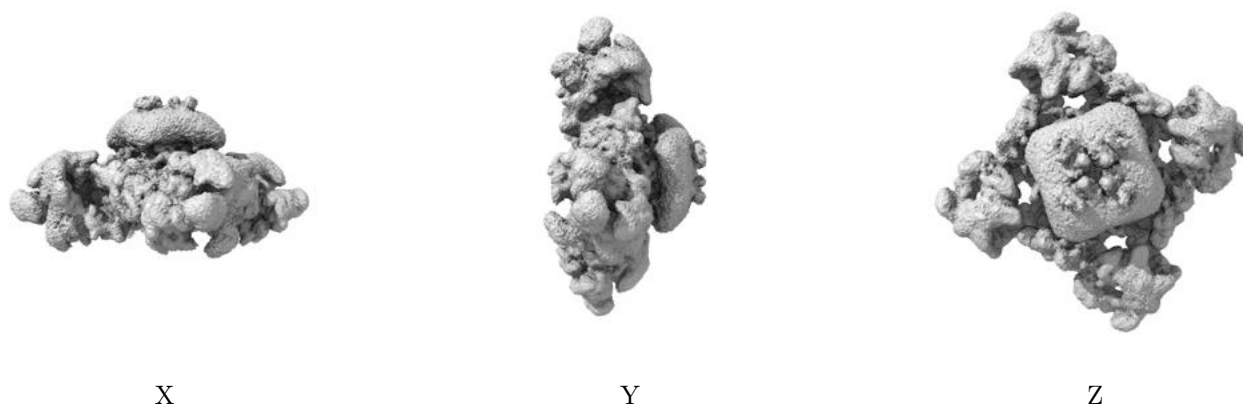
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

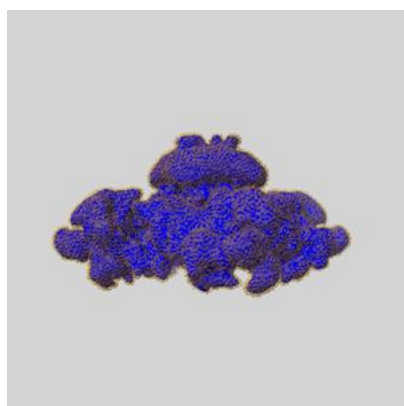
6.6 Mask visualisation [i](#)

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

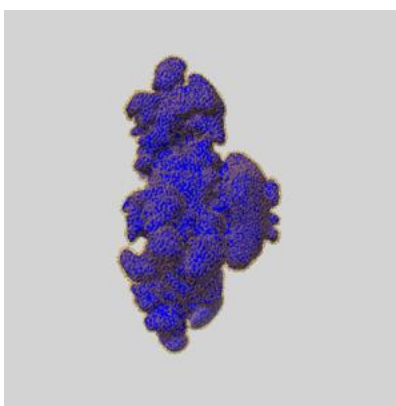
A mask typically either:

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

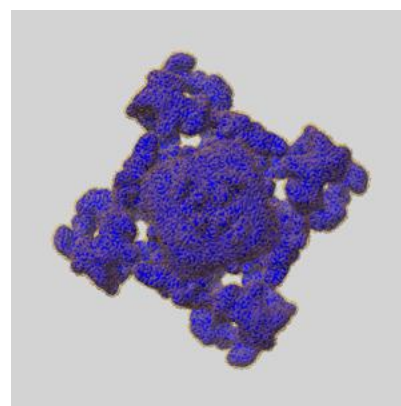
6.6.1 emd_25828_msk_1.map [i](#)



X



Y

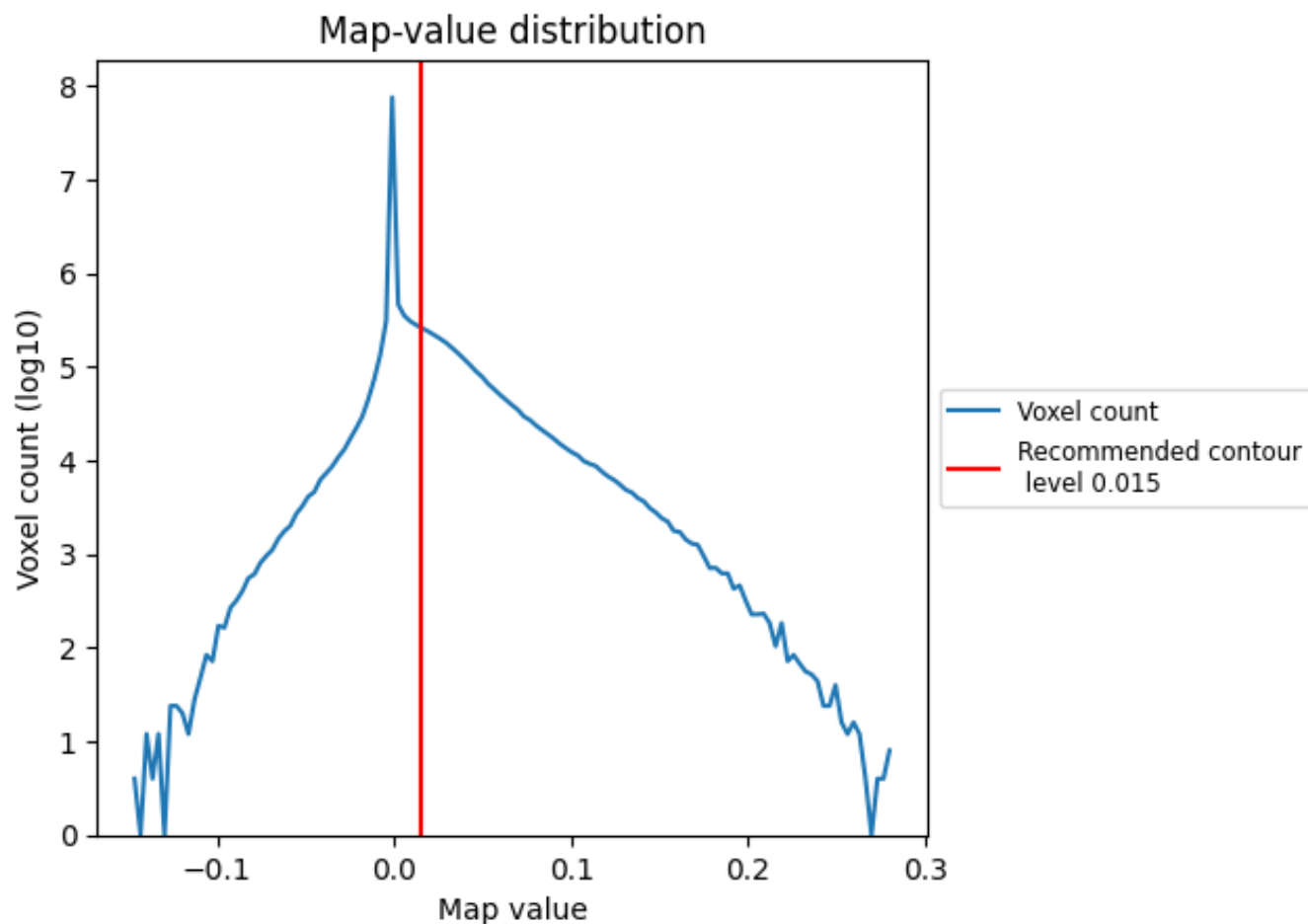


Z

7 Map analysis [i](#)

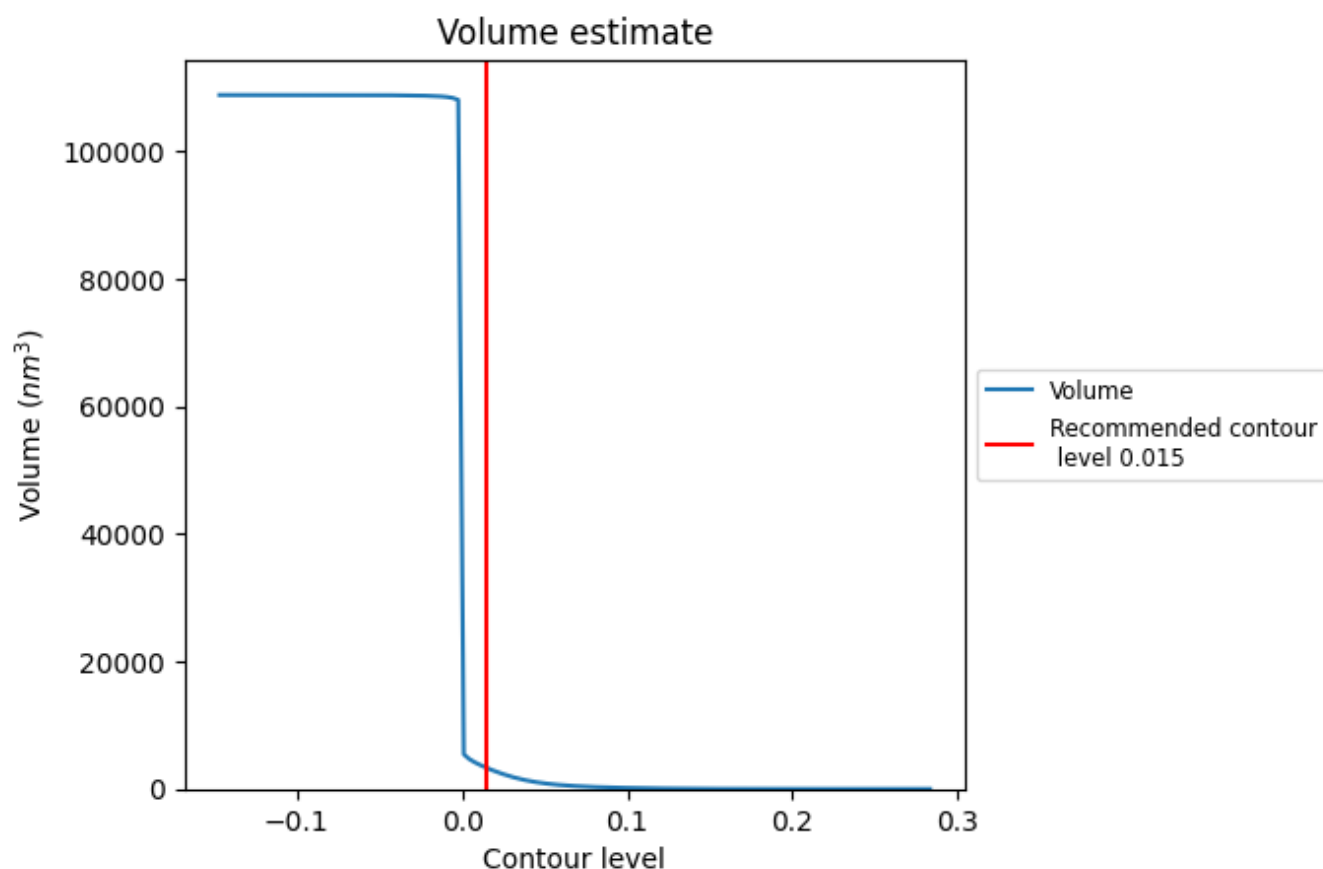
This section contains the results of statistical analysis of the map.

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.

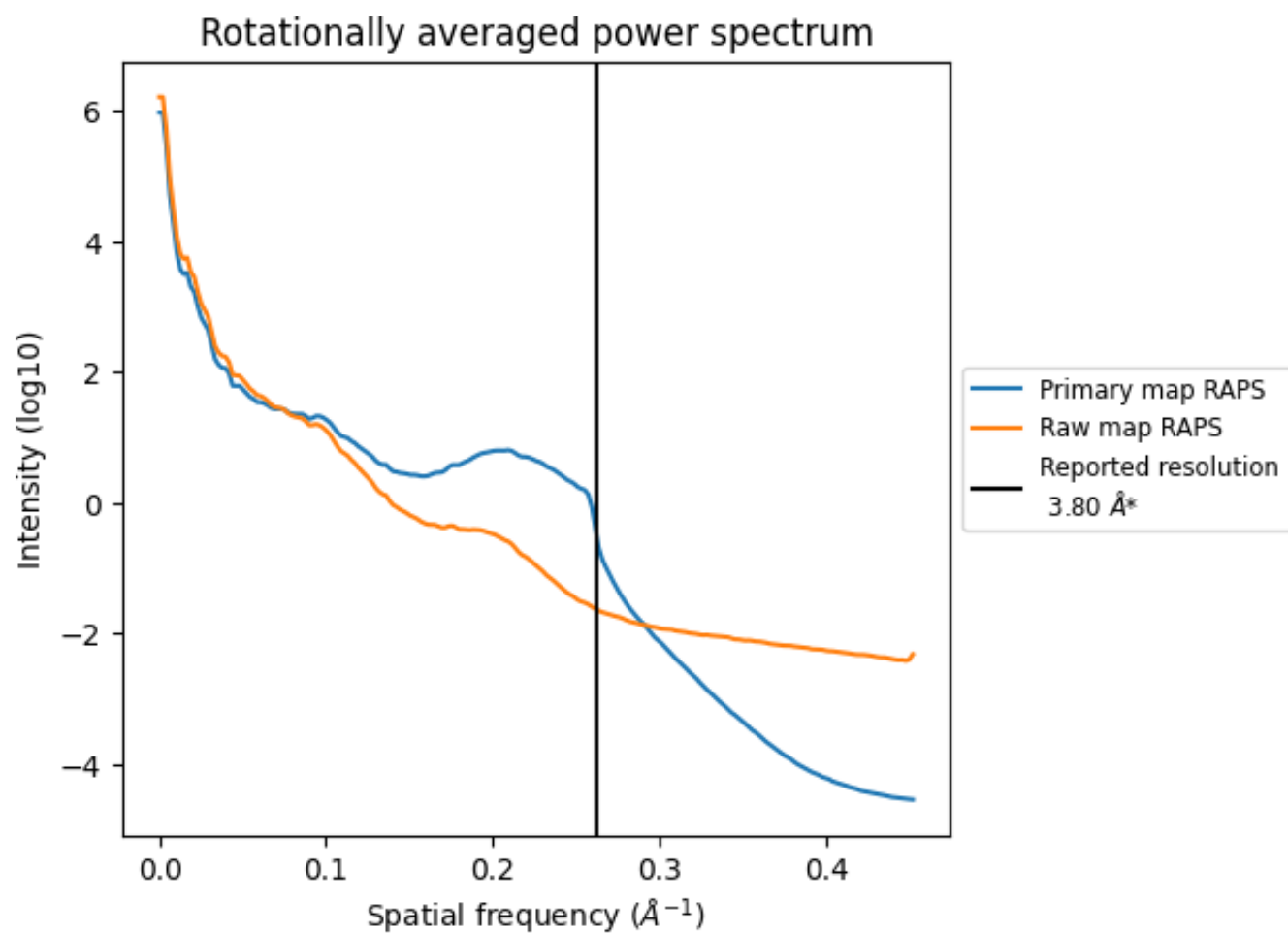
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3290 nm^3 ; this corresponds to an approximate mass of 2972 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 ⓘ

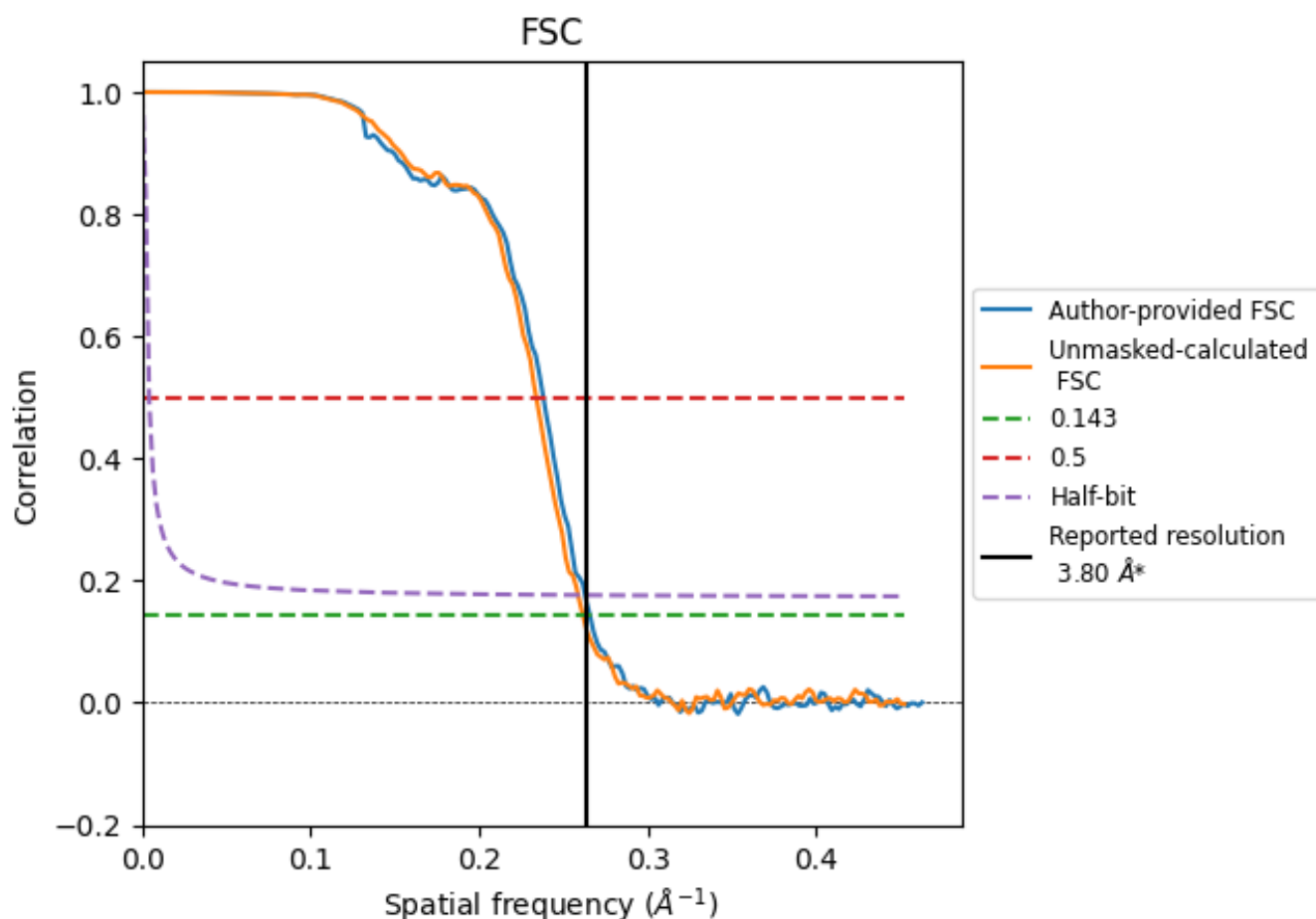


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 $0.263 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

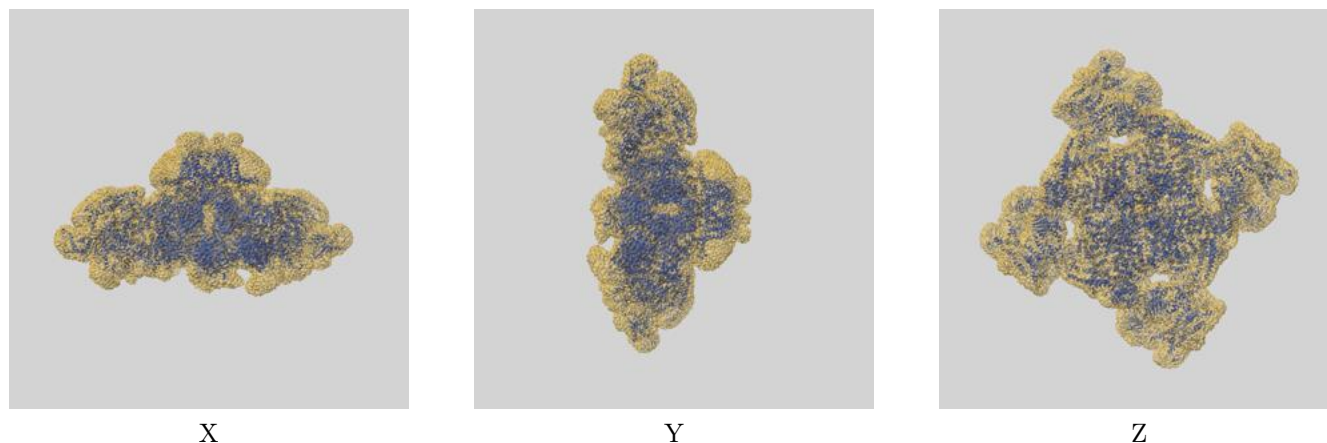
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	4.20	3.80
Unmasked-calculated*	3.82	4.28	3.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

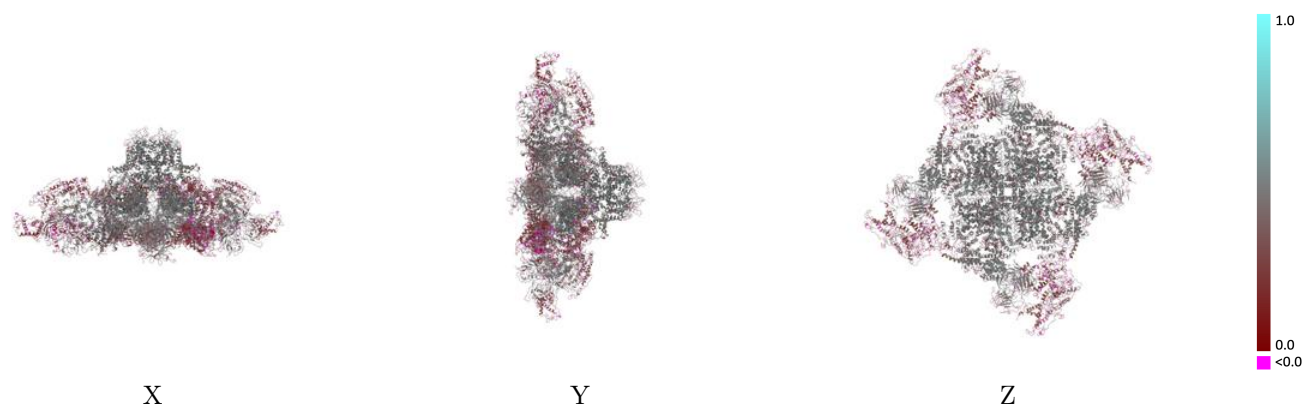
This section contains information regarding the fit between EMDB map EMD-25828 and PDB model 7TDG. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



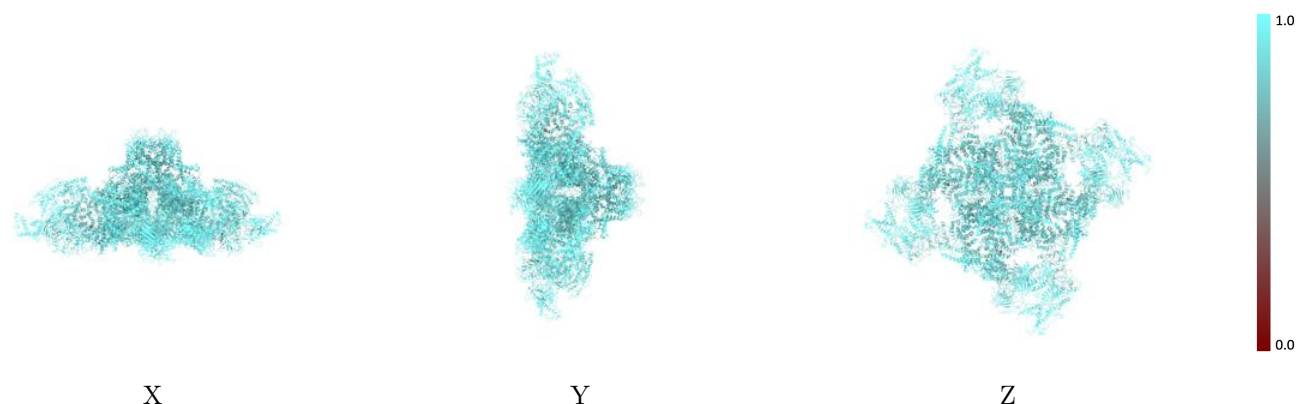
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



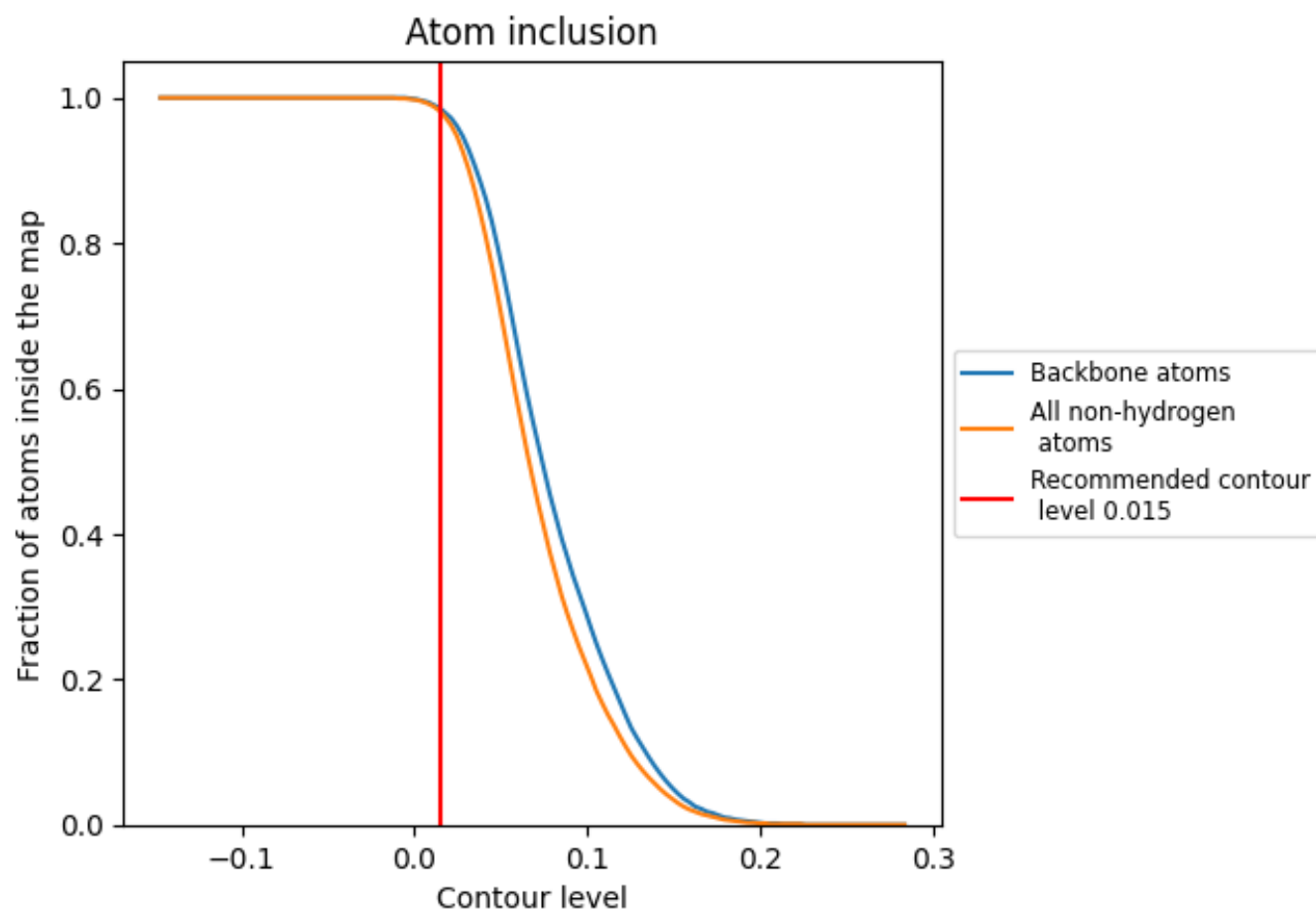
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9810	0.3860
A	0.9810	0.3860
B	0.9810	0.3860
C	0.9810	0.3860
D	0.9810	0.3850

