



## wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 01:41 AM EDT

PDB ID : 7TDG  
EMDB ID : EMD-25828  
Title : Rabbit RyR1 with AMP-PCP and high Ca<sup>2+</sup> 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.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39



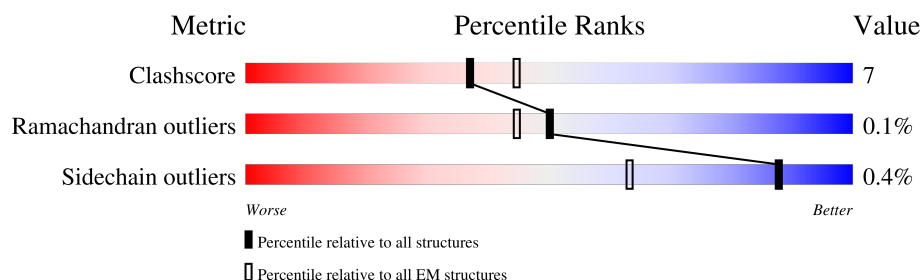
# 1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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 (three-letter code: 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	

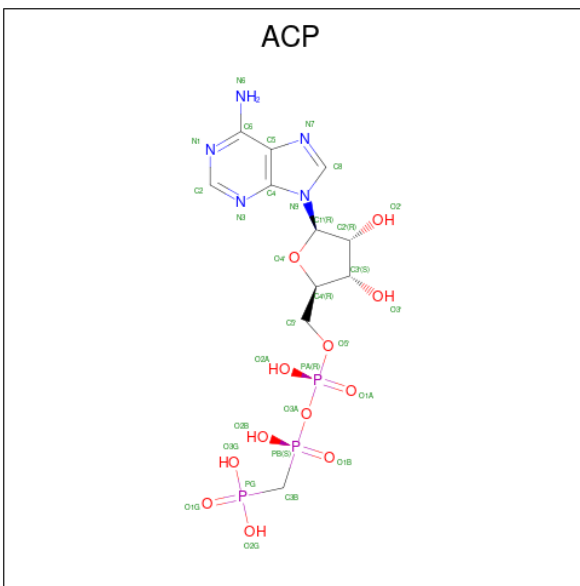
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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 (three-



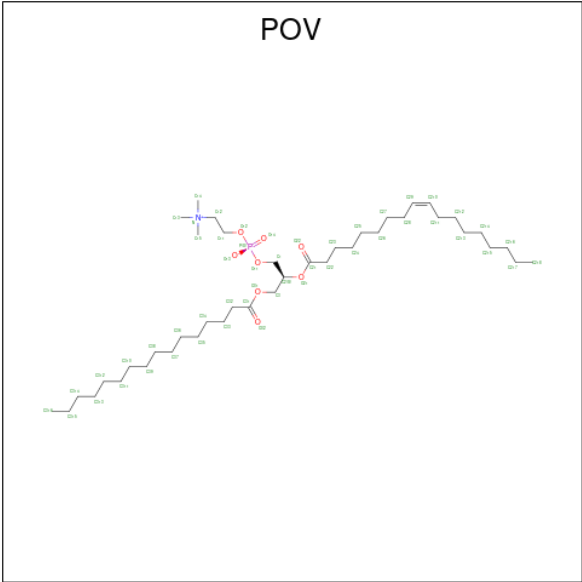
letter code: ACP) (formula:  $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$ ).



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 (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).





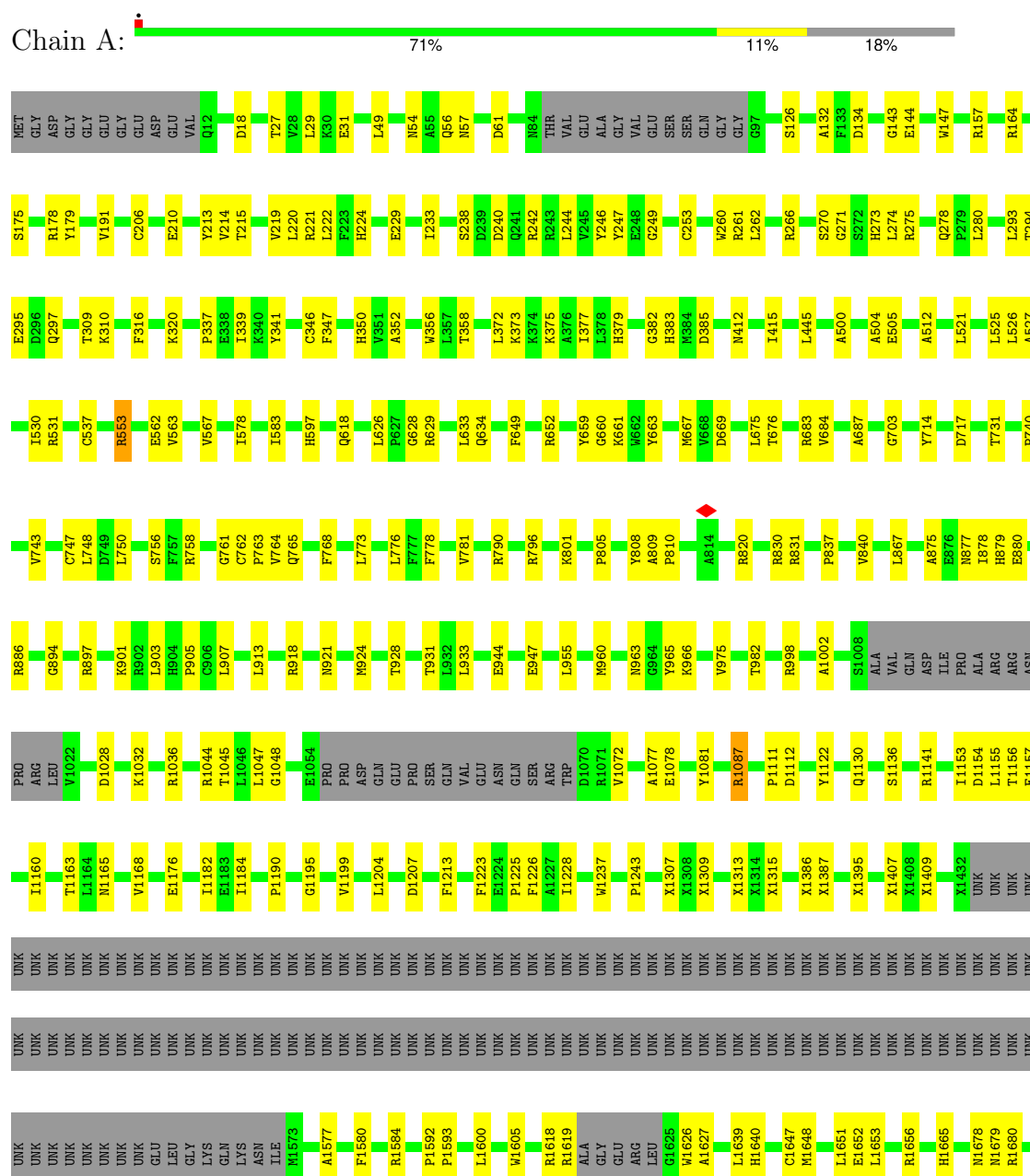
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C				0
			16	16				
5	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
5	C	1	Total	C				0
			16	16				
5	C	1	Total	C	N	O	P	0
			45	35	1	8	1	
5	C	1	Total	C				0
			16	16				
5	D	1	Total	C	N	O	P	0
			45	35	1	8	1	
5	B	1	Total	C				0
			16	16				
5	B	1	Total	C	N	O	P	0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



### 3 Residue-property plots

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

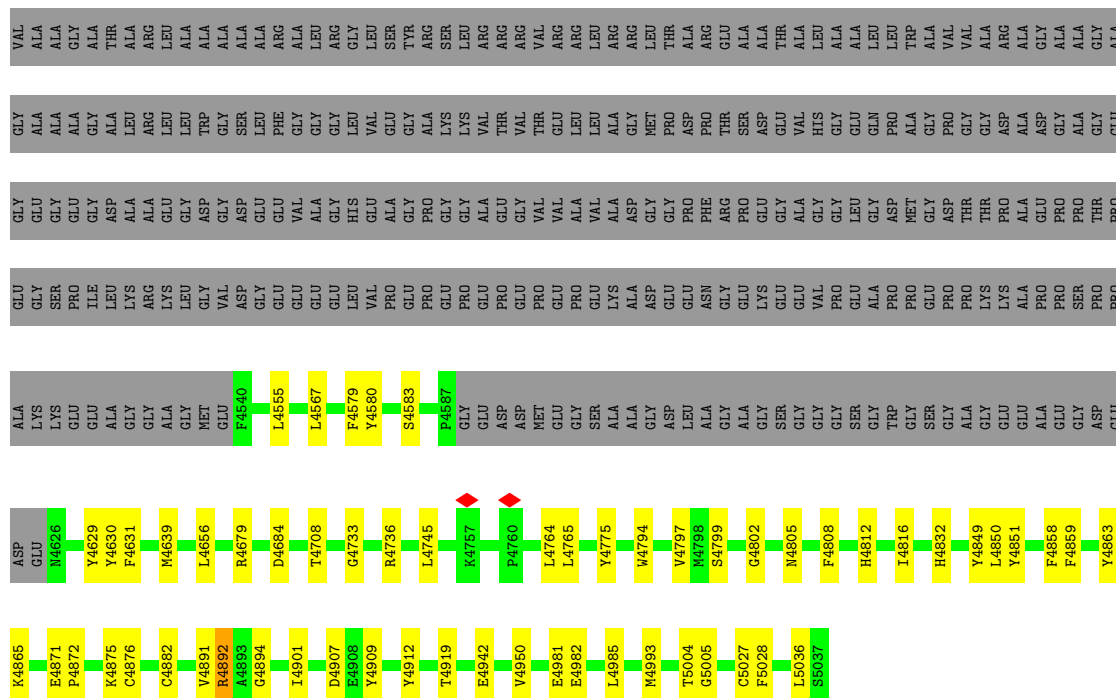
#### • Molecule 1: Ryanodine receptor 1, RyR1



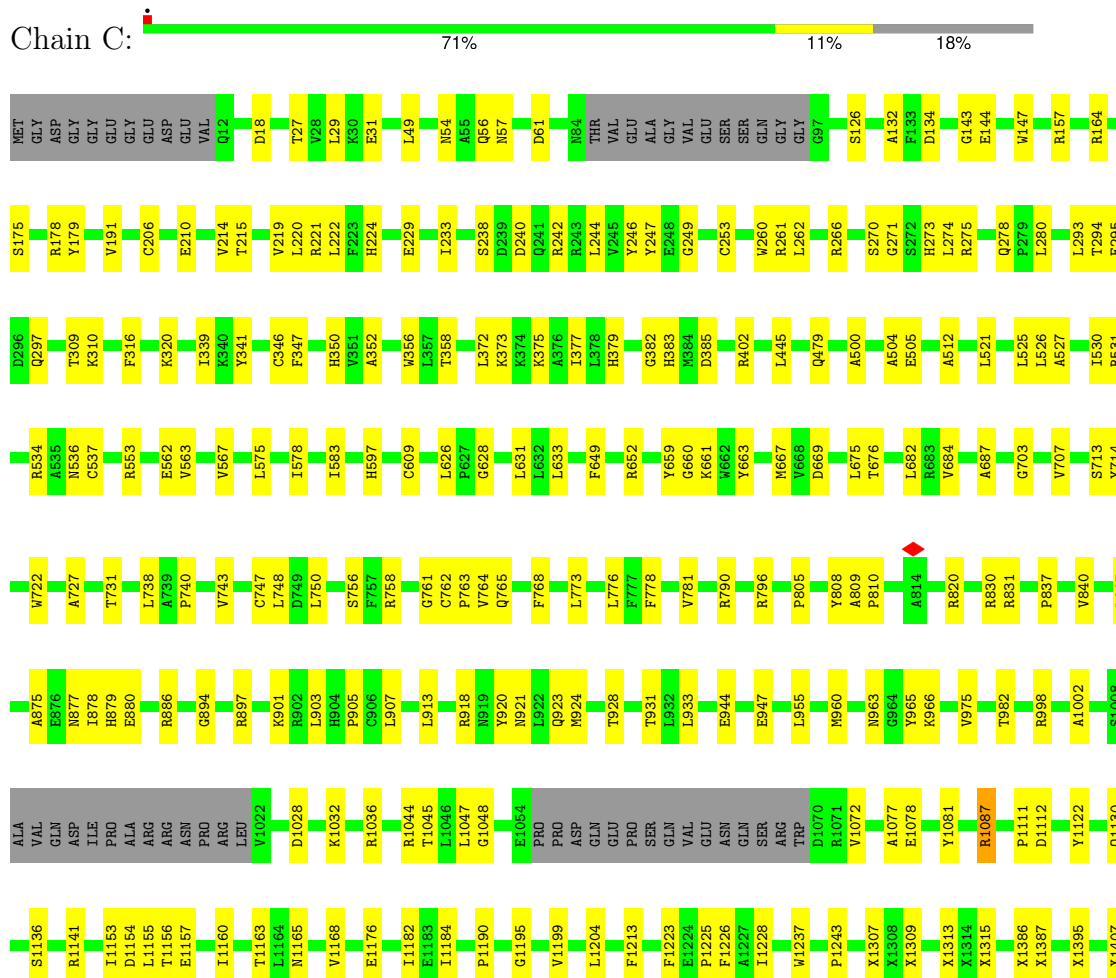


A4167	Y3937	E3747	X3562	UNK	R2869	I2809	X2695	GLY	A2200	SER	GLU	H1702
R4175	E3944	E3748	X3563	UNK	E2870	X2810	X2703	LYS	L2201	LEU	GLU	I1735
P4176	E3945	V3749	X3613	UNK	Q2872	E2811	CYS	ASP	F2239	THR	GLY	L1738
Y4177	Q3946	V3750	UNK	UNK	M2873	L2813	ALA	LEU	I2242	VAL	ASP	T1739
R4180	G3947	S3752	SER	UNK	M2874	X2814	ILE	VAL	L2288	ARG	ALA	T1742
R4198	K3948	E3755	LYS	UNK	E2876	X2815	ALA	X2487	L2288	LEU	GLU	T1742
Y4194	R3950	K3756	ALA	UNK	Q2877	ILE	GLY	X2506	Q2291	VAL	LYS	I1745
S4198	F3962	Q3761	TRP	UNK	E2880	TRP	ALA	ALA	E2292	LYS	GLU	F1748
E4199	T3966	R3762	HIS	UNK	M2881	GLU	PRO	X2511	R2336	LYS	GLU	P1749
T4200	E3967	Q3767	LYS	UNK	H2883	THR	ASP	X2568	R2336	GLU	ALA	P1750
N4201	Y3968	UNK	LEU	UNK	UNK	ILE	TYR	X2572	L2356	PRO	GLU	H1760
F4219	I3969	L3770	SER	UNK	W2886	GLU	VAL	X2579	R2359	LYS	GLU	T1769
C4238	Q3977	H3771	GLN	UNK	K2891	ALA	ALA	X2589	F2364	GLU	LYS	C1761
E4239	L3980	T3772	ARG	UNK	Q2892	ARG	SER	X2590	L2376	ALA	GLU	L1786
I4242	L3985	R3773	ARG	UNK	E2893	GLU	TYR	X2591	L1922	ASP	GLU	P1932
I4251	W3986	M3782	ARG	UNK	L2894	GLY	SER	X2592	P1932	ALA	ALA	E1933
S4252	T4252	T3790	ALA	UNK	E2895	GLU	SER	X2593	S1934	VAL	GLY	S1934
E4253	M4039	V3794	VAL	UNK	G2899	GLU	LYS	X2594	K1936	ALA	ALA	E1793
PRD	R4042	V3798	CYS	UNK	G2900	ARG	ALA	X2595	L1943	VAL	GLU	A1796
GLU	M4047	L3798	PHE	UNK	T2901	THR	LYS	X2606	V1966	GLU	GLU	R1797
GLY	M4047	L3804	ARG	UNK	H2902	THR	LYS	X2620	L1969	GLU	GLU	E1874
PRD	L4059	L3805	MET	UNK	L2911	GLN	ALA	X2626	R1974	GLU	GLU	GLU
GLU	K4060	N3806	T3639	UNK	T2912	ALA	THR	X2629	T1991	GLU	GLU	GLU
ALA	M4064	G3807	Y3642	UNK	A2913	THR	ASP	X2642	T1995	GLU	GLU	GLU
ASP	K4067	Q3812	A3649	UNK	E2915	ARG	ALA	X2644	L2009	GLU	GLU	GLU
ASP	L4068	Q3813	W3661	UNK	K2916	ILE	GLU	X2648	G2048	GLU	GLU	GLU
GLY	I4071	Q3814	I3662	UNK	R2920	SER	GLN	X2649	GLU	GLU	GLU	GLU
MET	D4079	X3815	L3663	UNK	E2921	THR	ALA	X2650	L2155	GLU	GLU	GLU
GLU	Y4080	D3818	F3669	UNK	Q2924	THR	THR	X2651	L2182	PRO	GLU	GLU
ALA	Q4094	Y3819	D3676	UNK	E2925	TYR	ASP	X2652	T2185	GLU	GLU	GLU
ALA	Q4094	L3835	X3458	UNK	K2928	PRO	PRO	X2658	N2188	GLU	GLU	GLU
GLU	Q4102	R3849	X3459	UNK	L2930	GLY	GLY	X2665	Y2192	GLU	GLU	GLU
GLY	I4108	L3856	X3491	UNK	Q2931	TYR	TYR	X2666	N2196	GLU	GLU	GLU
GLU	I4108	X3874	X3497	UNK	M2932	ASN	ASN	X2667	L2197	GLU	GLU	GLU
GLY	S4115	F3880	X3500	UNK	E2939	PRO	PRO	X2679	R2199	GLU	GLU	GLU
ALA	I4123	Q3889	X3501	UNK	GLY	GLN	GLN	X2680	L2479	GLU	GLU	GLU
GLY	E4152	L3890	X3502	UNK	LEU	PRO	PRO	X2681	L2433	GLU	GLU	GLU
GLU	H4153	L3891	X3503	UNK	UNK	ASP	ASP	X2682	G2434	GLU	GLU	GLU
GLY	V4154	C3892	X3504	UNK	UNK	LEU	LEU	X2683	R2435	THR	GLU	GLU
ALA	F4155	E3893	X3535	UNK	UNK	SER	SER	X2684	H2441	GLU	GLU	GLU
GLY	H4156	Q3906	X3536	UNK	UNK	GLY	E2799	X2685	L2463	SER	GLU	GLU
THR	R4161	UNK	X3537	UNK	UNK	VAL	K2802	X2686	D2464	ARG	GLU	GLU
			X3561	UNK	UNK	THR	R2806	X2687	L2479	ARG	GLU	GLU
				UNK	UNK		W2807	X2688				
				UNK	UNK		P2808	X2689				
				UNK	UNK			X2690				
				UNK	UNK			X2691				
				UNK	UNK			X2692				
				UNK	UNK			X2693				
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				UNK	UNK			X2796				
				UNK	UNK			X2797				
				UNK	UNK			X2798				
				UNK	UNK			X2799				
				UNK	UNK			X2800				
				UNK	UNK			X2801				





• Molecule 1: Ryanodine receptor 1, RyR1

























WORLDWIDE  
**PDB**  
PROTEIN DATA BANK







## 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: ZN, POV, ACP, CA

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	0.26	0/25300	0.49	2/34345 (0.0%)
1	B	0.26	0/25299	0.49	2/34344 (0.0%)
1	C	0.26	0/25297	0.50	3/34342 (0.0%)
1	D	0.26	0/25281	0.50	4/34322 (0.0%)
All	All	0.26	0/101177	0.50	11/137353 (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 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1618	ARG	O-C-N	-13.63	100.89	122.70
1	C	1618	ARG	O-C-N	-5.73	113.53	122.70
1	C	4985	LEU	CA-CB-CG	5.69	128.38	115.30
1	D	4895	GLY	C-N-CA	-5.34	111.09	122.30
1	B	4985	LEU	CA-CB-CG	5.24	127.35	115.30

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	396	0
1	B	29246	0	24757	415	0
1	C	29244	0	24747	378	0
1	D	29228	0	24714	404	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	1592	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 7.

The worst 5 of 1592 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

*Continued on next page...*



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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%)	50	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%)	2502 (100%)	10 (0%)	89	91
1	B	2512/3264 (77%)	2500 (100%)	12 (0%)	86	90
1	C	2512/3264 (77%)	2499 (100%)	13 (0%)	86	90
1	D	2508/3264 (77%)	2500 (100%)	8 (0%)	91	92
All	All	10044/13056 (77%)	10001 (100%)	43 (0%)	88	91

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3773	ARG
1	B	1786	LEU
1	D	4631	PHE
1	B	553	ARG
1	B	2920	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	634	GLN
1	B	921	ASN
1	B	2872	GLN
1	C	2127	GLN
1	C	1693	GLN

### 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
5	POV	D	5105	-	44,44,51	0.94	0	50,52,59	0.78	2 (4%)
4	ACP	C	5104	-	27,33,33	1.37	5 (18%)	33,52,52	1.70	6 (18%)
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%)
4	ACP	A	5104	-	27,33,33	1.37	5 (18%)	33,52,52	1.70	6 (18%)
5	POV	C	5106	-	44,44,51	0.94	0	50,52,59	0.77	2 (4%)
5	POV	A	5105	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
4	ACP	B	5104	-	27,33,33	1.37	5 (18%)	33,52,52	1.70	6 (18%)
5	POV	C	5105	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
5	POV	B	5105	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
4	ACP	D	5104	-	27,33,33	1.33	5 (18%)	33,52,52	1.63	5 (15%)
5	POV	A	5106	-	44,44,51	0.94	0	50,52,59	0.78	2 (4%)

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
5	POV	D	5105	-	-	20/48/48/55	-
4	ACP	C	5104	-	-	6/15/38/38	0/3/3/3
5	POV	B	5106	-	-	20/48/48/55	-
5	POV	C	5107	-	-	2/11/11/55	-
4	ACP	A	5104	-	-	6/15/38/38	0/3/3/3
5	POV	C	5106	-	-	20/48/48/55	-
5	POV	A	5105	-	-	2/11/11/55	-
4	ACP	B	5104	-	-	6/15/38/38	0/3/3/3

*Continued on next page...*



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	C	5105	-	-	2/11/11/55	-
5	POV	B	5105	-	-	2/11/11/55	-
4	ACP	D	5104	-	-	6/15/38/38	0/3/3/3
5	POV	A	5106	-	-	20/48/48/55	-

The worst 5 of 40 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 35 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	C	5104	ACP	PB-O3A-PA	-4.58	117.42	132.37

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
5	D	5105	POV	16	0
4	C	5104	ACP	2	0
5	B	5106	POV	17	0

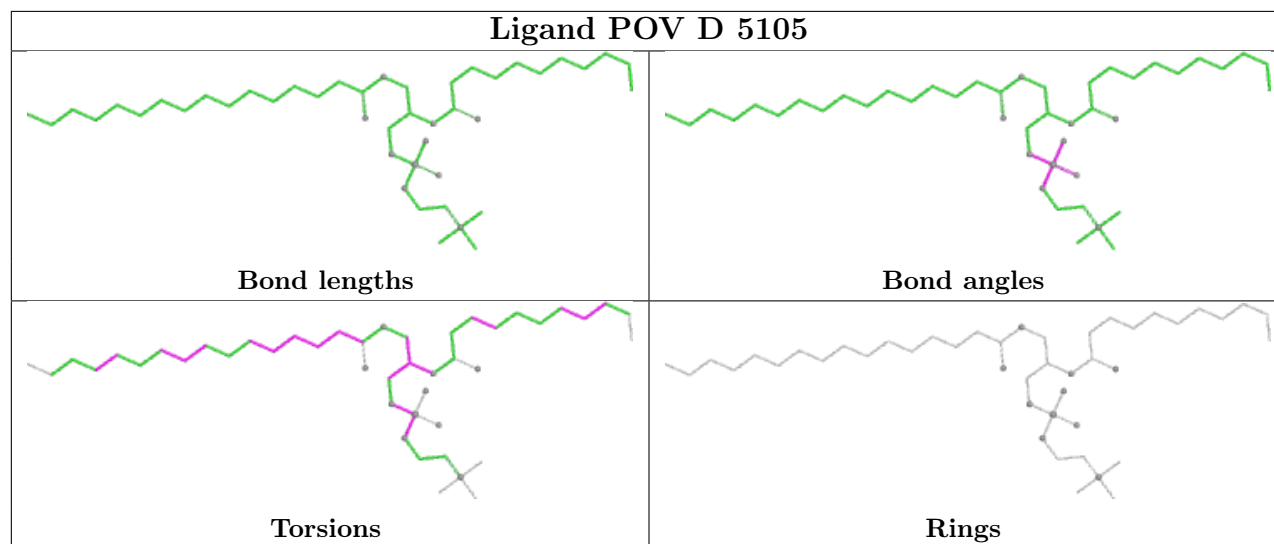
*Continued on next page...*



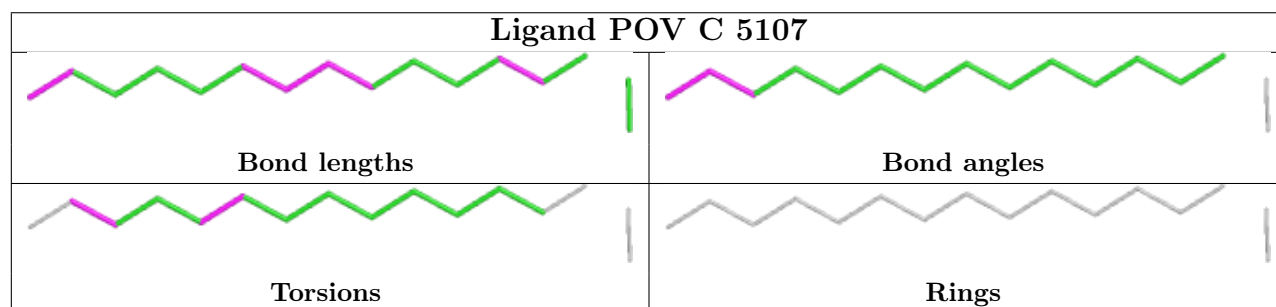
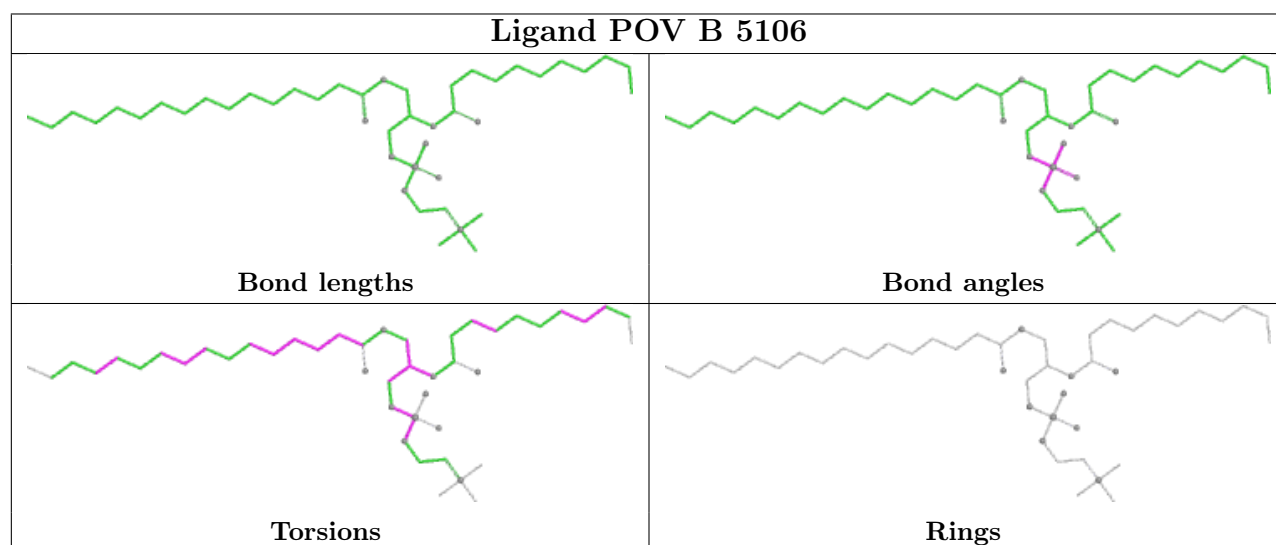
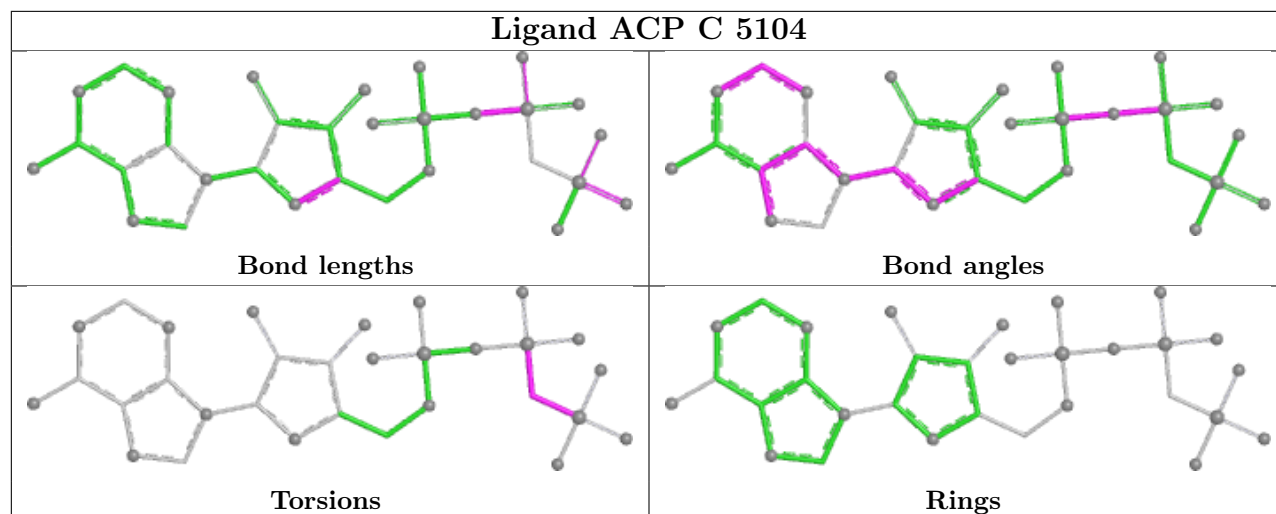
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5107	POV	4	0
4	A	5104	ACP	1	0
5	C	5106	POV	11	0
5	A	5105	POV	2	0
4	B	5104	ACP	1	0
5	C	5105	POV	2	0
5	B	5105	POV	2	0
4	D	5104	ACP	1	0
5	A	5106	POV	16	0

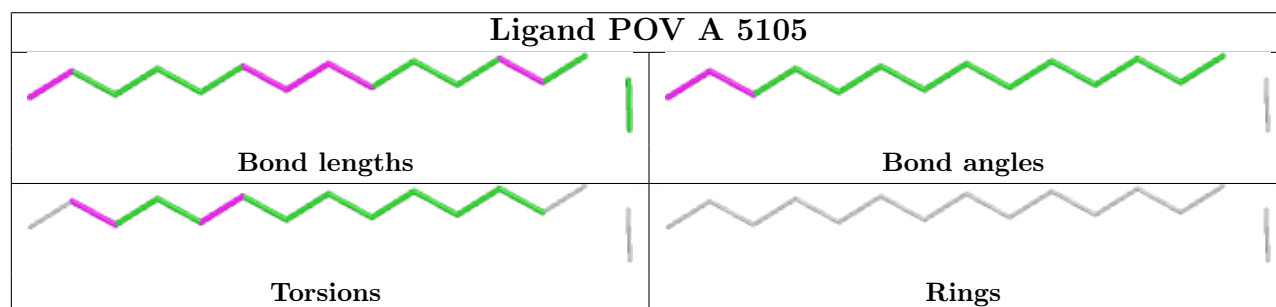
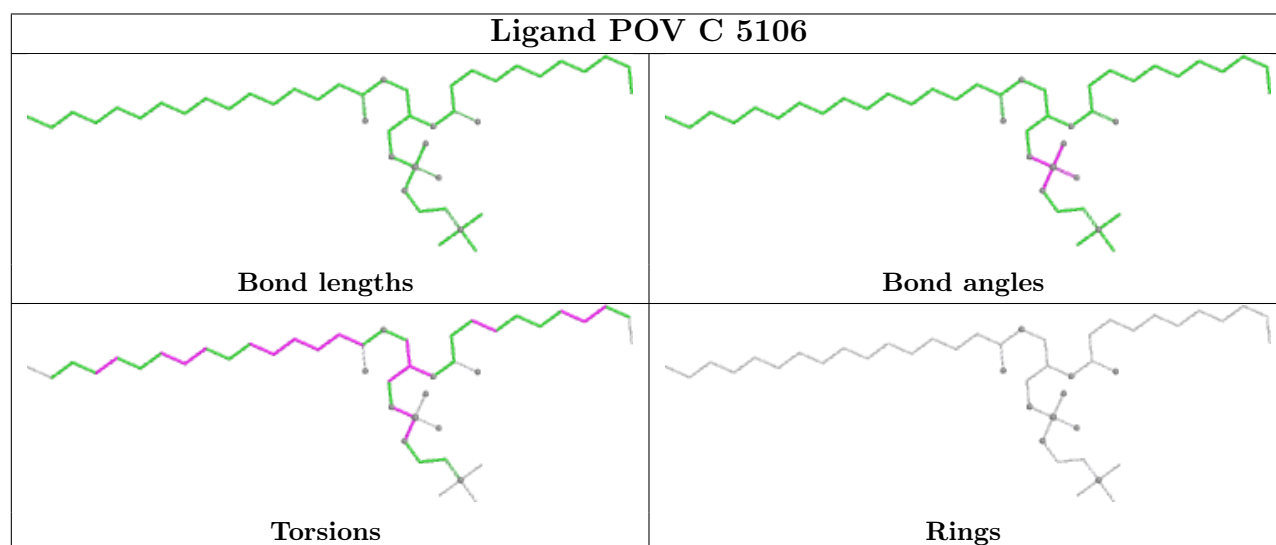
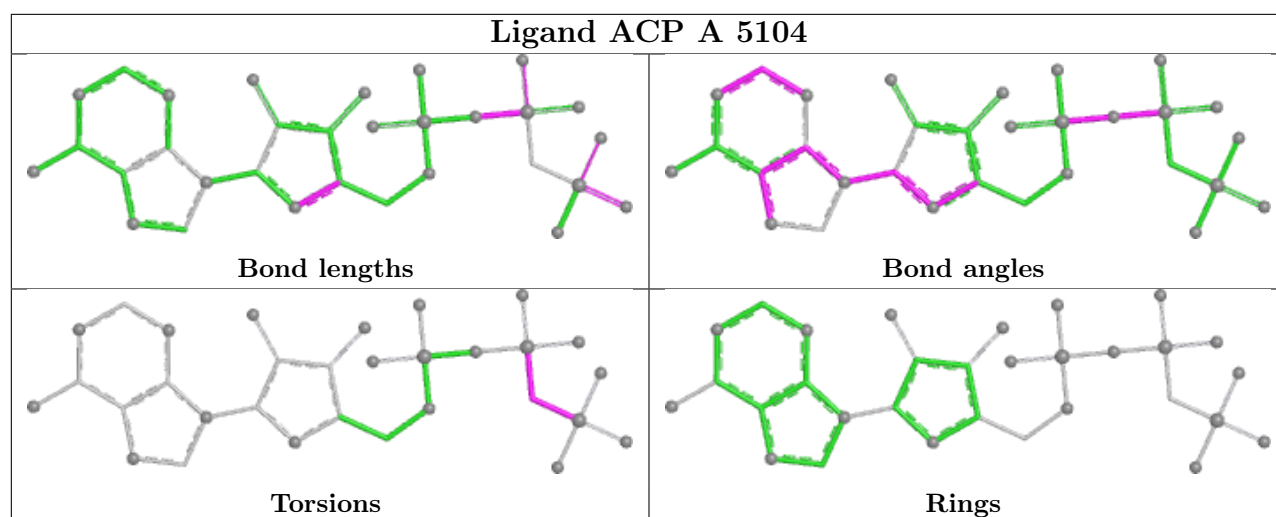
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



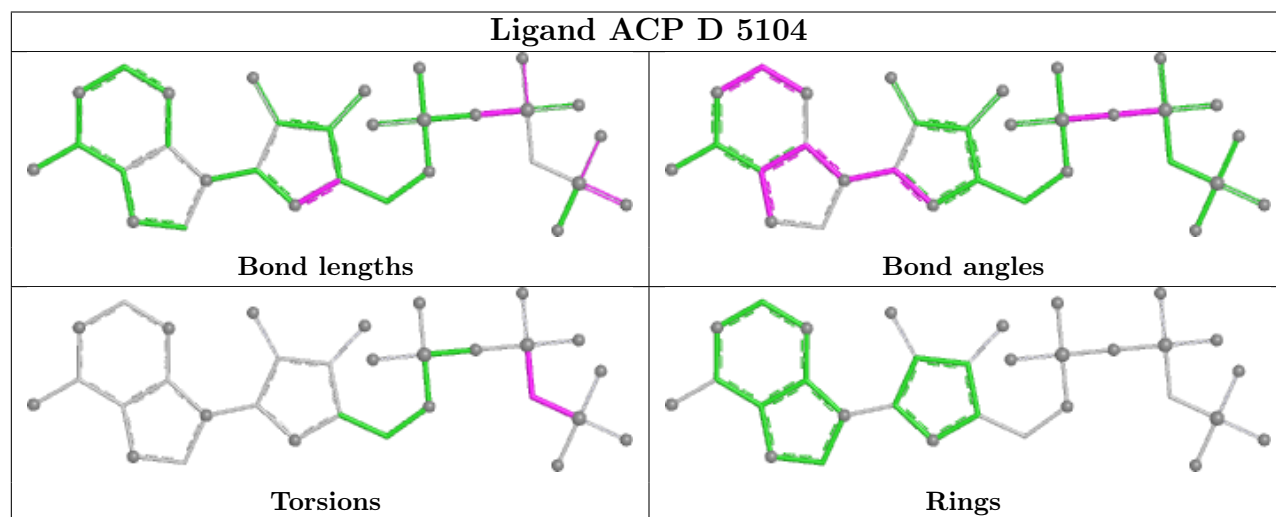
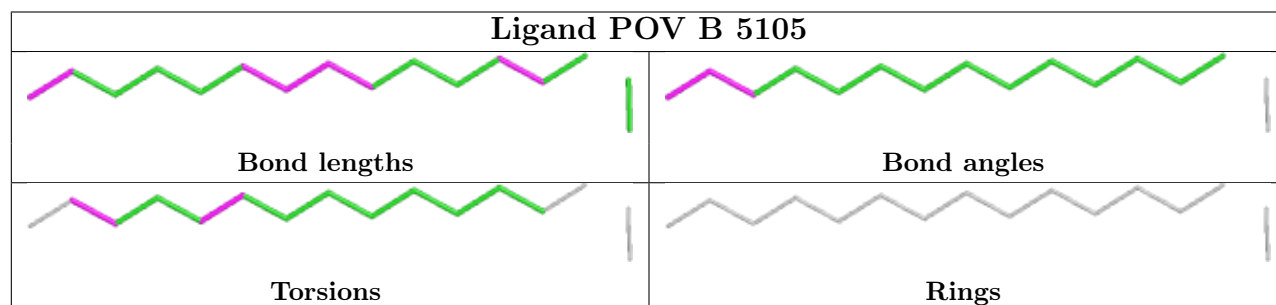
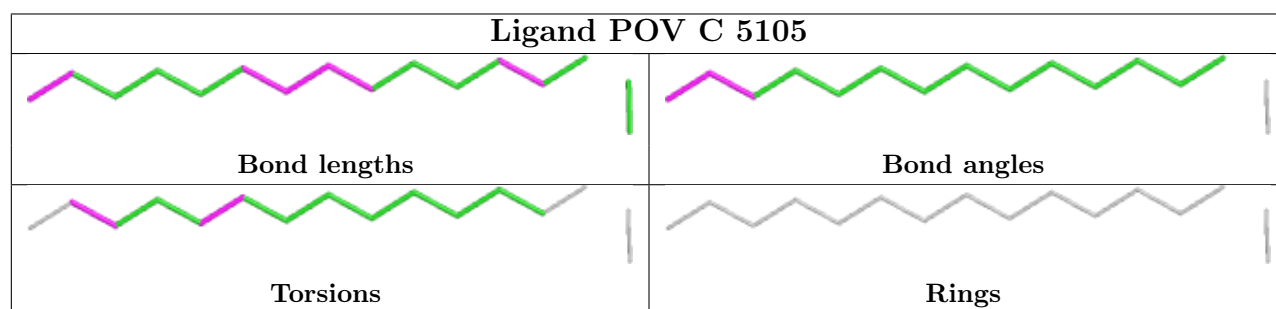
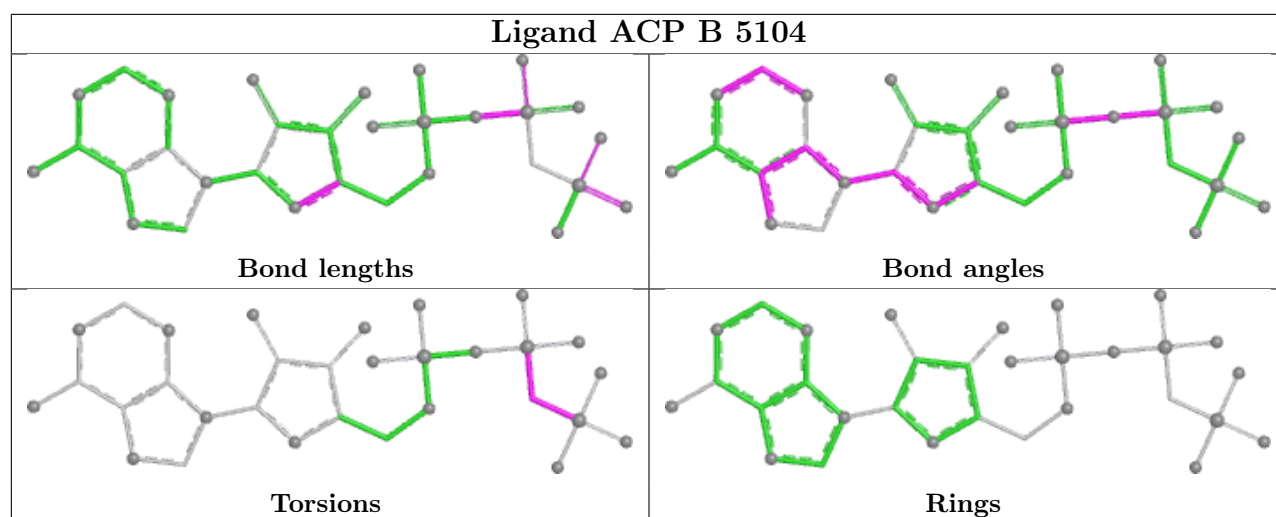




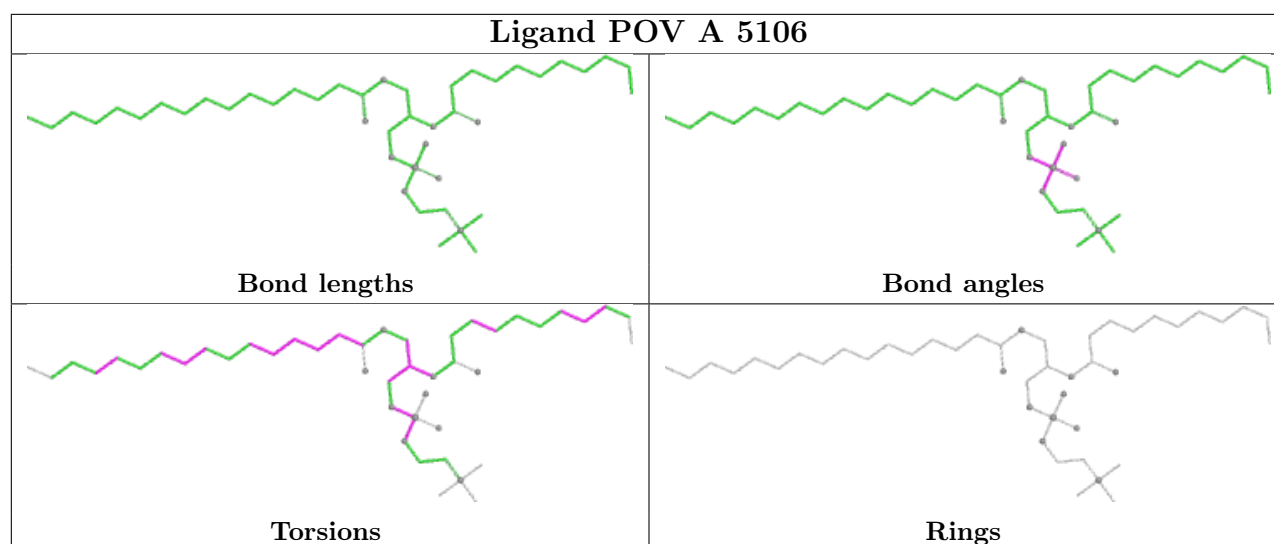












## 5.7 Other polymers [i](#)

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



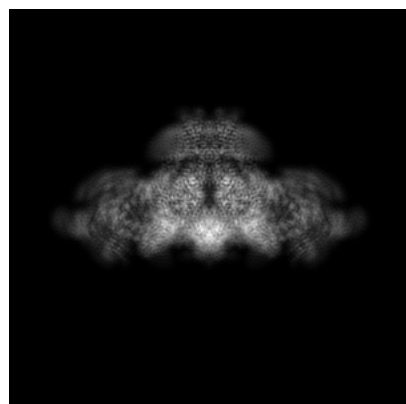
## 6 Map visualisation [i](#)

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.

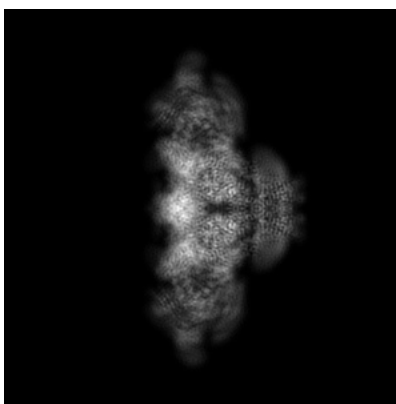
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

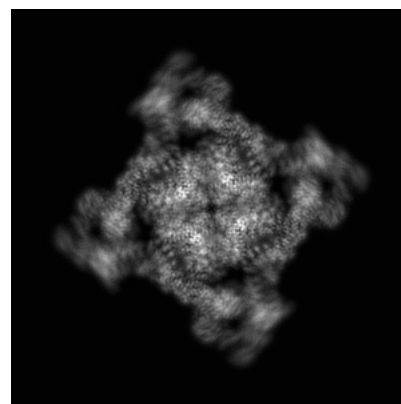
#### 6.1.1 Primary map



X

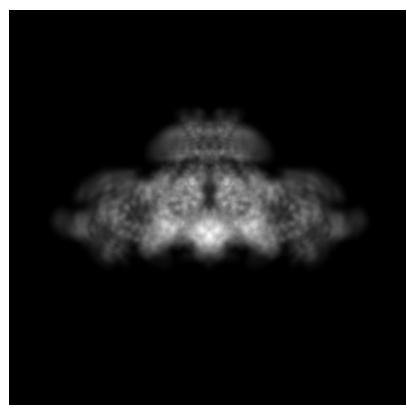


Y

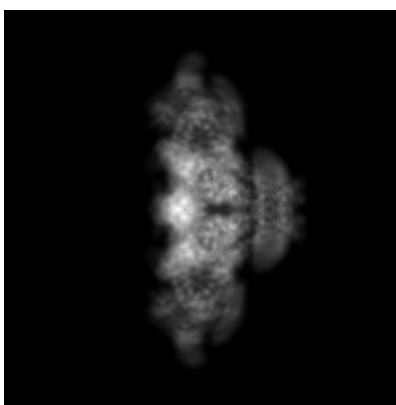


Z

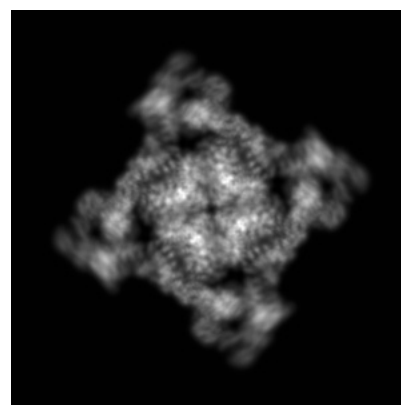
#### 6.1.2 Raw map



X



Y



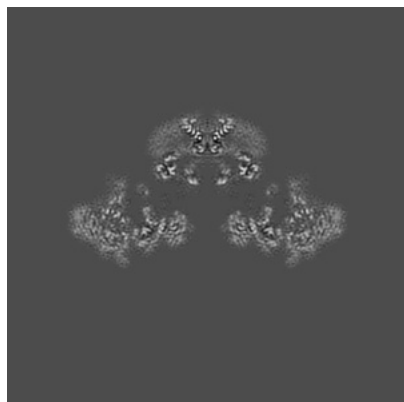
Z

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

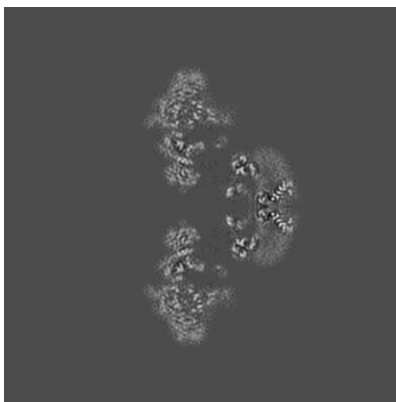


## 6.2 Central slices [i](#)

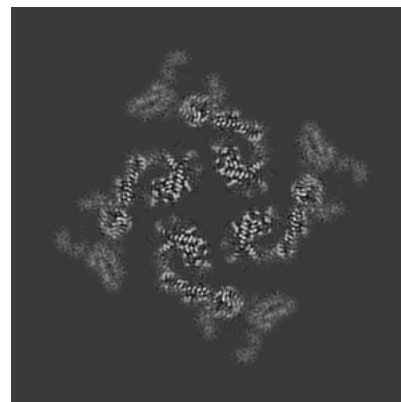
### 6.2.1 Primary map



X Index: 216

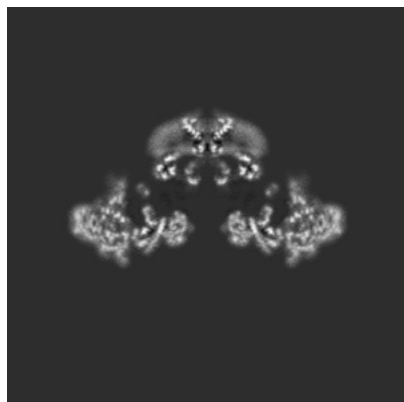


Y Index: 216

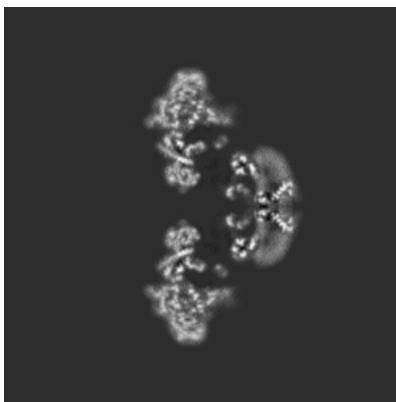


Z Index: 216

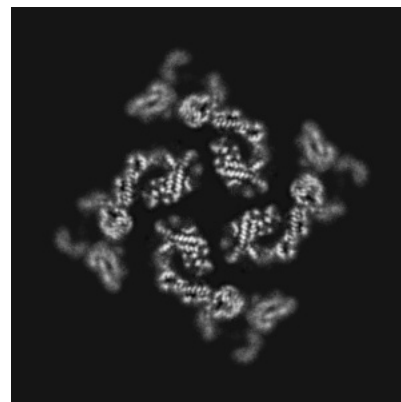
### 6.2.2 Raw map



X Index: 216



Y Index: 216



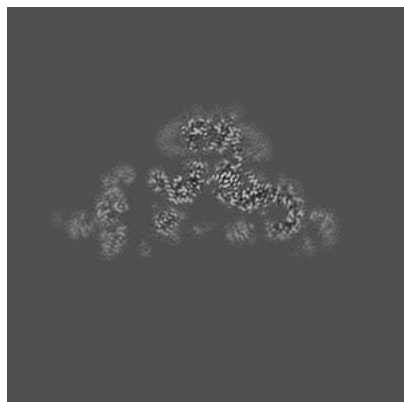
Z Index: 216

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

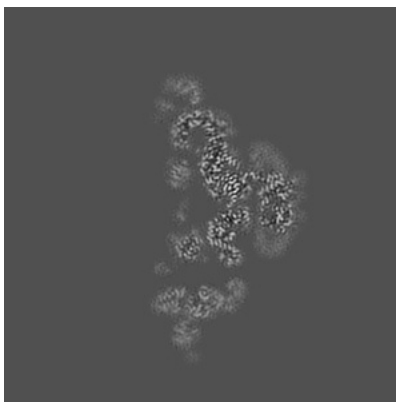


## 6.3 Largest variance slices [i](#)

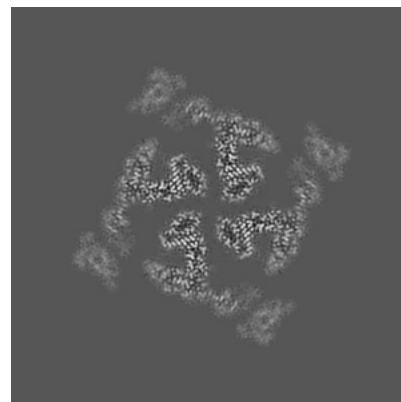
### 6.3.1 Primary map



X Index: 233

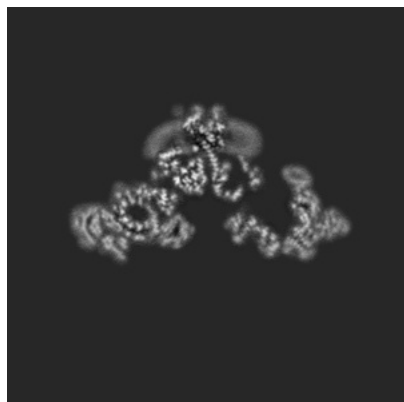


Y Index: 199

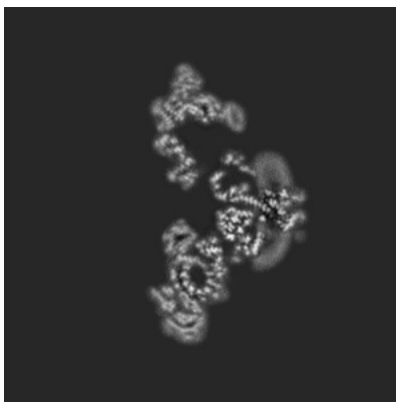


Z Index: 228

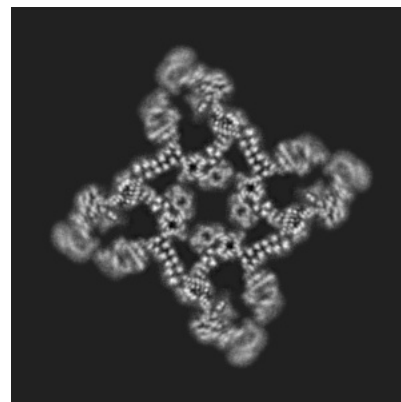
### 6.3.2 Raw map



X Index: 207



Y Index: 225



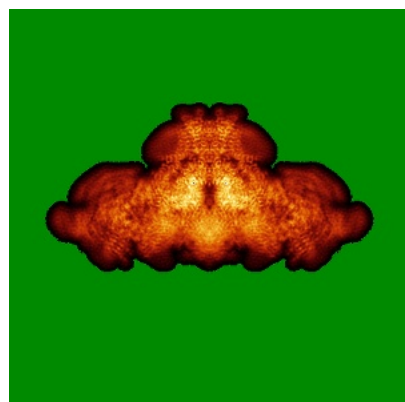
Z Index: 198

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

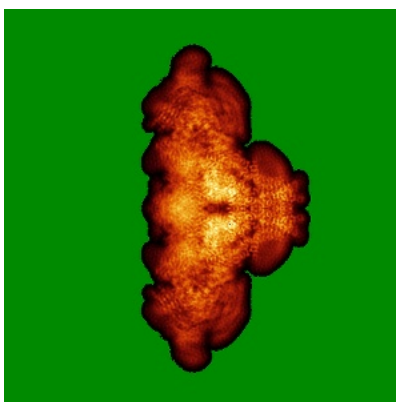


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

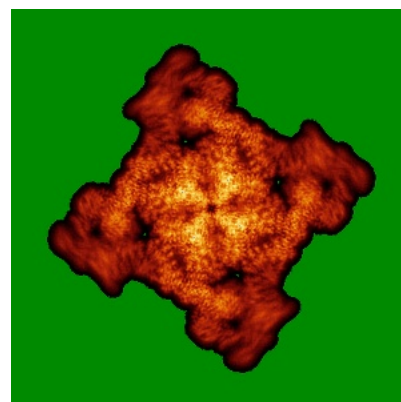
### 6.4.1 Primary map



X

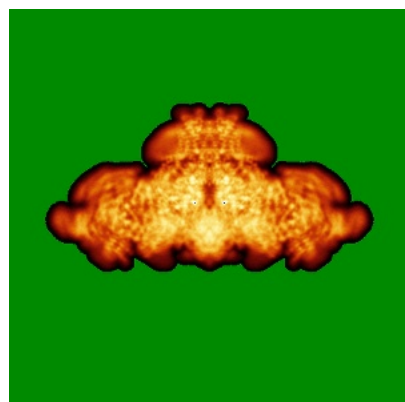


Y

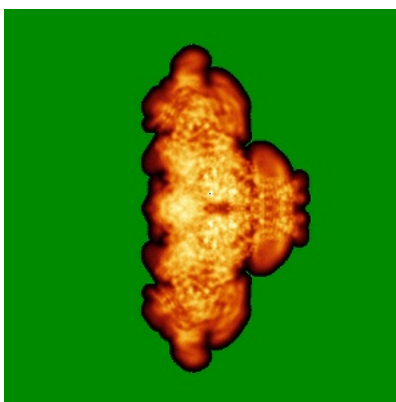


Z

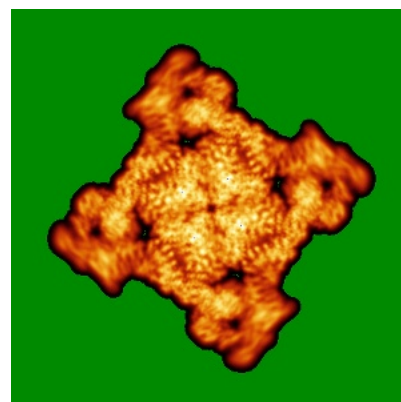
### 6.4.2 Raw map



X



Y



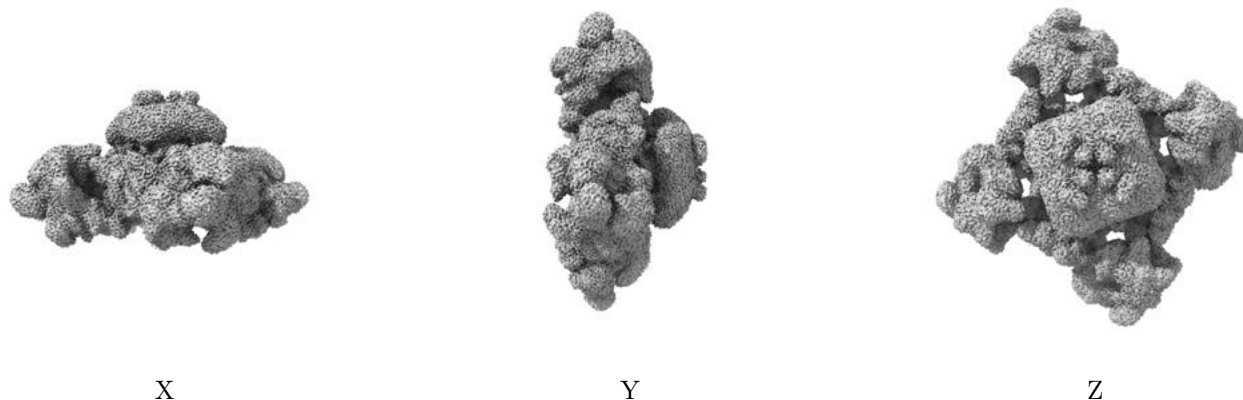
Z

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.



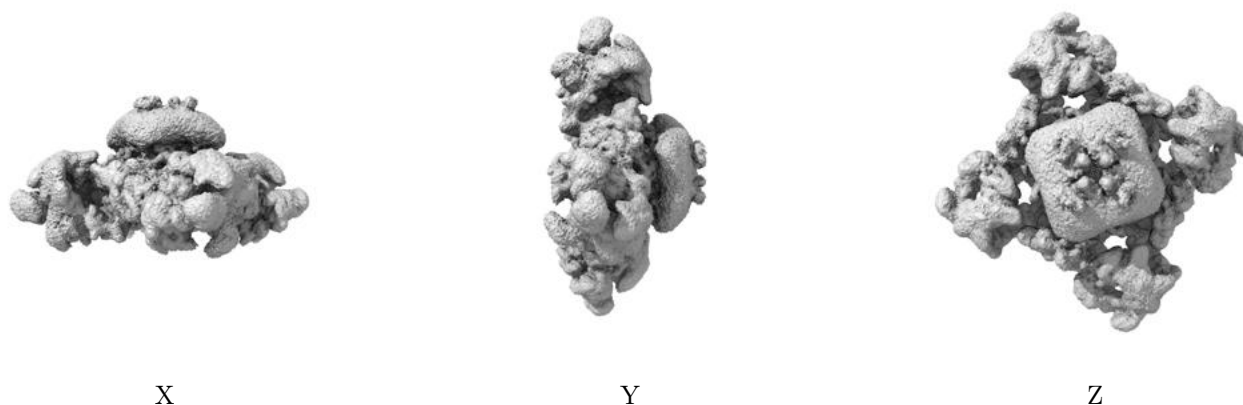
## 6.5 Orthogonal surface views [i](#)

### 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.



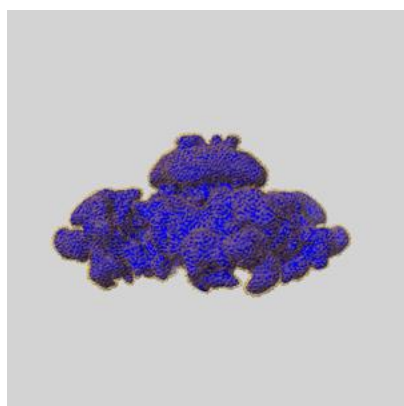
## 6.6 Mask visualisation [i](#)

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

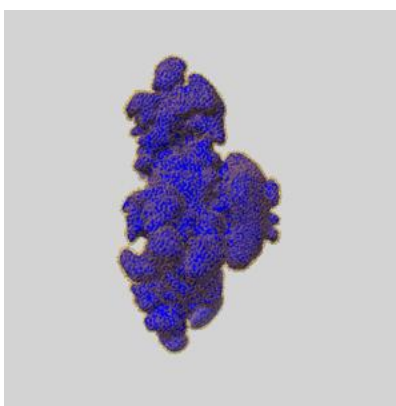
A mask typically either:

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

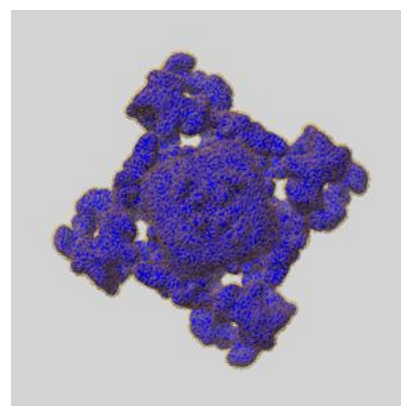
### 6.6.1 emd\_25828\_msk\_1.map [i](#)



X



Y



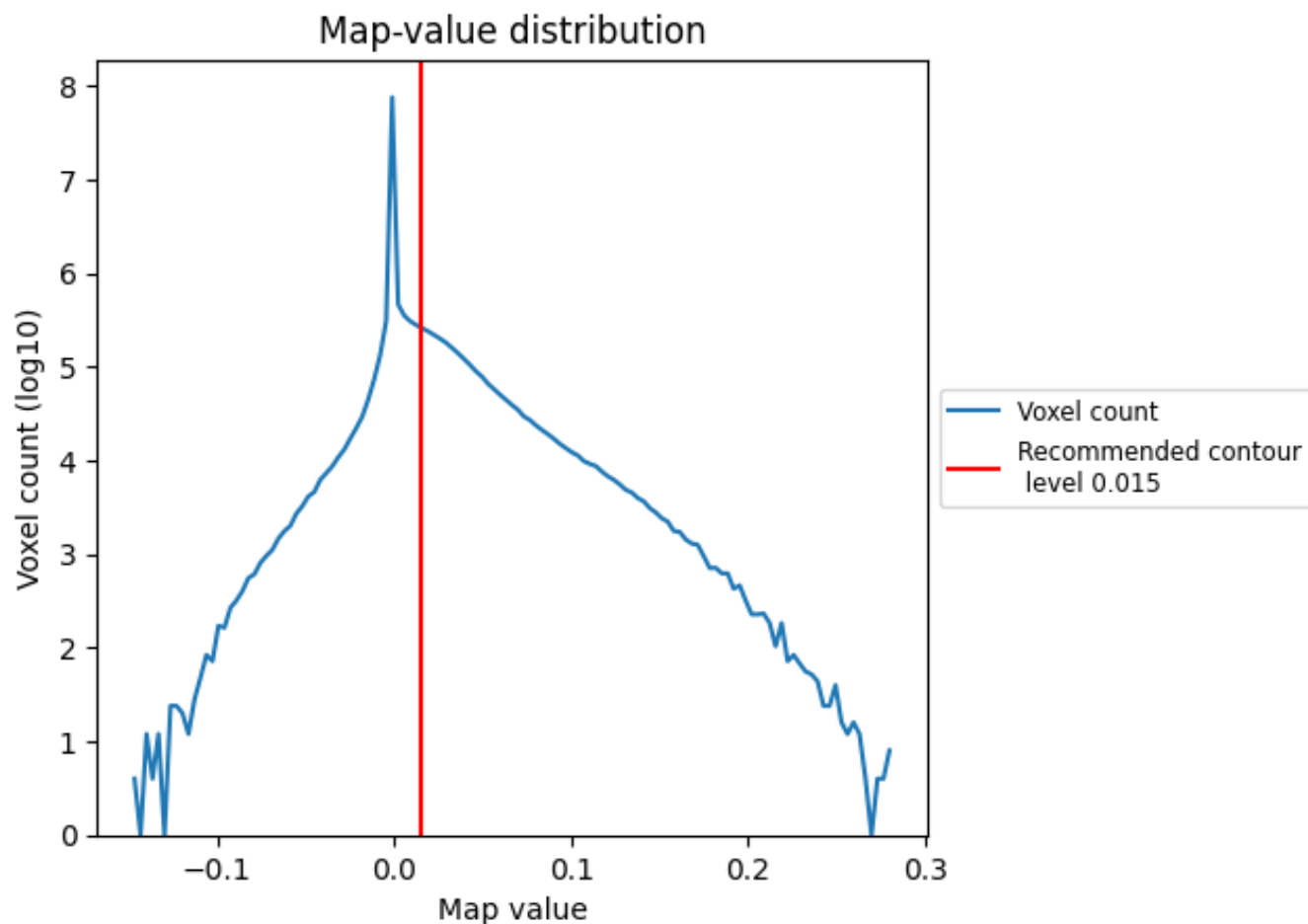
Z



## 7 Map analysis [i](#)

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

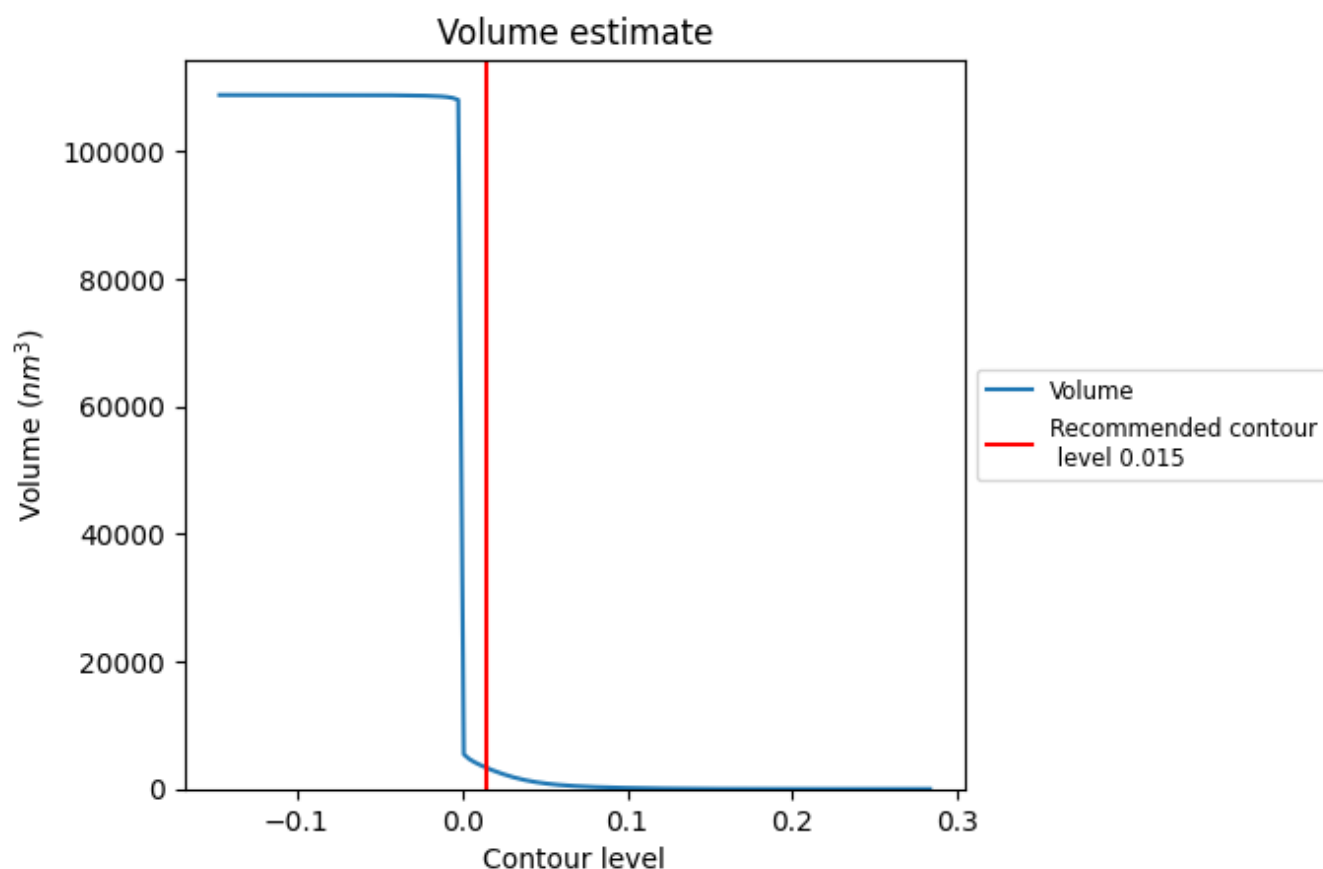
### 7.1 Map-value distribution [i](#)



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](#)

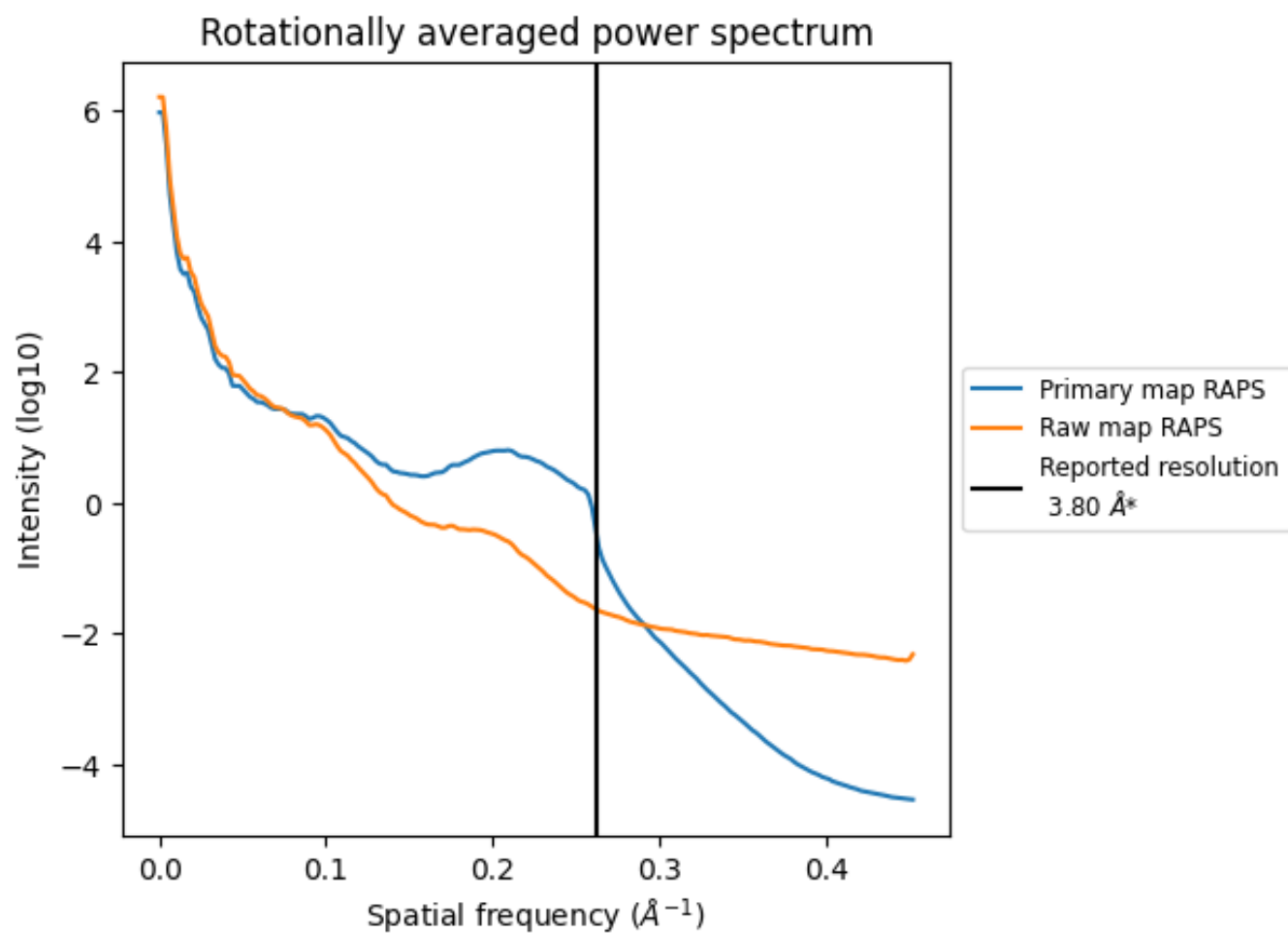


The volume at the recommended contour level is 3290  $\text{nm}^3$ ; this corresponds to an approximate mass of 2972 kDa.

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 ⓘ



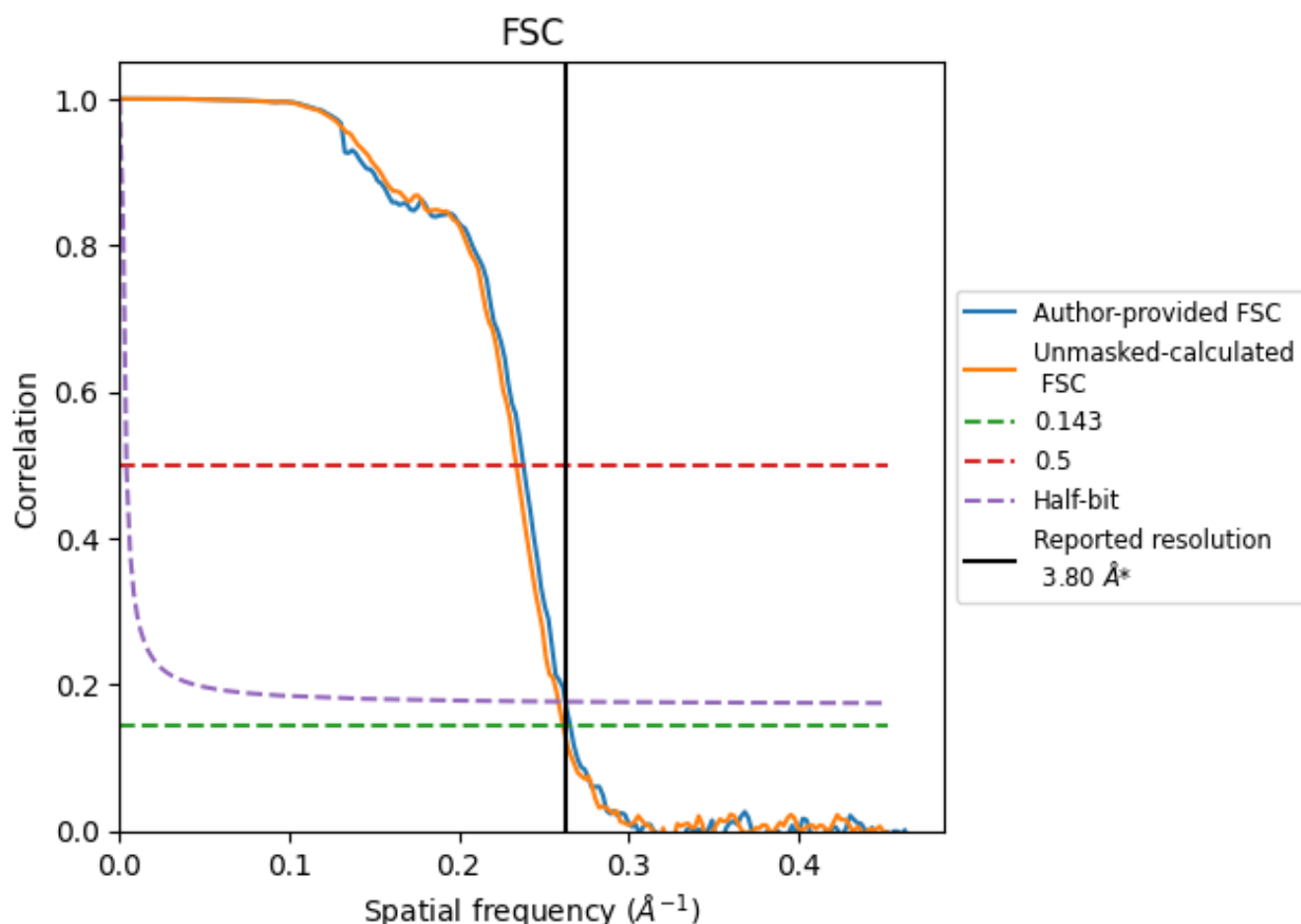
\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>



## 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 Å<sup>-1</sup>



## 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

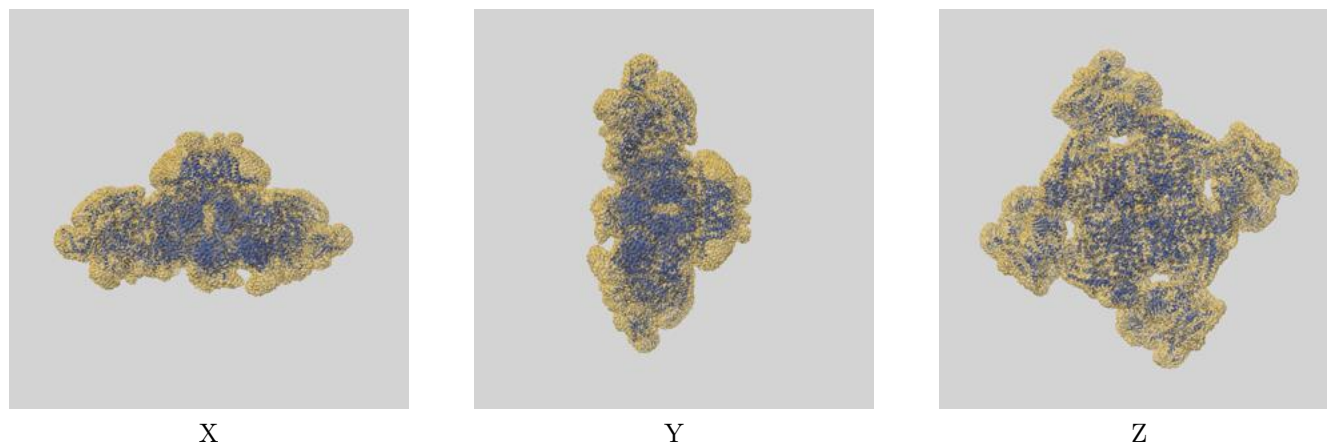
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 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](#).

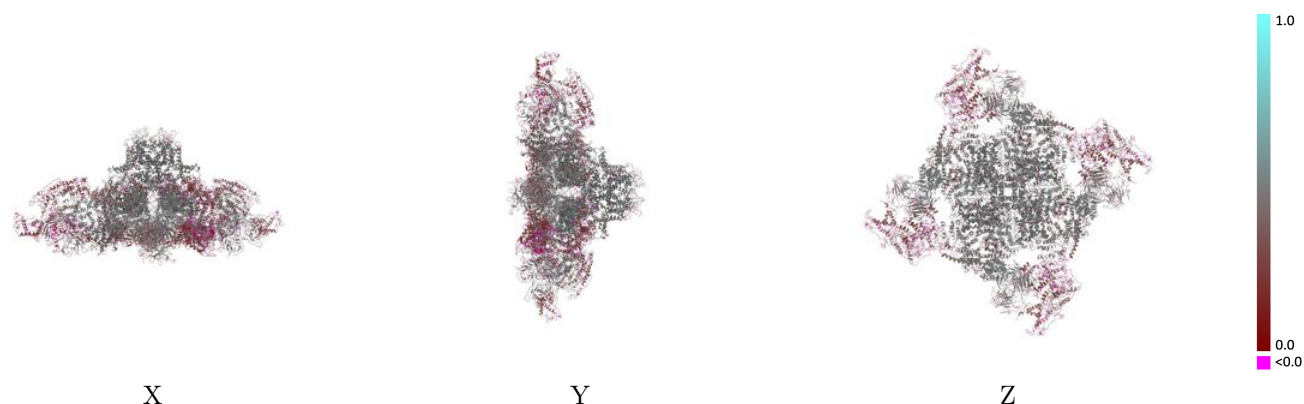
### 9.1 Map-model overlay [i](#)



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.

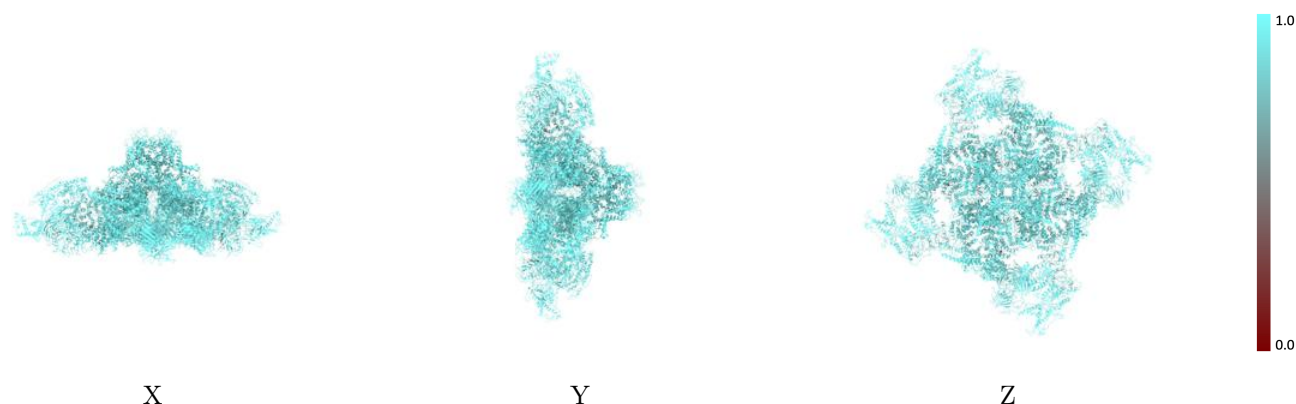


## 9.2 Q-score mapped to coordinate model [i](#)



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.

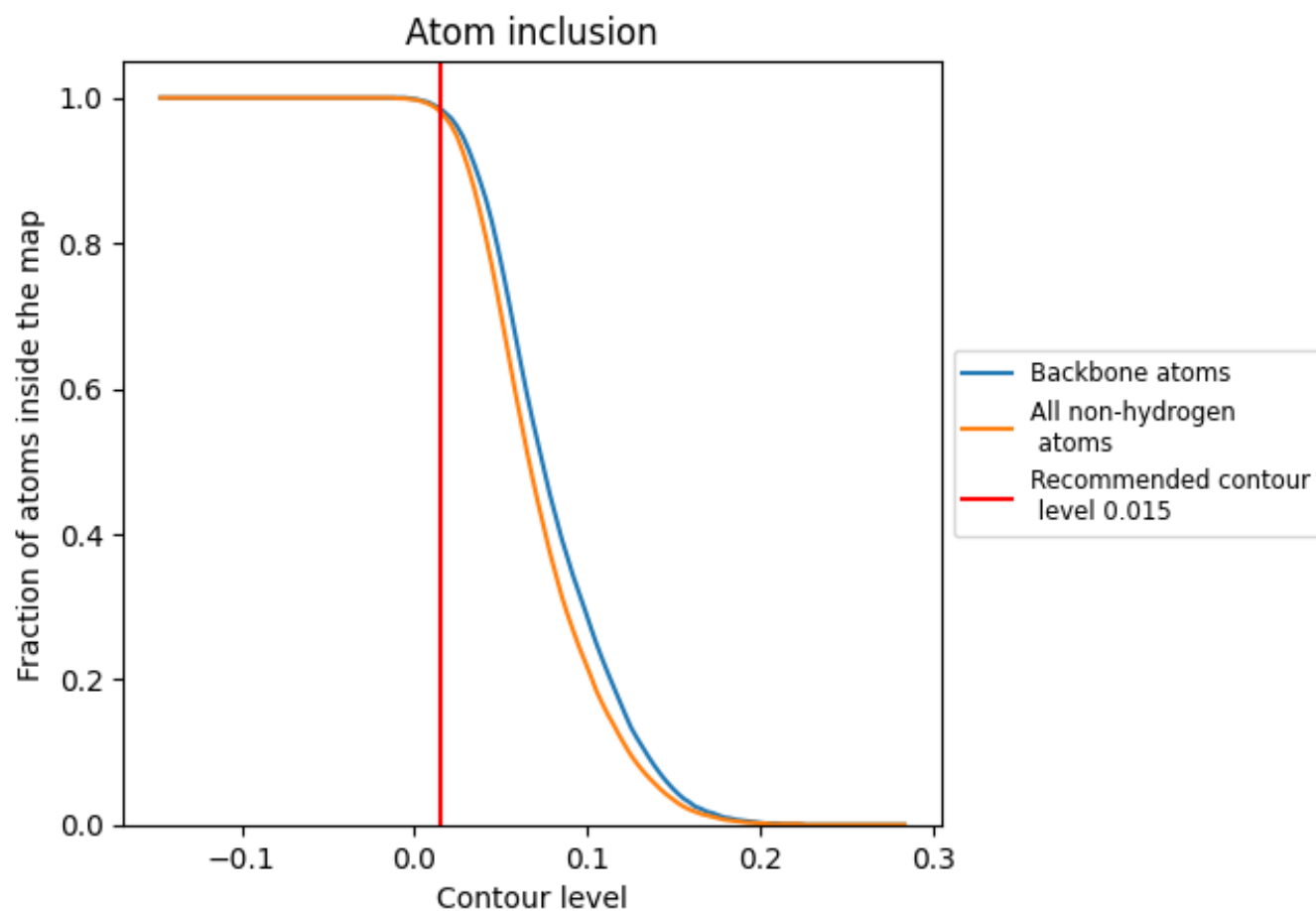
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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	<div></div> 0.9810	<div></div> 0.3860
A	<div></div> 0.9810	<div></div> 0.3860
B	<div></div> 0.9810	<div></div> 0.3860
C	<div></div> 0.9810	<div></div> 0.3860
D	<div></div> 0.9810	<div></div> 0.3850

