



## wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 05:32 AM EDT

PDB ID : 8E9Z  
EMDB ID : EMD-27969  
Title : CryoEM structure of miniGq-coupled hM3R in complex with Iperoxo  
Authors : Zhang, S.; Fay, J.F.; Roth, B.L.  
Deposited on : 2022-08-27  
Resolution : 2.69 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)

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<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

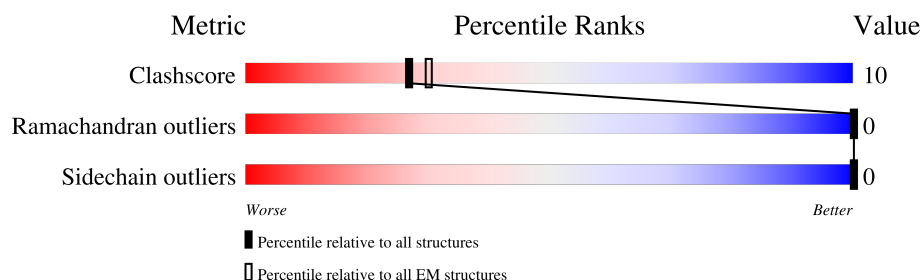
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*






The reported resolution of this entry is 2.69 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	568	
2	B	246	
3	C	368	
4	D	71	
5	E	251	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	IXO	A	801	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8566 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 Muscarinic acetylcholine receptor M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	278	Total	C	N	O	S	0	0
			2173	1450	339	368	16		

There are 203 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	591	GLY	-	expression tag	UNP P20309
A	592	GLY	-	expression tag	UNP P20309
A	593	SER	-	expression tag	UNP P20309
A	594	GLY	-	expression tag	UNP P20309
A	595	GLY	-	expression tag	UNP P20309
A	596	GLY	-	expression tag	UNP P20309
A	597	GLY	-	expression tag	UNP P20309
A	598	SER	-	expression tag	UNP P20309
A	599	GLY	-	expression tag	UNP P20309
A	600	GLY	-	expression tag	UNP P20309
A	601	SER	-	expression tag	UNP P20309
A	602	SER	-	expression tag	UNP P20309
A	603	SER	-	expression tag	UNP P20309
A	604	GLY	-	expression tag	UNP P20309
A	605	GLY	-	expression tag	UNP P20309
A	606	GLY	-	expression tag	UNP P20309
A	607	GLY	-	expression tag	UNP P20309
A	608	SER	-	expression tag	UNP P20309
A	609	GLY	-	expression tag	UNP P20309
A	610	GLY	-	expression tag	UNP P20309
A	611	GLY	-	expression tag	UNP P20309
A	612	GLY	-	expression tag	UNP P20309
A	613	SER	-	expression tag	UNP P20309
A	614	GLY	-	expression tag	UNP P20309
A	615	GLY	-	expression tag	UNP P20309
A	616	SER	-	expression tag	UNP P20309
A	617	SER	-	expression tag	UNP P20309
A	618	SER	-	expression tag	UNP P20309

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Chain	Residue	Modelled	Actual	Comment	Reference
A	619	GLY	-	expression tag	UNP P20309
A	620	GLY	-	expression tag	UNP P20309
A	621	VAL	-	expression tag	UNP P20309
A	622	PHE	-	expression tag	UNP P20309
A	623	THR	-	expression tag	UNP P20309
A	624	LEU	-	expression tag	UNP P20309
A	625	GLU	-	expression tag	UNP P20309
A	626	ASP	-	expression tag	UNP P20309
A	627	PHE	-	expression tag	UNP P20309
A	628	VAL	-	expression tag	UNP P20309
A	629	GLY	-	expression tag	UNP P20309
A	630	ASP	-	expression tag	UNP P20309
A	631	TRP	-	expression tag	UNP P20309
A	632	GLU	-	expression tag	UNP P20309
A	633	GLN	-	expression tag	UNP P20309
A	634	THR	-	expression tag	UNP P20309
A	635	ALA	-	expression tag	UNP P20309
A	636	ALA	-	expression tag	UNP P20309
A	637	TYR	-	expression tag	UNP P20309
A	638	ASN	-	expression tag	UNP P20309
A	639	LEU	-	expression tag	UNP P20309
A	640	ASP	-	expression tag	UNP P20309
A	641	GLN	-	expression tag	UNP P20309
A	642	VAL	-	expression tag	UNP P20309
A	643	LEU	-	expression tag	UNP P20309
A	644	GLU	-	expression tag	UNP P20309
A	645	GLN	-	expression tag	UNP P20309
A	646	GLY	-	expression tag	UNP P20309
A	647	GLY	-	expression tag	UNP P20309
A	648	VAL	-	expression tag	UNP P20309
A	649	SER	-	expression tag	UNP P20309
A	650	SER	-	expression tag	UNP P20309
A	651	LEU	-	expression tag	UNP P20309
A	652	LEU	-	expression tag	UNP P20309
A	653	GLN	-	expression tag	UNP P20309
A	654	ASN	-	expression tag	UNP P20309
A	655	LEU	-	expression tag	UNP P20309
A	656	ALA	-	expression tag	UNP P20309
A	657	VAL	-	expression tag	UNP P20309
A	658	SER	-	expression tag	UNP P20309
A	659	VAL	-	expression tag	UNP P20309
A	660	THR	-	expression tag	UNP P20309

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Chain	Residue	Modelled	Actual	Comment	Reference
A	661	PRO	-	expression tag	UNP P20309
A	662	ILE	-	expression tag	UNP P20309
A	663	GLN	-	expression tag	UNP P20309
A	664	ARG	-	expression tag	UNP P20309
A	665	ILE	-	expression tag	UNP P20309
A	666	VAL	-	expression tag	UNP P20309
A	667	ARG	-	expression tag	UNP P20309
A	668	SER	-	expression tag	UNP P20309
A	669	GLY	-	expression tag	UNP P20309
A	670	GLU	-	expression tag	UNP P20309
A	671	ASN	-	expression tag	UNP P20309
A	672	ALA	-	expression tag	UNP P20309
A	673	LEU	-	expression tag	UNP P20309
A	674	LYS	-	expression tag	UNP P20309
A	675	ILE	-	expression tag	UNP P20309
A	676	ASP	-	expression tag	UNP P20309
A	677	ILE	-	expression tag	UNP P20309
A	678	HIS	-	expression tag	UNP P20309
A	679	VAL	-	expression tag	UNP P20309
A	680	ILE	-	expression tag	UNP P20309
A	681	ILE	-	expression tag	UNP P20309
A	682	PRO	-	expression tag	UNP P20309
A	683	TYR	-	expression tag	UNP P20309
A	684	GLU	-	expression tag	UNP P20309
A	685	GLY	-	expression tag	UNP P20309
A	686	LEU	-	expression tag	UNP P20309
A	687	SER	-	expression tag	UNP P20309
A	688	ALA	-	expression tag	UNP P20309
A	689	ASP	-	expression tag	UNP P20309
A	690	GLN	-	expression tag	UNP P20309
A	691	MET	-	expression tag	UNP P20309
A	692	ALA	-	expression tag	UNP P20309
A	693	GLN	-	expression tag	UNP P20309
A	694	ILE	-	expression tag	UNP P20309
A	695	GLU	-	expression tag	UNP P20309
A	696	GLU	-	expression tag	UNP P20309
A	697	VAL	-	expression tag	UNP P20309
A	698	PHE	-	expression tag	UNP P20309
A	699	LYS	-	expression tag	UNP P20309
A	700	VAL	-	expression tag	UNP P20309
A	701	VAL	-	expression tag	UNP P20309
A	702	TYR	-	expression tag	UNP P20309

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Chain	Residue	Modelled	Actual	Comment	Reference
A	703	PRO	-	expression tag	UNP P20309
A	704	VAL	-	expression tag	UNP P20309
A	705	ASP	-	expression tag	UNP P20309
A	706	ASP	-	expression tag	UNP P20309
A	707	HIS	-	expression tag	UNP P20309
A	708	HIS	-	expression tag	UNP P20309
A	709	PHE	-	expression tag	UNP P20309
A	710	LYS	-	expression tag	UNP P20309
A	711	VAL	-	expression tag	UNP P20309
A	712	ILE	-	expression tag	UNP P20309
A	713	LEU	-	expression tag	UNP P20309
A	714	PRO	-	expression tag	UNP P20309
A	715	TYR	-	expression tag	UNP P20309
A	716	GLY	-	expression tag	UNP P20309
A	717	THR	-	expression tag	UNP P20309
A	718	LEU	-	expression tag	UNP P20309
A	719	VAL	-	expression tag	UNP P20309
A	720	ILE	-	expression tag	UNP P20309
A	721	ASP	-	expression tag	UNP P20309
A	722	GLY	-	expression tag	UNP P20309
A	723	VAL	-	expression tag	UNP P20309
A	724	THR	-	expression tag	UNP P20309
A	725	PRO	-	expression tag	UNP P20309
A	726	ASN	-	expression tag	UNP P20309
A	727	MET	-	expression tag	UNP P20309
A	728	LEU	-	expression tag	UNP P20309
A	729	ASN	-	expression tag	UNP P20309
A	730	TYR	-	expression tag	UNP P20309
A	731	PHE	-	expression tag	UNP P20309
A	732	GLY	-	expression tag	UNP P20309
A	733	ARG	-	expression tag	UNP P20309
A	734	PRO	-	expression tag	UNP P20309
A	735	TYR	-	expression tag	UNP P20309
A	736	GLU	-	expression tag	UNP P20309
A	737	GLY	-	expression tag	UNP P20309
A	738	ILE	-	expression tag	UNP P20309
A	739	ALA	-	expression tag	UNP P20309
A	740	VAL	-	expression tag	UNP P20309
A	741	PHE	-	expression tag	UNP P20309
A	742	ASP	-	expression tag	UNP P20309
A	743	GLY	-	expression tag	UNP P20309
A	744	LYS	-	expression tag	UNP P20309

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Chain	Residue	Modelled	Actual	Comment	Reference
A	745	LYS	-	expression tag	UNP P20309
A	746	ILE	-	expression tag	UNP P20309
A	747	THR	-	expression tag	UNP P20309
A	748	VAL	-	expression tag	UNP P20309
A	749	THR	-	expression tag	UNP P20309
A	750	GLY	-	expression tag	UNP P20309
A	751	THR	-	expression tag	UNP P20309
A	752	LEU	-	expression tag	UNP P20309
A	753	TRP	-	expression tag	UNP P20309
A	754	ASN	-	expression tag	UNP P20309
A	755	GLY	-	expression tag	UNP P20309
A	756	ASN	-	expression tag	UNP P20309
A	757	LYS	-	expression tag	UNP P20309
A	758	ILE	-	expression tag	UNP P20309
A	759	ILE	-	expression tag	UNP P20309
A	760	ASP	-	expression tag	UNP P20309
A	761	GLU	-	expression tag	UNP P20309
A	762	ARG	-	expression tag	UNP P20309
A	763	LEU	-	expression tag	UNP P20309
A	764	ILE	-	expression tag	UNP P20309
A	765	THR	-	expression tag	UNP P20309
A	766	PRO	-	expression tag	UNP P20309
A	767	ASP	-	expression tag	UNP P20309
A	768	GLY	-	expression tag	UNP P20309
A	769	SER	-	expression tag	UNP P20309
A	770	MET	-	expression tag	UNP P20309
A	771	LEU	-	expression tag	UNP P20309
A	772	PHE	-	expression tag	UNP P20309
A	773	ARG	-	expression tag	UNP P20309
A	774	VAL	-	expression tag	UNP P20309
A	775	THR	-	expression tag	UNP P20309
A	776	ILE	-	expression tag	UNP P20309
A	777	ASN	-	expression tag	UNP P20309
A	778	SER	-	expression tag	UNP P20309
A	779	GLY	-	expression tag	UNP P20309
A	780	GLY	-	expression tag	UNP P20309
A	781	SER	-	expression tag	UNP P20309
A	782	GLY	-	expression tag	UNP P20309
A	783	GLY	-	expression tag	UNP P20309
A	784	HIS	-	expression tag	UNP P20309
A	785	HIS	-	expression tag	UNP P20309
A	786	HIS	-	expression tag	UNP P20309

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Chain	Residue	Modelled	Actual	Comment	Reference
A	787	HIS	-	expression tag	UNP P20309
A	788	HIS	-	expression tag	UNP P20309
A	789	HIS	-	expression tag	UNP P20309
A	790	HIS	-	expression tag	UNP P20309
A	791	HIS	-	expression tag	UNP P20309
A	792	HIS	-	expression tag	UNP P20309
A	793	HIS	-	expression tag	UNP P20309

- Molecule 2 is a protein called miniGq.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	222	Total	C	N	O	S	0	0
			1698	1081	296	314	7		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	339	Total	C	N	O	S	0	0
			2504	1556	446	483	19		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	341	GLY	-	expression tag	UNP P62873
C	342	GLY	-	expression tag	UNP P62873
C	343	SER	-	expression tag	UNP P62873
C	344	GLY	-	expression tag	UNP P62873
C	345	GLY	-	expression tag	UNP P62873
C	346	GLY	-	expression tag	UNP P62873
C	347	GLY	-	expression tag	UNP P62873
C	348	SER	-	expression tag	UNP P62873
C	349	GLY	-	expression tag	UNP P62873
C	350	GLY	-	expression tag	UNP P62873
C	351	SER	-	expression tag	UNP P62873
C	352	SER	-	expression tag	UNP P62873
C	353	SER	-	expression tag	UNP P62873
C	354	GLY	-	expression tag	UNP P62873
C	355	GLY	-	expression tag	UNP P62873
C	356	VAL	-	expression tag	UNP P62873
C	357	SER	-	expression tag	UNP P62873
C	358	GLY	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
C	359	TRP	-	expression tag	UNP P62873
C	360	ARG	-	expression tag	UNP P62873
C	361	LEU	-	expression tag	UNP P62873
C	362	PHE	-	expression tag	UNP P62873
C	363	LYS	-	expression tag	UNP P62873
C	364	LYS	-	expression tag	UNP P62873
C	365	ILE	-	expression tag	UNP P62873
C	366	SER	-	expression tag	UNP P62873
C	367	GLY	-	expression tag	UNP P62873
C	368	GLY	-	expression tag	UNP P62873
C	369	SER	-	expression tag	UNP P62873

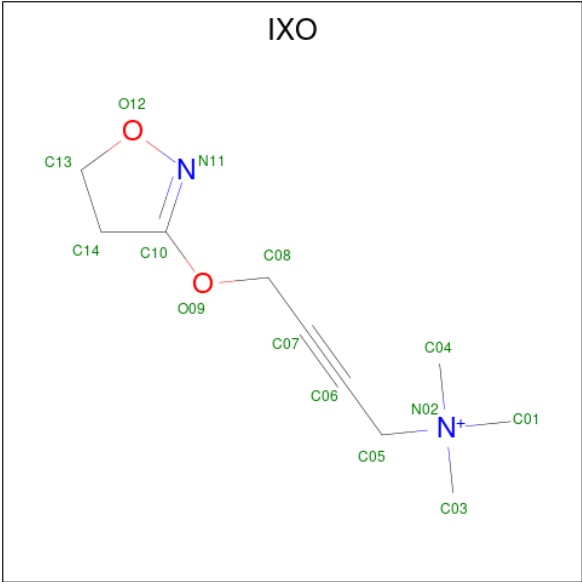
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	57	Total	C	N	O	S	0	0
			397	249	69	77	2		

- Molecule 5 is a protein called scFv16.

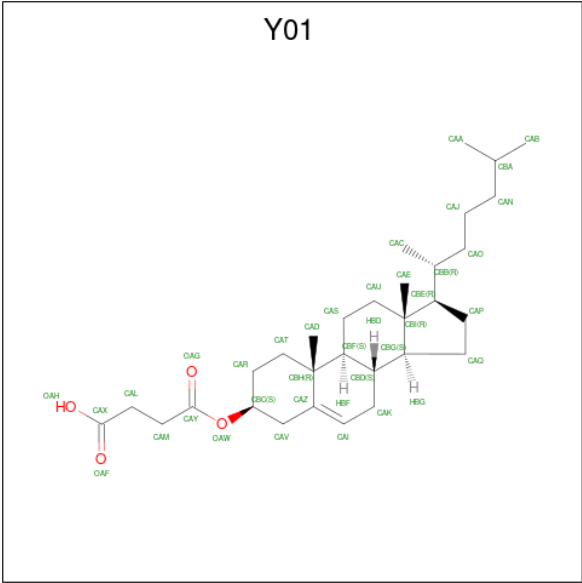
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	233	Total	C	N	O	S	0	0
			1745	1111	291	333	10		

- Molecule 6 is 4-(4,5-dihydro-1,2-oxazol-3-yloxy)-N,N,N-trimethylbut-2-yn-1-aminium (three-letter code: IXO) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



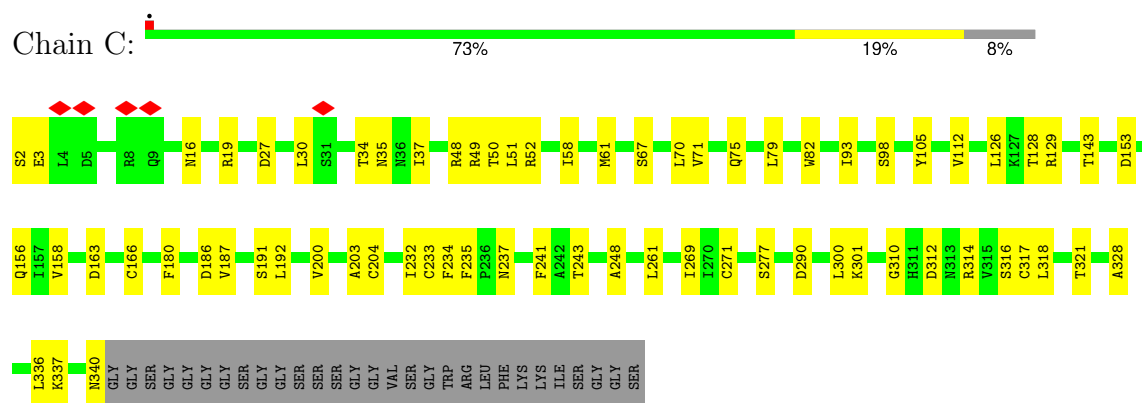
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	10	2	2	

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

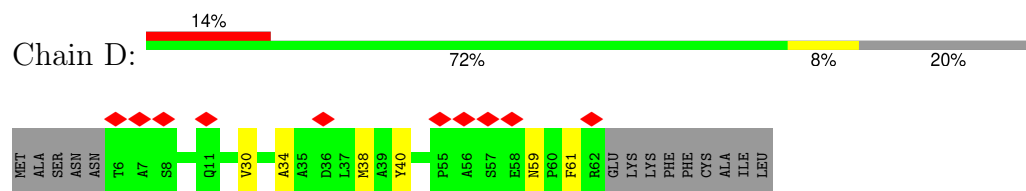


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	O		0
			35	31	4		

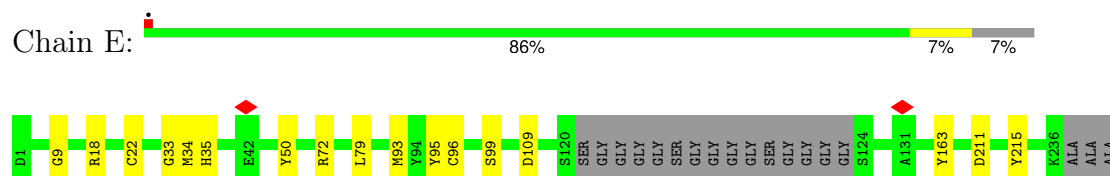




- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 5: scFv16



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	462349	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	59.00	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.862	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.06	Depositor
Map size ( $\text{\AA}$ )	253.44, 253.44, 253.44	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.88, 0.88, 0.88	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: IXO, Y01

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	0.28	0/2230	0.48	0/3057
2	B	0.28	0/1729	0.57	0/2344
3	C	0.26	0/2551	0.57	0/3473
4	D	0.23	0/403	0.43	0/552
5	E	0.32	0/1789	0.59	0/2431
All	All	0.28	0/8702	0.55	0/11857

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	2173	0	2173	52	0
2	B	1698	0	1609	34	0
3	C	2504	0	2337	58	0
4	D	397	0	370	20	0
5	E	1745	0	1651	18	0
6	A	14	0	17	8	0
7	A	35	0	49	5	0
All	All	8566	0	8206	162	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 10.

The worst 5 of 162 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:161:VAL:HG13	1:A:188:MET:CE	1.85	1.06
5:E:93:MET:HE2	5:E:95:TYR:CE1	1.96	1.00
3:C:34:THR:HG22	4:D:38:MET:SD	2.02	1.00
2:B:173:PRO:HA	2:B:188:ARG:HD3	1.02	0.98
1:A:125:PHE:CZ	1:A:129:ILE:HD11	1.98	0.97

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	274/568 (48%)	266 (97%)	8 (3%)	0	100	100
2	B	216/246 (88%)	207 (96%)	9 (4%)	0	100	100
3	C	337/368 (92%)	324 (96%)	13 (4%)	0	100	100
4	D	55/71 (78%)	55 (100%)	0	0	100	100
5	E	229/251 (91%)	224 (98%)	5 (2%)	0	100	100
All	All	1111/1504 (74%)	1076 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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



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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/478 (48%)	229 (100%)	0	100	100
2	B	170/213 (80%)	170 (100%)	0	100	100
3	C	253/298 (85%)	253 (100%)	0	100	100
4	D	36/58 (62%)	36 (100%)	0	100	100
5	E	184/201 (92%)	184 (100%)	0	100	100
All	All	872/1248 (70%)	872 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	514	ASN
1	A	527	ASN
4	D	59	ASN
5	E	35	HIS

### 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 ⓘ

2 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
7	Y01	A	802	-	38,38,38	0.81	1 (2%)	57,57,57	1.35	6 (10%)
6	IXO	A	801	-	13,14,14	0.98	1 (7%)	12,18,18	1.03	1 (8%)

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
7	Y01	A	802	-	-	13/19/77/77	0/4/4/4
6	IXO	A	801	-	-	5/9/16/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	IXO	C10-N11	2.88	1.32	1.29
7	A	802	Y01	OAW-CBC	-2.02	1.41	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	802	Y01	CBI-CBE-CBB	-4.50	112.54	119.50
7	A	802	Y01	CBH-CBF-CBD	-3.03	108.28	112.71
7	A	802	Y01	OAW-CAY-OAG	-2.66	117.49	123.70
7	A	802	Y01	CBI-CBG-CBD	-2.62	110.69	114.41
6	A	801	IXO	C13-O12-N11	2.25	110.33	108.13

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

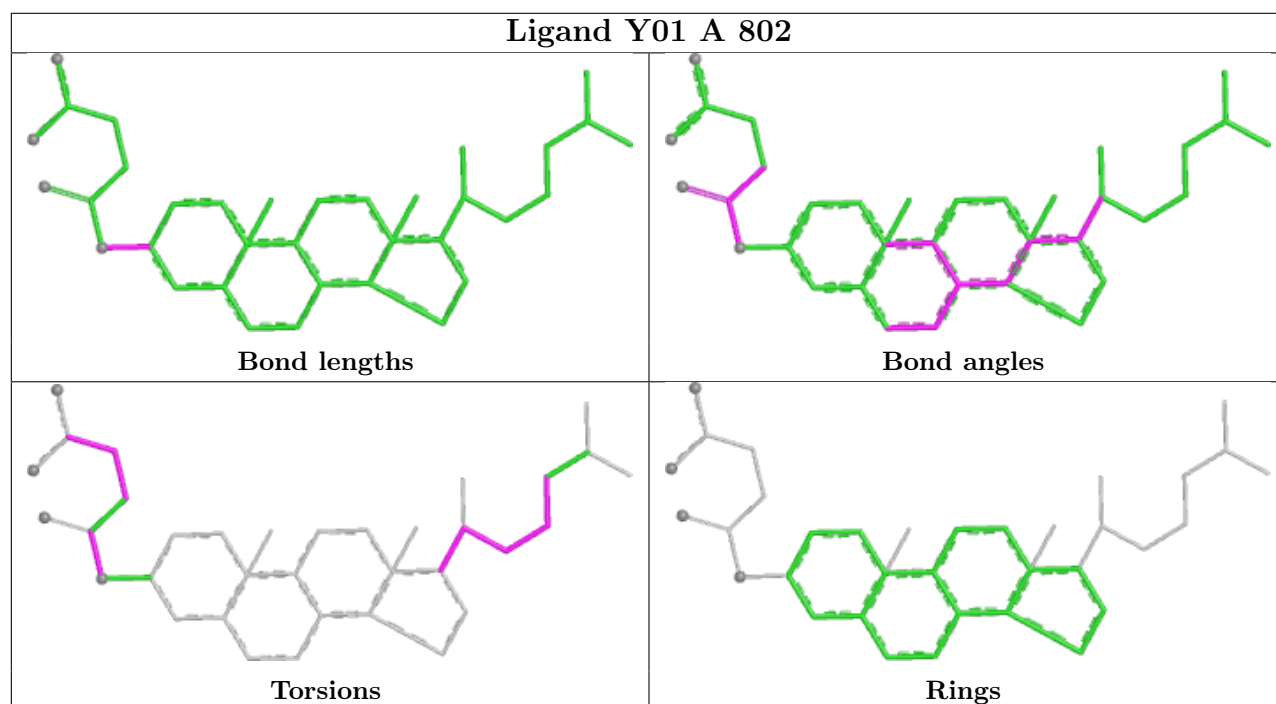
Mol	Chain	Res	Type	Atoms
6	A	801	IXO	N02-C05-C06-C07
6	A	801	IXO	C06-C07-C08-O09
6	A	801	IXO	N11-C10-O09-C08
7	A	802	Y01	CAC-CBB-CBE-CAP
7	A	802	Y01	CAC-CBB-CBE-CBI

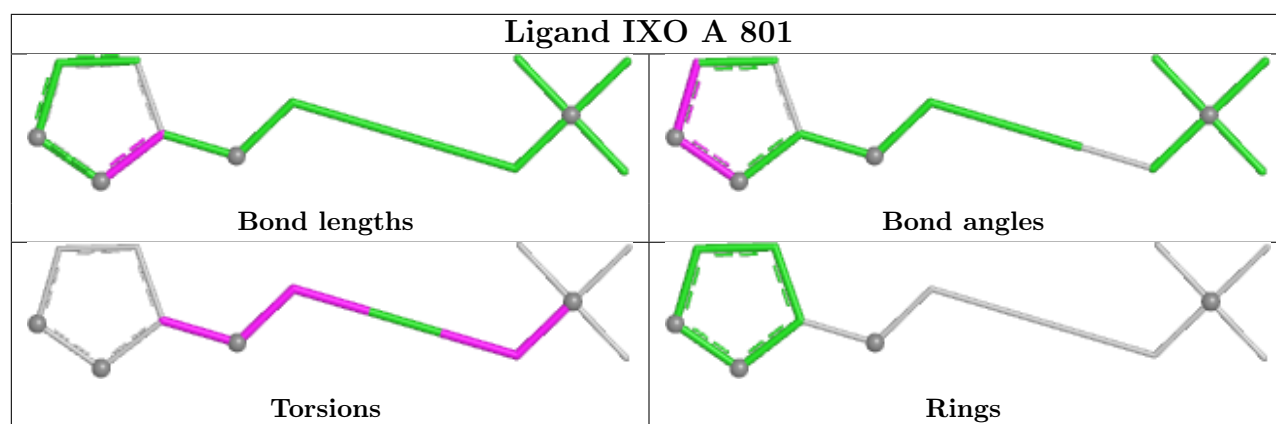
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	802	Y01	5	0
6	A	801	IXO	8	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.

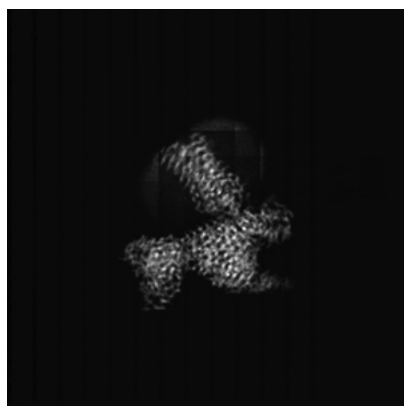
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27969. These allow visual inspection of the internal detail of the map and identification of artifacts.

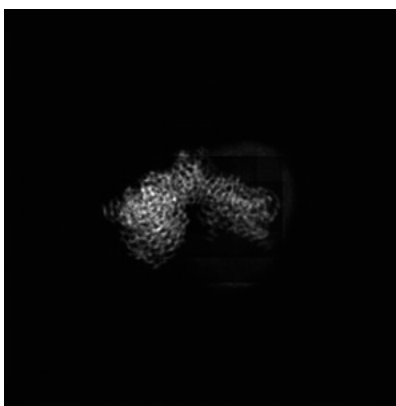
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

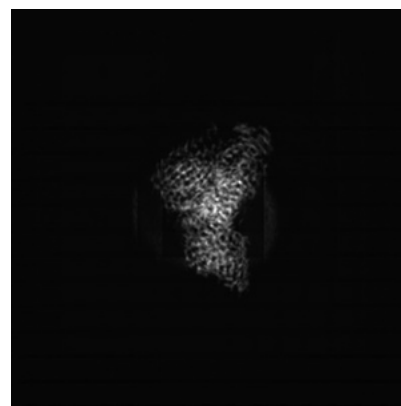
#### 6.1.1 Primary map



X

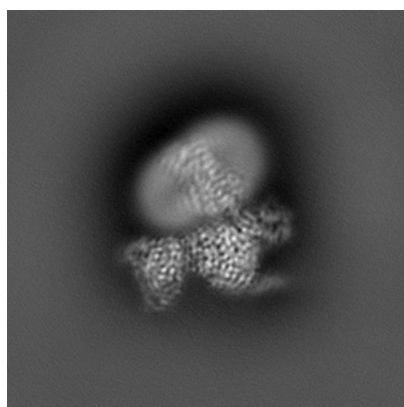


Y

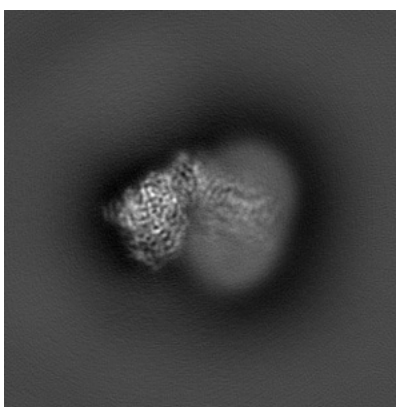


Z

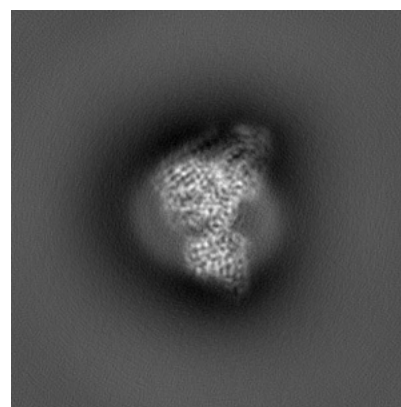
#### 6.1.2 Raw map



X



Y



Z

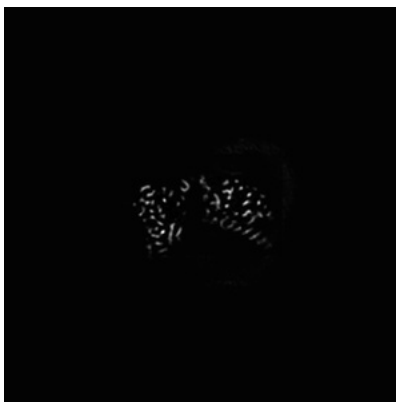
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

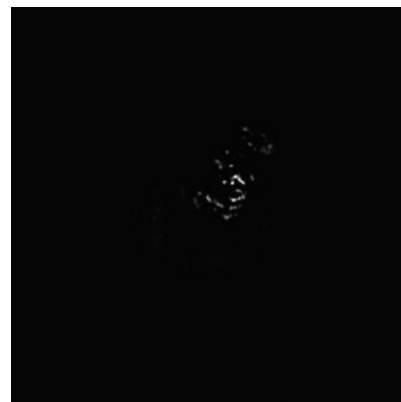
### 6.2.1 Primary map



X Index: 144

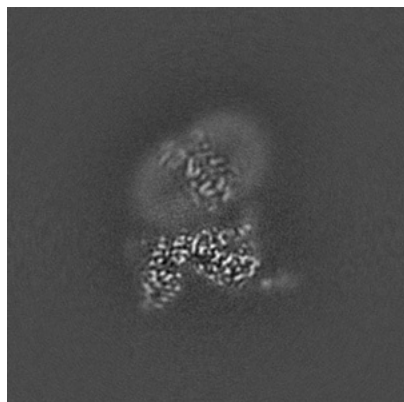


Y Index: 144

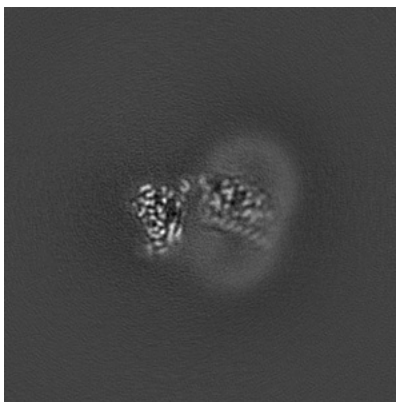


Z Index: 144

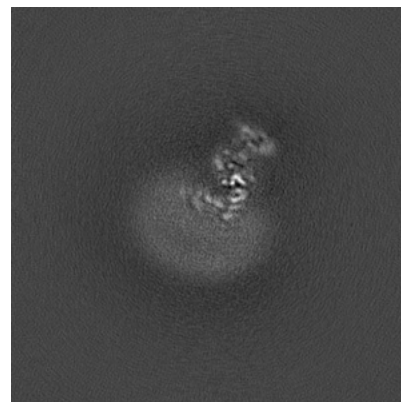
### 6.2.2 Raw map



X Index: 144



Y Index: 144

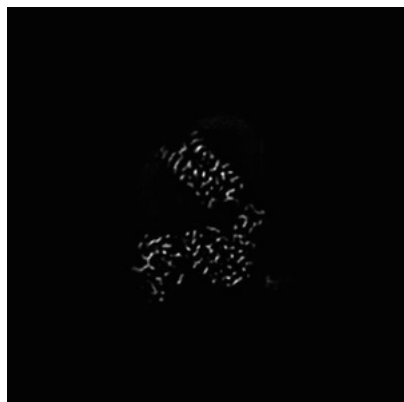


Z Index: 144

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: 149

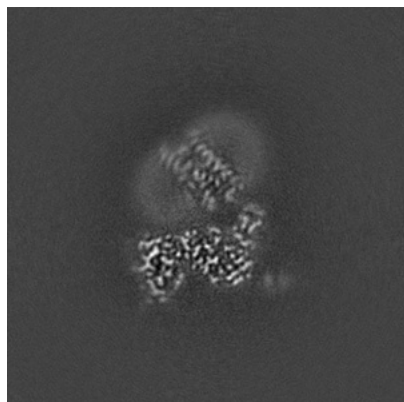


Y Index: 162

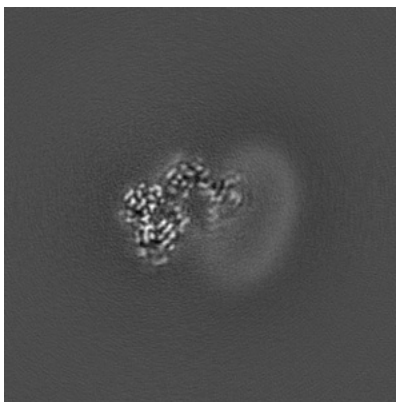


Z Index: 115

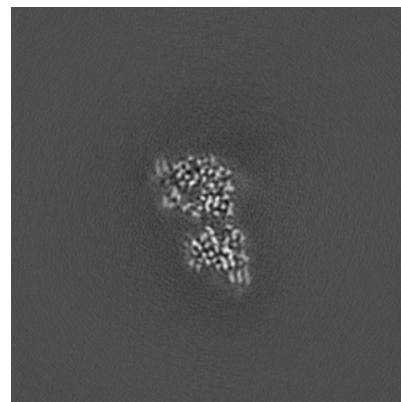
### 6.3.2 Raw map



X Index: 148



Y Index: 160

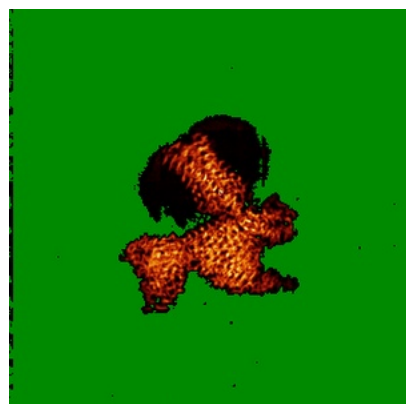


Z Index: 105

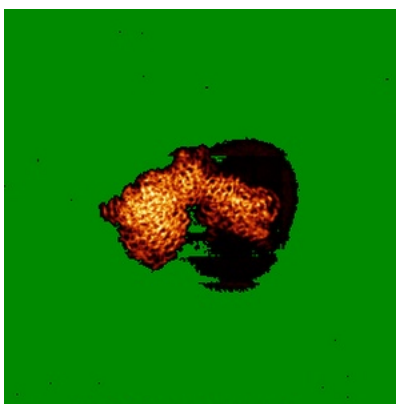
The images above show the largest variance slices of the map in three orthogonal directions.

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

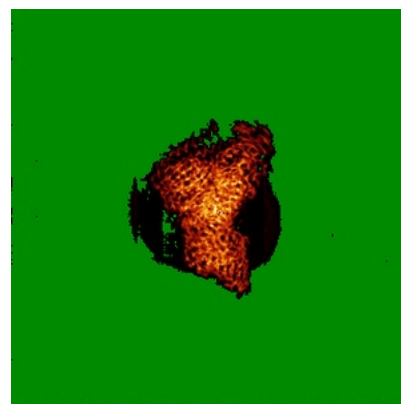
### 6.4.1 Primary map



X

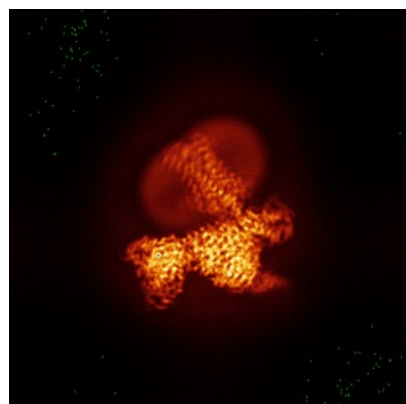


Y

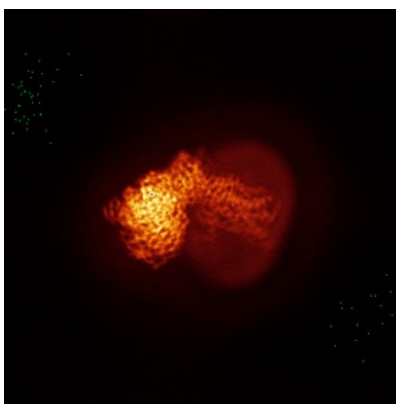


Z

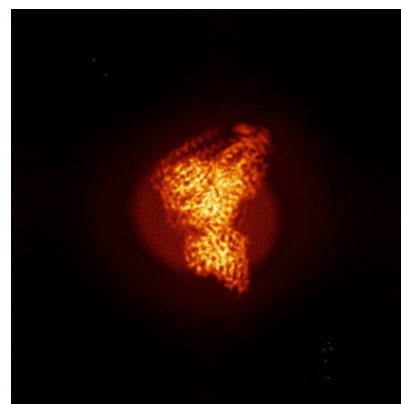
### 6.4.2 Raw map



X



Y



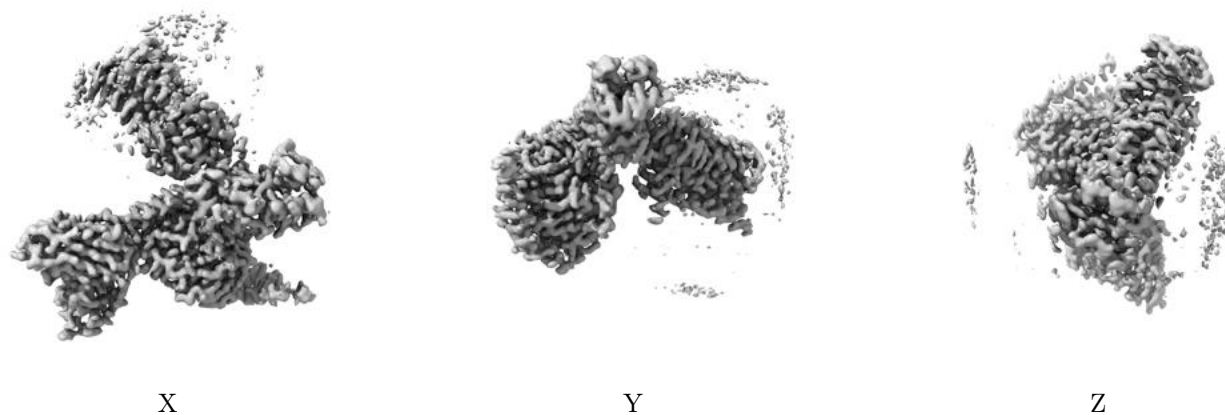
Z

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.



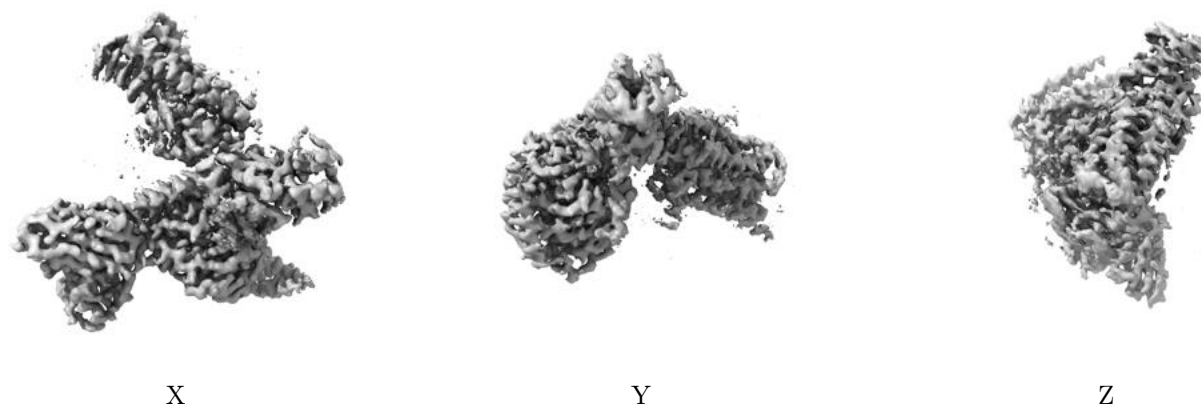
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

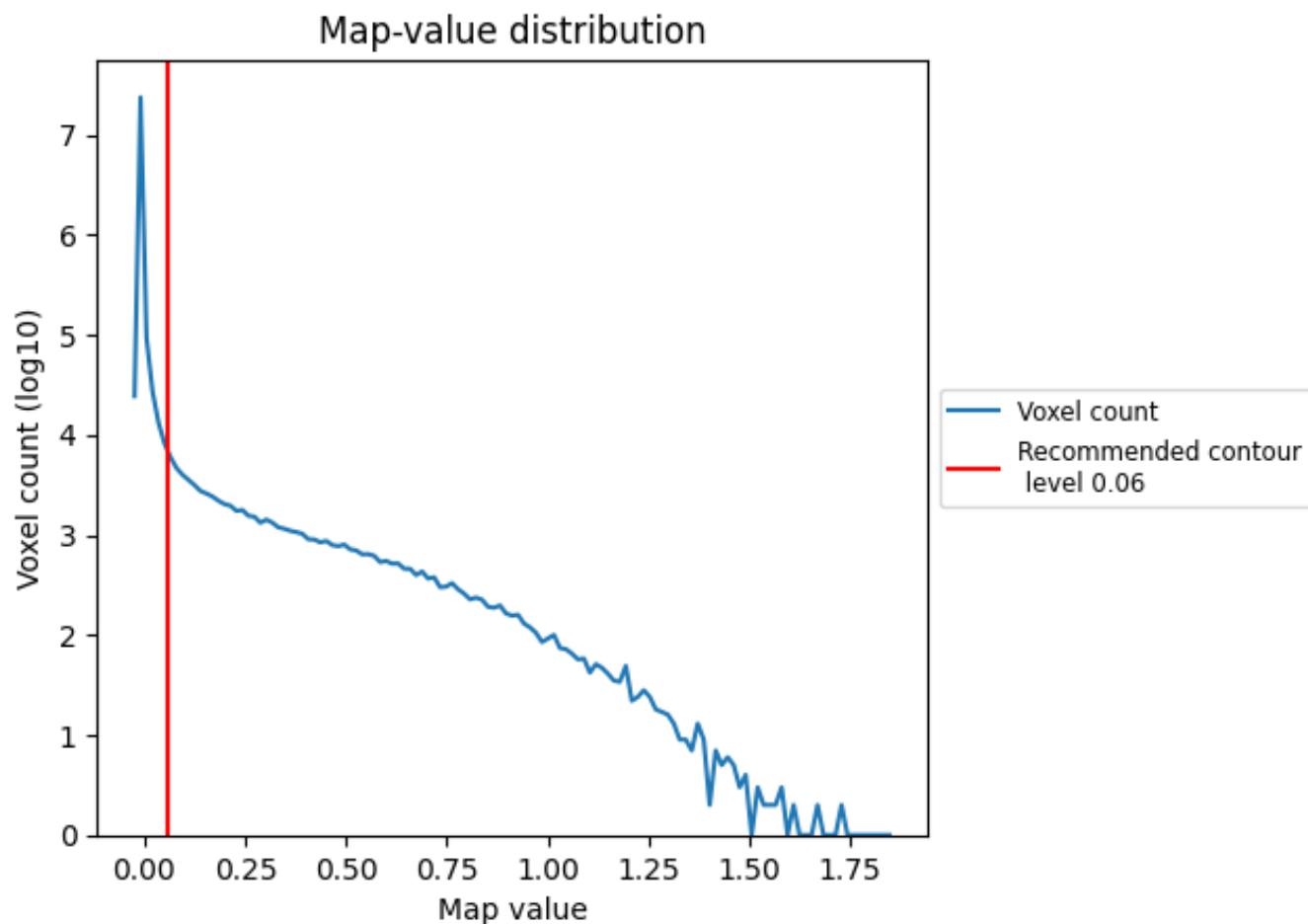
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

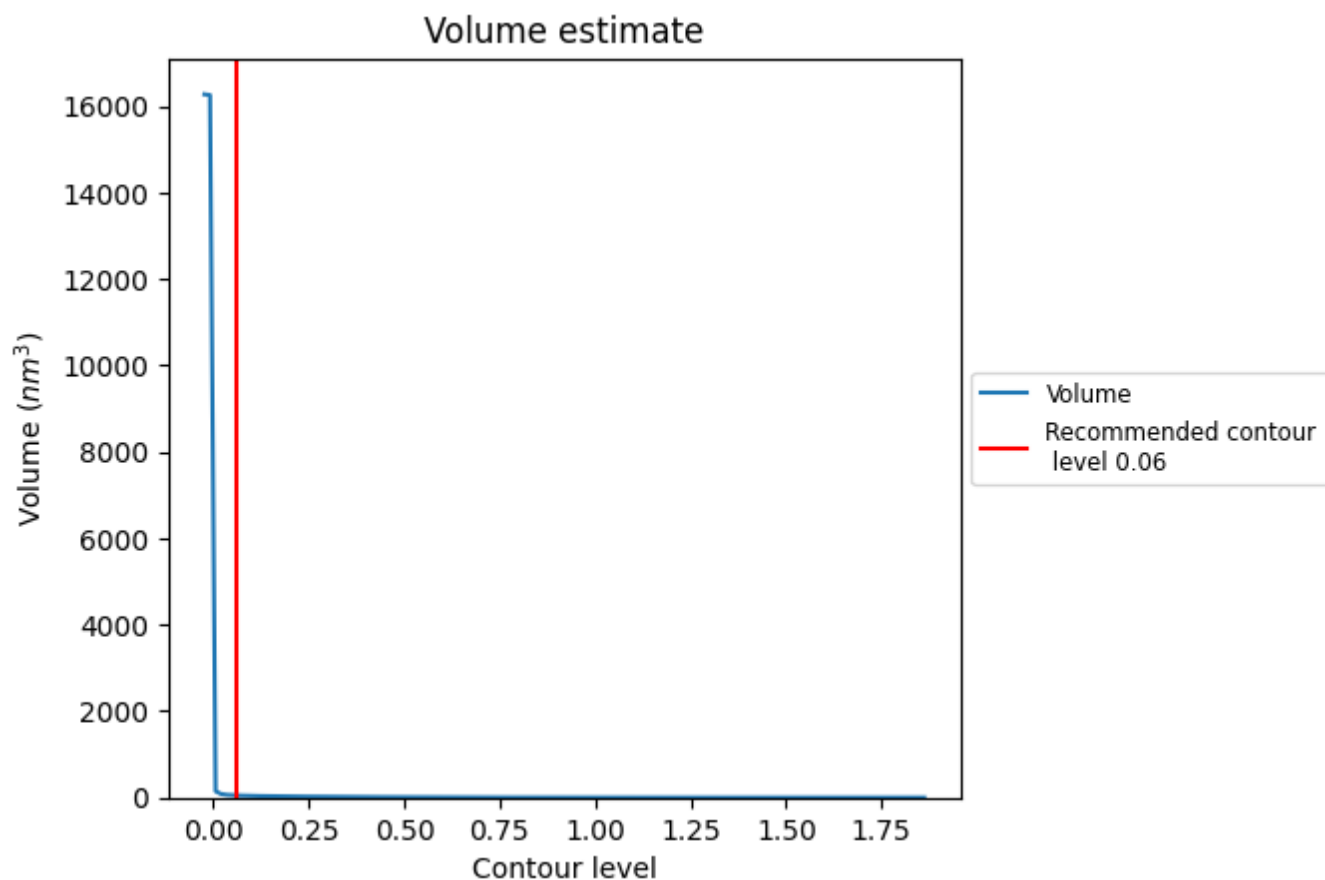
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

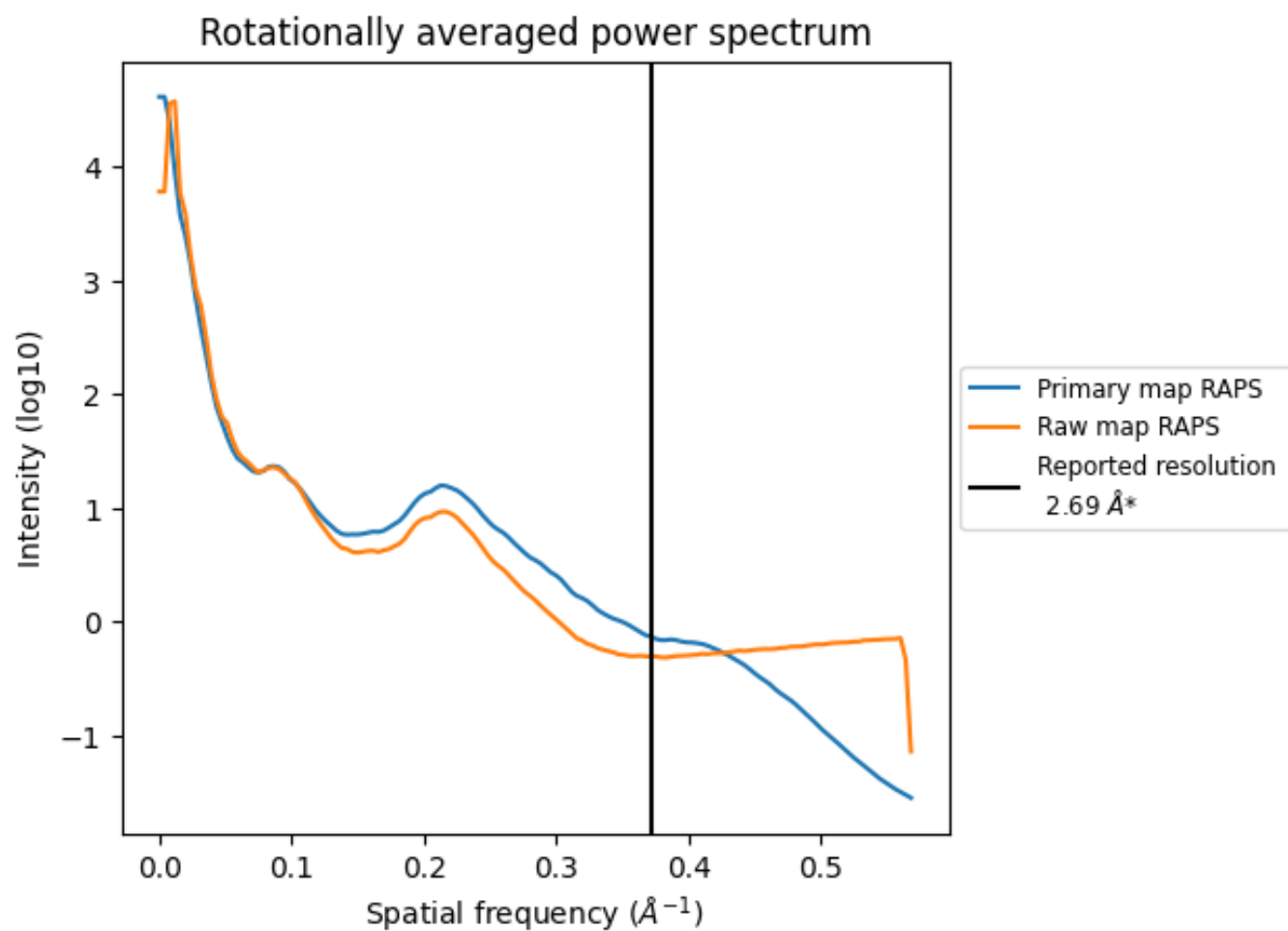
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50  $\text{nm}^3$ ; this corresponds to an approximate mass of 45 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 ⓘ

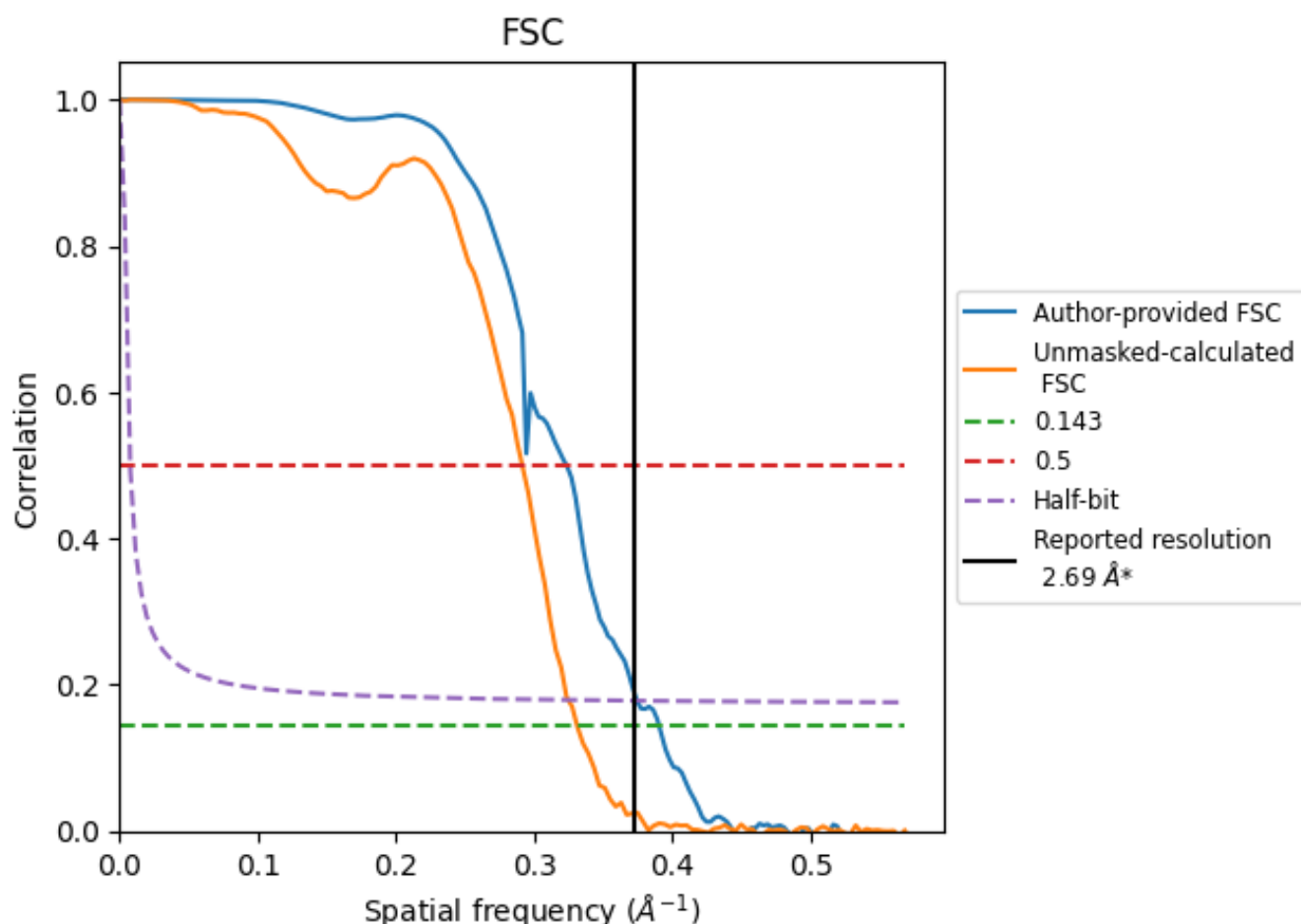


\*Reported resolution corresponds to spatial frequency of  $0.372 \text{ \AA}^{-1}$

## 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 0.372  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

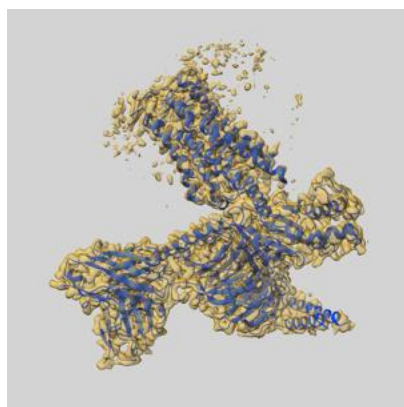
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.56	3.09	2.67
Unmasked-calculated*	3.02	3.43	3.08

\*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 3.02 differs from the reported value 2.69 by more than 10 %

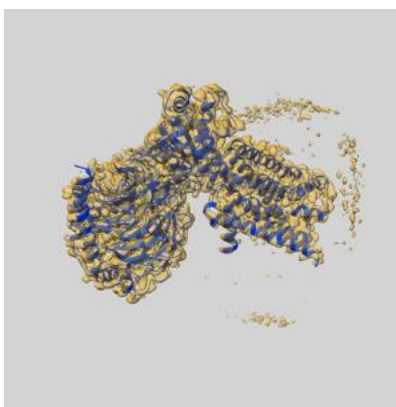
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27969 and PDB model 8E9Z. Per-residue inclusion information can be found in section [3](#) on page [12](#).

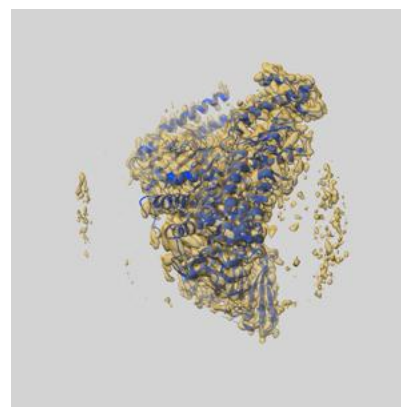
### 9.1 Map-model overlay [i](#)



X



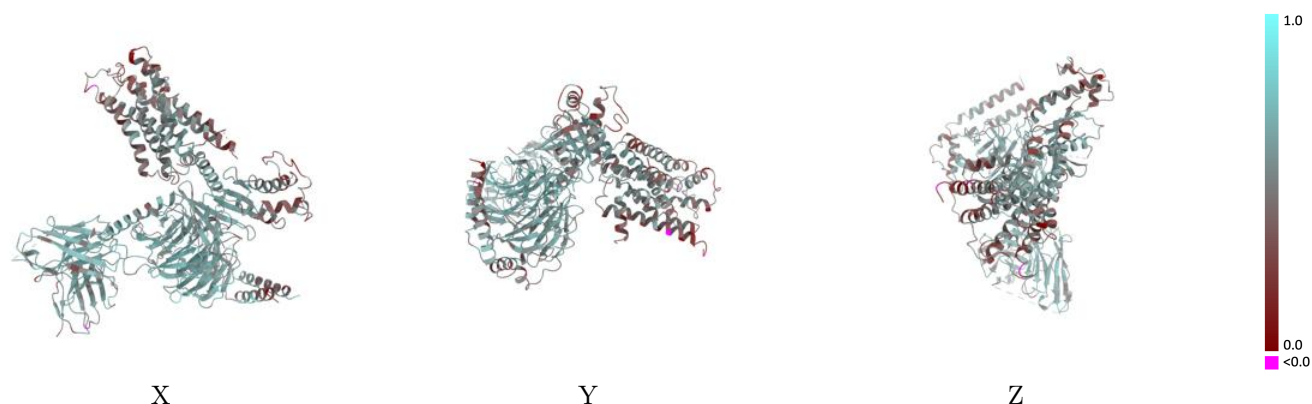
Y



Z

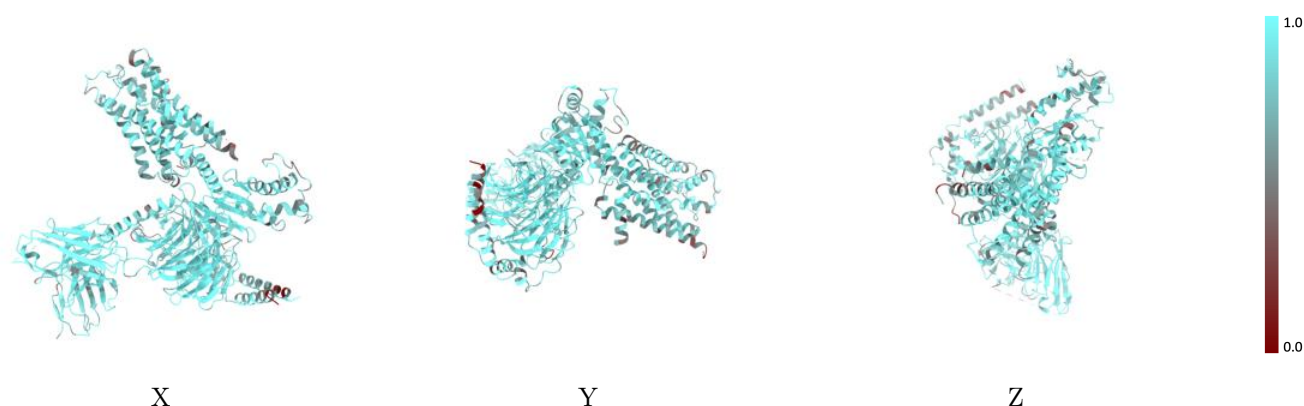
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

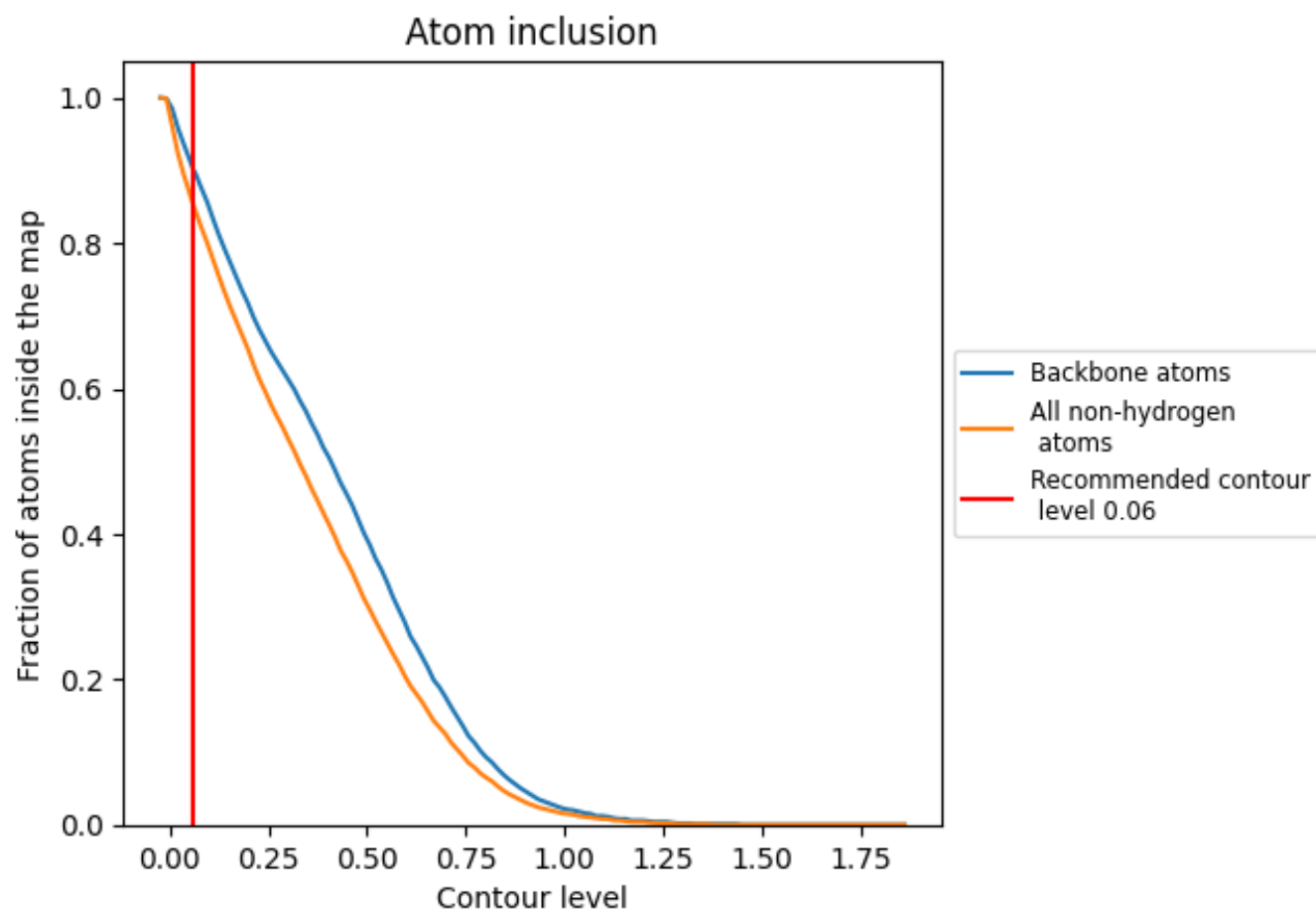
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8510	<div></div> 0.5310
A	<div></div> 0.7750	<div></div> 0.4330
B	<div></div> 0.8440	<div></div> 0.5190
C	<div></div> 0.9120	<div></div> 0.6010
D	<div></div> 0.6660	<div></div> 0.4310
E	<div></div> 0.9090	<div></div> 0.5890

