



## Full wwPDB EM Validation Report ⓘ

May 27, 2026 – 12:55 PM JST

PDB ID : 22BF / pdb\_000022bf  
EMDB ID : EMD-68148  
Title : XEN1101 bound KCNQ2/3 heteromer with 3:1 stoichiometry, state 2  
Authors : Lu, F.; Fan, X.; Huang, J.  
Deposited on : 2026-01-05  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

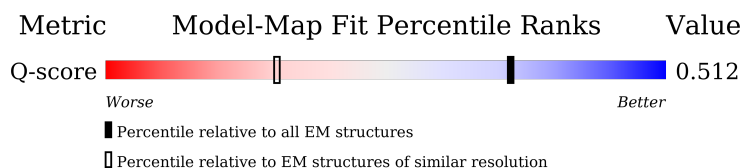
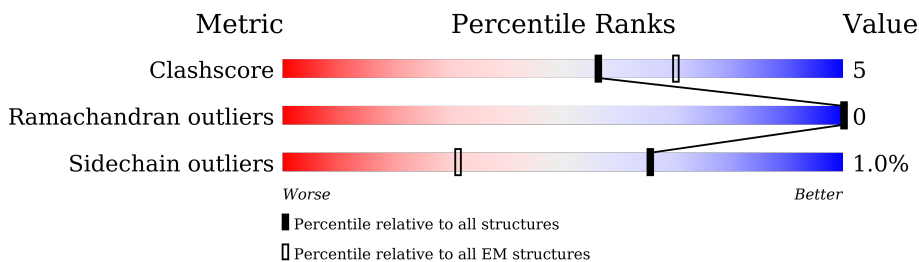
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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	7115 ( 2.00 - 3.00 )

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	872	 25% 71%
2	B	872	 24% 72%
2	C	872	 24% 72%
2	D	872	 25% 72%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8165 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 Potassium voltage-gated channel subfamily KQT member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	249	Total	C	N	O	S	0	0
			2006	1330	335	331	10		

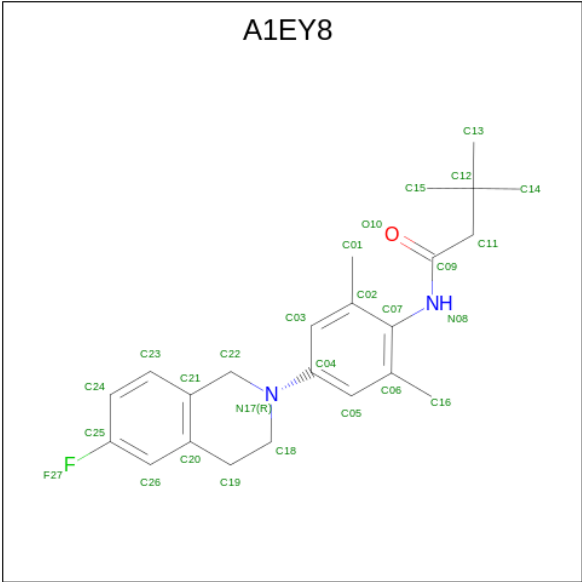
- Molecule 2 is a protein called Potassium voltage-gated channel subfamily KQT member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	248	Total	C	N	O	S	0	0
			2016	1339	339	329	9		
2	C	248	Total	C	N	O	S	0	0
			2016	1339	339	329	9		
2	D	248	Total	C	N	O	S	0	0
			2016	1339	339	329	9		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

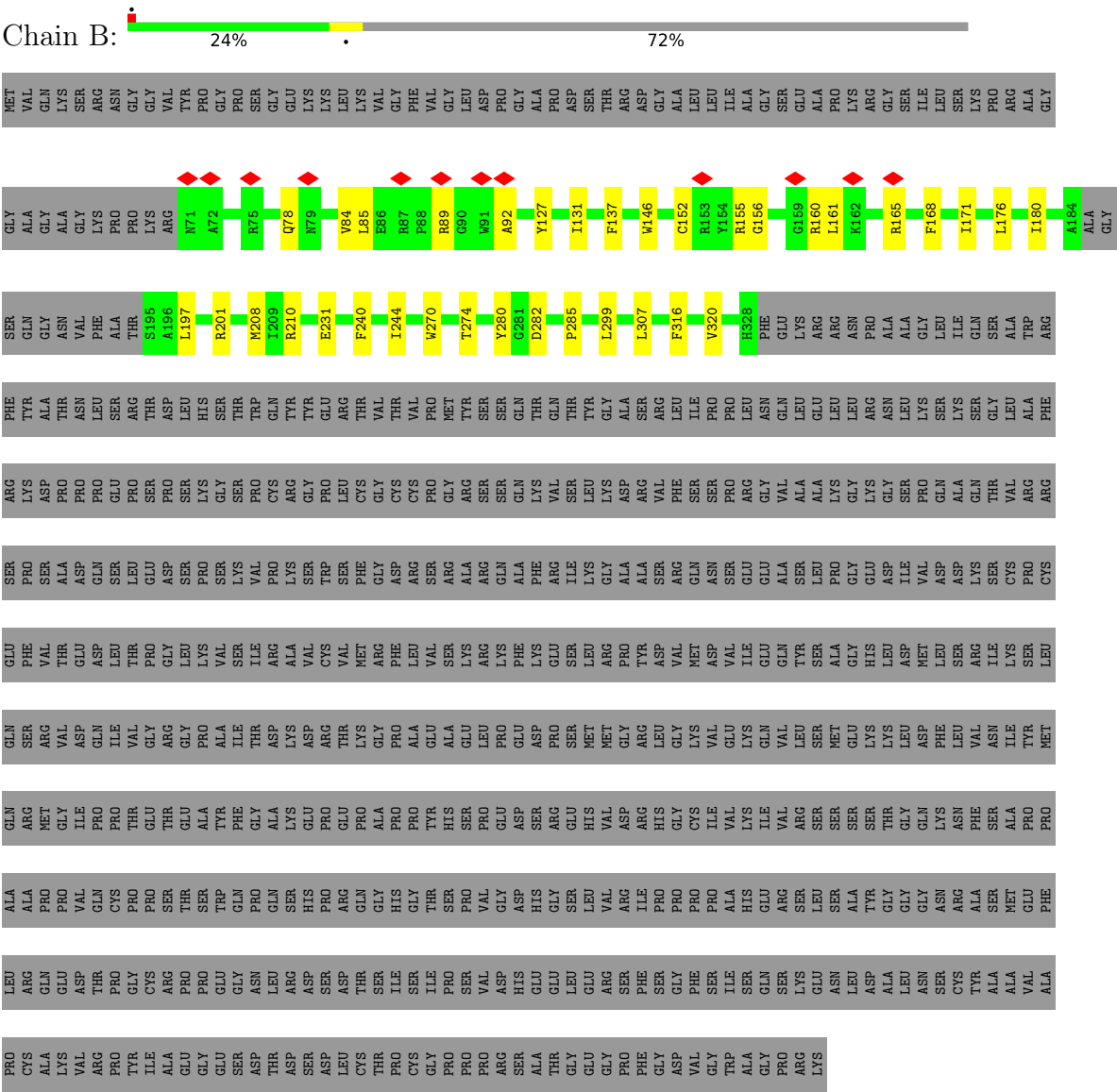
Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total	K	0
			3	3	

- Molecule 4 is Azetukalner (CCD ID: A1EY8) (formula: C<sub>23</sub>H<sub>29</sub>FN<sub>2</sub>O) (labeled as "Ligand of Interest" by depositor).

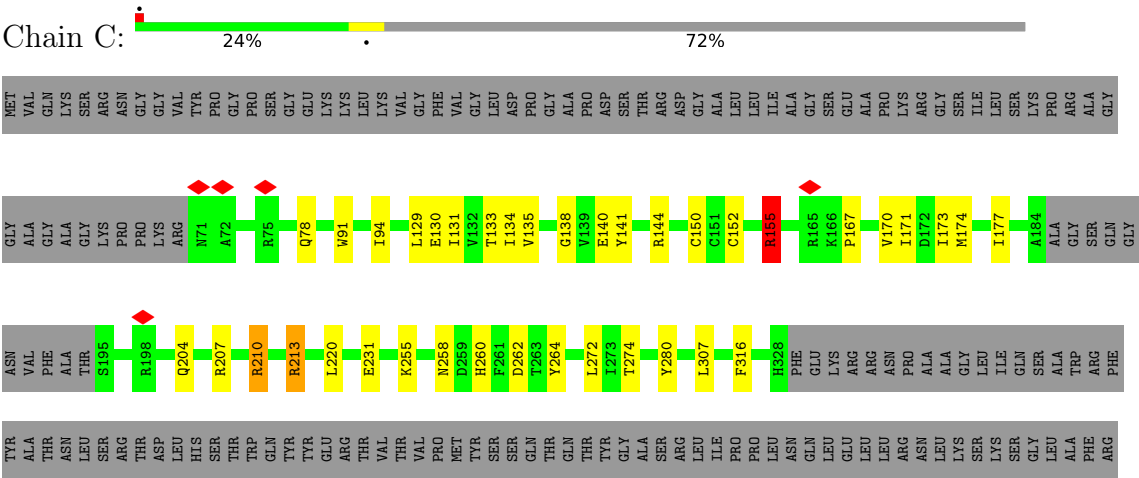


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	F	N	O	0
			27	23	1	2	1	
4	B	1	Total	C	F	N	O	0
			27	23	1	2	1	
4	C	1	Total	C	F	N	O	0
			27	23	1	2	1	
4	D	1	Total	C	F	N	O	0
			27	23	1	2	1	





• Molecule 2: Potassium voltage-gated channel subfamily KQT member 2



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

- Molecule 2: Potassium voltage-gated channel subfamily KQT member 2



GLY	THR	THR	GLY	PRO	ALA	LEU	ARG	CYS	VAL	R213	GLY	MET	VAL
THR	SER	SER	SER	HIS	ALA	VAL	ARG	GLY	PRO	L220	ALA	GLN	GLY
PRO	PRO	PRO	GLU	SER	GLU	SER	ALA	ARG	TYR	E231	ALA	SER	LYS
GLY	GLY	GLY	PRO	GLU	PRO	LYS	GLN	SER	SER	F240	LYS	ARG	ASN
ASP	ASP	ASP	GLU	ASP	GLU	PHE	ALA	SER	GLN	Y264	PRO	GLY	GLY
HIS	HIS	HIS	GLY	GLY	PRO	GLU	ARG	VAL	THR	G280	ARG	LYS	VAL
SER	SER	SER	SER	GLU	SER	SER	ILE	SER	THR	C281	THR	THR	THR
VAL	VAL	VAL	MET	HIS	MET	LEU	GLY	LYS	TYR	D282	GLY	TYR	TYR
ARG	ARG	ARG	GLY	ASP	PRO	ARG	ALA	ASP	ALA	N289	ALA	PRO	GLY
ILE	ILE	ILE	ARG	HIS	TYR	ASP	ALA	ARG	SER	G290	THR	PRO	PRO
PRO	PRO	PRO	GLY	GLY	VAL	VAL	ARG	PHE	LEU	F316	GLY	SER	LYS
PRO	PRO	PRO	LYS	CYS	ASP	MET	GLN	SER	ILE	H328	LYS	GLU	GLU
PRO	PRO	PRO	VAL	ILE	VAL	ASP	ASN	SER	PRO	PHE	LEU	LEU	LEU
ALA	ALA	ALA	GLU	VAL	GLU	ILE	GLU	ARG	PRO	S110	THR	VAL	VAL
HIS	HIS	HIS	LYS	LYS	GLN	GLU	ALA	GLY	LEU	S113	GLY	GLY	GLY
GLU	GLU	GLU	ILE	ILE	GLN	GLU	ALA	VAL	ASN	T114	GLY	LEU	LEU
ARG	ARG	ARG	VAL	VAL	VAL	TYR	ALA	ALA	GLY	E117	ASP	PRO	PRO
SER	SER	SER	LEU	ARG	LEU	SER	LEU	SER	LEU	Y116	GLY	ASP	ASP
LEU	LEU	LEU	SER	SER	MET	ASP	ILE	PRO	LYS	Y141	ALA	GLY	GLY
GLY	GLY	GLY	ASP	GLY	ASP	MET	VAL	GLN	SER	ILE	ALA	PRO	PRO
ASN	ASN	ASN	PHE	ASN	LEU	SER	ASP	ALA	LYS	I145	GLN	ASP	ASP
ARG	ARG	ARG	VAL	PHE	VAL	ARG	LYS	GLN	SER	W146	LYS	SER	SER
ALA	ALA	ALA	ASN	ASN	ILE	ILE	VAL	THR	GLY	V157	ALA	THR	THR
MET	MET	MET	ILE	ALA	ILE	LYS	CYS	VAL	LEU	R158	THR	ARG	ARG
GLU	GLU	GLU	THR	PRO	THR	SER	PRO	ARG	ALA	F168	GLY	ASP	ASP
PHE	PHE	PHE	MET	PRO	MET	LEU	CYS	ARG	PHE	I173	ALA	GLY	GLY
LEU	LEU	LEU	GLN	ALA	GLN	GLN	GLU	SER	ARG	ASN	LEU	ALA	ALA
GLN	GLN	GLN	VAL	ALA	ASP	ILE	THR	SER	ASP	LEU	LEU	LEU	LEU
ASP	ASP	ASP	ILE	VAL	ILE	ASP	GLU	ASP	PRO	THR	ILE	ILE	ILE
THR	THR	THR	PRO	CYS	PRO	GLN	ASP	GLN	PRO	A184	ALA	ALA	ALA
PRO	PRO	PRO	THR	THR	THR	ILE	LEU	SER	GLU	ALA	SER	SER	SER
GLY	GLY	GLY	PRO	PRO	PRO	VAL	THR	LEU	PRO	THR	GLY	GLU	GLU
ARG	ARG	ARG	THR	THR	THR	ARG	GLY	ASP	PRO	LEU	SER	ALA	ALA
PRO	PRO	PRO	GLU	SER	ALA	GLY	LEU	SER	SER	HIS	GLN	PRO	PRO
SER	SER	SER	PHE	THR	VAL	ILE	VAL	SER	GLY	LYS	ASN	ARG	ARG
LEU	LEU	LEU	THR	THR	ALA	THR	ILE	VAL	PRO	THR	THR	SER	SER
ARG	ARG	ARG	GLY	GLN	LYS	LYS	ALA	LYS	ARG	THR	THR	ILE	ILE
ASP	ASP	ASP	LYS	LYS	ASP	ASP	VAL	SER	GLY	S195	SER	SER	SER
SER	SER	SER	GLU	GLU	GLU	ARG	VAL	THR	PRO	A196	LYS	PRO	PRO
ASP	ASP	ASP	GLY	GLY	GLY	THR	MET	SER	LEU	I197	ARG	ARG	ARG
THR	THR	THR	PRO	PRO	PRO	LYS	VAL	PHE	CYS	R198	THR	GLY	GLY
SER	SER	SER	ALA	GLY	ALA	GLY	ARG	GLY	CYS	THR	VAL	VAL	VAL
SER	SER	SER	PRO	HIS	PRO	PRO	PHE	ASP	CYS	THR	THR	THR	THR

SER  
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LYS



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	189473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.272	Depositor
Minimum map value	-0.797	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	262.08, 262.08, 262.08	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93599993, 0.93599993, 0.93599993	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EY8, K

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	0.22	0/2055	0.34	0/2780
2	B	0.12	0/2071	0.26	0/2805
2	C	0.17	0/2071	0.28	0/2805
2	D	0.17	0/2071	0.29	0/2805
All	All	0.17	0/8268	0.30	0/11195

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	A	0	5
2	C	0	3
2	D	0	2
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	106	ARG	Sidechain
1	A	227	ARG	Sidechain
1	A	230	ARG	Sidechain
1	A	243	ARG	Sidechain
2	C	155	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	C	210	ARG	Sidechain
2	C	213	ARG	Sidechain
2	D	210	ARG	Sidechain
2	D	213	ARG	Sidechain

## 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	2006	0	2081	30	0
2	B	2016	0	2053	21	0
2	C	2016	0	2053	25	0
2	D	2016	0	2053	18	0
3	A	3	0	0	0	0
4	A	27	0	0	0	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	D	27	0	0	0	0
All	All	8165	0	8240	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (81) 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:117:ARG:NH1	1:A:243:ARG:HH22	1.67	0.92
1:A:230:ARG:CD	1:A:232:LEU:HD23	2.11	0.80
1:A:117:ARG:HD2	1:A:243:ARG:HH12	1.51	0.73
1:A:230:ARG:HD3	1:A:232:LEU:HD23	1.70	0.72
1:A:117:ARG:NH1	1:A:243:ARG:NH2	2.42	0.67
2:B:89:ARG:H	2:B:92:ALA:HB3	1.60	0.67
2:B:78:GLN:NE2	2:B:146:TRP:O	2.30	0.65
2:C:140:GLU:OE2	2:C:144:ARG:NH2	2.32	0.63
1:A:286:VAL:HG11	1:A:326:THR:HG21	1.81	0.61
2:C:170:VAL:HG12	2:C:174:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:255:LYS:NZ	2:C:262:ASP:O	2.32	0.58
2:C:231:GLU:HG3	2:D:220:LEU:HD21	1.86	0.56
1:A:196:LYS:HD2	1:A:197:PRO:HD2	1.89	0.54
2:C:264:TYR:H	2:D:114:THR:HG21	1.73	0.54
2:C:204:GLN:HE22	2:C:207:ARG:HH21	1.56	0.52
2:D:117:GLU:HG3	2:D:118:TYR:CD1	2.45	0.52
1:A:313:THR:OG1	2:B:280:TYR:OH	2.20	0.51
2:C:131:ILE:O	2:C:135:VAL:HG23	2.11	0.51
2:B:274:THR:OG1	2:C:280:TYR:OH	2.23	0.50
2:D:104:PHE:HA	2:D:107:LEU:HD12	1.94	0.50
2:D:141:TYR:CE2	2:D:173:ILE:HD11	2.46	0.50
2:C:130:GLU:O	2:C:134:ILE:HD12	2.12	0.49
1:A:187:TRP:HD1	1:A:190:ARG:HH21	1.61	0.49
2:C:141:TYR:CE2	2:C:173:ILE:HD11	2.48	0.49
1:A:237:MET:HE2	2:D:240:PHE:HE2	1.77	0.49
1:A:116:GLU:O	1:A:243:ARG:NH1	2.46	0.48
2:B:307:LEU:HD21	2:C:316:PHE:HE2	1.78	0.48
1:A:212:VAL:HG22	1:A:226:LEU:HD22	1.95	0.48
1:A:355:LEU:HB3	2:D:231:GLU:HG2	1.94	0.48
1:A:167:PHE:HE2	1:A:236:ARG:HD2	1.78	0.48
2:C:274:THR:OG1	2:D:280:TYR:OH	2.22	0.48
1:A:105:ARG:O	1:A:106:ARG:C	2.58	0.47
1:A:321:ASP:N	1:A:321:ASP:OD1	2.46	0.47
2:B:84:VAL:HG13	2:B:85:LEU:HG	1.97	0.47
1:A:117:ARG:HH11	1:A:243:ARG:HH22	1.54	0.47
1:A:208:ALA:HB3	1:A:232:LEU:HD11	1.97	0.47
2:B:127:TYR:O	2:B:131:ILE:HG12	2.15	0.47
1:A:128:LEU:O	1:A:132:ILE:HG12	2.16	0.46
2:B:152:CYS:HA	2:B:155:ARG:HB2	1.99	0.45
2:B:231:GLU:HG3	2:C:220:LEU:HD21	1.98	0.45
2:C:307:LEU:HD21	2:D:316:PHE:HE2	1.81	0.45
2:B:197:LEU:HB3	2:B:201:ARG:NH1	2.31	0.45
2:B:316:PHE:O	2:B:320:VAL:HG23	2.17	0.45
2:C:204:GLN:HE22	2:C:207:ARG:NH2	2.14	0.45
1:A:269:PHE:HE2	2:B:208:MET:HE2	1.82	0.45
2:B:168:PHE:HA	2:B:171:ILE:HG12	1.99	0.45
2:D:110:SER:O	2:D:113:SER:OG	2.29	0.45
2:C:91:TRP:CE3	2:C:94:ILE:HD11	2.51	0.44
2:C:134:ILE:O	2:C:138:GLY:N	2.41	0.44
2:D:78:GLN:NE2	2:D:146:TRP:O	2.50	0.44
2:D:117:GLU:HG3	2:D:118:TYR:HD1	1.82	0.44

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*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:TRP:HE1	2:B:285:PRO:HD3	1.82	0.44
1:A:103:LYS:HE2	1:A:103:LYS:HB3	1.75	0.44
2:B:161:LEU:HB3	2:B:165:ARG:HH21	1.83	0.44
2:B:176:LEU:O	2:B:180:ILE:HG13	2.18	0.44
2:C:141:TYR:CZ	2:C:173:ILE:HD11	2.53	0.44
1:A:105:ARG:HE	1:A:180:CYS:HA	1.83	0.43
1:A:196:LYS:HG3	1:A:198:LEU:H	1.83	0.43
2:B:137:PHE:HE1	2:B:210:ARG:CZ	2.31	0.43
2:C:129:LEU:O	2:C:133:THR:OG1	2.26	0.43
1:A:119:ARG:H	1:A:122:ALA:HB3	1.83	0.43
2:C:152:CYS:HA	2:C:155:ARG:HB2	2.00	0.43
2:C:167:PRO:O	2:C:171:ILE:HG12	2.17	0.43
1:A:117:ARG:CZ	1:A:243:ARG:HH22	2.28	0.43
2:C:78:GLN:HB3	2:C:150:CYS:HB3	2.01	0.43
1:A:230:ARG:HD2	1:A:232:LEU:HD23	1.97	0.42
2:C:258:ASN:ND2	2:C:260:HIS:HB2	2.34	0.42
1:A:105:ARG:HD3	1:A:105:ARG:HA	1.64	0.42
1:A:147:GLU:N	1:A:147:GLU:OE2	2.53	0.42
2:D:289:ASN:OD1	2:D:290:GLY:N	2.52	0.42
2:D:97:ALA:O	2:D:101:LEU:HG	2.20	0.42
2:B:240:PHE:O	2:B:244:ILE:HG12	2.21	0.41
2:B:282:ASP:N	2:B:282:ASP:OD1	2.53	0.41
1:A:147:GLU:HG2	1:A:148:TYR:CD1	2.55	0.41
2:D:141:TYR:O	2:D:145:ILE:HG12	2.21	0.41
1:A:144:THR:HG21	2:D:264:TYR:HB2	2.03	0.41
2:D:282:ASP:OD1	2:D:282:ASP:N	2.53	0.41
2:D:168:PHE:HD1	2:D:168:PHE:HA	1.74	0.41
2:B:156:GLY:O	2:B:160:ARG:HG2	2.21	0.40
2:C:173:ILE:O	2:C:177:ILE:HG12	2.21	0.40
2:B:299:LEU:HD21	2:C:272:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/872 (28%)	237 (98%)	6 (2%)	0	100	100
2	B	244/872 (28%)	242 (99%)	2 (1%)	0	100	100
2	C	244/872 (28%)	244 (100%)	0	0	100	100
2	D	244/872 (28%)	244 (100%)	0	0	100	100
All	All	975/3488 (28%)	967 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/725 (29%)	205 (99%)	2 (1%)	68	86
2	B	207/728 (28%)	207 (100%)	0	100	100
2	C	207/728 (28%)	204 (99%)	3 (1%)	59	81
2	D	207/728 (28%)	204 (99%)	3 (1%)	59	81
All	All	828/2909 (28%)	820 (99%)	8 (1%)	65	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LYS
1	A	105	ARG
2	C	155	ARG
2	C	210	ARG
2	C	213	ARG
2	D	168	PHE
2	D	198	ARG
2	D	210	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
2	C	204	GLN
2	C	286	GLN
2	D	83	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	A1EY8	D	901	-	29,29,29	0.14	0	43,43,43	0.57	1 (2%)
4	A1EY8	C	901	-	29,29,29	0.15	0	43,43,43	0.52	1 (2%)
4	A1EY8	B	901	-	29,29,29	0.15	0	43,43,43	0.55	1 (2%)
4	A1EY8	A	904	-	29,29,29	0.14	0	43,43,43	0.55	1 (2%)

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	A1EY8	D	901	-	-	0/13/22/22	0/3/3/3
4	A1EY8	C	901	-	-	0/13/22/22	0/3/3/3
4	A1EY8	B	901	-	-	0/13/22/22	0/3/3/3
4	A1EY8	A	904	-	-	0/13/22/22	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	A1EY8	C12-C11-C09	3.26	119.31	114.64
4	A	904	A1EY8	C12-C11-C09	3.08	119.05	114.64
4	B	901	A1EY8	C12-C11-C09	2.99	118.94	114.64
4	C	901	A1EY8	C12-C11-C09	2.86	118.75	114.64

There are no chirality outliers.

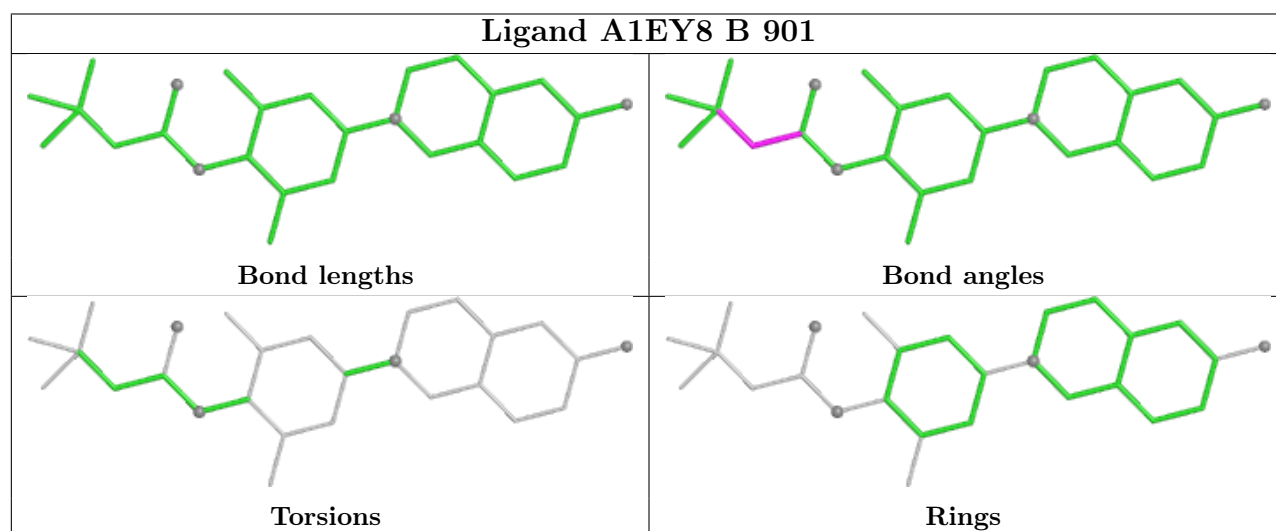
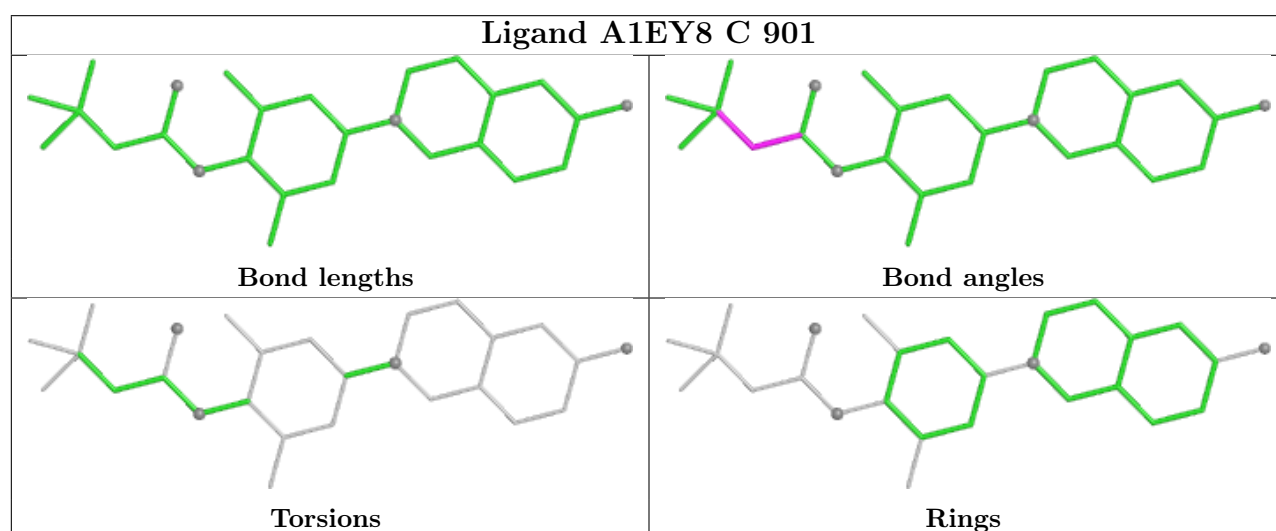
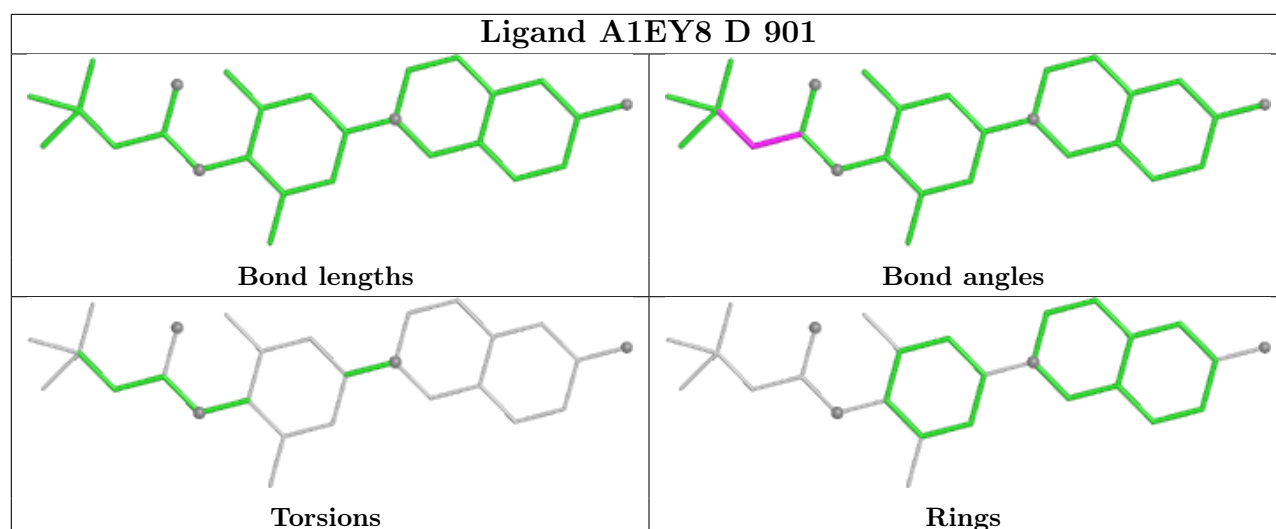
There are no torsion outliers.

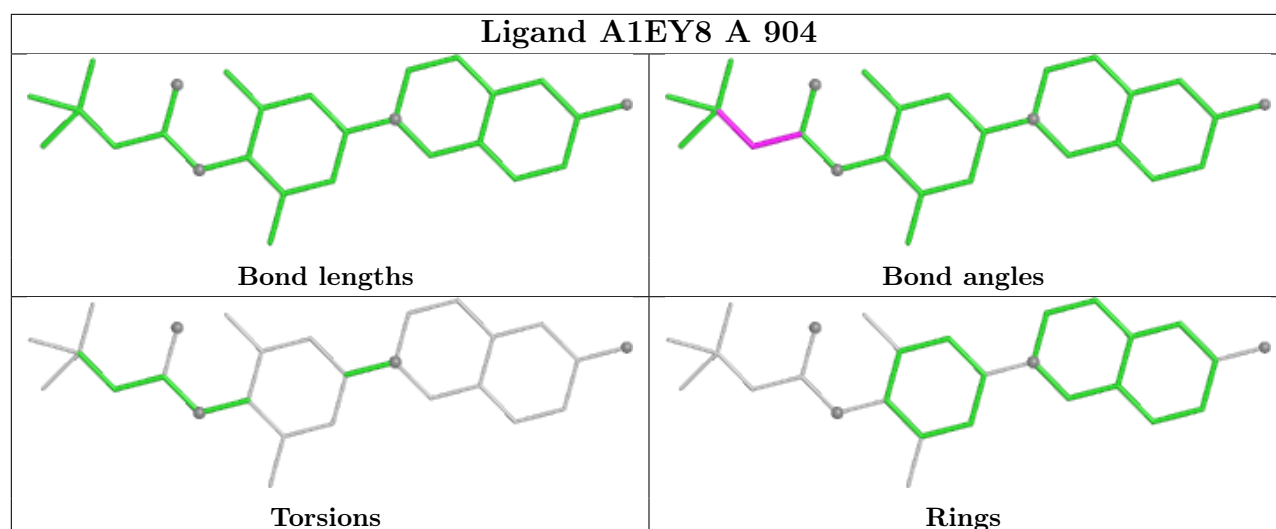
There are no ring outliers.

No monomer is involved in short contacts.

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

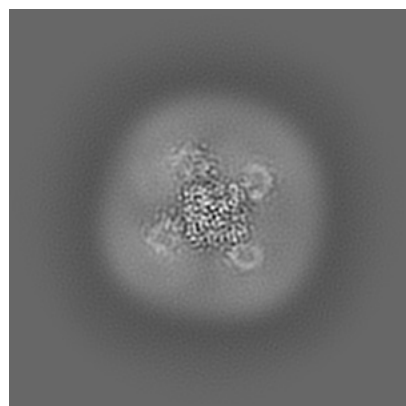
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68148. These allow visual inspection of the internal detail of the map and identification of artifacts.

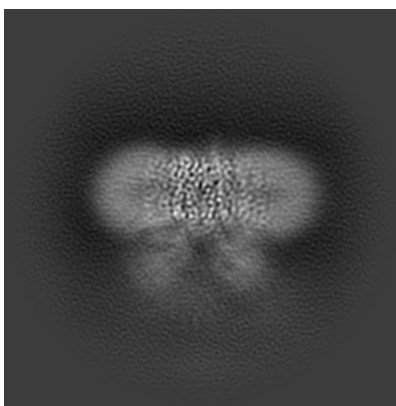
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

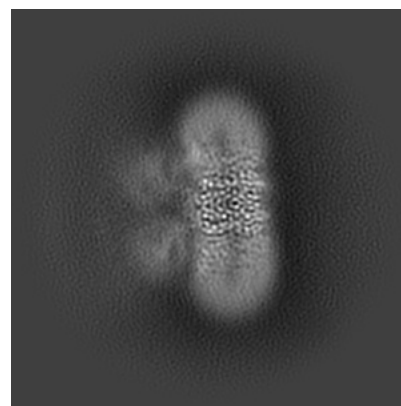
#### 6.1.1 Primary map



X

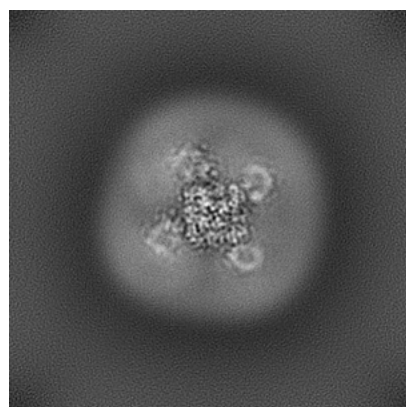


Y

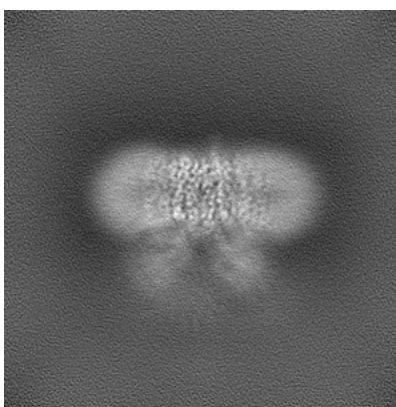


Z

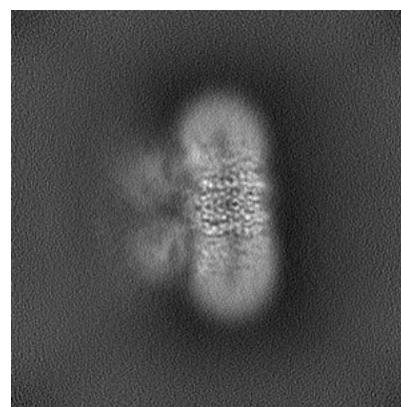
#### 6.1.2 Raw map



X



Y

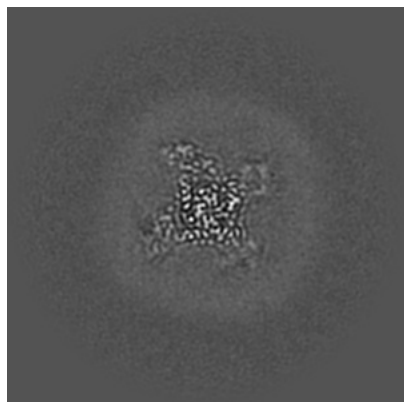


Z

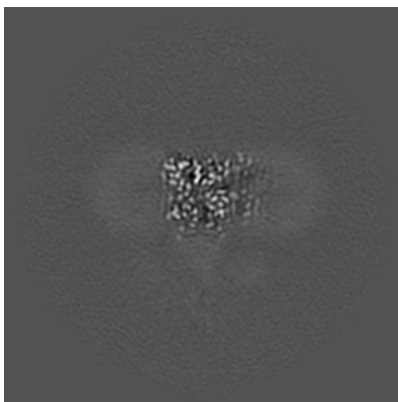
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

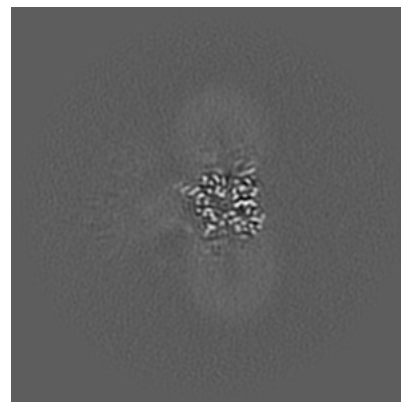
### 6.2.1 Primary map



X Index: 140

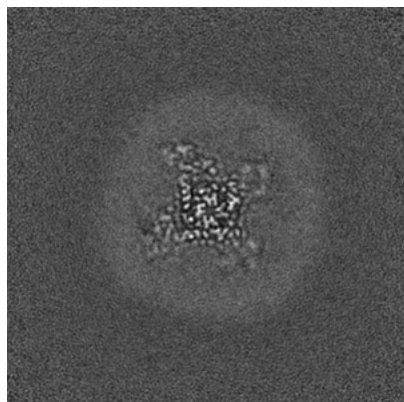


Y Index: 140

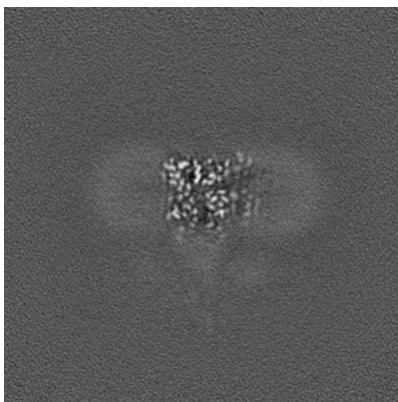


Z Index: 140

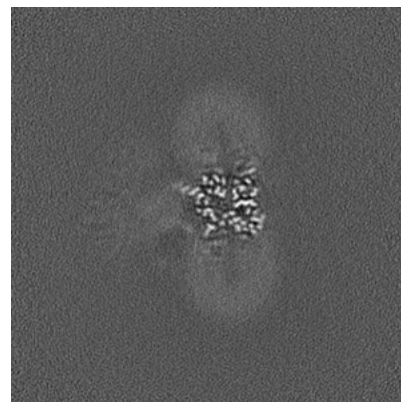
### 6.2.2 Raw map



X Index: 140



Y Index: 140

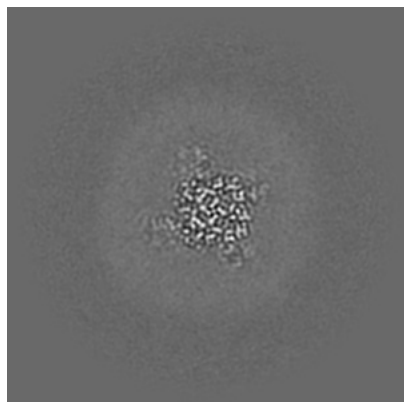


Z Index: 140

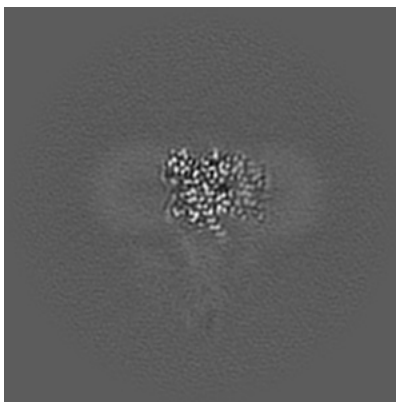
The images above show central slices of the map in three orthogonal directions.

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

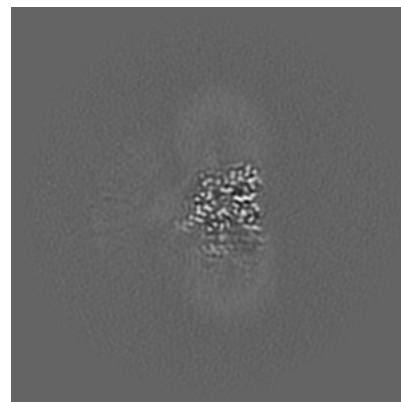
### 6.3.1 Primary map



X Index: 166

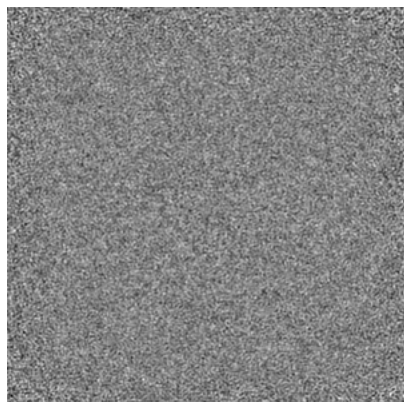


Y Index: 135

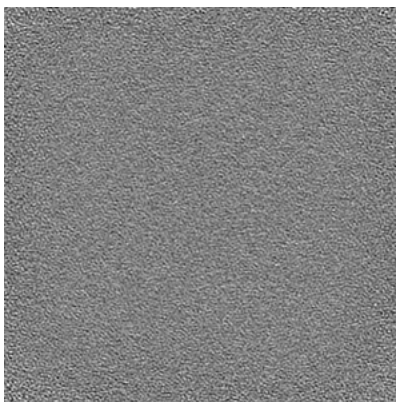


Z Index: 133

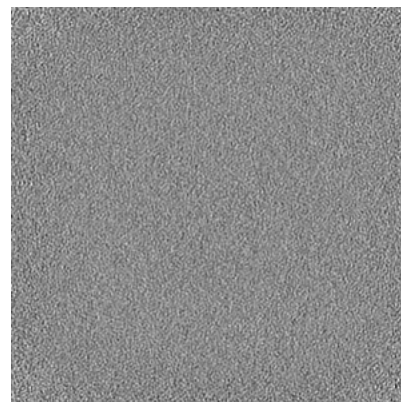
### 6.3.2 Raw map



X Index: 0



Y Index: 0



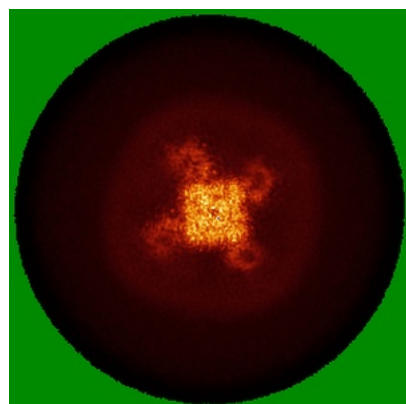
Z Index: 279

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

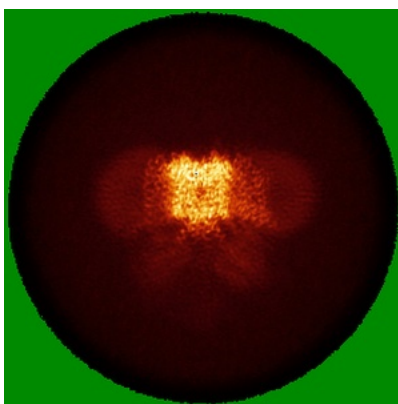


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

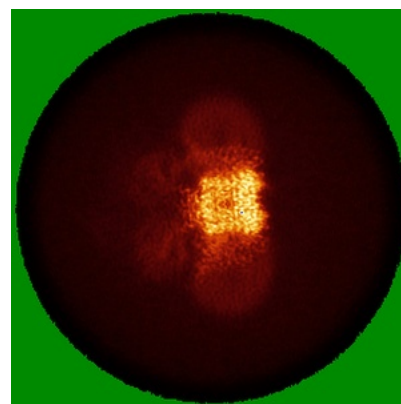
### 6.4.1 Primary map



X

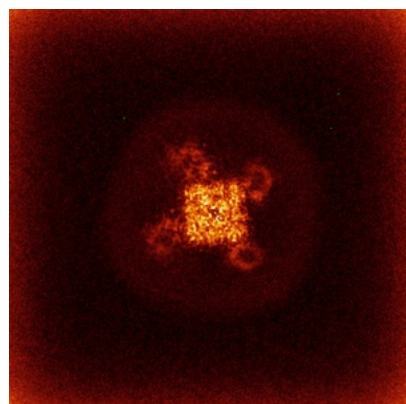


Y

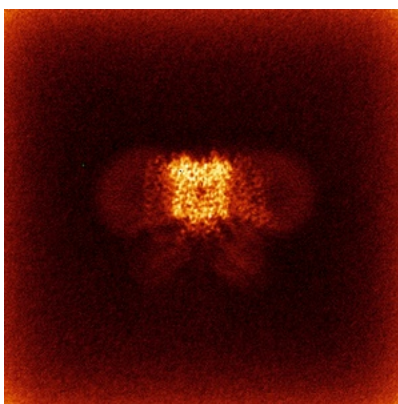


Z

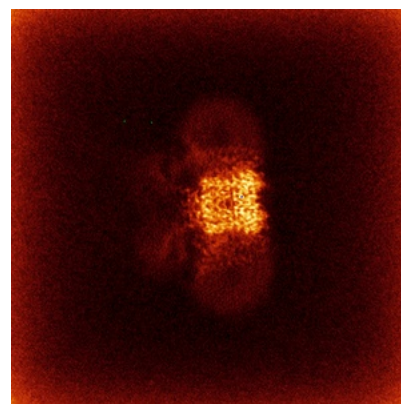
### 6.4.2 Raw map



X



Y

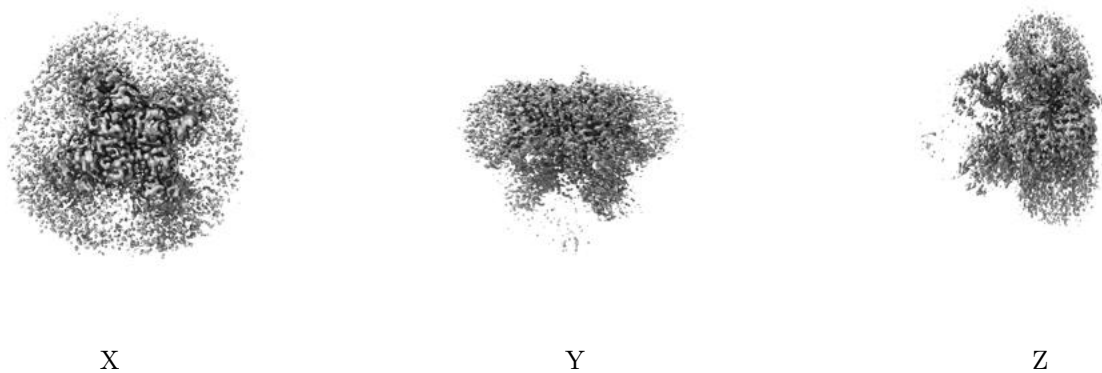


Z

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.

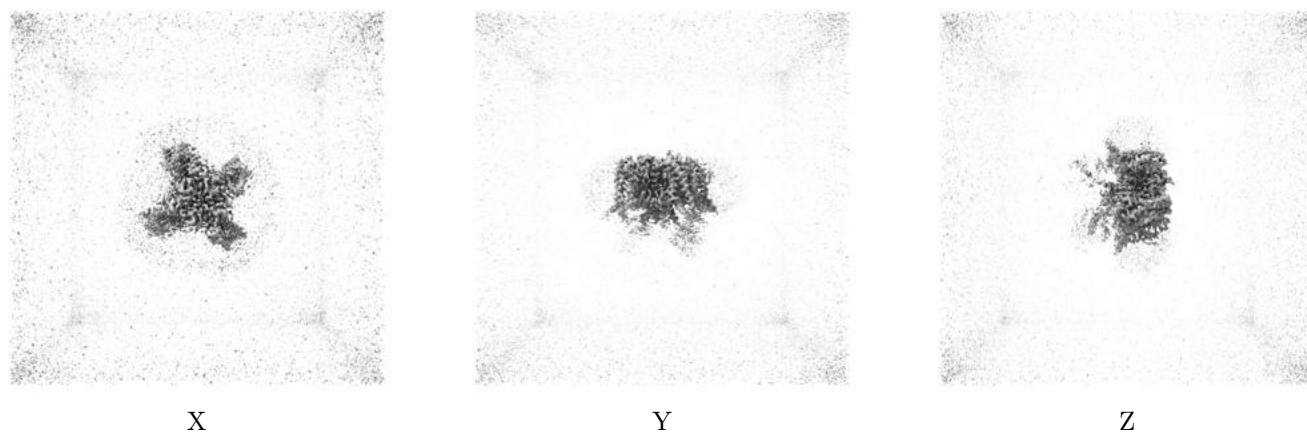
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

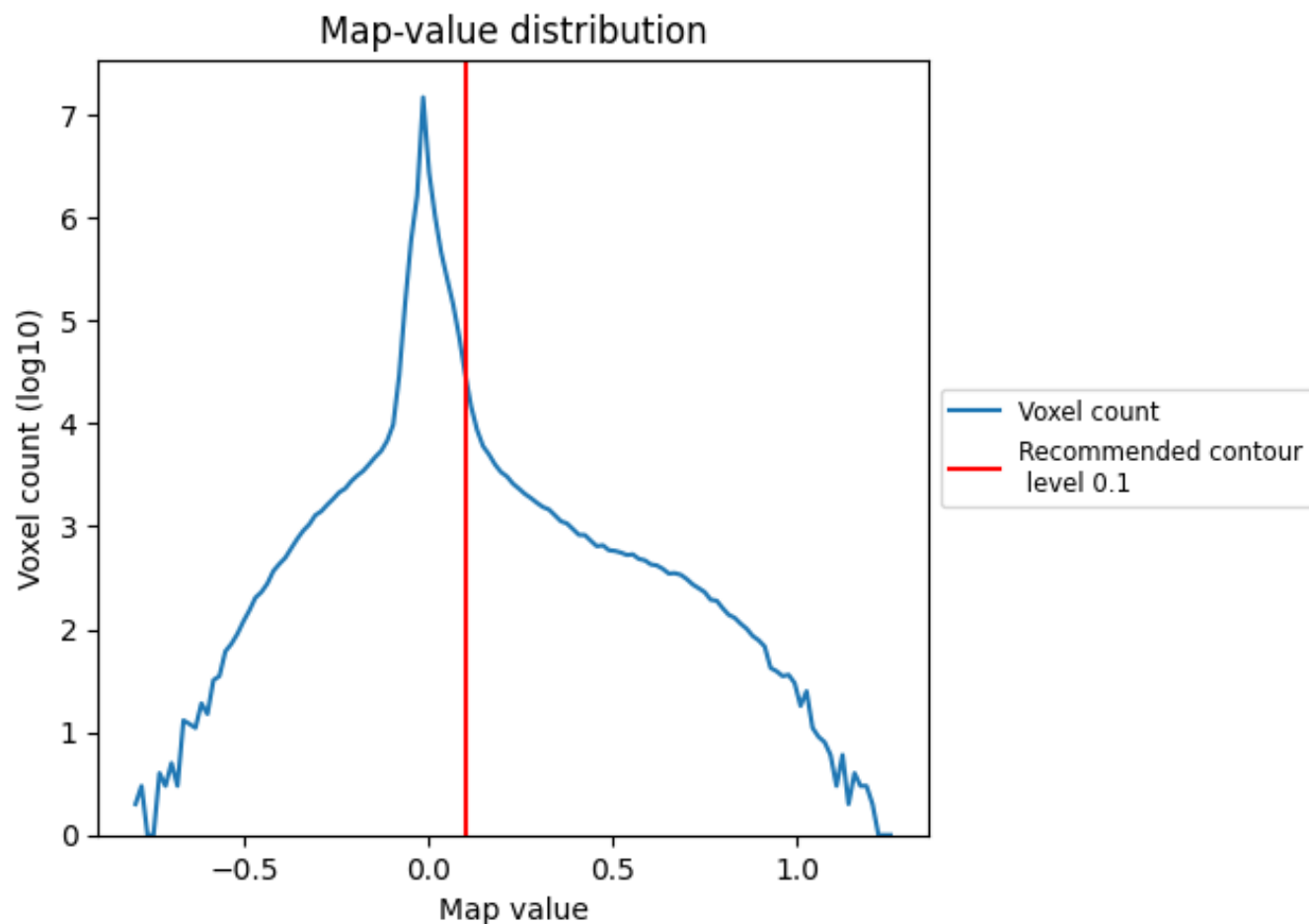
## 6.6 Mask visualisation [i](#)

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.

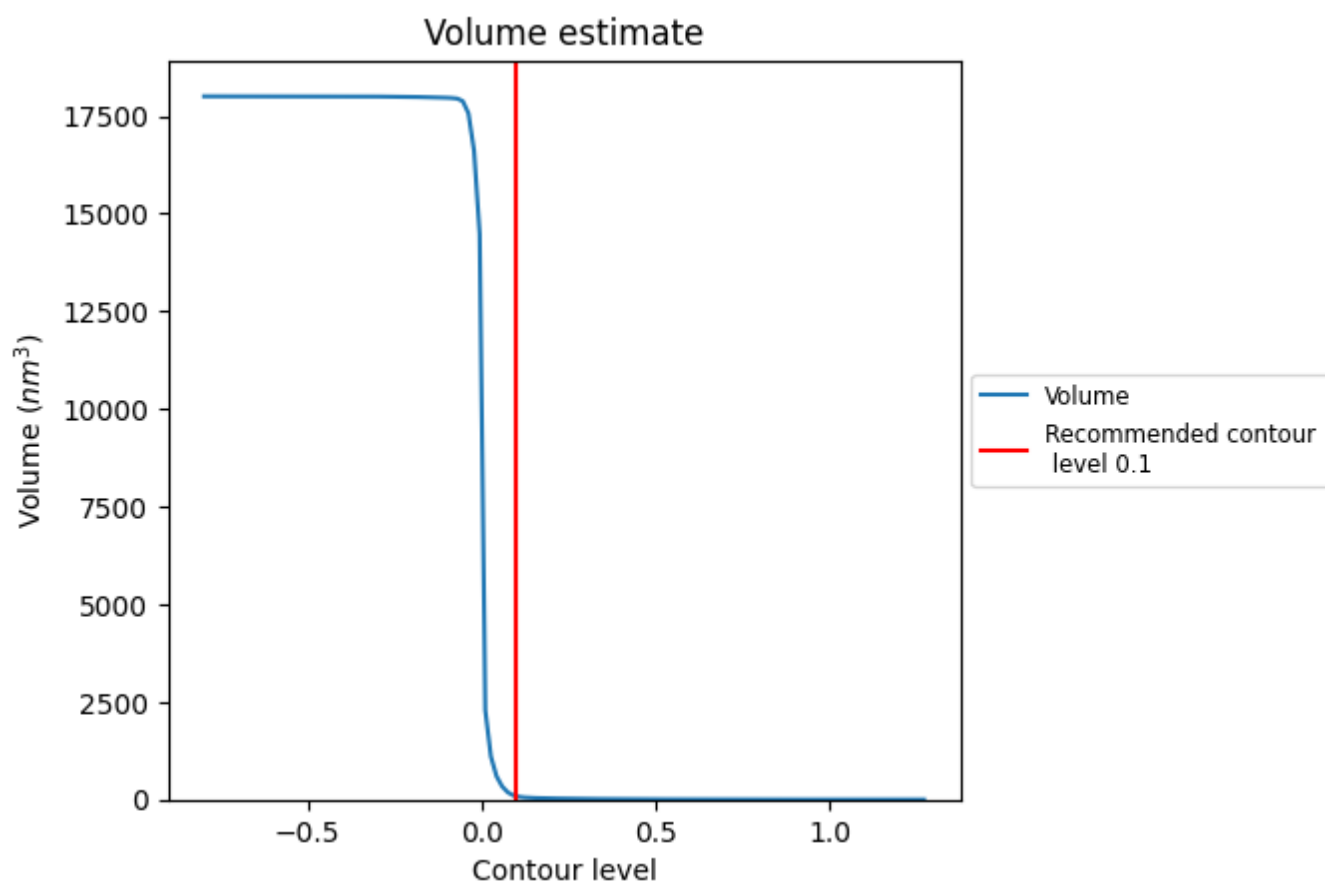
### 7.1 Map-value distribution [i](#)



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.



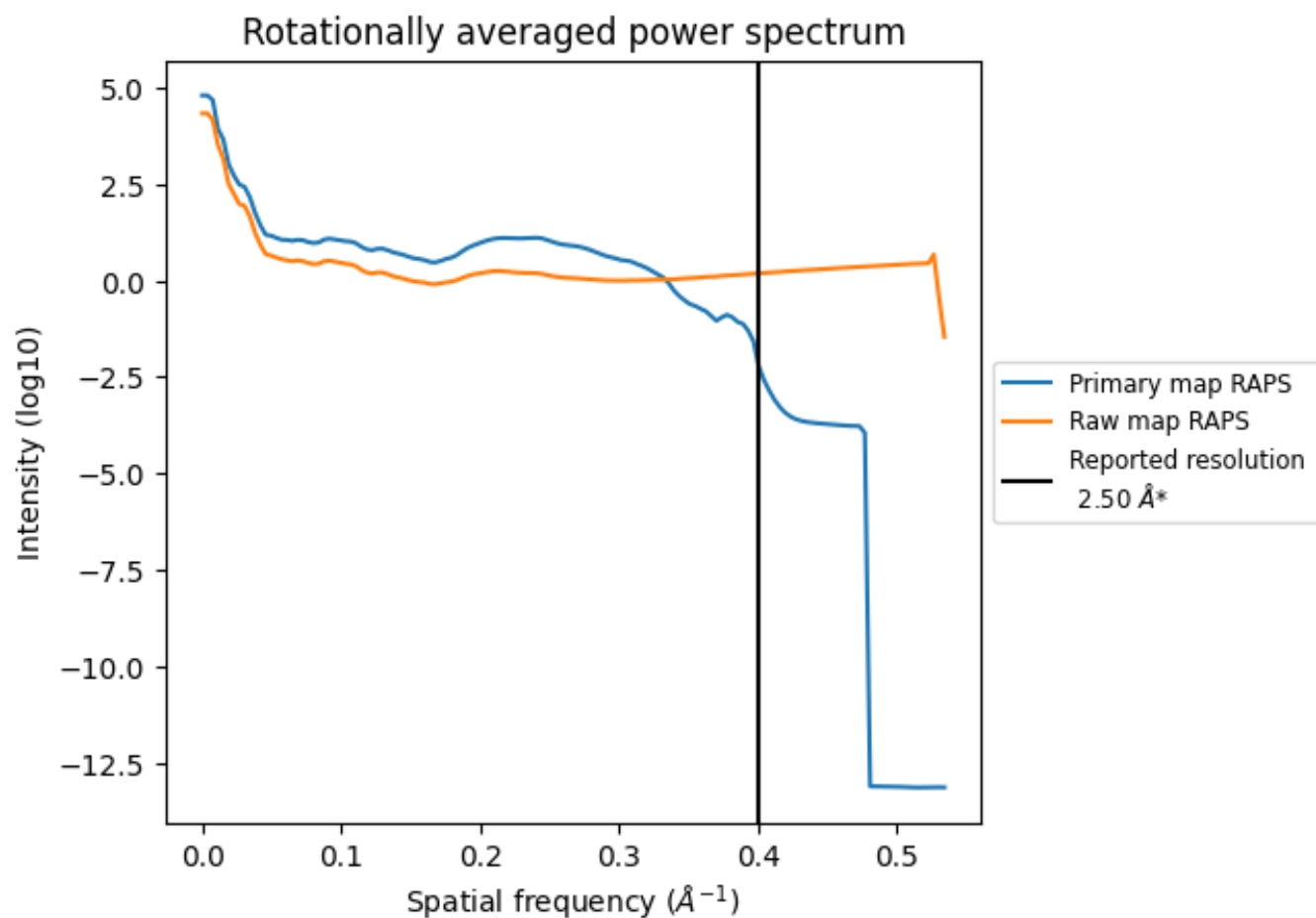
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88  $\text{nm}^3$ ; this corresponds to an approximate mass of 80 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 ⓘ

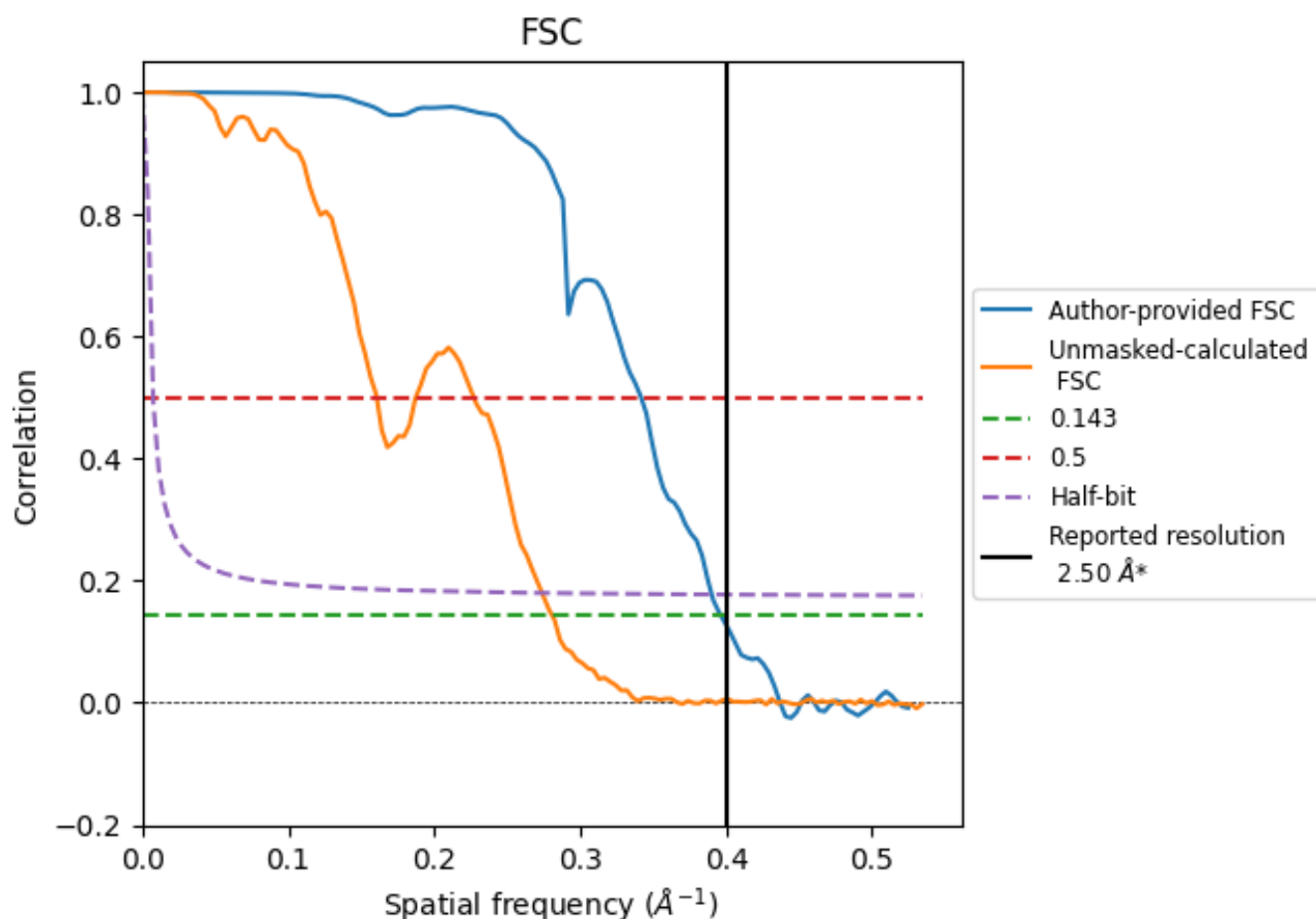


\*Reported resolution corresponds to spatial frequency of 0.400  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

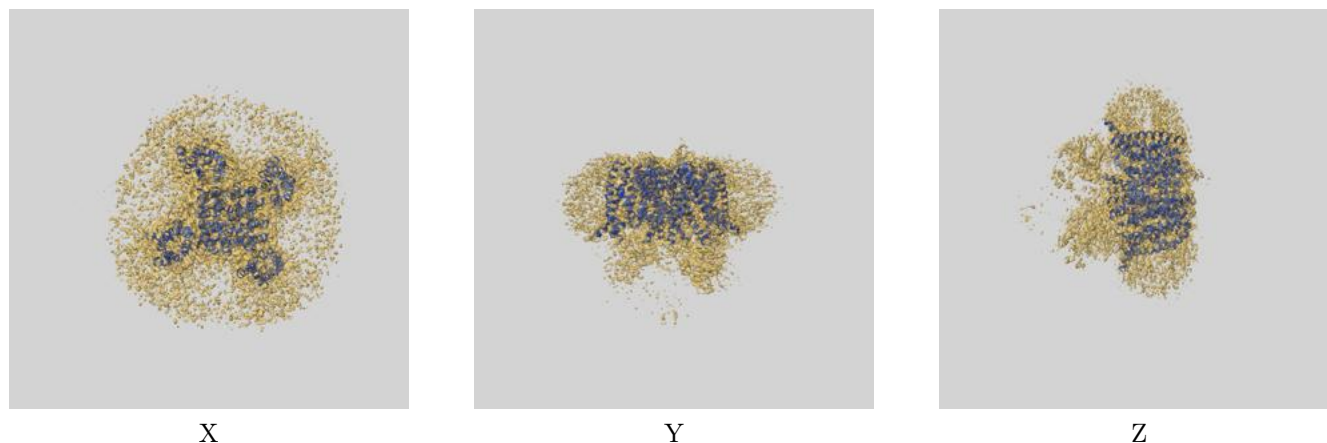
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.52	2.93	2.56
Unmasked-calculated*	3.56	6.23	3.65

\*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 3.56 differs from the reported value 2.5 by more than 10 %

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

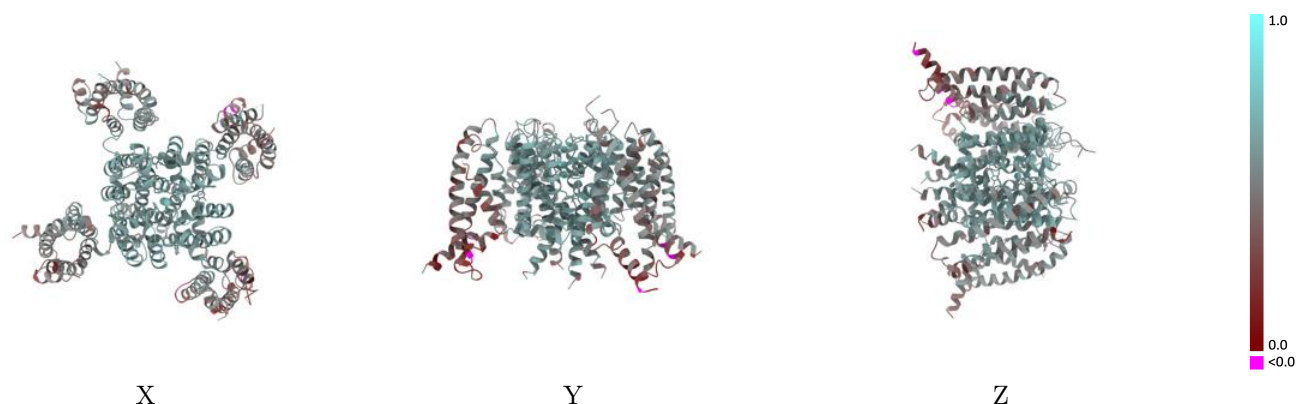
This section contains information regarding the fit between EMDB map EMD-68148 and PDB model 22BF. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



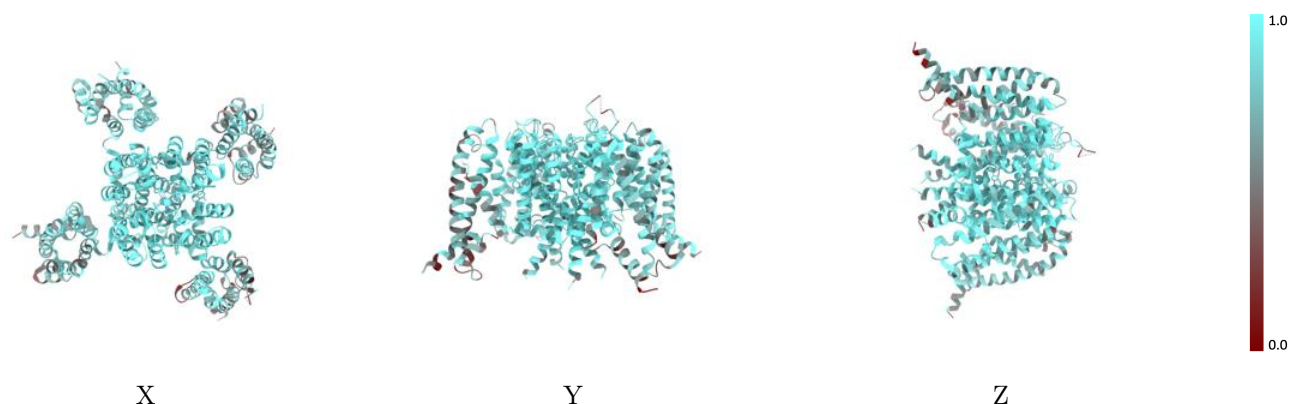
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



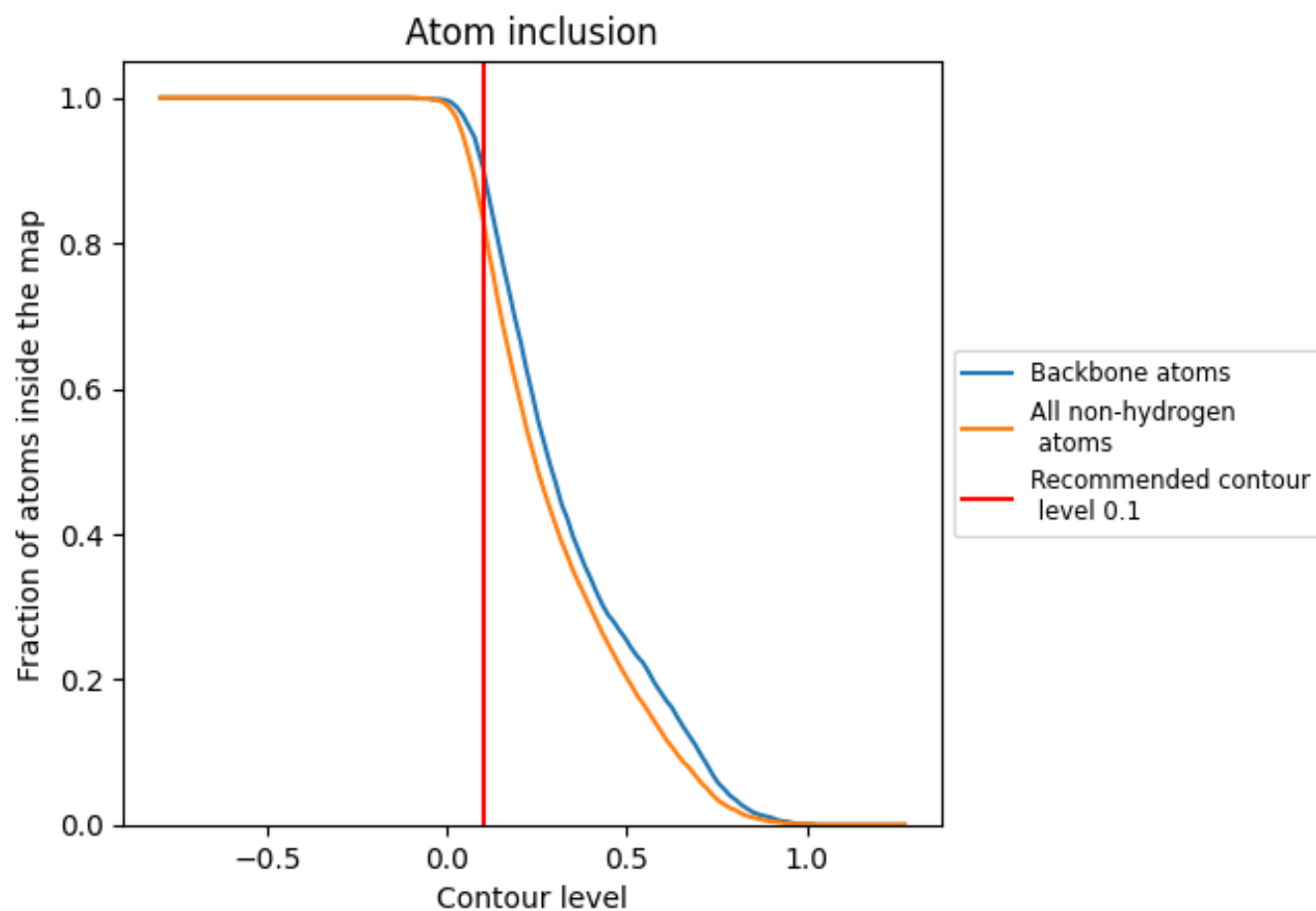
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8330	<div></div> 0.5120
A	<div></div> 0.7810	<div></div> 0.4790
B	<div></div> 0.8150	<div></div> 0.5010
C	<div></div> 0.8910	<div></div> 0.5420
D	<div></div> 0.8440	<div></div> 0.5270

