



## Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 12:16 PM JST

PDB ID : 9WXI / pdb\_00009wxi  
EMDB ID : EMD-66347  
Title : Cryo-EM structure of the type III-D2 CRISPR-Cas effector complex bound to a cognate target RNA in the post-cleavage state  
Authors : Mitsuda, Y.; Ishikawa, J.; Nagahata, N.; Hiraizumi, M.; Yamashita, K.; Nishimasu, H.  
Deposited on : 2025-09-25  
Resolution : 2.80 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>.

---

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

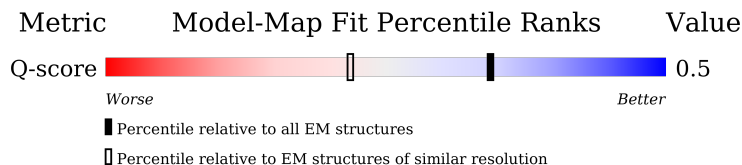
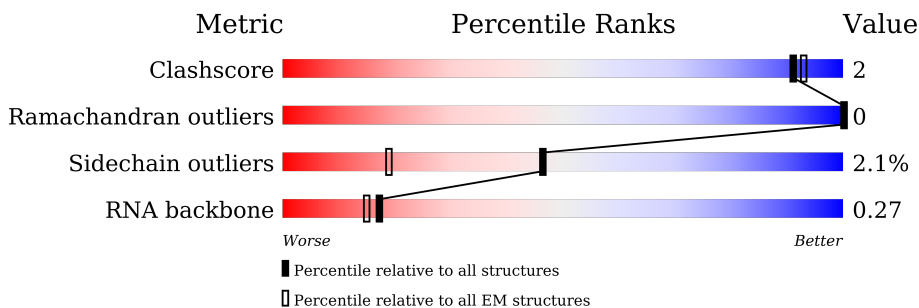
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 ( 2.30 - 3.30 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	43	
2	B	592	
3	C	635	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	1235	<div><div></div><div>12%</div><div>90%</div><div>6%</div><div></div><div></div></div>
5	E	32	<div><div></div><div>50%</div><div>22%</div><div></div><div>25%</div><div></div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19532 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 RNA chain called CRISPR RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	39	Total	C	N	O	P	0	0
			819	368	136	277	38		

- Molecule 2 is a protein called Cas10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	465	Total	C	N	O	S	0	0
			3796	2405	661	718	12		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP A0A9D0P2E0
B	-18	GLY	-	expression tag	UNP A0A9D0P2E0
B	-17	SER	-	expression tag	UNP A0A9D0P2E0
B	-16	SER	-	expression tag	UNP A0A9D0P2E0
B	-15	HIS	-	expression tag	UNP A0A9D0P2E0
B	-14	HIS	-	expression tag	UNP A0A9D0P2E0
B	-13	HIS	-	expression tag	UNP A0A9D0P2E0
B	-12	HIS	-	expression tag	UNP A0A9D0P2E0
B	-11	HIS	-	expression tag	UNP A0A9D0P2E0
B	-10	HIS	-	expression tag	UNP A0A9D0P2E0
B	-9	SER	-	expression tag	UNP A0A9D0P2E0
B	-8	SER	-	expression tag	UNP A0A9D0P2E0
B	-7	GLY	-	expression tag	UNP A0A9D0P2E0
B	-6	LEU	-	expression tag	UNP A0A9D0P2E0
B	-5	VAL	-	expression tag	UNP A0A9D0P2E0
B	-4	PRO	-	expression tag	UNP A0A9D0P2E0
B	-3	ARG	-	expression tag	UNP A0A9D0P2E0
B	-2	GLY	-	expression tag	UNP A0A9D0P2E0
B	-1	SER	-	expression tag	UNP A0A9D0P2E0
B	0	HIS	-	expression tag	UNP A0A9D0P2E0

- Molecule 3 is a protein called CRISPR type III-associated protein domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	626	Total	C	N	O	S	0	0
			4912	3132	828	935	17		

- Molecule 4 is a protein called TIGR03986 family CRISPR-associated RAMP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1194	Total	C	N	O	S	0	0
			9433	5911	1699	1791	32		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP A0A9D0P2B2

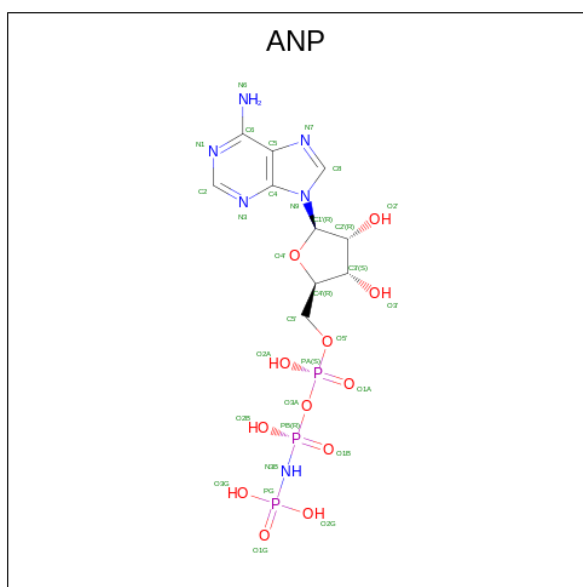
- Molecule 5 is a RNA chain called Cleaved cognate target RNA (CTR).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	24	Total	C	N	O	P	0	0
			511	229	93	165	24		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

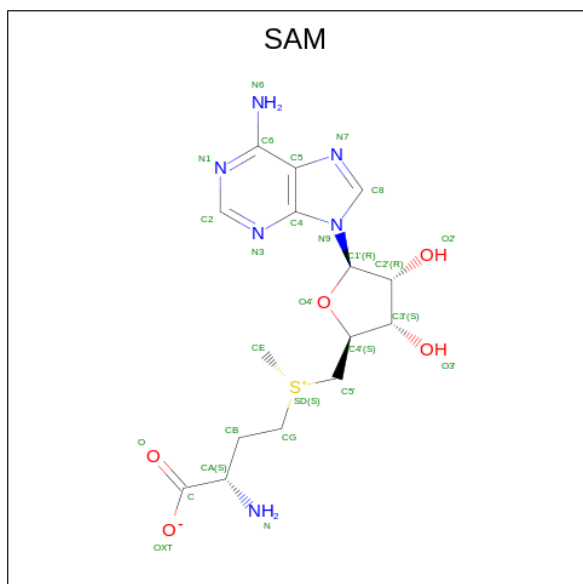
Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 8 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula:  $C_{15}H_{22}N_6O_5S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	N	O	S	0
			27	15	6	5	1	

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total 1	Zn 1	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total 1	O 1	0

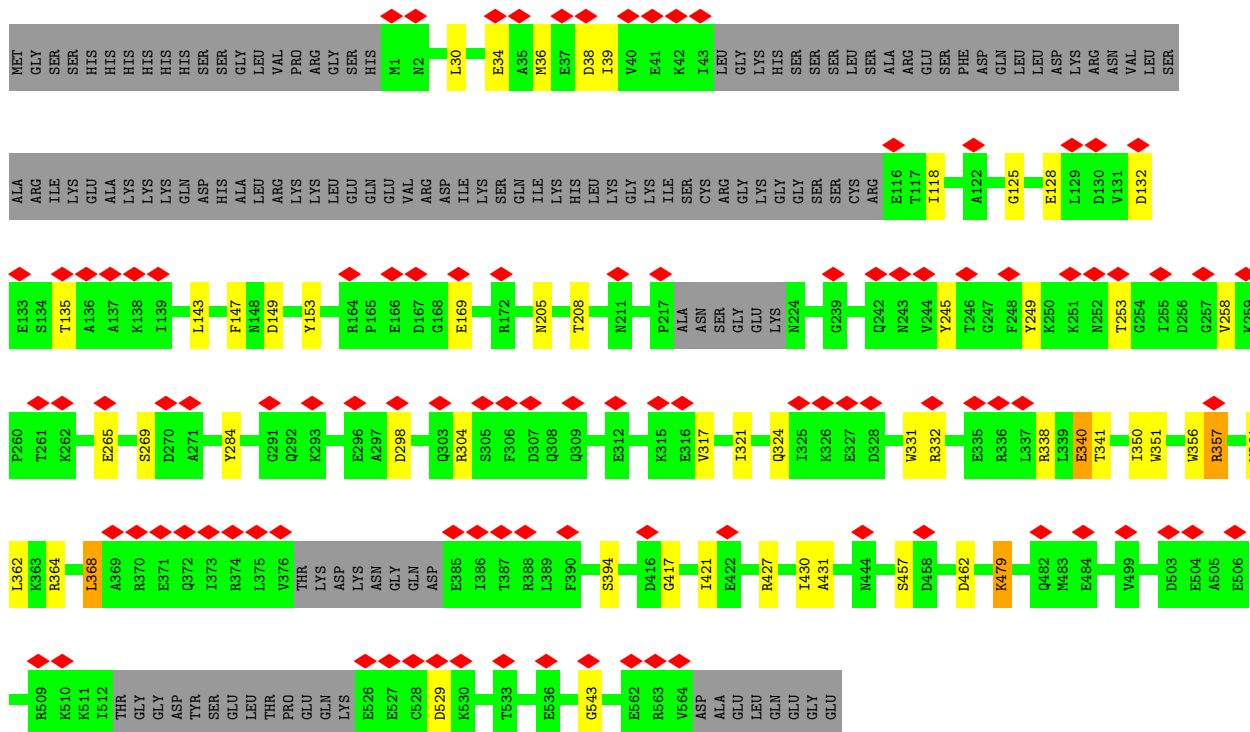
### 3 Residue-property plots [i](#)

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: CRISPR RNA



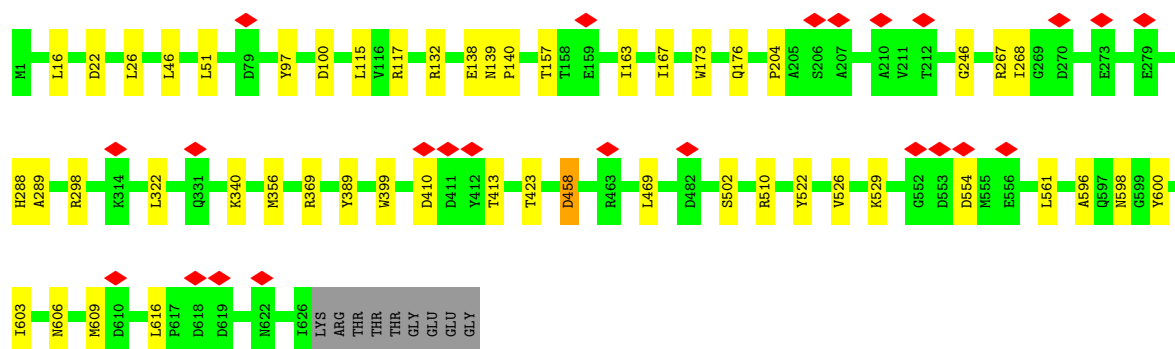
- Molecule 2: Cas10



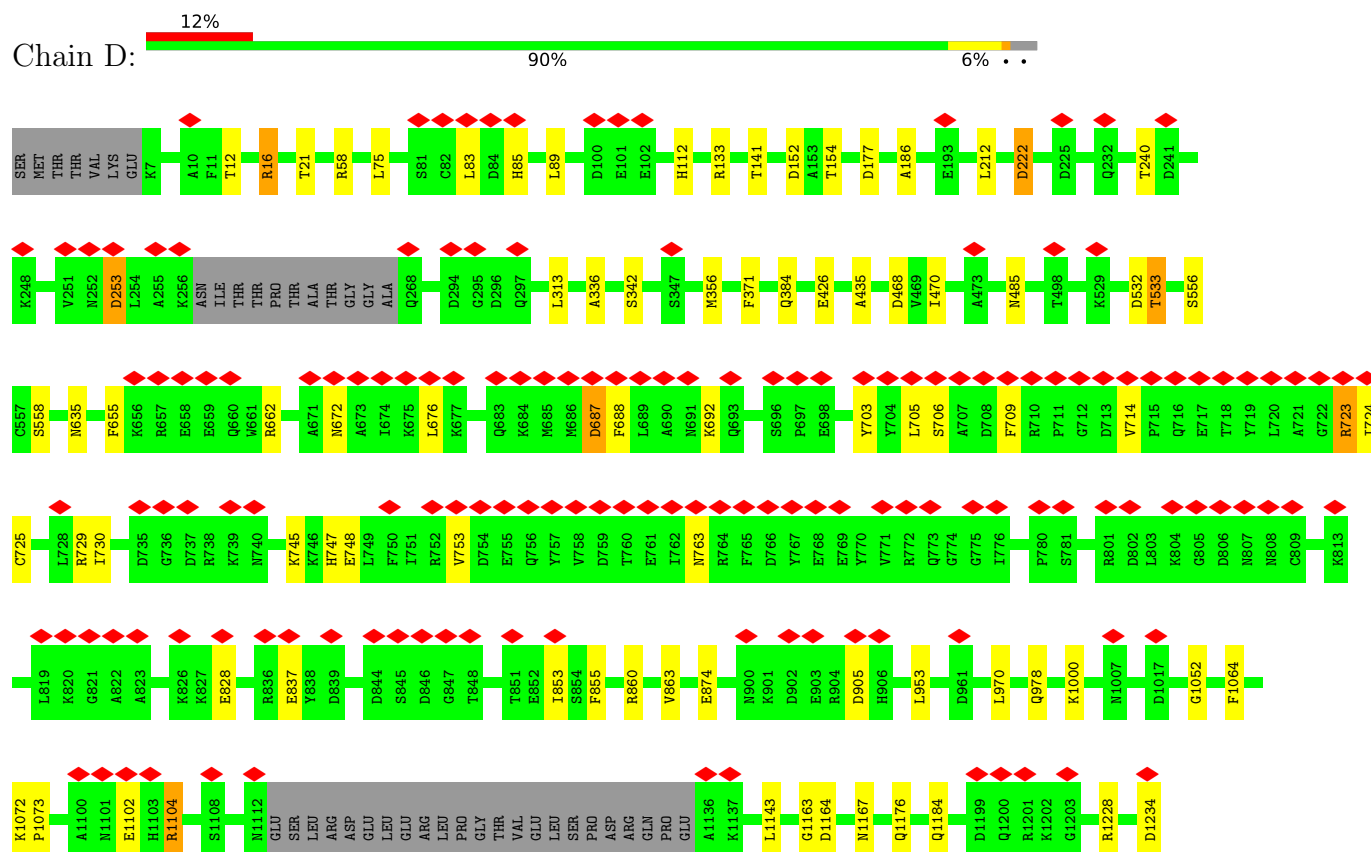
- Molecule 3: CRISPR type III-associated protein domain-containing protein



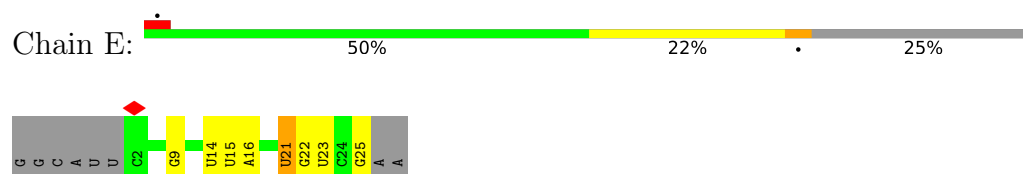




• Molecule 4: TIGR03986 family CRISPR-associated RAMP protein



• Molecule 5: Cleaved cognate target RNA (CTR)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	151530	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 ( $e^-/\text{\AA}^2$ )	49.833	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.474	Depositor
Minimum map value	-0.849	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.0967	Depositor
Map size (Å)	298.8, 298.8, 298.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.99599993, 0.99599993, 0.99599993	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAM, MG, ANP, ZN

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	0.60	0/913	1.24	4/1419 (0.3%)
2	B	0.56	0/3867	1.13	10/5205 (0.2%)
3	C	0.60	0/5032	1.09	8/6845 (0.1%)
4	D	0.60	0/9648	1.12	21/13041 (0.2%)
5	E	0.66	0/571	0.98	3/887 (0.3%)
All	All	0.60	0/20031	1.12	46/27397 (0.2%)

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
2	B	0	3
3	C	0	1
4	D	0	2
All	All	0	6

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	U	O3'-P-O5'	9.29	117.93	104.00
4	D	687	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	27	A	O3'-P-O5'	-7.29	93.06	104.00
3	C	458	ASP	CA-CB-CG	7.25	119.85	112.60
2	B	149	ASP	CA-CB-CG	6.99	119.59	112.60
4	D	152	ASP	CA-CB-CG	6.66	119.26	112.60
2	B	132	ASP	CA-CB-CG	6.35	118.95	112.60
4	D	532	ASP	CB-CA-C	6.34	120.72	110.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	340	GLU	CB-CG-CD	6.25	123.22	112.60
1	A	12	U	O3'-P-O5'	-6.24	94.63	104.00
4	D	714	VAL	N-CA-CB	6.22	116.88	110.23
5	E	21	U	O3'-P-O5'	-6.13	94.81	104.00
4	D	253	ASP	CA-CB-CG	6.03	118.62	112.60
5	E	14	U	O3'-P-O5'	-5.91	95.13	104.00
2	B	529	ASP	CA-CB-CG	5.78	118.38	112.60
3	C	97	TYR	N-CA-CB	5.78	119.66	110.65
3	C	554	ASP	CA-CB-CG	5.77	118.37	112.60
4	D	763	ASN	CB-CA-C	5.75	119.56	111.86
2	B	479	LYS	CB-CG-CD	5.64	124.27	111.30
1	A	10	U	C2'-C3'-O3'	-5.63	105.25	113.70
3	C	510	ARG	NE-CZ-NH2	5.62	124.26	119.20
4	D	723	ARG	CD-NE-CZ	5.61	132.25	124.40
4	D	723	ARG	CA-CB-CG	5.60	125.30	114.10
5	E	9	G	O3'-P-O5'	-5.55	95.68	104.00
4	D	222	ASP	CA-CB-CG	5.53	118.13	112.60
4	D	468	ASP	CA-CB-CG	5.53	118.12	112.60
4	D	426	GLU	CB-CG-CD	5.51	121.97	112.60
4	D	828	GLU	CB-CA-C	5.49	121.34	110.42
4	D	1104	ARG	NE-CZ-NH2	5.47	124.13	119.20
3	C	267	ARG	CB-CA-C	5.46	121.28	110.42
4	D	112	HIS	CB-CG-CD2	5.43	138.26	131.20
3	C	117	ARG	NE-CZ-NH2	5.34	124.01	119.20
3	C	22	ASP	CA-CB-CG	5.32	117.92	112.60
3	C	389	TYR	CA-CB-CG	5.29	123.42	113.90
4	D	905	ASP	CA-CB-CG	5.22	117.83	112.60
4	D	533	THR	N-CA-CB	5.21	119.30	110.49
2	B	265	GLU	N-CA-CB	5.16	117.49	110.01
2	B	332	ARG	CD-NE-CZ	5.12	131.57	124.40
4	D	635	ASN	CA-CB-CG	5.11	117.71	112.60
2	B	357	ARG	NE-CZ-NH2	5.08	123.77	119.20
4	D	1234	ASP	CA-CB-CG	5.08	117.68	112.60
2	B	304	ARG	NE-CZ-NH2	5.07	123.76	119.20
4	D	676	LEU	CA-C-N	5.05	128.84	121.31
4	D	676	LEU	C-N-CA	5.05	128.84	121.31
2	B	298	ASP	CA-CB-CG	5.04	117.64	112.60
4	D	662	ARG	NE-CZ-NH2	5.03	123.73	119.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	417	GLY	Peptide
2	B	421	ILE	Peptide
2	B	543	GLY	Peptide
3	C	609	MET	Peptide
4	D	558	SER	Peptide
4	D	672	ASN	Peptide

## 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	819	0	416	1	0
2	B	3796	0	3765	18	0
3	C	4912	0	4864	17	0
4	D	9433	0	9215	27	0
5	E	511	0	260	0	0
6	B	1	0	0	0	0
7	B	31	0	13	0	0
8	B	27	0	22	0	0
9	D	1	0	0	0	0
10	B	1	0	0	0	0
All	All	19532	0	18555	62	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 2.

All (62) 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)
2:B:362:LEU:HD21	2:B:430:ILE:HG12	1.77	0.67
4:D:435:ALA:HB2	4:D:470:ILE:HG21	1.80	0.64
2:B:245:TYR:OH	2:B:341:THR:O	2.16	0.63
4:D:688:PHE:O	4:D:692:LYS:HG2	1.98	0.63
4:D:1000:LYS:O	4:D:1228:ARG:NH1	2.26	0.61
2:B:118:ILE:HD11	2:B:128:GLU:HB2	1.81	0.60
3:C:289:ALA:HB1	3:C:399:TRP:HB3	1.84	0.60
2:B:331:TRP:CZ2	2:B:357:ARG:HB3	2.38	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:SER:HA	2:B:431:ALA:O	2.04	0.58
4:D:692:LYS:HD2	4:D:703:TYR:OH	2.02	0.58
2:B:36:MET:HE2	2:B:125:GLY:HA3	1.85	0.57
4:D:705:LEU:O	4:D:724:ILE:N	2.30	0.56
4:D:336:ALA:N	4:D:485:ASN:O	2.37	0.56
3:C:204:PRO:HA	3:C:423:THR:HG21	1.88	0.55
4:D:1176:GLN:NE2	4:D:1184:GLN:O	2.41	0.53
2:B:317:VAL:HG22	2:B:368:LEU:HB3	1.91	0.53
4:D:725:CYS:SG	4:D:753:VAL:O	2.64	0.53
2:B:356:TRP:CD1	2:B:357:ARG:HG2	2.45	0.52
4:D:655:PHE:HA	4:D:837:GLU:HG3	1.92	0.50
2:B:39:ILE:HD11	2:B:147:PHE:HZ	1.76	0.49
3:C:596:ALA:HA	3:C:600:TYR:O	2.14	0.48
2:B:38:ASP:OD2	2:B:153:TYR:OH	2.29	0.48
2:B:321:ILE:HG21	2:B:361:MET:HE1	1.96	0.48
3:C:157:THR:HG21	3:C:163:ILE:HD12	1.97	0.47
4:D:58:ARG:NH2	4:D:133:ARG:O	2.45	0.47
2:B:351:TRP:CE3	2:B:361:MET:HE3	2.50	0.46
3:C:522:TYR:CE1	3:C:526:VAL:HG21	2.50	0.46
3:C:288:HIS:O	3:C:298:ARG:NH1	2.47	0.46
2:B:324:GLN:OE1	2:B:364:ARG:NE	2.49	0.46
4:D:730:ILE:HA	4:D:748:GLU:OE1	2.16	0.46
4:D:313:LEU:HB3	4:D:371:PHE:HB2	1.97	0.45
3:C:115:LEU:HB3	3:C:139:ASN:O	2.17	0.45
4:D:141:THR:HA	4:D:154:THR:O	2.17	0.45
2:B:457:SER:OG	2:B:462:ASP:OD2	2.29	0.45
3:C:469:LEU:HD23	3:C:603:ILE:HG22	1.97	0.45
4:D:75:LEU:HD22	4:D:186:ALA:HB1	1.99	0.45
3:C:246:GLY:O	3:C:598:ASN:O	2.35	0.45
3:C:410:ASP:OD1	3:C:413:THR:OG1	2.33	0.45
3:C:100:ASP:OD2	3:C:369:ARG:NH1	2.49	0.44
4:D:688:PHE:CE1	4:D:692:LYS:HE2	2.52	0.44
3:C:522:TYR:CZ	3:C:526:VAL:HG21	2.53	0.44
4:D:85:HIS:O	4:D:89:LEU:HG	2.17	0.44
4:D:1164:ASP:HB3	4:D:1167:ASN:ND2	2.32	0.44
4:D:863:VAL:HG21	4:D:970:LEU:HD23	2.00	0.43
2:B:269:SER:O	2:B:338:ARG:NH2	2.50	0.43
2:B:284:TYR:HD1	2:B:350:ILE:HG12	1.82	0.43
2:B:205:ASN:ND2	2:B:208:THR:OG1	2.51	0.43
4:D:706:SER:O	4:D:709:PHE:HD2	2.02	0.43
3:C:138:GLU:HG2	3:C:140:PRO:HD3	2.02	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:A:OP1	4:D:860:ARG:NH1	2.51	0.41
4:D:16:ARG:NH2	4:D:240:THR:OG1	2.53	0.41
2:B:249:TYR:O	2:B:253:THR:OG1	2.36	0.41
4:D:1052:GLY:HA2	4:D:1143:LEU:HB3	2.02	0.41
4:D:1072:LYS:N	4:D:1073:PRO:HD2	2.36	0.41
3:C:163:ILE:O	3:C:167:ILE:HG12	2.21	0.41
3:C:502:SER:HA	3:C:561:LEU:HD13	2.03	0.41
4:D:21:THR:OG1	4:D:212:LEU:HD11	2.21	0.41
4:D:1064:PHE:CD1	4:D:1163:GLY:HA3	2.56	0.41
4:D:533:THR:HG21	4:D:874:GLU:HG3	2.03	0.41
3:C:458:ASP:O	3:C:606:ASN:ND2	2.54	0.40
4:D:729:ARG:NH1	4:D:855:PHE:O	2.50	0.40
3:C:51:LEU:HD21	3:C:167:ILE:HD12	2.03	0.40

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	
2	B	455/592 (77%)	447 (98%)	8 (2%)	0	100	100
3	C	624/635 (98%)	614 (98%)	10 (2%)	0	100	100
4	D	1188/1235 (96%)	1155 (97%)	33 (3%)	0	100	100
All	All	2267/2462 (92%)	2216 (98%)	51 (2%)	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	
2	B	406/514 (79%)	396 (98%)	10 (2%)	42	76
3	C	533/540 (99%)	521 (98%)	12 (2%)	44	78
4	D	1005/1041 (96%)	986 (98%)	19 (2%)	50	81
All	All	1944/2095 (93%)	1903 (98%)	41 (2%)	46	79

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	30	LEU
2	B	34	GLU
2	B	135	THR
2	B	143	LEU
2	B	169	GLU
2	B	258	VAL
2	B	340	GLU
2	B	368	LEU
2	B	427	ARG
2	B	479	LYS
3	C	16	LEU
3	C	26	LEU
3	C	46	LEU
3	C	132	ARG
3	C	173	TRP
3	C	176	GLN
3	C	268	ILE
3	C	322	LEU
3	C	340	LYS
3	C	356	MET
3	C	529	LYS
3	C	616	LEU
4	D	12	THR
4	D	16	ARG
4	D	83	LEU
4	D	177	ASP
4	D	222	ASP
4	D	253	ASP
4	D	342	SER
4	D	356	MET
4	D	384	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
4	D	556	SER
4	D	687	ASP
4	D	723	ARG
4	D	745	LYS
4	D	747	HIS
4	D	853	ILE
4	D	953	LEU
4	D	978	GLN
4	D	1102	GLU
4	D	1104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	11	ASN
2	B	197	GLN
2	B	205	ASN
2	B	288	ASN
2	B	495	GLN
3	C	2	GLN
3	C	385	GLN
3	C	470	GLN
3	C	567	GLN
4	D	78	HIS
4	D	421	ASN
4	D	499	ASN
4	D	517	HIS
4	D	635	ASN
4	D	773	GLN
4	D	880	GLN
4	D	900	ASN
4	D	906	HIS
4	D	929	GLN
4	D	995	GLN
4	D	1010	HIS
4	D	1040	HIS
4	D	1044	ASN
4	D	1167	ASN
4	D	1179	ASN
4	D	1227	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	38/43 (88%)	18 (47%)	9 (23%)
5	E	23/32 (71%)	5 (21%)	2 (8%)
All	All	61/75 (81%)	23 (37%)	11 (18%)

All (23) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	3	U
1	A	4	G
1	A	7	A
1	A	8	C
1	A	9	U
1	A	10	U
1	A	11	G
1	A	19	C
1	A	20	A
1	A	25	U
1	A	26	A
1	A	27	A
1	A	28	U
1	A	30	C
1	A	31	U
1	A	36	U
1	A	38	U
5	E	15	U
5	E	16	A
5	E	22	G
5	E	23	U
5	E	25	G

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	3	U
1	A	7	A
1	A	9	U
1	A	13	C
1	A	15	U
1	A	19	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	25	U
1	A	27	A
5	E	15	U
5	E	21	U

## 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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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$
8	SAM	B	603	-	27,29,29	0.41	0	36,42,42	0.61	1 (2%)
7	ANP	B	602	6	32,33,33	1.09	5 (15%)	44,52,52	0.94	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SAM	B	603	-	-	2/16/33/33	0/3/3/3
7	ANP	B	602	6	-	3/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	602	ANP	PG-O1G	2.98	1.50	1.46
7	B	602	ANP	PB-O1B	2.93	1.50	1.46
7	B	602	ANP	PG-O3G	-2.28	1.50	1.56
7	B	602	ANP	PB-O2B	-2.19	1.50	1.56
7	B	602	ANP	PG-O2G	-2.14	1.51	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	602	ANP	O2B-PB-O1B	4.08	118.48	109.92
7	B	602	ANP	O3G-PG-O1G	-2.26	107.76	113.45
8	B	603	SAM	CG-SD-C5'	-2.24	97.69	103.40
7	B	602	ANP	O2G-PG-O1G	-2.00	108.42	113.45

There are no chirality outliers.

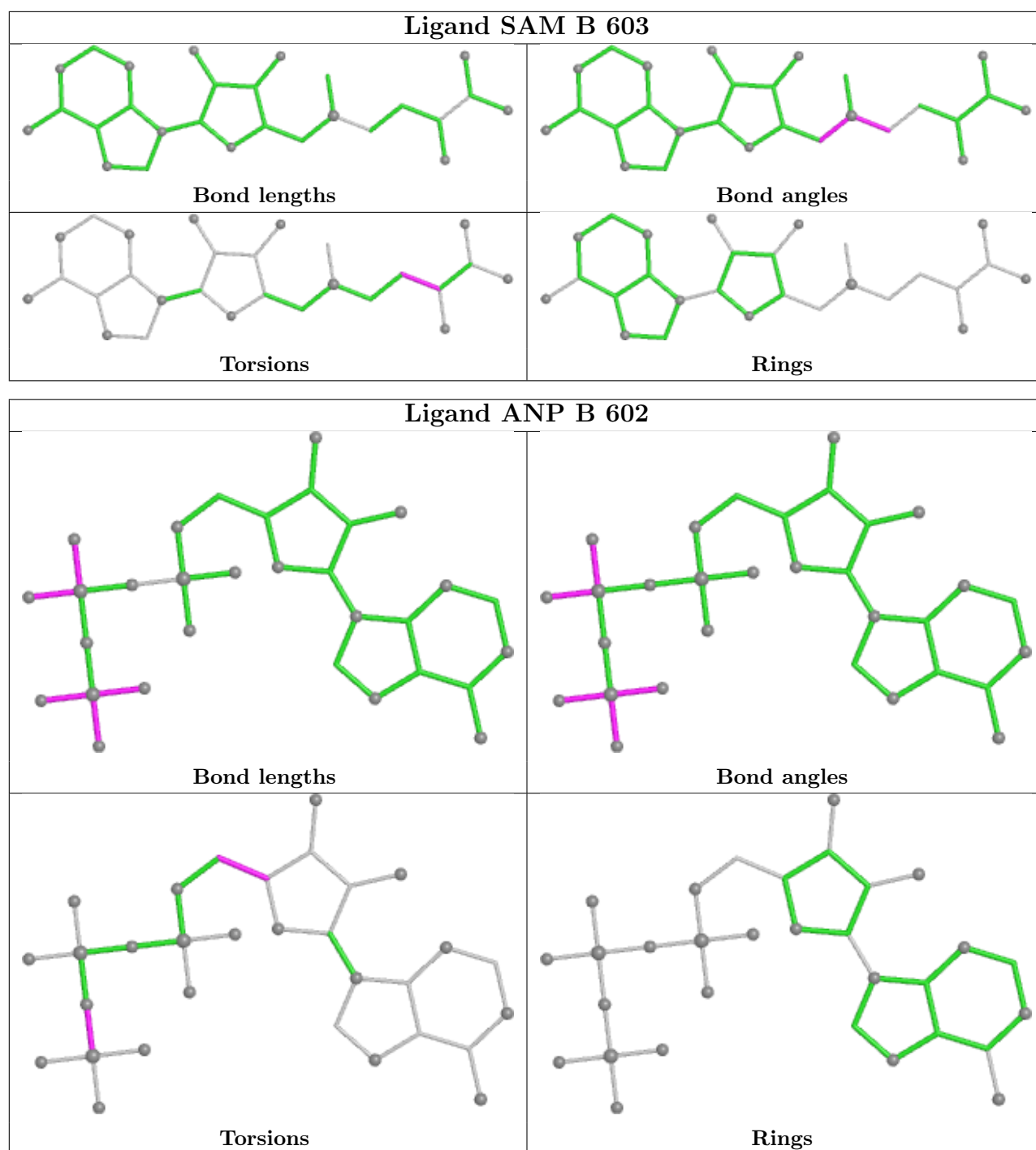
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	602	ANP	PB-N3B-PG-O1G
7	B	602	ANP	O4'-C4'-C5'-O5'
7	B	602	ANP	C3'-C4'-C5'-O5'
8	B	603	SAM	C-CA-CB-CG
8	B	603	SAM	N-CA-CB-CG

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.

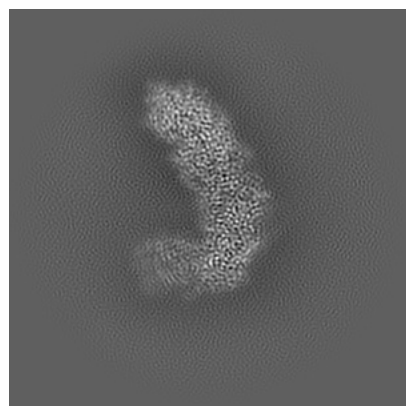
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66347. These allow visual inspection of the internal detail of the map and identification of artifacts.

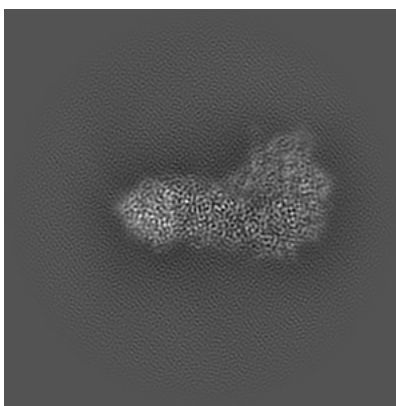
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

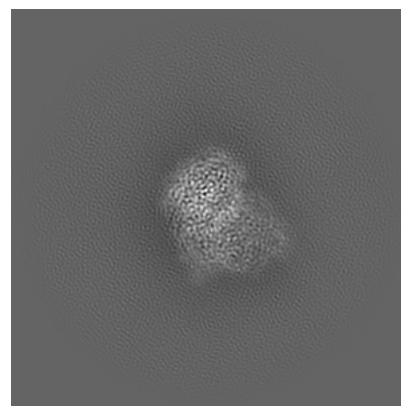
#### 6.1.1 Primary map



X

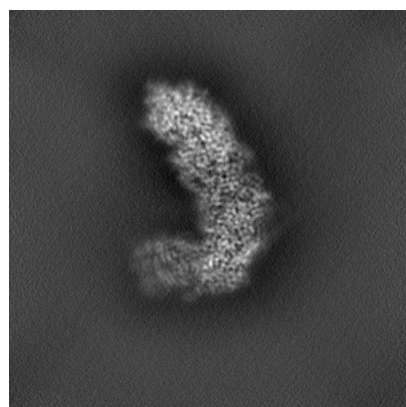


Y

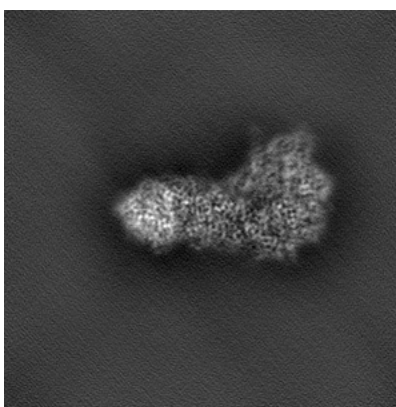


Z

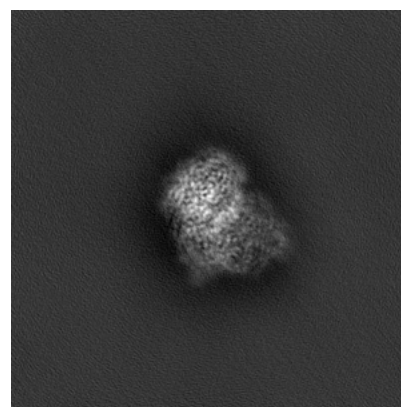
#### 6.1.2 Raw map



X



Y

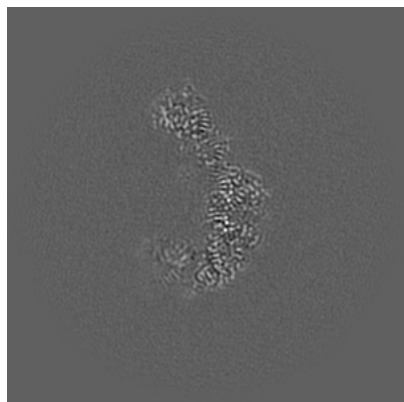


Z

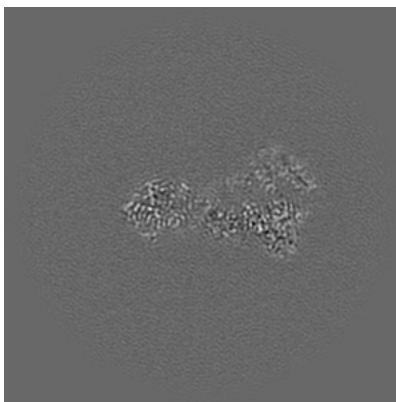
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

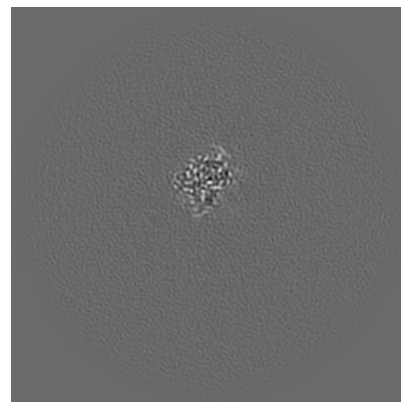
### 6.2.1 Primary map



X Index: 150

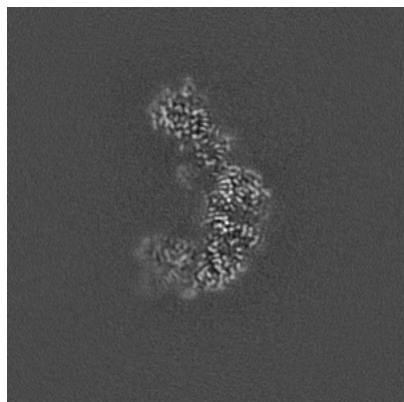


Y Index: 150

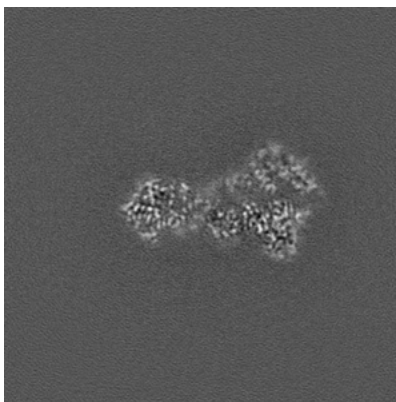


Z Index: 150

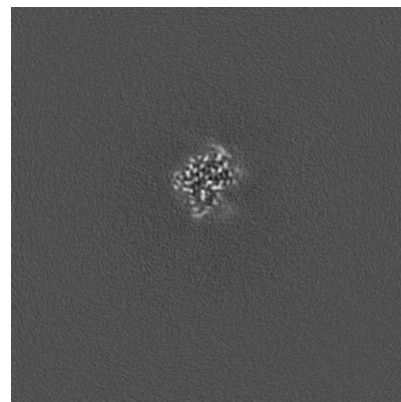
### 6.2.2 Raw map



X Index: 150



Y Index: 150



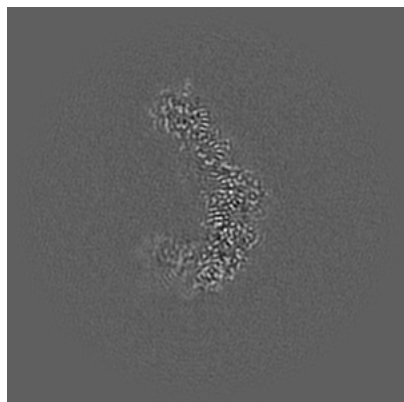
Z Index: 150

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

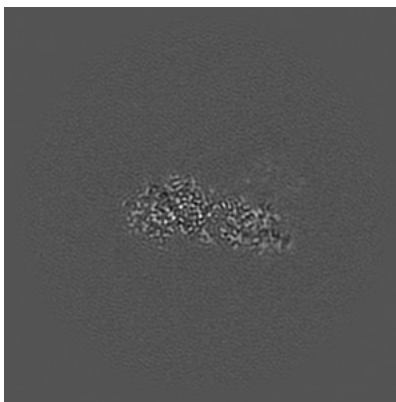


## 6.3 Largest variance slices [i](#)

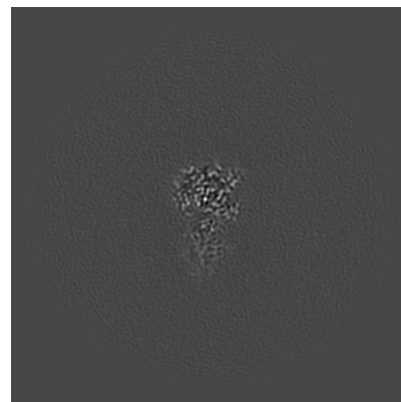
### 6.3.1 Primary map



X Index: 149

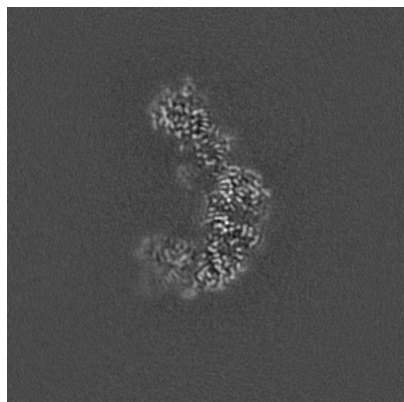


Y Index: 163

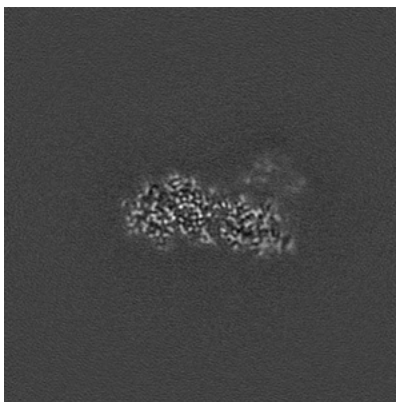


Z Index: 112

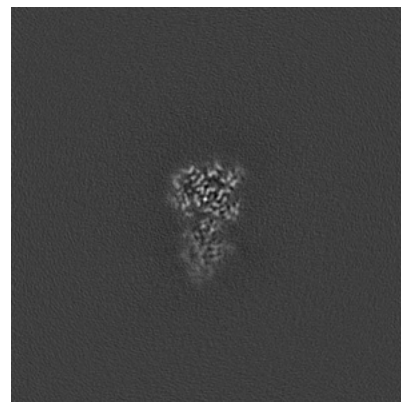
### 6.3.2 Raw map



X Index: 150



Y Index: 163



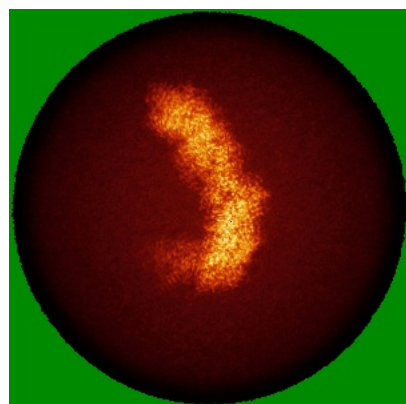
Z Index: 112

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

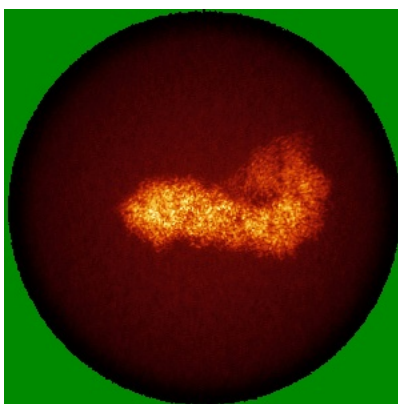


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

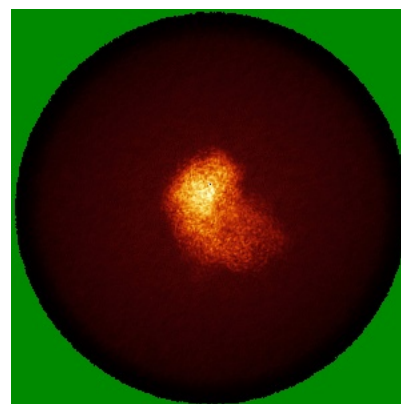
### 6.4.1 Primary map



X

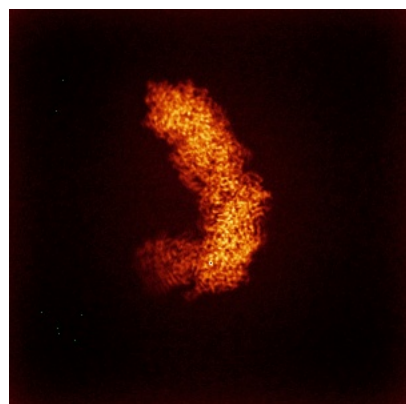


Y

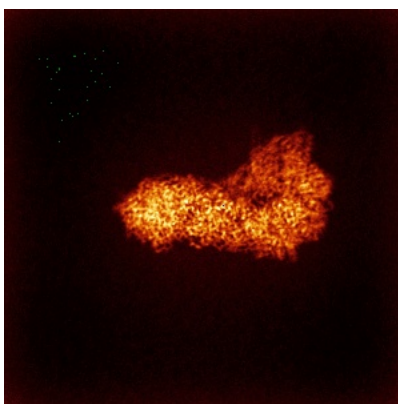


Z

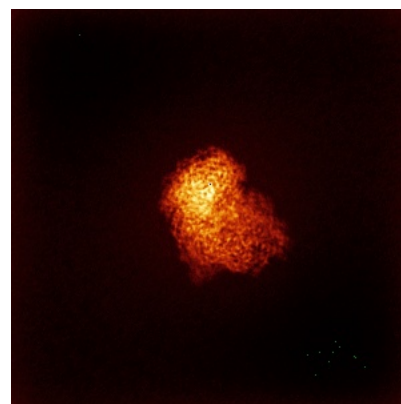
### 6.4.2 Raw map



X



Y

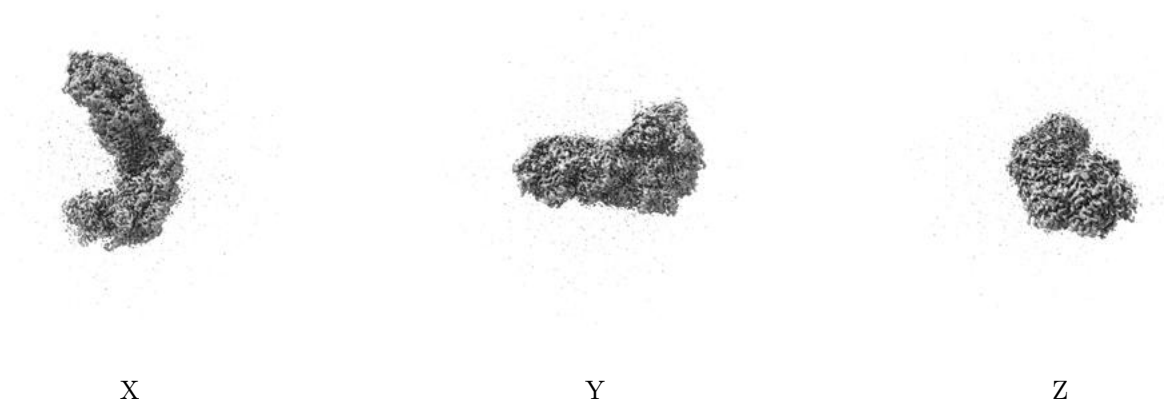


Z

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.

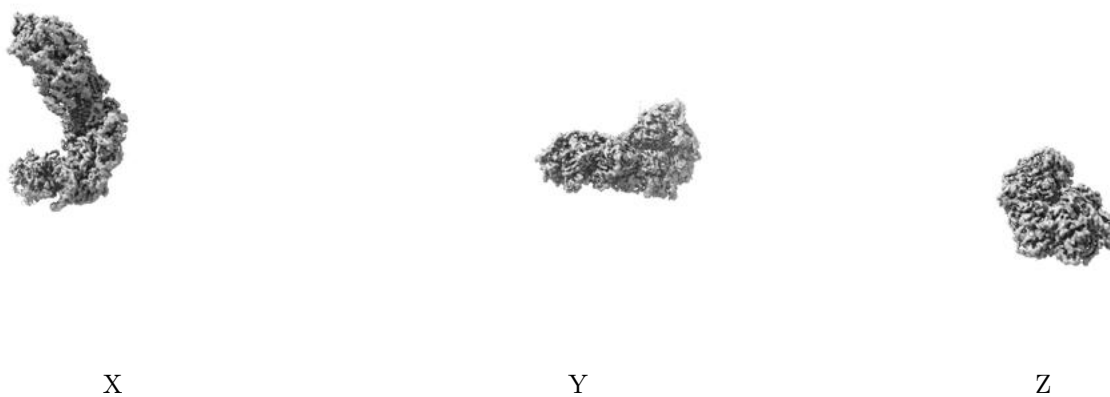
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0967. 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.

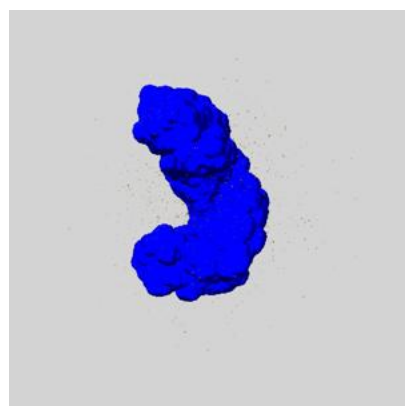
## 6.6 Mask visualisation [i](#)

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

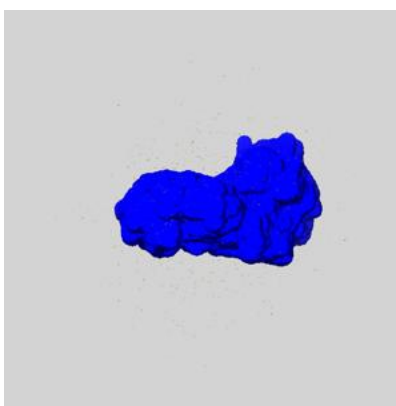
A mask typically either:

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

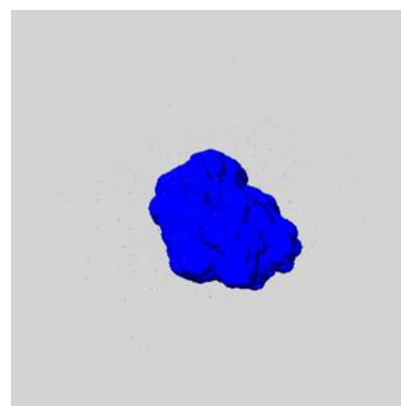
### 6.6.1 emd\_66347\_msk\_1.map [i](#)



X



Y

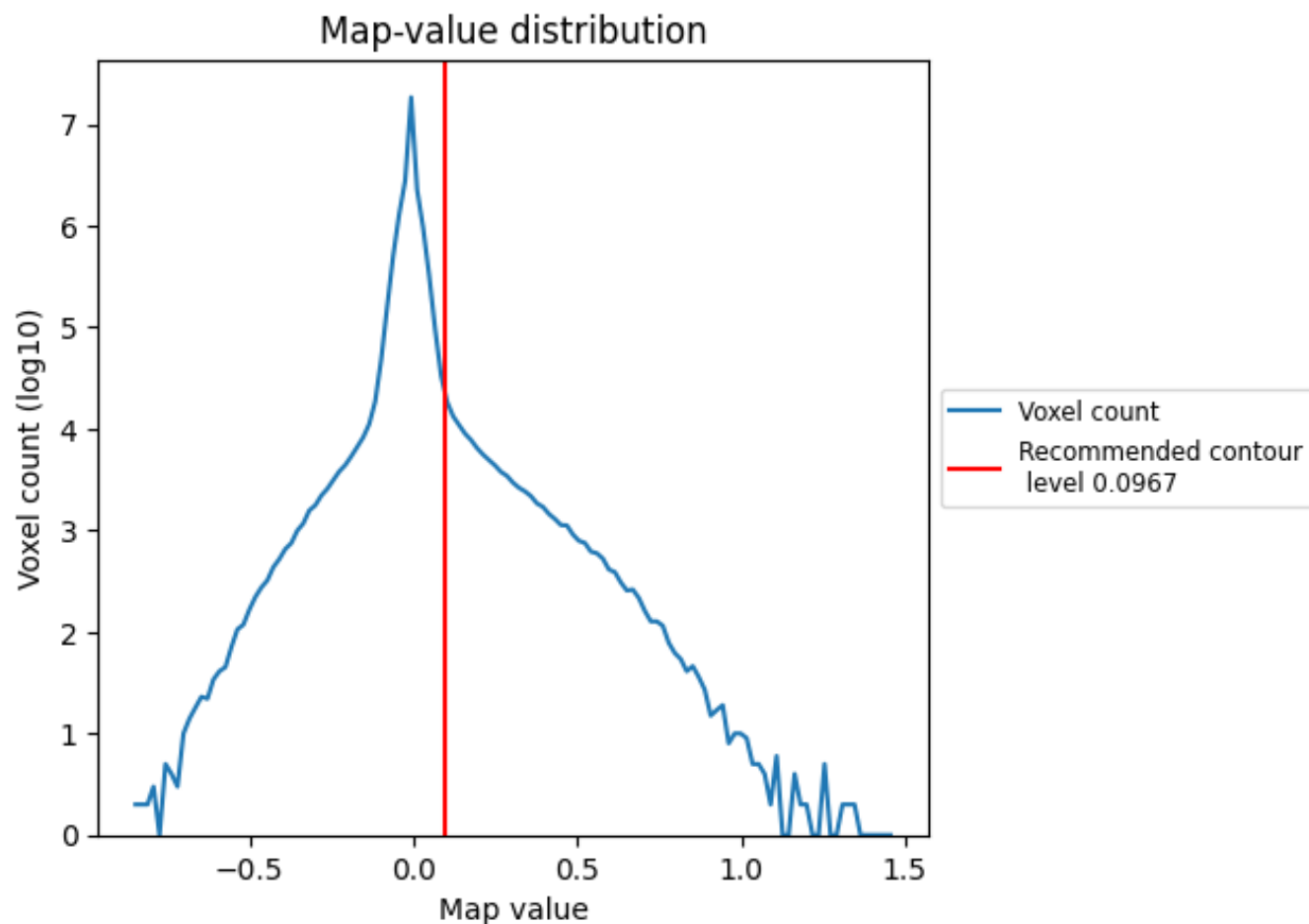


Z

## 7 Map analysis [i](#)

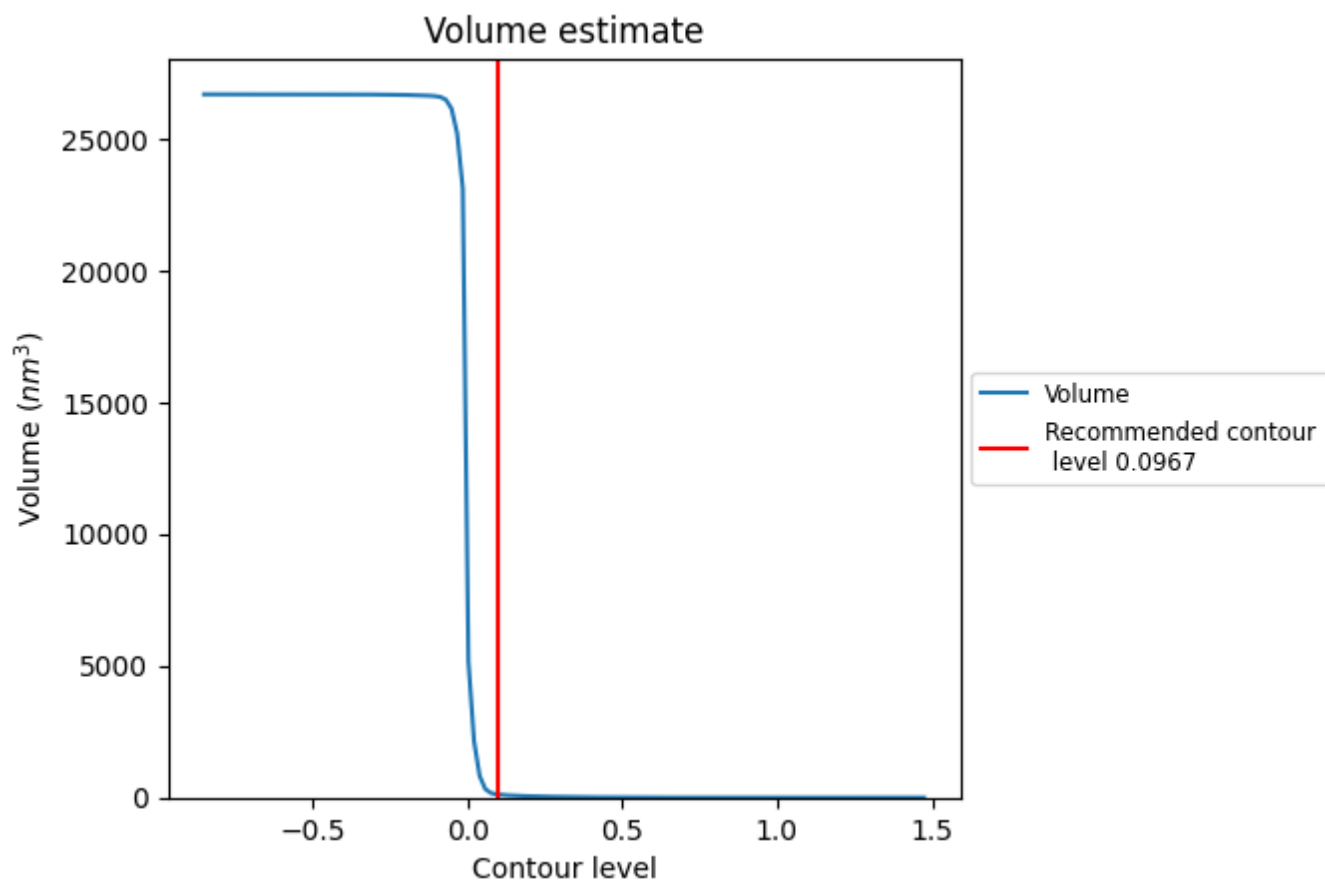
This section contains the results of statistical analysis of the map.

### 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.

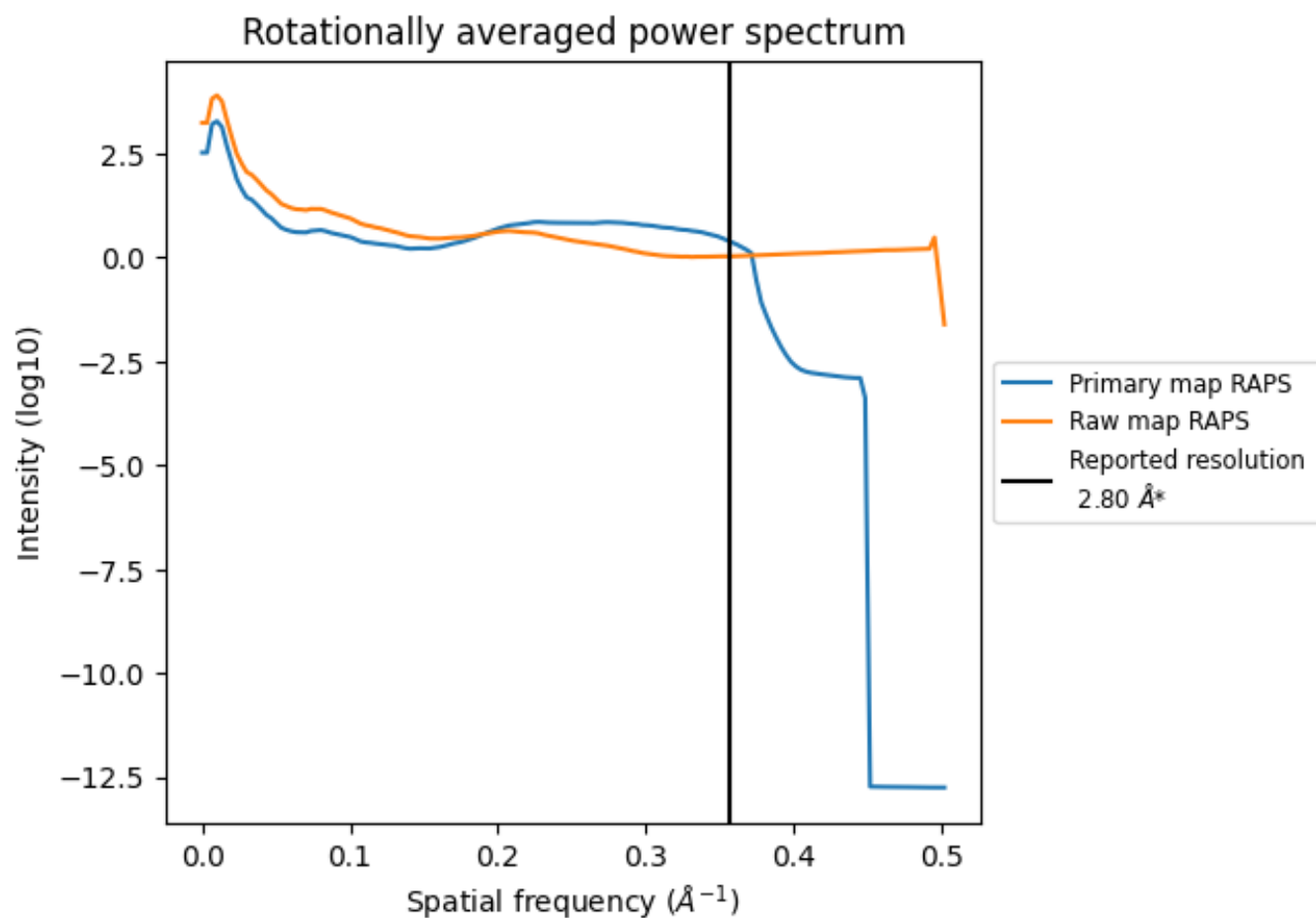
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121  $\text{nm}^3$ ; this corresponds to an approximate mass of 109 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 ⓘ

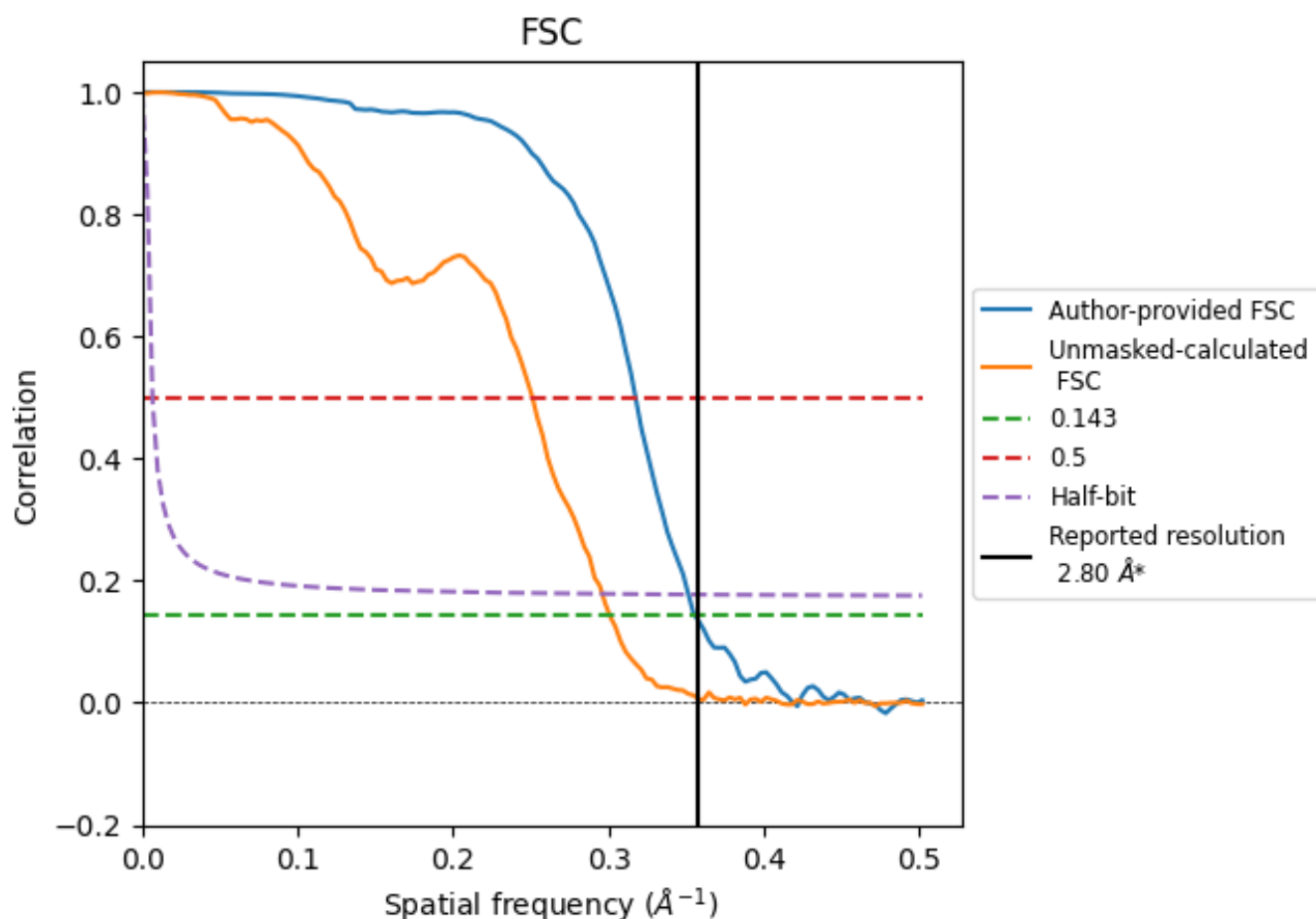


\*Reported resolution corresponds to spatial frequency of 0.357  $\text{\AA}^{-1}$

## 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 0.357 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	2.80	-	-
Author-provided FSC curve	2.81	3.15	2.84
Unmasked-calculated*	3.32	3.98	3.38

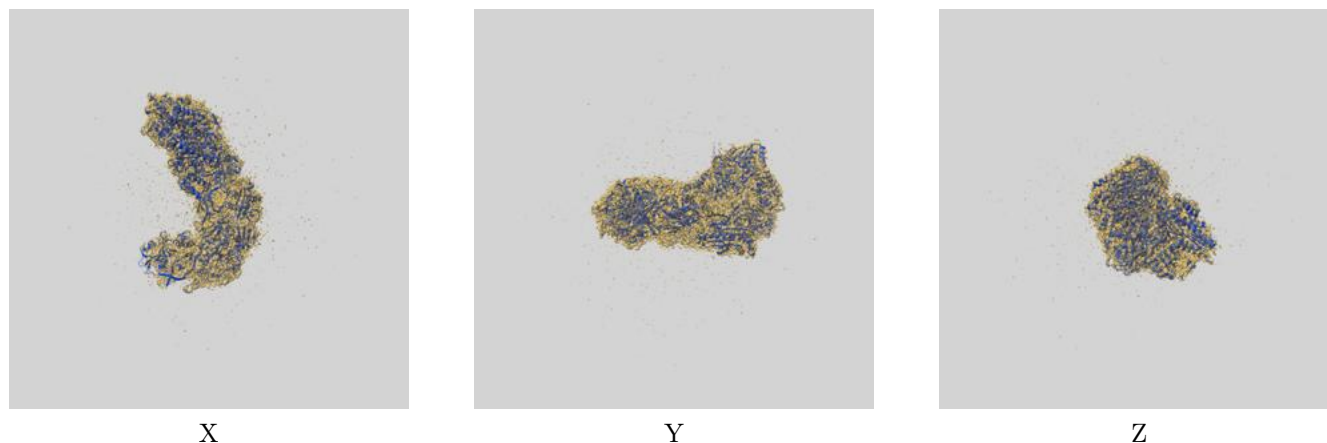
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.32 differs from the reported value 2.8 by more than 10 %



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

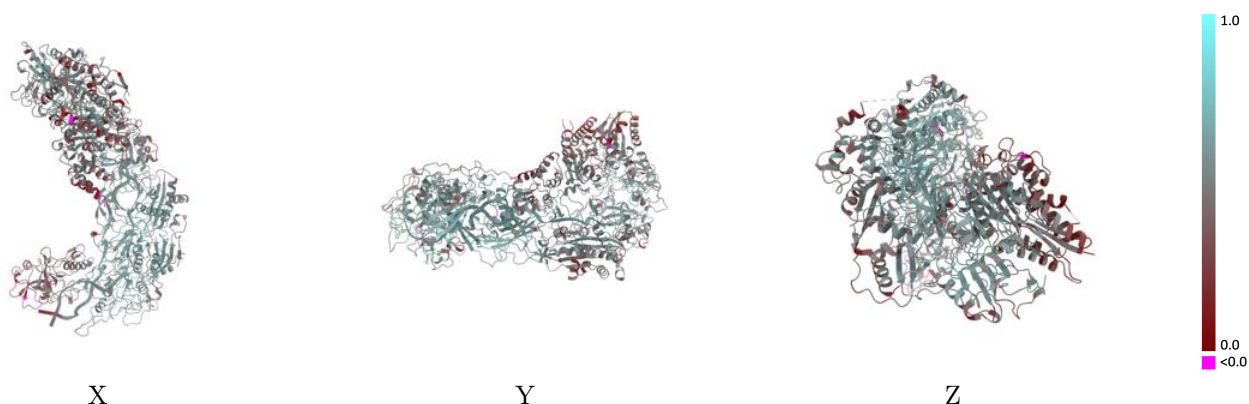
This section contains information regarding the fit between EMDB map EMD-66347 and PDB model 9WXI. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



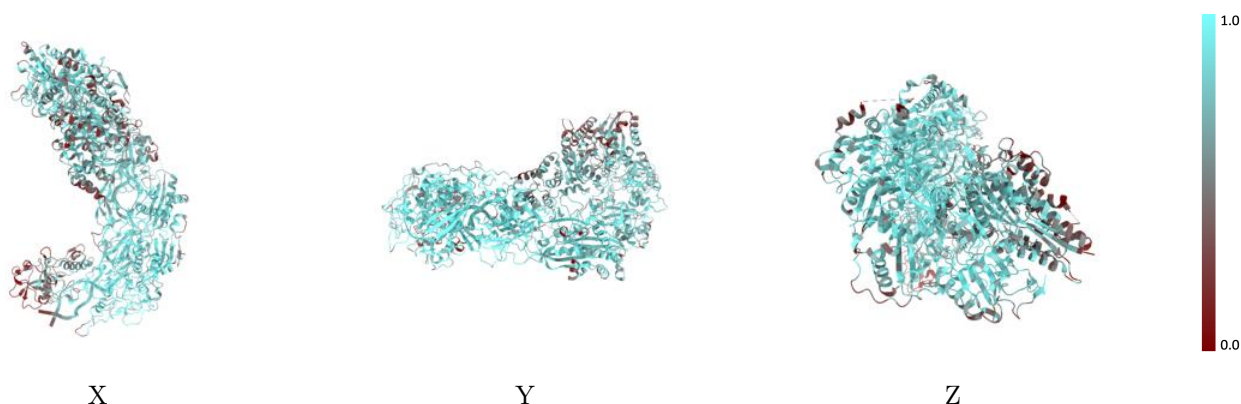
The images above show the 3D surface view of the map at the recommended contour level 0.0967 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



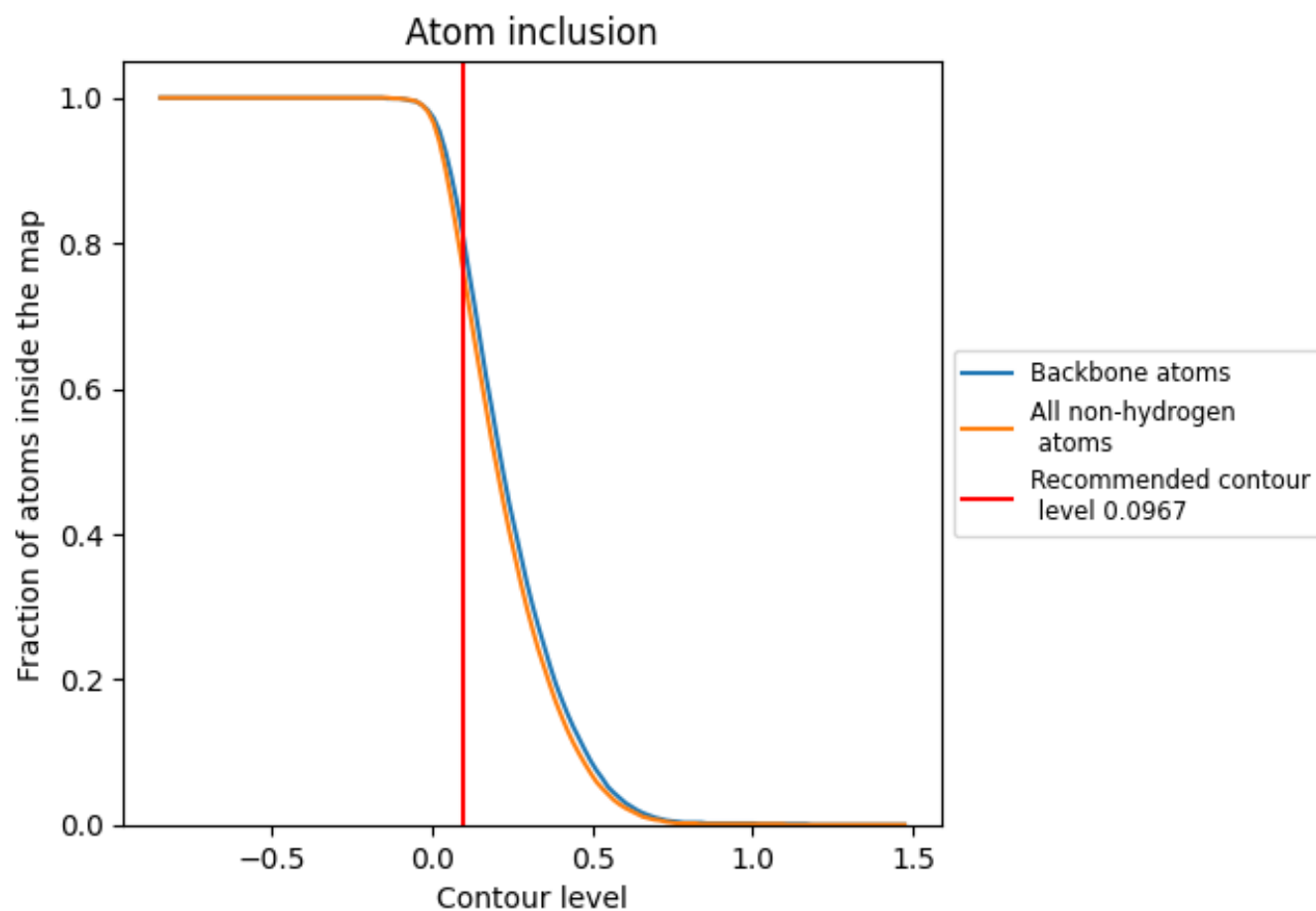
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0967).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 76% 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 (0.0967) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7620	<div></div> 0.5000
A	<div></div> 0.9430	<div></div> 0.6060
B	<div></div> 0.6200	<div></div> 0.4030
C	<div></div> 0.8270	<div></div> 0.5320
D	<div></div> 0.7710	<div></div> 0.5110
E	<div></div> 0.8060	<div></div> 0.5480

