



## Full wwPDB EM Validation Report ⓘ

May 6, 2023 – 12:37 PM EDT

PDB ID : 8DD7  
EMDB ID : EMD-27335  
Title : The Cryo-EM structure of Drosophila Cryptochrome in complex with Timeless  
Authors : Feng, S.; Lin, C.; DeOliveira, C.C.; Crane, B.R.  
Deposited on : 2022-06-17  
Resolution : 3.30 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.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

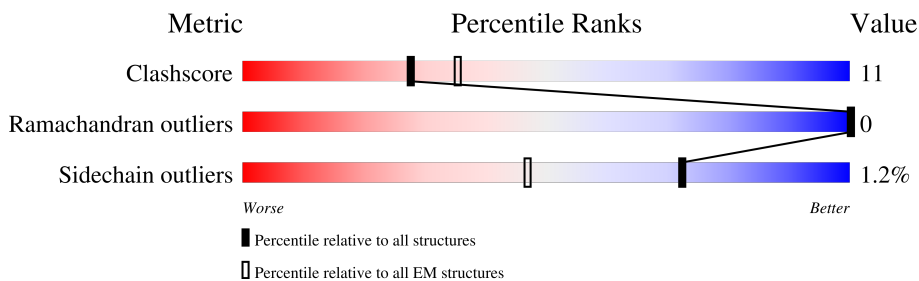
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	746	
2	B	1618	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10370 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 Methylated-DNA--protein-cysteine methyltransferase,Cryptochrome-1 fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	516	4192	2676	742	750	24	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-225	MET	-	initiating methionine	UNP E5BBQ0
A	-224	GLU	-	expression tag	UNP E5BBQ0
A	-223	GLN	-	expression tag	UNP E5BBQ0
A	-222	LYS	-	expression tag	UNP E5BBQ0
A	-221	LEU	-	expression tag	UNP E5BBQ0
A	-220	ILE	-	expression tag	UNP E5BBQ0
A	-219	SER	-	expression tag	UNP E5BBQ0
A	-218	GLU	-	expression tag	UNP E5BBQ0
A	-217	GLU	-	expression tag	UNP E5BBQ0
A	-216	ASP	-	expression tag	UNP E5BBQ0
A	-215	LEU	-	expression tag	UNP E5BBQ0
A	-214	GLY	-	expression tag	UNP E5BBQ0
A	-213	GLY	-	expression tag	UNP E5BBQ0
A	-212	GLY	-	expression tag	UNP E5BBQ0
A	-211	GLU	-	expression tag	UNP E5BBQ0
A	-210	GLN	-	expression tag	UNP E5BBQ0
A	-209	LYS	-	expression tag	UNP E5BBQ0
A	-208	LEU	-	expression tag	UNP E5BBQ0
A	-207	ILE	-	expression tag	UNP E5BBQ0
A	-206	SER	-	expression tag	UNP E5BBQ0
A	-205	GLU	-	expression tag	UNP E5BBQ0
A	-204	GLU	-	expression tag	UNP E5BBQ0
A	-203	ASP	-	expression tag	UNP E5BBQ0
A	-202	LEU	-	expression tag	UNP E5BBQ0
A	-201	GLY	-	expression tag	UNP E5BBQ0
A	-200	GLY	-	expression tag	UNP E5BBQ0
A	-199	GLY	-	expression tag	UNP E5BBQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-198	GLU	-	expression tag	UNP E5BBQ0
A	-197	GLN	-	expression tag	UNP E5BBQ0
A	-196	LYS	-	expression tag	UNP E5BBQ0
A	-195	LEU	-	expression tag	UNP E5BBQ0
A	-194	ILE	-	expression tag	UNP E5BBQ0
A	-193	SER	-	expression tag	UNP E5BBQ0
A	-192	GLU	-	expression tag	UNP E5BBQ0
A	-191	GLU	-	expression tag	UNP E5BBQ0
A	-190	ASP	-	expression tag	UNP E5BBQ0
A	-189	LEU	-	expression tag	UNP E5BBQ0
A	-187	GLY	PRO	conflict	UNP E5BBQ0
A	-185	MET	SER	conflict	UNP E5BBQ0
A	-156	ARG	GLU	conflict	UNP E5BBQ0
A	-126	ILE	MET	conflict	UNP E5BBQ0
A	-72	GLU	TYR	conflict	UNP E5BBQ0
A	-65	VAL	ALA	conflict	UNP E5BBQ0
A	-55	ASN	LYS	conflict	UNP E5BBQ0
A	-51	ASP	SER	conflict	UNP E5BBQ0
A	-33	SER	LEU	conflict	UNP E5BBQ0
A	-29	PRO	GLY	conflict	UNP E5BBQ0
A	-27	LEU	GLU	conflict	UNP E5BBQ0
A	-7	PRO	-	linker	UNP E5BBQ0
A	-6	GLY	-	linker	UNP E5BBQ0
A	-5	LEU	-	linker	UNP E5BBQ0
A	-4	GLY	-	linker	UNP E5BBQ0
A	-3	GLY	-	linker	UNP E5BBQ0
A	-2	GLY	-	linker	UNP E5BBQ0
A	-1	SER	-	linker	UNP E5BBQ0
A	0	GLY	-	linker	UNP E5BBQ0

- Molecule 2 is a protein called Protein timeless,Methylated-DNA--protein-cysteine methyltransferase fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	759	6125	3930	1029	1124	42	0	0

There are 44 discrepancies between the modelled and reference sequences:

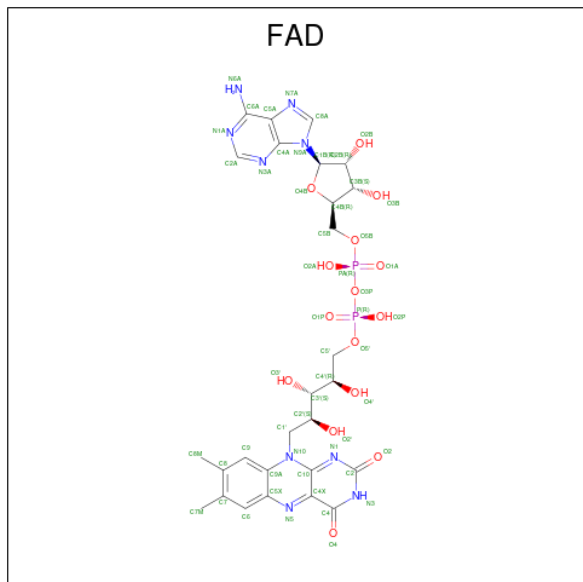
Chain	Residue	Modelled	Actual	Comment	Reference
B	1399	LEU	-	linker	UNP P49021
B	1400	GLU	-	linker	UNP P49021

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1401	GLY	-	linker	UNP P49021
B	1402	GLY	-	linker	UNP P49021
B	1403	SER	-	linker	UNP P49021
B	1404	GLY	-	linker	UNP P49021
B	1405	MET	-	linker	UNP P49021
B	1434	ARG	GLU	conflict	UNP E5BBQ0
B	1583	PRO	-	expression tag	UNP E5BBQ0
B	1584	GLY	-	expression tag	UNP E5BBQ0
B	1585	LEU	-	expression tag	UNP E5BBQ0
B	1586	GLY	-	expression tag	UNP E5BBQ0
B	1587	GLY	-	expression tag	UNP E5BBQ0
B	1588	GLY	-	expression tag	UNP E5BBQ0
B	1589	GLY	-	expression tag	UNP E5BBQ0
B	1590	TYR	-	expression tag	UNP E5BBQ0
B	1591	PRO	-	expression tag	UNP E5BBQ0
B	1592	TYR	-	expression tag	UNP E5BBQ0
B	1593	ASP	-	expression tag	UNP E5BBQ0
B	1594	VAL	-	expression tag	UNP E5BBQ0
B	1595	PRO	-	expression tag	UNP E5BBQ0
B	1596	ASP	-	expression tag	UNP E5BBQ0
B	1597	TYR	-	expression tag	UNP E5BBQ0
B	1598	ALA	-	expression tag	UNP E5BBQ0
B	1599	ARG	-	expression tag	UNP E5BBQ0
B	1600	THR	-	expression tag	UNP E5BBQ0
B	1601	GLY	-	expression tag	UNP E5BBQ0
B	1602	GLY	-	expression tag	UNP E5BBQ0
B	1603	GLY	-	expression tag	UNP E5BBQ0
B	1604	SER	-	expression tag	UNP E5BBQ0
B	1605	GLY	-	expression tag	UNP E5BBQ0
B	1606	SER	-	expression tag	UNP E5BBQ0
B	1607	ARG	-	expression tag	UNP E5BBQ0
B	1608	LEU	-	expression tag	UNP E5BBQ0
B	1609	GLU	-	expression tag	UNP E5BBQ0
B	1610	GLU	-	expression tag	UNP E5BBQ0
B	1611	GLU	-	expression tag	UNP E5BBQ0
B	1612	LEU	-	expression tag	UNP E5BBQ0
B	1613	ARG	-	expression tag	UNP E5BBQ0
B	1614	ARG	-	expression tag	UNP E5BBQ0
B	1615	ARG	-	expression tag	UNP E5BBQ0
B	1616	LEU	-	expression tag	UNP E5BBQ0
B	1617	THR	-	expression tag	UNP E5BBQ0
B	1618	GLU	-	expression tag	UNP E5BBQ0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).

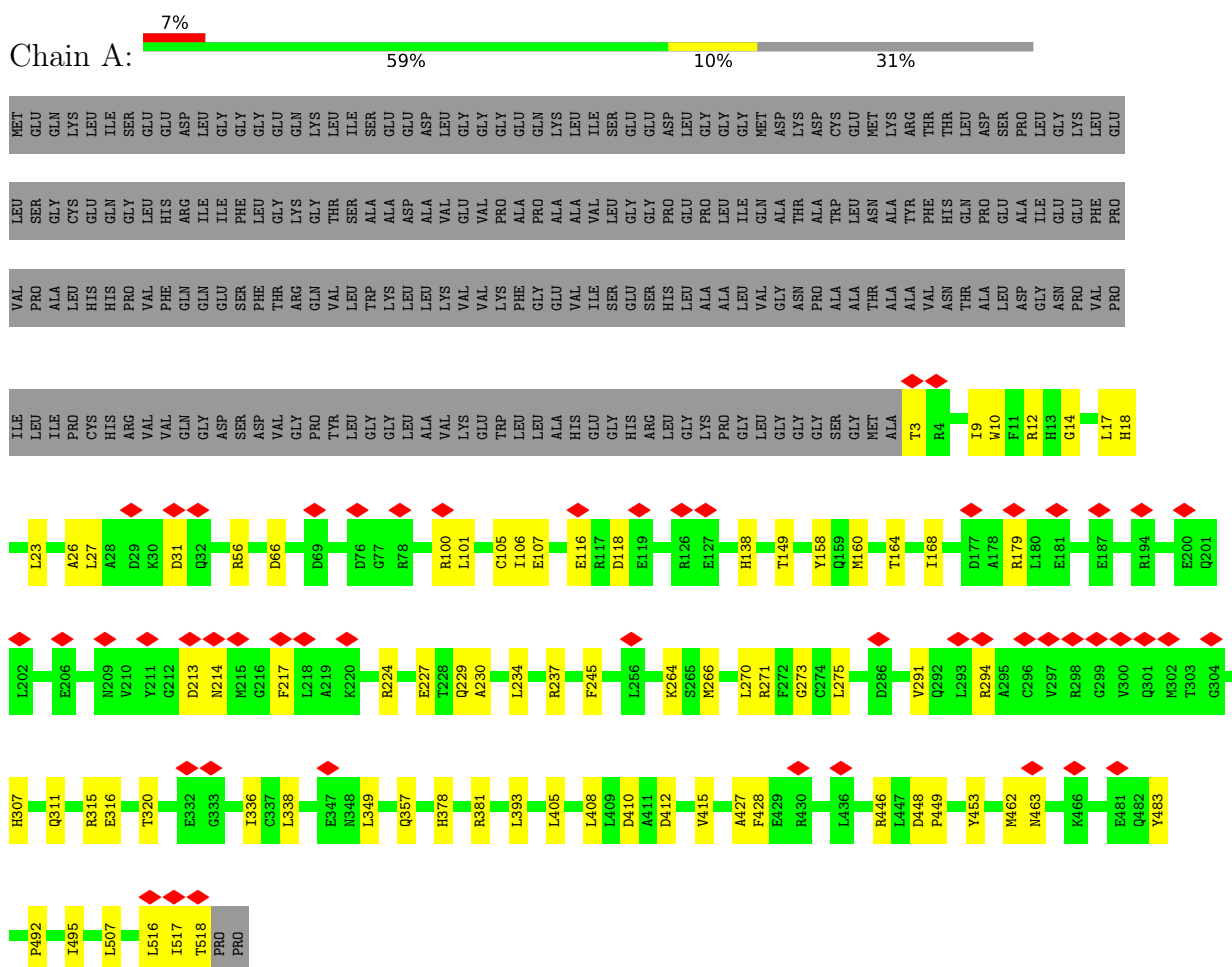


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	53	27	9	15	2	0

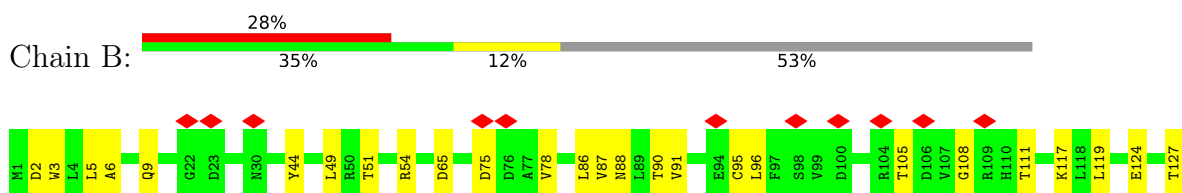
### 3 Residue-property plots

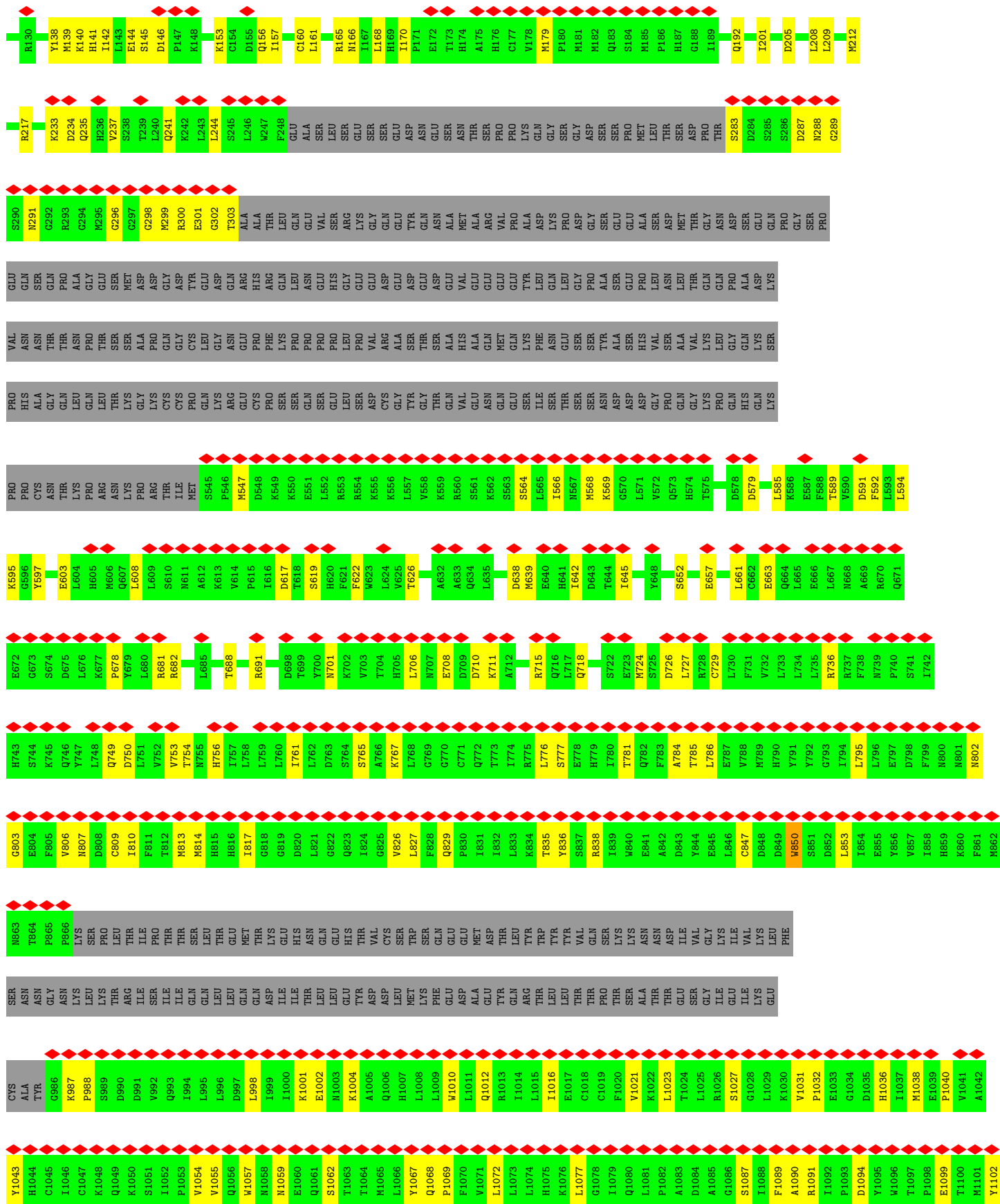
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Methylated-DNA--protein-cysteine methyltransferase,Cryptochrome-1 fusion



- Molecule 2: Protein timeless,Methylated-DNA--protein-cysteine methyltransferase fusion









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160000	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 ( $e^-/\text{\AA}^2$ )	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	53.328	Depositor
Minimum map value	-21.704	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	12.4	Depositor
Map size (Å)	309.59998, 309.59998, 309.59998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.032, 1.032, 1.032	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: FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/4303	0.53	0/5843
2	B	0.30	0/6255	0.60	0/8473
All	All	0.28	0/10558	0.57	0/14316

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1216	ARG	Sidechain

### 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	4192	0	4111	59	0
2	B	6125	0	6174	172	0
3	A	53	0	31	7	0
All	All	10370	0	10316	222	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 11.

All (222) 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:87:VAL:HG12	2:B:287:ASP:OD2	1.58	1.02
2:B:91:VAL:HG13	2:B:291:ASN:ND2	1.76	1.00
2:B:91:VAL:HG13	2:B:291:ASN:HD21	1.32	0.92
2:B:998:LEU:HD22	2:B:1069:PRO:HB3	1.61	0.81
2:B:91:VAL:CG1	2:B:291:ASN:HD21	1.94	0.80
2:B:141:HIS:O	2:B:145:SER:HB3	1.84	0.78
3:A:602:FAD:H5'1	3:A:602:FAD:O1A	1.84	0.77
1:A:158:TYR:CD2	2:B:2:ASP:HB3	2.21	0.76
2:B:91:VAL:HG13	2:B:291:ASN:CG	2.06	0.76
1:A:158:TYR:CE2	2:B:2:ASP:HB3	2.21	0.75
1:A:214:ASN:O	1:A:217:PHE:CD2	2.40	0.75
2:B:87:VAL:CG1	2:B:287:ASP:OD2	2.35	0.74
1:A:214:ASN:O	1:A:217:PHE:HD2	1.71	0.74
2:B:44:TYR:HH	2:B:283:SER:N	1.85	0.73
2:B:142:ILE:CG2	2:B:157:ILE:HD11	2.19	0.73
2:B:827:LEU:O	2:B:827:LEU:HG	1.89	0.72
2:B:1038:MET:H	2:B:1117:LYS:HE2	1.56	0.71
2:B:724:MET:SD	2:B:726:ASP:N	2.64	0.70
2:B:761:ILE:O	2:B:765:SER:HB3	1.91	0.70
2:B:998:LEU:HD23	2:B:998:LEU:O	1.93	0.69
2:B:142:ILE:HG21	2:B:157:ILE:HD11	1.75	0.68
2:B:688:THR:HG23	2:B:750:ASP:OD2	1.94	0.68
1:A:234:LEU:HA	1:A:266:MET:HE3	1.76	0.68
2:B:987:LYS:HB3	2:B:988:PRO:HD3	1.75	0.67
2:B:802:ASN:HB3	2:B:806:VAL:HB	1.78	0.66
1:A:234:LEU:HA	1:A:266:MET:CE	2.26	0.66
2:B:1031:VAL:HB	2:B:1032:PRO:HD2	1.78	0.66
2:B:853:LEU:C	2:B:853:LEU:HD23	2.17	0.65
2:B:1021:VAL:HG12	2:B:1038:MET:HG3	1.78	0.65
1:A:336:ILE:C	2:B:1214:VAL:HG11	2.18	0.64
2:B:826:VAL:O	2:B:829:GLN:NE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1038:MET:O	2:B:1038:MET:HG2	1.97	0.64
2:B:547:MET:SD	2:B:547:MET:N	2.70	0.64
2:B:91:VAL:CG1	2:B:291:ASN:OD1	2.45	0.63
1:A:427:ALA:O	2:B:1210:TRP:CE3	2.51	0.63
2:B:1038:MET:SD	2:B:1043:TYR:CD1	2.92	0.63
2:B:91:VAL:HG13	2:B:291:ASN:OD1	2.00	0.62
1:A:410:ASP:O	3:A:602:FAD:N3	2.30	0.61
1:A:234:LEU:CA	1:A:266:MET:HE3	2.30	0.61
2:B:1016:ILE:HD13	2:B:1105:ALA:HB1	1.83	0.60
2:B:1210:TRP:CE3	2:B:1211:LEU:N	2.69	0.60
2:B:91:VAL:HG22	2:B:291:ASN:HD21	1.66	0.60
2:B:724:MET:HE1	2:B:727:LEU:HB2	1.84	0.60
1:A:224:ARG:HB3	1:A:229:GLN:HG2	1.83	0.60
2:B:91:VAL:CG1	2:B:291:ASN:ND2	2.58	0.60
2:B:299:MET:C	2:B:301:GLU:H	2.04	0.59
2:B:1023:LEU:HD13	2:B:1123:LEU:HD22	1.84	0.59
1:A:462:MET:SD	1:A:462:MET:N	2.75	0.59
2:B:153:LYS:O	2:B:157:ILE:HG12	2.01	0.59
2:B:1059:ASN:HA	2:B:1062:SER:HB2	1.85	0.59
2:B:998:LEU:HD23	2:B:998:LEU:C	2.24	0.58
2:B:299:MET:O	2:B:299:MET:HG3	2.04	0.58
2:B:1210:TRP:O	2:B:1214:VAL:HG23	2.03	0.57
2:B:638:ASP:OD1	2:B:638:ASP:N	2.37	0.57
1:A:10:TRP:HB3	1:A:106:ILE:HG22	1.87	0.57
2:B:91:VAL:CG2	2:B:291:ASN:HD21	2.18	0.56
2:B:564:SER:O	2:B:568:MET:HG3	2.06	0.56
1:A:381:ARG:HE	1:A:408:LEU:HD11	1.70	0.56
1:A:378:HIS:CE1	3:A:602:FAD:HM81	2.41	0.55
2:B:1106:LYS:HG2	2:B:1111:LEU:HD21	1.87	0.55
1:A:357:GLN:HG3	1:A:492:PRO:HG3	1.87	0.55
2:B:165:ARG:NH2	2:B:166:ASN:OD1	2.40	0.55
2:B:287:ASP:OD1	2:B:288:ASN:N	2.40	0.55
2:B:711:LYS:O	2:B:715:ARG:HG2	2.07	0.55
2:B:749:GLN:OE1	2:B:802:ASN:ND2	2.38	0.55
2:B:1087:SER:OG	2:B:1091:ARG:NH2	2.39	0.55
2:B:1010:TRP:HZ2	2:B:1057:TRP:HB2	1.72	0.54
1:A:100:ARG:NH1	1:A:101:LEU:O	2.38	0.54
2:B:652:SER:HB2	2:B:1040:PRO:HB3	1.90	0.54
2:B:750:ASP:O	2:B:754:THR:HG23	2.07	0.54
2:B:814:MET:HB3	2:B:853:LEU:HD11	1.89	0.53
1:A:56:ARG:NH1	1:A:405:LEU:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:ASP:OD1	2:B:146:ASP:N	2.41	0.53
2:B:105:THR:HG23	2:B:108:GLY:H	1.73	0.53
1:A:266:MET:O	1:A:270:LEU:HB2	2.09	0.53
2:B:853:LEU:HD23	2:B:853:LEU:O	2.09	0.53
2:B:803:GLY:O	2:B:807:ASN:ND2	2.37	0.52
2:B:1099:GLU:HB2	2:B:1126:ALA:HB3	1.90	0.52
2:B:49:LEU:HB3	2:B:51:THR:HG23	1.91	0.51
2:B:777:SER:O	2:B:781:THR:OG1	2.28	0.51
2:B:1038:MET:O	2:B:1038:MET:CG	2.59	0.51
2:B:139:MET:CE	2:B:161:LEU:CD2	2.89	0.51
2:B:235:GLN:HE21	2:B:585:LEU:HD11	1.76	0.51
2:B:95:CYS:HB3	2:B:291:ASN:HA	1.93	0.50
2:B:987:LYS:HB3	2:B:988:PRO:CD	2.41	0.50
2:B:678:PRO:HA	2:B:681:ARG:HG2	1.92	0.50
1:A:230:ALA:HB1	1:A:275:LEU:HB2	1.93	0.50
2:B:1094:ASP:OD1	2:B:1094:ASP:N	2.44	0.50
2:B:708:GLU:HA	2:B:711:LYS:HB2	1.94	0.50
2:B:756:HIS:ND1	2:B:809:CYS:SG	2.78	0.50
1:A:12:ARG:NH1	1:A:118:ASP:OD1	2.45	0.49
2:B:566:ILE:HG22	2:B:569:LYS:HE3	1.95	0.49
2:B:591:ASP:HA	2:B:594:LEU:HD12	1.95	0.49
2:B:795:LEU:HD22	2:B:810:ILE:HG12	1.95	0.49
2:B:847:CYS:H	2:B:850:TRP:HE1	1.59	0.49
1:A:234:LEU:N	1:A:266:MET:HE3	2.27	0.49
1:A:291:VAL:HG23	1:A:294:ARG:HH12	1.77	0.49
2:B:724:MET:CE	2:B:727:LEU:CD1	2.91	0.49
2:B:209:LEU:HD13	2:B:595:LYS:HD3	1.94	0.48
2:B:1002:GLU:O	2:B:1004:LYS:NZ	2.41	0.48
1:A:307:HIS:H	1:A:307:HIS:CD2	2.32	0.48
1:A:349:LEU:HD13	1:A:393:LEU:HD22	1.94	0.48
2:B:241:GLN:HA	2:B:244:LEU:HD12	1.95	0.48
2:B:1099:GLU:O	2:B:1127:THR:OG1	2.31	0.48
2:B:619:SER:HB3	2:B:682:ARG:HG2	1.96	0.48
2:B:998:LEU:O	2:B:1001:LYS:HB2	2.13	0.48
2:B:179:MET:O	2:B:179:MET:HG3	2.14	0.48
2:B:724:MET:SD	2:B:727:LEU:HD12	2.54	0.48
2:B:1055:VAL:HA	2:B:1089:PHE:HB3	1.96	0.48
2:B:75:ASP:HB3	2:B:78:VAL:HG12	1.96	0.47
1:A:107:GLU:OE2	1:A:138:HIS:N	2.44	0.47
1:A:31:ASP:N	1:A:31:ASP:OD1	2.42	0.47
1:A:349:LEU:HD22	1:A:495:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:THR:HA	2:B:592:PHE:HB3	1.96	0.47
2:B:691:ARG:HB2	2:B:754:THR:HG22	1.96	0.47
2:B:619:SER:OG	2:B:681:ARG:NH2	2.46	0.47
2:B:701:ASN:ND2	2:B:718:GLN:OE1	2.30	0.47
2:B:729:CYS:HB2	2:B:1057:TRP:CE3	2.50	0.47
2:B:1068:GLN:HG3	2:B:1072:LEU:HG	1.96	0.47
2:B:296:GLY:HA3	2:B:617:ASP:OD2	2.14	0.47
2:B:566:ILE:HA	2:B:569:LYS:HG2	1.97	0.47
1:A:448:ASP:OD2	1:A:453:TYR:N	2.43	0.47
2:B:645:ILE:HD13	2:B:645:ILE:HA	1.81	0.47
2:B:88:ASN:OD1	2:B:287:ASP:OD2	2.33	0.46
1:A:412:ASP:HB3	1:A:415:VAL:HB	1.98	0.46
2:B:95:CYS:HB3	2:B:291:ASN:OD1	2.15	0.46
2:B:54:ARG:HD2	2:B:111:THR:HG23	1.97	0.46
2:B:300:ARG:O	2:B:301:GLU:C	2.53	0.46
2:B:724:MET:CE	2:B:727:LEU:HD12	2.45	0.46
2:B:139:MET:HE3	2:B:161:LEU:CD2	2.46	0.46
2:B:688:THR:CG2	2:B:750:ASP:OD2	2.62	0.46
2:B:998:LEU:CD2	2:B:1069:PRO:HB3	2.41	0.46
1:A:149:THR:HG21	1:A:168:ILE:HD11	1.97	0.45
2:B:124:GLU:O	2:B:127:THR:OG1	2.30	0.45
1:A:26:ALA:HB2	1:A:105:CYS:SG	2.56	0.45
2:B:205:ASP:OD1	2:B:205:ASP:N	2.49	0.45
2:B:639:MET:HA	2:B:642:ILE:HG22	1.98	0.45
1:A:17:LEU:N	1:A:227:GLU:OE2	2.49	0.45
1:A:428:PHE:HA	2:B:1210:TRP:CE2	2.51	0.45
2:B:299:MET:C	2:B:301:GLU:N	2.69	0.45
2:B:736:ARG:HH22	2:B:785:THR:HG21	1.81	0.45
2:B:767:LYS:HD3	2:B:776:LEU:HD11	1.99	0.45
2:B:786:LEU:HD21	2:B:826:VAL:HG22	1.98	0.45
2:B:1038:MET:SD	2:B:1043:TYR:HD1	2.39	0.45
1:A:27:LEU:HD13	1:A:179:ARG:HD2	1.99	0.45
2:B:998:LEU:C	2:B:998:LEU:CD2	2.86	0.44
1:A:516:LEU:CD1	2:B:1217:SER:HB3	2.47	0.44
2:B:1077:LEU:HD23	2:B:1077:LEU:H	1.82	0.44
2:B:827:LEU:O	2:B:827:LEU:CG	2.59	0.44
2:B:835:THR:HA	2:B:838:ARG:HG2	1.98	0.44
2:B:853:LEU:C	2:B:853:LEU:CD2	2.86	0.44
1:A:338:LEU:HD23	2:B:1217:SER:CB	2.48	0.44
2:B:736:ARG:NH1	2:B:1059:ASN:HB3	2.33	0.44
2:B:119:LEU:HB3	2:B:170:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:HG21	1:A:100:ARG:H	1.82	0.43
1:A:463:ASN:HD22	1:A:483:TYR:HA	1.83	0.43
2:B:299:MET:C	2:B:300:ARG:HG3	2.39	0.43
2:B:1012:GLN:O	2:B:1016:ILE:HG12	2.18	0.43
1:A:446:ARG:NH1	2:B:65:ASP:OD1	2.51	0.43
2:B:1123:LEU:HD12	2:B:1123:LEU:HA	1.88	0.43
2:B:234:ASP:N	2:B:235:GLN:OE1	2.50	0.43
2:B:298:GLY:O	2:B:299:MET:HB3	2.17	0.43
2:B:1077:LEU:HD13	2:B:1104:LEU:HD13	2.00	0.43
1:A:316:GLU:O	1:A:320:THR:OG1	2.32	0.43
2:B:140:LYS:O	2:B:144:GLU:HG3	2.18	0.43
1:A:18:HIS:ND1	1:A:227:GLU:OE1	2.41	0.43
2:B:814:MET:CB	2:B:853:LEU:HD11	2.48	0.43
1:A:14:GLY:HA2	1:A:273:GLY:HA3	2.01	0.43
1:A:214:ASN:O	1:A:217:PHE:CE2	2.72	0.43
2:B:217:ARG:NE	2:B:603:GLU:OE1	2.52	0.43
2:B:237:VAL:CG1	2:B:303:THR:OG1	2.67	0.43
1:A:237:ARG:NH1	1:A:264:LYS:O	2.51	0.42
2:B:91:VAL:HG22	2:B:291:ASN:ND2	2.33	0.42
2:B:622:PHE:HZ	2:B:657:GLU:HG2	1.83	0.42
1:A:336:ILE:HG12	1:A:427:ALA:HB1	2.00	0.42
1:A:446:ARG:HA	1:A:449:PRO:HG3	2.01	0.42
2:B:784:ALA:HB2	2:B:817:ILE:HD12	2.01	0.42
2:B:86:LEU:O	2:B:90:THR:HG22	2.19	0.42
2:B:96:LEU:HD12	2:B:96:LEU:HA	1.87	0.42
2:B:138:TYR:OH	2:B:156:GLN:NE2	2.49	0.42
2:B:302:GLY:O	2:B:303:THR:C	2.57	0.42
2:B:1089:PHE:HB2	2:B:1091:ARG:HH21	1.83	0.42
2:B:201:ILE:HD13	2:B:201:ILE:HA	1.86	0.42
1:A:338:LEU:HA	2:B:1218:LYS:HD3	2.00	0.42
2:B:1023:LEU:O	2:B:1027:SER:N	2.45	0.42
1:A:245:PHE:HB3	1:A:291:VAL:HG11	2.02	0.42
1:A:378:HIS:HE1	3:A:602:FAD:HM81	1.83	0.42
2:B:142:ILE:HG21	2:B:157:ILE:CD1	2.48	0.42
2:B:145:SER:OG	2:B:146:ASP:OD1	2.37	0.42
1:A:160:MET:O	1:A:164:THR:OG1	2.32	0.42
1:A:427:ALA:O	2:B:1210:TRP:CZ3	2.73	0.42
2:B:139:MET:CE	2:B:160:CYS:HB2	2.50	0.42
2:B:608:LEU:HD23	2:B:608:LEU:HA	1.93	0.42
1:A:315:ARG:HB3	3:A:602:FAD:H1B	2.02	0.41
1:A:517:ILE:HG22	1:A:518:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:579:ASP:OD1	2:B:579:ASP:N	2.53	0.41
2:B:168:LEU:HD13	2:B:168:LEU:HA	1.95	0.41
2:B:622:PHE:O	2:B:626:THR:HG23	2.20	0.41
2:B:1217:SER:OG	2:B:1218:LYS:N	2.53	0.41
2:B:208:LEU:O	2:B:212:MET:HG3	2.20	0.41
2:B:657:GLU:O	2:B:661:LEU:HB2	2.21	0.41
2:B:706:LEU:HD13	2:B:710:ASP:HB2	2.03	0.41
1:A:168:ILE:HD13	1:A:168:ILE:HA	1.97	0.41
2:B:138:TYR:CZ	2:B:142:ILE:HD11	2.55	0.41
1:A:311:GLN:HB2	3:A:602:FAD:C8A	2.50	0.41
2:B:117:LYS:HD2	2:B:117:LYS:HA	1.91	0.41
2:B:237:VAL:HG12	2:B:303:THR:OG1	2.19	0.41
2:B:691:ARG:HE	2:B:753:VAL:HG11	1.85	0.41
2:B:724:MET:HE1	2:B:727:LEU:CB	2.50	0.41
2:B:1209:ASN:HA	2:B:1212:GLN:HB2	2.02	0.41
2:B:95:CYS:CB	2:B:291:ASN:OD1	2.68	0.41
2:B:3:TRP:O	2:B:6:ALA:N	2.53	0.40
2:B:179:MET:O	2:B:179:MET:CG	2.70	0.40
2:B:987:LYS:HA	2:B:987:LYS:HD2	1.98	0.40
3:A:602:FAD:H62A	2:B:5:LEU:CD2	2.34	0.40
2:B:192:GLN:HE22	2:B:233:LYS:HD3	1.84	0.40
2:B:1054:VAL:HG23	2:B:1090:ALA:HB3	2.03	0.40
1:A:507:LEU:HD12	1:A:507:LEU:HA	1.94	0.40
2:B:663:GLU:OE2	2:B:1091:ARG:NH1	2.54	0.40
1:A:9:ILE:HD13	1:A:23:LEU:HD13	2.03	0.40
2:B:289:GLY:C	2:B:291:ASN:H	2.22	0.40
1:A:213:ASP:OD1	1:A:213:ASP:N	2.53	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	
1	A	514/746 (69%)	497 (97%)	17 (3%)	0	100	100
2	B	749/1618 (46%)	681 (91%)	68 (9%)	0	100	100
All	All	1263/2364 (53%)	1178 (93%)	85 (7%)	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	451/630 (72%)	448 (99%)	3 (1%)	84	90
2	B	694/1424 (49%)	683 (98%)	11 (2%)	62	79
All	All	1145/2054 (56%)	1131 (99%)	14 (1%)	72	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	116	GLU
1	A	271	ARG
2	B	9	GLN
2	B	597	TYR
2	B	813	MET
2	B	836	TYR
2	B	850	TRP
2	B	1036	HIS
2	B	1067	TYR
2	B	1102	TYR
2	B	1134	TYR
2	B	1210	TRP
2	B	1212	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	720	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

1 ligand is 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
3	FAD	A	602	-	53,58,58	1.29	5 (9%)	68,89,89	1.33	10 (14%)

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
3	FAD	A	602	-	-	8/30/50/50	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	FAD	C9A-C5X	5.09	1.49	1.41
3	A	602	FAD	C8-C7	3.35	1.49	1.40
3	A	602	FAD	C5A-C4A	2.51	1.47	1.40
3	A	602	FAD	C4X-N5	2.46	1.35	1.30
3	A	602	FAD	C4-N3	-2.42	1.34	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	FAD	P-O3P-PA	-3.71	120.10	132.83
3	A	602	FAD	N3A-C2A-N1A	-3.15	123.76	128.68
3	A	602	FAD	C3B-C2B-C1B	3.03	105.54	100.98
3	A	602	FAD	C4-C4X-N5	2.80	122.21	118.23
3	A	602	FAD	C4A-C5A-N7A	-2.68	106.61	109.40
3	A	602	FAD	C4X-C10-N1	-2.61	118.67	124.73
3	A	602	FAD	C10-N1-C2	2.22	121.33	116.90
3	A	602	FAD	O4-C4-C4X	-2.20	120.76	126.60
3	A	602	FAD	C4X-C4-N3	2.09	118.49	113.19
3	A	602	FAD	C4X-C10-N10	2.02	119.43	116.48

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	FAD	C5B-O5B-PA-O1A
3	A	602	FAD	C5'-O5'-P-O1P
3	A	602	FAD	C5'-O5'-P-O2P
3	A	602	FAD	C5'-O5'-P-O3P
3	A	602	FAD	O4'-C4'-C5'-O5'
3	A	602	FAD	C3'-C4'-C5'-O5'
3	A	602	FAD	O4B-C4B-C5B-O5B
3	A	602	FAD	C5B-O5B-PA-O3P

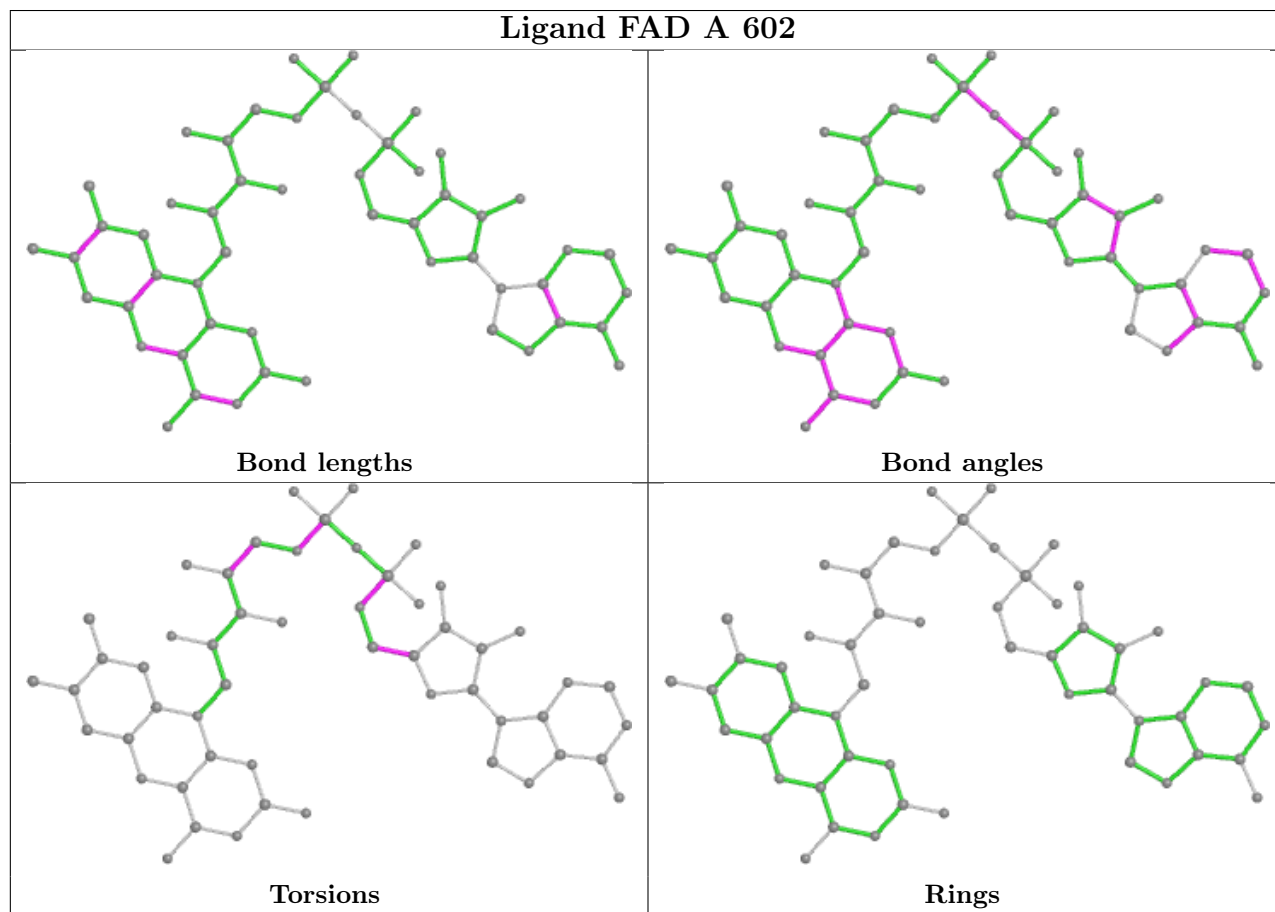
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	FAD	7	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.

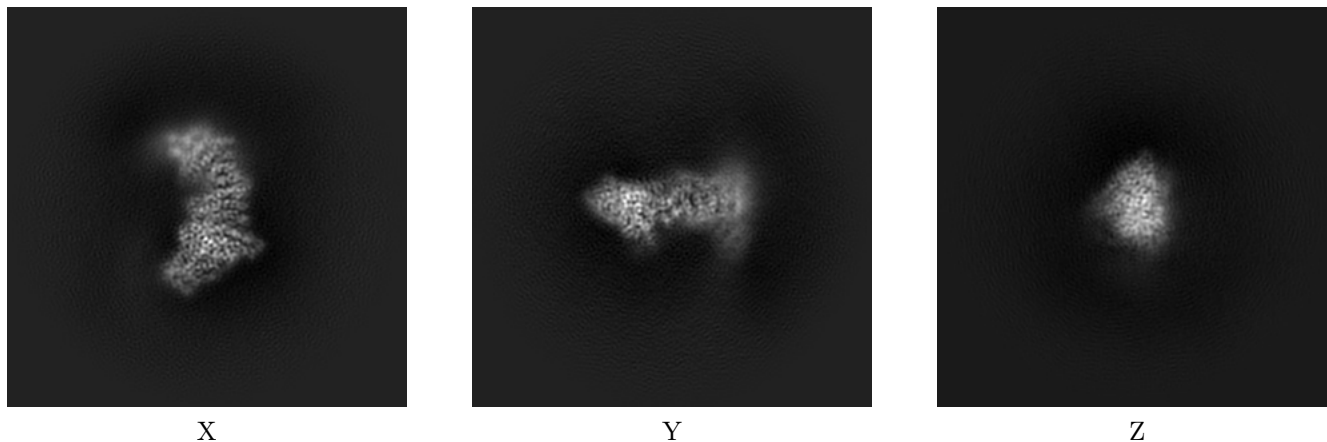
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27335. These allow visual inspection of the internal detail of the map and identification of artifacts.

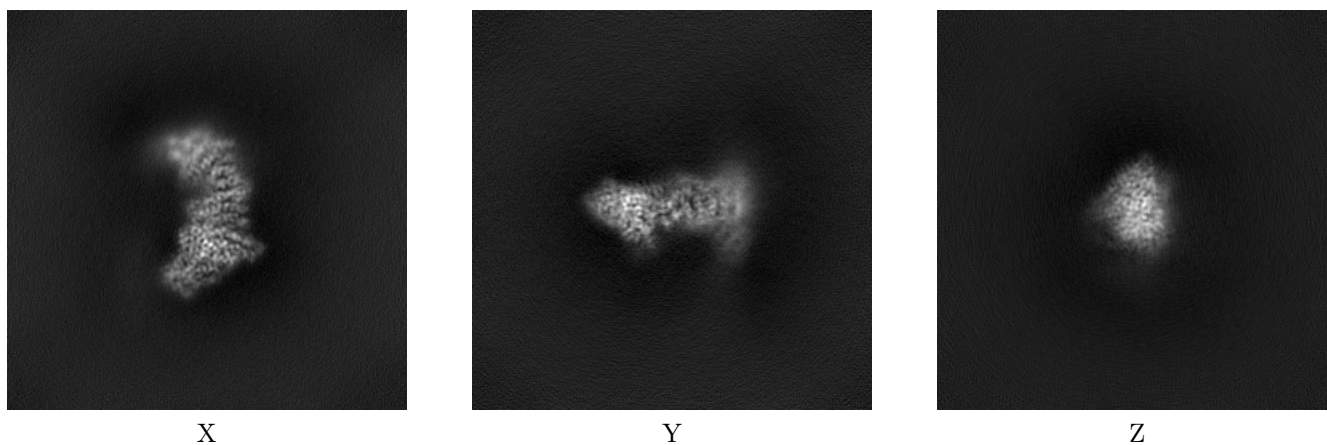
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



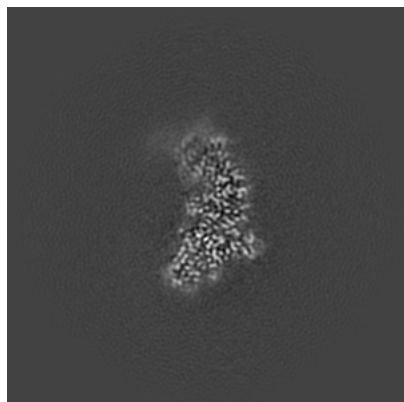
#### 6.1.2 Raw map



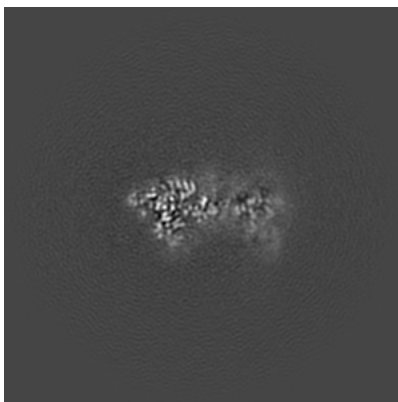
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

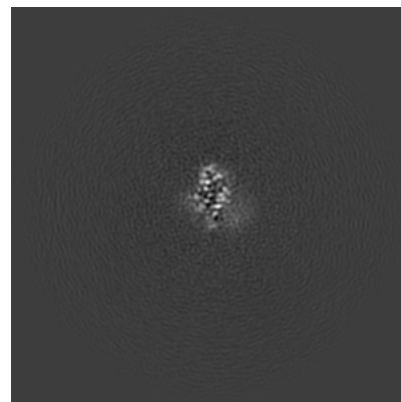
### 6.2.1 Primary map



X Index: 150

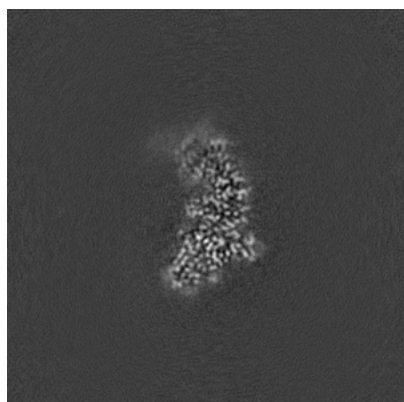


Y Index: 150

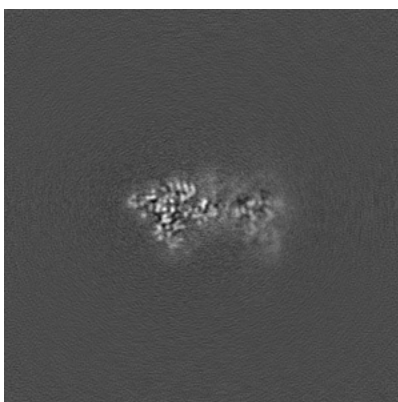


Z Index: 150

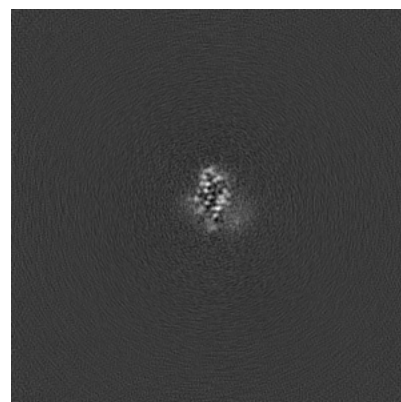
### 6.2.2 Raw map



X Index: 150



Y Index: 150



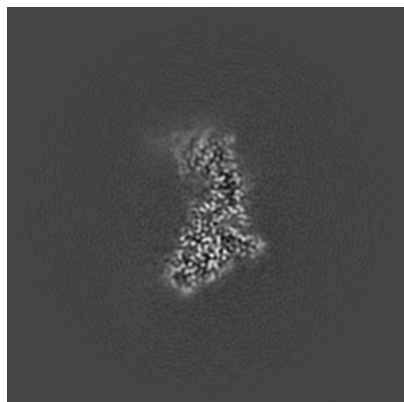
Z Index: 150

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

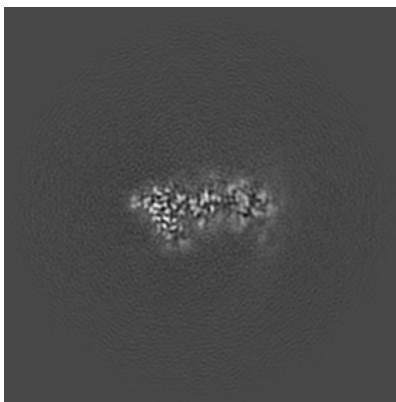


## 6.3 Largest variance slices [i](#)

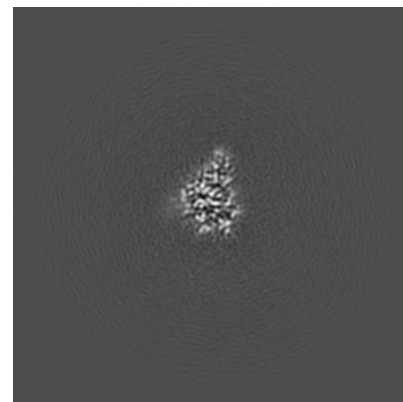
### 6.3.1 Primary map



X Index: 155

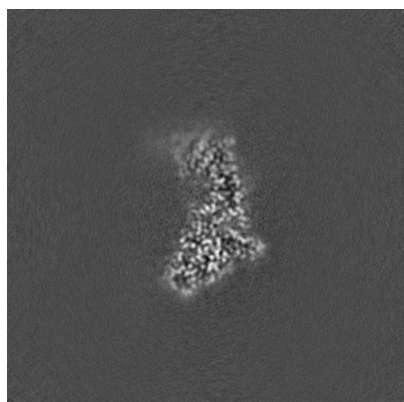


Y Index: 155

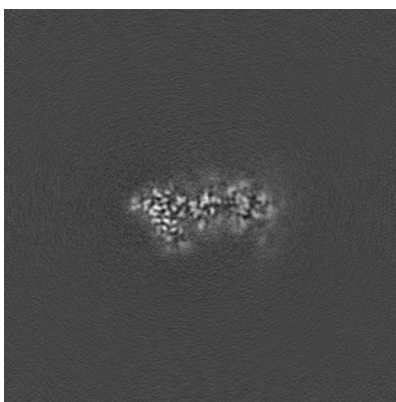


Z Index: 123

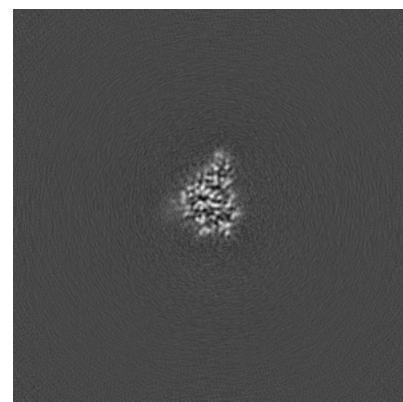
### 6.3.2 Raw map



X Index: 155



Y Index: 155



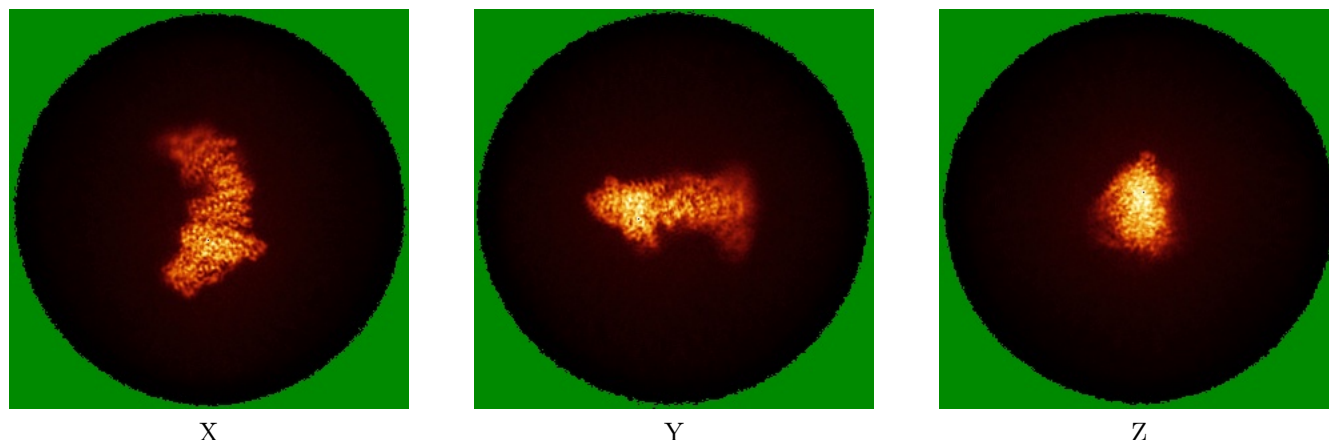
Z Index: 123

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

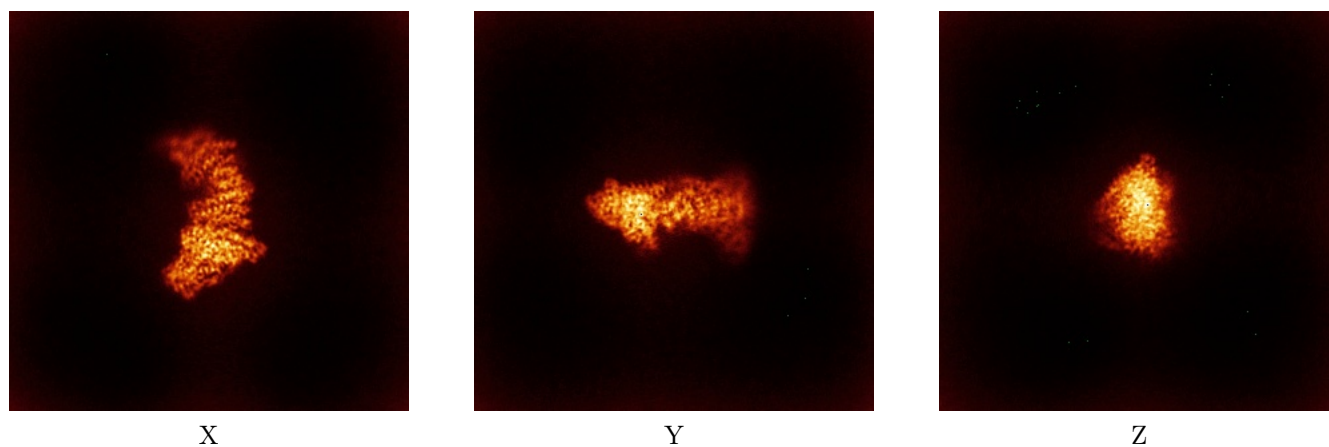


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



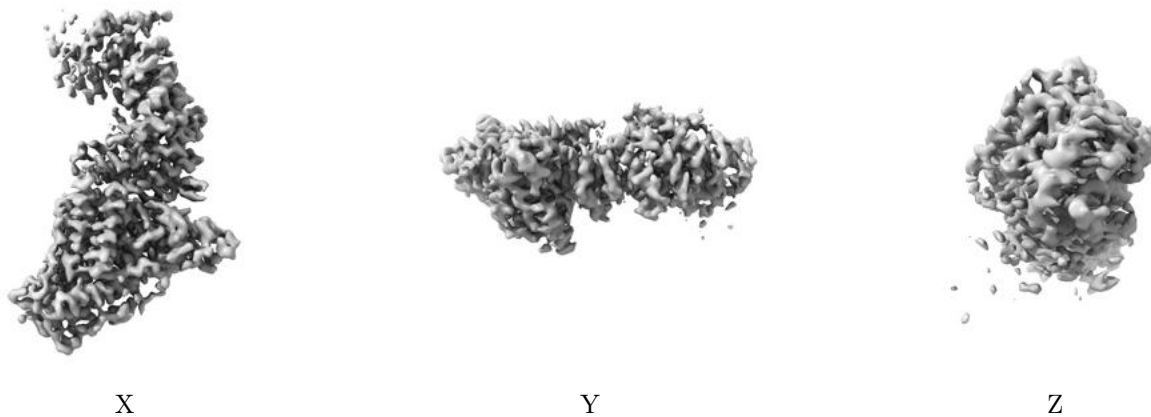
### 6.4.2 Raw map



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.

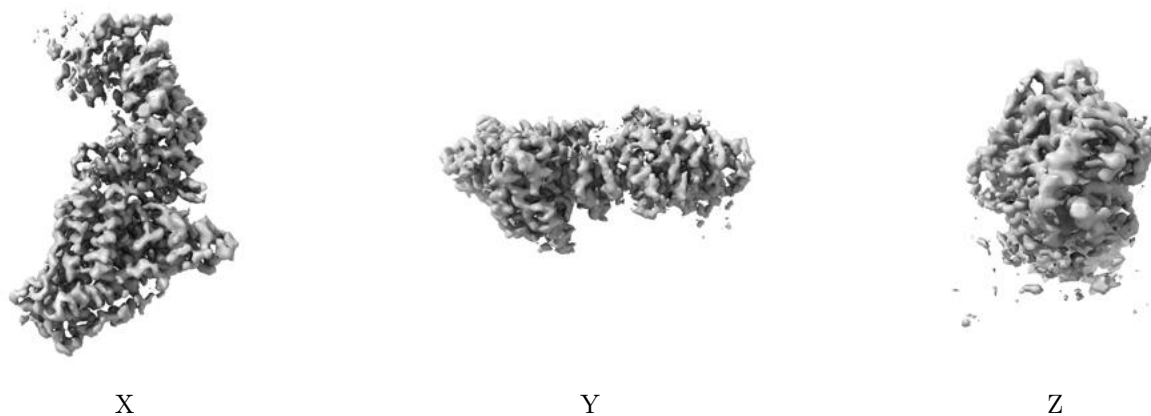
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 12.4. 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.

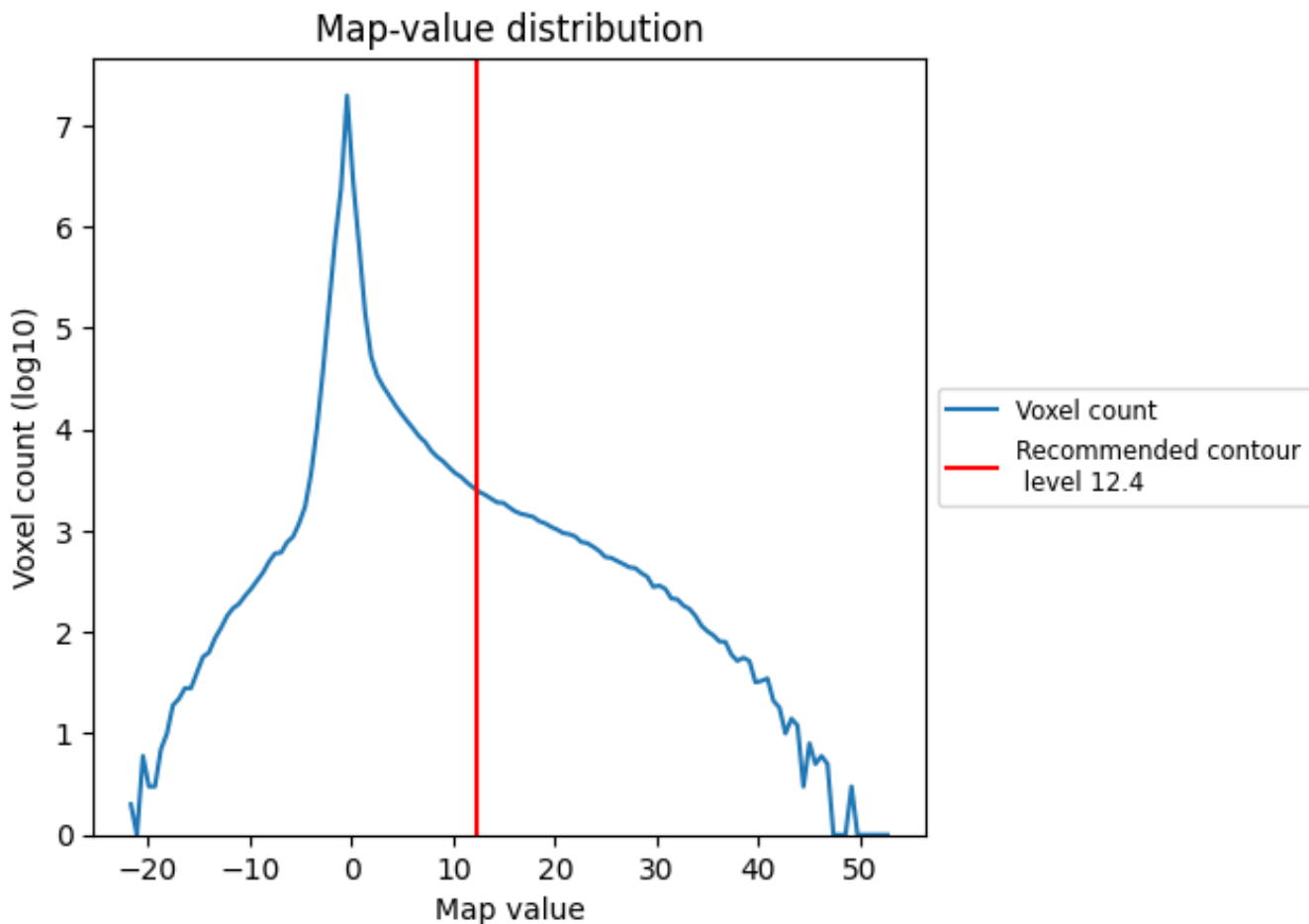
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

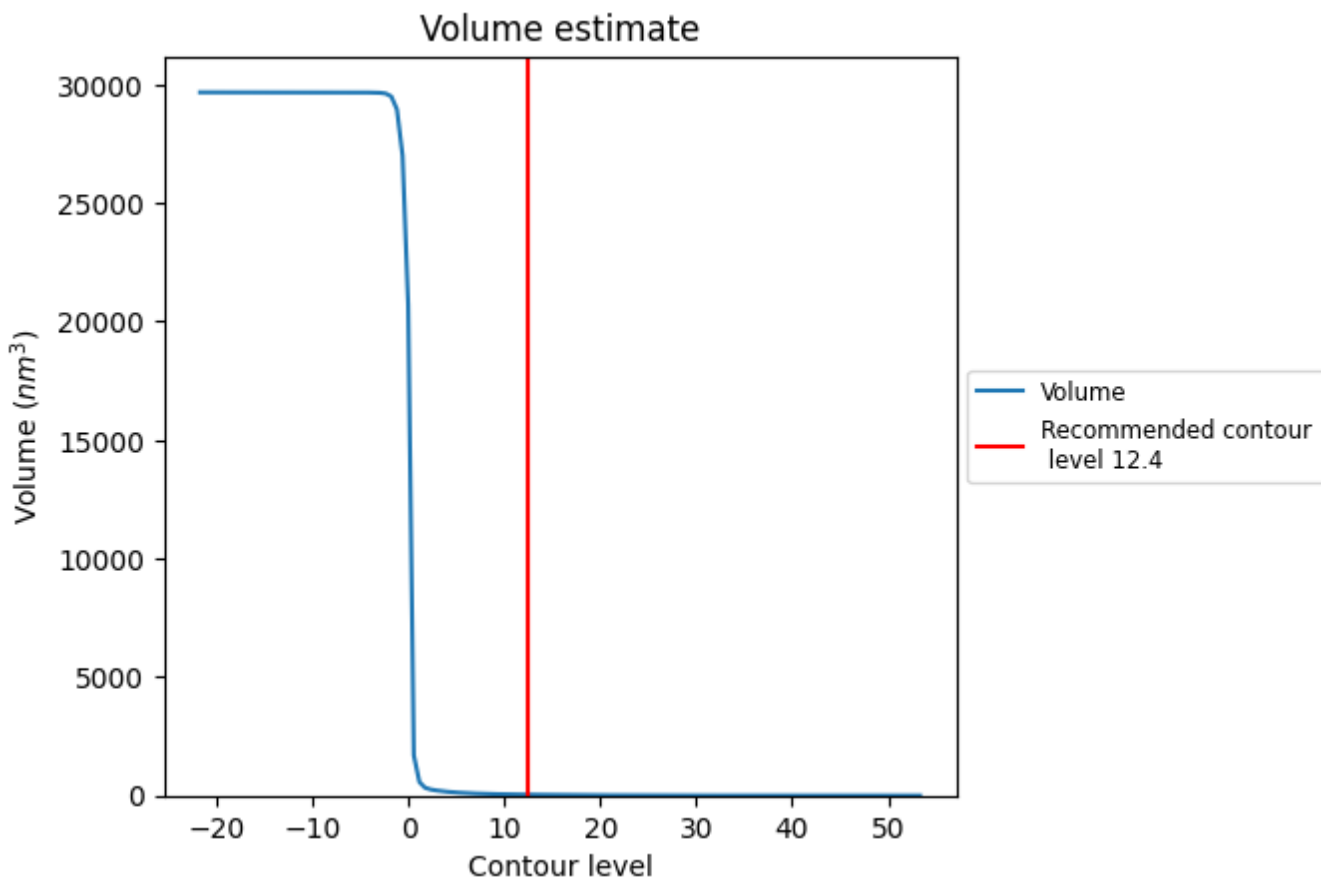
This section contains the results of statistical analysis of the map.

### 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.

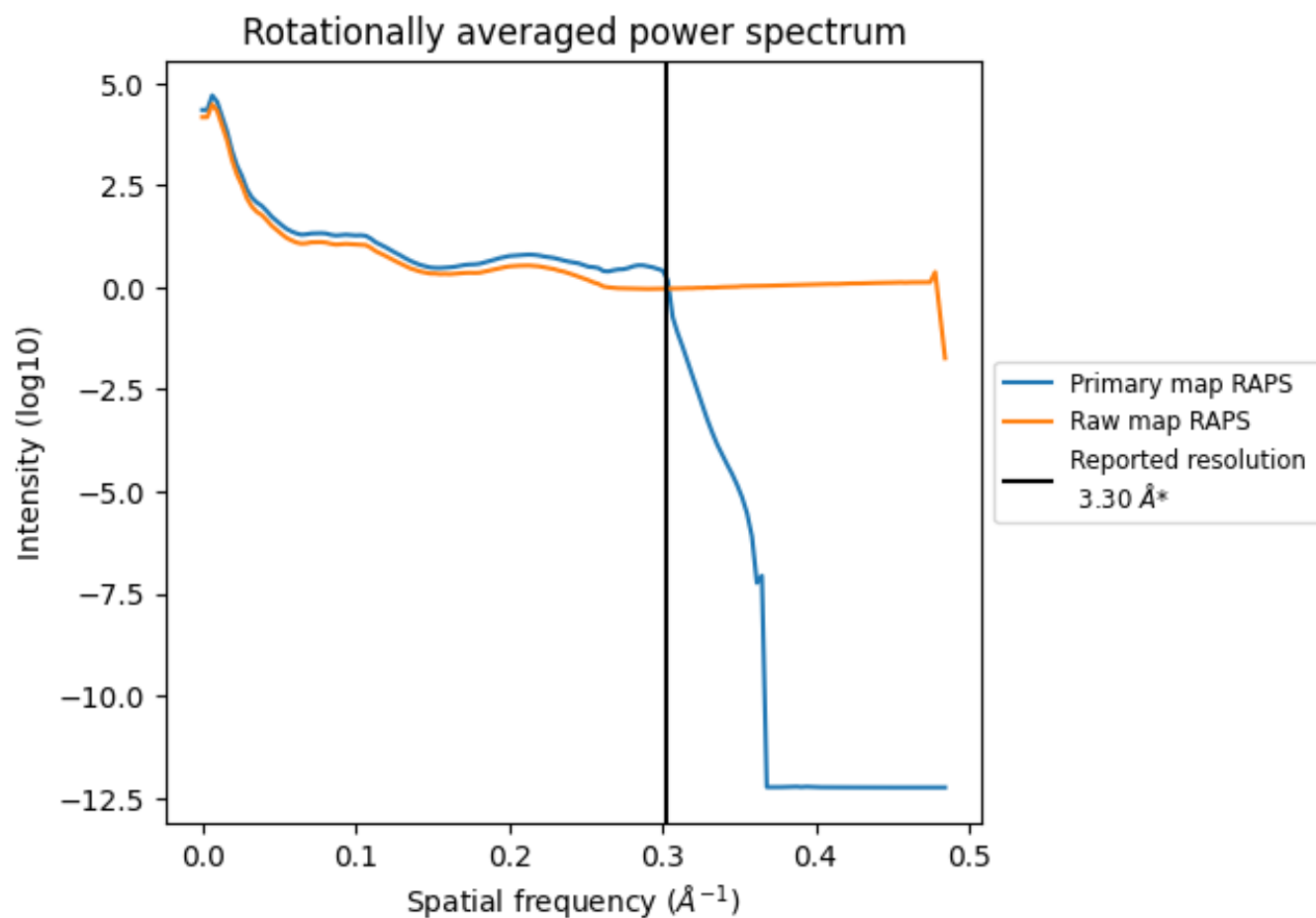
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm<sup>3</sup>; this corresponds to an approximate mass of 35 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 [i](#)

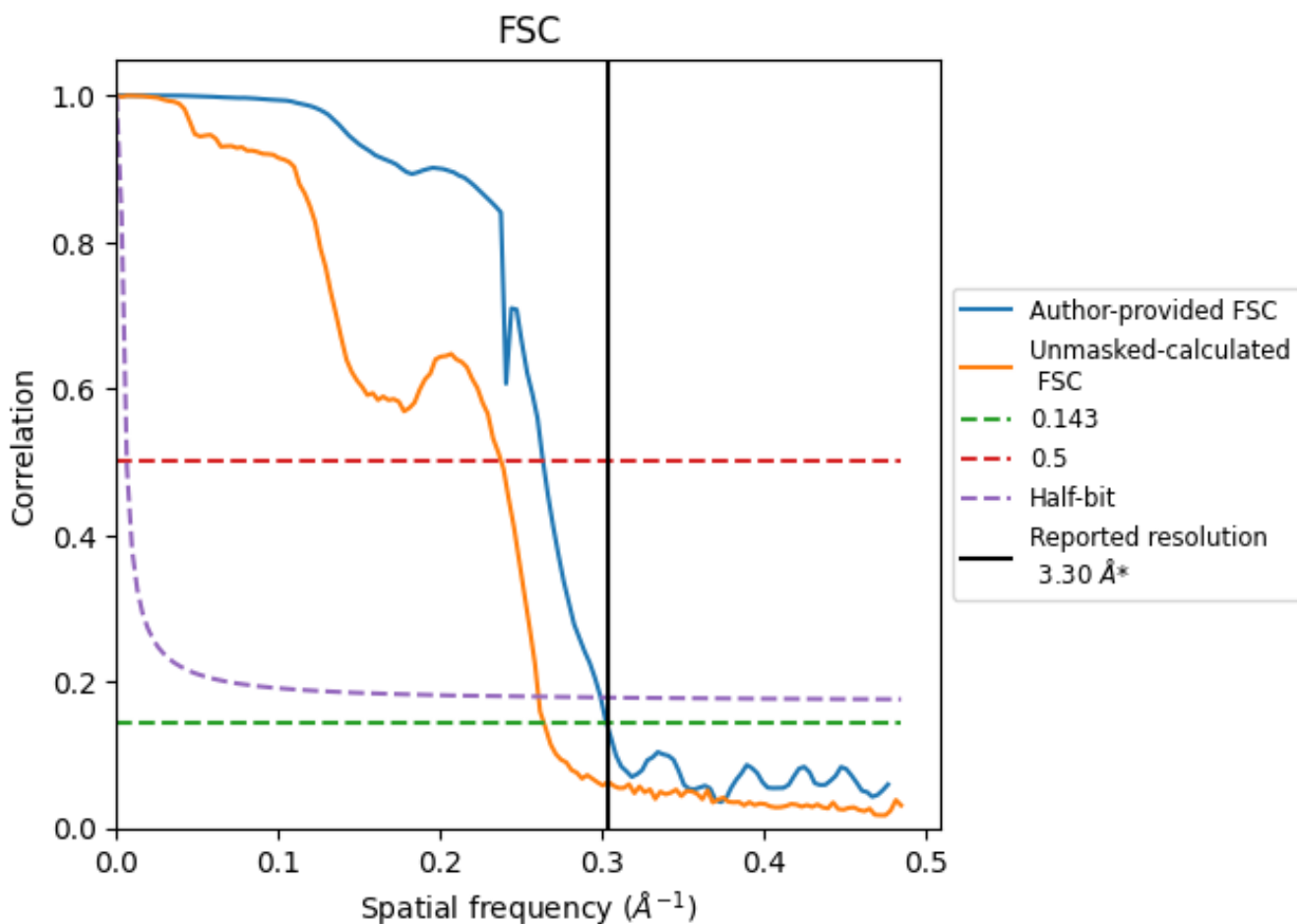


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

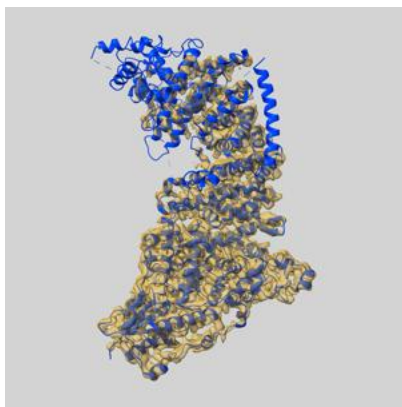
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.80	3.34
Unmasked-calculated*	3.79	4.21	3.84

\*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 3.79 differs from the reported value 3.3 by more than 10 %

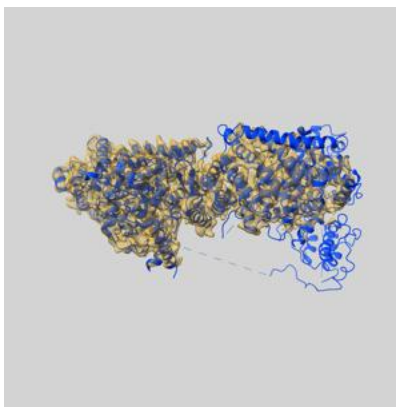
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27335 and PDB model 8DD7. Per-residue inclusion information can be found in section 3 on page 7.

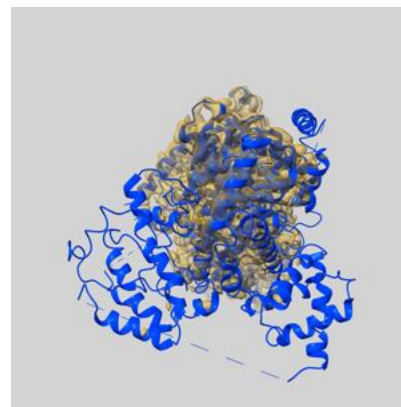
### 9.1 Map-model overlay [i](#)



X



Y

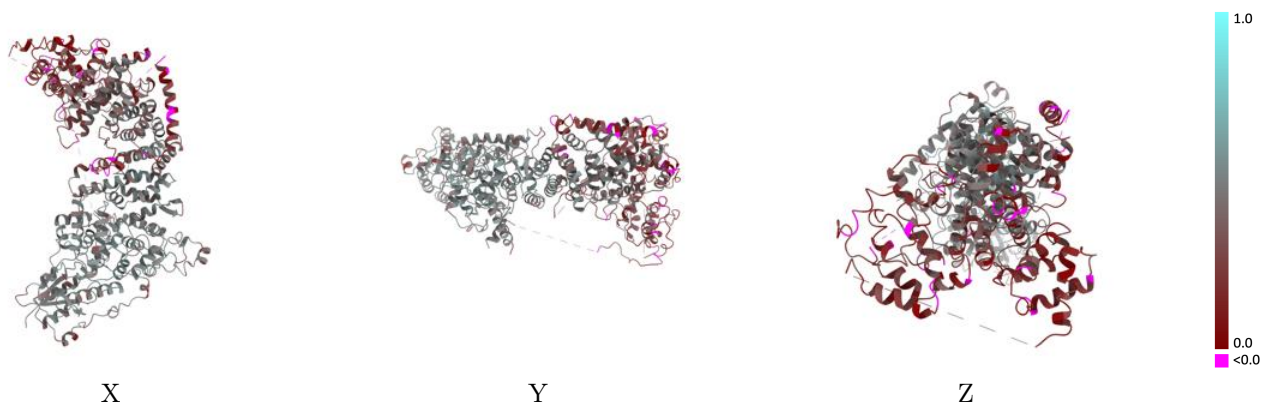


Z

The images above show the 3D surface view of the map at the recommended contour level 12.4 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.

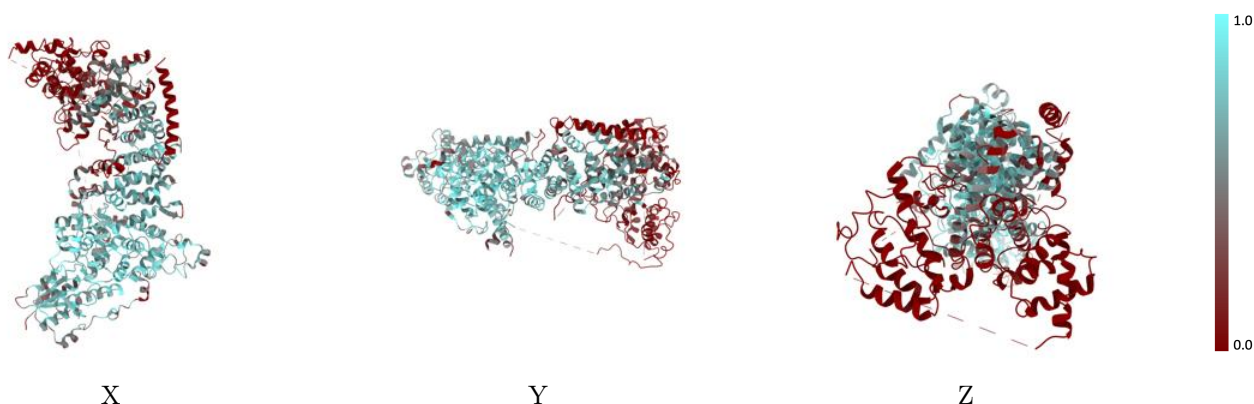


## 9.2 Q-score mapped to coordinate model [i](#)



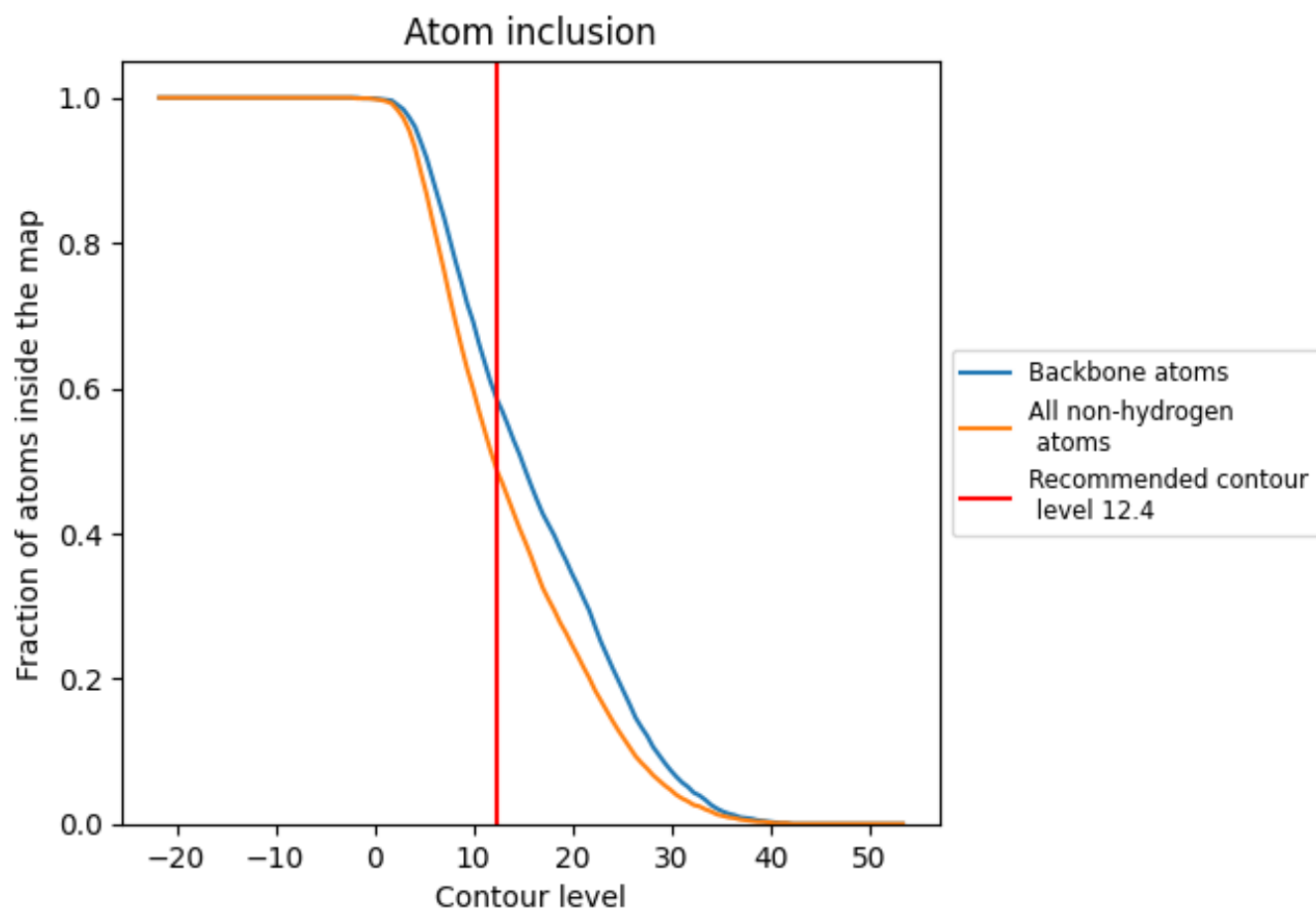
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (12.4).







## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (12.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4850	 0.3860
A	 0.7200	 0.4860
B	 0.3230	 0.3160

