Full wwPDB EM Validation Report (i)

May 12, 2024 – 08:19 pm BST

PDB ID	:	6RYR
EMDB ID	:	EMD-10058
Title	:	Nucleosome-CHD4 complex structure (single CHD4 copy)
Authors	:	Farnung, L.; Ochmann, M.; Cramer, P.
Deposited on	:	2019-06-11
Resolution	:	3.10 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

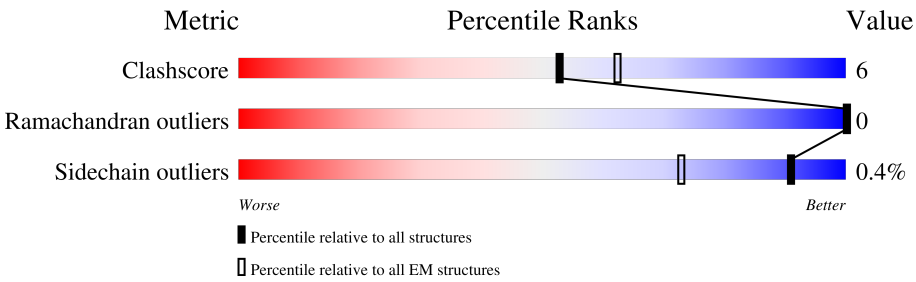
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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 >=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 <=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	136	57% 15% 29%
1	E	136	61% 10% 29%
2	B	103	7% 66% 17% 16%
2	F	103	71% 5% 24%
3	C	130	72% 8% 21%
3	G	130	72% 9% 19%
4	D	123	69% 8% 23%
4	H	123	62% 14% 24%

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Mol	Chain	Length	Quality of chain
5	I	149	90% 10%
6	J	149	5% 84% 16%
7	W	1927	6% 30% 7% 63%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 17834 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	97	802	506	155	138	3	0	0
1	E	97	801	504	155	139	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP P84233
E	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	87	703	442	142	118	1	0	0
2	F	78	619	391	120	107	1	0	0

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	103	795	501	155	139	0	0
3	G	105	809	510	158	141	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
C	123	SER	ALA	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897

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Chain	Residue	Modelled	Actual	Comment	Reference
G	123	SER	ALA	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	95	745	469	134	140	2	0	0
4	H	93	726	457	130	137	2	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P02281
D	29	THR	SER	conflict	UNP P02281
H	0	MET	-	initiating methionine	UNP P02281
H	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called DNA (149-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	149	3036	1443	555	890	148	0	0

- Molecule 6 is a DNA chain called DNA (149-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	149	3070	1454	571	896	149	0	0

- Molecule 7 is a protein called Chromodomain-helicase-DNA-binding protein 4,Chromodomain-helicase-DNA-binding protein 4,Chromodomain-helicase-DNA-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	W	708	5694	3638	990	1022	44	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-2	SER	-	expression tag	UNP Q14839

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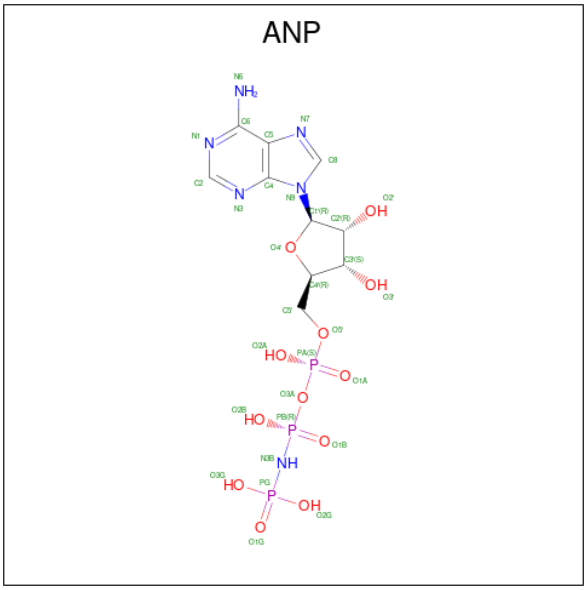
Chain	Residue	Modelled	Actual	Comment	Reference
W	-1	ASN	-	expression tag	UNP Q14839
W	0	ALA	-	expression tag	UNP Q14839

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	W	1	1	1	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

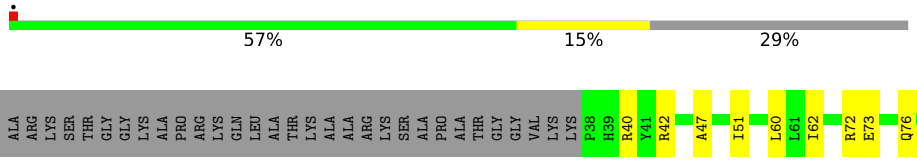
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	W	2	2	2	0

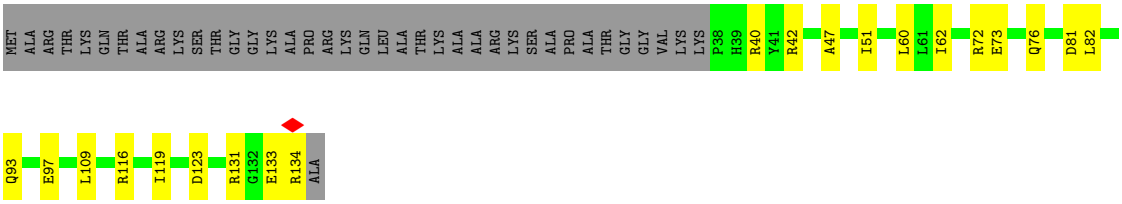
3 Residue-property plots (i)

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: Histone H3.2

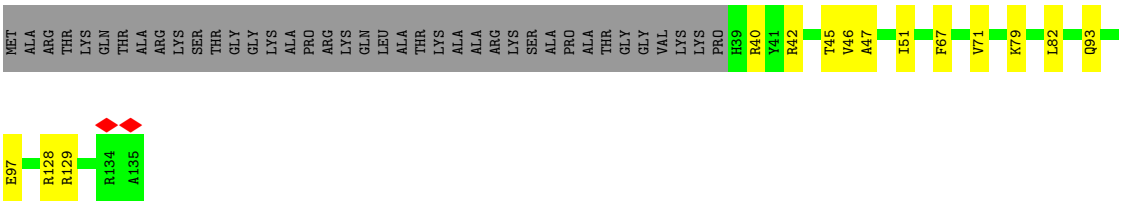
Chain A:





- Molecule 1: Histone H3.2

Chain E:

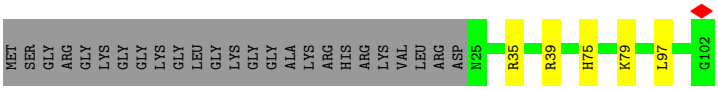


- Molecule 2: Histone H4

Chain B:

- Molecule 2: Histone H4

Chain F:



- Molecule 3: Histone H2A type 1

Chain C: 72% 8% 21%

MET SER GLY ARG GLY LYS GLN GLY GLY LYS THR ARG ALA LYS ALA LYS T16 R32 R35 L65 K75 A86 V87 R88 L97 T101 L116 P117 K118 LYS THR GLU SER SER LYS SER ALA LYS SER LYS

• Molecule 3: Histone H2A type 1

Chain G: 72% 9% 19%

MET SER GLY ARG GLY LYS GLN GLY GLY LYS THR ARG ALA LYS A14 V54 L65 T76 A86 V87 R88 E91 E92 L93 N94 G98 R99 V100 Q112 S113 P117 K118 LYS THR GLU SER SER LYS SER ALA LYS SER LYS

• Molecule 4: Histone H2B 1.1

Chain D: 69% 8% 23%

MET ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS ALA VAL THR LYS THR GLN LYS LYS ASP GLY LYS LYS ARG ARG K28 E32 I51 M56 N64 E68 L77 R89 T93 E102 H106 K122

• Molecule 4: Histone H2B 1.1

Chain H: 62% 14% 24%

MET ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS ALA VAL THR LYS THR GLN LYS LYS ASP GLY LYS LYS ARG ARG LYS T29 R30 K31 Y39 I51 D65 R69 R76 L77 A78 R89 E90 T93 A94 V95 L99 A104 V108 G111

V115 A121 LYS

• Molecule 5: DNA (149-MER)

Chain I: 90% 10%

A-72 G-34 C-23 C-18 G-7 G9 G28 C49 A50 G54 T55 C56 A61 A67 T68 C69 G70 A71 T72 A73 G74 G75 C76

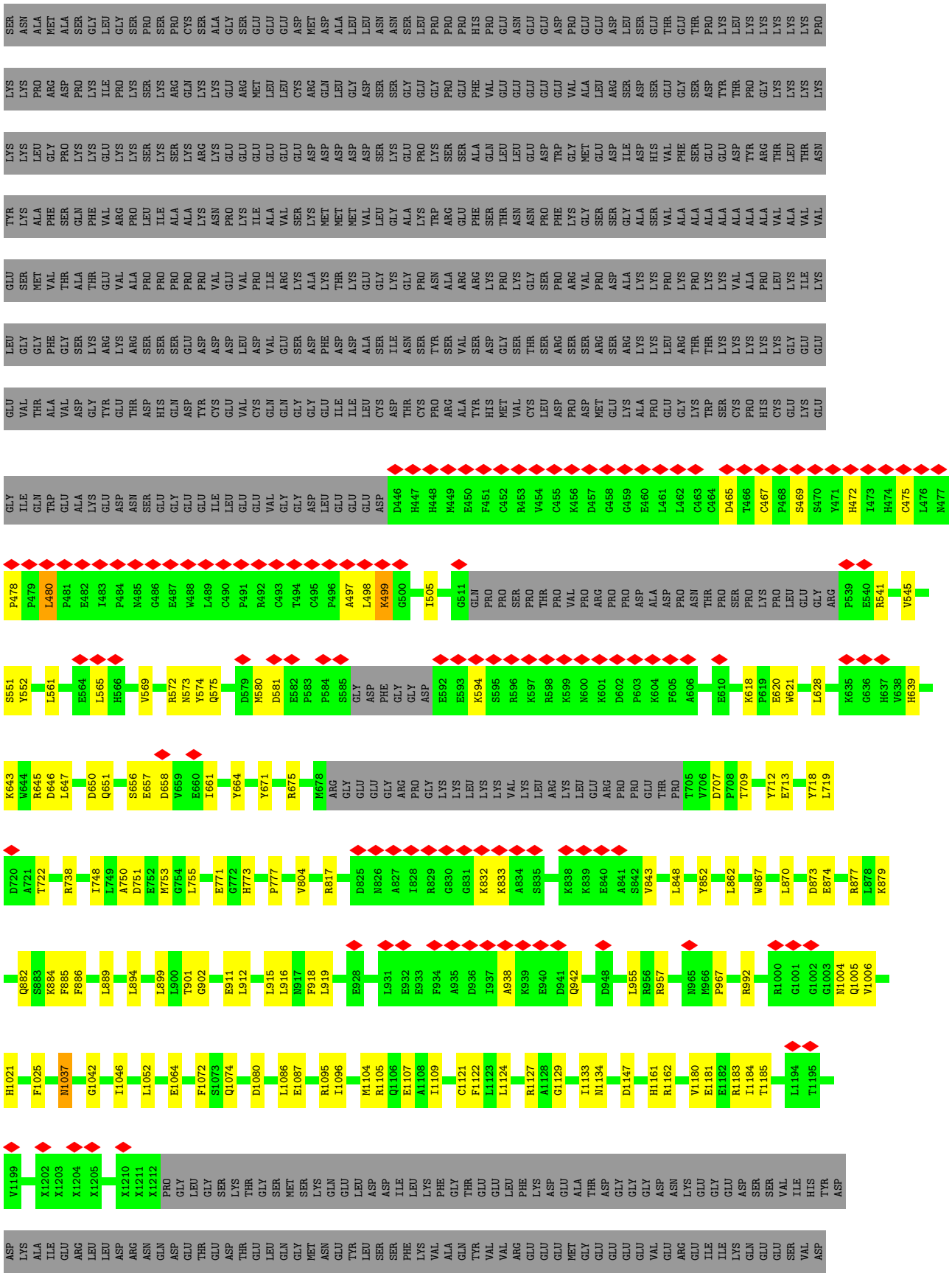
• Molecule 6: DNA (149-MER)

Chain J: 5% 84% 16%

G-76 C-75 C-74 T-73 A-72 T-71 C-70 G-69 A-68 T-67 G-66 A-62 T-61 T-57 G-56 A-55 T-17 T-16 A6 T9 G10 G21 T25 T35 A39 C58 G70 A71 T72

• Molecule 7: Chromodomain-helicase-DNA-binding protein 4,Chromodomain-helicase-DNA-binding protein 4,Chromodomain-helicase-DNA-binding protein 4

Chain W: 6% 30% 7% 63%


SER ASN ALA MET ALA SER GLY LEU GLY SER PRO SER PRO CYS SER ALA GLY SER GLU GLU GLU ASP MET ASP ALA LEU LEU ASN ASN SER LEU PRO PRO PRO HIS PRO GLU ASN GLU GLU ASP PRO GLU GLU ASP LEU SER GLU THR GLU THR PRO LYS LEU LYS LYS LYS LYS PRO
LYS LYS PRO ARG ASP PRO LYS ILE PRO LYS SER LYS ARG GLN LYS LYS GLU ARG MET LEU LEU CYS ARG GLN LEU LEU ASP SER SER GLY GLU GLY PRO GLU PHE VAL GLU GLU GLU GLU GLU GLU VAL ALA LEU ARG SER ASP SER GLY GLY SER ASP TYR THR PRO GLY LYS LYS LYS LYS
LYS LYS LEU GLY PRO LYS LYS GLU LYS LYS SER LYS SER LYS ARG LYS GLU GLU GLU GLU GLU GLU ASP ASP ASP ASP SER LYS GLU PRO LYS SER SER ALA GLN LEU LEU GLU ASP TRP GLY MET GLU ASP ILE ASP HIS VAL PHE SER GLU GLU ASP TYR ARG THR LEU THR ASN
TYR LYS ALA PHE SER GLN PHE VAL ARG PRO LEU ILE ALA ALA ALA LYS ASN PRO LYS ILE ALA VAL SER LYS MET MET MET VAL LEU LEU GLY ALA LYS TRP ARG GLU PHE SER THR ASN ASN PRO PHE LYS GLY SER SER GLY ALA SER VAL ALA ALA ALA ALA ALA ALA VAL ALA VAL VAL
GLU SER MET VAL THR ALA THR GLU VAL ALA PRO PRO PRO PRO VAL GLU VAL PRO ILE ALA ARG LYS ALA LYS THR LYS GLU GLY PRO ASN ALA ARG ARG LYS PRO LYS GLY SER THR SER ARG SER SER ARG SER ARG ARG LYS LYS PRO LYS PRO LYS LYS VAL ALA PRO LEU LYS ILE LYS
LEU GLY GLY PHE GLY SER LYS ARG LYS ARG SER SER SER GLU ASP ASP ASP LEU ASP VAL GLU SER ASP PHE ASP ASP ALA SER ILE ASN SER TYR SER VAL SER ASP GLY SER THR SER ARG SER SER ARG SER ARG ARG LYS LYS LYS LYS LEU ARG LYS LYS LYS LYS GLY GLU GLU
GLU VAL THR ALA VAL ASP GLY TYR GLU THR ASP HIS GLN ASP TYR CYS GLU VAL CYS GLN GLN GLY GLY GLU ILE ILE LEU CYS ASP THR CYS PRO ARG ALA TYR HIS MET VAL CYS LEU ASP PRO ASP MET GLU LYS ALA PRO GLU GLY LYS TRP SER CYS PRO HIS CYS GLU LYS ILE LYS GLU
GLY ILE GLN TRP GLU ALA LYS GLU ASP ASN SER GLU GLY GLU GLU ILE LEU GLU GLU GLU VAL GLY GLY ASP LEU GLU GLU GLU ASP D446 H447 H448 M449 E450 F451 C452 R453 V454 C455 K456 D457 G458 G459 E460 L461 L462 C463 C464 D465 T466 C467 P468 S469 S470 Y471 H472 I473 H474 C475 L476 N477
P478 P479 L480 P481 E482 I483 P484 N485 G486 E487 W488 L489 C490 P491 R492 C493 T494 C495 P496 A497 L498 K499 G500 I505 G511 GLN PRO PRO SER PRO THR PRO VAL PRO ARG PRO PRO ASP ALA ASP PRO ASN THR PRO SER PRO LYS PRO LEU GLU GLY ARG P539 E540 R541 V545
S551 Y552 L561 E564 L565 H566 V569 R572 N573 Y574 Q575 D579 M580 D581 E582 P583 P584 S585 GLY ASP PHE GLY GLY ASP E592 E593 K594 S595 R596 K597 R598 K599 N600 K601 D602 P603 K604 F605 A606 E610 K618 P619 E620 W621 L628 K635 G636 H637 V638 H639
K643 W644 R645 D646 L647 D650 Q651 S656 E657 D658 V659 E660 I661 Y664 Y671 R675 M678 ARG GLY GLU GLU GLY ARG PRO GLY LYS LYS LEU LYS LYS VAL LYS LEU ARG LYS LEU GLU ARG PRO PRO GLU THR PRO T705 V706 D707 P708 T709 Y712 E713 Y718 L719
D720 A721 T722 R738 I748 L749 A750 D751 E752 M753 G754 L755 E771 G772 H773 P777 V804 R817 D825 N826 A827 I828 R829 G830 G831 K832 K833 A834 S835 K838 K839 E840 A841 S842 V843 L848 Y852 L862 W867 L870 D873 E874 R877 L878 K879
Q882 S883 K884 F885 F886 L889 L894 L899 L900 T901 G902 E911 L912 L915 L916 N917 F918 L919 E928 L931 E932 E933 F934 A935 D936 I937 A938 K939 E940 D941 Q942 D948 L955 R956 R957 N965 M966 P967 R992 R1000 G1001 G1002 G1003 N1004 Q1005 V1006
H1021 F1025 N1037 G1042 I1046 L1052 E1064 F1072 S1073 Q1074 D1080 L1086 E1087 R1095 I1096 M1104 R1105 Q1106 E1107 A1108 I1109 C1121 F1122 L1123 L1124 R1127 A1128 G1129 I1133 N1134 D1147 H1161 R1162 V1180 E1181 E1182 R1183 I1184 T1185 L1194 T1195
V1199 X1202 X1203 X1204 X1205 X1210 X1211 X1212 PRO GLY LEU GLY SER LYS THR GLY SER MET SER LYS GLN GLU LEU ASP ASP ILE LEU LYS PHE GLY THR GLU GLU LEU PHE LYS ASP GLU ALA THR ASP GLY GLY GLY ASP ASN LYS GLU GLY GLU ASP SER SER VAL ILE HIS TYR ASP
ASP LYS ALA ILE GLU ARG LEU LEU ASP ARG ASN GLN ASP GLU THR GLU ASP THR GLU LEU GLN GLY MET ASN GLU TYR LEU ASP SER SER PHE LYS VAL ALA GLN TYR VAL VAL ARG GLU LYS GLU GLU MET GLY GLU GLU GLU GLU VAL GLU ARG GLU ILE ILE LYS GLN GLU GLU SER VAL ASP

PRO ASP TYR TRP GLU LYS LEU LEU ARG HIS HIS TYR GLU GLN GLN GLN GLU ASP LEU ALA ARG ASN LEU GLY LYS GLY LYS ARG ILE ARG LYS GLN VAL ASN TYR ASN ASP GLY SER GLN GLU ASP ARG ASP TRP GLN ASP ASP GLN SER ASP ASN GLN SER ASP TYR SER VAL ALA SER

GLU GLU GLY ASP GLU ASP PHE ASP GLU ARG SER GLU ALA PRO ARG ARG PRO SER ARG LYS GLY LEU ARG ASN ASP LYS ASP LYS PRO LEU PRO PRO LEU LEU ALA ARG VAL GLY GLY ASN ILE GLU VAL LEU GLY PHE ASN ALA ARG GLN ARG LYS ALA PHE LEU ASN ALA ILE MET ARG

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

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

PRO ASN THR PRO ALA PRO VAL PRO PRO ALA GLU ASP GLY ILE LYS ILE GLU GLU ASN SER LEU LYS GLU GLU GLU SER ILE GLU GLY GLU LYS GLU VAL LYS SER THR ALA PRO GLU THR ALA ILE GLU CYS THR GLN ALA PRO ALA PRO ALA SER GLU ASP GLU LYS VAL VAL GLU

PRO PRO GLU GLY GLU GLU LYS VAL GLU LYS ALA GLU VAL LYS GLU ARG THR GLU GLU PRO MET GLU THR GLU PRO LYS GLY ALA ALA ASP VAL GLU LYS VAL GLU GLU LYS SER ALA ILE ASP LEU THR PRO ILE VAL VAL GLU ASP LYS GLU GLU LYS LYS GLU GLU GLU LYS LYS

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

ARG ARG HIS ASP TYR TRP LEU LEU ALA GLY ILE ILE ASN HIS GLY TYR ALA ARG TRP GLN ASP ILE GLN ASN ASP PRO ARG TYR ALA ILE LEU ASN GLU PRO PHE LYS GLY GLU MET ASN ARG GLY ASN PHE LEU GLU ILE LYS ASN LYS PHE LEU ALA ARG ARG PHE LYS LEU LEU GLU

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

HIS LYS VAL LEU LYS GLN LEU GLU GLU LEU LEU SER ASP MET LYS ALA ASP VAL THR ARG LEU PRO ALA THR ILE ALA ARG ILE PRO PRO VAL ALA VAL ARG LEU GLN MET SER GLU ARG ASN ILE LEU SER ARG LEU ALA ASN ARG ALA PRO GLU PRO THR PRO GLN GLN VAL ALA GLN

GLN GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	89623	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.27	0/814	0.48	0/1092
1	E	0.25	0/812	0.49	0/1088
2	B	0.26	0/711	0.53	0/948
2	F	0.25	0/626	0.46	0/837
3	C	0.26	0/805	0.44	0/1088
3	G	0.24	0/819	0.46	0/1106
4	D	0.25	0/756	0.41	0/1015
4	H	0.26	0/737	0.45	0/993
5	I	0.50	0/3403	0.89	0/5246
6	J	0.51	0/3446	0.89	0/5321
7	W	0.26	0/5781	0.49	2/7806 (0.0%)
All	All	0.37	0/18710	0.67	2/26540 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	W	480	LEU	CB-CG-CD1	6.49	122.03	111.00
7	W	480	LEU	CB-CG-CD2	5.48	120.32	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	802	0	841	25	0
1	E	801	0	838	10	0
2	B	703	0	755	15	0
2	F	619	0	659	5	0
3	C	795	0	846	10	0
3	G	809	0	864	11	0
4	D	745	0	773	6	0
4	H	726	0	747	14	0
5	I	3036	0	1673	17	0
6	J	3070	0	1674	24	0
7	W	5694	0	5512	86	0
8	W	31	0	13	0	0
9	W	1	0	0	0	0
10	W	2	0	0	0	0
All	All	17834	0	15195	180	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 6.

All (180) 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)
7:W:852:TYR:OH	7:W:873:ASP:O	1.89	0.89
1:A:81:ASP:OD2	7:W:992:ARG:NH2	2.12	0.82
7:W:938:ALA:O	7:W:942:GLN:N	2.17	0.77
2:B:75:HIS:O	4:D:89:ARG:NH2	2.18	0.76
7:W:1037:ASN:O	7:W:1037:ASN:ND2	2.15	0.76
7:W:1134:ASN:OD1	7:W:1162:ARG:NH1	2.18	0.75
7:W:467:CYS:SG	7:W:469:SER:OG	2.42	0.75
5:I:74:DG:N2	6:J:-73:DT:O2	2.20	0.74
7:W:618:LYS:NZ	7:W:620:GLU:OE2	2.21	0.74
3:C:35:ARG:NH2	6:J:39:DA:OP2	2.20	0.73
7:W:912:LEU:O	7:W:916:LEU:HD12	1.88	0.73
7:W:873:ASP:OD1	7:W:874:GLU:N	2.24	0.71
7:W:817:ARG:NH2	7:W:832:LYS:O	2.23	0.71
7:W:712:TYR:OH	7:W:738:ARG:NH1	2.25	0.69
1:A:109:LEU:HD21	3:G:112:GLN:NE2	2.09	0.67
3:G:76:THR:O	3:G:76:THR:HG22	1.96	0.64
5:I:67:DA:N3	6:J:-66:DG:N2	2.45	0.64
1:A:109:LEU:HD21	3:G:112:GLN:HE22	1.63	0.64
7:W:478:PRO:HG2	7:W:480:LEU:HD11	1.79	0.64
2:B:17:ARG:NH2	7:W:1087:GLU:OE2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:NH2	5:I:-23:DC:OP1	2.33	0.62
7:W:1096:ILE:HG22	7:W:1122:PHE:HE1	1.64	0.61
7:W:561:LEU:O	7:W:565:LEU:HD12	2.00	0.61
3:C:88:ARG:NH1	3:C:97:LEU:O	2.34	0.61
5:I:-18:DC:OP2	7:W:1105:ARG:NH2	2.32	0.60
1:A:40:ARG:NH2	6:J:9:DT:O2	2.34	0.60
1:A:82:LEU:HD21	2:B:70:VAL:HG22	1.83	0.60
1:A:42:ARG:NH1	5:I:70:DG:O5'	2.36	0.59
2:B:68:ASP:OD1	2:B:93:GLN:NE2	2.35	0.58
1:A:47:ALA:O	1:A:51:ILE:HG13	2.04	0.58
7:W:505:ILE:HG12	7:W:545:VAL:HG12	1.84	0.58
7:W:719:LEU:O	7:W:722:THR:OG1	2.19	0.58
3:C:32:ARG:NH2	4:D:32:GLU:OE1	2.37	0.57
6:J:25:DT:OP1	7:W:1183:ARG:NH2	2.35	0.56
7:W:1096:ILE:CG2	7:W:1124:LEU:HD23	2.36	0.56
7:W:1080:ASP:OD1	7:W:1095:ARG:NH1	2.37	0.56
4:H:104:ALA:O	4:H:108:VAL:HG23	2.06	0.55
2:B:20:LYS:O	2:B:22:LEU:HD12	2.06	0.55
7:W:862:LEU:O	7:W:867:TRP:NE1	2.40	0.55
7:W:541:ARG:NH1	7:W:580:MET:O	2.39	0.55
7:W:569:VAL:O	7:W:573:ASN:OD1	2.25	0.55
7:W:804:VAL:HG23	7:W:848:LEU:HD12	1.88	0.54
7:W:1181:GLU:O	7:W:1185:THR:HG23	2.08	0.54
7:W:505:ILE:HG21	7:W:574:TYR:CE2	2.43	0.54
5:I:56:DC:N4	6:J:-57:DT:O4	2.41	0.54
7:W:707:ASP:OD2	7:W:709:THR:N	2.40	0.54
2:B:59:LYS:O	2:B:63:GLU:HG3	2.08	0.54
4:H:30:ARG:NH2	5:I:49:DC:O3'	2.29	0.53
7:W:646:ASP:O	7:W:647:LEU:HD12	2.08	0.53
7:W:899:LEU:HD23	7:W:915:LEU:HD11	1.89	0.53
6:J:21:DG:H21	7:W:1127[B]:ARG:HH12	1.55	0.53
2:B:16:LYS:O	2:B:17:ARG:HG3	2.09	0.52
3:G:88:ARG:NH2	3:G:100:VAL:O	2.43	0.52
1:A:62:ILE:N	1:A:97:GLU:OE2	2.42	0.52
2:F:75:HIS:O	4:H:89:ARG:NH2	2.42	0.52
4:H:30:ARG:HE	4:H:31:LYS:N	2.07	0.51
7:W:628:LEU:HD11	7:W:643:LYS:HB2	1.92	0.51
1:A:73:GLU:HG2	7:W:1004:ASN:HB2	1.93	0.51
4:H:39:TYR:HE1	4:H:51:ILE:HG22	1.76	0.51
7:W:817:ARG:HG3	7:W:817:ARG:HH11	1.76	0.51
3:C:75:LYS:NZ	6:J:58:DC:OP1	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:572:ARG:HA	7:W:575:GLN:HG2	1.94	0.50
6:J:-17:DT:H4'	6:J:-16:DT:OP1	2.12	0.49
7:W:618:LYS:HB3	7:W:621:TRP:CE2	2.48	0.49
7:W:1074:GLN:NE2	7:W:1147:ASP:OD1	2.46	0.49
2:B:73:THR:OG1	2:B:85:ASP:OD1	2.25	0.49
7:W:748:ILE:HG13	7:W:919:LEU:HD22	1.95	0.48
3:C:116:LEU:O	3:C:118:LYS:NZ	2.46	0.48
7:W:505:ILE:HG21	7:W:574:TYR:CD2	2.48	0.48
6:J:21:DG:OP1	7:W:877:ARG:NH2	2.47	0.48
2:F:79:LYS:N	5:I:28:DG:OP1	2.46	0.48
7:W:771:GLU:N	7:W:771:GLU:OE1	2.46	0.48
7:W:661:ILE:HG23	7:W:664:TYR:HB2	1.96	0.47
7:W:671:TYR:OH	7:W:675:ARG:NH1	2.48	0.47
5:I:61:DA:O5'	7:W:833:LYS:NZ	2.45	0.47
1:A:73:GLU:CD	2:B:25:ASN:HD21	2.17	0.47
4:H:30:ARG:NE	4:H:30:ARG:HA	2.30	0.47
7:W:581:ASP:O	7:W:581:ASP:OD1	2.33	0.47
1:A:40:ARG:NH1	6:J:10:DG:O4'	2.48	0.47
7:W:497:ALA:O	7:W:498:LEU:HD23	2.14	0.47
6:J:-72:DA:H2'	6:J:-71:DT:C4	2.50	0.46
1:E:40:ARG:NH2	5:I:9:DG:N3	2.61	0.46
2:F:75:HIS:ND1	4:H:93:THR:HG21	2.30	0.46
6:J:21:DG:OP2	7:W:884:LYS:N	2.49	0.46
7:W:879:LYS:HB2	7:W:911:GLU:HB3	1.98	0.45
1:E:67:PHE:O	1:E:71:VAL:HG23	2.16	0.45
7:W:771:GLU:HB3	7:W:773:HIS:CE1	2.52	0.45
7:W:1129:GLY:O	7:W:1133:ILE:HD11	2.17	0.45
7:W:505:ILE:CG1	7:W:545:VAL:HG12	2.47	0.45
7:W:1096:ILE:HG13	7:W:1105:ARG:HG2	1.97	0.45
3:C:65:LEU:HB3	3:C:86:ALA:HB1	1.99	0.45
7:W:777:PRO:HG3	7:W:843:VAL:HG21	1.99	0.45
1:A:62:ILE:O	1:A:93:GLN:NE2	2.50	0.45
1:E:47:ALA:O	1:E:51:ILE:HG13	2.17	0.45
4:H:76:ARG:HH11	4:H:76:ARG:HG3	1.82	0.45
7:W:1021:HIS:CD2	7:W:1052:LEU:HD12	2.52	0.45
7:W:751:ASP:OD2	7:W:755:LEU:HD12	2.17	0.45
4:D:77:LEU:CD1	4:D:93:THR:HG23	2.46	0.44
1:E:42:ARG:NH2	6:J:70:DG:P	2.90	0.44
7:W:657:GLU:O	7:W:658:ASP:OD1	2.35	0.44
7:W:1042:GLY:O	7:W:1046:ILE:HG13	2.17	0.44
3:C:35:ARG:HH22	6:J:39:DA:P	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:465:ASP:O	7:W:465:ASP:OD2	2.36	0.44
7:W:713:GLU:OE1	7:W:713:GLU:N	2.40	0.44
3:G:94:ASN:OD1	3:G:94:ASN:O	2.36	0.44
7:W:499:LYS:HD2	7:W:499:LYS:O	2.17	0.44
7:W:551:SER:OG	7:W:552:TYR:N	2.51	0.44
7:W:748:ILE:CD1	7:W:919:LEU:HD22	2.47	0.44
7:W:901:THR:O	7:W:901:THR:HG23	2.18	0.44
1:A:42:ARG:HH22	5:I:69:DC:H4'	1.83	0.44
1:A:76:GLN:HG3	7:W:1004:ASN:OD1	2.17	0.44
1:E:79:LYS:HD3	1:E:82:LEU:HD21	2.00	0.44
1:A:72:ARG:HH22	5:I:-23:DC:P	2.41	0.43
1:A:60:LEU:CD2	1:A:97:GLU:OE1	2.66	0.43
2:F:35:ARG:O	2:F:39:ARG:HG2	2.19	0.43
1:E:45:THR:HG23	1:E:46:VAL:N	2.33	0.43
5:I:-34:DG:N2	6:J:35:DT:O2	2.51	0.43
1:A:116:ARG:NH2	1:A:123:ASP:OD2	2.52	0.43
4:H:95:VAL:HG13	4:H:99:LEU:HD22	2.01	0.43
7:W:750:ALA:O	7:W:955:LEU:O	2.37	0.43
4:H:111:GLY:O	4:H:115:VAL:HG23	2.19	0.43
7:W:885:PHE:CE2	7:W:889:LEU:HD11	2.54	0.43
1:E:93:GLN:O	1:E:97:GLU:HG3	2.19	0.43
1:E:128:ARG:HH11	1:E:128:ARG:HG2	1.83	0.43
7:W:639:HIS:CD2	7:W:656:SER:HG	2.35	0.43
2:B:82:THR:HG22	2:B:83:ALA:N	2.34	0.42
4:D:102:GLU:OE1	4:D:106:HIS:NE2	2.52	0.42
6:J:-73:DT:H1'	6:J:-72:DA:C8	2.53	0.42
1:A:109:LEU:HD12	1:E:129:ARG:CZ	2.48	0.42
1:A:131:ARG:NH2	1:A:133:GLU:OE2	2.52	0.42
6:J:-69:DG:N3	6:J:-68:DA:N7	2.68	0.42
7:W:967:PRO:O	7:W:1161:HIS:NE2	2.52	0.42
1:A:119:ILE:O	1:A:119:ILE:HG13	2.20	0.42
5:I:54:DG:O6	6:J:-55:DA:N6	2.52	0.42
1:A:51:ILE:HG23	2:B:39:ARG:O	2.19	0.42
6:J:-75:DC:H2'	6:J:-74:DC:C6	2.55	0.42
6:J:-70:DC:H2"	6:J:-69:DG:C4	2.55	0.42
7:W:1109:ILE:HD11	7:W:1133:ILE:CG2	2.49	0.42
2:B:19:ARG:HH11	2:B:19:ARG:HG2	1.84	0.42
4:D:64:ASN:O	4:D:68:GLU:HG3	2.19	0.42
7:W:1096:ILE:CG2	7:W:1122:PHE:HE1	2.32	0.42
7:W:1180:VAL:O	7:W:1184:ILE:HG23	2.18	0.42
3:G:94:ASN:O	3:G:98:GLY:CA	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:THR:O	3:C:101:THR:OG1	2.37	0.42
1:A:134:ARG:HA	1:A:134:ARG:NE	2.35	0.42
7:W:870:LEU:HB2	7:W:894:LEU:HD22	2.02	0.42
1:A:109:LEU:HD12	1:E:129:ARG:NH1	2.35	0.42
7:W:886:PHE:CE1	7:W:918:PHE:HB2	2.55	0.41
4:D:51:ILE:HG21	4:D:56:MET:SD	2.61	0.41
6:J:-62:DA:H2'	6:J:-61:DT:C6	2.56	0.41
2:B:17:ARG:O	2:B:17:ARG:HD2	2.20	0.41
7:W:1104:MET:HA	7:W:1107:GLU:OE2	2.20	0.41
2:B:50:ILE:HG12	2:B:50:ILE:O	2.20	0.41
5:I:-7:DG:O6	6:J:6:DA:N6	2.53	0.41
7:W:882:GLN:HA	7:W:882:GLN:OE1	2.21	0.41
7:W:1064:GLU:N	7:W:1064:GLU:OE1	2.53	0.41
3:G:65:LEU:HB3	3:G:86:ALA:HB1	2.03	0.41
7:W:718:TYR:HD1	7:W:719:LEU:HD12	1.85	0.41
7:W:1005:GLN:HA	7:W:1005:GLN:OE1	2.21	0.41
1:A:42:ARG:HH11	5:I:70:DG:H4'	1.86	0.41
3:C:75:LYS:CA	3:C:75:LYS:HE3	2.51	0.41
4:H:39:TYR:CE1	4:H:51:ILE:HG22	2.53	0.41
5:I:49:DC:H2"	5:I:50:DA:C8	2.56	0.41
6:J:-74:DC:H1'	6:J:-73:DT:C6	2.56	0.41
7:W:472:HIS:HB3	7:W:475:CYS:SG	2.61	0.41
7:W:620:GLU:O	7:W:645:ARG:HB2	2.20	0.41
7:W:1086:LEU:HD13	7:W:1121:CYS:SG	2.61	0.41
7:W:753:MET:HG3	7:W:902:GLY:HA3	2.03	0.41
3:C:101:THR:OG1	2:F:97:LEU:HD12	2.21	0.40
3:G:99:ARG:O	3:G:99:ARG:HG2	2.20	0.40
4:H:78:ALA:HB2	4:H:90:GLU:OE1	2.21	0.40
7:W:1006:VAL:HG21	7:W:1025:PHE:HD1	1.86	0.40
7:W:1072:PHE:CE1	7:W:1124:LEU:HD13	2.56	0.40
2:B:35:ARG:O	2:B:39:ARG:HG2	2.21	0.40
3:G:54:VAL:HG21	4:H:95:VAL:HG21	2.03	0.40
4:H:65:ASP:OD1	4:H:69:ARG:NE	2.53	0.40
7:W:650:ASP:OD1	7:W:651:GLN:NE2	2.37	0.40
7:W:650:ASP:OD1	7:W:650:ASP:C	2.60	0.40
3:G:76:THR:O	3:G:76:THR:CG2	2.65	0.40
3:G:91:GLU:HG3	3:G:92:GLU:N	2.36	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	95/136 (70%)	95 (100%)	0	0	100	100
1	E	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
2	B	85/103 (82%)	82 (96%)	3 (4%)	0	100	100
2	F	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
3	C	101/130 (78%)	99 (98%)	2 (2%)	0	100	100
3	G	103/130 (79%)	102 (99%)	1 (1%)	0	100	100
4	D	93/123 (76%)	92 (99%)	1 (1%)	0	100	100
4	H	91/123 (74%)	89 (98%)	2 (2%)	0	100	100
7	W	690/1927 (36%)	652 (94%)	38 (6%)	0	100	100
All	All	1429/2911 (49%)	1379 (96%)	50 (4%)	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	85/111 (77%)	85 (100%)	0	100	100
1	E	84/111 (76%)	84 (100%)	0	100	100
2	B	72/79 (91%)	71 (99%)	1 (1%)	67	86
2	F	63/79 (80%)	63 (100%)	0	100	100
3	C	82/102 (80%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	83/102 (81%)	83 (100%)	0	100	100
4	D	81/103 (79%)	81 (100%)	0	100	100
4	H	79/103 (77%)	79 (100%)	0	100	100
7	W	600/1680 (36%)	596 (99%)	4 (1%)	84	93
All	All	1229/2470 (50%)	1224 (100%)	5 (0%)	91	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	16	LYS
7	W	499	LYS
7	W	594	LYS
7	W	957	ARG
7	W	1037	ASN

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

Mol	Chain	Res	Type
1	A	39	HIS
7	W	876	HIS
7	W	914	HIS
7	W	1151	HIS

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)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	ANP	W	2001	9	29,33,33	1.08	4 (13%)	31,52,52	1.10	2 (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	ANP	W	2001	9	-	4/14/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	2001	ANP	PG-O1G	2.41	1.50	1.46
8	W	2001	ANP	PB-O3A	-2.39	1.56	1.59
8	W	2001	ANP	PG-N3B	2.34	1.69	1.63
8	W	2001	ANP	PB-O1B	2.26	1.49	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	2001	ANP	PB-O3A-PA	-3.94	118.75	132.62
8	W	2001	ANP	C5-C6-N6	2.32	123.88	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	W	2001	ANP	O4'-C4'-C5'-O5'
8	W	2001	ANP	C3'-C4'-C5'-O5'

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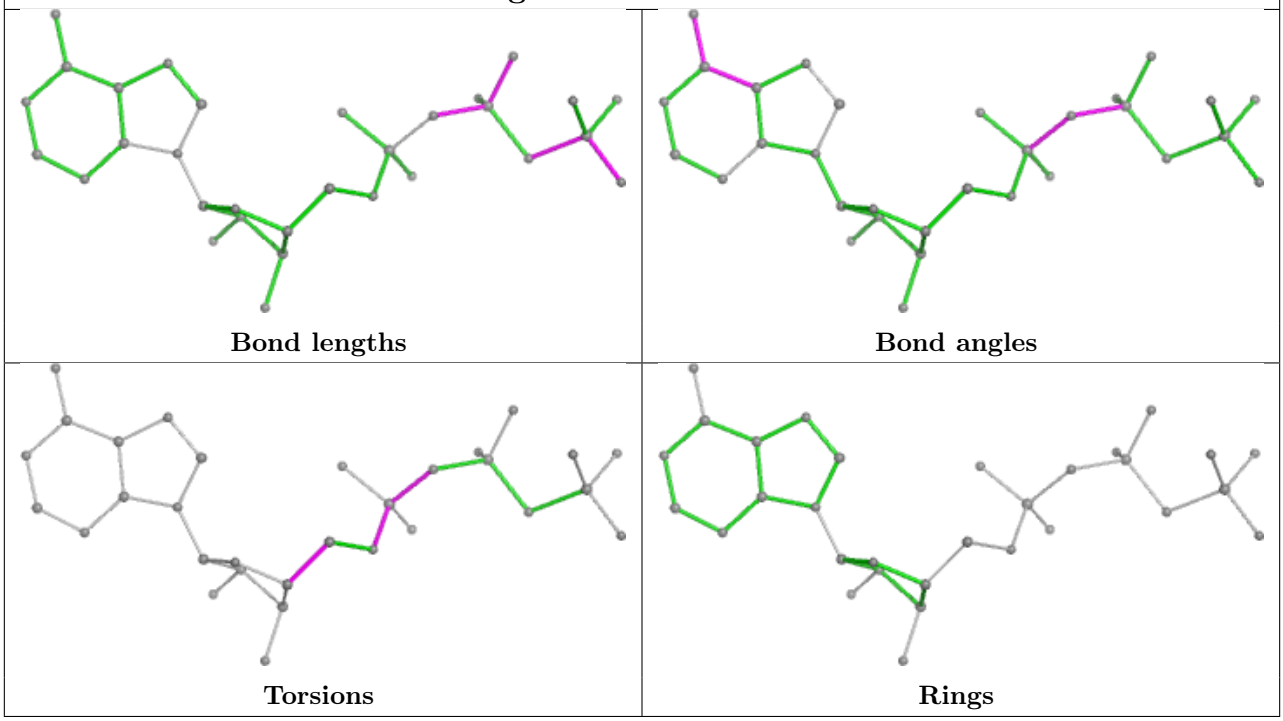
Mol	Chain	Res	Type	Atoms
8	W	2001	ANP	PB-O3A-PA-O2A
8	W	2001	ANP	C5'-O5'-PA-O1A

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 then 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.

Ligand ANP W 2001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	1200:ARG	C	1201:UNK	N	36.65

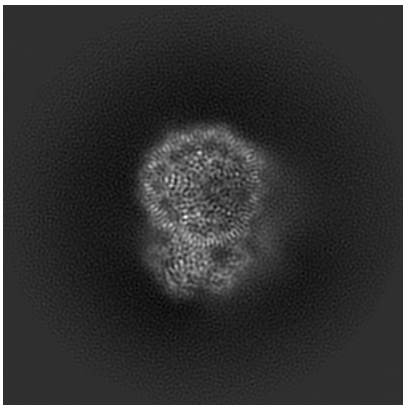
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10058. These allow visual inspection of the internal detail of the map and identification of artifacts.

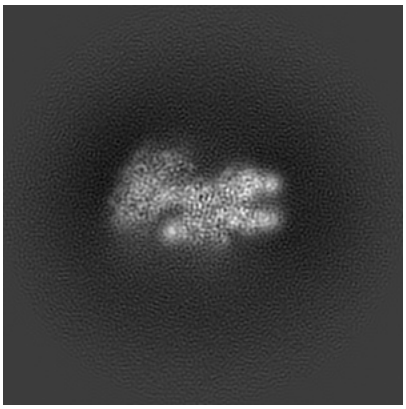
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

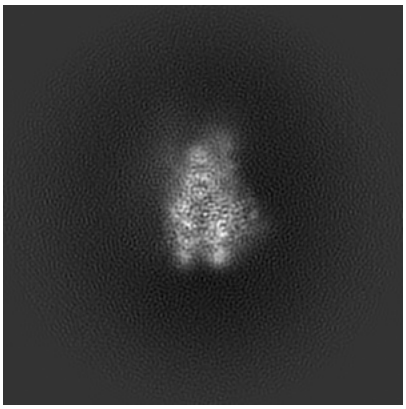
6.1.1 Primary map



X

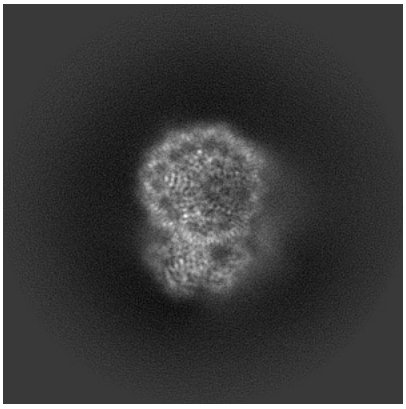


Y

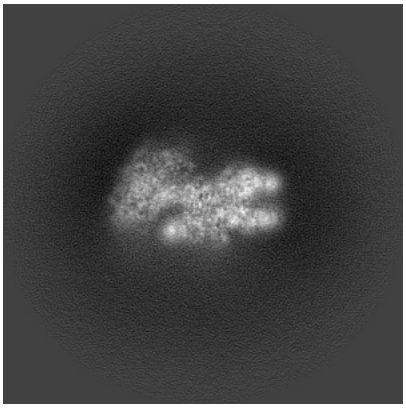


Z

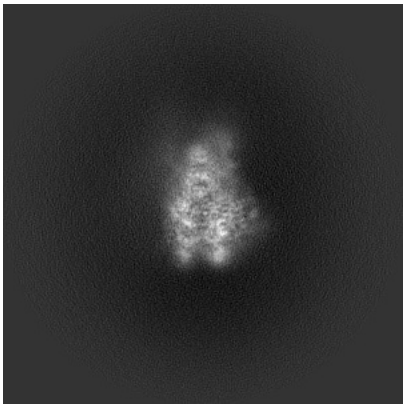
6.1.2 Raw map



X



Y

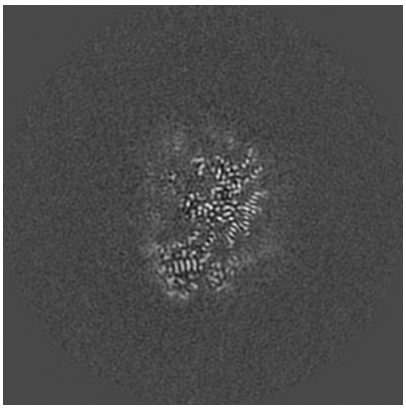


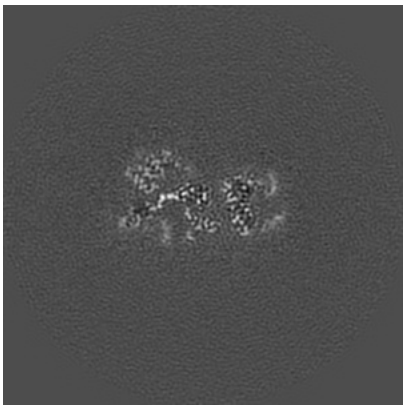
Z

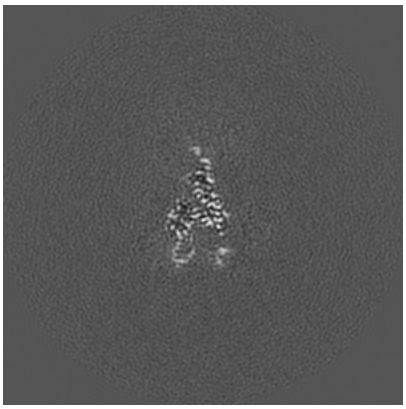
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

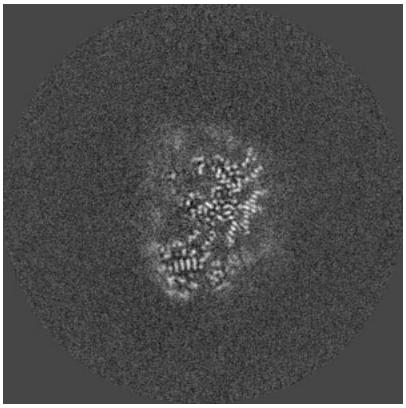
6.2.1 Primary map

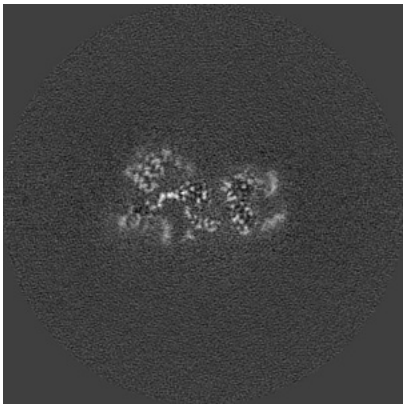

X Index: 150

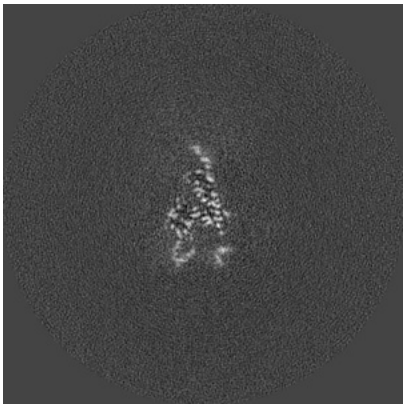

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

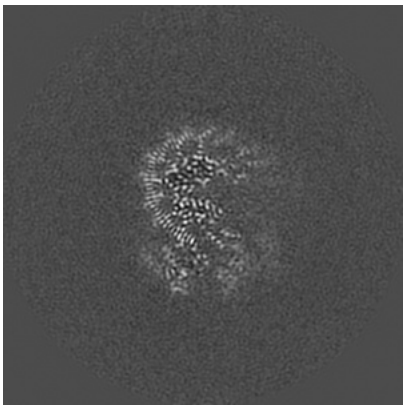

Y Index: 150

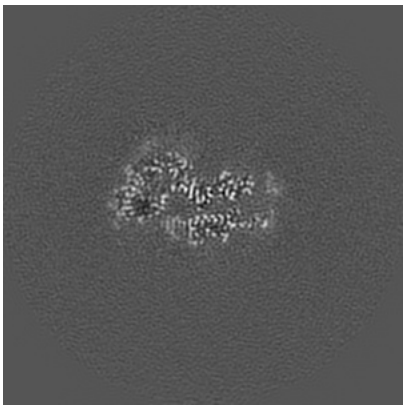

Z Index: 150

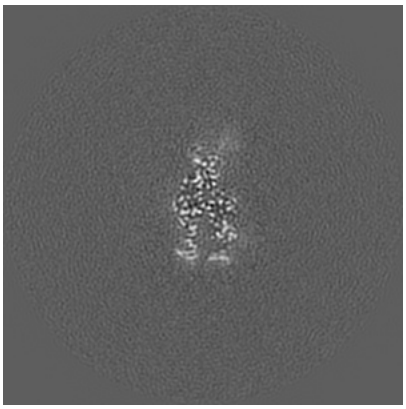
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

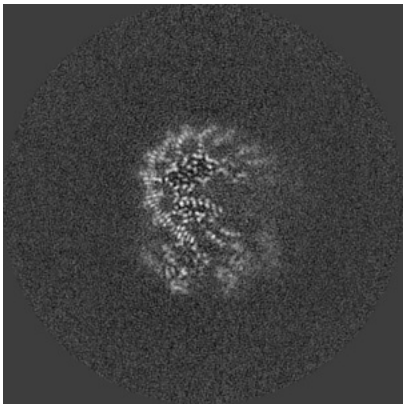
6.3.1 Primary map

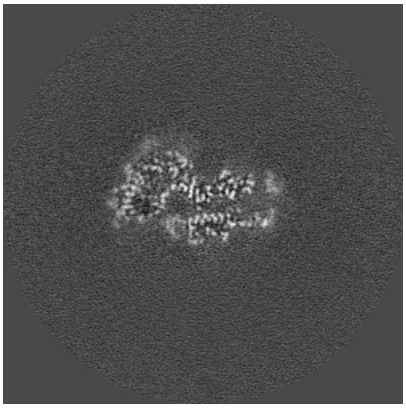

X Index: 161

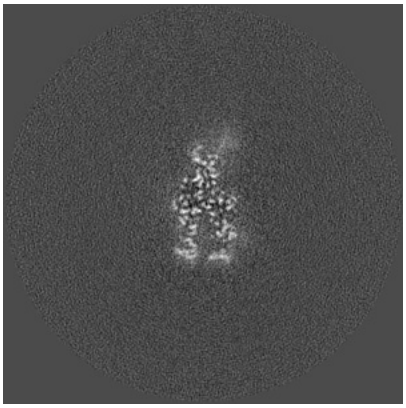

Y Index: 136


Z Index: 179

6.3.2 Raw map


X Index: 161

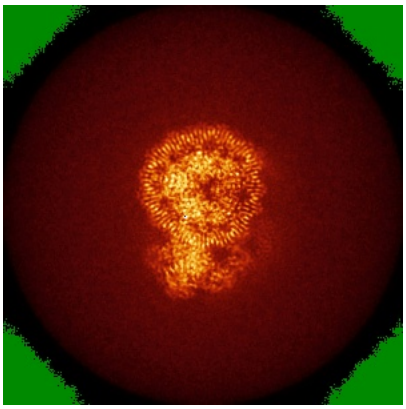

Y Index: 136

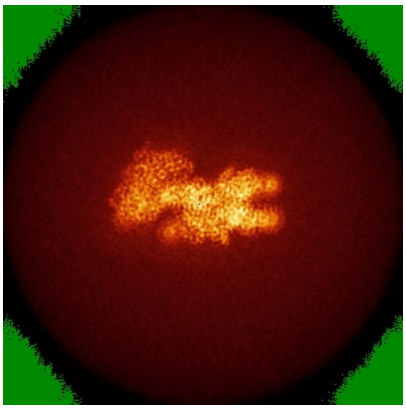

Z Index: 179

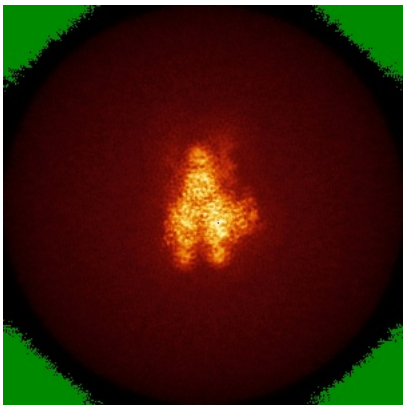
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

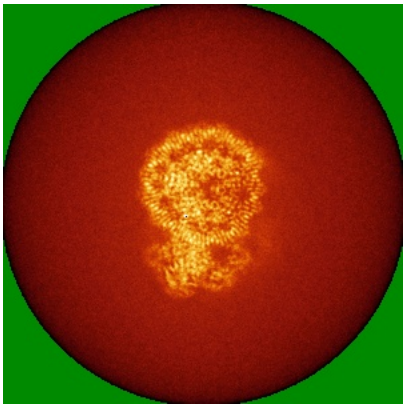
6.4.1 Primary map

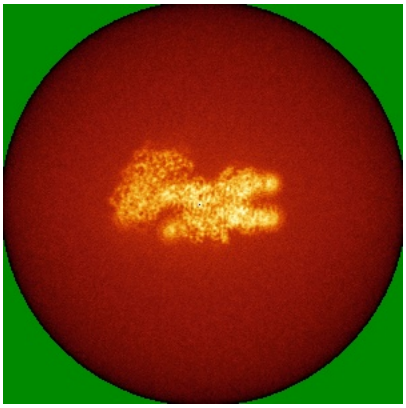

X

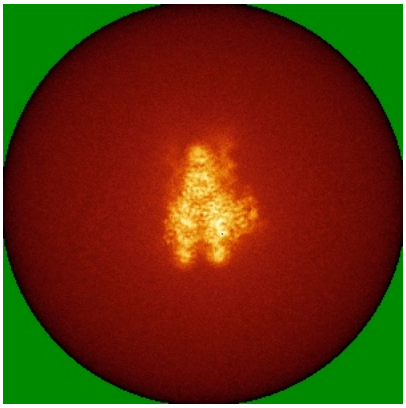

Y


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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. 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

X Y Z

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.

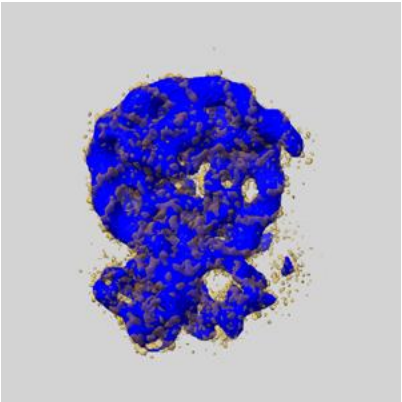
6.6 Mask visualisation (i)

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

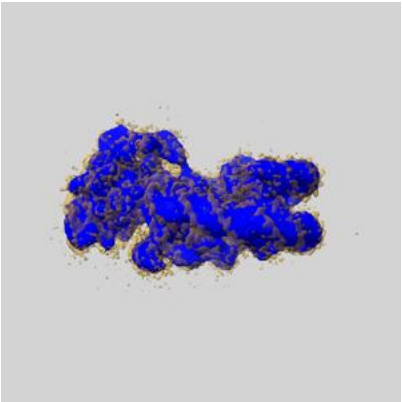
A mask typically either:

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

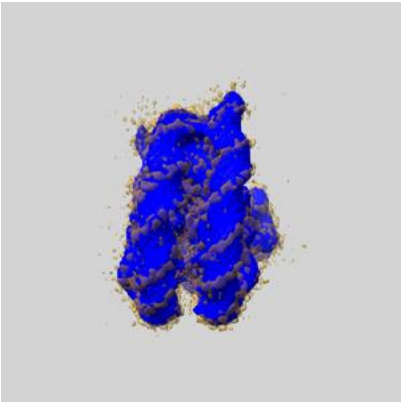
6.6.1 emd_10058_msk_1.map (i)



X



Y

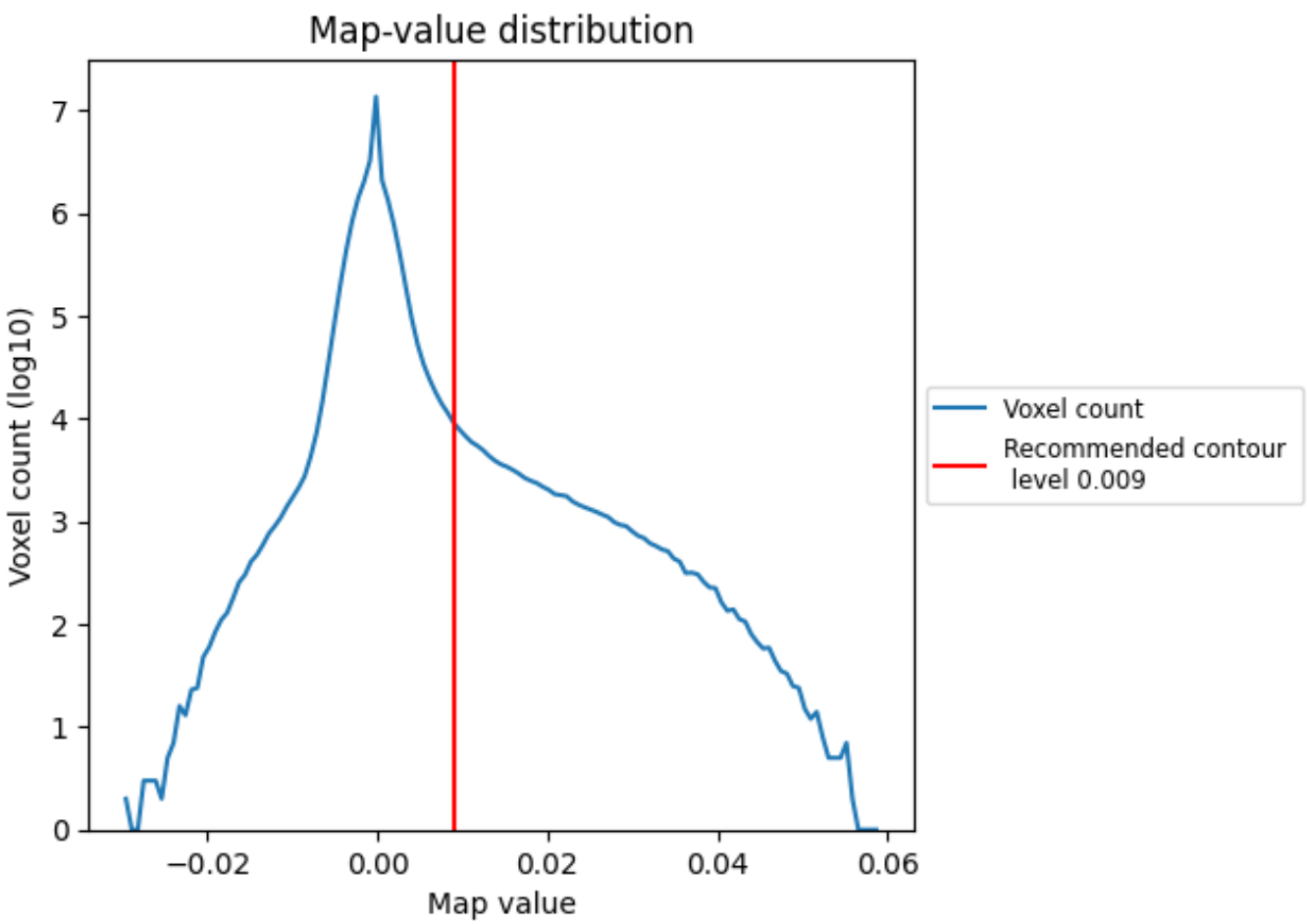


Z

7 Map analysis (i)

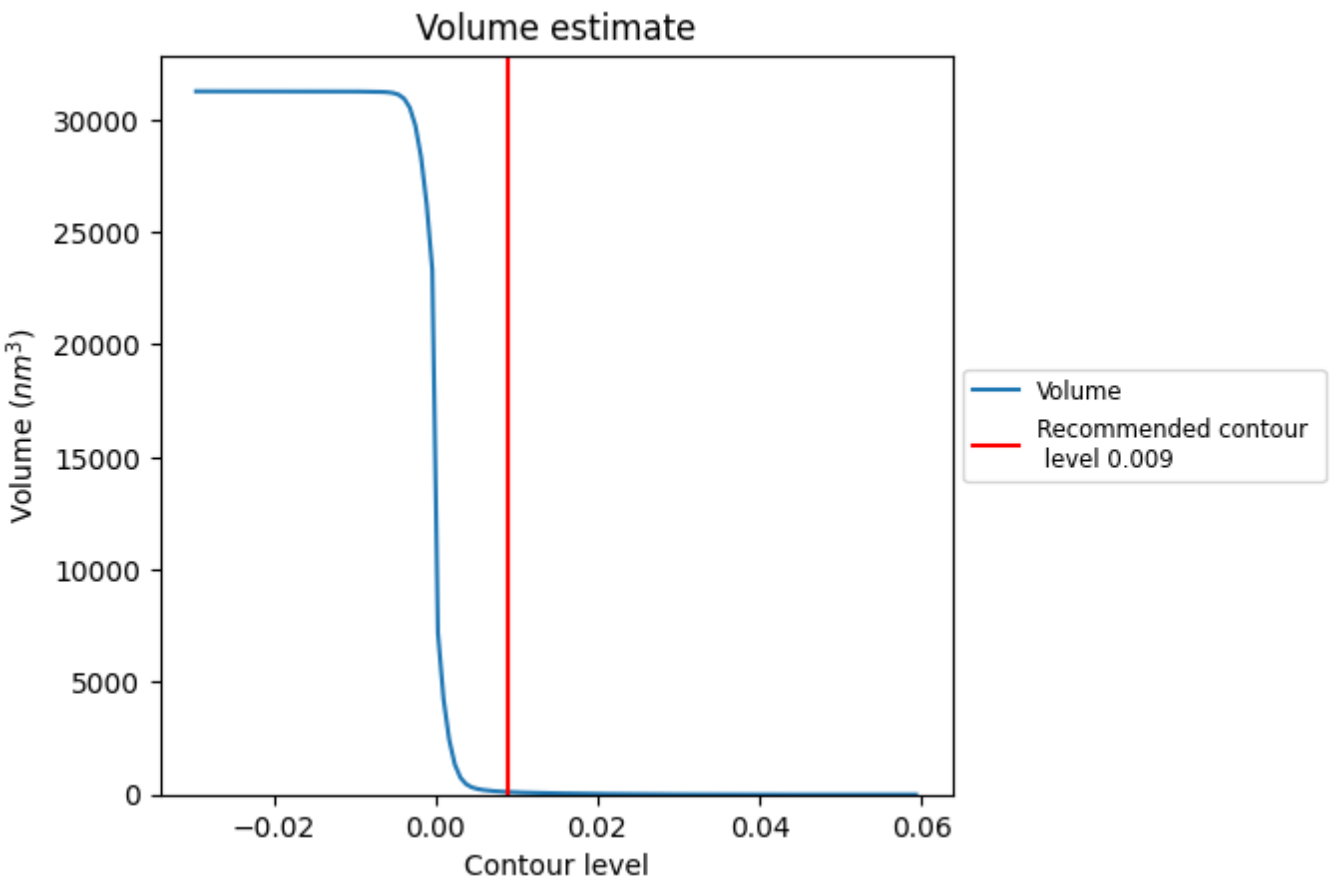
This section contains the results of statistical analysis of the map.

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.

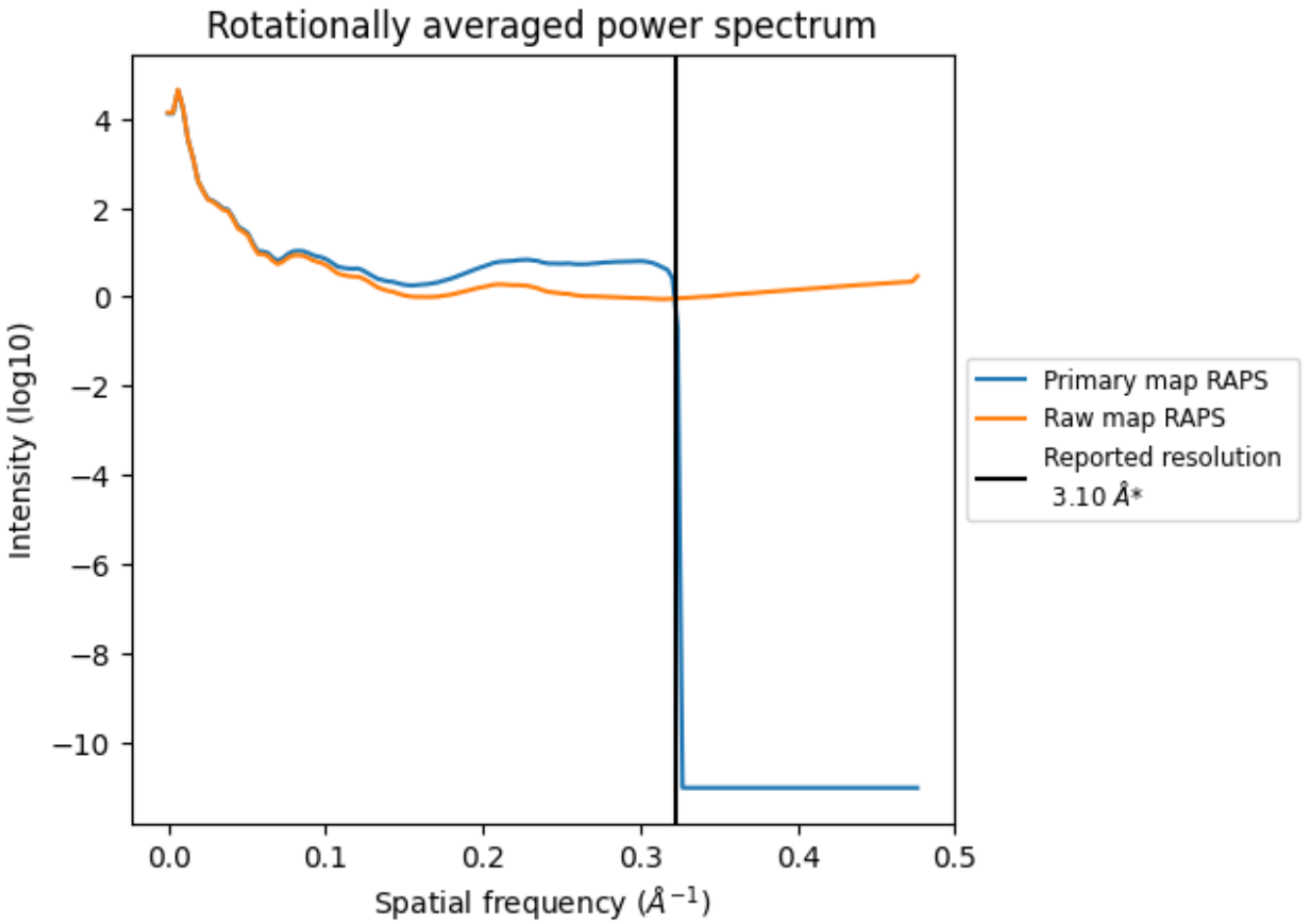
7.2 Volume estimate (i)



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 102 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)

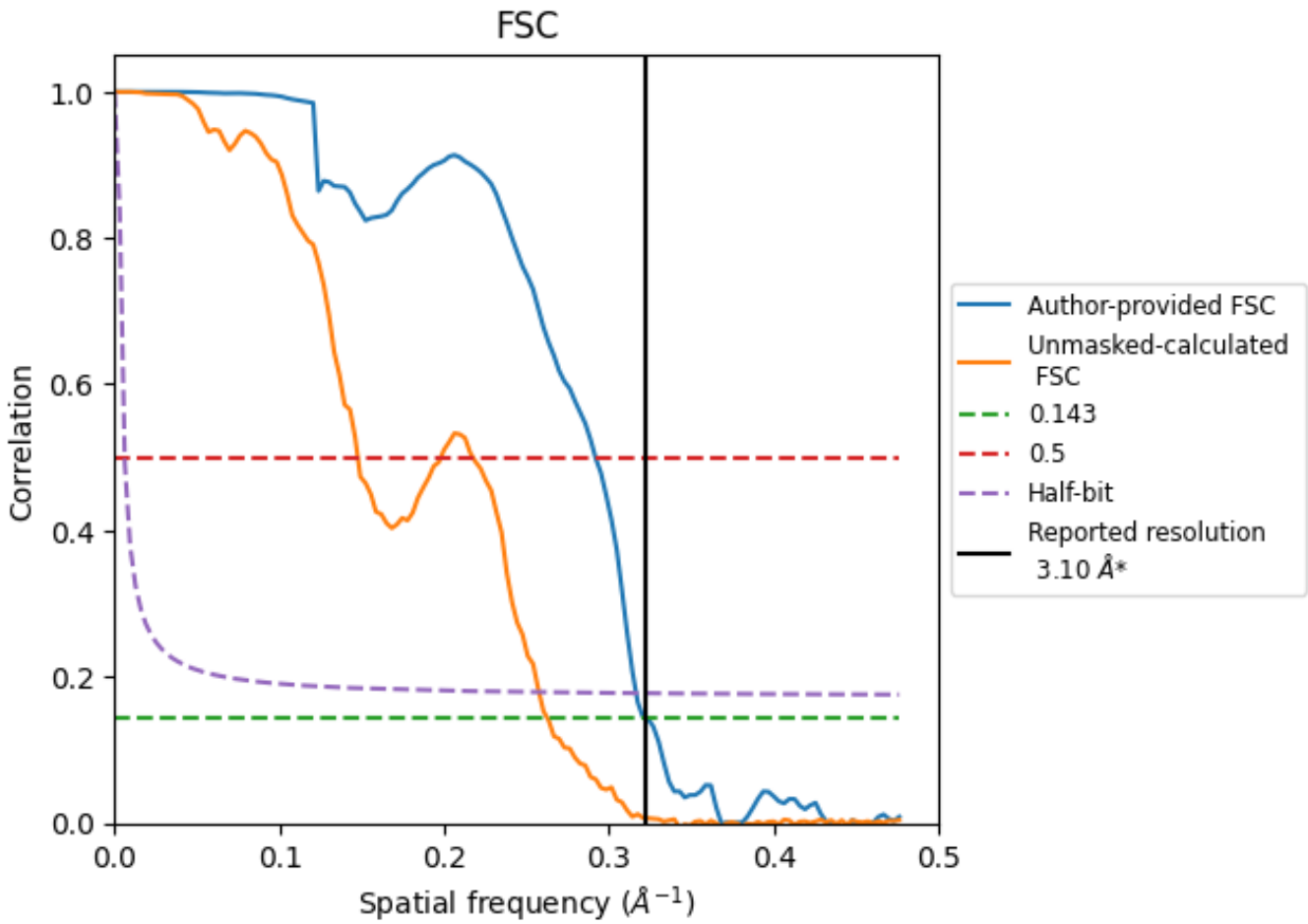


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

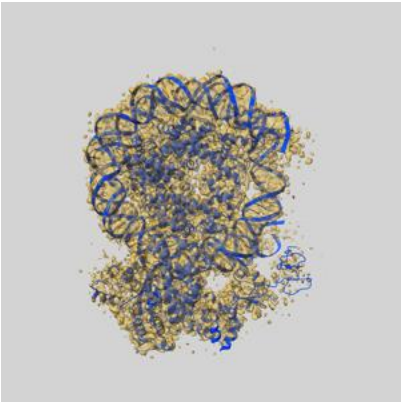
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.43	3.16
Unmasked-calculated*	3.81	6.77	3.88

*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 3.81 differs from the reported value 3.1 by more than 10 %

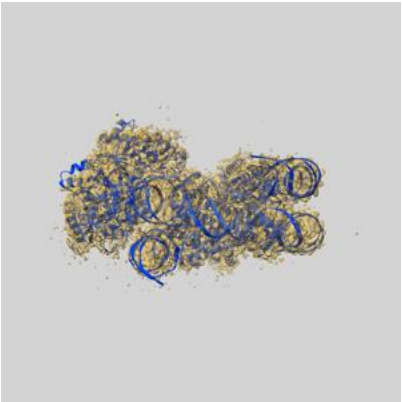
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10058 and PDB model 6RYR. Per-residue inclusion information can be found in section 3 on page 7.

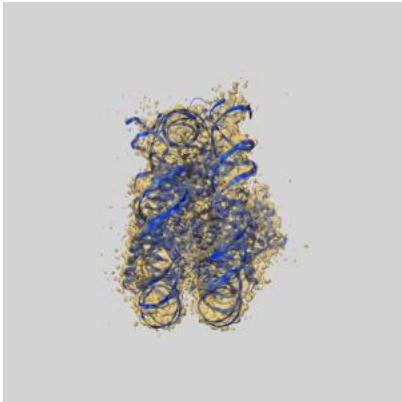
9.1 Map-model overlay (i)



X



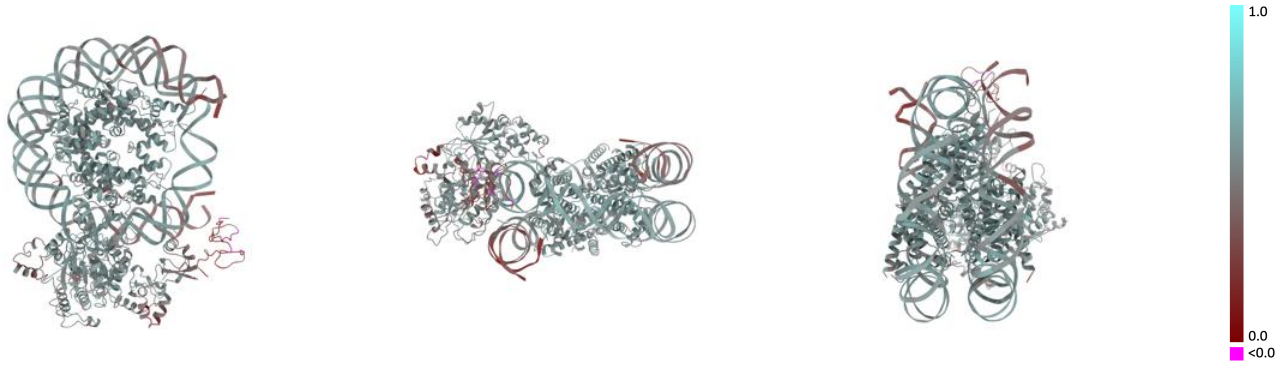
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

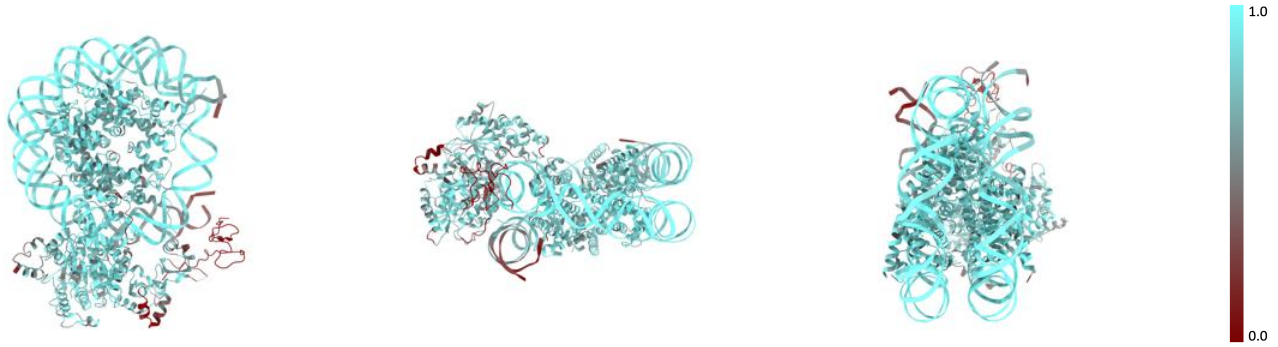
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

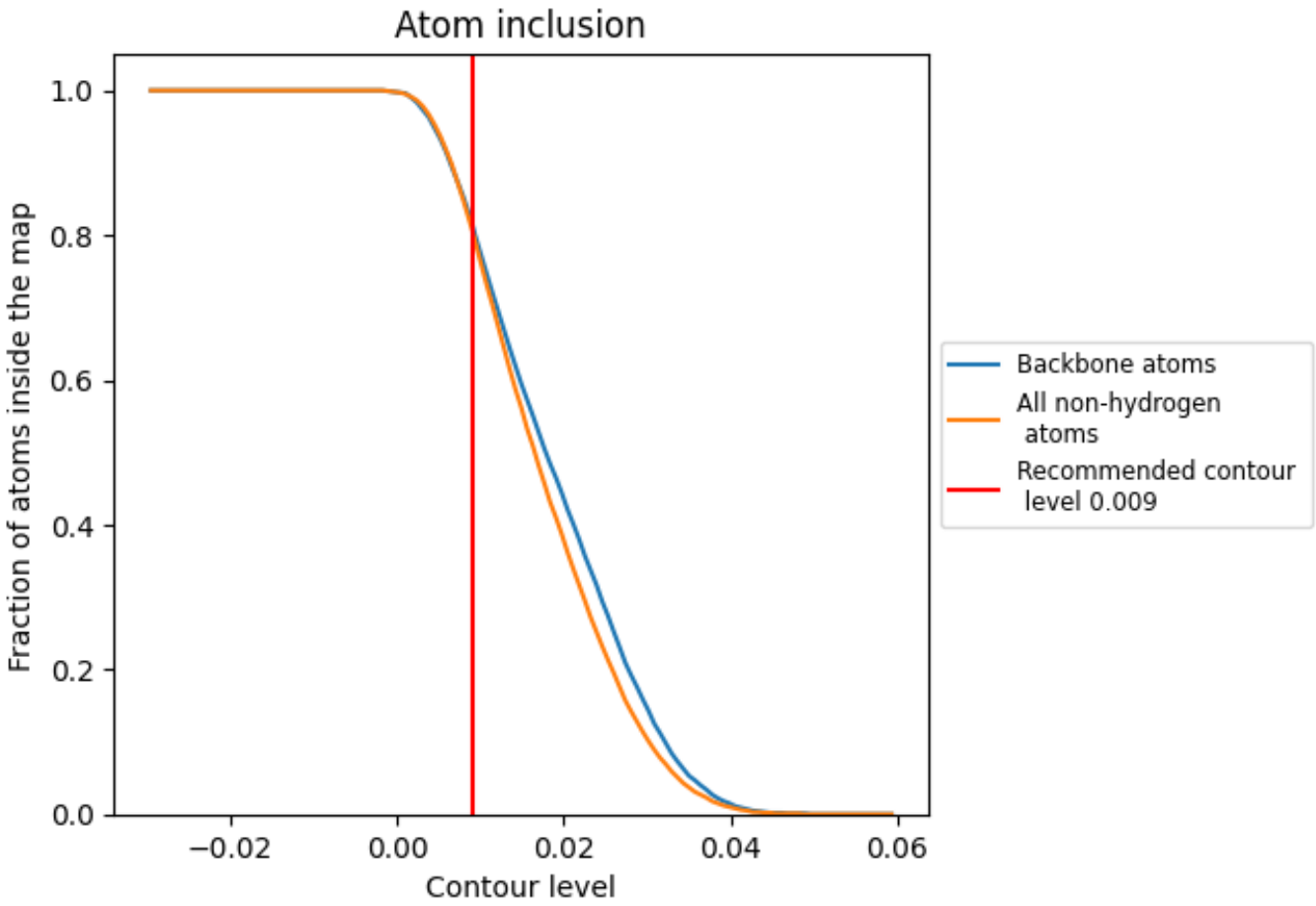
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.5200
A	0.8430	0.5630
B	0.8230	0.5710
C	0.8560	0.5670
D	0.8460	0.5450
E	0.8610	0.5690
F	0.8840	0.5750
G	0.8420	0.5670
H	0.8700	0.5590
I	0.8680	0.5110
J	0.8590	0.5120
W	0.6970	0.4840