wwPDB EM Validation Summary 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 wwPDB EM Validation Summary 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 ⓘ 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:

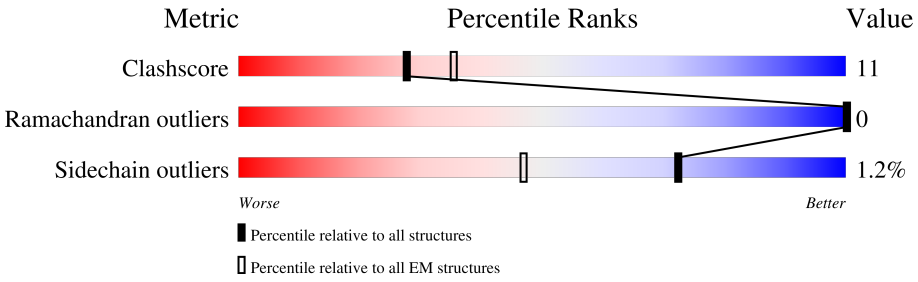
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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 >=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	746	7% 59% 10% 31%
2	B	1618	28% 35% 12% 53%

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
1	A	516	Total	C	N	O	S	0	0
			4192	2676	742	750	24		

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
2	B	759	Total	C	N	O	S	0	0
			6125	3930	1029	1124	42		

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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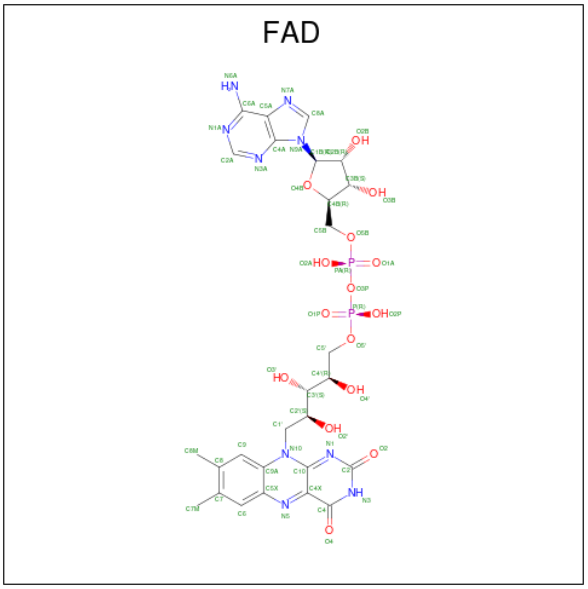
Chain	Residue	Modelled	Actual	Comment	Reference
B	1401	GLY	-	linker	UNP P49021
B	1402	GLY	-	linker	UNP P49021
B	1403	SER	-	linker	UNP P49021
B	1404	GLY	-	linker	UNP P49021
B	1405	MET	-	linker	UNP P49021
B	1434	ARG	GLU	conflict	UNP E5BBQ0
B	1583	PRO	-	expression tag	UNP E5BBQ0
B	1584	GLY	-	expression 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).



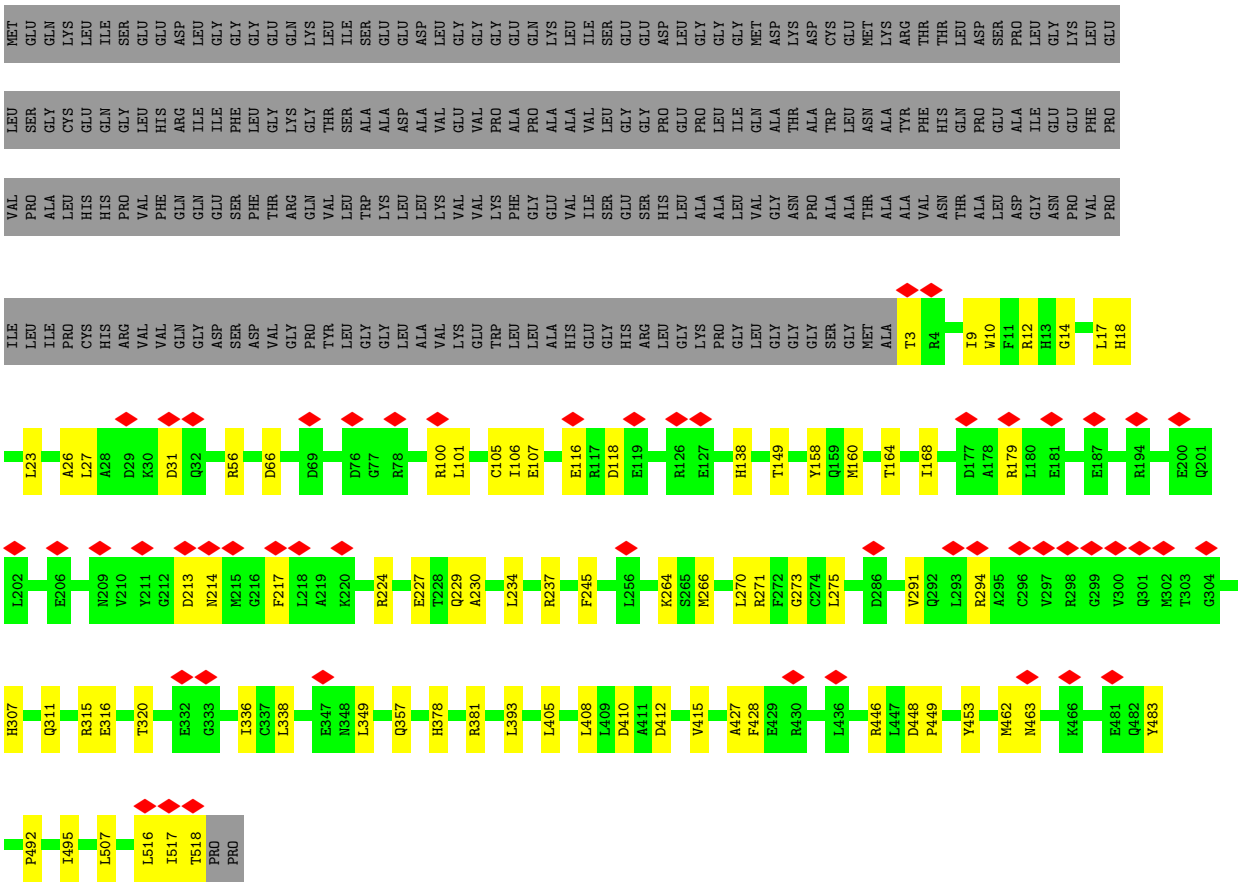
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	53	27	9	15	2	0

3 Residue-property plots (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.

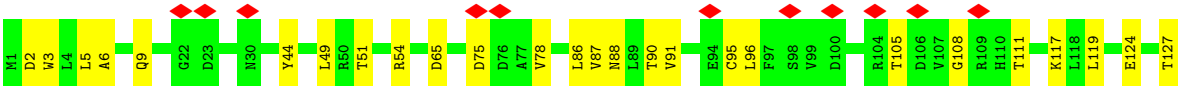
• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase,Cryptochrome-1 fusion

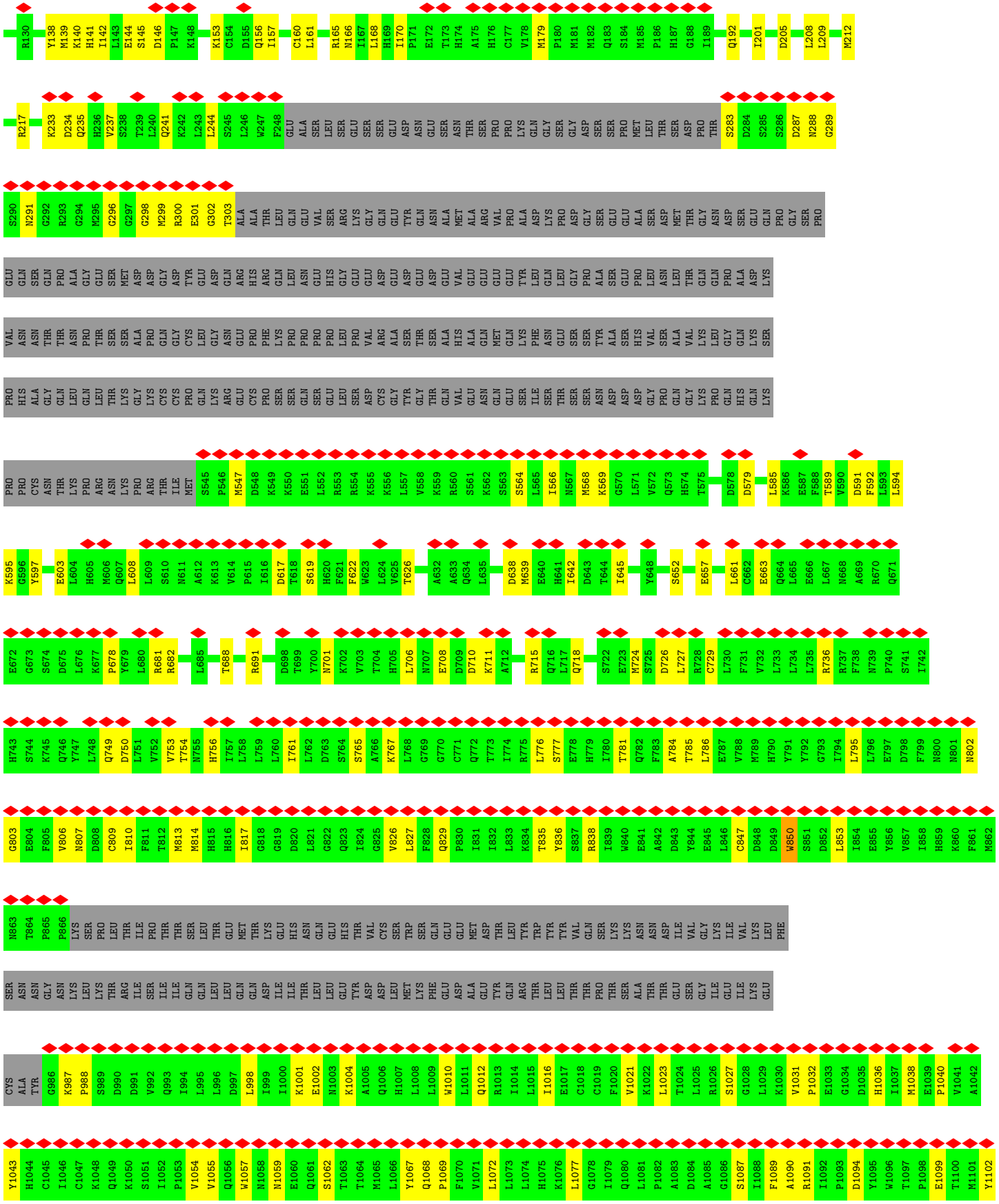
Chain A:

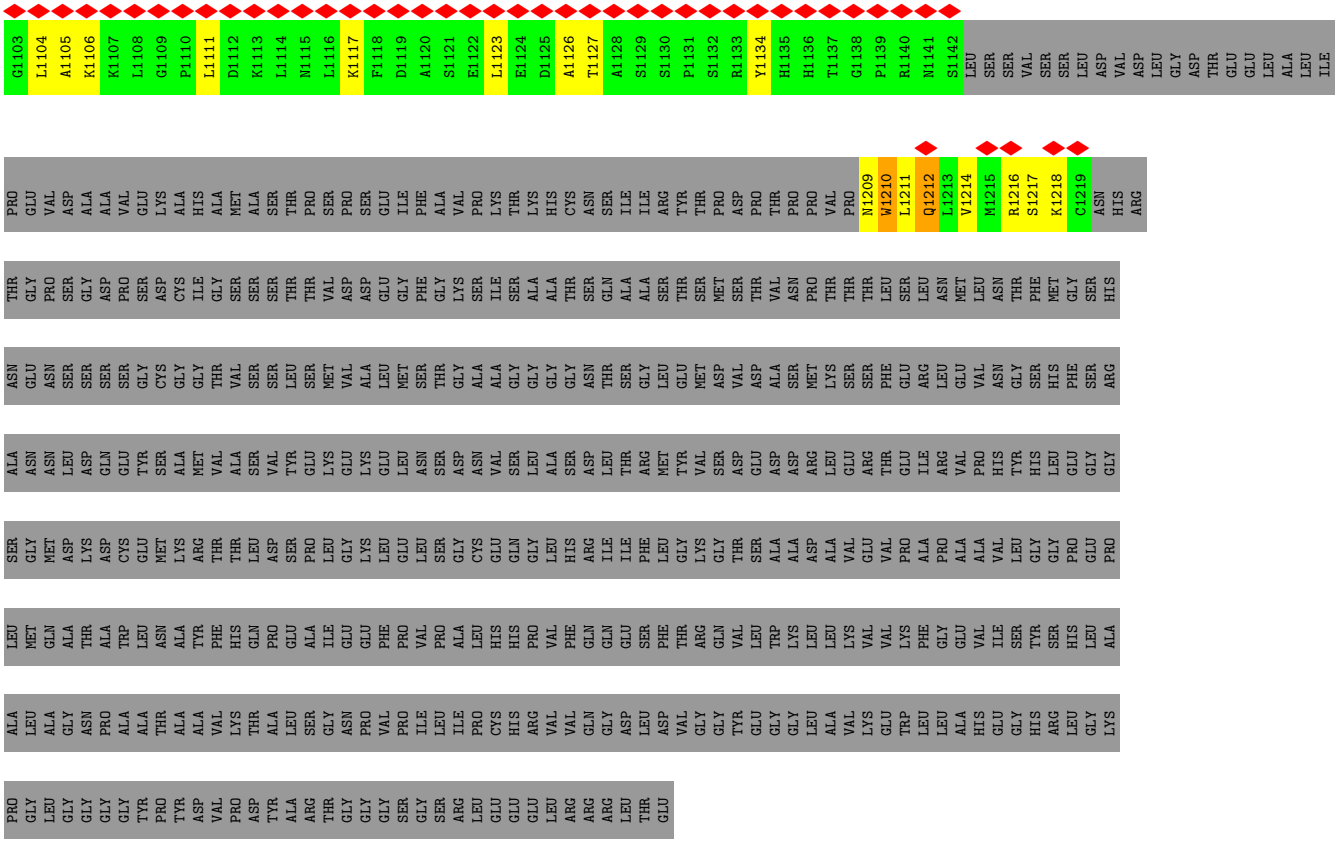


• Molecule 2: Protein timeless,Methylated-DNA--protein-cysteine methyltransferase fusion

Chain B:




R130 Y138 M139 K140 H141 I142 L143 E144 S145 D146 P147 K148 K153 C154 D155 Q156 I157 C160 L161 R165 N166 I167 L168 H169 I170 P171 E172 T173 H174 A175 H176 C177 V178 M179 P180 M181 M182 Q183 S184 M185 P186 H187 G188 I189 Q192 I201 D205 L208 L209 M212
R217 K233 D234 Q235 H236 V237 S238 T239 L240 Q241 K242 L243 L244 S245 L246 W247 F248 GLU ALA SER LEU SER GLU SER SER GLU ASP ASN GLU SER ASN THR SER PRO PRO LYS GLN GLY SER GLY ASP SER SER PRO MET LEU THR SER ASP PRO THR S283 D284 S285 S286 D287 N288 G289
S290 N291 G292 R293 G294 M295 G296 G297 G298 M299 R300 E301 G302 T303 ALA ALA THR LEU GLN GLU VAL SER ARG LYS GLY GLN GLU TYR GLN ASN ALA MET ALA ARG VAL PRO ALA ASP LYS PRO ASP GLY SER GLU GLU ALA SER ASP MET THR GLY ASN ASP SER GLU GLN PRO GLY SER PRO
GLU GLN SER GLN PRO ALA GLY GLU SER MET ASP ASP GLY ASP TYR GLU ASP GLN ARG HIS ARG GLN LEU ASN GLU HIS GLY GLU GLU ASP GLU ASP GLU ASP GLU VAL GLU GLU GLU GLU TYR LEU GLN LEU GLY PRO ALA SER GLU PRO LEU ASN LEU THR GLN GLN PRO ALA ASP LYS
VAL ASN ASN THR THR ASN PRO THR SER SER ALA PRO GLN GLY CYS LEU GLY ASN GLU PRO PHE LYS PRO PRO PRO PRO LEU PRO VAL ARG ALA SER THR SER ALA HIS ALA GLN MET GLN LYS PHE ASN GLU SER SER TYR ALA SER HIS VAL SER ALA VAL LYS LEU GLY GLN LYS SER
PRO HIS ALA GLY GLN LEU GLN LEU THR LYS GLY LYS CYS CYS PRO GLN LYS ARG GLU CYS PRO SER SER GLN SER GLU LEU SER ASP CYS GLY TYR GLY THR GLN VAL GLU ASN GLN GLU SER ILE SER THR THR SER SER ASN ASP ASP GLY PRO GLN GLY LYS PRO GLN HIS GLN LYS
PRO PRO CYS ASN THR LYS PRO ARG ASN LYS PRO ARG THR ILE MET S545 P546 M547 D548 K549 K550 E551 L552 R553 R554 K555 K556 L557 V558 K559 R560 S561 K562 S563 S564 L565 I566 N567 M568 K569 G570 L571 V572 Q573 H574 T575 D578 D579 L585 K586 E587 F588 T589 V590 D591 F592 L593 L594
K595 G596 Y597 E603 L604 H605 M606 Q607 L608 L609 S610 N611 A612 K613 V614 P615 I616 D617 T618 S619 H620 F621 F622 W623 L624 V625 T626 A632 A633 Q634 L635 D638 M639 E640 H641 I642 D643 T644 I645 Y648 S652 E657 L661 C662 E663 Q664 L665 E666 L667 N668 A669 R670 Q671
E672 G673 S674 D675 L676 K677 P678 Y679 L680 R681 R682 L685 T688 R691 D698 T699 Y700 N701 K702 V703 T704 H705 L706 N707 E708 D709 D710 K711 A712 R715 Q716 L717 Q718 S722 E723 M724 S725 D726 L727 R728 C729 L730 F731 V732 L733 L734 L735 R736 R737 F738 N739 P740 S741 I742
H743 S744 K745 Q746 Y747 L748 Q749 D750 L751 V752 V753 T754 N755 H756 I757 L758 L759 L760 I761 L762 D763 S764 S765 A766 K767 L768 G769 G770 C771 Q772 T773 I774 R775 L776 S777 E778 H779 I780 T781 Q782 F783 A784 T785 L786 E787 V788 M789 H790 Y791 Y792 G793 I794 L795 L796 E797 D798 F799 N800 N801 N802
G803 E804 F805 V806 N807 D808 C809 I810 F811 T812 M813 M814 H815 H816 I817 G818 G819 D820 L821 G822 Q823 I824 G825 V826 L827 F828 Q829 P830 I831 I832 L833 K834 T835 Y836 S837 R838 I839 W840 E841 A842 D843 Y844 E845 L846 C847 D848 D849 W850 S851 D852 L853 I854 E855 Y856 V857 I858 H859 K860 F861 M862
N863 T864 P865 P866 LYS SER PRO LEU THR ILE PRO THR THR SER LEU THR GLU MET THR LYS GLU HIS ASN GLN GLU HIS THR VAL CYS SER TRP SER GLN GLU GLU MET ASP THR LEU TYR TRP TYR TYR VAL GLN SER LYS LYS ASN ASN ASP ILE VAL GLY LYS ILE VAL LYS LEU PHE
SER ASN ASN GLY ASN LYS LEU LYS THR ARG ILE SER ILE ILE GLN GLN LEU LEU GLN GLN ASP ILE ILE THR LEU LEU GLU LEU LEU GLU TYR ASP ASP LEU MET LYS PHE GLU ASP ALA GLU TYR GLN ARG THR LEU LEU LEU THR THR PRO THR SER ALA THR THR GLU SER GLY ILE GLU ILE LYS GLU
CYS ALA TYR G986 K987 P988 S989 D990 D991 V992 Q993 I994 L995 L996 D997 L998 I999 I1000 K1001 E1002 N1003 K1004 A1005 Q1006 H1007 L1008 L1009 W1010 L1011 Q1012 R1013 I1014 L1015 I1016 E1017 C1018 C1019 F1020 V1021 K1022 L1023 T1024 L1025 R1026 S1027 G1028 L1029 K1030 V1031 P1032 E1033 G1034 D1035 H1036 I1037 M1038 E1039 P1040 V1041 A1042
Y1043 H1044 C1045 I1046 C1047 K1048 Q1049 K1050 S1051 I1052 P1053 V1054 V1055 Q1056 W1057 N1058 N1059 E1060 Q1061 S1062 T1063 T1064 M1065 L1066 Y1067 Q1068 P1069 F1070 V1071 L1072 L1073 L1074 H1075 K1076 L1077 G1078 I1079 Q1080 L1081 P1082 A1083 D1084 A1085 G1086 S1087 I1088 F1089 A1090 R1091 I1092 P1093 D1094 Y1095 W1096 T1097 P1098 E1099 T1100 M1101 Y1102


G1103 L1104 A1105 K1106 K1107 L1108 G1109 P1110 L1111 D1112 K1113 L1114 N1115 L1116 K1117 F1118 D1119 A1120 S1121 E1122 L1123 E1124 D1125 A1126 T1127 A1128 S1129 S1130 P1131 S1132 R1133 Y1134 H1135 H1136 T1137 G1138 P1139 R1140 N1141 S1142 LEU SER SER VAL SER SER LEU ASP VAL ASP LEU GLY ASP THR GLU GLU LEU ALA LEU ILE
PRO GLU VAL ASP ALA ALA VAL GLU LYS ALA HIS ALA MET ALA SER THR PRO SER PRO SER GLU ILE PHE ALA VAL PRO LYS THR LYS HIS CYS ASN SER ILE ARG TYR THR PRO ASP PRO THR PRO VAL PRO N1209 W1210 L1211 Q1212 L1213 V1214 M1215 R1216 S1217 K1218 G1219 ASN HIS ARG
THR GLY PRO SER GLY ASP PRO SER ASP CYS ILE GLY SER SER SER THR THR VAL ASP ASP GLU GLY PHE GLY LYS SER ILE SER ALA ALA THR SER GLN ALA ALA SER THR SER MET SER THR VAL ASN PRO THR THR THR LEU SER LEU ASN MET LEU ASN THR PHE MET GLY SER HIS
ASN GLU ASN SER SER SER SER GLY CYS GLY GLY THR VAL SER SER LEU SER MET VAL ALA LEU MET SER THR GLY ALA ALA GLY GLY GLY GLY ASN THR SER GLY LEU GLU MET ASP VAL ASP ALA SER MET LYS SER SER PHE GLU ARG LEU GLU VAL ASN GLY SER HIS PHE SER ARG
ALA ASN ASN LEU ASP GLN GLU TYR SER ALA MET VAL ALA SER VAL TYR GLU LYS GLU LYS GLU LEU LEU ASN SER ASP ASN VAL SER LEU ALA SER ASP LEU THR ARG MET TYR VAL SER ASP GLU ASP ASP ARG LEU GLU GLU ARG THR GLU ILE ARG VAL PRO HIS TYR HIS LEU GLU GLY GLY
SER GLY MET ASP LYS ASP CYS GLU MET LYS ARG THR THR LEU ASP SER PRO LEU GLY LYS LEU GLU LEU SER GLY CYS GLU GLN GLY LEU HIS ARG ILE ILE PHE LEU GLY LYS GLY THR SER ALA ALA ASP ALA VAL GLU VAL PRO ALA PRO ALA ALA VAL LEU LEU GLY GLY PRO GLU PRO
LEU MET GLN ALA THR ALA TRP LEU ASN ALA TYR PHE HIS GLN PRO GLU ALA ILE GLU GLU PHE PRO VAL PRO ALA LEU HIS HIS PRO VAL PHE GLN GLN GLU SER PHE THR ARG GLN VAL LEU TRP LYS LEU LEU LYS VAL VAL LYS PHE GLY GLU VAL ILE SER TYR SER HIS LEU ALA
ALA LEU ALA GLY ASN PRO ALA ALA THR ALA VAL LYS THR ALA LEU SER GLY ASN PRO VAL PRO ILE LEU ILE PRO CYS HIS ARG VAL VAL GLN GLY ASP LEU ASP VAL GLY GLY TYR GLU GLY GLY LEU ALA VAL LYS GLU TRP LEU LEU HIS GLU GLY HIS ARG LEU GLY LYS
PRO GLY LEU GLY GLY GLY TYR PRO TYR ASP VAL PRO ASP TYR ALA ARG THR GLY GLY GLY SER GLY SER ARG LEU GLU GLU LEU ARG ARG ARG LEU THR GLU

4 Experimental information (i)

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 ($e^-/Å^2$)	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

5.1 Standard geometry

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

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.

The worst 5 of 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

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

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	850	TRP
2	B	1036	HIS
2	B	1212	GLN
2	B	1134	TYR
2	B	1210	TRP

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

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 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'

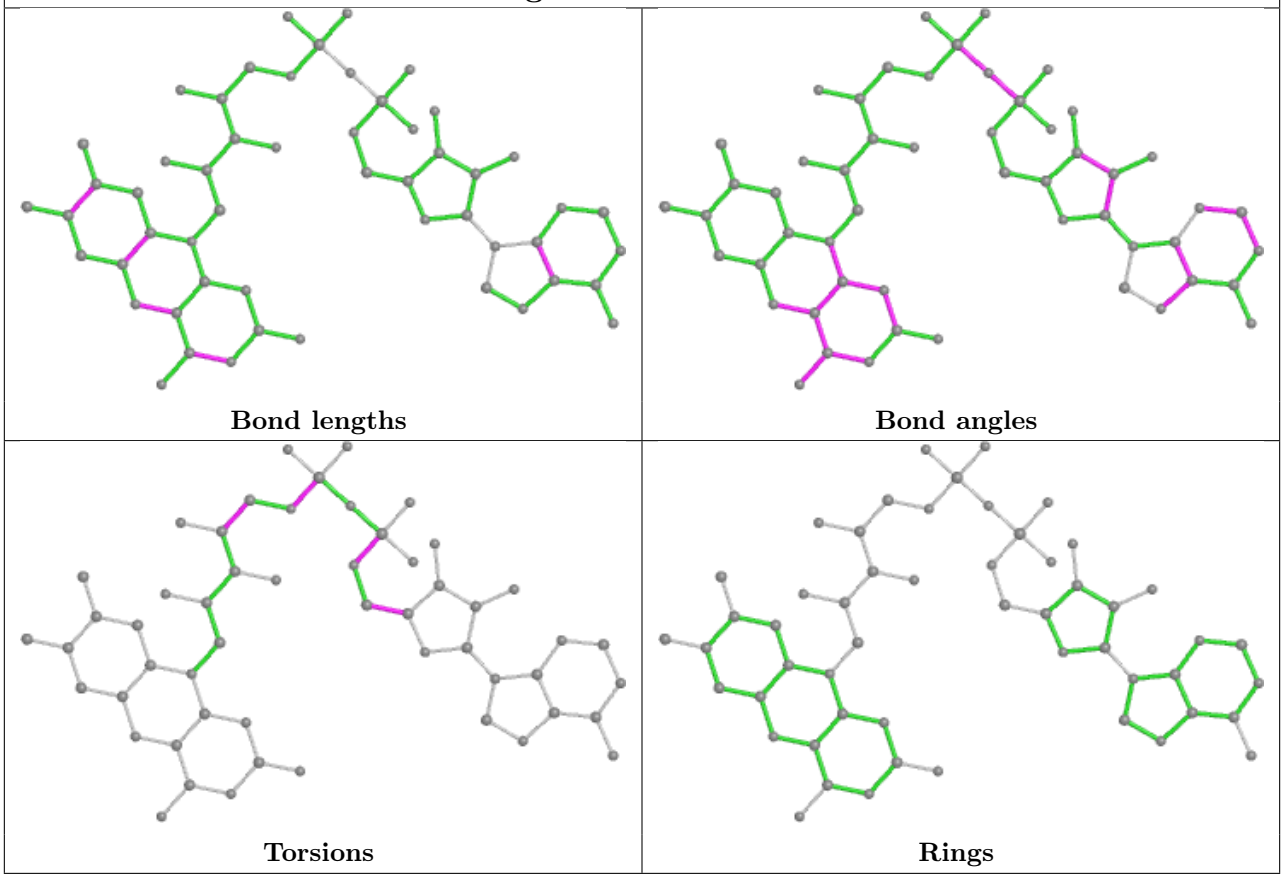
There are no ring outliers.

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 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 FAD A 602



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.

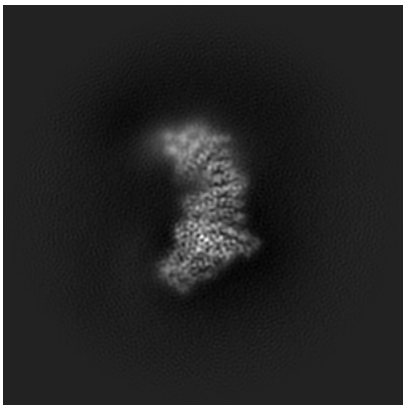
6 Map visualisation

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.

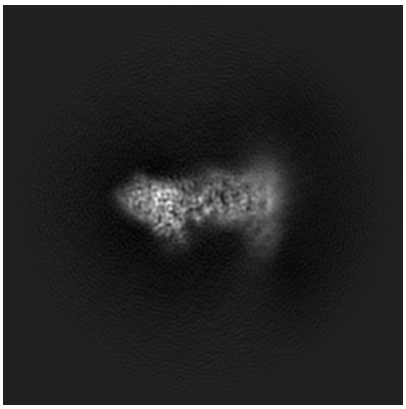
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

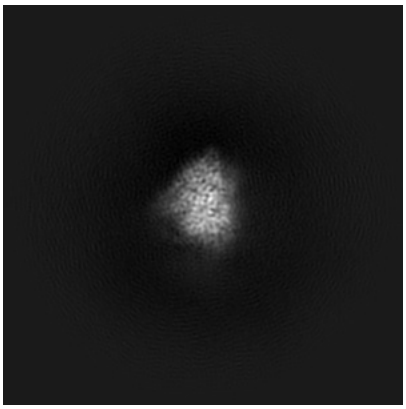
6.1.1 Primary map



X

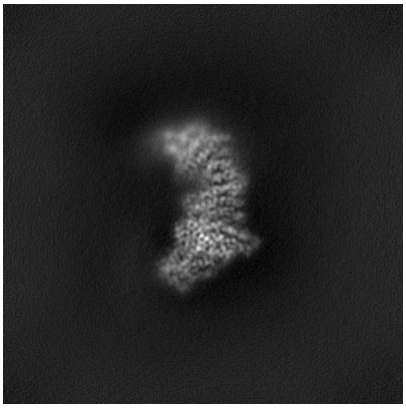


Y

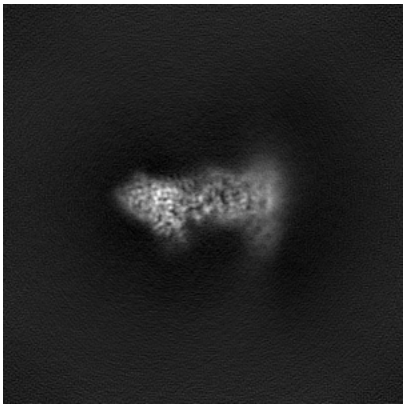


Z

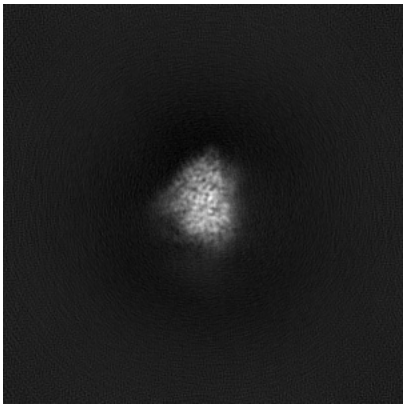
6.1.2 Raw map



X



Y

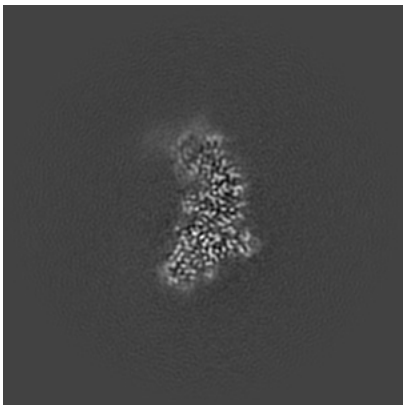


Z

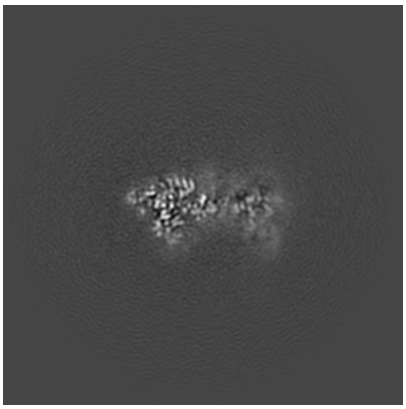
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

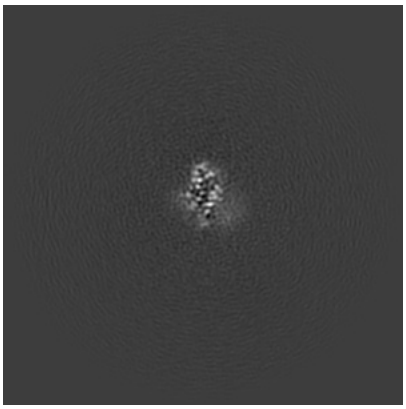
6.2.1 Primary map



X Index: 150

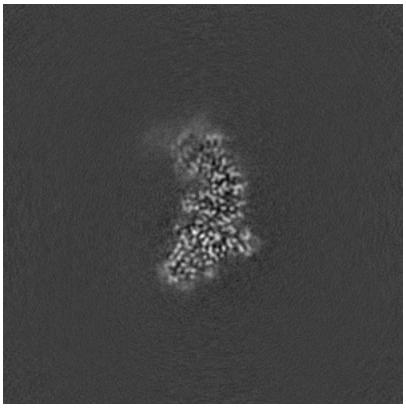


Y Index: 150

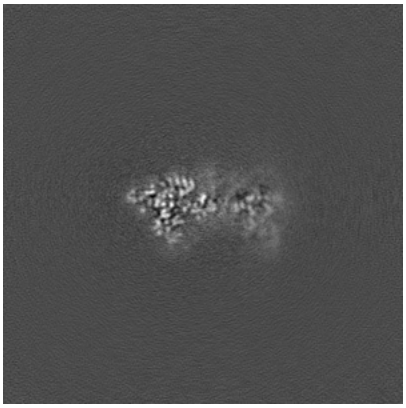


Z Index: 150

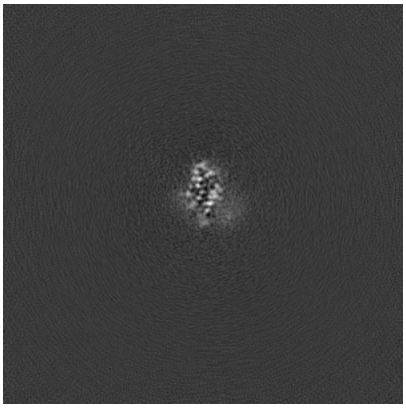
6.2.2 Raw map



X Index: 150



Y Index: 150

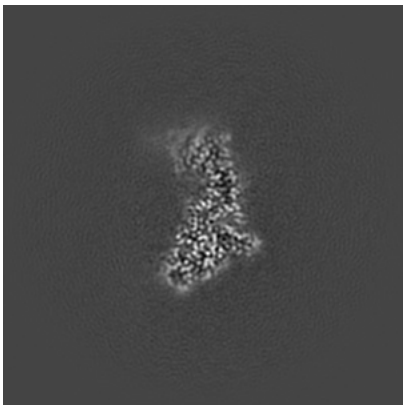


Z Index: 150

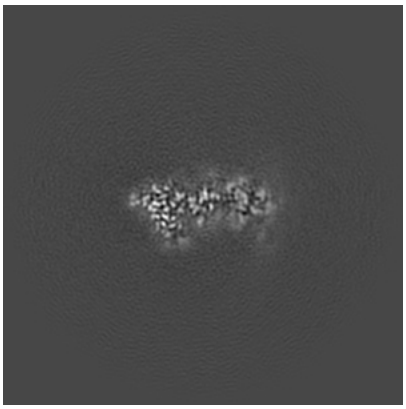
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

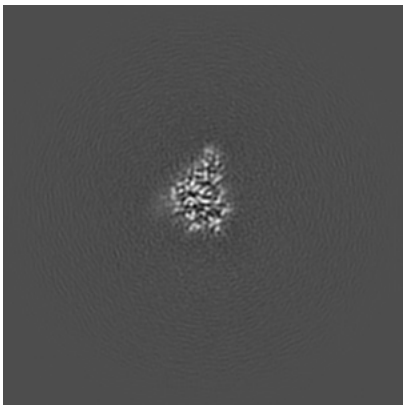
6.3.1 Primary map



X Index: 155

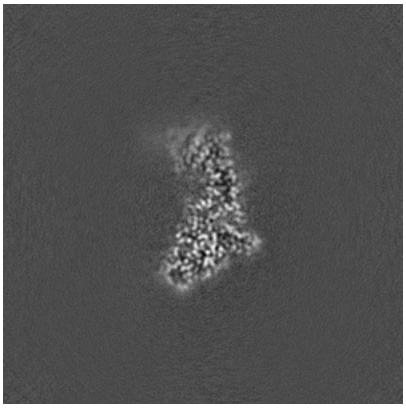


Y Index: 155

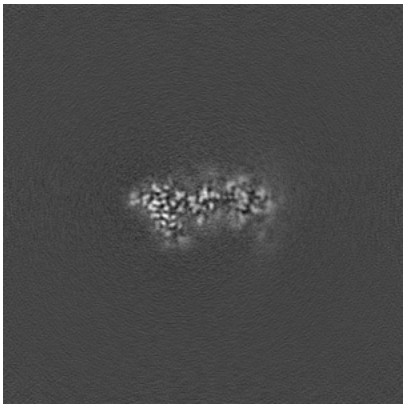


Z Index: 123

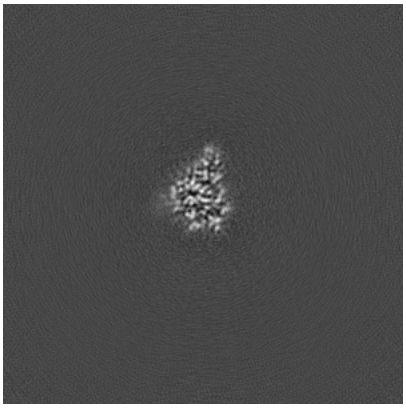
6.3.2 Raw map



X Index: 155



Y Index: 155

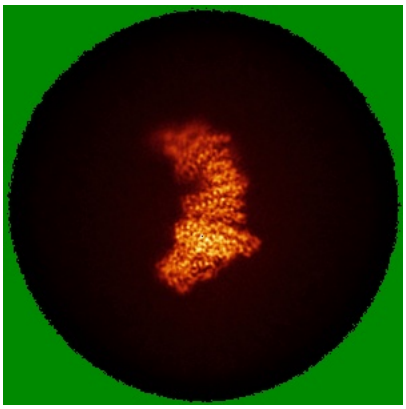


Z Index: 123

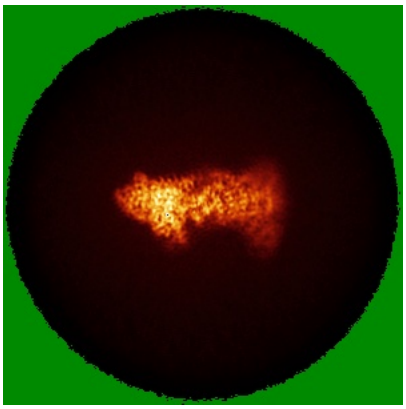
The images above show the largest variance slices of the map in three orthogonal directions.

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

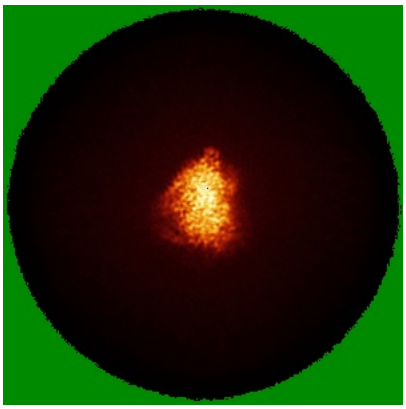
6.4.1 Primary map



X

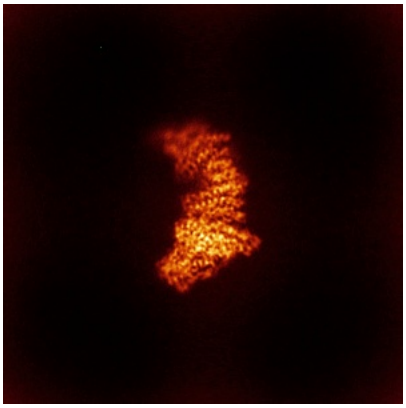


Y

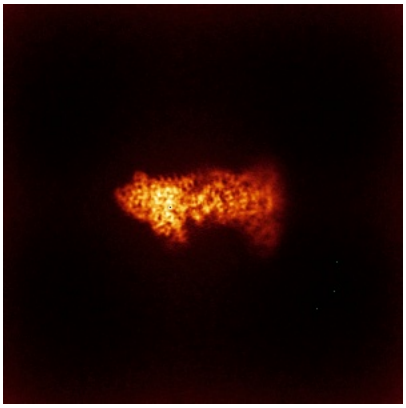


Z

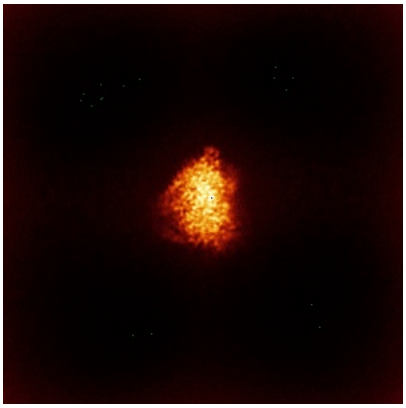
6.4.2 Raw map



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 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

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.

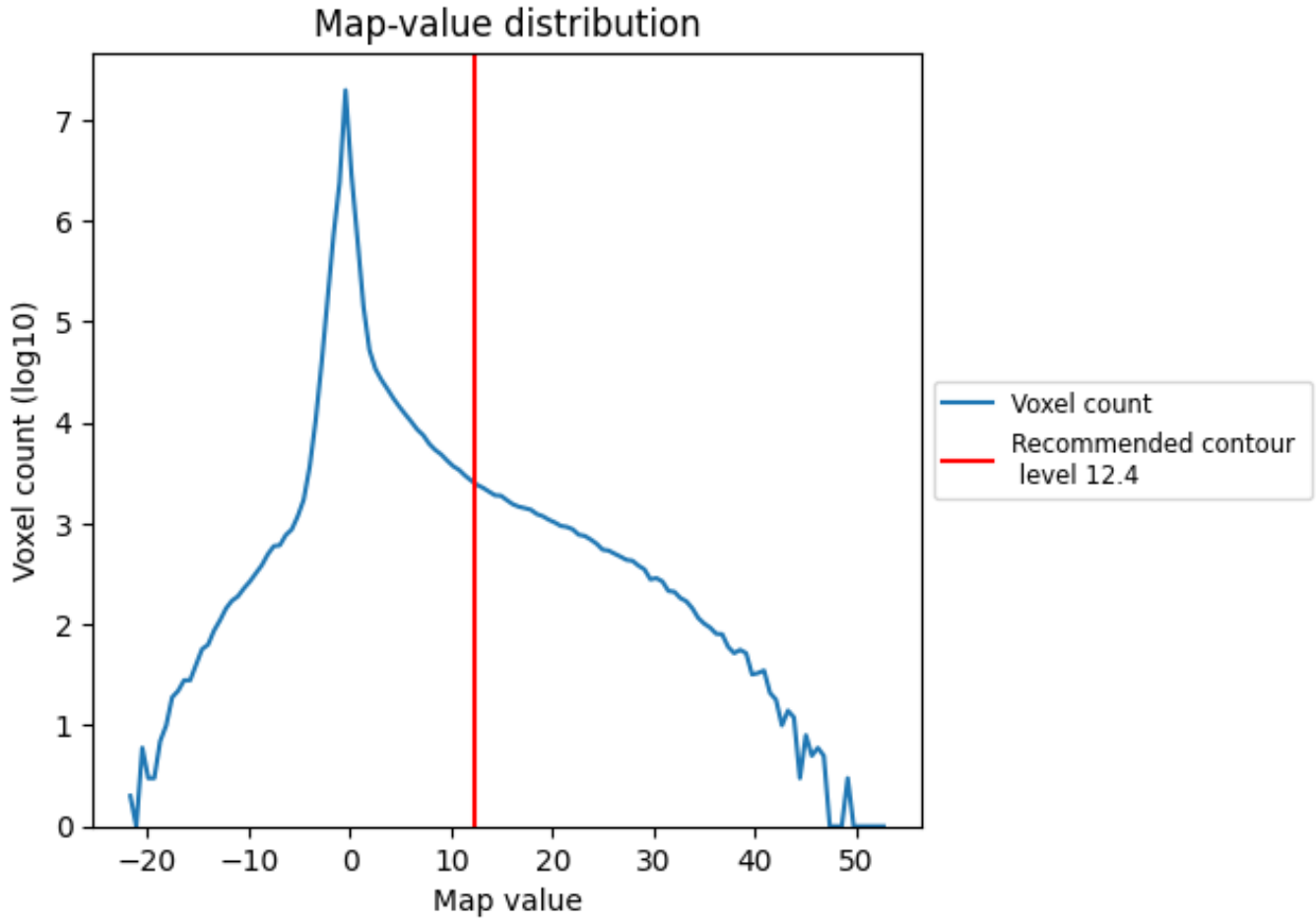
6.6 Mask visualisation (i)

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

7 Map analysis

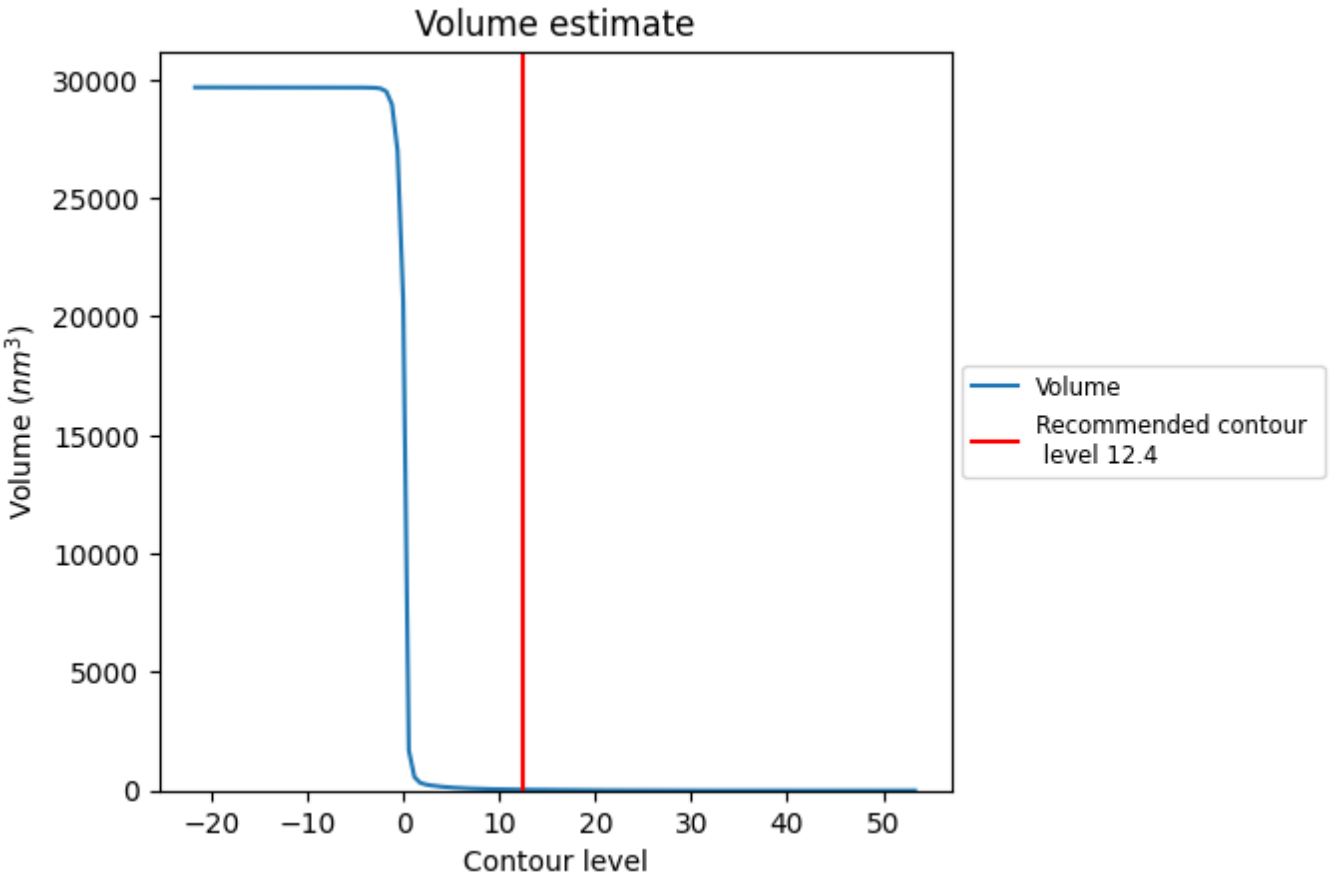
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

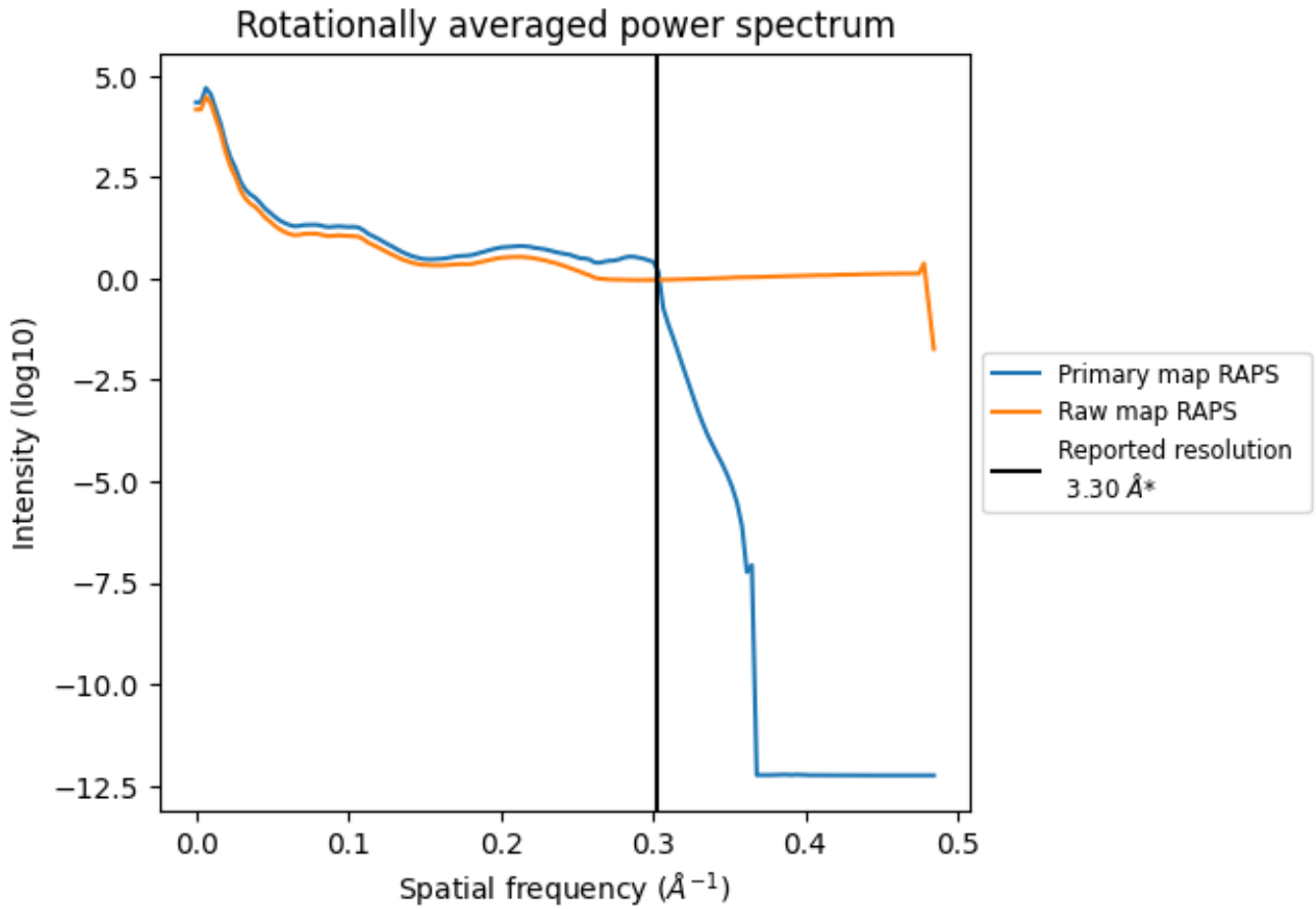
7.2 Volume estimate (i)



The volume at the recommended contour level is 39 nm^3; 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)

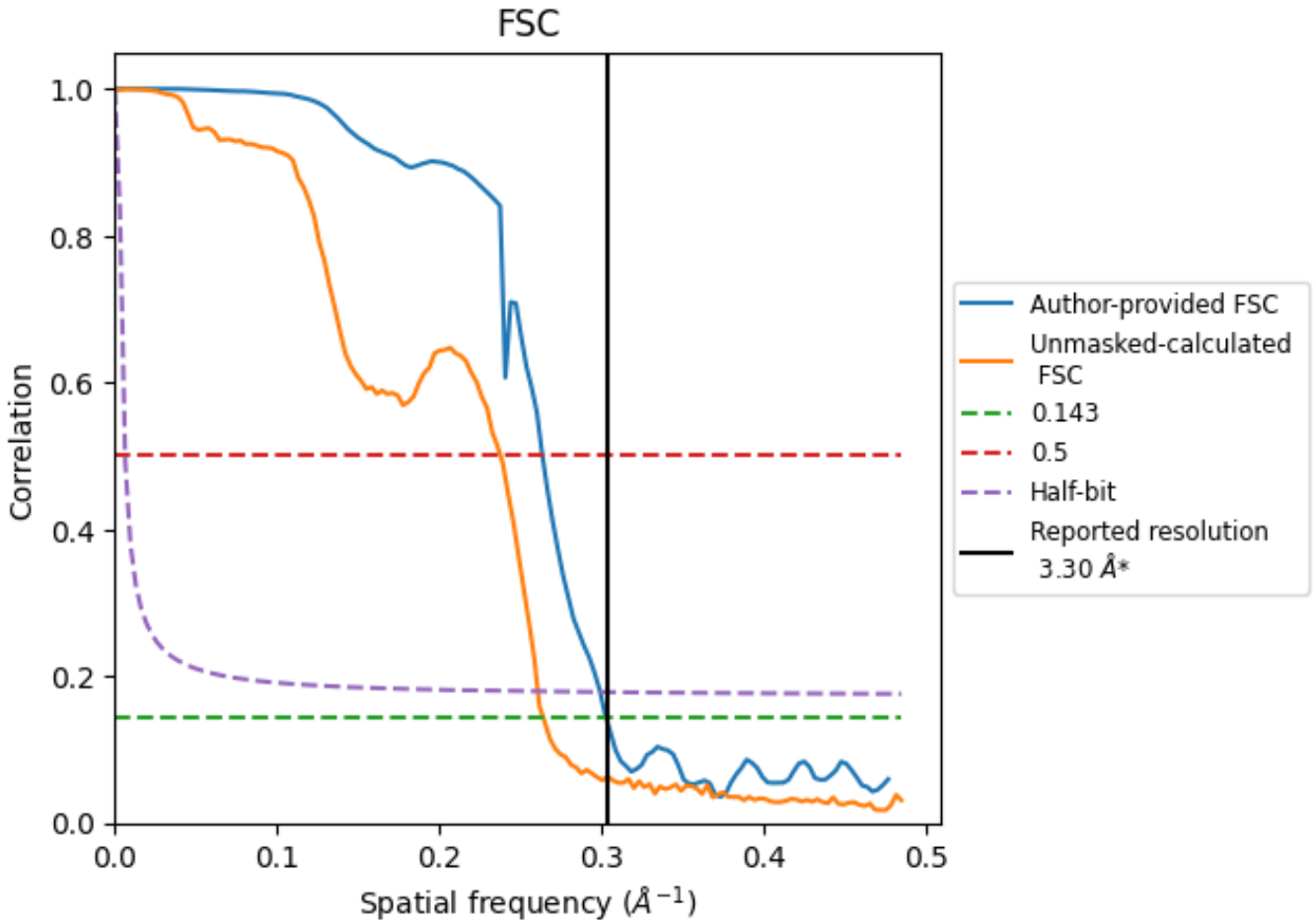


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

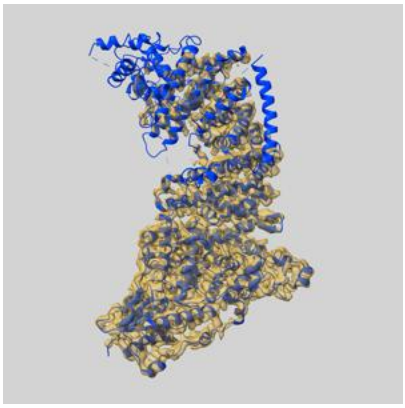
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.80	3.34
Unmasked-calculated*	3.79	4.21	3.84

*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 %

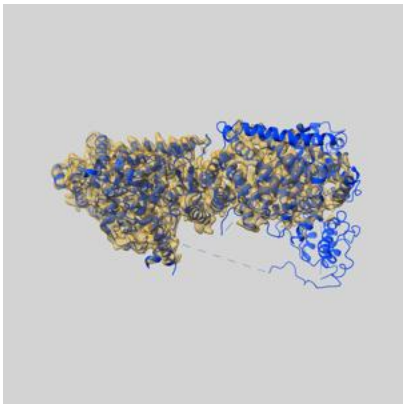
9 Map-model fit

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.

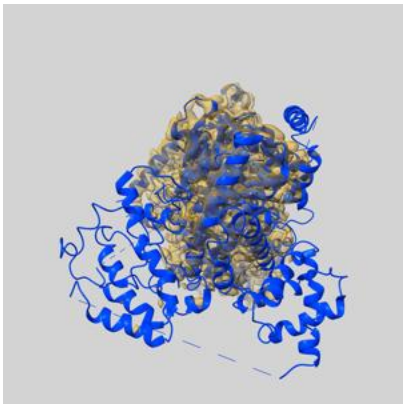
9.1 Map-model overlay



X



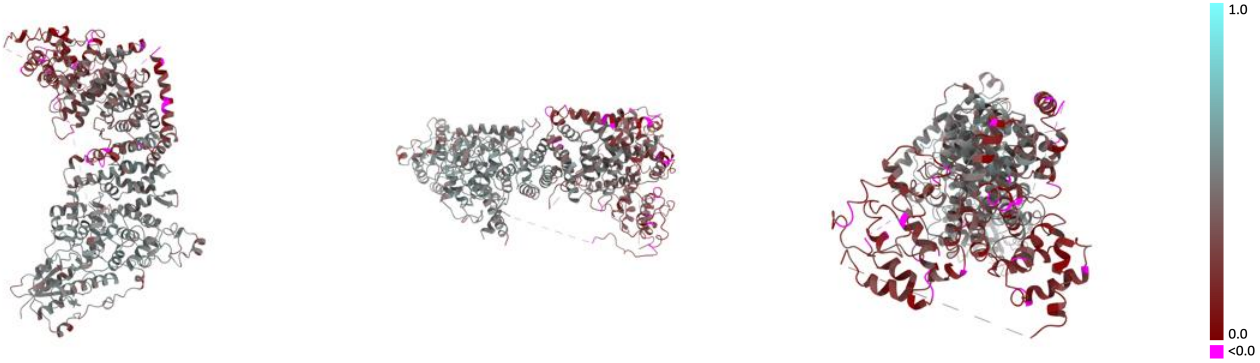
Y



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.

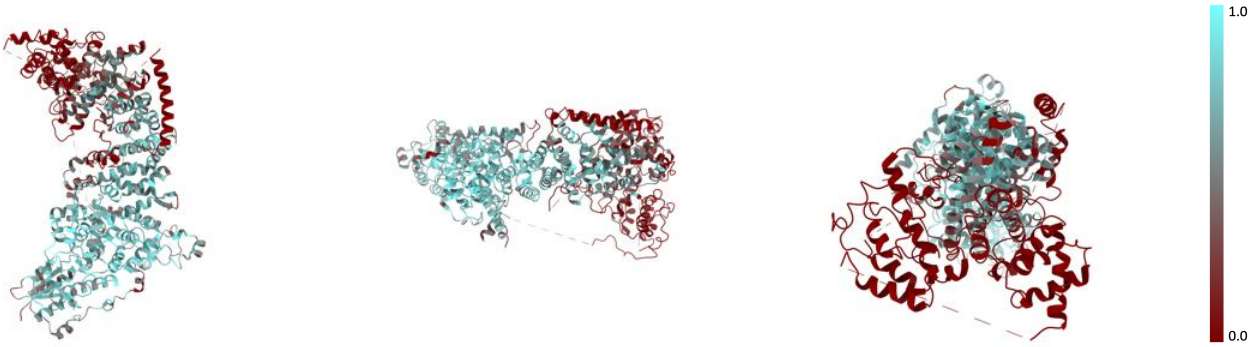
9.2 Q-score mapped to coordinate model



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.

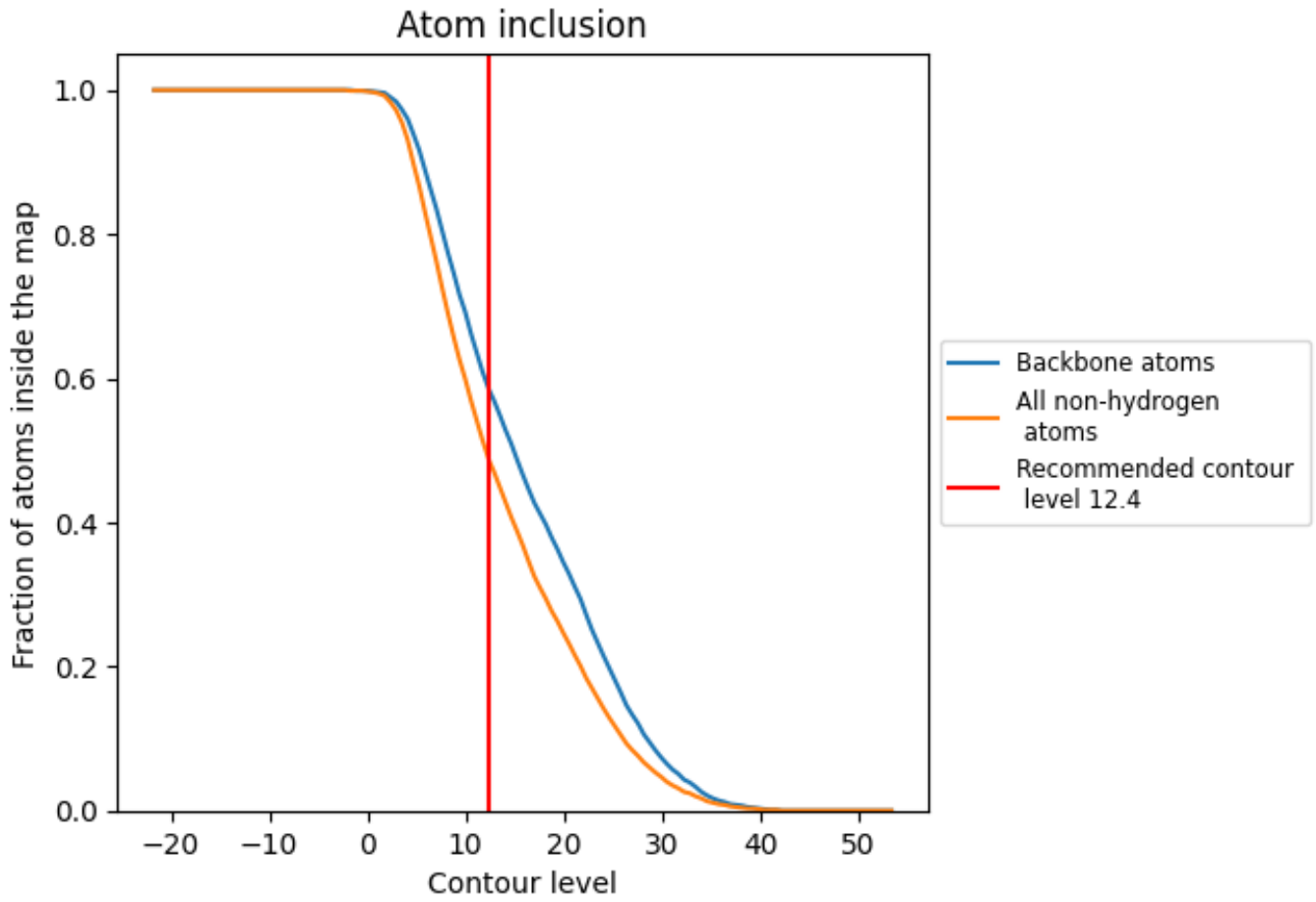
9.3 Atom inclusion mapped to coordinate model



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 (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

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