Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 12:34 PM JST

PDB ID	:	7VPI
EMDB ID	:	EMD-32066
Title	:	Cryo-EM structure of the human ATP13A2 (E1-ATP state)
Authors	:	Tomita, A.; Yamashita, K.; Nishizawa, T.; Nureki, O.
Deposited on	:	2021-10-17
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

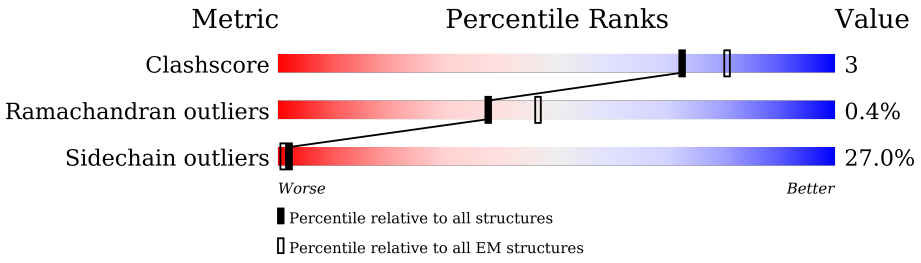
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1184	19% 57% 21% • 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7375 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.

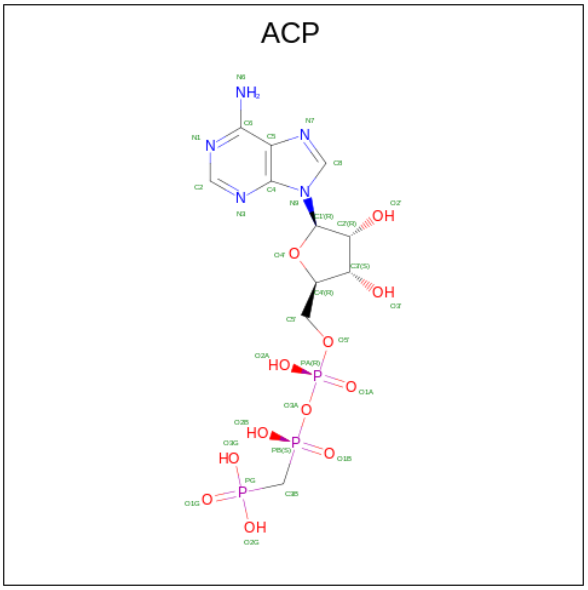
- Molecule 1 is a protein called Polyamine-transporting ATPase 13A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	959	7343	4738	1252	1303	50	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9NQ11
A	-2	PRO	-	expression tag	UNP Q9NQ11
A	-1	SER	-	expression tag	UNP Q9NQ11
A	0	ARG	-	expression tag	UNP Q9NQ11

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	11	5	12	3	0

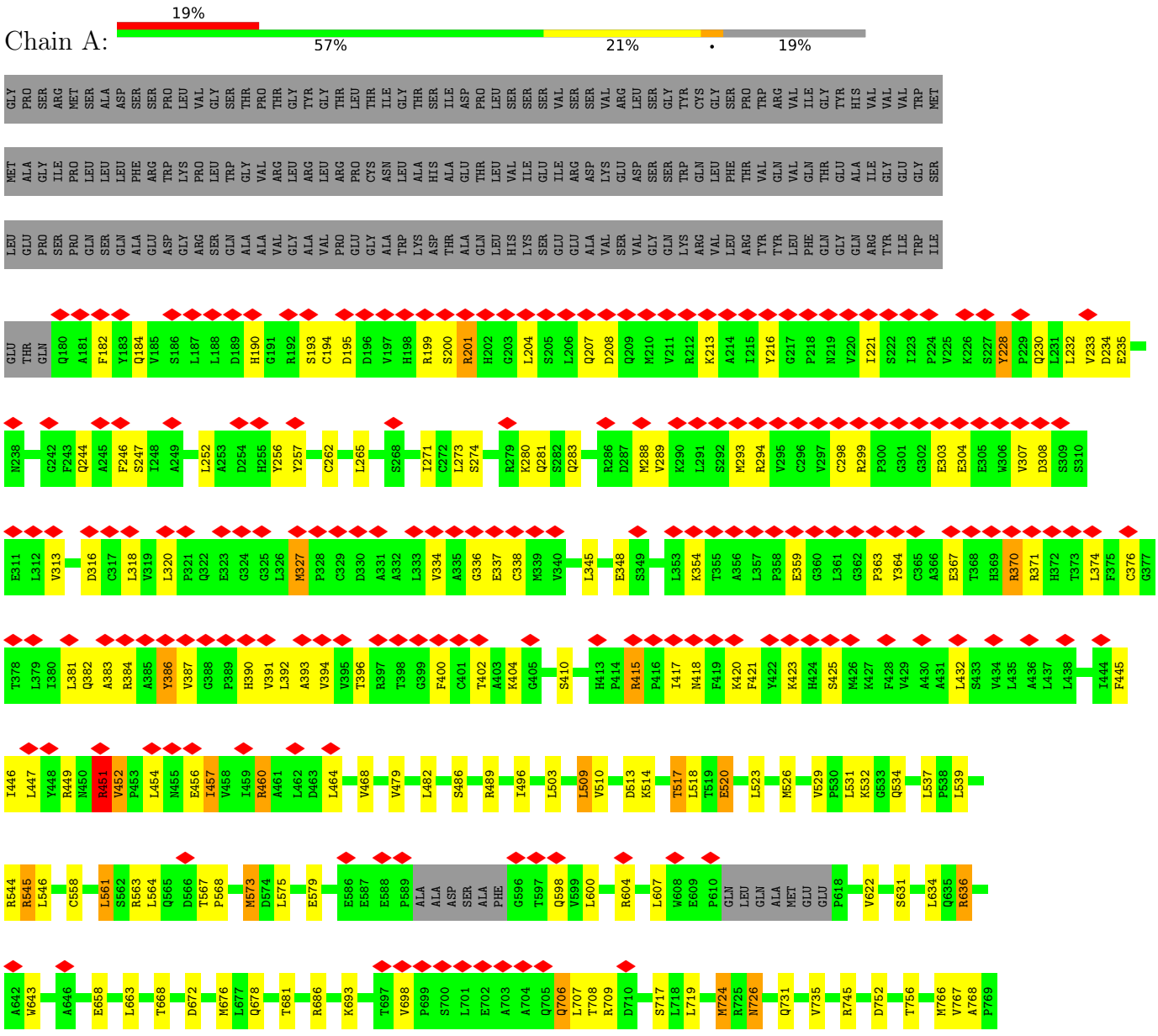
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

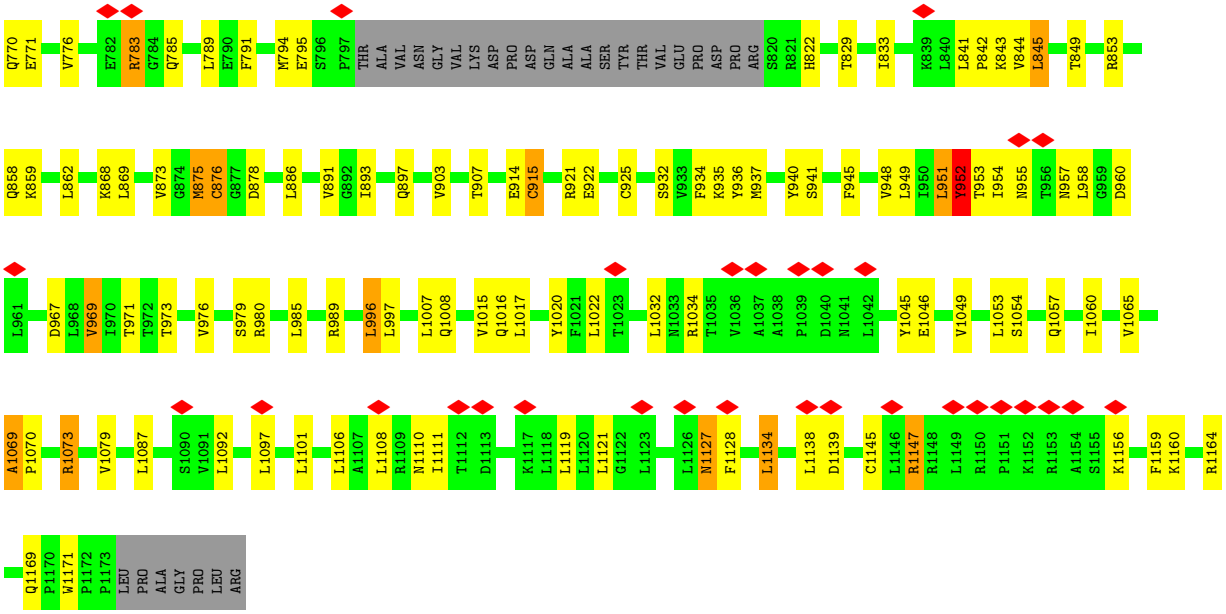
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	1	1	1	0

3 Residue-property plots (i)

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

- Molecule 1: Polyamine-transporting ATPase 13A2




Q770 E771 V776 E782 R783 G784 Q785 L789 E790 F791 M794 E795 S796 P797 THR ALA VAL ASN GLY VAL LYS ASP PRO ASP GLN ALA ALA SER TYR THR VAL GLU PRO ASP PRO ARG S820 R821 H822 T829 I833 K839 L840 L841 P842 K843 V844 L845 T849 R853
Q858 K859 L862 K868 L869 V873 G874 M875 C876 G877 D878 L886 V891 G892 I893 Q897 V903 T907 E914 C915 R921 E922 C925 S932 Y933 F934 K935 Y936 M937 Y940 S941 F945 V948 L949 I950 L951 Y952 T953 I954 N955 T956 N957 L958 G959 D960
L961 D967 L968 V969 I970 T971 T972 T973 V976 S979 R980 L985 R989 L996 L997 L1007 Q1008 V1015 Q1016 L1017 Y1020 F1021 L1022 T1023 L1032 N1033 R1034 T1035 V1036 A1037 A1038 P1039 D1040 N1041 L1042 Y1045 E1046 V1049 L1053 S1054 Q1057 I1060 V1065
A1069 P1070 R1073 V1079 L1087 S1090 V1091 L1092 L1097 L1101 L1106 A1107 L1108 R1109 N1110 I1111 T1112 D1113 K1117 L1118 L1119 L1120 L1121 G1122 L1123 L1126 N1127 F1128 L1134 L1138 D1139 C1145 L1146 R1147 R1148 L1149 R1150 P1151 K1152 R1153 A1154 S1155 K1156 F1159 K1160 R1164
Q1169 P1170 W1171 P1172 P1173 LEU PRO ALA GLY PRO LEU ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3114	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.588	Depositor
Minimum map value	-0.414	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0359	Depositor
Map size (Å)	179.08978, 179.08978, 179.08978	wwPDB
Map dimensions	118, 118, 118	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.51771, 1.51771, 1.51771	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.84	0/7507	1.14	11/10235 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1147	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	1073	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	199	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	256	TYR	CB-CG-CD1	5.39	124.23	121.00
1	A	451	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	A	783	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	952	TYR	CB-CG-CD1	5.11	124.06	121.00
1	A	449	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	636	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	A	370	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	A	545	ARG	NE-CZ-NH2	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	7343	0	7611	51	0
2	A	31	0	14	0	0
3	A	1	0	0	0	0
All	All	7375	0	7625	51	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 3.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:SER:HA	1:A:363:PRO:HA	1.64	0.79
1:A:383:ALA:HB1	1:A:391:VAL:HG21	1.72	0.72
1:A:523:LEU:HD11	1:A:573:MET:HA	1.72	0.71
1:A:193:SER:HA	1:A:363:PRO:CA	2.23	0.69
1:A:235:GLU:HB3	1:A:271:ILE:HD11	1.78	0.66
1:A:221:ILE:HG21	1:A:289:VAL:HB	1.76	0.66
1:A:425:SER:HB2	1:A:996:LEU:HD12	1.80	0.64
1:A:1007:LEU:HB3	1:A:1134:LEU:HD11	1.81	0.62
1:A:876:CYS:SG	1:A:876:CYS:O	2.60	0.59
1:A:1060:ILE:HG21	1:A:1128:PHE:HA	1.84	0.59
1:A:523:LEU:HD13	1:A:724:MET:HB3	1.84	0.58
1:A:844:VAL:HG23	1:A:845:LEU:HD23	1.85	0.57
1:A:776:VAL:HG13	1:A:789:LEU:HD21	1.90	0.54
1:A:509:LEU:HD21	1:A:873:VAL:HG12	1.91	0.53
1:A:517:THR:HG21	1:A:876:CYS:O	2.08	0.53
1:A:1015:VAL:HG21	1:A:1127:ASN:HB3	1.91	0.52
1:A:622:VAL:HG12	1:A:643:TRP:HB3	1.91	0.52
1:A:989:ARG:O	1:A:989:ARG:NH1	2.43	0.51
1:A:686:ARG:NH1	1:A:752:ASP:OD2	2.44	0.50
1:A:1069:ALA:HB3	1:A:1070:PRO:HD3	1.93	0.49
1:A:386:TYR:HB2	1:A:598:GLN:HA	1.95	0.48
1:A:897:GLN:HB2	1:A:907:THR:HG23	1.96	0.48
1:A:893:ILE:HG21	1:A:915:CYS:SG	2.54	0.48
1:A:875:MET:HB3	1:A:886:LEU:HD23	1.96	0.47
1:A:523:LEU:HD12	1:A:523:LEU:O	2.13	0.47
1:A:327:MET:HA	1:A:327:MET:HE2	1.95	0.47
1:A:452:VAL:HG23	1:A:457:ILE:HG22	1.97	0.46
1:A:842:PRO:HA	1:A:869:LEU:HD21	1.97	0.46
1:A:479:VAL:HG21	1:A:976:VAL:HG22	1.97	0.46
1:A:822:HIS:ND1	1:A:849:THR:HG21	2.30	0.46
1:A:415:ARG:NE	1:A:415:ARG:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LEU:HD11	1:A:575:LEU:HA	1.97	0.45
1:A:520:GLU:O	1:A:726:ASN:ND2	2.50	0.45
1:A:948:VAL:HG22	1:A:958:LEU:HD22	1.98	0.45
1:A:460:ARG:HD3	1:A:952:TYR:CE1	2.52	0.44
1:A:446:ILE:HG13	1:A:953:THR:HG22	2.00	0.44
1:A:200:SER:HB2	1:A:394:VAL:HG21	2.00	0.43
1:A:336:GLY:HA3	1:A:391:VAL:HG12	2.00	0.43
1:A:845:LEU:HD13	1:A:862:LEU:HD12	2.00	0.43
1:A:451:ARG:HA	1:A:451:ARG:NH2	2.33	0.43
1:A:936:TYR:HB2	1:A:1065:VAL:HG11	1.99	0.43
1:A:193:SER:HA	1:A:363:PRO:CB	2.48	0.43
1:A:451:ARG:HA	1:A:451:ARG:CZ	2.48	0.43
1:A:969:VAL:O	1:A:973:THR:HB	2.19	0.42
1:A:706:GLN:O	1:A:706:GLN:NE2	2.54	0.41
1:A:951:LEU:HB3	1:A:957:ASN:O	2.20	0.41
1:A:768:ALA:HB3	1:A:771:GLU:HG2	2.03	0.41
1:A:517:THR:HG23	1:A:878:ASP:HB3	2.02	0.40
1:A:320:LEU:HD21	1:A:393:ALA:HB3	2.03	0.40
1:A:383:ALA:HB1	1:A:391:VAL:CG2	2.47	0.40
1:A:201:ARG:HB2	1:A:334:VAL:HG21	2.02	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	951/1184 (80%)	909 (96%)	38 (4%)	4 (0%)	34 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	TYR

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Mol	Chain	Res	Type
1	A	1079	VAL
1	A	1069	ALA
1	A	568	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	819/1005 (82%)	598 (73%)	221 (27%)	0 3

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	PHE
1	A	184	GLN
1	A	190	HIS
1	A	194	CYS
1	A	195	ASP
1	A	201	ARG
1	A	204	LEU
1	A	207	GLN
1	A	208	ASP
1	A	213	LYS
1	A	216	TYR
1	A	228	TYR
1	A	230	GLN
1	A	232	LEU
1	A	233	VAL
1	A	234	ASP
1	A	244	GLN
1	A	246	PHE
1	A	247	SER
1	A	252	LEU
1	A	257	TYR
1	A	262	CYS
1	A	265	LEU

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Mol	Chain	Res	Type
1	A	273	LEU
1	A	274	SER
1	A	280	LYS
1	A	281	GLN
1	A	283	GLN
1	A	288	MET
1	A	293	MET
1	A	294	ARG
1	A	298	CYS
1	A	299	ARG
1	A	303	GLU
1	A	304	GLU
1	A	307	VAL
1	A	308	ASP
1	A	313	VAL
1	A	316	ASP
1	A	318	LEU
1	A	327	MET
1	A	337	GLU
1	A	338	CYS
1	A	345	LEU
1	A	348	GLU
1	A	354	LYS
1	A	359	GLU
1	A	364	TYR
1	A	367	GLU
1	A	370	ARG
1	A	371	ARG
1	A	374	LEU
1	A	376	CYS
1	A	381	LEU
1	A	382	GLN
1	A	384	ARG
1	A	386	TYR
1	A	387	VAL
1	A	390	HIS
1	A	392	LEU
1	A	396	THR
1	A	400	PHE
1	A	402	THR
1	A	404	LYS
1	A	410	SER

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Mol	Chain	Res	Type
1	A	415	ARG
1	A	417	ILE
1	A	418	ASN
1	A	420	LYS
1	A	421	PHE
1	A	423	LYS
1	A	432	LEU
1	A	445	PHE
1	A	447	LEU
1	A	451	ARG
1	A	452	VAL
1	A	454	LEU
1	A	456	GLU
1	A	457	ILE
1	A	460	ARG
1	A	464	LEU
1	A	468	VAL
1	A	482	LEU
1	A	486	SER
1	A	489	ARG
1	A	496	ILE
1	A	503	LEU
1	A	509	LEU
1	A	510	VAL
1	A	513	ASP
1	A	514	LYS
1	A	517	THR
1	A	518	LEU
1	A	520	GLU
1	A	526	MET
1	A	529	VAL
1	A	531	LEU
1	A	532	LYS
1	A	534	GLN
1	A	537	LEU
1	A	539	LEU
1	A	544	ARG
1	A	545	ARG
1	A	546	LEU
1	A	558	CYS
1	A	561	LEU
1	A	563	ARG

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Mol	Chain	Res	Type
1	A	564	LEU
1	A	567	THR
1	A	573	MET
1	A	579	GLU
1	A	600	LEU
1	A	604	ARG
1	A	607	LEU
1	A	631	SER
1	A	634	LEU
1	A	636	ARG
1	A	658	GLU
1	A	663	LEU
1	A	668	THR
1	A	672	ASP
1	A	676	MET
1	A	678	GLN
1	A	681	THR
1	A	693	LYS
1	A	698	VAL
1	A	706	GLN
1	A	707	LEU
1	A	708	THR
1	A	709	ARG
1	A	717	SER
1	A	719	LEU
1	A	724	MET
1	A	726	ASN
1	A	731	GLN
1	A	735	VAL
1	A	745	ARG
1	A	756	THR
1	A	766	MET
1	A	767	VAL
1	A	770	GLN
1	A	783	ARG
1	A	785	GLN
1	A	791	PHE
1	A	794	MET
1	A	795	GLU
1	A	829	THR
1	A	833	ILE
1	A	841	LEU

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Mol	Chain	Res	Type
1	A	843	LYS
1	A	845	LEU
1	A	853	ARG
1	A	858	GLN
1	A	859	LYS
1	A	868	LYS
1	A	875	MET
1	A	876	CYS
1	A	891	VAL
1	A	903	VAL
1	A	914	GLU
1	A	915	CYS
1	A	921	ARG
1	A	922	GLU
1	A	925	CYS
1	A	932	SER
1	A	934	PHE
1	A	935	LYS
1	A	937	MET
1	A	940	TYR
1	A	941	SER
1	A	945	PHE
1	A	949	LEU
1	A	951	LEU
1	A	952	TYR
1	A	954	ILE
1	A	955	ASN
1	A	960	ASP
1	A	967	ASP
1	A	969	VAL
1	A	971	THR
1	A	979	SER
1	A	980	ARG
1	A	985	LEU
1	A	996	LEU
1	A	997	LEU
1	A	1008	GLN
1	A	1016	GLN
1	A	1017	LEU
1	A	1020	TYR
1	A	1022	LEU
1	A	1032	LEU

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Mol	Chain	Res	Type
1	A	1034	ARG
1	A	1045	TYR
1	A	1046	GLU
1	A	1049	VAL
1	A	1053	LEU
1	A	1054	SER
1	A	1057	GLN
1	A	1073	ARG
1	A	1087	LEU
1	A	1092	LEU
1	A	1097	LEU
1	A	1101	LEU
1	A	1106	LEU
1	A	1108	LEU
1	A	1110	ASN
1	A	1111	ILE
1	A	1119	LEU
1	A	1121	LEU
1	A	1127	ASN
1	A	1134	LEU
1	A	1138	LEU
1	A	1139	ASP
1	A	1145	CYS
1	A	1147	ARG
1	A	1156	LYS
1	A	1159	PHE
1	A	1160	LYS
1	A	1164	ARG
1	A	1169	GLN
1	A	1171	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	534	GLN
1	A	706	GLN
1	A	726	ASN
1	A	731	GLN
1	A	962	GLN
1	A	1041	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
2	ACP	A	1201	3	27,33,33	0.89	2 (7%)	32,52,52	0.85	0

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
2	ACP	A	1201	3	-	4/15/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ACP	PB-O2B	-2.37	1.50	1.56
2	A	1201	ACP	C8-N7	-2.04	1.31	1.34

There are no bond angle outliers.

There are no chirality outliers.

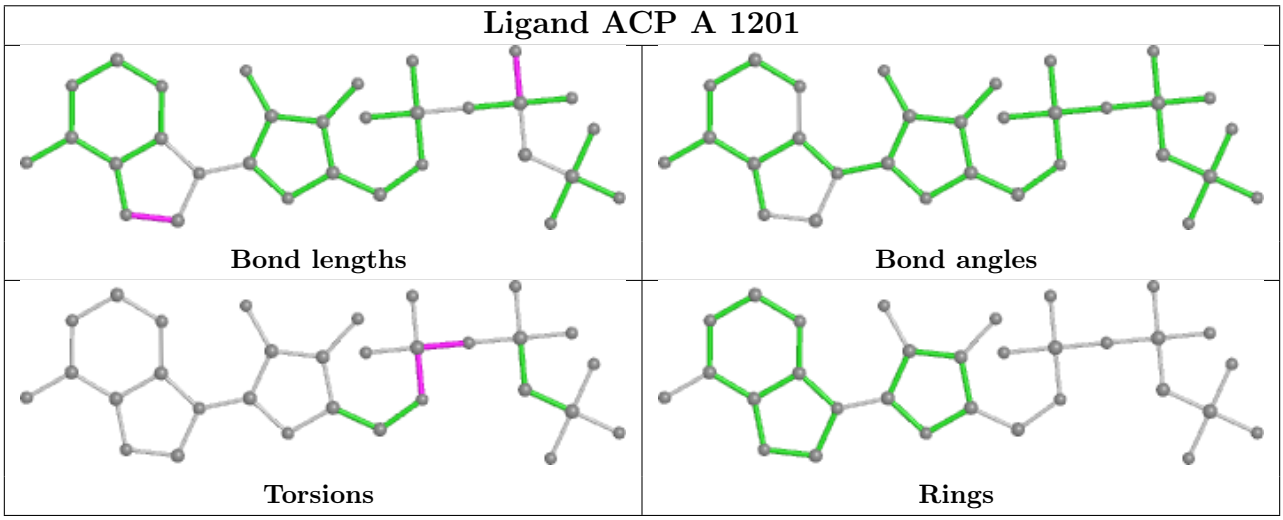
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ACP	C5'-O5'-PA-O1A
2	A	1201	ACP	C5'-O5'-PA-O2A
2	A	1201	ACP	PB-O3A-PA-O5'
2	A	1201	ACP	C5'-O5'-PA-O3A

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.



5.7 Other polymers

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

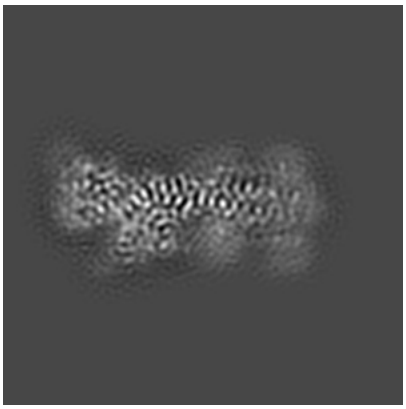
This section contains visualisations of the EMDB entry EMD-32066. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

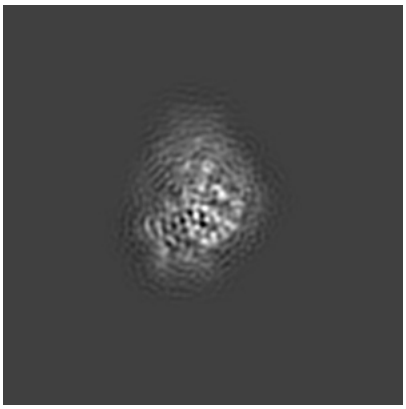
6.1 Orthogonal projections

6.1.1 Primary map

X

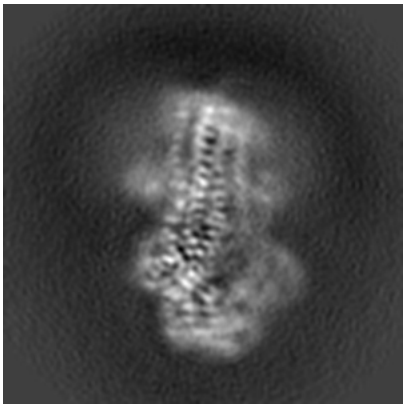


Y

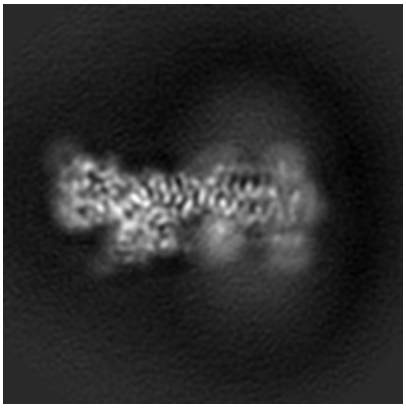


Z

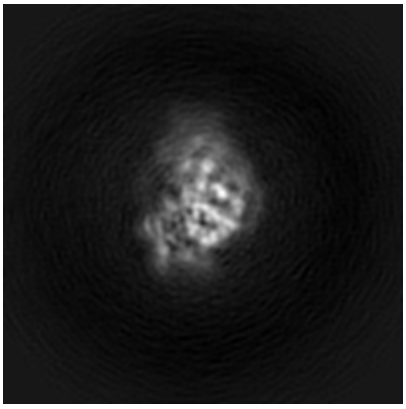
6.1.2 Raw map



X



Y



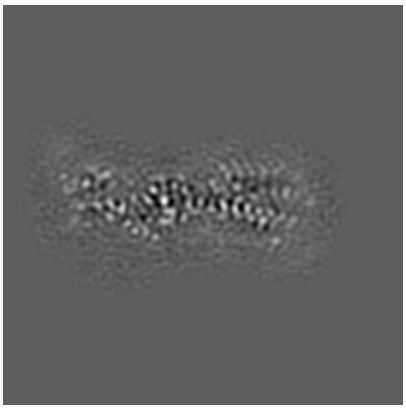
Z

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

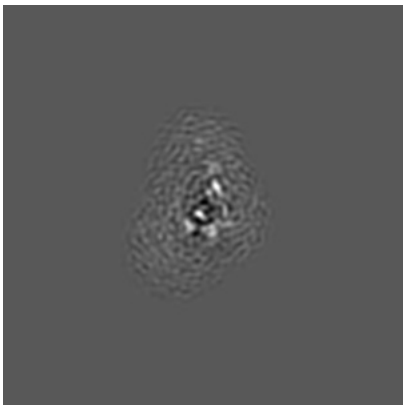
6.2 Central slices (i)

6.2.1 Primary map

X Index: 59

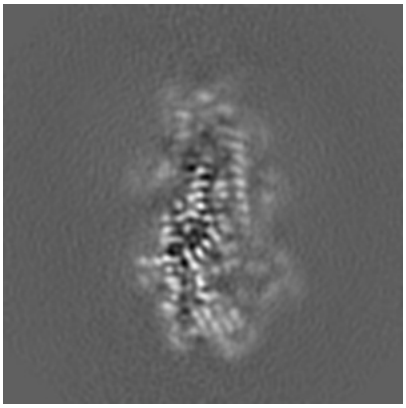


Y Index: 59

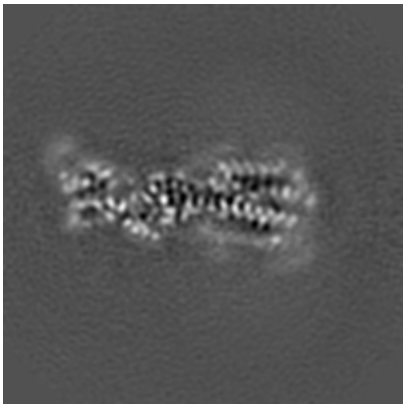


Z Index: 59

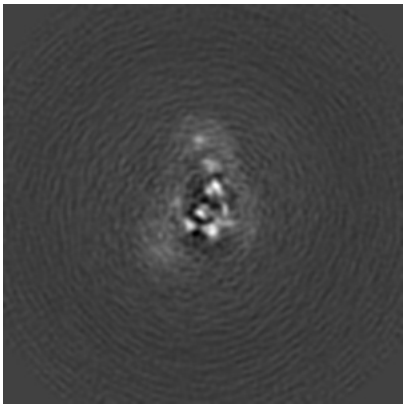
6.2.2 Raw map



X Index: 59



Y Index: 59



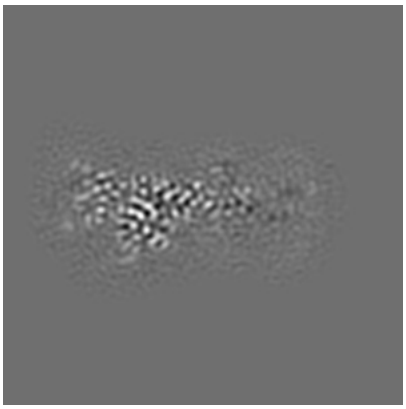
Z Index: 59

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

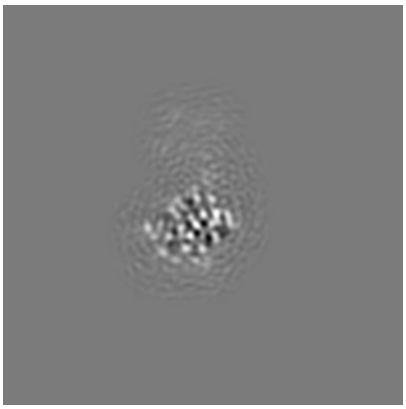
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 59

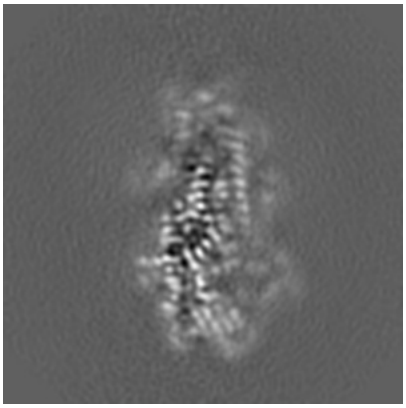


Y Index: 55

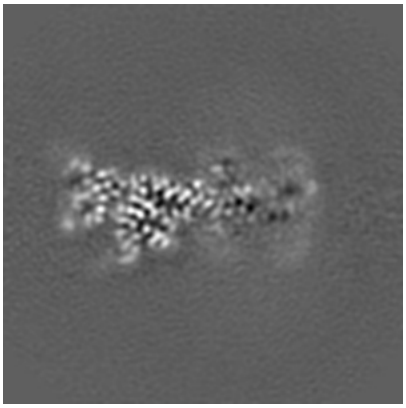


Z Index: 41

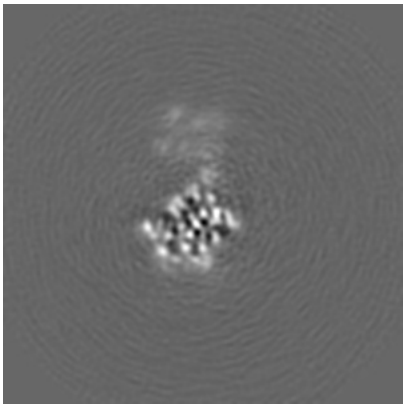
6.3.2 Raw map



X Index: 59



Y Index: 55



Z Index: 41

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

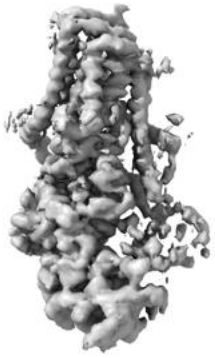
X

Y

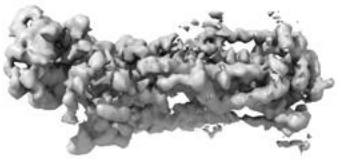
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0359. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

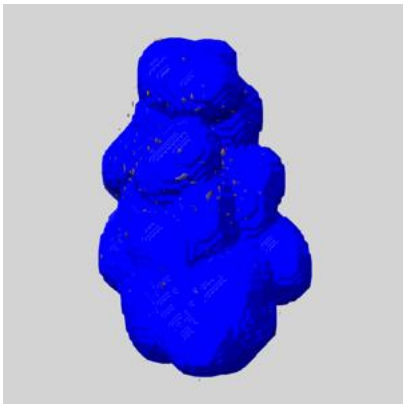
6.5 Mask visualisation (i)

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

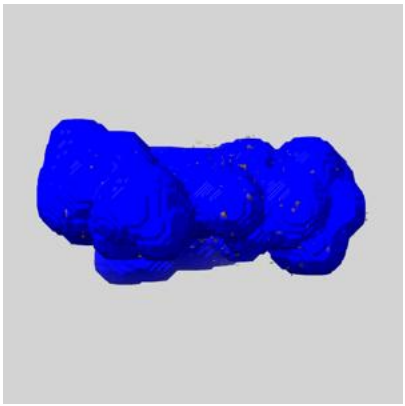
A mask typically either:

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

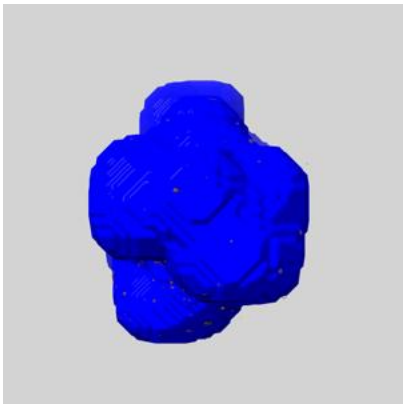
6.5.1 emd_32066_msk_1.map (i)



X



Y

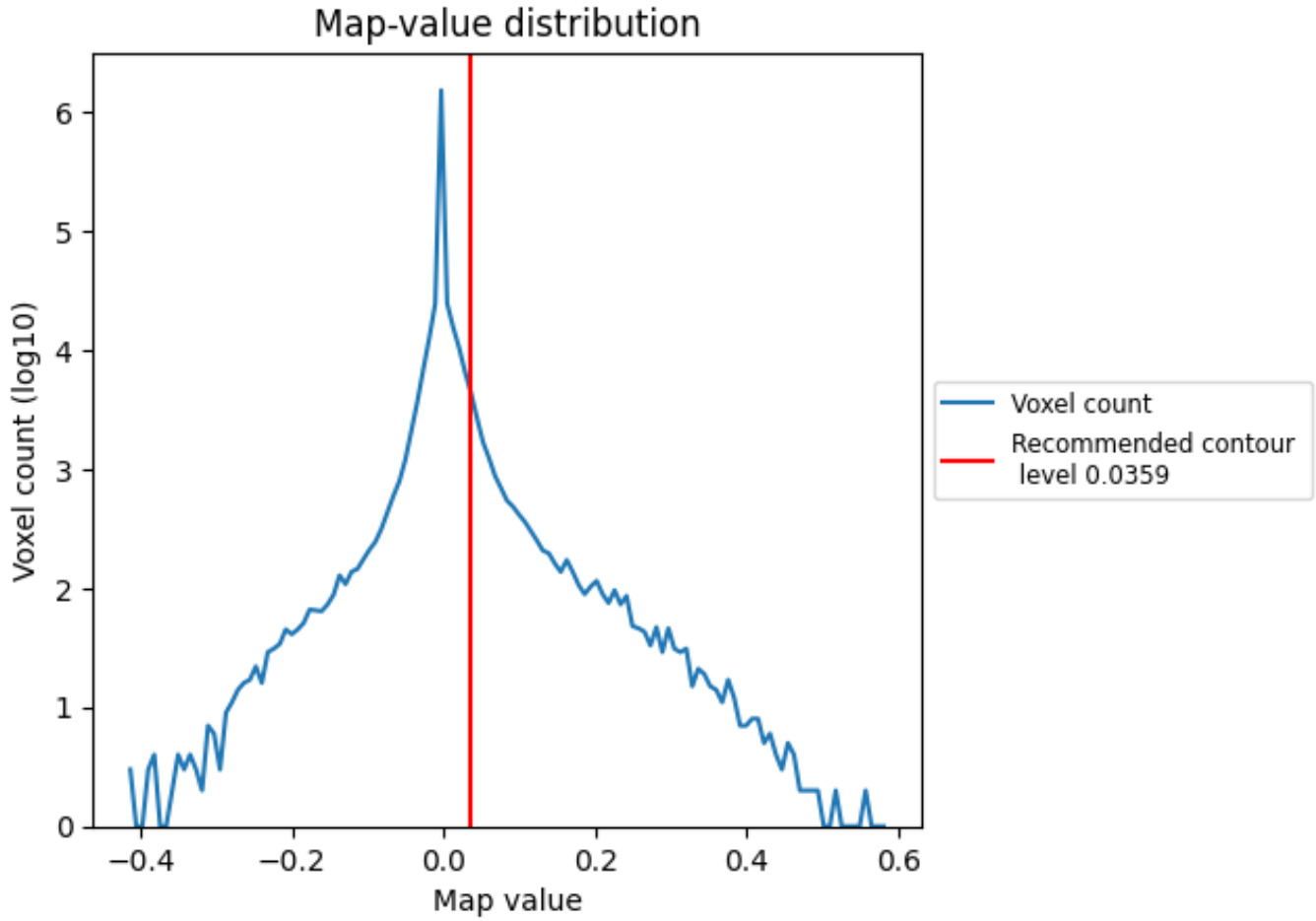


Z

7 Map analysis

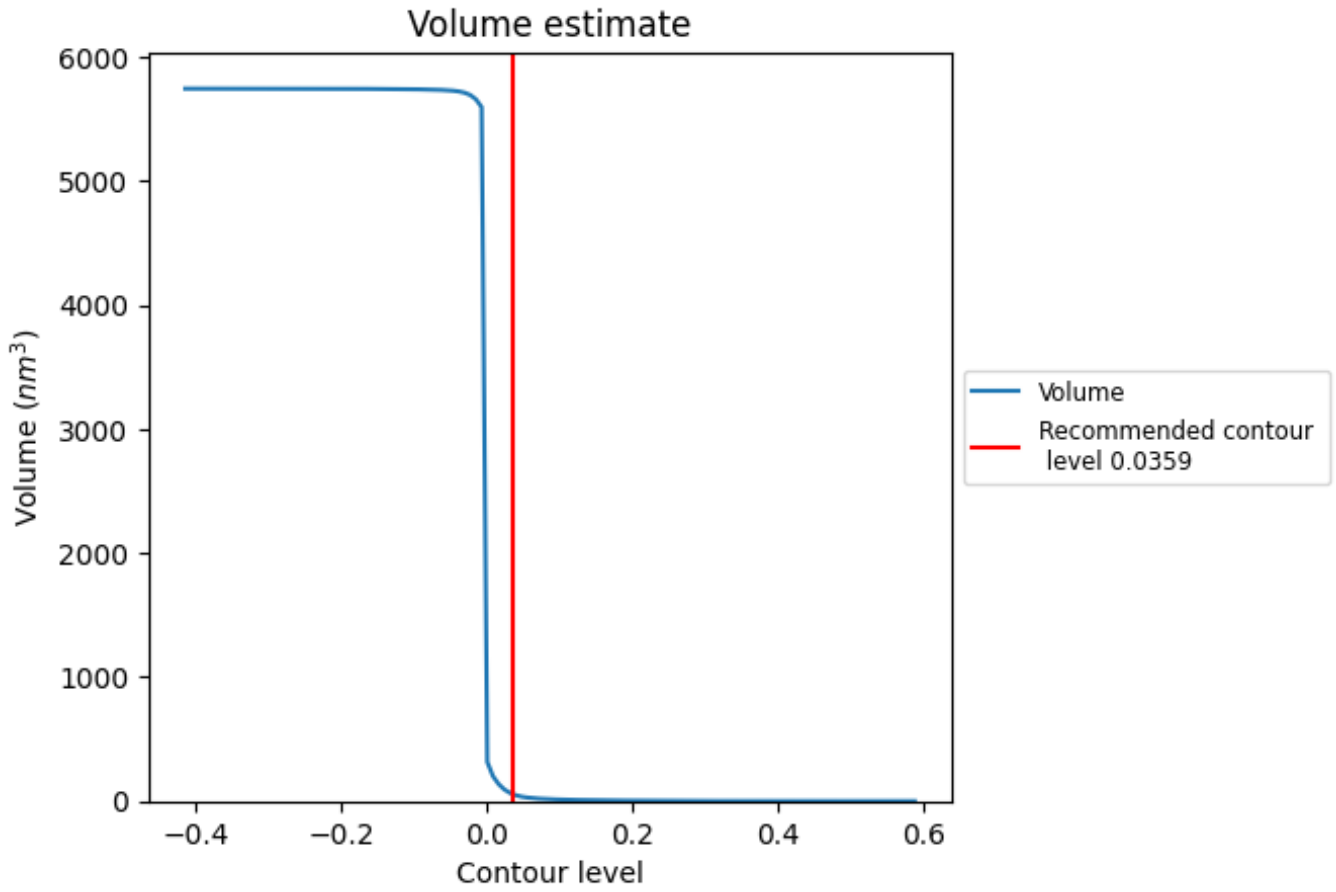
This section contains the results of statistical analysis of the map.

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.

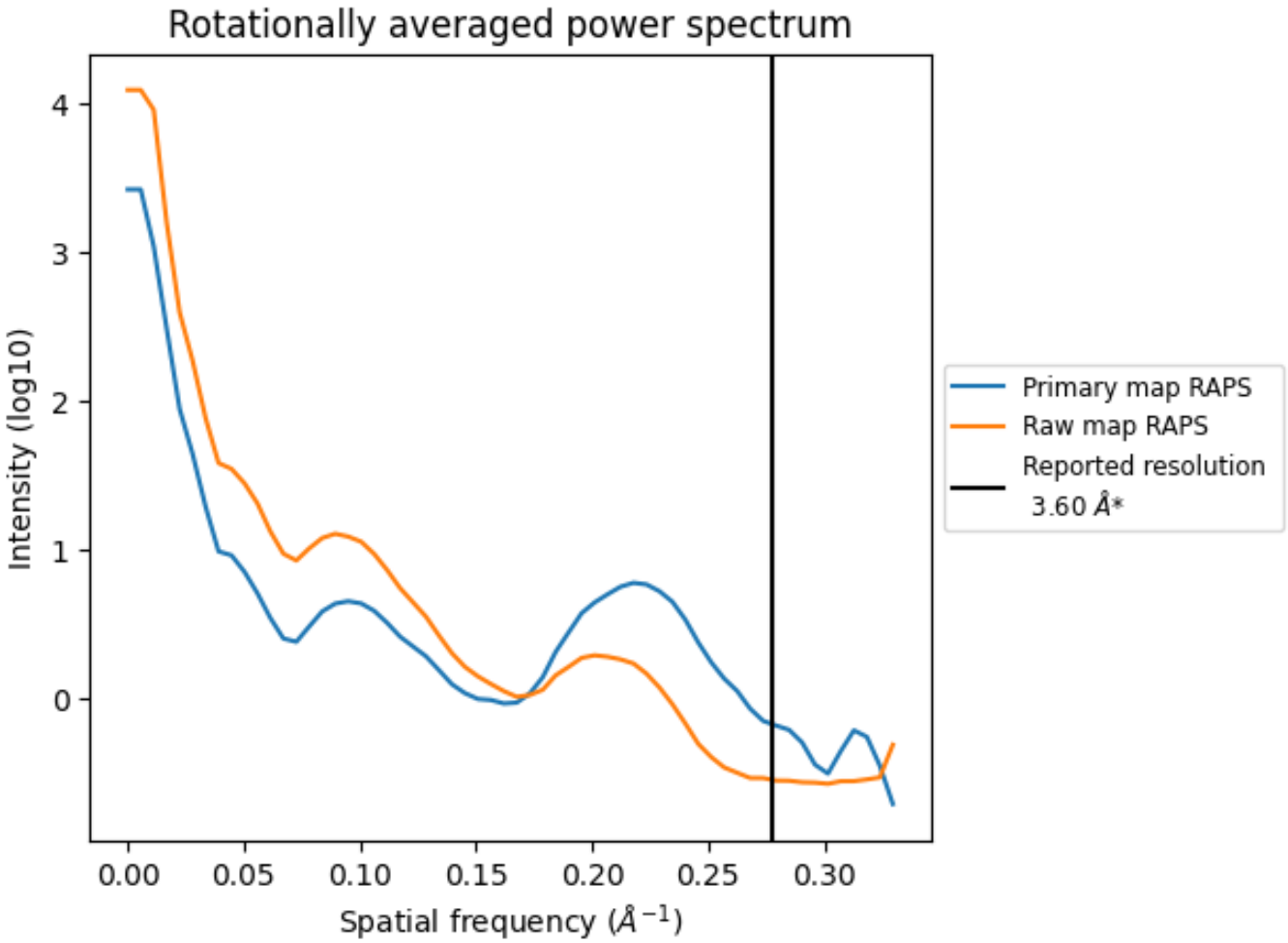
7.2 Volume estimate



The volume at the recommended contour level is 58 nm^3; this corresponds to an approximate mass of 53 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)

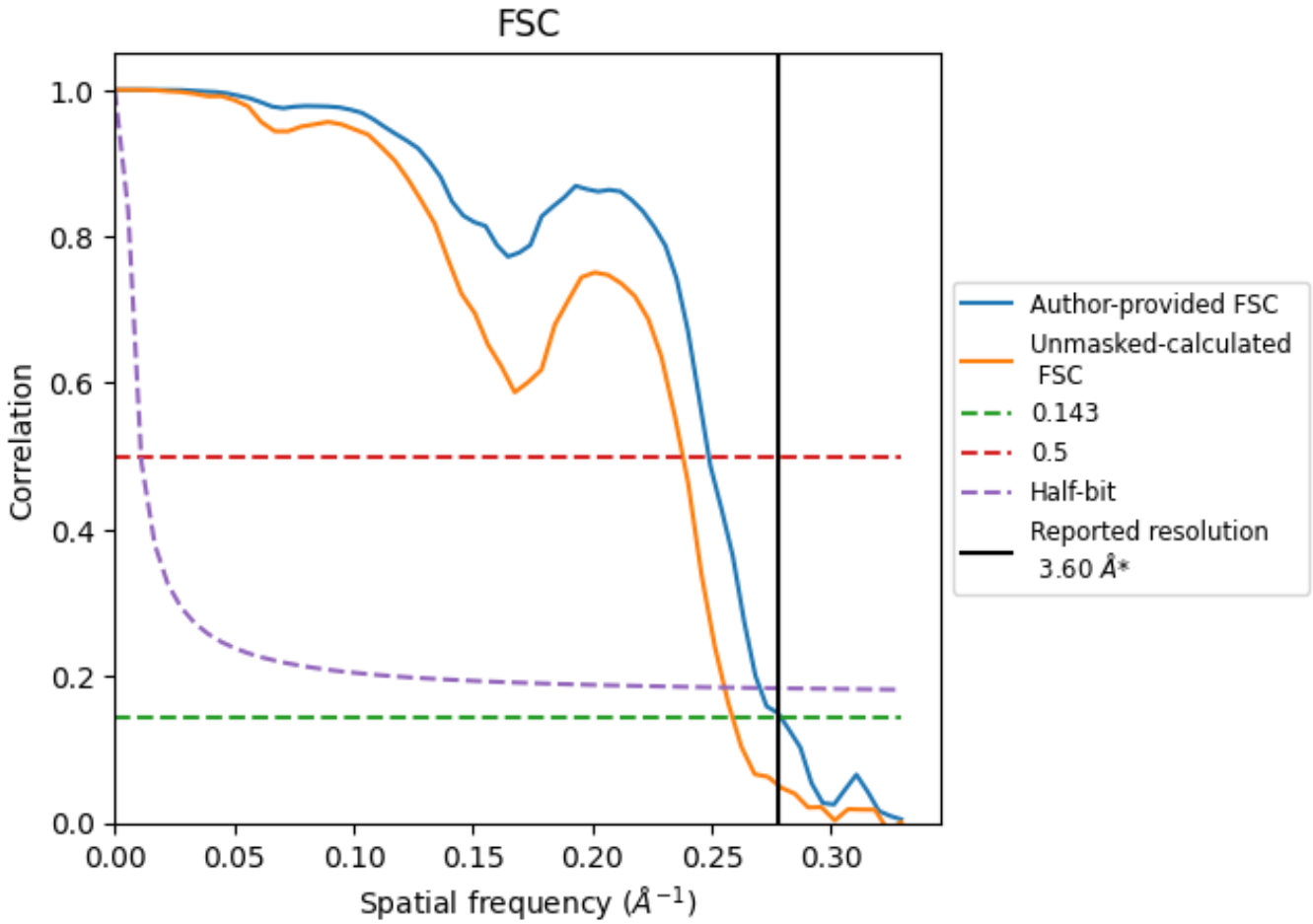


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

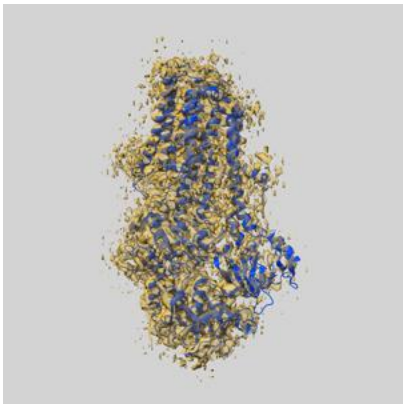
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.02	3.70
Unmasked-calculated*	3.86	4.20	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

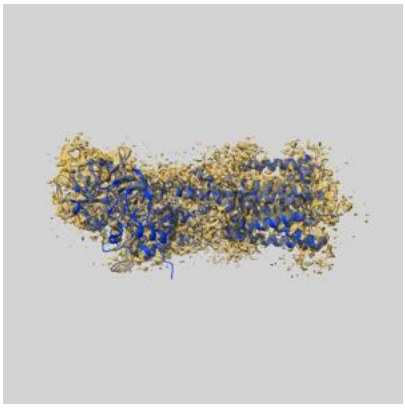
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32066 and PDB model 7VPI. Per-residue inclusion information can be found in section 3 on page 5.

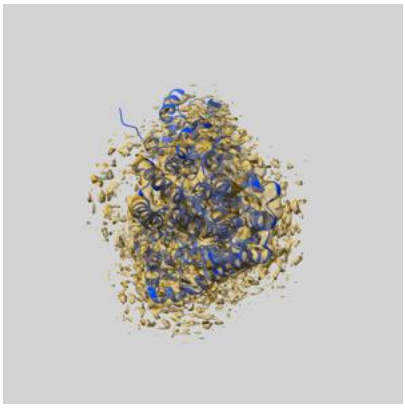
9.1 Map-model overlay



X



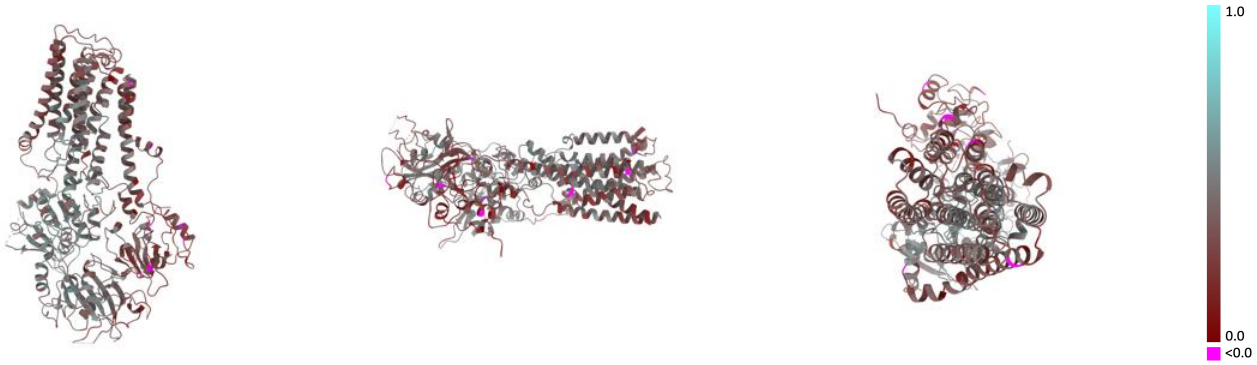
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0359 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.

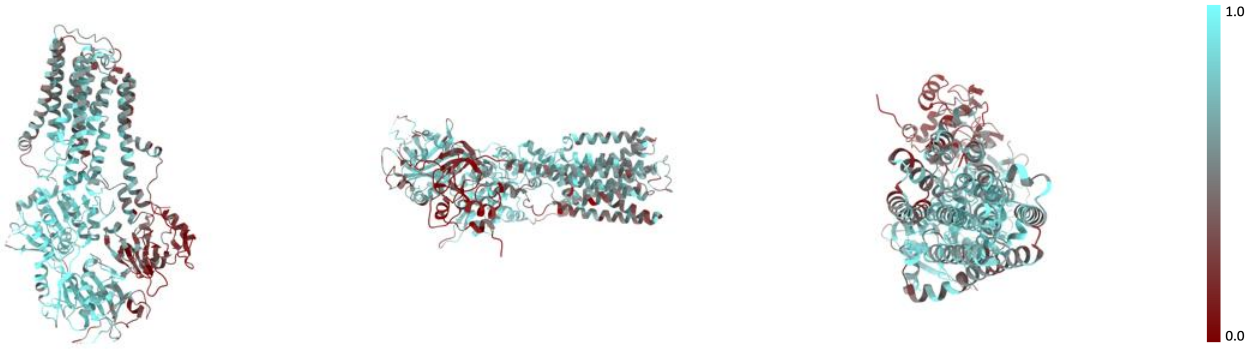
9.2 Q-score mapped to coordinate model (i)



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.

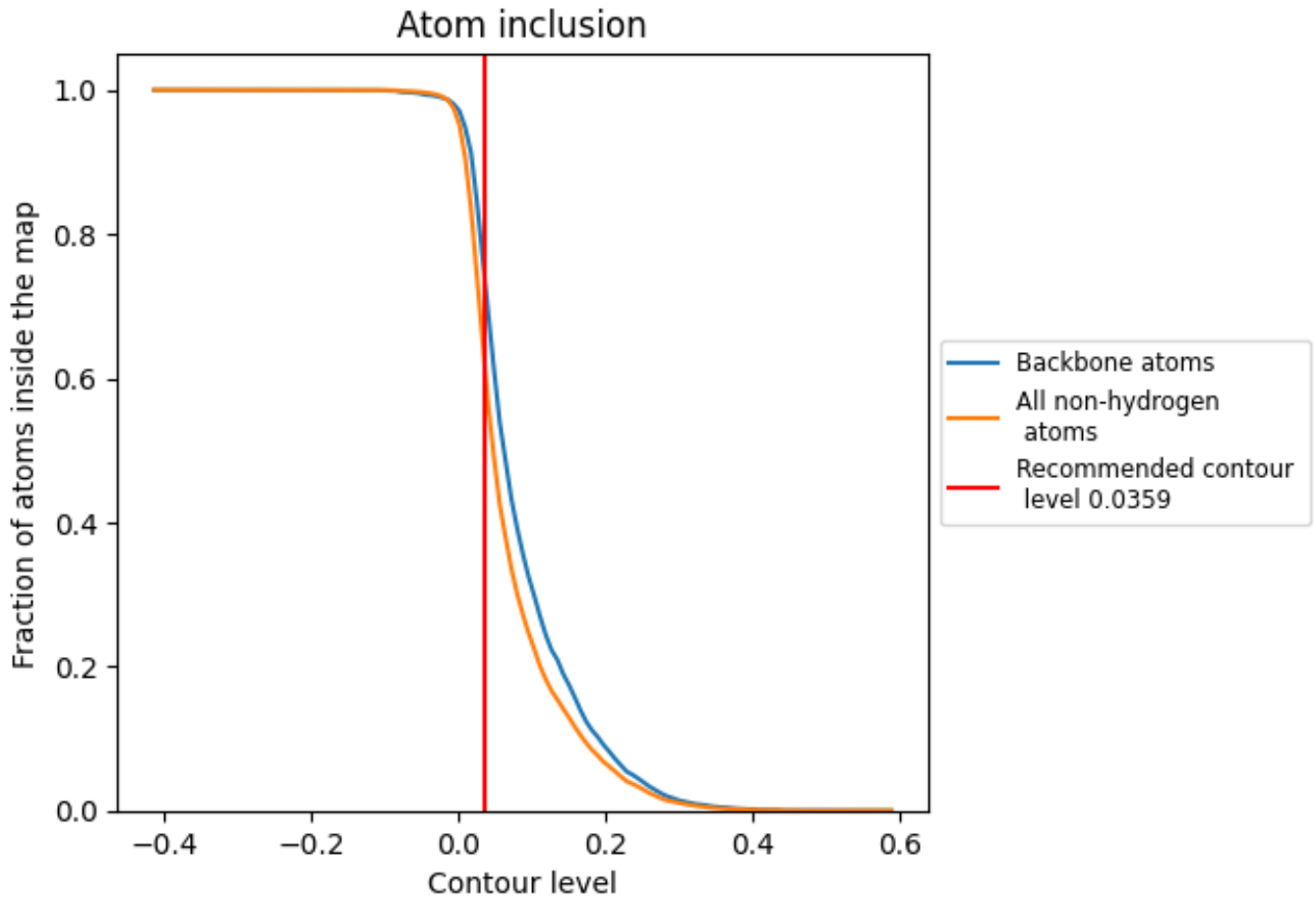
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0359).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0359) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6102	0.3720
A	0.6102	0.3720