Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 04:44 pm BST

PDB ID	:	7OP1 / pdb_00007op1
EMDB ID	:	EMD-13011
Title	:	Cryo-EM structure of P5B-ATPase E2PiAlF/SPM
Authors	:	Li, P.; Gourdon, P.
Deposited on	:	2021-05-28
Resolution	:	3.70 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:

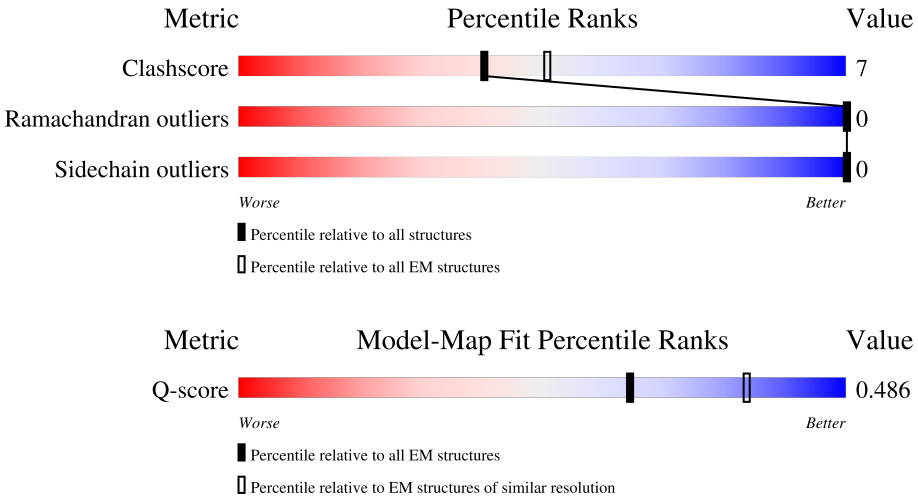
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	1393	14% 65% 14% 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8744 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 Cation-transporting ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1098	Total	C	N	O	S	0	0
			8724	5673	1448	1550	53		

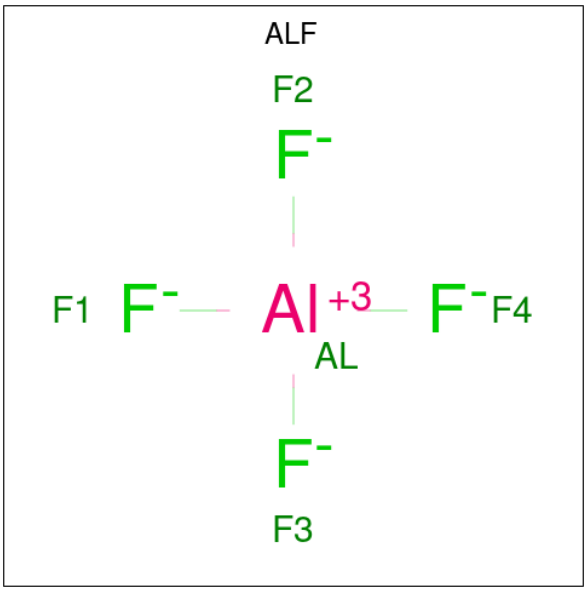
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1389	GLU	-	expression tag	UNP G0S7G9
A	1390	ASN	-	expression tag	UNP G0S7G9
A	1391	LEU	-	expression tag	UNP G0S7G9
A	1392	TYR	-	expression tag	UNP G0S7G9
A	1393	PHE	-	expression tag	UNP G0S7G9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

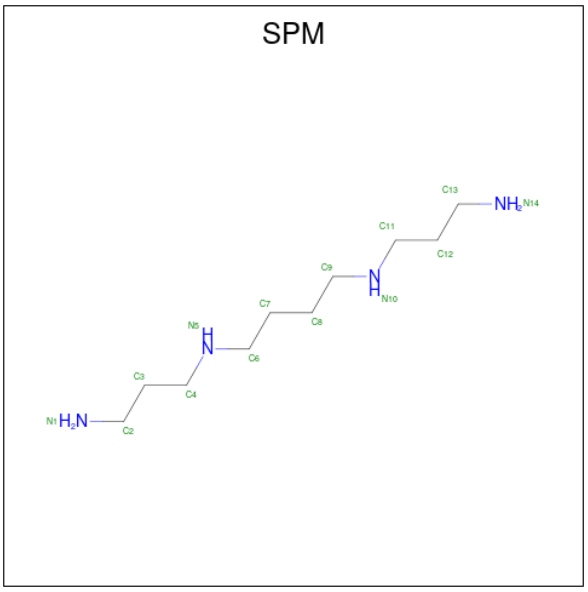
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mg	0
			1	1	

- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
3	A	1	5	1	4	0

- Molecule 4 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



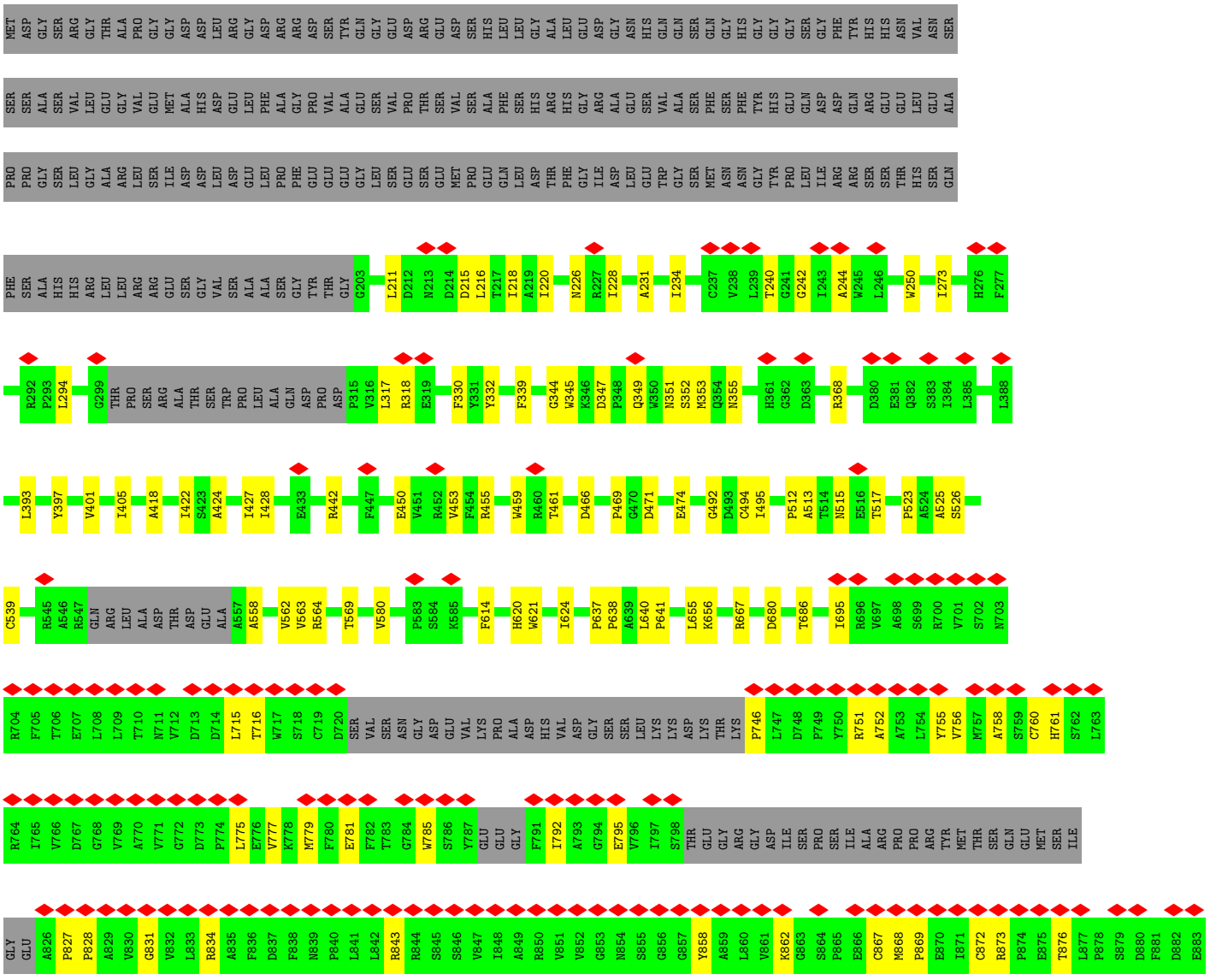
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
4	A	1	14	10	4	0

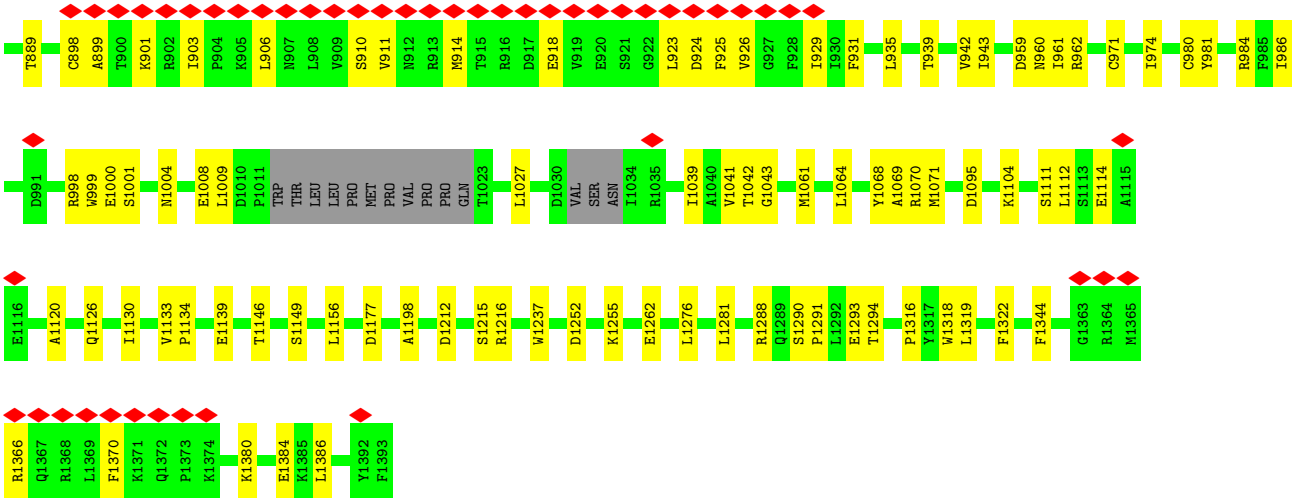
3 Residue-property plots (i)

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: Cation-transporting ATPase

Chain A:




T889
C898 A899 T900 K901 R902 I903 P904 K905 L906 N907 L908 V909 S910 V911 N912 R913 M914 T915 R916 D917 E918 V919 E920 S921 G922 L923 D924 F925 V926 G927 F928 I929 I930 F931 L935 T939 V942 I943 D959 N960 I961 R962 C971 I974 C980 Y981 R984 F985 I986
D991 R998 W999 E1000 S1001 N1004 E1008 L1009 D1010 P1011 TRP THR LEU LEU PRO MET PRO VAL PRO PRO GLN T1023 L1027 D1030 VAL SER ASN I1034 R1035 I1039 A1040 V1041 T1042 G1043 M1061 L1064 Y1068 A1069 R1070 M1071 D1095 K1104 S1111 L1112 S1113 E1114 A1115
E1116 A1120 Q1126 I1130 V1133 P1134 E1139 T1146 S1149 L1156 D1177 A1198 D1212 S1215 R1216 W1237 D1252 K1255 E1262 L1276 L1281 R1288 Q1289 S1290 P1291 L1292 E1293 T1294 P1316 Y1317 W1318 L1319 F1322 F1344 G1363 R1364 M1365
R1366 Q1367 R1368 L1369 F1370 K1371 Q1372 P1373 K1374 K1380 E1384 K1385 L1386 Y1392 F1393

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59345	Depositor
Resolution determination method	FSC 0.5 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 (6k x 4k)	Depositor
Maximum map value	2.387	Depositor
Minimum map value	-1.403	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	275.744, 275.744, 275.744	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86169994, 0.86169994, 0.86169994	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/8939	0.37	0/12141

There are no bond length outliers.

There are no bond angle outliers.

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	8724	0	8801	123	0
2	A	1	0	0	0	0
3	A	5	0	0	1	0
4	A	14	0	26	0	0
All	All	8744	0	8827	123	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 7.

All (123) 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:843:ARG:NH1	1:A:867:CYS:SG	2.61	0.73
1:A:939:THR:HG23	1:A:1130:ILE:HD11	1.72	0.72
1:A:353:MET:HE3	1:A:515:ASN:HA	1.73	0.71
1:A:889:THR:O	1:A:962:ARG:NH1	2.25	0.69
1:A:1316:PRO:HD2	1:A:1319:LEU:HD12	1.76	0.66
1:A:1068:TYR:HB3	1:A:1071:MET:HE3	1.77	0.66
1:A:1290:SER:OG	1:A:1293:GLU:OE1	2.13	0.65
1:A:901:LYS:HB2	1:A:923:LEU:HD23	1.78	0.65
1:A:655:LEU:HD21	1:A:1139:GLU:HG3	1.80	0.63
1:A:347:ASP:OD2	1:A:349:GLN:HG2	1.99	0.62
1:A:998:ARG:NH2	1:A:1008:GLU:OE2	2.30	0.62
1:A:1237:TRP:NE1	1:A:1262:GLU:OE2	2.30	0.62
1:A:614:PHE:HB3	1:A:624:ILE:HG12	1.80	0.62
1:A:211:LEU:HD11	1:A:218:ILE:HD13	1.83	0.60
1:A:834:ARG:NH2	1:A:911:VAL:O	2.35	0.60
1:A:695:ILE:HG12	1:A:929:ILE:HG22	1.83	0.60
1:A:686:THR:HA	1:A:935:LEU:HA	1.84	0.59
1:A:250:TRP:NE1	1:A:393:LEU:O	2.34	0.59
1:A:1095:ASP:HB3	1:A:1112:LEU:HB2	1.85	0.58
1:A:1380:LYS:O	1:A:1384:GLU:HG2	2.04	0.58
1:A:695:ILE:HD12	1:A:715:LEU:HD11	1.85	0.58
1:A:1198:ALA:HB3	1:A:1288:ARG:HH21	1.70	0.57
1:A:943:ILE:HG13	1:A:971:CYS:SG	2.45	0.56
1:A:455:ARG:NH2	1:A:466:ASP:O	2.39	0.56
1:A:876:THR:HG21	1:A:924:ASP:HA	1.87	0.56
1:A:640:LEU:HB3	1:A:641:PRO:HD3	1.88	0.56
1:A:777:VAL:O	1:A:781:GLU:HG3	2.06	0.55
1:A:914:MET:HE2	1:A:918:GLU:HB2	1.89	0.55
1:A:368:ARG:NH1	1:A:469:PRO:O	2.40	0.54
1:A:459:TRP:CZ3	1:A:474:GLU:HB2	2.43	0.54
1:A:240:THR:HG21	1:A:244:ALA:H	1.73	0.53
1:A:345:TRP:CE2	1:A:347:ASP:HB2	2.44	0.53
1:A:792:ILE:HG22	1:A:831:GLY:HA2	1.91	0.53
1:A:903:ILE:HG21	1:A:906:LEU:HD13	1.91	0.52
1:A:450:GLU:OE2	1:A:461:THR:HG22	2.10	0.52
1:A:220:ILE:HG13	1:A:273:ILE:HG12	1.90	0.52
1:A:873:ARG:NH1	1:A:924:ASP:OD1	2.43	0.52
1:A:1041:VAL:HG12	1:A:1042:THR:O	2.11	0.50
1:A:1276:LEU:HD13	1:A:1344:PHE:HB2	1.93	0.50
1:A:680:ASP:OD1	3:A:1402:ALF:F4	2.20	0.49
1:A:746:PRO:HG2	1:A:858:TYR:CG	2.46	0.49
1:A:492:GLY:O	1:A:512:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:VAL:HG12	1:A:564:ARG:HG3	1.95	0.49
1:A:758:ALA:O	1:A:761:HIS:NE2	2.43	0.49
1:A:294:LEU:HD12	1:A:317:LEU:HD12	1.95	0.49
1:A:332:TYR:HB2	1:A:339:PHE:HE1	1.78	0.48
1:A:453:VAL:HG23	1:A:455:ARG:HG2	1.95	0.48
1:A:211:LEU:HD21	1:A:330:PHE:HZ	1.78	0.48
1:A:216:LEU:HD11	1:A:580:VAL:HG11	1.96	0.48
1:A:899:ALA:HA	1:A:926:VAL:HG23	1.95	0.48
1:A:1237:TRP:HE1	1:A:1262:GLU:CD	2.22	0.47
1:A:775:LEU:HD13	1:A:931:PHE:HE2	1.79	0.47
1:A:984:ARG:NH1	1:A:1000:GLU:OE2	2.47	0.47
1:A:1114:GLU:OE2	1:A:1126:GLN:NE2	2.47	0.47
1:A:751:ARG:HG2	1:A:755:TYR:CZ	2.50	0.47
1:A:424:ALA:O	1:A:428:ILE:HG12	2.15	0.46
1:A:1212:ASP:OD2	1:A:1215:SER:HB2	2.16	0.46
1:A:513:ALA:HB1	1:A:517:THR:HG21	1.98	0.46
1:A:492:GLY:HA3	1:A:558:ALA:HB2	1.98	0.46
1:A:525:ALA:O	1:A:526:SER:OG	2.28	0.46
1:A:756:VAL:O	1:A:760:CYS:HB2	2.16	0.46
1:A:494:CYS:SG	1:A:495:ILE:N	2.89	0.46
1:A:716:THR:O	1:A:751:ARG:NH2	2.41	0.46
1:A:935:LEU:H	1:A:935:LEU:HD23	1.81	0.46
1:A:1291:PRO:HA	1:A:1294:THR:HG22	1.97	0.46
1:A:942:VAL:HG21	1:A:1130:ILE:O	2.16	0.46
1:A:986:ILE:HD12	1:A:998:ARG:HD2	1.97	0.45
1:A:1061:MET:HE2	1:A:1061:MET:HB3	1.91	0.45
1:A:1068:TYR:HB3	1:A:1071:MET:CE	2.45	0.45
1:A:418:ALA:O	1:A:422:ILE:HG23	2.16	0.45
1:A:1064:LEU:HD11	1:A:1386:LEU:HD13	1.99	0.45
1:A:1318:TRP:O	1:A:1322:PHE:CB	2.65	0.45
1:A:1104:LYS:HB2	1:A:1120:ALA:HB1	1.98	0.44
1:A:1133:VAL:HB	1:A:1134:PRO:HD3	1.99	0.44
1:A:471:ASP:O	1:A:562:VAL:HG12	2.18	0.44
1:A:1146:THR:OG1	1:A:1288:ARG:NH1	2.51	0.44
1:A:620:HIS:CE1	1:A:621:TRP:CD1	3.06	0.44
1:A:981:TYR:O	1:A:1039:ILE:HA	2.18	0.44
1:A:756:VAL:HG11	1:A:898:CYS:HB3	2.00	0.44
1:A:1177:ASP:OD1	1:A:1177:ASP:N	2.47	0.44
1:A:215:ASP:OD1	1:A:216:LEU:N	2.44	0.43
1:A:442:ARG:O	1:A:442:ARG:HD2	2.18	0.43
1:A:1215:SER:OG	1:A:1216:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASN:HB3	1:A:228:ILE:HG22	1.99	0.43
1:A:1149:SER:OG	1:A:1281:LEU:O	2.30	0.43
1:A:1156:LEU:HD12	1:A:1281:LEU:HD11	1.99	0.43
1:A:397:TYR:CZ	1:A:427:ILE:HD11	2.54	0.43
1:A:397:TYR:CE2	1:A:427:ILE:HD11	2.53	0.43
1:A:868:MET:N	1:A:869:PRO:HD2	2.34	0.43
1:A:1111:SER:OG	1:A:1112:LEU:N	2.51	0.43
1:A:401:VAL:O	1:A:405:ILE:HG12	2.19	0.43
1:A:959:ASP:OD1	1:A:960:ASN:N	2.46	0.43
1:A:1041:VAL:HG21	1:A:1061:MET:SD	2.58	0.42
1:A:211:LEU:HD21	1:A:330:PHE:CZ	2.54	0.42
1:A:351:ASN:OD1	1:A:352:SER:N	2.52	0.42
1:A:1043:GLY:HA3	1:A:1070:ARG:O	2.19	0.42
1:A:539:CYS:HB3	1:A:569:THR:HG21	2.01	0.42
1:A:827:PRO:HA	1:A:828:PRO:HD3	1.92	0.42
1:A:344:GLY:HA3	1:A:523:PRO:HG2	2.01	0.42
1:A:1318:TRP:O	1:A:1322:PHE:HB3	2.20	0.42
1:A:910:SER:O	1:A:914:MET:HG3	2.19	0.42
1:A:1001:SER:HB3	1:A:1004:ASN:O	2.20	0.42
1:A:1252:ASP:HB3	1:A:1255:LYS:O	2.20	0.42
1:A:317:LEU:HD23	1:A:318:ARG:N	2.35	0.41
1:A:351:ASN:OD1	1:A:355:ASN:ND2	2.54	0.41
1:A:656:LYS:HB2	1:A:656:LYS:HE2	1.79	0.41
1:A:779:MET:HE1	1:A:862:LYS:NZ	2.36	0.41
1:A:226:ASN:C	1:A:228:ILE:H	2.28	0.41
1:A:1130:ILE:O	1:A:1130:ILE:HG13	2.21	0.41
1:A:999:TRP:HB2	1:A:1009:LEU:HB2	2.03	0.41
1:A:240:THR:HG23	1:A:242:GLY:H	1.86	0.41
1:A:637:PRO:HA	1:A:638:PRO:HD3	1.89	0.41
1:A:974:ILE:HD13	1:A:980:CYS:SG	2.60	0.41
1:A:785:TRP:CZ3	1:A:795:GLU:HG2	2.56	0.41
1:A:876:THR:HB	1:A:925:PHE:H	1.85	0.41
1:A:872:CYS:SG	1:A:923:LEU:HB2	2.62	0.40
1:A:1027:LEU:HD23	1:A:1027:LEU:HA	1.90	0.40
1:A:231:ALA:HA	1:A:234:ILE:HG22	2.03	0.40
1:A:353:MET:HE2	1:A:353:MET:N	2.36	0.40
1:A:961:ILE:HD13	1:A:1069:ALA:HB3	2.03	0.40
1:A:667:ARG:HA	1:A:667:ARG:HD3	1.83	0.40
1:A:752:ALA:O	1:A:756:VAL:HG23	2.21	0.40
1:A:1366:ARG:HG2	1:A:1370:PHE:HD2	1.86	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	1082/1393 (78%)	1031 (95%)	51 (5%)	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	959/1204 (80%)	959 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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	355	ASN
1	A	620	HIS
1	A	1233	GLN
1	A	1372	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ALF	A	1402	1	0,4,4	-	-	-		
4	SPM	A	1403	-	13,13,13	0.34	0	12,12,12	0.72	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
4	SPM	A	1403	-	-	6/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1403	SPM	C7-C8-C9-N10
4	A	1403	SPM	N5-C6-C7-C8
4	A	1403	SPM	C12-C11-N10-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1403	SPM	C6-C7-C8-C9
4	A	1403	SPM	C8-C9-N10-C11
4	A	1403	SPM	C7-C6-N5-C4

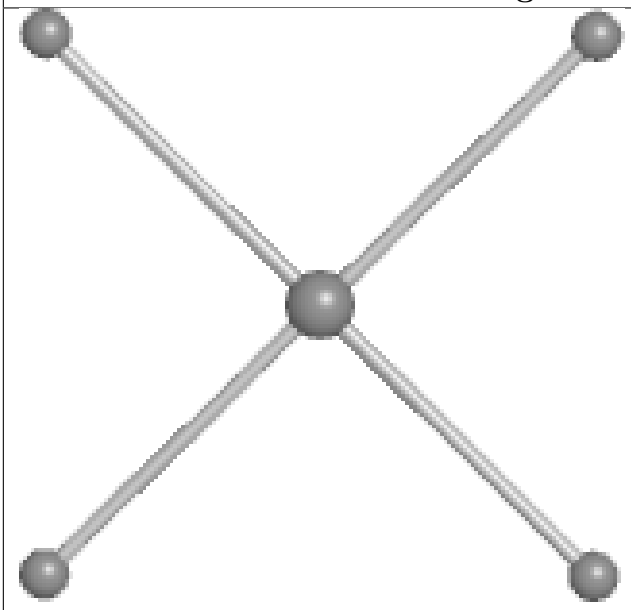
There are no ring outliers.

1 monomer is involved in 1 short contact:

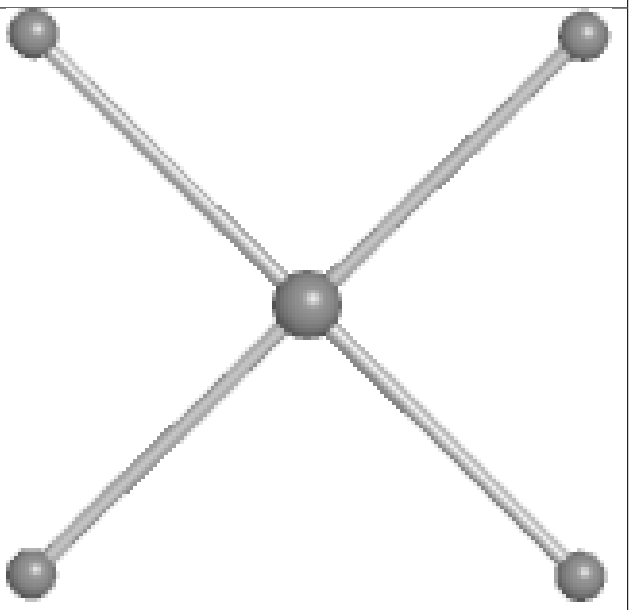
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	ALF	1	0

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.

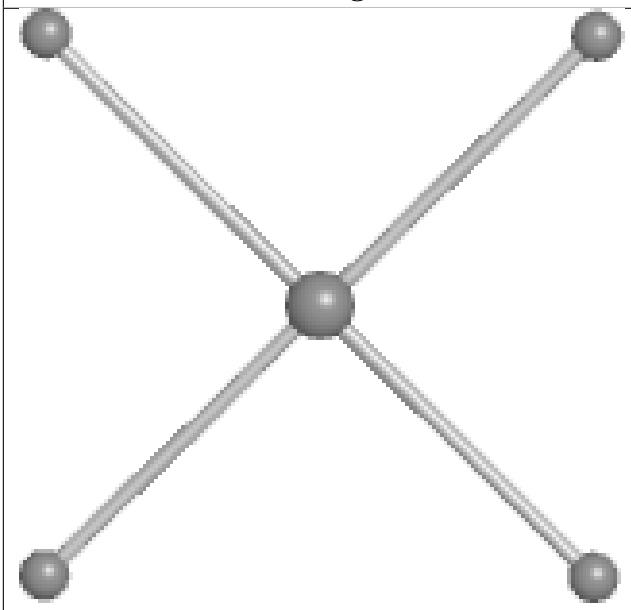
Ligand ALF A 1402



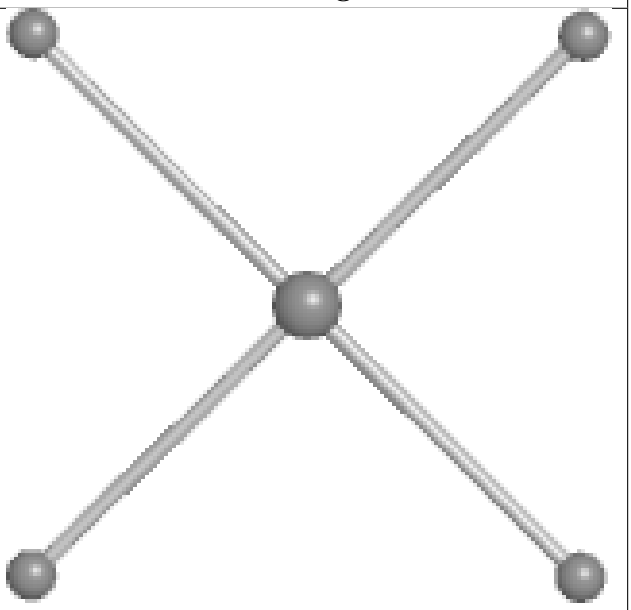
Bond lengths



Bond angles



Torsions

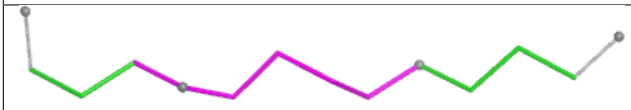


Rings

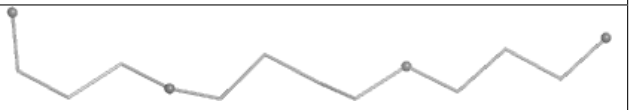
Ligand SPM A 1403

Bond lengths

Bond angles



Torsions



Rings

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.

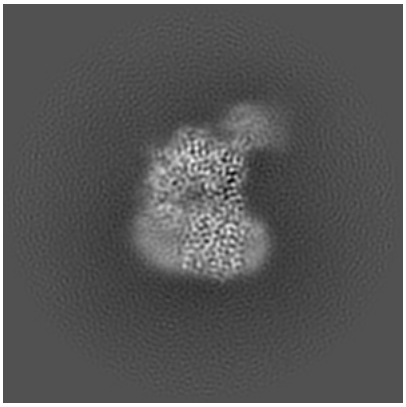
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13011. These allow visual inspection of the internal detail of the map and identification of artifacts.

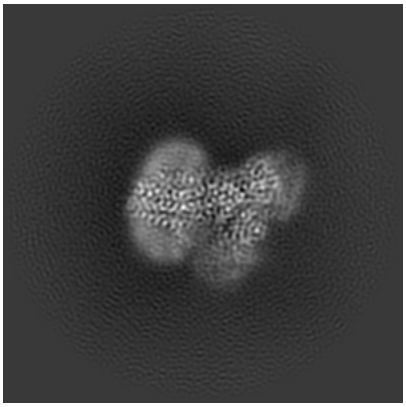
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

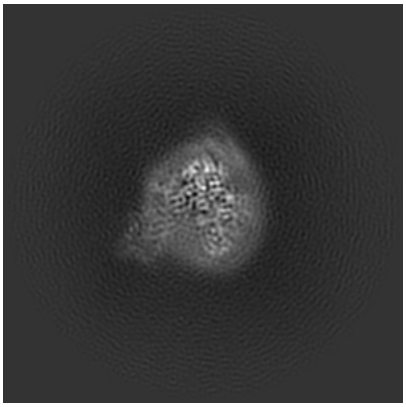
6.1.1 Primary map



X



Y

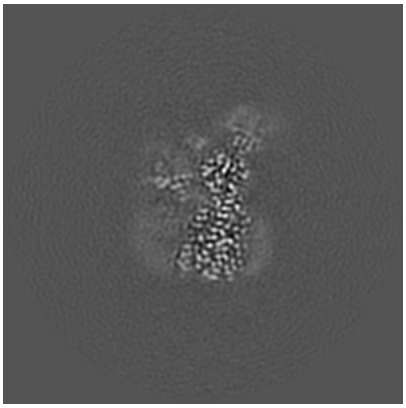


Z

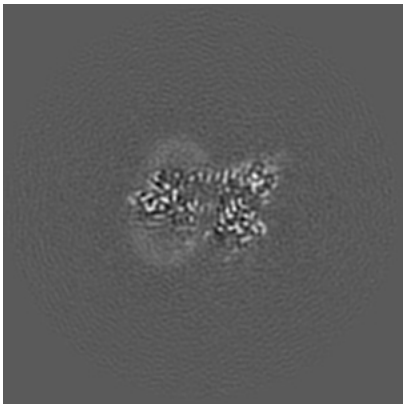
The images above show the map projected in three orthogonal directions.

6.2 Central slices

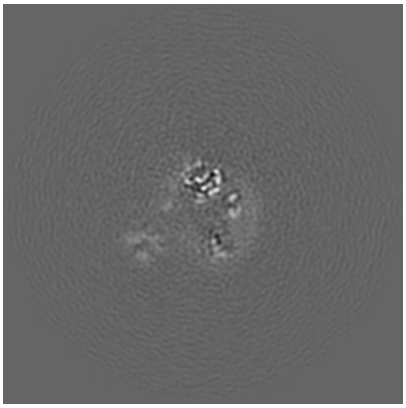
6.2.1 Primary map



X Index: 160



Y Index: 160

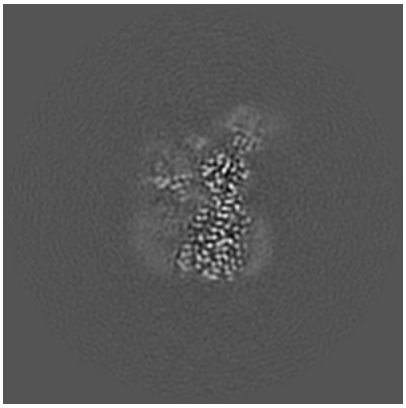


Z Index: 160

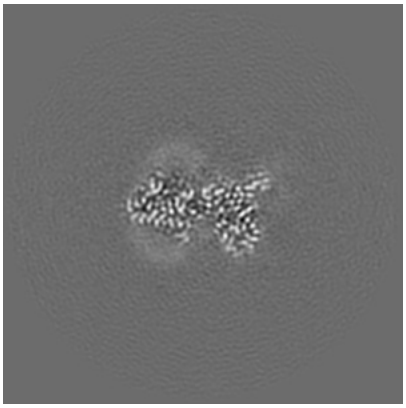
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

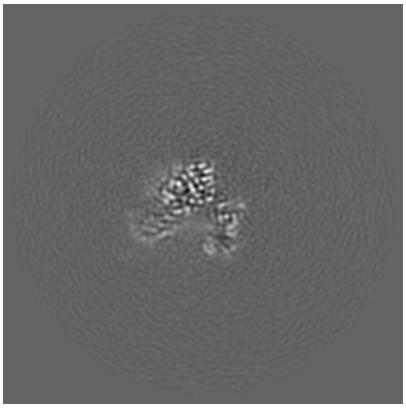
6.3.1 Primary map



X Index: 160



Y Index: 170

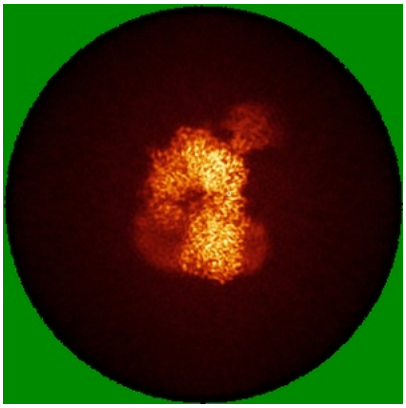


Z Index: 191

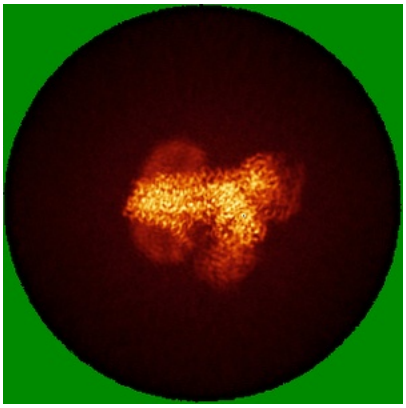
The images above show the largest variance slices of the map in three orthogonal directions.

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

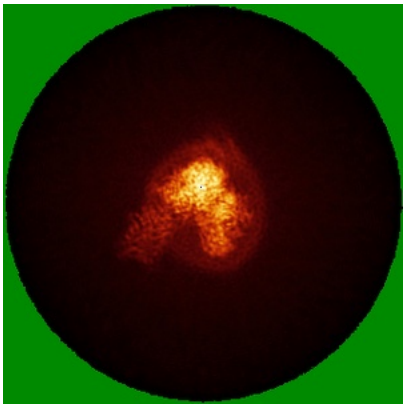
6.4.1 Primary map



X



Y



Z

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 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

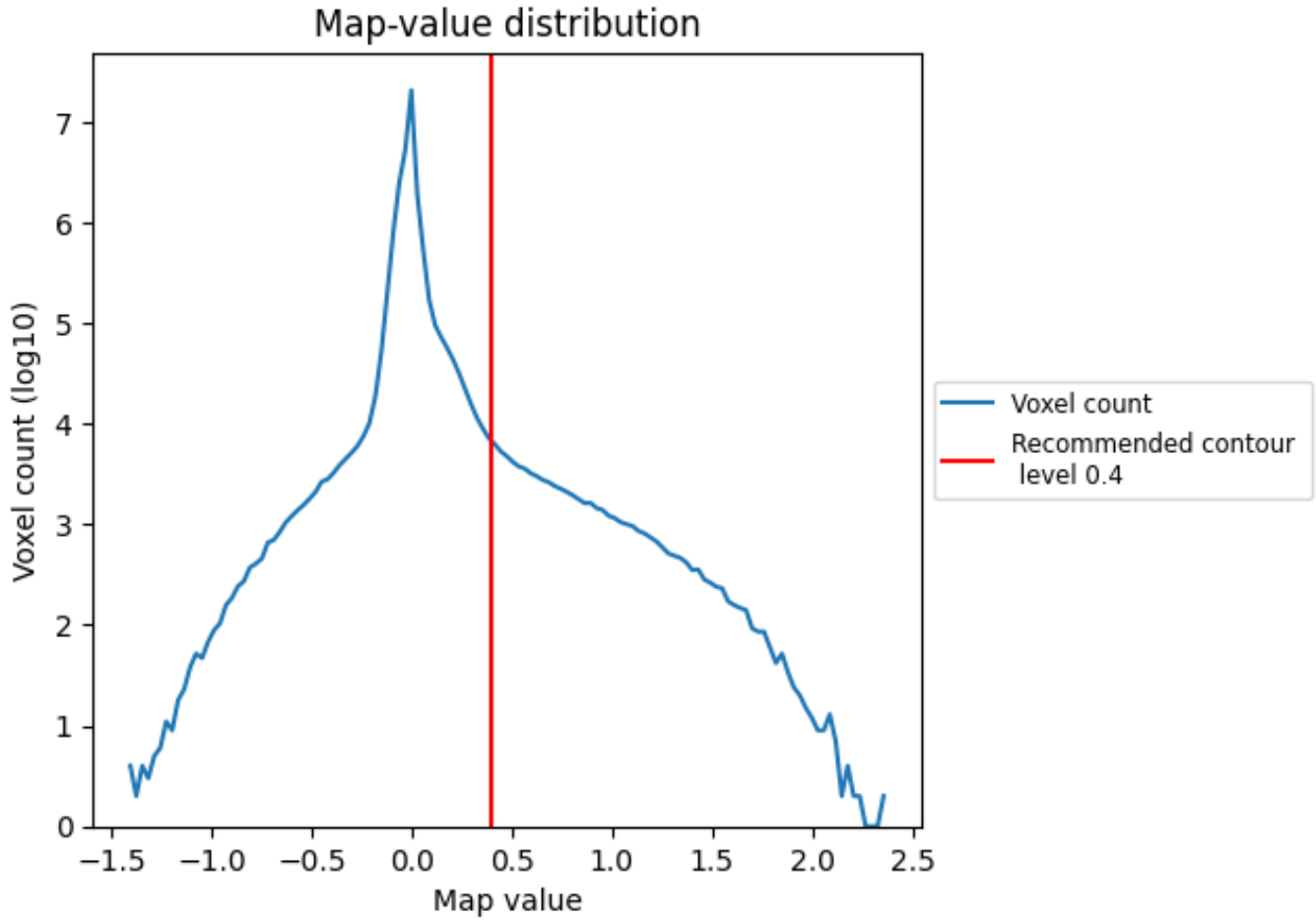
6.6 Mask visualisation (i)

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

7 Map analysis

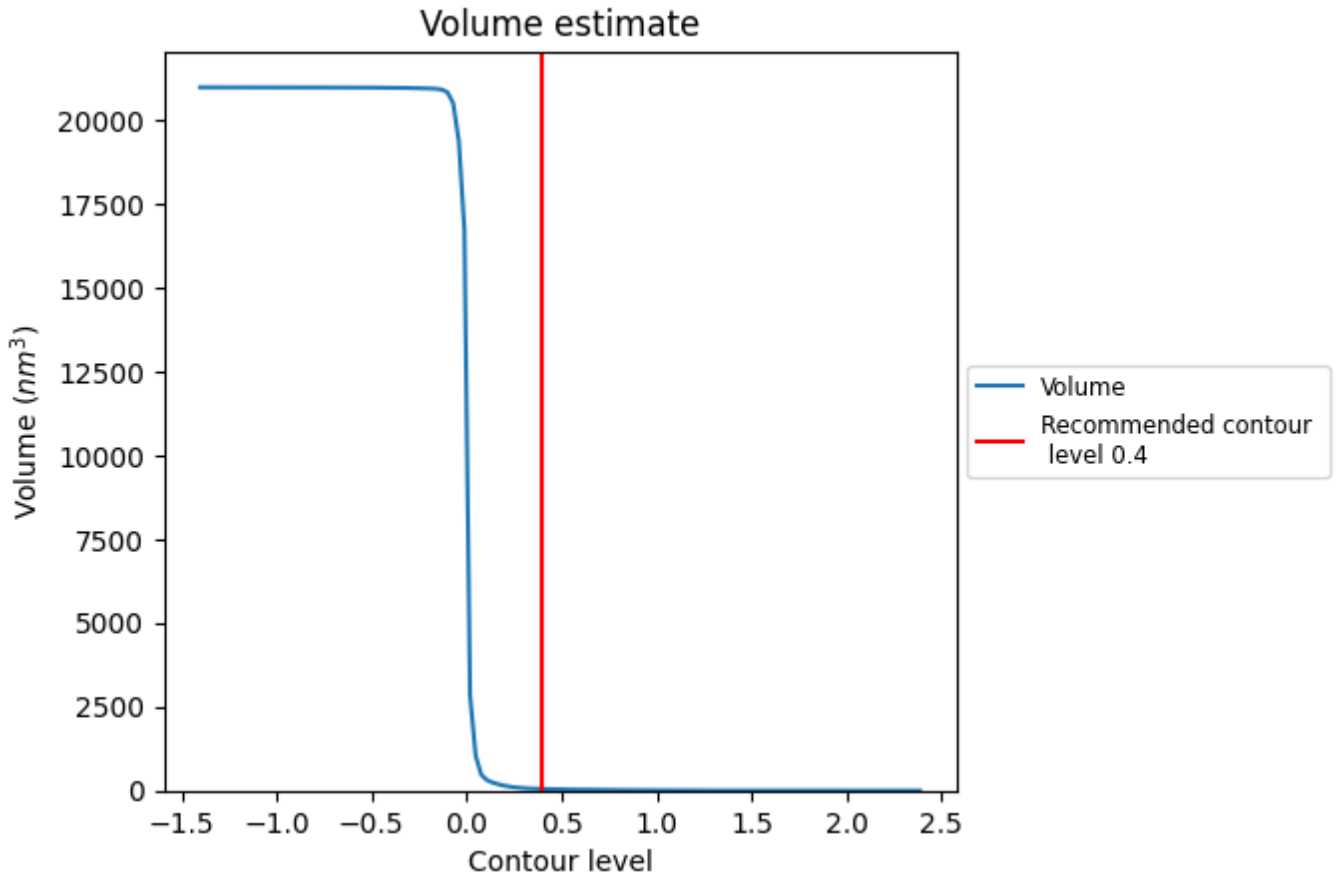
This section contains the results of statistical analysis of the map.

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.

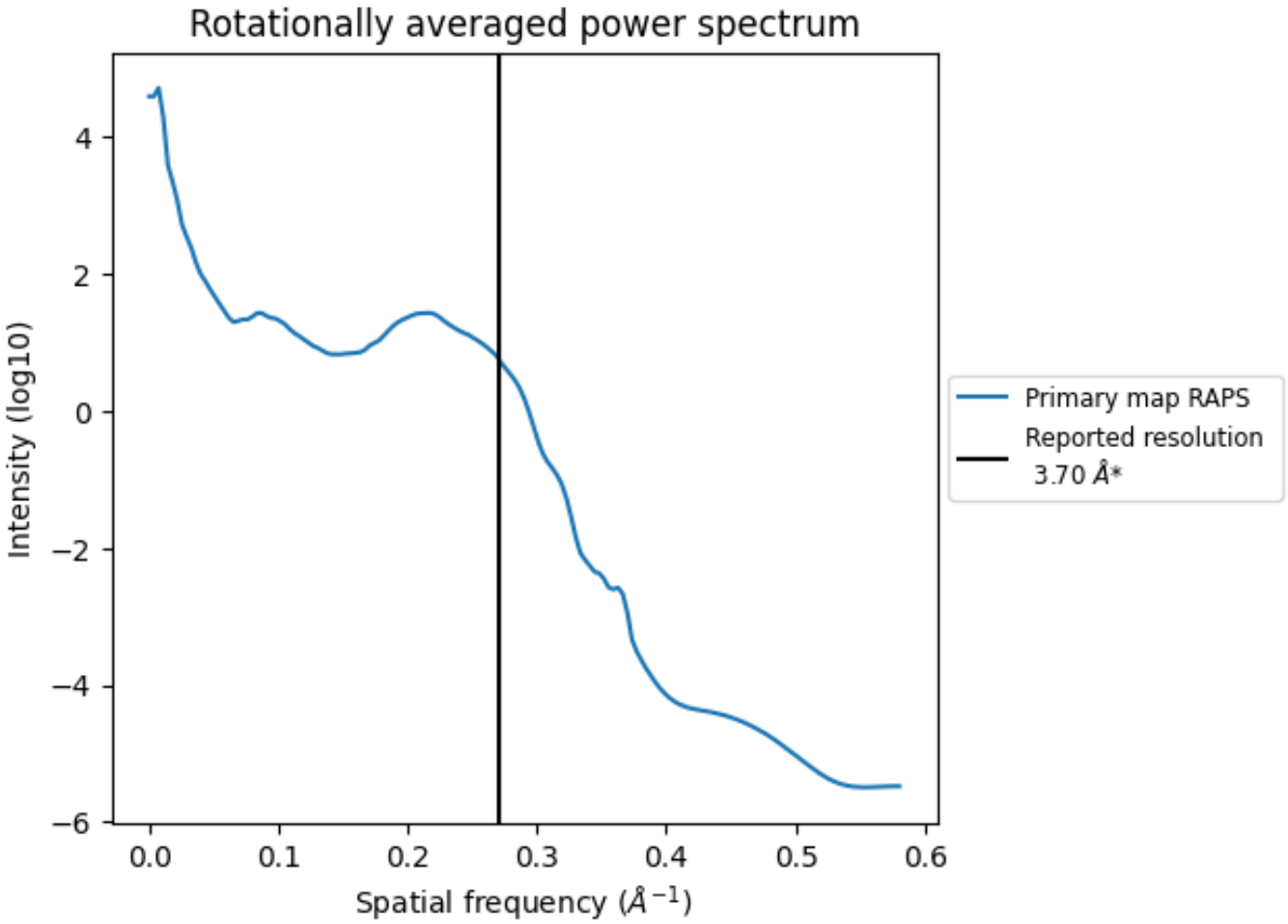
7.2 Volume estimate



The volume at the recommended contour level is 47 nm^3; this corresponds to an approximate mass of 43 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 0.270 Å^{-1}

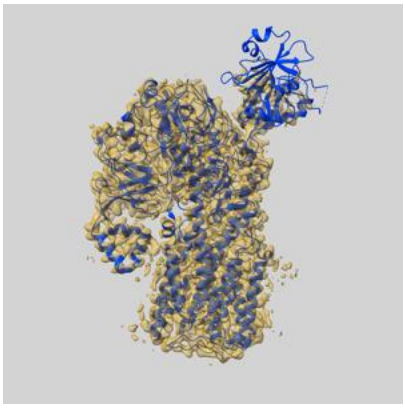
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

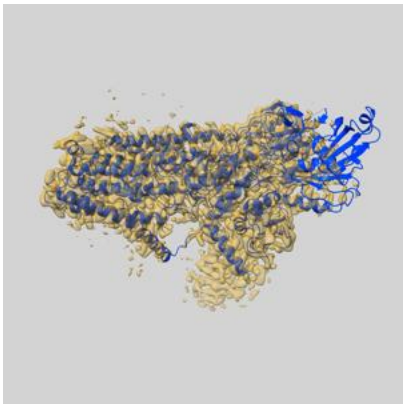
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13011 and PDB model 7OP1. Per-residue inclusion information can be found in section 3 on page 5.

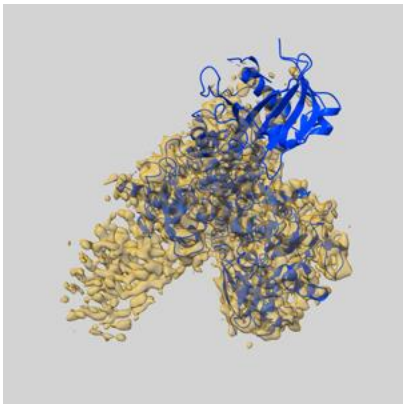
9.1 Map-model overlay



X



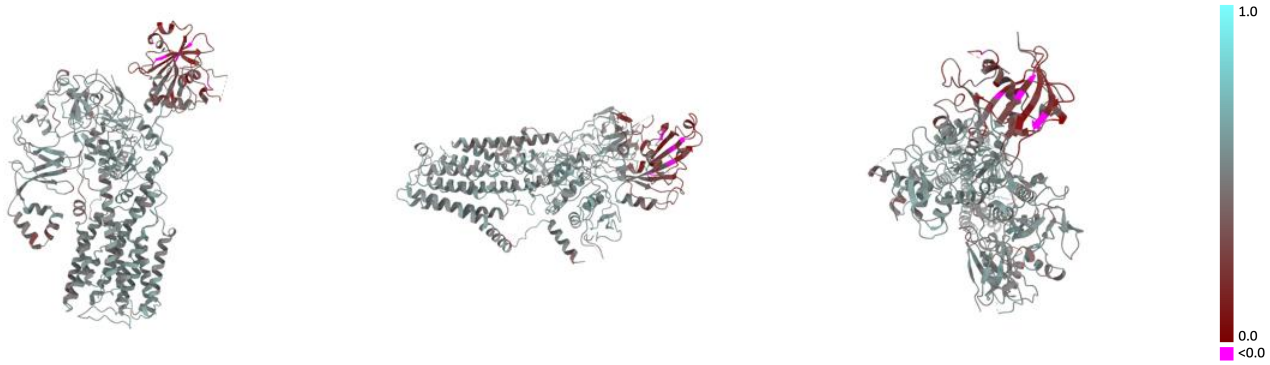
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

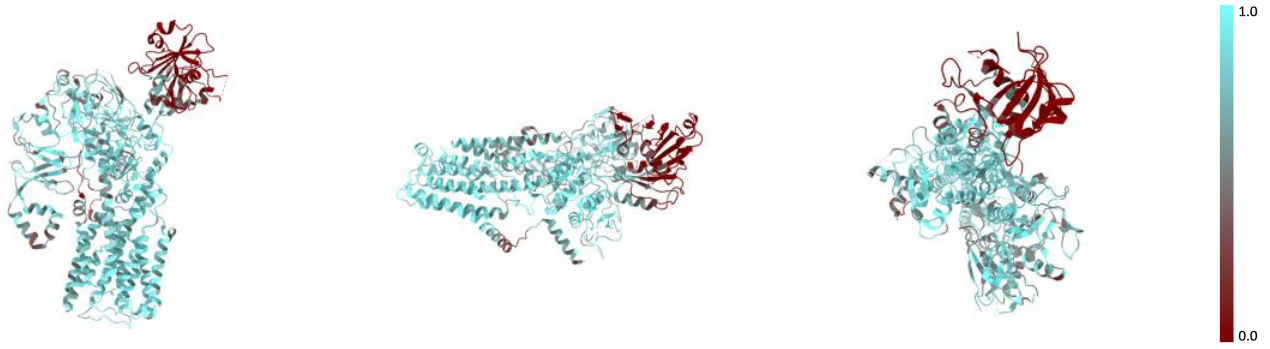
9.2 Q-score mapped to coordinate model (i)



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.

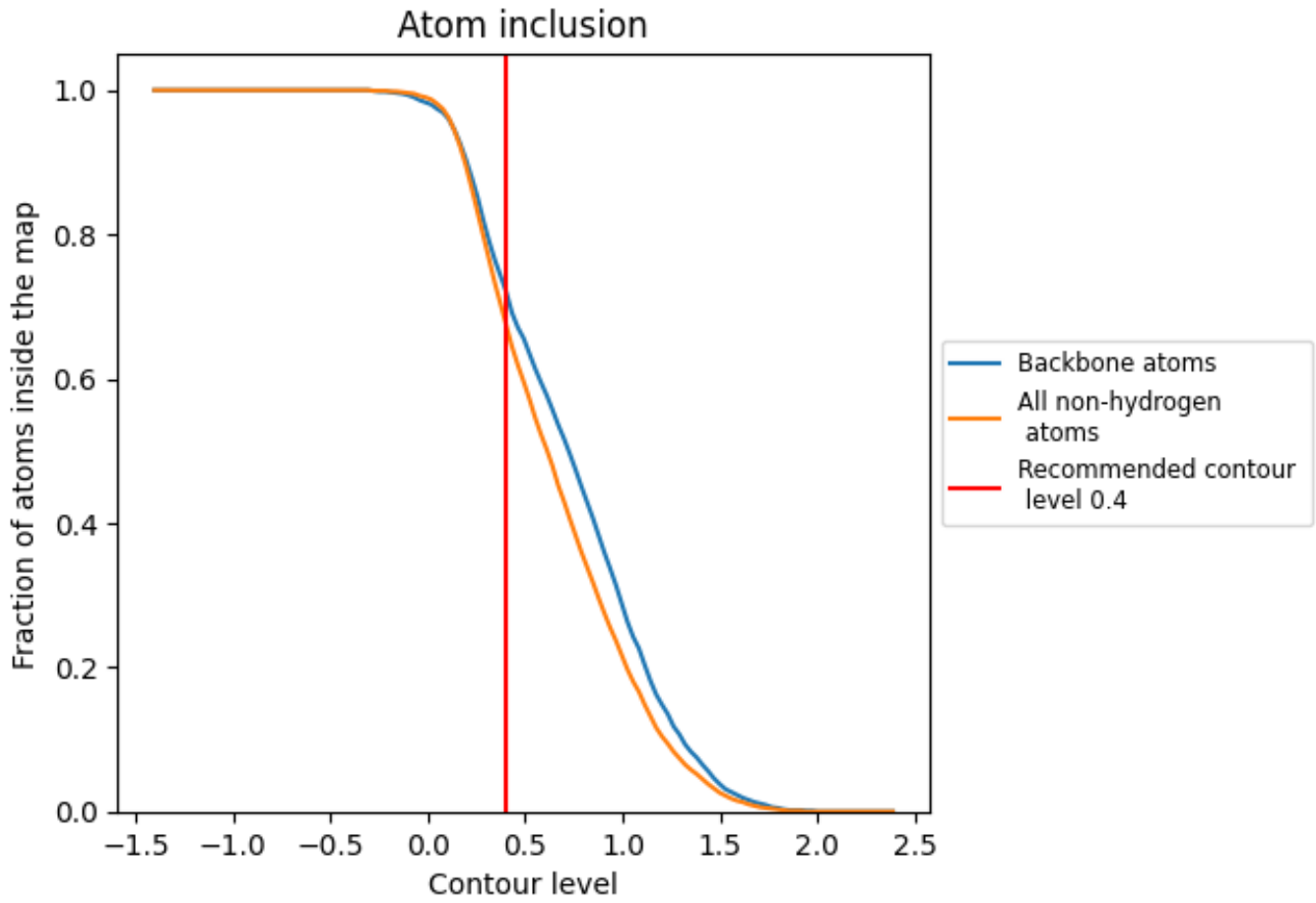
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 68% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6770	0.4860
A	0.6770	0.4860