Full wwPDB EM Validation Report ⓘ

Jul 9, 2024 – 10:15 PM JST

PDB ID	:	8XQ7
EMDB ID	:	EMD-38568
Title	:	Structure of the sea urchin spSLC9C1 in state-1 w/ cAMP dimer
Authors	:	Qu, H.; Zheng, X.
Deposited on	:	2024-01-04
Resolution	:	3.15 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:

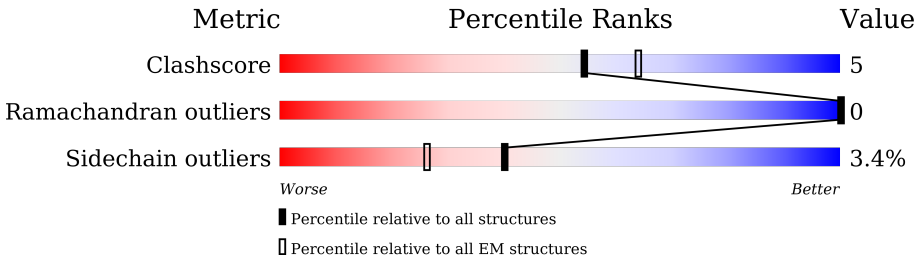
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.15 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	1196	5% 74% 12% 13%
1	B	1196	5% 73% 13% 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16430 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.

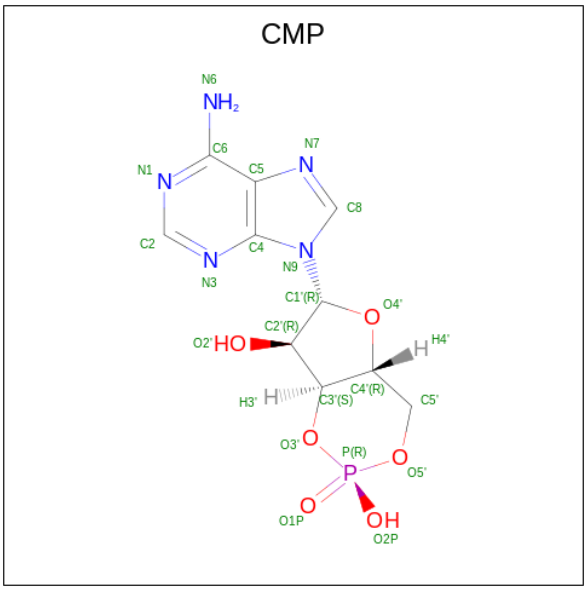
- Molecule 1 is a protein called Sperm-specific sodium proton exchanger.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1041	Total	C	N	O	S	0	0
			8193	5337	1357	1455	44		
1	B	1041	Total	C	N	O	S	0	0
			8193	5337	1357	1455	44		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	-	expression tag	UNP A3RL54
A	29	SER	-	expression tag	UNP A3RL54
B	28	GLY	-	expression tag	UNP A3RL54
B	29	SER	-	expression tag	UNP A3RL54

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$) (labeled as "Ligand of Interest" by depositor).

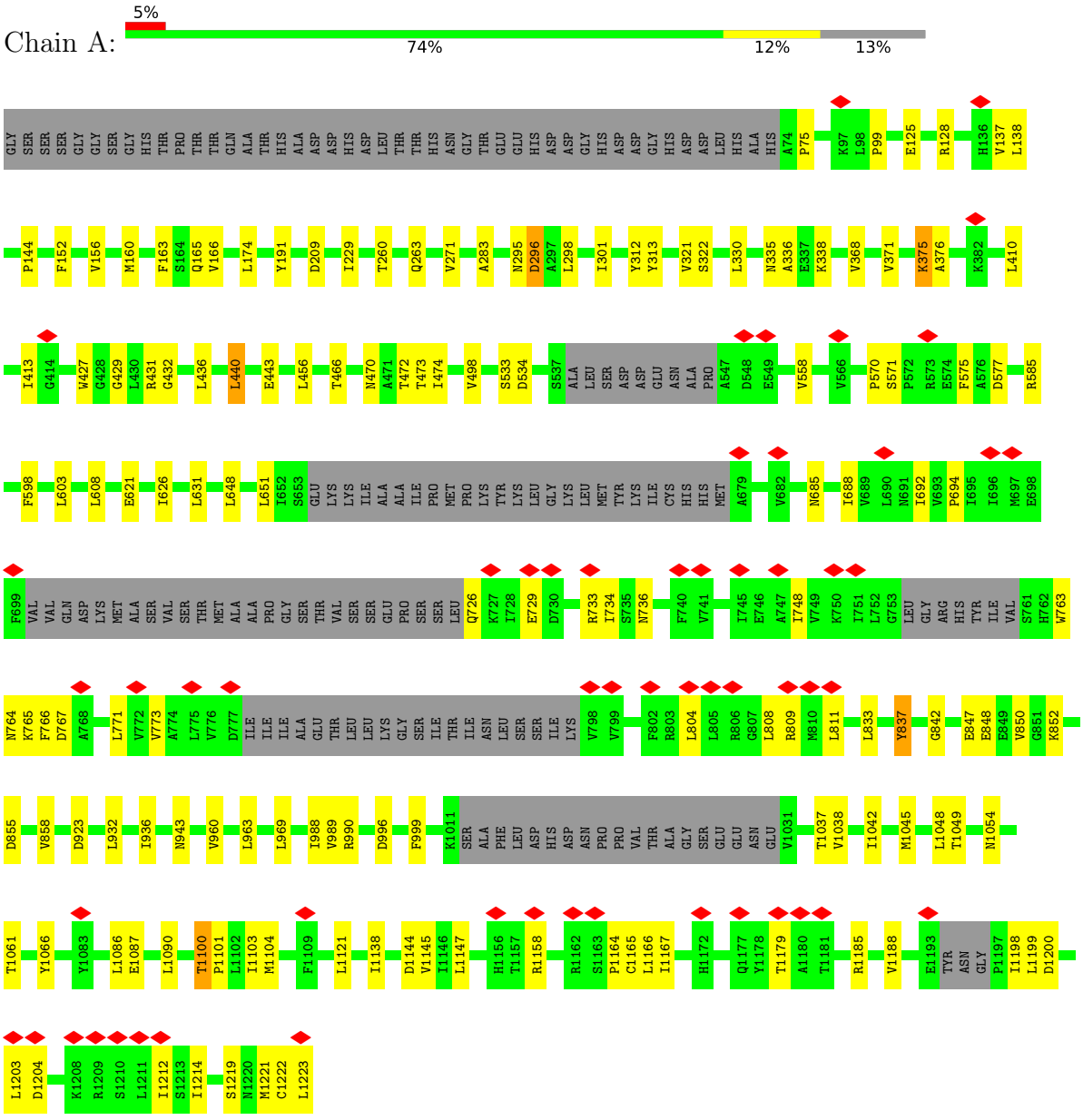


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	B	1	Total	C	N	O	P	0
			22	10	5	6	1	

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.

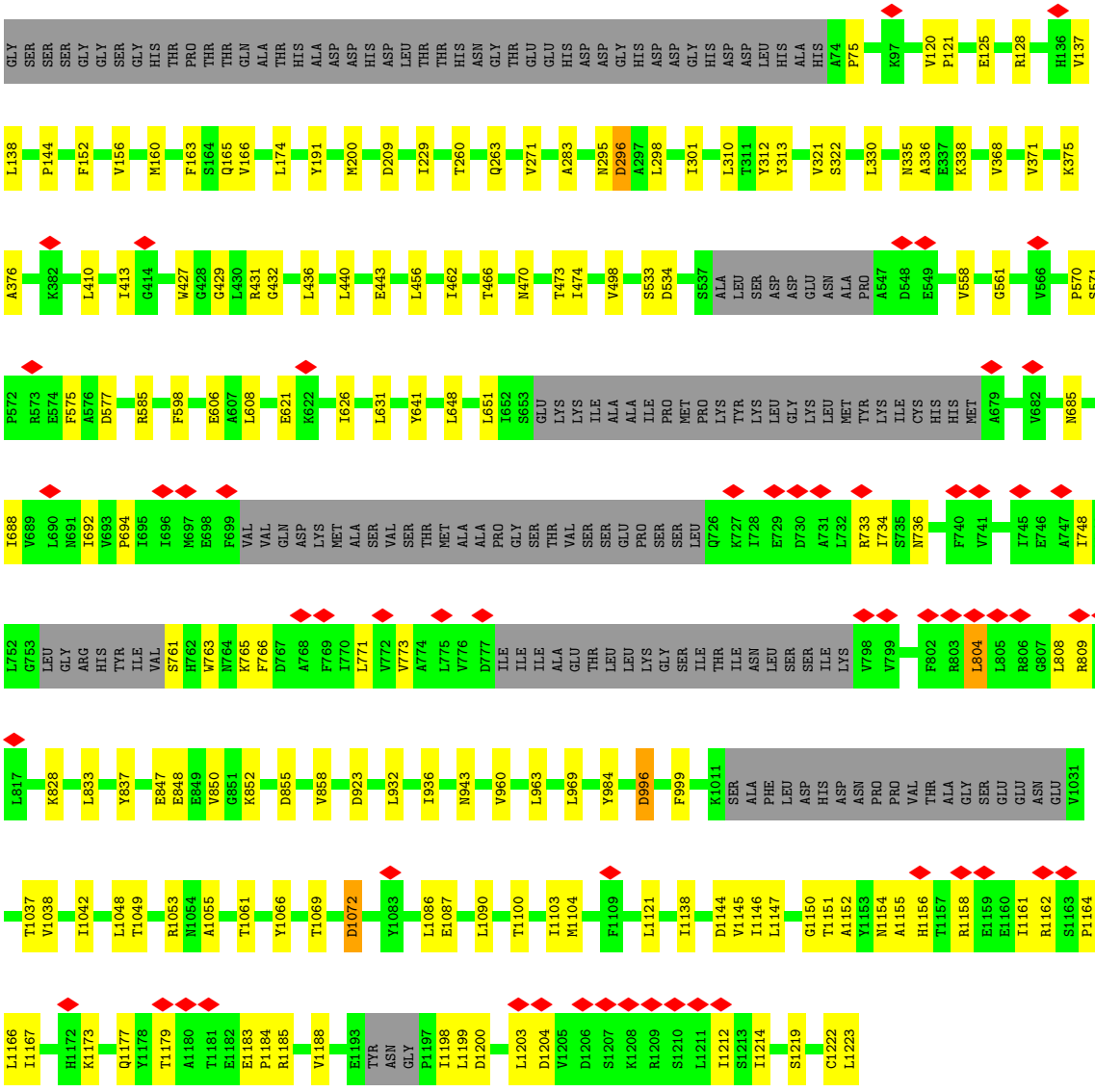
• Molecule 1: Sperm-specific sodium proton exchanger



• Molecule 1: Sperm-specific sodium proton exchanger

Chain B:


5%
73%
13%
13%


GLY SER SER SER GLY GLY SER GLY HIS THR PRO THR THR GLN ALA THR HIS ALA ASP ASP HIS ASP LEU THR THR HIS ASN GLY THR GLU GLU HIS ASP ASP GLY HIS ASP ASP GLY HIS ASP ASP LEU HIS ALA HIS A74 P75 K97 V120 P121 E125 R128 H136 V137
L138 P144 F152 V156 M160 F163 S164 Q165 V166 L174 Y191 M200 D209 I229 T260 Q263 V271 A283 N295 D296 A297 L298 I301 L310 T311 Y312 Y313 V321 S322 L330 N335 A336 E337 K338 V368 V371 K375
A376 K382 L410 I413 G414 W427 G428 G429 L430 R431 G432 L436 L440 E443 L456 I462 T466 N470 T473 I474 V498 S533 D534 S537 ALA LEU SER ASP ASP GLU ASN ALA PRO A547 D548 E549 V558 G561 V566 P570 S571
P572 R573 E574 F575 A576 D577 R585 F598 E606 A607 L608 E621 K622 I626 L631 Y641 L648 L651 I652 S653 GLU LYS LYS ILE ALA ALA ILE PRO MET PRO LYS TYR LYS LEU GLY LYS LEU MET TYR LYS ILE CYS HIS HIS MET A679 V682 N685
I688 V689 L690 N691 I692 V693 P694 I695 I696 M697 E698 F699 VAL VAL GLN ASP LYS MET ALA SER VAL SER THR MET ALA ALA PRO GLY SER THR VAL SER SER GLU PRO SER SER LEU Q726 K727 I728 E729 D730 A731 L732 R733 I734 S735 N736 F740 V741 I745 E746 A747 I748 V749 K750 I751
L752 G753 LEU GLY ARG HIS TYR ILE VAL S761 H762 W763 N764 K765 F766 D767 A768 F769 I770 L771 V772 V773 A774 L775 V776 D777 ILE ILE ILE ALA GLU THR LEU LEU LYS GLY SER ILE THR ILE ASN LEU SER SER ILE LYS V798 V799 F802 R803 L804 L805 R806 G807 L808 R809 M810 L811
L817 K828 L833 Y837 E847 E848 E849 V850 G851 K852 D855 V858 D923 L932 I936 N943 V960 L963 L969 Y984 D996 F999 K1011 SER ALA PHE LEU ASP HIS ASP ASN PRO PRO VAL THR ALA GLY SER GLU GLU ASN GLU V1031
T1037 V1038 I1042 L1048 T1049 R1053 N1054 A1055 T1061 Y1066 T1069 D1072 Y1083 L1086 E1087 L1090 T1100 I1103 M1104 F1109 L1121 I1138 D1144 V1145 I1146 L1147 G1150 T1151 A1152 Y1153 N1154 A1155 H1156 T1157 R1158 E1159 E1160 I1161 R1162 S1163 P1164 C1165
L1166 I1167 H1172 K1173 Q1177 Y1178 T1179 A1180 T1181 E1182 E1183 P1184 R1185 V1188 E1193 TYR ASN GLY P1197 I1198 L1199 D1200 L1203 D1204 V1205 D1206 S1207 K1208 R1209 S1210 L1211 I1212 S1213 I1214 S1219 C1222 L1223

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125603	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.712	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/8345	0.52	2/11314 (0.0%)
1	B	0.27	0/8345	0.52	2/11314 (0.0%)
All	All	0.27	0/16690	0.52	4/22628 (0.0%)

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
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	570	PRO	C-N-CA	5.50	135.44	121.70
1	A	570	PRO	C-N-CA	5.40	135.21	121.70
1	B	771	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	771	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	621	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8193	0	8513	90	0
1	B	8193	0	8513	99	0
2	A	22	0	11	2	0
2	B	22	0	11	2	0
All	All	16430	0	17048	180	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2001:CMP:C2	2:B:2001:CMP:H2	0.97	1.49
2:A:2001:CMP:H2	2:A:2001:CMP:C2	0.97	1.49
1:B:1147:LEU:CD2	1:B:1161:ILE:HG21	1.69	1.20
1:B:1147:LEU:HD21	1:B:1161:ILE:HG21	1.17	1.09
1:B:1147:LEU:HD21	1:B:1161:ILE:CG2	1.84	1.07
1:B:1147:LEU:HD11	1:B:1164:PRO:HA	1.51	0.90
1:B:1147:LEU:CD1	1:B:1164:PRO:HA	2.05	0.85
1:A:1147:LEU:CD1	1:A:1164:PRO:HA	2.14	0.77
1:A:1147:LEU:O	1:A:1147:LEU:HD12	1.85	0.76
1:A:1147:LEU:HD11	1:A:1164:PRO:HA	1.68	0.75
1:B:1198:ILE:HD12	1:B:1199:LEU:N	2.03	0.74
1:A:1198:ILE:HD12	1:A:1199:LEU:N	2.03	0.73
1:A:466:THR:O	1:A:470:ASN:HB2	1.90	0.71
1:B:466:THR:O	1:B:470:ASN:HB2	1.91	0.69
1:B:1147:LEU:CD2	1:B:1161:ILE:CG2	2.53	0.69
1:B:1147:LEU:HD12	1:B:1147:LEU:O	1.92	0.69
1:A:858:VAL:HG13	1:B:1223:LEU:HD11	1.77	0.67
1:A:368:VAL:HG21	1:A:436:LEU:HB3	1.78	0.66
1:A:1223:LEU:HD11	1:B:858:VAL:HG13	1.76	0.66
1:B:368:VAL:HG21	1:B:436:LEU:HB3	1.78	0.65
1:B:1198:ILE:HG13	1:B:1199:LEU:H	1.62	0.64
1:A:1198:ILE:HG13	1:A:1199:LEU:H	1.61	0.63
1:A:969:LEU:HD21	1:A:1086:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1103:ILE:HG13	1:B:1121:LEU:HD21	1.82	0.61
1:B:969:LEU:HD21	1:B:1086:LEU:HD13	1.83	0.60
1:A:1198:ILE:CG1	1:A:1199:LEU:H	2.14	0.60
1:A:1203:LEU:HB3	1:A:1214:ILE:HD13	1.84	0.60
1:B:1198:ILE:CG1	1:B:1199:LEU:H	2.15	0.59
1:B:1147:LEU:HD23	1:B:1161:ILE:HG21	1.78	0.59
1:B:1198:ILE:HD11	1:B:1219:SER:HA	1.85	0.59
1:B:1150:GLY:HA3	1:B:1184:PRO:HB3	1.85	0.59
1:B:1203:LEU:HB3	1:B:1214:ILE:HD13	1.85	0.58
1:A:1147:LEU:HD23	1:A:1167:ILE:HD11	1.86	0.58
1:A:1147:LEU:HD12	1:A:1164:PRO:HA	1.86	0.57
1:A:694:PRO:HB3	1:A:733:ARG:HD2	1.86	0.56
1:B:996:ASP:H	1:B:1053:ARG:HH22	1.54	0.56
1:A:1222:CYS:SG	1:A:1223:LEU:N	2.79	0.56
1:B:296:ASP:N	1:B:296:ASP:OD1	2.38	0.56
1:A:470:ASN:O	1:A:474:ILE:HB	2.05	0.56
1:A:1198:ILE:HD11	1:A:1219:SER:HA	1.88	0.56
1:B:999:PHE:HB2	1:B:1042:ILE:HB	1.88	0.56
1:B:1222:CYS:SG	1:B:1223:LEU:N	2.78	0.56
1:A:296:ASP:N	1:A:296:ASP:OD1	2.38	0.55
1:B:470:ASN:O	1:B:474:ILE:HB	2.06	0.55
1:B:694:PRO:HB3	1:B:733:ARG:HD2	1.88	0.55
1:B:1165:CYS:SG	1:B:1166:LEU:N	2.80	0.55
1:A:165:GLN:HG3	1:A:410:LEU:HG	1.89	0.54
1:B:165:GLN:HG3	1:B:410:LEU:HG	1.89	0.54
1:B:1048:LEU:HD11	1:B:1090:LEU:HB3	1.88	0.54
1:A:692:ILE:HG12	1:A:809:ARG:HE	1.73	0.54
1:A:1198:ILE:CG1	1:A:1199:LEU:N	2.71	0.54
1:B:626:ILE:HD11	1:B:631:LEU:HD21	1.90	0.54
1:A:1198:ILE:CD1	1:A:1199:LEU:N	2.70	0.53
1:A:558:VAL:HG23	1:A:577:ASP:HB3	1.90	0.53
1:A:626:ILE:HD11	1:A:631:LEU:HD21	1.90	0.53
1:A:1103:ILE:HG13	1:A:1121:LEU:HD21	1.90	0.53
1:B:1198:ILE:CG1	1:B:1199:LEU:N	2.71	0.53
1:A:166:VAL:HG23	1:A:229:ILE:HD13	1.90	0.53
1:B:558:VAL:HG23	1:B:577:ASP:HB3	1.91	0.53
1:B:1087:GLU:OE2	1:B:1185:ARG:NH2	2.42	0.53
1:B:848:GLU:OE1	1:B:852:LYS:NZ	2.42	0.52
1:B:1198:ILE:CD1	1:B:1199:LEU:N	2.70	0.52
1:B:923:ASP:OD1	1:B:923:ASP:N	2.39	0.52
1:A:295:ASN:HD21	1:A:932:LEU:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:ILE:HG12	1:B:809:ARG:HE	1.73	0.52
1:B:295:ASN:HD21	1:B:932:LEU:HD13	1.75	0.52
1:B:1183:GLU:O	1:B:1185:ARG:NH1	2.43	0.52
1:A:999:PHE:HB2	1:A:1042:ILE:HB	1.90	0.52
1:B:166:VAL:HG23	1:B:229:ILE:HD13	1.92	0.52
1:A:75:PRO:HD2	1:B:313:TYR:HE2	1.75	0.51
1:A:209:ASP:HB2	1:A:432:GLY:HA3	1.92	0.51
1:B:209:ASP:HB2	1:B:432:GLY:HA3	1.92	0.51
1:B:1147:LEU:HD12	1:B:1164:PRO:HA	1.88	0.51
1:A:1045:MET:O	1:A:1049:THR:OG1	2.26	0.51
1:A:848:GLU:OE1	1:A:852:LYS:NZ	2.43	0.51
1:A:298:LEU:HA	1:A:301:ILE:HD12	1.93	0.51
1:A:313:TYR:HE2	1:B:75:PRO:HD2	1.76	0.51
1:A:988:ILE:HG22	1:A:989:VAL:HG23	1.92	0.50
1:B:298:LEU:HA	1:B:301:ILE:HD12	1.92	0.50
1:B:1072:ASP:OD1	1:B:1072:ASP:N	2.44	0.50
1:A:152:PHE:O	1:A:335:ASN:ND2	2.45	0.50
1:A:371:VAL:HG23	1:A:456:LEU:HD21	1.92	0.50
1:A:648:LEU:HD23	1:A:651:LEU:HD12	1.94	0.50
1:B:152:PHE:O	1:B:335:ASN:ND2	2.45	0.50
1:B:371:VAL:HG23	1:B:456:LEU:HD21	1.93	0.50
1:A:1138:ILE:HD12	1:A:1145:VAL:HG21	1.93	0.50
1:A:1048:LEU:HD11	1:A:1090:LEU:HB3	1.94	0.49
1:B:1037:THR:OG1	1:B:1038:VAL:N	2.45	0.49
1:B:1138:ILE:HD12	1:B:1145:VAL:HG21	1.95	0.49
1:B:648:LEU:HD23	1:B:651:LEU:HD12	1.95	0.49
1:B:1152:ALA:HB3	1:B:1161:ILE:HD12	1.94	0.49
1:A:1147:LEU:HD12	1:A:1147:LEU:C	2.34	0.48
1:A:1199:LEU:HD12	1:A:1219:SER:HB3	1.95	0.48
1:A:1037:THR:OG1	1:A:1038:VAL:N	2.44	0.48
1:A:1087:GLU:OE2	1:A:1185:ARG:NH2	2.46	0.48
1:B:1198:ILE:CD1	1:B:1199:LEU:H	2.27	0.48
1:B:1199:LEU:HD12	1:B:1219:SER:HB3	1.95	0.48
1:A:1054:ASN:ND2	2:A:2001:CMP:O1P	2.40	0.47
1:B:1147:LEU:HD12	1:B:1147:LEU:C	2.35	0.47
1:B:427:TRP:NE1	1:B:473:THR:OG1	2.42	0.47
1:A:138:LEU:HD11	1:A:440:LEU:HD13	1.96	0.47
1:A:335:ASN:O	1:A:338:LYS:NZ	2.45	0.47
1:A:271:VAL:HG13	1:A:322:SER:HB3	1.97	0.47
1:B:271:VAL:HG13	1:B:322:SER:HB3	1.96	0.46
1:B:1147:LEU:HD21	1:B:1161:ILE:HG22	1.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:SER:O	1:B:575:PHE:N	2.45	0.46
1:A:726:GLN:HG2	1:A:729:GLU:H	1.81	0.46
1:A:766:PHE:HE1	1:A:811:LEU:HB3	1.80	0.46
1:A:1198:ILE:HG21	1:B:585:ARG:NH2	2.30	0.46
1:B:766:PHE:HE1	1:B:811:LEU:HB3	1.80	0.46
1:A:923:ASP:OD1	1:A:923:ASP:N	2.39	0.46
1:A:156:VAL:HG11	1:A:336:ALA:HA	1.97	0.46
1:B:1144:ASP:N	1:B:1144:ASP:OD1	2.49	0.46
1:A:376:ALA:HB2	1:A:456:LEU:HD23	1.98	0.46
1:A:429:GLY:O	1:A:431:ARG:NH1	2.49	0.46
1:A:858:VAL:HA	1:B:1223:LEU:HD21	1.96	0.46
1:A:1198:ILE:CD1	1:A:1199:LEU:H	2.27	0.45
1:A:427:TRP:NE1	1:A:473:THR:OG1	2.42	0.45
1:A:571:SER:O	1:A:575:PHE:N	2.45	0.45
1:B:156:VAL:HG11	1:B:336:ALA:HA	1.98	0.45
1:B:160:MET:HA	1:B:163:PHE:HB2	1.98	0.45
1:B:1145:VAL:HG22	1:B:1188:VAL:HG12	1.98	0.45
1:A:1198:ILE:HD12	1:A:1200:ASP:H	1.80	0.45
1:B:1147:LEU:HB3	1:B:1167:ILE:HD11	1.99	0.45
1:B:375:LYS:NZ	1:B:443:GLU:OE2	2.48	0.45
1:B:1204:ASP:OD1	1:B:1204:ASP:N	2.48	0.45
1:A:773:VAL:HG12	1:A:804:LEU:HD13	1.98	0.45
1:B:773:VAL:HG12	1:B:804:LEU:HD13	1.99	0.45
1:A:1204:ASP:N	1:A:1204:ASP:OD1	2.49	0.45
1:B:138:LEU:HD11	1:B:440:LEU:HD13	1.99	0.45
1:B:1151:THR:OG1	1:B:1177:GLN:NE2	2.49	0.45
1:B:125:GLU:HG2	1:B:128:ARG:HH21	1.83	0.44
1:B:1198:ILE:HD12	1:B:1200:ASP:H	1.81	0.44
1:A:160:MET:HA	1:A:163:PHE:HB2	2.00	0.44
1:A:1144:ASP:OD1	1:A:1144:ASP:N	2.50	0.44
1:B:283:ALA:HB2	1:B:330:LEU:HA	2.00	0.44
1:B:295:ASN:HB2	1:B:936:ILE:HD11	1.99	0.44
1:B:1055:ALA:HB3	2:B:2001:CMP:H5'1	2.00	0.44
1:A:685:ASN:HA	1:A:688:ILE:HD12	1.98	0.44
1:B:429:GLY:O	1:B:431:ARG:NH1	2.51	0.44
1:A:1165:CYS:SG	1:A:1166:LEU:N	2.91	0.44
1:A:1100:THR:HG23	1:A:1101:PRO:HD3	2.00	0.43
1:B:641:TYR:OH	1:B:828:LYS:NZ	2.44	0.43
1:A:295:ASN:HB2	1:A:936:ILE:HD11	2.00	0.43
1:B:376:ALA:HB2	1:B:456:LEU:HD23	1.99	0.43
1:B:144:PRO:HG3	1:B:312:TYR:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:ASN:HA	1:B:688:ILE:HD12	1.99	0.43
1:A:144:PRO:HG3	1:A:312:TYR:CG	2.54	0.43
1:A:283:ALA:HB2	1:A:330:LEU:HA	2.00	0.42
1:B:260:THR:HG23	1:B:263:GLN:H	1.85	0.42
1:A:837:TYR:HD1	1:A:837:TYR:HA	1.71	0.42
1:A:498:VAL:HG21	1:A:534:ASP:HA	2.01	0.42
1:B:335:ASN:O	1:B:338:LYS:NZ	2.46	0.42
1:A:99:PRO:HB2	1:A:472:THR:HG22	2.02	0.42
1:A:1145:VAL:HG22	1:A:1188:VAL:HG12	2.02	0.42
1:B:1103:ILE:HD11	1:B:1146:ILE:HD11	2.01	0.42
1:A:990:ARG:HD3	1:A:990:ARG:HA	1.71	0.42
1:A:585:ARG:NH2	1:B:1198:ILE:HG21	2.34	0.42
1:A:764:ASN:HA	1:A:767:ASP:HB2	2.02	0.42
1:A:847:GLU:HA	1:A:850:VAL:HG12	2.01	0.42
1:B:847:GLU:HA	1:B:850:VAL:HG12	2.02	0.42
1:A:75:PRO:HG3	1:B:137:VAL:HG12	2.02	0.41
1:A:260:THR:HG23	1:A:263:GLN:H	1.85	0.41
1:B:498:VAL:HG21	1:B:534:ASP:HA	2.01	0.41
1:A:137:VAL:HG12	1:B:75:PRO:HG3	2.02	0.41
1:A:375:LYS:NZ	1:A:443:GLU:OE2	2.49	0.41
1:A:1198:ILE:HG21	1:B:585:ARG:CZ	2.51	0.41
1:B:598:PHE:CG	1:B:608:LEU:HD22	2.56	0.41
1:A:765:LYS:HD3	1:A:765:LYS:HA	1.89	0.41
1:A:533:SER:OG	1:A:534:ASP:N	2.54	0.41
1:A:603:LEU:HD21	1:A:842:GLY:HA3	2.01	0.41
1:A:125:GLU:HG2	1:A:128:ARG:HH21	1.86	0.41
1:B:120:VAL:HA	1:B:121:PRO:HD3	1.95	0.41
1:B:1155:ALA:HB2	1:B:1173:LYS:HB2	2.03	0.41
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.88	0.40
1:B:533:SER:OG	1:B:534:ASP:N	2.54	0.40
1:B:761:SER:O	1:B:765:LYS:N	2.54	0.40
1:A:598:PHE:CG	1:A:608:LEU:HD22	2.57	0.40
1:A:1221:MET:HA	1:B:561:GLY:HA3	2.03	0.40
1:B:462:ILE:HD13	1:B:462:ILE:HA	1.94	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	1025/1196 (86%)	983 (96%)	42 (4%)	0	100	100
1	B	1025/1196 (86%)	981 (96%)	44 (4%)	0	100	100
All	All	2050/2392 (86%)	1964 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	896/1025 (87%)	870 (97%)	26 (3%)	42	72
1	B	896/1025 (87%)	861 (96%)	35 (4%)	32	64
All	All	1792/2050 (87%)	1731 (97%)	61 (3%)	40	68

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LEU
1	A	191	TYR
1	A	296	ASP
1	A	321	VAL
1	A	375	LYS
1	A	413	ILE
1	A	440	LEU
1	A	734	ILE

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Mol	Chain	Res	Type
1	A	736	ASN
1	A	748	ILE
1	A	763	TRP
1	A	808	LEU
1	A	833	LEU
1	A	837	TYR
1	A	855	ASP
1	A	943	ASN
1	A	960	VAL
1	A	963	LEU
1	A	996	ASP
1	A	1061	THR
1	A	1066	TYR
1	A	1100	THR
1	A	1104	MET
1	A	1158	ARG
1	A	1179	THR
1	A	1212	ILE
1	B	174	LEU
1	B	191	TYR
1	B	200	MET
1	B	296	ASP
1	B	321	VAL
1	B	413	ILE
1	B	606	GLU
1	B	621	GLU
1	B	734	ILE
1	B	736	ASN
1	B	748	ILE
1	B	763	TRP
1	B	804	LEU
1	B	808	LEU
1	B	833	LEU
1	B	837	TYR
1	B	855	ASP
1	B	943	ASN
1	B	960	VAL
1	B	963	LEU
1	B	984	TYR
1	B	996	ASP
1	B	1049	THR
1	B	1061	THR

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Mol	Chain	Res	Type
1	B	1066	TYR
1	B	1069	THR
1	B	1072	ASP
1	B	1100	THR
1	B	1104	MET
1	B	1154	ASN
1	B	1156	HIS
1	B	1158	ARG
1	B	1162	ARG
1	B	1179	THR
1	B	1212	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	ASN
1	A	421	ASN
1	A	736	ASN
1	B	295	ASN
1	B	421	ASN
1	B	736	ASN

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)

2 ligands are 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	$\#\|Z\| > 2$
2	CMP	B	2001	-	22,25,25	1.42	5 (22%)	24,39,39	1.75	4 (16%)
2	CMP	A	2001	-	22,25,25	1.44	5 (22%)	24,39,39	1.77	4 (16%)

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	CMP	B	2001	-	-	0/0/31/31	0/4/4/4
2	CMP	A	2001	-	-	0/0/31/31	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	CMP	C6-N6	3.16	1.45	1.34
2	B	2001	CMP	C6-N6	3.15	1.45	1.34
2	A	2001	CMP	P-O3'	2.67	1.62	1.57
2	B	2001	CMP	P-O3'	2.61	1.62	1.57
2	A	2001	CMP	P-O5'	2.53	1.60	1.57
2	B	2001	CMP	P-O5'	2.35	1.60	1.57
2	B	2001	CMP	O5'-C5'	-2.35	1.42	1.46
2	A	2001	CMP	O5'-C5'	-2.35	1.42	1.46
2	A	2001	CMP	P-O2P	2.13	1.65	1.55
2	B	2001	CMP	P-O2P	2.11	1.65	1.55

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	CMP	O5'-P-O3'	4.81	112.30	105.68
2	A	2001	CMP	N3-C2-N1	-4.61	121.47	128.68
2	B	2001	CMP	N3-C2-N1	-4.55	121.57	128.68
2	B	2001	CMP	O5'-P-O3'	4.40	111.73	105.68
2	B	2001	CMP	O2P-P-O1P	2.68	117.12	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	CMP	C4-C5-N7	-2.65	106.63	109.40
2	A	2001	CMP	O2P-P-O1P	2.63	116.95	108.73
2	A	2001	CMP	C4-C5-N7	-2.63	106.66	109.40

There are no chirality outliers.

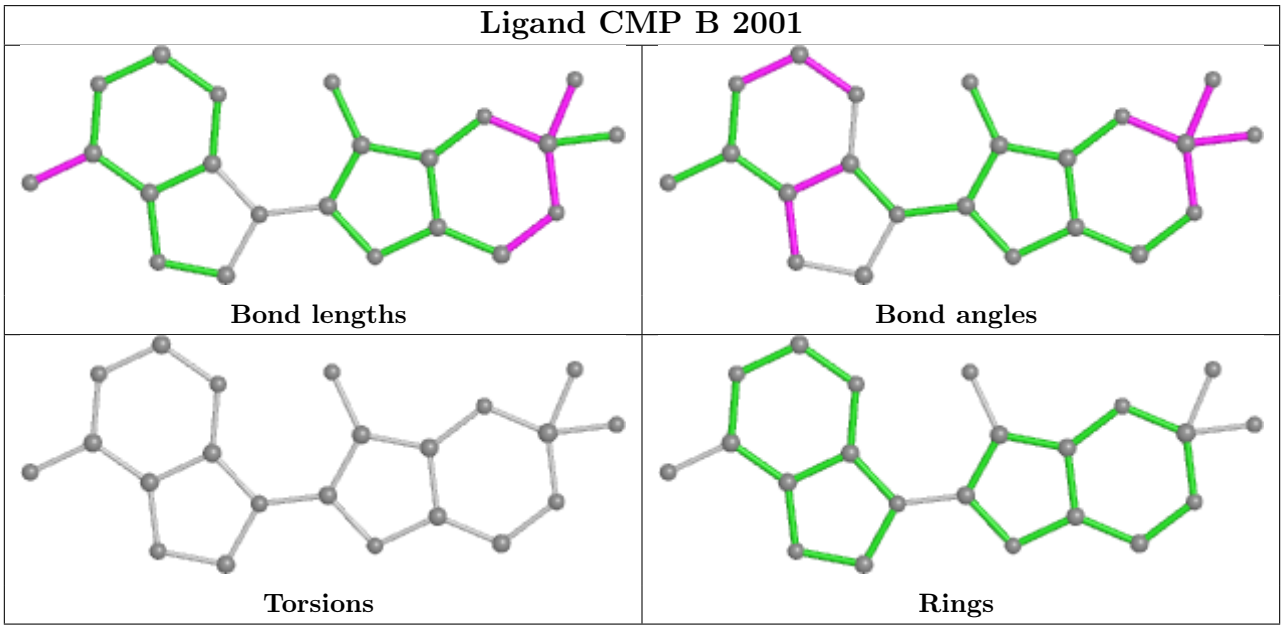
There are no torsion outliers.

There are no ring outliers.

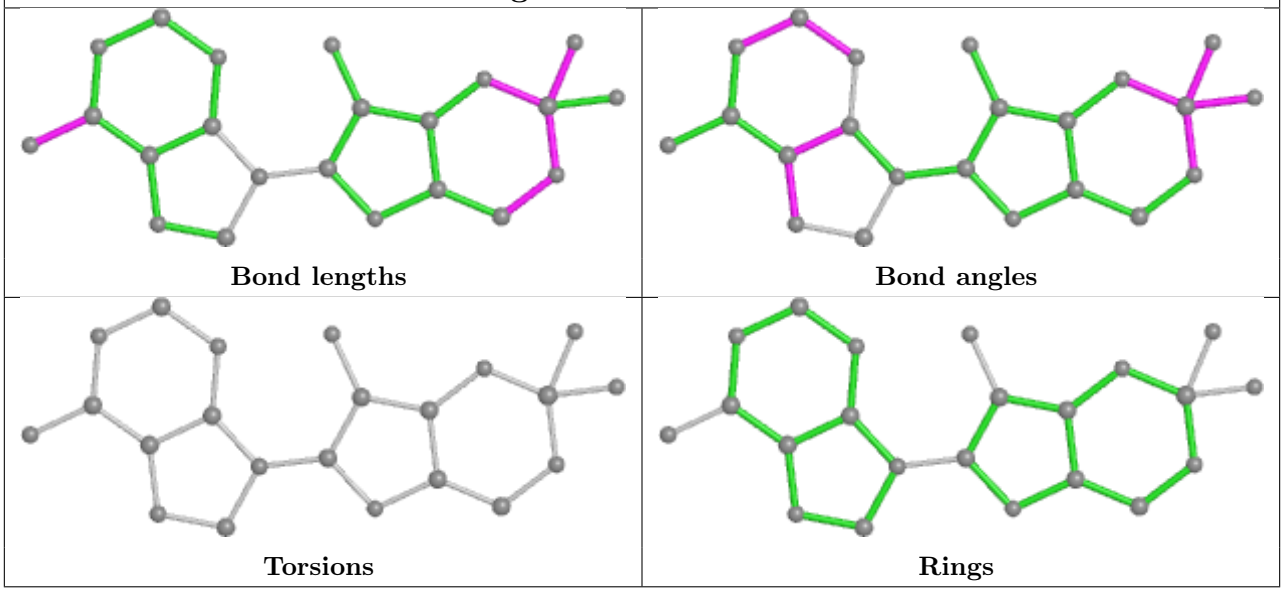
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	CMP	2	0
2	A	2001	CMP	2	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 CMP A 2001



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.

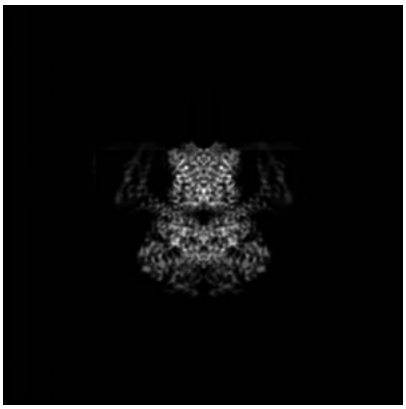
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38568. These allow visual inspection of the internal detail of the map and identification of artifacts.

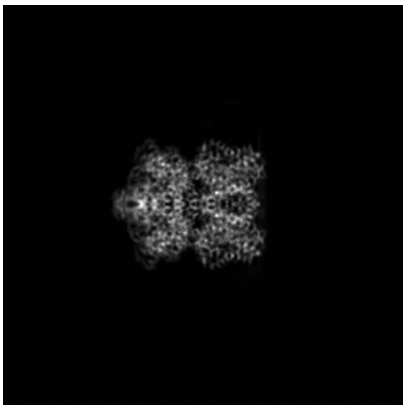
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

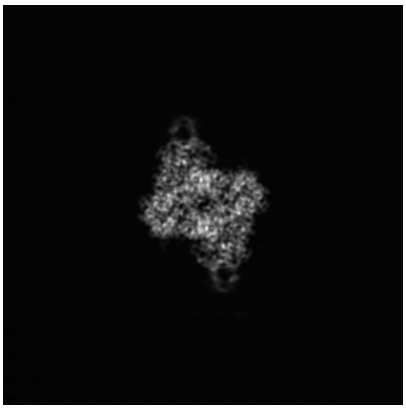
6.1.1 Primary map



X

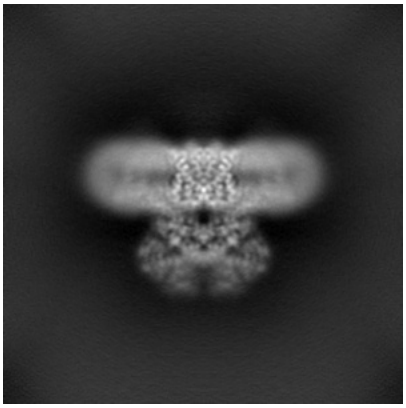


Y

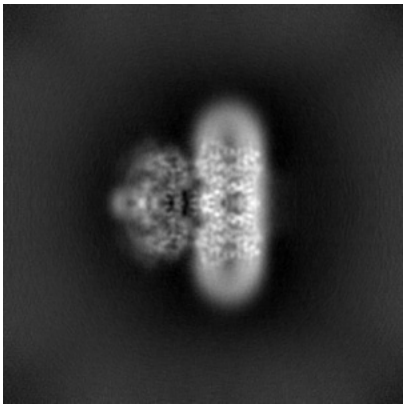


Z

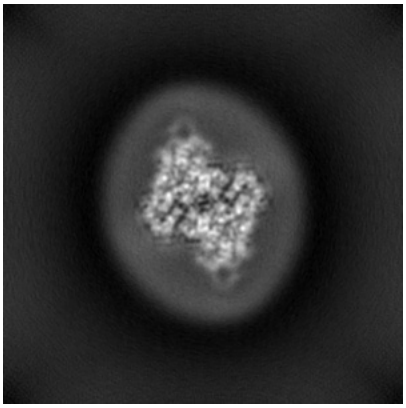
6.1.2 Raw map



X



Y



Z

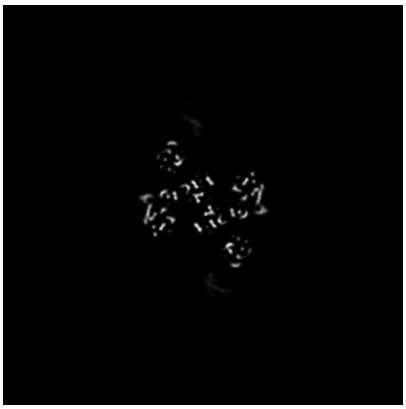
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

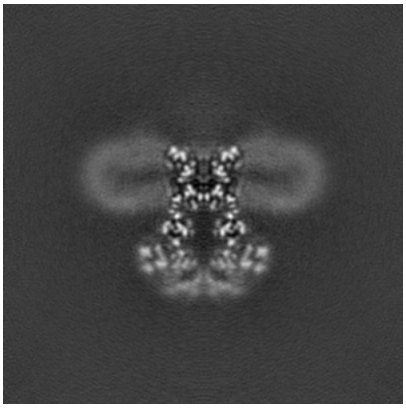
X Index: 128

Y Index: 128

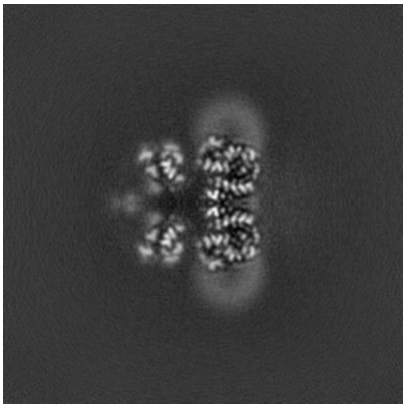


Z Index: 128

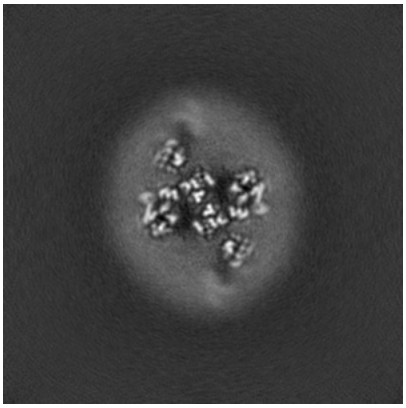
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

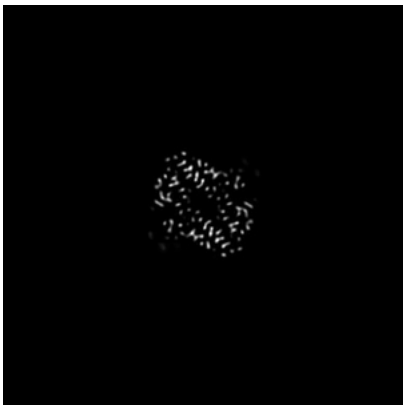
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

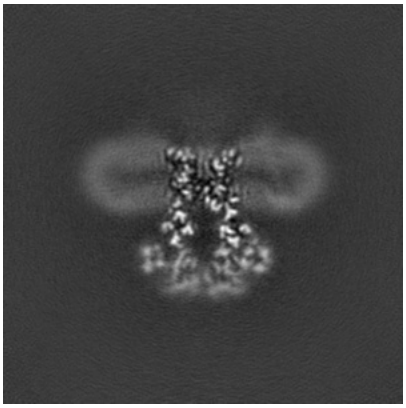
X Index: 126

Y Index: 112

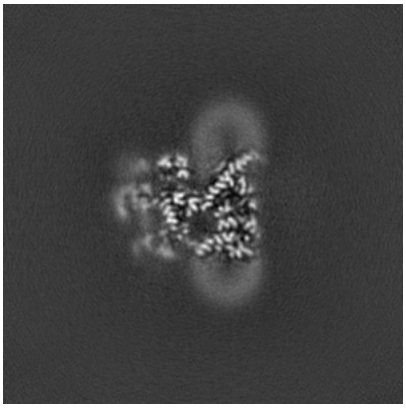


Z Index: 113

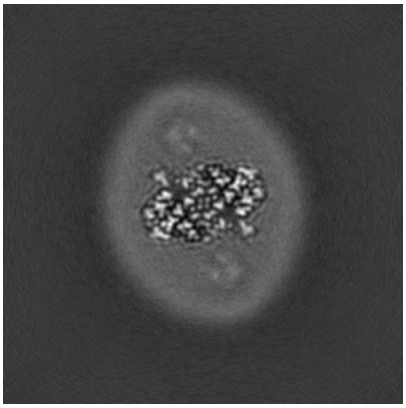
6.3.2 Raw map



X Index: 126



Y Index: 112

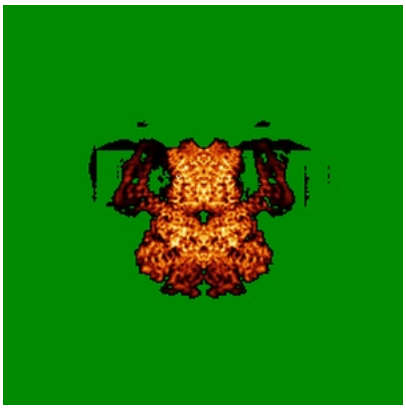


Z Index: 155

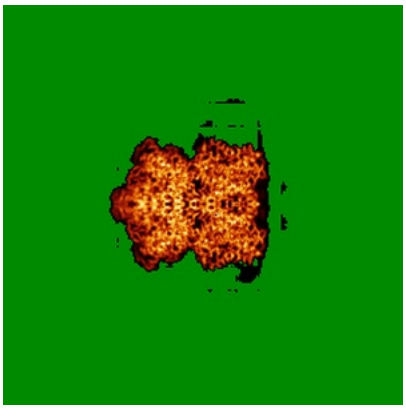
The images above show the largest variance slices of the map in three orthogonal directions.

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

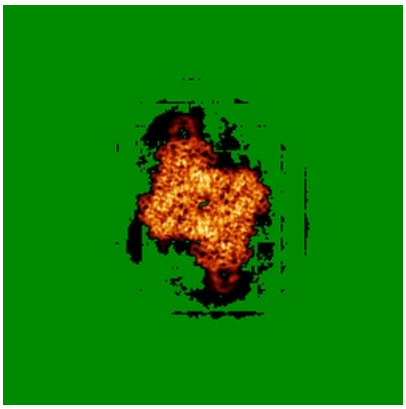
6.4.1 Primary map



X

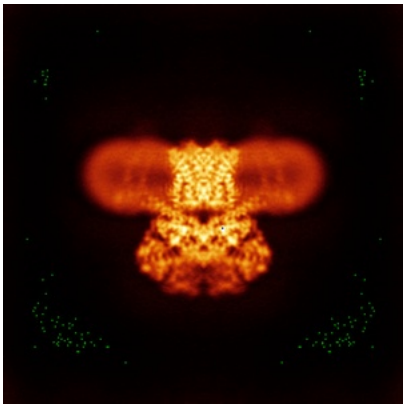


Y

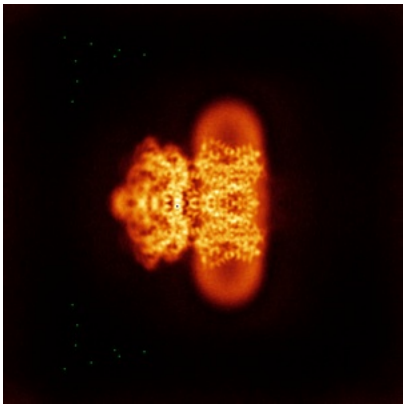


Z

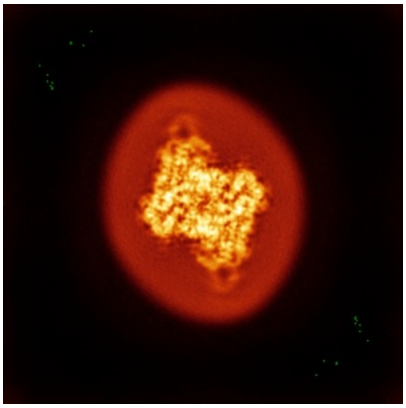
6.4.2 Raw map



X



Y

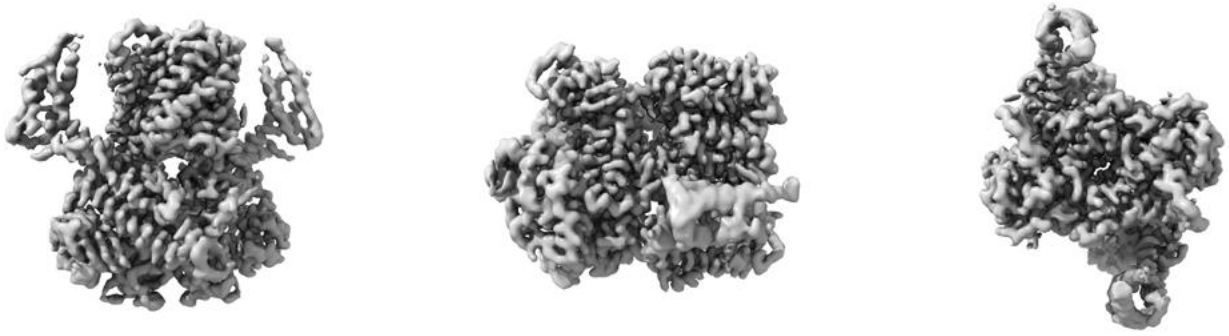


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

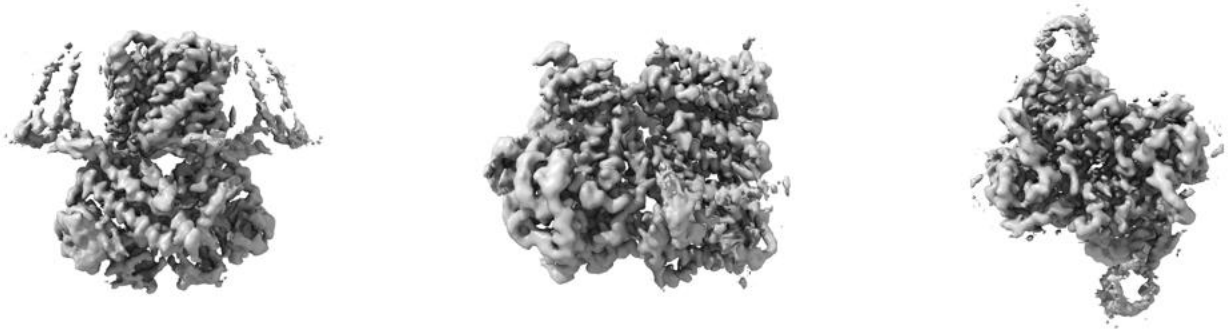
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

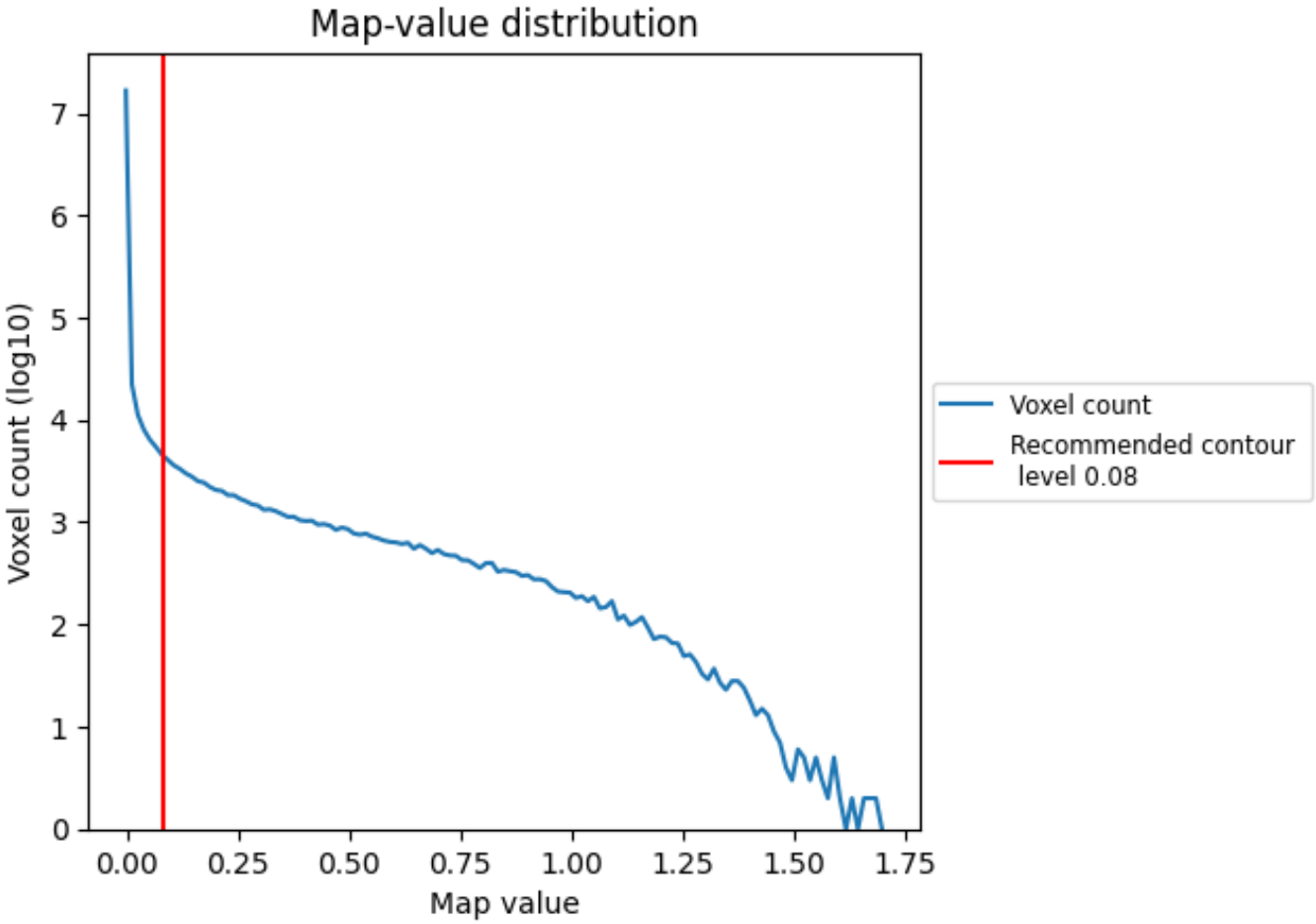
6.6 Mask visualisation (i)

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

7 Map analysis

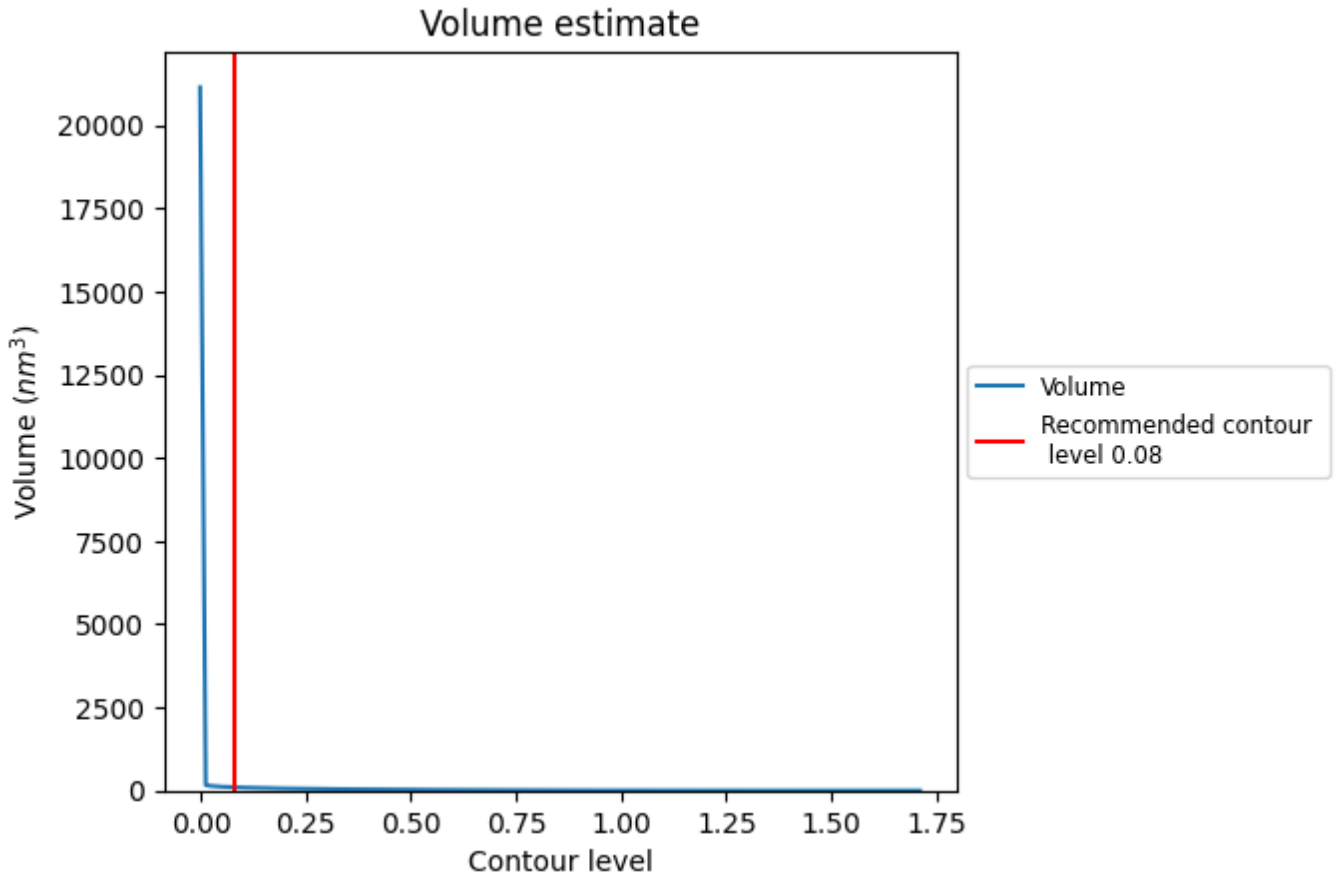
This section contains the results of statistical analysis of the map.

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.

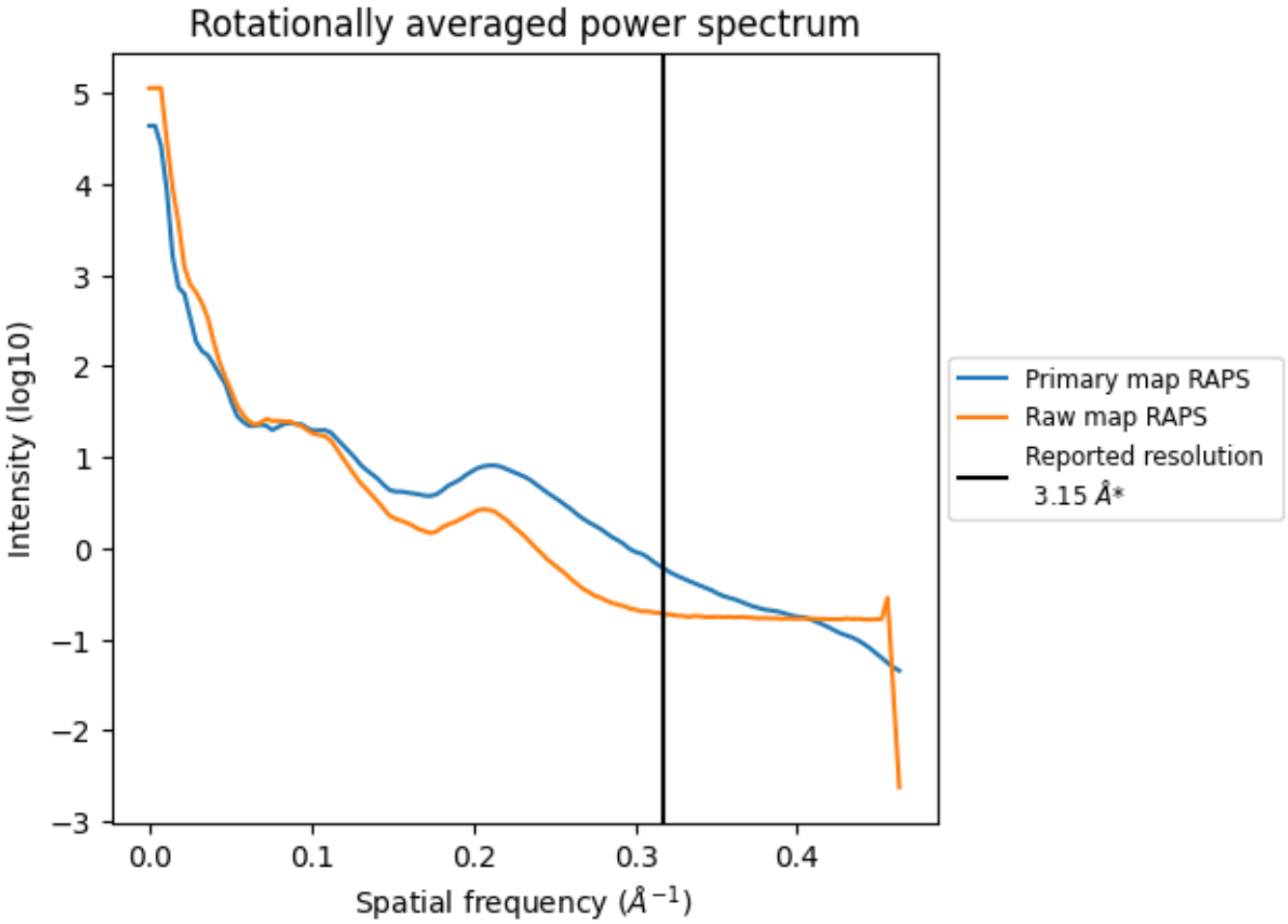
7.2 Volume estimate



The volume at the recommended contour level is 98 nm^3; this corresponds to an approximate mass of 89 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)

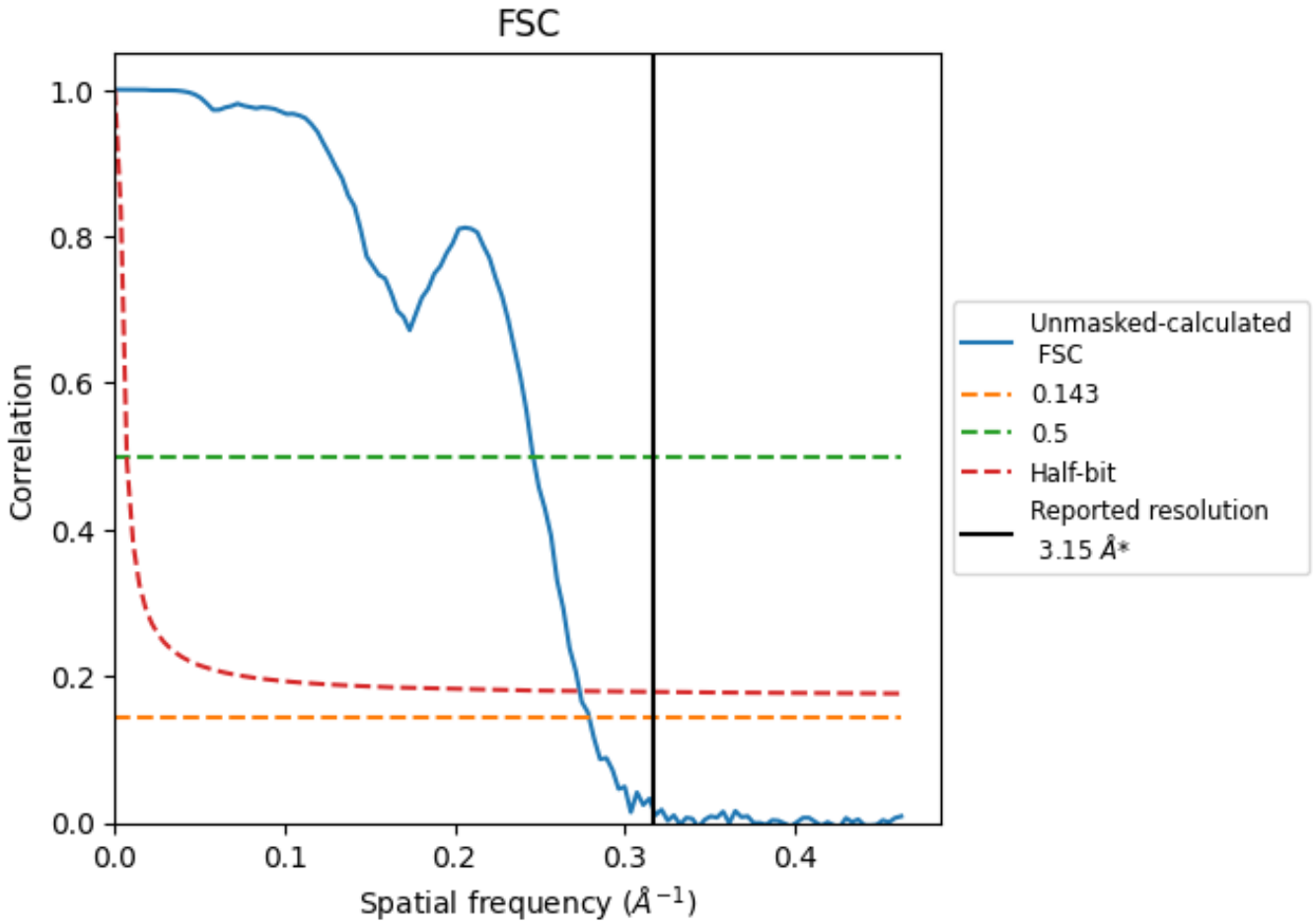


*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

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 0.317 Å^{-1}

8.2 Resolution estimates (i)

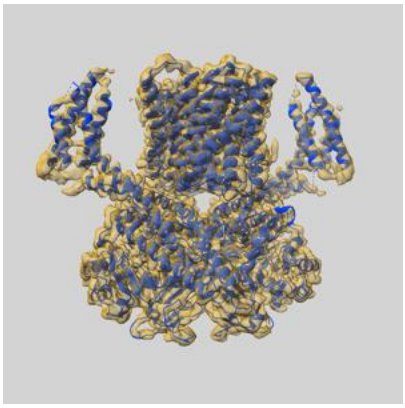
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.06	3.65

*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 3.58 differs from the reported value 3.15 by more than 10 %

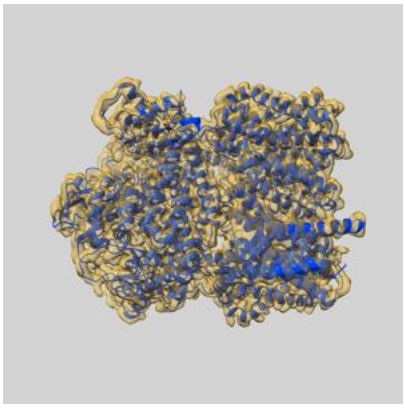
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38568 and PDB model 8XQ7. Per-residue inclusion information can be found in section 3 on page 5.

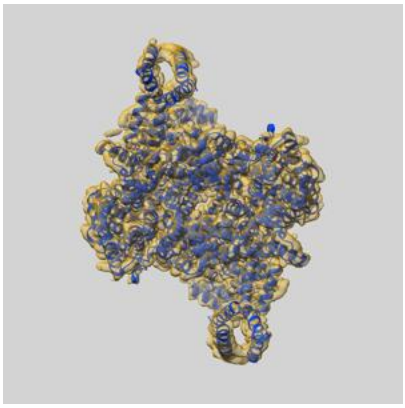
9.1 Map-model overlay



X



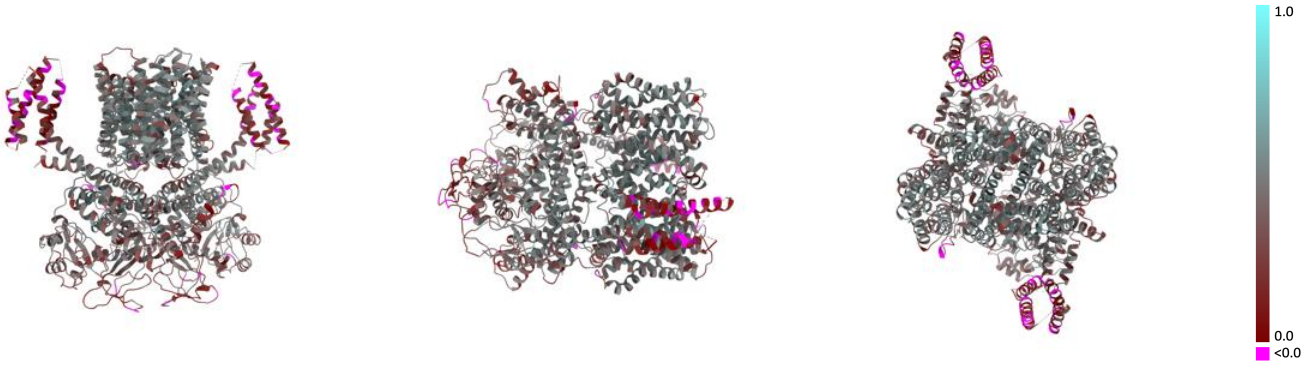
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

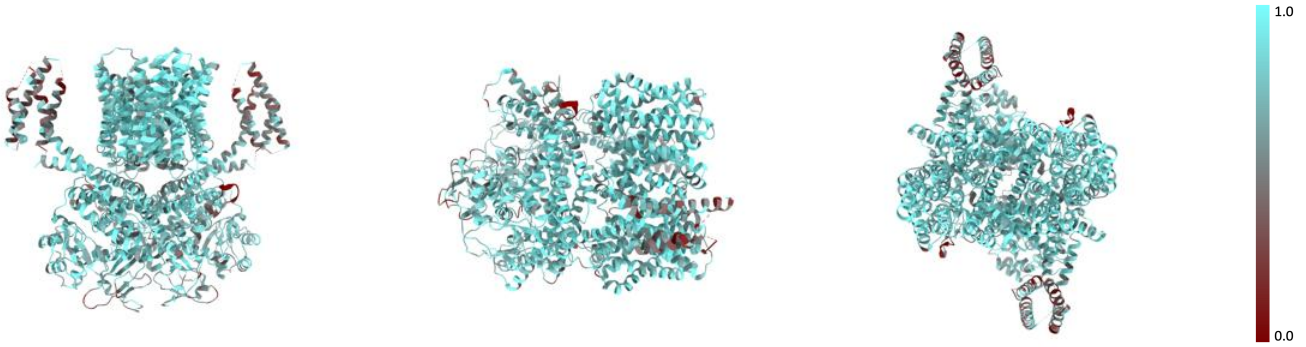
9.2 Q-score mapped to coordinate model (i)



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.

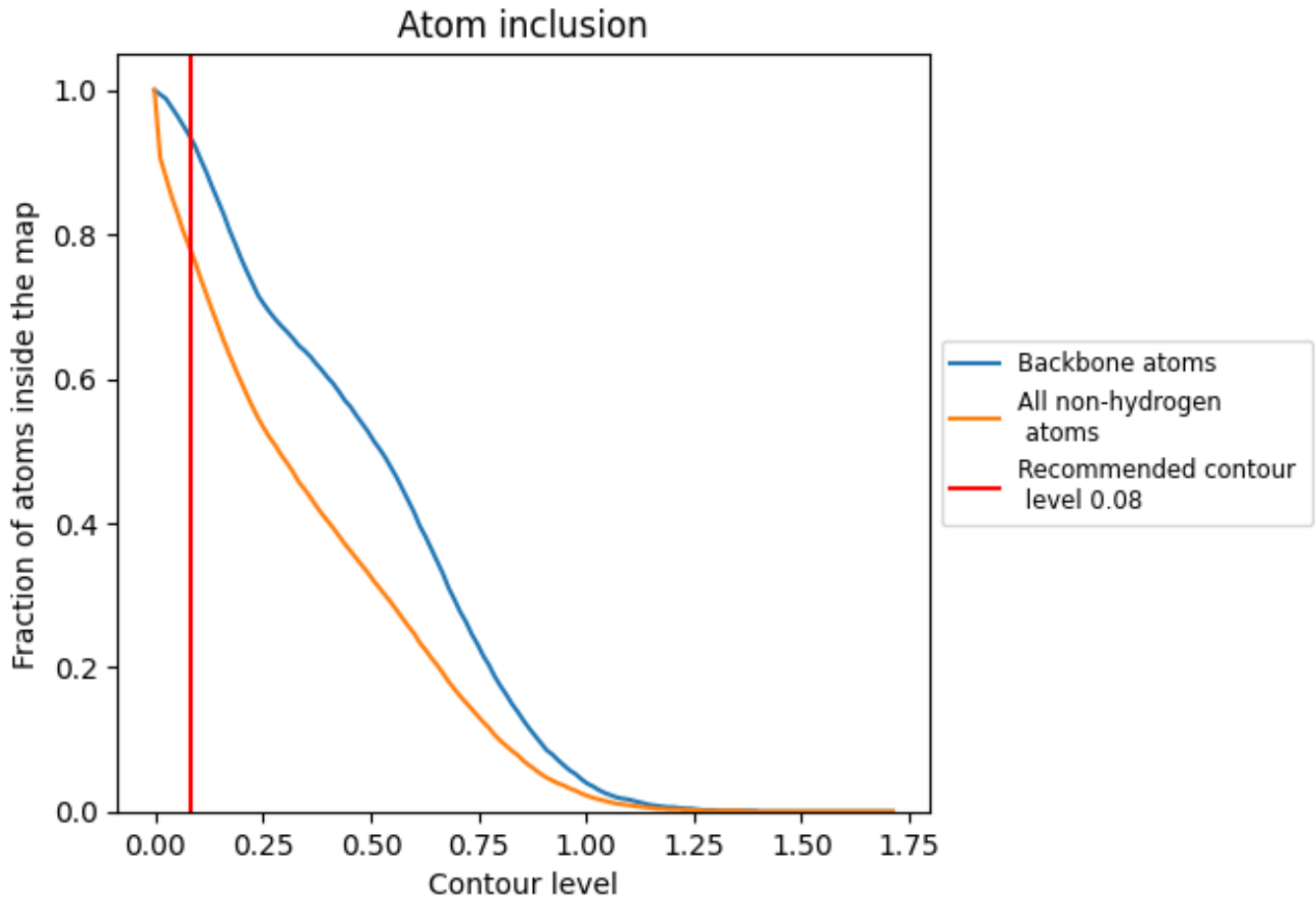
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 78% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7810	0.3900
A	0.7810	0.3890
B	0.7820	0.3910