Full wwPDB EM Validation Report ⓘ

Feb 17, 2024 – 06:26 am GMT

PDB ID	:	8C8G
EMDB ID	:	EMD-16475
Title	:	Cryo-EM structure of BoNT/Wo-NTNH complex
Authors	:	Kosenina, S.; Skerlova, J.; Stenmark, P.
Deposited on	:	2023-01-20
Resolution	:	2.98 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:

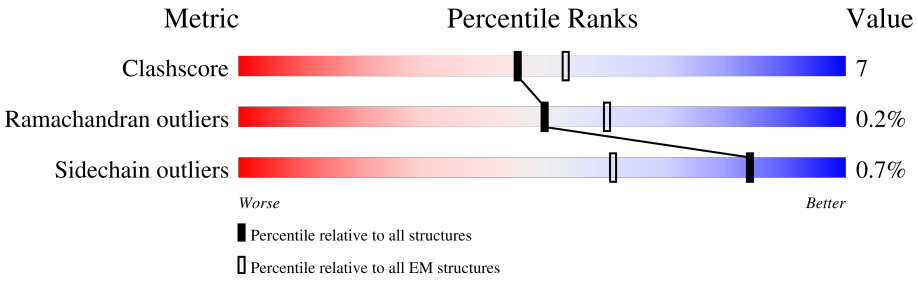
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.98 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	1371	82% 15%
2	B	1458	68% 13% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20362 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 Putative botulinum-like toxin Wo.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1335	10790	6867	1786	2104	33	0	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1337	GLY	-	expression tag	UNP A0A069CUU9
A	1338	SER	-	expression tag	UNP A0A069CUU9
A	1339	TYR	-	expression tag	UNP A0A069CUU9
A	1340	PRO	-	expression tag	UNP A0A069CUU9
A	1341	TYR	-	expression tag	UNP A0A069CUU9
A	1342	ASP	-	expression tag	UNP A0A069CUU9
A	1343	VAL	-	expression tag	UNP A0A069CUU9
A	1344	PRO	-	expression tag	UNP A0A069CUU9
A	1345	ASP	-	expression tag	UNP A0A069CUU9
A	1346	TYR	-	expression tag	UNP A0A069CUU9
A	1347	ALA	-	expression tag	UNP A0A069CUU9
A	1348	LEU	-	expression tag	UNP A0A069CUU9
A	1349	GLU	-	expression tag	UNP A0A069CUU9
A	1350	SER	-	expression tag	UNP A0A069CUU9
A	1351	GLY	-	expression tag	UNP A0A069CUU9
A	1352	LYS	-	expression tag	UNP A0A069CUU9
A	1353	GLU	-	expression tag	UNP A0A069CUU9
A	1354	THR	-	expression tag	UNP A0A069CUU9
A	1355	ALA	-	expression tag	UNP A0A069CUU9
A	1356	ALA	-	expression tag	UNP A0A069CUU9
A	1357	ALA	-	expression tag	UNP A0A069CUU9
A	1358	LYS	-	expression tag	UNP A0A069CUU9
A	1359	PHE	-	expression tag	UNP A0A069CUU9
A	1360	GLU	-	expression tag	UNP A0A069CUU9
A	1361	ARG	-	expression tag	UNP A0A069CUU9
A	1362	GLN	-	expression tag	UNP A0A069CUU9
A	1363	HIS	-	expression tag	UNP A0A069CUU9
A	1364	MET	-	expression tag	UNP A0A069CUU9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1365	ASP	-	expression tag	UNP A0A069CUU9
A	1366	SER	-	expression tag	UNP A0A069CUU9
A	1367	SER	-	expression tag	UNP A0A069CUU9
A	1368	THR	-	expression tag	UNP A0A069CUU9
A	1369	SER	-	expression tag	UNP A0A069CUU9
A	1370	ALA	-	expression tag	UNP A0A069CUU9
A	1371	ALA	-	expression tag	UNP A0A069CUU9

- Molecule 2 is a protein called Structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1195	Total	C	N	O	S	0	0
			9572	6128	1517	1909	18		

There are 21 discrepancies between the modelled and reference sequences:

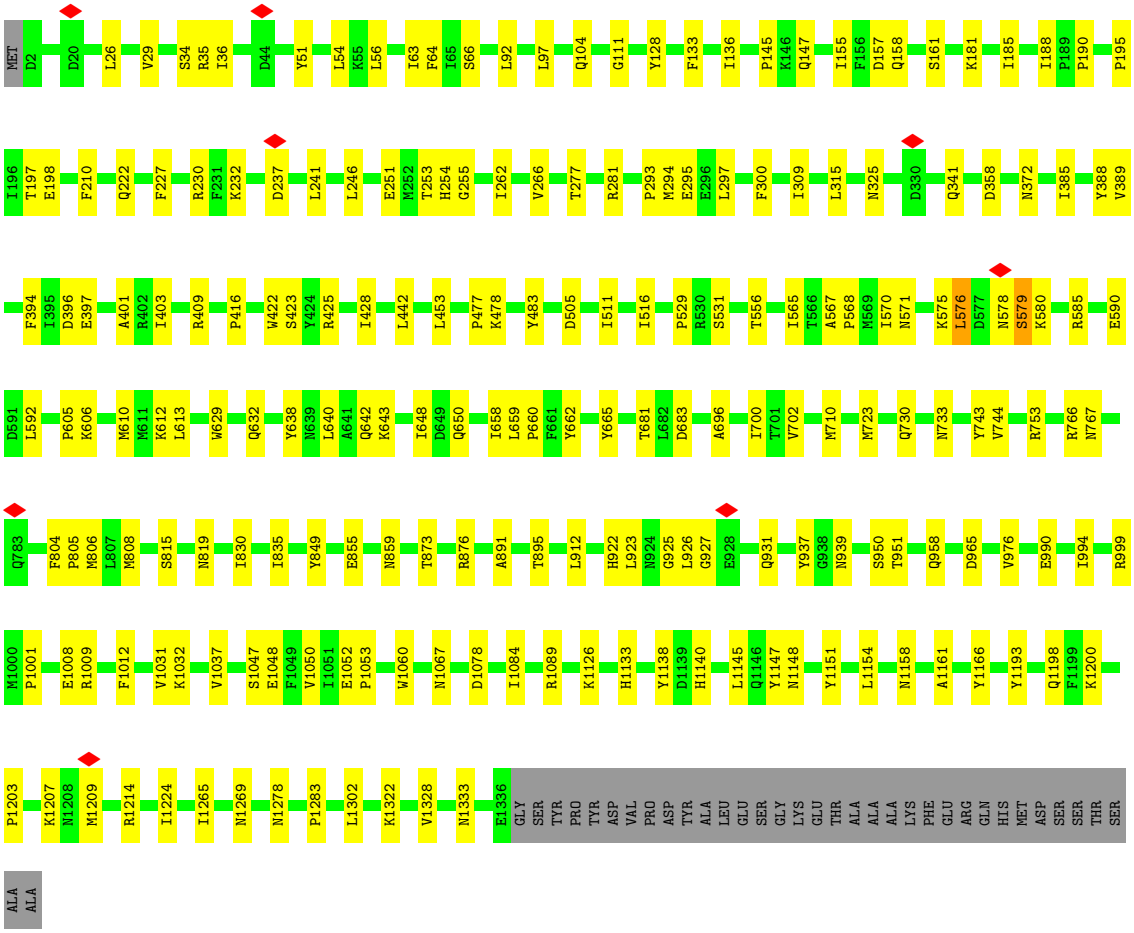
Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	MET	-	initiating methionine	UNP A0A069CVS9
B	-11	GLY	-	expression tag	UNP A0A069CVS9
B	-10	SER	-	expression tag	UNP A0A069CVS9
B	-9	ASP	-	expression tag	UNP A0A069CVS9
B	-8	TYR	-	expression tag	UNP A0A069CVS9
B	-7	LYS	-	expression tag	UNP A0A069CVS9
B	-6	ASP	-	expression tag	UNP A0A069CVS9
B	-5	ASP	-	expression tag	UNP A0A069CVS9
B	-4	ASP	-	expression tag	UNP A0A069CVS9
B	-3	ASP	-	expression tag	UNP A0A069CVS9
B	-2	LYS	-	expression tag	UNP A0A069CVS9
B	-1	SER	-	expression tag	UNP A0A069CVS9
B	0	GLY	-	expression tag	UNP A0A069CVS9
B	1438	SER	-	expression tag	UNP A0A069CVS9
B	1439	GLY	-	expression tag	UNP A0A069CVS9
B	1440	HIS	-	expression tag	UNP A0A069CVS9
B	1441	HIS	-	expression tag	UNP A0A069CVS9
B	1442	HIS	-	expression tag	UNP A0A069CVS9
B	1443	HIS	-	expression tag	UNP A0A069CVS9
B	1444	HIS	-	expression tag	UNP A0A069CVS9
B	1445	HIS	-	expression tag	UNP A0A069CVS9

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.

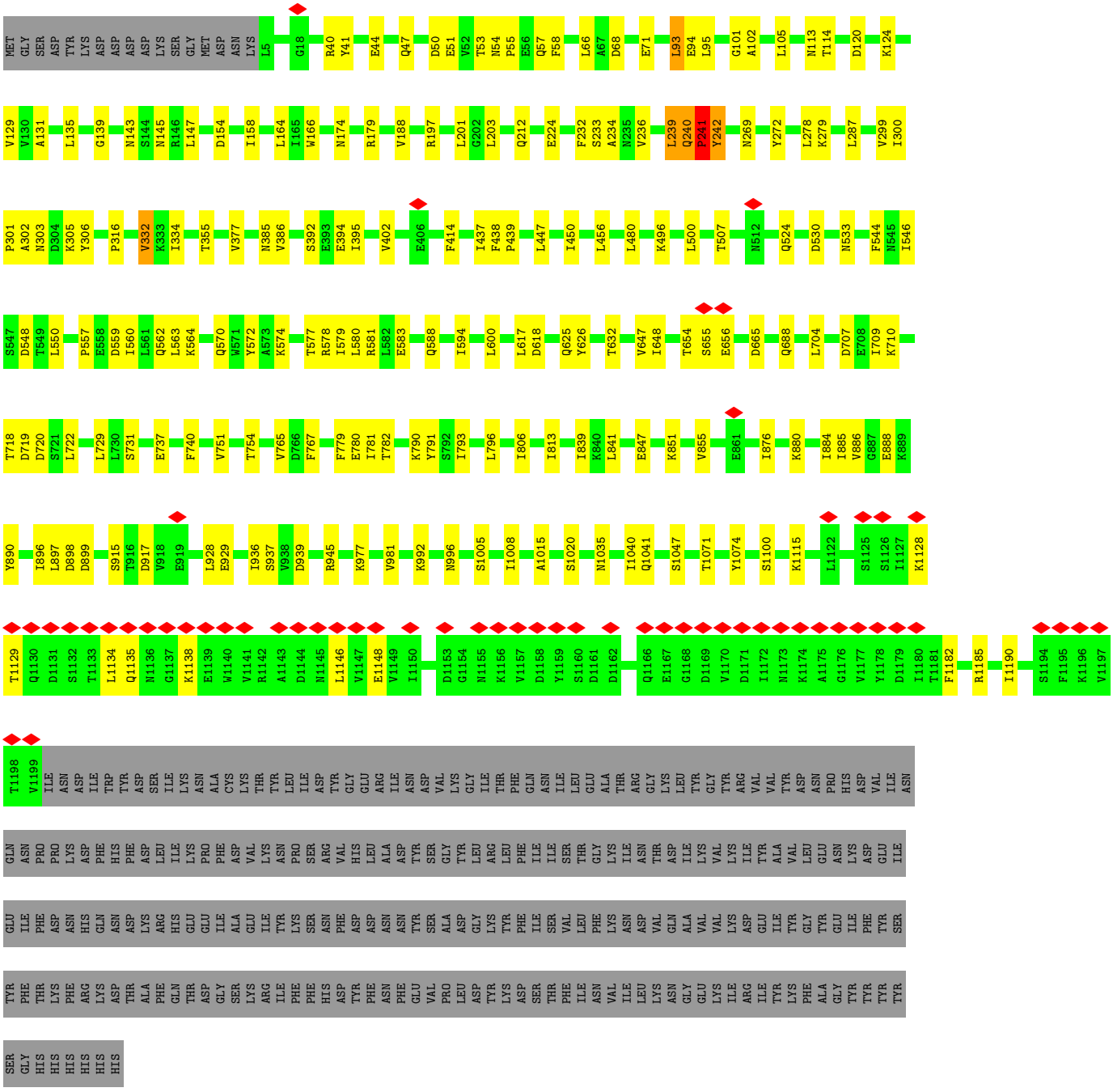
• Molecule 1: Putative botulinum-like toxin Wo

Chain A:



• Molecule 2: Structural protein

Chain B:


MET GLY SER ASP TYR LYS ASP ASP ASP ASP LYS SER GLY MET ASP ASN LYS L5 G18 R40 Y41 E44 Q47 D50 E51 V52 T53 N54 P55 E56 Q57 F58 L66 A67 D68 E71 L93 E94 L95 G101 A102 L105 N113 T114 D120 K124
V129 V130 A131 L135 G139 N143 S144 N145 R146 L147 D154 I158 L164 I165 W166 N174 R179 V188 R197 L201 G202 L203 Q212 E224 F232 S233 A234 N235 V236 L239 Q240 P241 Y242 N269 Y272 L278 K279 L287 V299 I300
P301 A302 N303 D304 K305 Y306 P316 V332 K333 I334 T355 V377 N385 V386 S392 E393 E394 I395 V402 E406 F414 I437 F438 P439 L447 I450 L456 L480 K496 L500 T507 N512 Q524 D530 N533 F544 N545 I546
S547 D548 T549 L550 P557 E558 D559 I560 L561 Q562 L563 K564 Q570 W571 Y572 A573 K574 T577 R578 I579 L580 R581 L582 E583 Q588 I594 L600 L617 D618 Q625 Y626 T632 V647 I648 T654 S655 E656 D665 Q688 L704 D707 E708 I709 K710
T718 D719 D720 S721 L722 L729 L730 S731 E737 F740 V751 T754 V765 D766 F767 F779 E780 I781 T782 K790 Y791 S792 I793 L796 I806 I813 I839 K840 L841 E847 K851 V855 E861 I876 K880 I884 I885 V886 G887 E888 K889
Y890 I896 L897 D898 D899 S915 T916 D917 V918 E919 L928 E929 I936 S937 V938 D939 R945 K977 V981 K992 N996 S1005 I1008 A1015 S1020 N1035 I1040 Q1041 S1047 T1071 Y1074 S1100 K1115 L1122 S1125 S1126 I1127 K1128
T1129 Q1130 D1131 S1132 T1133 L1134 Q1135 N1136 G1137 K1138 E1139 W1140 V1141 R1142 A1143 D1144 N1145 L1146 V1147 E1148 V1149 I1150 D1153 G1154 N1155 K1156 V1157 D1158 Y1159 S1160 D1161 D1162 Q1166 E1167 G1168 D1169 V1170 D1171 I1172 N1173 K1174 A1175 G1176 V1177 Y1178 D1179 I1180 T1181 F1182 R1185 I1190 S1194 F1195 K1196 V1197
T1198 V1199 ILE ASN ASP ILE TRP TYR ASP SER ILE LYS ASN ALA CYS LYS THR TYR LEU ILE ASP TYR GLY GLU ARG ILE ASN ASP VAL LYS GLY ILE THR PHE GLN ASN ILE LEU GLU ALA THR ARG GLY LYS LEU TYR GLY TYR ARG VAL VAL TYR ASP ASN PRO HIS ASP VAL ILE ASN
GLN ASN PRO PRO LYS ASP PHE HIS PHE ASP LEU ILE LYS PRO PHE ASP VAL LYS ASN PRO SER ARG VAL HIS LEU ALA ASP TYR SER GLY TYR LEU ARG LEU PHE ILE ILE SER THR GLY LYS ILE ASN ILE THR ASP ILE LYS VAL LYS ASP GLY LYS TYR PHE ILE SER VAL LEU PHE LYS ASN ASP VAL GLN ALA VAL VAL LYS ASP GLU ILE TYR ILE VAL LEU GLU ASN LYS ASP GLU ILE PHE TYR SER
GLU ILE PHE ASP ASN HIS GLN ASN ASP LYS ARG HIS GLU GLU ILE ALA GLU ILE TYR LYS SER ASN PHE ASP ASP ASN ASN TYR SER ALA ASP GLY LYS TYR PHE ILE SER VAL LEU PHE LYS ASN ASP VAL GLN ALA VAL VAL LYS ASP GLU ILE TYR ILE VAL LEU GLU ASN LYS ASP GLU ILE PHE TYR SER
TYR PHE THR LYS PHE ARG LYS ASP THR ALA PHE GLN THR ASP GLY SER LYS ARG ILE PHE PHE HIS ASP TYR PHE ASN PHE GLU VAL PRO LEU ASP TYR LYS ASP SER THR PHE ILE ASN VAL ILE LEU LYS ASN GLY GLU LYS ILE ARG ILE TYR LYS PHE ALA GLY TYR TYR TYR
SER GLY HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	283452	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.246	Depositor
Minimum map value	-0.856	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.124	Depositor
Map size (Å)	262.4, 262.4, 262.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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	0.65	0/11018	0.74	0/14897
2	B	0.64	0/9759	0.72	1/13242 (0.0%)
All	All	0.65	0/20777	0.73	1/28139 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	241	PRO	N-CA-CB	-8.62	92.95	103.30

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	10790	0	10543	143	0
2	B	9572	0	9465	142	0
All	All	20362	0	20008	266	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 (266) 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:1129:THR:CG2	2:B:1146:LEU:HD23	1.65	1.23
2:B:1129:THR:HG22	2:B:1146:LEU:HD23	1.28	1.06
2:B:560:ILE:HG23	2:B:563:LEU:HD21	1.49	0.93
2:B:1129:THR:CG2	2:B:1146:LEU:CD2	2.53	0.86
2:B:239:LEU:O	2:B:240:GLN:C	2.20	0.80
2:B:93:LEU:HD12	2:B:93:LEU:C	2.03	0.79
1:A:1302:LEU:CB	2:B:93:LEU:HD11	2.13	0.77
2:B:1134:LEU:HB3	2:B:1138:LYS:HB3	1.68	0.75
2:B:1146:LEU:HD11	2:B:1182:PHE:CG	2.23	0.74
1:A:766:ARG:CG	1:A:808:MET:HE1	2.21	0.70
2:B:1129:THR:HG23	2:B:1146:LEU:HD23	1.67	0.70
1:A:1302:LEU:HD11	2:B:392:SER:HB2	1.75	0.69
1:A:766:ARG:HB2	1:A:808:MET:HE1	1.76	0.68
1:A:1302:LEU:HB3	2:B:93:LEU:HD11	1.74	0.67
2:B:740:PHE:HB2	2:B:839:ILE:HD11	1.75	0.67
1:A:1302:LEU:HB2	2:B:93:LEU:HD11	1.74	0.67
1:A:29:VAL:O	1:A:181:LYS:NZ	2.29	0.66
1:A:516:ILE:HD13	2:B:981:VAL:HG21	1.77	0.66
1:A:36:ILE:HG12	1:A:54:LEU:HD21	1.78	0.65
1:A:659:LEU:HD11	1:A:815:SER:HA	1.78	0.65
1:A:612:LYS:O	1:A:629:TRP:NE1	2.30	0.65
2:B:105:LEU:HB2	2:B:158:ILE:HG23	1.79	0.65
1:A:743:TYR:HH	1:A:895:THR:HG1	1.44	0.65
1:A:766:ARG:CB	1:A:808:MET:HE1	2.27	0.65
2:B:496:LYS:HG3	2:B:500:LEU:HD12	1.78	0.64
2:B:299:VAL:HG12	2:B:300:ILE:HD12	1.80	0.64
2:B:438:PHE:HB3	2:B:439:PRO:HD3	1.81	0.63
2:B:570:GLN:HG3	2:B:574:LYS:HD2	1.81	0.63
1:A:659:LEU:HD11	1:A:815:SER:CA	2.27	0.63
1:A:766:ARG:HB2	1:A:808:MET:CE	2.29	0.63
1:A:648:ILE:HG22	1:A:650:GLN:H	1.64	0.62
1:A:766:ARG:HG3	1:A:808:MET:HE1	1.82	0.61
1:A:1140:HIS:O	1:A:1269:ASN:ND2	2.34	0.61
1:A:958:GLN:HE22	2:B:996:ASN:HD21	1.47	0.61
1:A:638:TYR:O	1:A:642:GLN:NE2	2.34	0.61
1:A:640:LEU:HA	1:A:660:PRO:HB2	1.83	0.60
2:B:233:SER:OG	2:B:234:ALA:N	2.34	0.60
1:A:1148:ASN:HA	1:A:1200:LYS:HE3	1.84	0.60
1:A:36:ILE:HG12	1:A:54:LEU:CD2	2.32	0.59
2:B:301:PRO:HG2	2:B:625:GLN:HB3	1.84	0.59
2:B:977:LYS:HD3	2:B:992:LYS:HD3	1.85	0.59
2:B:93:LEU:C	2:B:93:LEU:CD1	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD12	1:A:66:SER:HB2	1.84	0.58
2:B:594:ILE:HG23	2:B:617:LEU:HD22	1.85	0.58
1:A:1214:ARG:NH2	2:B:939:ASP:OD2	2.36	0.58
2:B:1135:GLN:H	2:B:1138:LYS:HB2	1.69	0.57
2:B:58:PHE:O	2:B:143:ASN:ND2	2.34	0.57
1:A:111:GLY:HA3	1:A:428:ILE:HD11	1.86	0.56
1:A:585:ARG:NH2	1:A:613:LEU:O	2.38	0.56
1:A:1052:GLU:N	1:A:1053:PRO:HD2	2.20	0.56
1:A:66:SER:HB3	1:A:188:ILE:HG22	1.88	0.56
1:A:990:GLU:O	1:A:1089:ARG:NH1	2.35	0.56
2:B:765:VAL:HG22	2:B:841:LEU:HD12	1.87	0.56
1:A:232:LYS:HD2	1:A:237:ASP:HA	1.87	0.56
2:B:524:GLN:HE21	2:B:530:ASP:HB3	1.71	0.56
1:A:925:GLY:HA3	1:A:951:THR:HG21	1.88	0.56
2:B:896:ILE:HD11	2:B:1035:ASN:HA	1.88	0.55
2:B:95:LEU:HD22	2:B:188:VAL:HG23	1.88	0.55
1:A:1145:LEU:HD22	1:A:1151:TYR:CE2	2.41	0.55
1:A:54:LEU:HD12	1:A:66:SER:CB	2.37	0.55
1:A:1148:ASN:HB2	1:A:1209:MET:HA	1.89	0.55
1:A:702:VAL:HG11	1:A:835:ILE:HD11	1.88	0.55
2:B:102:ALA:HA	2:B:279:LYS:HG3	1.89	0.54
2:B:135:LEU:HD21	2:B:166:TRP:HE3	1.72	0.54
1:A:262:ILE:HG21	1:A:389:VAL:HG13	1.89	0.54
1:A:253:THR:HG21	1:A:396:ASP:HA	1.89	0.54
2:B:718:THR:HG22	2:B:720:ASP:H	1.71	0.54
2:B:559:ASP:OD1	2:B:559:ASP:N	2.40	0.54
1:A:1278:ASN:HA	1:A:1283:PRO:HA	1.90	0.54
2:B:239:LEU:O	2:B:241:PRO:N	2.41	0.54
2:B:557:PRO:HD2	2:B:563:LEU:HD23	1.89	0.54
1:A:958:GLN:HE22	2:B:996:ASN:ND2	2.05	0.54
2:B:145:ASN:HD22	2:B:166:TRP:HA	1.73	0.54
2:B:240:GLN:HG2	2:B:564:LYS:HD3	1.91	0.53
1:A:632:GLN:HE21	2:B:533:ASN:HB3	1.74	0.53
2:B:240:GLN:O	2:B:241:PRO:C	2.47	0.53
1:A:643:LYS:HA	1:A:659:LEU:HD23	1.90	0.52
2:B:239:LEU:HD22	2:B:377:VAL:HB	1.92	0.52
1:A:396:ASP:OD1	1:A:396:ASP:N	2.43	0.52
1:A:195:PRO:HG2	1:A:198:GLU:HB2	1.91	0.52
1:A:590:GLU:HB3	1:A:606:LYS:HG2	1.93	0.51
2:B:212:GLN:HE22	2:B:548:ASP:HB2	1.75	0.51
1:A:965:ASP:O	1:A:1009:ARG:NH1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:LYS:NZ	1:A:1048:GLU:OE2	2.44	0.51
2:B:301:PRO:CG	2:B:625:GLN:HB3	2.40	0.51
2:B:550:LEU:HD22	2:B:570:GLN:HG2	1.92	0.51
2:B:1128:LYS:HB2	2:B:1148:GLU:HB3	1.93	0.51
1:A:926:LEU:HB3	2:B:1015:ALA:HB1	1.93	0.51
1:A:230:ARG:HG2	1:A:422:TRP:HA	1.93	0.51
2:B:1146:LEU:HD11	2:B:1182:PHE:CB	2.41	0.51
1:A:63:ILE:HG23	1:A:185:ILE:HB	1.93	0.50
1:A:325:ASN:O	1:A:341:GLN:NE2	2.44	0.50
1:A:294:MET:HG2	1:A:297:LEU:HD12	1.93	0.50
2:B:179:ARG:NH2	2:B:618:ASP:OD2	2.45	0.50
1:A:56:LEU:HD22	1:A:64:PHE:HB3	1.94	0.50
1:A:111:GLY:CA	1:A:428:ILE:HD11	2.42	0.50
2:B:880:LYS:NZ	2:B:1074:TYR:O	2.45	0.50
1:A:1265:ILE:HG21	1:A:1322:LYS:HD3	1.92	0.50
1:A:1158:ASN:ND2	2:B:385:ASN:O	2.44	0.49
2:B:57:GLN:NE2	2:B:334:ILE:O	2.44	0.49
1:A:155:ILE:HD11	1:A:529:PRO:HG2	1.94	0.49
2:B:1185:ARG:HA	2:B:1190:ILE:HG12	1.93	0.49
1:A:1207:LYS:NZ	2:B:937:SER:OG	2.41	0.49
1:A:516:ILE:CD1	2:B:981:VAL:HG21	2.42	0.49
1:A:1302:LEU:CD1	2:B:392:SER:HB2	2.43	0.49
1:A:638:TYR:CZ	2:B:507:THR:HG21	2.48	0.49
2:B:101:GLY:HA3	2:B:395:ILE:HD12	1.94	0.49
1:A:181:LYS:HA	1:A:531:SER:HA	1.95	0.49
2:B:447:LEU:HD21	2:B:480:LEU:HB3	1.94	0.49
2:B:174:ASN:ND2	2:B:299:VAL:O	2.46	0.49
2:B:583:GLU:HB2	2:B:632:THR:HG21	1.96	0.48
2:B:1041:GLN:HB3	2:B:1074:TYR:HB3	1.95	0.48
2:B:269:ASN:HB2	2:B:272:TYR:H	1.78	0.48
2:B:1005:SER:HB2	2:B:1008:ILE:HB	1.95	0.48
1:A:133:PHE:HA	1:A:136:ILE:HG22	1.94	0.48
2:B:839:ILE:HD13	2:B:855:VAL:HG11	1.95	0.48
1:A:385:ILE:HA	1:A:388:TYR:HB3	1.95	0.48
2:B:93:LEU:HD12	2:B:94:GLU:N	2.28	0.48
2:B:1047:SER:HB3	2:B:1071:THR:HB	1.94	0.48
1:A:92:LEU:H	1:A:104:GLN:NE2	2.12	0.48
2:B:68:ASP:HB3	2:B:71:GLU:HG2	1.94	0.48
1:A:570:ILE:HD13	1:A:665:TYR:HA	1.96	0.48
2:B:884:ILE:HG21	2:B:928:LEU:HD12	1.96	0.48
1:A:277:THR:HA	1:A:293:PRO:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1198:GLN:HB3	1:A:1224:ILE:HD12	1.96	0.47
2:B:241:PRO:O	2:B:242:TYR:C	2.52	0.47
1:A:927:GLY:HA3	1:A:931:GLN:HA	1.96	0.47
2:B:232:PHE:HZ	2:B:236:VAL:HG23	1.79	0.47
2:B:707:ASP:OD1	2:B:707:ASP:N	2.47	0.47
1:A:128:TYR:OH	1:A:394:PHE:O	2.31	0.47
1:A:662:TYR:OH	1:A:819:ASN:ND2	2.47	0.47
1:A:567:ALA:HB3	1:A:568:PRO:HD3	1.95	0.47
2:B:779:PHE:O	2:B:791:TYR:N	2.47	0.47
1:A:251:GLU:O	1:A:255:GLY:N	2.48	0.47
1:A:958:GLN:NE2	2:B:996:ASN:HD21	2.12	0.47
1:A:51:TYR:OH	1:A:158:GLN:NE2	2.47	0.47
1:A:145:PRO:O	1:A:147:GLN:NE2	2.44	0.47
1:A:681:THR:HG23	1:A:683:ASP:H	1.80	0.47
2:B:58:PHE:CE1	2:B:316:PRO:HB3	2.49	0.47
2:B:560:ILE:HG21	2:B:654:THR:HG21	1.97	0.47
2:B:665:ASP:OD1	2:B:665:ASP:N	2.41	0.47
2:B:793:ILE:HD12	2:B:796:LEU:HD13	1.97	0.47
2:B:688:GLN:HB2	2:B:855:VAL:HG23	1.97	0.47
2:B:129:VAL:HG12	2:B:402:VAL:HG12	1.97	0.47
2:B:718:THR:OG1	2:B:729:LEU:HB2	2.15	0.47
1:A:1154:LEU:HD23	1:A:1161:ALA:HB2	1.96	0.47
2:B:437:ILE:HG12	2:B:456:LEU:HD11	1.96	0.47
2:B:876:ILE:HD12	2:B:936:ILE:HG22	1.97	0.47
2:B:710:LYS:HE3	2:B:737:GLU:HB3	1.97	0.46
2:B:55:PRO:HB2	2:B:332:VAL:HG21	1.98	0.46
2:B:239:LEU:HG	2:B:242:TYR:CZ	2.50	0.46
2:B:240:GLN:H	2:B:240:GLN:NE2	2.13	0.46
2:B:886:VAL:HG13	2:B:929:GLU:HA	1.96	0.46
2:B:915:SER:OG	2:B:917:ASP:OD1	2.32	0.46
2:B:929:GLU:OE1	2:B:945:ARG:NH1	2.47	0.46
1:A:478:LYS:NZ	1:A:556:THR:OG1	2.47	0.46
1:A:1008:GLU:HA	1:A:1031:VAL:O	2.15	0.46
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.77	0.46
2:B:40:ARG:HG3	2:B:66:LEU:HB2	1.97	0.46
2:B:120:ASP:OD1	2:B:124:LYS:N	2.49	0.46
1:A:999:ARG:HB2	1:A:1060:TRP:CD2	2.52	0.45
2:B:557:PRO:CD	2:B:563:LEU:HD23	2.46	0.45
2:B:767:PHE:HD2	2:B:806:ILE:HD13	1.81	0.45
2:B:780:GLU:OE2	2:B:790:LYS:NZ	2.50	0.45
1:A:34:SER:OG	1:A:35:ARG:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:HD2	1:A:403:ILE:HD11	1.80	0.45
1:A:950:SER:OG	1:A:951:THR:N	2.49	0.45
1:A:994:ILE:HD12	1:A:1012:PHE:HZ	1.81	0.45
2:B:114:THR:OG1	2:B:131:ALA:O	2.35	0.45
2:B:44:GLU:HB3	2:B:414:PHE:HE2	1.80	0.45
2:B:154:ASP:N	2:B:154:ASP:OD1	2.48	0.45
1:A:565:ILE:HG22	1:A:570:ILE:HG13	1.98	0.45
2:B:41:TYR:HB3	2:B:139:GLY:HA2	1.99	0.45
2:B:303:ASN:HA	2:B:306:TYR:CZ	2.52	0.45
1:A:1001:PRO:HB3	1:A:1333:ASN:HB3	1.98	0.45
1:A:1147:TYR:HB3	1:A:1203:PRO:HD3	1.99	0.45
2:B:241:PRO:HB2	2:B:562:GLN:HA	1.98	0.45
1:A:232:LYS:O	1:A:409:ARG:NH2	2.49	0.45
1:A:511:ILE:HG21	1:A:891:ALA:HB2	1.99	0.45
1:A:605:PRO:HD2	1:A:610:MET:HG3	1.98	0.45
1:A:246:LEU:HD21	1:A:401:ALA:HB2	1.98	0.44
1:A:804:PHE:O	1:A:805:PRO:C	2.55	0.44
2:B:143:ASN:OD1	2:B:143:ASN:N	2.51	0.44
1:A:190:PRO:HA	1:A:222:GLN:HB3	1.99	0.44
1:A:710:MET:HG3	1:A:849:TYR:HE2	1.82	0.44
2:B:201:LEU:HD11	2:B:287:LEU:HD13	1.98	0.44
1:A:197:THR:HG22	1:A:227:PHE:HB3	2.00	0.44
1:A:650:GLN:NE2	1:A:681:THR:OG1	2.51	0.44
1:A:1200:LYS:HG3	1:A:1224:ILE:HD11	1.98	0.44
2:B:647:VAL:HG13	2:B:648:ILE:HG23	2.00	0.44
1:A:210:PHE:HB3	1:A:266:VAL:HG11	2.00	0.44
1:A:157:ASP:N	1:A:157:ASP:OD1	2.51	0.44
1:A:251:GLU:HA	1:A:254:HIS:HB2	1.99	0.44
1:A:35:ARG:HB3	1:A:51:TYR:HD2	1.83	0.44
1:A:766:ARG:NE	1:A:808:MET:HE1	2.32	0.44
2:B:546:ILE:HG12	2:B:578:ARG:HB2	2.00	0.44
1:A:700:ILE:HD12	1:A:830:ILE:HG21	2.00	0.43
2:B:731:SER:HA	2:B:847:GLU:HG2	2.00	0.43
2:B:754:THR:HB	2:B:851:LYS:HB3	2.00	0.43
2:B:147:LEU:O	2:B:197:ARG:NH1	2.51	0.43
2:B:577:THR:HA	2:B:580:LEU:HB3	2.00	0.43
1:A:300:PHE:HD1	1:A:397:GLU:HB3	1.83	0.43
2:B:50:ASP:OD1	2:B:50:ASP:N	2.51	0.43
2:B:719:ASP:OD1	2:B:719:ASP:N	2.51	0.43
1:A:423:SER:HB3	1:A:453:LEU:HD12	1.99	0.43
1:A:1078:ASP:HB2	1:A:1126:LYS:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:LEU:O	2:B:242:TYR:N	2.52	0.43
2:B:688:GLN:HG3	2:B:740:PHE:HE1	1.84	0.43
1:A:505:ASP:O	1:A:733:ASN:ND2	2.44	0.43
2:B:233:SER:HB3	2:B:572:TYR:CE2	2.53	0.43
1:A:1067:ASN:OD1	1:A:1089:ARG:NH2	2.51	0.43
2:B:899:ASP:OD1	2:B:1041:GLN:NE2	2.45	0.43
1:A:576:LEU:HD11	1:A:578:ASN:ND2	2.33	0.43
2:B:203:LEU:HB2	2:B:224:GLU:HG3	2.00	0.43
1:A:1193:TYR:HB3	1:A:1328:VAL:HG21	2.00	0.43
2:B:751:VAL:HG22	2:B:855:VAL:HG12	2.00	0.43
2:B:781:ILE:HD11	2:B:813:ILE:HD11	2.00	0.43
2:B:105:LEU:O	2:B:113:ASN:ND2	2.48	0.42
2:B:438:PHE:CE2	2:B:588:GLN:HB3	2.54	0.42
2:B:239:LEU:HA	2:B:242:TYR:CE1	2.54	0.42
2:B:450:ILE:HG12	2:B:600:LEU:HD11	2.01	0.42
1:A:766:ARG:CB	1:A:808:MET:CE	2.94	0.42
1:A:912:LEU:HD22	1:A:939:ASN:HB3	2.01	0.42
1:A:453:LEU:HA	1:A:453:LEU:HD23	1.84	0.42
1:A:97:LEU:HD13	1:A:425:ARG:HD2	2.00	0.42
2:B:300:ILE:HG21	2:B:306:TYR:OH	2.20	0.42
2:B:305:LYS:HB3	2:B:580:LEU:HD21	2.01	0.42
2:B:544:PHE:HD2	2:B:579:ILE:HA	1.84	0.42
1:A:315:LEU:HD11	1:A:744:VAL:HG13	2.02	0.42
1:A:730:GLN:HA	1:A:733:ASN:HB2	2.00	0.42
2:B:53:THR:OG1	2:B:54:ASN:N	2.52	0.41
1:A:157:ASP:O	1:A:161:SER:OG	2.30	0.41
1:A:855:GLU:O	1:A:859:ASN:ND2	2.47	0.41
1:A:923:LEU:HD11	1:A:976:VAL:HG21	2.01	0.41
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.85	0.41
1:A:571:ASN:O	1:A:767:ASN:ND2	2.44	0.41
1:A:1302:LEU:HD11	2:B:392:SER:CB	2.47	0.41
2:B:278:LEU:HD21	2:B:394:GLU:HB3	2.02	0.41
2:B:655:SER:OG	2:B:656:GLU:OE1	2.36	0.41
1:A:297:LEU:HD23	1:A:309:ILE:HG23	2.02	0.41
2:B:438:PHE:HB3	2:B:439:PRO:CD	2.49	0.41
1:A:696:ALA:O	1:A:753:ARG:NH2	2.47	0.41
1:A:1302:LEU:HD12	2:B:94:GLU:HG2	2.01	0.41
2:B:239:LEU:HG	2:B:242:TYR:CE2	2.55	0.41
2:B:1100:SER:HB2	2:B:1115:LYS:HD2	2.03	0.41
1:A:922:HIS:CD2	2:B:1020:SER:O	2.74	0.41
1:A:1047:SER:HB2	1:A:1084:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:885:ILE:HB	2:B:888:GLU:HG3	2.01	0.41
1:A:26:LEU:HD12	1:A:26:LEU:HA	1.95	0.41
1:A:254:HIS:ND1	1:A:295:GLU:OE2	2.54	0.41
2:B:47:GLN:HB3	2:B:51:GLU:HB2	2.02	0.41
2:B:578:ARG:HE	2:B:581:ARG:HD3	1.85	0.41
1:A:241:LEU:HD12	1:A:241:LEU:HA	1.95	0.41
1:A:579:SER:OG	1:A:580:LYS:HD2	2.20	0.41
1:A:570:ILE:HG12	1:A:592:LEU:HD21	2.02	0.40
2:B:704:LEU:HB2	2:B:709:ILE:HD13	2.03	0.40
1:A:281:ARG:H	1:A:483:TYR:HB3	1.86	0.40
1:A:1133:HIS:O	1:A:1138:TYR:OH	2.28	0.40
2:B:890:TYR:HB3	2:B:1040:ILE:HG23	2.04	0.40
1:A:416:PRO:HD2	1:A:477:PRO:HB3	2.03	0.40
1:A:372:ASN:OD1	1:A:372:ASN:N	2.53	0.40
1:A:1037:VAL:HG22	1:A:1050:VAL:HG22	2.02	0.40
1:A:358:ASP:OD1	1:A:358:ASP:N	2.54	0.40
1:A:710:MET:HE2	1:A:723:MET:HG2	2.04	0.40
1:A:873:THR:HG22	1:A:876:ARG:HH22	1.86	0.40
1:A:922:HIS:HB2	1:A:937:TYR:CZ	2.57	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	1333/1371 (97%)	1215 (91%)	116 (9%)	2 (0%)	47	80
2	B	1193/1458 (82%)	1104 (92%)	85 (7%)	4 (0%)	41	74
All	All	2526/2829 (89%)	2319 (92%)	201 (8%)	6 (0%)	50	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	SER
2	B	241	PRO
2	B	302	ALA
2	B	242	TYR
1	A	1166	TYR
2	B	898	ASP

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	1190/1218 (98%)	1186 (100%)	4 (0%)	92 97
2	B	1090/1330 (82%)	1078 (99%)	12 (1%)	73 90
All	All	2280/2548 (90%)	2264 (99%)	16 (1%)	84 93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	575	LYS
1	A	576	LEU
1	A	658	ILE
1	A	806	MET
2	B	93	LEU
2	B	164	LEU
2	B	239	LEU
2	B	240	GLN
2	B	241	PRO
2	B	332	VAL
2	B	355	THR
2	B	386	VAL
2	B	626	TYR
2	B	722	LEU
2	B	782	THR
2	B	897	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	104	GLN
1	A	158	GLN
1	A	184	ASN
1	A	303	HIS
1	A	390	GLN
1	A	445	GLN
1	A	572	HIS
1	A	632	GLN
1	A	650	GLN
1	A	730	GLN
1	A	819	ASN
1	A	931	GLN
1	A	958	GLN
1	A	1076	GLN
2	B	145	ASN
2	B	212	GLN
2	B	344	ASN
2	B	362	GLN
2	B	524	GLN
2	B	570	GLN
2	B	591	ASN
2	B	643	GLN
2	B	688	GLN
2	B	733	ASN
2	B	777	ASN
2	B	825	HIS
2	B	865	ASN
2	B	996	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)

There are no ligands in this entry.

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.

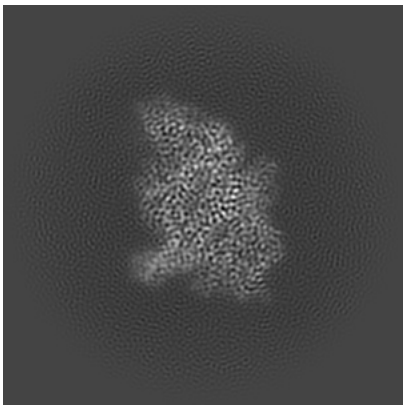
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16475. These allow visual inspection of the internal detail of the map and identification of artifacts.

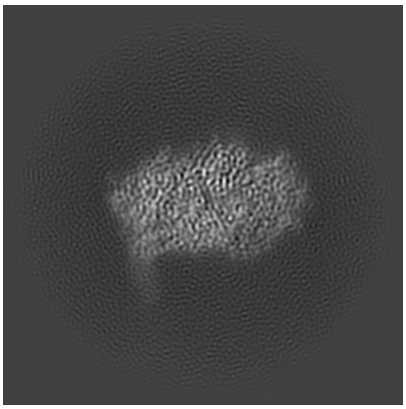
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

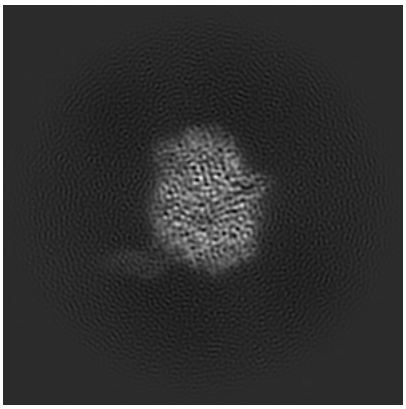
6.1.1 Primary map



X

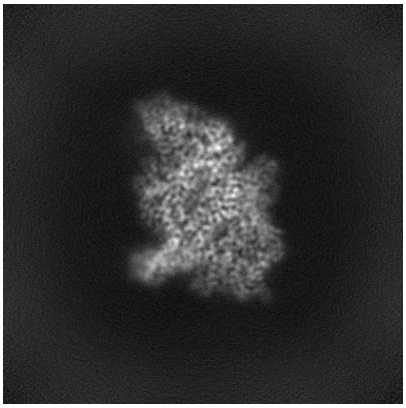


Y

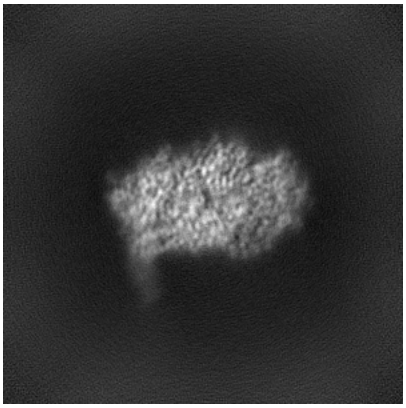


Z

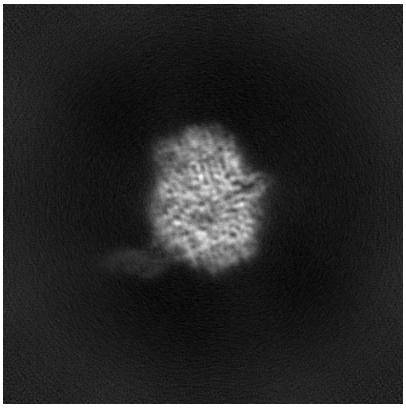
6.1.2 Raw map



X



Y

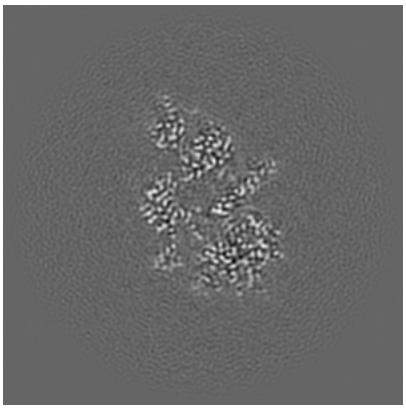


Z

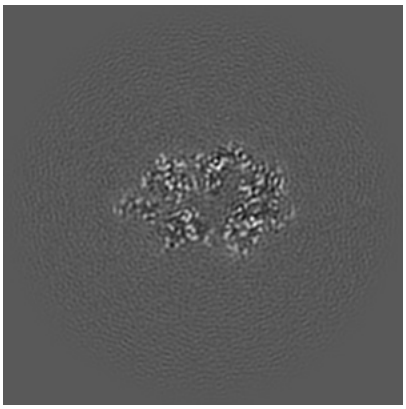
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

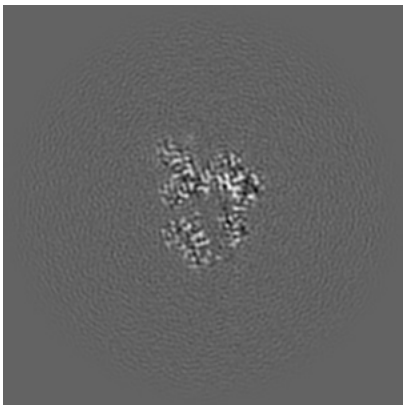
6.2.1 Primary map



X Index: 160

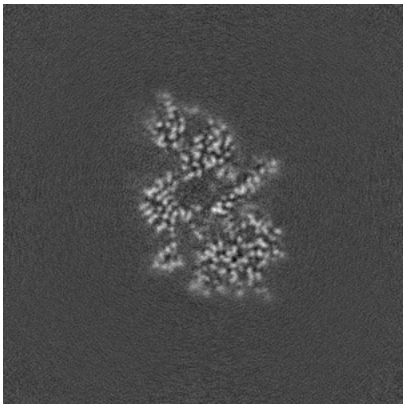


Y Index: 160

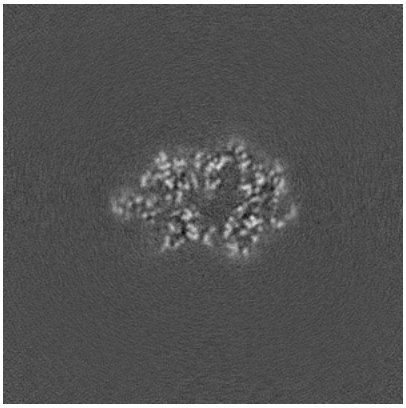


Z Index: 160

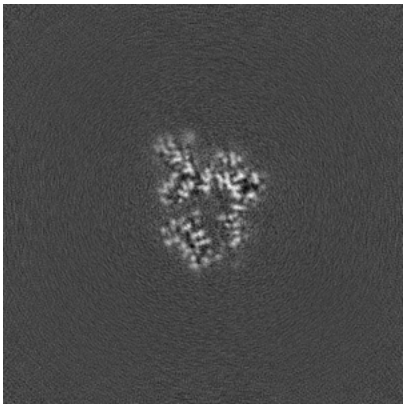
6.2.2 Raw map



X Index: 160



Y Index: 160

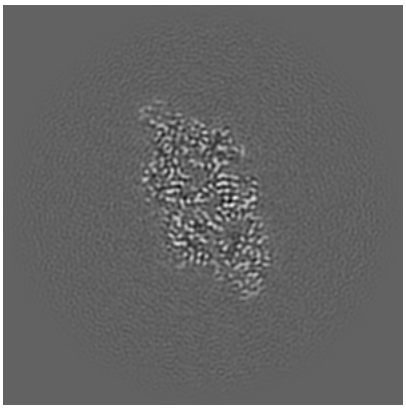


Z Index: 160

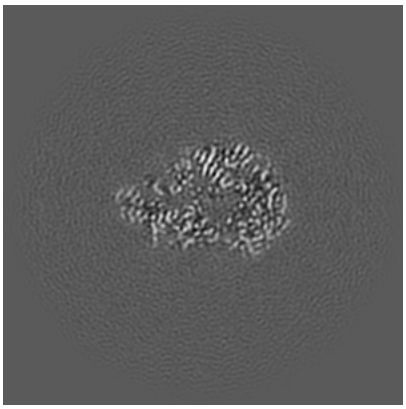
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

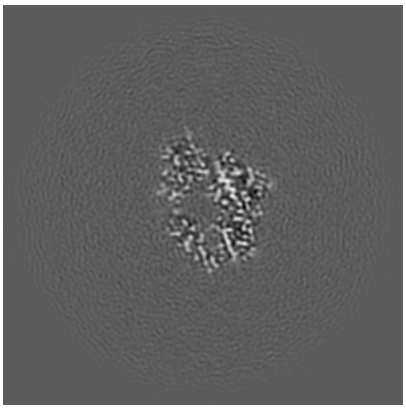
6.3.1 Primary map



X Index: 178

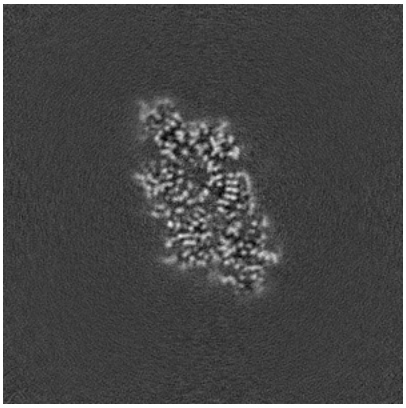


Y Index: 166

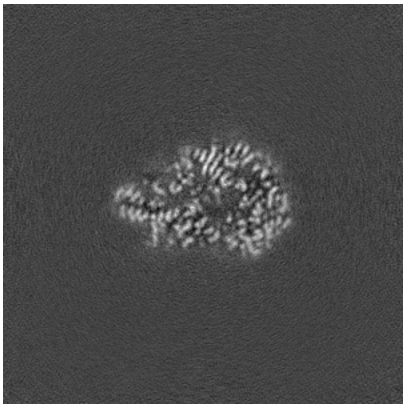


Z Index: 171

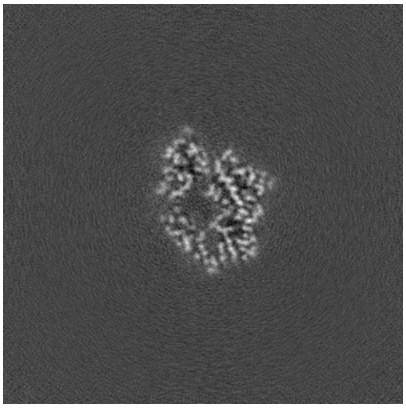
6.3.2 Raw map



X Index: 175



Y Index: 166

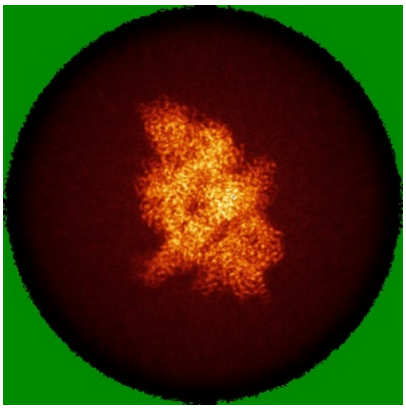


Z Index: 172

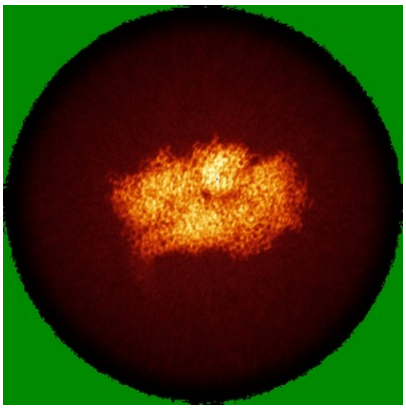
The images above show the largest variance slices of the map in three orthogonal directions.

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

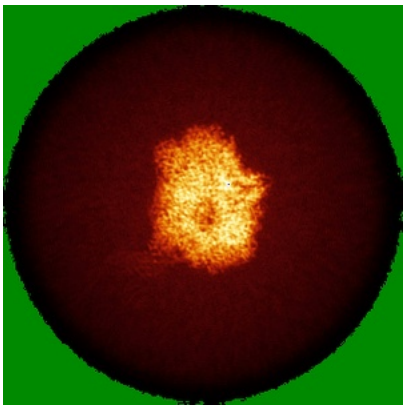
6.4.1 Primary map



X

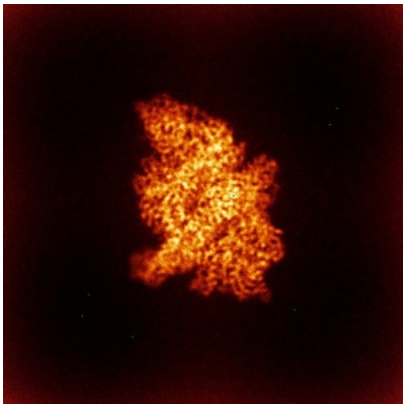


Y

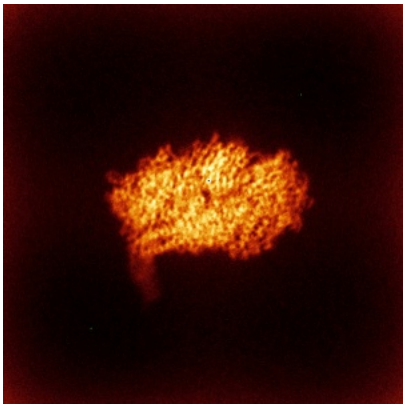


Z

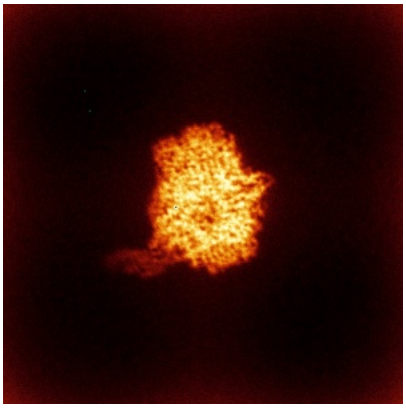
6.4.2 Raw map



X



Y

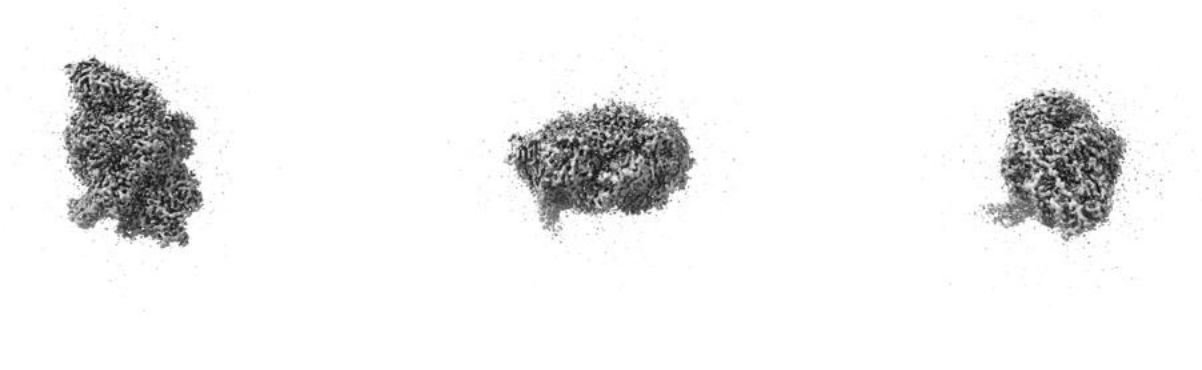


Z

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 0.124. 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.

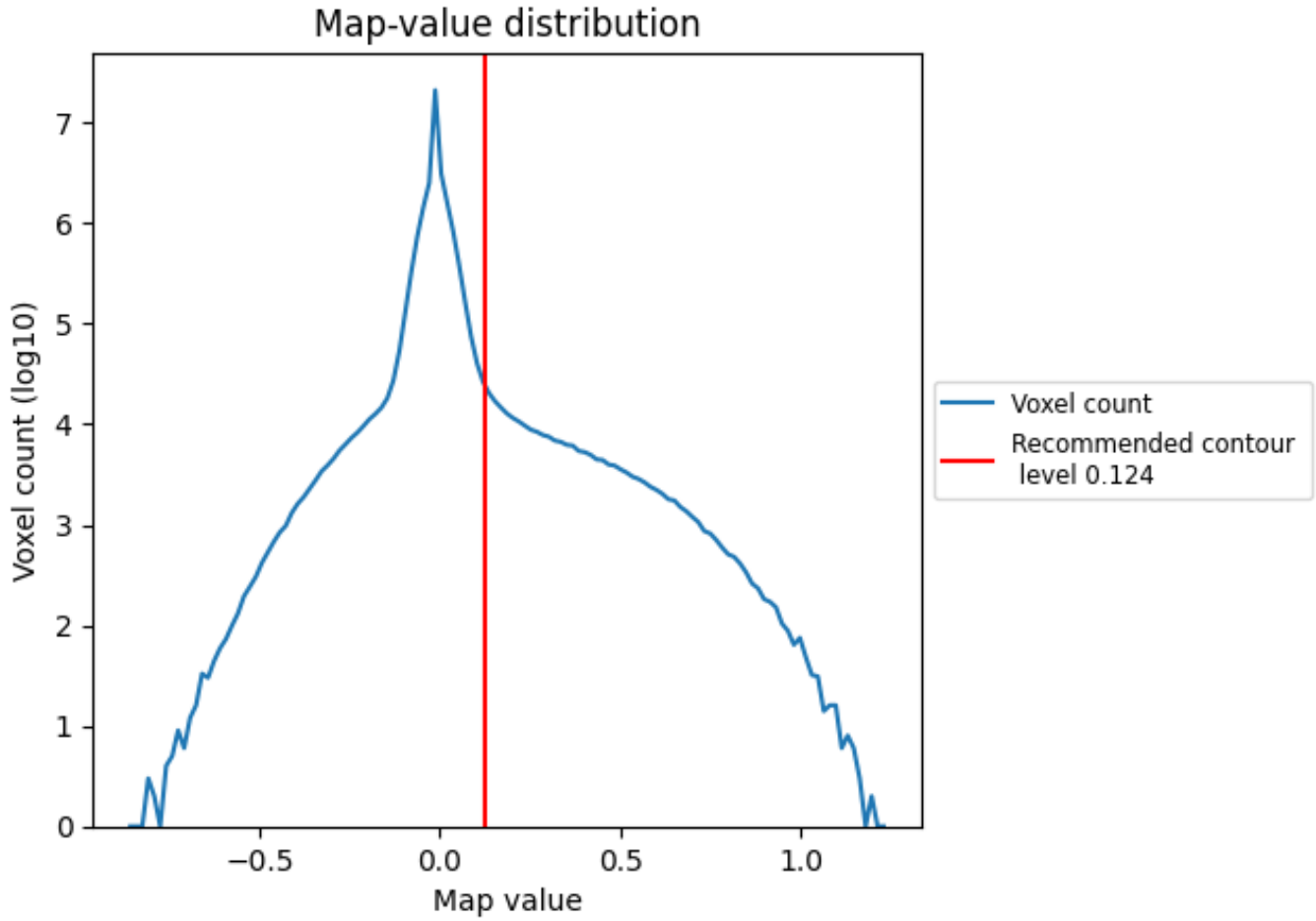
6.6 Mask visualisation (i)

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

7 Map analysis

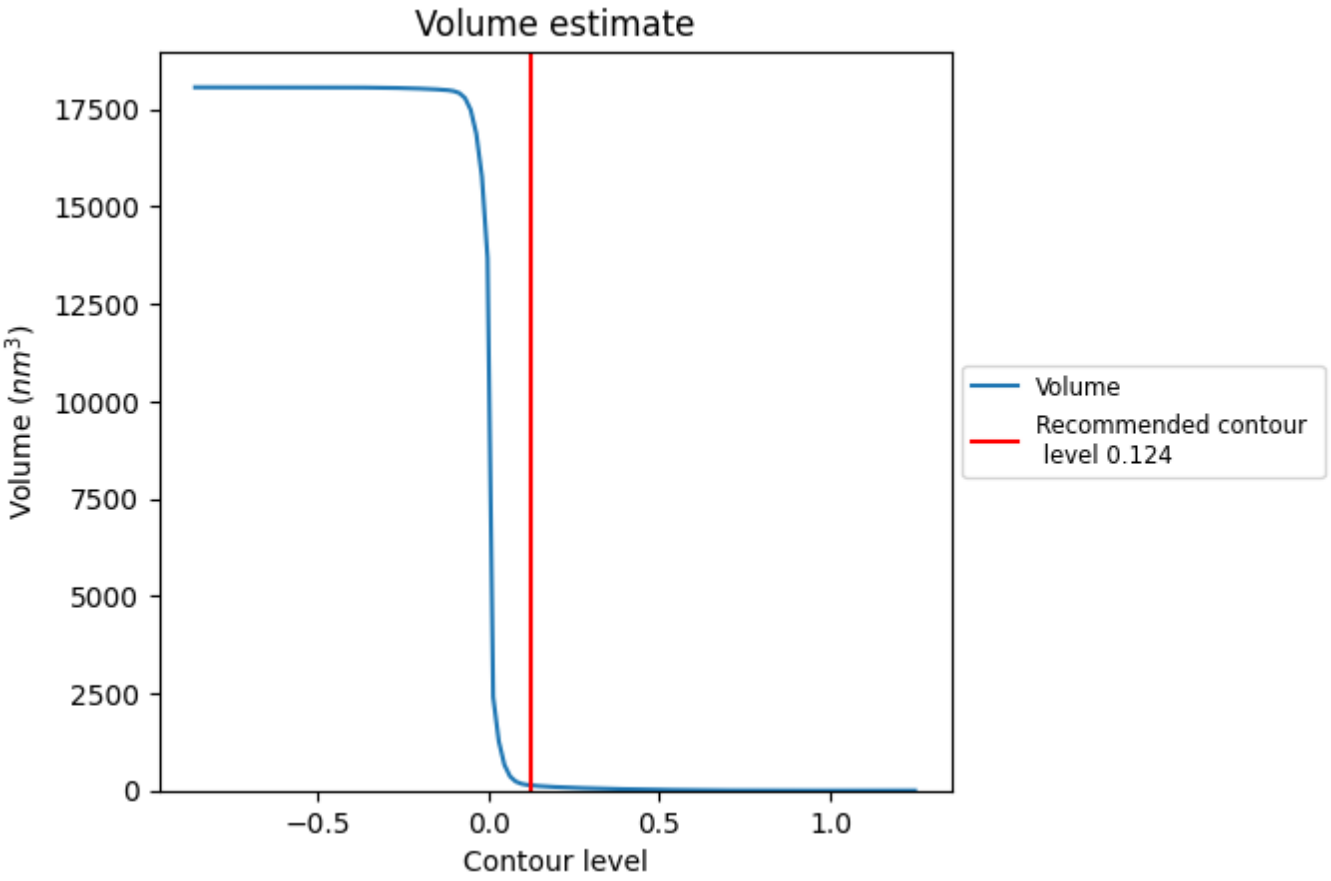
This section contains the results of statistical analysis of the map.

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.

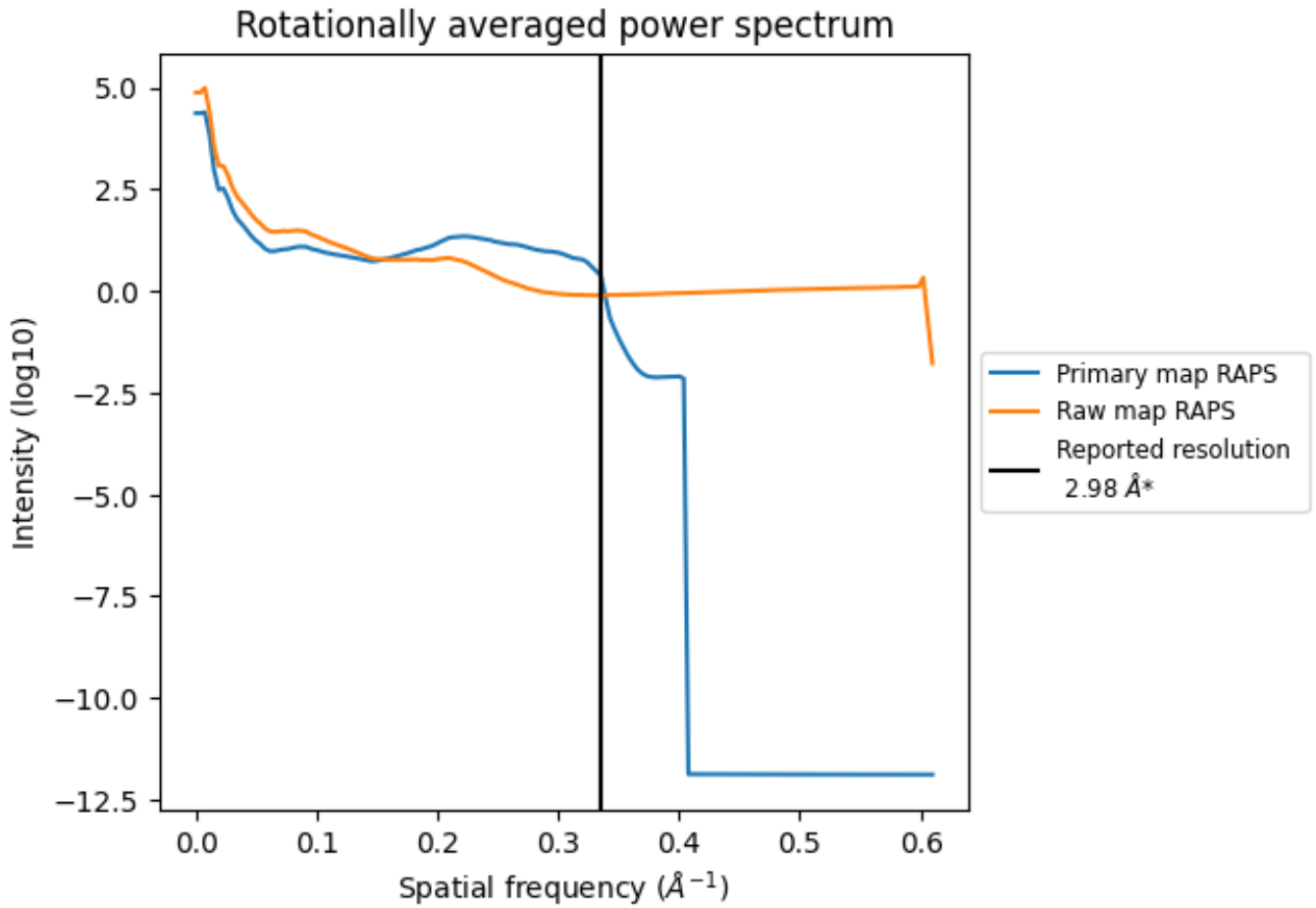
7.2 Volume estimate



The volume at the recommended contour level is 135 nm^3; this corresponds to an approximate mass of 122 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)

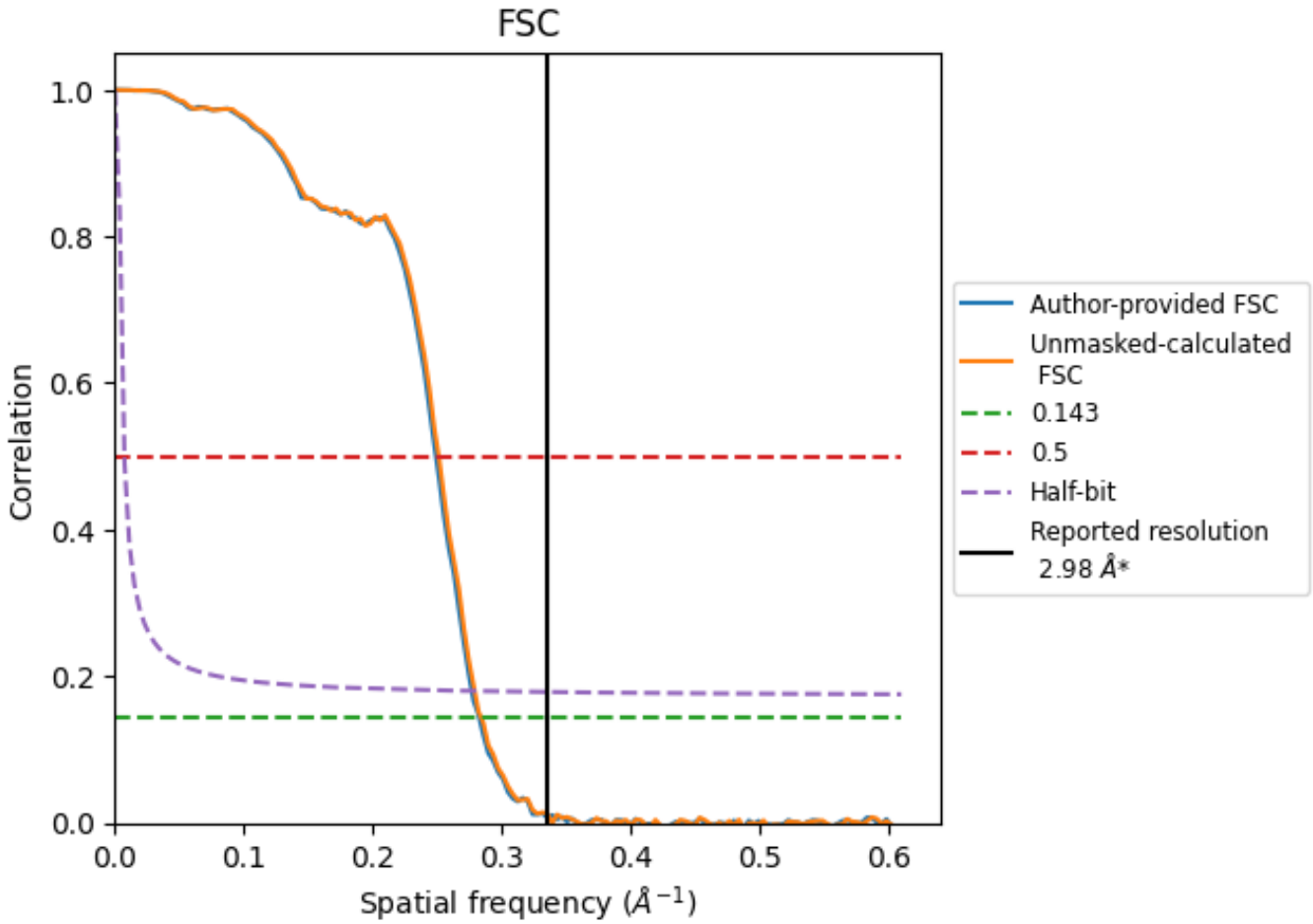


*Reported resolution corresponds to spatial frequency of 0.336 $Å^{-1}$

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 0.336 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	3.54	4.02	3.61
Unmasked-calculated*	3.52	3.98	3.58

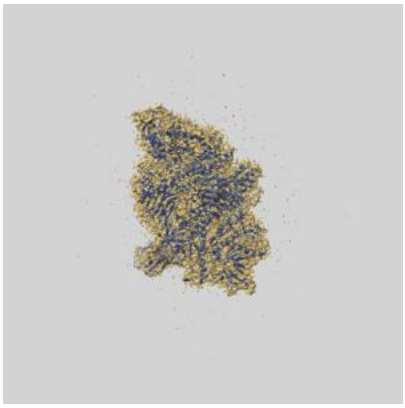
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.54 differs from the reported value 2.98 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.52 differs from the reported value 2.98 by more than 10 %

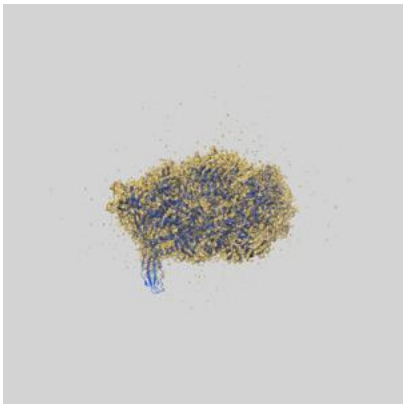
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16475 and PDB model 8C8G. Per-residue inclusion information can be found in section 3 on page 5.

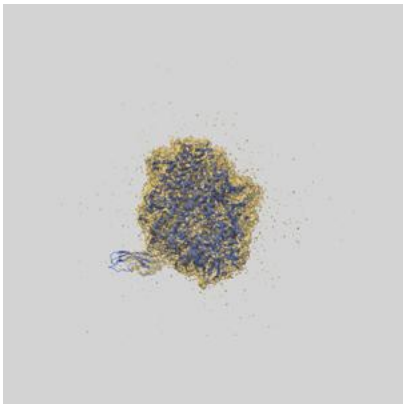
9.1 Map-model overlay



X



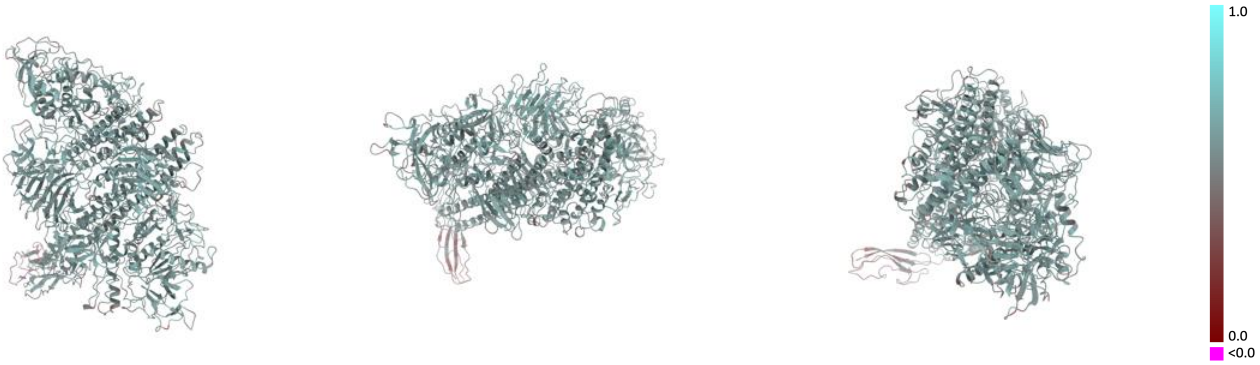
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.124 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

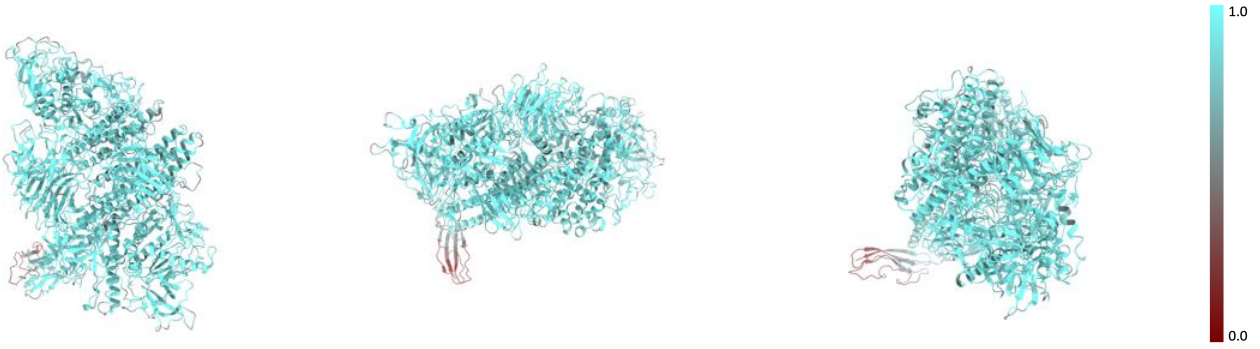
9.2 Q-score mapped to coordinate model



X Y Z

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

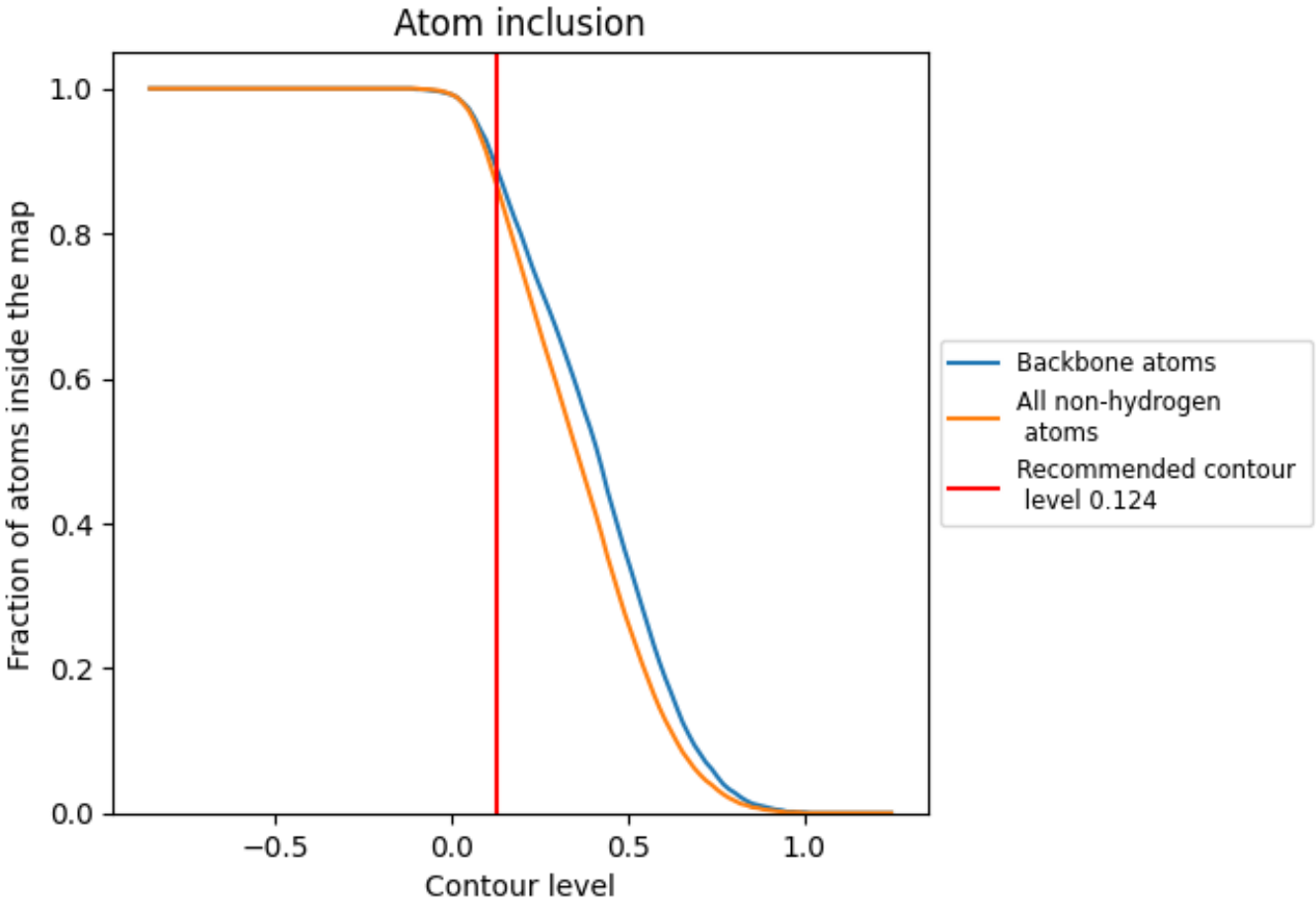
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.124).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.124) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.5630
A	0.8920	0.5710
B	0.8490	0.5530