Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 05:45 pm GMT

PDB ID	:	6YRK
EMDB ID	:	EMD-10890
Title	:	P140-P110 complex fitted into the cryo-electron density map of the heterodimer
Authors	:	Scheffer, M.P.; Aparicio, D.
Deposited on	:	2020-04-20
Resolution	:	4.10 Å(reported)
Based on initial models	:	6RUT, 6R3T

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

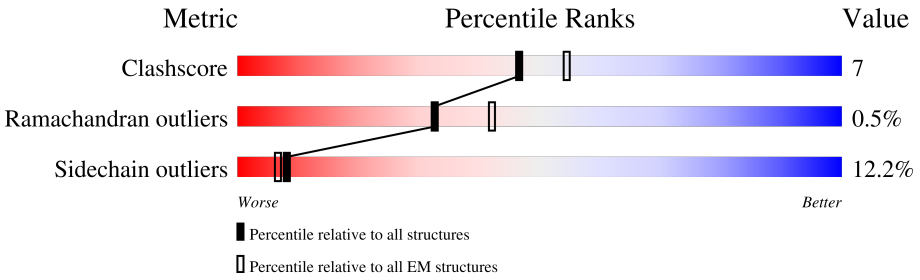
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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	777	15% 82% 15% .
2	B	1160	17% 73% 23% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15058 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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	777	5982	3740	1003	1233	6	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P22747
A	?	-	ILE	deletion	UNP P22747
A	?	-	GLY	deletion	UNP P22747
A	?	-	GLY	deletion	UNP P22747
A	?	-	GLY	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747

- Molecule 2 is a protein called Adhesin P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1160	9076	5750	1541	1772	13	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	ASP	deletion	UNP P20796
B	?	-	LYS	deletion	UNP P20796
B	?	-	ALA	deletion	UNP P20796

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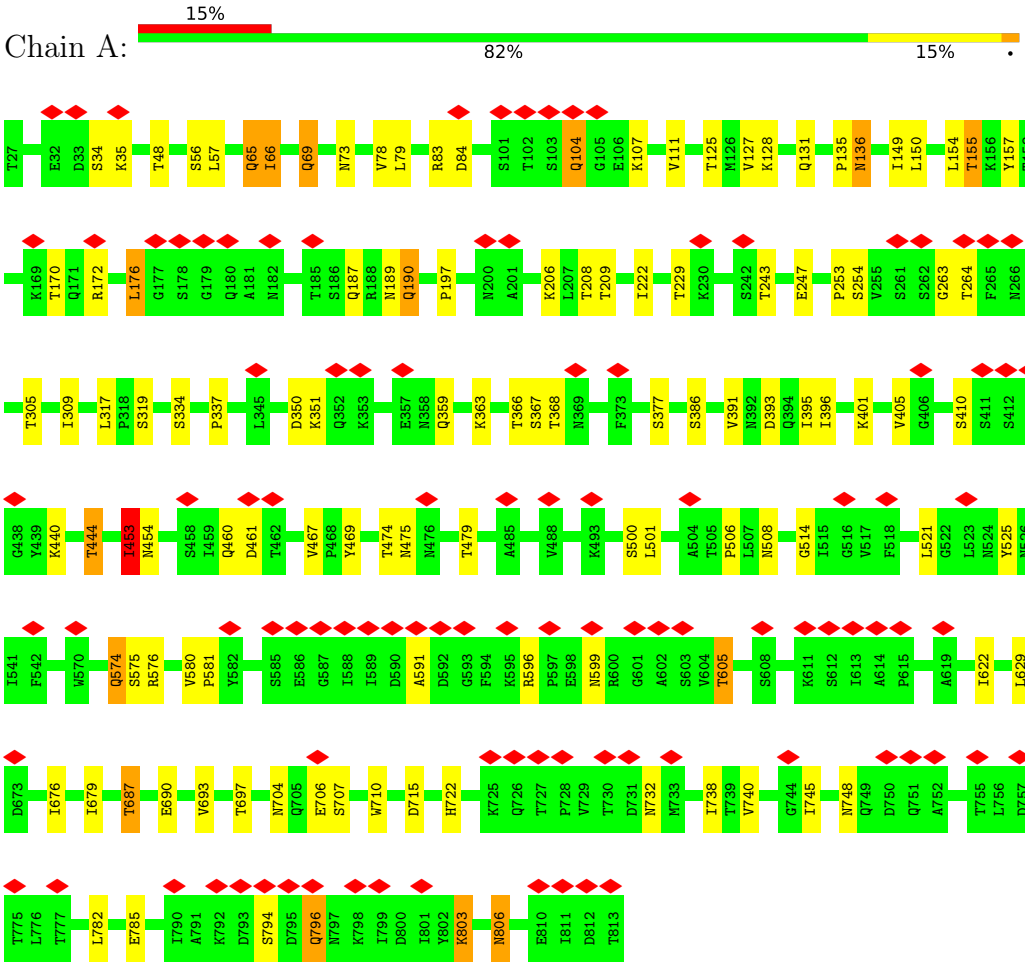
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P20796
B	?	-	GLN	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	PRO	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	THR	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	ALA	deletion	UNP P20796
B	789	ALA	SER	conflict	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	THR	deletion	UNP P20796
B	?	-	THR	deletion	UNP P20796
B	?	-	TYR	deletion	UNP P20796
B	?	-	ASP	deletion	UNP P20796
B	?	-	THR	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	GLN	deletion	UNP P20796
B	?	-	GLY	deletion	UNP P20796
B	?	-	ASN	deletion	UNP P20796

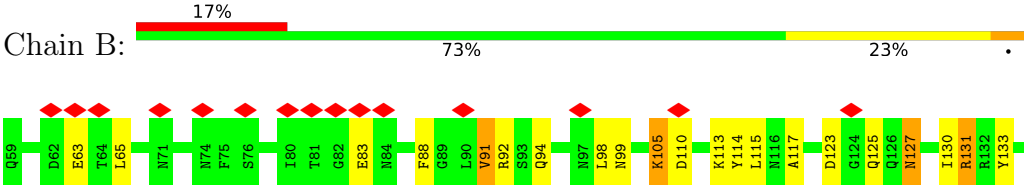
3 Residue-property plots (i)

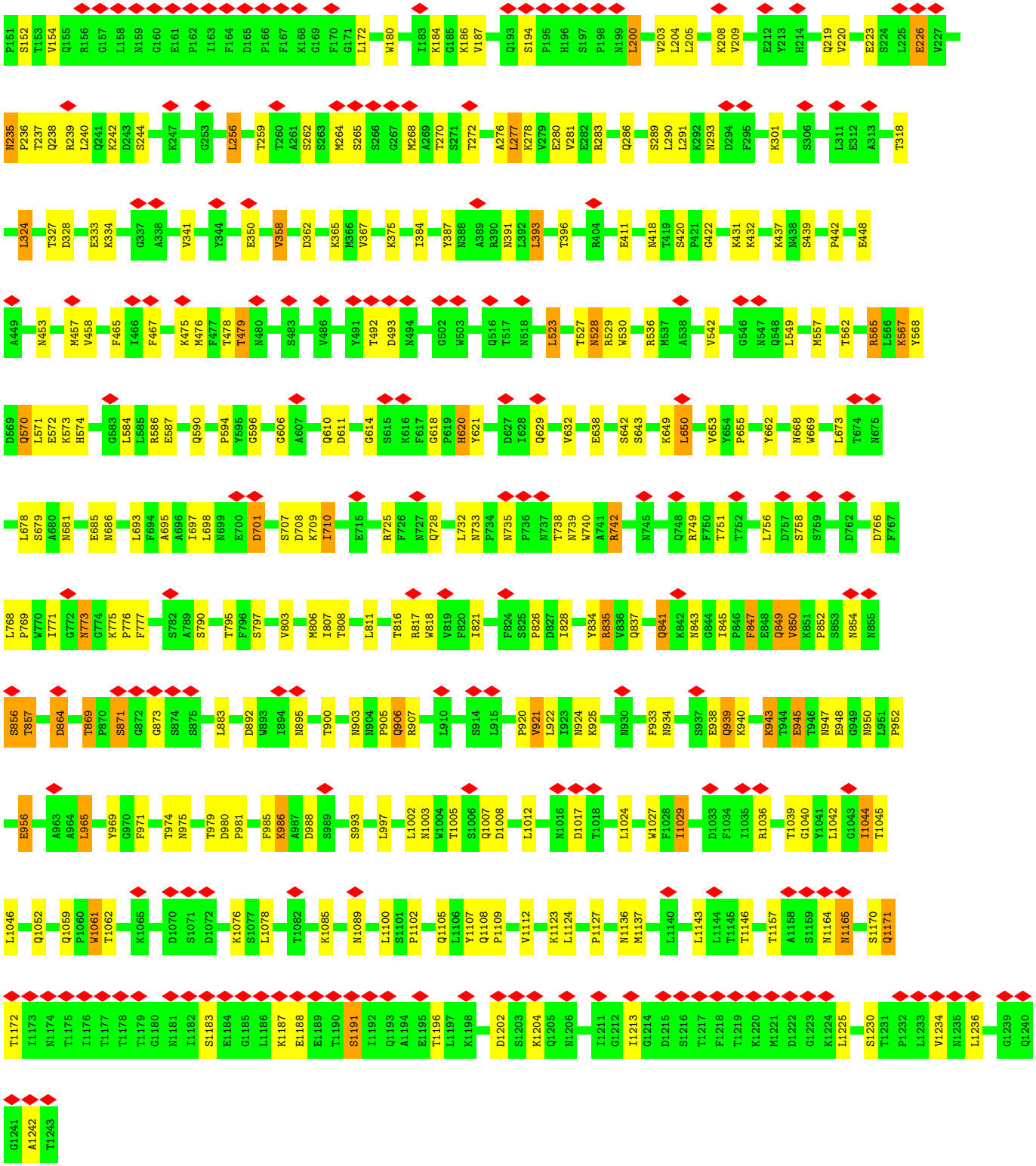
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Mgp-operon protein 3



• Molecule 2: Adhesin P1




P151 S152 T153 V154 Q155 R156 G157 L158 N159 G160 E161 P162 I163 F164 D165 P166 F167 K168 G169 F170 G171 L172 W180 I183 K184 G185 K186 V187 Q193 S194 P195 H196 S197 P198 N199 L200 V203 L204 L205 K208 V209 E212 Y213 H214 Q219 V220 E223 S224 L225 E226 V227
N235 P236 T237 Q238 R239 L240 Q241 K242 D243 S244 K247 G253 L256 T259 T260 A261 S262 S263 M264 S265 S266 G267 M268 A269 T270 S271 T272 A276 L277 K278 V279 E280 V281 E282 R283 Q286 S289 L290 L291 K292 N293 D294 F295 K301 S306 L311 E312 A313 T318
L324 T327 D328 E333 K334 G337 A338 V341 Y344 E350 V358 D362 K365 M366 V367 K375 I384 Y387 N388 A389 R390 N391 L392 L393 T396 R404 E411 N418 T419 S420 P421 G422 K431 K432 K437 N438 S439 P442 E448
A449 N453 M457 V458 F465 I466 F467 K475 M476 F477 T478 T479 N480 S483 V486 Y491 T492 D493 N494 G502 W503 Q516 T517 N518 L523 T527 N528 R529 W530 R536 M537 A538 V542 G546 N547 Q548 L549 M557 T562 R565 L566 K567 Y568
D569 Q570 L571 E572 K573 H574 G583 L584 L585 R586 E587 Q590 P594 Y595 G596 G606 A607 Q610 D611 G614 S615 K616 F617 G618 P619 H620 Y621 D627 I628 Q629 V632 E638 S642 S643 K649 L650 V653 Y654 P655 Y662 N668 W669 L673 T674 N675
L678 S679 A680 N681 E685 N686 L693 F694 A695 A696 I697 L698 N699 E700 D701 S707 D708 K709 T710 E715 R725 F726 N727 Q728 L732 N733 P734 N735 P736 N737 T738 N739 W740 A741 R742 N745 Q748 R749 F750 T751 T752 L756 D757 S758 S759 D762 D766 F767
L768 P769 W770 I771 G772 N773 G774 K775 P776 F777 S782 A789 S790 T795 F796 S797 V803 M806 I807 T808 L811 T816 R817 W818 V819 F820 I821 F824 S825 P826 D827 I828 Y834 R835 V836 Q837 Q841 K842 N843 G844 I845 P846 F847 E848 Q849 V850 K851 P852 S853 N854 N855
S856 T857 D864 T869 P870 S871 G872 G873 S874 S875 L883 D892 W893 I894 N895 T900 N903 N904 P905 Q906 R907 L910 S914 L915 P920 V921 L922 I923 N924 K925 N930 F933 N934 S937 E938 Q939 K940 K943 T944 E945 T946 N947 E948 G949 N950 L951 P952
E956 A963 A964 L965 Y969 G970 F971 T974 N975 T979 D980 P981 F985 K986 A987 D988 S989 S993 L997 L1002 N1003 W1004 T1005 S1006 Q1007 D1008 L1012 N1016 D1017 T1018 L1024 W1027 F1028 I1029 D1033 F1034 I1035 R1036 T1039 G1040 Y1041 L1042 G1043 I1044 T1045
L1046 Q1052 Q1059 P1060 W1061 T1062 K1065 D1070 S1071 D1072 K1076 S1077 L1078 T1082 K1085 N1089 L1100 S1101 P1102 Q1105 L1106 Y1107 Q1108 P1109 V1112 K1123 L1124 P1127 N1136 M1137 L1140 L1143 L1144 T1145 T1146 T1157 A1158 S1159 N1164 N1165 S1170 Q1171
T1172 I1173 N1174 T1175 I1176 T1177 T1178 T1179 G1180 N1181 I1182 S1183 E1184 G1185 L1186 K1187 E1188 E1189 T1190 S1191 I1192 Q1193 A1194 E1195 T1196 L1197 K1198 D1202 S1203 K1204 Q1205 N1206 I1211 G1212 I1213 G1214 D1215 S1216 T1217 F1218 T1219 K1220 M1221 D1222 G1223 K1224 L1225 S1230 T1231 P1232 L1233 V1234 N1235 L1236 G1239 Q1240
G1241 A1242 T1243

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37009	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 ($e^-/Å^2$)	7.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	283.5, 283.5, 283.5	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.48	0/6105	0.74	0/8298
2	B	0.51	0/9303	0.76	1/12656 (0.0%)
All	All	0.50	0/15408	0.75	1/20954 (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	856	SER	C-N-CA	5.39	135.17	121.70

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	5982	0	5775	62	0
2	B	9076	0	8814	141	0
All	All	15058	0	14589	193	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 (193) 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:440:LYS:O	1:A:444:THR:HG23	1.63	0.97
2:B:527:THR:HG23	2:B:678:LEU:HD23	1.46	0.94
1:A:66:ILE:HD11	1:A:69:GLN:HG3	1.54	0.90
2:B:280:GLU:HG3	2:B:650:LEU:HD12	1.59	0.85
2:B:766:ASP:OD2	2:B:797:SER:HB3	1.84	0.78
2:B:924:ASN:HB2	2:B:985:PHE:HA	1.67	0.77
1:A:596:ARG:HB2	1:A:599:ASN:ND2	2.00	0.76
2:B:988:ASP:OD1	2:B:993:SER:HB2	1.86	0.75
1:A:66:ILE:HD12	1:A:78:VAL:HG13	1.67	0.75
1:A:474:THR:HG21	1:A:479:THR:CG2	2.18	0.74
2:B:65:LEU:HB3	2:B:91:VAL:HG13	1.70	0.73
1:A:474:THR:HG21	1:A:479:THR:HG21	1.70	0.73
1:A:65:GLN:HE22	1:A:83:ARG:HG3	1.55	0.72
1:A:136:ASN:HD22	1:A:136:ASN:H	1.37	0.71
1:A:687:THR:HG23	1:A:690:GLU:OE1	1.90	0.70
1:A:104:GLN:HA	1:A:104:GLN:OE1	1.91	0.70
2:B:773:ASN:HD22	2:B:775:LYS:HB2	1.55	0.70
1:A:596:ARG:HB2	1:A:599:ASN:HD22	1.54	0.69
1:A:155:THR:HG22	1:A:157:TYR:H	1.58	0.69
2:B:835:ARG:HD3	2:B:845:ILE:HG21	1.76	0.68
2:B:262:SER:HB2	2:B:643:SER:HB3	1.76	0.67
2:B:286:GLN:OE1	2:B:289:SER:HB3	1.97	0.65
2:B:1005:THR:HG22	2:B:1007:GLN:H	1.63	0.64
1:A:794:SER:H	1:A:796:GLN:HE22	1.45	0.63
1:A:187:GLN:O	1:A:190:GLN:HG2	1.99	0.62
2:B:226:GLU:HB2	2:B:239:ARG:CZ	2.29	0.62
1:A:460:GLN:HG3	2:B:895:ASN:HB2	1.82	0.62
2:B:278:LYS:HB2	2:B:650:LEU:HD11	1.82	0.62
2:B:1109:PRO:HB3	2:B:1137:MET:HE1	1.81	0.61
2:B:527:THR:HG23	2:B:678:LEU:CD2	2.25	0.61
2:B:921:VAL:HG13	2:B:965:LEU:HD13	1.83	0.61
2:B:341:VAL:HG22	2:B:358:VAL:HB	1.83	0.60
1:A:475:ASN:O	2:B:817:ARG:HD2	2.01	0.60
1:A:166:GLU:HG3	1:A:206:LYS:HB2	1.83	0.60
2:B:110:ASP:HA	2:B:220:VAL:HG13	1.83	0.59
1:A:475:ASN:ND2	2:B:817:ARG:H	2.00	0.59
2:B:934:ASN:O	2:B:938:GLU:HB2	2.01	0.59
1:A:135:PRO:HB3	1:A:337:PRO:HG2	1.85	0.59
2:B:268:MET:HB2	2:B:871:SER:OG	2.02	0.58
1:A:670:SER:HA	1:A:679:ILE:HG22	1.85	0.58
2:B:611:ASP:OD1	2:B:614:GLY:HA2	2.03	0.57
2:B:237:THR:HG22	2:B:1108:GLN:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:LEU:HB2	2:B:584:LEU:HD22	1.86	0.57
2:B:115:LEU:HD11	2:B:324:LEU:HD22	1.87	0.57
2:B:807:ILE:HG21	2:B:828:ILE:HD12	1.86	0.57
1:A:475:ASN:HD22	2:B:817:ARG:H	1.51	0.57
2:B:849:GLN:HE22	2:B:883:LEU:HD12	1.69	0.57
2:B:590:GLN:CD	2:B:906:GLN:HG2	2.26	0.56
1:A:66:ILE:HD12	1:A:78:VAL:CG1	2.35	0.56
1:A:197:PRO:HD2	1:A:453:ILE:HD11	1.88	0.55
2:B:590:GLN:OE1	2:B:906:GLN:HG2	2.06	0.55
1:A:66:ILE:HD11	1:A:69:GLN:CG	2.31	0.55
2:B:695:ALA:HB3	2:B:751:THR:HG22	1.88	0.55
2:B:1046:LEU:HD12	2:B:1213:ILE:HD12	1.87	0.55
2:B:773:ASN:HB3	2:B:775:LYS:H	1.72	0.55
2:B:773:ASN:HD21	2:B:975:ASN:HB3	1.72	0.54
2:B:777:PHE:O	2:B:795:THR:HG22	2.07	0.54
2:B:391:ASN:HD22	2:B:418:ASN:HD22	1.56	0.53
1:A:766:GLN:O	2:B:742:ARG:HD2	2.07	0.53
2:B:1234:VAL:HG13	2:B:1236:LEU:HG	1.89	0.53
2:B:194:SER:HB2	2:B:200:LEU:HB3	1.91	0.53
2:B:235:ASN:HD22	2:B:236:PRO:HD2	1.73	0.53
2:B:1003:ASN:HB3	2:B:1102:PRO:HG2	1.91	0.53
2:B:98:LEU:HD12	2:B:125:GLN:HG2	1.90	0.52
1:A:111:VAL:HG11	1:A:309:ILE:HG21	1.91	0.52
1:A:514:GLY:HA2	1:A:605:THR:HG23	1.92	0.52
2:B:852:PRO:HB2	2:B:857:THR:HG22	1.89	0.52
2:B:476:MET:H	2:B:479:THR:HG22	1.74	0.51
2:B:1008:ASP:HB3	2:B:1061:TRP:CD1	2.45	0.51
2:B:283:ARG:HD2	2:B:290:LEU:HD23	1.91	0.51
2:B:528:ASN:ND2	2:B:530:TRP:HE3	2.09	0.51
2:B:769:PRO:HA	2:B:776:PRO:HA	1.93	0.50
1:A:281:LEU:H	1:A:293:GLN:HE22	1.59	0.50
2:B:693:LEU:HD21	2:B:1024:LEU:HD22	1.94	0.50
2:B:244:SER:HB2	2:B:568:TYR:O	2.12	0.50
1:A:693:VAL:HG21	1:A:738:ILE:HD11	1.93	0.49
2:B:952:PRO:HG2	2:B:956:GLU:HG2	1.93	0.49
2:B:362:ASP:HB3	2:B:365:LYS:HG2	1.93	0.49
2:B:268:MET:HG3	2:B:638:GLU:OE1	2.13	0.49
2:B:277:LEU:HB2	2:B:653:VAL:HB	1.94	0.49
2:B:920:PRO:HB2	2:B:997:LEU:HG	1.94	0.49
2:B:1029:ILE:HD11	2:B:1044:ILE:HG12	1.95	0.49
1:A:521:LEU:HD23	1:A:580:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:903:ASN:O	2:B:907:ARG:HG3	2.12	0.49
2:B:969:TYR:HB3	2:B:971:PHE:CD1	2.47	0.49
2:B:492:THR:HG22	2:B:493:ASP:N	2.28	0.49
2:B:742:ARG:HG2	2:B:742:ARG:HH11	1.78	0.48
2:B:892:ASP:HA	2:B:900:THR:HG23	1.96	0.48
2:B:138:ARG:HG2	2:B:1242:ALA:HB1	1.94	0.48
1:A:710:TRP:HB2	1:A:740:VAL:HB	1.96	0.48
1:A:704:ASN:HB3	1:A:707:SER:HB2	1.95	0.48
1:A:273:GLN:HG2	1:A:722:HIS:HD2	1.79	0.47
2:B:939:GLN:HE21	2:B:950:ASN:HB2	1.80	0.47
1:A:806:ASN:ND2	2:B:701:ASP:O	2.48	0.47
2:B:180:TRP:O	2:B:184:LYS:HB2	2.15	0.47
2:B:570:GLN:HG3	2:B:573:LYS:HE3	1.96	0.47
2:B:549:LEU:HD23	2:B:698:LEU:HB2	1.97	0.47
2:B:92:ARG:HD3	2:B:94:GLN:NE2	2.30	0.46
1:A:475:ASN:ND2	2:B:816:THR:H	2.13	0.46
2:B:523:LEU:HG	2:B:557:MET:HE1	1.96	0.46
2:B:1078:LEU:HD22	2:B:1225:LEU:HD23	1.97	0.46
2:B:1027:TRP:CE3	2:B:1046:LEU:HB3	2.51	0.46
2:B:393:LEU:HD23	2:B:565:ARG:HD2	1.97	0.46
2:B:837:GLN:HB3	2:B:841:GLN:HB3	1.98	0.46
1:A:127:VAL:HG12	1:A:128:LYS:HG3	1.97	0.46
2:B:808:THR:HG23	2:B:826:PRO:CG	2.46	0.46
2:B:259:THR:HG22	2:B:278:LYS:HD3	1.96	0.46
1:A:222:ILE:HD12	1:A:270:ASN:HD21	1.81	0.46
2:B:668:ASN:HB2	2:B:669:TRP:CE3	2.50	0.46
2:B:924:ASN:ND2	2:B:986:LYS:H	2.14	0.46
2:B:223:GLU:HG3	2:B:478:THR:OG1	2.16	0.46
2:B:945:GLU:H	2:B:945:GLU:HG3	1.38	0.46
1:A:454:ASN:ND2	1:A:467:VAL:H	2.14	0.45
1:A:525:TYR:CE1	1:A:591:ALA:HB1	2.50	0.45
2:B:697:ILE:HD12	2:B:749:ARG:HB2	1.98	0.45
2:B:841:GLN:HE21	2:B:841:GLN:HA	1.81	0.45
1:A:461:ASP:HB3	2:B:811:LEU:HD13	1.99	0.45
1:A:506:PRO:HB2	1:A:540:GLN:HA	1.99	0.45
2:B:735:ASN:HB2	2:B:738:THR:HG23	1.98	0.45
2:B:1112:VAL:HA	2:B:1127:PRO:HA	1.98	0.45
2:B:1191:SER:HB3	2:B:1196:THR:HG23	1.97	0.45
1:A:135:PRO:HA	1:A:337:PRO:HD2	1.98	0.45
2:B:65:LEU:HD21	2:B:127:ASN:HB3	1.99	0.45
2:B:272:THR:HG21	2:B:864:ASP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:777:PHE:HB3	2:B:795:THR:CG2	2.46	0.45
1:A:574:GLN:HE21	1:A:575:SER:H	1.64	0.45
2:B:105:LYS:H	2:B:105:LYS:HD2	1.81	0.45
2:B:114:TYR:O	2:B:117:ALA:HB3	2.17	0.45
1:A:405:VAL:HG11	1:A:426:ALA:HB2	1.98	0.45
1:A:410:SER:HB2	1:A:421:LYS:HG3	1.97	0.44
2:B:834:TYR:CZ	2:B:945:GLU:HG2	2.53	0.44
2:B:933:PHE:HZ	2:B:939:GLN:HG2	1.82	0.44
2:B:457:MET:HA	2:B:465:PHE:O	2.17	0.44
1:A:785:GLU:HG3	1:A:803:LYS:HZ3	1.83	0.44
2:B:276:ALA:HB2	2:B:655:PRO:HD3	1.99	0.44
1:A:275:LEU:HD12	1:A:275:LEU:HA	1.88	0.44
2:B:186:LYS:HB3	2:B:205:LEU:HB3	2.00	0.44
2:B:422:GLY:HA2	2:B:439:SER:HB2	2.00	0.44
2:B:387:TYR:O	2:B:391:ASN:HB2	2.18	0.43
2:B:1040:GLY:HA3	2:B:1183:SER:HB3	2.00	0.43
2:B:467:PHE:CG	2:B:542:VAL:HG21	2.53	0.43
2:B:574:HIS:CE1	2:B:596:GLY:HA3	2.53	0.43
2:B:1165:ASN:C	2:B:1165:ASN:HD22	2.21	0.43
2:B:492:THR:CG2	2:B:493:ASP:N	2.81	0.43
2:B:1062:THR:HG21	2:B:1085:LYS:HB2	2.01	0.43
1:A:155:THR:CG2	1:A:157:TYR:H	2.27	0.43
2:B:620:HIS:CD2	2:B:620:HIS:H	2.36	0.43
2:B:847:PHE:CE1	2:B:850:VAL:HB	2.54	0.43
1:A:172:ARG:O	1:A:176:LEU:HB2	2.19	0.43
2:B:152:SER:HB2	2:B:172:LEU:HD22	2.00	0.43
2:B:131:ARG:HD2	2:B:133:TYR:CE1	2.53	0.43
1:A:253:PRO:HD2	1:A:263:GLY:HA3	2.01	0.43
2:B:758:SER:HA	2:B:907:ARG:NH1	2.33	0.43
2:B:92:ARG:HD3	2:B:94:GLN:HE22	1.83	0.42
2:B:742:ARG:HG2	2:B:742:ARG:NH1	2.35	0.42
1:A:460:GLN:NE2	2:B:816:THR:OG1	2.51	0.42
2:B:567:LYS:HD3	2:B:621:TYR:CE2	2.53	0.42
2:B:834:TYR:OH	2:B:945:GLU:HG2	2.18	0.42
2:B:1234:VAL:CG1	2:B:1236:LEU:HG	2.50	0.42
1:A:396:ILE:HG22	1:A:629:LEU:HD21	2.00	0.42
2:B:375:LYS:HA	2:B:442:PRO:HB3	2.02	0.42
2:B:536:ARG:NH1	2:B:686:ASN:HB3	2.34	0.42
1:A:474:THR:CG2	1:A:479:THR:CG2	2.94	0.42
2:B:256:LEU:HD13	2:B:606:GLY:HA3	2.02	0.42
2:B:327:THR:HG21	2:B:367:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1003:ASN:ND2	2:B:1146:THR:HG21	2.34	0.42
1:A:163:LEU:HD23	1:A:622:ILE:HD11	2.01	0.41
1:A:34:SER:HB2	1:A:65:GLN:HB2	2.01	0.41
1:A:359:GLN:HG2	1:A:405:VAL:HG12	2.02	0.41
1:A:469:TYR:CE1	2:B:818:TRP:HD1	2.38	0.41
2:B:475:LYS:HD2	2:B:479:THR:O	2.19	0.41
2:B:739:ASN:O	2:B:742:ARG:HB2	2.21	0.41
2:B:1076:LYS:HE3	2:B:1171:GLN:HG3	2.03	0.41
2:B:821:ILE:HD11	2:B:828:ILE:HD11	2.02	0.41
2:B:943:LYS:HB3	2:B:948:GLU:HB2	2.03	0.41
1:A:697:THR:HB	1:A:715:ASP:O	2.21	0.41
1:A:293:GLN:NE2	1:A:293:GLN:HA	2.36	0.41
1:A:639:MET:HB2	1:A:748:ASN:O	2.21	0.41
2:B:115:LEU:HD22	2:B:209:VAL:HG11	2.01	0.41
2:B:123:ASP:OD1	2:B:208:LYS:HE2	2.21	0.41
2:B:223:GLU:HG2	2:B:1100:LEU:HD23	2.03	0.41
2:B:1105:GLN:HB2	2:B:1107:TYR:CE2	2.55	0.41
1:A:581:PRO:HG3	1:A:654:GLY:HA3	2.03	0.41
2:B:594:PRO:HG2	2:B:1124:LEU:HD22	2.03	0.41
2:B:869:THR:HG22	2:B:873:GLY:HA2	2.02	0.41
2:B:244:SER:HB3	2:B:571:LEU:HB2	2.02	0.40
2:B:281:VAL:HG22	2:B:293:ASN:HA	2.03	0.40
2:B:710:ILE:HD12	2:B:740:TRP:HA	2.03	0.40
1:A:405:VAL:HG22	1:A:501:LEU:HD11	2.04	0.40
2:B:467:PHE:CD1	2:B:542:VAL:HG21	2.56	0.40
2:B:980:ASP:HA	2:B:981:PRO:HD3	1.98	0.40
2:B:903:ASN:HB2	2:B:905:PRO:HD2	2.03	0.40
2:B:940:LYS:HB2	2:B:948:GLU:HB3	2.03	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	769/777 (99%)	715 (93%)	51 (7%)	3 (0%)	34	71
2	B	1148/1160 (99%)	1071 (93%)	71 (6%)	6 (0%)	29	67
All	All	1917/1937 (99%)	1786 (93%)	122 (6%)	9 (0%)	32	67

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	THR
2	B	618	GLY
2	B	847	PHE
2	B	1188	GLU
2	B	854	ASN
1	A	367	SER
2	B	586	ARG
1	A	453	ILE
2	B	143	ILE

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	681/681 (100%)	612 (90%)	69 (10%)	7	28
2	B	1011/1011 (100%)	874 (86%)	137 (14%)	3	20
All	All	1692/1692 (100%)	1486 (88%)	206 (12%)	8	23

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	48	THR
1	A	56	SER
1	A	57	LEU
1	A	65	GLN
1	A	66	ILE
1	A	69	GLN

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Mol	Chain	Res	Type
1	A	73	ASN
1	A	79	LEU
1	A	84	ASP
1	A	104	GLN
1	A	107	LYS
1	A	125	THR
1	A	131	GLN
1	A	136	ASN
1	A	149	ILE
1	A	150	LEU
1	A	154	LEU
1	A	155	THR
1	A	163	LEU
1	A	170	THR
1	A	176	LEU
1	A	189	ASN
1	A	190	GLN
1	A	208	THR
1	A	209	THR
1	A	229	THR
1	A	243	THR
1	A	247	GLU
1	A	254	SER
1	A	264	THR
1	A	275	LEU
1	A	305	THR
1	A	317	LEU
1	A	319	SER
1	A	334	SER
1	A	350	ASP
1	A	351	LYS
1	A	363	LYS
1	A	366	THR
1	A	377	SER
1	A	386	SER
1	A	391	VAL
1	A	393	ASP
1	A	395	ILE
1	A	401	LYS
1	A	419	SER
1	A	421	LYS
1	A	444	THR

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Mol	Chain	Res	Type
1	A	453	ILE
1	A	500	SER
1	A	508	ASN
1	A	537	ARG
1	A	574	GLN
1	A	576	ARG
1	A	605	THR
1	A	657	VAL
1	A	665	ASN
1	A	670	SER
1	A	676	ILE
1	A	687	THR
1	A	706	GLU
1	A	732	ASN
1	A	745	ILE
1	A	770	GLN
1	A	782	LEU
1	A	796	GLN
1	A	803	LYS
1	A	806	ASN
2	B	63	GLU
2	B	83	GLU
2	B	88	PHE
2	B	91	VAL
2	B	99	ASN
2	B	105	LYS
2	B	113	LYS
2	B	127	ASN
2	B	130	ILE
2	B	131	ARG
2	B	142	ASP
2	B	148	MET
2	B	150	ASN
2	B	154	VAL
2	B	187	VAL
2	B	200	LEU
2	B	203	VAL
2	B	204	LEU
2	B	219	GLN
2	B	226	GLU
2	B	235	ASN
2	B	238	GLN

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Mol	Chain	Res	Type
2	B	242	LYS
2	B	256	LEU
2	B	264	MET
2	B	265	SER
2	B	270	THR
2	B	277	LEU
2	B	291	LEU
2	B	301	LYS
2	B	318	THR
2	B	324	LEU
2	B	328	ASP
2	B	333	GLU
2	B	334	LYS
2	B	350	GLU
2	B	358	VAL
2	B	384	ILE
2	B	393	LEU
2	B	396	THR
2	B	411	GLU
2	B	420	SER
2	B	431	LYS
2	B	432	LYS
2	B	437	LYS
2	B	448	GLU
2	B	453	ASN
2	B	458	VAL
2	B	479	THR
2	B	523	LEU
2	B	528	ASN
2	B	529	ARG
2	B	562	THR
2	B	565	ARG
2	B	567	LYS
2	B	570	GLN
2	B	572	GLU
2	B	587	GLU
2	B	610	GLN
2	B	620	HIS
2	B	629	GLN
2	B	632	VAL
2	B	642	SER
2	B	649	LYS

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Mol	Chain	Res	Type
2	B	650	LEU
2	B	662	TYR
2	B	673	LEU
2	B	679	SER
2	B	681	ASN
2	B	685	GLU
2	B	701	ASP
2	B	707	SER
2	B	708	ASP
2	B	709	LYS
2	B	710	ILE
2	B	725	ARG
2	B	728	GLN
2	B	732	LEU
2	B	733	ASN
2	B	742	ARG
2	B	756	LEU
2	B	768	LEU
2	B	771	ILE
2	B	773	ASN
2	B	790	SER
2	B	803	VAL
2	B	806	MET
2	B	835	ARG
2	B	841	GLN
2	B	843	ASN
2	B	849	GLN
2	B	850	VAL
2	B	856	SER
2	B	857	THR
2	B	864	ASP
2	B	869	THR
2	B	871	SER
2	B	906	GLN
2	B	921	VAL
2	B	922	LEU
2	B	925	LYS
2	B	939	GLN
2	B	943	LYS
2	B	945	GLU
2	B	947	ASN
2	B	956	GLU

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Mol	Chain	Res	Type
2	B	965	LEU
2	B	974	THR
2	B	979	THR
2	B	986	LYS
2	B	1002	LEU
2	B	1012	LEU
2	B	1017	ASP
2	B	1029	ILE
2	B	1036	ARG
2	B	1039	THR
2	B	1042	LEU
2	B	1044	ILE
2	B	1045	THR
2	B	1052	GLN
2	B	1059	GLN
2	B	1061	TRP
2	B	1089	ASN
2	B	1123	LYS
2	B	1136	ASN
2	B	1143	LEU
2	B	1157	THR
2	B	1164	ASN
2	B	1165	ASN
2	B	1170	SER
2	B	1171	GLN
2	B	1172	THR
2	B	1187	LYS
2	B	1191	SER
2	B	1202	ASP
2	B	1204	LYS
2	B	1230	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	136	ASN
1	A	194	ASN
1	A	211	ASN
1	A	270	ASN
1	A	293	GLN
1	A	394	GLN

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Mol	Chain	Res	Type
1	A	454	ASN
1	A	460	GLN
1	A	475	ASN
1	A	530	ASN
1	A	531	GLN
1	A	574	GLN
1	A	599	ASN
1	A	662	ASN
1	A	665	ASN
1	A	722	HIS
1	A	796	GLN
1	A	797	ASN
1	A	806	ASN
2	B	99	ASN
2	B	127	ASN
2	B	144	ASN
2	B	235	ASN
2	B	302	HIS
2	B	360	HIS
2	B	381	HIS
2	B	391	ASN
2	B	395	GLN
2	B	528	ASN
2	B	548	GLN
2	B	570	GLN
2	B	582	GLN
2	B	620	HIS
2	B	684	ASN
2	B	728	GLN
2	B	733	ASN
2	B	735	ASN
2	B	745	ASN
2	B	773	ASN
2	B	841	GLN
2	B	849	GLN
2	B	908	ASN
2	B	924	ASN
2	B	932	GLN
2	B	939	GLN
2	B	947	ASN
2	B	1011	ASN
2	B	1119	ASN

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Mol	Chain	Res	Type
2	B	1165	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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	5
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	227:VAL	C	232:SER	N	11.85
1	B	782:SER	C	789:ALA	N	11.65
1	B	1089:ASN	C	1097:ASN	N	10.05
1	B	105:LYS	C	110:ASP	N	8.60
1	A	255:VAL	C	261:SER	N	8.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	412:SER	C	416:SER	N	6.36
1	A	118:THR	C	121:GLY	N	6.20
1	B	1159:SER	C	1164:ASN	N	5.28

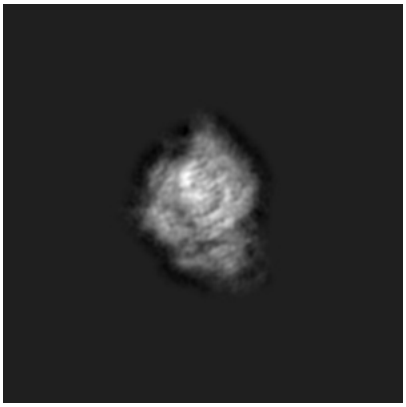
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10890. These allow visual inspection of the internal detail of the map and identification of artifacts.

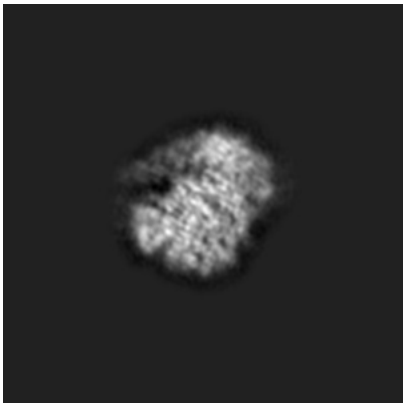
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

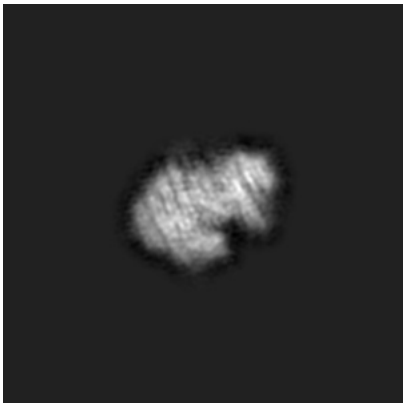
6.1.1 Primary map



X



Y

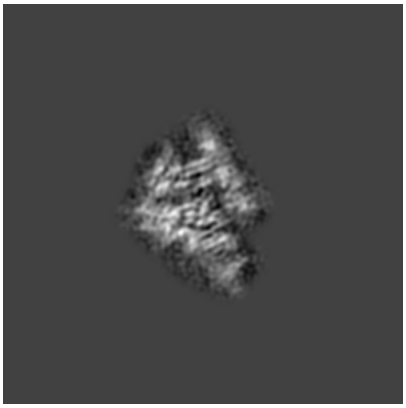


Z

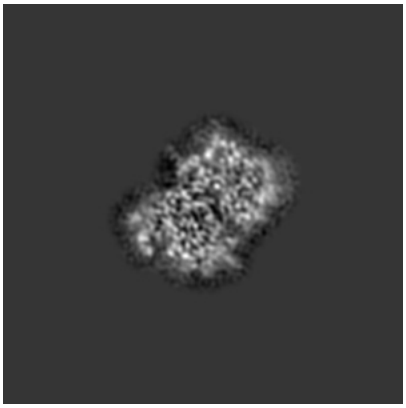
The images above show the map projected in three orthogonal directions.

6.2 Central slices

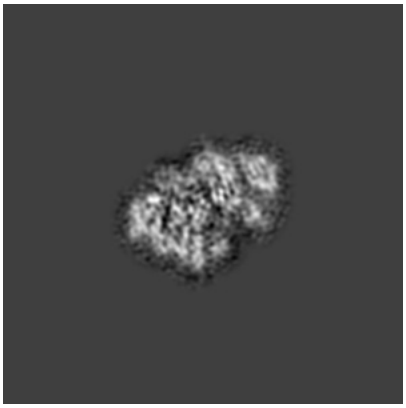
6.2.1 Primary map



X Index: 135



Y Index: 135

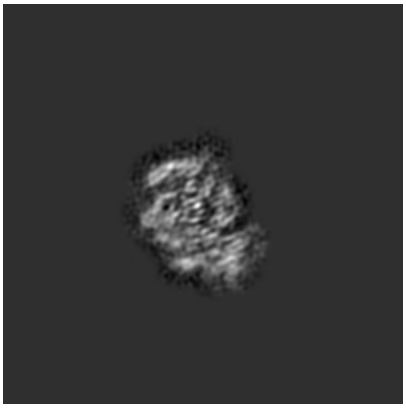


Z Index: 135

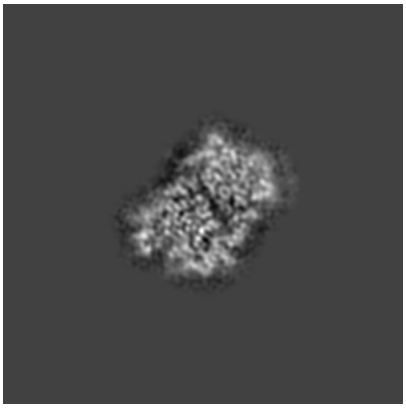
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

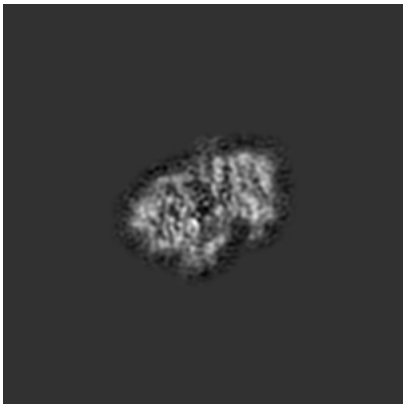
6.3.1 Primary map



X Index: 117



Y Index: 131

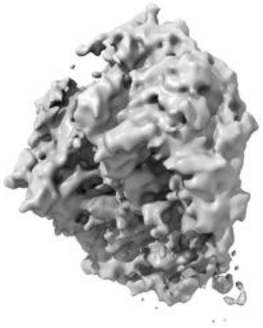


Z Index: 140

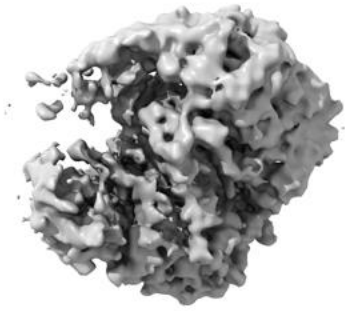
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

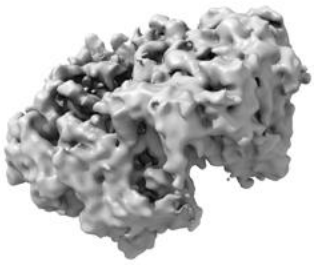
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

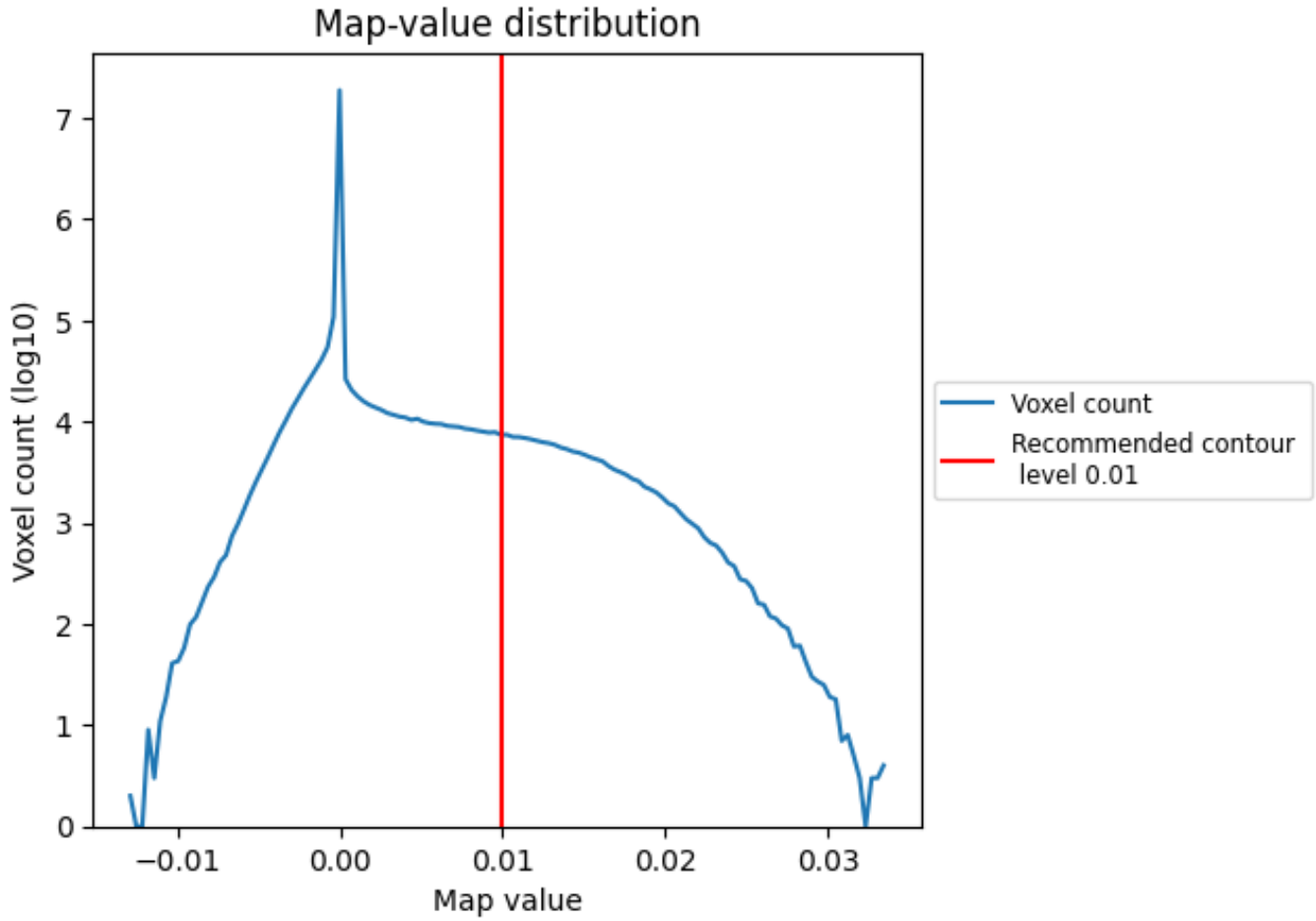
6.5 Mask visualisation (i)

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

7 Map analysis

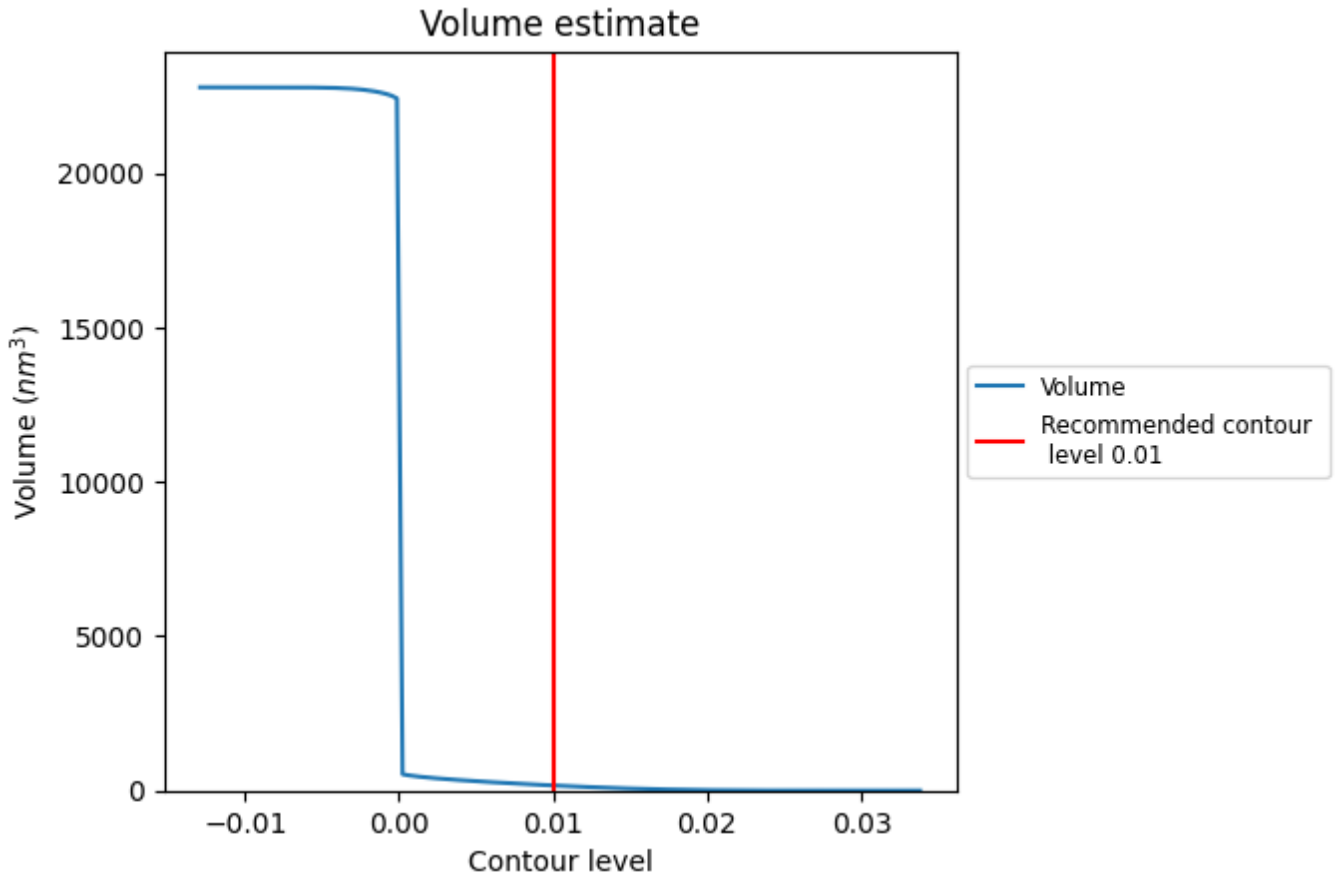
This section contains the results of statistical analysis of the map.

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.

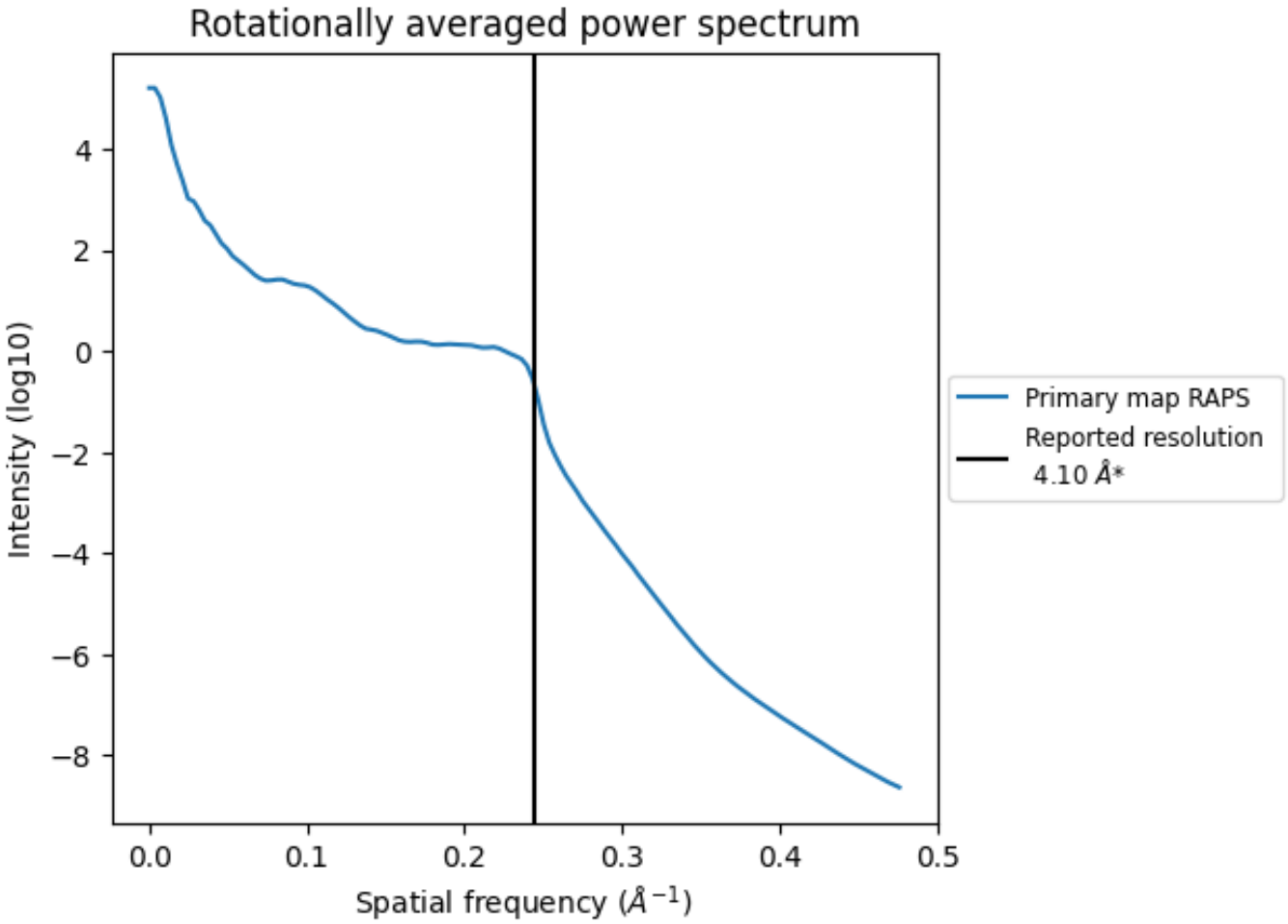
7.2 Volume estimate



The volume at the recommended contour level is 165 nm^3; this corresponds to an approximate mass of 149 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)

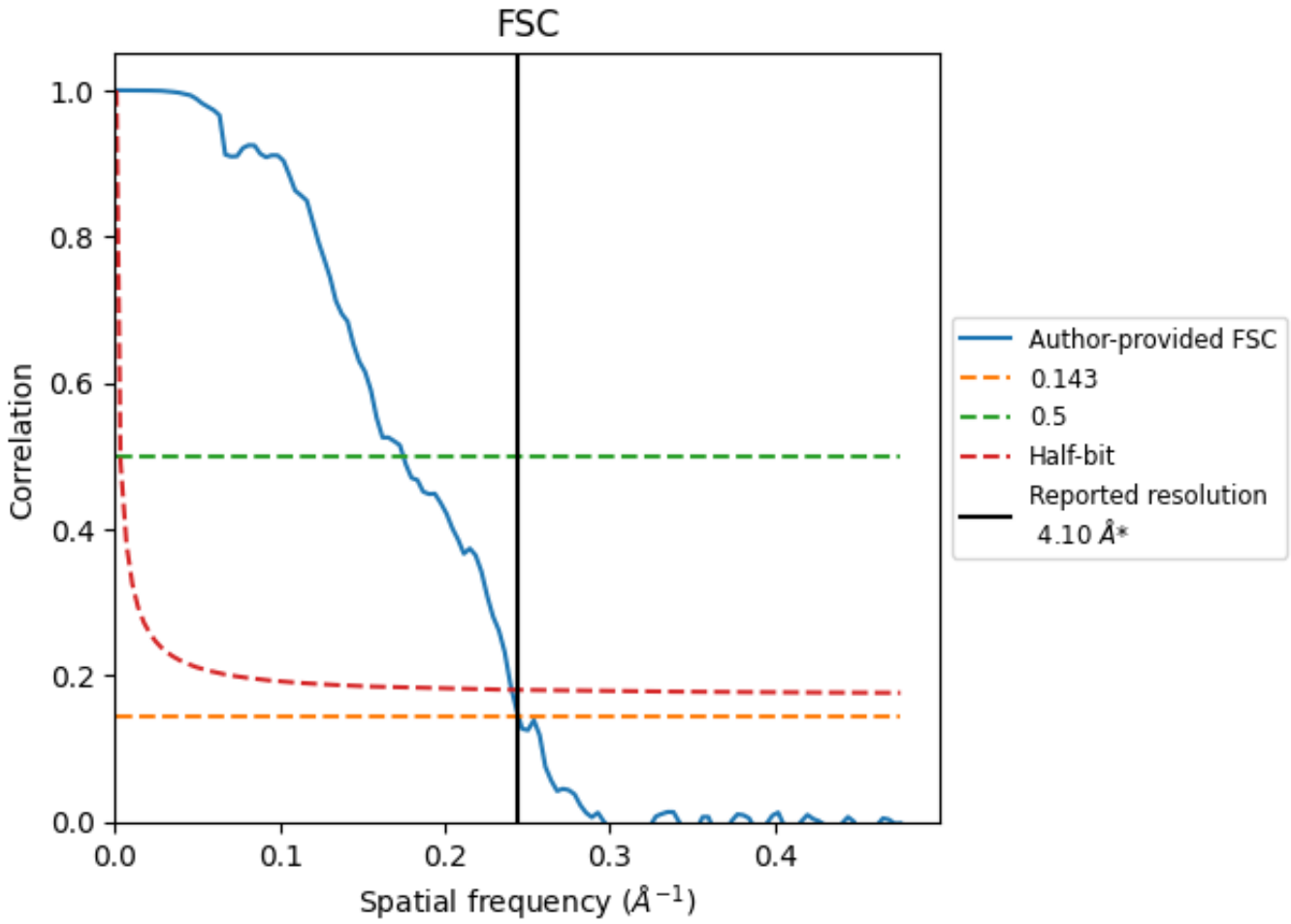


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

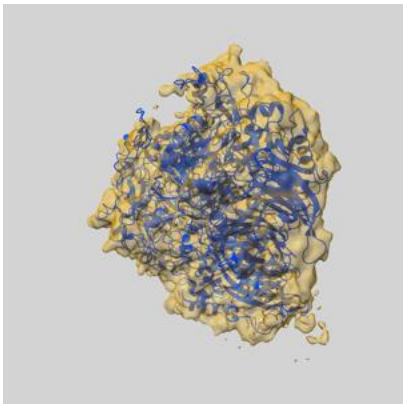
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.08	5.72	4.16
Unmasked-calculated*	-	-	-

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

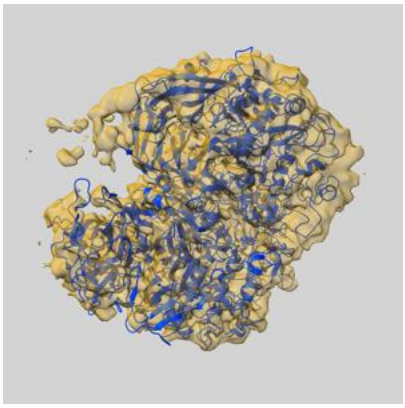
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10890 and PDB model 6YRK. Per-residue inclusion information can be found in section 3 on page 5.

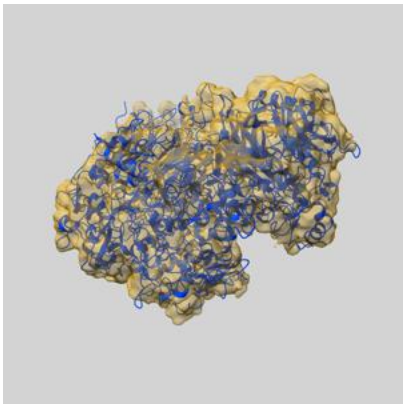
9.1 Map-model overlay



X



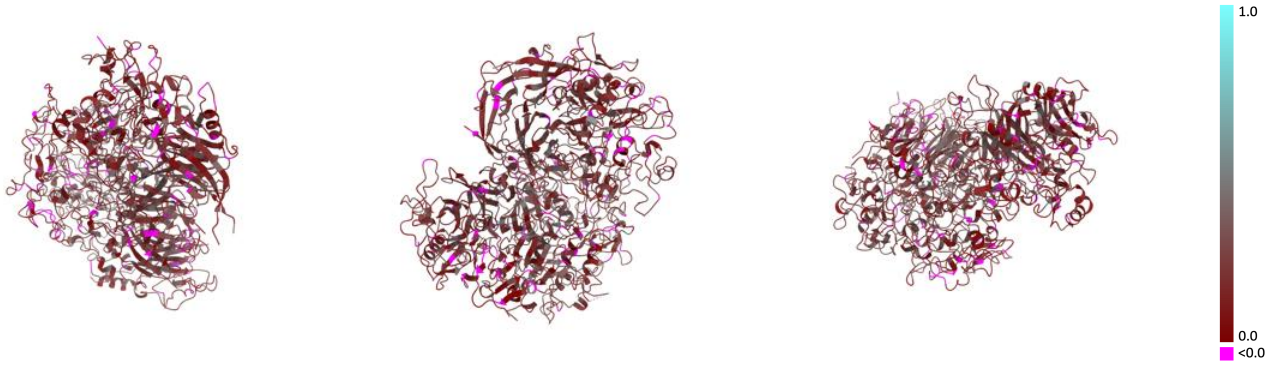
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

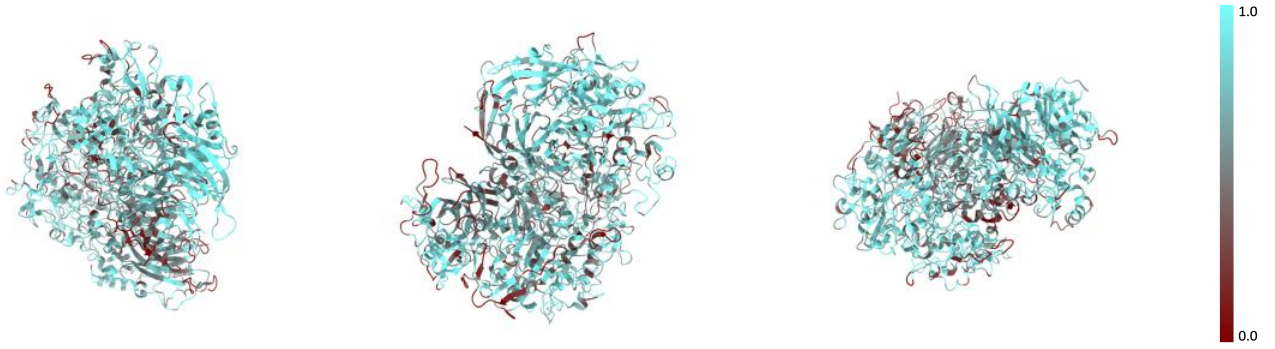
9.2 Q-score mapped to coordinate model (i)



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.

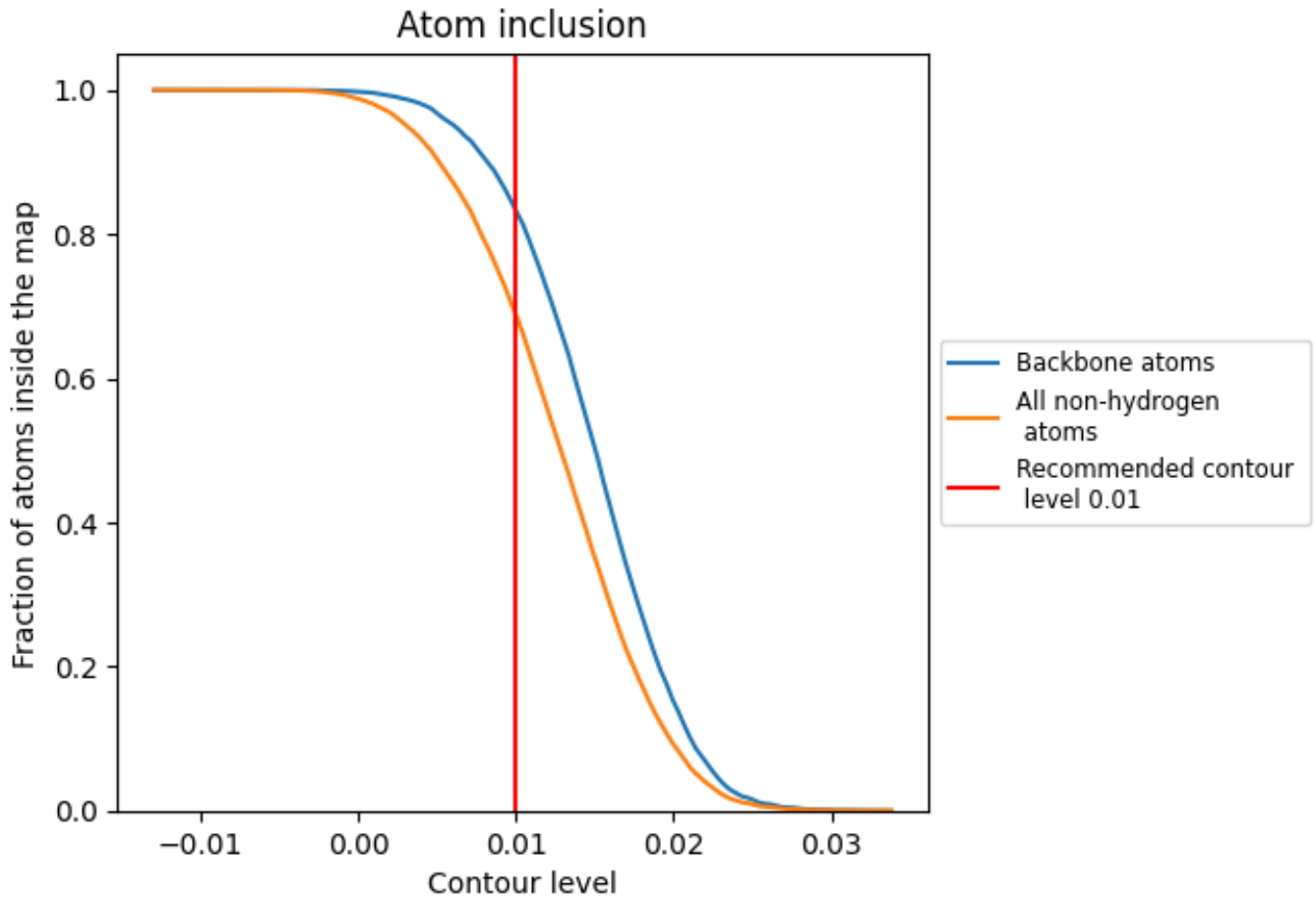
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6876	0.2060
A	0.7056	0.2030
B	0.6758	0.2090