WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Mar 10, 2024 – 09:52 PM EDT

PDB ID	:	6P18
EMDB ID	:	EMD-20233
Title	:	Q21 transcription antitermination complex: loading complex
Authors	:	Yin, Z.; Ebright, R.H.
Deposited on	:	2019-05-19
Resolution	:	3.50 Å(reported)
Based on initial models	:	4MEY, 4YLN, 5IPL

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
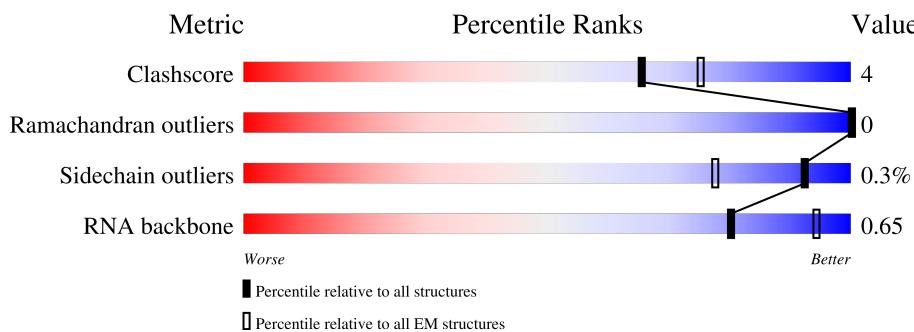
1　Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
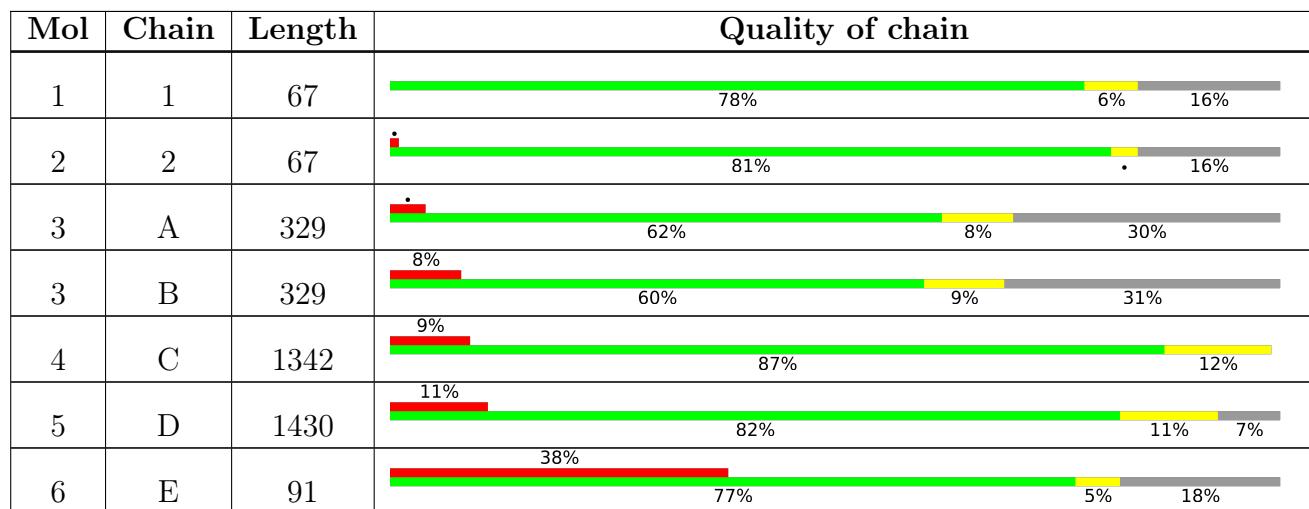
The reported resolution of this entry is 3.50 Å.

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

Metric	Percentile Ranks	Value
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0.3%
RNA backbone		0.65

Worse　　　　　*Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
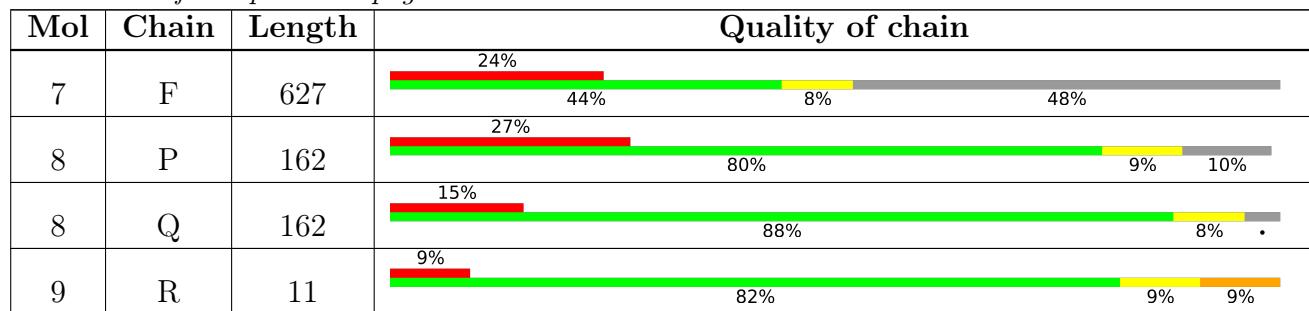
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1	67	78% 6% 16%
2	2	67	81% · 16%
3	A	329	62% 8% 30%
3	B	329	8% 60% 9% 31%
4	C	1342	9% 87% 12%
5	D	1430	11% 82% 11% 7%
6	E	91	38% 77% 5% 18%

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Mol	Chain	Length	Quality of chain
7	F	627	24% ▬▬▬ 44% 8% 48%
8	P	162	27% ▬▬▬ 80% 9% 10%
8	Q	162	15% ▬▬▬ 88% 8% •
9	R	11	9% ▬▬▬ 82% 9% 9%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 32673 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 DNA chain called DNA (67-MER) fragment carrying phage-21 pR' promoter and pause element, nontemplate strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	56	Total	C	N	O	P	0	0
			1153	551	211	335	56		

- Molecule 2 is a DNA chain called DNA (67-MER) fragment carrying phage-21 pR' promoter and pause element, template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	56	Total	C	N	O	P	0	0
			1142	548	199	339	56		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		
3	B	228	Total	C	N	O	S	0	0
			1767	1100	312	349	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1340	Total	C	N	O	S	0	0
			10568	6629	1841	2055	43		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1327	Total	C	N	O	S	0	0
			10319	6484	1839	1947	49		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	expression tag	UNP P0A8T7
D	1409	GLU	-	expression tag	UNP P0A8T7
D	1410	ARG	-	expression tag	UNP P0A8T7
D	1411	ARG	-	expression tag	UNP P0A8T7
D	1412	ALA	-	expression tag	UNP P0A8T7
D	1413	SER	-	expression tag	UNP P0A8T7
D	1414	GLU	-	expression tag	UNP P0A8T7
D	1415	ASN	-	expression tag	UNP P0A8T7
D	1416	LEU	-	expression tag	UNP P0A8T7
D	1417	TYR	-	expression tag	UNP P0A8T7
D	1418	PHE	-	expression tag	UNP P0A8T7
D	1419	GLN	-	expression tag	UNP P0A8T7
D	1420	GLY	-	expression tag	UNP P0A8T7
D	1421	HIS	-	expression tag	UNP P0A8T7
D	1422	HIS	-	expression tag	UNP P0A8T7
D	1423	HIS	-	expression tag	UNP P0A8T7
D	1424	HIS	-	expression tag	UNP P0A8T7
D	1425	HIS	-	expression tag	UNP P0A8T7
D	1426	HIS	-	expression tag	UNP P0A8T7
D	1427	HIS	-	expression tag	UNP P0A8T7
D	1428	HIS	-	expression tag	UNP P0A8T7
D	1429	HIS	-	expression tag	UNP P0A8T7
D	1430	HIS	-	expression tag	UNP P0A8T7

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	75	600	365	114	120	1	0	0

- Molecule 7 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	325	2665	1679	476	494	16	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	MET	-	initiating methionine	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	SER	-	expression tag	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	HIS	-	expression tag	UNP P00579
F	-3	SER	-	expression tag	UNP P00579
F	-2	SER	-	expression tag	UNP P00579
F	-1	GLY	-	expression tag	UNP P00579
F	0	HIS	-	expression tag	UNP P00579
F	541	CYS	ARG	engineered mutation	UNP P00579
F	607	PRO	LEU	engineered mutation	UNP P00579

- Molecule 8 is a protein called Q protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	145	Total 1165	C 743	N 206	O 205	S 11	0	0
8	Q	156	Total 1261	C 801	N 229	O 220	S 11	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	SER	-	expression tag	UNP Q9XJQ6
P	24	GLY	-	insertion	UNP Q9XJQ6
P	26	TRP	HIS	conflict	UNP Q9XJQ6
P	27	VAL	GLY	conflict	UNP Q9XJQ6
P	28	TYR	LEU	conflict	UNP Q9XJQ6
P	47	VAL	ILE	conflict	UNP Q9XJQ6
Q	1	SER	-	expression tag	UNP Q9XJQ6
Q	24	GLY	-	insertion	UNP Q9XJQ6
Q	26	TRP	HIS	conflict	UNP Q9XJQ6
Q	27	VAL	GLY	conflict	UNP Q9XJQ6
Q	28	TYR	LEU	conflict	UNP Q9XJQ6
Q	47	VAL	ILE	conflict	UNP Q9XJQ6

- Molecule 9 is a RNA chain called RNA (5'-R(P*UP*GP*GP*GP*AP*GP*AP*GP*GP*U P*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	R	11	244	108	49	76	11	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	D	2	2	2	0
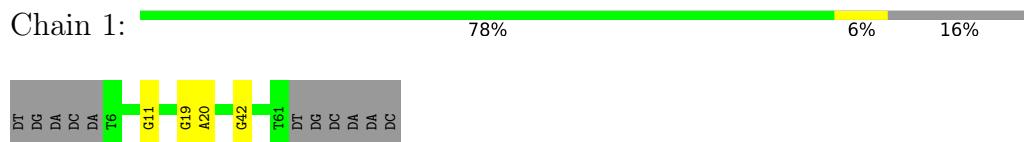
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
11	D	1	1	1	0
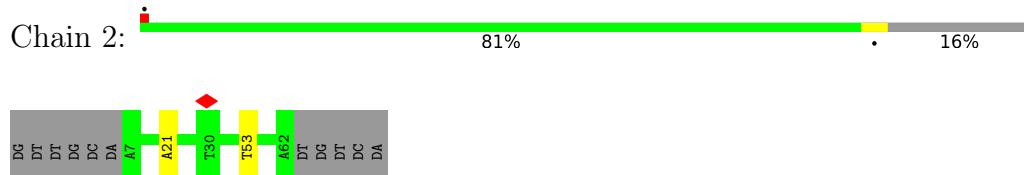
3   Residue-property plots ⓘ

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: DNA (67-MER) fragment carrying phage-21 pR' promoter and pause element, nontemplate strand

Chain 1:

• Molecule 2: DNA (67-MER) fragment carrying phage-21 pR' promoter and pause element, template strand

Chain 2:

• Molecule 3: DNA-directed RNA polymerase subunit alpha

Chain A:

• Molecule 3: DNA-directed RNA polymerase subunit alpha

Chain B:

• Molecule 4: DNA-directed RNA polymerase subunit beta

Chain C:

• Molecule 5: DNA-directed RNA polymerase subunit beta'

Chain D:

R220 P234 L242 L249 R250 P251 D256 R259 D289 R312 R339 Q340 N341 L342 L343 G344 H364 K371 M372 I381 L412 T416 R425 L432 P439 D462 M466 L472 E475 A476 Q477 L478 T487 N488 I499 P502

S503 Q504 D505 V506 L510 R515 D516 C517 V518 T528 G529 P530 R535 L536 Y537 H545 A546 R547 R551 N560 G561 T573 R576 M581 I582 V583 P584 I591 V592 N593 M604 K615 I624 G628 A633 R634 V639 M644 Q665 E677

L701 E704 I707 N708 G711 Q712 E713 E714 F719 Y723 R731 K749 I755 R764 D785 K789 Q805 D806 L807 V825 I826 E827 K832 T844 L849 G852 T853 A854 D855 I856 N875 V882 V894 L903 A904 R905 G912

T928 Q929 L930 THR MET ARG THR PHE HIS ILE GLY ALA ALA SER ARG ALA ALA ALA GLU SER SER ILE GLN VAL LYS ASN LYS GLY S957 I958 K959 L960 S961 N962 V963 K964 S965 V966 V967 N968 S969 S970 G971 K972 L973 T976 S977 R978 N979 T980 E981 I985 D986 E987 S994

L1003 A1004 K1005 G1006 D1007 G1008 E1009 E1015 P1026 V1027 I1028 T1029 E1030 V1031 S1032 G1033 F1034 V1035 R1036 F1037 T1038 D1039 M1040 I1041 L1042 G1043 Q1044 T1045 I1046 T1047 R1048 Q1049 T1050 D1051 E1052 L1053 T1054 G1055 L1056 S1057 S1058 L1059 V1060 V1061 L1062 D1063 S1064 A1065 E1066 R1067 T1068 A1069 G1070 G1071 K1072 D1073 L1074

R1075 P1076 A1077 L1078 K1079 I1080 V1081 D1082 A1083 Q1084 G1085 N1086 D1087 V1088 L1089 I1090 P1091 G1092 T1093 D1094 M1095 P1096 A1097 F1100 K1104 A1105 I1106 V1107 Q1108 L1109 E1110 D1111 G1112 V1113 Q1114 I1115 S1116 S1117 D1118 D1119 T1120 R1123 Q1126 GLU SER GLY THR LYS ASP ILE THR G1136 D1143 L1144

R1148 G1161 I1162 V1163 S1164 F1165 G1166 K1167 E1168 T1169 K1170 G1171 K1172 R1173 I1177 D1181 G1182 S1183 D1184 P1185 M1189 Q1195 R1203 V1204 E1205 D1212 E1215 D1219 I1220 E1236 D1239 N1249 L1275 E1276 Q1279 A1294 D1305 L1306 L1307 K1311 A1323

T1328 R1341 D1342 E1343 G1346 N1350 L1356 G1360 T1361 H1366 A1374 A1375 G1376 GLU ALA PRO ALA ALA PRO GLN VAL THR ALA GLU ASP ALA SER ALA SER LEU ALA GLU LEU LEU ASN ALA GLY LEU GLY GLY SER ASP ASN GLU LEU GLU ARG ALA SER GLU ASN

LEU TYR PHE GLN GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

- **Molecule 6: DNA-directed RNA polymerase subunit omega**

Chain E:
38%
77% 5% 18%

MET A2 R3 D8 E11 K12 I13 G14 F17 V20 R28 K35 D36 P37 L38 V39 P40 E41 E42 N43 D44 R52 E55 E56 G57 N60 N61 Q62 I63 L64 D65 V66 R67 E68 R69 Q70 E71 Q72 Q73 E74 Q75 E76 ALA ALA GLU LEU GLN ALA VAL THR ALA

ILE ALA GLU GLY ARG ARG

- **Molecule 7: RNA polymerase sigma factor RpoD**

Chain F:
24%
44% 8% 48%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY HIS MET GLU GLN ASN PRO GLN SER GLN LEU LYS LEU LEU VAL THR ARG GLY LYS GLU GLN GLY TYR LEU THR TYR ALA GLU VAL ASN ASP HIS LEU PRO GLU ASP ILE VAL ASP SER ASP GLN ILE GLU ASP ILE ILE GLN

• Molecule 8: Q protein

Chain P:

• Molecule 8: Q protein

Chain Q:

• Molecule 9: RNA (5'-R(P*UP*GP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3')

Chain R:

9%

82%

9% 9%

U1 G2 A11

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	150310	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 $(e^-/Å^2)$	1.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	47608	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.324	Depositor
Minimum map value	-0.205	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0286	Depositor
Map size (Å)	272.896, 272.896, 272.896	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	Depositor

5   Model quality (i)

5.1   Standard geometry (i)

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

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	1	0.49	0/1294	0.97	0/1996
2	2	0.50	0/1278	0.98	0/1969
3	A	0.24	0/1808	0.45	0/2450
3	B	0.26	0/1789	0.51	0/2425
4	C	0.26	0/10737	0.50	0/14486
5	D	0.26	0/10476	0.50	0/14146
6	E	0.27	0/602	0.49	0/810
7	F	0.27	0/2701	0.57	0/3627
8	P	0.25	0/1192	0.53	0/1605
8	Q	0.27	0/1289	0.47	0/1731
9	R	0.21	0/274	0.73	0/427
All	All	0.29	0/33440	0.56	0/45672

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (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	1	1153	0	634	4	0
2	2	1142	0	636	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1786	0	1813	16	0
3	B	1767	0	1789	21	0
4	C	10568	0	10575	103	0
5	D	10319	0	10527	98	0
6	E	600	0	607	4	0
7	F	2665	0	2721	27	0
8	P	1165	0	1170	10	0
8	Q	1261	0	1277	8	0
9	R	244	0	119	2	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
All	All	32673	0	31868	265	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 4.

All (265) 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)
4:C:992:LEU:HD12	4:C:993:PRO:HD2	1.33	1.06
4:C:992:LEU:HD12	4:C:993:PRO:CD	2.01	0.91
4:C:992:LEU:CD1	4:C:993:PRO:HD2	2.12	0.78
4:C:238:GLN:HB3	4:C:284:LEU:HD11	1.76	0.67
4:C:975:ILE:HG22	4:C:1014:LEU:HD13	1.79	0.64
4:C:1117:LEU:HD13	4:C:1195:ILE:HG12	1.81	0.63
4:C:533:LEU:HD21	4:C:571:LEU:HD13	1.84	0.59
4:C:691:PRO:HB3	4:C:788:SER:HB3	1.84	0.59
3:B:176:CYS:SG	5:D:535:ARG:NH2	2.76	0.59
3:A:158:ARG:NH2	3:A:173:VAL:O	2.36	0.58
8:P:70:VAL:HG23	8:P:141:ILE:HD11	1.85	0.58
4:C:221:LEU:HD13	4:C:336:LEU:HD11	1.87	0.57
5:D:1144:LEU:HD11	5:D:1236:GLU:HG3	1.86	0.57
7:F:138:PRO:HA	7:F:141:ILE:HD12	1.87	0.57
7:F:401:PHE:HA	7:F:404:LEU:HD12	1.86	0.57
7:F:311:THR:O	7:F:345:GLN:NE2	2.37	0.56
7:F:283:GLN:HE21	7:F:343:LYS:HD2	1.70	0.56
5:D:591:ILE:HG23	5:D:604:MET:HG2	1.87	0.56
8:P:117:ARG:NH2	8:Q:87:TYR:O	2.39	0.56
5:D:1143:ASP:OD1	5:D:1148:ARG:NH1	2.39	0.56
3:A:32:GLU:OE2	3:A:195:ARG:NH2	2.39	0.56
4:C:176:ILE:HD12	4:C:184:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:92:VAL:HG22	3:B:121:VAL:HG22	1.88	0.56
5:D:502:PRO:HB3	5:D:506:VAL:HB	1.89	0.55
5:D:517:CYS:H	5:D:545:HIS:HB3	1.72	0.55
3:B:92:VAL:O	3:B:148:ARG:NH2	2.40	0.55
4:C:817:LEU:HD21	4:C:1080:ASN:HD22	1.71	0.55
5:D:1054:THR:HG23	5:D:1056:LEU:H	1.72	0.54
5:D:1167:LYS:HZ2	5:D:1170:LYS:HB3	1.73	0.54
5:D:807:LEU:HD11	5:D:894:VAL:HG13	1.89	0.54
5:D:1275:LEU:O	5:D:1276:GLU:HG3	2.08	0.54
4:C:1269:ARG:NH1	5:D:344:GLY:O	2.40	0.54
5:D:381:ILE:HD11	5:D:412:LEU:HD13	1.89	0.54
5:D:1165:PHE:HE2	5:D:1173:ARG:HB3	1.73	0.54
3:B:27:THR:HG23	3:B:202:VAL:HG22	1.90	0.54
8:P:48:GLU:O	8:P:51:ARG:NH1	2.40	0.54
5:D:1346:GLY:O	5:D:1350:ASN:ND2	2.41	0.54
5:D:1026:PRO:HB2	5:D:1028:ILE:HG23	1.90	0.54
5:D:1062:LEU:HD11	5:D:1066:GLU:HB2	1.90	0.53
5:D:825:VAL:HG13	5:D:832:LYS:HB2	1.91	0.53
7:F:152:GLU:OE2	7:F:218:ARG:NH1	2.41	0.53
3:A:182:ARG:NH1	4:C:1090:ASN:O	2.41	0.53
3:B:86:LYS:NZ	3:B:174:ASP:OD2	2.40	0.53
4:C:213:LEU:HD13	4:C:422:LYS:HG3	1.91	0.53
4:C:591:TYR:OH	4:C:637:ARG:NH2	2.42	0.53
4:C:444:ASP:O	4:C:450:ASN:ND2	2.42	0.53
8:Q:16:LEU:HD22	8:Q:142:TYR:HB2	1.90	0.52
5:D:42:GLU:OE2	7:F:451:ARG:NH1	2.42	0.52
5:D:979:ASN:ND2	5:D:1205:GLU:OE2	2.42	0.52
4:C:358:ASP:N	4:C:358:ASP:OD1	2.43	0.52
5:D:844:THR:HA	5:D:882:VAL:HG12	1.91	0.52
3:A:166:ARG:NH1	3:A:170:ARG:O	2.43	0.52
4:C:276:GLN:HA	4:C:279:LYS:HE3	1.92	0.52
7:F:102:MET:HA	7:F:105:MET:HG2	1.92	0.52
5:D:827:GLU:O	5:D:832:LYS:NZ	2.43	0.52
5:D:1049:GLN:NE2	5:D:1058:SER:O	2.43	0.52
7:F:94:THR:HG21	7:F:103:ARG:HH12	1.74	0.51
3:B:124:VAL:HG21	3:B:209:GLY:HA3	1.93	0.51
7:F:320:ILE:HA	7:F:327:SER:HB3	1.92	0.51
4:C:528:ARG:NH2	4:C:576:SER:O	2.38	0.51
4:C:530:ILE:HD11	4:C:575:LEU:HD13	1.90	0.51
4:C:660:VAL:HG13	4:C:661:VAL:HG13	1.93	0.51
4:C:607:SER:OG	4:C:608:ALA:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:227:GLN:OE1	7:F:251:LYS:NZ	2.41	0.51
3:A:235:ARG:HA	3:B:218:ARG:HH21	1.75	0.51
5:D:425:ARG:HB2	5:D:466:MET:HG2	1.93	0.51
5:D:432:LEU:HD13	5:D:499:ILE:HG21	1.93	0.51
5:D:854:ALA:HB3	5:D:875:ASN:HD21	1.76	0.51
4:C:548:ARG:HH11	4:C:569:ILE:HG22	1.76	0.50
4:C:576:SER:OG	4:C:577:VAL:N	2.43	0.50
4:C:28:LEU:HD21	4:C:524:ILE:HG13	1.93	0.50
4:C:820:GLU:HB3	4:C:1082:ILE:HG23	1.93	0.50
3:A:58:GLU:HB2	3:A:145:LYS:HD2	1.93	0.50
5:D:573:THR:OG1	5:D:576:ARG:NH1	2.44	0.50
4:C:758:ARG:NH1	4:C:762:ASN:OD1	2.45	0.50
5:D:1028:ILE:HG22	5:D:1120:THR:HA	1.93	0.50
5:D:69:GLU:HG2	5:D:76:LYS:HG2	1.93	0.50
4:C:565:GLU:OE1	4:C:684:ASN:ND2	2.44	0.50
3:B:80:GLU:O	3:B:84:ASN:ND2	2.44	0.49
4:C:14:ASP:HA	4:C:1183:ALA:HB3	1.93	0.49
4:C:998:LEU:HD11	4:C:1015:ALA:HB2	1.94	0.49
1:1:11:DG:OP1	8:Q:119:GLN:NE2	2.45	0.49
5:D:644:MET:O	5:D:764:ARG:NH1	2.46	0.49
5:D:960:LEU:HB3	5:D:963:VAL:HG11	1.94	0.49
7:F:294:GLN:HE22	7:F:333:VAL:HG21	1.77	0.49
3:A:211:ILE:HD11	3:A:219:ARG:HH12	1.77	0.49
5:D:339:ARG:HA	5:D:343:LEU:HD12	1.94	0.49
5:D:1323:ALA:HB1	5:D:1328:THR:HG23	1.95	0.49
5:D:194:LEU:HD11	5:D:234:PRO:HD3	1.95	0.49
4:C:692:THR:HA	4:C:830:THR:HG22	1.95	0.48
3:B:83:LEU:HD22	5:D:551:ARG:HH21	1.78	0.48
7:F:113:ARG:O	7:F:113:ARG:NH1	2.44	0.48
1:1:20:DA:OP2	8:Q:51:ARG:NH2	2.44	0.48
4:C:373:GLY:O	7:F:103:ARG:NH1	2.43	0.48
4:C:397:LEU:HB3	4:C:401:GLY:HA3	1.95	0.48
5:D:749:LYS:HG3	5:D:755:ILE:HG12	1.96	0.48
8:P:23:TRP:HE1	8:P:67:SER:HB3	1.78	0.48
4:C:972:PHE:HA	4:C:975:ILE:HG12	1.96	0.48
3:B:62:ASP:N	3:B:62:ASP:OD1	2.47	0.48
4:C:39:ILE:O	4:C:73:TYR:OH	2.32	0.48
4:C:786:GLY:N	4:C:789:THR:OG1	2.46	0.47
4:C:811:ASN:ND2	4:C:1098:LEU:O	2.46	0.47
5:D:105:ILE:HD12	5:D:242:LEU:HD23	1.96	0.47
4:C:662:SER:OG	4:C:663:VAL:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:124:ILE:HG22	5:D:135:ILE:HD13	1.95	0.47
4:C:1325:VAL:HG22	5:D:249:LEU:HD22	1.96	0.47
5:D:1279:GLN:NE2	5:D:1305:ASP:OD2	2.46	0.47
5:D:48:THR:HG23	5:D:50:LYS:HG2	1.97	0.47
3:A:158:ARG:HH21	3:A:172:LEU:HG	1.79	0.47
4:C:106:GLU:HB2	4:C:112:GLY:HA3	1.97	0.47
3:B:86:LYS:HD3	3:B:174:ASP:HB2	1.97	0.47
4:C:988:LYS:HA	4:C:991:LYS:HG2	1.97	0.47
5:D:128:LEU:HD13	5:D:188:LEU:HD23	1.96	0.47
3:B:93:GLN:HB2	3:B:120:ASP:HB2	1.97	0.47
7:F:112:THR:OG1	7:F:113:ARG:N	2.48	0.47
4:C:702:THR:HG23	4:C:1185:PRO:HA	1.97	0.46
4:C:1005:GLU:H	4:C:1008:GLN:HB2	1.80	0.46
4:C:617:ALA:HB2	4:C:650:VAL:HG11	1.98	0.46
3:A:78:ILE:HA	3:A:81:ILE:HD12	1.96	0.46
4:C:3:TYR:O	4:C:8:LYS:NZ	2.45	0.46
4:C:363:LEU:HB3	4:C:381:ALA:HB1	1.98	0.46
4:C:211:ARG:HH12	4:C:217:THR:HG23	1.81	0.46
4:C:1103:VAL:HG21	5:D:639:VAL:HG21	1.97	0.46
4:C:1257:GLN:HB3	4:C:1296:ASP:HB3	1.98	0.46
5:D:537:TYR:OH	5:D:634:ARG:NE	2.48	0.46
5:D:903:LEU:HD11	5:D:1249:ASN:HD22	1.81	0.46
5:D:1046:ILE:HD12	5:D:1059:LEU:HD12	1.98	0.46
3:B:83:LEU:HD21	5:D:528:THR:HA	1.98	0.46
7:F:324:LYS:HD2	7:F:325:PRO:HD2	1.98	0.46
2:2:53:DT:H5"	8:P:115:GLY:HA2	1.97	0.46
4:C:1308:ILE:HD11	5:D:472:LEU:HB3	1.97	0.46
5:D:156:ARG:HG2	5:D:157:GLN:HG3	1.97	0.46
3:B:98:VAL:HG11	3:B:121:VAL:HG21	1.98	0.46
5:D:973:LEU:N	5:D:1003:LEU:O	2.49	0.46
4:C:1134:GLN:OE1	4:C:1136:GLN:NE2	2.46	0.46
4:C:59:ILE:HD13	4:C:472:GLU:HB2	1.98	0.45
4:C:678:ARG:NH2	4:C:1071:GLY:O	2.43	0.45
6:E:40:PRO:O	6:E:52:ARG:NH2	2.49	0.45
4:C:1004:ASP:HA	4:C:1008:GLN:HG3	1.99	0.45
5:D:1119:ASP:OD1	5:D:1119:ASP:N	2.47	0.45
5:D:416:ILE:HG12	5:D:439:PRO:HG2	1.97	0.45
5:D:1162:ILE:HG22	5:D:1203:ARG:HB2	1.98	0.45
4:C:732:ILE:HD11	4:C:769:PRO:HB3	1.98	0.45
4:C:185:ASP:OD2	4:C:200:ARG:NH2	2.50	0.45
4:C:171:LEU:HD21	4:C:190:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:141:SER:O	3:A:141:SER:OG	2.35	0.45
3:B:61:ILE:HG12	3:B:142:MET:HB3	1.99	0.45
4:C:902:LEU:HD23	4:C:905:ILE:HD12	1.99	0.45
4:C:933:VAL:HG13	4:C:1050:VAL:HG22	1.99	0.45
4:C:987:GLU:HG3	4:C:991:LYS:CE	2.46	0.45
5:D:127:LEU:O	5:D:220:ARG:NH2	2.50	0.45
8:P:61:ASP:OD1	8:P:61:ASP:N	2.50	0.45
5:D:157:GLN:HG2	5:D:188:LEU:HD21	1.98	0.44
7:F:147:GLN:OE1	7:F:265:GLN:NE2	2.50	0.44
4:C:149:LEU:HB2	4:C:530:ILE:HG22	1.99	0.44
4:C:509:SER:OG	4:C:510:GLN:N	2.49	0.44
4:C:1257:GLN:NE2	5:D:341:ASN:OD1	2.47	0.44
4:C:1303:LYS:HA	4:C:1303:LYS:HD3	1.82	0.44
5:D:488:ASN:HB3	5:D:905:ARG:HH12	1.83	0.44
7:F:412:LEU:HD13	7:F:435:ILE:HD11	1.99	0.44
3:B:131:CYS:SG	3:B:132:HIS:N	2.91	0.44
5:D:912:GLY:O	5:D:1360:GLY:N	2.46	0.44
1:1:42:DG:N2	4:C:374:GLU:OE1	2.51	0.44
4:C:520:PRO:HG3	4:C:714:VAL:HG11	1.99	0.44
5:D:504:GLN:HB2	5:D:731:ARG:HG2	2.00	0.44
5:D:1341:ARG:NH1	5:D:1343:GLU:OE2	2.51	0.44
4:C:86:GLN:NE2	4:C:142:GLU:OE1	2.51	0.43
5:D:472:LEU:O	5:D:477:GLN:NE2	2.51	0.43
8:P:122:SER:OG	8:P:123:LEU:N	2.51	0.43
4:C:296:VAL:HG23	4:C:336:LEU:HD13	2.00	0.43
4:C:318:SER:OG	4:C:319:LEU:N	2.49	0.43
5:D:826:ILE:HD12	5:D:826:ILE:HA	1.91	0.43
7:F:235:ILE:HD12	7:F:245:ALA:HB1	2.01	0.43
3:A:46:ILE:HD11	3:A:224:LEU:HD13	2.01	0.43
5:D:194:LEU:HD21	5:D:234:PRO:HG3	2.00	0.43
5:D:957:SER:N	5:D:985:ILE:O	2.52	0.43
4:C:808:ASN:H	5:D:633:ALA:HB2	1.84	0.43
4:C:1279:GLU:OE1	5:D:805:GLN:NE2	2.52	0.43
5:D:1163:VAL:HG23	5:D:1177:ILE:HG12	2.01	0.43
7:F:217:ALA:HA	7:F:220:LYS:HG2	2.00	0.43
3:A:45:ARG:NH1	4:C:1084:ASP:OD1	2.36	0.43
4:C:262:TYR:O	4:C:267:ARG:NH2	2.51	0.43
4:C:1254:VAL:HG22	5:D:251:PRO:HG3	2.00	0.43
5:D:1106:ILE:HB	5:D:1123:ARG:HB2	2.00	0.43
4:C:568:ASN:HB3	4:C:572:ILE:HG12	2.01	0.43
5:D:506:VAL:HG13	5:D:628:GLY:HA3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:701:LEU:HG	5:D:723:TYR:HB2	2.00	0.43
7:F:303:ILE:O	7:F:307:THR:OG1	2.34	0.43
4:C:160:ASP:OD1	4:C:160:ASP:N	2.52	0.42
4:C:4:SER:OG	4:C:781:ASP:OD2	2.31	0.42
5:D:981:GLU:OE2	5:D:994:SER:OG	2.30	0.42
7:F:339:ARG:HG2	7:F:342:GLN:HE21	1.83	0.42
8:Q:9:THR:OG1	8:Q:10:LYS:N	2.52	0.42
4:C:1259:LEU:HD23	4:C:1259:LEU:HA	1.93	0.42
5:D:515:ARG:HH12	5:D:719:PHE:HA	1.84	0.42
5:D:516:ASP:OD1	5:D:516:ASP:N	2.52	0.42
5:D:583:VAL:HA	5:D:584:PRO:HD3	1.93	0.42
3:B:111:THR:OG1	3:B:112:ALA:N	2.53	0.42
4:C:231:GLU:HB3	4:C:238:GLN:HB2	2.02	0.42
5:D:364:HIS:HB3	5:D:487:THR:HG23	2.00	0.42
5:D:789:LYS:NZ	5:D:928:THR:O	2.40	0.42
5:D:1195:GLN:NE2	5:D:1212:ASP:OD2	2.48	0.42
1:1:19:DG:OP1	8:P:119:GLN:NE2	2.53	0.42
4:C:886:LYS:NZ	4:C:916:SER:OG	2.44	0.42
7:F:227:GLN:HB3	7:F:252:LEU:HD21	2.02	0.42
7:F:291:CYS:SG	7:F:299:LYS:NZ	2.93	0.42
8:P:22:LEU:HD12	8:P:58:CYS:HB3	2.02	0.42
8:Q:42:LYS:NZ	9:R:2:G:O6	2.42	0.42
4:C:720:ARG:NH2	4:C:749:ASP:OD1	2.53	0.42
5:D:1356:LEU:O	5:D:1366:HIS:NE2	2.43	0.42
5:D:518:VAL:HA	5:D:547:ARG:HH12	1.85	0.42
5:D:576:ARG:HD3	5:D:593:ASN:HA	2.02	0.42
2:2:21:DA:OP1	4:C:1269:ARG:NE	2.50	0.42
3:A:28:LEU:N	3:A:201:LEU:O	2.53	0.42
5:D:371:LYS:H	5:D:371:LYS:HG3	1.67	0.42
5:D:530:PRO:HB2	5:D:581:MET:HG2	2.02	0.42
5:D:1361:THR:HA	6:E:17:PHE:HB3	2.02	0.42
4:C:772:SER:OG	4:C:775:GLU:OE1	2.37	0.42
5:D:1275:LEU:O	5:D:1276:GLU:CG	2.68	0.42
5:D:1307:LEU:HD22	5:D:1311:LYS:HE2	2.02	0.42
7:F:274:ARG:HD2	7:F:274:ARG:HA	1.78	0.42
4:C:1247:SER:OG	4:C:1248:THR:N	2.53	0.42
5:D:826:ILE:HG23	5:D:994:SER:HB2	2.02	0.42
4:C:421:SER:OG	4:C:422:LYS:N	2.53	0.41
4:C:1141:LEU:HD23	4:C:1141:LEU:HA	1.94	0.41
4:C:1150:ASP:OD2	4:C:1158:LYS:NZ	2.48	0.41
5:D:708:ASN:ND2	5:D:714:GLU:O	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:69:SER:OG	3:A:70:THR:N	2.52	0.41
4:C:75:LEU:HD21	4:C:127:ILE:HD11	2.02	0.41
4:C:75:LEU:HD23	4:C:75:LEU:HA	1.92	0.41
5:D:475:GLU:OE1	6:E:28:ARG:NH2	2.53	0.41
5:D:615:LYS:HB3	5:D:615:LYS:HE2	1.79	0.41
4:C:1073:LYS:HD2	5:D:462:ASP:HB2	2.02	0.41
5:D:478:LEU:HB3	6:E:20:VAL:HG13	2.02	0.41
5:D:259:ARG:HA	5:D:259:ARG:HD3	1.84	0.41
4:C:1245:ALA:HB2	5:D:372:MET:HG3	2.02	0.41
3:B:166:ARG:HB2	3:B:170:ARG:HD2	2.02	0.41
4:C:1020:GLU:HA	4:C:1023:HIS:HB2	2.03	0.41
4:C:1073:LYS:NZ	9:R:11:A:OP1	2.40	0.41
5:D:1215:GLU:HG3	5:D:1220:ILE:HD11	2.03	0.41
4:C:243:PRO:HB3	4:C:277:LEU:HB3	2.03	0.41
4:C:1253:LEU:HD23	4:C:1253:LEU:HA	1.95	0.41
4:C:229:ILE:HB	4:C:240:GLU:HB3	2.02	0.41
5:D:136:GLU:OE1	5:D:312:ARG:NH2	2.54	0.41
5:D:510:LEU:HD11	5:D:624:ILE:HG12	2.02	0.41
7:F:151:VAL:HB	7:F:161:LEU:HD21	2.02	0.41
8:P:127:ARG:HE	8:P:127:ARG:HB3	1.72	0.41
8:Q:158:ILE:HD12	8:Q:158:ILE:HA	1.97	0.41
3:B:112:ALA:HB1	3:B:123:ILE:HG21	2.03	0.41
4:C:496:LYS:HD2	4:C:496:LYS:HA	1.82	0.41
3:B:102:LEU:HD13	3:B:115:ILE:HG22	2.03	0.40
4:C:69:GLN:OE1	4:C:101:ARG:NH2	2.42	0.40
5:D:44:ILE:HG22	5:D:51:PRO:HA	2.03	0.40
3:A:158:ARG:HE	3:A:172:LEU:HD11	1.85	0.40
4:C:200:ARG:HA	4:C:200:ARG:HD3	1.83	0.40
4:C:726:TYR:HB3	4:C:733:VAL:HB	2.03	0.40
4:C:226:GLU:OE1	4:C:245:ARG:NH2	2.54	0.40
4:C:1142:ARG:NH1	4:C:1161:LEU:O	2.55	0.40
7:F:157:ARG:H	7:F:157:ARG:HG2	1.69	0.40
8:Q:134:LEU:HD23	8:Q:134:LEU:HA	1.91	0.40
3:A:102:LEU:HB3	3:A:142:MET:HG3	2.03	0.40
3:B:47:LEU:HB3	3:B:180:VAL:HG11	2.03	0.40
4:C:890:LYS:HD2	4:C:913:VAL:HB	2.03	0.40
5:D:1275:LEU:C	5:D:1276:GLU:HG3	2.41	0.40
7:F:392:LYS:HB3	7:F:392:LYS:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
3	A	228/329 (69%)	225 (99%)	3 (1%)	0	100	100
3	B	226/329 (69%)	217 (96%)	9 (4%)	0	100	100
4	C	1338/1342 (100%)	1278 (96%)	60 (4%)	0	100	100
5	D	1321/1430 (92%)	1251 (95%)	70 (5%)	0	100	100
6	E	73/91 (80%)	71 (97%)	2 (3%)	0	100	100
7	F	319/627 (51%)	302 (95%)	17 (5%)	0	100	100
8	P	143/162 (88%)	137 (96%)	6 (4%)	0	100	100
8	Q	154/162 (95%)	152 (99%)	2 (1%)	0	100	100
All	All	3802/4472 (85%)	3633 (96%)	169 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	198/286 (69%)	198 (100%)	0	100	100
3	B	196/286 (68%)	196 (100%)	0	100	100
4	C	1154/1157 (100%)	1151 (100%)	3 (0%)	92	97
5	D	1110/1189 (93%)	1110 (100%)	0	100	100
6	E	65/75 (87%)	65 (100%)	0	100	100
7	F	288/552 (52%)	284 (99%)	4 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	P	125/140 (89%)	125 (100%)	0	100	100
8	Q	135/140 (96%)	132 (98%)	3 (2%)	52	78
All	All	3271/3825 (86%)	3261 (100%)	10 (0%)	92	97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	114	VAL
4	C	539	THR
4	C	988	LYS
7	F	150	ARG
7	F	277	MET
7	F	300	LYS
7	F	329	LYS
8	Q	11	GLU
8	Q	31	ARG
8	Q	155	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	75	GLN
4	C	120	GLN
4	C	447	HIS
4	C	490	GLN
4	C	622	ASN
4	C	673	HIS
4	C	1237	HIS
5	D	196	GLN
5	D	232	ASN
5	D	477	GLN
5	D	777	HIS
5	D	875	ASN
5	D	1019	ASN
5	D	1049	GLN
5	D	1238	GLN
5	D	1259	GLN
7	F	128	ASN
7	F	258	GLN
7	F	283	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	F	294	GLN
7	F	342	GLN
7	F	409	ASN
8	P	68	GLN
8	P	90	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	R	10/11 (90%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	R	2	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.
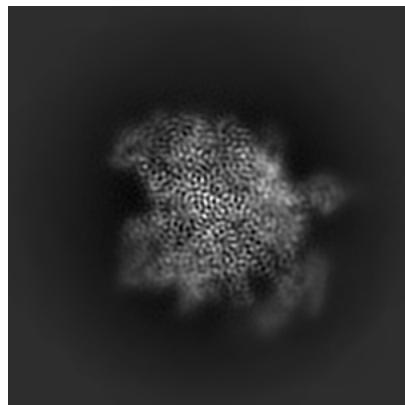
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-20233. These allow visual inspection of the internal detail of the map and identification of artifacts.
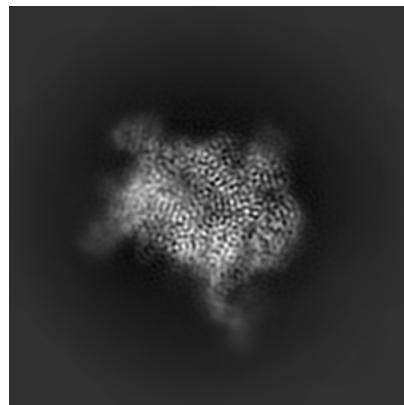
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ
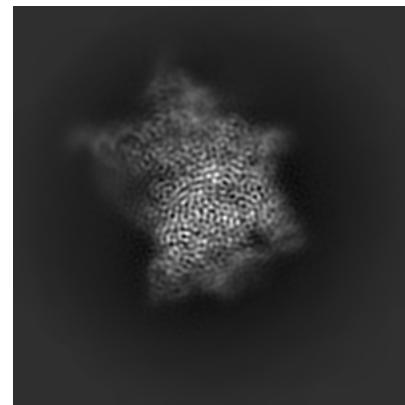
6.1.1 Primary map

X

Y

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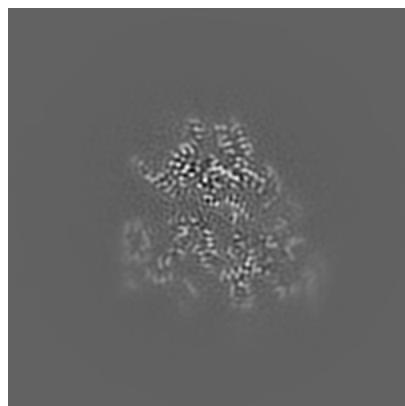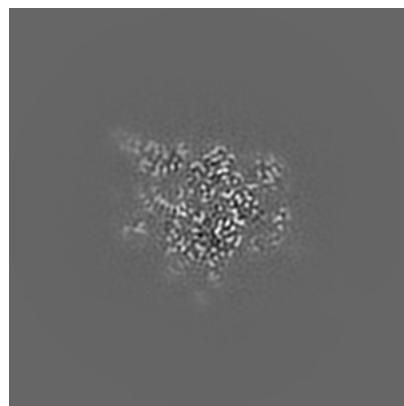
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
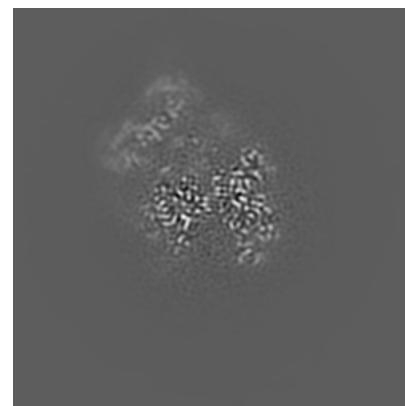
6.2.1 Primary map

X Index: 128

Y Index: 128
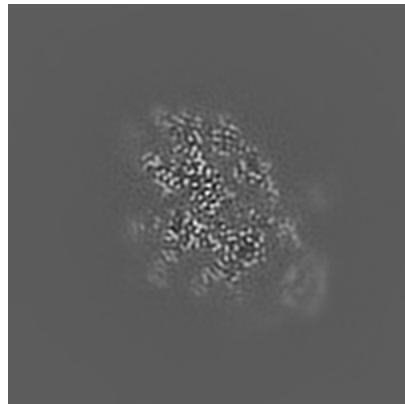
Z Index: 128
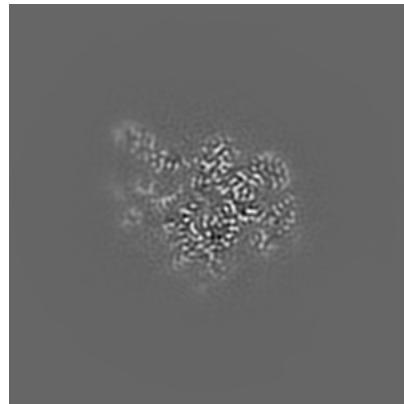
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices (i)
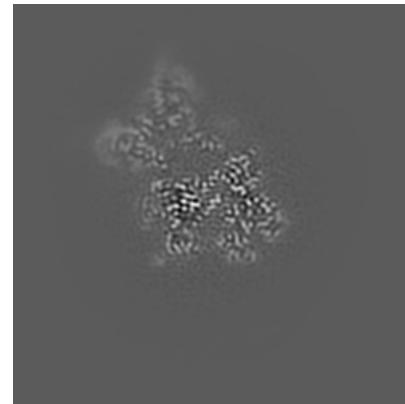
6.3.1   Primary map

| X Index: 118 | Y Index: 123 | Z Index: 134 |
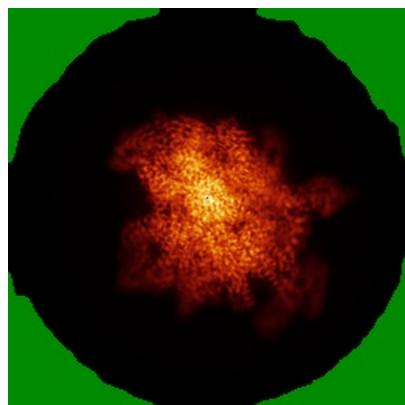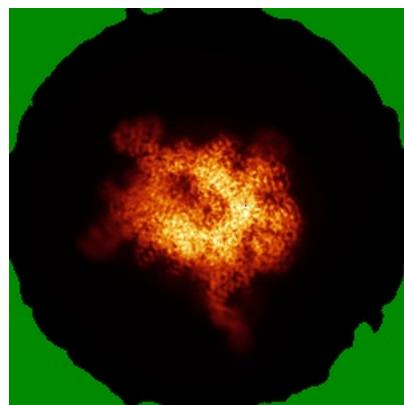
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal standard-deviation projections (False-color) (i)
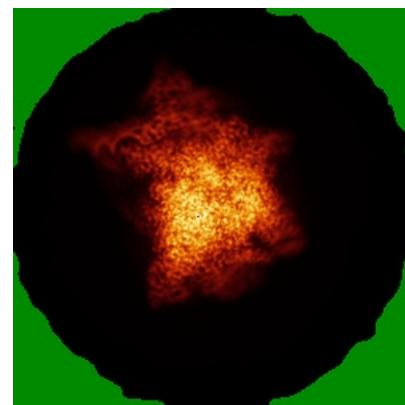
6.4.1   Primary map

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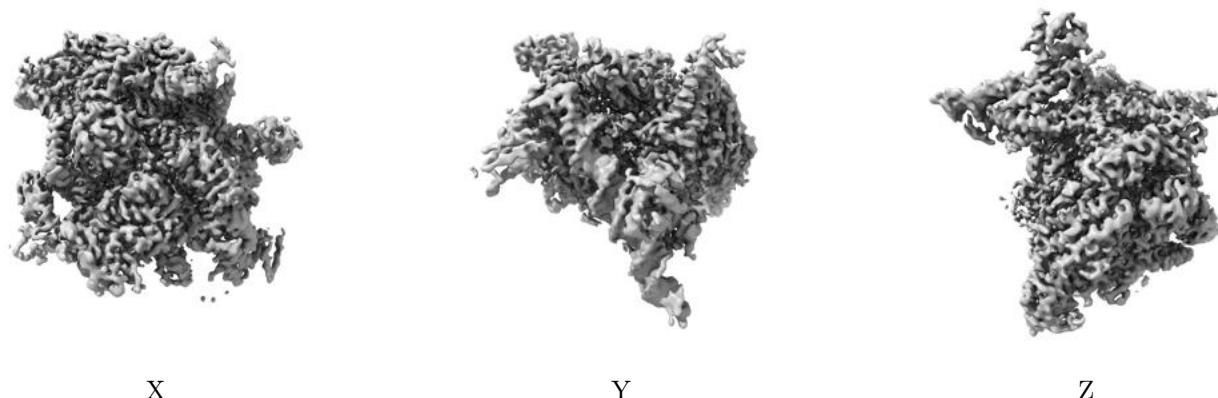
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.0286. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.
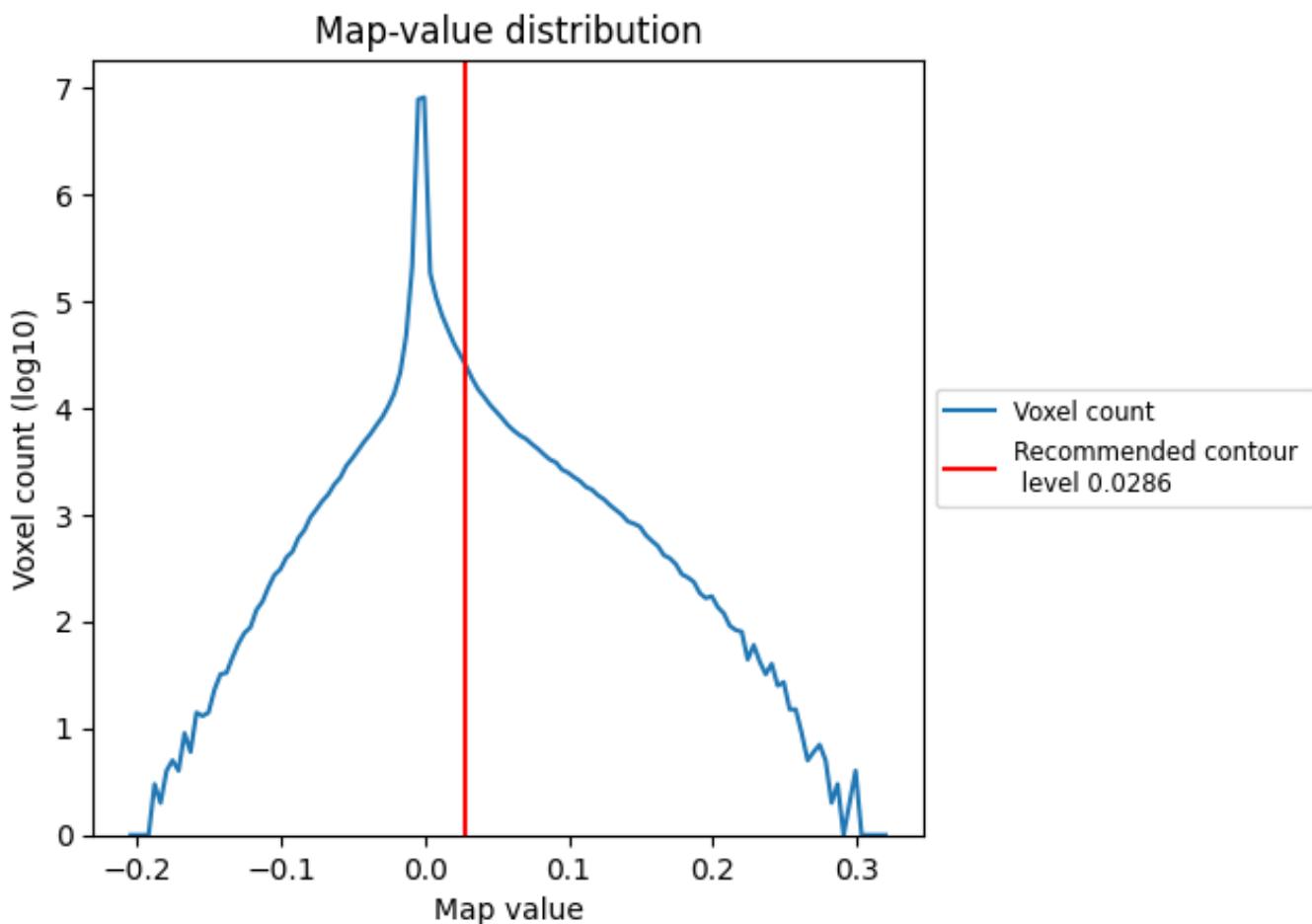
6.6 Mask visualisation (i)

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

7 Map analysis ⓘ
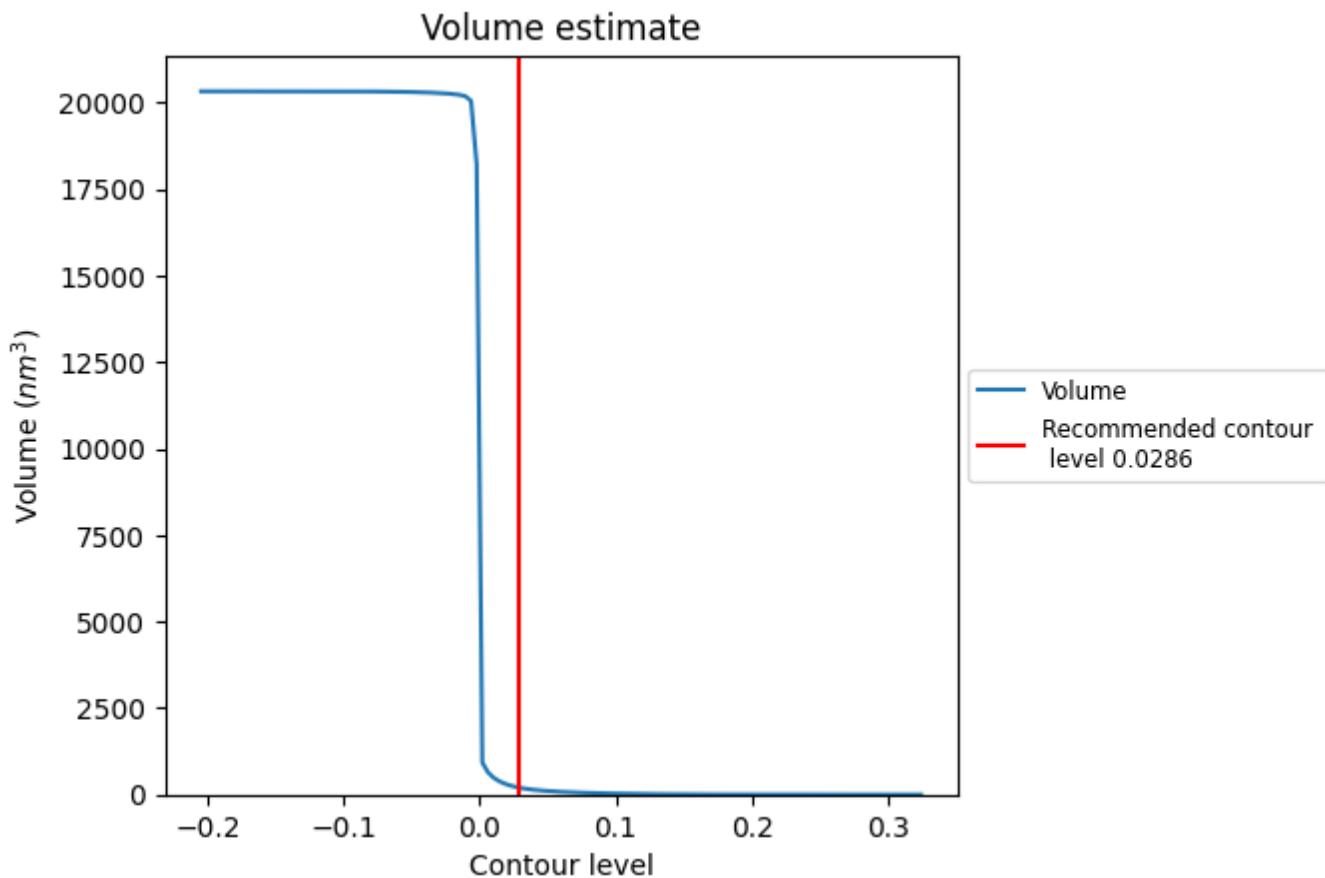
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.
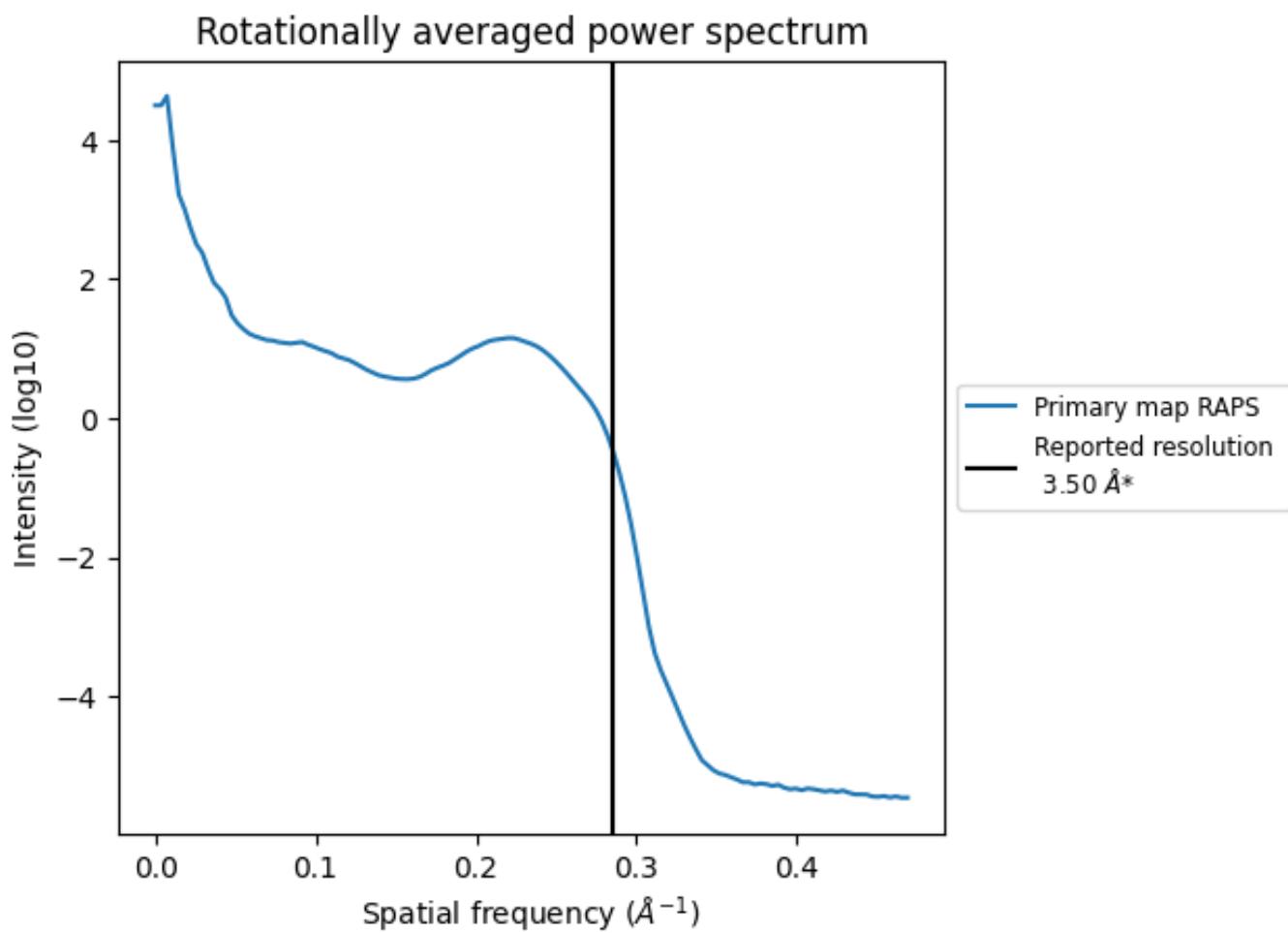
7.2　Volume estimate　ⓘ

Volume estimate

The volume at the recommended contour level is 204 nm^3; this corresponds to an approximate mass of 185 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 ⓘ
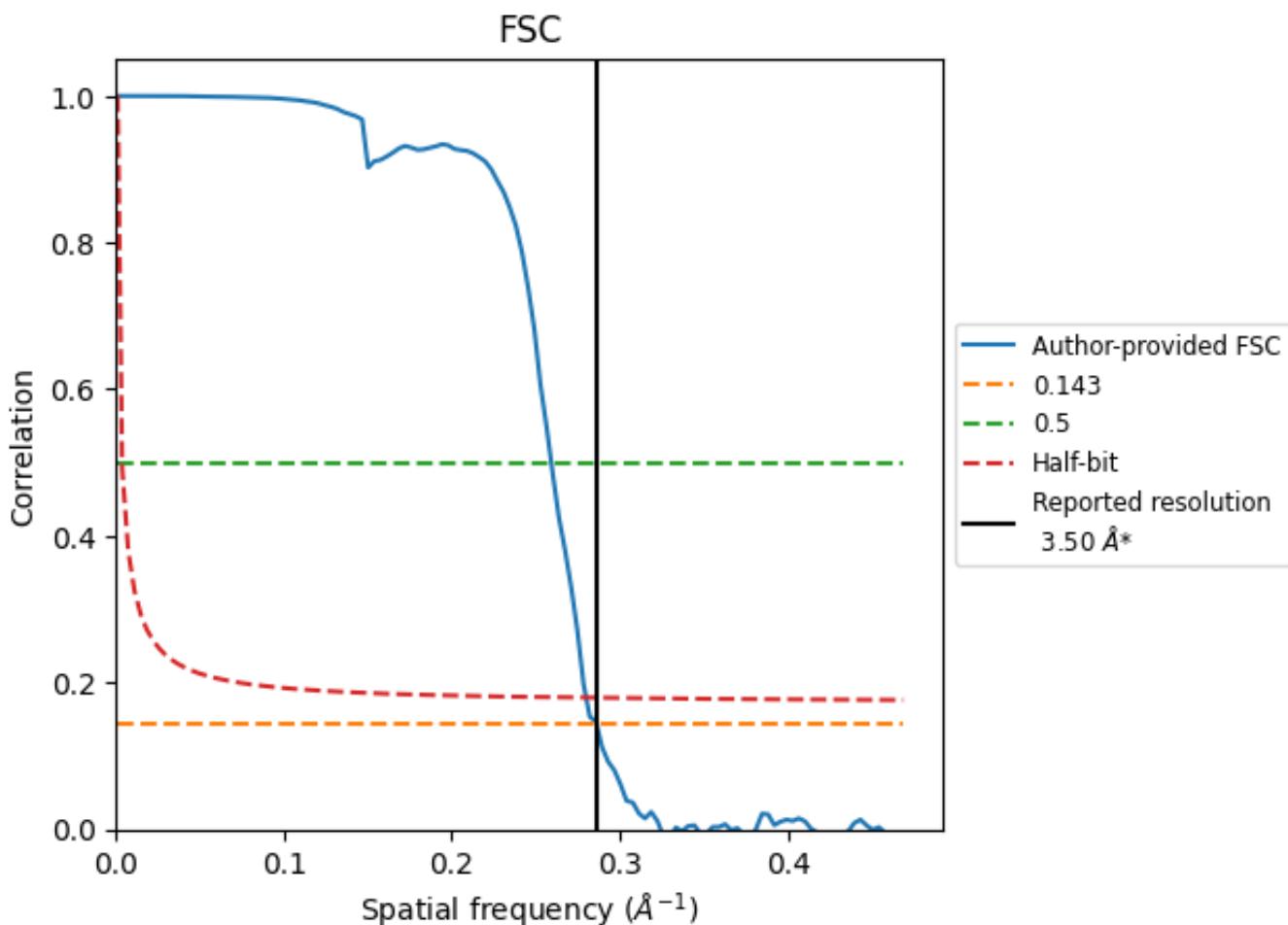
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)
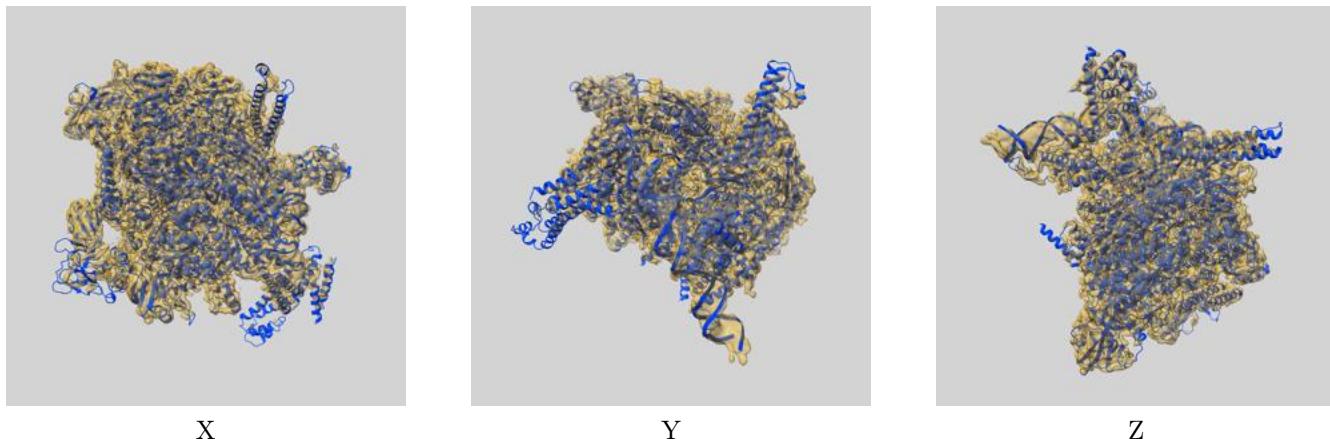
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	3.86	3.57
Unmasked-calculated*	-	-	-

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

9 Map-model fit ⓘ
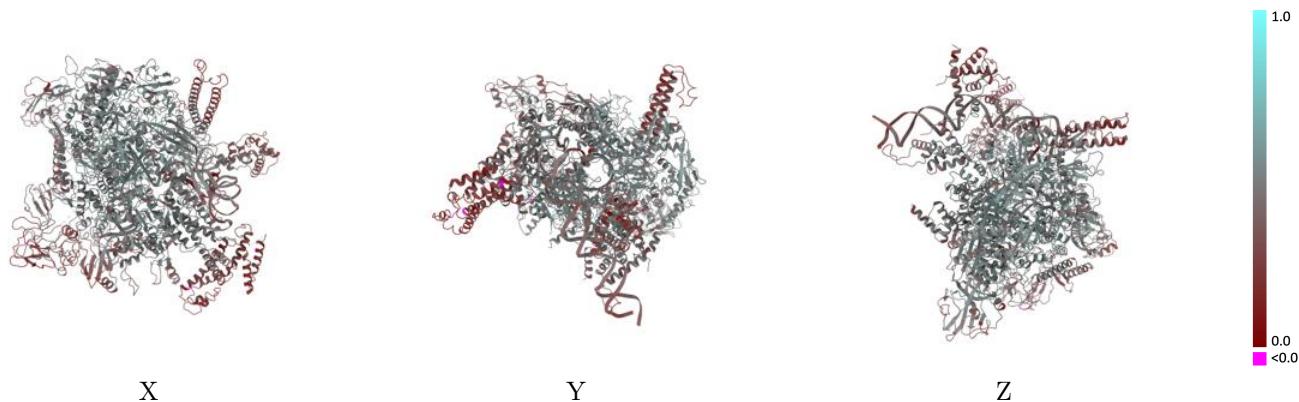
This section contains information regarding the fit between EMDB map EMD-20233 and PDB model 6P18. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay ⓘ
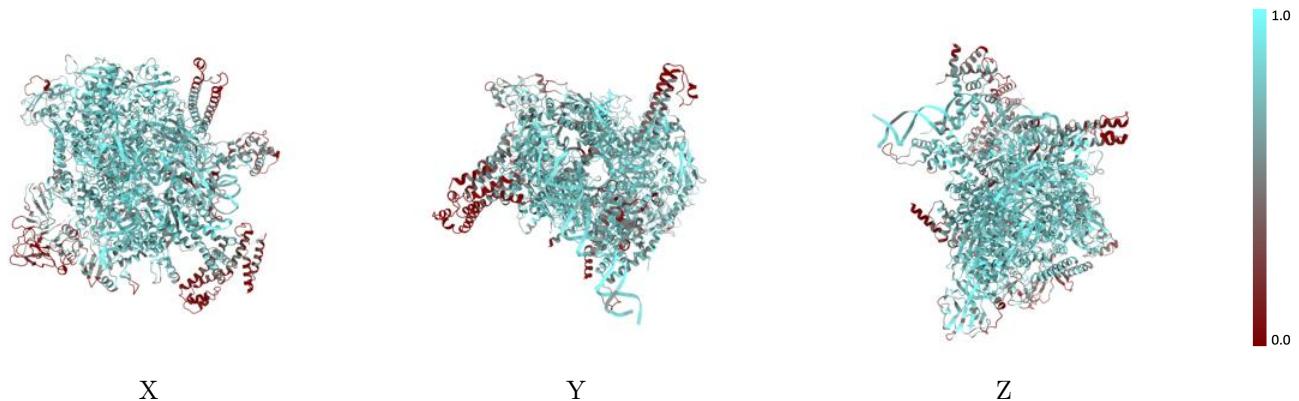
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0286 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
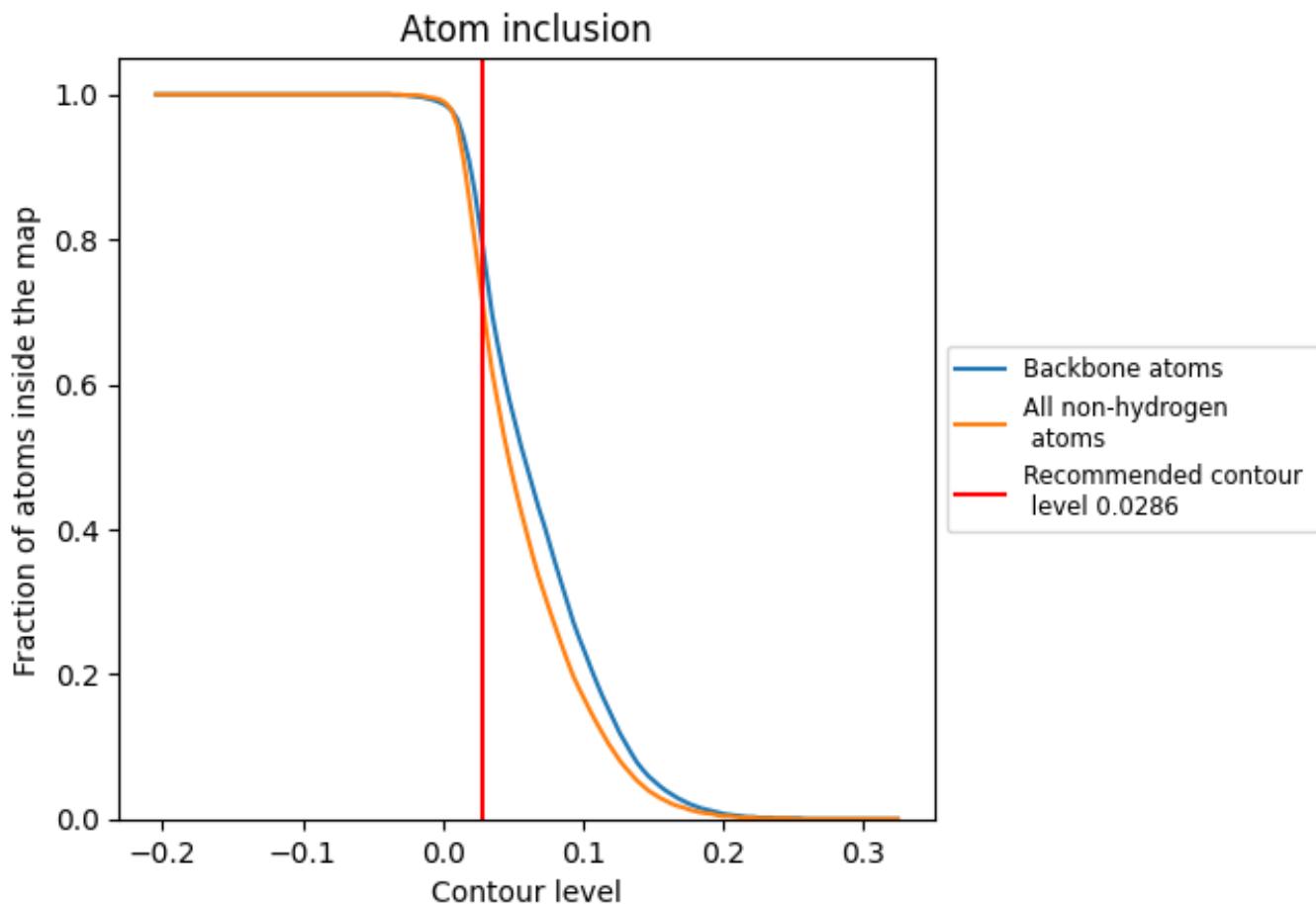
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0286).

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9.4 Atom inclusion ⓘ

At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.0286) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.4470
1	0.8450	0.4070
2	0.8300	0.4010
A	0.7740	0.4940
B	0.7070	0.4510
C	0.7500	0.4730
D	0.7320	0.4650
E	0.3870	0.4280
F	0.4190	0.3220
P	0.5390	0.3520
Q	0.6850	0.4390
R	0.8650	0.5020

1.0

0.0
<0.0