Full wwPDB EM Validation Report (i)

Mar 9, 2024 – 10:12 AM EST

PDB ID	:	6NMA
EMDB ID	:	EMD-0445
Title	:	CryoEM structure of the LbCas12a-crRNA-AcrVA4 complex
Authors	:	Chang, L.; Li, Z.; Zhang, H.
Deposited on	:	2019-01-10
Resolution	:	3.38 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 (i) 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 (i)) were used in the production of this report:
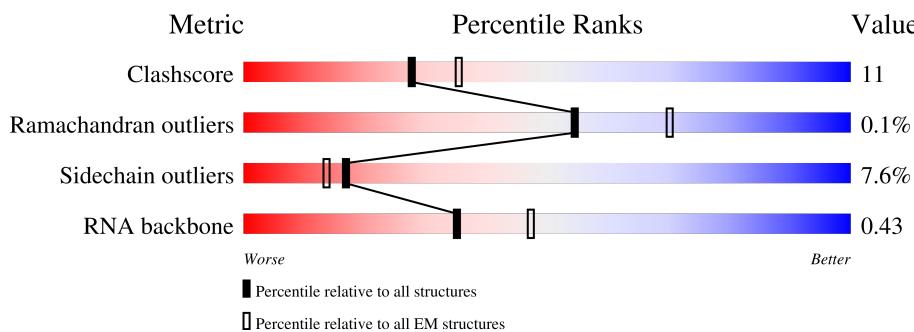
|		
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 3.38 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		11
Ramachandran outliers		0.1%
Sidechain outliers		7.6%
RNA backbone		0.43

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	A	234	33% 15% • 51%
1	C	234	14% 35% 13% • 51%
2	B	1227	17% 69% 26% • •
3	G	40	30% 32% 38%

WORLDWIDE wwPDB PROTEIN DATA BANK

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12404 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 AcrVA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total 951	C 606	N 161	O 178	S 6	0	0
1	C	114	Total 942	C 600	N 159	O 177	S 6	0	0

- Molecule 2 is a protein called Cpf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1206	Total 9974	C 6424	N 1632	O 1889	S 29	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP A0A182DWE3
B	112	ASN	ALA	conflict	UNP A0A182DWE3
B	113	GLU	ALA	conflict	UNP A0A182DWE3
B	131	PHE	ALA	conflict	UNP A0A182DWE3
B	132	LEU	ALA	conflict	UNP A0A182DWE3
B	264	GLN	ALA	conflict	UNP A0A182DWE3
B	269	LYS	ALA	conflict	UNP A0A182DWE3
B	357	VAL	LEU	conflict	UNP A0A182DWE3
B	1076	ARG	ALA	conflict	UNP A0A182DWE3
B	1077	ASN	ALA	conflict	UNP A0A182DWE3
B	1078	PRO	ALA	conflict	UNP A0A182DWE3
B	1085	ASP	ALA	conflict	UNP A0A182DWE3

- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	25	Total 535	C 240	N 97	O 173	P 25	0	0
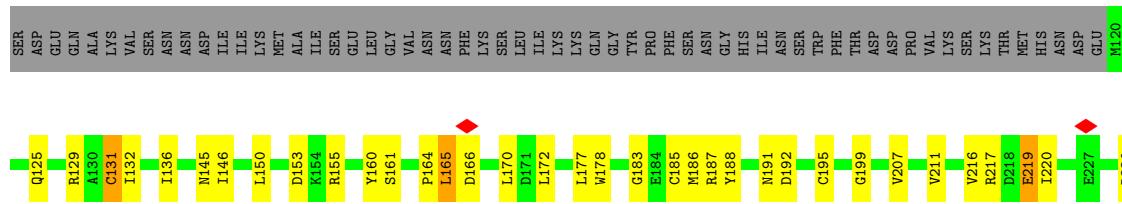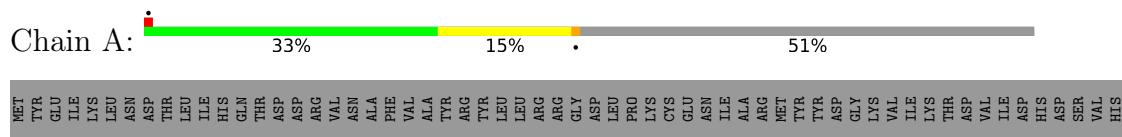
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	0
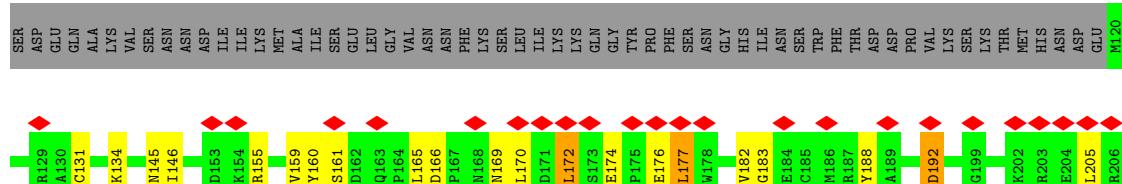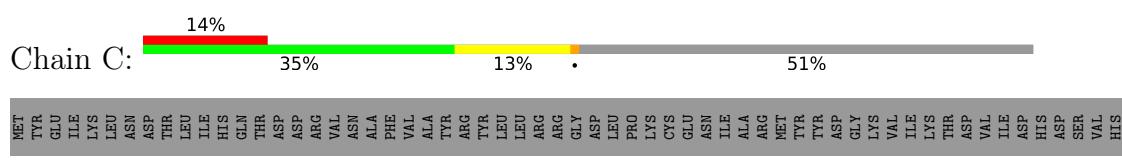
3 Residue-property plots ⓘ

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: AcrVA1

Chain A:
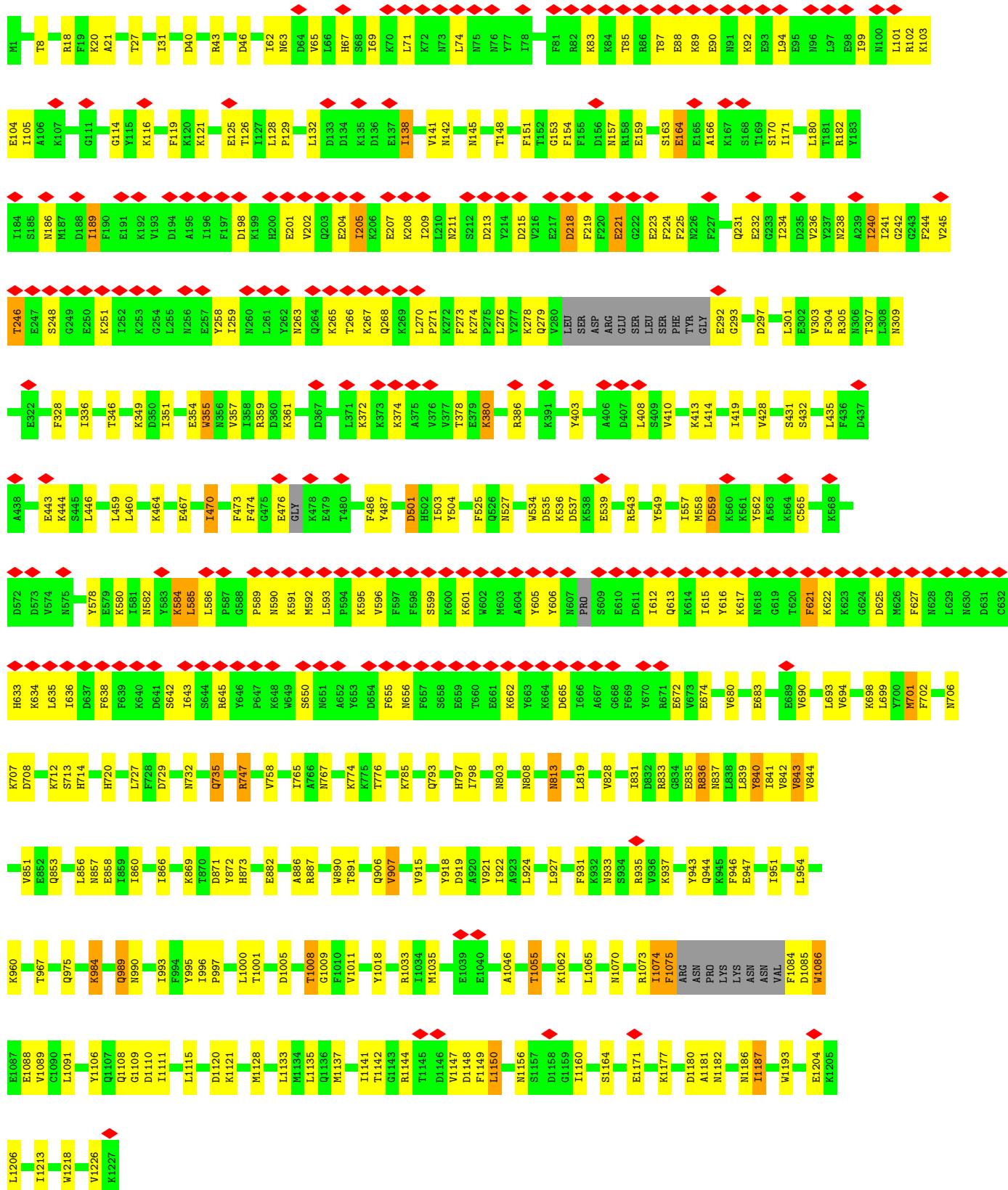
- Molecule 1: AcrVA1
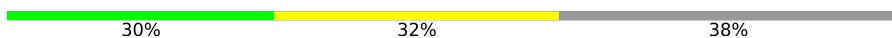
Chain C:

- Molecule 2: Cpf1

Chain B:

• Molecule 3: RNA

Chain G:

30%   32%   38%

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	297026	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	0.85	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	0.207	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0226	Depositor
Map size (Å)	255.84, 255.84, 255.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z|>5$	RMSZ	$\#|Z|>5$
1	A	0.58	0/970	0.52	0/1318
1	C	0.31	0/961	0.45	0/1307
2	B	0.48	0/10180	0.48	0/13668
3	G	1.39	0/599	1.04	0/931
All	All	0.56	0/12710	0.53	0/17224

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	951	0	951	30	0
1	C	942	0	938	22	0
2	B	9974	0	9918	210	0
3	G	535	0	268	13	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
All	All	12404	0	12075	261	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 11.

All (261) 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:837:ASN:HA	2:B:857:ASN:HD21	1.46	0.80
2:B:20:LYS:HD3	2:B:793:GLN:HE21	1.49	0.78
1:A:187:ARG:HH11	1:A:192:ASP:HB3	1.49	0.77
1:C:160:TYR:HB2	1:C:207:VAL:HG11	1.69	0.74
2:B:605:TYR:HB3	2:B:645:ARG:HH22	1.53	0.73
1:C:155:ARG:NH1	1:C:183:GLY:O	2.22	0.73
2:B:142:ASN:O	2:B:145:ASN:ND2	2.25	0.70
1:A:178:TRP:CZ3	1:A:217:ARG:HB2	2.28	0.69
2:B:211:ASN:ND2	2:B:213:ASP:O	2.26	0.69
2:B:1055:THR:O	2:B:1055:THR:OG1	2.10	0.68
2:B:1111:ILE:HG13	2:B:1115:LEU:HD23	1.73	0.68
2:B:182:ARG:O	2:B:186:ASN:ND2	2.22	0.67
2:B:204:GLU:O	2:B:208:LYS:NZ	2.27	0.67
1:C:192:ASP:N	1:C:192:ASP:OD1	2.25	0.66
2:B:157:ASN:ND2	3:G:27:A:O2'	2.29	0.66
2:B:712:LYS:NZ	3:G:16:U:OP2	2.29	0.65
1:A:136:ILE:HD11	1:A:166:ASP:HA	1.79	0.65
2:B:616:TYR:HA	2:B:621:PHE:HE1	1.62	0.65
1:A:155:ARG:NH1	1:A:183:GLY:O	2.28	0.65
2:B:83:LYS:HD3	2:B:85:THR:HA	1.76	0.65
1:C:169:ASN:OD1	1:C:170:LEU:N	2.30	0.64
1:A:178:TRP:HZ3	1:A:217:ARG:HB2	1.61	0.64
2:B:67:HIS:NE2	2:B:232:GLU:OE2	2.31	0.63
2:B:589:PRO:HG3	2:B:674:GLU:HB2	1.80	0.63
2:B:593:LEU:HA	2:B:596:VAL:HG12	1.80	0.63
2:B:706:ASN:HD22	3:G:6:U:H5	1.45	0.63
2:B:633:HIS:HA	2:B:636:ILE:HB	1.81	0.62
2:B:301:LEU:HD11	2:B:435:LEU:HD11	1.80	0.62
2:B:872:TYR:OH	2:B:906:GLN:NE2	2.33	0.62
2:B:201:GLU:HG2	2:B:202:VAL:HG13	1.82	0.62
2:B:354:GLU:HB2	2:B:357:VAL:HG23	1.81	0.61
2:B:464:LYS:NZ	2:B:501:ASP:OD1	2.21	0.61
2:B:443:GLU:HG3	2:B:444:LYS:HG3	1.83	0.61
1:A:186:MET:HE3	3:G:3:A:H5'	1.82	0.61
1:C:159:VAL:HG21	1:C:170:LEU:HD21	1.83	0.61
2:B:537:ASP:OD2	2:B:584:LYS:NZ	2.35	0.60
2:B:613:GLN:OE1	2:B:617:LYS:NZ	2.34	0.60
2:B:856:LEU:HD13	2:B:907:VAL:HG22	1.82	0.60
2:B:278:LYS:NZ	2:B:279:GLN:O	2.35	0.60
2:B:245:VAL:HG22	2:B:251:LYS:HZ3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:PRO:HA	2:B:138:ILE:HD11	1.82	0.60
2:B:924:LEU:HD13	2:B:947:GLU:HG2	1.83	0.60
2:B:189:ILE:HD11	2:B:271:PRO:HB2	1.83	0.59
2:B:828:VAL:HG22	2:B:921:VAL:HG22	1.83	0.59
2:B:1000:LEU:HD22	2:B:1011:VAL:HG21	1.83	0.59
2:B:693:LEU:HD23	2:B:698:LYS:HE3	1.85	0.59
2:B:803:ASN:HD22	2:B:975:GLN:NE2	1.99	0.59
2:B:836:ARG:NH2	2:B:1144:ARG:O	2.23	0.58
2:B:1001:THR:HG21	2:B:1187:ILE:HG13	1.85	0.58
2:B:706:ASN:O	2:B:708:ASP:N	2.37	0.58
2:B:592:MET:O	2:B:596:VAL:N	2.31	0.58
2:B:612:ILE:HD13	2:B:634:LYS:HE3	1.86	0.58
1:C:161:SER:HB3	1:C:165:LEU:HD11	1.85	0.58
2:B:767:ASN:ND2	2:B:774:LYS:O	2.37	0.57
2:B:774:LYS:NZ	3:G:15:G:O6	2.37	0.57
2:B:662:LYS:NZ	2:B:672:GLU:OE1	2.38	0.57
2:B:1070:ASN:ND2	2:B:1088:GLU:OE2	2.38	0.57
2:B:268:GLN:HG3	2:B:270:LEU:HG	1.86	0.57
2:B:305:ARG:O	2:B:309:ASN:ND2	2.25	0.57
2:B:536:LYS:HG2	2:B:582:ASN:HB2	1.87	0.57
1:C:219:GLU:N	1:C:219:GLU:OE1	2.38	0.56
2:B:246:THR:O	2:B:246:THR:OG1	2.20	0.56
1:A:216:VAL:HG22	1:A:217:ARG:H	1.71	0.56
1:C:174:GLU:HG2	1:C:176:GLU:H	1.71	0.56
2:B:374:LYS:NZ	2:B:378:THR:OG1	2.38	0.56
2:B:785:LYS:NZ	3:G:3:A:OP1	2.28	0.56
1:C:215:GLY:HA3	1:C:220:ILE:HA	1.88	0.56
1:A:188:TYR:CE2	1:A:195:CYS:HB3	2.42	0.55
2:B:151:PHE:O	2:B:154:PHE:N	2.39	0.55
2:B:40:ASP:OD1	2:B:43:ARG:NH1	2.35	0.55
2:B:153:GLY:HA3	3:G:26:A:O2'	2.06	0.55
2:B:927:LEU:HD11	2:B:943:TYR:HD2	1.72	0.55
1:C:155:ARG:HB3	1:C:182:VAL:HG12	1.88	0.54
2:B:835:GLU:N	2:B:835:GLU:OE1	2.40	0.54
2:B:871:ASP:OD1	2:B:872:TYR:N	2.41	0.54
3:G:26:A:N6	3:G:27:A:N1	2.55	0.54
1:A:125:GLN:O	1:A:129:ARG:NH2	2.41	0.54
2:B:915:VAL:HG21	2:B:922:ILE:HD11	1.90	0.54
1:C:172:LEU:HA	1:C:177:LEU:HD21	1.89	0.54
2:B:707:LYS:N	3:G:6:U:OP1	2.36	0.54
2:B:871:ASP:OD1	2:B:873:HIS:N	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:ASN:OD1	2:B:274:LYS:N	2.39	0.53
2:B:954:LEU:HD22	2:B:993:ILE:HD11	1.90	0.53
2:B:943:TYR:O	2:B:946:PHE:N	2.41	0.53
2:B:1033:ARG:HB2	2:B:1046:ALA:HB3	1.88	0.53
2:B:486:PHE:HD2	2:B:487:TYR:CD1	2.27	0.53
2:B:933:ASN:O	2:B:935:ARG:N	2.41	0.53
2:B:349:LYS:HD2	2:B:355:TRP:CD1	2.44	0.53
2:B:525:PHE:HD2	2:B:557:ILE:HG21	1.72	0.53
2:B:1108:GLN:O	2:B:1108:GLN:HG3	2.07	0.53
2:B:87:THR:O	2:B:90:GLU:N	2.41	0.52
2:B:63:ASN:HD21	2:B:231:GLN:HB3	1.73	0.52
2:B:198:ASP:N	2:B:201:GLU:OE2	2.42	0.52
2:B:238:ASN:O	2:B:242:GLY:N	2.41	0.52
2:B:535:ASP:HA	2:B:584:LYS:HB3	1.92	0.52
2:B:1120:ASP:OD1	2:B:1120:ASP:N	2.42	0.52
1:A:150:LEU:HD22	1:A:233:HIS:HB2	1.92	0.52
2:B:119:PHE:CE2	2:B:159:GLU:HG2	2.45	0.52
2:B:590:ASN:OD1	2:B:591:LYS:NZ	2.42	0.52
2:B:1193:TRP:CD2	2:B:1213:ILE:HD12	2.45	0.52
2:B:71:LEU:HB3	2:B:101:LEU:HD11	1.92	0.52
2:B:595:LYS:O	2:B:599:SER:OG	2.20	0.52
2:B:99:ILE:O	2:B:103:LYS:HG2	2.10	0.52
2:B:268:GLN:HG2	2:B:270:LEU:H	1.75	0.52
2:B:1008:THR:OG1	2:B:1009:GLY:N	2.43	0.51
2:B:219:PHE:HD2	2:B:240:ILE:HD11	1.75	0.51
2:B:589:PRO:HA	2:B:592:MET:HB3	1.92	0.51
2:B:486:PHE:HD2	2:B:487:TYR:HD1	1.58	0.51
2:B:927:LEU:HD13	2:B:944:GLN:HG3	1.93	0.51
2:B:351:ILE:HA	2:B:413:LYS:HG2	1.93	0.51
2:B:612:ILE:HD11	2:B:635:LEU:HD13	1.93	0.51
2:B:1065:LEU:HD21	2:B:1135:LEU:HD21	1.93	0.51
2:B:1073:ARG:HB2	2:B:1133:LEU:HD21	1.94	0.50
1:A:187:ARG:NH1	1:A:192:ASP:O	2.44	0.50
2:B:218:ASP:HA	2:B:221:GLU:HB3	1.94	0.50
3:G:25:A:H2'	3:G:26:A:O4'	2.12	0.50
2:B:1171:GLU:H	2:B:1171:GLU:CD	2.15	0.50
1:C:213:VAL:HG12	1:C:223:VAL:HA	1.93	0.49
2:B:559:ASP:CG	2:B:562:TYR:H	2.15	0.49
2:B:292:GLU:HG3	2:B:293:GLY:H	1.77	0.49
2:B:297:ASP:CG	2:B:446:LEU:HB2	2.33	0.49
1:A:178:TRP:HZ3	1:A:217:ARG:HE	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:837:ASN:ND2	2:B:1180:ASP:OD2	2.44	0.48
2:B:539:GLU:OE2	2:B:580:LYS:NZ	2.38	0.48
2:B:843:VAL:O	2:B:851:VAL:HG12	2.13	0.48
2:B:234:ILE:HG13	2:B:276:LEU:HB2	1.95	0.48
2:B:747:ARG:HE	2:B:747:ARG:HB3	1.39	0.48
1:A:165:LEU:HD13	1:A:170:LEU:HD11	1.95	0.48
2:B:1089:VAL:HG11	2:B:1133:LEU:HD23	1.95	0.48
2:B:234:ILE:HD13	2:B:278:LYS:HB2	1.96	0.48
2:B:163:SER:O	2:B:170:SER:OG	2.22	0.47
2:B:1137:MET:O	2:B:1150:LEU:HB2	2.14	0.47
2:B:1150:LEU:N	2:B:1164:SER:OG	2.41	0.47
2:B:18:ARG:HG2	2:B:797:HIS:CD2	2.50	0.47
2:B:585:LEU:HD12	2:B:585:LEU:H	1.78	0.47
2:B:951:ILE:HD11	2:B:995:TYR:OH	2.15	0.47
1:A:136:ILE:HG21	1:A:164:PRO:HB3	1.97	0.47
2:B:125:GLU:HG2	2:B:126:THR:HG23	1.96	0.47
1:C:146:ILE:HG21	1:C:229:VAL:HG13	1.97	0.47
1:A:187:ARG:NH1	1:A:192:ASP:HB3	2.25	0.47
2:B:231:GLN:HB2	2:B:278:LYS:HE3	1.97	0.47
2:B:460:LEU:HB3	2:B:504:TYR:HD1	1.80	0.47
2:B:665:ASP:N	2:B:665:ASP:OD1	2.48	0.47
1:A:199:GLY:HA3	2:B:882:GLU:OE2	2.15	0.47
2:B:1213:ILE:HD11	2:B:1218:TRP:HA	1.96	0.47
1:A:216:VAL:HG12	1:A:219:GLU:HG2	1.97	0.47
2:B:83:LYS:O	2:B:83:LYS:HG2	2.14	0.47
2:B:361:LYS:NZ	2:B:403:TYR:O	2.48	0.46
2:B:121:LYS:HB2	2:B:148:THR:HG21	1.97	0.46
2:B:886:ALA:O	2:B:887:ARG:HG2	2.15	0.46
1:A:131:CYS:SG	1:C:134:LYS:NZ	2.77	0.46
2:B:351:ILE:HD13	2:B:410:VAL:HG13	1.97	0.46
2:B:1156:ASN:ND2	2:B:1160:ILE:O	2.46	0.46
2:B:245:VAL:HG13	2:B:251:LYS:HD3	1.98	0.46
1:A:161:SER:HB3	1:A:165:LEU:HG	1.96	0.46
2:B:259:ILE:O	2:B:268:GLN:NE2	2.48	0.46
2:B:858:GLU:OE1	2:B:869:LYS:HD2	2.16	0.46
2:B:559:ASP:OD2	2:B:562:TYR:N	2.49	0.45
2:B:735:GLN:H	2:B:735:GLN:HG2	1.35	0.45
2:B:74:LEU:HD22	2:B:223:GLU:HB2	1.97	0.45
2:B:102:ARG:HH12	2:B:166:ALA:HB2	1.82	0.45
2:B:578:TYR:CD2	2:B:690:VAL:HG21	2.50	0.45
3:G:7:U:H2'	3:G:8:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:GLU:HG2	2:B:215:ASP:HB3	1.98	0.45
2:B:69:ILE:HD11	2:B:105:ILE:HA	1.98	0.45
2:B:1164:SER:HB2	2:B:1177:LYS:O	2.16	0.45
1:C:165:LEU:HD13	1:C:170:LEU:HD11	1.98	0.45
2:B:128:LEU:HD23	2:B:141:VAL:HG21	1.98	0.45
2:B:656:ASN:ND2	2:B:656:ASN:O	2.49	0.45
1:A:160:TYR:HB2	1:A:207:VAL:HG21	1.99	0.45
2:B:549:TYR:HB2	2:B:578:TYR:CD1	2.52	0.45
2:B:612:ILE:HD12	2:B:615:ILE:HD11	1.99	0.45
2:B:1091:LEU:HD23	2:B:1091:LEU:HA	1.79	0.45
2:B:69:ILE:HG12	2:B:105:ILE:HG13	1.98	0.44
2:B:643:ILE:O	2:B:650:SER:OG	2.35	0.44
2:B:101:LEU:O	2:B:104:GLU:HG2	2.17	0.44
2:B:960:LYS:HD2	3:G:21:A:OP2	2.18	0.44
2:B:414:LEU:HD13	2:B:473:PHE:CZ	2.53	0.44
2:B:839:LEU:HB3	2:B:856:LEU:HD12	2.00	0.44
2:B:840:TYR:CE1	2:B:1181:ALA:HB2	2.52	0.44
2:B:151:PHE:O	2:B:153:GLY:N	2.51	0.44
2:B:359:ARG:HH21	2:B:386:ARG:HE	1.64	0.44
2:B:372:LYS:HA	2:B:372:LYS:HD2	1.66	0.44
2:B:470:ILE:HD13	2:B:470:ILE:HA	1.69	0.44
2:B:21:ALA:HB1	2:B:702:PHE:HB3	2.00	0.44
2:B:62:ILE:HD13	2:B:171:ILE:HD11	2.00	0.44
1:A:146:ILE:HD11	1:A:230:ARG:HB2	2.00	0.43
2:B:1182:ASN:OD1	2:B:1186:ASN:ND2	2.51	0.43
1:A:145:ASN:ND2	1:C:145:ASN:OD1	2.51	0.43
2:B:103:LYS:HZ3	2:B:164:GLU:HB2	1.83	0.43
2:B:263:ASN:HD22	2:B:268:GLN:HB3	1.83	0.43
2:B:265:LYS:HE2	2:B:268:GLN:HA	2.00	0.43
2:B:582:ASN:O	2:B:680:VAL:HA	2.18	0.43
2:B:984:LYS:HB2	2:B:984:LYS:NZ	2.32	0.43
2:B:1062:LYS:HE3	2:B:1062:LYS:HB3	1.87	0.43
1:A:230:ARG:NH2	1:C:192:ASP:OD2	2.51	0.43
2:B:180:LEU:HD23	2:B:180:LEU:HA	1.87	0.43
2:B:218:ASP:OD1	2:B:218:ASP:N	2.50	0.43
2:B:558:MET:HA	2:B:699:LEU:HD12	2.01	0.43
2:B:414:LEU:HD13	2:B:473:PHE:HZ	1.84	0.43
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.89	0.43
1:A:191:ASN:OD1	1:A:191:ASN:N	2.44	0.43
2:B:304:PHE:CZ	2:B:459:LEU:HD23	2.54	0.43
2:B:1035:MET:HA	2:B:1109:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:THR:HG22	2:B:380:LYS:HG3	2.01	0.43
2:B:527:ASN:HB2	2:B:543:ARG:HH21	1.84	0.43
2:B:586:LEU:HA	2:B:586:LEU:HD12	1.78	0.42
1:A:186:MET:HE2	1:A:186:MET:HB3	1.78	0.42
2:B:1108:GLN:HA	2:B:1108:GLN:OE1	2.19	0.42
2:B:27:THR:O	2:B:31:ILE:HG13	2.18	0.42
2:B:419:ILE:HD13	2:B:419:ILE:HA	1.85	0.42
2:B:831:ILE:HD12	2:B:924:LEU:HD21	2.01	0.42
2:B:1075:PHE:HB3	2:B:1085:ASP:HB3	2.01	0.42
2:B:431:SER:O	2:B:431:SER:OG	2.35	0.42
2:B:202:VAL:HG12	2:B:258:TYR:CZ	2.54	0.42
2:B:1074:ILE:HD13	2:B:1074:ILE:HA	1.81	0.42
1:C:214:ILE:HD11	1:C:222:ARG:HE	1.85	0.42
2:B:727:LEU:HA	2:B:727:LEU:HD23	1.77	0.42
2:B:241:ILE:HD13	2:B:273:PHE:HB3	2.02	0.42
2:B:694:VAL:HG21	2:B:701:MET:HE2	2.01	0.42
2:B:432:SER:O	2:B:432:SER:OG	2.31	0.42
2:B:622:LYS:HE2	2:B:622:LYS:HB2	1.88	0.42
2:B:503:ILE:HD13	2:B:503:ILE:HA	1.83	0.42
2:B:584:LYS:H	2:B:584:LYS:HG3	1.57	0.42
2:B:732:ASN:O	2:B:732:ASN:ND2	2.53	0.42
2:B:808:ASN:N	2:B:808:ASN:HD22	2.17	0.42
2:B:114:GLY:C	2:B:116:LYS:H	2.24	0.41
2:B:142:ASN:ND2	2:B:145:ASN:HD21	2.18	0.41
2:B:1085:ASP:OD1	2:B:1086:TRP:N	2.44	0.41
2:B:89:LYS:HE2	2:B:92:LYS:HG3	2.02	0.41
2:B:813:ASN:OD1	2:B:813:ASN:N	2.53	0.41
1:C:160:TYR:CE2	1:C:205:LEU:HD21	2.55	0.41
1:A:131:CYS:HB2	1:C:131:CYS:SG	2.61	0.41
2:B:444:LYS:HE2	2:B:444:LYS:HB3	1.93	0.41
2:B:860:ILE:HG12	2:B:869:LYS:HB3	2.03	0.41
2:B:1008:THR:HA	2:B:1226:VAL:HG21	2.01	0.41
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.75	0.41
2:B:989:GLN:HG3	2:B:990:ASN:N	2.33	0.41
1:C:214:ILE:HD11	1:C:222:ARG:HB3	2.02	0.41
2:B:638:PHE:O	2:B:642:SER:OG	2.24	0.41
3:G:8:C:N3	3:G:21:A:C2	2.89	0.41
2:B:1033:ARG:HA	2:B:1110:ASP:OD1	2.21	0.41
2:B:1141:ILE:O	2:B:1142:THR:OG1	2.32	0.41
2:B:1206:LEU:HD23	2:B:1206:LEU:HA	1.82	0.41
1:A:136:ILE:HD13	1:A:136:ILE:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HB2	1:A:155:ARG:HD3	2.02	0.41
2:B:205:ILE:O	2:B:209:ILE:HG12	2.21	0.40
2:B:562:TYR:HB3	2:B:565:CYS:HB3	2.03	0.40
2:B:937:LYS:HD3	2:B:937:LYS:HA	1.83	0.40
1:A:234:LYS:HD3	1:A:234:LYS:HA	1.96	0.40
2:B:87:THR:O	2:B:88:GLU:HG2	2.22	0.40
2:B:428:VAL:HG11	2:B:459:LEU:HA	2.04	0.40
2:B:843:VAL:HG21	2:B:918:TYR:CD2	2.57	0.40
2:B:1106:TYR:HA	2:B:1111:ILE:HG21	2.04	0.40
2:B:74:LEU:HD11	2:B:225:PHE:HB3	2.03	0.40
2:B:616:TYR:HA	2:B:621:PHE:CE1	2.49	0.40
2:B:292:GLU:N	2:B:303:VAL:HG11	2.35	0.40
2:B:853:GLN:NE2	2:B:1177:LYS:HG3	2.36	0.40
2:B:606:TYR:HD1	2:B:606:TYR:HA	1.78	0.40
2:B:996:ILE:HG13	2:B:997:PRO:HD2	2.02	0.40
2:B:1018:TYR:OH	2:B:1121:LYS:HG3	2.21	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	113/234 (48%)	97 (86%)	16 (14%)	0	100	100
1	C	112/234 (48%)	97 (87%)	15 (13%)	0	100	100
2	B	1196/1227 (98%)	1070 (90%)	125 (10%)	1 (0%)	51	82
All	All	1421/1695 (84%)	1264 (89%)	156 (11%)	1 (0%)	54	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	559	ASP

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	
1	A	108/217 (50%)	98 (91%)	10 (9%)	9	31
1	C	107/217 (49%)	100 (94%)	7 (6%)	17	48
2	B	1095/1114 (98%)	1012 (92%)	83 (8%)	13	41
All	All	1310/1548 (85%)	1210 (92%)	100 (8%)	17	41

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	CYS
1	A	132	ILE
1	A	153	ASP
1	A	165	LEU
1	A	177	LEU
1	A	185	CYS
1	A	211	VAL
1	A	219	GLU
1	A	220	ILE
1	A	232	LEU
2	B	8	THR
2	B	46	ASP
2	B	65	VAL
2	B	94	LEU
2	B	132	LEU
2	B	138	ILE
2	B	164	GLU
2	B	189	ILE
2	B	205	ILE
2	B	218	ASP
2	B	221	GLU
2	B	224	PHE
2	B	236	VAL
2	B	240	ILE
2	B	244	PHE
2	B	246	THR

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Mol	Chain	Res	Type
2	B	248	SER
2	B	266	THR
2	B	267	LYS
2	B	307	THR
2	B	328	PHE
2	B	336	ILE
2	B	346	THR
2	B	355	TRP
2	B	380	LYS
2	B	408	LEU
2	B	467	GLU
2	B	470	ILE
2	B	474	PHE
2	B	476	GLU
2	B	501	ASP
2	B	534	TRP
2	B	584	LYS
2	B	585	LEU
2	B	601	LYS
2	B	621	PHE
2	B	625	ASP
2	B	627	PHE
2	B	655	PHE
2	B	683	GLU
2	B	701	MET
2	B	713	SER
2	B	714	HIS
2	B	720	HIS
2	B	729	ASP
2	B	735	GLN
2	B	747	ARG
2	B	758	VAL
2	B	765	ILE
2	B	776	THR
2	B	798	ILE
2	B	813	ASN
2	B	819	LEU
2	B	833	ARG
2	B	836	ARG
2	B	840	TYR
2	B	841	ILE
2	B	842	VAL

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Mol	Chain	Res	Type
2	B	843	VAL
2	B	844	VAL
2	B	866	ILE
2	B	890	TRP
2	B	891	THR
2	B	907	VAL
2	B	919	ASP
2	B	931	PHE
2	B	967	THR
2	B	984	LYS
2	B	989	GLN
2	B	1005	ASP
2	B	1008	THR
2	B	1055	THR
2	B	1074	ILE
2	B	1075	PHE
2	B	1084	PHE
2	B	1086	TRP
2	B	1128	MET
2	B	1147	VAL
2	B	1148	ASP
2	B	1149	PHE
2	B	1150	LEU
2	B	1187	ILE
2	B	1204	GLU
1	C	166	ASP
1	C	172	LEU
1	C	177	LEU
1	C	188	TYR
1	C	192	ASP
1	C	216	VAL
1	C	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	157	ASN
1	A	168	ASN
1	A	208	ASN
2	B	28	GLN
2	B	33	ASN

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Mol	Chain	Res	Type
2	B	63	ASN
2	B	142	ASN
2	B	145	ASN
2	B	157	ASN
2	B	263	ASN
2	B	340	ASN
2	B	567	GLN
2	B	651	ASN
2	B	676	GLN
2	B	735	GLN
2	B	793	GLN
2	B	808	ASN
2	B	861	ASN
2	B	906	GLN
2	B	975	GLN
1	C	145	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	24/40 (60%)	3 (12%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	G	13	A
3	G	14	A
3	G	17	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 2 ligands modelled in this entry, 2 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.
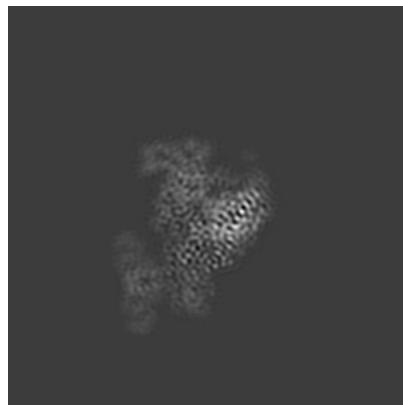
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-0445. These allow visual inspection of the internal detail of the map and identification of artifacts.
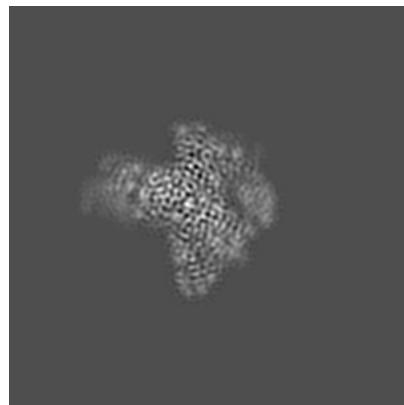
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ
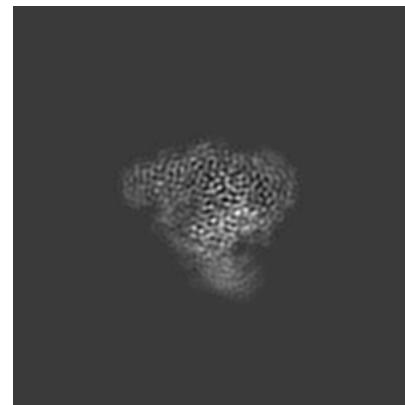
6.1.1 Primary map

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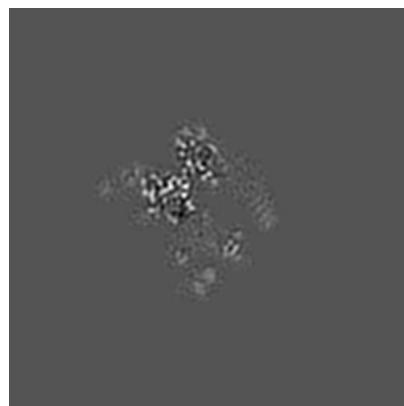
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
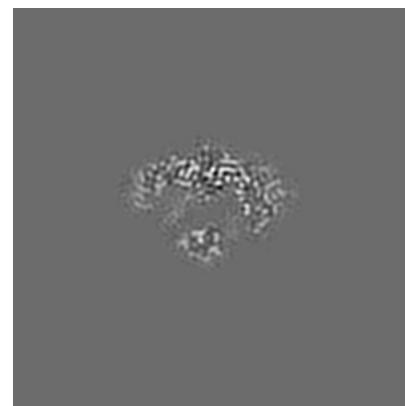
6.2.1 Primary map

X Index: 120	Y Index: 120	Z Index: 120
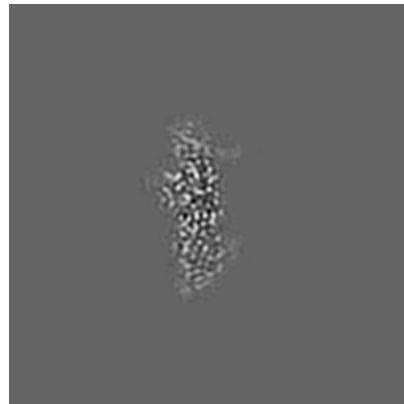
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ

6.3.1   Primary map

| X Index: 120 | Y Index: 137 | Z Index: 107 |
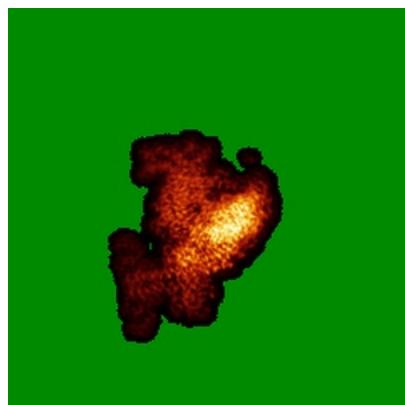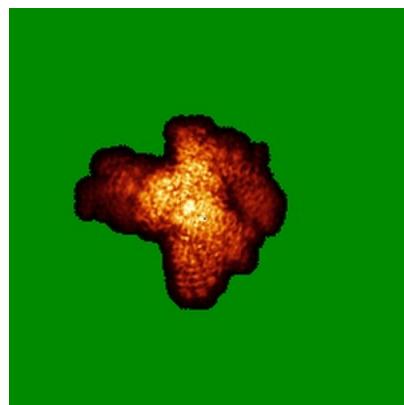
The images above show the largest variance slices of the map in three orthogonal directions.

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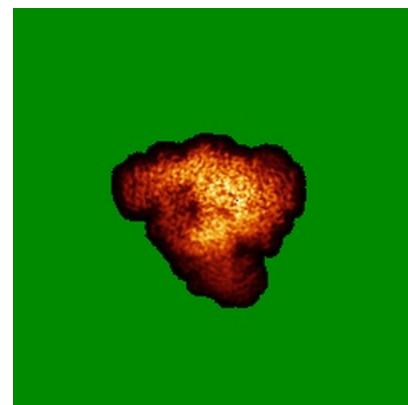
6.4.1   Primary map

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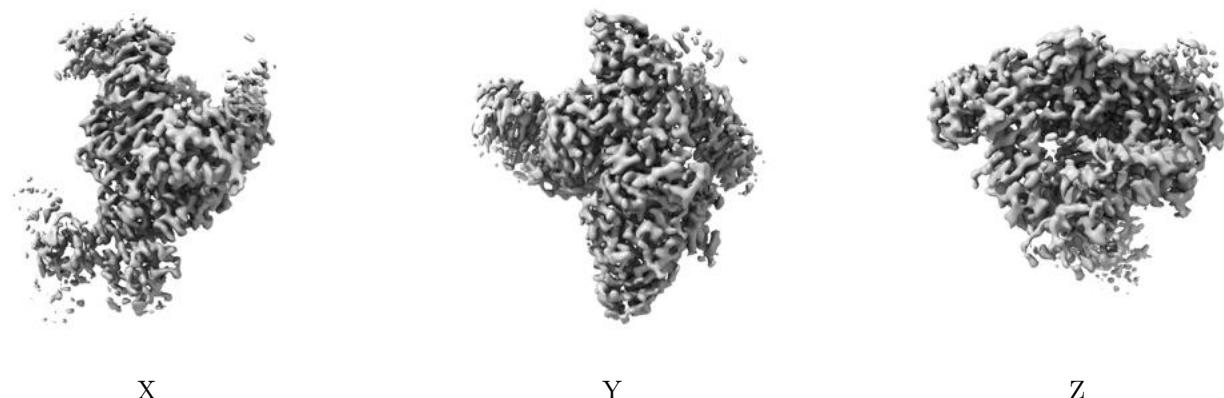
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.0226. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.
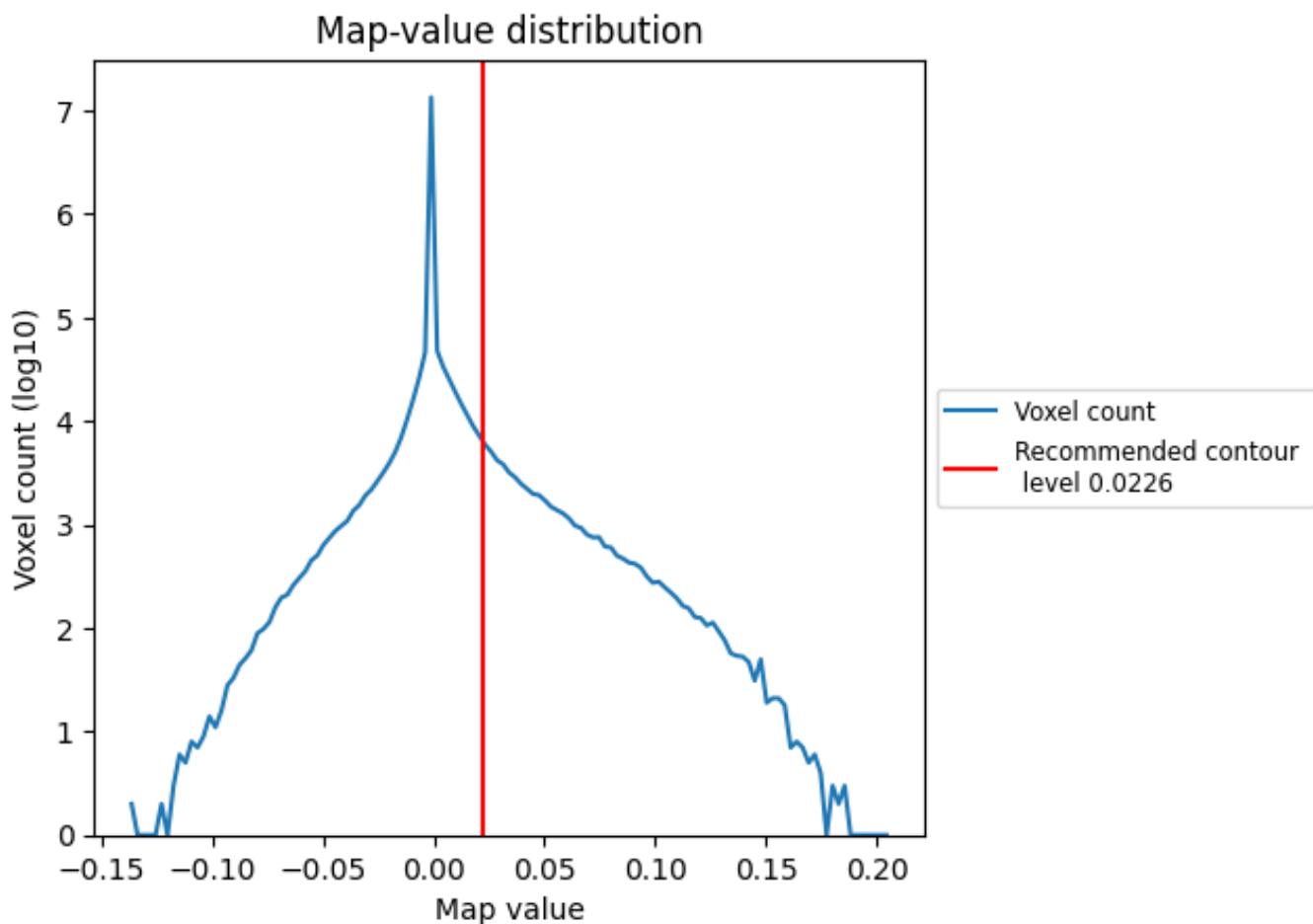
6.6 Mask visualisation ⓘ

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

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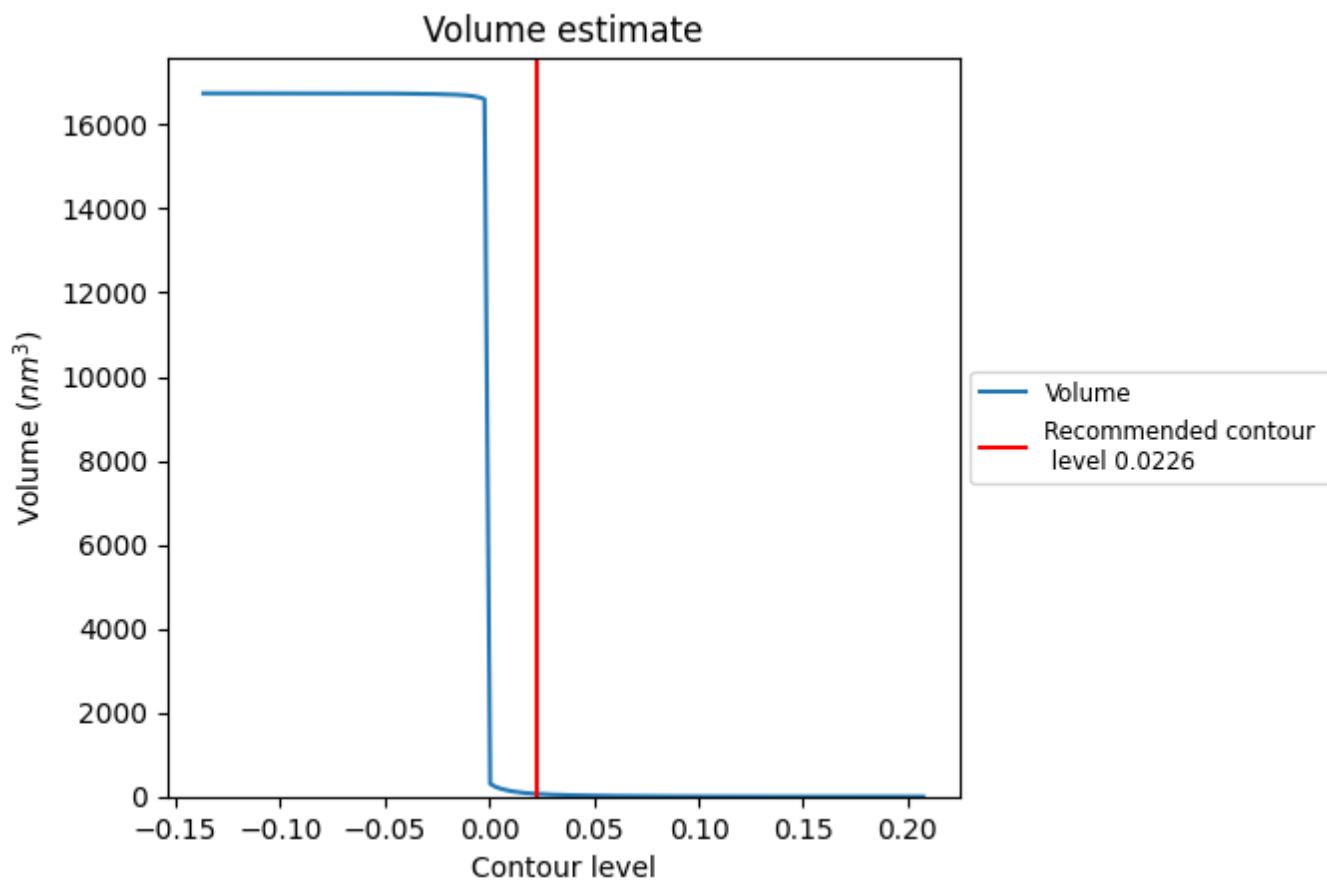
This section contains the results of statistical analysis of the map.

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.
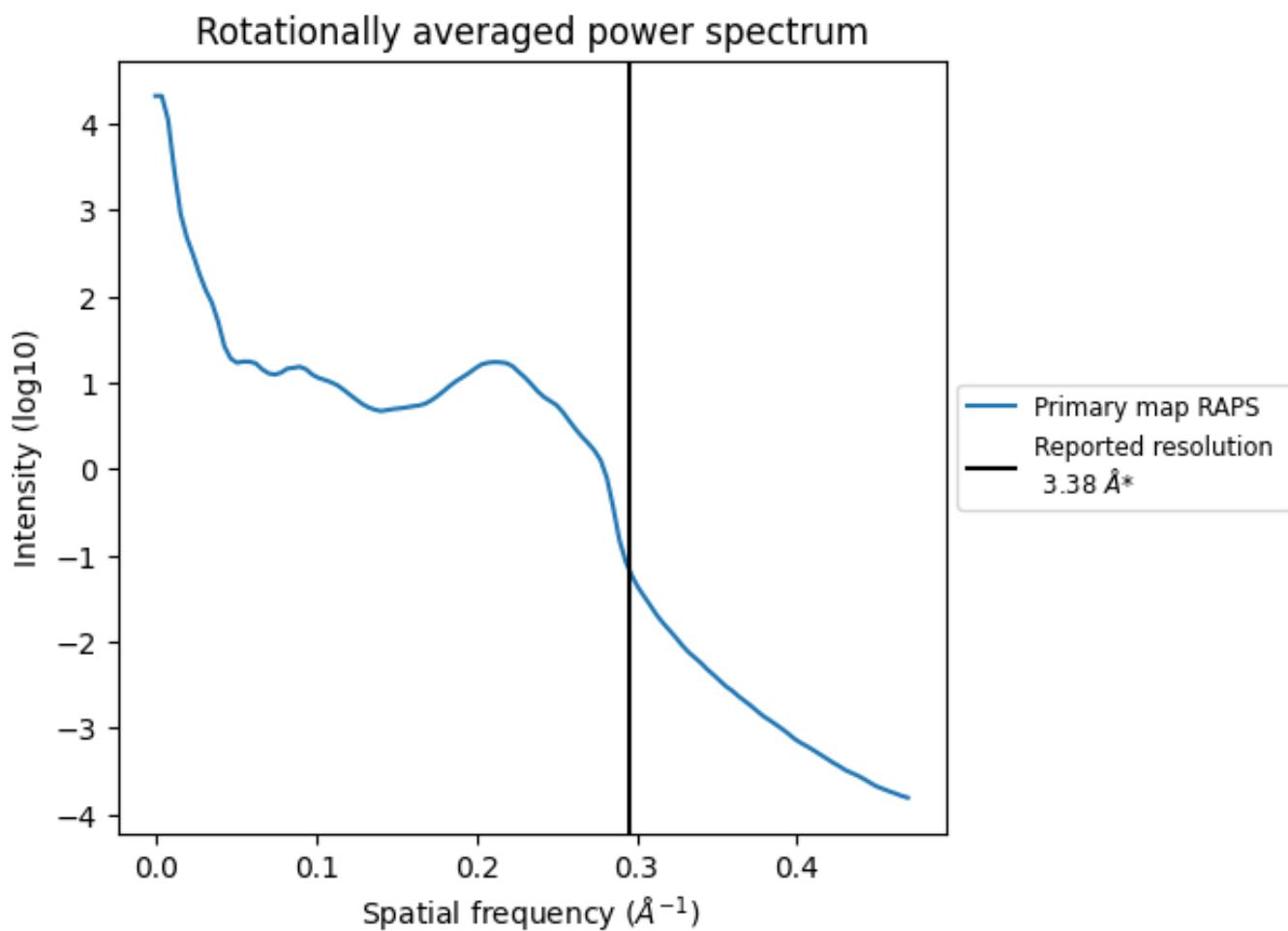
7.2   Volume estimate ⓘ

The volume at the recommended contour level is 64 nm^3; this corresponds to an approximate mass of 58 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 0.296 Å^{-1}
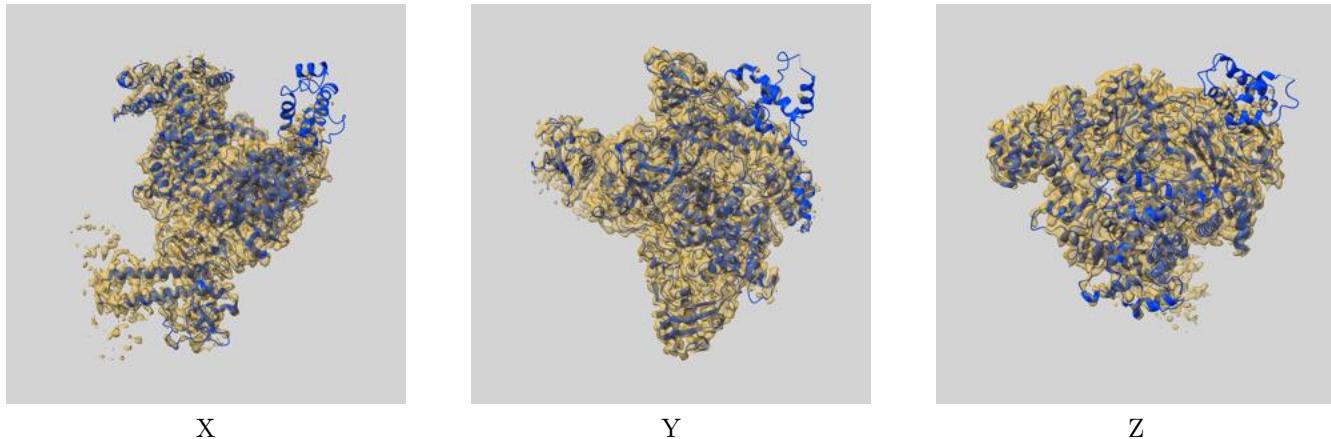
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit (i)
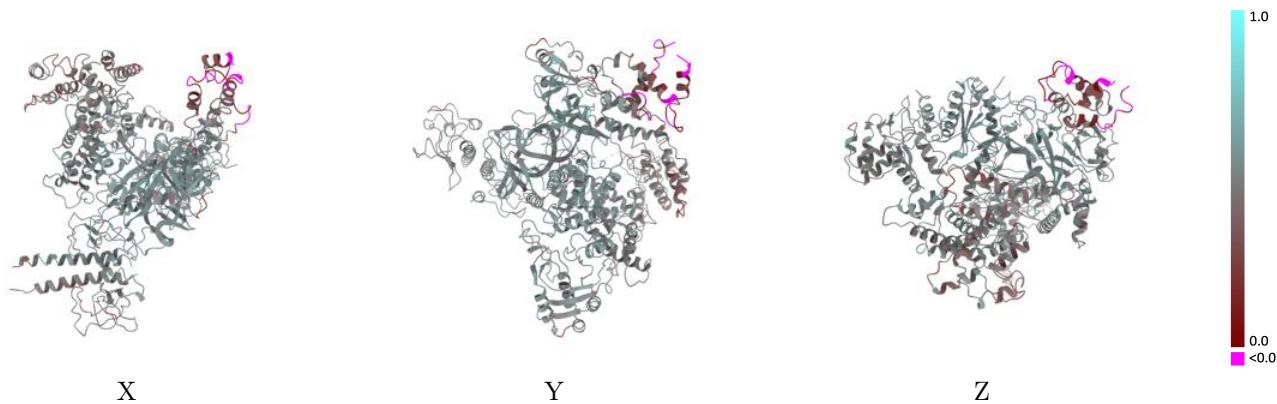
This section contains information regarding the fit between EMDB map EMD-0445 and PDB model 6NMA. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay (i)
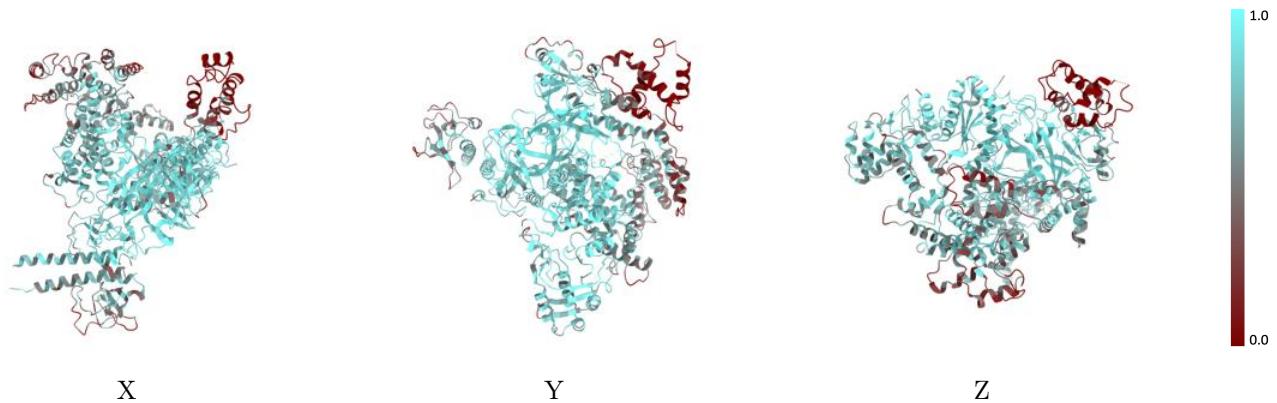
X　　　　　　　　　　Y　　　　　　　　　　Z

The images above show the 3D surface view of the map at the recommended contour level 0.0226 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 ⓘ
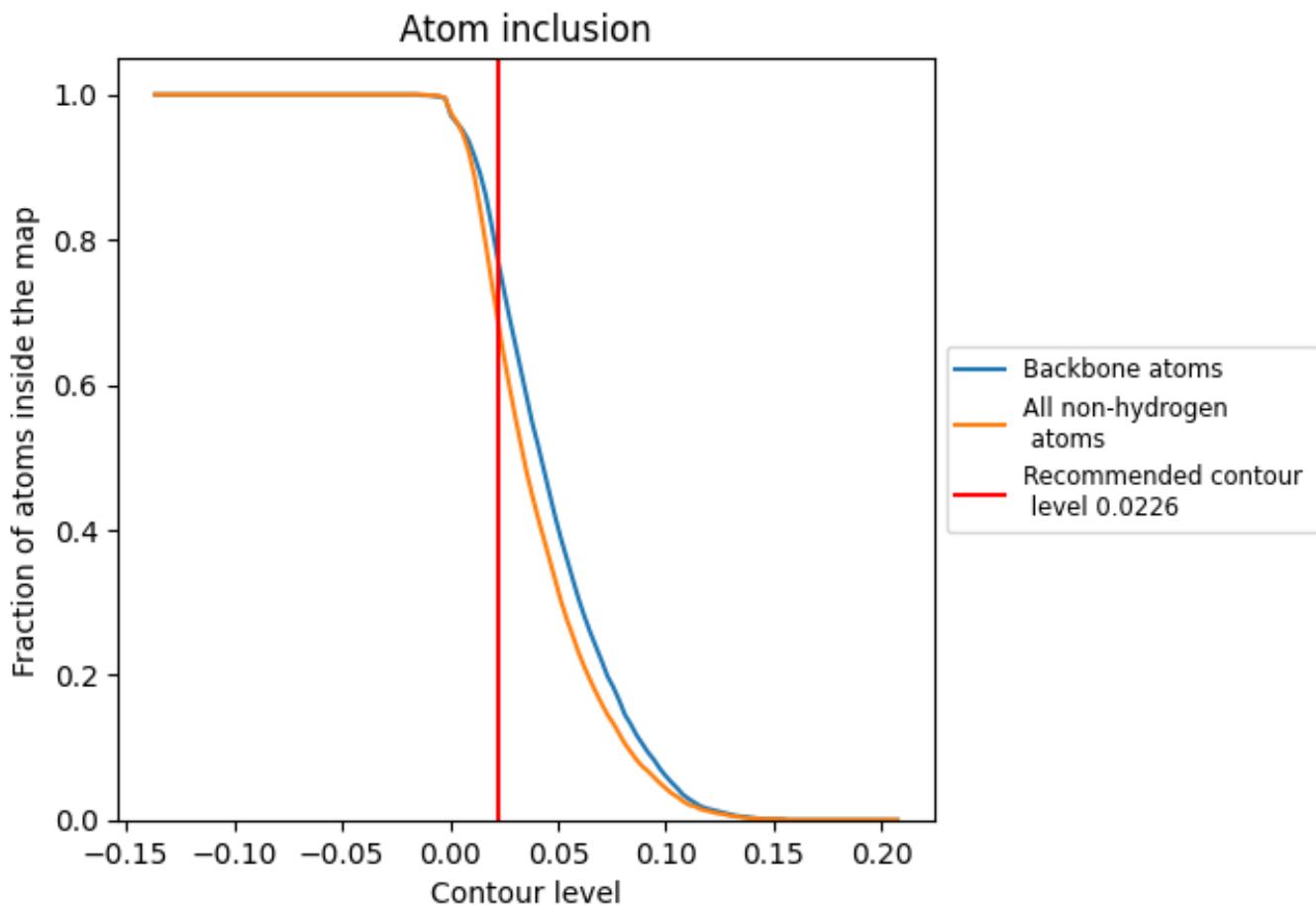
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ

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 (0.0226).

9.4　Atom inclusion ⓘ

At the recommended contour level, 77% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary   ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0226) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6810	0.4890
A	0.7950	0.5280
B	0.6710	0.4850
C	0.5310	0.4710
G	0.9100	0.5270

1.0

0.0

<0.0