Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 11:37 AM EDT

PDB ID	:	7L7K / pdb_0000717k
EMDB ID	:	EMD-23215
Title	:	Cryo-EM structure of protein encoded by vaccine candidate BNT162b2
Authors	:	Lees, J.A.; Han, S.
Deposited on	:	2020-12-28
Resolution	:	3.29 Å(reported)

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

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

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

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

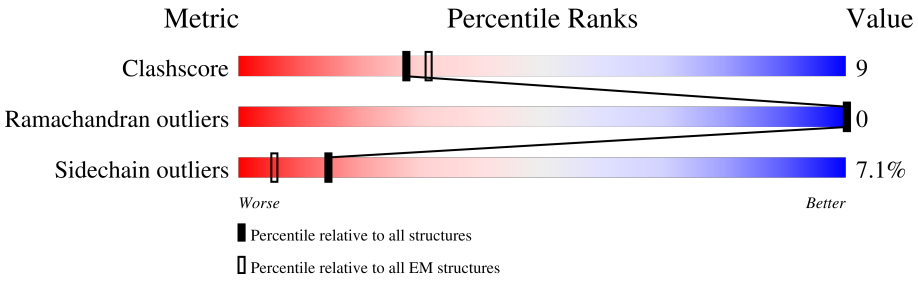
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.29 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1273	56% 19% • 24%
1	B	1273	57% 18% • 24%
1	C	1273	57% 18% • 24%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22124 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	973	Total	C	N	O	S	0	0
			7370	4708	1225	1403	34		
1	C	973	Total	C	N	O	S	0	0
			7384	4720	1225	1405	34		
1	A	973	Total	C	N	O	S	0	0
			7370	4708	1225	1403	34		

There are 6 discrepancies between the modelled and reference sequences:

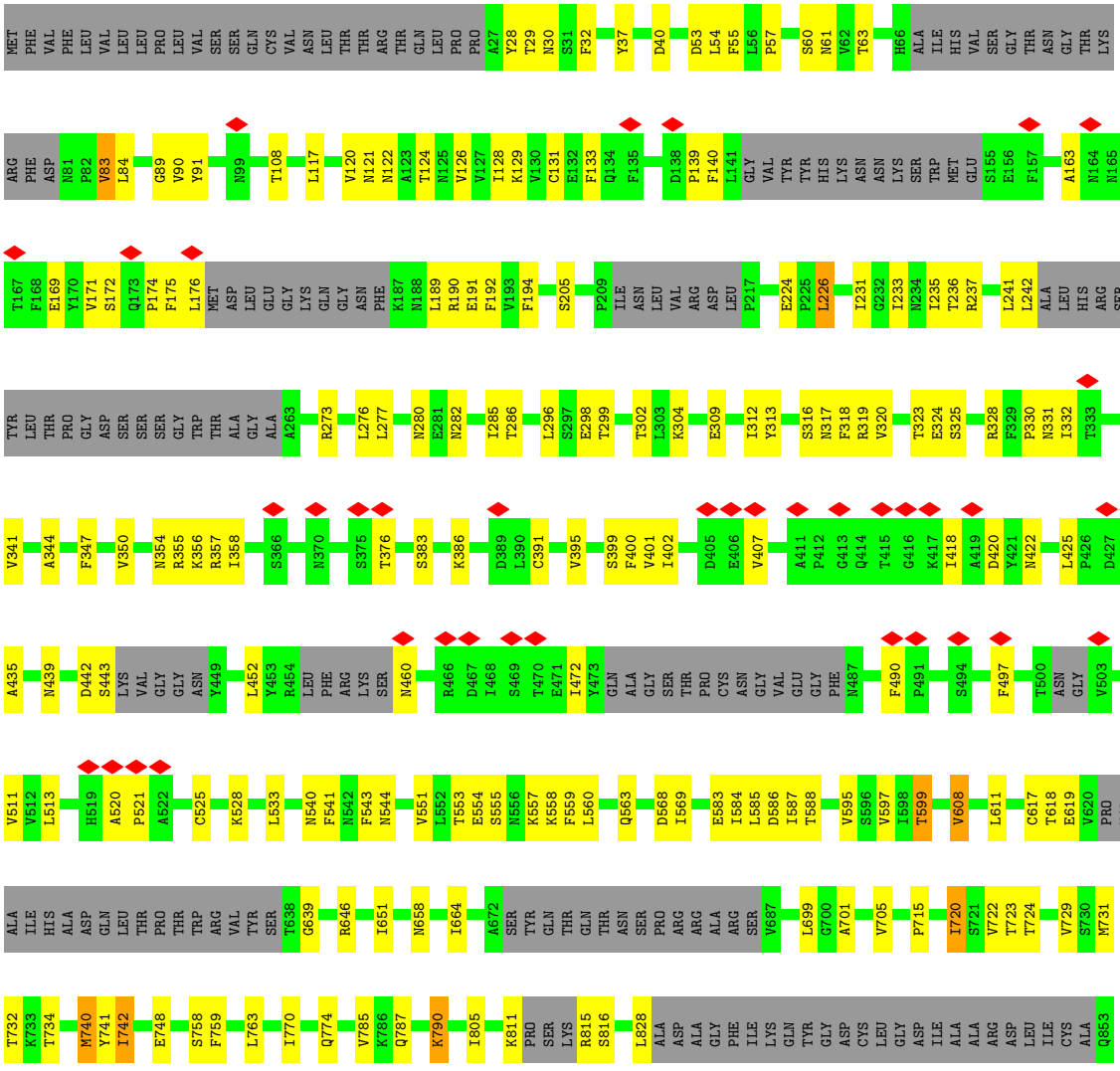
Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2

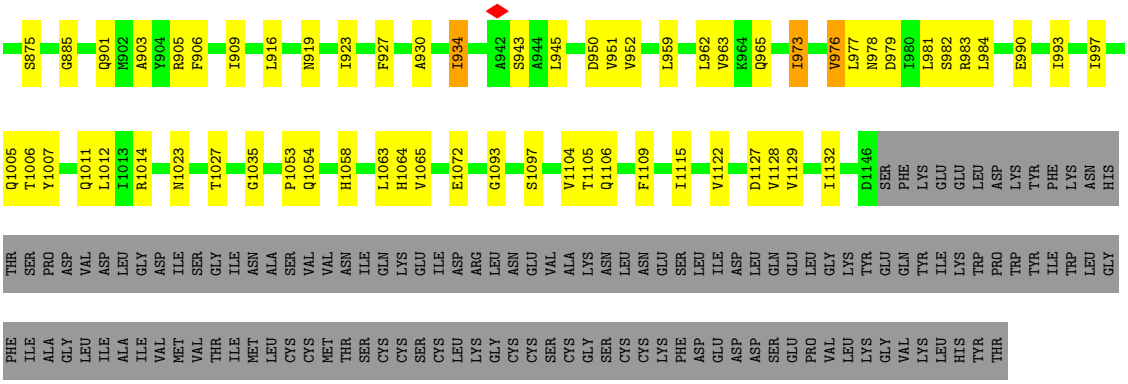
3 Residue-property plots (i)

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: Spike glycoprotein

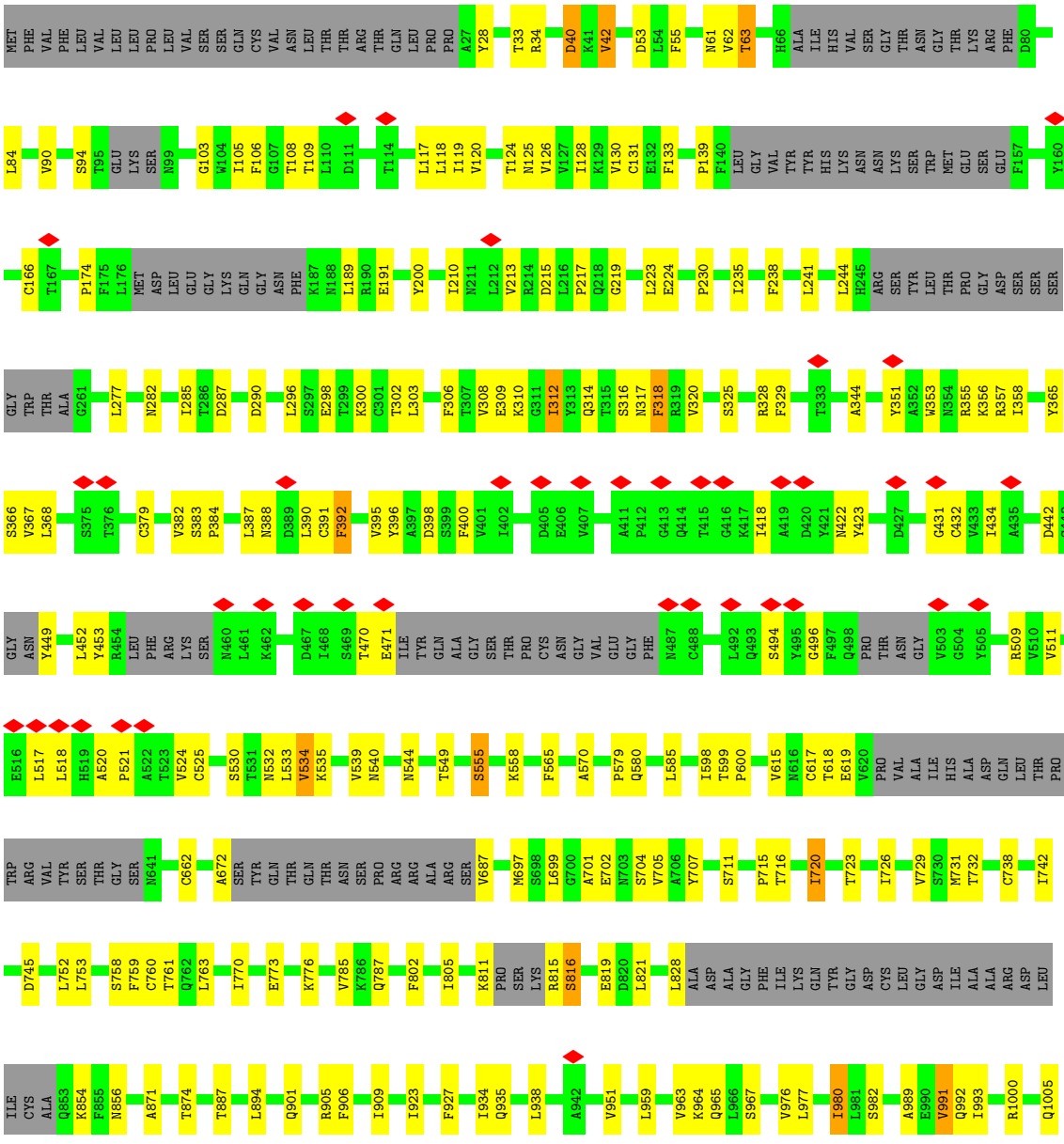
Chain B:

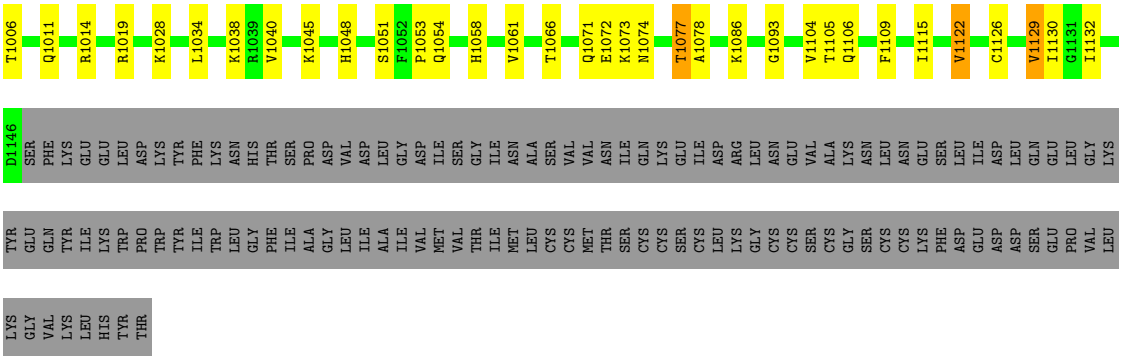




• Molecule 1: Spike glycoprotein

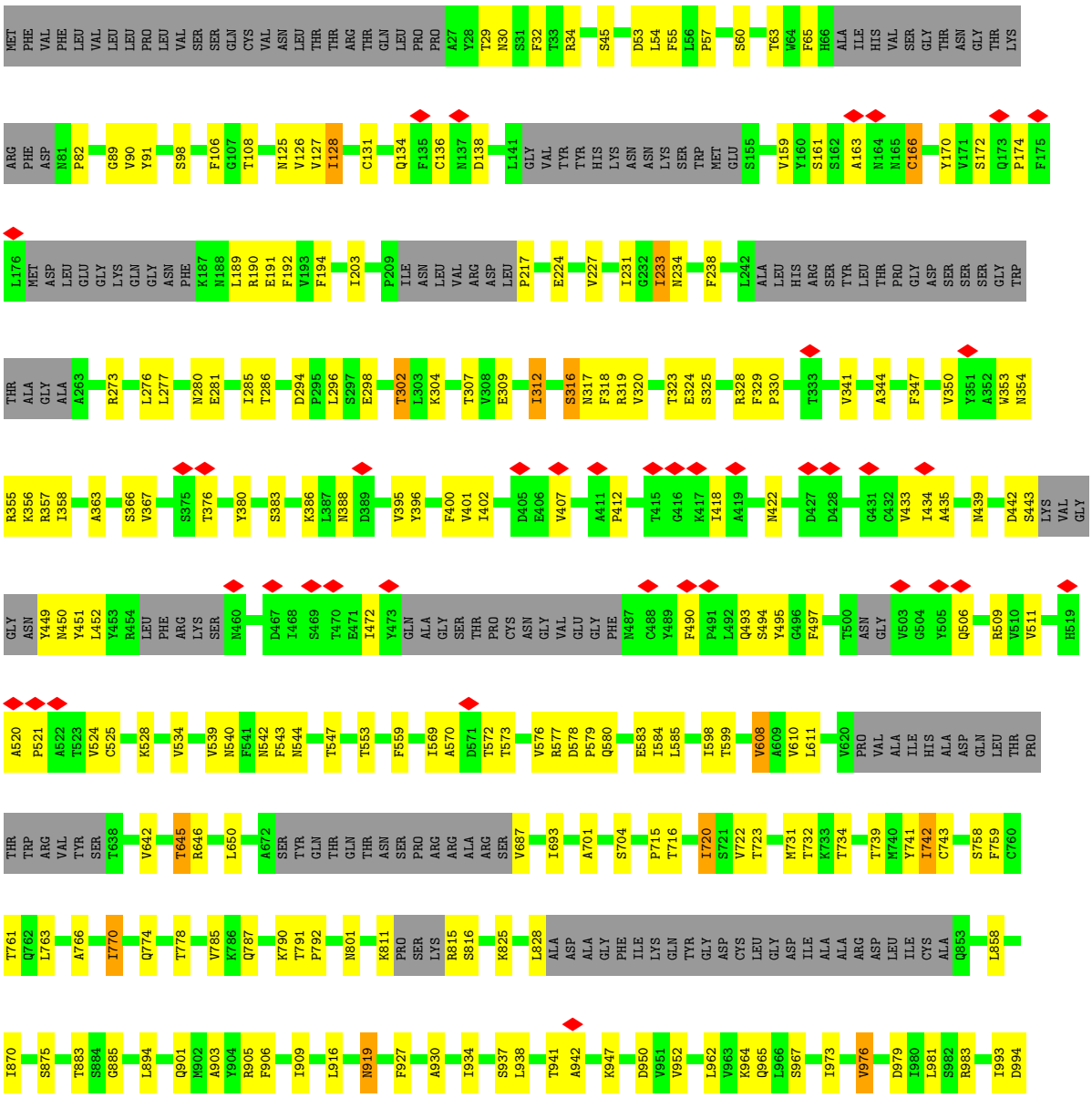
Chain C:

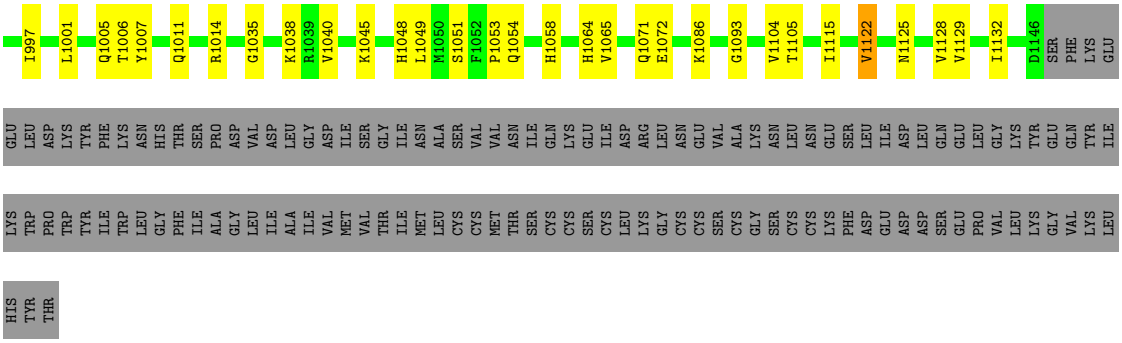




• Molecule 1: Spike glycoprotein

Chain A: 56% 19% 24%




I997 L1001 Q1005 T1006 Y1007 Q1011 R1014 G1035 K1038 R1039 V1040 K1045 H1048 L1049 M1050 S1051 F1052 P1053 Q1054 H1058 H1064 V1065 Q1071 E1072 K1086 G1093 V1104 T1105 I1115 V1122 N1125 V1128 V1129 I1132 D1146 SER PHE LYS GLU
GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN TYR ILE
LYS TRP PRO TRP TYR ILE TRP LEU GLY PHE ILE ALA GLY LEU ILE ALA ILE VAL MET VAL THR ILE MET LEU CYS CYS MET THR SER CYS CYS SER CYS LEU LYS GLY CYS CYS SER CYS GLY SER CYS CYS LYS PHE ASP GLU ASP ASP SER GLU PRO VAL LEU LYS GLY VAL LYS LEU
HIS TYR THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	58295	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 ($e^-/Å^2$)	50.22	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	0.002	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0003	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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	0.16	0/7527	0.36	0/10258
1	B	0.16	0/7527	0.37	0/10258
1	C	0.15	0/7540	0.36	0/10279
All	All	0.16	0/22594	0.36	0/30795

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	7370	0	7024	155	0
1	B	7370	0	7024	139	0
1	C	7384	0	7061	143	0
All	All	22124	0	21109	410	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 9.

All (410) 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:C:103:GLY:HA3	1:C:119:ILE:O	1.53	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.53	0.91
1:C:105:ILE:HG12	1:C:241:LEU:HD11	1.58	0.85
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.59	0.85
1:A:347:PHE:HD2	1:A:509:ARG:HD3	1.48	0.78
1:B:646:ARG:O	1:B:646:ARG:NH1	2.21	0.73
1:A:126:VAL:HG23	1:A:174:PRO:HA	1.70	0.72
1:A:646:ARG:O	1:A:646:ARG:NH1	2.22	0.71
1:A:131:CYS:HA	1:A:166:CYS:HB3	1.76	0.68
1:A:1093:GLY:HA3	1:A:1105:THR:O	1.92	0.67
1:A:277:LEU:HD23	1:A:285:ILE:HG21	1.76	0.67
1:A:442:ASP:OD1	1:A:509:ARG:NH1	2.28	0.67
1:C:384:PRO:HA	1:C:387:LEU:HD13	1.75	0.67
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.60	0.67
1:A:901:GLN:HE21	1:A:905:ARG:HH21	1.43	0.66
1:A:578:ASP:HB2	1:A:583:GLU:H	1.61	0.66
1:B:296:LEU:HD13	1:B:608:VAL:HG21	1.77	0.66
1:C:367:VAL:HG23	1:C:368:LEU:HD12	1.78	0.66
1:C:28:TYR:HA	1:C:62:VAL:O	1.95	0.65
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.59	0.65
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.29	0.65
1:A:53:ASP:OD1	1:A:54:LEU:N	2.30	0.64
1:C:344:ALA:O	1:C:509:ARG:NH1	2.30	0.64
1:B:977:LEU:HD11	1:B:993:ILE:HG12	1.80	0.64
1:C:296:LEU:HG	1:C:300:LYS:HE3	1.80	0.64
1:B:981:LEU:HD21	1:B:993:ILE:HD11	1.79	0.63
1:C:392:PHE:HD2	1:C:517:LEU:HD11	1.63	0.63
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.63	0.63
1:B:139:PRO:HG2	1:B:241:LEU:HD23	1.81	0.63
1:B:901:GLN:HE21	1:B:905:ARG:HH21	1.47	0.63
1:B:401:VAL:HG12	1:B:509:ARG:HG3	1.80	0.62
1:C:1006:THR:OG1	1:A:1005:GLN:OE1	2.17	0.62
1:C:1129:VAL:HG13	1:C:1132:ILE:HD13	1.81	0.62
1:A:134:GLN:H	1:A:161:SER:HB2	1.62	0.62
1:C:126:VAL:HG23	1:C:174:PRO:HA	1.80	0.62
1:C:1011:GLN:OE1	1:C:1014:ARG:NH1	2.33	0.62
1:A:366:SER:HB3	1:A:388:ASN:HD21	1.63	0.62
1:B:1005:GLN:OE1	1:A:1006:THR:OG1	2.18	0.62
1:C:901:GLN:HE21	1:C:905:ARG:HH21	1.46	0.62
1:A:34:ARG:NH1	1:A:217:PRO:O	2.33	0.62
1:B:790:LYS:HE3	1:A:704:SER:HB3	1.82	0.62
1:B:442:ASP:OD1	1:B:509:ARG:NH1	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:PHE:HD2	1:B:509:ARG:HD3	1.66	0.61
1:B:358:ILE:HB	1:B:395:VAL:HB	1.82	0.61
1:B:978:ASN:OD1	1:A:547:THR:OG1	2.19	0.61
1:A:316:SER:OG	1:A:317:ASN:N	2.33	0.61
1:A:341:VAL:HG22	1:A:356:LYS:HZ2	1.65	0.61
1:B:420:ASP:O	1:B:460:ASN:N	2.34	0.61
1:C:328:ARG:HH11	1:C:530:SER:HB3	1.66	0.61
1:A:280:ASN:ND2	1:A:286:THR:OG1	2.34	0.61
1:C:701:ALA:HB3	1:A:787:GLN:HG3	1.81	0.61
1:A:131:CYS:HB3	1:A:163:ALA:HA	1.82	0.61
1:A:402:ILE:HD11	1:A:407:VAL:HA	1.82	0.61
1:C:119:ILE:HG13	1:C:128:ILE:HD12	1.83	0.60
1:B:57:PRO:HG3	1:B:273:ARG:HD2	1.83	0.60
1:C:434:ILE:HB	1:C:511:VAL:HG23	1.83	0.60
1:B:1006:THR:OG1	1:C:1005:GLN:OE1	2.18	0.60
1:B:108:THR:HG23	1:B:236:THR:HB	1.83	0.60
1:B:1011:GLN:OE1	1:B:1014:ARG:NH1	2.35	0.60
1:C:358:ILE:HB	1:C:395:VAL:HB	1.84	0.60
1:C:131:CYS:HA	1:C:166:CYS:HB3	1.84	0.59
1:A:363:ALA:N	1:A:525:CYS:O	2.34	0.59
1:A:434:ILE:HB	1:A:511:VAL:HG23	1.83	0.59
1:B:280:ASN:ND2	1:B:286:THR:OG1	2.35	0.59
1:A:296:LEU:HD13	1:A:608:VAL:HG21	1.84	0.59
1:C:672:ALA:O	1:C:687:VAL:N	2.36	0.59
1:C:977:LEU:HD11	1:C:993:ILE:HG12	1.85	0.59
1:A:358:ILE:HB	1:A:395:VAL:HB	1.83	0.59
1:B:722:VAL:HG22	1:B:930:ALA:HB1	1.85	0.59
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.85	0.58
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.36	0.58
1:A:1104:VAL:HG23	1:A:1115:ILE:HG12	1.84	0.58
1:C:540:ASN:HB3	1:C:549:THR:HG22	1.85	0.58
1:C:244:LEU:HD23	1:C:244:LEU:H	1.69	0.58
1:A:1129:VAL:HB	1:A:1132:ILE:HD11	1.84	0.57
1:B:126:VAL:HB	1:B:174:PRO:HB3	1.86	0.57
1:B:787:GLN:HG3	1:A:701:ALA:HB3	1.86	0.57
1:C:442:ASP:OD2	1:C:509:ARG:NE	2.30	0.57
1:B:701:ALA:HB3	1:C:787:GLN:HG2	1.86	0.57
1:A:298:GLU:O	1:A:302:THR:OG1	2.23	0.57
1:B:402:ILE:HD11	1:B:407:VAL:HA	1.86	0.57
1:B:316:SER:OG	1:B:317:ASN:N	2.35	0.56
1:B:233:ILE:HG22	1:B:235:ILE:HG13	1.85	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:LEU:HD21	1:A:983:ARG:HB2	1.86	0.56
1:B:341:VAL:HG13	1:B:356:LYS:HD2	1.86	0.56
1:A:731:MET:HG3	1:A:774:GLN:HG3	1.87	0.56
1:B:319:ARG:NH2	1:C:745:ASP:OD1	2.39	0.56
1:A:347:PHE:CD2	1:A:509:ARG:HD3	2.36	0.56
1:B:328:ARG:HH21	1:B:533:LEU:HB2	1.71	0.56
1:B:560:LEU:H	1:B:563:GLN:HG3	1.70	0.56
1:A:325:SER:HA	1:A:540:ASN:O	2.05	0.56
1:A:543:PHE:CZ	1:A:579:PRO:HD3	2.41	0.56
1:C:760:CYS:SG	1:C:761:THR:N	2.79	0.56
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.88	0.55
1:C:618:THR:OG1	1:C:619:GLU:OE1	2.24	0.55
1:A:57:PRO:HG3	1:A:273:ARG:HD2	1.87	0.55
1:B:741:TYR:HD2	1:B:742:ILE:HG22	1.72	0.55
1:A:449:TYR:O	1:A:494:SER:OG	2.25	0.55
1:A:828:LEU:H	1:A:828:LEU:HD12	1.72	0.55
1:C:1093:GLY:HA3	1:C:1105:THR:O	2.06	0.55
1:B:722:VAL:HG12	1:B:1065:VAL:HG22	1.87	0.55
1:A:439:ASN:HA	1:A:442:ASP:HB2	1.87	0.55
1:B:1093:GLY:HA3	1:B:1105:THR:O	2.07	0.54
1:B:731:MET:HG3	1:B:774:GLN:HG3	1.89	0.54
1:A:534:VAL:HG21	1:A:539:VAL:HG11	1.88	0.54
1:C:329:PHE:O	1:C:580:GLN:NE2	2.32	0.54
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.26	0.54
1:B:108:THR:O	1:B:237:ARG:NH1	2.38	0.54
1:A:108:THR:OG1	1:A:234:ASN:O	2.26	0.54
1:A:323:THR:OG1	1:A:324:GLU:N	2.41	0.54
1:A:722:VAL:HG12	1:A:1065:VAL:HG22	1.90	0.54
1:B:347:PHE:CD2	1:B:509:ARG:HD3	2.42	0.54
1:C:887:THR:HG21	1:C:894:LEU:HG	1.89	0.54
1:B:758:SER:H	1:A:965:GLN:HE22	1.56	0.54
1:C:210:ILE:HG21	1:C:217:PRO:HG3	1.90	0.54
1:B:277:LEU:HD23	1:B:285:ILE:HG21	1.89	0.53
1:B:740:MET:HG3	1:A:319:ARG:HH22	1.73	0.53
1:A:309:GLU:OE2	1:A:309:GLU:N	2.41	0.53
1:B:472:ILE:HA	1:B:490:PHE:HA	1.90	0.53
1:B:553:THR:HG22	1:B:554:GLU:H	1.74	0.53
1:C:34:ARG:NE	1:C:191:GLU:OE1	2.41	0.53
1:C:312:ILE:HD12	1:C:598:ILE:HG12	1.89	0.53
1:C:707:TYR:HB2	1:A:883:THR:HG23	1.90	0.53
1:A:559:PHE:HB2	1:A:577:ARG:HH21	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:TYR:HD2	1:C:387:LEU:HB3	1.74	0.53
1:A:45:SER:HB3	1:A:281:GLU:HA	1.91	0.53
1:A:125:ASN:OD1	1:A:125:ASN:N	2.42	0.53
1:B:205:SER:HB3	1:B:226:LEU:HD13	1.89	0.52
1:B:89:GLY:HA2	1:B:194:PHE:O	2.10	0.52
1:B:828:LEU:HD12	1:B:828:LEU:H	1.73	0.52
1:A:443:SER:HA	1:A:497:PHE:HB2	1.91	0.52
1:B:174:PRO:HG2	1:B:176:LEU:HG	1.90	0.52
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.91	0.52
1:C:773:GLU:OE2	1:C:1019:ARG:NH1	2.43	0.52
1:B:175:PHE:O	1:B:190:ARG:NH2	2.43	0.51
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.91	0.51
1:A:578:ASP:N	1:A:583:GLU:O	2.41	0.51
1:C:366:SER:OG	1:C:388:ASN:ND2	2.41	0.51
1:B:298:GLU:O	1:B:302:THR:OG1	2.26	0.51
1:B:965:GLN:HE22	1:C:758:SER:H	1.56	0.51
1:A:231:ILE:HG22	1:A:233:ILE:HG12	1.91	0.51
1:A:741:TYR:HD2	1:A:742:ILE:HG22	1.76	0.51
1:C:351:TYR:HB3	1:C:453:TYR:HA	1.91	0.51
1:B:53:ASP:OD2	1:B:54:LEU:N	2.44	0.51
1:B:618:THR:OG1	1:B:619:GLU:OE2	2.20	0.51
1:C:139:PRO:HB3	1:C:241:LEU:HD23	1.91	0.51
1:B:29:THR:HG22	1:B:30:ASN:H	1.75	0.51
1:B:331:ASN:OD1	1:B:332:ILE:N	2.44	0.51
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.93	0.51
1:C:533:LEU:HD13	1:C:535:LYS:HZ3	1.76	0.50
1:B:323:THR:C	1:B:324:GLU:HG3	2.36	0.50
1:C:316:SER:OG	1:C:317:ASN:N	2.42	0.50
1:C:742:ILE:HG21	1:C:753:LEU:HD13	1.94	0.50
1:A:190:ARG:HB3	1:A:192:PHE:HE2	1.76	0.50
1:C:131:CYS:HB2	1:C:133:PHE:CE1	2.47	0.50
1:C:353:TRP:HB3	1:C:400:PHE:HB3	1.94	0.50
1:B:599:THR:HB	1:B:608:VAL:HG22	1.94	0.50
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.94	0.49
1:B:885:GLY:HA2	1:B:901:GLN:NE2	2.26	0.49
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.47	0.49
1:C:517:LEU:HB3	1:C:518:LEU:HD23	1.93	0.49
1:C:418:ILE:HG23	1:C:422:ASN:HB2	1.94	0.49
1:B:325:SER:HA	1:B:540:ASN:O	2.13	0.49
1:C:828:LEU:HD12	1:C:828:LEU:H	1.77	0.49
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:THR:HG22	1:B:597:VAL:HG21	1.94	0.49
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.94	0.49
1:C:353:TRP:NE1	1:C:422:ASN:O	2.42	0.49
1:C:555:SER:O	1:C:555:SER:OG	2.30	0.49
1:A:741:TYR:CD2	1:A:742:ILE:HG22	2.48	0.49
1:C:532:ASN:OD1	1:C:532:ASN:N	2.46	0.49
1:A:29:THR:HG22	1:A:30:ASN:H	1.77	0.49
1:A:312:ILE:HD12	1:A:598:ILE:HG12	1.95	0.49
1:C:40:ASP:HB3	1:C:42:VAL:HG13	1.95	0.48
1:B:439:ASN:HA	1:B:442:ASP:HB2	1.95	0.48
1:C:33:THR:OG1	1:C:219:GLY:O	2.17	0.48
1:C:398:ASP:O	1:C:511:VAL:HA	2.13	0.48
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.46	0.48
1:B:555:SER:HB2	1:B:557:LYS:HG2	1.94	0.48
1:A:350:VAL:HG22	1:A:402:ILE:HG22	1.94	0.48
1:B:166:CYS:HB2	1:B:169:GLU:OE2	2.14	0.48
1:A:128:ILE:HG23	1:A:170:TYR:HB3	1.96	0.48
1:A:328:ARG:NH2	1:A:578:ASP:OD2	2.46	0.48
1:B:122:ASN:C	1:B:124:THR:H	2.22	0.48
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.95	0.48
1:C:452:LEU:HA	1:C:494:SER:HA	1.95	0.48
1:C:821:LEU:HD23	1:C:938:LEU:HB3	1.96	0.48
1:A:203:ILE:HB	1:A:227:VAL:HG22	1.95	0.48
1:A:366:SER:HB3	1:A:388:ASN:ND2	2.29	0.48
1:B:959:LEU:O	1:B:963:VAL:HG23	2.14	0.48
1:C:325:SER:HB3	1:C:540:ASN:ND2	2.28	0.48
1:C:871:ALA:HA	1:C:874:THR:HG22	1.95	0.48
1:A:981:LEU:HD21	1:A:993:ILE:HD11	1.96	0.48
1:A:277:LEU:HD23	1:A:285:ILE:HD13	1.96	0.47
1:A:687:VAL:N	1:A:693:ILE:H	2.12	0.47
1:A:716:THR:OG1	1:A:1071:GLN:O	2.27	0.47
1:A:1093:GLY:CA	1:A:1105:THR:O	2.59	0.47
1:B:309:GLU:N	1:B:309:GLU:OE1	2.46	0.47
1:C:738:CYS:HB3	1:C:760:CYS:HB2	1.95	0.47
1:A:330:PRO:HD3	1:A:544:ASN:ND2	2.29	0.47
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.42	0.47
1:A:170:TYR:CE1	1:A:172:SER:HB2	2.50	0.47
1:B:354:ASN:OD1	1:B:355:ARG:N	2.47	0.47
1:B:741:TYR:CD2	1:B:742:ILE:HG22	2.49	0.47
1:C:224:GLU:N	1:C:224:GLU:OE1	2.44	0.47
1:C:619:GLU:OE1	1:C:619:GLU:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:TYR:HB3	1:A:792:PRO:HG3	1.96	0.47
1:A:276:LEU:HD11	1:A:304:LYS:HA	1.97	0.47
1:C:379:CYS:HA	1:C:432:CYS:HA	1.97	0.47
1:C:534:VAL:HG21	1:C:539:VAL:HG21	1.96	0.47
1:B:1035:GLY:HA3	1:A:1040:VAL:HG21	1.96	0.47
1:A:1086:LYS:HD2	1:A:1122:VAL:HG21	1.95	0.47
1:A:885:GLY:HA2	1:A:901:GLN:NE2	2.29	0.47
1:C:53:ASP:HB2	1:C:55:PHE:CE2	2.50	0.47
1:A:354:ASN:OD1	1:A:355:ARG:N	2.48	0.47
1:B:299:THR:CG2	1:B:597:VAL:HG21	2.45	0.46
1:C:418:ILE:HD13	1:C:422:ASN:ND2	2.30	0.46
1:A:720:ILE:HD11	1:A:927:PHE:HB2	1.96	0.46
1:B:559:PHE:HB3	1:B:563:GLN:HB2	1.97	0.46
1:B:934:ILE:HD13	1:B:1063:LEU:HD22	1.97	0.46
1:C:705:VAL:HB	1:A:883:THR:HG21	1.96	0.46
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.97	0.46
1:B:740:MET:HG3	1:A:319:ARG:NH2	2.31	0.46
1:B:83:VAL:O	1:B:84:LEU:HD13	2.15	0.46
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.79	0.46
1:B:140:PHE:HA	1:B:242:LEU:C	2.41	0.46
1:C:716:THR:OG1	1:C:1071:GLN:O	2.25	0.46
1:B:330:PRO:HD3	1:B:544:ASN:ND2	2.31	0.46
1:C:277:LEU:HD22	1:C:285:ILE:HD13	1.97	0.46
1:C:811:LYS:O	1:C:815:ARG:N	2.49	0.46
1:A:383:SER:HB3	1:A:386:LYS:HD2	1.98	0.46
1:B:224:GLU:OE1	1:B:224:GLU:N	2.46	0.46
1:C:309:GLU:OE1	1:C:309:GLU:N	2.47	0.46
1:A:811:LYS:HD2	1:A:815:ARG:HB2	1.98	0.46
1:C:379:CYS:HB3	1:C:431:GLY:O	2.16	0.45
1:C:470:THR:OG1	1:C:471:GLU:N	2.50	0.45
1:C:959:LEU:O	1:C:963:VAL:HG23	2.17	0.45
1:A:542:ASN:HA	1:A:547:THR:HG22	1.99	0.45
1:C:449:TYR:HA	1:C:496:GLY:HA2	1.98	0.45
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.33	0.45
1:A:329:PHE:O	1:A:580:GLN:NE2	2.31	0.45
1:C:106:PHE:HD1	1:C:238:PHE:HB2	1.81	0.45
1:C:704:SER:HB3	1:A:790:LYS:HE3	1.98	0.45
1:A:739:THR:O	1:A:743:CYS:HB2	2.17	0.45
1:A:451:TYR:HB2	1:A:495:TYR:HB2	1.98	0.45
1:A:472:ILE:HA	1:A:490:PHE:HA	1.98	0.45
1:B:131:CYS:HB2	1:B:133:PHE:CZ	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:TYR:CD2	1:C:387:LEU:HB3	2.52	0.45
1:C:356:LYS:HE3	1:C:356:LYS:HB2	1.85	0.45
1:C:991:VAL:HG22	1:C:992:GLN:HE21	1.82	0.45
1:B:583:GLU:OE1	1:B:584:ILE:N	2.47	0.44
1:C:200:TYR:HA	1:C:230:PRO:HA	1.99	0.44
1:A:376:THR:OG1	1:A:435:ALA:HB3	2.17	0.44
1:A:400:PHE:HD1	1:A:402:ILE:HG23	1.82	0.44
1:C:418:ILE:HD13	1:C:422:ASN:HD22	1.82	0.44
1:A:350:VAL:HG12	1:A:422:ASN:HB3	2.00	0.44
1:C:965:GLN:HE22	1:A:758:SER:H	1.64	0.44
1:C:1073:LYS:HB3	1:C:1073:LYS:HE2	1.72	0.44
1:C:1093:GLY:CA	1:C:1105:THR:O	2.66	0.44
1:B:126:VAL:O	1:B:171:VAL:HA	2.18	0.44
1:B:383:SER:HB3	1:B:386:LYS:HD2	1.99	0.44
1:B:431:GLY:N	1:B:513:LEU:O	2.50	0.44
1:C:117:LEU:HD12	1:C:130:VAL:HG12	2.00	0.44
1:A:722:VAL:HA	1:A:1064:HIS:O	2.18	0.44
1:B:586:ASP:OD1	1:B:587:ILE:N	2.50	0.44
1:C:759:PHE:O	1:C:763:LEU:HG	2.18	0.44
1:A:825:LYS:NZ	1:A:942:ALA:HA	2.33	0.44
1:A:1005:GLN:HE21	1:A:1005:GLN:HB2	1.56	0.44
1:B:276:LEU:HD11	1:B:304:LYS:HA	2.00	0.44
1:B:350:VAL:HG12	1:B:422:ASN:HB3	2.00	0.44
1:B:386:LYS:HD3	1:C:982:SER:O	2.18	0.44
1:A:766:ALA:O	1:A:770:ILE:HG23	2.17	0.44
1:A:825:LYS:NZ	1:A:941:THR:O	2.33	0.44
1:B:1005:GLN:HE21	1:B:1005:GLN:HB2	1.56	0.43
1:C:108:THR:HG23	1:C:109:THR:H	1.82	0.43
1:C:570:ALA:HB2	1:A:964:LYS:HA	1.99	0.43
1:A:57:PRO:O	1:A:60:SER:HB2	2.18	0.43
1:B:344:ALA:HB3	1:B:347:PHE:CZ	2.53	0.43
1:C:287:ASP:HB3	1:C:306:PHE:CE2	2.53	0.43
1:C:815:ARG:HG2	1:C:819:GLU:HB2	2.00	0.43
1:A:543:PHE:CE1	1:A:579:PRO:HD3	2.52	0.43
1:C:357:ARG:HG3	1:C:396:TYR:HE2	1.84	0.43
1:A:344:ALA:HB3	1:A:347:PHE:CZ	2.53	0.43
1:A:901:GLN:NE2	1:A:905:ARG:HH21	2.14	0.43
1:A:1045:LYS:HA	1:A:1045:LYS:HD3	1.86	0.43
1:B:277:LEU:HD22	1:B:285:ILE:HD13	1.99	0.43
1:B:976:VAL:HG13	1:B:979:ASP:HB3	1.99	0.43
1:B:982:SER:O	1:A:386:LYS:HD3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HH21	1:A:579:PRO:HD2	1.83	0.43
1:C:1040:VAL:HG21	1:A:1035:GLY:HA3	1.99	0.43
1:C:1086:LYS:HD2	1:C:1122:VAL:HG21	1.99	0.43
1:A:964:LYS:HE3	1:A:964:LYS:HB2	1.89	0.43
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.83	0.43
1:A:136:CYS:HB3	1:A:159:VAL:HA	2.01	0.43
1:B:37:TYR:OH	1:B:53:ASP:OD2	2.36	0.43
1:B:568:ASP:O	1:B:569:ILE:HG13	2.19	0.43
1:B:984:LEU:O	1:A:386:LYS:NZ	2.37	0.43
1:A:570:ALA:O	1:A:572:THR:HG23	2.19	0.43
1:B:117:LEU:HA	1:B:129:LYS:O	2.19	0.43
1:A:53:ASP:HB3	1:A:55:PHE:HE2	1.84	0.43
1:B:1129:VAL:HB	1:B:1132:ILE:HG13	2.00	0.43
1:A:323:THR:O	1:A:324:GLU:HG2	2.18	0.43
1:B:943:SER:O	1:B:943:SER:OG	2.36	0.42
1:A:65:PHE:CD2	1:A:82:PRO:HB3	2.54	0.42
1:B:30:ASN:HB3	1:B:32:PHE:CE1	2.54	0.42
1:B:57:PRO:O	1:B:60:SER:HB2	2.19	0.42
1:B:376:THR:OG1	1:B:435:ALA:HB3	2.19	0.42
1:B:973:ILE:HD11	1:B:983:ARG:NH2	2.34	0.42
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	2.01	0.42
1:A:962:LEU:HD13	1:A:1007:TYR:HB2	2.01	0.42
1:B:309:GLU:O	1:B:313:TYR:OH	2.31	0.42
1:B:231:ILE:HG22	1:B:233:ILE:HG13	2.01	0.42
1:B:399:SER:HB3	1:B:511:VAL:HG12	2.01	0.42
1:B:720:ILE:HD11	1:B:927:PHE:HB2	2.02	0.42
1:A:903:ALA:HB2	1:A:916:LEU:HD23	2.01	0.42
1:B:722:VAL:HA	1:B:1064:HIS:O	2.19	0.42
1:B:1093:GLY:CA	1:B:1105:THR:O	2.68	0.42
1:C:964:LYS:HE2	1:C:964:LYS:HB2	1.76	0.42
1:C:1077:THR:HG22	1:C:1078:ALA:H	1.84	0.42
1:A:439:ASN:ND2	1:A:506:GLN:HE21	2.16	0.42
1:A:906:PHE:O	1:A:909:ILE:HG12	2.20	0.42
1:C:303:LEU:HD12	1:C:308:VAL:HG12	2.02	0.42
1:C:318:PHE:CE1	1:C:615:VAL:HG21	2.55	0.42
1:C:662:CYS:HB2	1:C:697:MET:SD	2.60	0.42
1:B:962:LEU:HD13	1:B:1007:TYR:HB2	2.02	0.42
1:B:945:LEU:HD23	1:B:945:LEU:HA	1.85	0.42
1:A:353:TRP:HB3	1:A:400:PHE:HB3	2.01	0.42
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.82	0.42
1:B:759:PHE:O	1:B:763:LEU:HG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:HA2	1:A:194:PHE:O	2.20	0.42
1:A:106:PHE:HA	1:A:238:PHE:HA	2.01	0.42
1:A:1125:ASN:OD1	1:A:1125:ASN:N	2.49	0.42
1:B:83:VAL:HG22	1:B:237:ARG:HB3	2.00	0.42
1:B:553:THR:HG22	1:B:554:GLU:N	2.35	0.42
1:C:854:LYS:HE3	1:C:854:LYS:HB3	1.94	0.42
1:B:906:PHE:O	1:B:909:ILE:HG12	2.20	0.41
1:C:353:TRP:HZ3	1:C:355:ARG:HD2	1.85	0.41
1:C:520:ALA:HB1	1:C:521:PRO:HD2	2.02	0.41
1:C:906:PHE:O	1:C:909:ILE:HG12	2.20	0.41
1:C:1048:HIS:HE2	1:C:1051:SER:HG	1.64	0.41
1:A:610:VAL:O	1:A:650:LEU:HD12	2.20	0.41
1:C:901:GLN:NE2	1:C:905:ARG:HH21	2.16	0.41
1:A:380:TYR:HE2	1:A:412:PRO:HD2	1.85	0.41
1:A:947:LYS:HB3	1:A:947:LYS:HE2	1.85	0.41
1:A:976:VAL:HG13	1:A:979:ASP:HB3	2.02	0.41
1:A:981:LEU:HD23	1:A:981:LEU:HA	1.84	0.41
1:B:357:ARG:HB3	1:B:357:ARG:HH11	1.85	0.41
1:B:811:LYS:HD2	1:B:815:ARG:HB2	2.02	0.41
1:C:418:ILE:HG22	1:C:423:TYR:O	2.20	0.41
1:A:138:ASP:N	1:A:138:ASP:OD1	2.51	0.41
1:A:190:ARG:HB3	1:A:192:PHE:CE2	2.54	0.41
1:C:106:PHE:HB3	1:C:235:ILE:HD13	2.02	0.41
1:B:28:TYR:HD2	1:B:61:ASN:HD22	1.69	0.41
1:B:443:SER:HA	1:B:497:PHE:HB2	2.02	0.41
1:B:520:ALA:HB1	1:B:521:PRO:HD2	2.03	0.41
1:C:53:ASP:HB2	1:C:55:PHE:HE2	1.84	0.41
1:C:124:THR:O	1:C:125:ASN:ND2	2.53	0.41
1:C:816:SER:OG	1:C:819:GLU:HG3	2.21	0.41
1:C:1126:CYS:O	1:C:1132:ILE:HD11	2.20	0.41
1:A:34:ARG:HH12	1:A:217:PRO:HG2	1.85	0.41
1:A:905:ARG:HD3	1:A:1049:LEU:O	2.21	0.41
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.54	0.41
1:C:357:ARG:HG3	1:C:396:TYR:CE2	2.56	0.41
1:C:715:PRO:HD3	1:A:894:LEU:HD13	2.03	0.41
1:C:856:ASN:OD1	1:C:856:ASN:N	2.53	0.41
1:C:938:LEU:HD23	1:C:938:LEU:HA	1.82	0.41
1:C:980:ILE:HD11	1:C:989:ALA:HA	2.03	0.41
1:A:233:ILE:HD13	1:A:233:ILE:HA	1.83	0.41
1:A:357:ARG:HG3	1:A:396:TYR:HE1	1.86	0.41
1:A:759:PHE:O	1:A:763:LEU:HG	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.85	0.41
1:C:702:GLU:OE2	1:A:790:LYS:HG3	2.20	0.41
1:C:720:ILE:HD11	1:C:927:PHE:HB2	2.02	0.41
1:A:645:THR:OG1	1:A:646:ARG:N	2.54	0.41
1:B:400:PHE:HD1	1:B:402:ILE:HG23	1.85	0.41
1:C:720:ILE:HG21	1:C:923:ILE:HG23	2.02	0.41
1:A:520:ALA:HB1	1:A:521:PRO:HD2	2.03	0.41
1:A:1048:HIS:HE2	1:A:1051:SER:HG	1.66	0.41
1:B:120:VAL:HG12	1:B:121:ASN:N	2.35	0.41
1:B:131:CYS:HB3	1:B:163:ALA:HA	2.02	0.41
1:B:639:GLY:H	1:B:651:ILE:HG21	1.86	0.41
1:B:901:GLN:NE2	1:B:905:ARG:HH21	2.18	0.41
1:B:1023:ASN:O	1:B:1027:THR:HG23	2.21	0.41
1:C:28:TYR:HD2	1:C:61:ASN:HD22	1.68	0.41
1:C:215:ASP:OD1	1:C:215:ASP:N	2.54	0.41
1:A:452:LEU:HD13	1:A:493:GLN:O	2.21	0.41
1:B:190:ARG:HB3	1:B:192:PHE:HE2	1.86	0.41
1:B:528:LYS:HA	1:B:528:LYS:HD2	1.74	0.41
1:A:30:ASN:HB3	1:A:32:PHE:CE1	2.56	0.41
1:A:224:GLU:OE1	1:A:224:GLU:N	2.50	0.41
1:B:541:PHE:HD1	1:B:543:PHE:HB2	1.86	0.40
1:B:916:LEU:HD12	1:B:923:ILE:HD12	2.03	0.40
1:B:959:LEU:HD12	1:B:959:LEU:HA	1.91	0.40
1:C:63:THR:O	1:C:63:THR:OG1	2.39	0.40
1:C:118:LEU:HD11	1:C:120:VAL:HG23	2.02	0.40
1:C:318:PHE:HE1	1:C:615:VAL:HG21	1.86	0.40
1:A:1038:LYS:HE2	1:A:1038:LYS:HB3	1.95	0.40
1:A:341:VAL:HG22	1:A:356:LYS:HD2	2.04	0.40
1:A:528:LYS:HA	1:A:528:LYS:HD2	1.78	0.40
1:A:919:ASN:OD1	1:A:919:ASN:N	2.54	0.40
1:A:1001:LEU:HD12	1:A:1001:LEU:HA	1.92	0.40
1:C:776:LYS:HE2	1:C:776:LYS:HB2	1.73	0.40
1:B:323:THR:OG1	1:B:324:GLU:N	2.54	0.40
1:B:903:ALA:HB2	1:B:916:LEU:HD23	2.04	0.40
1:C:544:ASN:HD21	1:C:579:PRO:HB3	1.86	0.40
1:C:1028:LYS:HE3	1:C:1028:LYS:HB2	1.94	0.40
1:A:577:ARG:HA	1:A:584:ILE:HA	2.04	0.40
1:B:328:ARG:HA	1:B:328:ARG:HD3	1.75	0.40
1:B:919:ASN:OD1	1:B:919:ASN:N	2.54	0.40
1:C:1038:LYS:HE2	1:C:1038:LYS:HB3	1.93	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	945/1273 (74%)	897 (95%)	48 (5%)	0	100	100
1	B	945/1273 (74%)	890 (94%)	55 (6%)	0	100	100
1	C	945/1273 (74%)	895 (95%)	50 (5%)	0	100	100
All	All	2835/3819 (74%)	2682 (95%)	153 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	792/1112 (71%)	734 (93%)	58 (7%)	11	35
1	B	792/1112 (71%)	737 (93%)	55 (7%)	13	38
1	C	796/1112 (72%)	741 (93%)	55 (7%)	13	38
All	All	2380/3336 (71%)	2212 (93%)	168 (7%)	15	37

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	ASP
1	B	63	THR
1	B	83	VAL
1	B	90	VAL
1	B	128	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	166	CYS
1	B	172	SER
1	B	189	LEU
1	B	226	LEU
1	B	282	ASN
1	B	312	ILE
1	B	318	PHE
1	B	320	VAL
1	B	425	LEU
1	B	452	LEU
1	B	551	VAL
1	B	558	LYS
1	B	585	LEU
1	B	588	THR
1	B	595	VAL
1	B	599	THR
1	B	608	VAL
1	B	611	LEU
1	B	617	CYS
1	B	658	ASN
1	B	664	ILE
1	B	699	LEU
1	B	705	VAL
1	B	720	ILE
1	B	723	THR
1	B	724	THR
1	B	729	VAL
1	B	732	THR
1	B	734	THR
1	B	740	MET
1	B	742	ILE
1	B	748	GLU
1	B	785	VAL
1	B	790	LYS
1	B	805	ILE
1	B	816	SER
1	B	875	SER
1	B	934	ILE
1	B	950	ASP
1	B	951	VAL
1	B	952	VAL
1	B	973	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	976	VAL
1	B	990	GLU
1	B	997	ILE
1	B	1058	HIS
1	B	1097	SER
1	B	1122	VAL
1	B	1127	ASP
1	B	1128	VAL
1	C	40	ASP
1	C	42	VAL
1	C	63	THR
1	C	84	LEU
1	C	90	VAL
1	C	94	SER
1	C	189	LEU
1	C	213	VAL
1	C	223	LEU
1	C	282	ASN
1	C	290	ASP
1	C	298	GLU
1	C	302	THR
1	C	312	ILE
1	C	314	GLN
1	C	318	PHE
1	C	320	VAL
1	C	382	VAL
1	C	383	SER
1	C	392	PHE
1	C	514	SER
1	C	524	VAL
1	C	534	VAL
1	C	555	SER
1	C	558	LYS
1	C	565	PHE
1	C	585	LEU
1	C	599	THR
1	C	617	CYS
1	C	699	LEU
1	C	711	SER
1	C	720	ILE
1	C	723	THR
1	C	729	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	731	MET
1	C	732	THR
1	C	752	LEU
1	C	770	ILE
1	C	785	VAL
1	C	816	SER
1	C	934	ILE
1	C	935	GLN
1	C	951	VAL
1	C	967	SER
1	C	976	VAL
1	C	980	ILE
1	C	991	VAL
1	C	1034	LEU
1	C	1045	LYS
1	C	1058	HIS
1	C	1074	ASN
1	C	1077	THR
1	C	1122	VAL
1	C	1129	VAL
1	C	1130	ILE
1	A	63	THR
1	A	90	VAL
1	A	98	SER
1	A	127	VAL
1	A	128	ILE
1	A	166	CYS
1	A	189	LEU
1	A	233	ILE
1	A	294	ASP
1	A	302	THR
1	A	307	THR
1	A	312	ILE
1	A	316	SER
1	A	318	PHE
1	A	320	VAL
1	A	367	VAL
1	A	401	VAL
1	A	433	VAL
1	A	450	ASN
1	A	524	VAL
1	A	553	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	569	ILE
1	A	573	THR
1	A	576	VAL
1	A	585	LEU
1	A	599	THR
1	A	608	VAL
1	A	611	LEU
1	A	642	VAL
1	A	645	THR
1	A	720	ILE
1	A	723	THR
1	A	732	THR
1	A	734	THR
1	A	742	ILE
1	A	761	THR
1	A	770	ILE
1	A	778	THR
1	A	785	VAL
1	A	791	THR
1	A	801	ASN
1	A	816	SER
1	A	858	LEU
1	A	870	ILE
1	A	875	SER
1	A	919	ASN
1	A	934	ILE
1	A	937	SER
1	A	950	ASP
1	A	952	VAL
1	A	967	SER
1	A	973	ILE
1	A	976	VAL
1	A	994	ASP
1	A	997	ILE
1	A	1058	HIS
1	A	1122	VAL
1	A	1128	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	81	ASN
1	B	134	GLN
1	B	280	ASN
1	B	317	ASN
1	B	536	ASN
1	B	544	ASN
1	B	644	GLN
1	B	755	GLN
1	B	774	GLN
1	B	801	ASN
1	B	901	GLN
1	B	954	GLN
1	B	965	GLN
1	B	1002	GLN
1	B	1010	GLN
1	B	1101	HIS
1	B	1108	ASN
1	B	1135	ASN
1	C	66	HIS
1	C	125	ASN
1	C	137	ASN
1	C	239	GLN
1	C	388	ASN
1	C	409	GLN
1	C	422	ASN
1	C	437	ASN
1	C	644	GLN
1	C	751	ASN
1	C	755	GLN
1	C	901	GLN
1	C	914	ASN
1	C	965	GLN
1	C	969	ASN
1	C	992	GLN
1	C	1002	GLN
1	C	1101	HIS
1	C	1106	GLN
1	C	1134	ASN
1	A	271	GLN
1	A	280	ASN
1	A	388	ASN
1	A	439	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	506	GLN
1	A	536	ASN
1	A	644	GLN
1	A	755	GLN
1	A	774	GLN
1	A	804	GLN
1	A	901	GLN
1	A	965	GLN
1	A	1101	HIS
1	A	1134	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

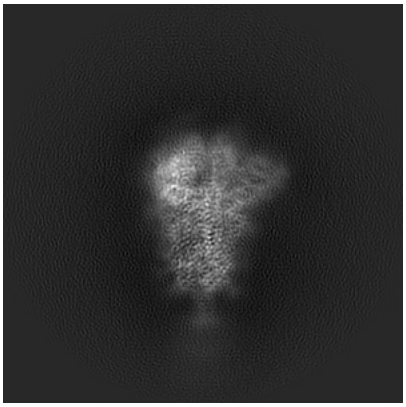
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23215. These allow visual inspection of the internal detail of the map and identification of artifacts.

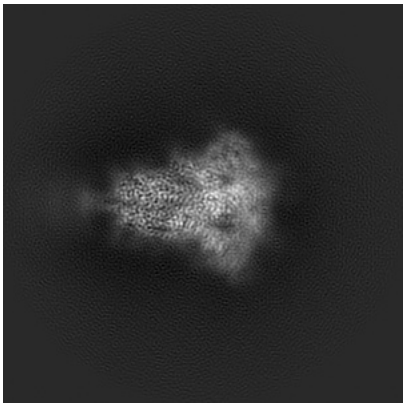
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

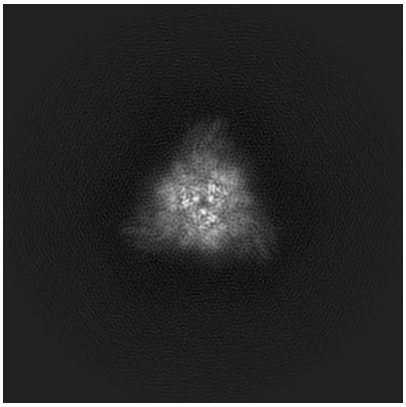
6.1.1 Primary map



X



Y

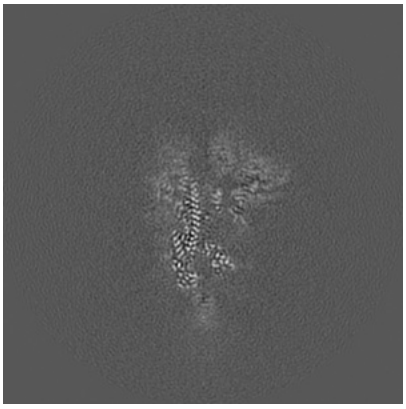


Z

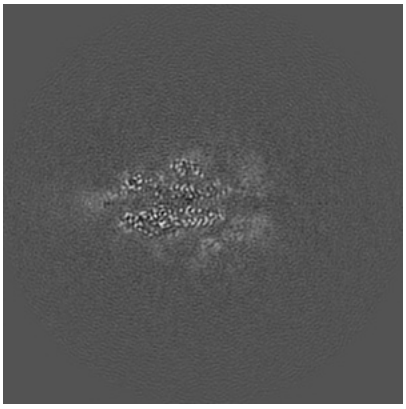
The images above show the map projected in three orthogonal directions.

6.2 Central slices

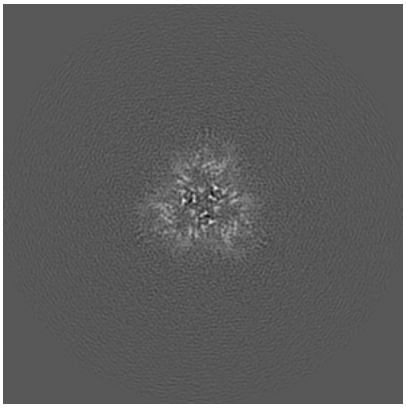
6.2.1 Primary map



X Index: 225



Y Index: 225

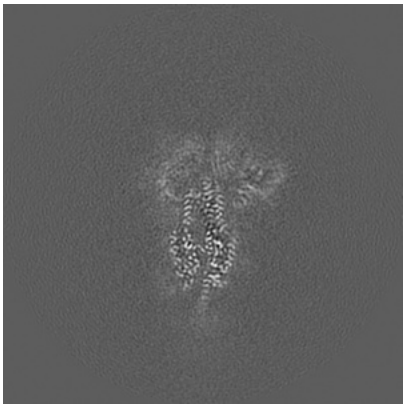


Z Index: 225

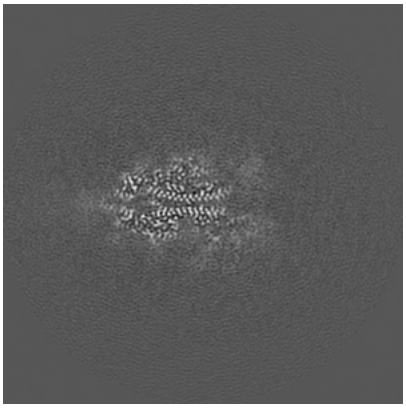
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

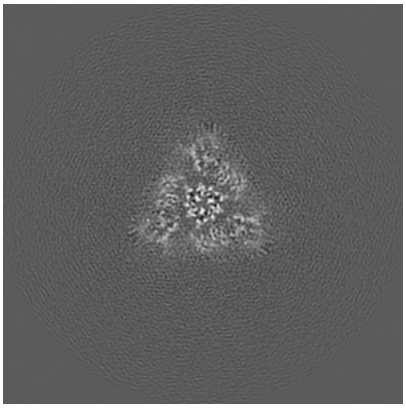
6.3.1 Primary map



X Index: 236



Y Index: 230

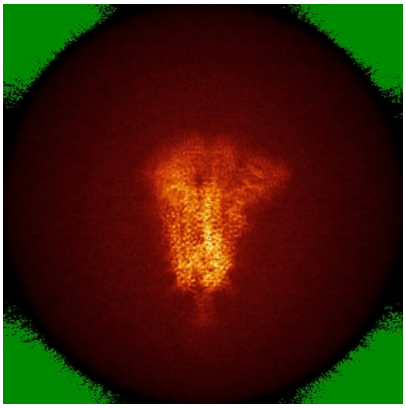


Z Index: 235

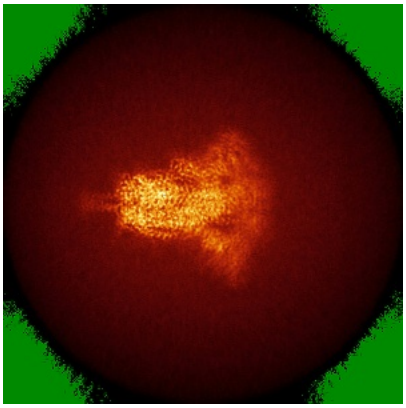
The images above show the largest variance slices of the map in three orthogonal directions.

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

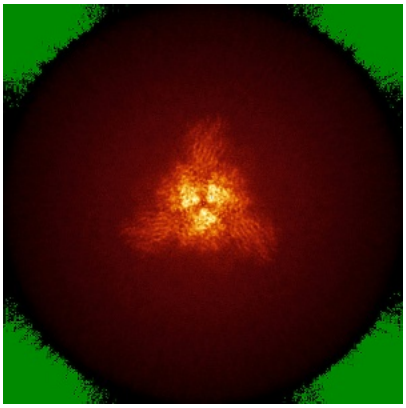
6.4.1 Primary map



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 0.0003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

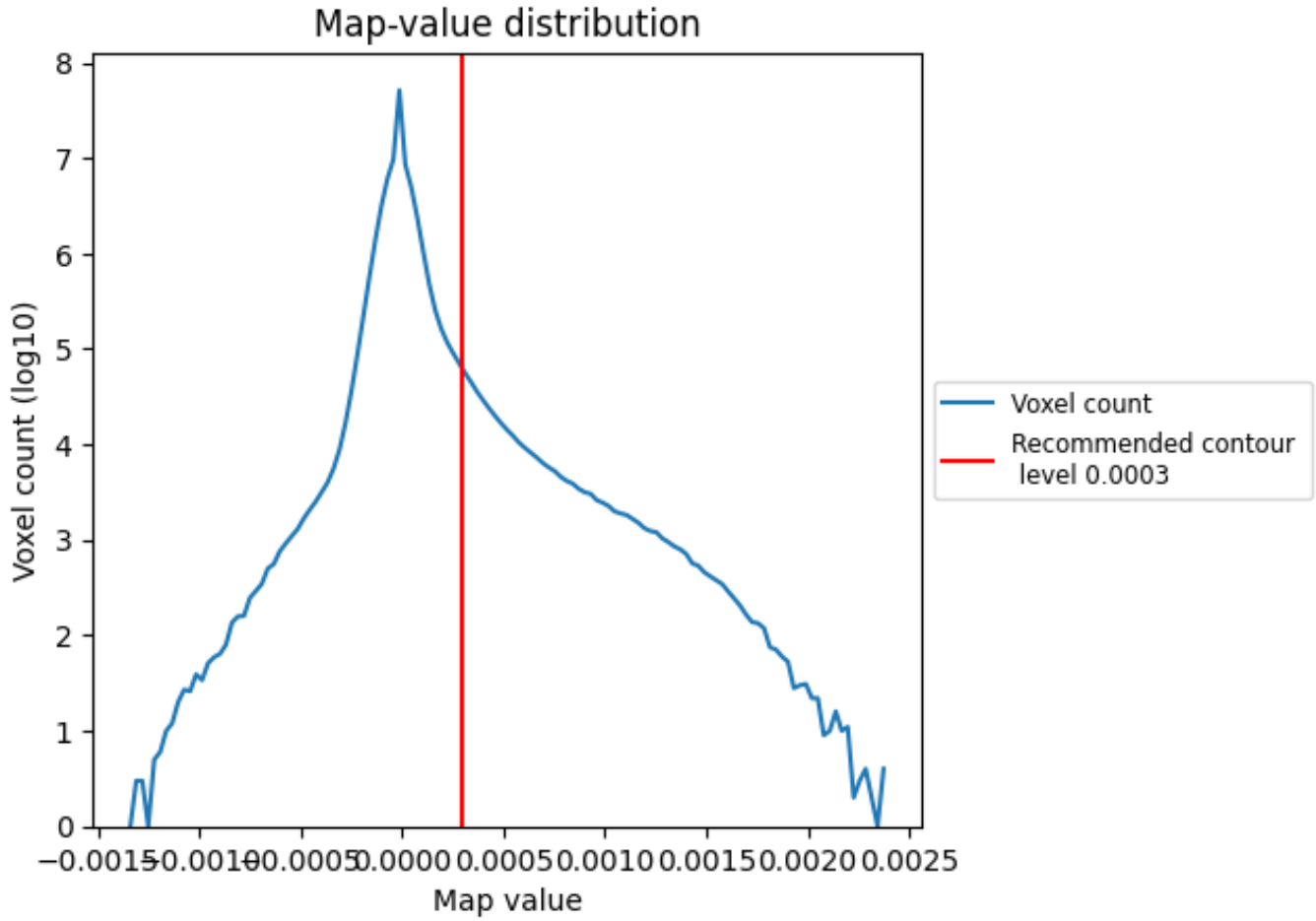
6.6 Mask visualisation (i)

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

7 Map analysis

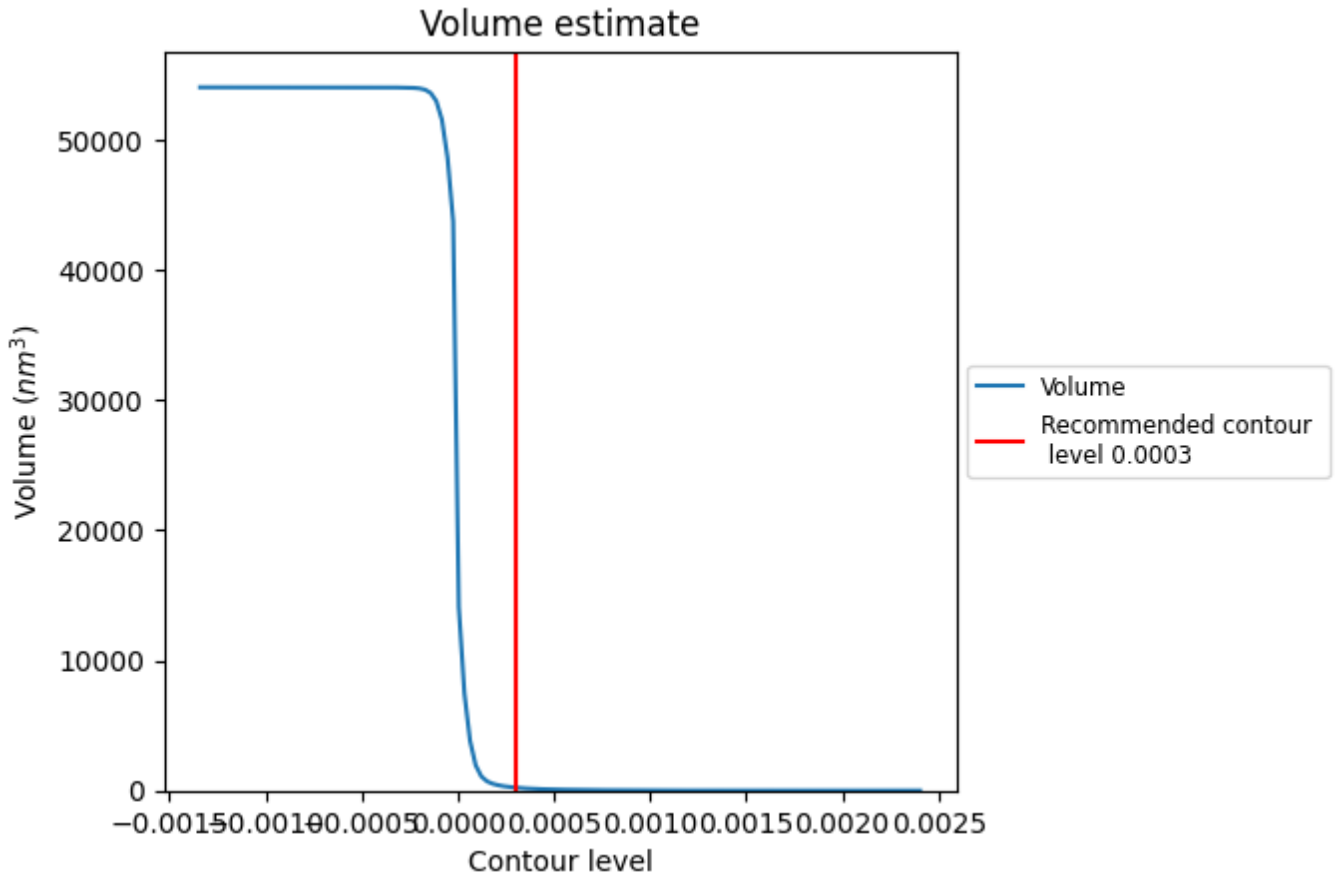
This section contains the results of statistical analysis of the map.

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.

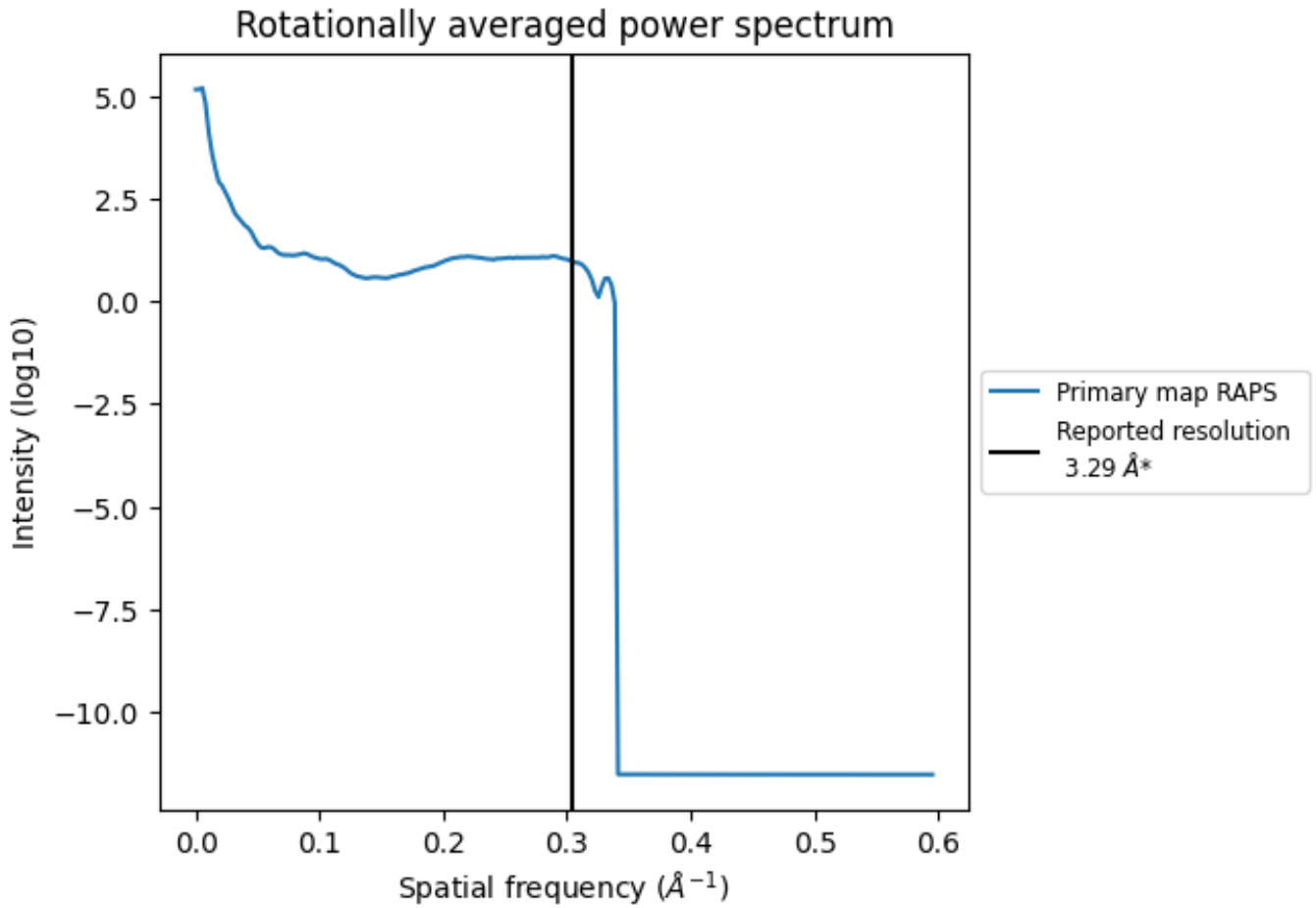
7.2 Volume estimate



The volume at the recommended contour level is 226 nm^3; this corresponds to an approximate mass of 204 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 0.304 $Å^{-1}$

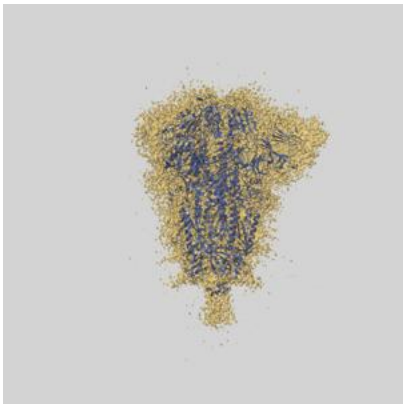
8 Fourier-Shell correlation (i)

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

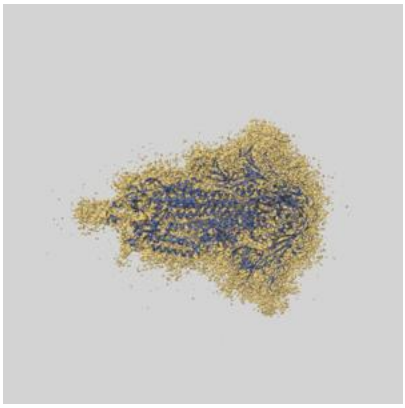
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23215 and PDB model 7L7K. Per-residue inclusion information can be found in section 3 on page 4.

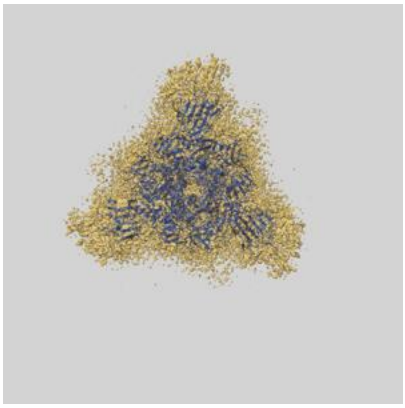
9.1 Map-model overlay



X



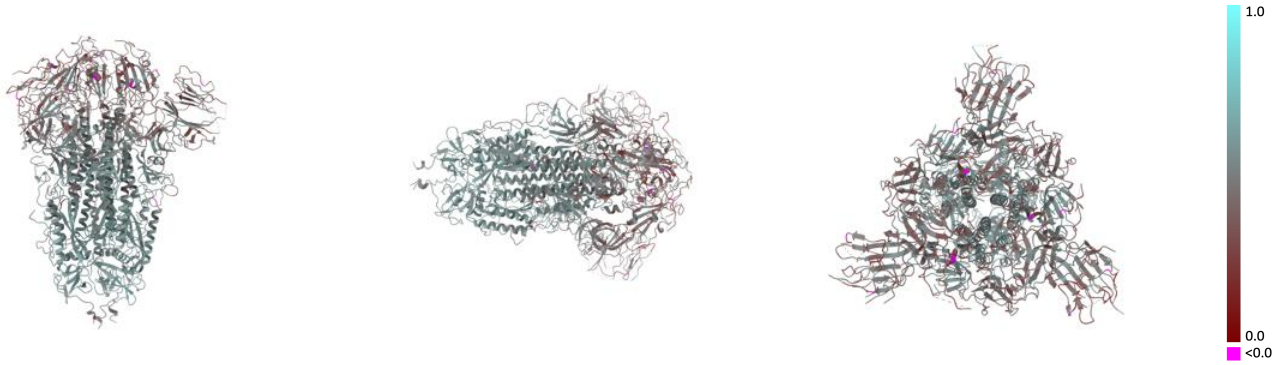
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0003 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.

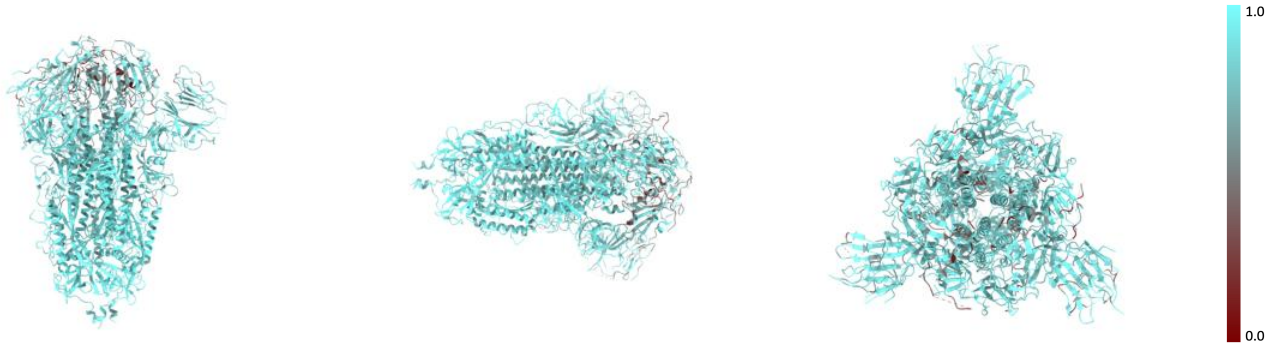
9.2 Q-score mapped to coordinate model (i)



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.

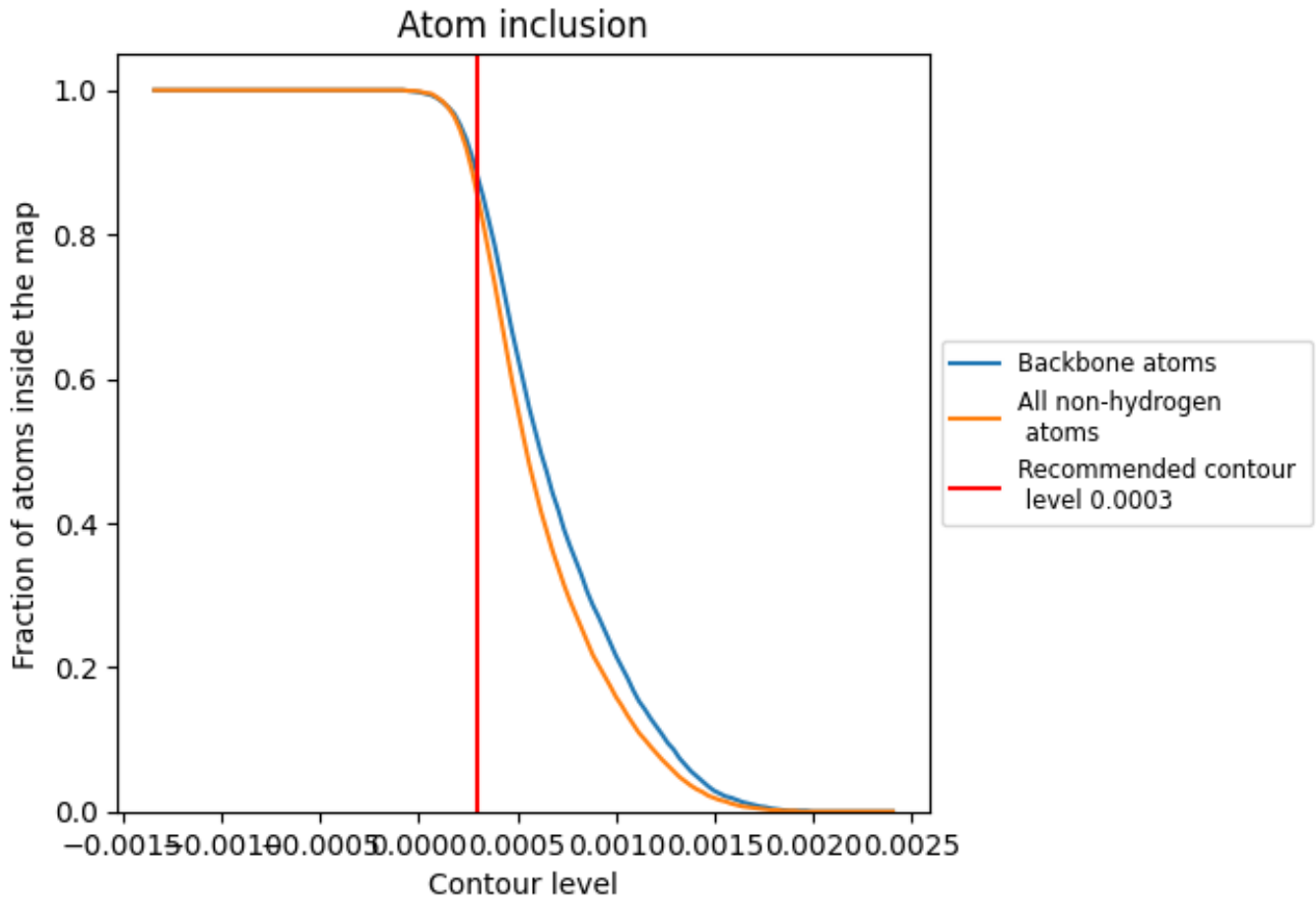
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0003).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.4840
A	0.8520	0.4850
B	0.8490	0.4820
C	0.8530	0.4850