



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 02:37 PM JST

PDB ID : 7V6Y
EMDB ID : EMD-31753
Title : Cryo-EM structure of Patched in lipid nanodisc - the wildtype, 3.5 angstrom
(re-processed with dataset of 7dzq)
Authors : Luo, Y.; Zhao, Y.; Qu, Q.; Li, D.
Deposited on : 2021-08-20
Resolution : 3.50 Å(reported)
Based on initial model : 6MG8

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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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) : 2.39

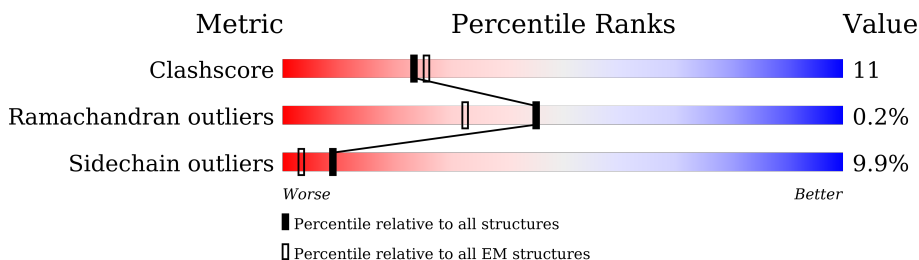
1 Overall quality at a glance

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	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 $\leq 5\%$. 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	1090	
2	B	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7484 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 Protein patched homolog 1, Protein patched homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	990	7326	4809	1215	1264	38	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q61115
A	0	GLY	-	expression tag	UNP Q61115
A	1	SER	-	expression tag	UNP Q61115
A	1176	THR	-	expression tag	UNP Q61115
A	1177	LEU	-	expression tag	UNP Q61115
A	1178	GLU	-	expression tag	UNP Q61115
A	1179	VAL	-	expression tag	UNP Q61115
A	1180	LEU	-	expression tag	UNP Q61115
A	1181	PHE	-	expression tag	UNP Q61115
A	1182	GLN	-	expression tag	UNP Q61115
A	1183	GLY	-	expression tag	UNP Q61115

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



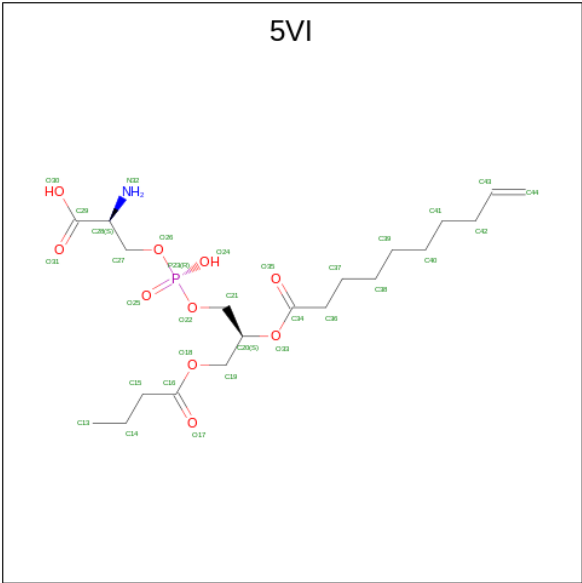
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	2	28	16	2	10	0	0

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	

- Molecule 4 is (2S)-2-azanyl-3-[[[(2S)-3-butanoyloxy-2-dec-9-enoyloxy-propoxy]-oxidanyl-phosphoryl]oxy-propanoic acid (three-letter code: 5VI) (formula: C₂₀H₃₆NO₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	20	1	10	1	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

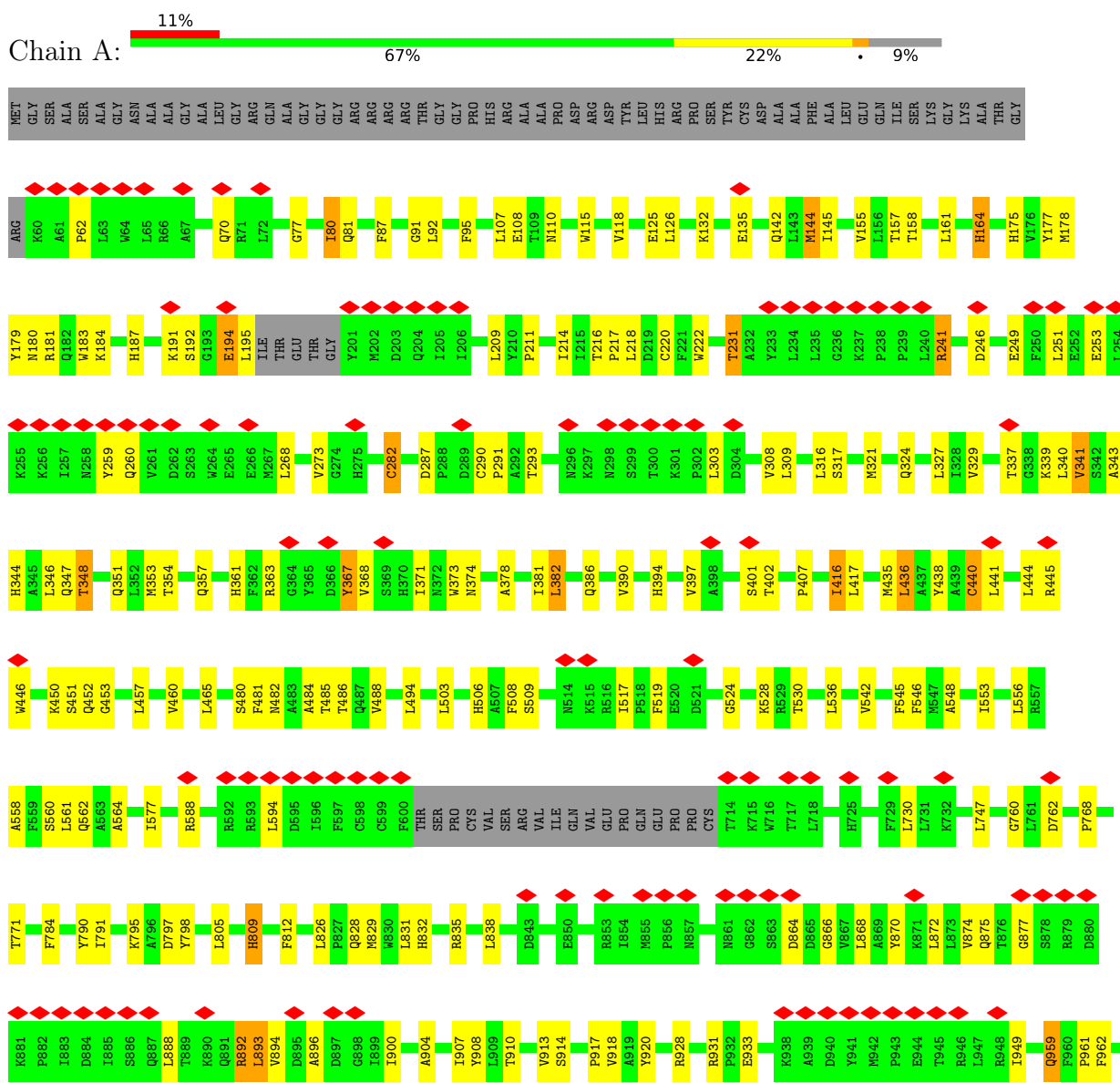


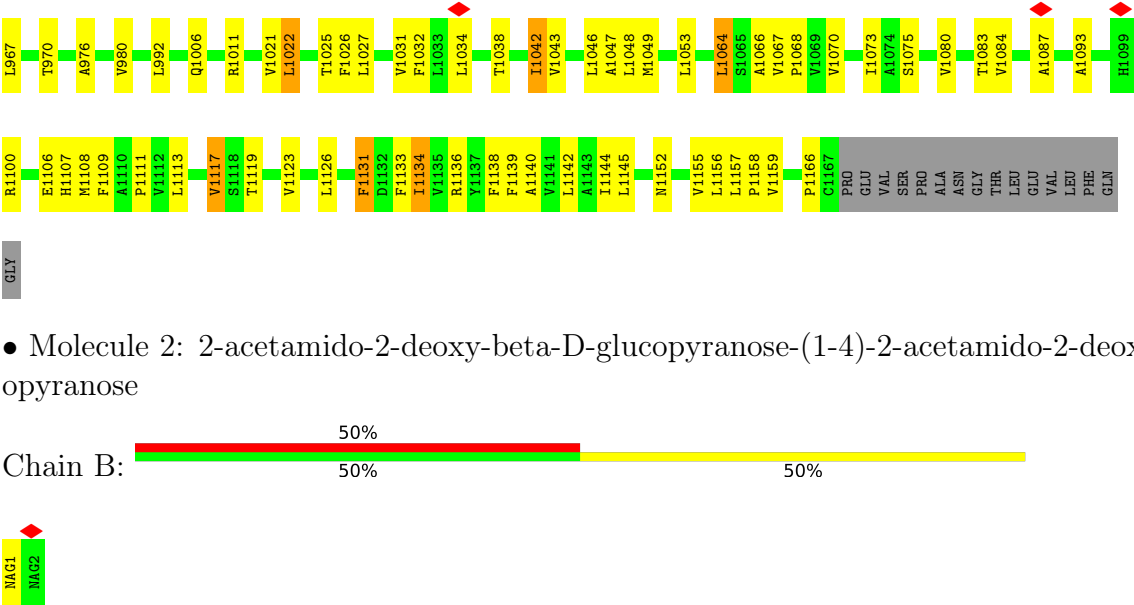
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	

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: Protein patched homolog 1, Protein patched homolog 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	172299	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	120000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.252	Depositor
Minimum map value	-2.573	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.355	Depositor
Map size (\AA)	216.48, 216.48, 216.48	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	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: NAG, 5VI, CLR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	0/7511	0.81	0/10283

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	A	7326	0	7047	155	0
2	B	28	0	25	0	0
3	A	56	0	92	10	0
4	A	32	0	0	0	0
5	A	42	0	39	2	0
All	All	7484	0	7203	159	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 (159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TRP:CZ3	1:A:381:ILE:HG12	1.81	1.15
1:A:486:THR:HG23	3:A:1202:CLR:H6	1.43	1.01
1:A:183:TRP:HZ3	1:A:381:ILE:HG12	1.24	0.99
1:A:339:LYS:HA	5:A:1205:NAG:H61	1.59	0.84
1:A:108:GLU:OE2	1:A:480:SER:CB	2.26	0.84
1:A:1026:PHE:HB2	1:A:1043:VAL:HG21	1.58	0.84
1:A:183:TRP:CE3	1:A:381:ILE:CG2	2.63	0.82
1:A:183:TRP:CE3	1:A:381:ILE:HG23	2.15	0.81
1:A:183:TRP:HE3	1:A:381:ILE:HG23	1.46	0.80
1:A:144:MET:HG3	1:A:348:THR:HG23	1.65	0.77
1:A:251:LEU:HD11	1:A:268:LEU:HD12	1.66	0.77
1:A:183:TRP:CZ3	1:A:381:ILE:CG1	2.64	0.76
1:A:195:LEU:HD13	3:A:1201:CLR:H182	1.67	0.75
1:A:536:LEU:HD22	1:A:1084:VAL:HG21	1.69	0.75
1:A:195:LEU:HD22	3:A:1201:CLR:H181	1.73	0.70
1:A:826:LEU:HD13	1:A:962:PHE:HE1	1.59	0.67
1:A:164:HIS:HB3	1:A:218:LEU:HD21	1.76	0.66
1:A:77:GLY:HA3	1:A:524:GLY:HA2	1.79	0.65
1:A:440:CYS:HB3	1:A:457:LEU:HD21	1.79	0.65
1:A:1107:HIS:O	1:A:1111:PRO:HD2	1.96	0.64
1:A:894:VAL:C	1:A:896:ALA:H	2.00	0.64
1:A:435:MET:HG2	1:A:494:LEU:HD21	1.82	0.62
1:A:183:TRP:CE3	1:A:381:ILE:HG21	2.34	0.62
1:A:1106:GLU:O	1:A:1109:PHE:HB3	2.00	0.61
1:A:790:TYR:HB3	1:A:959:GLN:HG2	1.82	0.61
1:A:503:LEU:HD21	1:A:530:THR:HB	1.83	0.60
1:A:378:ALA:HB1	1:A:381:ILE:HD12	1.84	0.60
1:A:1140:ALA:O	1:A:1144:ILE:HG22	2.03	0.59
1:A:211:PRO:HG3	1:A:316:LEU:HD12	1.85	0.58
1:A:805:LEU:HD23	1:A:992:LEU:HD21	1.86	0.58
1:A:917:PRO:O	1:A:918:VAL:C	2.40	0.58
1:A:1156:LEU:HA	1:A:1159:VAL:HG22	1.85	0.57
1:A:155:VAL:HG22	1:A:343:ALA:O	2.05	0.56
1:A:216:THR:HG22	1:A:348:THR:HB	1.87	0.56
1:A:1046:LEU:HD13	1:A:1080:VAL:HG22	1.87	0.56
1:A:145:ILE:HG22	1:A:347:GLN:HG3	1.88	0.56
1:A:324:GLN:HB2	1:A:327:LEU:HD13	1.88	0.55
1:A:231:THR:HB	1:A:241:ARG:HA	1.88	0.55
1:A:508:PHE:O	1:A:509:SER:C	2.42	0.55
1:A:760:GLY:HA3	1:A:970:THR:HG21	1.88	0.55
1:A:835:ARG:HB3	1:A:900:ILE:HD11	1.88	0.54
1:A:829:MET:HG2	1:A:832:HIS:ND1	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HG22	1:A:216:THR:HG23	1.88	0.54
1:A:558:ALA:O	1:A:562:GLN:HG2	2.08	0.53
1:A:1067:VAL:HB	1:A:1068:PRO:HD3	1.90	0.53
1:A:179:TYR:HB3	1:A:371:ILE:HD12	1.89	0.53
1:A:809:HIS:CE1	1:A:829:MET:HB3	2.44	0.53
1:A:70:GLN:HB3	1:A:528:LYS:HG3	1.92	0.52
1:A:378:ALA:HB1	1:A:381:ILE:CD1	2.40	0.52
1:A:339:LYS:CA	5:A:1205:NAG:H61	2.36	0.52
1:A:91:GLY:HA3	1:A:577:ILE:HD12	1.91	0.51
1:A:553:ILE:HD11	1:A:1006:GLN:OE1	2.11	0.51
1:A:95:PHE:HB3	1:A:465:LEU:CD2	2.40	0.51
1:A:440:CYS:SG	1:A:441:LEU:N	2.84	0.51
1:A:894:VAL:C	1:A:896:ALA:N	2.64	0.51
1:A:95:PHE:HB3	1:A:465:LEU:HD21	1.93	0.51
1:A:485:THR:OG1	1:A:562:GLN:HG3	2.11	0.50
1:A:209:LEU:HD21	1:A:231:THR:HA	1.93	0.50
1:A:536:LEU:HD12	1:A:1032:PHE:HB2	1.92	0.50
1:A:1042:ILE:O	1:A:1046:LEU:HG	2.11	0.50
1:A:1126:LEU:HD21	1:A:1138:PHE:HB2	1.93	0.50
1:A:401:SER:O	1:A:402:THR:OG1	2.27	0.50
1:A:1022:LEU:HD11	1:A:1046:LEU:HB2	1.94	0.50
1:A:904:ALA:HB1	1:A:907:ILE:HD12	1.93	0.50
1:A:179:TYR:HB3	1:A:371:ILE:CD1	2.42	0.50
1:A:317:SER:O	1:A:321:MET:HB2	2.12	0.50
1:A:870:TYR:CE1	1:A:888:LEU:HD21	2.46	0.50
1:A:273:VAL:HG21	3:A:1201:CLR:H161	1.93	0.49
1:A:484:ALA:O	1:A:488:VAL:HG12	2.11	0.49
1:A:892:ARG:HG2	1:A:893:LEU:N	2.26	0.49
1:A:556:LEU:HB3	1:A:1070:VAL:HG21	1.94	0.49
1:A:913:VAL:HG23	1:A:920:TYR:CD2	2.47	0.49
1:A:287:ASP:HA	1:A:290:CYS:HB2	1.95	0.49
1:A:178:MET:O	1:A:179:TYR:C	2.51	0.49
1:A:546:PHE:CE2	1:A:564:ALA:HB1	2.48	0.49
1:A:877:GLY:HA3	1:A:904:ALA:HB2	1.95	0.49
1:A:1075:SER:HB3	1:A:1145:LEU:HD13	1.94	0.49
1:A:184:LYS:HG2	1:A:187:HIS:CE1	2.48	0.48
1:A:416:ILE:HG23	1:A:768:PRO:HD2	1.95	0.48
1:A:62:PRO:CB	1:A:1034:LEU:HD13	2.44	0.48
1:A:829:MET:HG3	1:A:831:LEU:H	1.77	0.48
1:A:1107:HIS:O	1:A:1108:MET:C	2.50	0.48
1:A:910:THR:HA	1:A:913:VAL:HG12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLN:O	1:A:390:VAL:HG23	2.15	0.47
1:A:1131:PHE:CE1	1:A:1134:ILE:HB	2.50	0.47
1:A:339:LYS:CB	1:A:341:VAL:HG13	2.45	0.46
1:A:1049:MET:HG3	1:A:1152:ASN:HD22	1.79	0.46
1:A:1087:ALA:HB2	1:A:1157:LEU:HD21	1.97	0.46
1:A:195:LEU:HD22	3:A:1201:CLR:C18	2.43	0.46
1:A:142:GLN:NE2	1:A:386:GLN:HG2	2.31	0.46
1:A:444:LEU:HD12	1:A:453:GLY:HA3	1.97	0.46
1:A:347:GLN:HB2	1:A:784:PHE:CZ	2.51	0.46
1:A:273:VAL:HA	1:A:316:LEU:O	2.16	0.46
1:A:545:PHE:O	1:A:560:SER:OG	2.34	0.45
1:A:875:GLN:HG2	1:A:907:ILE:HD13	1.97	0.45
1:A:826:LEU:HD13	1:A:962:PHE:CE1	2.46	0.45
1:A:892:ARG:HB2	1:A:908:TYR:CE2	2.51	0.45
1:A:382:LEU:HA	1:A:382:LEU:HD13	1.68	0.45
1:A:222:TRP:HB3	1:A:282:CYS:HA	1.98	0.44
1:A:561:LEU:HD23	1:A:561:LEU:HA	1.80	0.44
1:A:1022:LEU:HD12	1:A:1022:LEU:HA	1.71	0.44
1:A:353:MET:HE1	1:A:361:HIS:HB2	1.99	0.44
1:A:80:ILE:O	1:A:81:GLN:C	2.56	0.44
1:A:1113:LEU:O	1:A:1117:VAL:HG12	2.17	0.44
1:A:812:PHE:HE1	1:A:980:VAL:HG13	1.82	0.44
1:A:1064:LEU:HD23	1:A:1068:PRO:HB2	1.99	0.44
1:A:194:GLU:H	1:A:194:GLU:HG2	1.71	0.44
3:A:1202:CLR:H162	3:A:1202:CLR:H212	1.29	0.44
1:A:436:LEU:HD12	1:A:460:VAL:CG1	2.48	0.44
1:A:1021:VAL:O	1:A:1025:THR:HG23	2.18	0.44
1:A:1038:THR:CG2	1:A:1166:PRO:HB3	2.48	0.44
1:A:1119:THR:O	1:A:1123:VAL:HG23	2.18	0.44
1:A:747:LEU:HD13	1:A:1048:LEU:HD12	1.98	0.43
1:A:291:PRO:C	1:A:293:THR:H	2.21	0.43
1:A:828:GLN:O	1:A:961:PRO:HG2	2.18	0.43
1:A:1053:LEU:HD11	1:A:1144:ILE:HG23	1.99	0.43
1:A:1093:ALA:O	1:A:1100:ARG:HD3	2.18	0.43
1:A:1031:VAL:O	1:A:1034:LEU:HG	2.18	0.43
3:A:1201:CLR:H182	3:A:1201:CLR:H8	1.33	0.43
1:A:451:SER:O	1:A:452:GLN:C	2.57	0.43
1:A:798:TYR:HD2	1:A:805:LEU:HD11	1.84	0.43
1:A:809:HIS:HE1	1:A:829:MET:HB3	1.84	0.43
1:A:864:ASP:C	1:A:866:GLY:H	2.22	0.43
1:A:874:VAL:HG22	1:A:888:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TRP:HE1	1:A:367:TYR:HD2	1.66	0.42
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.75	0.42
1:A:588:ARG:HD3	1:A:594:LEU:HA	2.00	0.42
1:A:373:TRP:O	1:A:374:ASN:C	2.57	0.42
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.88	0.42
1:A:482:ASN:HD21	1:A:558:ALA:HB3	1.83	0.42
1:A:1022:LEU:HD21	1:A:1047:ALA:HA	2.02	0.42
1:A:351:GLN:HE21	1:A:351:GLN:HB3	1.59	0.42
1:A:548:ALA:HB2	1:A:1073:ILE:HB	2.01	0.42
1:A:542:VAL:HG13	1:A:546:PHE:CE2	2.55	0.42
3:A:1201:CLR:H191	3:A:1201:CLR:H111	1.79	0.42
1:A:542:VAL:HG13	1:A:546:PHE:HE2	1.84	0.42
1:A:192:SER:O	3:A:1201:CLR:H42	2.20	0.41
1:A:445:ARG:HH22	1:A:506:HIS:HE1	1.67	0.41
1:A:450:LYS:HB3	1:A:450:LYS:HE2	1.81	0.41
1:A:730:LEU:HD11	1:A:1155:VAL:HG13	2.02	0.41
1:A:914:SER:HB2	1:A:933:GLU:HA	2.02	0.41
1:A:249:GLU:O	1:A:253:GLU:HG2	2.20	0.41
1:A:831:LEU:HD11	1:A:900:ILE:HD13	2.02	0.41
1:A:1123:VAL:CG1	1:A:1139:PHE:HA	2.50	0.41
1:A:217:PRO:HG2	1:A:346:LEU:HB3	2.03	0.41
1:A:340:LEU:HD13	1:A:340:LEU:HA	1.71	0.41
1:A:812:PHE:CE1	1:A:980:VAL:HG13	2.56	0.41
1:A:354:THR:HG22	1:A:357:GLN:CD	2.41	0.41
1:A:760:GLY:CA	1:A:970:THR:HG21	2.51	0.41
1:A:913:VAL:HG11	1:A:931:ARG:HG3	2.02	0.41
1:A:178:MET:C	1:A:180:ASN:N	2.71	0.41
1:A:438:TYR:OH	1:A:1117:VAL:HG11	2.20	0.41
1:A:107:LEU:HA	1:A:481:PHE:O	2.21	0.40
1:A:1126:LEU:HD21	1:A:1138:PHE:CB	2.51	0.40
1:A:967:LEU:HD21	1:A:976:ALA:HB2	2.04	0.40
1:A:1156:LEU:O	1:A:1157:LEU:C	2.58	0.40
1:A:553:ILE:HD12	1:A:1066:ALA:HB3	2.02	0.40
3:A:1202:CLR:H231	3:A:1202:CLR:H211	1.73	0.40
1:A:132:LYS:HB3	1:A:928:ARG:HG3	2.04	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	984/1090 (90%)	930 (94%)	52 (5%)	2 (0%)	44 75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	ARG
1	A	407	PRO

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	705/917 (77%)	635 (90%)	70 (10%)	6 27

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	87	PHE
1	A	92	LEU
1	A	110	ASN
1	A	115	TRP
1	A	118	VAL
1	A	125	GLU
1	A	135	GLU
1	A	144	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	157	THR
1	A	158	THR
1	A	161	LEU
1	A	164	HIS
1	A	175	HIS
1	A	177	TYR
1	A	181	ARG
1	A	191	LYS
1	A	194	GLU
1	A	220	CYS
1	A	231	THR
1	A	246	ASP
1	A	259	TYR
1	A	260	GLN
1	A	282	CYS
1	A	303	LEU
1	A	308	VAL
1	A	309	LEU
1	A	329	VAL
1	A	337	THR
1	A	341	VAL
1	A	344	HIS
1	A	348	THR
1	A	363	ARG
1	A	367	TYR
1	A	368	VAL
1	A	382	LEU
1	A	394	HIS
1	A	397	VAL
1	A	416	ILE
1	A	417	LEU
1	A	436	LEU
1	A	440	CYS
1	A	446	TRP
1	A	517	ILE
1	A	519	PHE
1	A	762	ASP
1	A	771	THR
1	A	791	ILE
1	A	795	LYS
1	A	797	ASP
1	A	809	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	868	LEU
1	A	872	LEU
1	A	892	ARG
1	A	893	LEU
1	A	949	ILE
1	A	959	GLN
1	A	1011	ARG
1	A	1022	LEU
1	A	1027	LEU
1	A	1042	ILE
1	A	1064	LEU
1	A	1083	THR
1	A	1117	VAL
1	A	1131	PHE
1	A	1133	PHE
1	A	1134	ILE
1	A	1136	ARG
1	A	1142	LEU
1	A	1158	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	163	GLN
1	A	180	ASN
1	A	244	ASN
1	A	269	ASN
1	A	275	HIS
1	A	296	ASN
1	A	351	GLN
1	A	452	GLN
1	A	506	HIS
1	A	562	GLN
1	A	780	GLN
1	A	891	GLN
1	A	926	ASN
1	A	959	GLN
1	A	985	ASN
1	A	1085	HIS
1	A	1152	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 ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	2	14,14,15	0.60	0	17,19,21	2.09	5 (29%)
2	NAG	B	2	2	14,14,15	0.22	0	17,19,21	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C3-C4-C5	4.33	117.96	110.24
2	B	1	NAG	C1-O5-C5	3.94	117.54	112.19
2	B	1	NAG	O5-C1-C2	-3.45	105.83	111.29
2	B	1	NAG	O5-C5-C6	3.19	112.20	107.20
2	B	1	NAG	O4-C4-C5	-2.50	103.10	109.30

There are no chirality outliers.

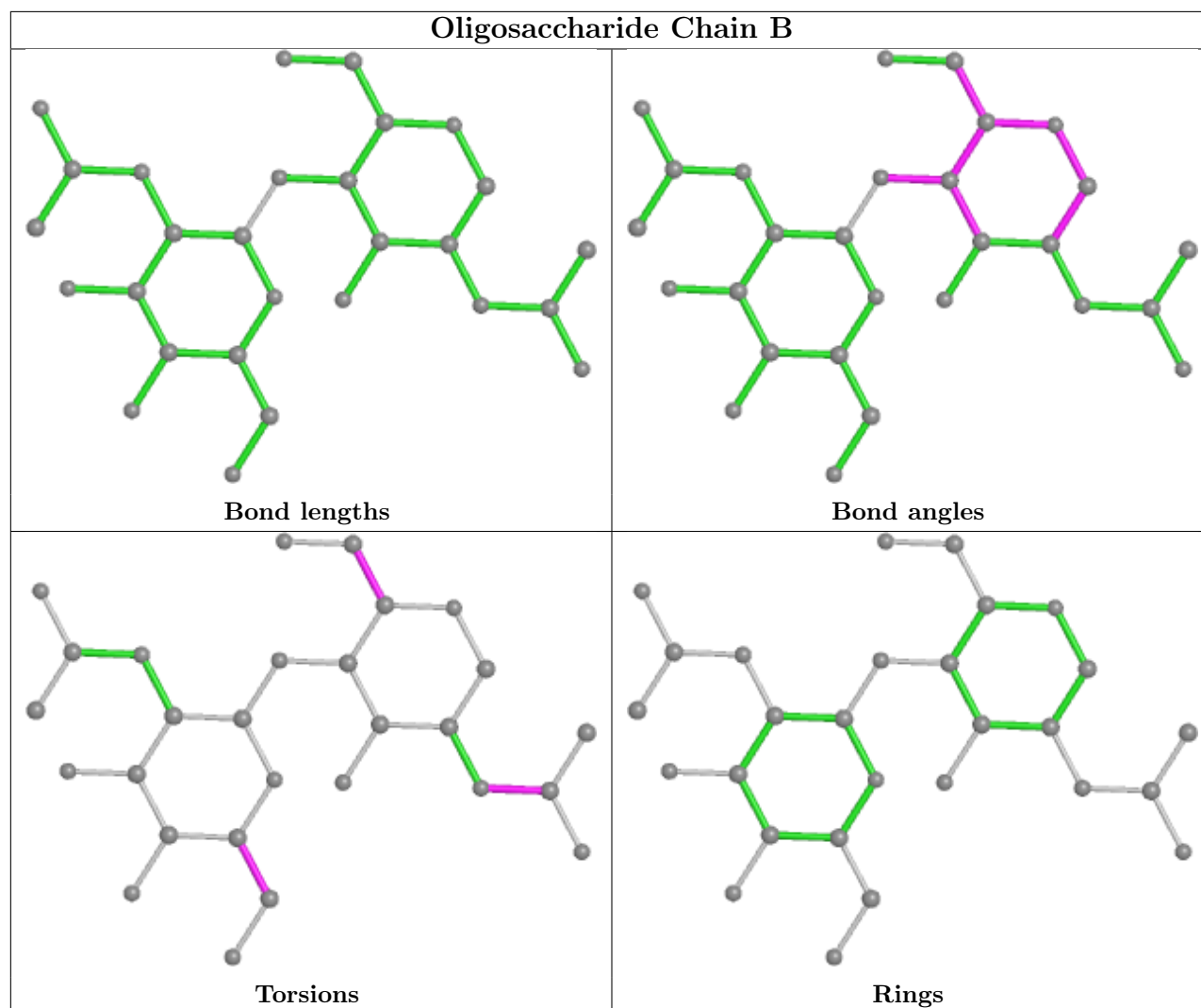
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLR	A	1201	-	31,31,31	1.05	3 (9%)	48,48,48	3.03	21 (43%)
5	NAG	A	1206	1	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	A	1205	-	14,14,15	0.22	0	17,19,21	0.39	0
4	5VI	A	1203	-	30,31,31	1.15	3 (10%)	34,38,38	1.37	3 (8%)
5	NAG	A	1204	1	14,14,15	0.40	0	17,19,21	0.82	0
3	CLR	A	1202	-	31,31,31	0.84	1 (3%)	48,48,48	2.26	16 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	A	1201	-	-	0/10/68/68	0/4/4/4
5	NAG	A	1206	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1205	-	-	2/6/23/26	0/1/1/1
4	5VI	A	1203	-	-	21/37/37/37	-
5	NAG	A	1204	1	-	0/6/23/26	0/1/1/1
3	CLR	A	1202	-	-	6/10/68/68	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	5VI	O33-C20	-2.95	1.39	1.46
3	A	1201	CLR	C13-C14	-2.82	1.49	1.55
4	A	1203	5VI	O18-C19	-2.34	1.39	1.45
3	A	1201	CLR	C13-C17	-2.29	1.50	1.55
4	A	1203	5VI	O18-C16	2.25	1.39	1.33
3	A	1202	CLR	C13-C14	-2.04	1.51	1.55
3	A	1201	CLR	C18-C13	-2.04	1.50	1.54

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1201	CLR	C13-C14-C8	-8.16	102.29	114.38
3	A	1201	CLR	C17-C13-C14	7.59	109.06	100.07
3	A	1201	CLR	C8-C7-C6	-7.17	102.42	112.73
3	A	1202	CLR	C8-C7-C6	-7.01	102.66	112.73
3	A	1201	CLR	C18-C13-C12	6.35	120.61	110.59
3	A	1201	CLR	C18-C13-C17	-6.15	100.25	111.71
3	A	1202	CLR	C16-C17-C20	-5.90	103.01	112.15
3	A	1201	CLR	C18-C13-C14	-5.11	102.17	111.71
4	A	1203	5VI	O33-C34-C36	4.76	121.76	111.50
3	A	1202	CLR	C22-C20-C17	4.64	119.88	110.28
3	A	1201	CLR	C11-C9-C8	-4.15	105.77	111.75
3	A	1201	CLR	C15-C14-C13	-4.04	98.97	103.84
3	A	1202	CLR	C19-C10-C9	-3.95	106.97	111.68
3	A	1202	CLR	C13-C17-C20	3.84	125.51	119.49
3	A	1201	CLR	C7-C8-C14	3.80	116.41	110.91
3	A	1201	CLR	C16-C17-C13	-3.68	99.41	103.84
4	A	1203	5VI	C20-O33-C34	-3.51	109.16	117.79
3	A	1202	CLR	C23-C22-C20	-3.48	105.03	115.03
3	A	1201	CLR	C13-C17-C20	-3.34	114.25	119.49
3	A	1201	CLR	C7-C6-C5	-3.17	119.22	125.06
3	A	1202	CLR	C4-C5-C10	3.14	120.59	116.42
3	A	1202	CLR	C21-C20-C17	-2.84	108.57	112.92
3	A	1201	CLR	C1-C10-C5	-2.82	103.58	108.75
3	A	1202	CLR	C18-C13-C14	-2.77	106.55	111.71
3	A	1202	CLR	C11-C9-C8	-2.77	107.77	111.75
3	A	1201	CLR	C21-C20-C17	2.76	117.14	112.92
3	A	1201	CLR	C9-C10-C5	2.62	113.76	109.65
3	A	1201	CLR	C3-C4-C5	-2.62	107.59	112.03
3	A	1202	CLR	C15-C14-C8	-2.60	114.81	119.08
3	A	1202	CLR	C2-C3-C4	-2.55	106.81	110.31
3	A	1202	CLR	C4-C5-C6	-2.48	117.03	120.61
3	A	1202	CLR	C19-C10-C5	2.44	112.29	108.34
3	A	1201	CLR	C10-C9-C8	2.44	116.39	112.73
3	A	1201	CLR	C1-C10-C9	2.39	112.06	108.73
3	A	1202	CLR	C3-C4-C5	-2.37	108.01	112.03
3	A	1201	CLR	C11-C12-C13	2.27	116.67	112.78
4	A	1203	5VI	O18-C16-C15	2.18	118.75	111.91
3	A	1201	CLR	C15-C16-C17	2.16	109.41	105.13
3	A	1202	CLR	C7-C6-C5	-2.14	121.12	125.06
3	A	1201	CLR	C16-C17-C20	-2.12	108.87	112.15

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	CLR	C13-C17-C20-C22
4	A	1203	5VI	C21-O22-P23-O24
4	A	1203	5VI	C21-O22-P23-O25
4	A	1203	5VI	C21-O22-P23-O26
4	A	1203	5VI	C27-O26-P23-O25
4	A	1203	5VI	O26-C27-C28-C29
4	A	1203	5VI	O26-C27-C28-N32
3	A	1202	CLR	C16-C17-C20-C22
5	A	1205	NAG	O5-C5-C6-O6
4	A	1203	5VI	O17-C16-O18-C19
3	A	1202	CLR	C16-C17-C20-C21
5	A	1205	NAG	C4-C5-C6-O6
4	A	1203	5VI	C15-C16-O18-C19
3	A	1202	CLR	C21-C20-C22-C23
4	A	1203	5VI	C27-O26-P23-O22
4	A	1203	5VI	C20-C21-O22-P23
4	A	1203	5VI	C36-C37-C38-C39
4	A	1203	5VI	C37-C38-C39-C40
4	A	1203	5VI	C19-C20-C21-O22
4	A	1203	5VI	C40-C41-C42-C43
4	A	1203	5VI	O18-C19-C20-C21
3	A	1202	CLR	C13-C17-C20-C21
4	A	1203	5VI	O33-C20-C21-O22
4	A	1203	5VI	O18-C19-C20-O33
4	A	1203	5VI	C36-C34-O33-C20
4	A	1203	5VI	O35-C34-O33-C20
4	A	1203	5VI	C14-C15-C16-O18
3	A	1202	CLR	C23-C24-C25-C26
4	A	1203	5VI	C14-C15-C16-O17

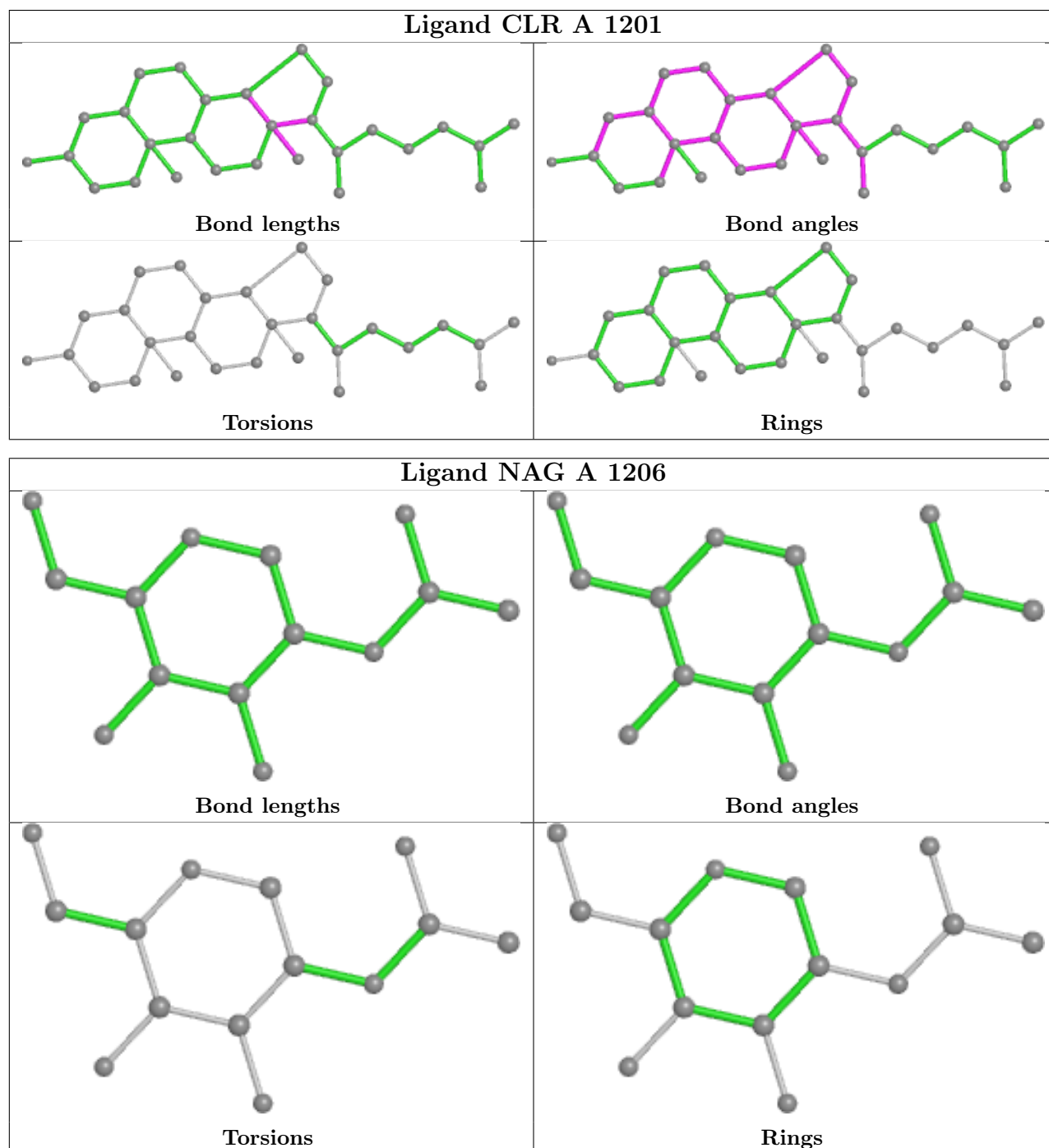
There are no ring outliers.

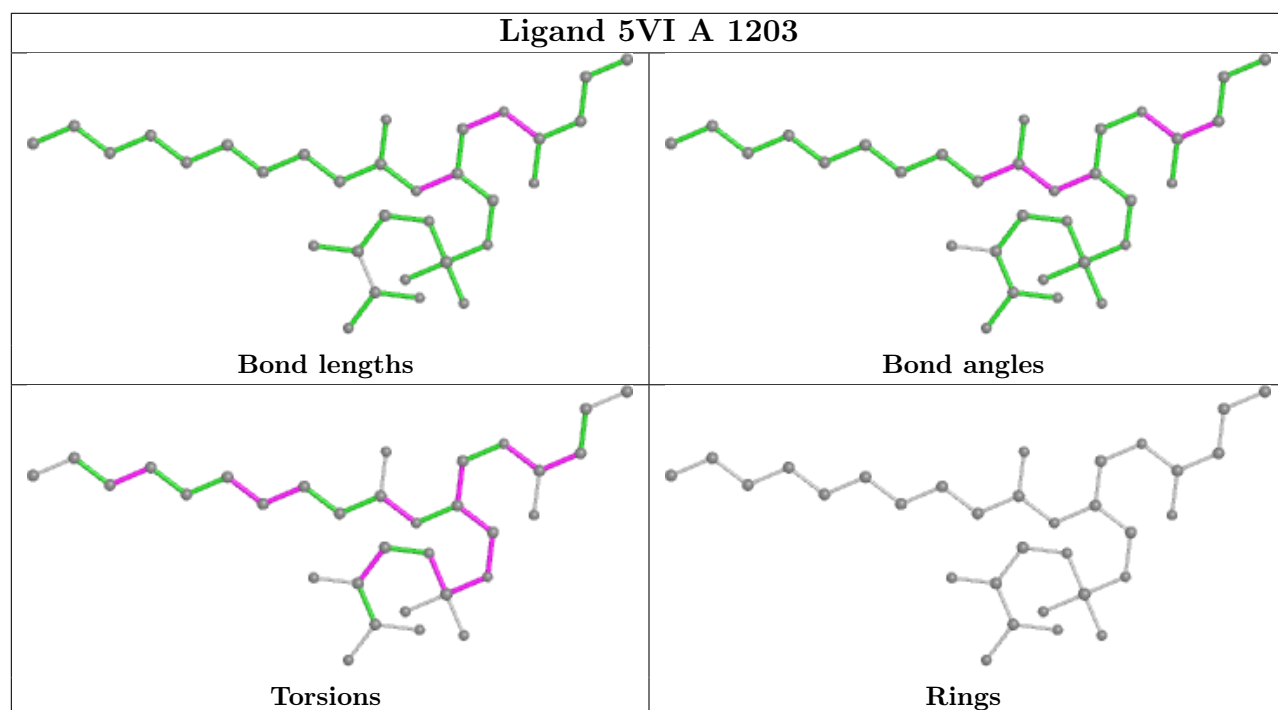
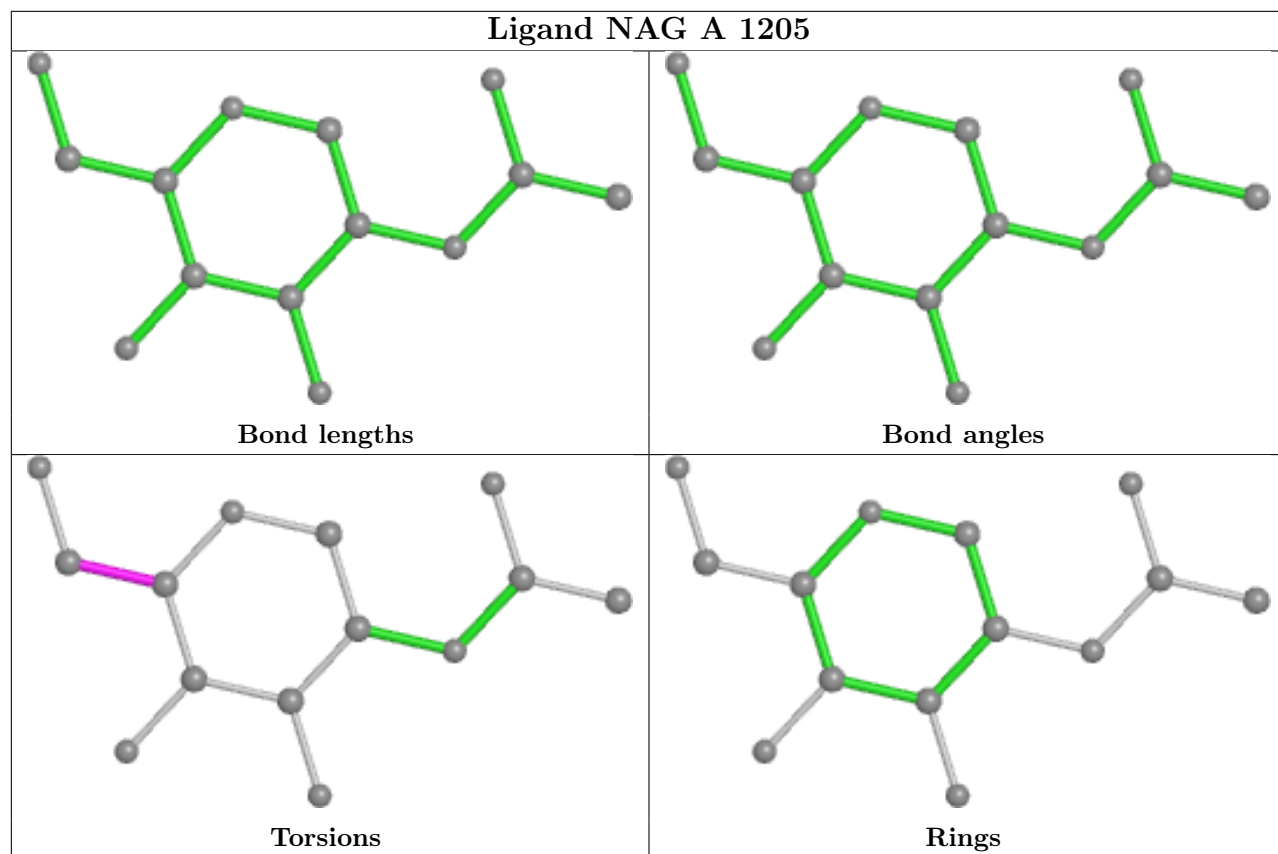
3 monomers are involved in 12 short contacts:

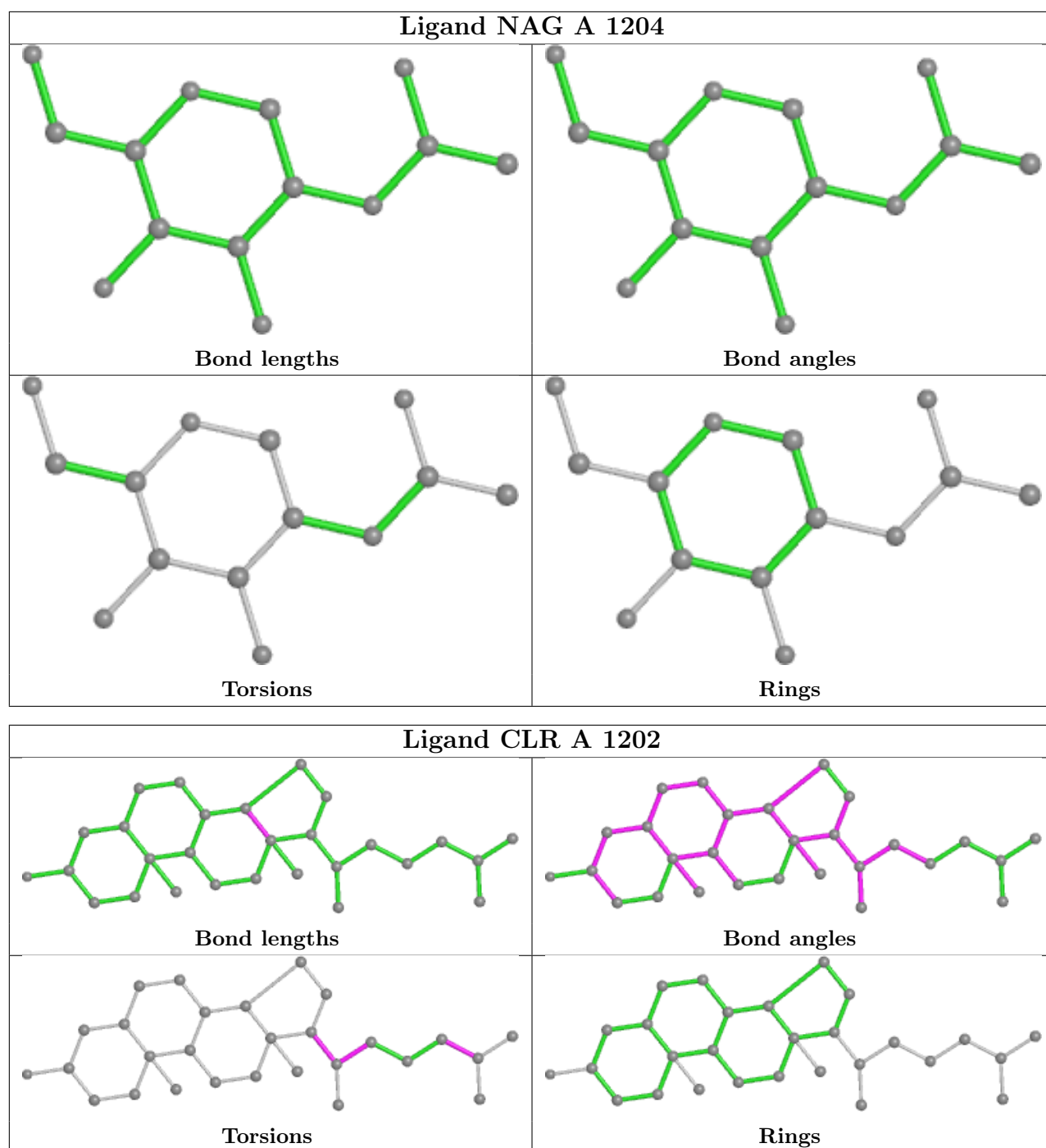
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1201	CLR	7	0
5	A	1205	NAG	2	0
3	A	1202	CLR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

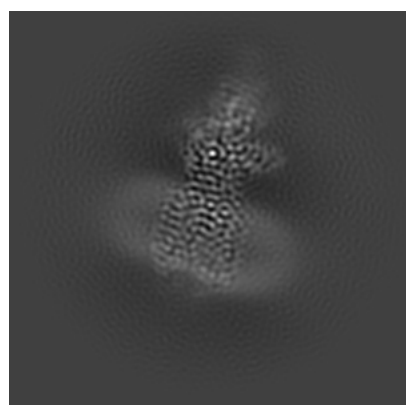
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31753. These allow visual inspection of the internal detail of the map and identification of artifacts.

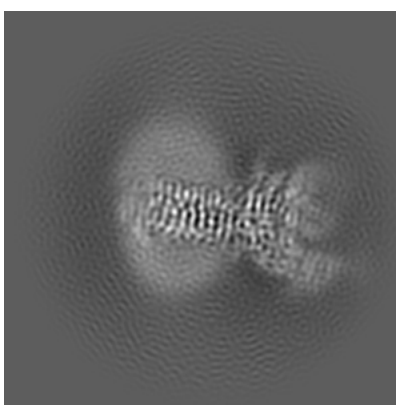
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

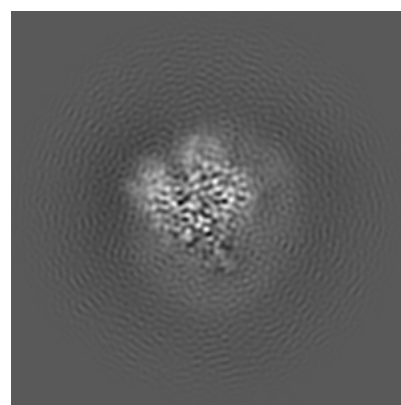
6.1.1 Primary map



X



Y

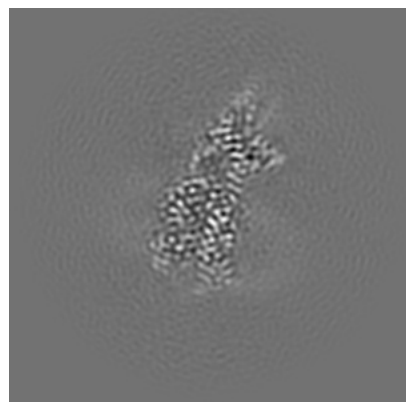


Z

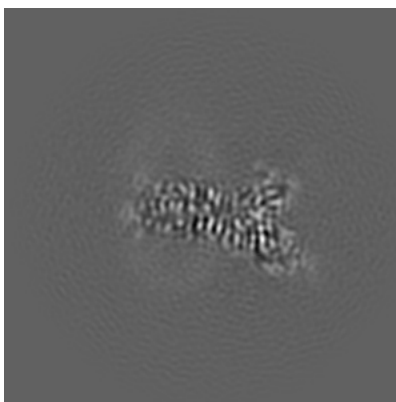
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

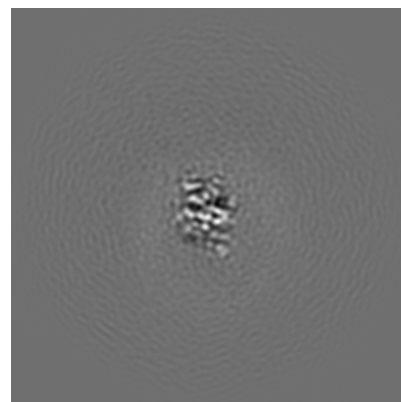
6.2.1 Primary map



X Index: 132



Y Index: 132

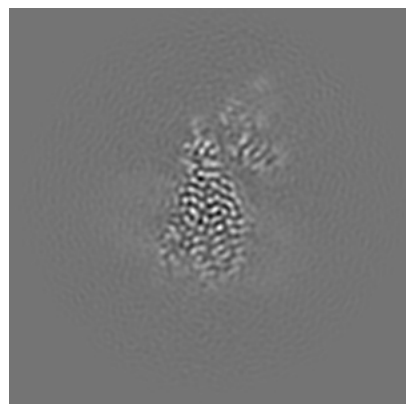


Z Index: 132

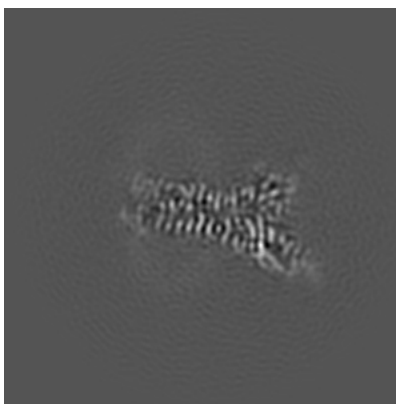
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

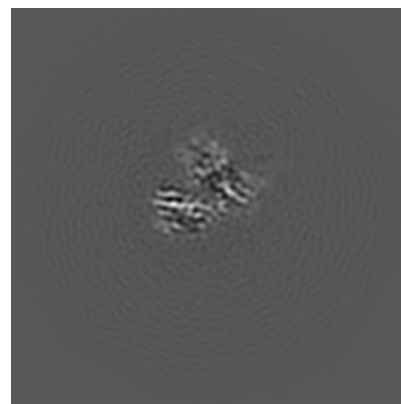
6.3.1 Primary map



X Index: 123



Y Index: 134

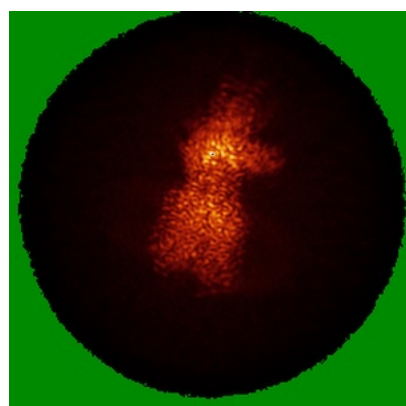


Z Index: 169

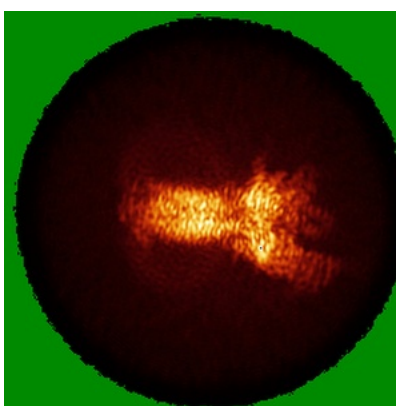
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

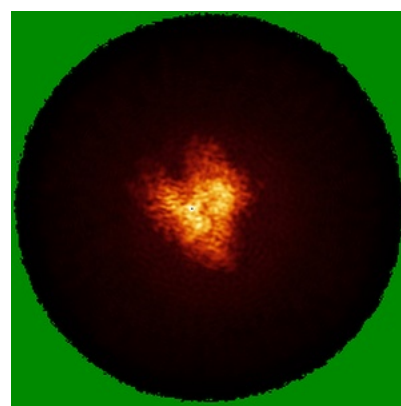
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.355. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

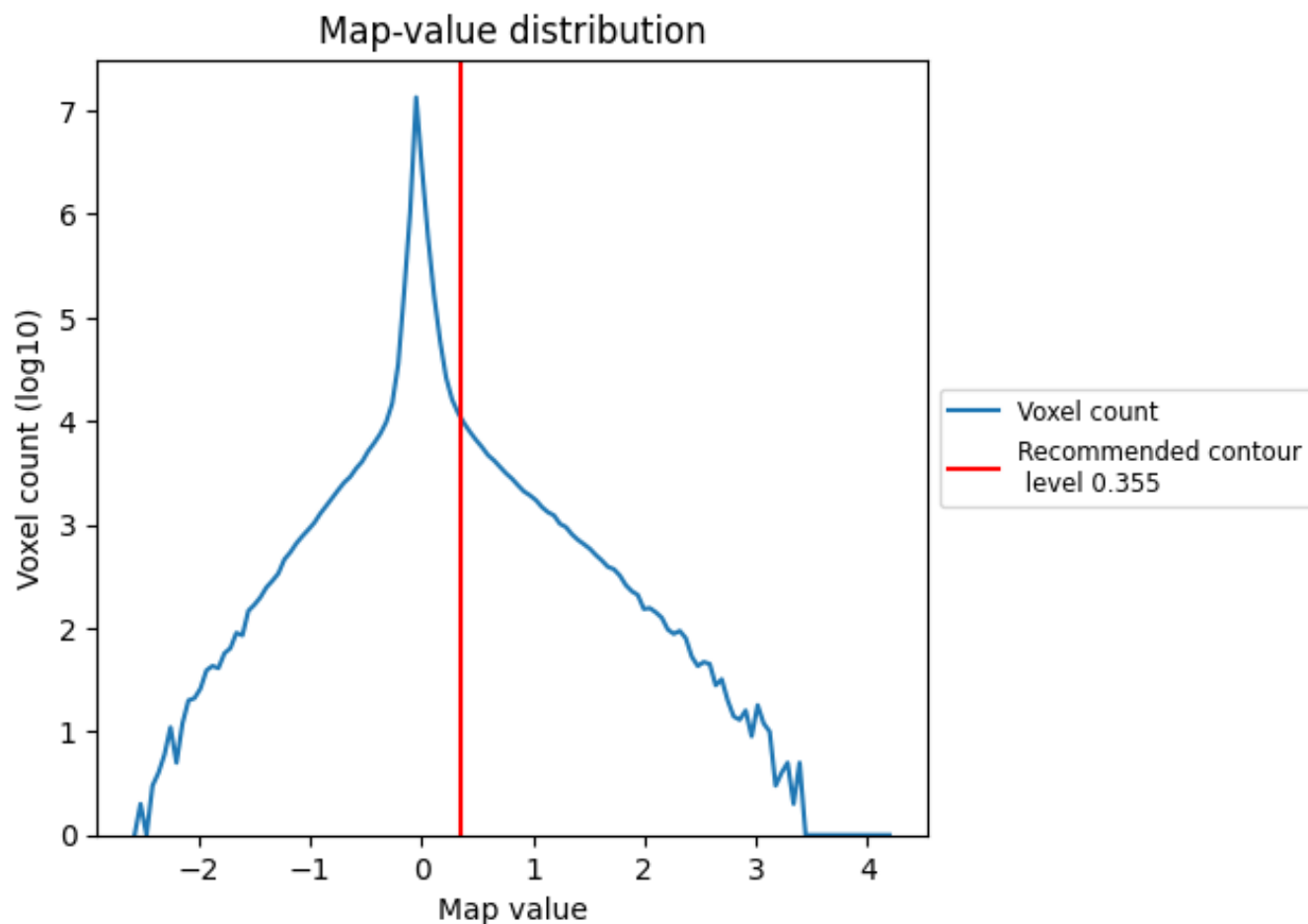
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

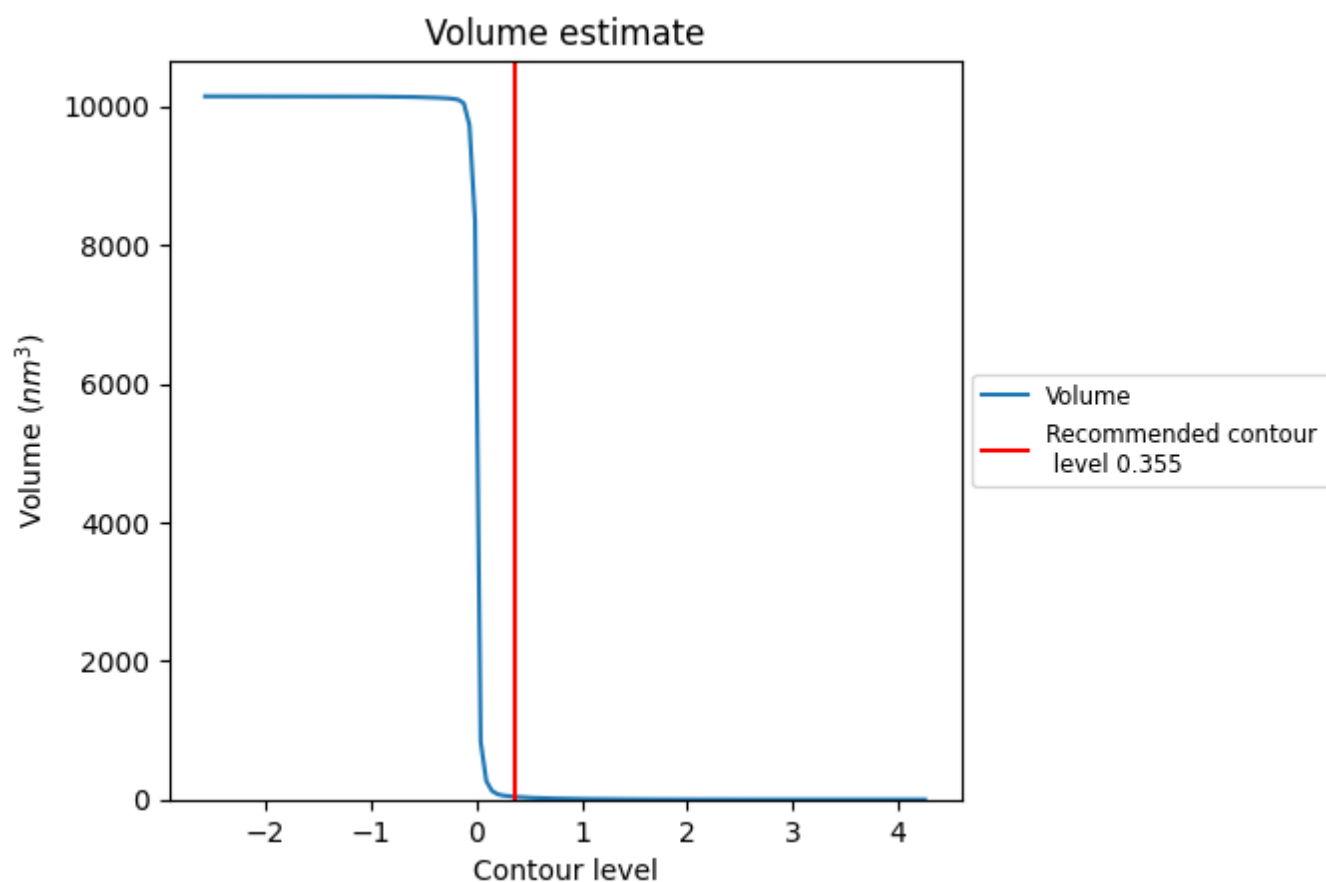
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

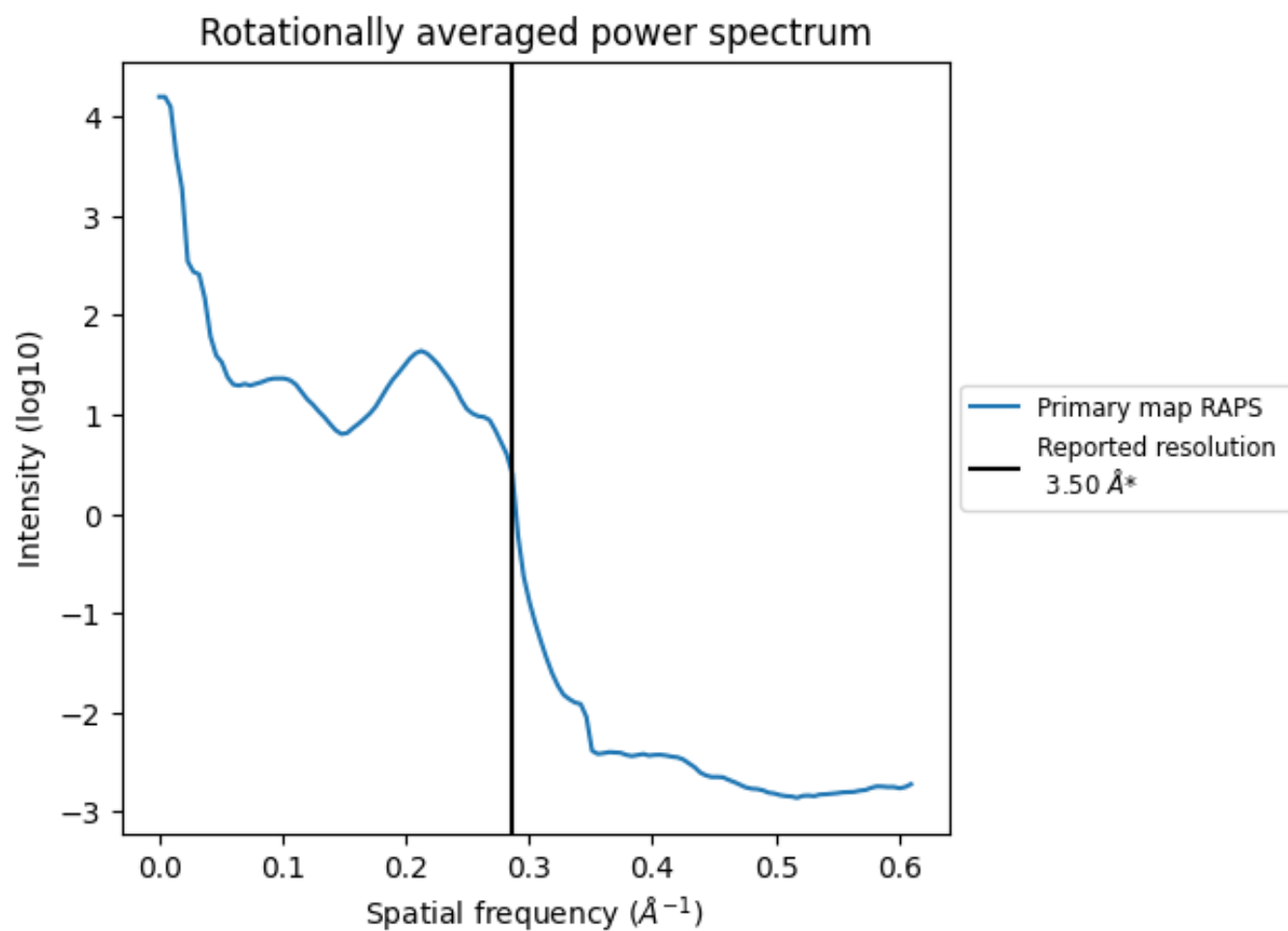
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 41 nm^3 ; this corresponds to an approximate mass of 37 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

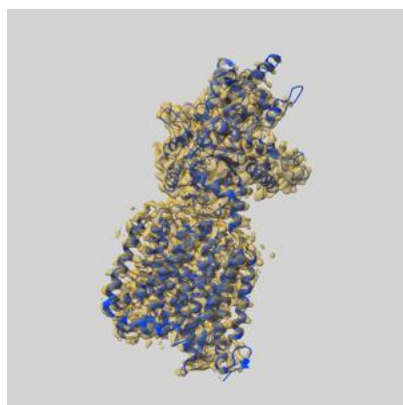
8 Fourier-Shell correlation ⓘ

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

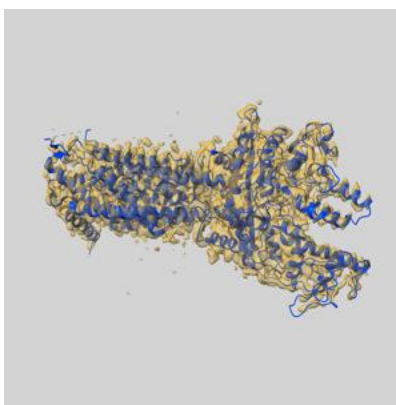
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31753 and PDB model 7V6Y. Per-residue inclusion information can be found in section [3](#) on page [6](#).

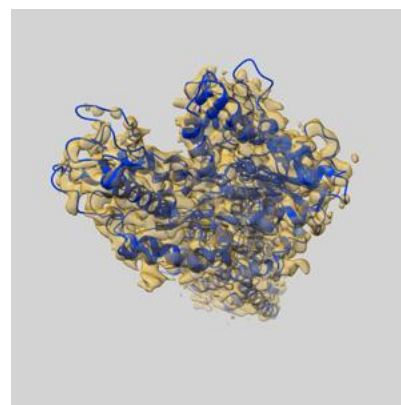
9.1 Map-model overlay [i](#)



X



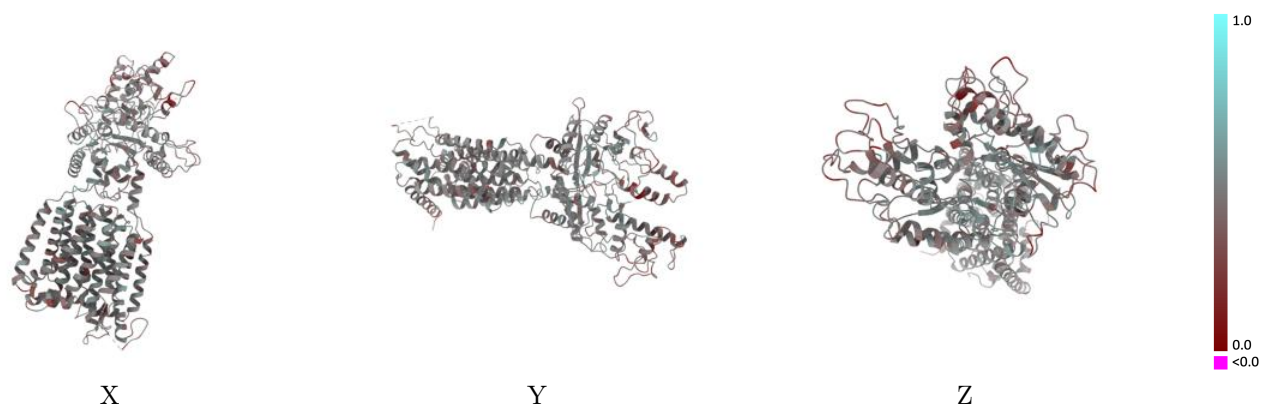
Y



Z

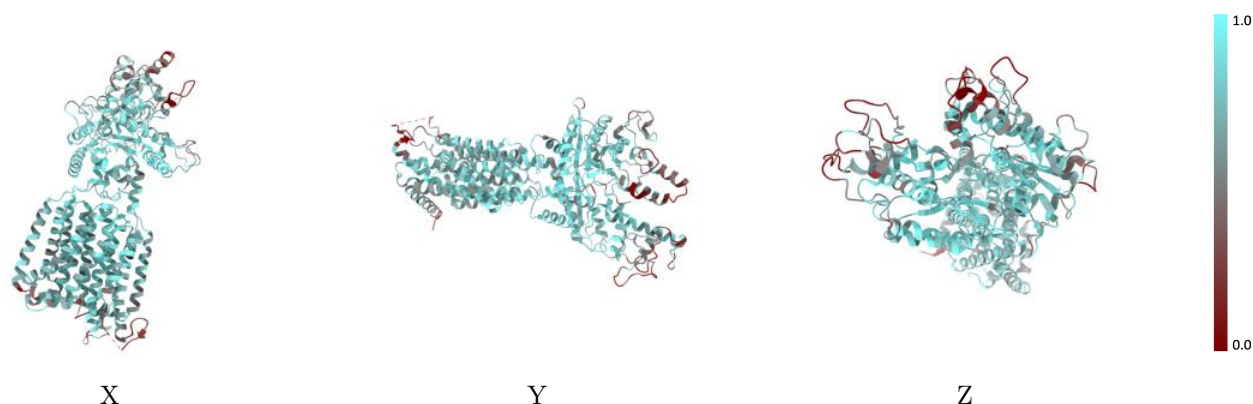
The images above show the 3D surface view of the map at the recommended contour level 0.355 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



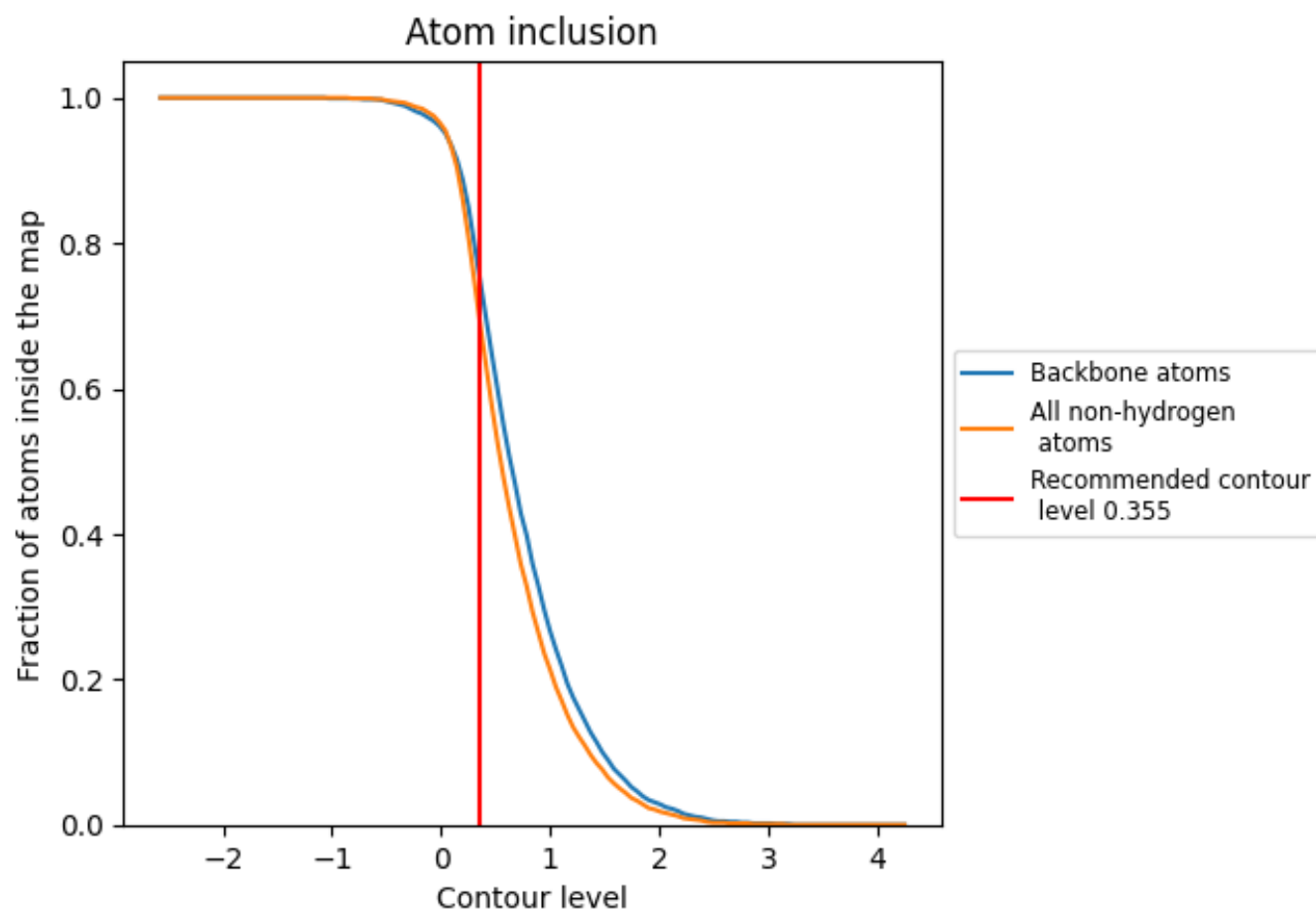
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.355).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.355) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6930	<div></div> 0.4480
A	<div></div> 0.6940	<div></div> 0.4480
B	<div></div> 0.4290	<div></div> 0.4010

