



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:02 PM UTC

PDB ID : 7KY6 / pdb_00007ky6
EMDB ID : EMD-23069
Title : Structure of the *S. cerevisiae* phosphatidylcholine flippase Dnf1-Lem3 complex in the apo E1 state
Authors : Bai, L.; You, Q.; Jain, B.K.; Duan, H.D.; Kovach, A.; Graham, T.R.; Li, H.
Deposited on : 2020-12-07
Resolution : 3.10 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:

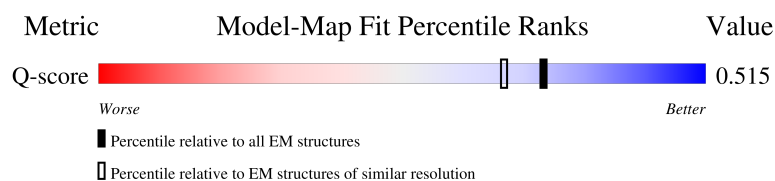
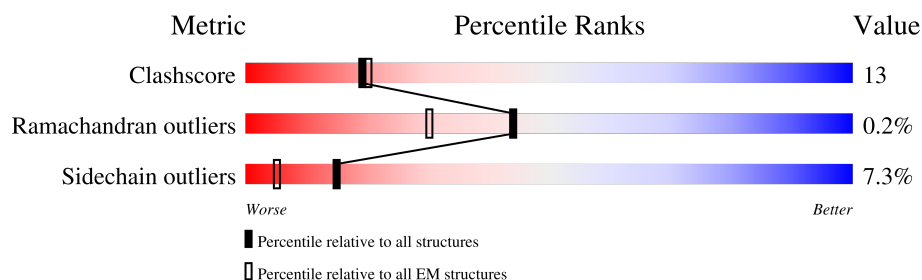
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1571	
2	B	414	
3	C	3	
4	D	2	

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Mol	Chain	Length	Quality of chain
4	E	2	50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10729 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.

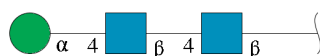
- Molecule 1 is a protein called Phospholipid-transporting ATPase DNF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	957	Total	C	N	O	S	0	0
			7646	4964	1250	1396	36		

- Molecule 2 is a protein called Alkylphosphocholine resistance protein LEM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	365	Total	C	N	O	S	0	0
			2959	1899	499	547	14		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	3	Total	C	N	O	0	0
			39	22	2	15		

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

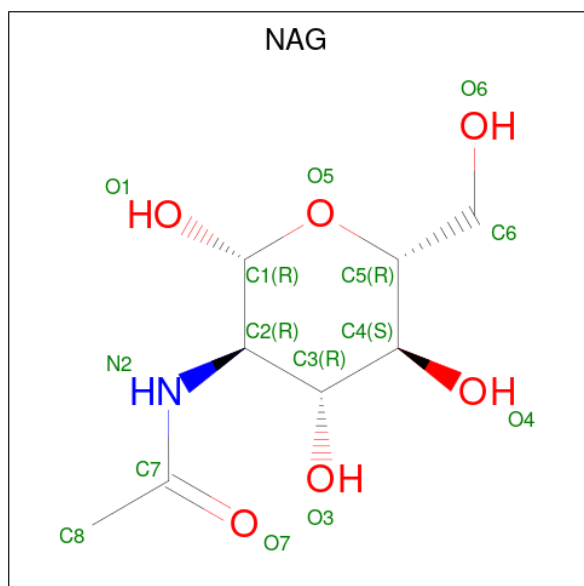


Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

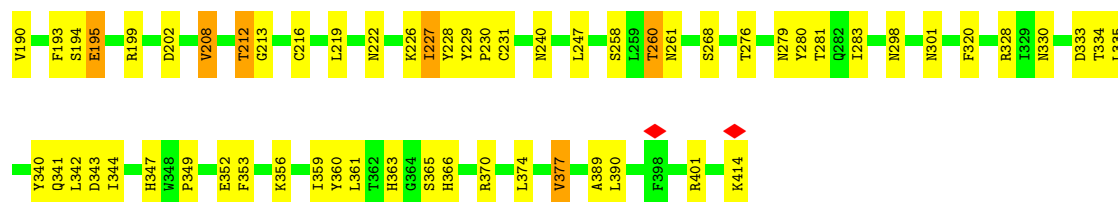
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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



- Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50%
100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50%
50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	473761	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.017	Depositor
Map size ($\text{\AA}$)	231.28, 231.28, 231.28	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.826, 0.826, 0.826	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, MG, MAN

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	0.25	0/7820	0.43	0/10592
2	B	0.29	0/3042	0.39	1/4136 (0.0%)
All	All	0.26	0/10862	0.42	1/14728 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	170	LYS	CB-CA-C	-5.34	110.40	116.54

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	7646	0	7644	215	0
2	B	2959	0	2866	71	0
3	C	39	0	34	2	0
4	D	28	0	25	0	0
4	E	28	0	25	1	0
5	A	1	0	0	0	0
6	B	28	0	26	1	0
All	All	10729	0	10620	272	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 13.

All (272) 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:169:MET:SD	2:B:335:LEU:HD23	1.89	1.11
2:B:170:LYS:O	2:B:334:THR:HG23	1.58	1.04
1:A:1353:THR:HG21	1:A:1373:TYR:CE2	1.96	1.01
1:A:1350:PHE:O	1:A:1353:THR:HG22	1.63	0.97
1:A:1320:VAL:HG11	1:A:1349:VAL:HG21	1.53	0.91
1:A:1353:THR:HG21	1:A:1373:TYR:HE2	1.34	0.87
1:A:1353:THR:CG2	1:A:1373:TYR:HE2	1.89	0.85
1:A:819:THR:HG23	1:A:824:ILE:HD11	1.69	0.74
1:A:723:ARG:NH2	1:A:744:VAL:O	2.23	0.72
1:A:855:ILE:O	1:A:864:PRO:HA	1.88	0.71
1:A:1266:ASN:N	1:A:1266:ASN:OD1	2.24	0.70
1:A:909:ARG:HB2	1:A:963:ILE:HD12	1.74	0.70
1:A:1237:LEU:HD12	1:A:1327:VAL:HG13	1.74	0.70
1:A:1353:THR:HG21	1:A:1373:TYR:CZ	2.26	0.70
2:B:169:MET:HB2	2:B:335:LEU:HB3	1.71	0.70
2:B:170:LYS:O	2:B:334:THR:HA	1.91	0.70
1:A:671:THR:O	1:A:968:GLN:NE2	2.25	0.69
1:A:1331:GLN:HE22	1:A:1338:SER:HB3	1.56	0.68
1:A:1176:HIS:O	1:A:1177:GLY:C	2.36	0.68
1:A:1209:ASN:ND2	1:A:1214:SER:OG	2.27	0.68
1:A:1007:ASN:ND2	1:A:1008:ASN:O	2.27	0.67
2:B:170:LYS:O	2:B:334:THR:CG2	2.40	0.67
1:A:835:GLU:HB2	1:A:854:LYS:HB2	1.77	0.66
1:A:1195:ASN:OD1	1:A:1196:MET:N	2.28	0.66
1:A:840:LEU:HB3	1:A:846:ARG:HH22	1.61	0.66
1:A:1107:PRO:HB3	1:A:1133:ASN:HB3	1.78	0.66
2:B:180:GLU:HB2	2:B:356:LYS:HB2	1.78	0.65
1:A:1145:ILE:HD13	1:A:1161:TYR:HB2	1.78	0.65
1:A:1133:ASN:OD1	1:A:1133:ASN:N	2.29	0.65
2:B:154:LYS:NZ	2:B:352:GLU:OE2	2.27	0.65
2:B:194:SER:OG	2:B:231:CYS:SG	2.51	0.65
1:A:702:LYS:HE3	1:A:708:VAL:HG21	1.79	0.64
1:A:1014:VAL:HG12	1:A:1016:LYS:H	1.63	0.64
1:A:671:THR:HG23	1:A:1147:ILE:HG13	1.80	0.63
2:B:169:MET:CE	2:B:361:LEU:HD23	2.28	0.63
1:A:585:TYR:HE2	2:B:353:PHE:HE1	1.46	0.63
2:B:169:MET:CE	2:B:361:LEU:CD2	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:VAL:O	2:B:370:ARG:NH1	2.31	0.63
1:A:782:VAL:HB	1:A:792:LEU:HD12	1.81	0.63
1:A:1384:VAL:HG21	2:B:377:VAL:HG13	1.80	0.63
2:B:301:ASN:HD22	6:B:1001:NAG:H61	1.65	0.62
1:A:924:GLU:O	1:A:928:GLU:HG2	2.00	0.62
1:A:1350:PHE:O	1:A:1353:THR:CG2	2.43	0.62
1:A:1196:MET:O	1:A:1197:ILE:C	2.41	0.61
1:A:1353:THR:HG21	1:A:1373:TYR:OH	2.01	0.61
1:A:764:GLN:O	1:A:768:GLU:HG2	2.01	0.61
1:A:1138:ILE:HG23	1:A:1144:GLY:HA3	1.83	0.60
1:A:1095:LYS:HD3	1:A:1121:LEU:HD21	1.81	0.60
1:A:1194:LYS:HG3	1:A:1195:ASN:N	2.15	0.60
1:A:865:ARG:HD2	1:A:919:SER:HA	1.82	0.60
2:B:258:SER:O	2:B:330:ASN:ND2	2.35	0.60
1:A:749:LYS:HA	1:A:752:VAL:HG12	1.84	0.59
1:A:752:VAL:O	1:A:756:LYS:NZ	2.36	0.59
1:A:1332:TYR:O	1:A:1412:ARG:NH2	2.34	0.59
1:A:1174:LEU:O	1:A:1175:VAL:C	2.43	0.59
2:B:169:MET:HE2	2:B:361:LEU:CD2	2.33	0.59
1:A:655:SER:O	1:A:658:LEU:HB2	2.03	0.58
1:A:1353:THR:HG23	1:A:1354:GLY:N	2.18	0.58
2:B:154:LYS:NZ	3:C:2:NAG:O7	2.31	0.58
1:A:1028:GLU:HG2	1:A:1029:PRO:HD2	1.85	0.58
2:B:169:MET:HE1	2:B:361:LEU:HD23	1.84	0.58
1:A:710:THR:HA	1:A:713:ARG:HG2	1.85	0.57
1:A:1022:VAL:HG22	1:A:1032:ILE:HD13	1.86	0.57
2:B:151:ASP:OD1	2:B:151:ASP:N	2.37	0.57
1:A:788:ASN:HB3	1:A:791:LYS:HD2	1.85	0.57
1:A:984:LYS:HG2	1:A:1098:ARG:HA	1.87	0.57
2:B:103:VAL:HG13	2:B:128:PHE:HE1	1.69	0.57
1:A:754:ASP:HA	1:A:758:ALA:HB3	1.86	0.57
2:B:105:ILE:HD12	2:B:359:ILE:HD11	1.87	0.57
2:B:176:ASN:HD22	2:B:360:TYR:HD2	1.52	0.57
2:B:79:TYR:HB3	2:B:389:ALA:HB2	1.86	0.57
1:A:1054:ILE:HD13	1:A:1092:LEU:HD12	1.86	0.56
1:A:1030:SER:HB3	1:A:1079:LEU:HD22	1.85	0.56
1:A:774:LEU:HD23	1:A:808:ALA:HB2	1.88	0.56
2:B:143:ARG:NH2	2:B:160:GLN:OE1	2.38	0.56
1:A:1324:ASN:HB3	1:A:1342:ILE:HG23	1.87	0.55
1:A:1353:THR:CG2	1:A:1373:TYR:CE2	2.71	0.55
2:B:169:MET:HE1	2:B:361:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:LEU:O	1:A:1175:VAL:O	2.24	0.55
1:A:866:ALA:HB3	1:A:918:LEU:HB2	1.87	0.55
1:A:1412:ARG:HH21	2:B:67:ASN:HD22	1.55	0.55
1:A:1021:ASP:HA	1:A:1024:GLU:HG2	1.88	0.54
1:A:1218:GLU:OE2	1:A:1356:TRP:NE1	2.39	0.54
1:A:1393:ARG:NH1	1:A:1397:ASP:OD1	2.40	0.54
1:A:237:VAL:HG11	2:B:187:ARG:HD3	1.89	0.54
1:A:733:LEU:HD22	1:A:756:LYS:HE3	1.89	0.54
1:A:798:SER:OG	1:A:800:ASP:OD1	2.24	0.54
1:A:571:ASN:HD22	1:A:601:SER:HB3	1.72	0.53
1:A:774:LEU:HD11	1:A:804:LEU:HD22	1.89	0.53
2:B:162:ARG:HE	2:B:341:GLN:HE21	1.55	0.53
1:A:701:ARG:HE	1:A:706:ILE:HD13	1.74	0.53
1:A:679:PHE:HE2	1:A:961:THR:HB	1.73	0.53
1:A:1377:SER:O	1:A:1381:VAL:HG23	2.08	0.53
1:A:601:SER:HA	1:A:604:VAL:HG12	1.89	0.53
1:A:726:MET:HG3	1:A:752:VAL:HG11	1.90	0.53
1:A:706:ILE:HD12	1:A:706:ILE:H	1.73	0.53
1:A:206:PHE:O	1:A:210:ASN:HB2	2.08	0.53
1:A:878:TYR:HA	1:A:881:LEU:HD21	1.90	0.53
1:A:914:ALA:HB1	1:A:955:LEU:HB3	1.91	0.53
1:A:610:GLN:O	1:A:613:VAL:HG12	2.09	0.52
2:B:170:LYS:HG2	2:B:363:HIS:NE2	2.23	0.52
1:A:237:VAL:O	1:A:238:THR:OG1	2.23	0.52
1:A:738:GLN:HE22	1:A:792:LEU:H	1.58	0.52
2:B:162:ARG:HE	2:B:341:GLN:NE2	2.07	0.52
1:A:729:GLU:OE2	1:A:749:LYS:NZ	2.42	0.52
1:A:1128:ILE:HD11	1:A:1147:ILE:HD11	1.91	0.52
1:A:223:PHE:O	1:A:227:ILE:HG13	2.10	0.51
1:A:668:LYS:HD3	1:A:989:THR:HG22	1.92	0.51
1:A:1246:ASP:OD1	1:A:1246:ASP:N	2.41	0.51
1:A:780:VAL:HG21	1:A:805:VAL:HG21	1.92	0.51
1:A:780:VAL:HG22	1:A:796:ALA:HB2	1.92	0.51
1:A:1016:LYS:HG2	1:A:1018:THR:HG23	1.93	0.51
1:A:1176:HIS:O	1:A:1177:GLY:O	2.28	0.51
1:A:1258:VAL:HG22	1:A:1263:LYS:HB2	1.93	0.51
1:A:1047:LEU:HD11	1:A:1092:LEU:HD21	1.91	0.51
1:A:256:ILE:O	1:A:260:ILE:HG13	2.11	0.50
1:A:922:GLU:HA	1:A:925:LYS:HE2	1.92	0.50
1:A:654:ILE:HD11	1:A:1160:ASP:HB3	1.93	0.50
1:A:1155:ALA:O	1:A:1159:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1296:MET:HE1	2:B:320:PHE:HD2	1.76	0.50
1:A:625:LYS:HE3	1:A:1184:LEU:HD11	1.94	0.50
1:A:1381:VAL:HG22	2:B:374:LEU:HD21	1.92	0.50
1:A:596:THR:O	1:A:600:VAL:HG23	2.11	0.50
1:A:723:ARG:O	1:A:727:ILE:HG13	2.12	0.50
1:A:776:LEU:HD22	1:A:869:ILE:HD11	1.94	0.50
1:A:549:LEU:HD11	1:A:617:LEU:HD21	1.94	0.49
1:A:1243:ASP:OD2	1:A:1243:ASP:N	2.39	0.49
1:A:257:LYS:O	1:A:261:GLU:HG2	2.12	0.49
1:A:1051:GLU:CD	1:A:1051:GLU:H	2.20	0.49
2:B:260:THR:OG1	4:E:1:NAG:H83	2.13	0.49
2:B:342:LEU:HD23	2:B:344:ILE:HD11	1.95	0.49
2:B:365:SER:OG	2:B:366:HIS:N	2.46	0.49
1:A:608:LEU:HD12	1:A:1215:TYR:CE1	2.48	0.49
1:A:943:GLU:O	1:A:947:VAL:HG23	2.12	0.49
1:A:797:GLN:OE1	1:A:797:GLN:N	2.46	0.49
1:A:1179:TRP:O	1:A:1180:SER:C	2.56	0.49
2:B:194:SER:OG	2:B:216:CYS:SG	2.70	0.49
1:A:969:ASP:HB3	1:A:1432:PRO:HG2	1.95	0.49
1:A:843:ASN:ND2	1:A:846:ARG:HD3	2.28	0.48
1:A:1371:ARG:HH21	2:B:268:SER:HG	1.56	0.48
2:B:208:VAL:HG13	2:B:216:CYS:SG	2.53	0.48
1:A:549:LEU:HD13	1:A:1188:ILE:HD13	1.96	0.48
1:A:1184:LEU:O	1:A:1185:ALA:C	2.55	0.48
2:B:193:PHE:HE1	2:B:195:GLU:HG2	1.78	0.48
1:A:809:ARG:HG3	1:A:814:SER:HB3	1.95	0.48
1:A:943:GLU:HA	1:A:946:VAL:HG12	1.96	0.48
1:A:640:ASN:HB2	1:A:1168:TYR:HE2	1.79	0.48
1:A:790:LYS:HA	1:A:790:LYS:HD2	1.78	0.48
1:A:1225:TYR:HA	1:A:1229:PHE:HB2	1.95	0.48
1:A:257:LYS:HE2	1:A:622:GLU:HB3	1.96	0.47
1:A:779:SER:OG	1:A:797:GLN:NE2	2.47	0.47
2:B:175:LEU:HB3	2:B:328:ARG:HB2	1.96	0.47
2:B:261:ASN:HB3	2:B:328:ARG:NH2	2.28	0.47
1:A:223:PHE:HB3	1:A:247:LEU:HD13	1.97	0.47
1:A:796:ALA:HB3	1:A:802:ALA:HB2	1.96	0.47
2:B:101:ASP:HA	2:B:129:VAL:O	2.13	0.47
1:A:744:VAL:HG22	1:A:810:ASP:HB3	1.94	0.47
1:A:1186:GLU:OE2	1:A:1273:TYR:OH	2.26	0.47
1:A:717:ALA:O	1:A:721:LYS:HG2	2.14	0.47
1:A:1020:ASP:OD2	1:A:1020:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:ILE:HA	1:A:1036:LEU:HD13	1.97	0.47
2:B:146:ASP:OD2	2:B:147:ASP:N	2.47	0.47
2:B:162:ARG:HA	2:B:340:TYR:O	2.15	0.47
2:B:222:ASN:HB3	2:B:228:TYR:CE1	2.50	0.46
1:A:832:LYS:NZ	1:A:833:GLU:O	2.48	0.46
2:B:169:MET:CE	2:B:361:LEU:HD21	2.45	0.46
1:A:940:ARG:O	1:A:943:GLU:HG2	2.15	0.46
1:A:1063:PHE:CD2	1:A:1064:PRO:HD2	2.51	0.46
1:A:1353:THR:CG2	1:A:1354:GLY:N	2.77	0.46
1:A:250:ILE:HD12	1:A:615:ILE:HG12	1.98	0.46
1:A:636:VAL:H	2:B:60:GLN:HE22	1.62	0.45
1:A:222:TYR:CE2	1:A:226:LEU:HD11	2.51	0.45
1:A:697:LEU:O	1:A:701:ARG:HG2	2.16	0.45
1:A:1035:ALA:O	1:A:1039:LYS:HG2	2.17	0.45
1:A:1438:THR:OG1	1:A:1439:LYS:N	2.49	0.45
1:A:1086:ILE:HD12	1:A:1086:ILE:H	1.81	0.45
1:A:713:ARG:HG3	1:A:714:ARG:N	2.31	0.45
1:A:727:ILE:HG23	1:A:739:PHE:HZ	1.81	0.45
1:A:249:VAL:HG11	1:A:1227:LEU:HD21	1.99	0.45
1:A:977:LEU:HD11	1:A:1429:PRO:HG2	1.98	0.45
2:B:142:TRP:HA	2:B:160:GLN:O	2.17	0.45
1:A:954:GLU:O	1:A:955:LEU:HD23	2.16	0.45
1:A:776:LEU:HD11	1:A:853:VAL:HG21	1.99	0.44
2:B:186:HIS:O	2:B:190:VAL:HG23	2.16	0.44
1:A:725:THR:O	1:A:729:GLU:HG3	2.17	0.44
1:A:1064:PRO:O	1:A:1098:ARG:NH2	2.50	0.44
1:A:770:PHE:HB3	1:A:771:MET:HE2	1.99	0.44
1:A:942:ASP:O	1:A:945:GLU:HG3	2.18	0.44
1:A:1001:PHE:HE2	1:A:1012:LEU:HD11	1.83	0.44
2:B:414:LYS:HD3	2:B:414:LYS:N	2.32	0.44
1:A:795:LYS:HA	1:A:795:LYS:HD3	1.86	0.44
1:A:973:ASP:HA	1:A:976:GLU:HG2	2.00	0.44
1:A:1073:ASP:OD2	1:A:1073:ASP:N	2.50	0.44
1:A:767:CYS:O	1:A:771:MET:HG2	2.18	0.44
1:A:679:PHE:HZ	1:A:682:CYS:HB3	1.82	0.44
1:A:1345:SER:O	1:A:1348:VAL:HG12	2.18	0.44
2:B:128:PHE:CZ	2:B:140:PRO:HG3	2.53	0.43
1:A:1353:THR:HG23	1:A:1373:TYR:HE2	1.80	0.43
2:B:111:MET:HE2	2:B:111:MET:HB3	1.78	0.43
1:A:800:ASP:OD1	1:A:800:ASP:N	2.51	0.43
1:A:925:LYS:O	1:A:929:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:THR:O	1:A:1022:VAL:HG23	2.19	0.43
1:A:748:SER:HB3	1:A:751:PHE:HB3	2.00	0.43
1:A:801:GLU:O	1:A:805:VAL:HG22	2.19	0.43
1:A:1110:LYS:O	1:A:1114:VAL:HG23	2.18	0.43
2:B:229:TYR:HB3	2:B:230:PRO:HD3	2.00	0.43
1:A:1070:ILE:HB	1:A:1100:VAL:HG22	2.01	0.43
1:A:696:ALA:HB3	1:A:906:GLU:O	2.19	0.43
1:A:822:GLY:HA3	1:A:834:PHE:O	2.19	0.43
1:A:874:ASP:HA	1:A:912:CYS:SG	2.59	0.43
1:A:877:ILE:HG21	1:A:957:LEU:HD12	2.01	0.43
2:B:240:ASN:HB3	2:B:347:HIS:HB3	2.01	0.43
1:A:585:TYR:OH	2:B:349:PRO:O	2.33	0.43
1:A:815:PHE:HD2	1:A:823:LEU:HD13	1.84	0.43
1:A:1391:LEU:HD22	1:A:1391:LEU:HA	1.82	0.43
2:B:279:ASN:C	2:B:281:THR:H	2.27	0.43
1:A:1243:ASP:HB2	1:A:1408:VAL:HG21	2.01	0.42
1:A:557:PHE:CE1	1:A:613:VAL:HG23	2.54	0.42
1:A:582:ARG:NH2	1:A:589:THR:O	2.52	0.42
1:A:1191:PHE:HA	1:A:1194:LYS:HG2	2.00	0.42
1:A:1195:ASN:O	1:A:1196:MET:C	2.62	0.42
1:A:1308:ARG:CZ	2:B:190:VAL:HG11	2.49	0.42
1:A:800:ASP:O	1:A:804:LEU:HG	2.19	0.42
1:A:1376:PRO:HG2	2:B:366:HIS:O	2.20	0.42
2:B:195:GLU:O	2:B:199:ARG:HG3	2.20	0.42
1:A:222:TYR:O	1:A:226:LEU:HG	2.20	0.42
1:A:1201:ALA:HB3	1:A:1217:TYR:OH	2.20	0.42
1:A:1305:LEU:HD21	1:A:1371:ARG:HB3	2.01	0.42
2:B:212:THR:HG22	2:B:213:GLY:H	1.84	0.42
2:B:227:ILE:O	2:B:283:ILE:HA	2.19	0.42
1:A:856:PRO:HA	1:A:864:PRO:HB3	2.02	0.42
2:B:202:ASP:OD1	2:B:202:ASP:N	2.36	0.42
1:A:821:LYS:NZ	1:A:836:ILE:O	2.49	0.42
1:A:725:THR:HB	1:A:749:LYS:HE3	2.02	0.42
1:A:840:LEU:HB3	1:A:846:ARG:NH2	2.31	0.42
1:A:719:ILE:HD12	1:A:719:ILE:HA	1.77	0.42
1:A:818:LYS:NZ	1:A:823:LEU:HB3	2.35	0.41
1:A:1029:PRO:HA	1:A:1032:ILE:HD12	2.02	0.41
1:A:1128:ILE:HA	1:A:1145:ILE:O	2.20	0.41
1:A:1189:PRO:O	1:A:1190:GLU:C	2.62	0.41
1:A:1242:GLN:NE2	2:B:61:GLN:HB3	2.35	0.41
1:A:587:PHE:CE2	2:B:219:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ARG:NH2	1:A:711:GLU:OE2	2.53	0.41
1:A:915:GLN:HG2	1:A:958:LEU:HD21	2.01	0.41
1:A:688:SER:HB2	1:A:899:HIS:CD2	2.55	0.41
1:A:1237:LEU:HG	1:A:1331:GLN:HG2	2.03	0.41
2:B:222:ASN:HD21	2:B:226:LYS:HD2	1.86	0.41
1:A:989:THR:O	1:A:1105:VAL:HG22	2.20	0.41
1:A:1107:PRO:HB3	1:A:1133:ASN:CB	2.47	0.41
1:A:1200:LEU:HD13	1:A:1278:LEU:HD12	2.02	0.41
2:B:170:LYS:O	2:B:334:THR:CA	2.65	0.41
1:A:265:ARG:HD3	1:A:265:ARG:HA	1.94	0.41
1:A:1184:LEU:HD23	1:A:1184:LEU:HA	1.80	0.41
1:A:1413:GLU:CD	2:B:401:ARG:HH12	2.28	0.41
1:A:617:LEU:HB2	1:A:1191:PHE:CE2	2.56	0.41
1:A:640:ASN:HB2	1:A:1168:TYR:CE2	2.54	0.41
1:A:738:GLN:HG3	1:A:809:ARG:HD2	2.03	0.41
2:B:240:ASN:ND2	3:C:1:NAG:O7	2.54	0.41
1:A:738:GLN:NE2	1:A:792:LEU:H	2.17	0.41
1:A:1137:MET:HE2	1:A:1137:MET:HB3	1.95	0.41
1:A:1177:GLY:O	1:A:1178:ARG:C	2.64	0.41
2:B:135:THR:O	2:B:135:THR:OG1	2.37	0.41
1:A:769:HIS:NE2	1:A:915:GLN:OE1	2.54	0.40
1:A:814:SER:OG	1:A:826:GLU:HB3	2.21	0.40
1:A:874:ASP:OD1	1:A:874:ASP:N	2.53	0.40
2:B:56:ASP:HB3	2:B:59:THR:HG23	2.02	0.40
1:A:989:THR:OG1	1:A:1102:CYS:O	2.33	0.40
1:A:1058:LYS:HA	1:A:1121:LEU:HD12	2.03	0.40
2:B:170:LYS:HB2	2:B:363:HIS:CD2	2.57	0.40
1:A:941:GLU:OE1	1:A:941:GLU:N	2.55	0.40
1:A:1299:THR:OG1	1:A:1303:LEU:O	2.31	0.40
1:A:1357:SER:O	1:A:1359:ALA:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	951/1571 (60%)	884 (93%)	65 (7%)	2 (0%)	43	73
2	B	363/414 (88%)	337 (93%)	26 (7%)	0	100	100
All	All	1314/1985 (66%)	1221 (93%)	91 (7%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1098	ARG
1	A	1175	VAL

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	823/1367 (60%)	768 (93%)	55 (7%)	15	43
2	B	321/364 (88%)	292 (91%)	29 (9%)	9	33
All	All	1144/1731 (66%)	1060 (93%)	84 (7%)	15	40

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	LEU
1	A	228	ILE
1	A	229	LEU
1	A	251	VAL
1	A	256	ILE
1	A	543	SER
1	A	548	GLU
1	A	566	VAL
1	A	569	ILE
1	A	606	VAL
1	A	607	ILE

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Mol	Chain	Res	Type
1	A	612	LEU
1	A	622	GLU
1	A	683	THR
1	A	687	VAL
1	A	695	GLU
1	A	715	GLU
1	A	719	ILE
1	A	747	VAL
1	A	801	GLU
1	A	840	LEU
1	A	855	ILE
1	A	869	ILE
1	A	920	TRP
1	A	963	ILE
1	A	964	GLU
1	A	975	ILE
1	A	985	LEU
1	A	995	THR
1	A	1006	LEU
1	A	1048	THR
1	A	1101	LEU
1	A	1108	SER
1	A	1133	ASN
1	A	1145	ILE
1	A	1150	GLU
1	A	1151	GLU
1	A	1193	TYR
1	A	1227	LEU
1	A	1234	VAL
1	A	1246	ASP
1	A	1258	VAL
1	A	1266	ASN
1	A	1291	VAL
1	A	1295	ASN
1	A	1299	THR
1	A	1323	CYS
1	A	1344	LEU
1	A	1348	VAL
1	A	1360	ILE
1	A	1362	SER
1	A	1377	SER
1	A	1391	LEU

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Mol	Chain	Res	Type
1	A	1400	GLN
1	A	1434	ARG
2	B	69	VAL
2	B	71	THR
2	B	78	LEU
2	B	81	LEU
2	B	87	VAL
2	B	101	ASP
2	B	112	THR
2	B	113	ASN
2	B	135	THR
2	B	150	ASP
2	B	151	ASP
2	B	165	THR
2	B	169	MET
2	B	170	LYS
2	B	171	ASN
2	B	176	ASN
2	B	195	GLU
2	B	208	VAL
2	B	212	THR
2	B	227	ILE
2	B	247	LEU
2	B	260	THR
2	B	276	THR
2	B	280	TYR
2	B	298	ASN
2	B	333	ASP
2	B	343	ASP
2	B	377	VAL
2	B	390	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	ASN
1	A	640	ASN
1	A	660	GLN
1	A	738	GLN
1	A	843	ASN
1	A	927	ASN
1	A	939	ASN

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Mol	Chain	Res	Type
1	A	1046	ASN
1	A	1165	GLN
1	A	1267	GLN
1	A	1293	HIS
1	A	1330	HIS
1	A	1331	GLN
1	A	1419	HIS
2	B	60	GLN
2	B	67	ASN
2	B	125	HIS
2	B	186	HIS
2	B	341	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

7 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	$\# Z > 2$
3	NAG	C	1	3,2	14,14,15	0.56	0	17,19,21	0.54	0
3	NAG	C	2	3	14,14,15	0.39	0	17,19,21	0.48	0
3	MAN	C	3	3	11,11,12	0.77	0	15,15,17	1.24	2 (13%)
4	NAG	D	1	2,4	14,14,15	0.44	0	17,19,21	0.56	0
4	NAG	D	2	4	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	E	1	2,4	14,14,15	0.35	0	17,19,21	0.40	0
4	NAG	E	2	4	14,14,15	0.22	0	17,19,21	0.41	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
3	NAG	C	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	MAN	C	3	3	-	2/2/19/22	1/1/1/1
4	NAG	D	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	MAN	C1-O5-C5	3.60	117.01	112.19
3	C	3	MAN	O2-C2-C3	-2.51	104.94	110.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	C	3	MAN	O5-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

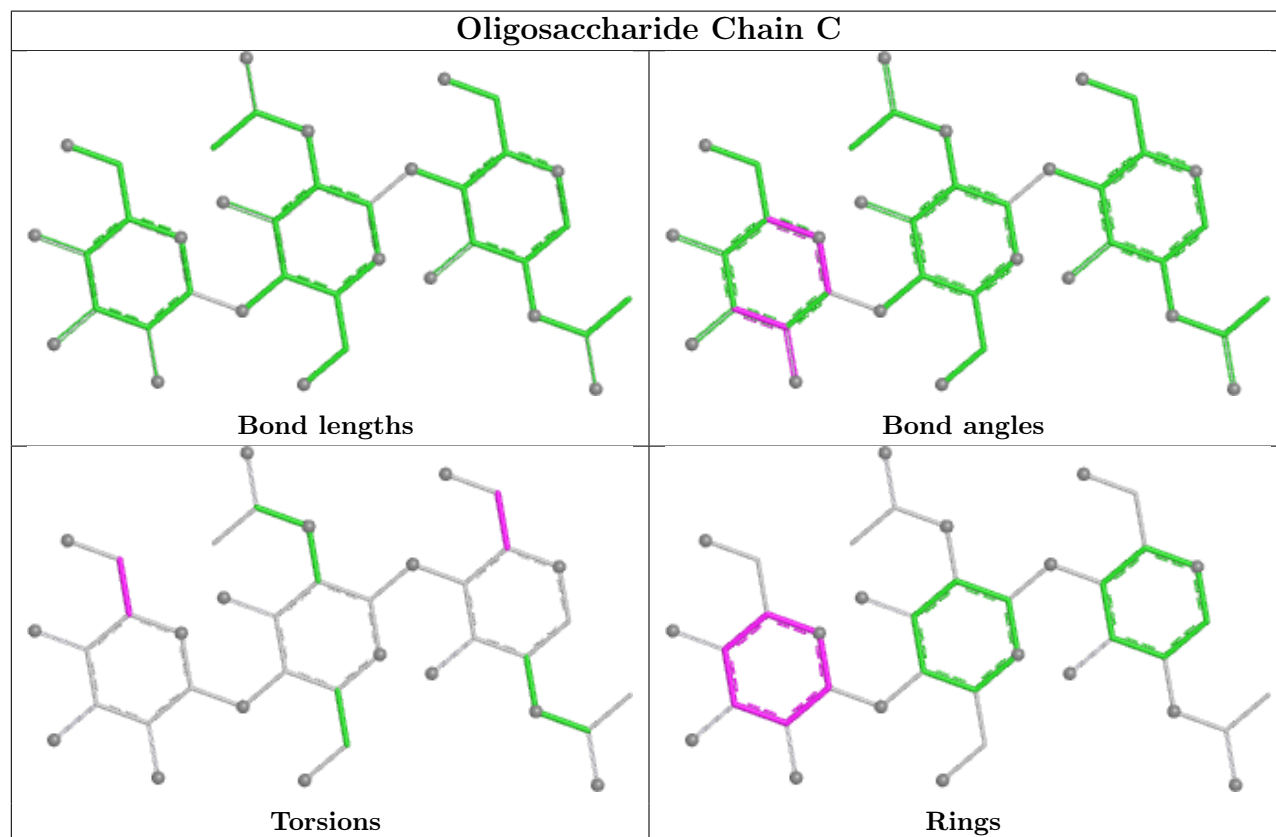
All (1) ring outliers are listed below:

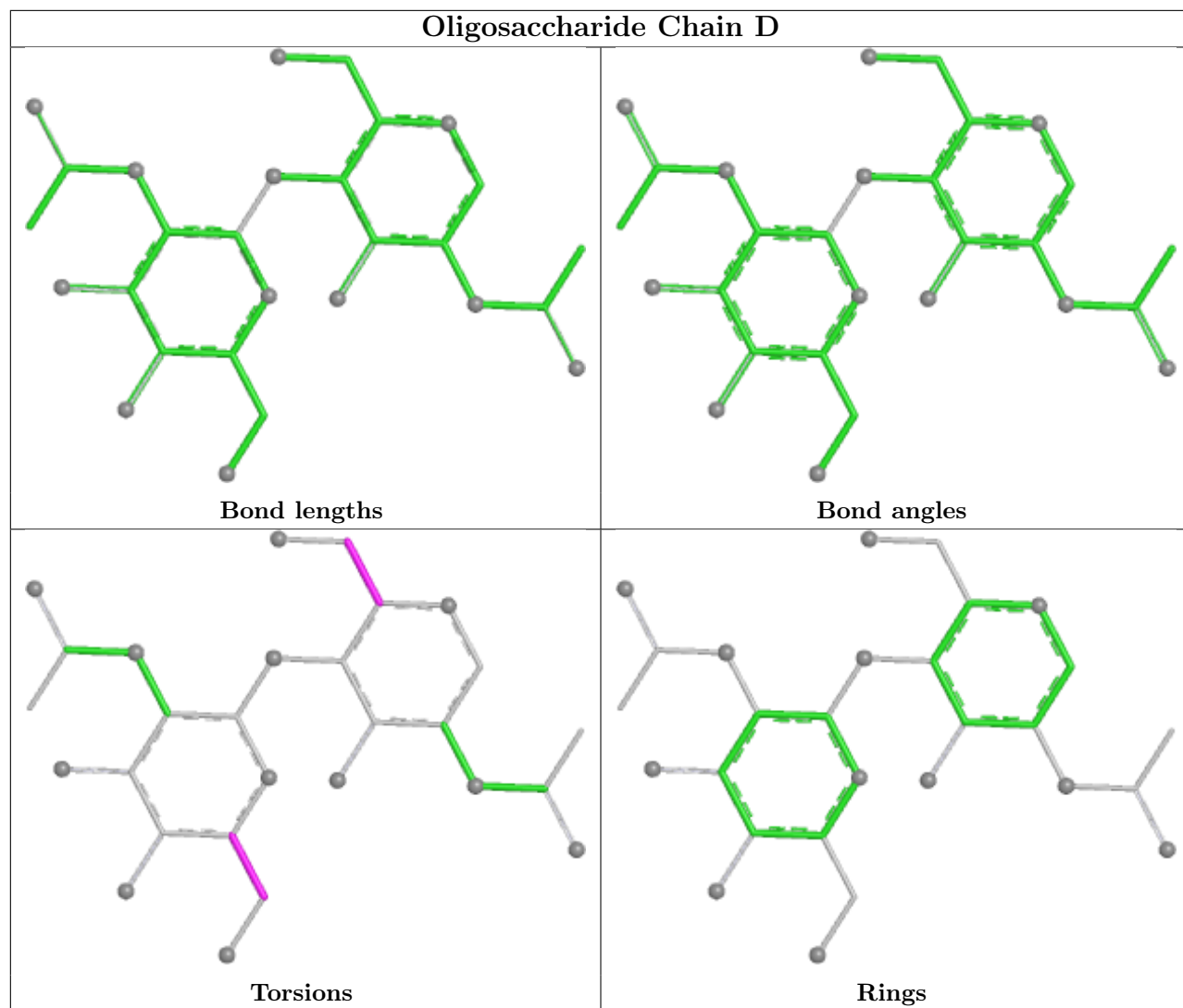
Mol	Chain	Res	Type	Atoms
3	C	3	MAN	C1-C2-C3-C4-C5-O5

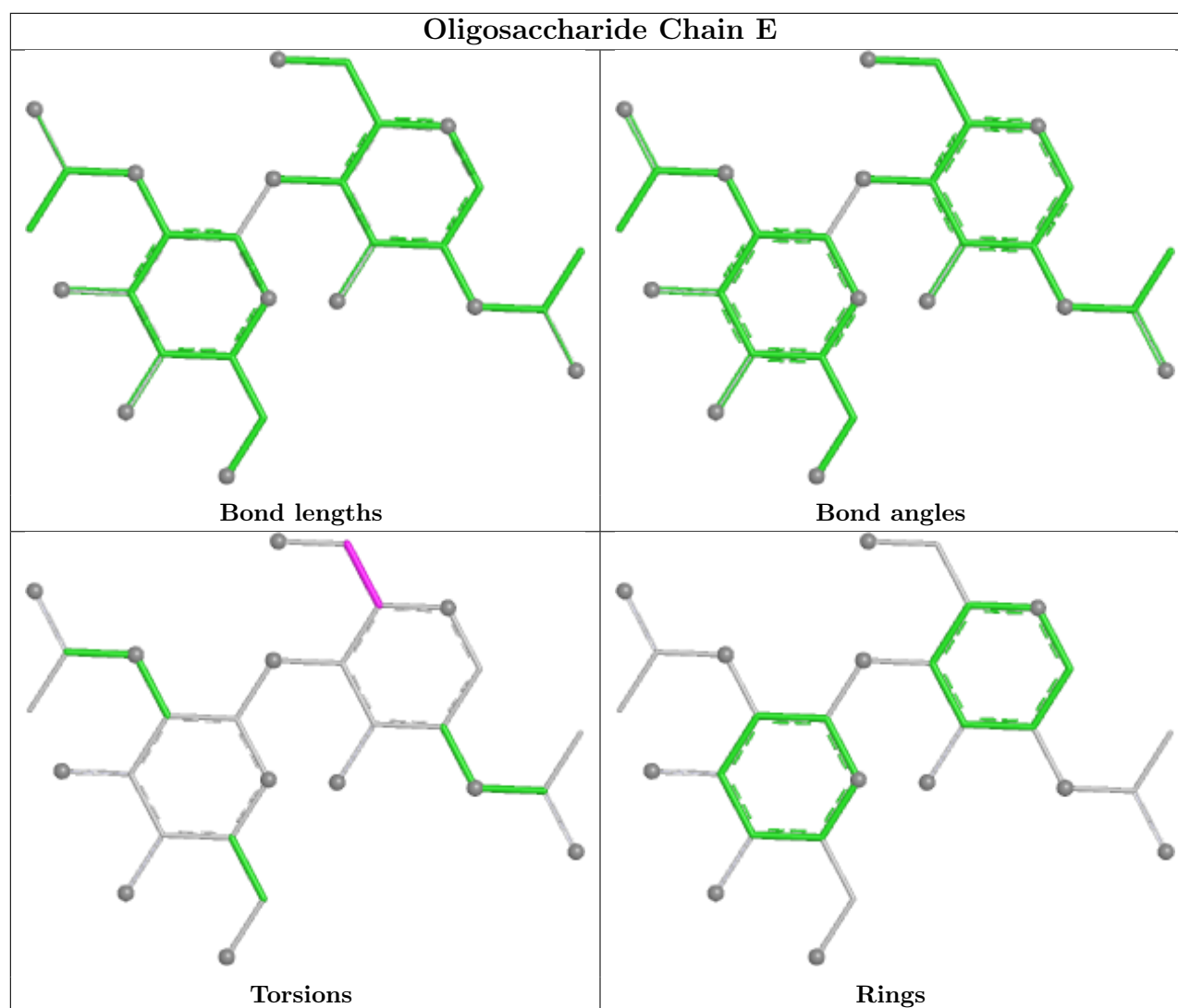
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0
3	C	1	NAG	1	0
3	C	2	NAG	1	0

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 [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
6	NAG	B	1002	2	14,14,15	0.16	0	17,19,21	0.51	0
6	NAG	B	1001	2	14,14,15	0.31	0	17,19,21	0.50	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
6	NAG	B	1002	2	-	0/6/23/26	0/1/1/1
6	NAG	B	1001	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1001	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1001	NAG	1	0

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.

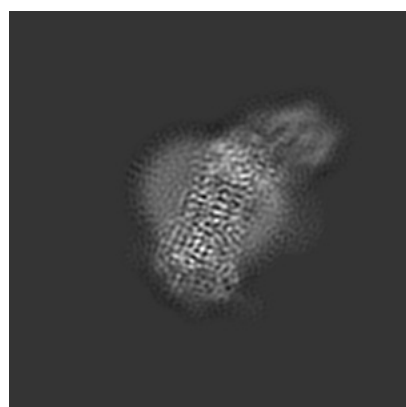
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23069. These allow visual inspection of the internal detail of the map and identification of artifacts.

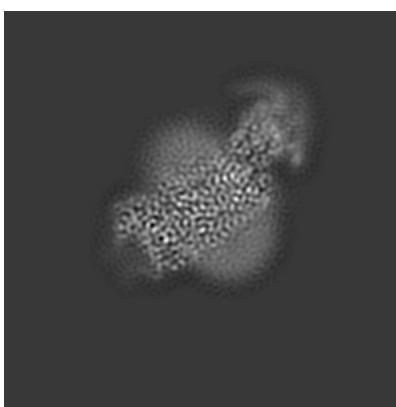
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

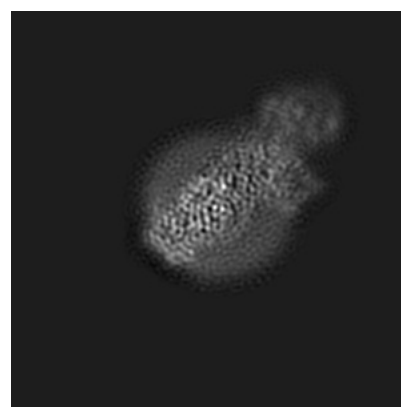
6.1.1 Primary map



X



Y

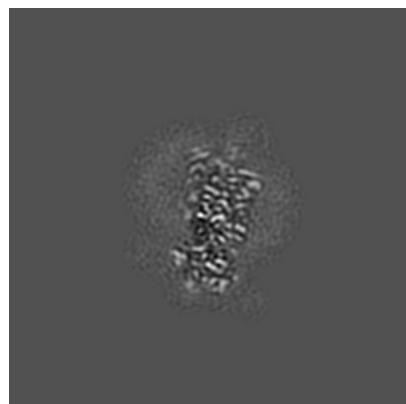


Z

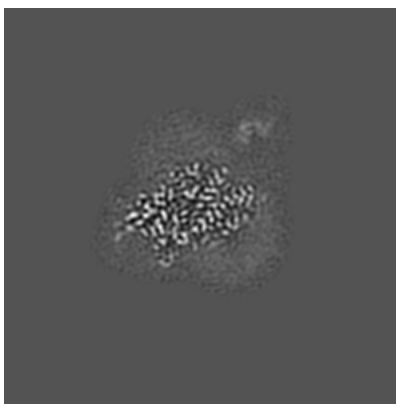
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

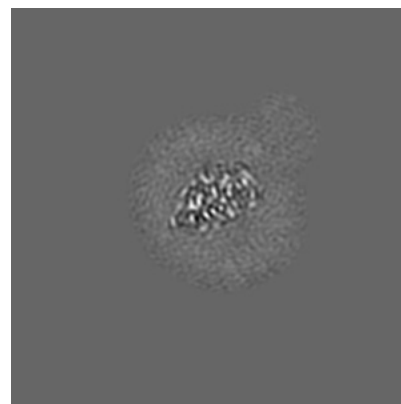
6.2.1 Primary map



X Index: 140



Y Index: 140

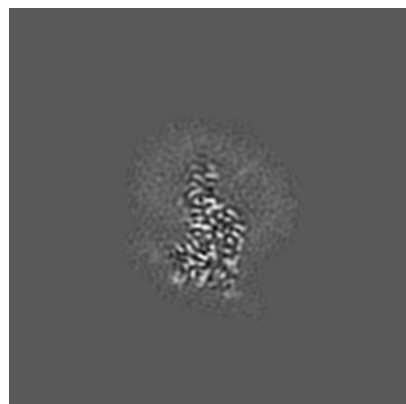


Z Index: 140

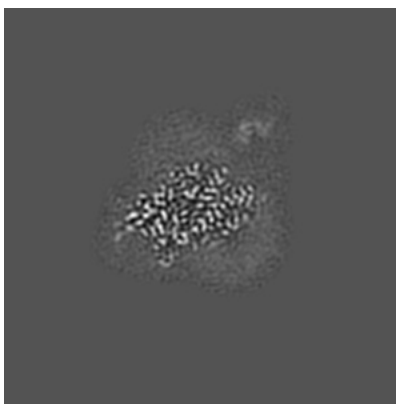
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

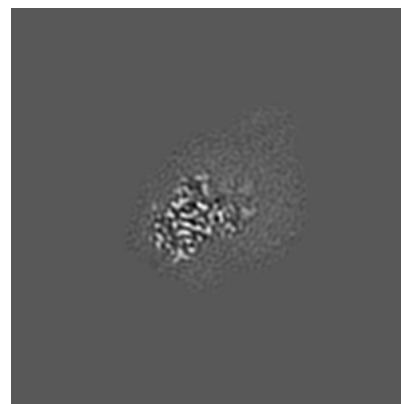
6.3.1 Primary map



X Index: 131



Y Index: 140

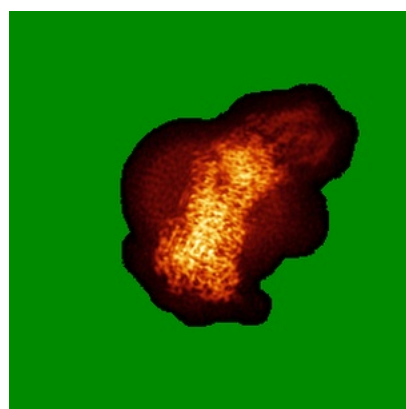


Z Index: 112

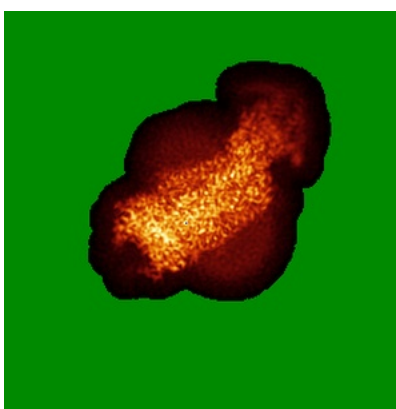
The images above show the largest variance slices of the map in three orthogonal directions.

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

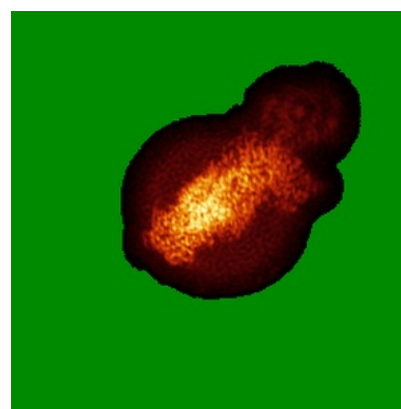
6.4.1 Primary map



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

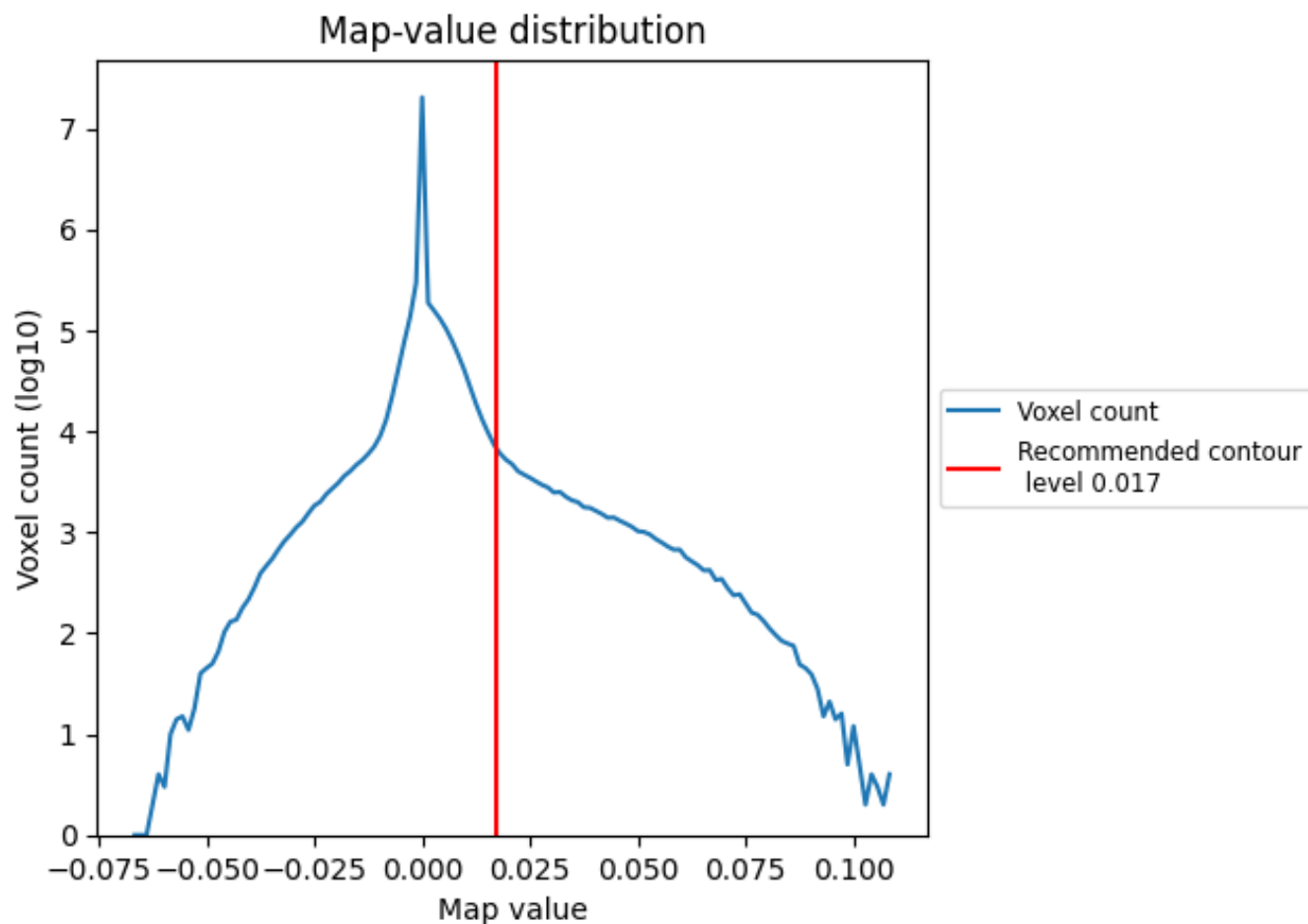
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

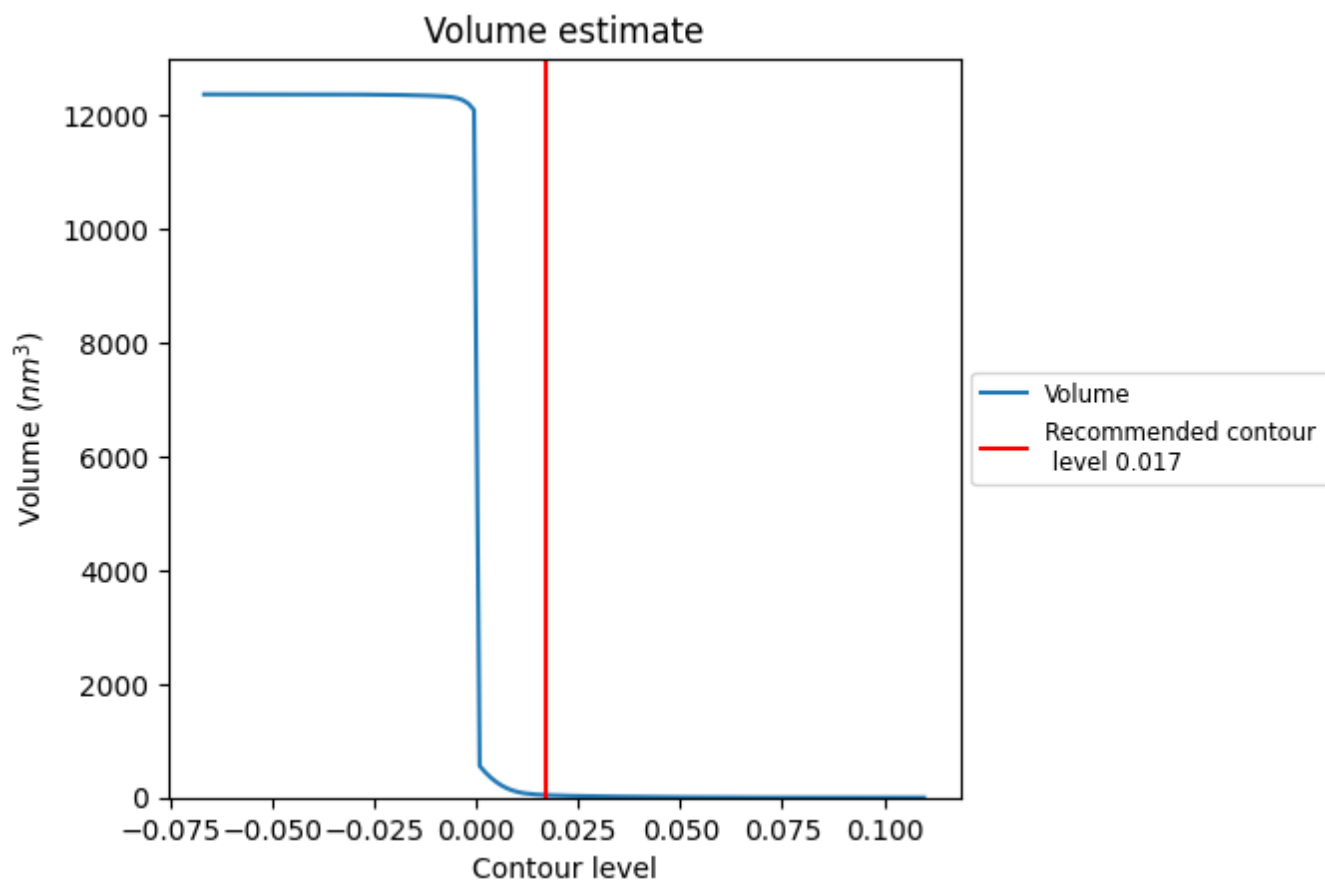
This section contains the results of statistical analysis of the map.

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.

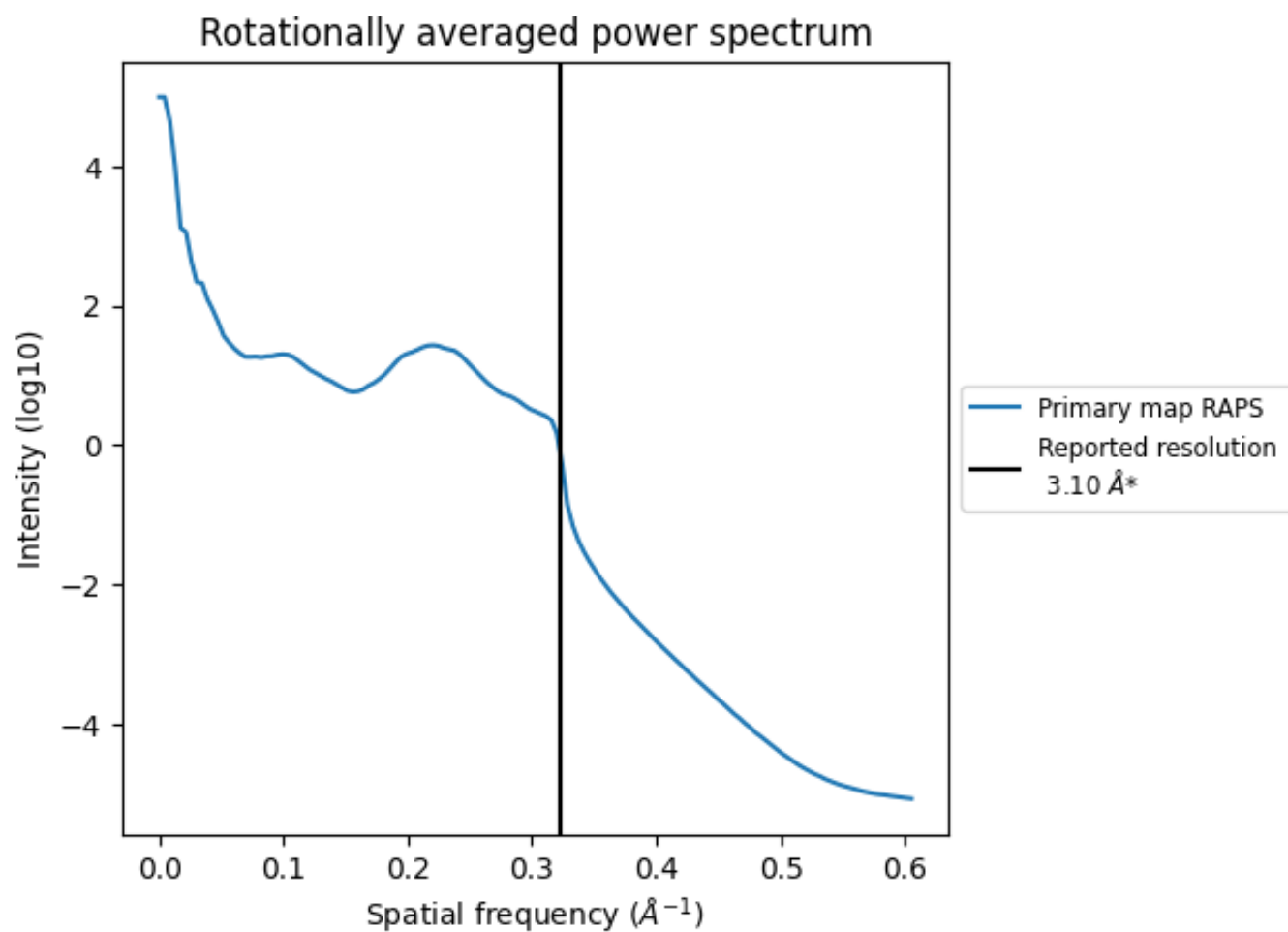
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 44 nm³; this corresponds to an approximate mass of 40 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 0.323 Å⁻¹

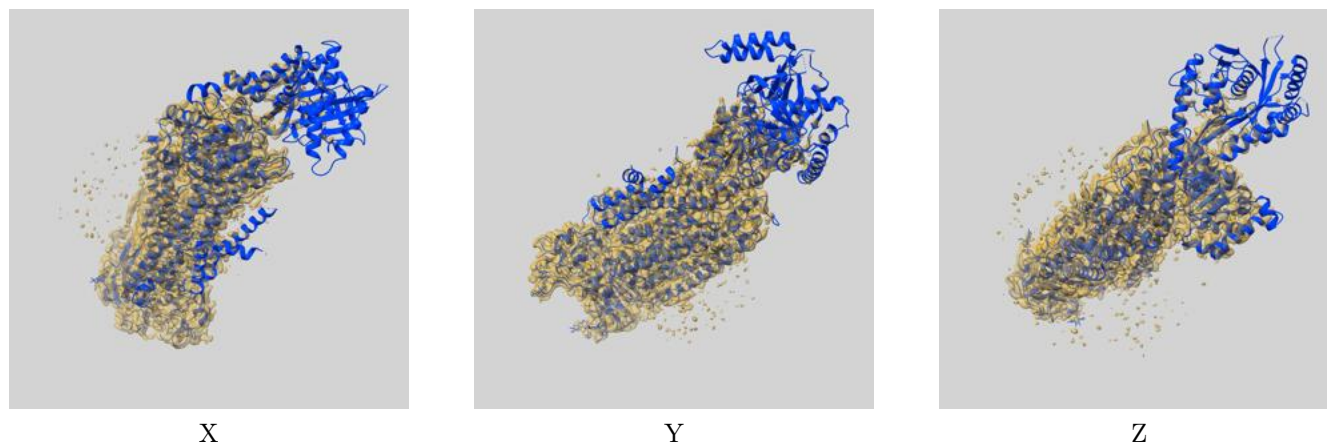
8 Fourier-Shell correlation

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-23069 and PDB model 7KY6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



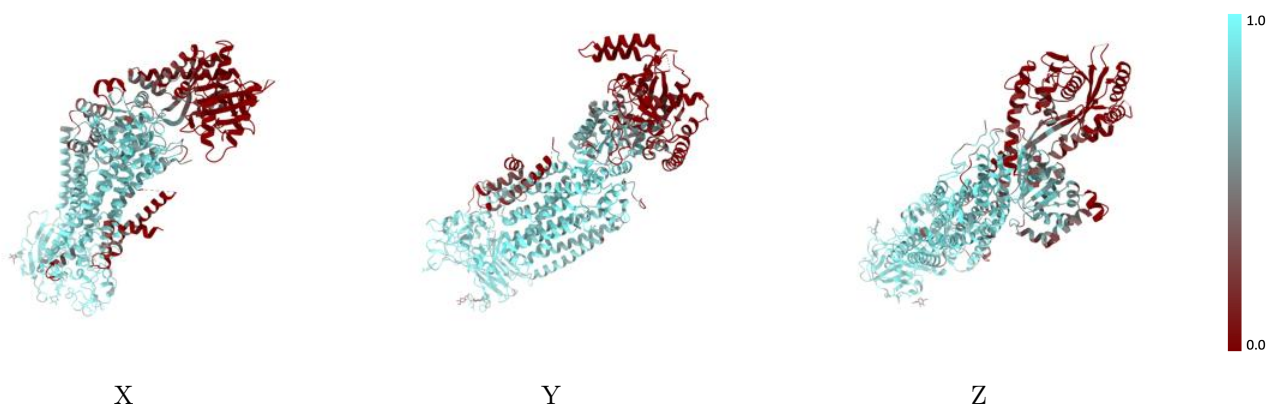
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



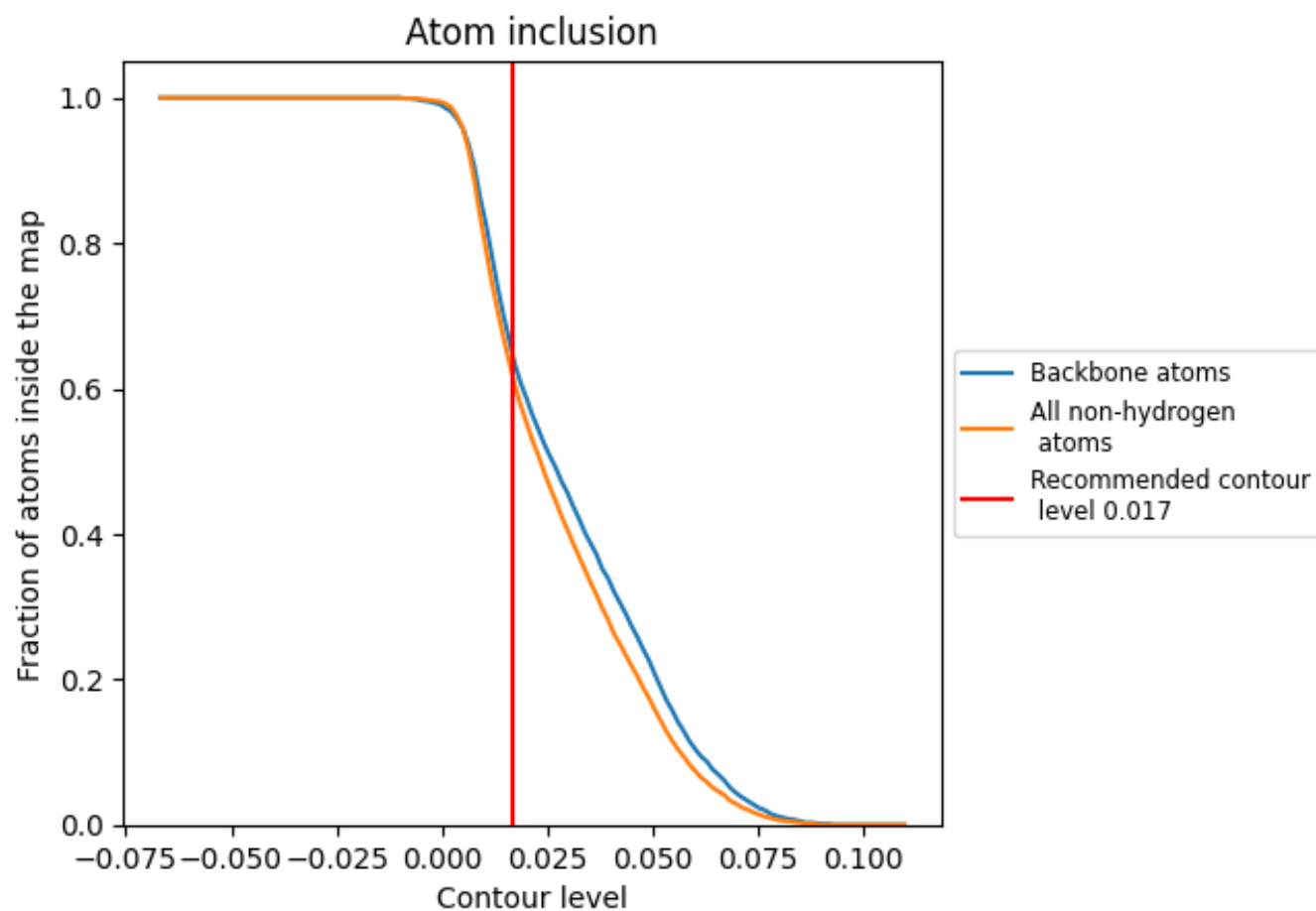
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 61% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6120	0.5150
A	0.5250	0.4930
B	0.8340	0.5710
C	0.8720	0.5560
D	0.5000	0.4840
E	0.5360	0.5360

