



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:08 AM UTC

PDB ID : 7KY5 / pdb_00007ky5
EMDB ID : EMD-23068
Title : Structure of the *S. cerevisiae* phosphatidylcholine flippase Dnf2-Lem3 complex in the E2P transition 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 : 3.98 Å(reported)

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

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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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

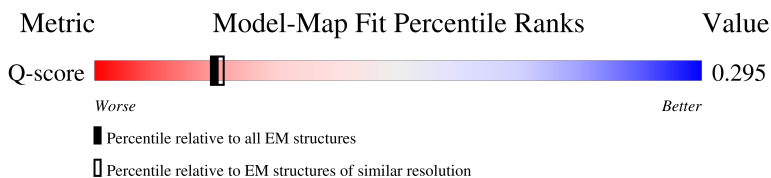
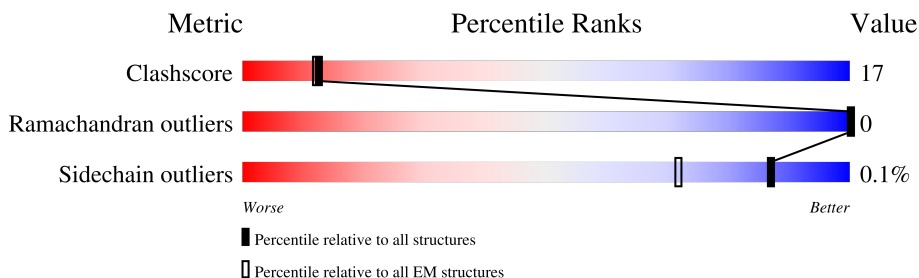
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.98 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	7512 (3.48 - 4.48)

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	1612	31% 47% 25% 28%
2	B	414	18% 59% 30% 11%
3	C	3	100%
3	D	3	100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12483 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.

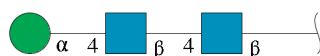
- Molecule 1 is a protein called Phospholipid-transporting ATPase DNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1165	9297	5976	1543	1730	48	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	369	2974	1908	501	551	14	0	0

- 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.



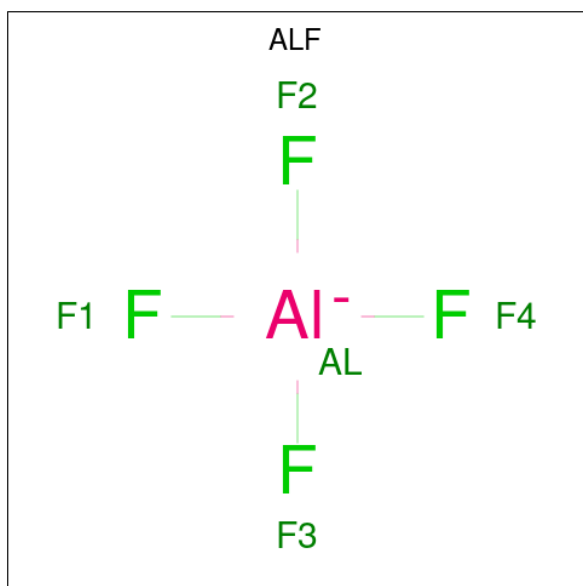
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	3	39	22	2	15	0	0
3	D	3	39	22	2	15	0	0

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 5 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Al	F	0
			5	1	4	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



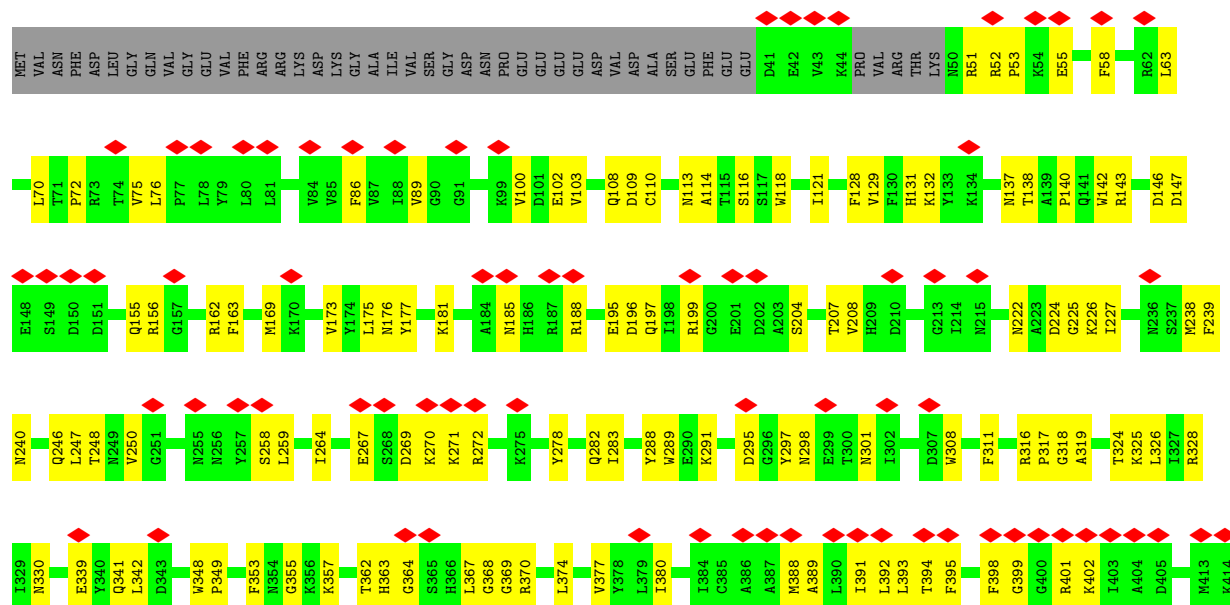
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			15	8	1	6	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			15	8	1	6	

ASN	ASN	ASP	A1417	V1340	F1260	G1187	A1119	G1046	N952	D919	G857	D788	E723	F644
LEU	LEU	PHE	Q1418	V1341	E1261	V1188	A1123	N1047	R983	S920	N958	D789	F724	F644
PRO	PRO	GLY	P1419	T1342	Y1262	G1192	L1124	V1048	E984	V921	S959	L789	K725	W648
ARG	ARG	ILE	W1422	L1346	Y1263	G1193	N1126	L1049	E985	I922	F960	V649	K726	V649
SER	SER	SER	A1423	L1347	T1265	E1194	G1126	N1051	E986	R925	G862	V791	K727	I652
MET	MET	LEU	V1424	G1347	F1267	G1195	E1127	D1052	N987	L926	S863	V792	I728	L653
ALA	ALA	ASP	V1427	L1348	F1267	G1195	E1128	D1052	N988	D927	S864	K794	I729	L653
SER	SER	THR	G1428	N1268	M1200	M1200	M1129	L1056	K989	R928	K865	V795	N730	L657
SER	SER	THR	V1429	D1349	N1269	C1201	R1130	V1057	G989	T929	K865	V796	Y734	L657
GLY	GLY	PHE	L1430	H1350	L1270	S1202	R1131	V1058	T991	Q930	S866	V797	G735	V658
ASN	ASN	ASP	F1431	R1351	A1271	D1203	K1132	K1059	D992	N931	S867	V798	R736	V659
LYS	LYS	GLY	C1432	F1352	F1272	Y1204	F1133	A1060	V993	D932	L868	V799	L741	I660
LEU	LEU	VAL	C1433	V1354	T1273	A1205	F1136	S1061	I994	A933	L869	L800	A742	S861
SER	SER	SER	L1434	G1355	S1274	I1206	L1136	G1062	E995	T934	V870	L801	A743	L862
ARG	ARG	HIS	L1435	V1356	G1207	G1207	C1137	E1063	R996	R935	I871	K801	A744	L863
THR	THR	SER	P1435	F1357	Q1208	F1208	L1144	E1064	R997	L936	E872	G802	E740	I664
SER	SER	GLN	R1436	V1358	F1209	F1209	K1141	D1065	E998	L937	G874	S903	E741	E667
ASP	ASP	THR	I1439	A1360	Y1211	V1212	A1142	V1066	I999	K938	Q877	S904	L742	I668
THR	THR	ILE	I1442	V1363	V1216	V1216	V1143	E1067	L1000	T939	Q877	G905	A743	I669
ARG	ARG	VAL	R1443	F1368	L1217	L1217	L1144	F1068	L1001	A940	E878	D806	G744	Q673
GLY	GLY	GLY	K1444	Y1369	V1218	V1218	C1145	G1069	G1002	L941	F879	Q808	L745	A674
GLY	GLY	ILE	I1445	V1370	H1219	H1219	C1147	S1070	I1006	H942	Q880	Q809	R746	I675
LEU	LEU	PRO	F1446	F1371	K1221	K1221	P1150	D1071	I1007	L943	V881	L832	L746	Y678
ASN	ASN	MET	Y1447	M1372	W1222	W1222	A1151	L1079	D1008	E945	N884	K810	ARG	Y678
SER	SER	ILE	P1448	E1373	Y1224	Y1224	Q1152	K1082	R1009	Y946	N884	H814	GLN	V681
LEU	LEU	ILE	D1450	Q1374	Y1301	Y1301	A1154	E1085	Q1011	A947	L885	F815	GLY	V681
ASP	ASP	ASN	I1453	Y1375	G1302	G1302	A1155	E1086	D1012	T948	E886	L817	D752	K687
THR	THR	GLY	W1377	R1376	R1226	R1226	V1156	F1087	G1013	R952	N888	L819	E754	L688
GLY	GLY	GLY	F1380	W1377	A1228	A1228	V1157	F1088	V1014	R952	S889	A820	E755	D689
VAL	VAL	SER	C1381	R1380	E1229	E1229	K1158	G1089	D1015	C955	R891	L821	E756	P691
ARG	ARG	ARG	G1382	K1305	Q1233	Q1233	V1159	M1090	D1016	L955	K892	V825	G757	C892
GLY	GLY	TYR	L1383	K1306	F1234	F1234	V1160	S1091	S1017	L957	R893	K331	G758	P694
ALA	ALA	ALA	F1384	N1307	F1235	F1235	K1161	E1094	I1018	A957	M894	D832	R759	I699
SER	SER	VAL	L1387	N1309	Y1236	Y1236	G1092	E1095	A1019	Q958	R893	D833	E760	S700
LEU	LEU	SER	G1387	Q1310	K1237	K1237	S1093	E1096	L1020	R959	I897	P834	K761	D701
LEU	LEU	THR	A1390	F1312	N1238	N1238	E1094	E1097	A1022	E960	I898	D835	E762	D702
ASP	ASP	THR	V1391	K1313	V1239	V1239	E1095	E1097	E1023	L961	I898	P834	E763	L703
PRO	PRO	LEU	D1471	L1314	F1239	F1239	T1168	L1097	A1024	T962	K999	K335	I764	G704
GLY	GLY	GLY	P1472	W1315	I1240	I1240	L1169	K1098	G1025	W963	I900	K336	A765	I706
ILE	ILE	ARG	G1394	Y1316	I1243	I1243	A1170	E1099	G1025	S964	P901	L837	A766	I706
ASN	ASN	ARG	M1317	M1317	L1243	L1243	A1170	E1099	L1028	E965	G902	D838	D767	I709
ASP	ASP	GLN	L1318	L1318	F1246	F1246	D1173	K1101	W1029	Y966	THR	I839	R768	F710
HIS	HIS	LEU	D1319	D1319	W1247	W1247	G1174	K1101	V1030	E967	THR	K340	E769	S711
GLY	GLY	LEU	Q1323	Q1323	Y1248	Y1248	S1175	L1031	L1031	R968	LYS	A841	T770	D712
THR	THR	PRO	M1252	M1252	N1252	N1252	N1176	D1034	D1034	W969	ASP	Q842	M771	K713
VAL	VAL	VAL	F1253	F1253	V1176	V1176	V1176	K1035	K1035	S970	E908	S943	I772	T771
THR	THR	THR	F1254	F1254	A1179	A1179	P1107	V1036	P909	K971	P909	P944	D773	D773
THR	THR	THR	D1255	D1255	M1180	M1180	Q1108	E1037	K910	T972	K910	D845	E774	L717
GLN	GLN	THR	P1331	P1331	I1181	I1181	Q1108	T1038	A911	Y973	A911	E946	L775	Q719
			N1338	N1338	G1256	G1256	M1110	A1039	L912	D974	L912	V850	S777	N720
			M1339	M1339	S1257	S1257	F1111	I1040	L913	V975	L913	S851	M778	V721
			V1415	V1415	Y1258	Y1258	A1112	N1041	F1044	A976	I914	T852	S779	N721
			F1416	F1416	L1259	L1259	V1113	S1045	S1045	A977	C915	A853	D780	M722
							I1114			S978	K916	R854	T782	
							D1118			S979		Q855	Q783	
										V980		L856	F784	
										T981				

ARG
SER
ARG
ASP
ARG

• Molecule 2: Alkylphosphocholine resistance protein LEM3

Chain B:  18% 59% 30% 11%

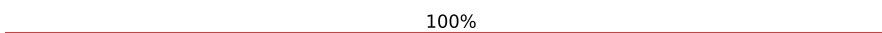


• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
MAG2
MAN3

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

Chain D:  100% 100%

MAG1
MAG2
MAN3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127442	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	0.037	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	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: ALF, NAG, MG, MAN, 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	0.15	0/9490	0.41	1/12865 (0.0%)
2	B	0.14	0/3055	0.36	0/4153
All	All	0.14	0/12545	0.40	1/17018 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	ILE	N-CA-C	5.49	115.15	106.32

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	9297	0	9301	332	0
2	B	2974	0	2868	115	0
3	C	39	0	34	3	0
3	D	39	0	32	3	0
4	A	56	0	92	2	0
5	A	5	0	0	0	0
6	A	1	0	0	0	0
7	B	72	0	69	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12483	0	12396	419	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 17.

The worst 5 of 419 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:1409:TYR:HD1	2:B:272:ARG:NH2	1.45	1.12
1:A:1127:GLU:HG2	1:A:1130:ARG:HH11	1.02	1.09
1:A:941:LEU:HA	1:A:944:GLU:OE1	1.54	1.08
1:A:941:LEU:HA	1:A:944:GLU:CD	1.78	1.08
1:A:1409:TYR:CD1	2:B:272:ARG:NH2	2.20	1.06

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	1155/1612 (72%)	1077 (93%)	78 (7%)	0	100	100
2	B	365/414 (88%)	343 (94%)	22 (6%)	0	100	100
All	All	1520/2026 (75%)	1420 (93%)	100 (7%)	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	1027/1426 (72%)	1026 (100%)	1 (0%)	88	89
2	B	320/364 (88%)	320 (100%)	0	100	100
All	All	1347/1790 (75%)	1346 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1099	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1011	GLN
2	B	282	GLN
1	A	1041	ASN
2	B	301	ASN
2	B	131	HIS

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](#)

6 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	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	C	2	3	14,14,15	0.24	0	17,19,21	0.40	0
3	MAN	C	3	3	11,11,12	0.63	0	15,15,17	1.06	2 (13%)
3	NAG	D	1	3,2	14,14,15	0.47	0	17,19,21	0.49	0
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	0.49	0
3	MAN	D	3	3	11,11,12	0.64	0	15,15,17	0.90	1 (6%)

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	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	MAN	D	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	MAN	C1-O5-C5	2.77	115.90	112.19
3	D	3	MAN	O2-C2-C3	-2.18	105.64	110.15
3	C	3	MAN	O2-C2-C3	-2.17	105.65	110.15

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

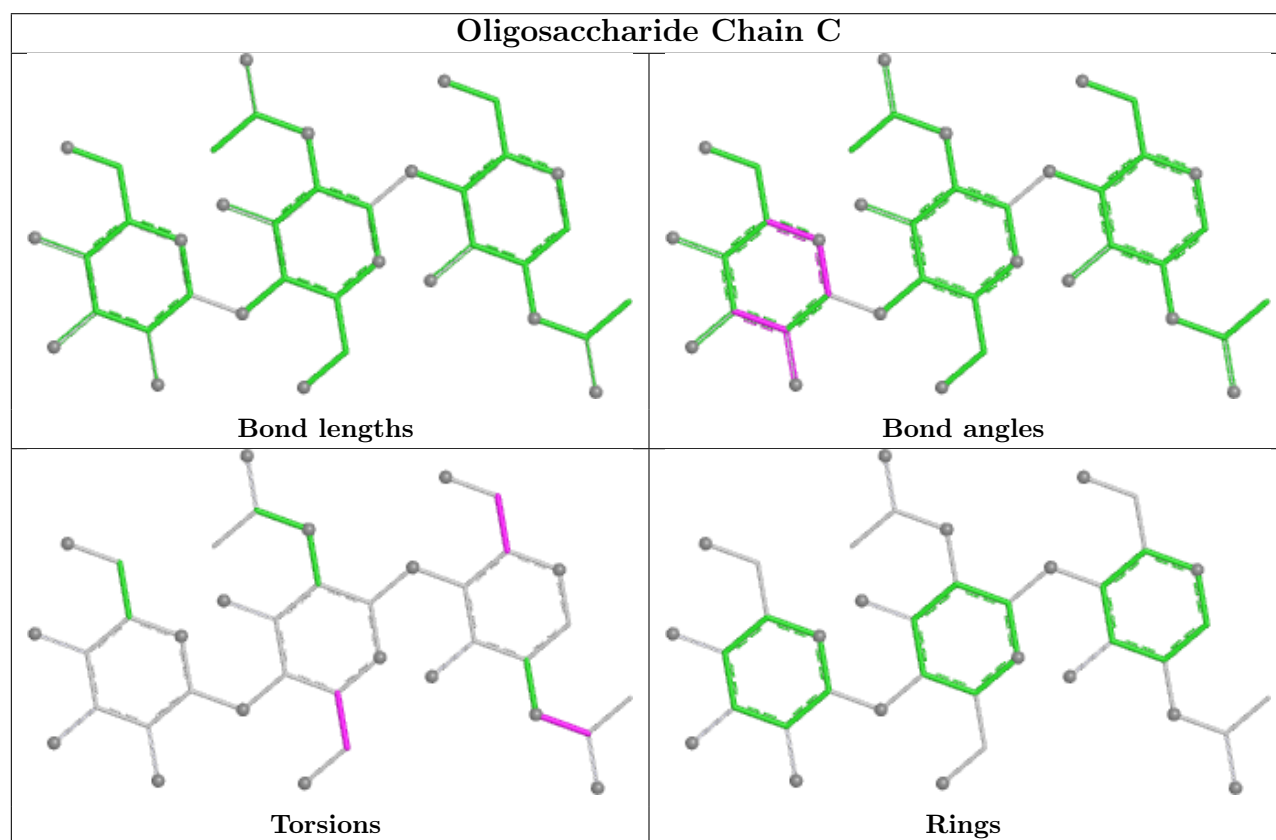
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

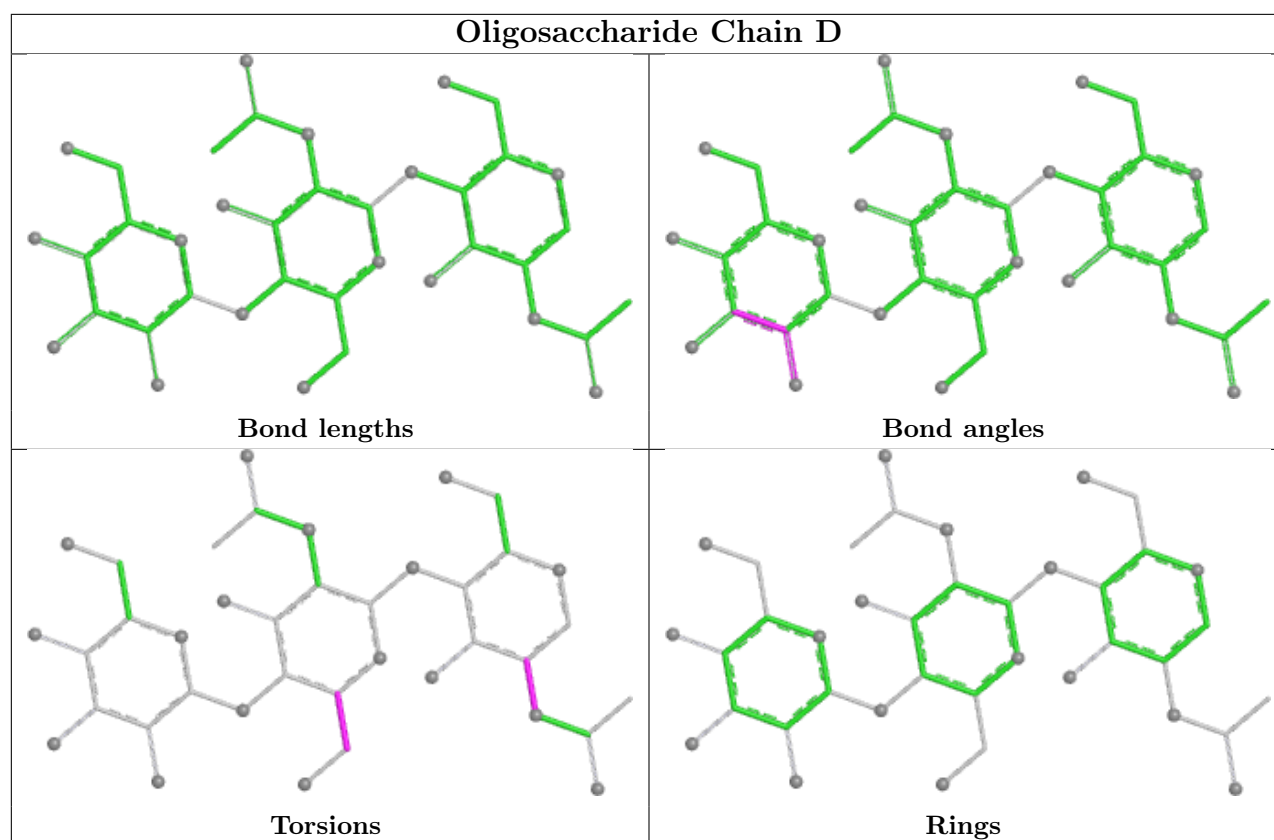
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	3	0
3	C	2	NAG	2	0
3	D	2	NAG	1	0
3	C	1	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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
7	NAG	B	504	2	14,14,15	0.22	0	17,19,21	0.38	0
7	NAG	B	505	-	15,15,15	0.10	0	21,21,21	0.11	0
7	NAG	B	503	-	15,15,15	0.11	0	21,21,21	0.10	0
4	CLR	A	1702	-	31,31,31	0.52	0	48,48,48	1.36	5 (10%)
7	NAG	B	502	2	14,14,15	0.28	0	17,19,21	0.42	0
5	ALF	A	1703	-	4,4,4	1.38	0	-		
7	NAG	B	501	2	14,14,15	0.21	0	17,19,21	0.42	0
4	CLR	A	1701	-	31,31,31	0.54	0	48,48,48	1.33	6 (12%)

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
7	NAG	B	504	2	-	1/6/23/26	0/1/1/1
7	NAG	B	505	-	-	0/6/26/26	0/1/1/1
7	NAG	B	503	-	-	2/6/26/26	0/1/1/1
4	CLR	A	1702	-	-	7/10/68/68	0/4/4/4
7	NAG	B	502	2	-	2/6/23/26	0/1/1/1
7	NAG	B	501	2	-	2/6/23/26	0/1/1/1
4	CLR	A	1701	-	-	7/10/68/68	0/4/4/4

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1702	CLR	C13-C17-C20	-4.49	112.56	119.50
4	A	1701	CLR	C13-C17-C20	-4.35	112.77	119.50
4	A	1701	CLR	C13-C14-C8	-2.92	110.26	114.41
4	A	1702	CLR	C13-C14-C8	-2.92	110.28	114.41
4	A	1702	CLR	C8-C7-C6	-2.48	109.33	112.76

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1702	CLR	C13-C17-C20-C21
4	A	1702	CLR	C16-C17-C20-C21
4	A	1701	CLR	C13-C17-C20-C21
4	A	1701	CLR	C13-C17-C20-C22
4	A	1702	CLR	C13-C17-C20-C22

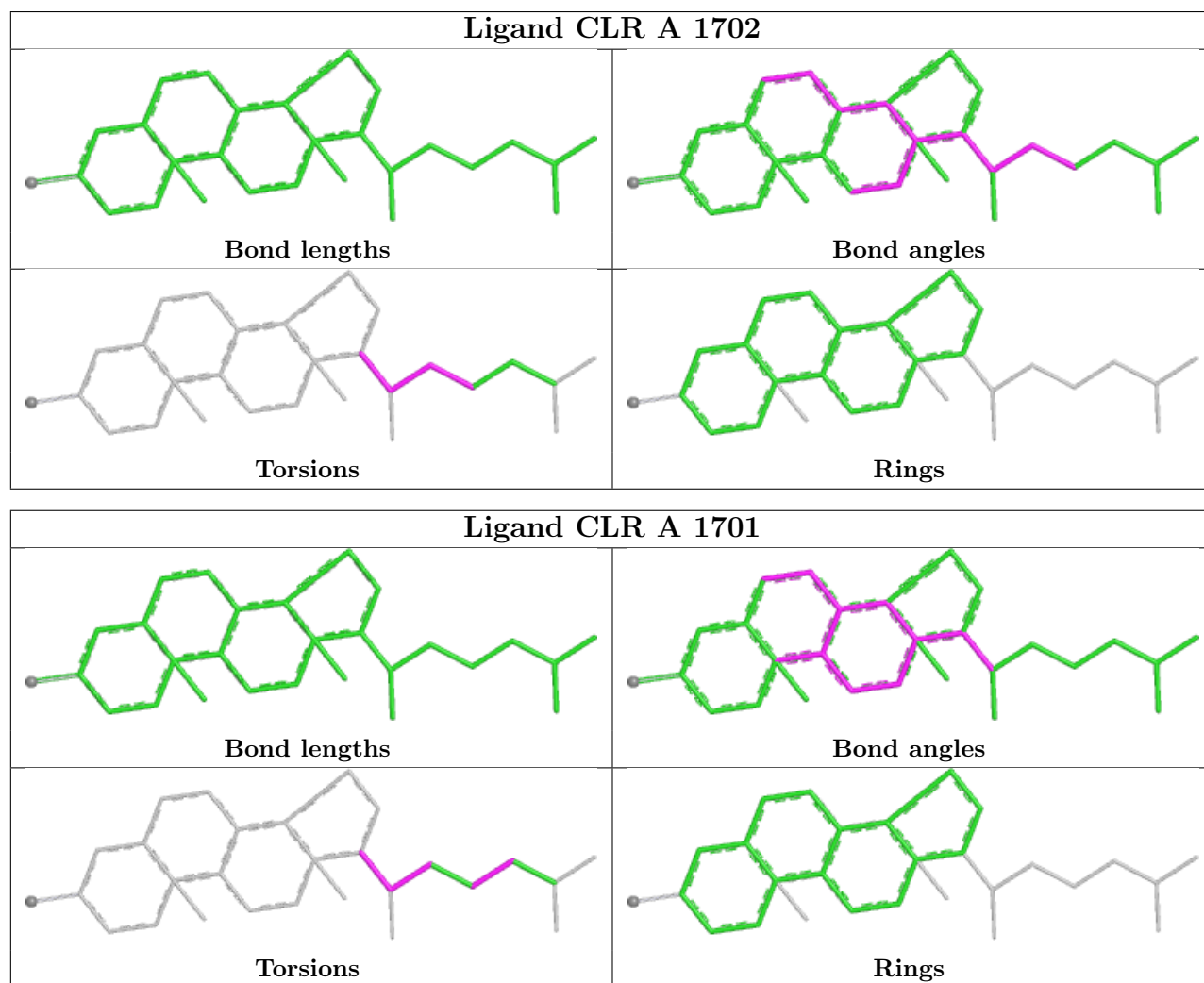
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1702	CLR	1	0
4	A	1701	CLR	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 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 ⓘ

There are no chain breaks in this entry.

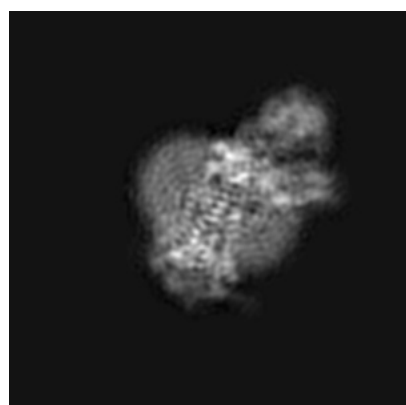
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23068. These allow visual inspection of the internal detail of the map and identification of artifacts.

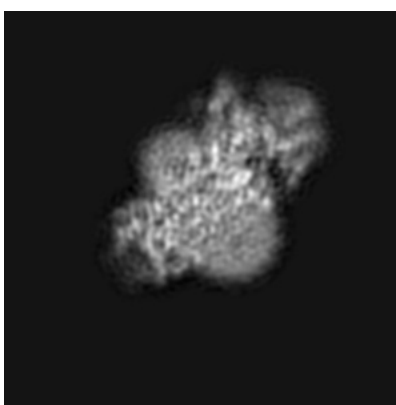
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

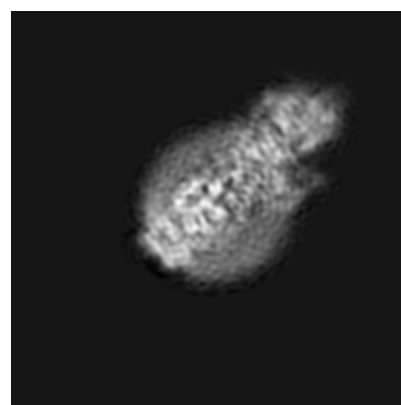
6.1.1 Primary map



X



Y

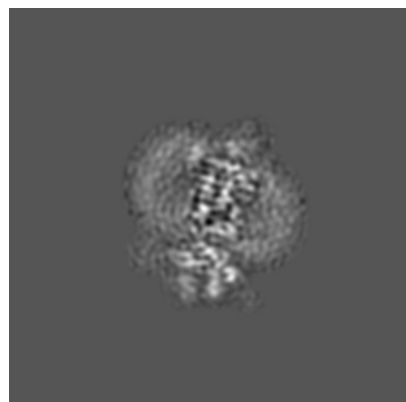


Z

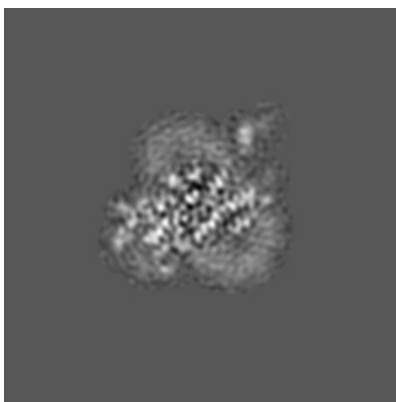
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

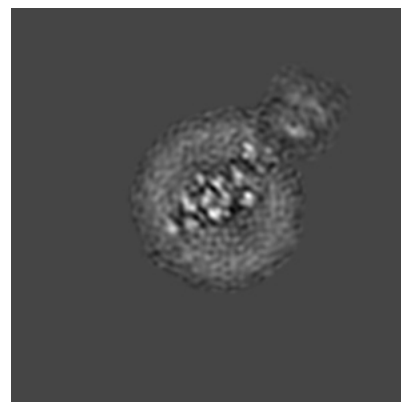
6.2.1 Primary map



X Index: 140



Y Index: 140

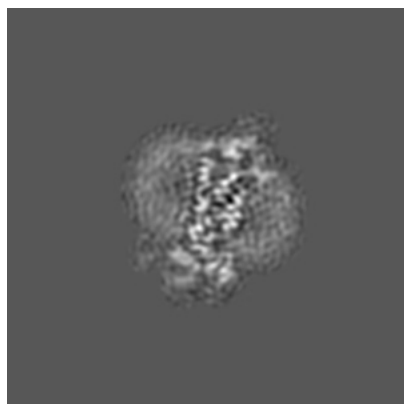


Z Index: 140

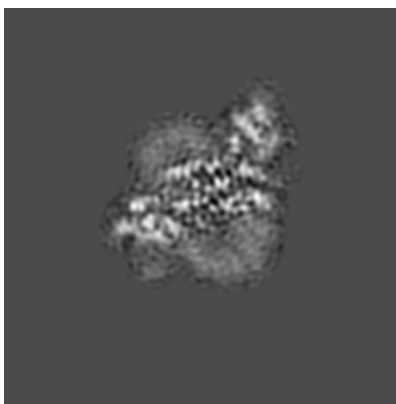
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 144



Y Index: 154

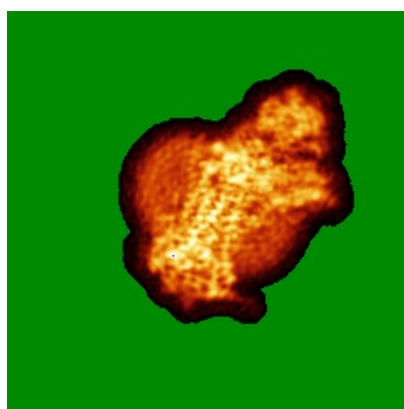


Z Index: 163

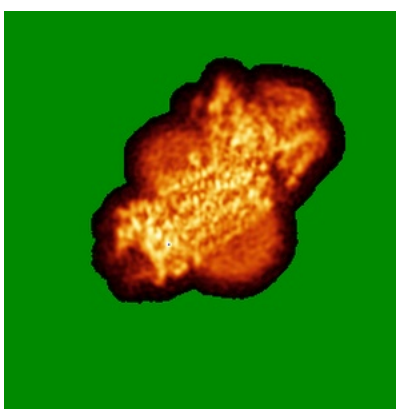
The images above show the largest variance slices of the map in three orthogonal directions.

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

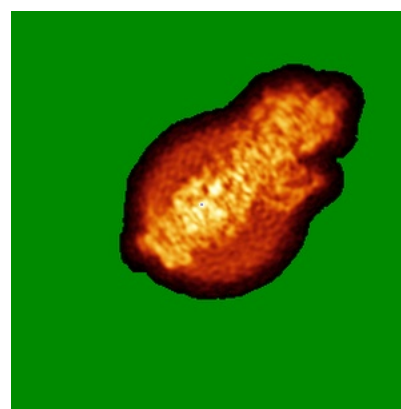
6.4.1 Primary map



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

This section was not generated.

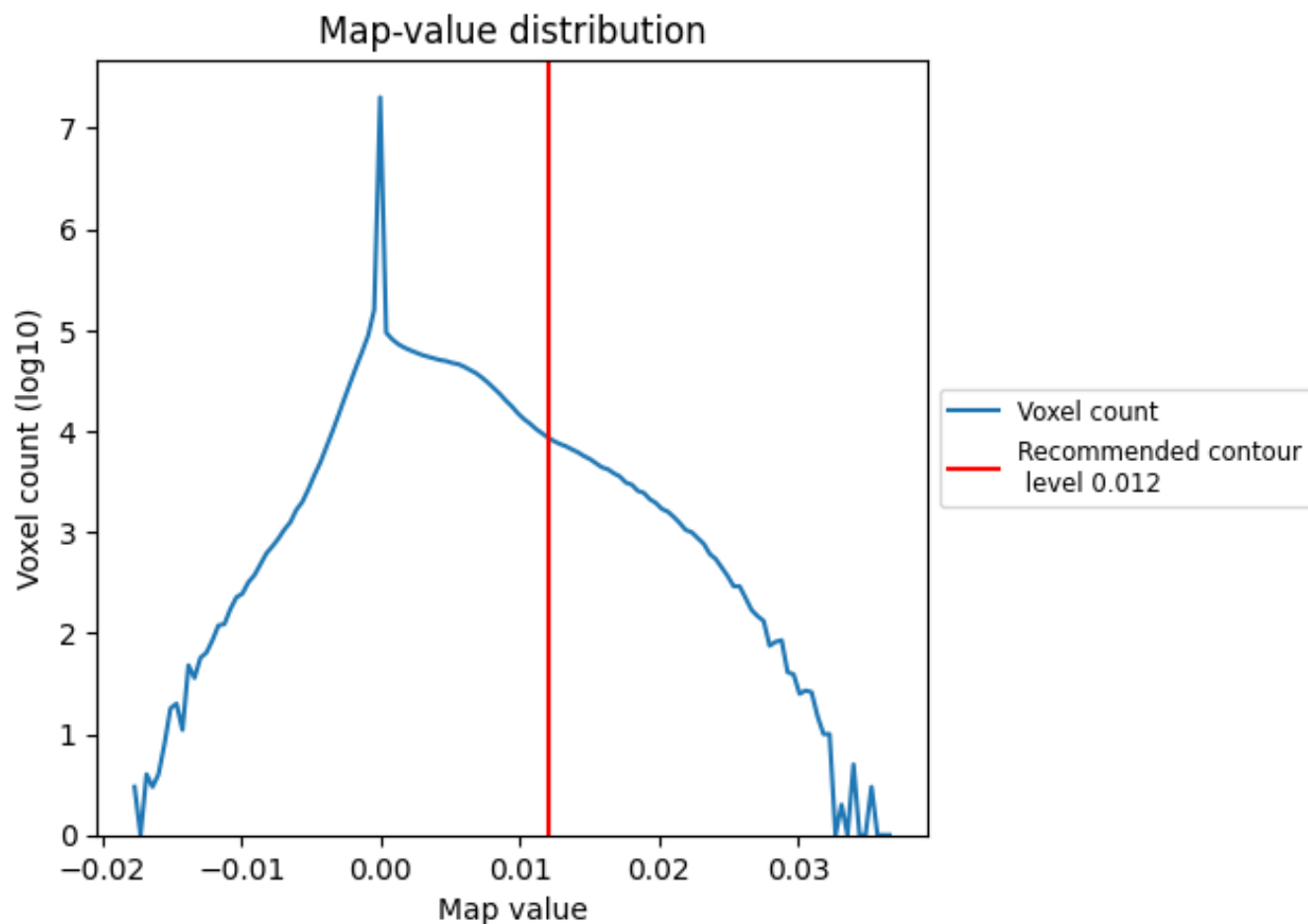
6.6 Mask visualisation

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

7 Map analysis [i](#)

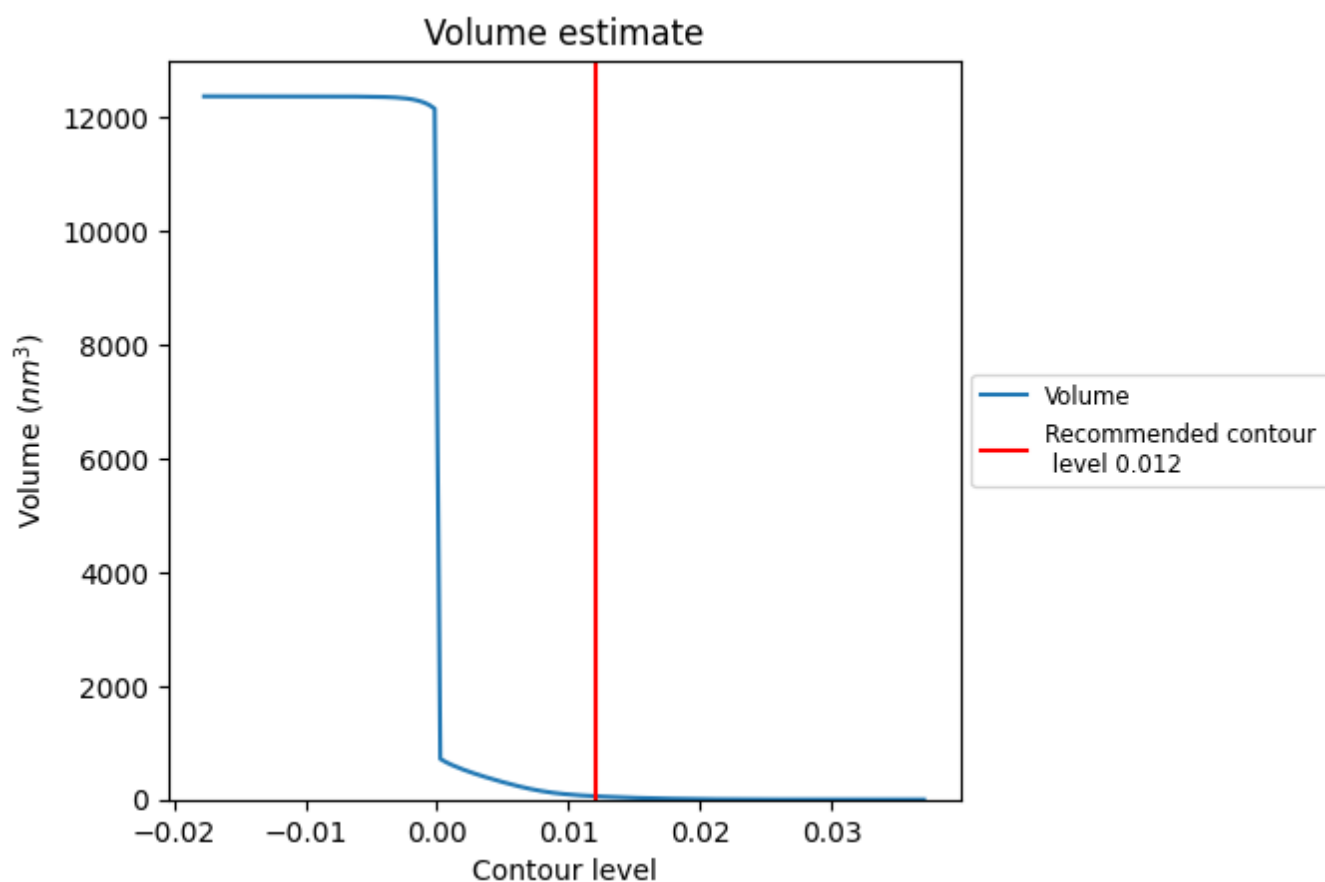
This section contains the results of statistical analysis of the map.

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.

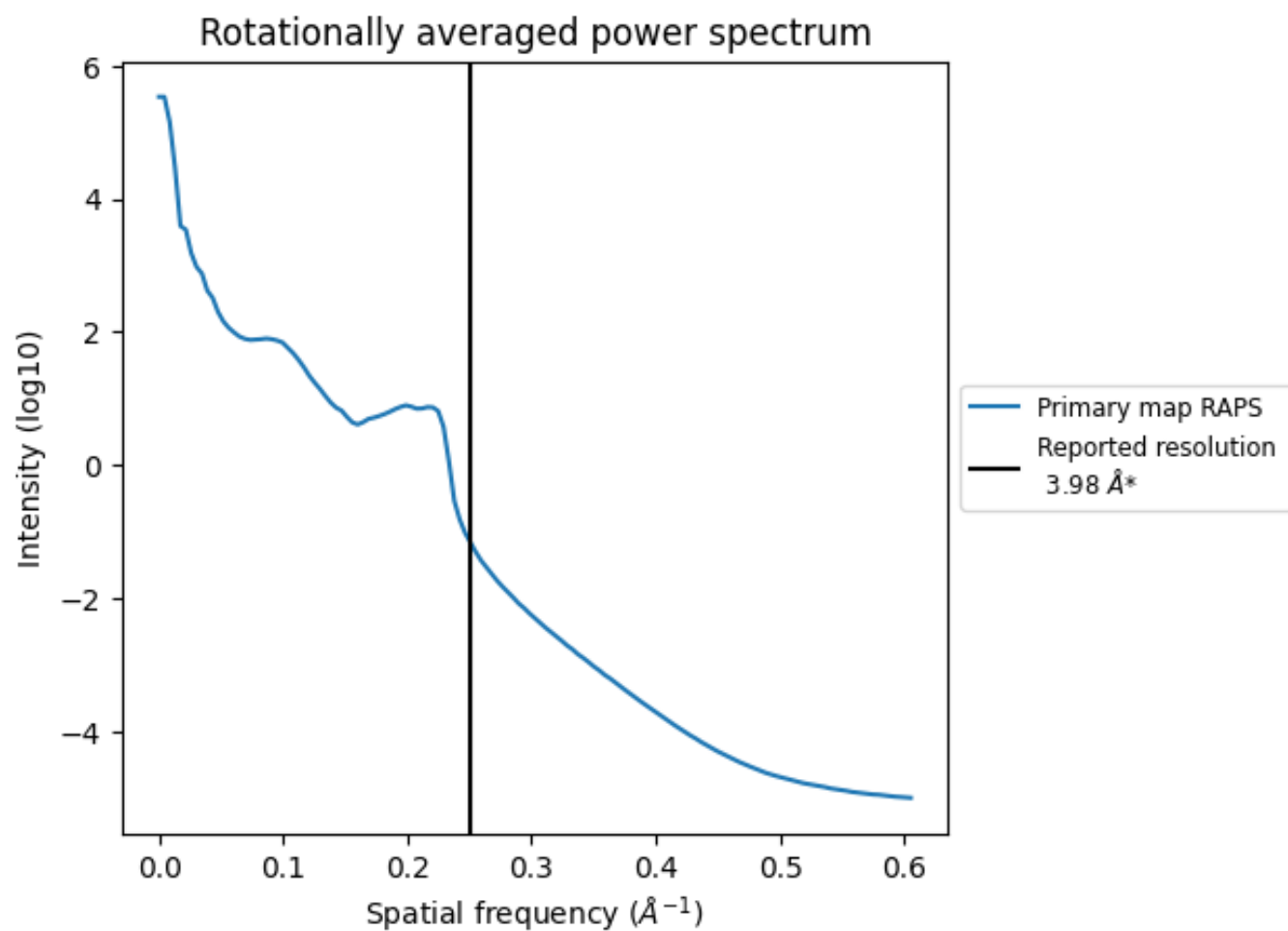
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm³; this corresponds to an approximate mass of 53 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 0.251 Å⁻¹

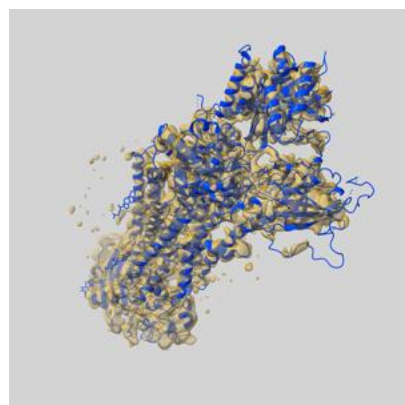
8 Fourier-Shell correlation

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

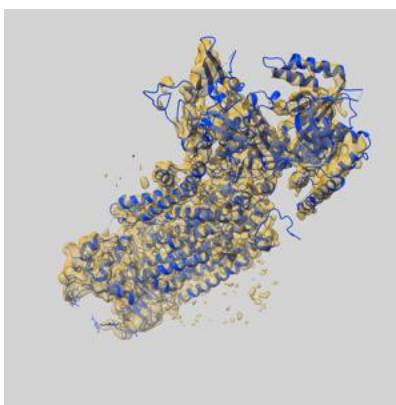
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23068 and PDB model 7KY5. Per-residue inclusion information can be found in section [3](#) on page [6](#).

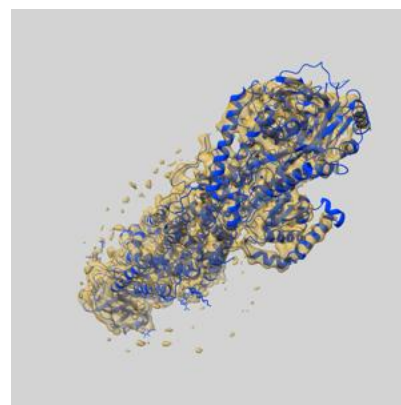
9.1 Map-model overlay [i](#)



X



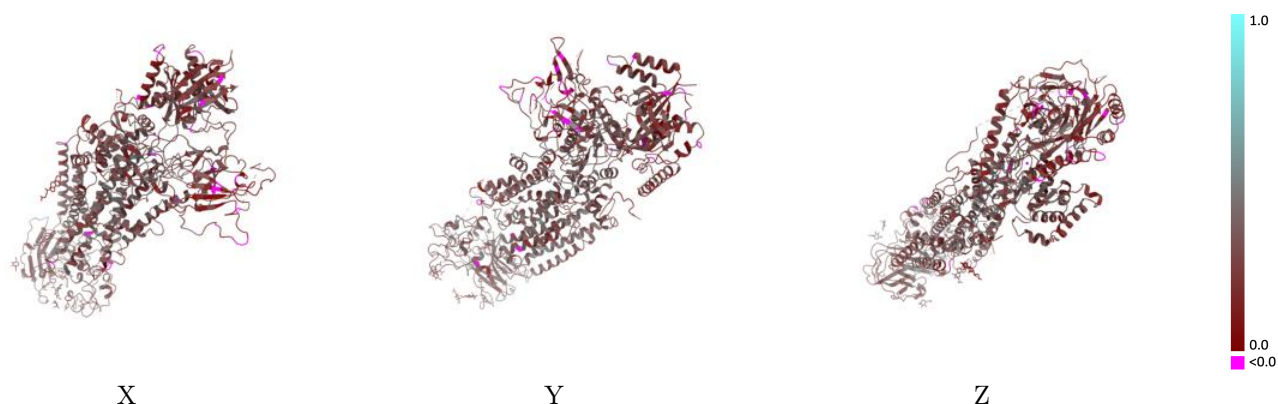
Y



Z

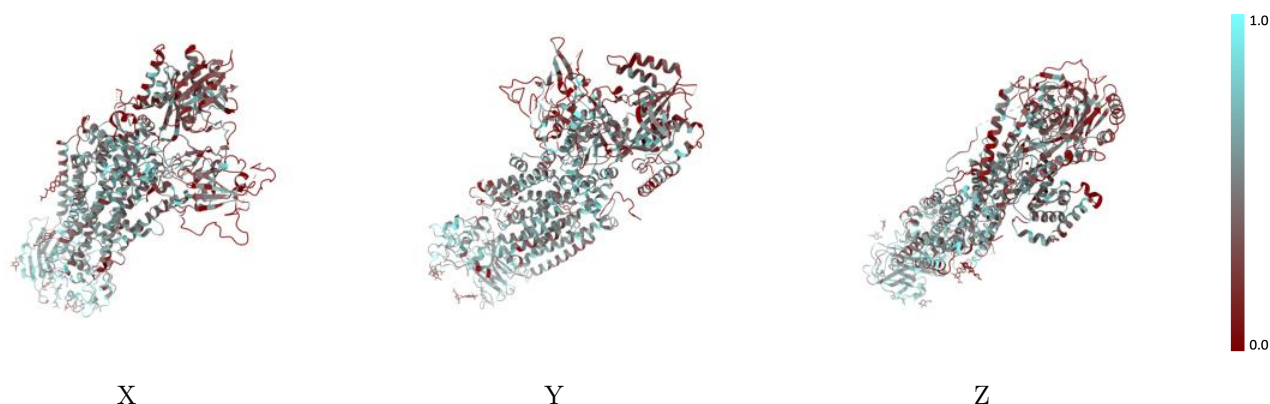
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



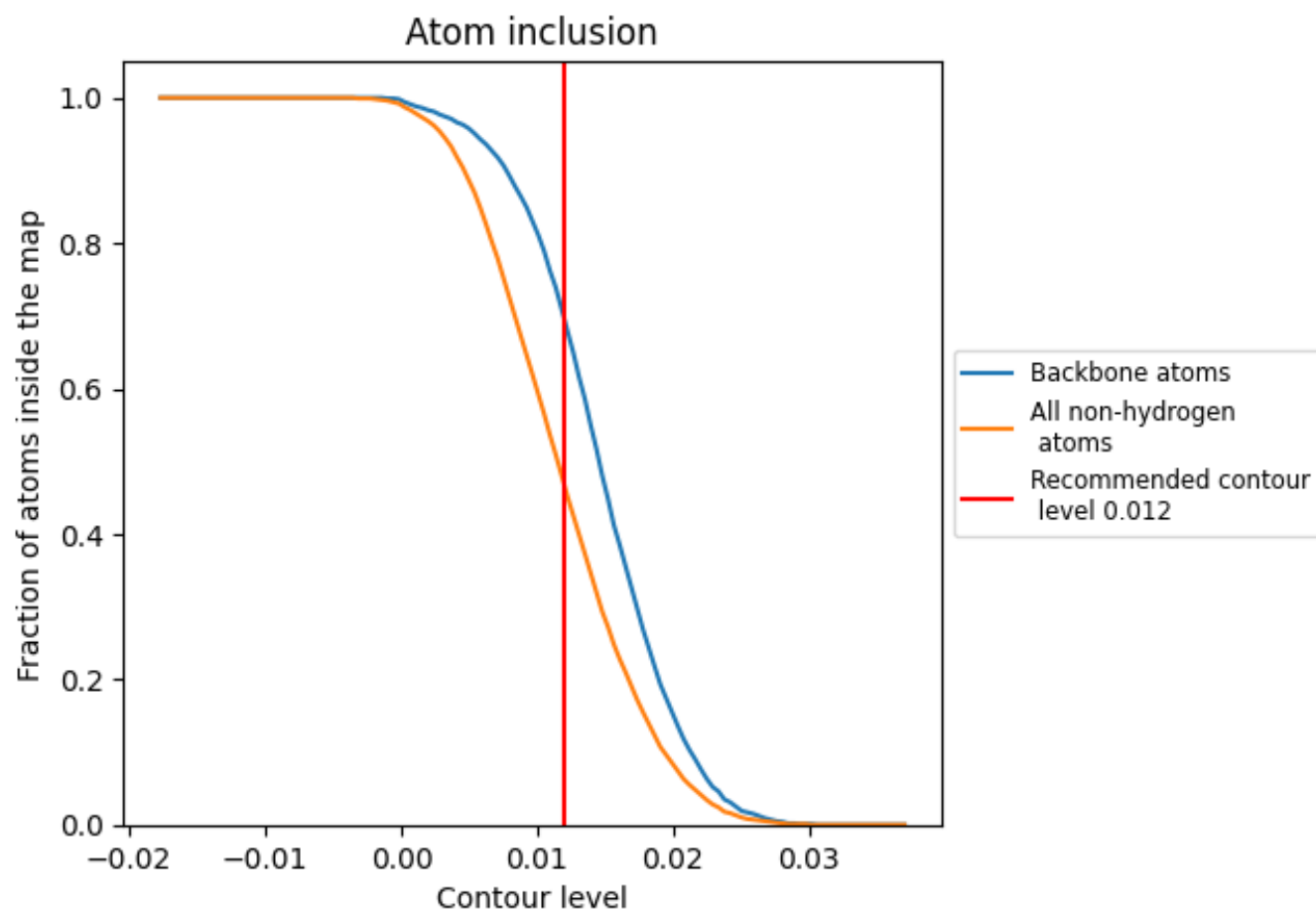
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 47% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4670	0.2950
A	0.4320	0.2850
B	0.5740	0.3260
C	0.6150	0.3380
D	0.2310	0.2730

