



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 06:47 AM EDT

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)

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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:

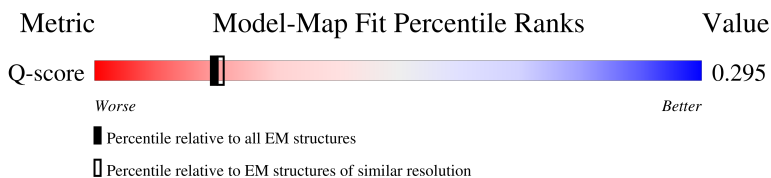
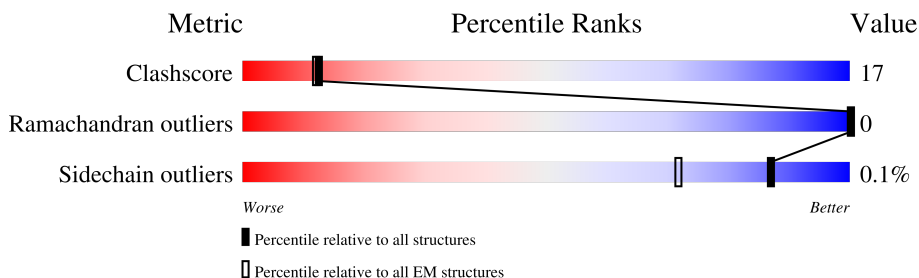
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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	
2	B	414	
3	C	3	
3	D	3	

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.

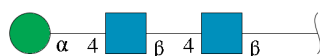
- Molecule 1 is a protein called Phospholipid-transporting ATPase DNF2.

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.

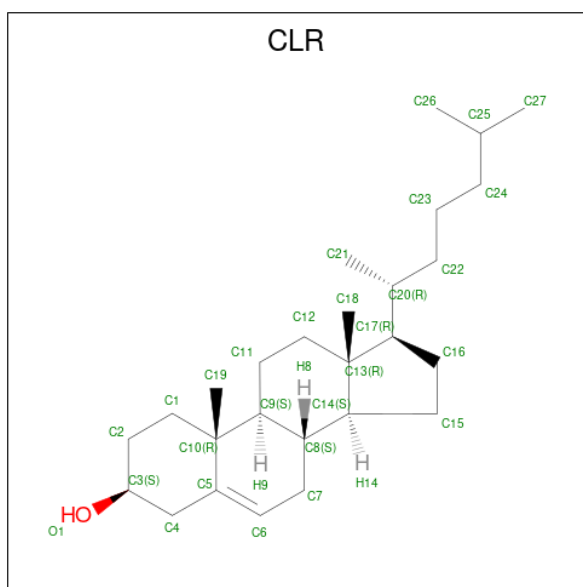
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	369	2974	1908	501	551	14	0	0

- 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.



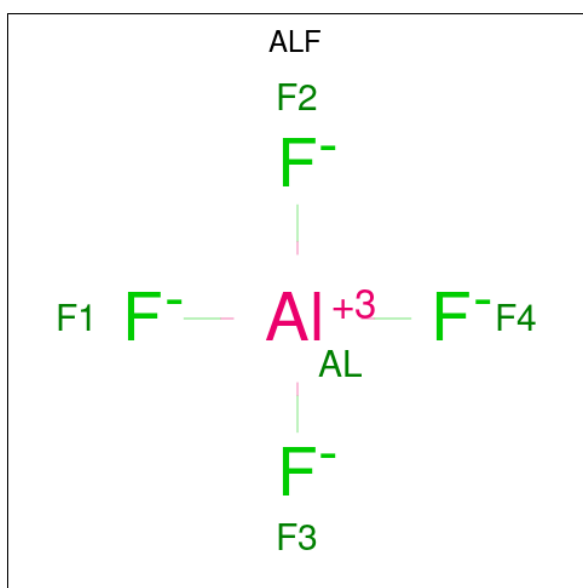
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	3	39	22	2	15	0	0
3	D	3	39	22	2	15	0	0

- 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).

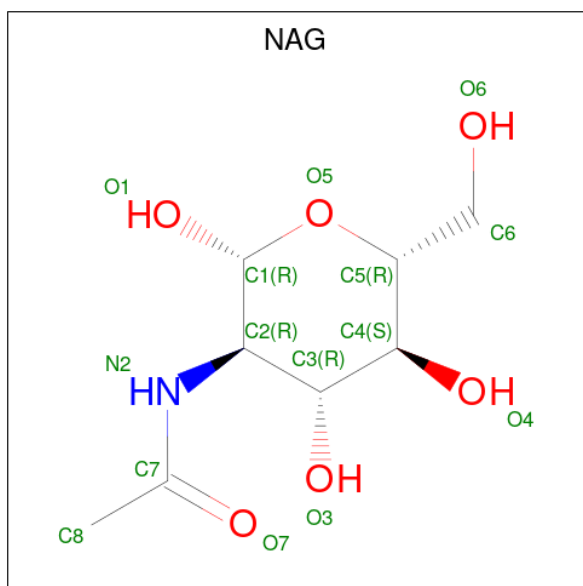


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Al	F	0
			5	1	4	

- 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: $C_8H_{15}NO_6$).



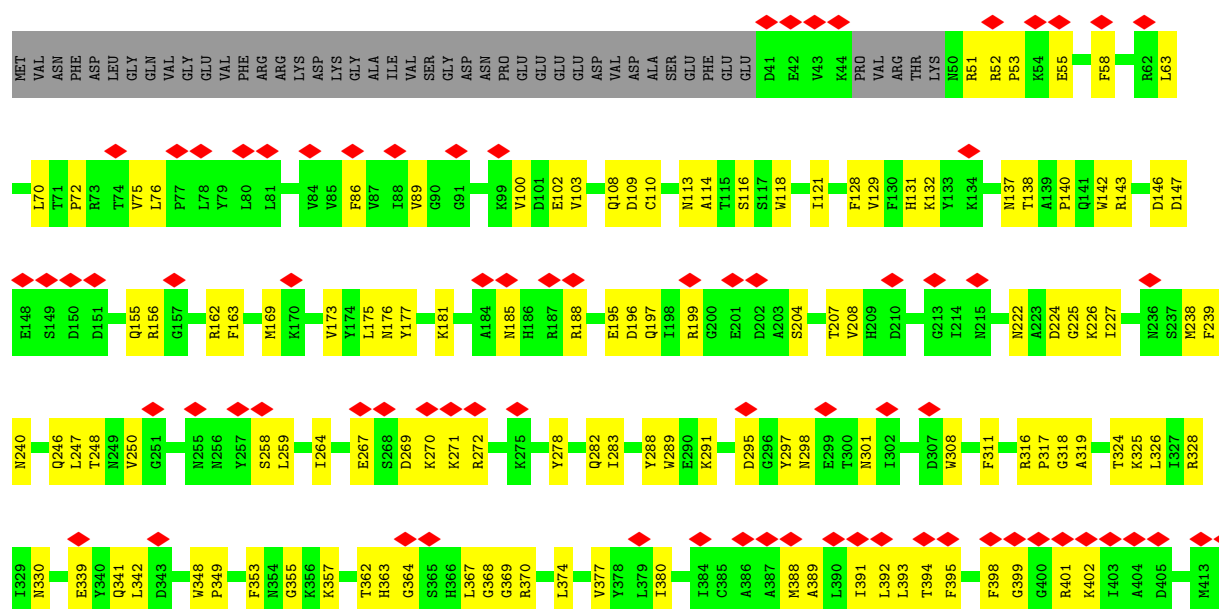
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			15	8	1	6	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			15	8	1	6	

ASN	ASN	ASP	A1417	V1340	F1260	G1187	A1119	G1046	N952	D919	G857	D788	E723	F644	ASN	ASN	ASP	A1418	V1341	F1261	G1188	A1120	G1047	N953	D920	G858	F724	ASN	ASN	ASP	A1419	V1342	F1262	G1189	A1121	G1048	N954	D921	G859	F725	ASN	ASN	ASP	A1420	V1343	F1263	G1190	A1122	G1049	N955	D922	G860	F726	ASN	ASN	ASP	A1421	V1344	F1264	G1191	A1123	G1050	N956	D923	G861	F727	ASN	ASN	ASP	A1422	V1345	F1265	G1192	A1124	G1051	N957	D924	G862	F728	ASN	ASN	ASP	A1423	V1346	F1266	G1193	A1125	G1052	N958	D925	G863	F729	ASN	ASN	ASP	A1424	V1347	F1267	G1194	A1126	G1053	N959	D926	G864	F730	ASN	ASN	ASP	A1425	V1348	F1268	G1195	A1127	G1054	N960	D927	G865	F731	ASN	ASN	ASP	A1426	V1349	F1269	G1196	A1128	G1055	N961	D928	G866	F732	ASN	ASN	ASP	A1427	V1350	F1270	G1197	A1129	G1056	N962	D929	G867	F733	ASN	ASN	ASP	A1428	V1351	F1271	G1198	A1130	G1057	N963	D930	G868	F734	ASN	ASN	ASP	A1429	V1352	F1272	G1199	A1131	G1058	N964	D931	G869	F735	ASN	ASN	ASP	A1430	V1353	F1273	G1200	A1132	G1059	N965	D932	G870	F736	ASN	ASN	ASP	A1431	V1354	F1274	G1201	A1133	G1060	N966	D933	G871	F737	ASN	ASN	ASP	A1432	V1355	F1275	G1202	A1134	G1061	N967	D934	G872	F738	ASN	ASN	ASP	A1433	V1356	F1276	G1203	A1135	G1062	N968	D935	G873	F739	ASN	ASN	ASP	A1434	V1357	F1277	G1204	A1136	G1063	N969	D936	G874	F740	ASN	ASN	ASP	A1435	V1358	F1278	G1205	A1137	G1064	N970	D937	G875	F741	ASN	ASN	ASP	A1436	V1359	F1279	G1206	A1138	G1065	N971	D938	G876	F742	ASN	ASN	ASP	A1437	V1360	F1280	G1207	A1139	G1066	N972	D939	G877	F743	ASN	ASN	ASP	A1438	V1361	F1281	G1208	A1140	G1067	N973	D940	G878	F744	ASN	ASN	ASP	A1439	V1362	F1282	G1209	A1141	G1068	N974	D941	G879	F745	ASN	ASN	ASP	A1440	V1363	F1283	G1210	A1142	G1069	N975	D942	G880	F746	ASN	ASN	ASP	A1441	V1364	F1284	G1211	A1143	G1070	N976	D943	G881	F747	ASN	ASN	ASP	A1442	V1365	F1285	G1212	A1144	G1071	N977	D944	G882	F748	ASN	ASN	ASP	A1443	V1366	F1286	G1213	A1145	G1072	N978	D945	G883	F749	ASN	ASN	ASP	A1444	V1367	F1287	G1214	A1146	G1073	N979	D946	G884	F750	ASN	ASN	ASP	A1445	V1368	F1288	G1215	A1147	G1074	N980	D947	G885	F751	ASN	ASN	ASP	A1446	V1369	F1289	G1216	A1148	G1075	N981	D948	G886	F752	ASN	ASN	ASP	A1447	V1370	F1290	G1217	A1149	G1076	N982	D949	G887	F753	ASN	ASN	ASP	A1448	V1371	F1291	G1218	A1150	G1077	N983	D950	G888	F754	ASN	ASN	ASP	A1449	V1372	F1292	G1219	A1151	G1078	N984	D951	G889	F755	ASN	ASN	ASP	A1450	V1373	F1293	G1220	A1152	G1079	N985	D952	G890	F756	ASN	ASN	ASP	A1451	V1374	F1294	G1221	A1153	G1080	N986	D953	G891	F757	ASN	ASN	ASP	A1452	V1375	F1295	G1222	A1154	G1081	N987	D954	G892	F758	ASN	ASN	ASP	A1453	V1376	F1296	G1223	A1155	G1082	N988	D955	G893	F759	ASN	ASN	ASP	A1454	V1377	F1297	G1224	A1156	G1083	N989	D956	G894	F760	ASN	ASN	ASP	A1455	V1378	F1298	G1225	A1157	G1084	N990	D957	G895	F761	ASN	ASN	ASP	A1456	V1379	F1299	G1226	A1158	G1085	N991	D958	G896	F762	ASN	ASN	ASP	A1457	V1380	F1300	G1227	A1159	G1086	N992	D959	G897	F763	ASN	ASN	ASP	A1458	V1381	F1301	G1228	A1160	G1087	N993	D960	G898	F764	ASN	ASN	ASP	A1459	V1382	F1302	G1229	A1161	G1088	N994	D961	G899	F765	ASN	ASN	ASP	A1460	V1383	F1303	G1230	A1162	G1089	N995	D962	G900	F766	ASN	ASN	ASP	A1461	V1384	F1304	G1231	A1163	G1090	N996	D963	G901	F767	ASN	ASN	ASP	A1462	V1385	F1305	G1232	A1164	G1091	N997	D964	G902	F768	ASN	ASN	ASP	A1463	V1386	F1306	G1233	A1165	G1092	N998	D965	G903	F769	ASN	ASN	ASP	A1464	V1387	F1307	G1234	A1166	G1093	N999	D966	G904	F770	ASN	ASN	ASP	A1465	V1388	F1308	G1235	A1167	G1094	N1000	D967	G905	F771	ASN	ASN	ASP	A1466	V1389	F1309	G1236	A1168	G1095	N1001	D968	G906	F772	ASN	ASN	ASP	A1467	V1390	F1310	G1237	A1169	G1096	N1002	D969	G907	F773	ASN	ASN	ASP	A1468	V1391	F1311	G1238	A1170	G1097	N1003	D970	G908	F774	ASN	ASN	ASP	A1469	V1392	F1312	G1239	A1171	G1098	N1004	D971	G909	F775	ASN	ASN	ASP	A1470	V1393	F1313	G1240	A1172	G1099	N1005	D972	G910	F776	ASN	ASN	ASP	A1471	V1394	F1314	G1241	A1173	G1100	N1006	D973	G911	F777	ASN	ASN	ASP	A1472	V1395	F1315	G1242	A1174	G1101	N1007	D974	G912	F778	ASN	ASN	ASP	A1473	V1396	F1316	G1243	A1175	G1102	N1008	D975	G913	F779	ASN	ASN	ASP	A1474	V1397	F1317	G1244	A1176	G1103	N1009	D976	G914	F780	ASN	ASN	ASP	A1475	V1398	F1318	G1245	A1177	G1104	N1010	D977	G915	F781	ASN	ASN	ASP	A1476	V1399	F1319	G1246	A1178	G1105	N1011	D978	G916	F782	ASN	ASN	ASP	A1477	V1400	F1320	G1247	A1179	G1106	N1012	D979	G917	F783	ASN	ASN	ASP	A1478	V1401	F1321	G1248	A1180	G1107	N1013	D980	G918	F784	ASN	ASN	ASP	A1479	V1402	F1322	G1249	A1181	G1108	N1014	D981	G919	F785	ASN	ASN	ASP	A1480	V1403	F1323	G1250	A1182	G1109	N1015	D982	G920	F786	ASN	ASN	ASP	A1481	V1404	F1324	G1251	A1183	G1110	N1016	D983	G921	F787	ASN	ASN	ASP	A1482	V1405	F1325	G1252	A1184	G1111	N1017	D984	G922	F788	ASN	ASN	ASP	A1483	V1406	F1326	G1253	A1185	G1112	N1018	D985	G923	F789	ASN	ASN	ASP	A1484	V1407	F1327	G1254	A1186	G1113	N1019	D986	G924	F790	ASN	ASN	ASP	A1485	V1408	F1328	G1255	A1187	G1114	N1020	D987	G925	F791	ASN	ASN	ASP	A1486	V1409	F1329	G1256	A1188	G1115	N1021	D988	G926	F792	ASN	ASN	ASP	A1487	V1410	F1330	G1257	A1189	G1116	N1022	D989	G927	F793	ASN	ASN	ASP	A1488	V1411	F1331	G1258	A1190	G1117	N1023	D990	G928	F794	ASN	ASN	ASP	A1489	V1412	F1332	G1259	A1191	G1118	N1024	D991	G929	F795	A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ARG
SER
ARG
ASP
ARG

• Molecule 2: Alkylphosphocholine resistance protein LEM3

Chain B: 

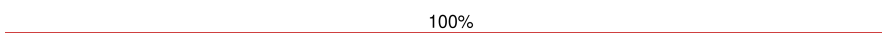


• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 

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: 

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: MG, MAN, NAG, CLR, ALF

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	2,3	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	2,3	-	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:

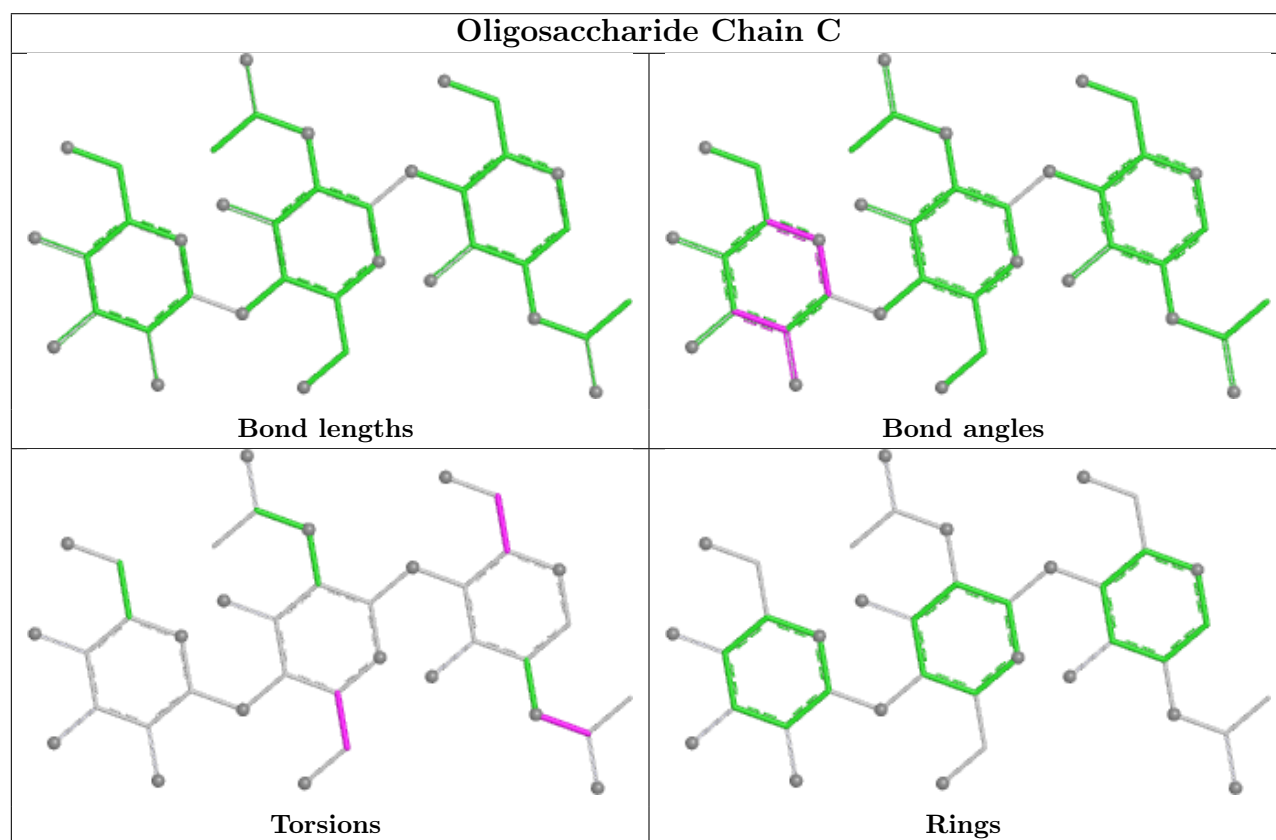
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

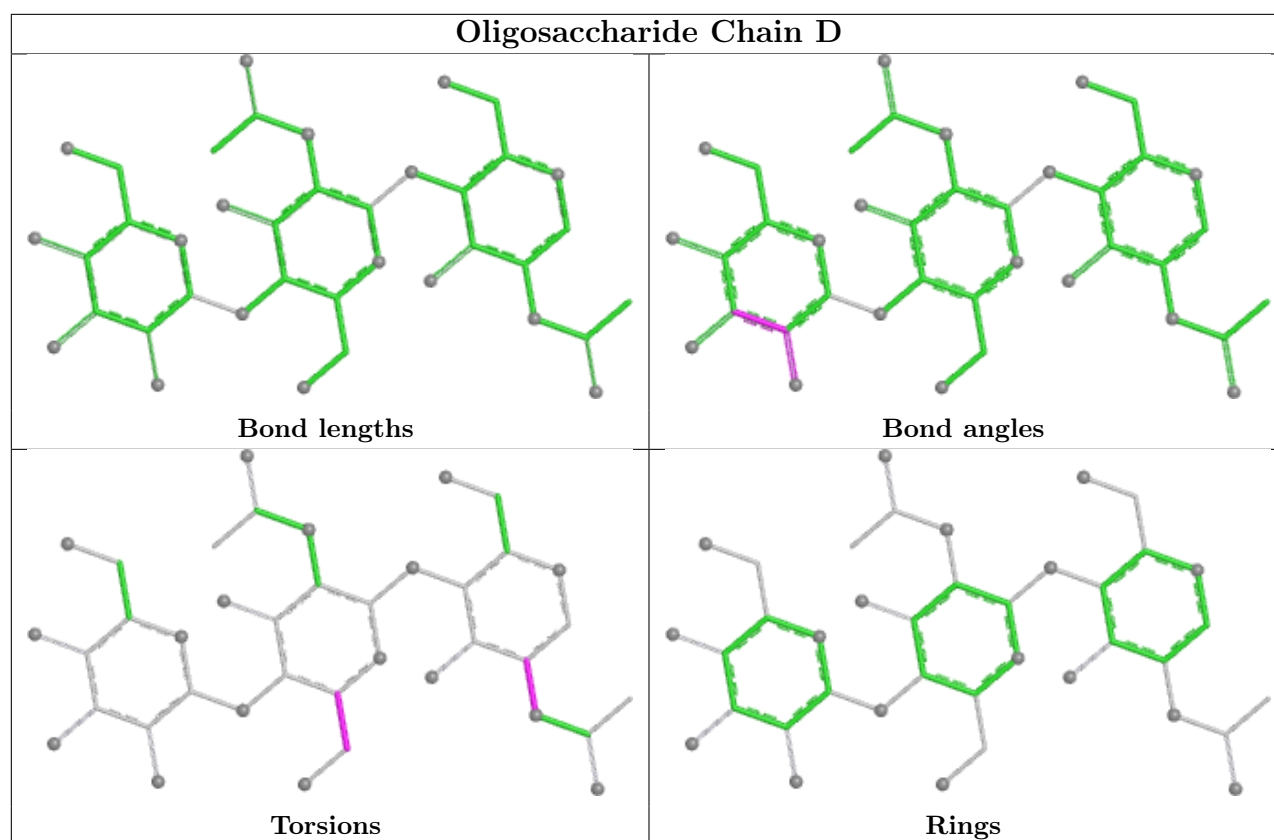
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	C	1	NAG	1	0
3	C	2	NAG	2	0
3	D	1	NAG	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 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	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%)
5	ALF	A	1703	-	4,4,4	1.38	0	-		
4	CLR	A	1702	-	31,31,31	0.52	0	48,48,48	1.36	5 (10%)
7	NAG	B	503	-	15,15,15	0.11	0	21,21,21	0.10	0
7	NAG	B	505	-	15,15,15	0.10	0	21,21,21	0.11	0
7	NAG	B	504	2	14,14,15	0.22	0	17,19,21	0.38	0
7	NAG	B	502	2	14,14,15	0.28	0	17,19,21	0.42	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
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
4	CLR	A	1702	-	-	7/10/68/68	0/4/4/4
7	NAG	B	503	-	-	2/6/26/26	0/1/1/1
7	NAG	B	505	-	-	0/6/26/26	0/1/1/1
7	NAG	B	504	2	-	1/6/23/26	0/1/1/1
7	NAG	B	502	2	-	2/6/23/26	0/1/1/1

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

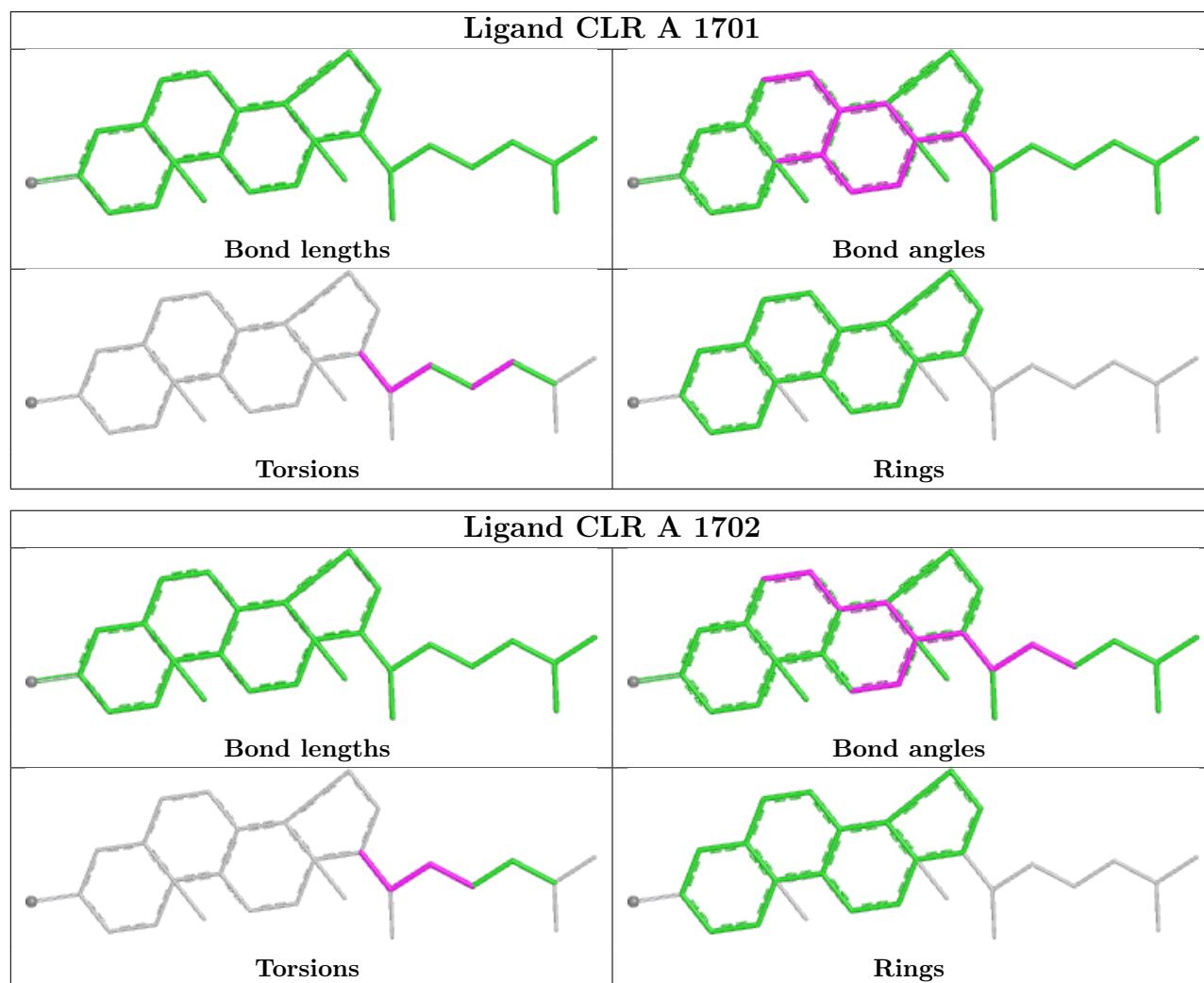
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

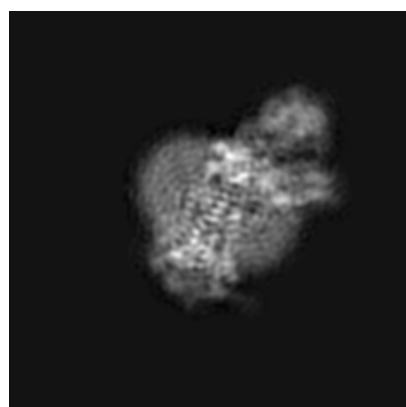
6 Map visualisation [i](#)

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.

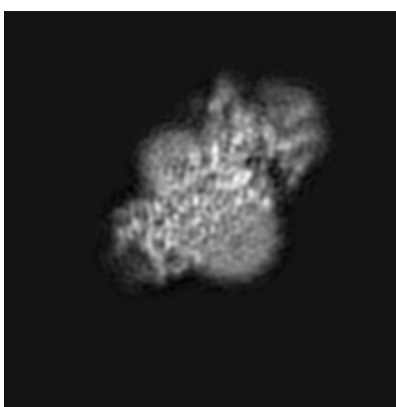
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

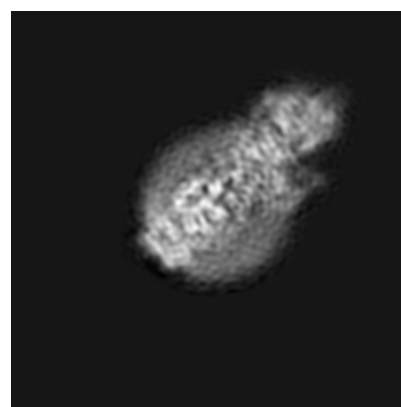
6.1.1 Primary map



X



Y

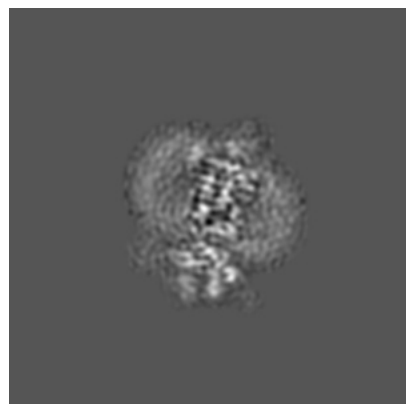


Z

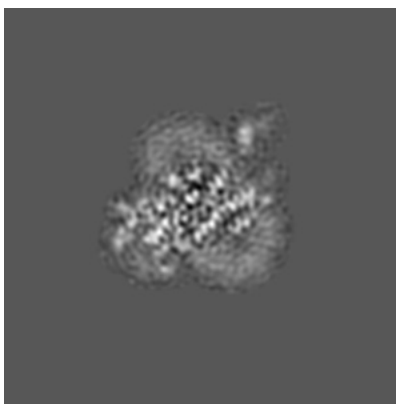
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

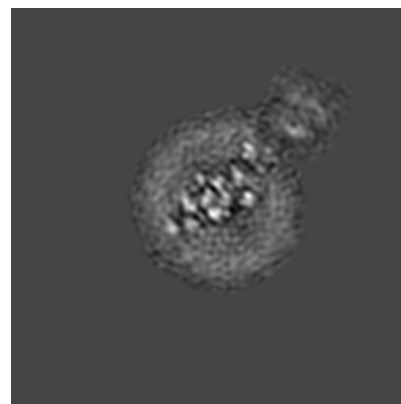
6.2.1 Primary map



X Index: 140



Y Index: 140

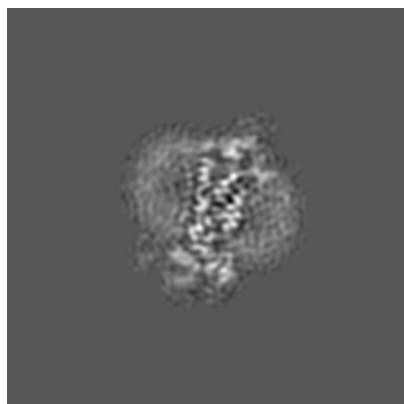


Z Index: 140

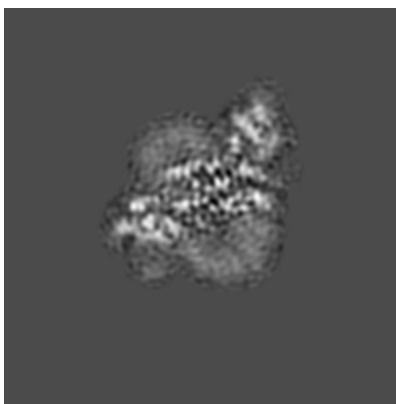
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 144



Y Index: 154

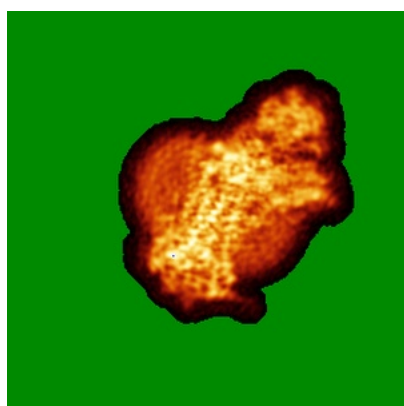


Z Index: 163

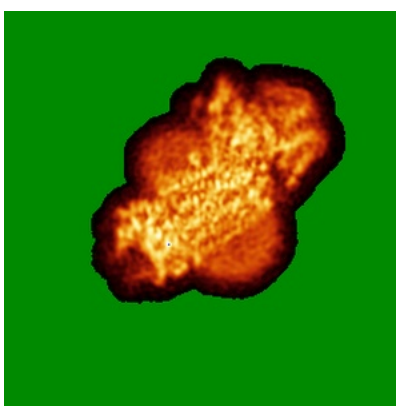
The images above show the largest variance slices of the map in three orthogonal directions.

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

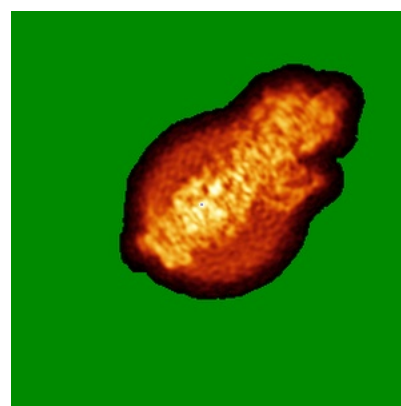
6.4.1 Primary map



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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

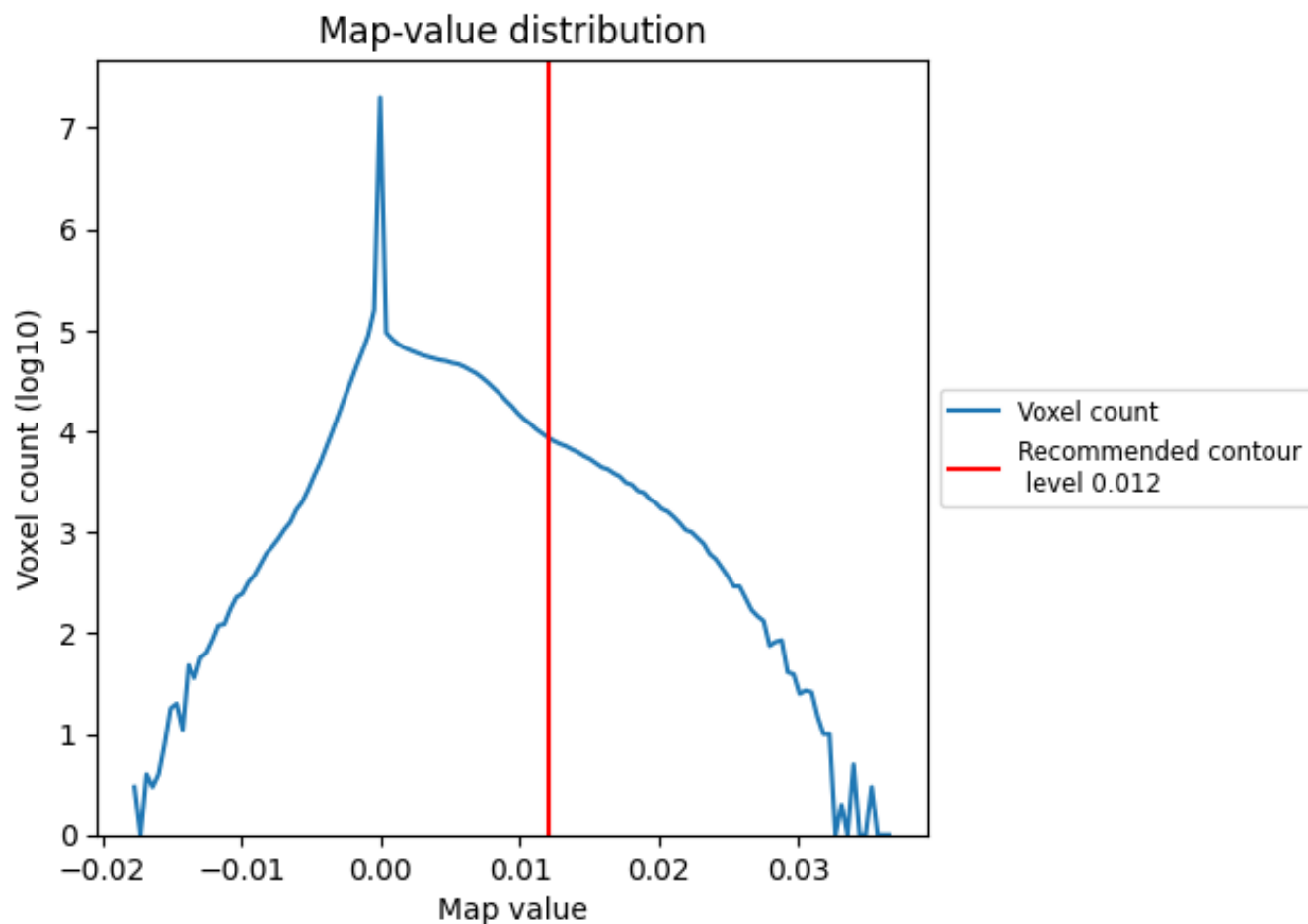
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

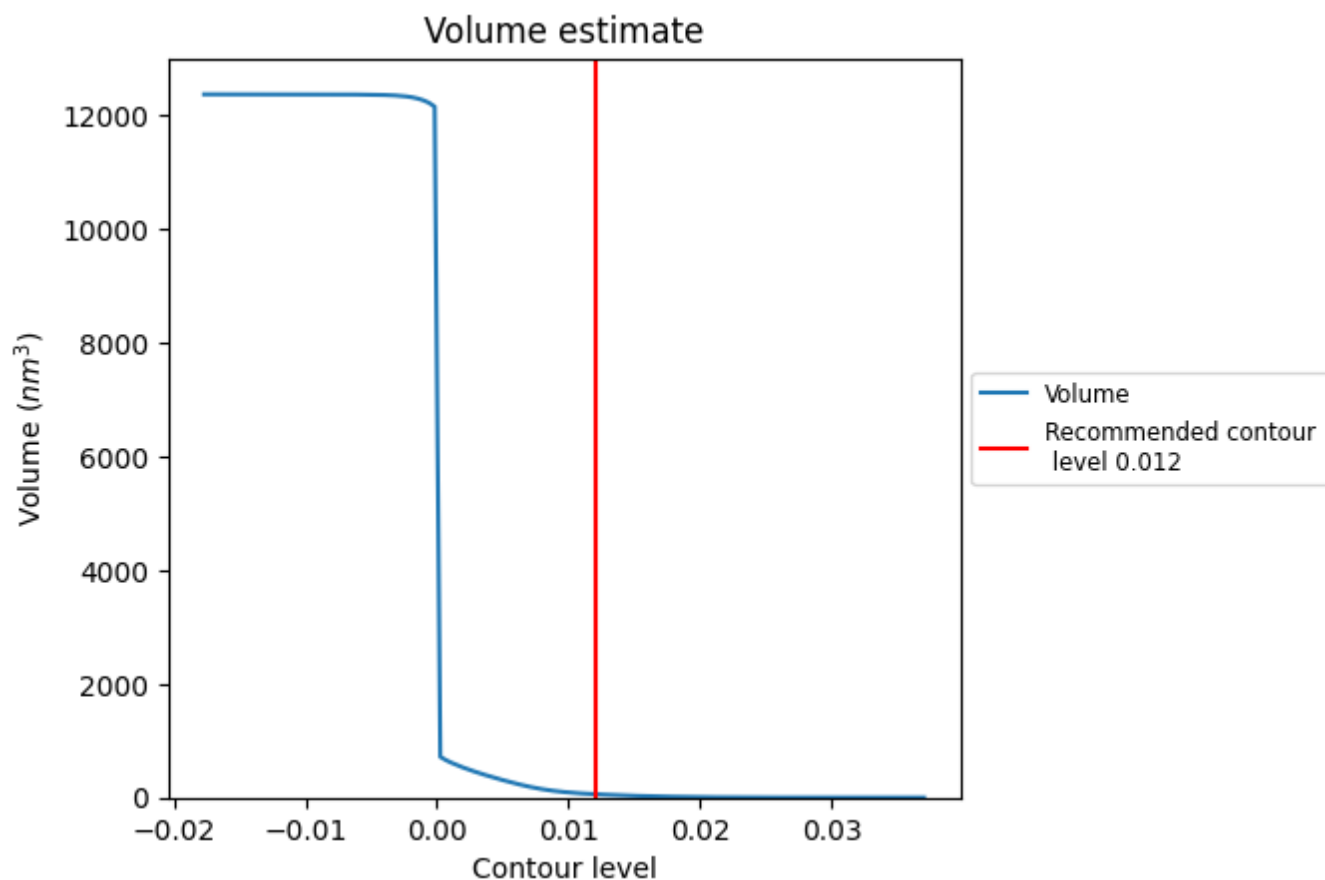
This section contains the results of statistical analysis of the map.

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.

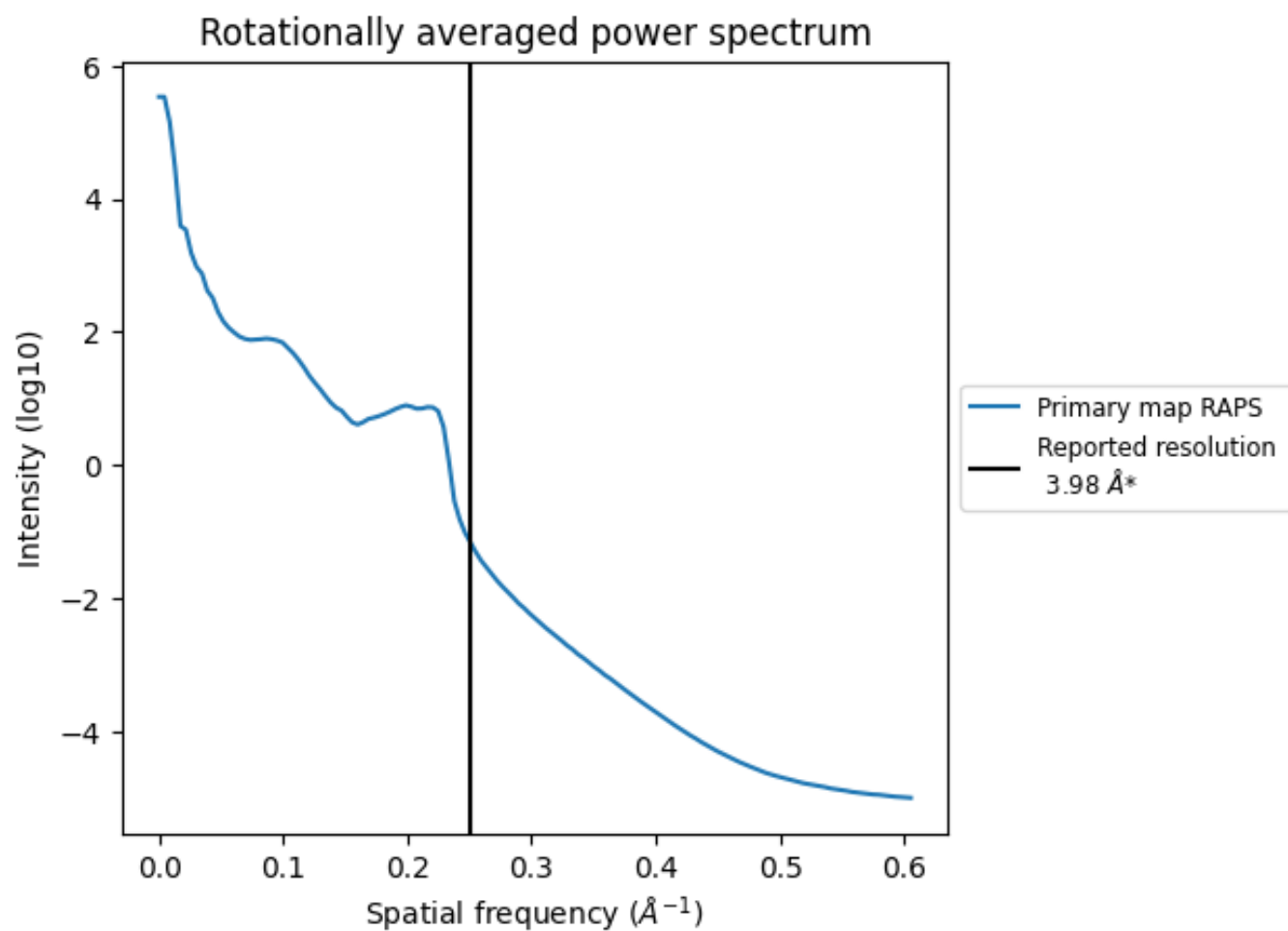
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 $\text{\AA}^{-1}$

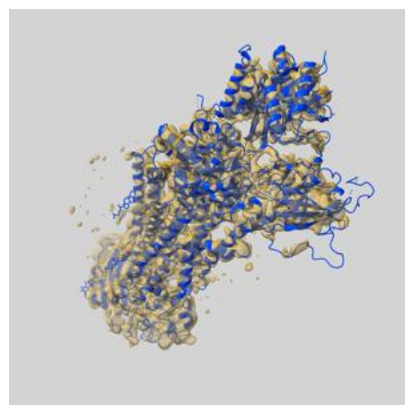
8 Fourier-Shell correlation

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

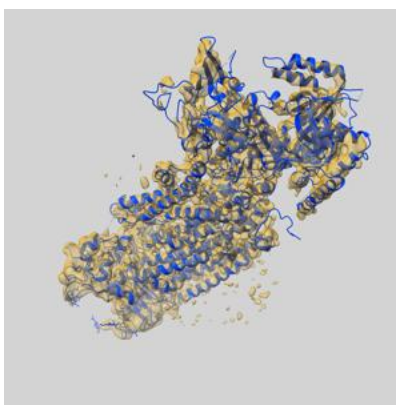
9 Map-model fit [i](#)

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](#).

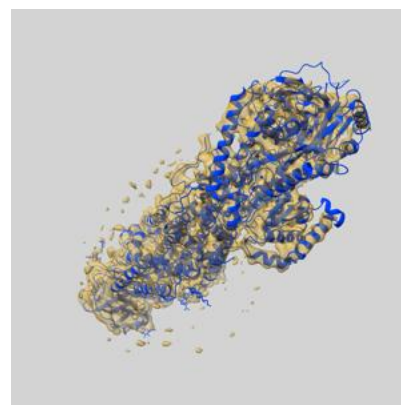
9.1 Map-model overlay [i](#)



X



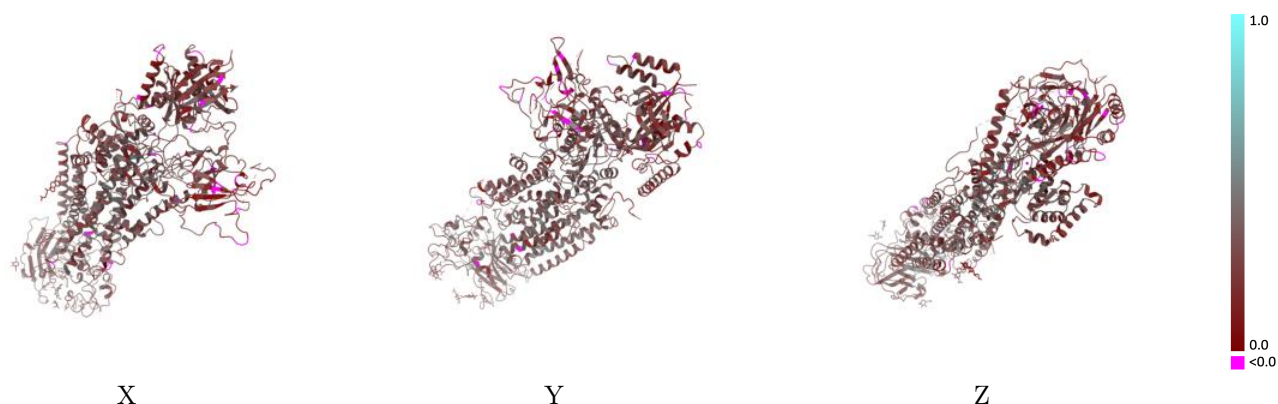
Y



Z

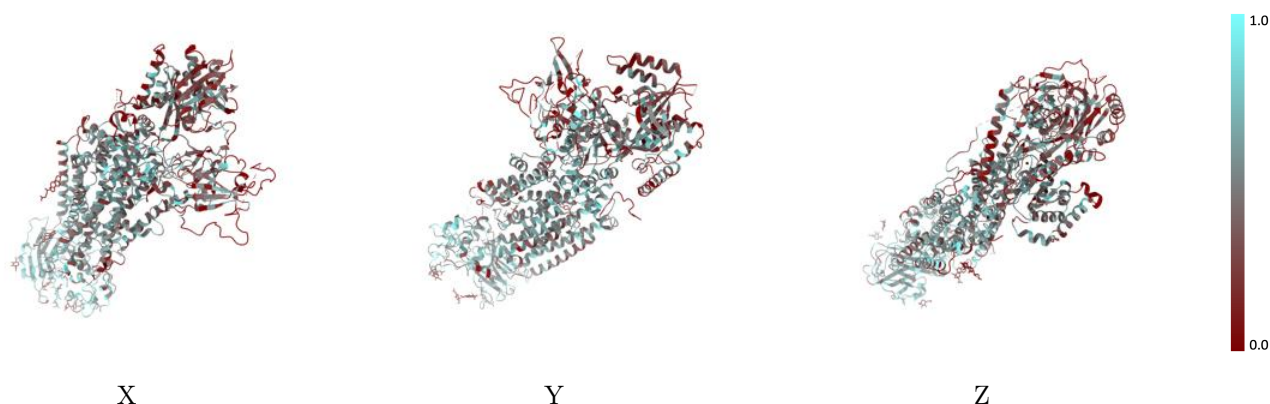
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



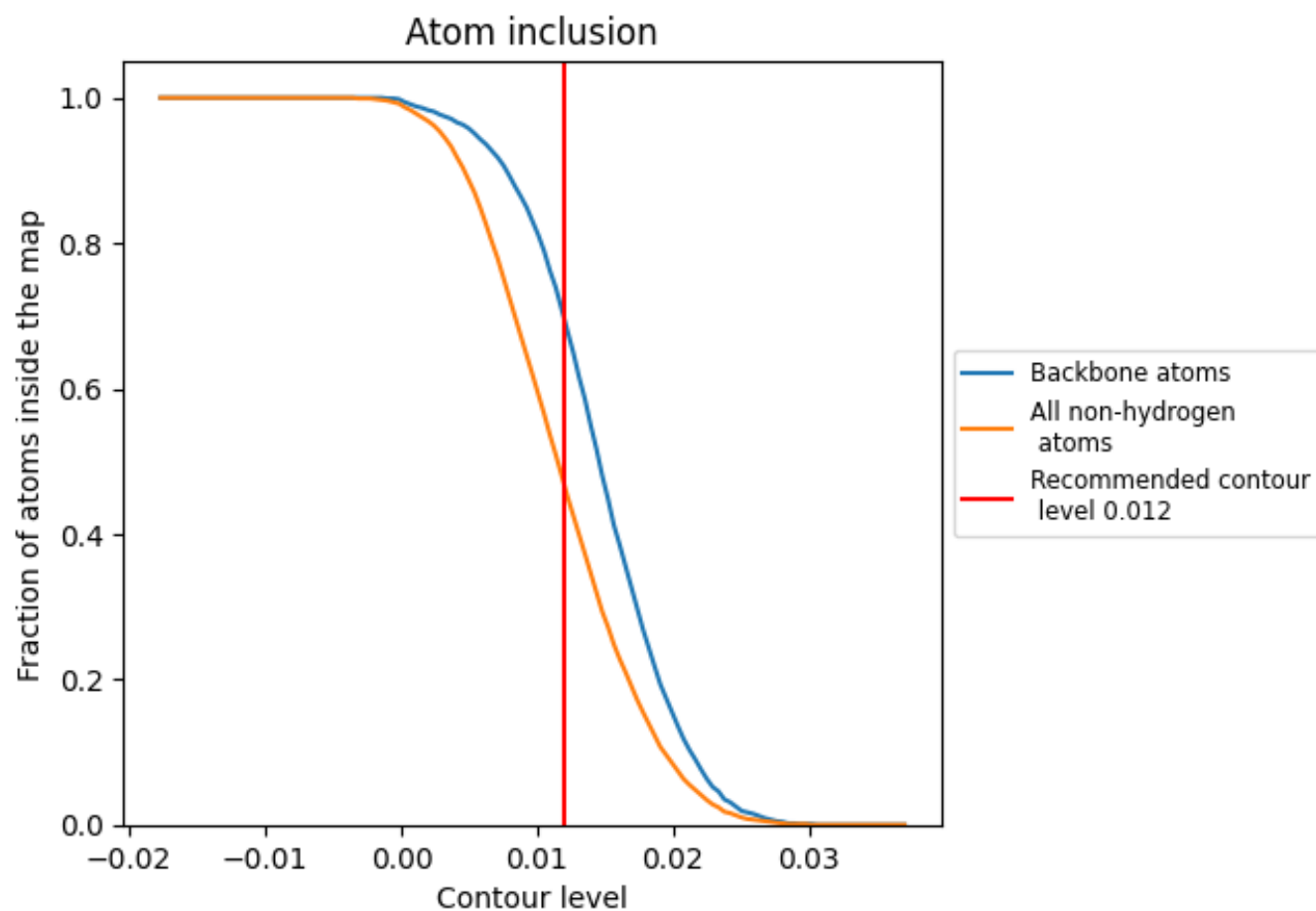
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

