



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2025 – 09:00 PM JST

PDB ID : 8WEA / pdb_00008wea
EMDB ID : EMD-37476
Title : Human L-type voltage-gated calcium channel Cav1.2 (Class II) in the presence of pinaverium at 3.2 Angstrom resolution
Authors : Gao, S.; Yao, X.; Fan, X.; Yan, N.
Deposited on : 2023-09-17
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

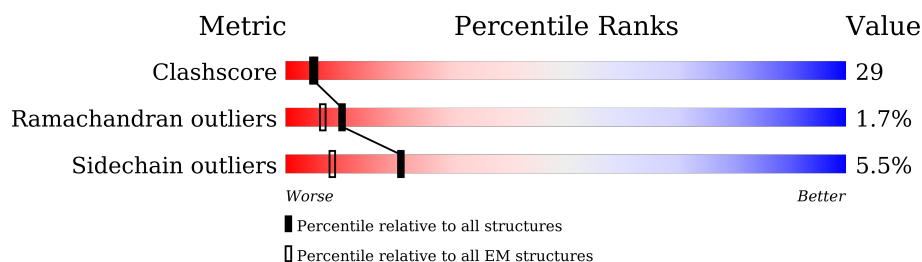
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2201	 22% 22% 27% 5% • 45%
2	D	1103	 7% 65% 20% • 14%
3	B	3	 33% 67% 33%
4	C	2	 50% 50% 50%
4	F	2	 50% 100%
4	G	2	 50% 50% 50%
5	E	4	 25% 75%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 17188 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 Voltage-dependent L-type calcium channel subunit alpha-1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1206	Total	C	N	O	S	0	0
			9335	6116	1541	1617	61		

- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	948	Total	C	N	O	S	0	0
			7570	4803	1269	1467	31		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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	B	3	Total	C	N	O	0	0
			42	24	3	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	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

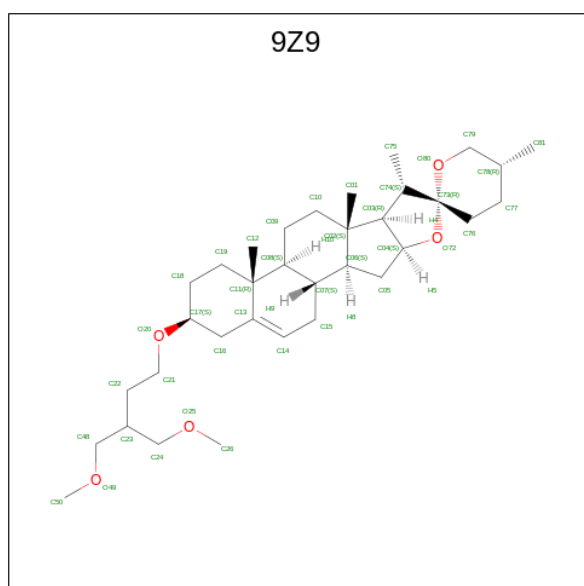


Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

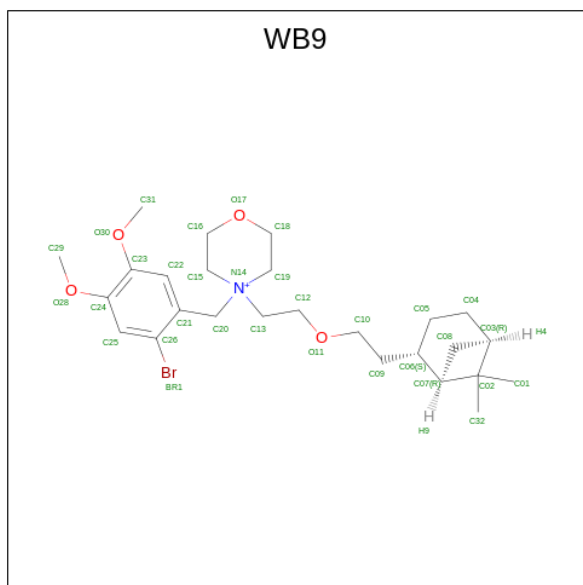
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	

- Molecule 7 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



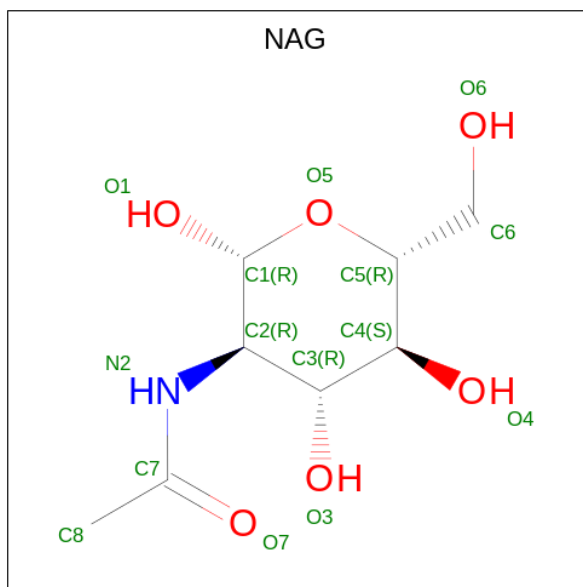
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			39	34	5	

- Molecule 8 is 4-[(2-bromanyl-4,5-dimethoxy-phenyl)methyl]-4-[2-[2-[(1 {R},2 {S},5 {R})-6,6-dimethyl-2-bicyclo[3.1.1]heptanyl]ethoxy]ethyl]morpholin-4-ium (CCD ID: WB9) (formula: $C_{26}H_{41}BrNO_4$) (labeled as "Ligand of Interest" by depositor).



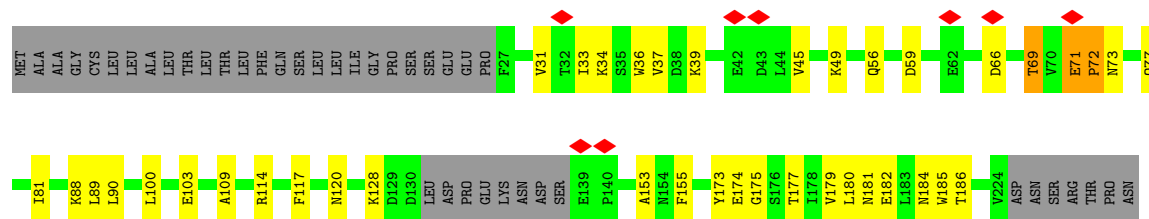
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	Br	C	N	O	0
			32	1	26	1	4	

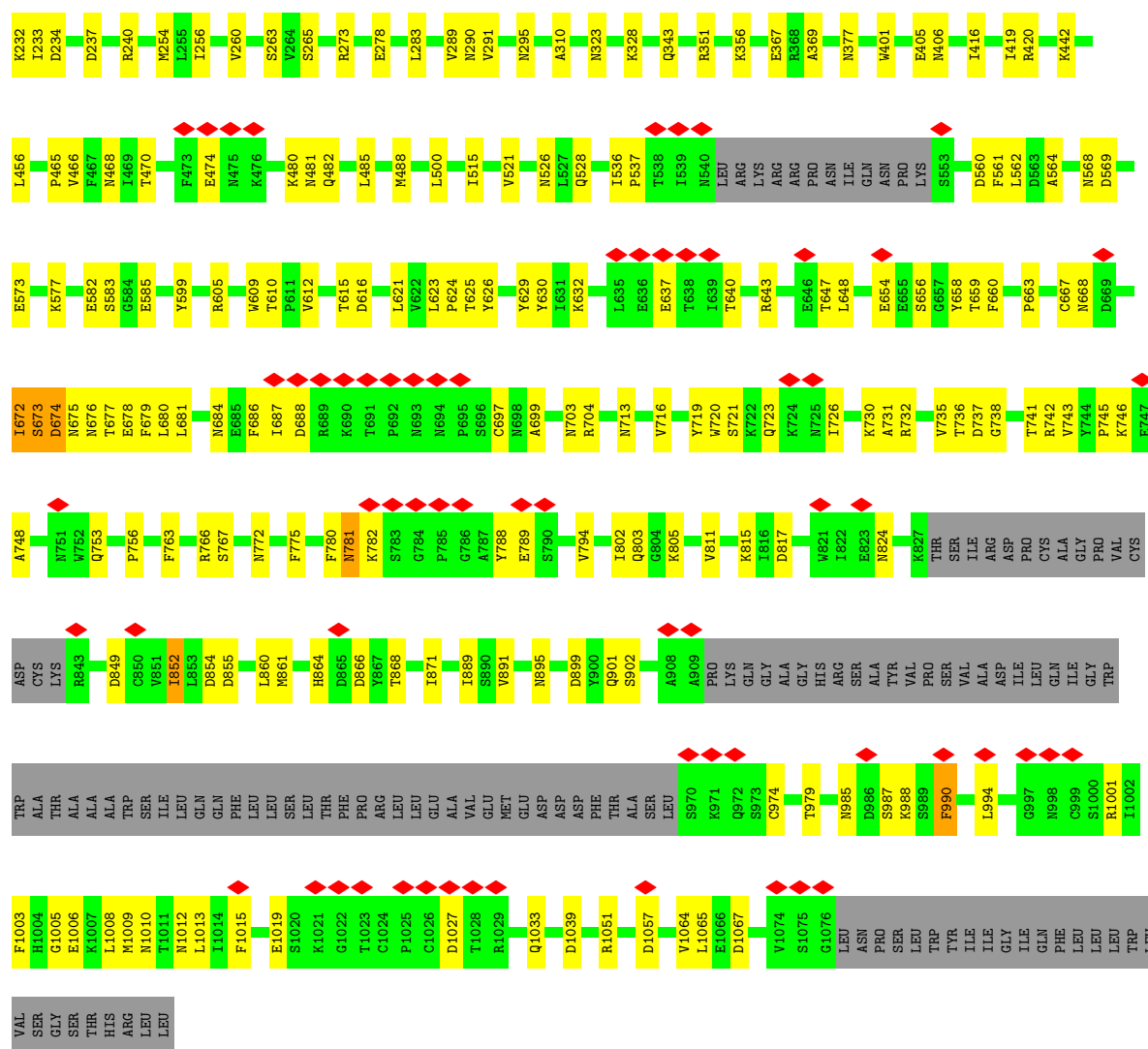
- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

ARG	ILE	S1372	I1373	T1374	F1375	F1376	R1377	L1378	F1379	R1380	M1381	M1382	R1383	L1384	V1385	K1386	L1387	L1388	S1389	R1390	G1391	E1392	G1393	I1394	R1395	T1396	L1397	L1398	L1399	F1400	T1401	I1402	K1403	S1404	F1405	Q1406	A1407	P1408	Y1410	A1412	L1413	L1414	V1415	V1416	F1420	I1421	I1422	A1423	V1424	I1425	V1429	F1430	G1431	K1432	I1433			
L1309	I1310	V1311	I1312	G1313	S1314	I1315	I1316	I1319	L1320	S1321	E1322	T1323	ASN	HIS	TRP	PHE	CYS	ASP	ALA	TRP	ASN	THR	PHE	ASP	ALA	LEU	ILE	VAL	GLY	VAL	ILE	VAL	ASP	ILE	A1408	A1409	THR	THR	ASN	ALA	ALA	HIS	THR	GLN	CYS	SER	PRO	SER	MET	ASN	ALA	GLU	GLU	ASN	SER			
Y1243	L1244	M1245	F1246	V1247	L1248	I1249	L1250	L1251	I1254	G1255	L1256	H1260	Q1263	S1264	C1265	L1266	F1267	K1268	M1271	M1272	I1273	L1274	M1275	M1276	L1277	F1278	L1281	F1282	T1283	V1284	E1285	M1286	I1287	L1288	K1289	L1290	I1291	A1292	F1293	K1294	P1295	K1296	G1297	Y1298	F1299	S1300	D1301	P1302	W1303	M1304	V1305	F1306	D1307	F1308				
V1121	L1122	A1123	A1124	M1125	M1126	A1127	L1128	F1129	T1133	PHE	GLU	GLY	TRP	PRO	GLU	LEU	LEU	TRP	ARG	SER	ILE	ASP	SER	HIS	THR	GLU	ASP	LYS	P1154	I1155	Y1156	M1157	Y1158	R1159	V1160	E1161	S1162	S1163	F1164	F1165	F1166	I1167	I1168	Y1169	I1170	I1171	I1172	I1173	A1174	F1175	F1176	M1177	M1178	N1179	I1180	F1181	V1182	
I1052	V1053	I1054	T1057	Q1060	F1061	M1062	F1063	A1064	C1065	I1066	G1067	V1068	Q1069	L1070	F1071	K1072	G1073	K1074	L1075	C1078	S1079	K1083	Q1084	T1085	E1086	A1087	E1088	C1089	K1090	Y1093	Y1096	K1097	D1098	D1102	H1103	P1104	I1105	I1106	Q1107	P1108	R1109	S1110	W1111	E1112	N1113	S1114	K1115	F1116	D1117	F1118	D1119	N1120						
PHE	CYS	ARG	ASN	TVR	F989	N990	N991	L994	V997	S998	V999	L1000	L1001	I1002	S1003	F1004	Q1007	S1008	S1009	ALA	ILE	M1012	V1013	V1014	V1019	L1020	L1023	K1024	P1025	L1026	K1027	A1028	I1029	M1030	R1031	A1032	K1033	G1034	LEU	LYS	HIS	V1038	V1039	Q1040	C1041	V1042	F1043	V1044	R1047	T1048	I1049	G1050	M1051					
N904	L905	I906	L907	F908	F909	L910	L911	L912	S913	S914	L915	S916	L917	A918	A919	E920	D921	P922	V923	Q924	H925	T926	S927	F928	R929	N930	H931	L932	L933	G934	N935	A936	D937	Y938	V939	F960	T961	S962	L963	F964	T965	L966	E967	I968	L969	L970	K971	M972	T973	A974	G975	ALA	PHE	LEU	HIS	LYS	GLY	SER
GLY	GLU	GLU	ASP	GLU	GLU	GLU	PRO	GLU	PRO	GLU	MET	VAL	GLY	PRO	ARG	ARG	PRO	LEU	HIS	LEU	LYS	GLU	LYS	VAL	ALA	VAL	PRO	PRO	PRO	ALA	SER	PHE	PHE	ILE	PHE	SER	ASN	ASN	R888	R889	L891	Q892	C893	H894	R895	I896	V897	N898	D899	T900	L901	F902	T903					
PRO	GLU	LYS	LYS	GLN	GLU	LEU	VAL	GLU	LYS	PRO	PRO	ALA	VAL	GLY	GLU	SER	LYS	ILE	THR	ALA	ASP	GLY	GLU	THR	PRO	PRO	PRO	PRO	ALA	ALA	LYS	THR	ILE	LYS	ASN	MET	LEU	THR	ASP	ASP	GLN	PRO	ASN	GLU	GLU	GLU	LYS	PRO	ARG	TVR	PRO	LYS	LEU	GLU	PRO	THR	ALA	SER
F584	V585	S586	M587	F588	N589	R590	F591	D592	C593	F594	V595	C597	G598	G599	I600	L601	E602	T603	I604	L605	V606	E607	THR	LYS	ILE	MET	S612	P613	L614	G615	I616	S617	V618	L619	R620	C621	V622	R623	L624	L625	R626	I627	F628	K629	I630	T631	R632	Y633	W634	S635	L636	S638	N639	L640	V641	A642		
L645	N646	S647	V648	R649	S650	I651	L654	L655	L656	L657	L658	F659	L660	F661	I662	G663	I664	F665	S666	M670	Q671	L672	F673	G674	G675	K676	F677	E681	M682	Q683	T684	R685	R686	M691	F692	P693	Q694	S695	L696	V699	F700	I702	L703	T704	G705	E706	D707	W708	N709	S710	M712	Y713						
D714	G715	I716	M717	Y718	Y719	F724	P725	G726	M727	L728	W729	C730	I731	F732	F733	I734	I735	L736	F737	N746	F747	F748	L749	A750	I751	A752	V753	D754	M755	L756	A757	D758	A759	E760	S761	LEU	THR	SER	ASP	ASP	GLN	PRO	ASN	GLU	GLU	GLU	LYS	PRO	ARG	TVR	PRO	LYS	LEU	GLU	PRO	THR	ALA	SER





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



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



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



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	299035	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.106	Depositor
Minimum map value	-2.750	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	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: WB9, NAG, CA, 9Z9

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	0.76	13/9535 (0.1%)	0.97	47/12941 (0.4%)
2	D	0.15	0/7728	0.37	0/10477
All	All	0.58	13/17263 (0.1%)	0.76	47/23418 (0.2%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	ASP	CA-C	-8.17	1.47	1.52
1	A	146	PRO	CA-CB	-7.83	1.45	1.54
1	A	316	CYS	CA-C	-6.93	1.44	1.52
1	A	145	ILE	CA-C	-6.89	1.45	1.52
1	A	147	PHE	CA-C	-6.50	1.44	1.52

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1032	ALA	N-CA-C	-12.01	99.40	113.21
1	A	1406	GLN	N-CA-C	-9.36	103.95	114.62
1	A	1030	ASN	N-CA-C	-8.85	101.54	111.71
1	A	379	ASP	N-CA-C	8.27	119.92	111.07
1	A	375	ALA	N-CA-C	8.00	119.78	111.14

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	9335	0	9194	817	0
2	D	7570	0	7371	173	0
3	B	42	0	37	4	0
4	C	28	0	25	1	0
4	F	28	0	25	1	0
4	G	28	0	25	1	0
5	E	56	0	49	4	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	39	0	0	0	0
8	A	32	0	0	1	0
9	D	28	0	26	2	0
All	All	17188	0	16752	990	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 29.

The worst 5 of 990 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:511:ARG:CZ	1:A:512:PHE:CE1	1.97	1.46
1:A:511:ARG:NH2	1:A:512:PHE:HE1	1.00	1.44
1:A:511:ARG:NH2	1:A:512:PHE:CE1	1.93	1.36
1:A:511:ARG:CZ	1:A:512:PHE:HE1	1.32	1.28
1:A:282:TYR:CD2	1:A:384:TYR:HE1	1.55	1.25

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	1180/2201 (54%)	998 (85%)	148 (12%)	34 (3%)	3	24
2	D	936/1103 (85%)	883 (94%)	51 (5%)	2 (0%)	44	75
All	All	2116/3304 (64%)	1881 (89%)	199 (9%)	36 (2%)	10	36

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	PRO
1	A	304	ILE
1	A	309	ALA
1	A	752	ALA
1	A	929	ARG

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	961/1896 (51%)	870 (90%)	91 (10%)	7	28
2	D	837/971 (86%)	829 (99%)	8 (1%)	73	87
All	All	1798/2867 (63%)	1699 (94%)	99 (6%)	20	51

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	906	ILE
1	A	1128	LEU
1	A	955	ASN
1	A	969	ILE
1	A	1260	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1260	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	1010	ASN
2	D	73	ASN
2	D	725	ASN
1	A	1445	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

13 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	B	1	2,3	14,14,15	0.88	1 (7%)	17,19,21	1.20	1 (5%)
3	NAG	B	2	3	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	B	3	3	14,14,15	0.30	0	17,19,21	0.39	0
4	NAG	C	1	2,4	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	C	2	4	14,14,15	0.57	0	17,19,21	0.77	0
5	NAG	E	1	2,5	14,14,15	0.28	0	17,19,21	0.41	0
5	NAG	E	2	5	14,14,15	0.71	0	17,19,21	1.96	7 (41%)
5	NAG	E	3	5	14,14,15	0.69	0	17,19,21	1.43	3 (17%)
5	NAG	E	4	5	14,14,15	0.45	0	17,19,21	0.91	1 (5%)
4	NAG	F	1	2,4	14,14,15	0.47	0	17,19,21	0.52	0
4	NAG	F	2	4	14,14,15	0.27	0	17,19,21	0.43	0
4	NAG	G	1	2,4	14,14,15	0.48	0	17,19,21	0.39	0
4	NAG	G	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	B	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	NAG	B	3	3	-	2/6/23/26	0/1/1/1
4	NAG	C	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	E	3	5	-	6/6/23/26	0/1/1/1
5	NAG	E	4	5	-	5/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	NAG	O5-C1	3.03	1.48	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C1-O5-C5	4.72	118.58	112.19
5	E	2	NAG	C2-N2-C7	-3.85	117.41	122.90
5	E	3	NAG	O4-C4-C3	-3.42	102.43	110.35
5	E	2	NAG	C1-C2-N2	-3.22	104.98	110.49
5	E	2	NAG	O5-C1-C2	3.07	116.14	111.29

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	3	NAG	C3-C2-N2-C7
5	E	3	NAG	C8-C7-N2-C2
5	E	3	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

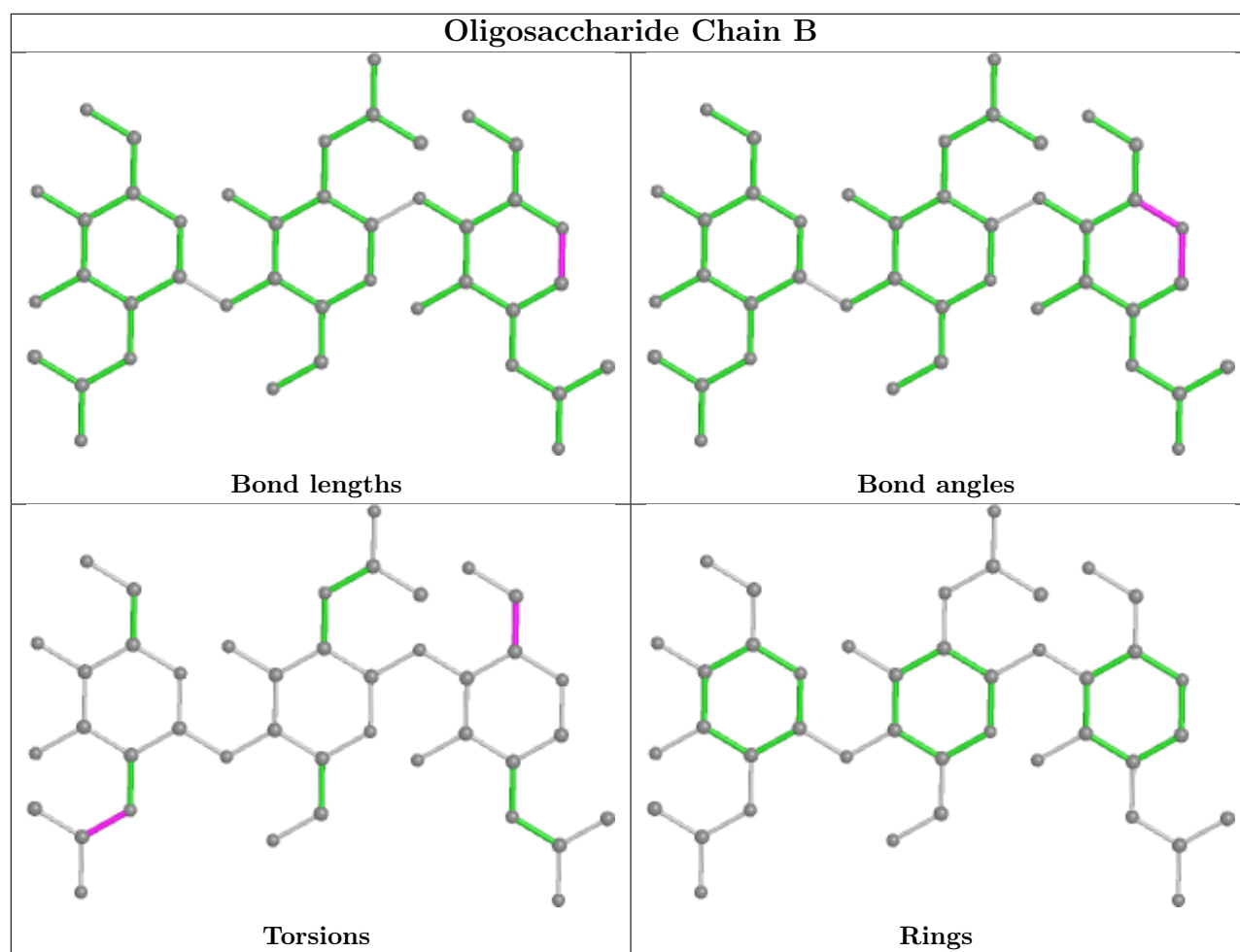
Mol	Chain	Res	Type	Atoms
5	E	4	NAG	C8-C7-N2-C2
5	E	4	NAG	O7-C7-N2-C2

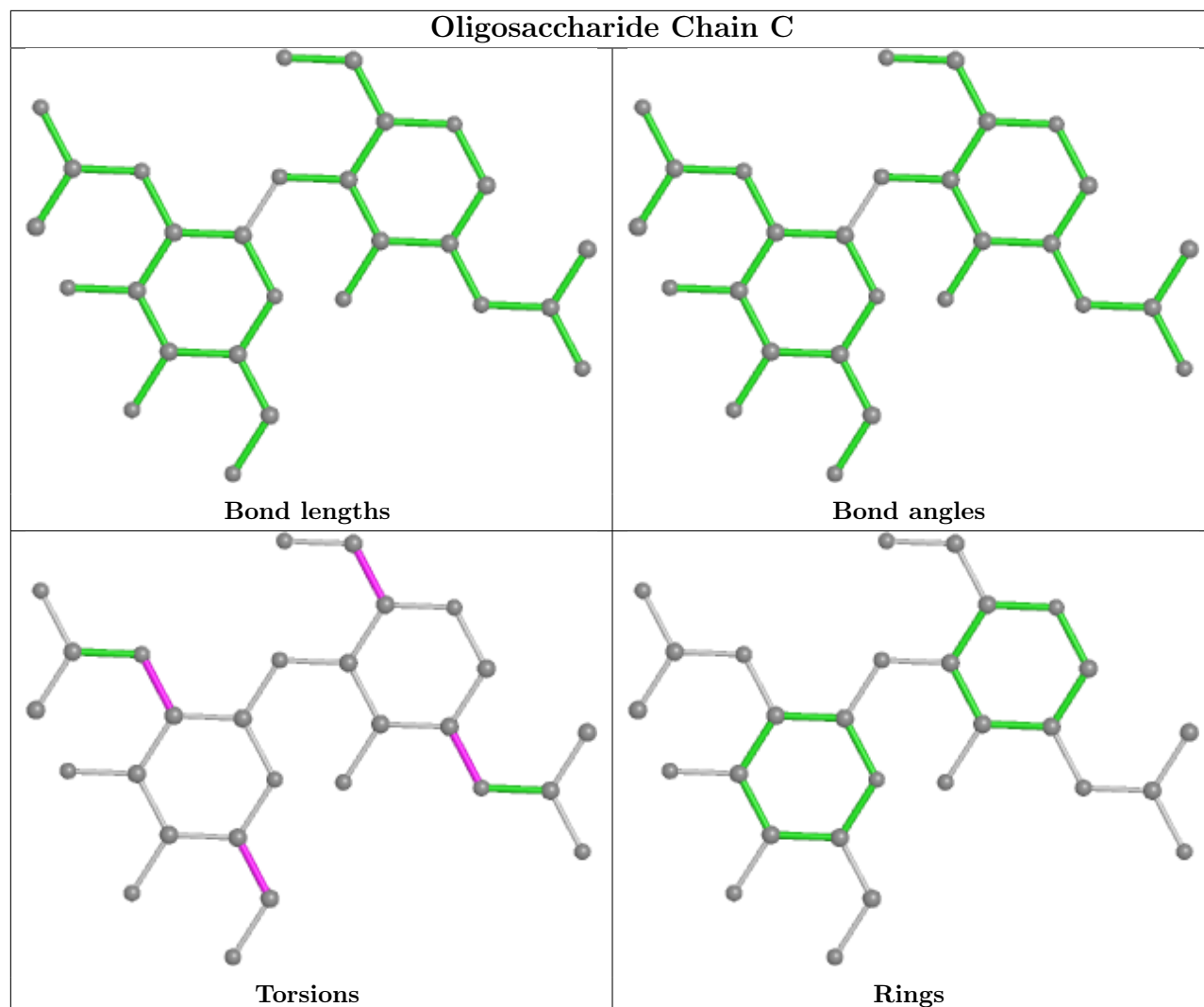
There are no ring outliers.

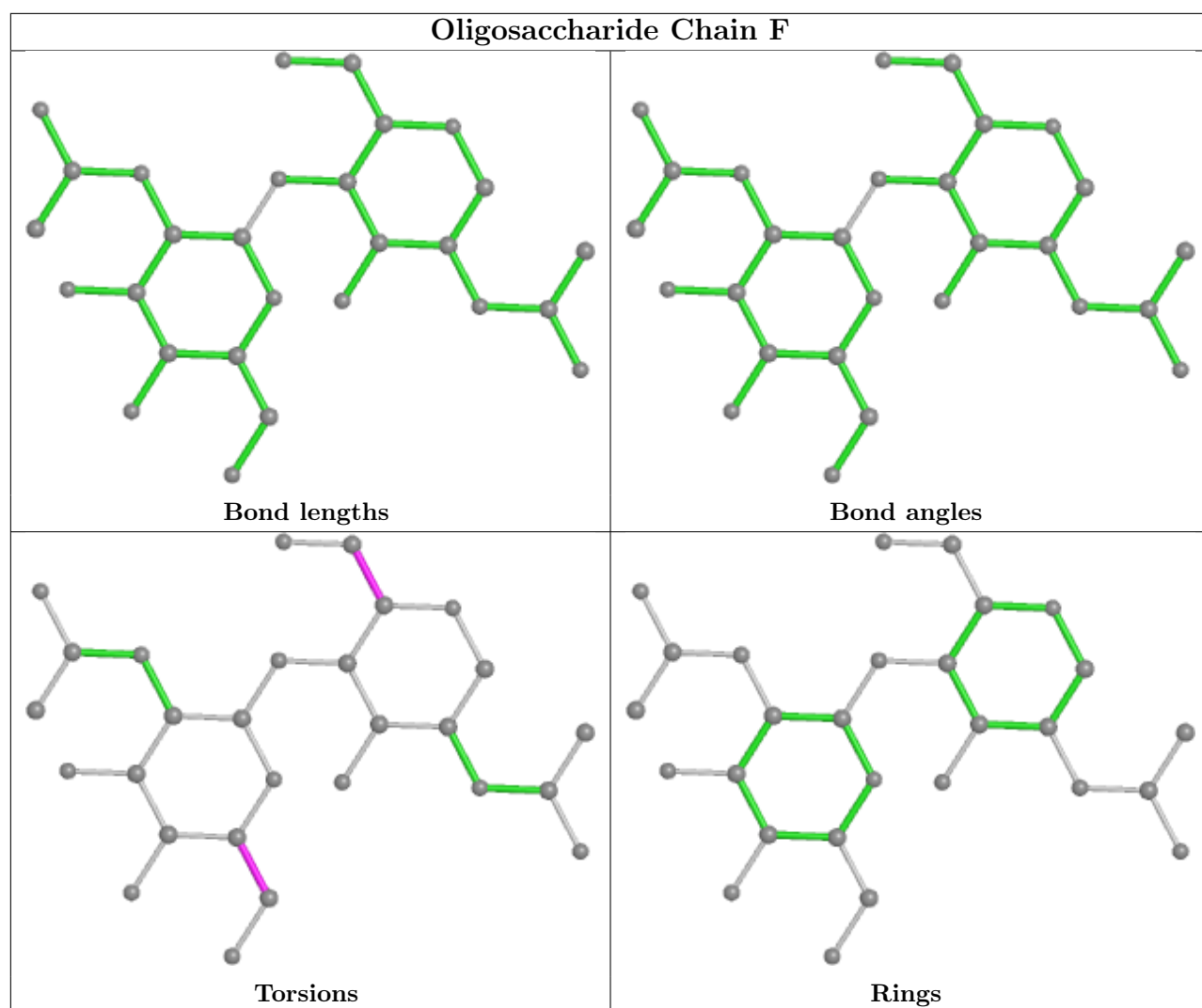
9 monomers are involved in 11 short contacts:

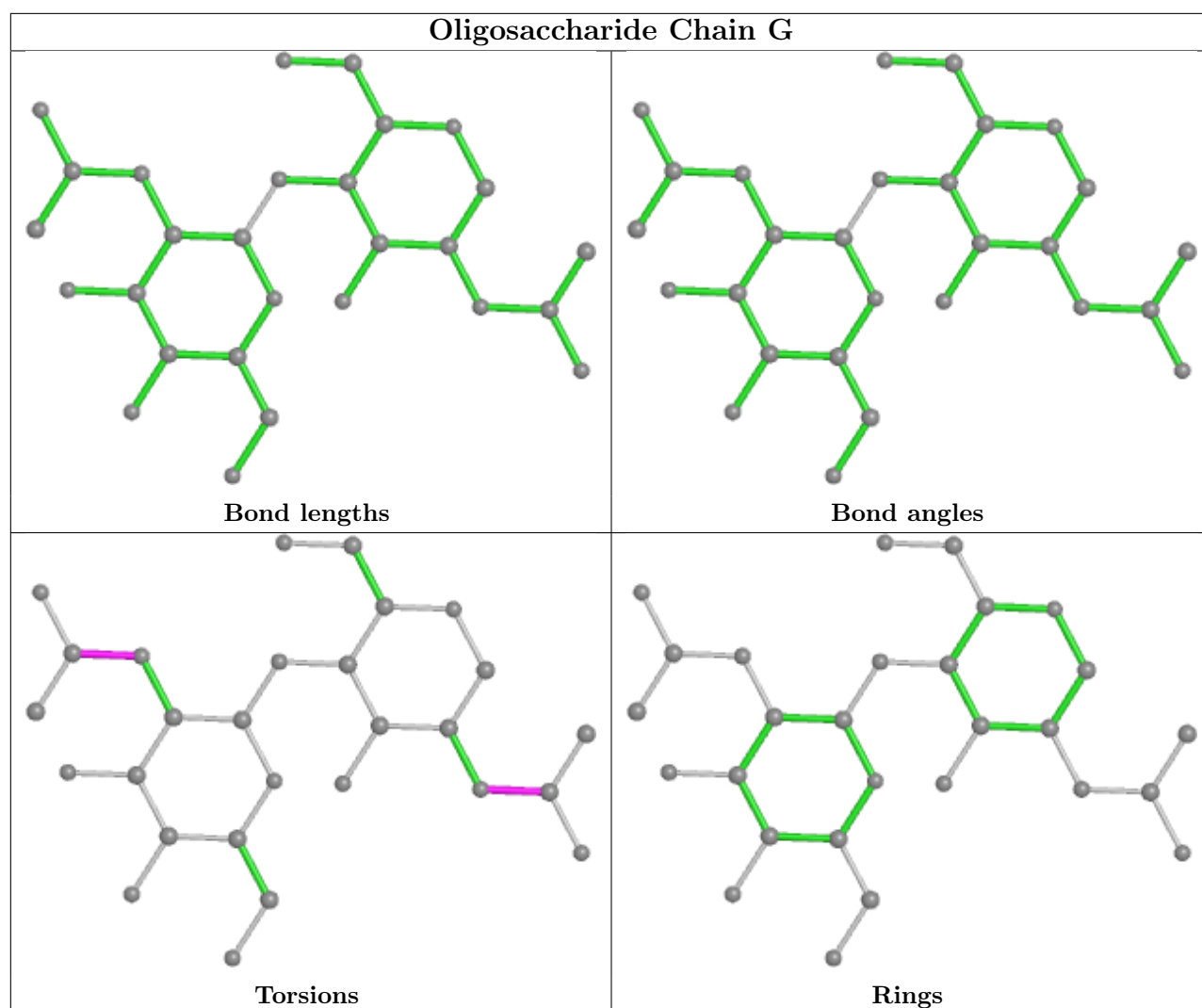
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	2	0
5	E	3	NAG	2	0
4	G	1	NAG	1	0
4	F	1	NAG	1	0
4	F	2	NAG	1	0
3	B	1	NAG	4	0
5	E	4	NAG	1	0
5	E	2	NAG	1	0
4	C	2	NAG	1	0

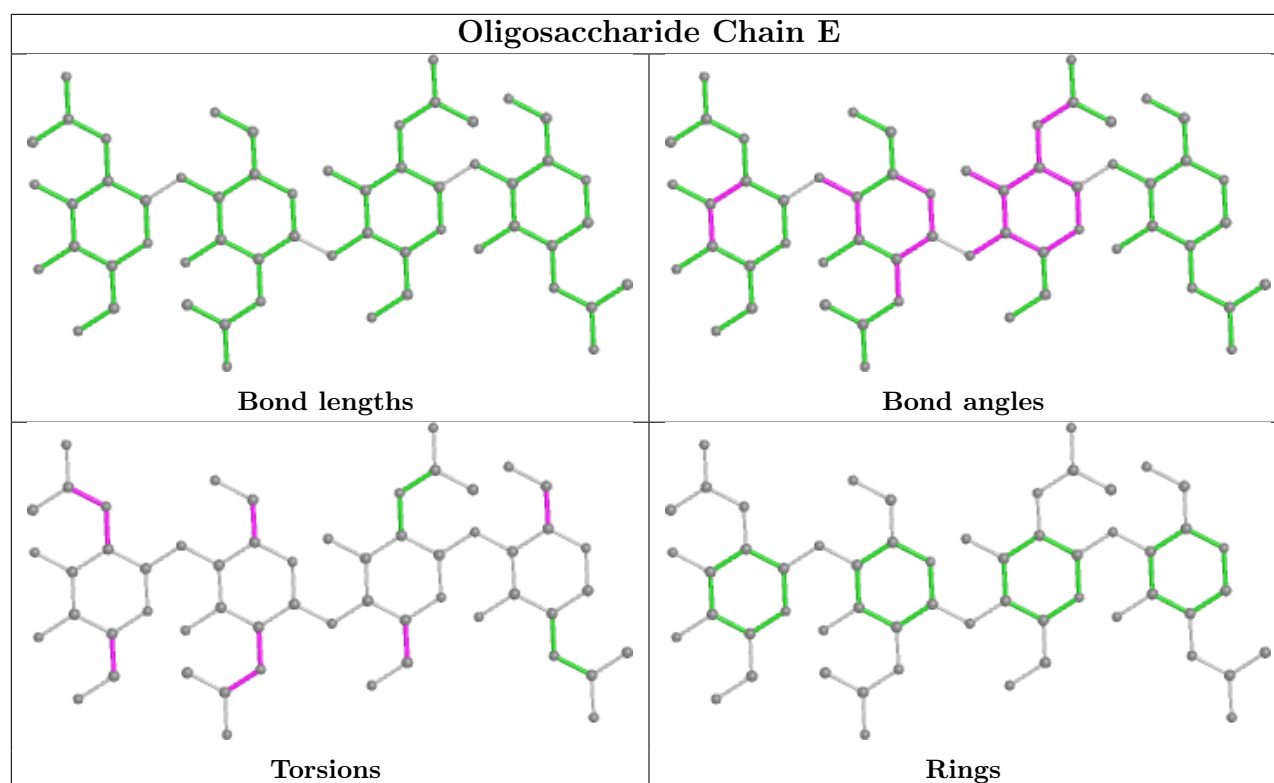
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
9	NAG	D	1203	2	14,14,15	1.14	1 (7%)	17,19,21	1.19	1 (5%)
8	WB9	A	2303	-	35,35,35	1.54	7 (20%)	48,51,51	6.99	21 (43%)
7	9Z9	A	2302	-	44,44,44	1.69	11 (25%)	66,68,68	1.57	14 (21%)
9	NAG	D	1202	2	14,14,15	0.44	0	17,19,21	0.40	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
9	NAG	D	1203	2	-	1/6/23/26	0/1/1/1
8	WB9	A	2303	-	-	15/18/53/53	0/5/4/4
7	9Z9	A	2302	-	-	5/12/100/100	0/6/6/6
9	NAG	D	1202	2	-	4/6/23/26	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2302	9Z9	C11-C08	-3.90	1.49	1.56
9	D	1203	NAG	O5-C1	3.86	1.49	1.43
7	A	2302	9Z9	C11-C13	-3.80	1.45	1.52
7	A	2302	9Z9	O80-C79	-3.77	1.38	1.43
7	A	2302	9Z9	C09-C08	-3.58	1.47	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2303	WB9	C02-C07-C06	-25.98	67.13	113.91
8	A	2303	WB9	C04-C03-C02	-22.51	66.33	111.51
8	A	2303	WB9	C08-C03-C04	19.70	134.76	108.69
8	A	2303	WB9	C08-C07-C06	15.88	135.21	107.66
8	A	2303	WB9	C32-C02-C01	-14.72	74.81	108.67

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2302	9Z9	C24-C23-C48-O49
8	A	2303	WB9	C05-C06-C09-C10
8	A	2303	WB9	C07-C06-C09-C10
8	A	2303	WB9	O11-C12-C13-N14
8	A	2303	WB9	C12-C13-N14-C15

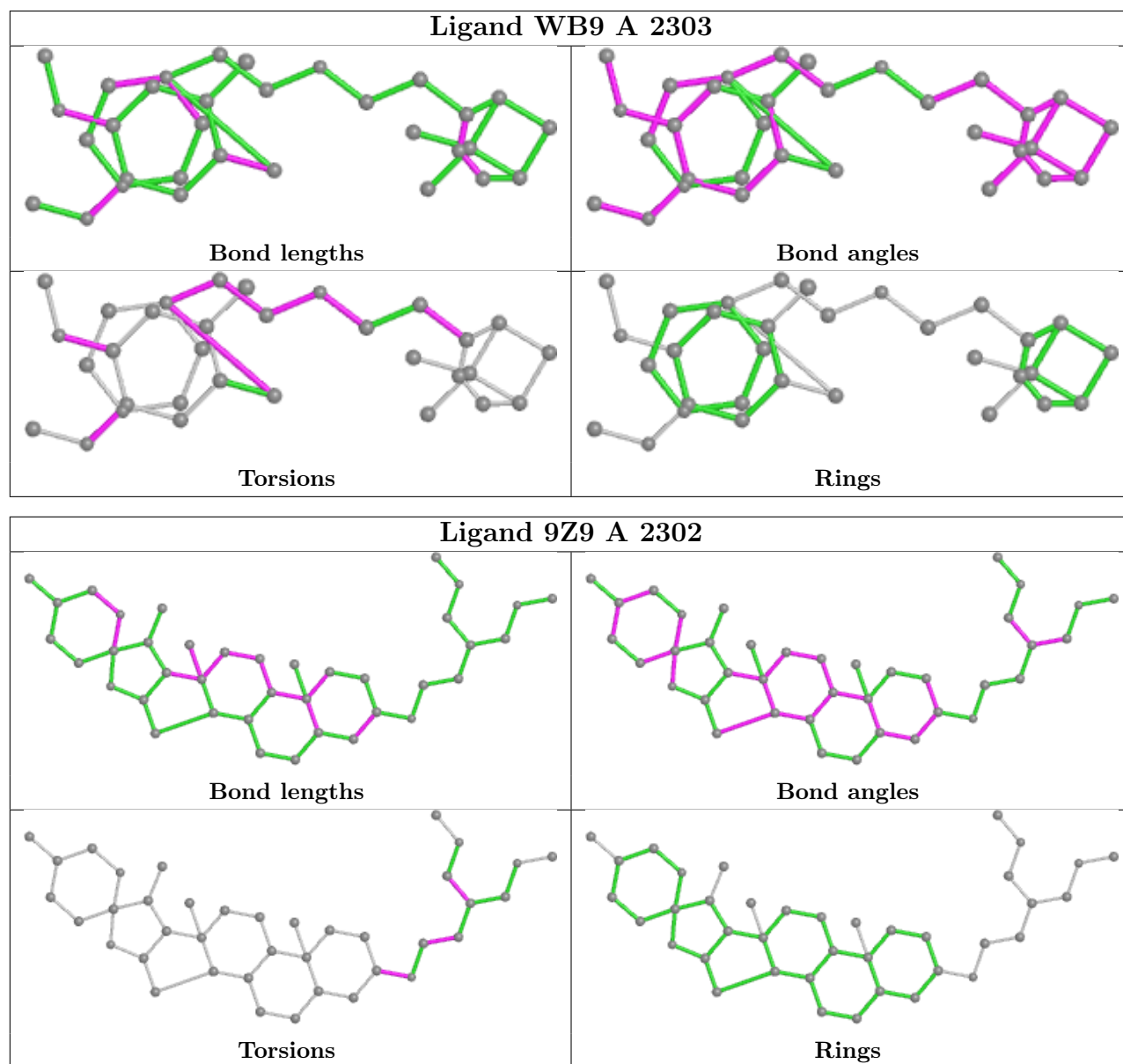
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	1203	NAG	2	0
8	A	2303	WB9	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 [i](#)

There are no chain breaks in this entry.

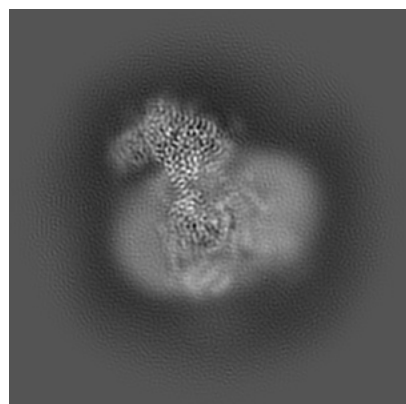
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37476. These allow visual inspection of the internal detail of the map and identification of artifacts.

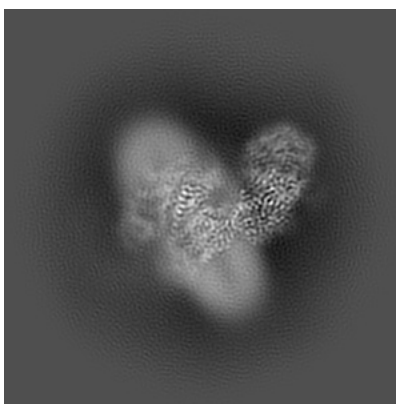
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

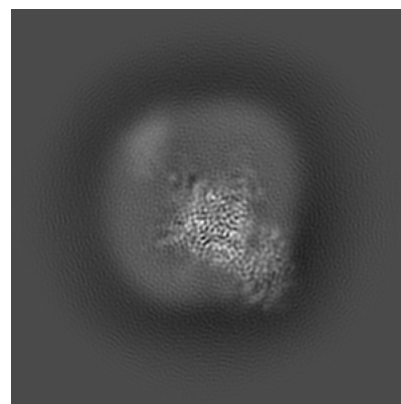
6.1.1 Primary map



X

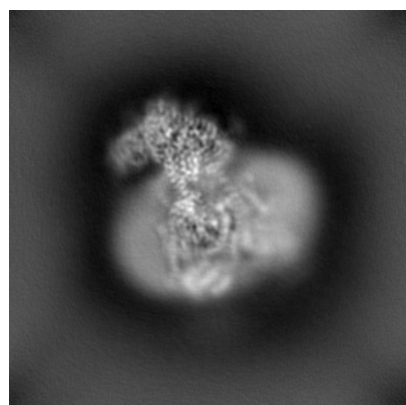


Y

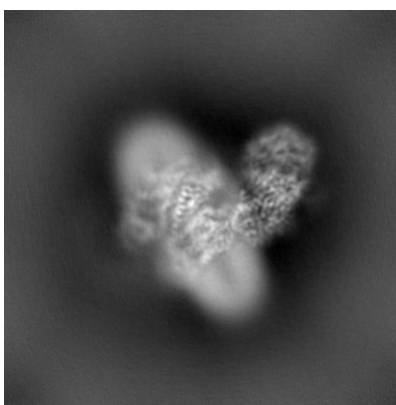


Z

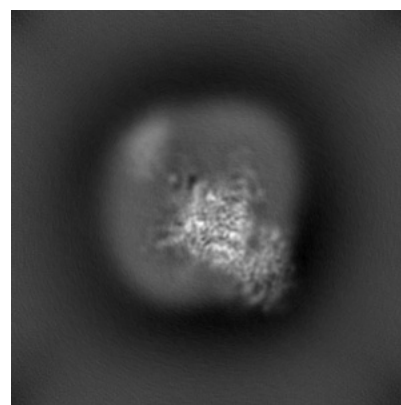
6.1.2 Raw map



X



Y

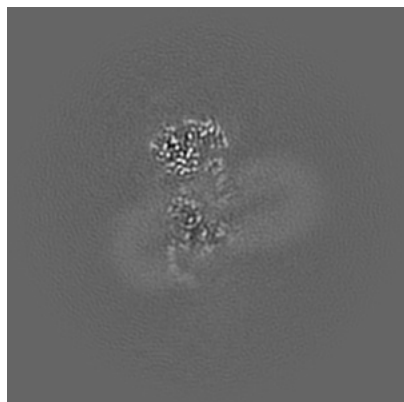


Z

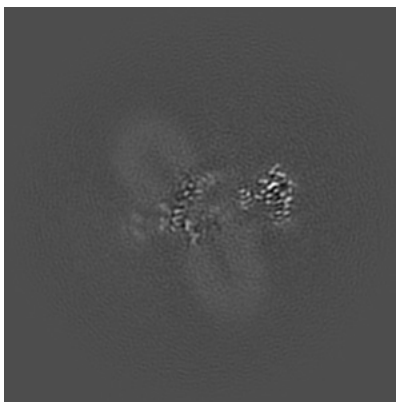
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

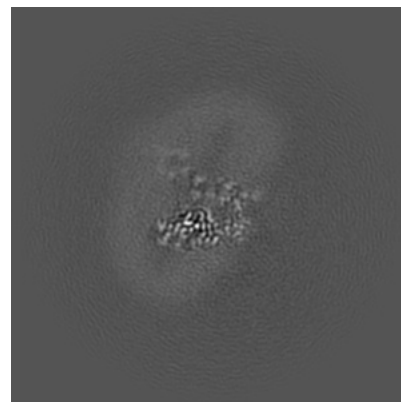
6.2.1 Primary map



X Index: 140

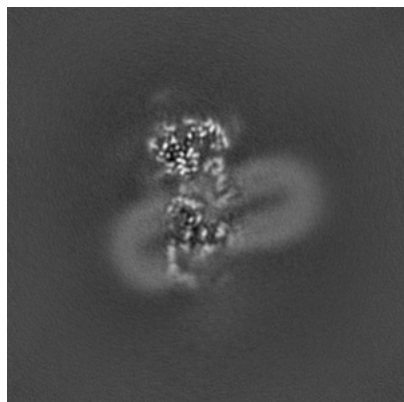


Y Index: 140

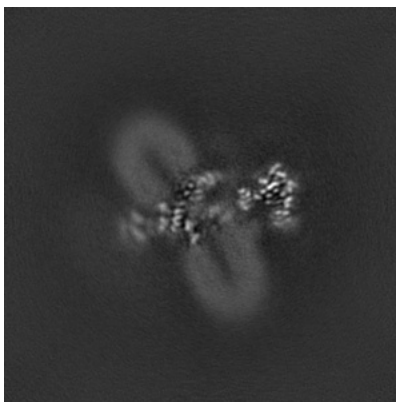


Z Index: 140

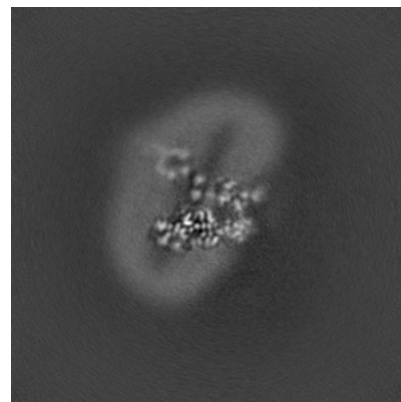
6.2.2 Raw map



X Index: 140



Y Index: 140

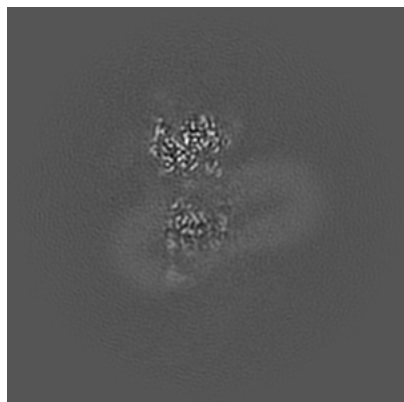


Z Index: 140

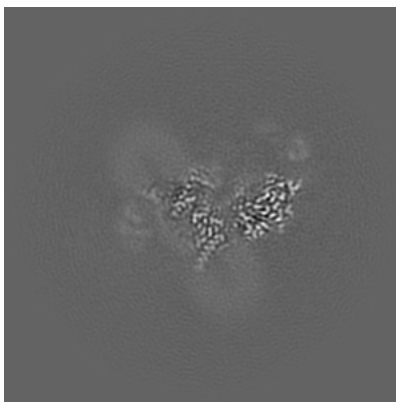
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

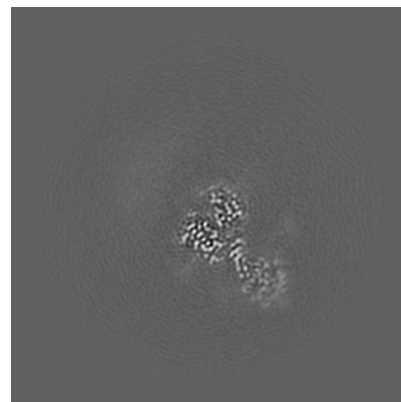
6.3.1 Primary map



X Index: 143

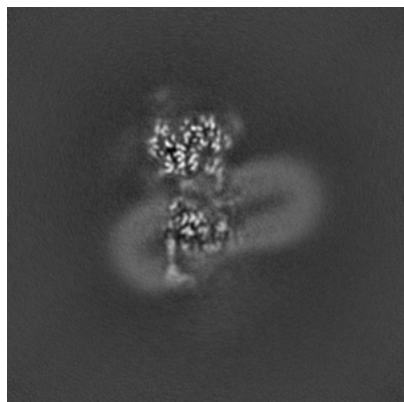


Y Index: 127

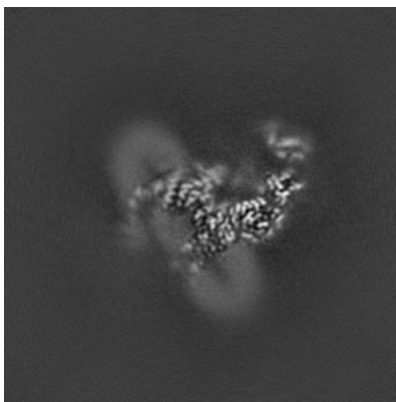


Z Index: 182

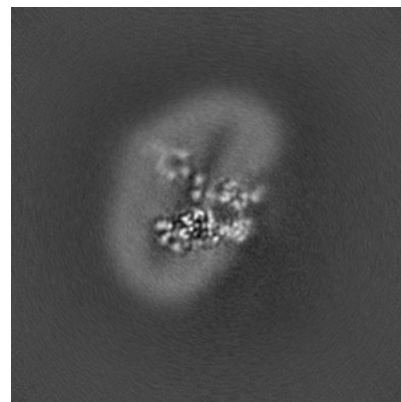
6.3.2 Raw map



X Index: 142



Y Index: 122

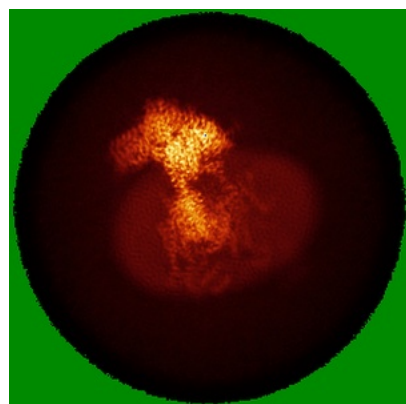


Z Index: 141

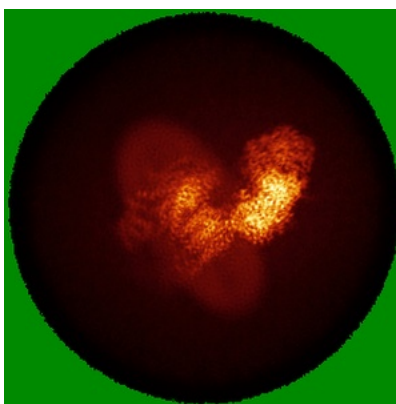
The images above show the largest variance slices of the map in three orthogonal directions.

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

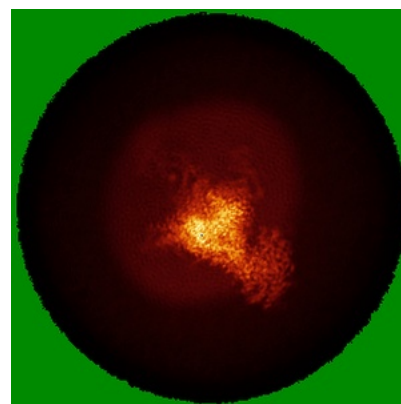
6.4.1 Primary map



X

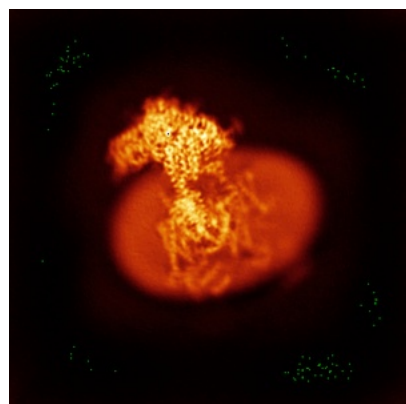


Y

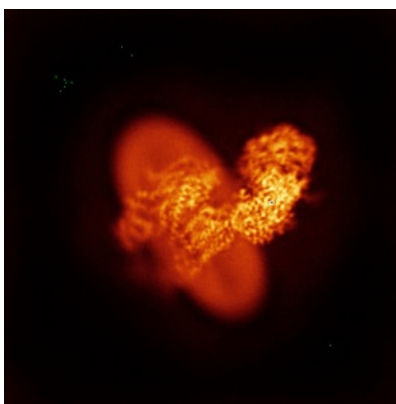


Z

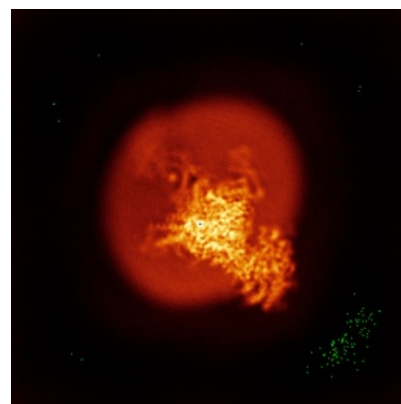
6.4.2 Raw map



X



Y

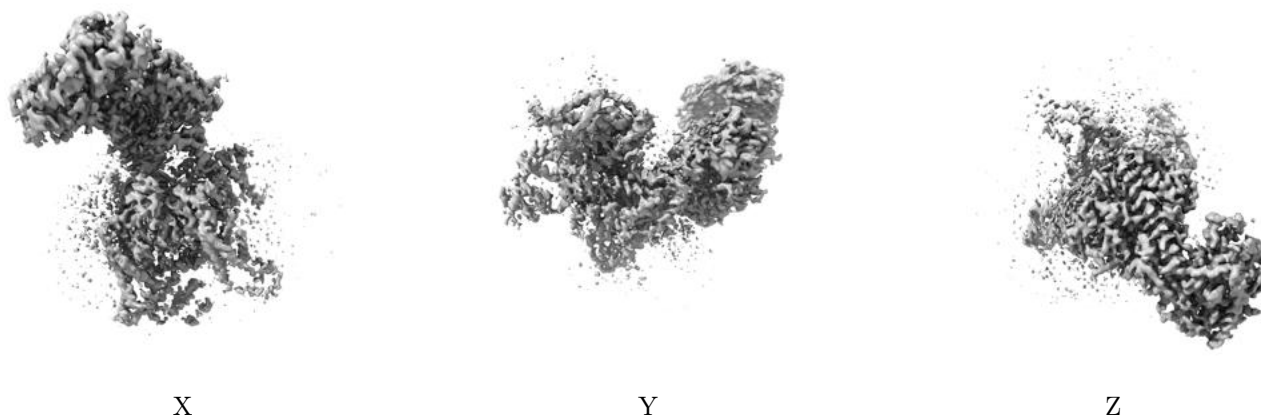


Z

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.

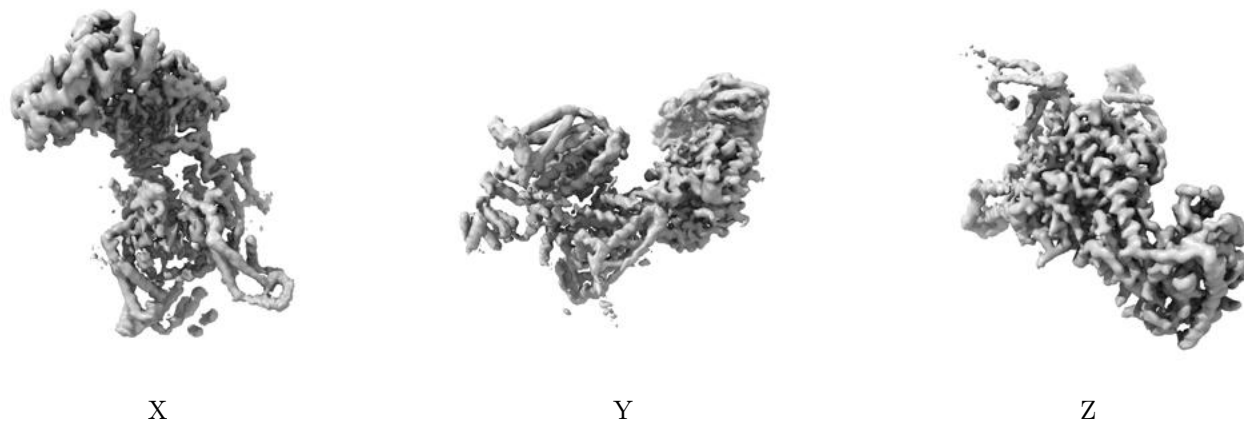
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

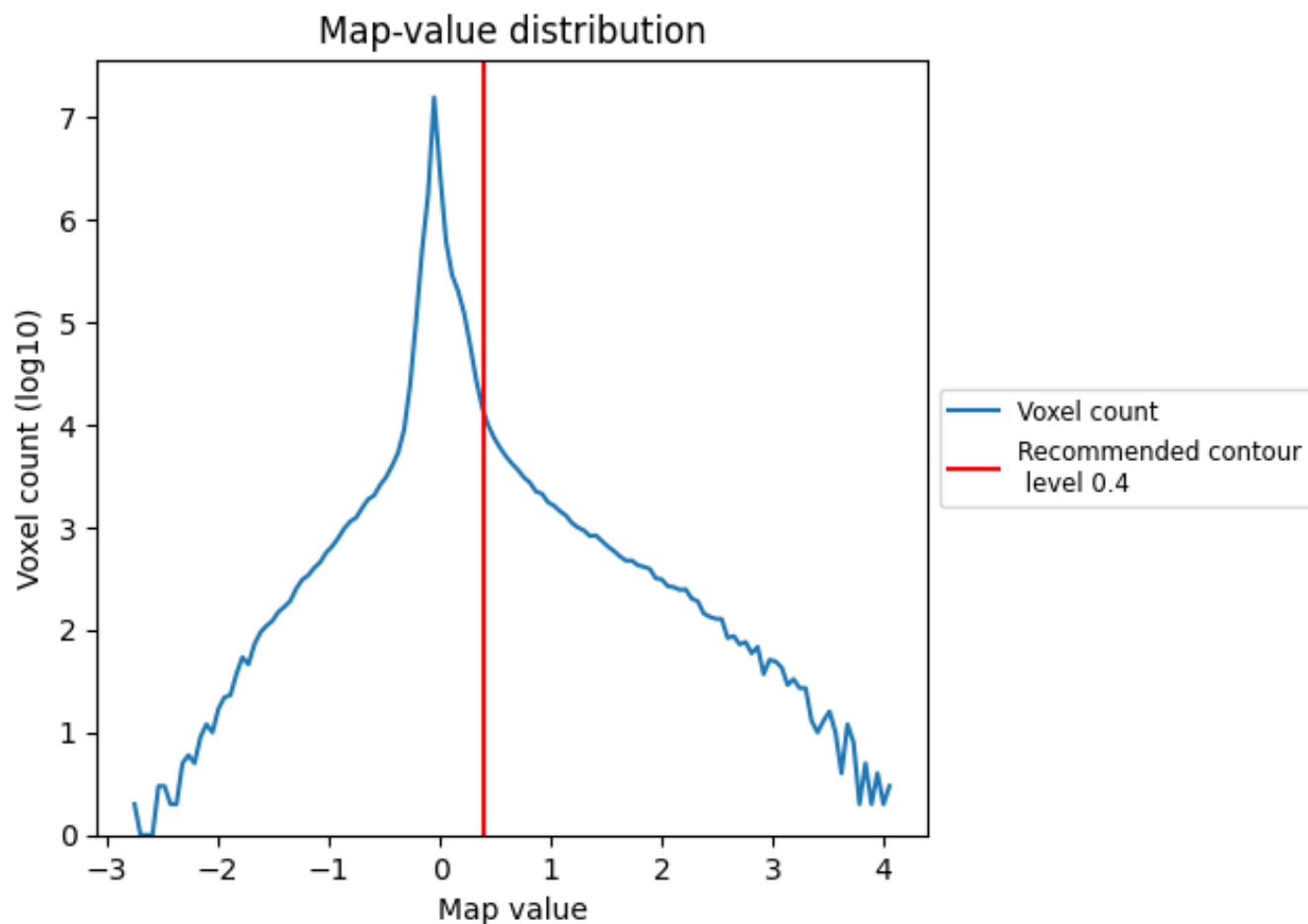
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

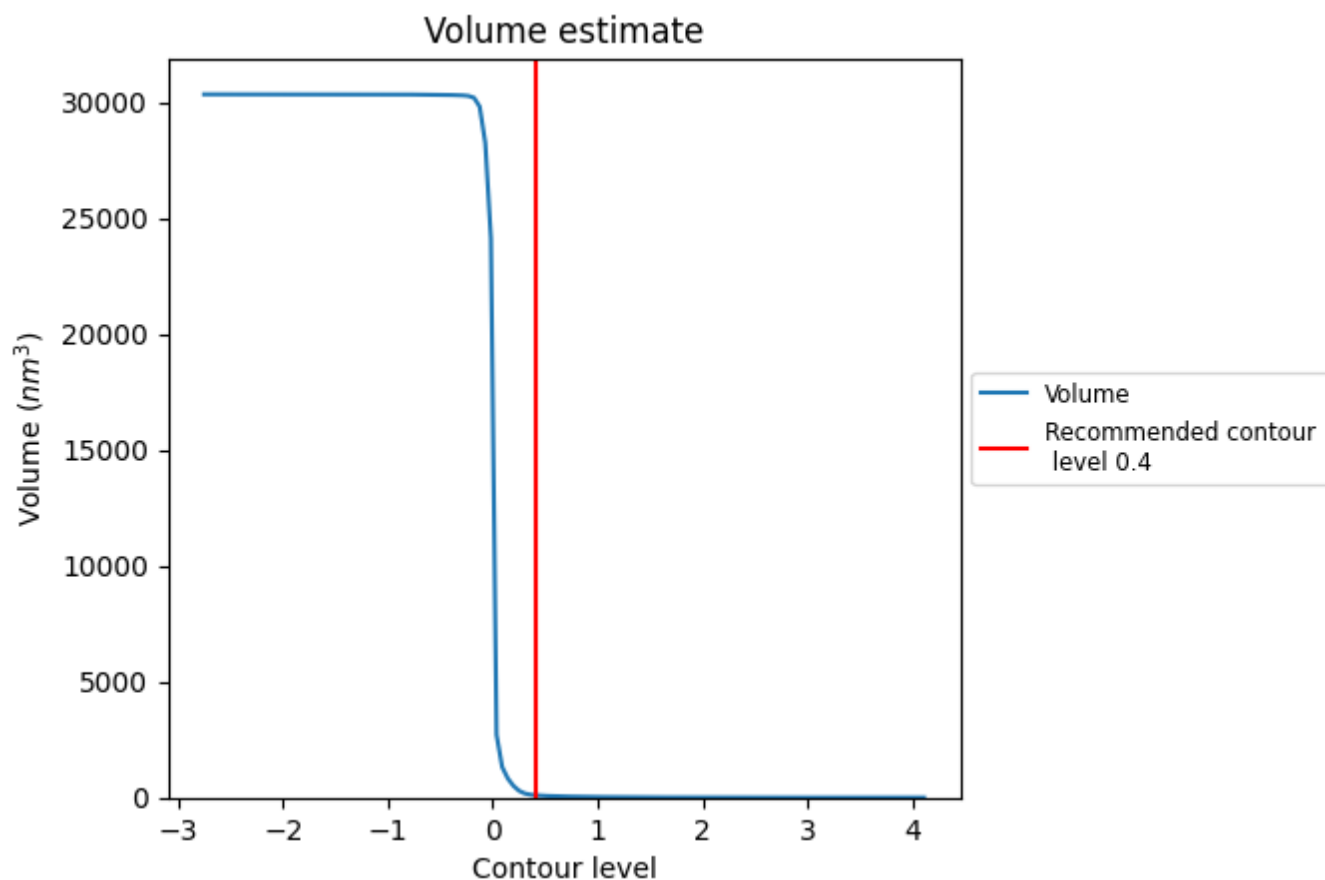
This section contains the results of statistical analysis of the map.

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.

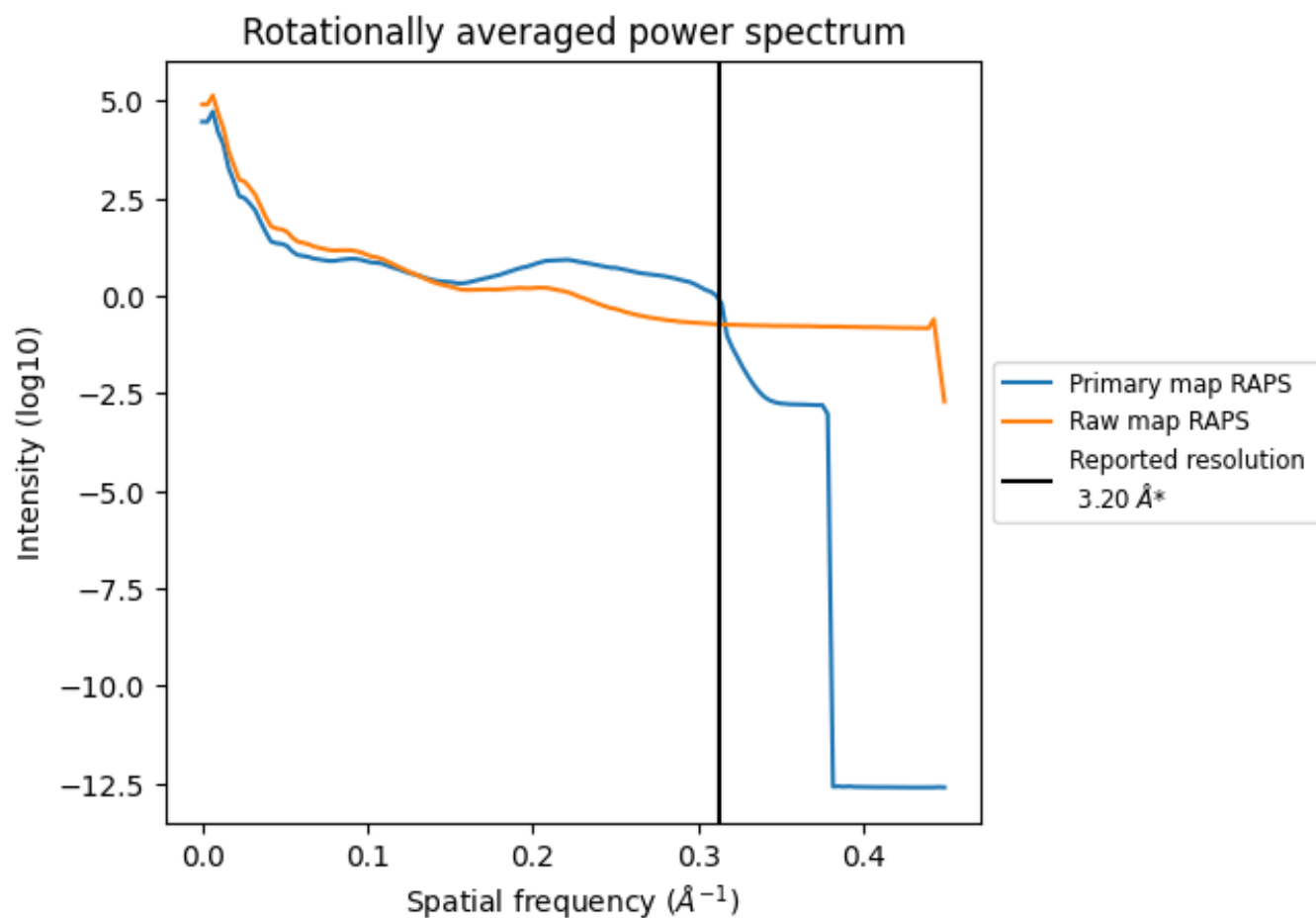
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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 ⓘ

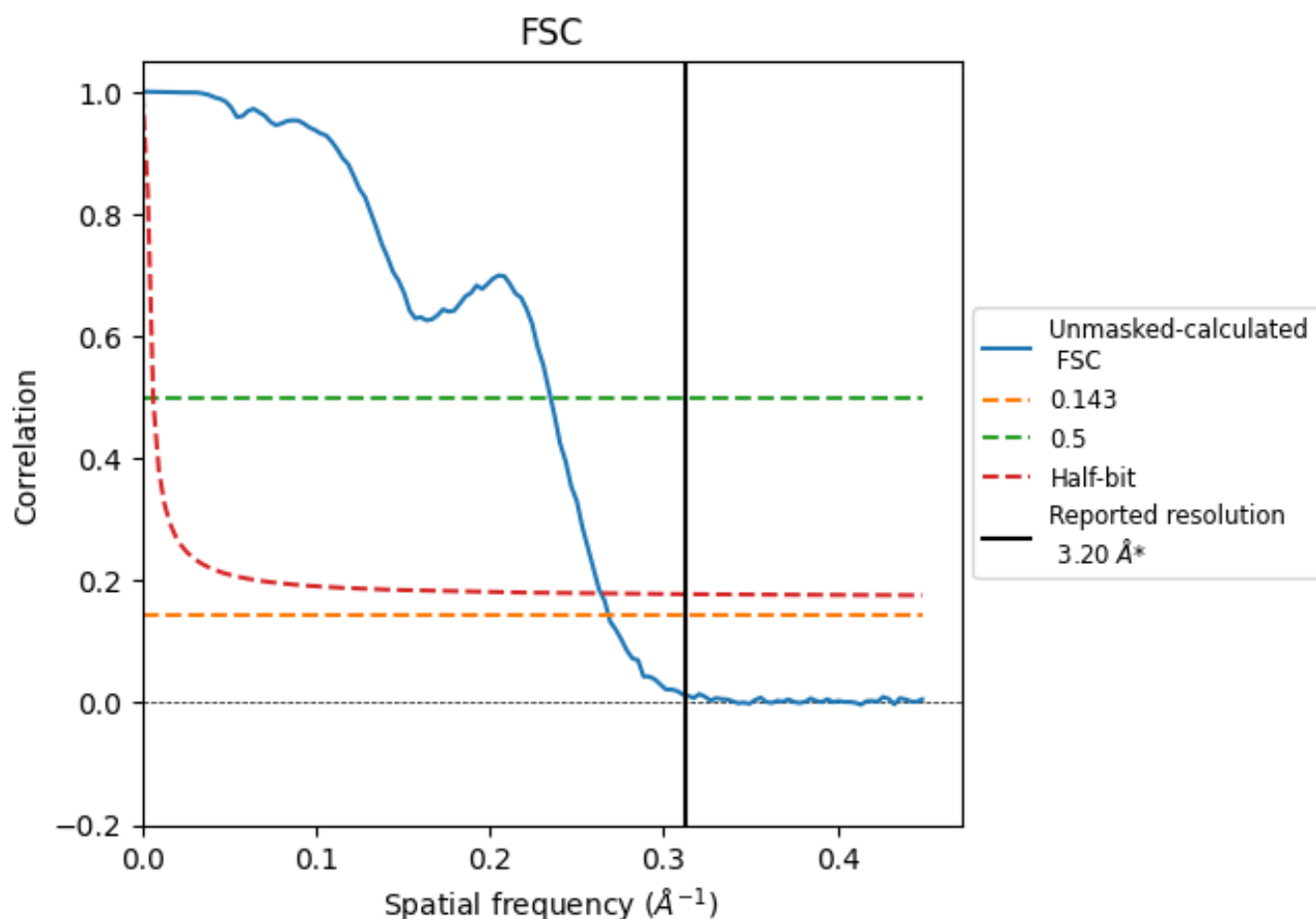


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

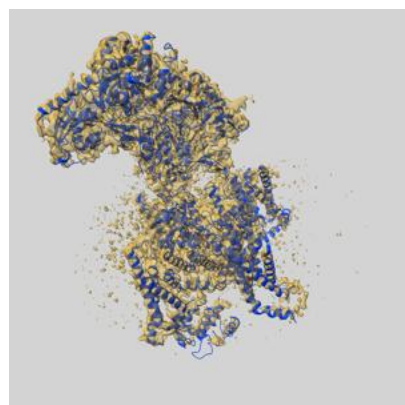
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.26	3.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.73 differs from the reported value 3.2 by more than 10 %

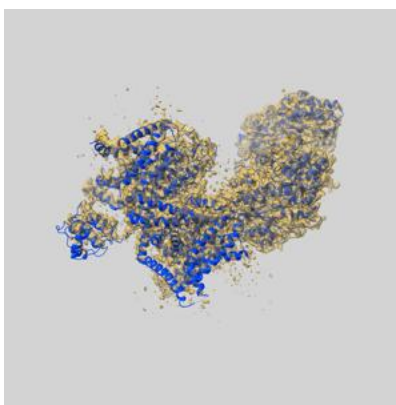
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37476 and PDB model 8WEA. Per-residue inclusion information can be found in section [3](#) on page [7](#).

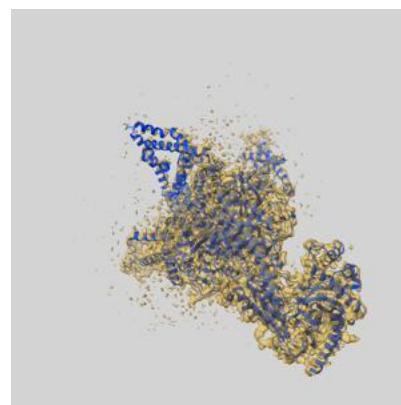
9.1 Map-model overlay [i](#)



X



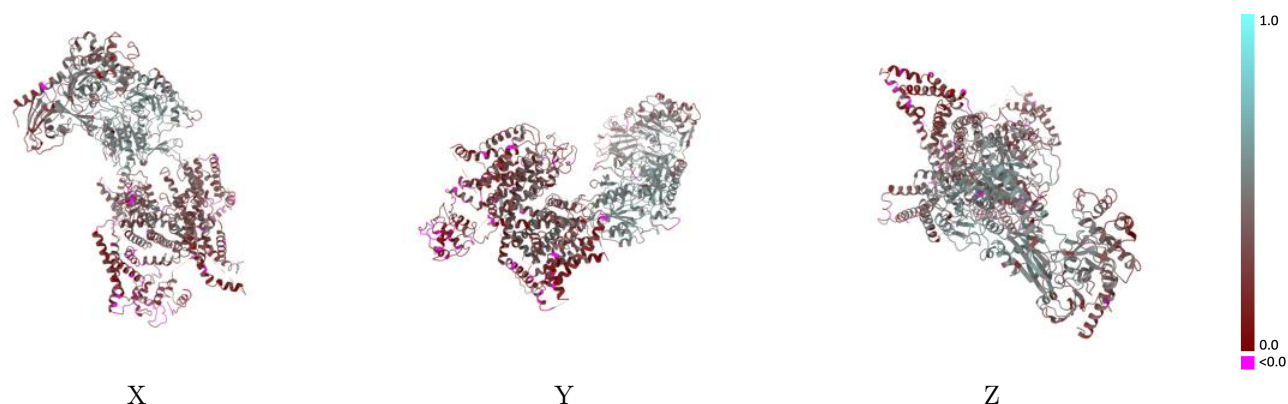
Y



Z

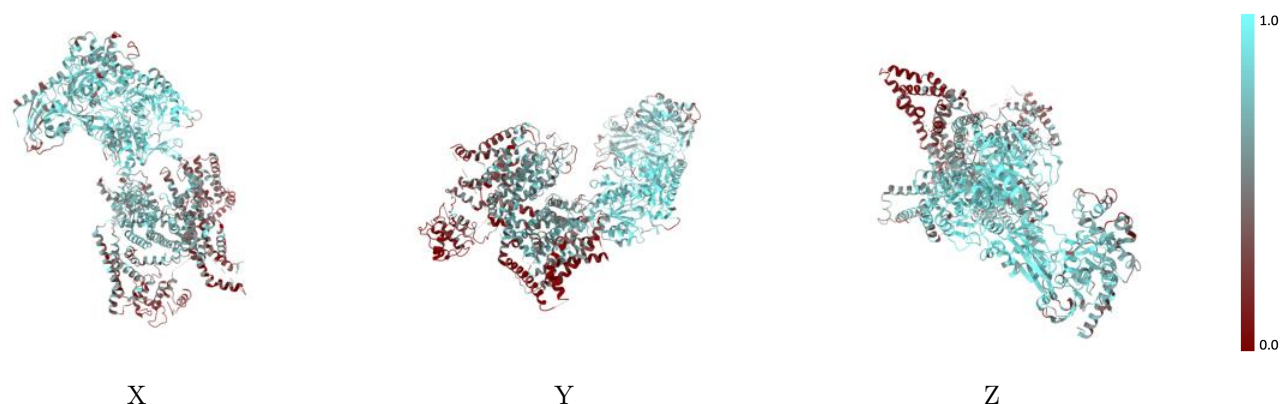
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



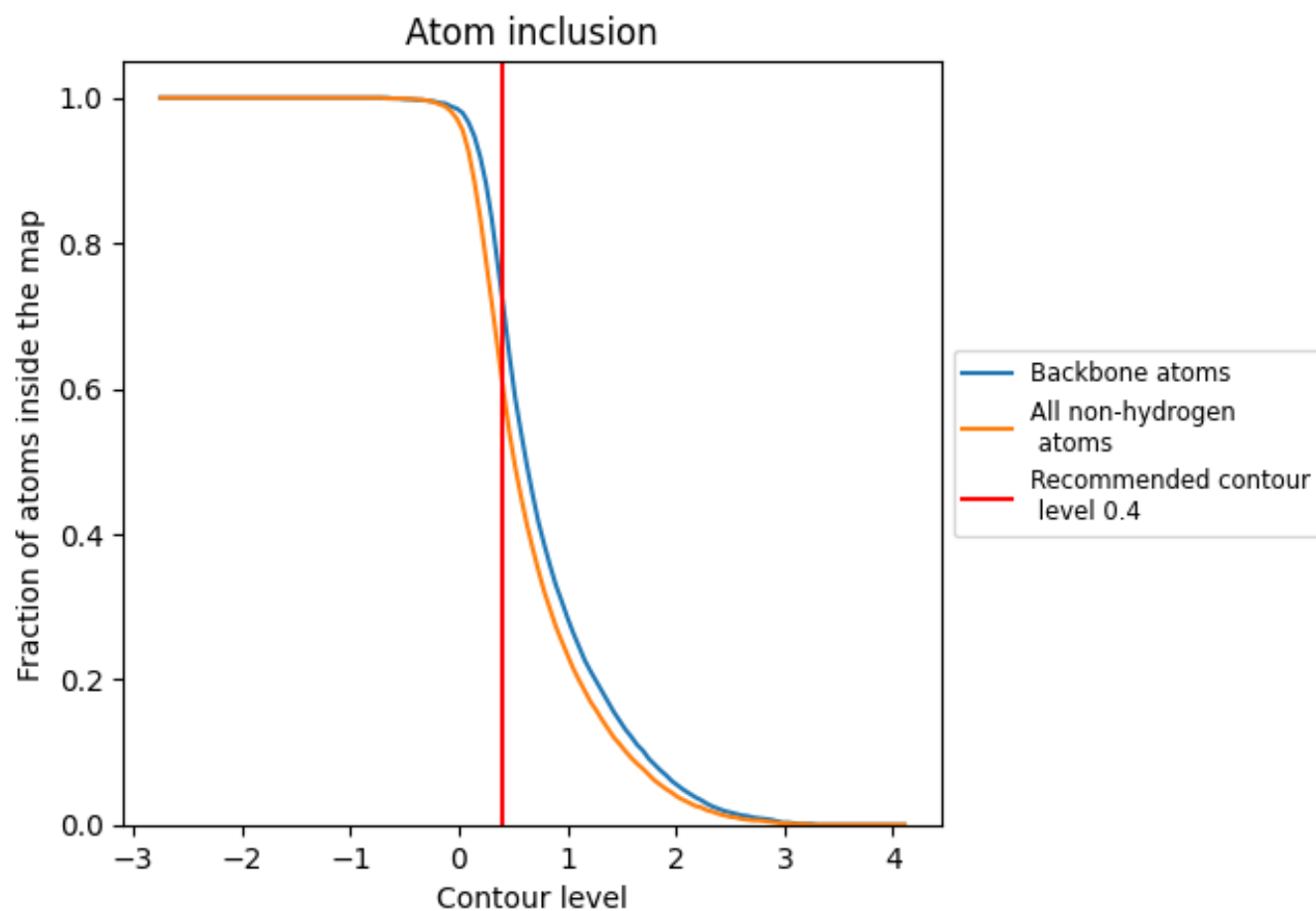
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6080	<div></div> 0.3490
A	<div></div> 0.4720	<div></div> 0.2600
B	<div></div> 0.4290	<div></div> 0.3350
C	<div></div> 0.2860	<div></div> 0.3440
D	<div></div> 0.7790	<div></div> 0.4590
E	<div></div> 0.7860	<div></div> 0.5040
F	<div></div> 0.3210	<div></div> 0.2010
G	<div></div> 0.5360	<div></div> 0.3500

1.0

0.0

<0.0