



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 12:36 AM UTC

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:

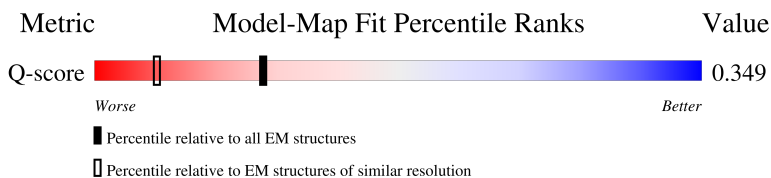
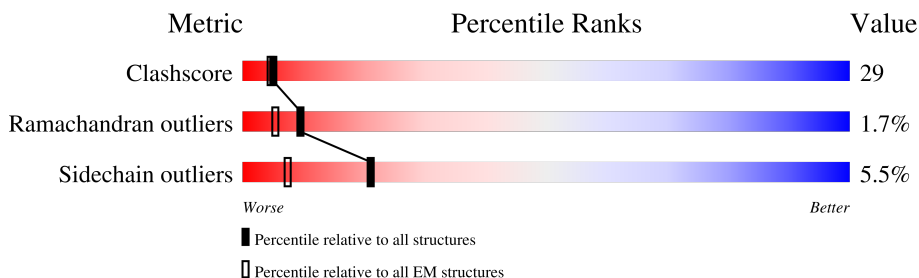
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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.



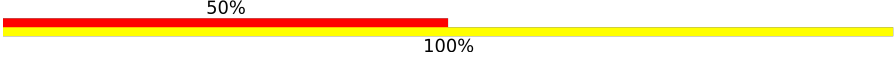


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	<p>22% (red), 22% (orange), 27% (yellow), 5% (green), 45% (grey)</p>
2	D	1103	<p>7% (red), 65% (orange), 20% (yellow), 14% (grey)</p>
3	B	3	<p>33% (red), 67% (orange), 33% (yellow)</p>
4	C	2	<p>50% (red), 50% (orange), 50% (yellow)</p>

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Mol	Chain	Length	Quality of chain
4	F	2	 50% 100%
4	G	2	 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.

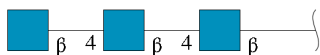
- Molecule 1 is a protein called Voltage-dependent L-type calcium channel subunit alpha-1C.

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

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

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

- 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
			Total	C	N	O		
3	B	3	42	24	3	15	0	0

- 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
			Total	C	N	O		
4	C	2	28	16	2	10	0	0
4	F	2	28	16	2	10	0	0

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

- 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.

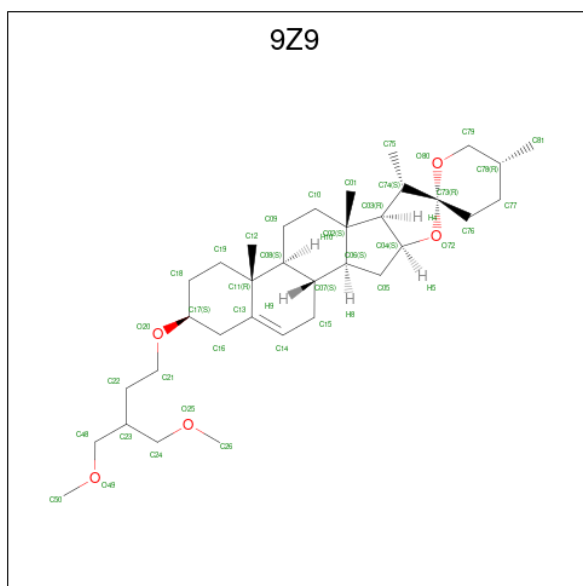


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	4	56	32	4	20	0	0

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

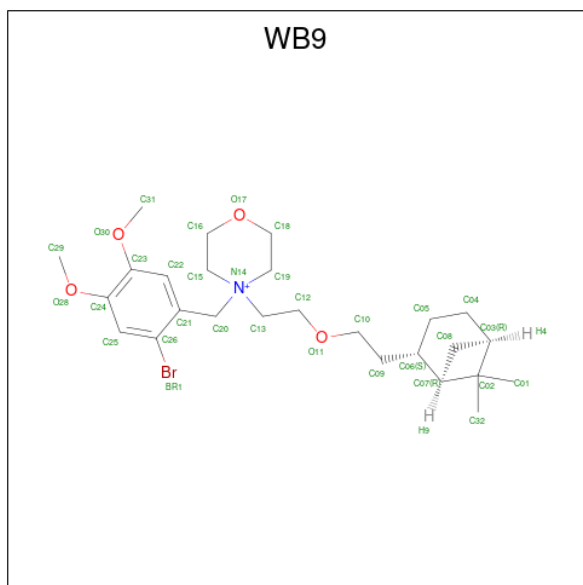
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	

- 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).



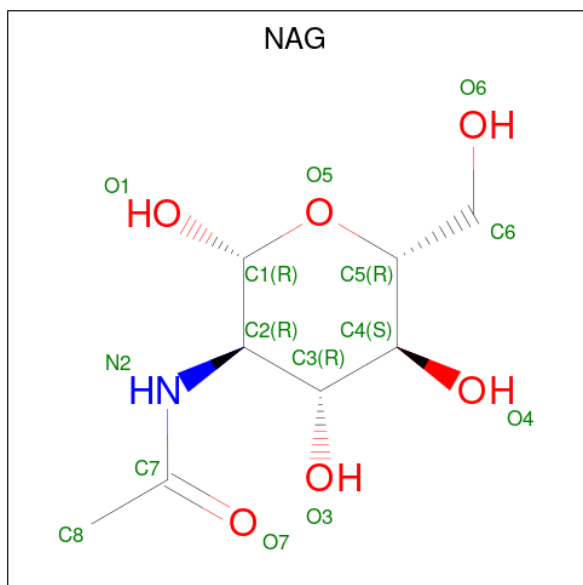
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			39	34	5	

- 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).



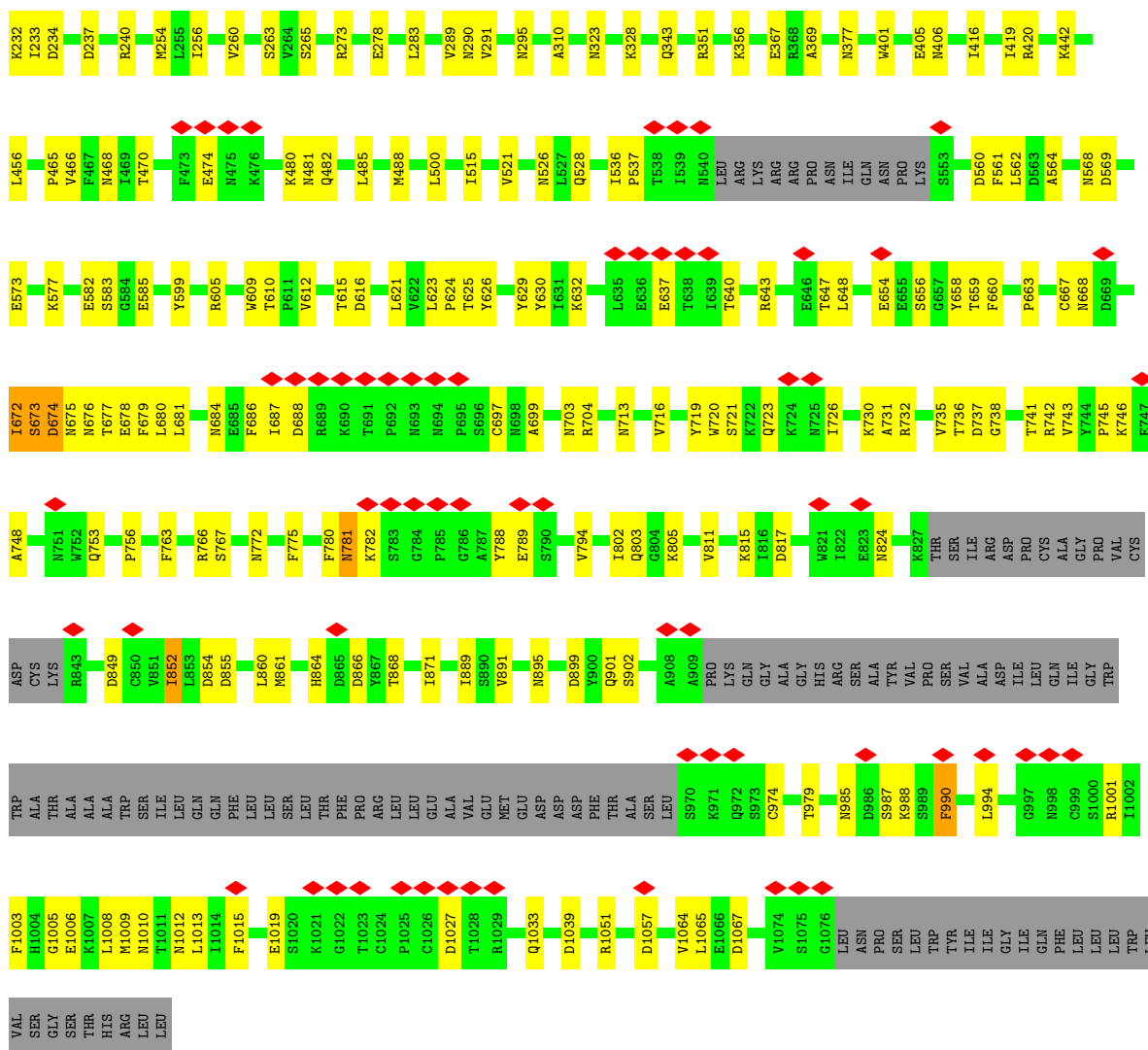
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	Br	C	N	O	0
			32	1	26	1	4	

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
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	L1309	Y1243	G1183	V1121	I1052	PHE	N904	L645	F584
ILE	I1310	L1244	F1184	L1122	V1053	CYS	L905	M646	V685
S1372	I1311	M1245	V1185	A1123	I1054	ASN	I906	S647	S686
I1373	I1312	F1246	I1186	A1124	I1057	ARG	L907	V648	S687
I1374	G1313	V1247	V1187	M1125	T1057	TVR	L908	R649	L688
F1375	I1314	L1248	T1188	M1126	Q1060	F989	F908	S650	F689
R1376	I1315	A1127	F1189	A1127	F1061	N990	L910	I651	R690
R1377	I1316	L1250	F1190	L1128	M1062	N991	L911		R691
F1378	L1317	L1251	Q1190	F1129	F1063	L994	L912		R692
F1379	I1318	T1133	E1191	T1133	A1064	PHE	L913		R693
R1380	L1320	GLY	Q1192	GLY	C1065	GLY	L914		R694
M1381	E1321	GLY	GLY	GLY	C1066	V997	L915		R695
M1382	E1322	GLY	GLY	TRP	I1067	S998	L916		R696
R1383	T1323	H1260	GLN	V1068	V1067	S999	L917		R697
L1384	ASN	Q1263	TRP	Q1069	Q1068	V999	L918		R698
V1385	HIS	S1264	PRO	L1070	Q1069	S1000	A918		R699
K1386	TVR	C1265	GLY	L1071	L1070	L1001	A919		R700
L1387	PHE	L1266	LEU	F1071	K1072	S1002	E920		R701
L1388	CYS	F1267	LEU	I1002	K1073	I1002	D921		R702
S1389	ASP	F1267	TVR	S1003	G1074	S1003	D922		R703
R1390	ALA	K1268	ARG	F1004	K1074	F1004	P923		R704
G1391	TRP	M1271	SER	L1075	L1075	Q1007	Q924		R705
E1392	ASN	M1272	ILE	C1078	C1078	S1008	H925		R706
E1393	THR	I1273	ASP	S1079	S1079	S1009	T926		R707
I1394	PHE	L1274	SER	K1083	K1083	ALA	S927		R708
R1395	ASP	L1275	HIS	Q1084	Q1084	ILE	F928		R709
T1396	ALA	M1275	GLU	L1085	L1085	PRO	R929		R710
L1397	LEU	M1276	ASP	E1086	E1086	M1012	N930		R711
L1398	ILE	L1277	LYS	A1087	A1087	V1013	H931		R712
L1399	VAL	F1278	GLY	E1088	E1088	V1014	I932		R713
L1400	GLY	L1281	GLY	K1089	K1089	V1019	L933		R714
F1401	VAL	F1282	ILE	K1090	K1090	L1020	G934		R715
I1402	ILE	T1283	Y1093	Y1093	Y1093	L1023	N955		R716
K1403	ASP	V1284	Y1096	Y1096	Y1096	R1024	A956		R717
S1404	ILE	E1285	K1097	K1097	K1097	P1025	D957		R718
F1405	ILE	M1286	D1098	D1098	D1098	L1026	V959		R719
Q1406	THR	I1287	D1102	D1102	D1102	R1027	F960		R720
A1407	GLU	L1288	H1103	H1103	H1103	A1028	T961		R721
L1408	VAL	K1289	P1104	P1104	P1104	I1029	S962		R722
P1409	ASN	L1290	I1105	I1105	I1105	M1030	F964		R723
Y1410	ALA	I1291	I1106	I1106	I1106	R1031	T965		R724
V1411	ALA	A1292	Q1107	Q1107	Q1107	A1032	L966		R725
L1412	HIS	P1293	P1108	P1108	P1108	A1032	E967		R726
L1413	THR	F1294	R1109	R1109	R1109	K1033	I968		R727
L1414	THR	P1295	E1112	E1112	E1112	G1034	L969		R728
V1415	GLM	K1296	W1111	W1111	W1111	LEU	L970		R729
F1420	SER	K1296	N1113	N1113	N1113	LYS	R971		R730
I1421	PRO	G1297	S1114	S1114	S1114	HIS	M972		R731
I1422	PRO	F1299	K1115	K1115	K1115	V1038	T973		R732
A1423	ASN	S1300	F1176	F1176	F1176	V1039	N974		R733
V1424	ALA	D1301	M1177	M1177	M1177	Q1040	A974		R734
I1425	GLU	P1302	D1117	D1117	D1117	C1041	F975		R735
V1429	ASN	W1303	D1118	D1118	D1118	V1042	G976		R736
F1430	SER	M1304	D1119	D1119	D1119	F1043	L901		R737
G1431	GLU	V1305	I1180	I1180	I1180	V1044	ALA		R738
K1432	GLU	F1306	V1182	V1182	V1182	R1047	PHE		R739
I1433	GLU	F1308	W1120	W1120	W1120	T1048	LEU		R740
						I1049	HIS		R741
						G1050	GLY		R742
						M1051	SER		R743
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- 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-(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: NAG, 9Z9, WB9, CA

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%)	43	73
All	All	2116/3304 (64%)	1881 (89%)	199 (9%)	36 (2%)	9	35

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 [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	961/1896 (51%)	870 (90%)	91 (10%)	8	32
2	D	837/971 (86%)	829 (99%)	8 (1%)	68	80
All	All	1798/2867 (63%)	1699 (94%)	99 (6%)	21	52

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

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

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](#)

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	0.85	1 (7%)	17,19,21	1.21	1 (5%)
3	NAG	B	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	B	3	3	14,14,15	0.30	0	17,19,21	0.41	0
4	NAG	C	1	2,4	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	C	2	4	14,14,15	0.54	0	17,19,21	0.80	0
5	NAG	E	1	2,5	14,14,15	0.28	0	17,19,21	0.43	0
5	NAG	E	2	5	14,14,15	0.72	0	17,19,21	2.00	7 (41%)
5	NAG	E	3	5	14,14,15	0.70	0	17,19,21	1.43	3 (17%)
5	NAG	E	4	5	14,14,15	0.44	0	17,19,21	0.88	1 (5%)
4	NAG	F	1	2,4	14,14,15	0.51	0	17,19,21	0.53	0
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	G	1	2,4	14,14,15	0.51	0	17,19,21	0.41	0
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.43	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	-	4/6/23/26	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	-	5/6/23/26	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	2.89	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	4.77	118.58	112.19
5	E	2	NAG	C2-N2-C7	-4.09	117.41	122.90
5	E	2	NAG	C1-C2-N2	-3.46	104.98	110.43
5	E	3	NAG	O4-C4-C3	-3.37	102.43	110.38
5	E	2	NAG	O5-C1-C2	3.13	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...

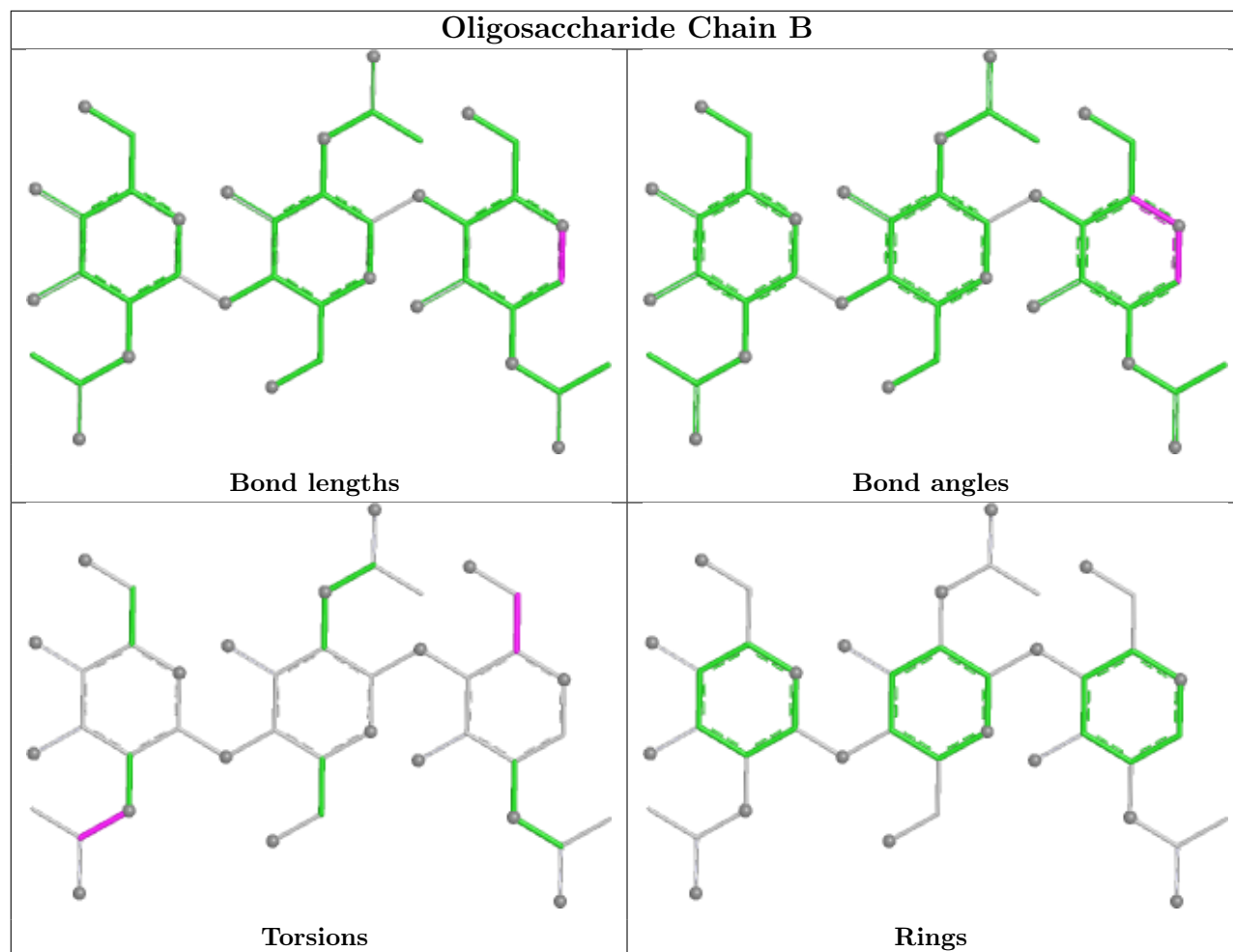
Mol	Chain	Res	Type	Atoms
5	E	4	NAG	C1-C2-N2-C7
5	E	4	NAG	C8-C7-N2-C2

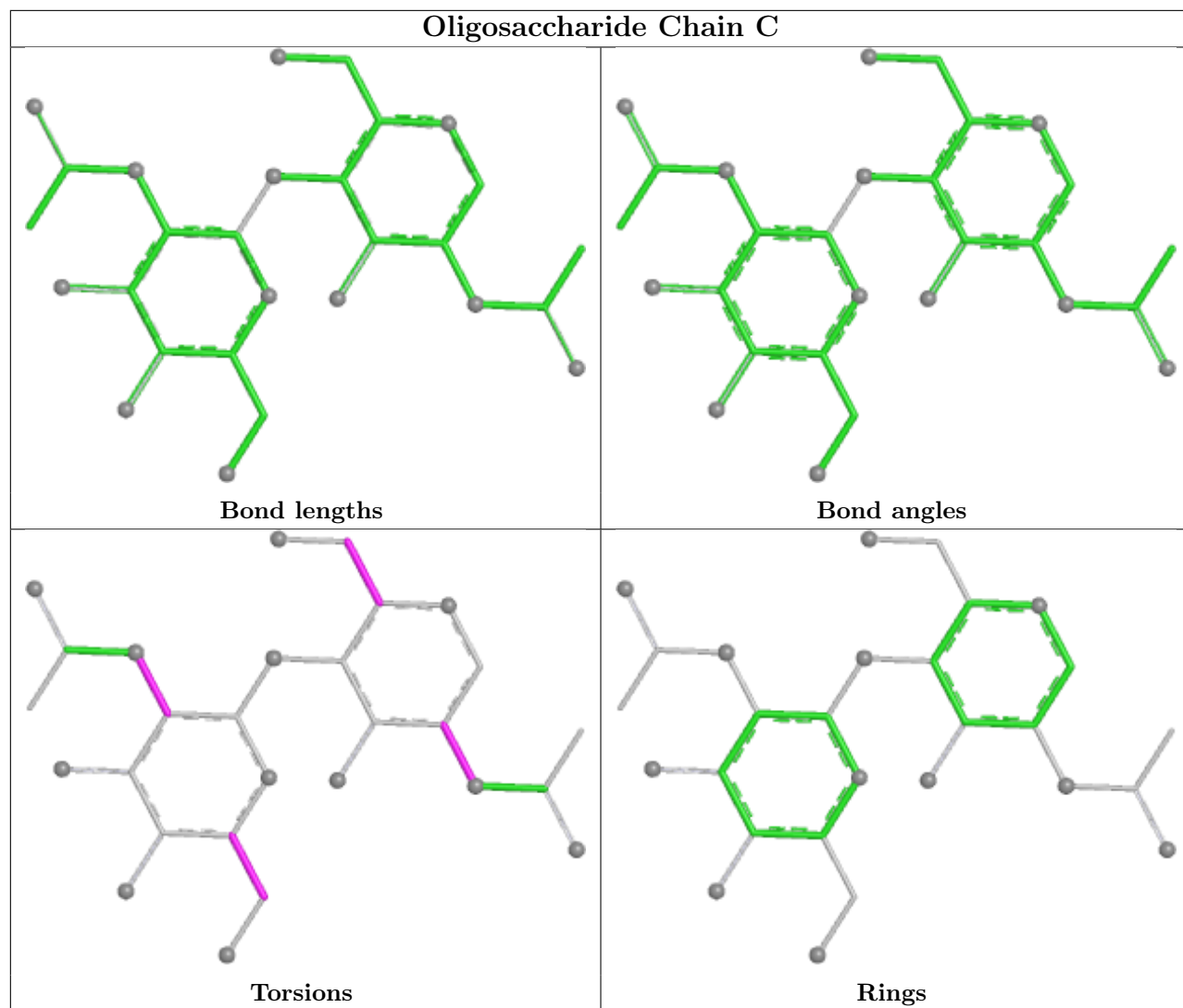
There are no ring outliers.

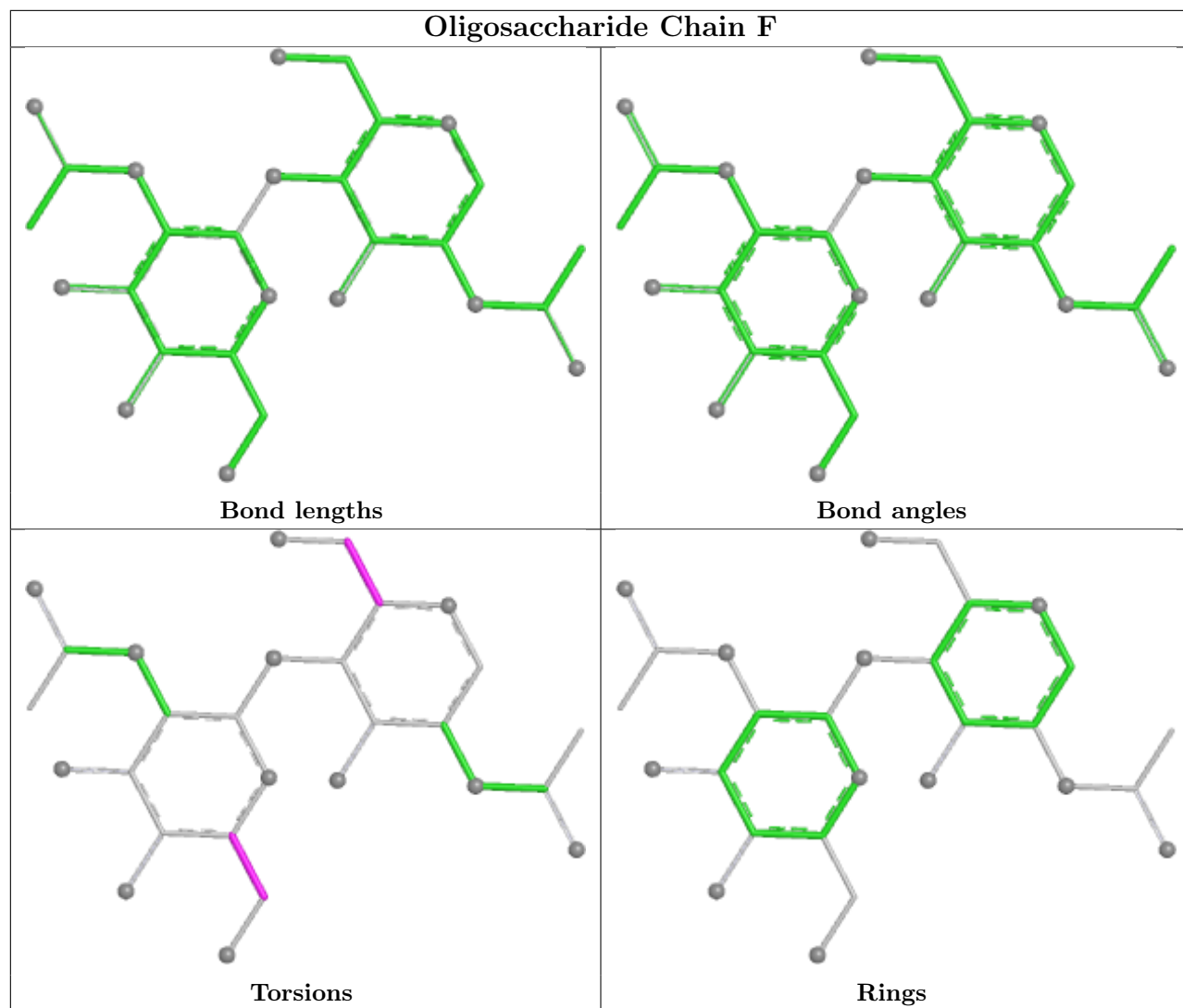
9 monomers are involved in 11 short contacts:

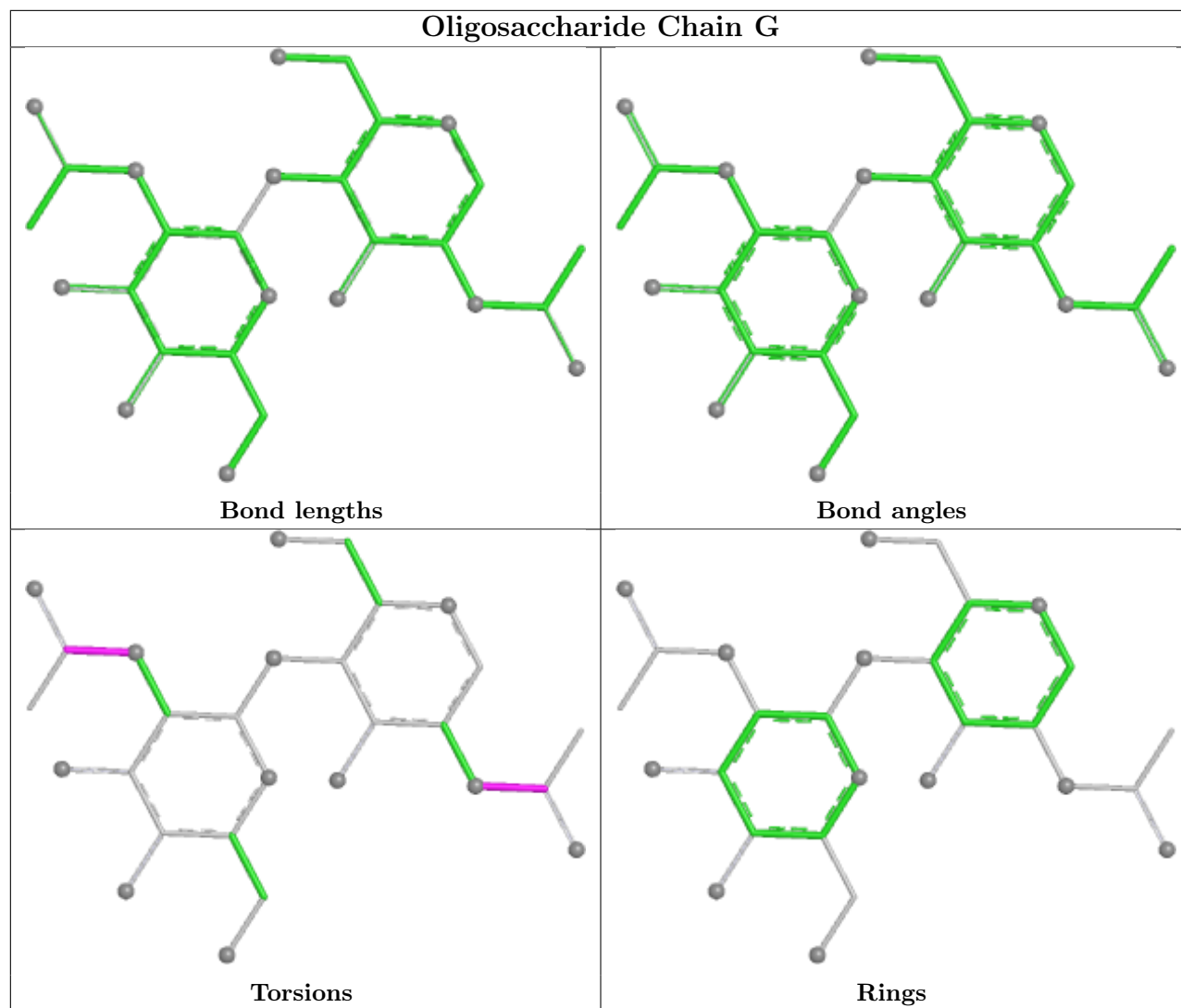
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0
4	F	2	NAG	1	0
5	E	4	NAG	1	0
4	F	1	NAG	1	0
5	E	3	NAG	2	0
3	B	1	NAG	4	0
5	E	1	NAG	2	0
4	C	2	NAG	1	0
5	E	2	NAG	1	0

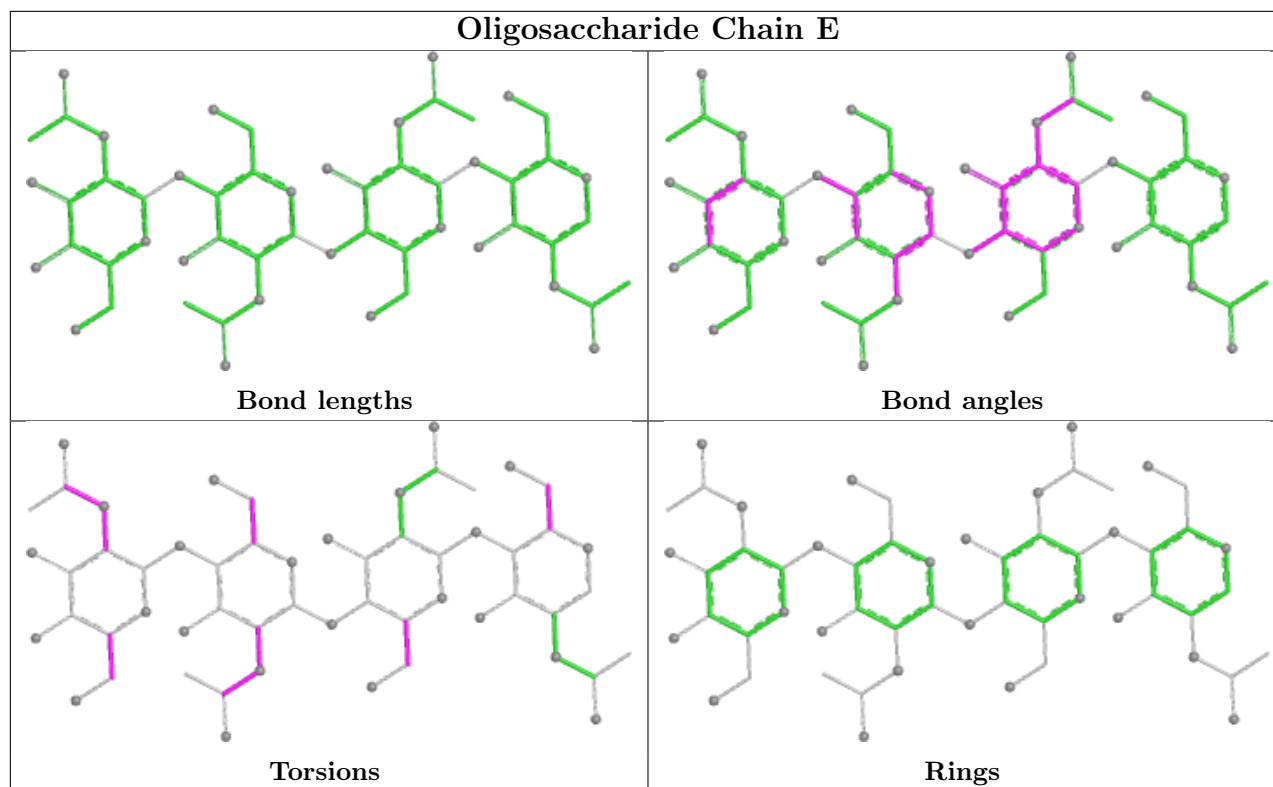
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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
7	9Z9	A	2302	-	44,44,44	1.75	11 (25%)	64,68,68	1.69	17 (26%)
8	WB9	A	2303	-	35,35,35	1.54	8 (22%)	47,51,51	7.04	21 (44%)
9	NAG	D	1202	2	14,14,15	0.43	0	17,19,21	0.42	0
9	NAG	D	1203	2	14,14,15	1.11	1 (7%)	17,19,21	1.21	1 (5%)

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	9Z9	A	2302	-	-	5/12/100/100	0/6/6/6
8	WB9	A	2303	-	-	15/18/53/53	0/5/4/4
9	NAG	D	1202	2	-	4/6/23/26	0/1/1/1
9	NAG	D	1203	2	-	1/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2302	9Z9	C11-C08	-4.12	1.49	1.56
7	A	2302	9Z9	C11-C13	-3.96	1.45	1.52
7	A	2302	9Z9	O80-C79	-3.70	1.38	1.43
9	D	1203	NAG	O5-C1	3.68	1.49	1.43
7	A	2302	9Z9	C09-C08	-3.64	1.47	1.53

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2303	WB9	C02-C07-C06	-27.07	67.13	114.03
8	A	2303	WB9	C08-C03-C04	19.81	134.76	108.67
8	A	2303	WB9	C04-C03-C02	-19.28	66.33	111.41
8	A	2303	WB9	C08-C07-C06	16.79	135.21	107.63
8	A	2303	WB9	C32-C02-C01	-15.31	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

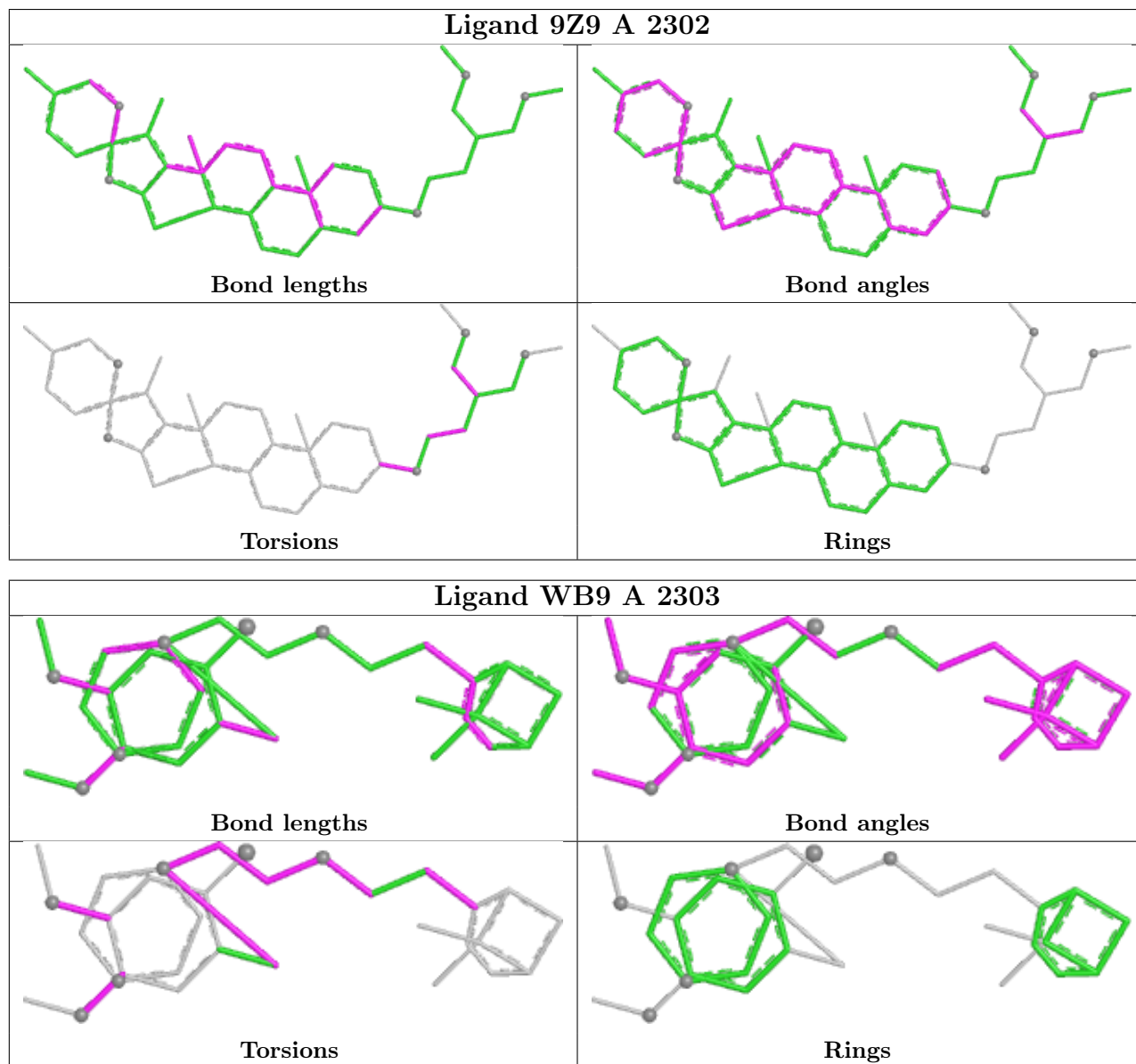
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2303	WB9	1	0
9	D	1203	NAG	2	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.

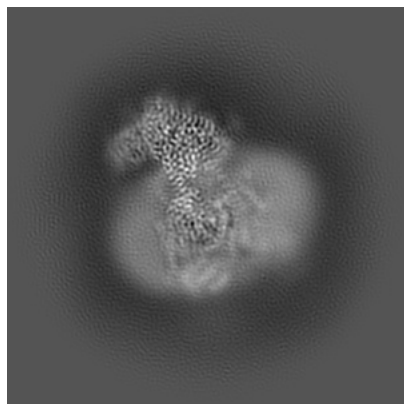
6 Map visualisation [i](#)

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.

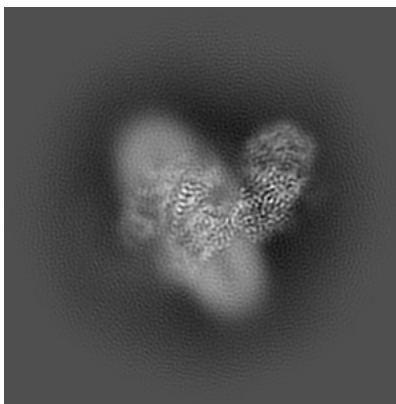
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

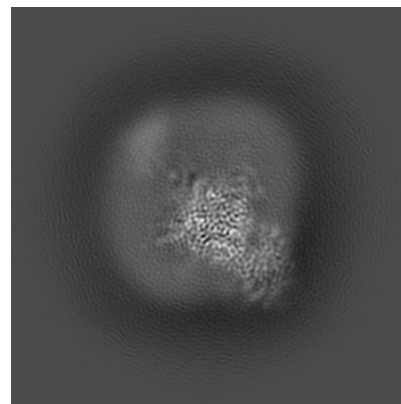
6.1.1 Primary map



X

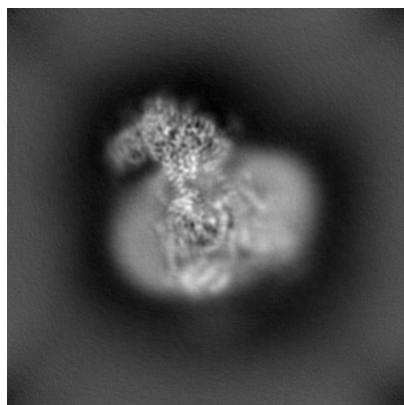


Y

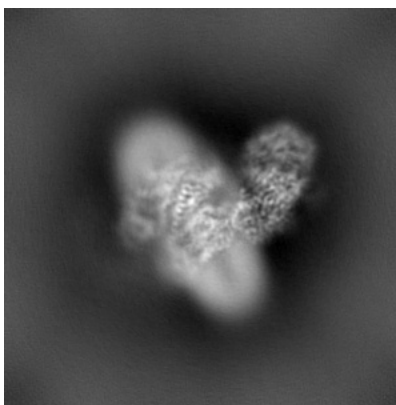


Z

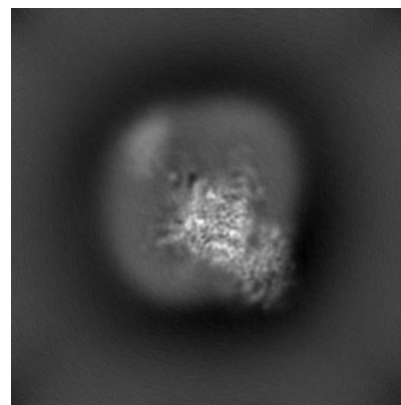
6.1.2 Raw map



X



Y

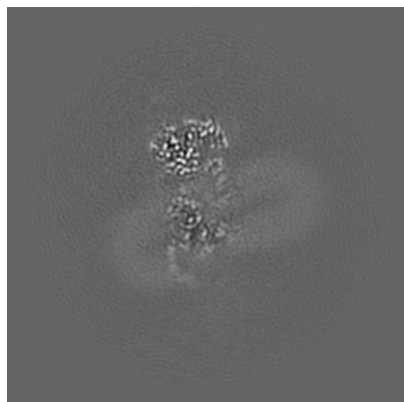


Z

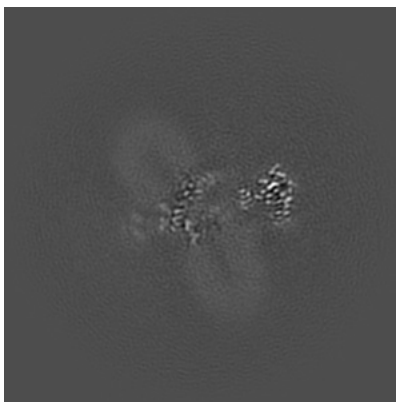
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

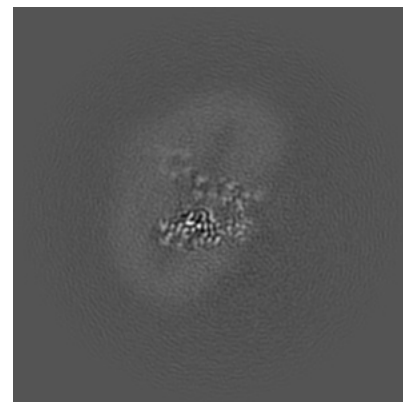
6.2.1 Primary map



X Index: 140

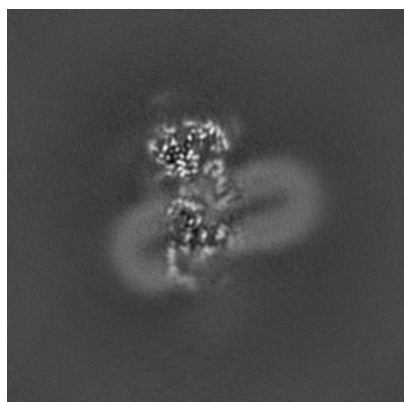


Y Index: 140

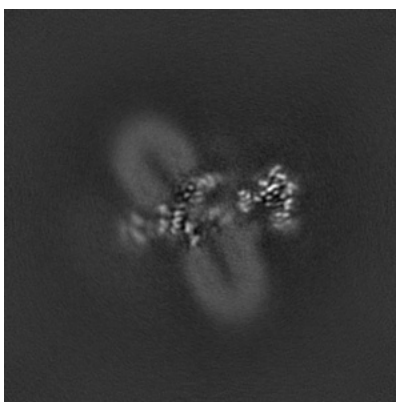


Z Index: 140

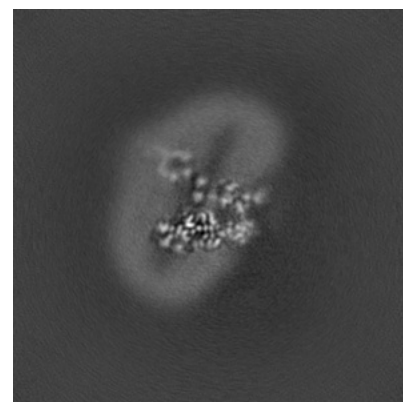
6.2.2 Raw map



X Index: 140



Y Index: 140

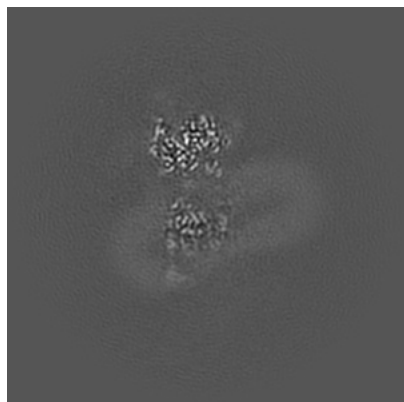


Z Index: 140

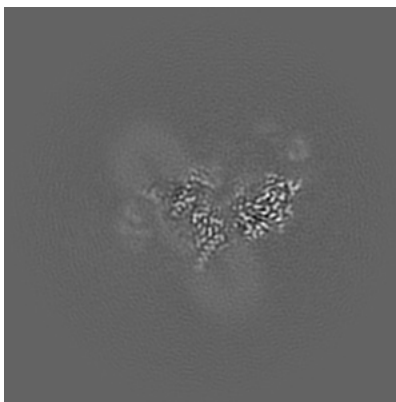
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

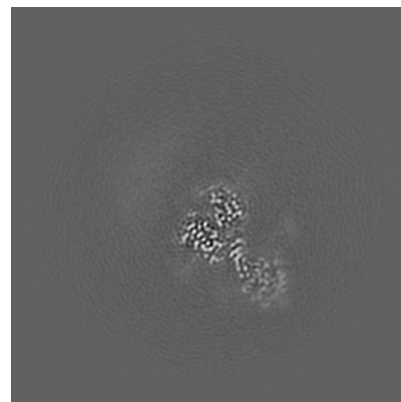
6.3.1 Primary map



X Index: 143

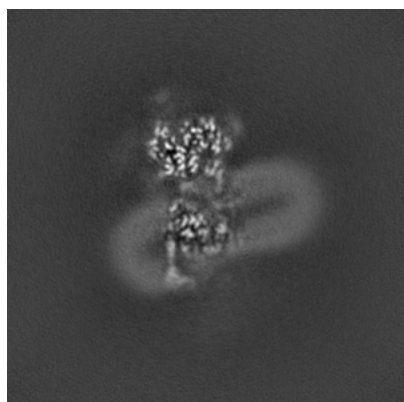


Y Index: 127

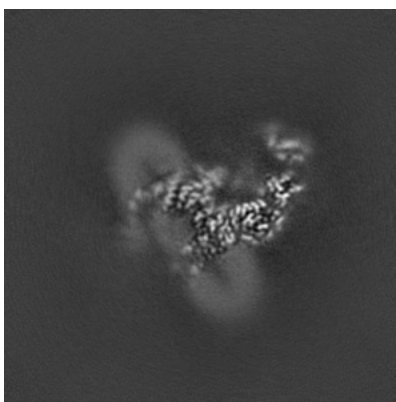


Z Index: 182

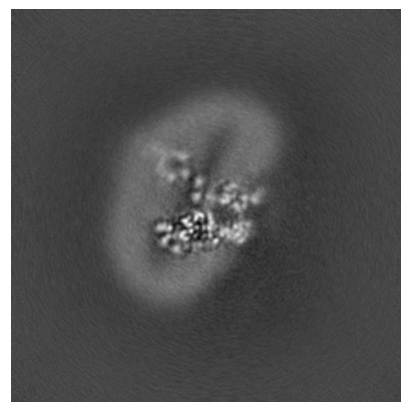
6.3.2 Raw map



X Index: 142



Y Index: 122

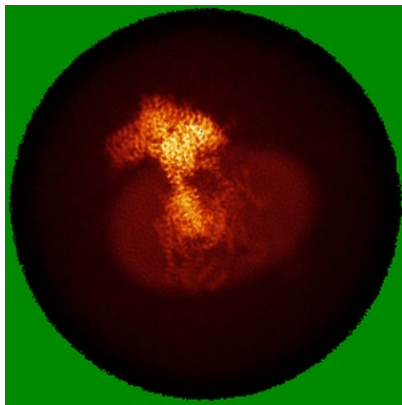


Z Index: 141

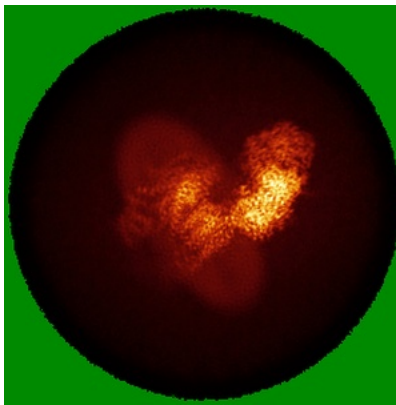
The images above show the largest variance slices of the map in three orthogonal directions.

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

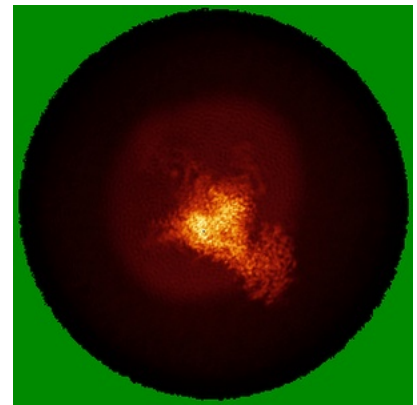
6.4.1 Primary map



X

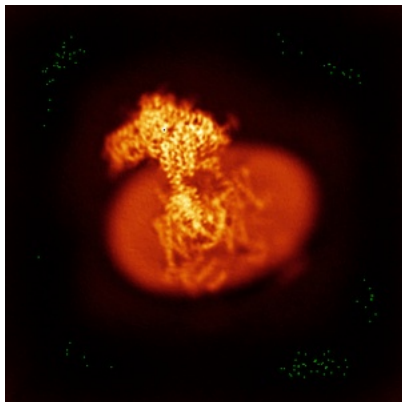


Y

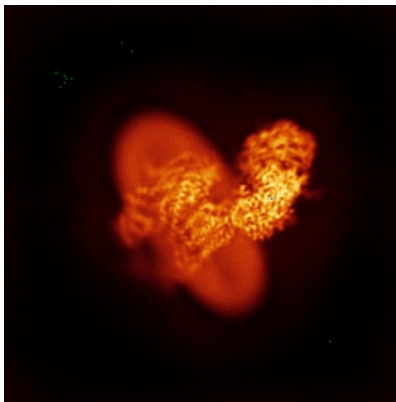


Z

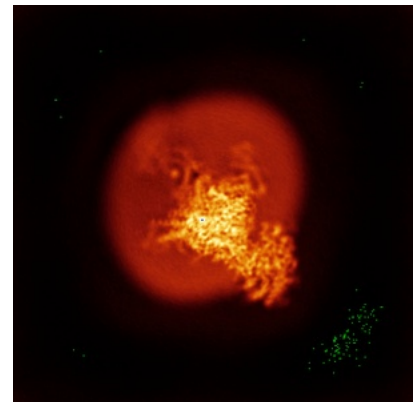
6.4.2 Raw map



X



Y

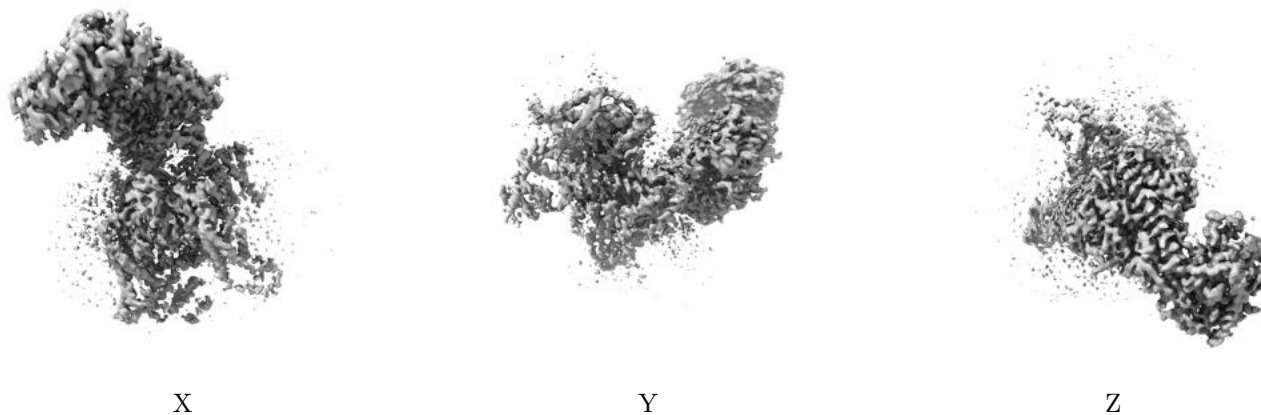


Z

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.

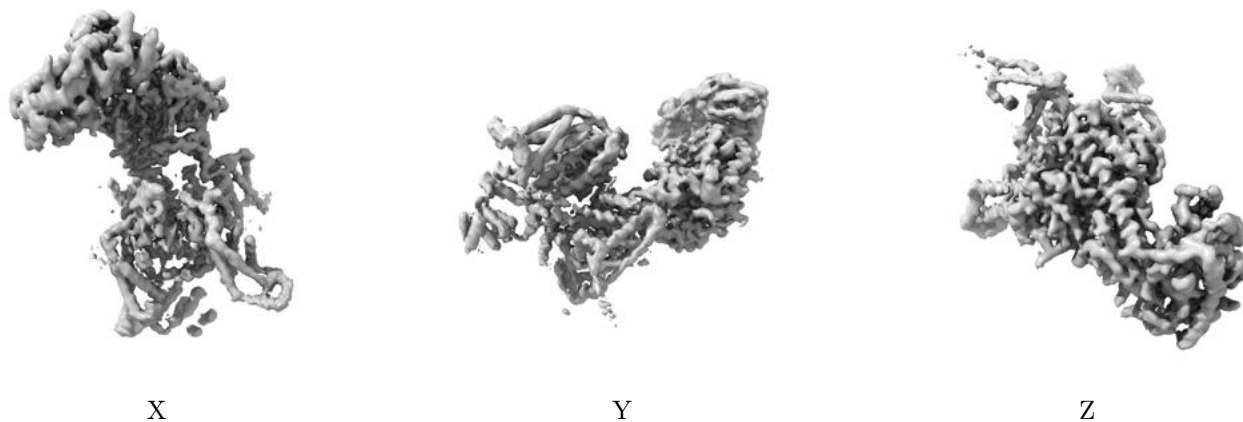
6.5 Orthogonal surface views [i](#)

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.

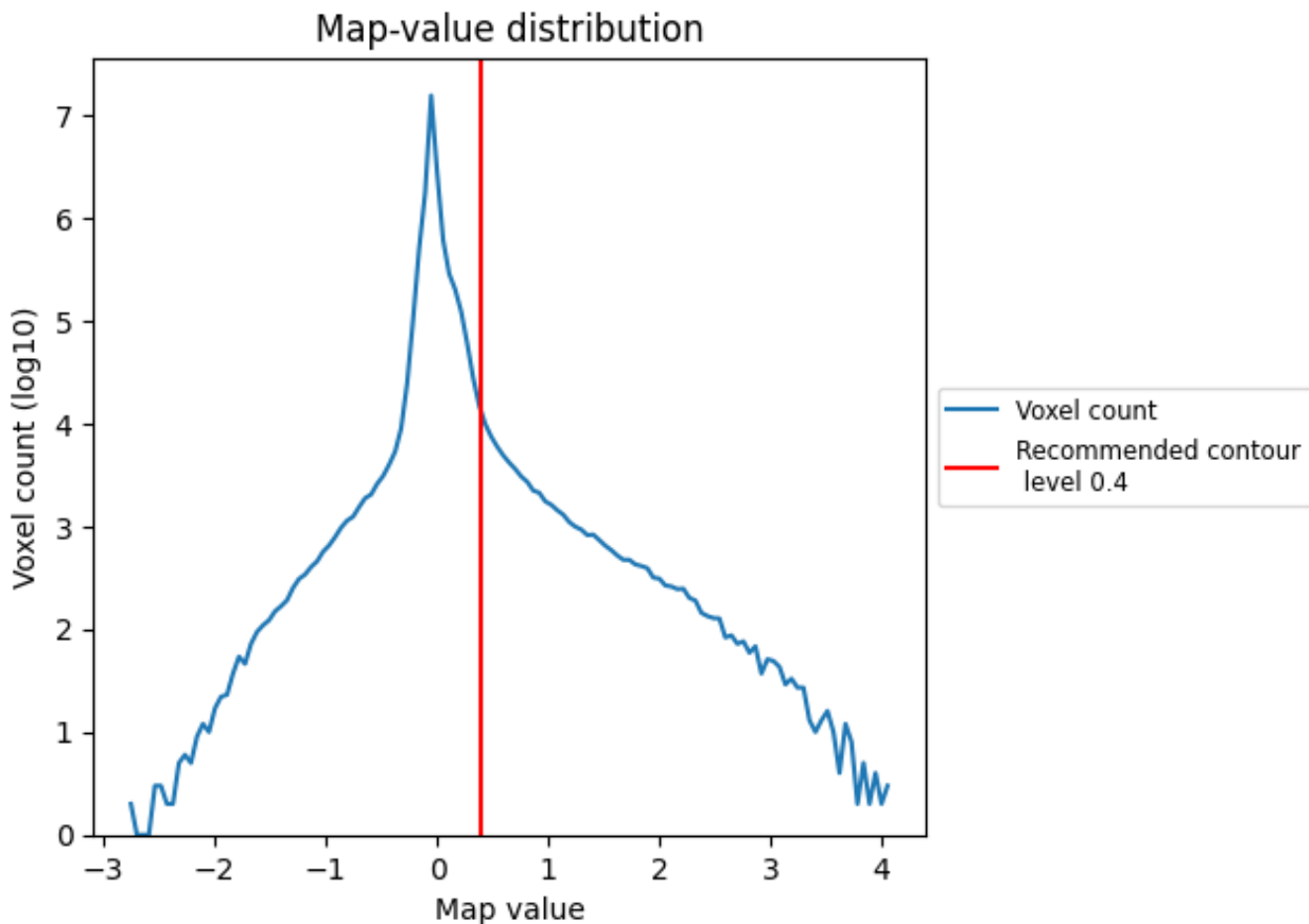
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

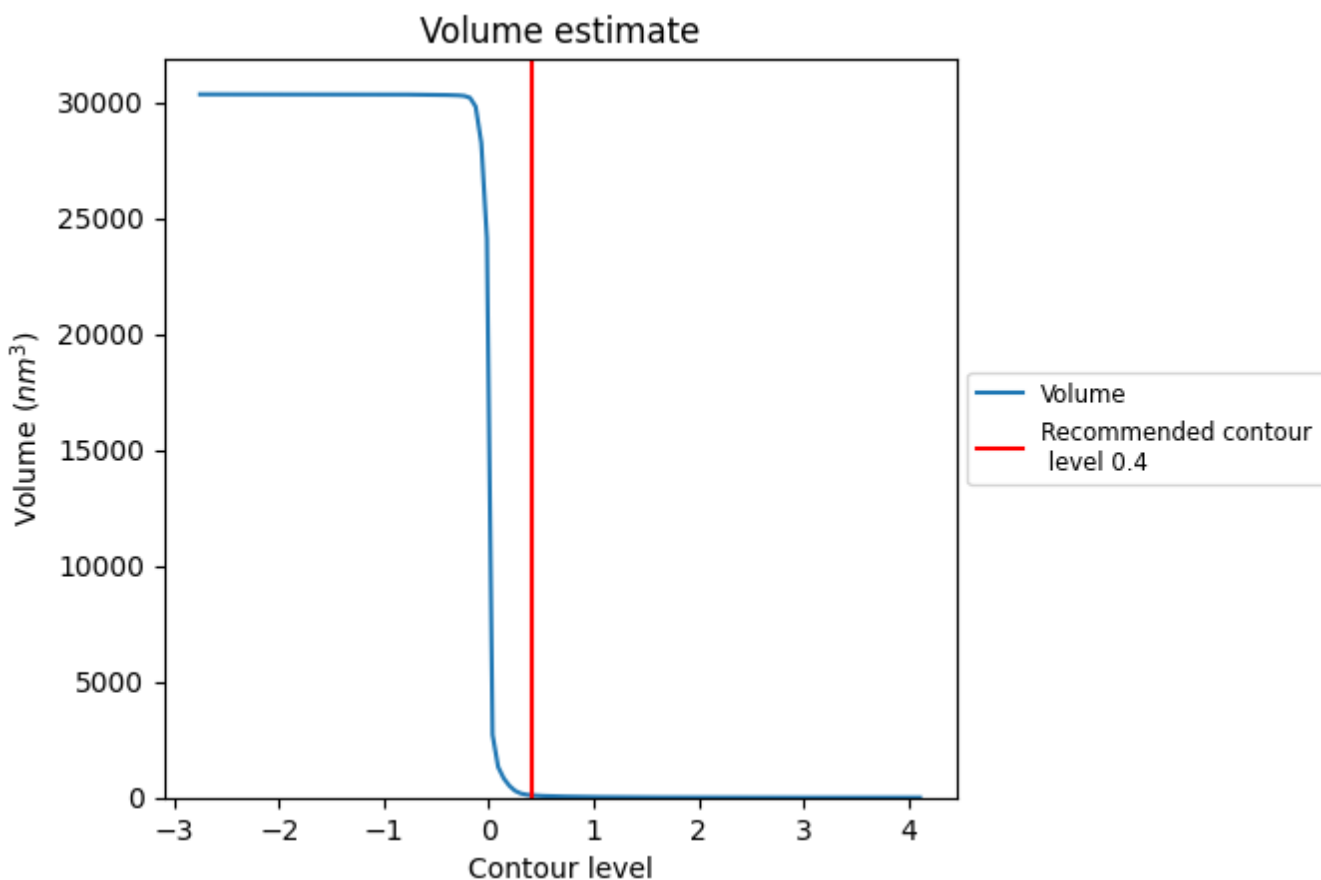
This section contains the results of statistical analysis of the map.

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.

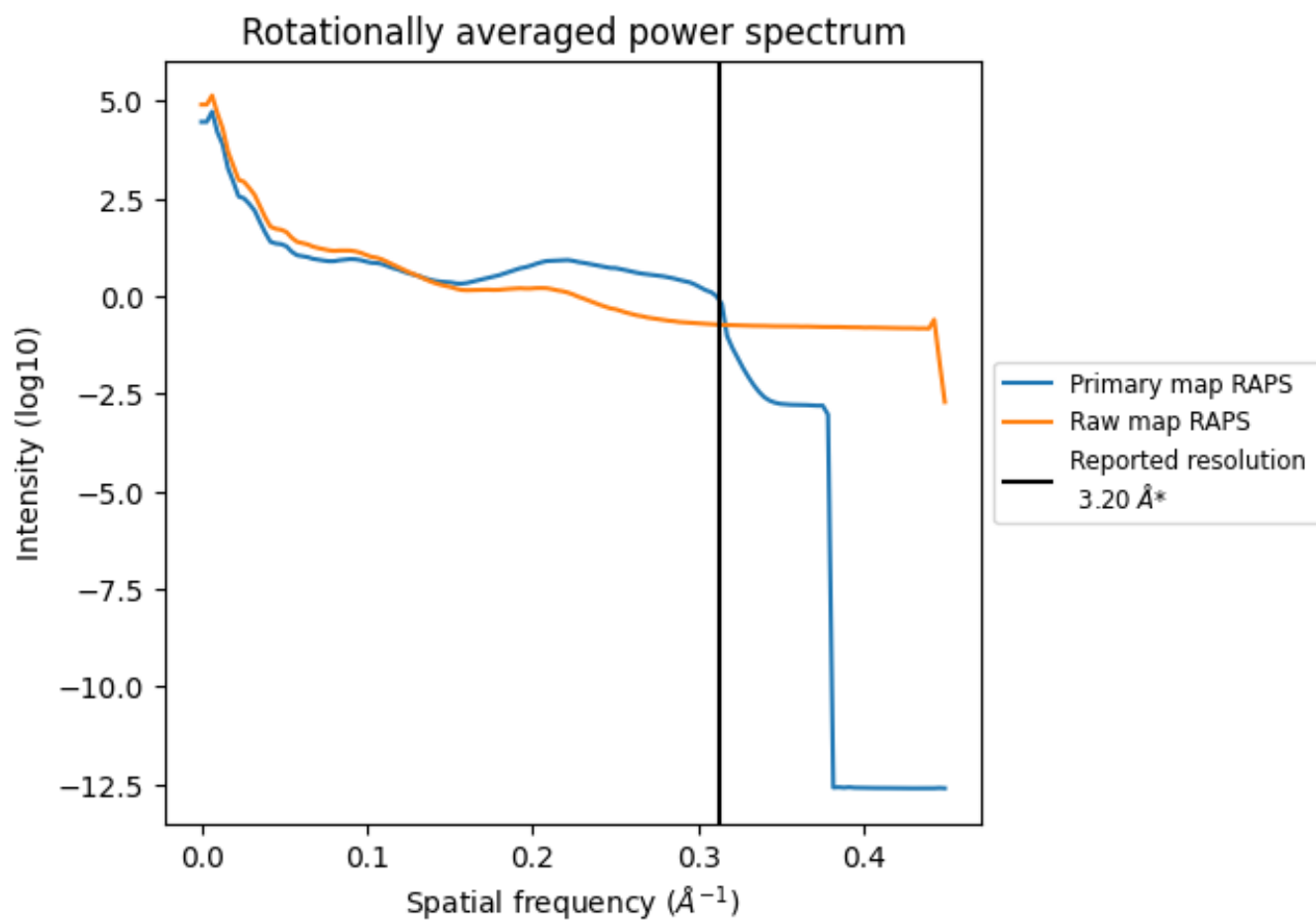
7.2 Volume estimate [i](#)



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 [i](#)

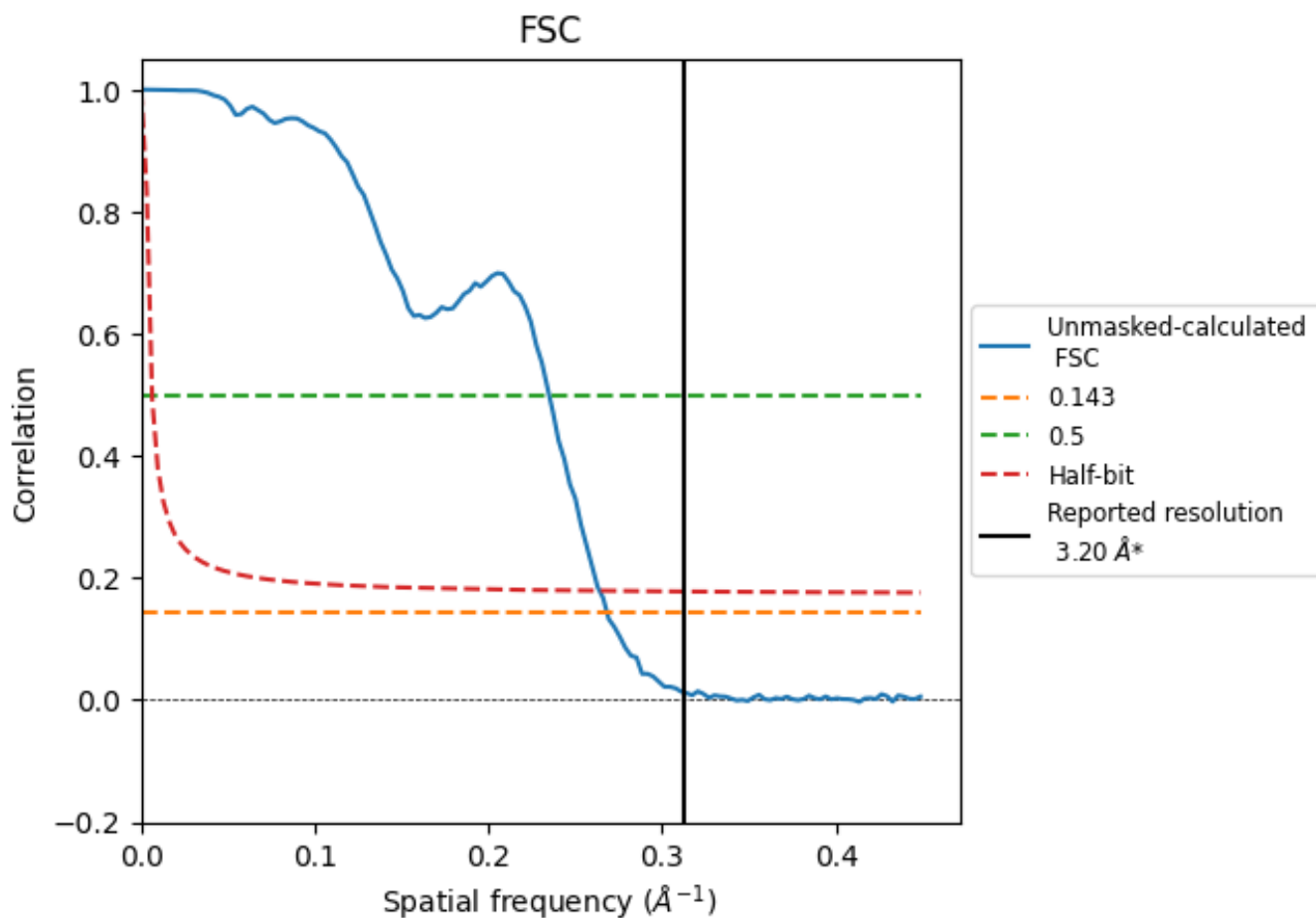


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

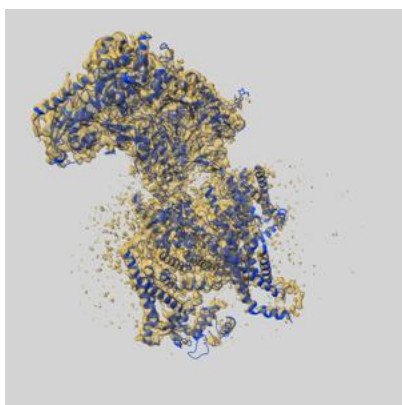
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.26	3.79

*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 %

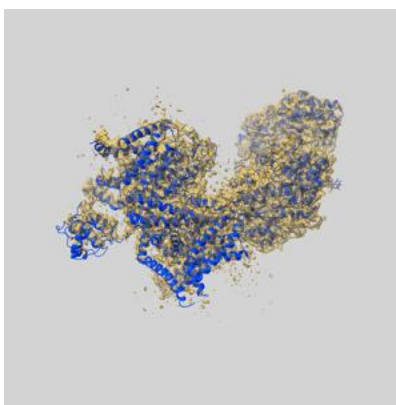
9 Map-model fit [i](#)

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 [8](#).

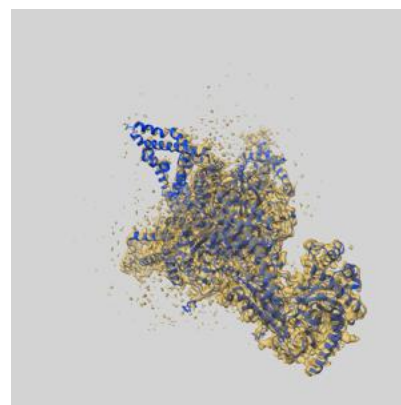
9.1 Map-model overlay [i](#)



X



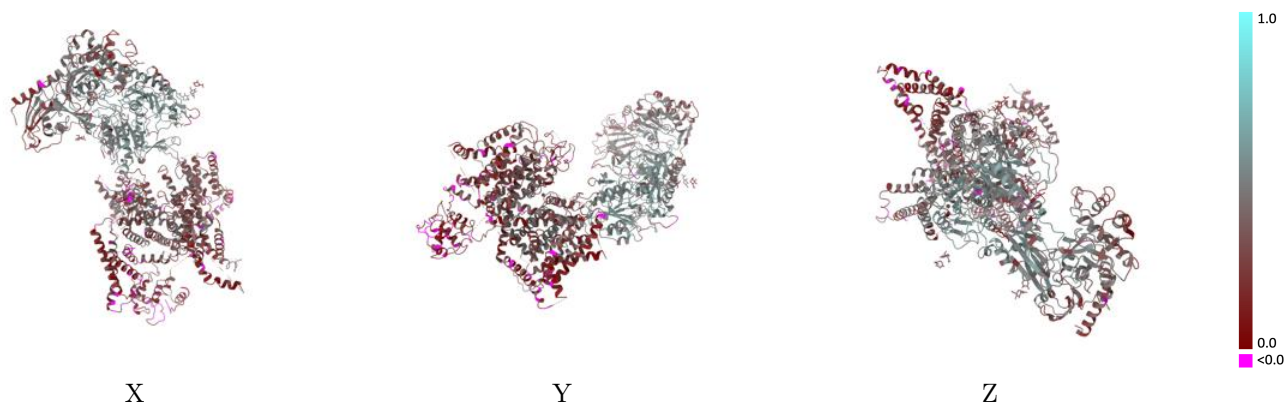
Y



Z

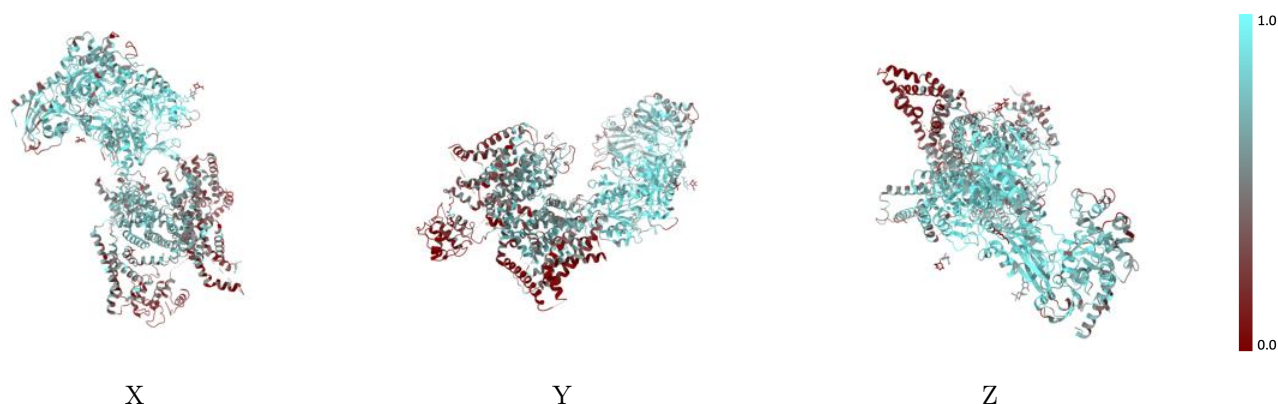
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



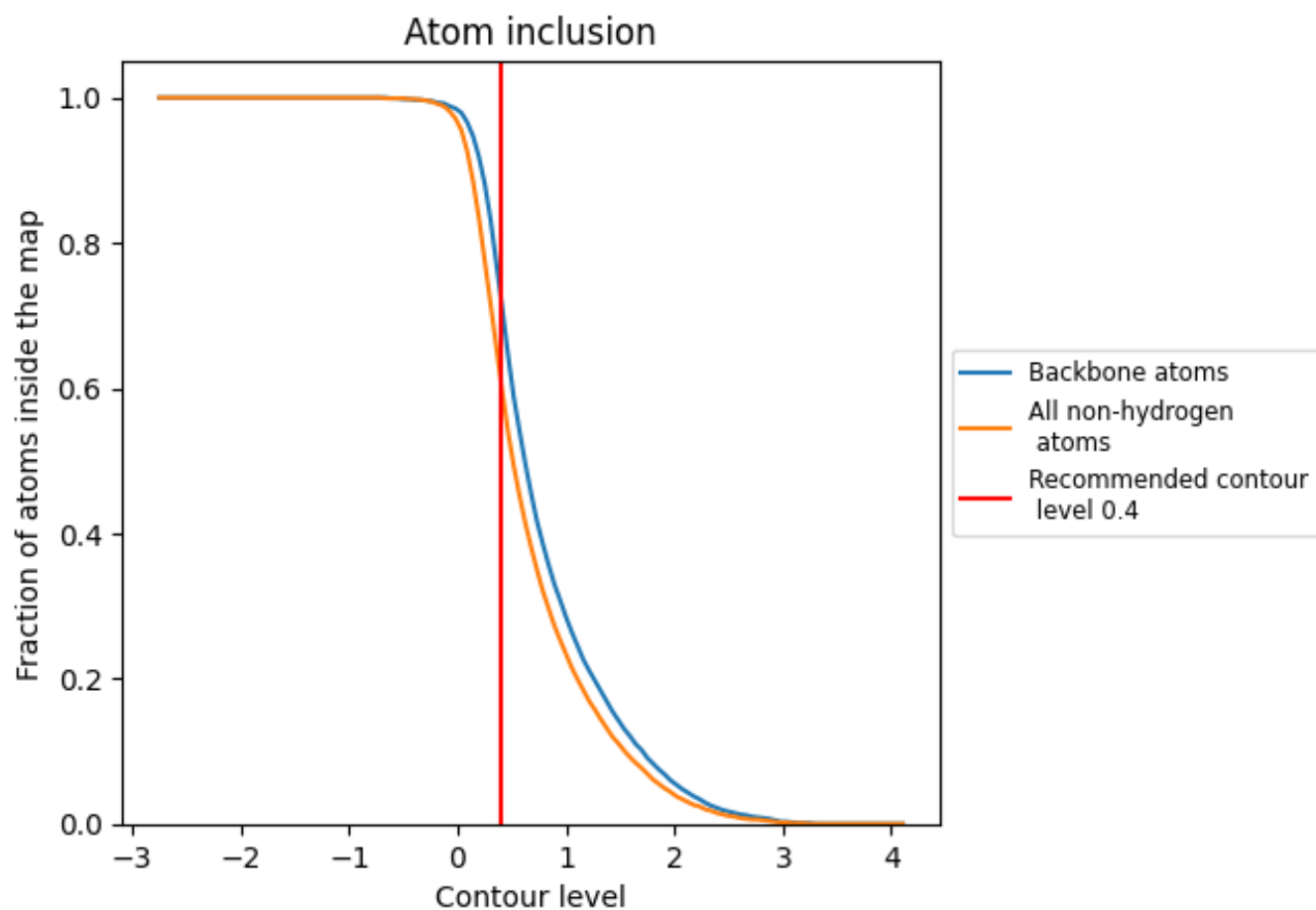
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.6080	 0.3490
A	 0.4720	 0.2600
B	 0.4290	 0.3350
C	 0.2860	 0.3440
D	 0.7790	 0.4590
E	 0.7860	 0.5040
F	 0.3210	 0.2010
G	 0.5360	 0.3500

