



wwPDB EM Validation Summary Report ⓘ

May 18, 2026 – 01:32 PM EDT

PDB ID : 9ON3 / pdb_00009on3
EMDB ID : EMD-70628
Title : Cryo-EM structure of the salivary protein complex Saglin-SGS4 from Anopheles gambiae
Authors : Su, T.; Liu, S.; Williams, A.E.; Calvo, E.; Zhou, Z.H.
Deposited on : 2025-05-14
Resolution : 3.40 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:

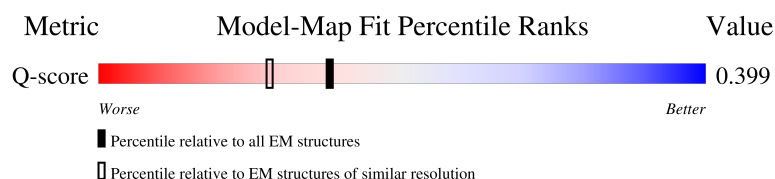
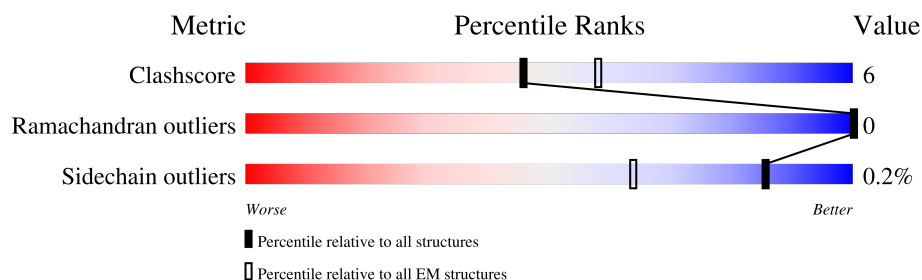
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	3398	<div> <div>15%</div> <div>67%</div> <div>13%</div> <div>20%</div> </div>
2	B	392	<div> <div>80%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	C	392	<div> <div>83%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>
3	D	2	<div> <div>100%</div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	2	<div><div></div><div>100%</div></div>
3	G	2	<div><div></div><div>100%</div></div>
3	I	2	<div><div></div><div>100%</div></div>
3	J	2	<div><div></div><div>100%</div></div>
4	E	3	<div><div></div><div>67%</div></div>
4	H	3	<div><div></div><div>33%</div><div>67%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 28611 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 SGS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2734	Total	C	N	O	S	0	0
			22154	14120	3783	4167	84		

- Molecule 2 is a protein called Saglin.

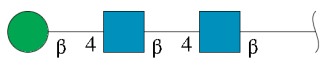
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	388	Total	C	N	O	S	0	0
			3126	1943	573	598	12		
2	C	378	Total	C	N	O	S	0	0
			3071	1914	567	579	11		

- Molecule 3 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
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is an oligosaccharide called beta-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
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

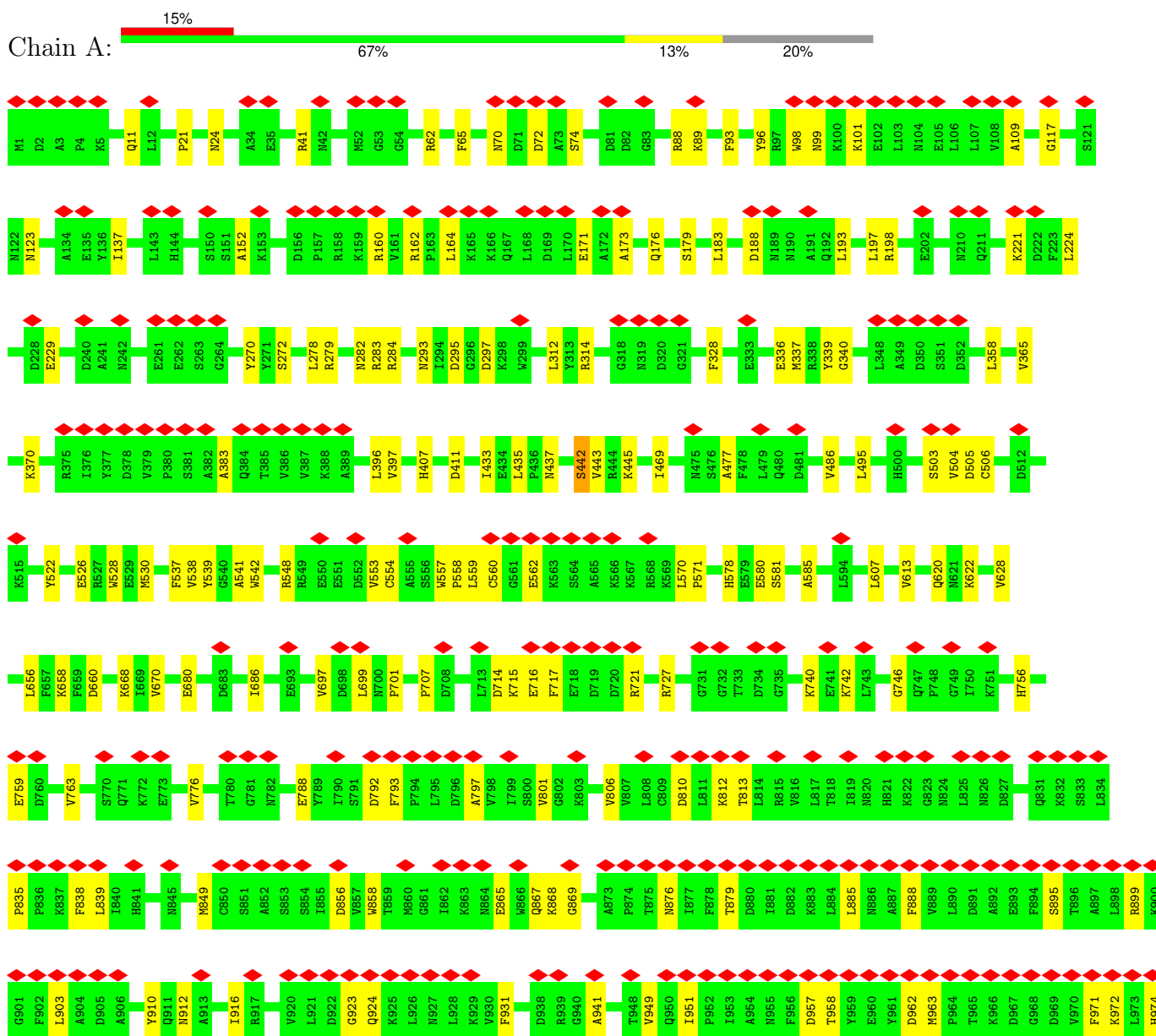


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

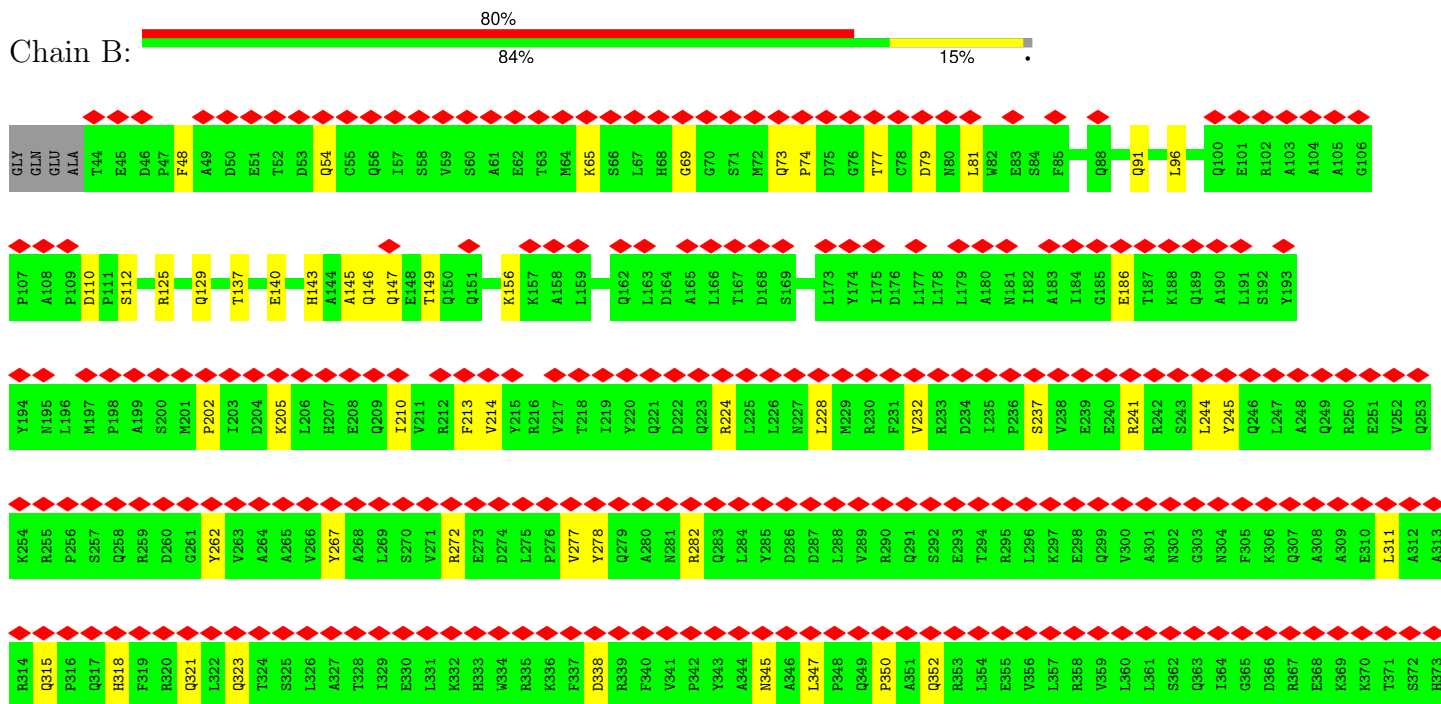
• Molecule 1: SGS4



D2733	G2734	GLU	L2643	L2377	L2383	T2145	V1973	T1760	F1625	E1435	R1291	R1181	A1102	Y975
PHE	ALA	ALA	E2649	L2383	L2383	K2154	S1978	Q1761	C1626	I1438	D1292	H1182	Y1104	K976
THR	ALA	ALA	I2658	T2387	T2387	D2157	M1984	G1771	T1628	H1442	D1294	V1183	S1105	Q978
LEU	ALA	ALA	R1985	R1985	R1985	R1817	G1629	R1817	G1629	T1443	V1295	E1185	Y1106	Q979
ALA	ALA	ALA	A1987	A1987	A1987	E1823	S1630	S1630	S1630	A1444	W1303	T1186	Q1107	N980
VAL	ALA	ALA	N1990	N1990	N1990	E1823	S1631	S1631	S1631	D1445	K1307	S1187	D1108	K981
LEU	ALA	ALA	I1841	I1841	I1841	E1823	N1632	N1632	N1632	G1446	K1310	V1190	T1109	Y982
ILE	ALA	ALA	R1993	R1993	R1993	E1823	S1633	S1633	S1633	S1447	K1313	V1191	Y1113	Y983
LEU	ALA	ALA	E1994	E1994	E1994	E1823	C1634	C1634	C1634	K1448	D1313	E1114	E1114	L984
LEU	ALA	ALA	Q1998	Q1998	Q1998	E1823	R1636	R1636	R1636	N1452	L1317	S1197	M1115	K985
VAL	ALA	ALA	I1999	I1999	I1999	E1823	P1637	P1637	P1637	T1455	L1317	L1199	P1116	L986
ALA	ALA	ALA	T2002	T2002	T2002	E1823	E1642	E1642	E1642	E1459	V1323	T1207	R1117	K987
ALA	ALA	ALA	I2012	I2012	I2012	E1823	T1648	T1648	T1648	D1465	W1339	K1208	H1118	S988
ALA	ALA	ALA	V2019	V2019	V2019	E1823	E1649	E1649	E1649	D1465	K1340	K1208	A1119	K990
ALA	ALA	ALA	R2034	R2034	R2034	E1823	L1650	L1650	L1650	H1468	K1341	L1213	Y1120	G991
ALA	ALA	ALA	K2085	K2085	K2085	E1823	R1651	R1651	R1651	V1469	W1342	L1213	Y1121	P992
ASN	ALA	ALA	I2036	I2036	I2036	E1823	H1659	H1659	H1659	R1470	W1343	Q1215	Y1122	L993
ASN	ALA	ALA	G2037	G2037	G2037	E1823	K1667	K1667	K1667	D1486	S1344	L1218	Q1125	N994
CYS	ALA	ALA	K2038	K2038	K2038	E1823	P1668	P1668	P1668	T1487	A1348	R1219	T1126	S996
TRP	ALA	ALA	E2043	E2043	E2043	E1823	P1670	P1670	P1670	V1533	R1354	K1229	M1127	L997
PRO	ALA	ALA	K2291	K2291	K2291	E1823	R1671	R1671	R1671	E1553	Y1358	D1230	P1129	T998
LEU	ALA	ALA	H2296	H2296	H2296	E1823	T1904	T1904	T1904	E1566	L1367	V1230	Q1130	E999
LYS	ALA	ALA	G2297	G2297	G2297	E1823	R1905	R1905	R1905	E1566	K1368	G1236	E1131	Q1000
TRP	ALA	ALA	L2298	L2298	L2298	E1823	F1907	F1907	F1907	E1566	L1367	G1236	Q1131	K1001
TRP	ALA	ALA	L2306	L2306	L2306	E1823	L1908	L1908	L1908	E1566	K1368	G1236	Q1132	Q1002
ARG	ALA	ALA	L2310	L2310	L2310	E1823	G1910	G1910	G1910	E1566	K1368	G1236	Q1133	K1003
SER	ALA	ALA	F2311	F2311	F2311	E1823	L1681	L1681	L1681	E1566	K1368	G1236	Q1134	Q1004
SER	ALA	ALA	T2311	T2311	T2311	E1823	P1682	P1682	P1682	E1566	K1368	G1236	Q1135	S1004
THR	ALA	ALA	I2315	I2315	I2315	E1823	T1686	T1686	T1686	E1566	K1368	G1236	Q1136	Y1005
TRP	ALA	ALA	K2316	K2316	K2316	E1823	K1687	K1687	K1687	E1566	K1368	G1236	Q1137	S1070
ILE	ALA	ALA	G2317	G2317	G2317	E1823	I1688	I1688	I1688	E1566	K1368	G1236	Q1138	Q1006
GLY	ALA	ALA	E2072	E2072	E2072	E1823	I1915	I1915	I1915	E1566	K1368	G1236	Q1139	Q1007
LEU	ALA	ALA	S2030	S2030	S2030	E1823	I1917	I1917	I1917	E1566	K1368	G1236	Q1140	I1008
THR	ALA	ALA	M2085	M2085	M2085	E1823	E1928	E1928	E1928	E1566	K1368	G1236	Q1141	D1009
GLY	ALA	ALA	D2086	D2086	D2086	E1823	D1936	D1936	D1936	E1566	K1368	G1236	Q1142	A1010
ALA	ALA	ALA	S2087	S2087	S2087	E1823	I1948	I1948	I1948	E1566	K1368	G1236	Q1143	S1011
VAL	ALA	ALA	A2088	A2088	A2088	E1823	Y1949	Y1949	Y1949	E1566	K1368	G1236	Q1144	G1012
THR	ALA	ALA	S2090	S2090	S2090	E1823	S1952	S1952	S1952	E1566	K1368	G1236	Q1145	E1013
GLY	ALA	ALA	D2097	D2097	D2097	E1823	L1955	L1955	L1955	E1566	K1368	G1236	Q1146	A1014
ALA	ALA	ALA	S2106	S2106	S2106	E1823	R1956	R1956	R1956	E1566	K1368	G1236	Q1147	V1015
VAL	ALA	ALA	R2113	R2113	R2113	E1823	F1957	F1957	F1957	E1566	K1368	G1236	Q1148	E1016
THR	ALA	ALA	G2351	G2351	G2351	E1823	R1966	R1966	R1966	E1566	K1368	G1236	Q1149	I1017
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1150	K1018
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1151	A1019
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1152	Q1020
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1153	Y1021
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THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1155	K1023
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1156	E1024
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1157	V1025
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1158	D1026
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1159	E1027
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1160	K1028
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1161	F1029
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1162	A1030
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1163	E1031
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1164	E1032
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1165	V1033
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1166	D1034
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1167	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1168	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1169	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1170	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1171	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1172	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1173	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1174	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1175	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1176	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1177	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1178	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1179	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1180	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1181	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1182	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1183	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1184	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1185	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1186	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1187	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1188	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1189	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1190	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1191	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1192	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1193	
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GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1195	
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GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1198	
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THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1200	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1201	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1202	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1203	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1204	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1205	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1206	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1207	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1208	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1209	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1210	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1211	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1212	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1213	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1214	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1215	
GLY	ALA	ALA				E1823				E1566	K1368	G1236	Q1216	
ALA	ALA	ALA				E1823				E1566	K1368	G1236	Q1217	
THR	ALA	ALA				E1823				E1566	K1368	G1236	Q1218	

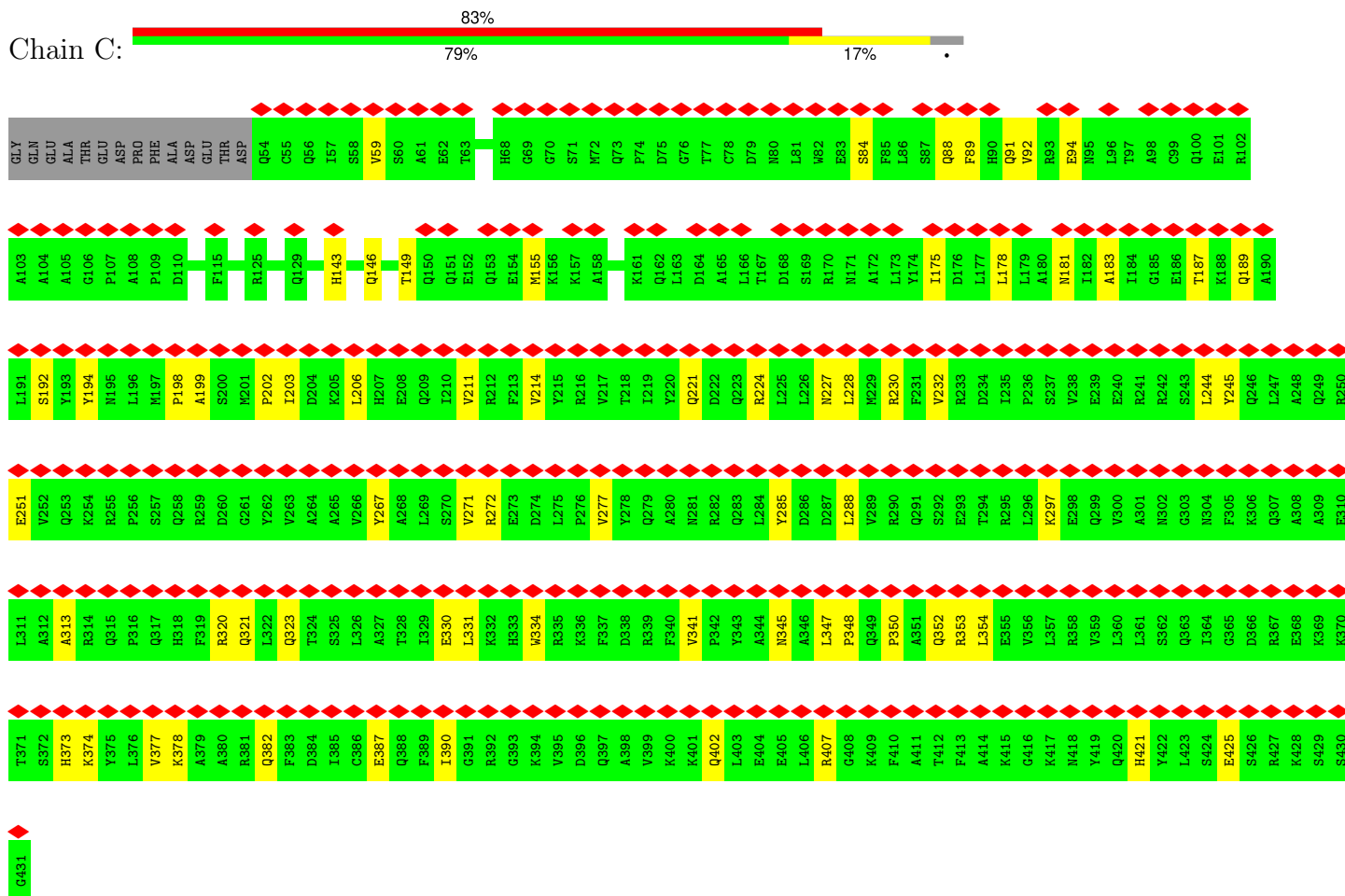
[illegible]

- Molecule 2: Saglin





• Molecule 2: Saglin



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



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



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



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



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



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



- Molecule 4: beta-D-mannopyranose-(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, C1	Depositor
Number of particles used	91242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.333	Depositor
Minimum map value	-2.176	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: BMA, NAG

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	0/22685	0.33	0/30719
2	B	0.10	0/3181	0.25	0/4288
2	C	0.12	0/3124	0.27	0/4208
All	All	0.14	0/28990	0.31	0/39215

There are no bond length outliers.

There are no bond angle outliers.

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	22154	0	21715	271	0
2	B	3126	0	3046	41	0
2	C	3071	0	3043	49	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
3	I	28	0	25	0	0
3	J	28	0	25	1	0
4	E	39	0	34	0	0
4	H	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	26	0	0
5	B	14	0	13	1	0
All	All	28611	0	28036	352	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 6.

The worst 5 of 352 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:2561:GLN:HB2	1:A:2570:PHE:HB3	1.67	0.77
1:A:2625:VAL:HG22	1:A:2634:GLY:HA2	1.68	0.76
2:C:341:VAL:HG12	2:C:382:GLN:HG3	1.68	0.74
1:A:1136:ALA:HB1	1:A:1138:ARG:HG3	1.69	0.74
1:A:869:GLY:HA3	1:A:941:ALA:HB3	1.71	0.73

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	2732/3398 (80%)	2606 (95%)	126 (5%)	0	100	100
2	B	386/392 (98%)	381 (99%)	5 (1%)	0	100	100
2	C	376/392 (96%)	373 (99%)	3 (1%)	0	100	100
All	All	3494/4182 (84%)	3360 (96%)	134 (4%)	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	2417/3004 (80%)	2411 (100%)	6 (0%)	87	85
2	B	329/339 (97%)	329 (100%)	0	100	100
2	C	327/339 (96%)	327 (100%)	0	100	100
All	All	3073/3682 (84%)	3067 (100%)	6 (0%)	85	85

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1134	VAL
1	A	1135	VAL
1	A	1138	ARG
1	A	1132	ILE
1	A	442	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
2	C	160	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

16 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	D	1	3,1	14,14,15	0.71	0	17,19,21	0.92	1 (5%)
3	NAG	D	2	3	14,14,15	0.72	0	17,19,21	0.80	0
4	NAG	E	1	1,4	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
4	NAG	E	2	4	14,14,15	0.72	0	17,19,21	0.95	1 (5%)
4	BMA	E	3	4	11,11,12	0.83	0	15,15,17	2.11	3 (20%)
3	NAG	F	1	3,1	14,14,15	0.71	0	17,19,21	0.86	1 (5%)
3	NAG	F	2	3	14,14,15	0.71	0	17,19,21	0.93	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.76	0	17,19,21	2.00	5 (29%)
3	NAG	G	2	3	14,14,15	0.70	0	17,19,21	0.89	0
4	NAG	H	1	1,4	14,14,15	0.73	0	17,19,21	0.85	0
4	NAG	H	2	4	14,14,15	0.69	0	17,19,21	0.84	1 (5%)
4	BMA	H	3	4	11,11,12	0.84	0	15,15,17	2.12	3 (20%)
3	NAG	I	1	3,1	14,14,15	0.77	0	17,19,21	1.31	1 (5%)
3	NAG	I	2	3	14,14,15	0.73	0	17,19,21	0.84	0
3	NAG	J	1	3,1	14,14,15	0.74	0	17,19,21	1.05	0
3	NAG	J	2	3	14,14,15	0.68	0	17,19,21	1.33	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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	3	BMA	C1-O5-C5	6.30	120.63	112.19
4	E	3	BMA	C1-O5-C5	6.23	120.53	112.19
3	G	1	NAG	C1-O5-C5	-4.63	105.99	112.19
3	J	2	NAG	O5-C1-C2	-4.27	104.68	111.29
3	G	1	NAG	O5-C1-C2	-3.94	105.20	111.29

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

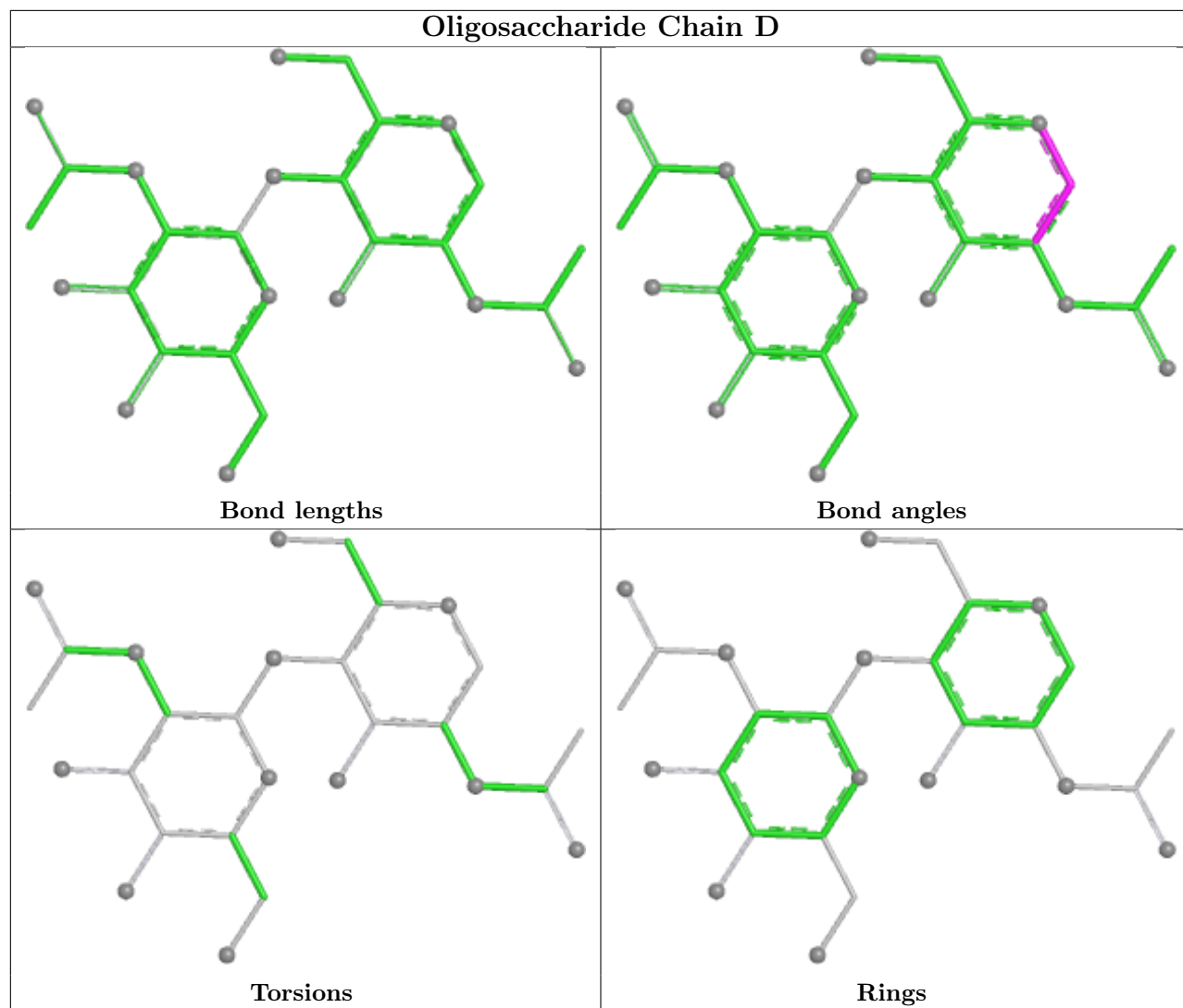
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	J	1	NAG	O5-C5-C6-O6

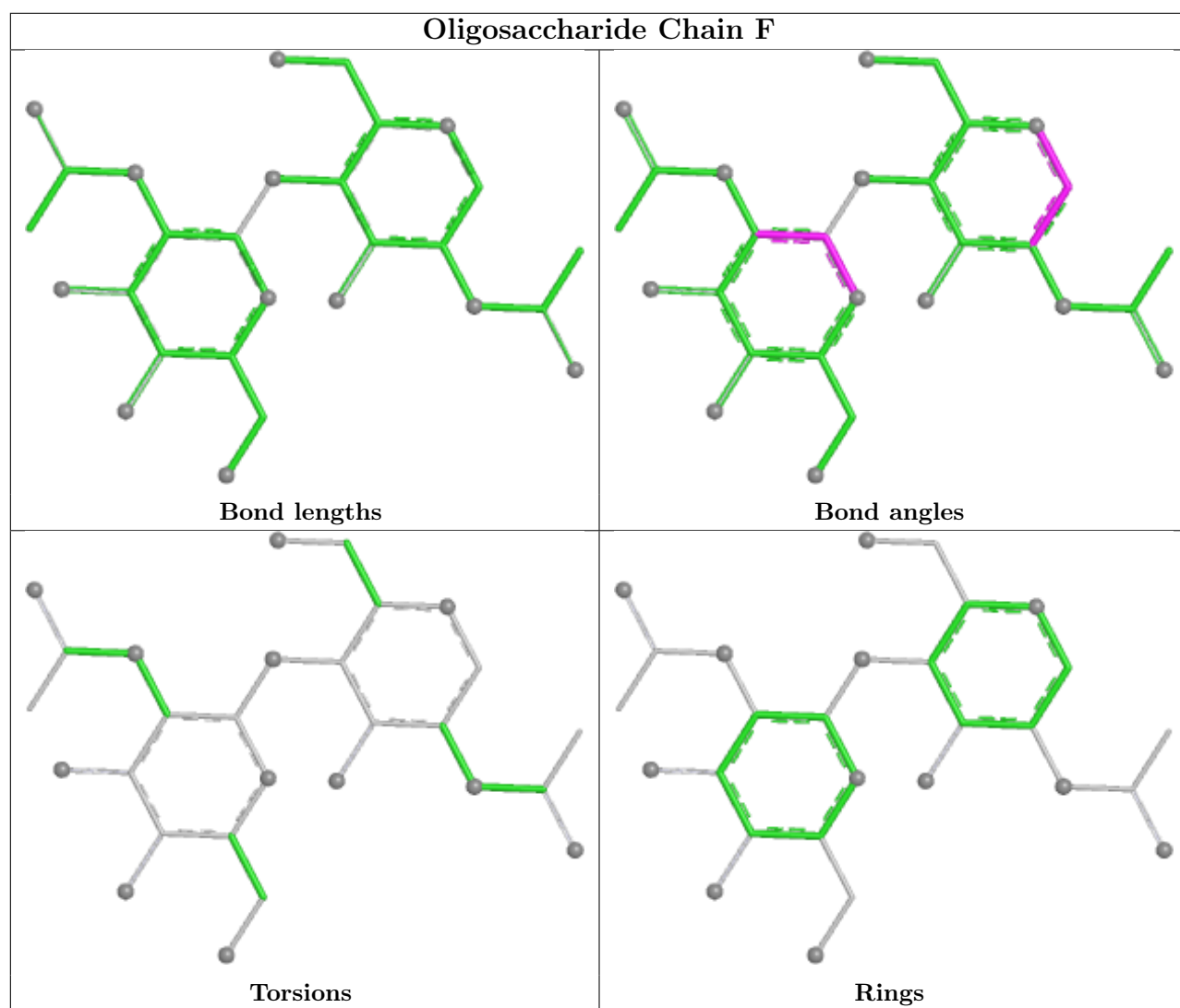
There are no ring outliers.

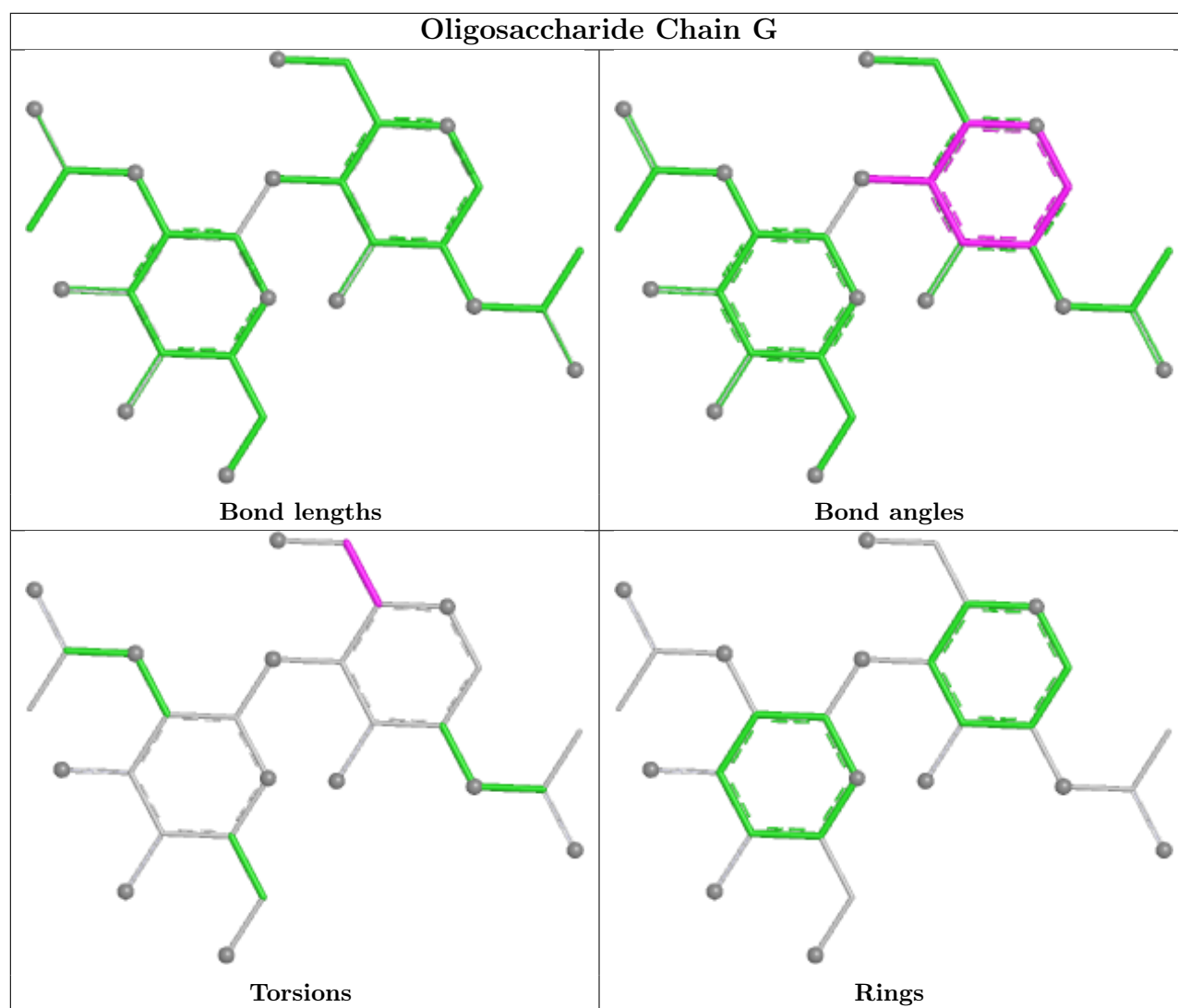
2 monomers are involved in 2 short contacts:

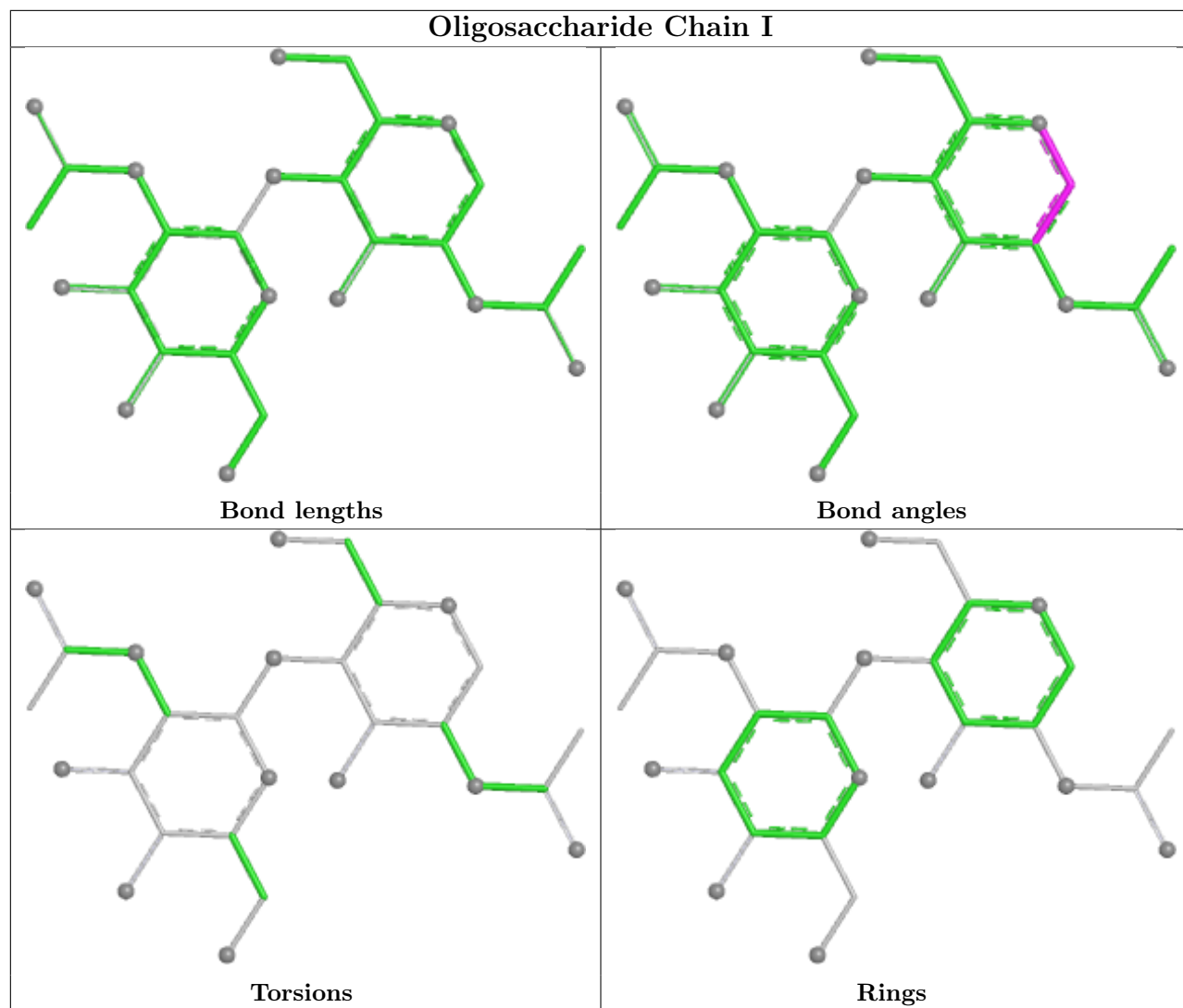
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	J	1	NAG	1	0

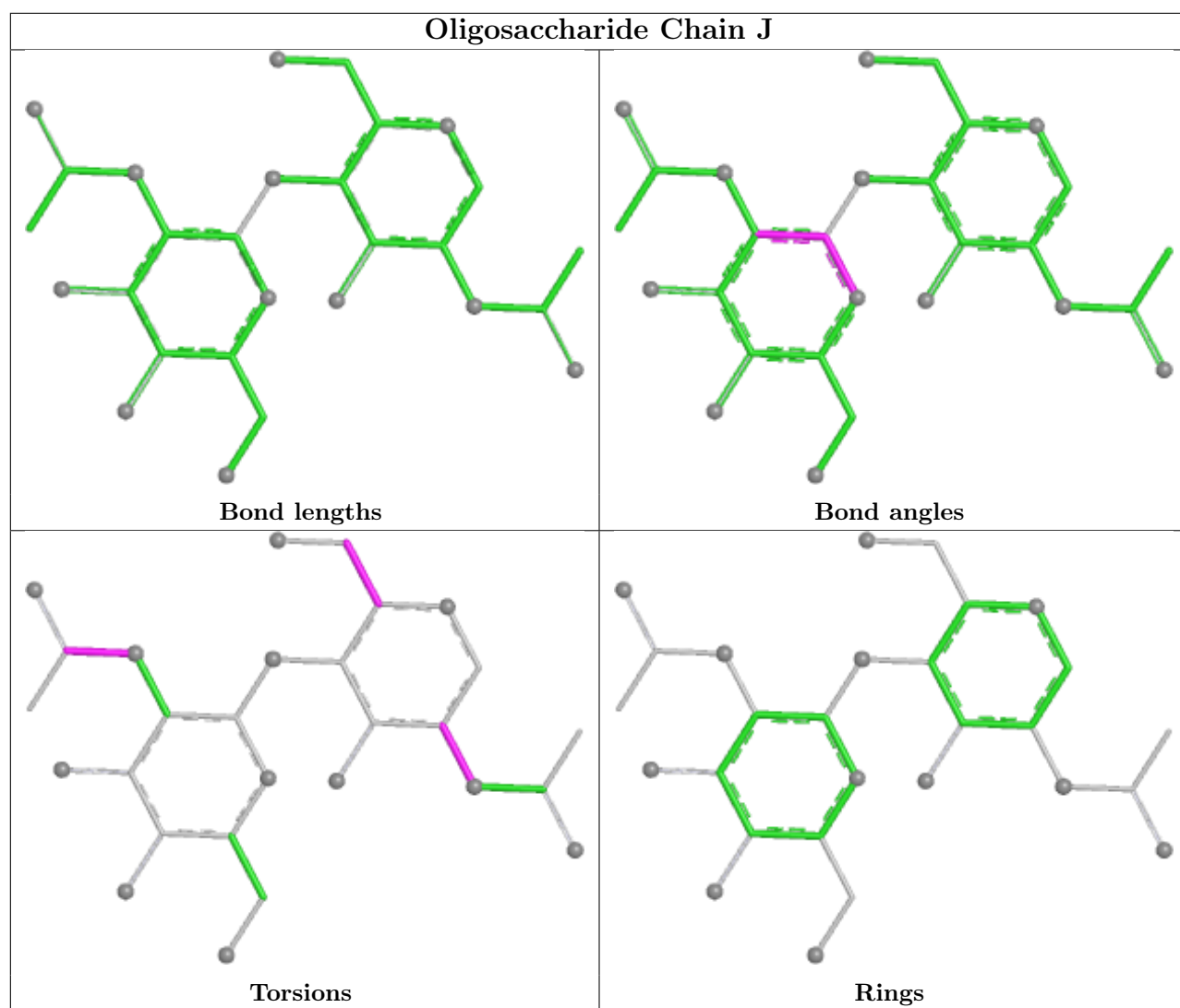
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

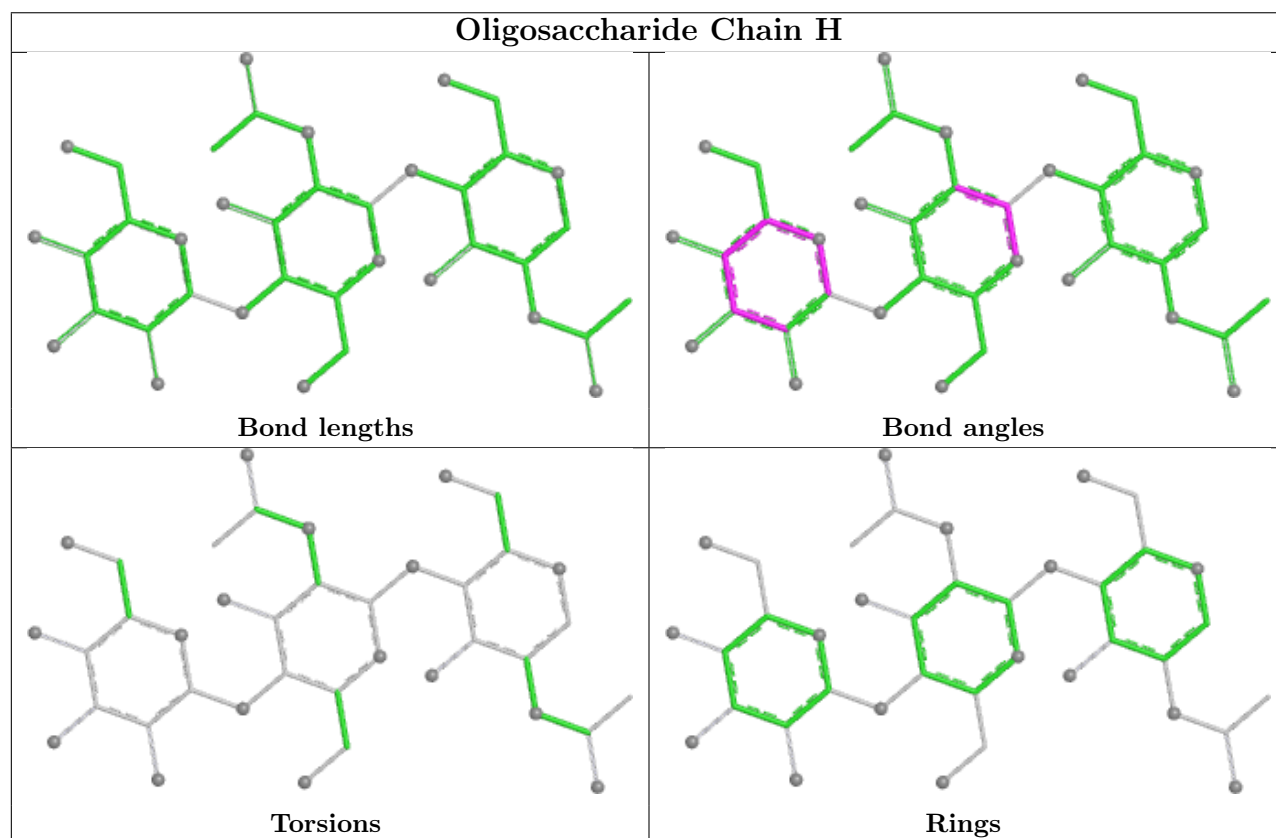
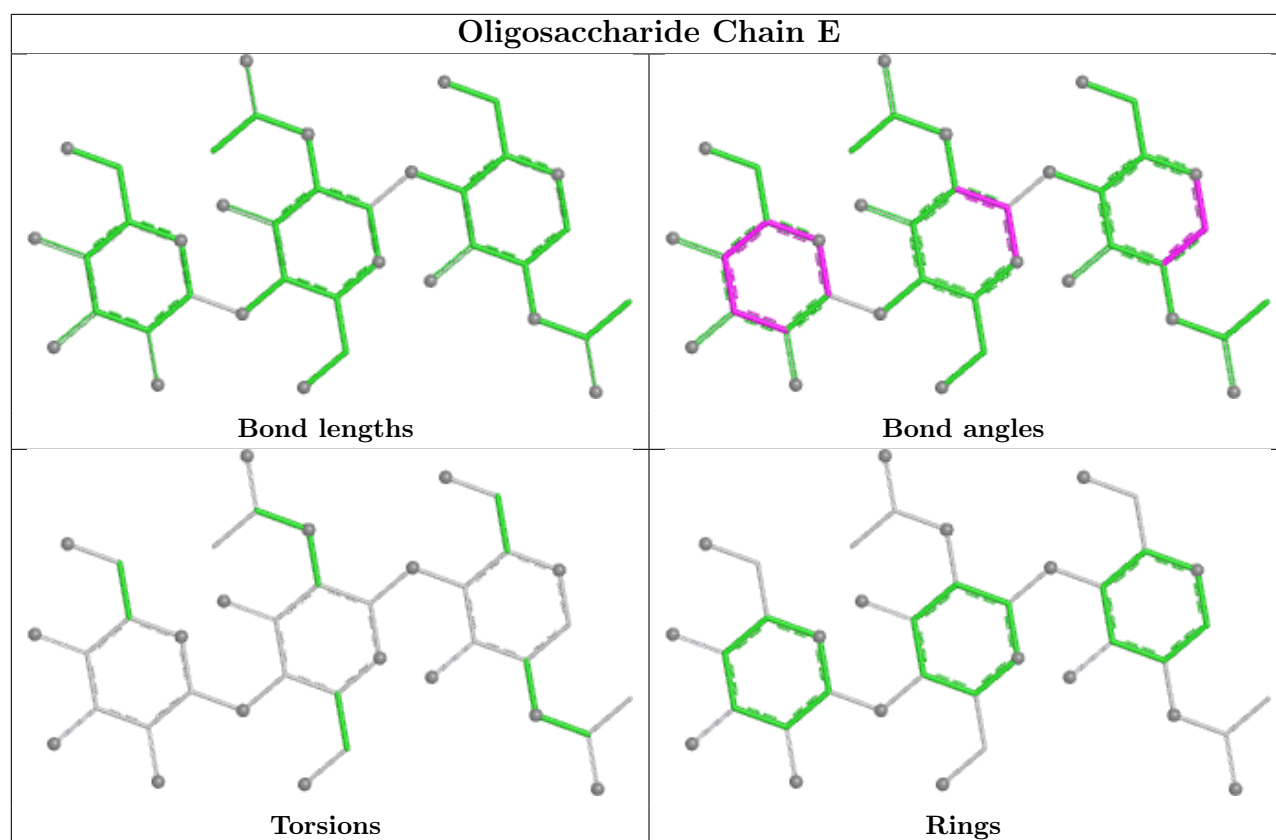












5.6 Ligand geometry

3 ligands 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	$\# Z > 2$
5	NAG	A	3401	1	14,14,15	0.74	0	17,19,21	0.90	0
5	NAG	A	3402	1	14,14,15	0.68	0	17,19,21	0.95	1 (5%)
5	NAG	B	501	2	14,14,15	0.76	0	17,19,21	0.94	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
5	NAG	A	3401	1	-	1/6/23/26	0/1/1/1
5	NAG	A	3402	1	-	1/6/23/26	0/1/1/1
5	NAG	B	501	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3402	NAG	O5-C1-C2	-2.82	106.92	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

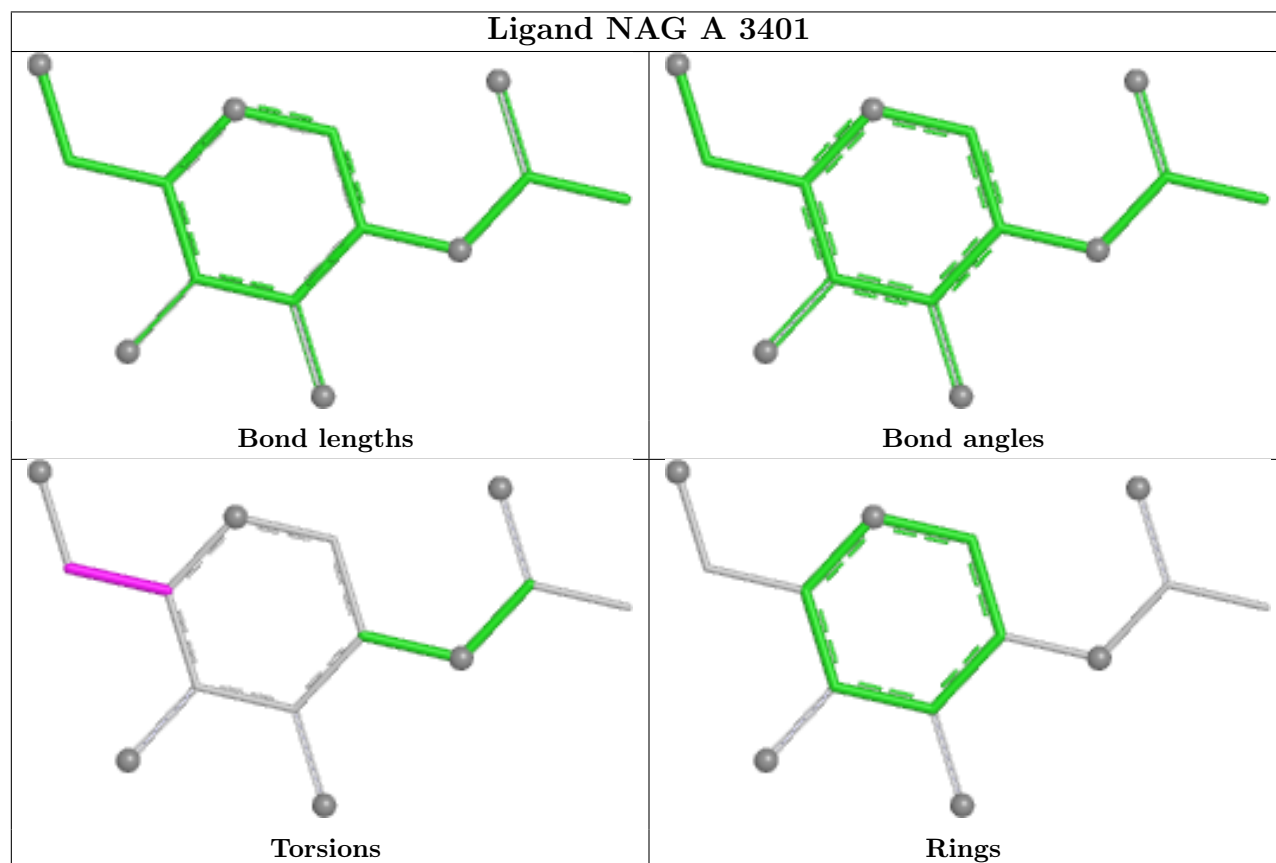
Mol	Chain	Res	Type	Atoms
5	A	3401	NAG	O5-C5-C6-O6
5	A	3402	NAG	O5-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6

There are no ring outliers.

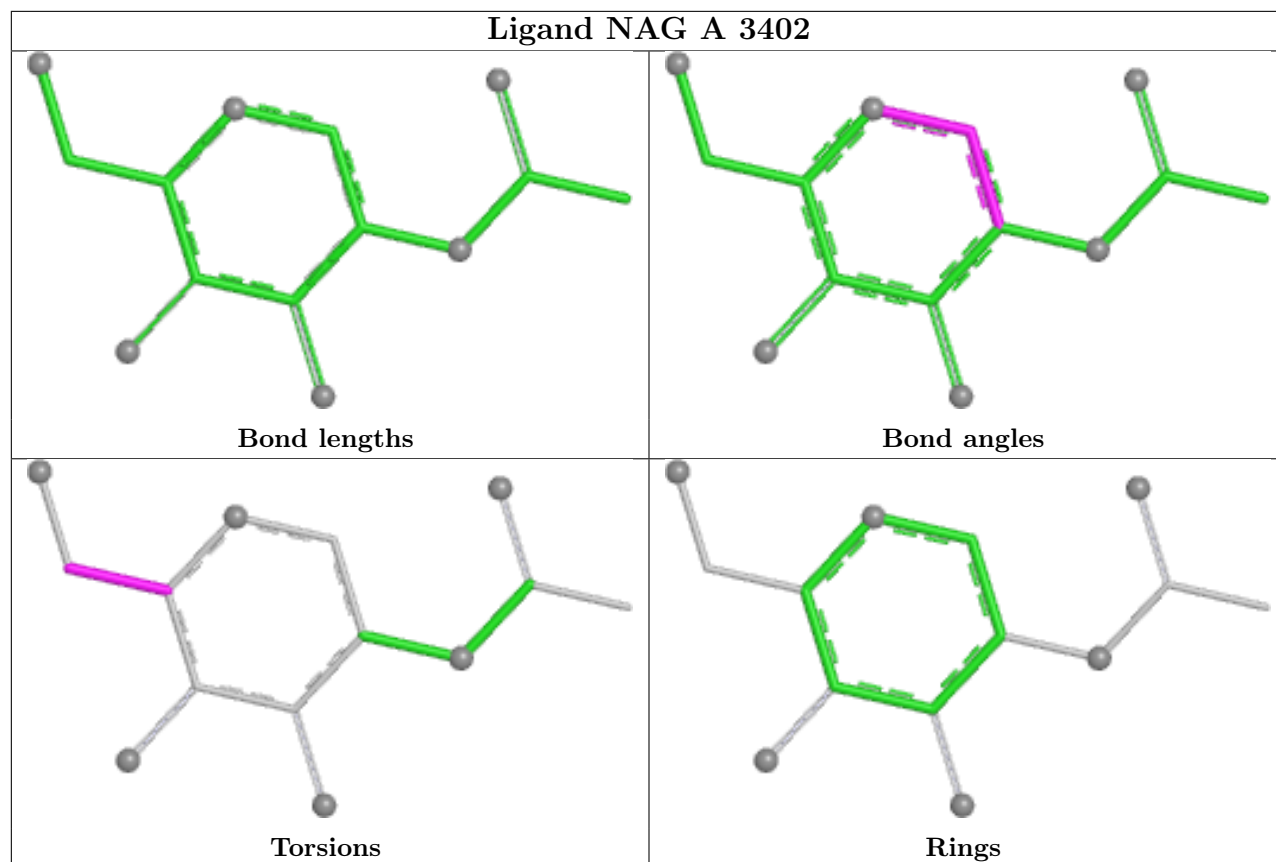
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	NAG	1	0

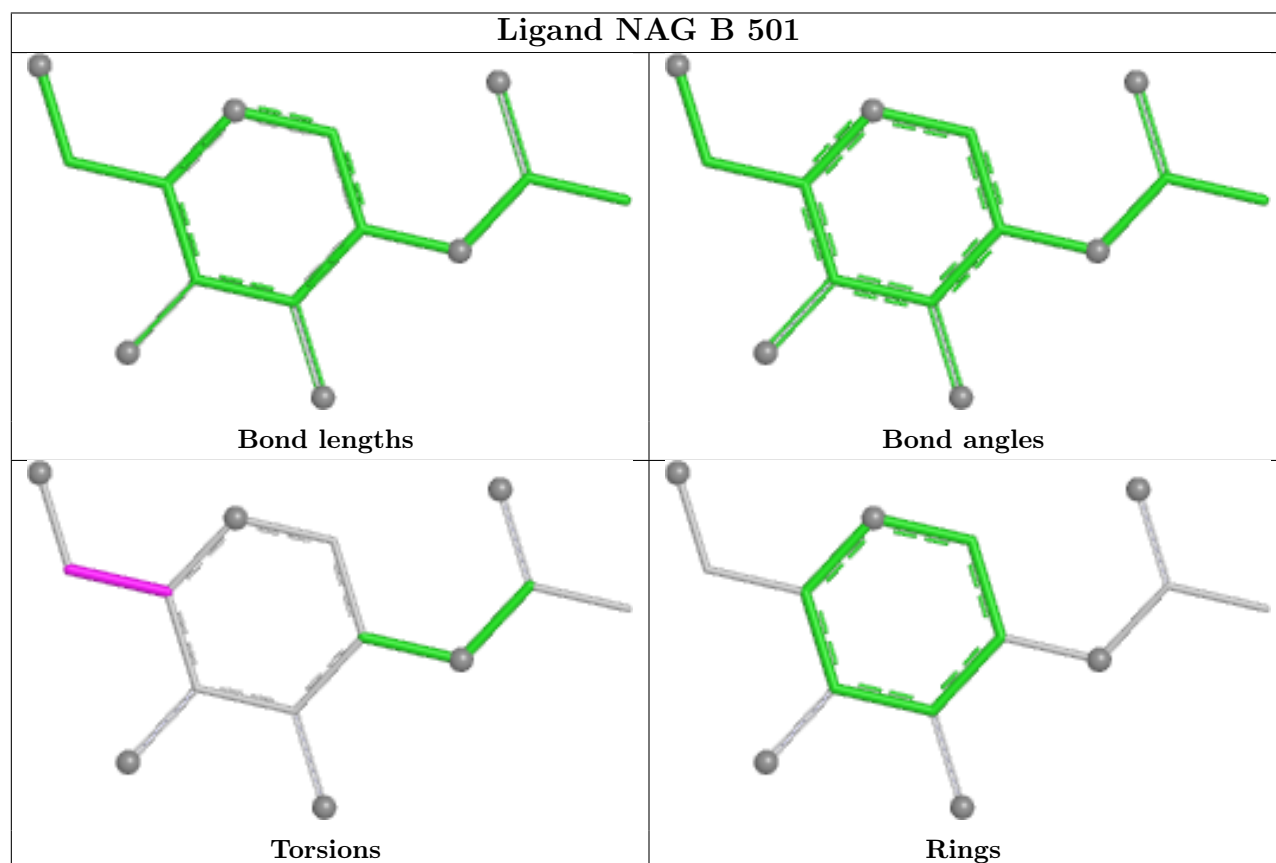
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand NAG A 3402



Ligand NAG B 501



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-70628. These allow visual inspection of the internal detail of the map and identification of artifacts.

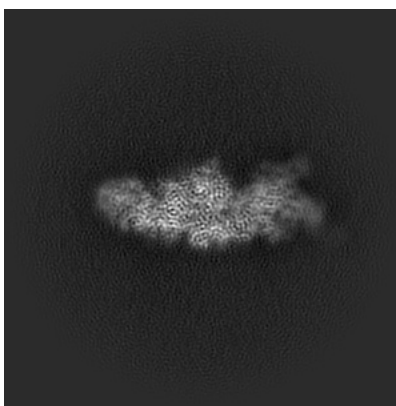
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

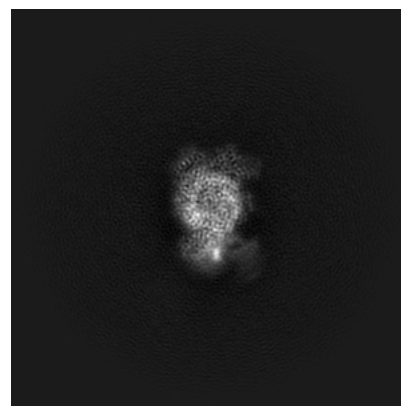
6.1.1 Primary map



X



Y

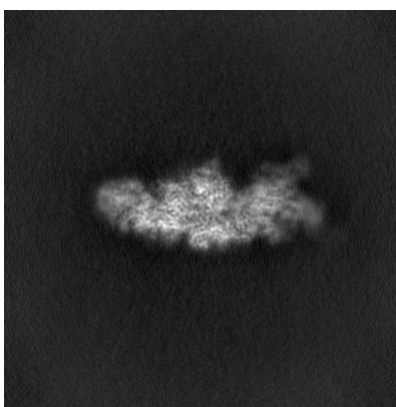


Z

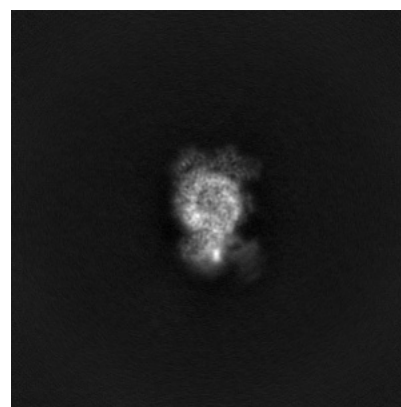
6.1.2 Raw map



X



Y

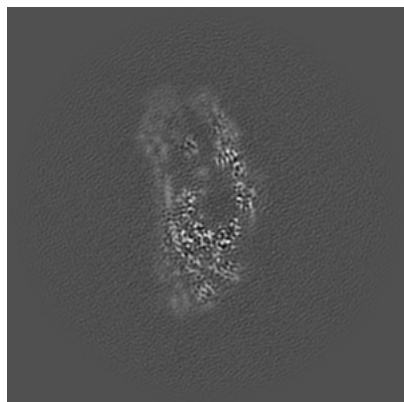


Z

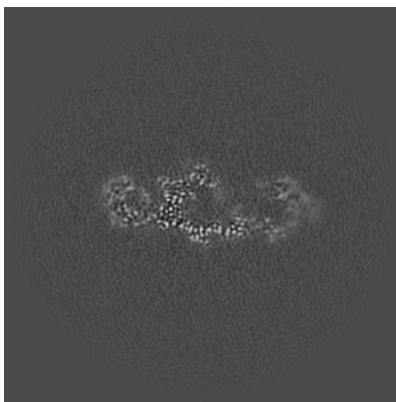
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

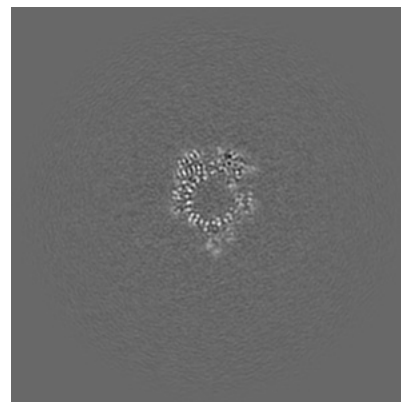
6.2.1 Primary map



X Index: 180

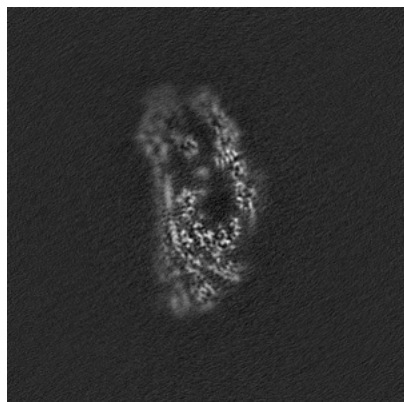


Y Index: 180

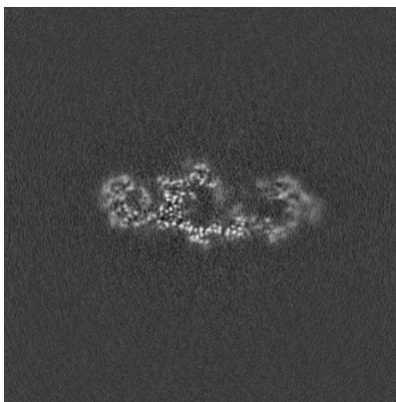


Z Index: 180

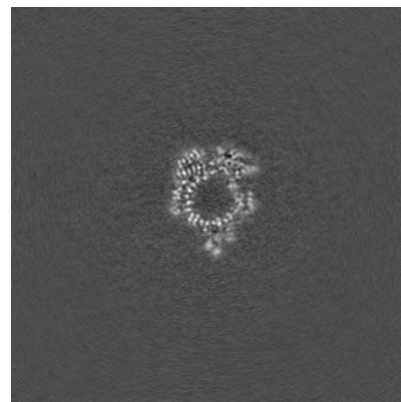
6.2.2 Raw map



X Index: 180



Y Index: 180

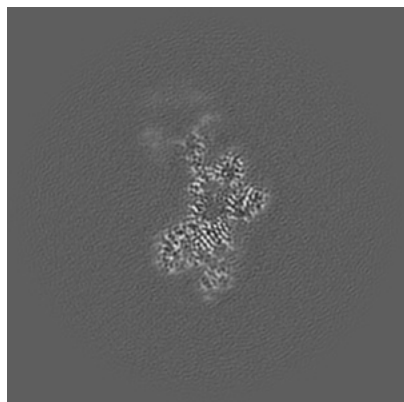


Z Index: 180

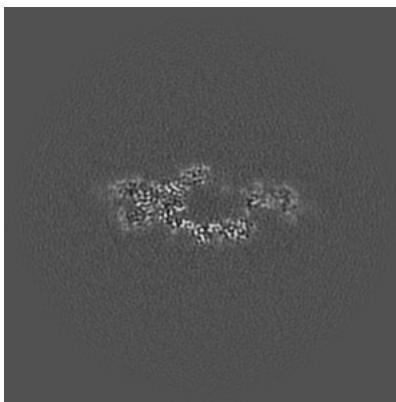
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

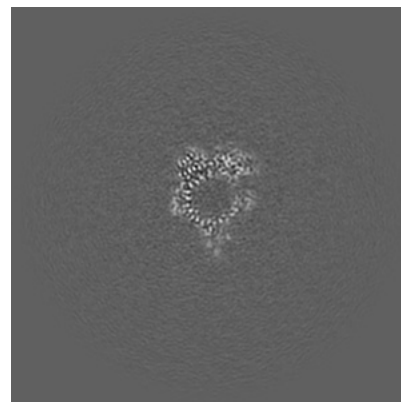
6.3.1 Primary map



X Index: 165

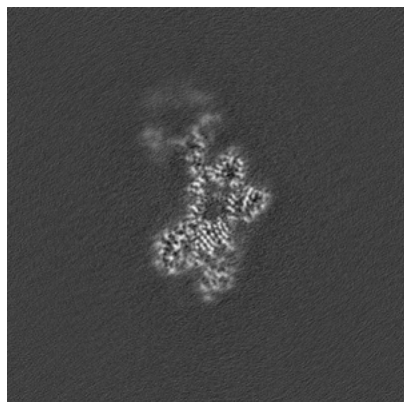


Y Index: 191

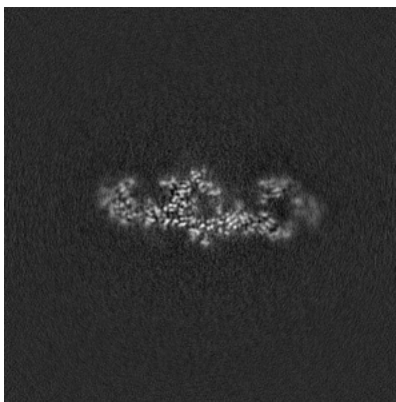


Z Index: 182

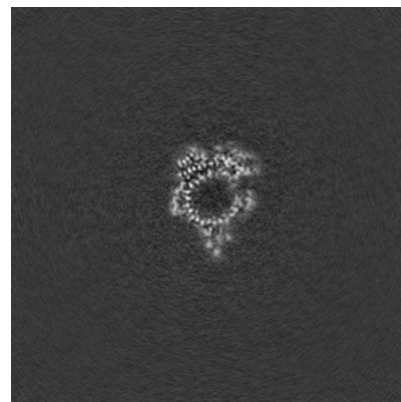
6.3.2 Raw map



X Index: 165



Y Index: 174

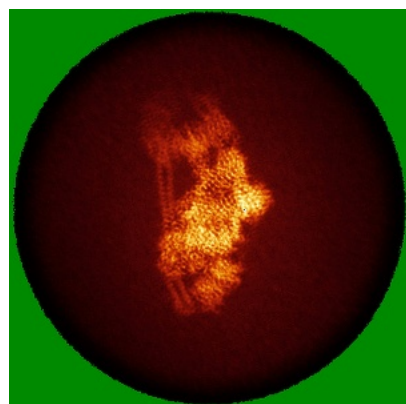


Z Index: 182

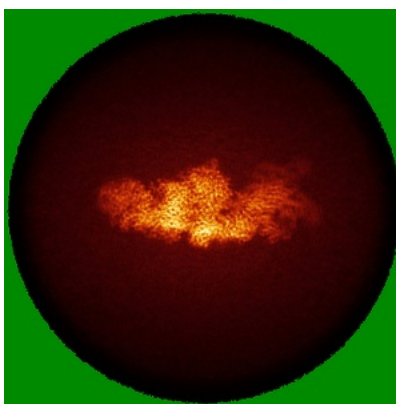
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

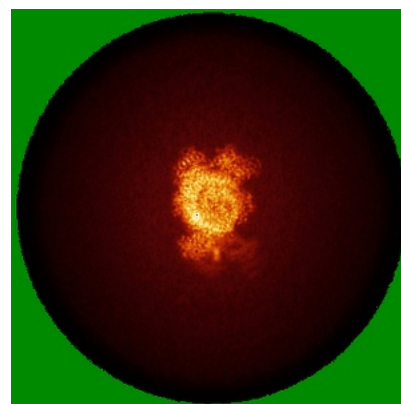
6.4.1 Primary map



X

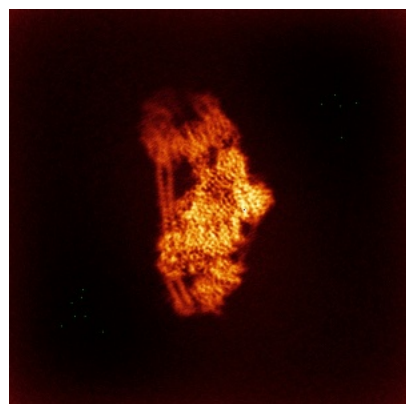


Y

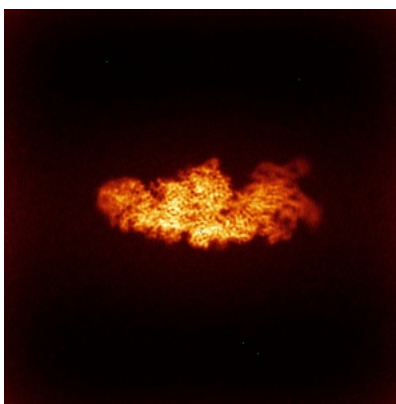


Z

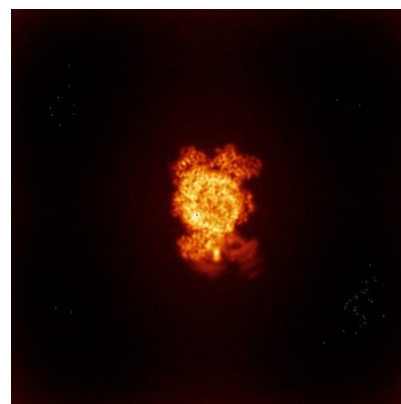
6.4.2 Raw map



X



Y

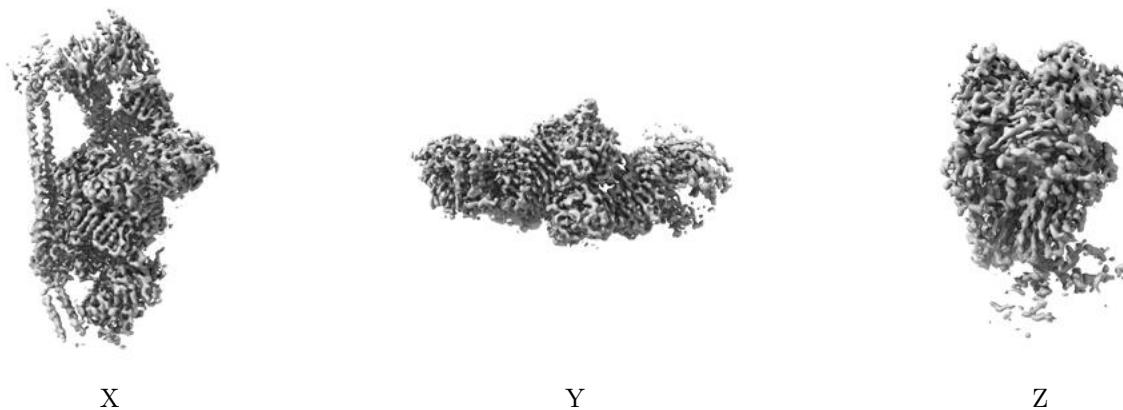


Z

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 0.6. 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.

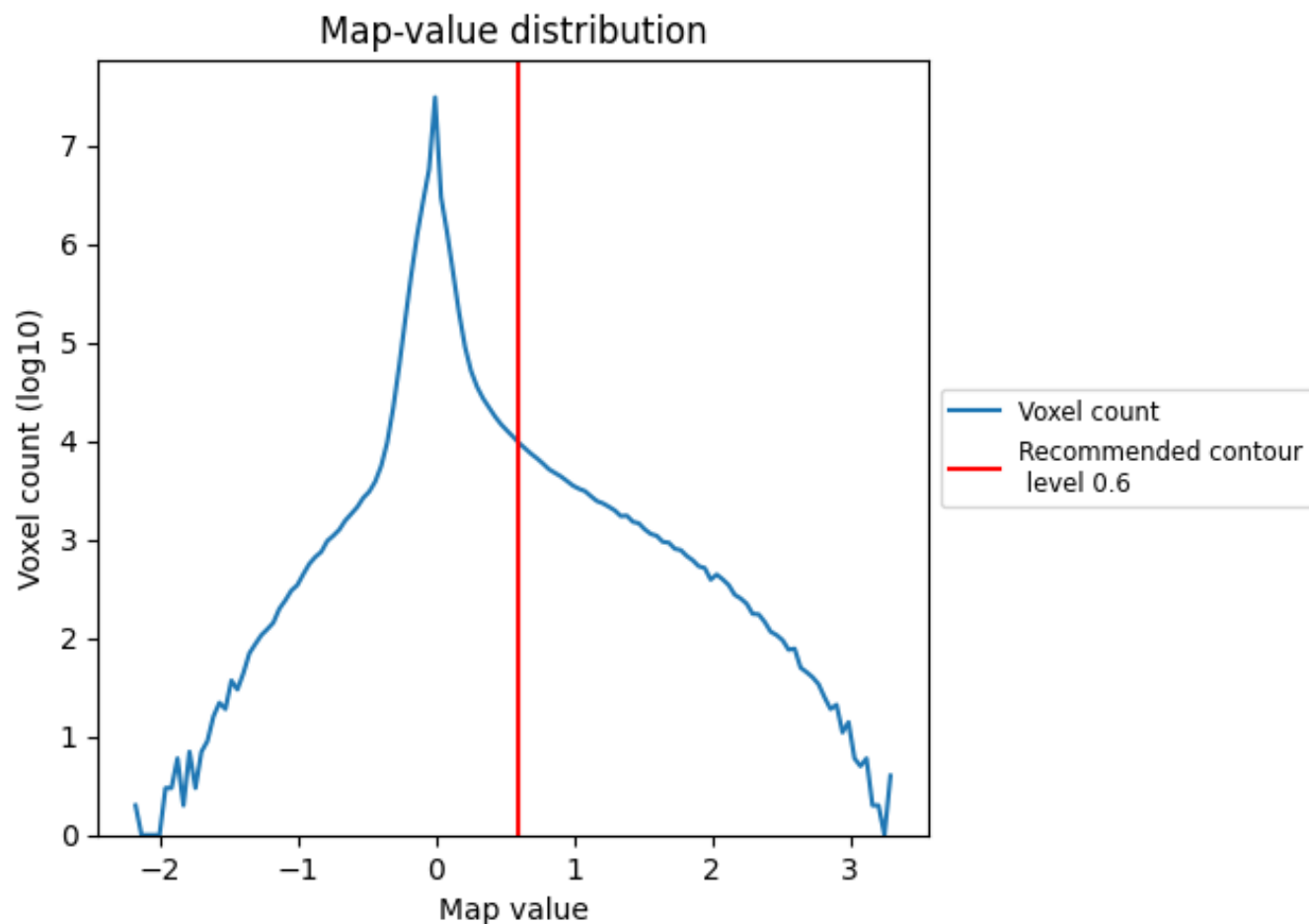
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

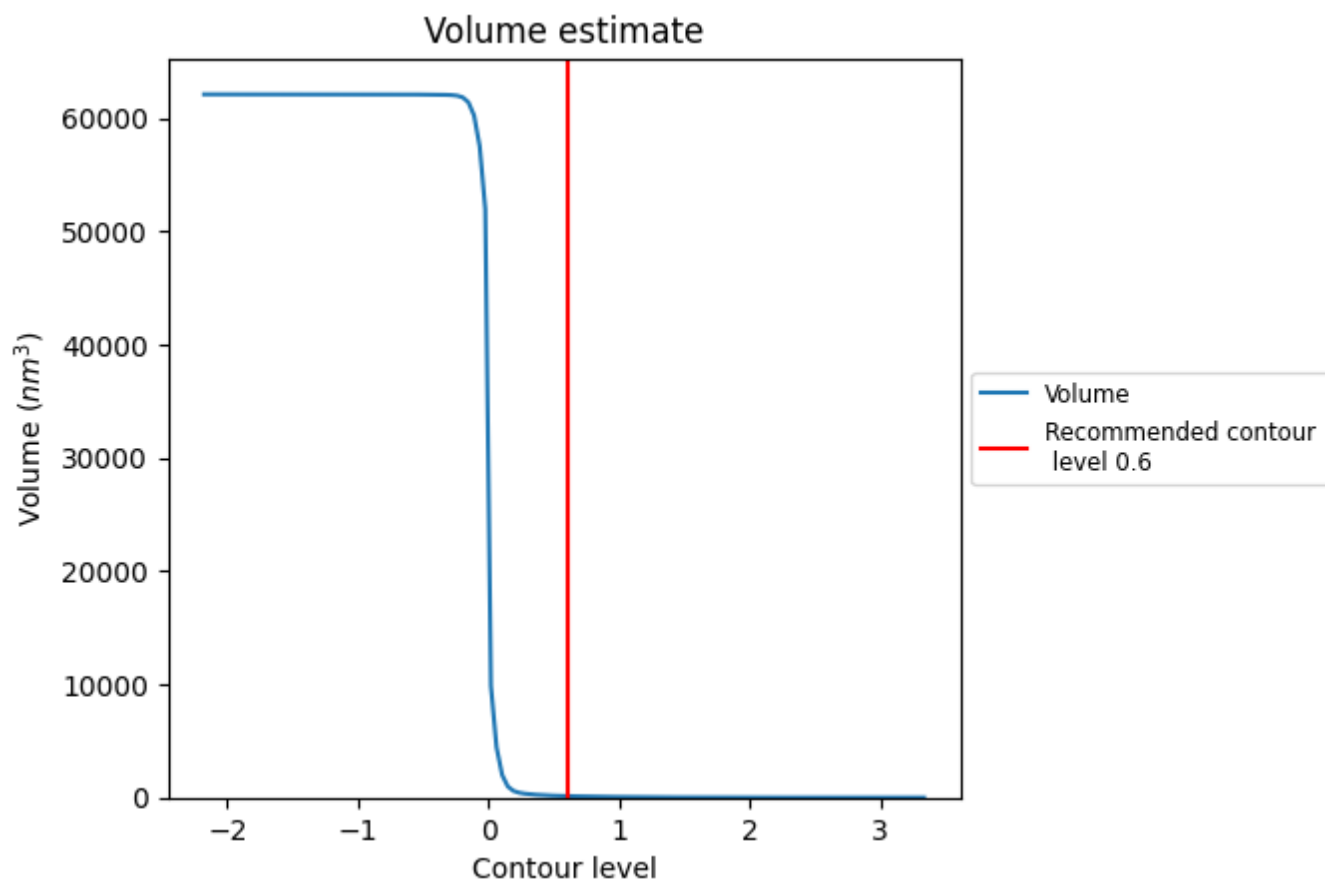
This section contains the results of statistical analysis of the map.

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.

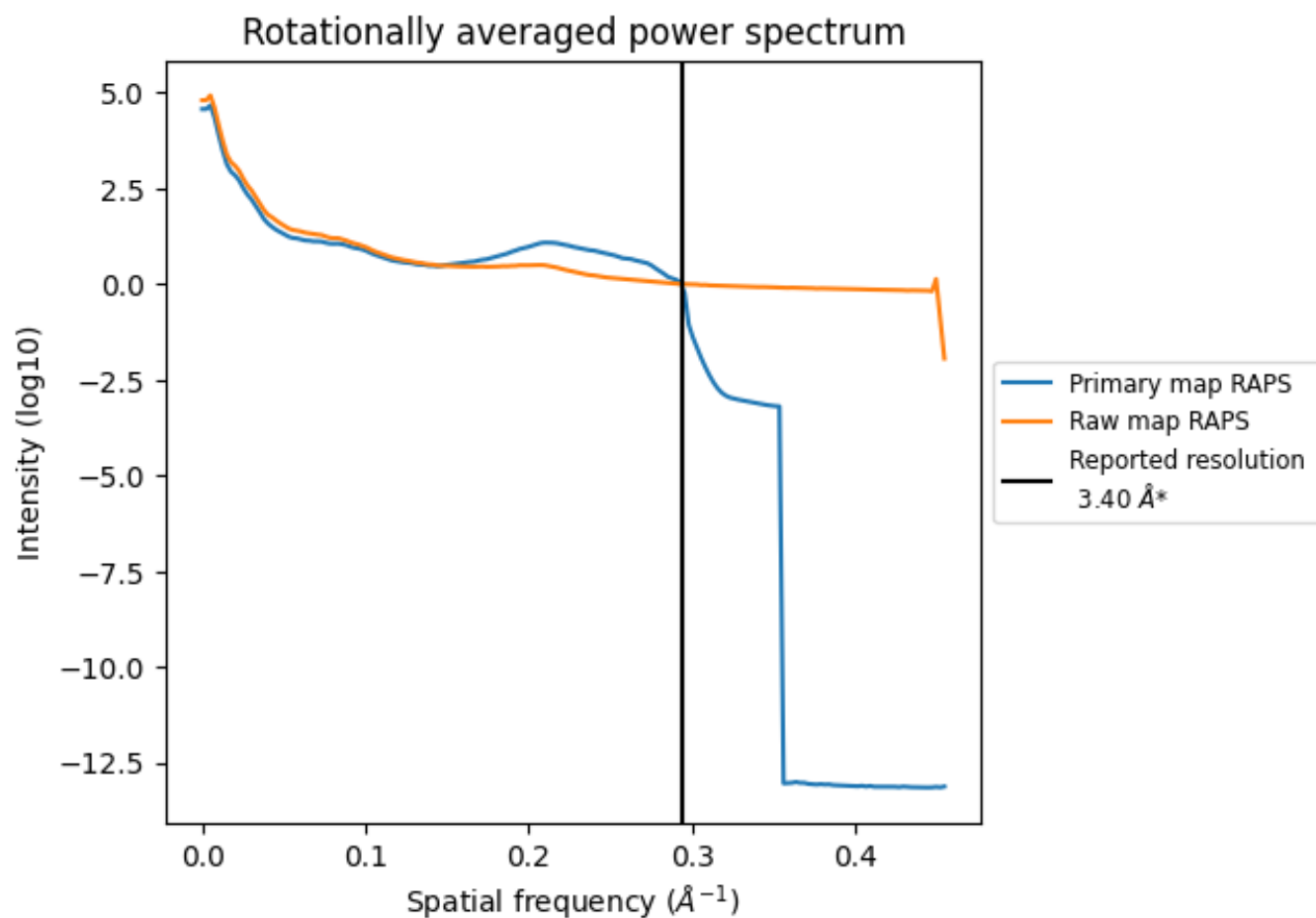
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm³; this corresponds to an approximate mass of 117 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 ⓘ

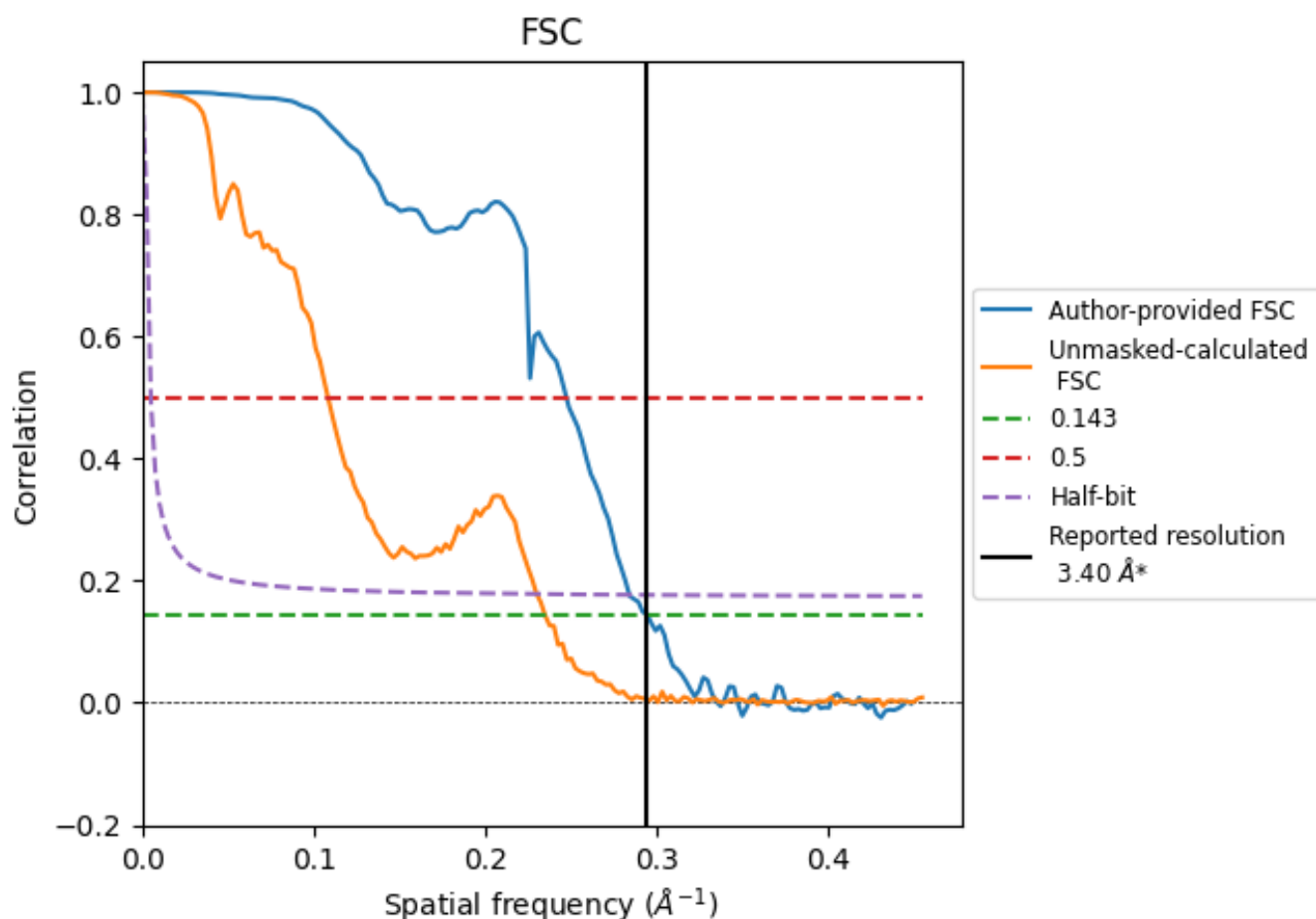


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

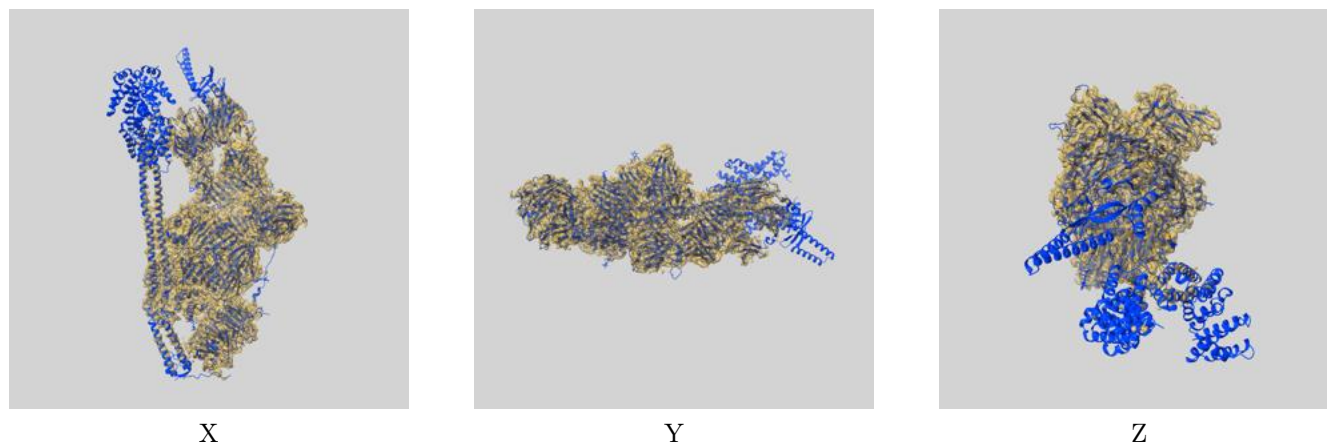
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	4.05	3.52
Unmasked-calculated*	4.26	9.24	4.35

*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 4.26 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

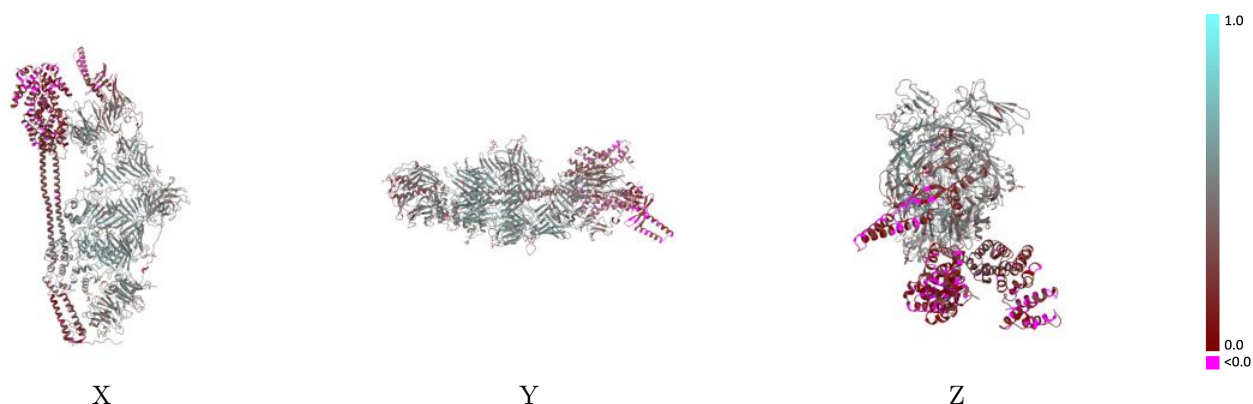
This section contains information regarding the fit between EMDB map EMD-70628 and PDB model 9ON3. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



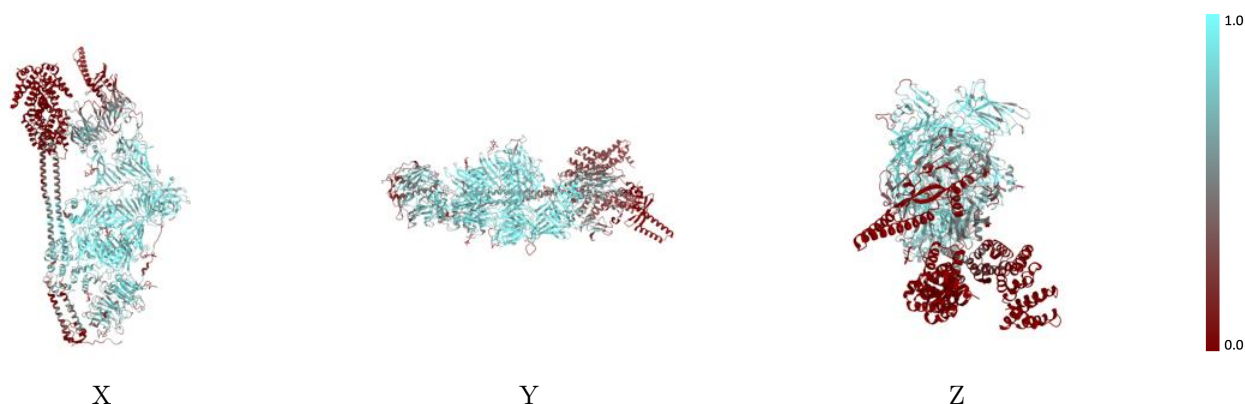
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



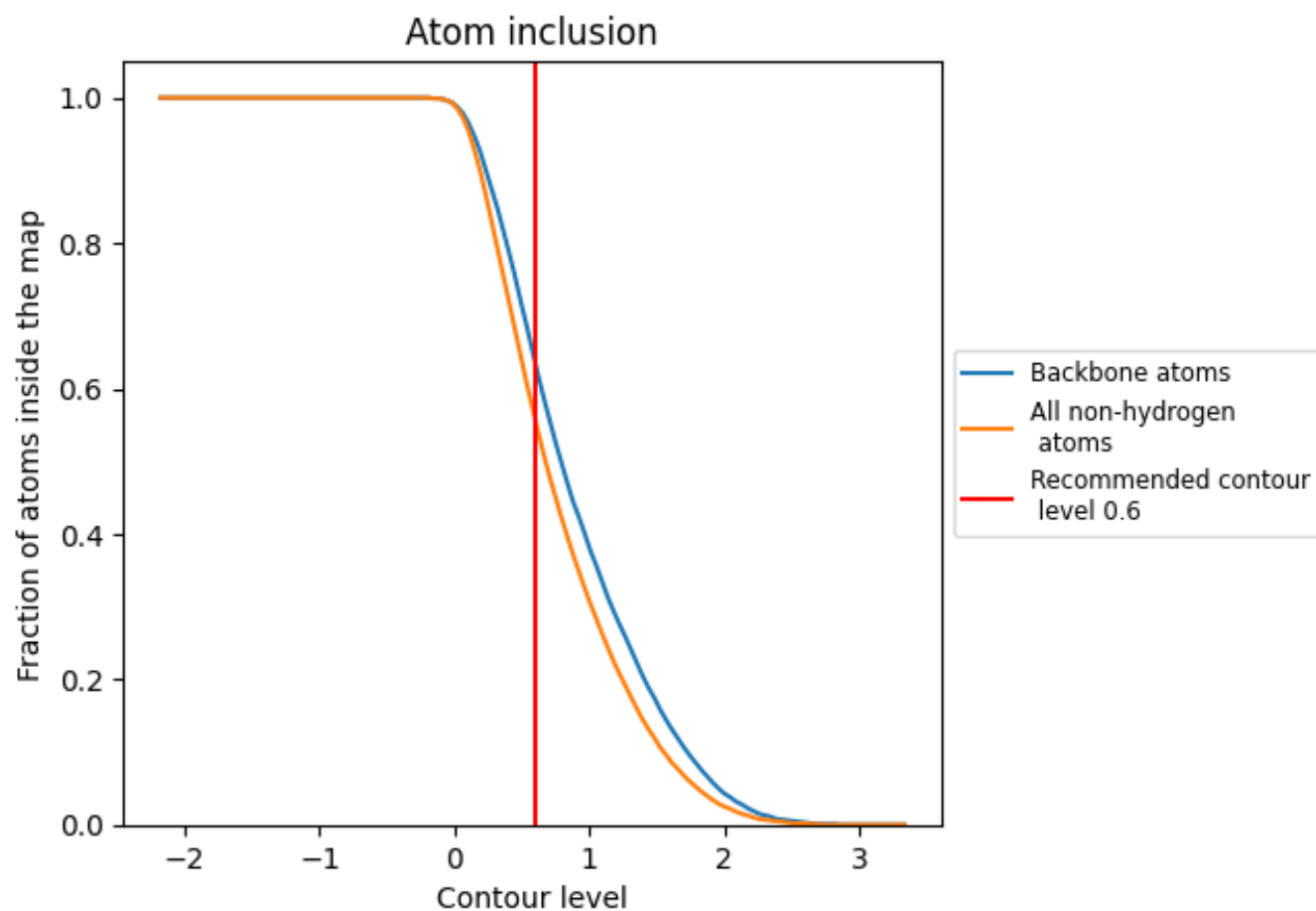
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 56% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5560	<div></div> 0.3990
A	<div></div> 0.6740	<div></div> 0.4580
B	<div></div> 0.1720	<div></div> 0.2100
C	<div></div> 0.1230	<div></div> 0.1710
D	<div></div> 0.0000	<div></div> 0.2060
E	<div></div> 0.3080	<div></div> 0.3890
F	<div></div> 0.1430	<div></div> 0.3630
G	<div></div> 0.1070	<div></div> 0.2580
H	<div></div> 0.0000	<div></div> 0.2180
I	<div></div> 0.0360	<div></div> 0.3210
J	<div></div> 0.3930	<div></div> 0.2810

