



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 01:33 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 Full wwPDB EM Validation 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:

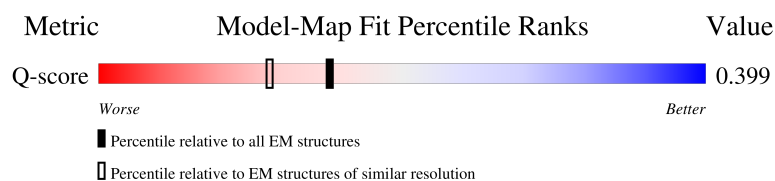
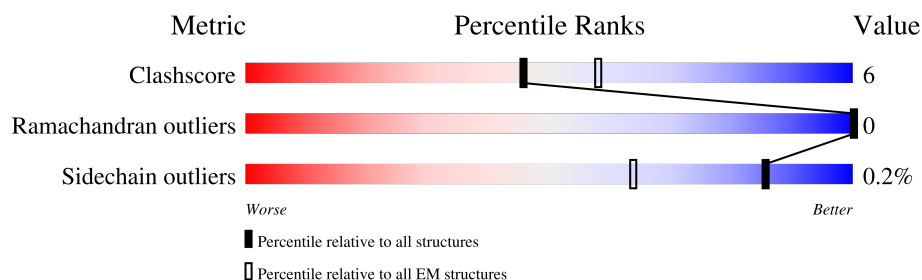
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

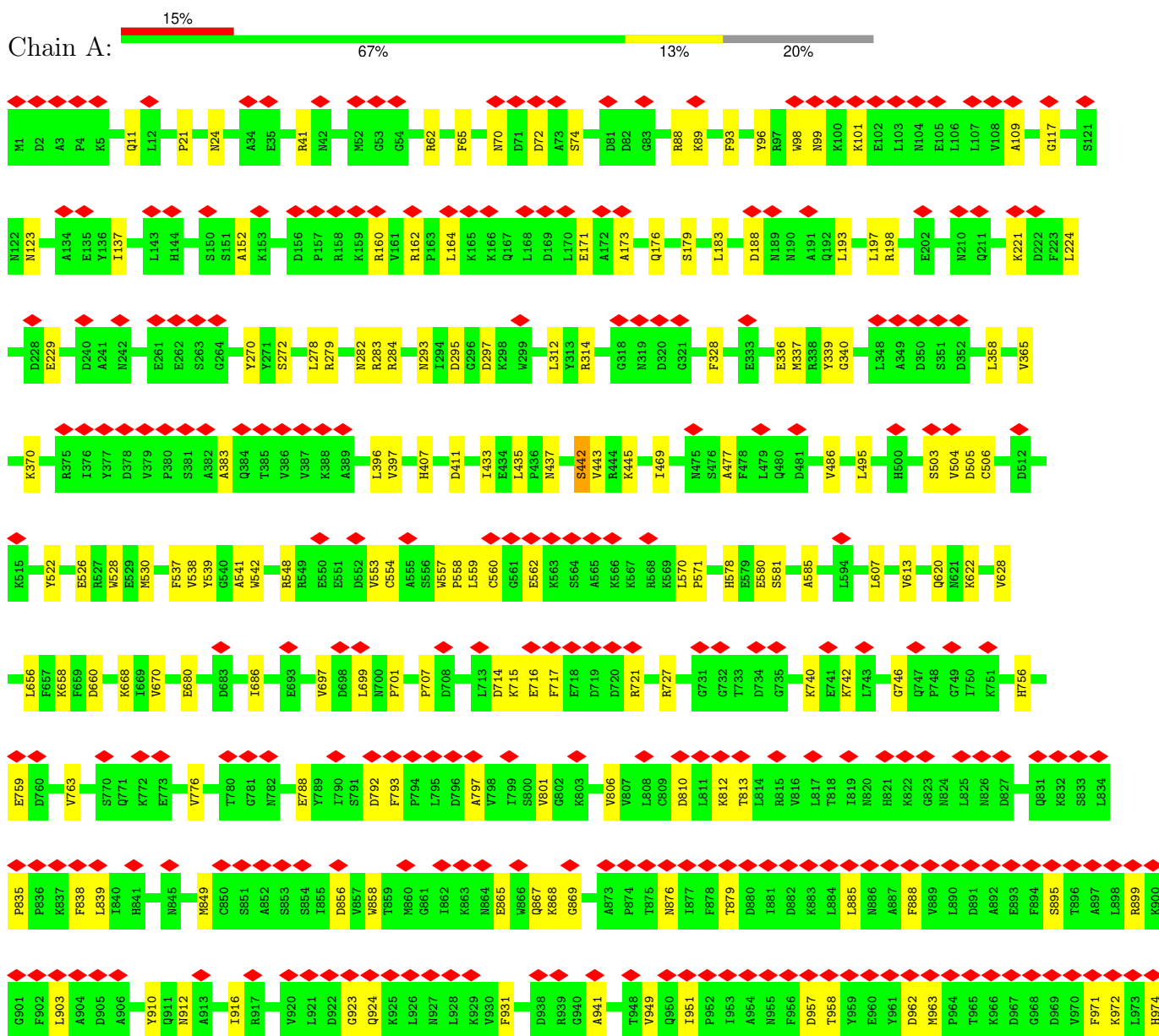


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

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.

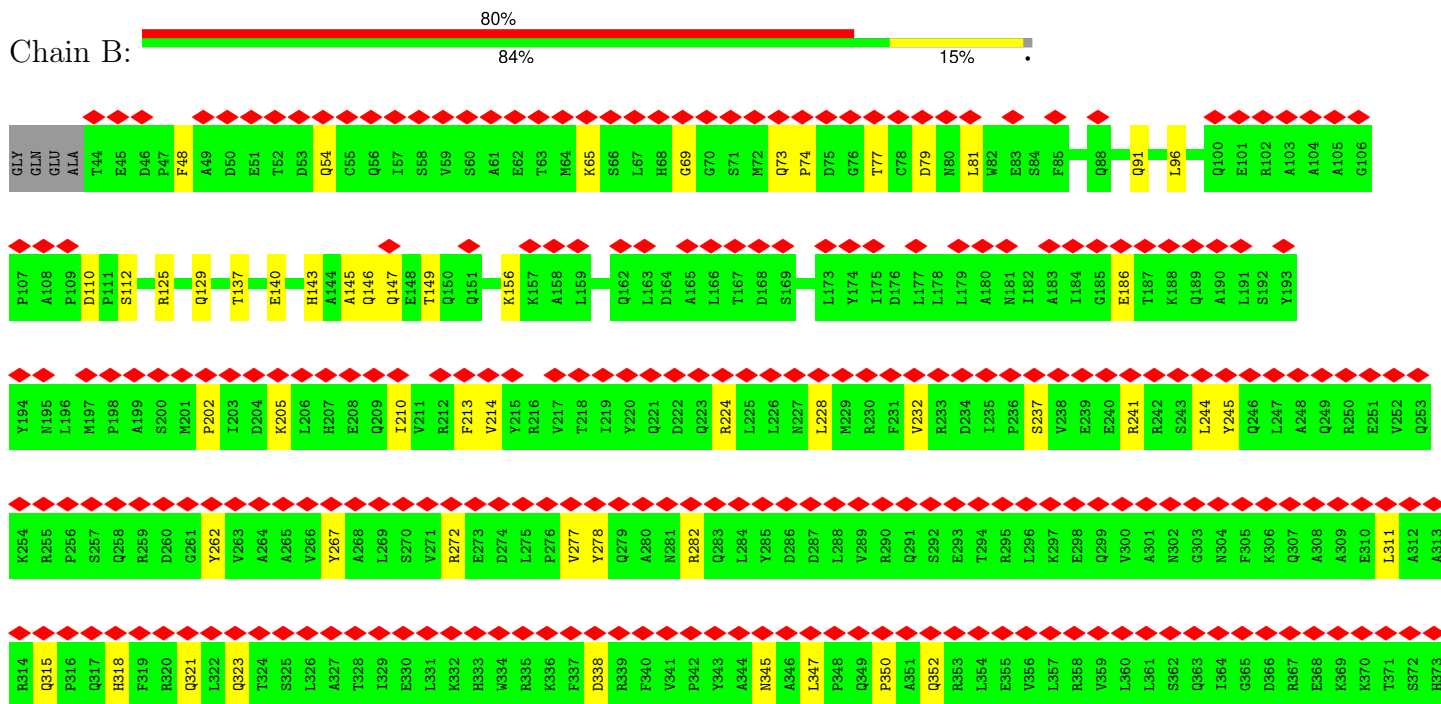
• Molecule 1: SGS4

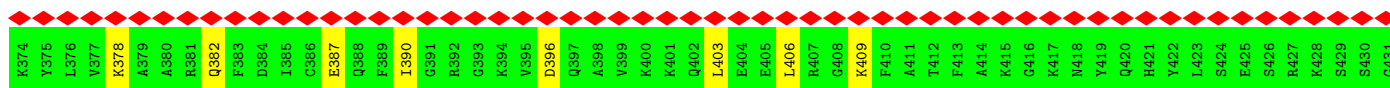


D2733	G2734	L2543	I2377	T2145	V1973	T1760	F1625	E1435	R1291	R1181	A1102	N1035
GLU	PHE	E2549	L2383	K2154	S1978	Q1761	C1626	I1438	D1292	H1182	K1103	I1036
ALA	ALA	I2558	T2387	D2157	M1984	G1771	T1628	I1438	D1293	V1183	Y1104	S1037
THR	THR	Q2561	K2391	R2158	R1985	R1817	G1629	H1442	D1294	N1184	S1105	Q1038
LEU	LEU	Y2562	T2198	T2198	E1986	R1817	S1630	T1443	V1295	E1185	Y1106	T1039
ALA	ALA	V2563	S2199	A1987	S1631	E1823	S1630	A1444	W1303	T1186	Q1107	V1040
VAL	VAL	R2565	P2200	E1987	N1632	E1823	S1631	A1444	W1303	T1186	Q1107	V1040
LEU	LEU	D2213	D2213	N1990	N1632	E1823	S1632	G1446	K1307	D1108	D1108	V1041
ILE	ILE	K2404	E2412	I1841	S1633	I1841	S1633	G1446	K1307	T1109	T1109	K1042
LEU	LEU	T2669	L2227	R1950	C1634	I1849	C1634	S1447	K1310	Y1113	Y1113	K1043
ALA	ALA	P2670	L2227	R1950	N1635	R1950	N1635	K1448	D1313	E1114	E1114	A1044
VAL	VAL	K2417	D2249	V1953	P1637	V1953	P1637	N1452	L1317	M1115	P1115	Q1045
GLY	GLY	Q2416	K2266	A1862	E1642	E1642	E1642	I1455	V1323	P1116	A1047	F1046
ALA	ALA	Q2417	T2270	V1867	T1648	V1867	T1648	E1459	W1339	R1117	R1117	M1048
TYR	TYR	E2421	P2274	G1868	E1649	G1868	E1649	D1465	K1340	L1200	L1200	D1049
LEU	LEU	S2422	Y2277	N1869	L1650	N1869	L1650	H1468	K1341	L1213	G991	L1050
ALA	ALA	A2423	Y2277	S1880	R1651	S1880	R1651	V1469	W1342	D1214	Y1121	Q1052
SER	SER	D2424	D2282	H1885	H1659	H1885	H1659	R1470	W1343	Q1215	Y1122	F1053
ASN	ASN	A2425	D2282	L1890	K1667	L1890	K1667	D1466	S1344	L1218	Q1125	G1054
ASN	ASN	P2426	D2285	F1894	P1668	F1894	P1668	T1467	F1345	R1219	T1126	V1055
CYS	CYS	S2429	K2291	H2296	E2043	H2296	E2043	V1533	A1348	D1229	T1127	L1056
TRP	TRP	N2431	H2296	G2297	E2043	G2297	E2043	E1553	R1354	V1230	N1127	Q1059
LEU	LEU	E2432	G2297	L2298	L2054	L2298	L2054	E1556	Y1358	D1236	M1128	H1060
LYS	LYS	F2434	L2298	L2306	V2060	L2306	V2060	V1567	L1367	Q1130	P1129	G1061
TRP	TRP	P2446	L2306	L2310	I2063	L2310	I2063	S1568	K1368	E1131	E1131	G1065
TRP	TRP	D2632	F2311	F2311	N2064	F2311	N2064	I1569	A1369	Q1132	Q1132	N1066
SER	SER	Y2625	I2315	I2315	R2065	I2315	R2065	E1573	K1369	W1134	V1134	Q1067
SER	SER	F2626	K2316	K2316	T2066	K2316	T2066	E1574	F1384	V1135	A1136	S1004
THR	THR	V2627	G2317	G2317	E2072	E1915	E1915	E1575	W1385	A1136	P1137	Q1068
THR	THR	R2628	D2317	D2317	S2030	I1917	I1917	E1576	K1377	R1138	Y1139	Y1005
THR	THR	L2636	I2318	I2318	M2085	A1689	A1689	G1579	S1383	Q1140	T1140	Q1006
ILE	ILE	L2645	E2319	E2319	D2086	E1948	E1948	V1581	F1384	Q1141	Q1141	Q1007
LEU	LEU	D2657	A2321	A2321	S2087	Y1949	Y1949	A1582	W1385	S1142	S1142	I1008
LEU	LEU	Y2661	K2322	K2322	M2085	D1936	D1936	Q1583	V1406	D1072	G1073	D1009
GLY	GLY	R2666	T2326	T2326	D2086	I1948	I1948	R1589	V1409	Q1074	Q1074	A1010
VAL	VAL	L2672	T2326	T2326	S2087	Y1949	Y1949	T1590	N1410	T1075	T1075	S1011
THR	THR	D2673	K2333	K2333	A2089	Y1949	Y1949	R1589	L1411	Q1076	W1076	G1012
GLY	GLY	Y2692	T2337	T2337	S2106	R1956	R1956	Q1583	V1406	Q1078	Q1077	E1013
ALA	ALA	G2513	F2338	F2338	D2087	L1955	L1955	Q1583	V1406	Q1079	Q1079	A1014
SER	SER	E2713	D2339	D2339	D2087	P1719	P1719	R1601	N1412	P1080	P1080	V1015
ILE	ILE	P2726	R2349	R2349	S2106	R1956	R1956	F1602	Q1414	I1081	I1081	E1016
PRO	PRO	D2522	E2350	E2350	R2113	F1957	F1957	V1604	K1415	D1082	D1082	K1017
PHE	PHE	G2523	G2351	G2351		R1966	R1966	N1605	L1419	Q1083	Q1083	A1019
ASN	ASN	A2539						D1609	V1424	A1084	A1084	Q1020
ALA	ALA							D1610		T1085	T1085	Y1021
										Q1086	Q1086	K1022
										R1087	R1087	K1023
										E1089	E1089	E1024
										K1090	K1090	V1025
										V1091	V1091	D1026
										E1027	E1027	E1027
										D1092	D1092	K1028
										Q1093	Q1093	F1029
										A1097	A1097	A1030
										G1098	G1098	E1031
										F1099	F1099	E1032
												V1033
												D1034

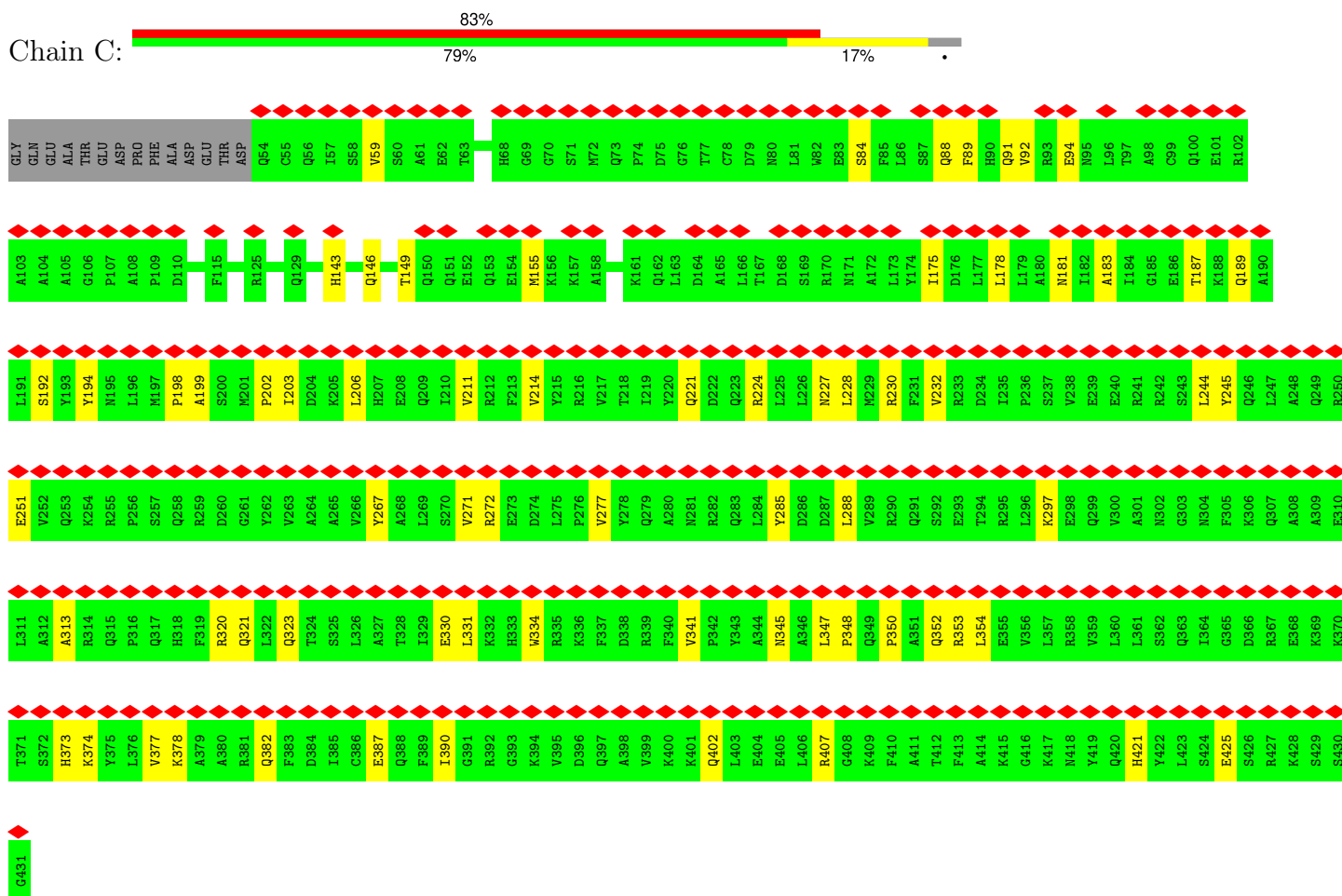
[illegible]

- 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.

All (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
1:A:397:VAL:HG22	1:A:1354:ARG:HH21	1.54	0.72
1:A:1367:LEU:HD23	1:A:1455:ILE:HD11	1.70	0.72
1:A:164:LEU:HD13	2:B:48:PHE:HB3	1.72	0.71
1:A:1134:VAL:HB	1:A:1140:ILE:HG13	1.72	0.71
2:B:213:PHE:O	2:B:224:ARG:NH1	2.25	0.70
1:A:383:ALA:HB3	1:A:2113:ARG:HE	1.57	0.69
1:A:1136:ALA:C	1:A:1138:ARG:H	1.98	0.69
1:A:469:ILE:HG12	1:A:486:VAL:HG22	1.75	0.69
1:A:1345:PHE:HB3	1:A:1367:LEU:HD13	1.75	0.69
1:A:336:GLU:HA	1:A:2200:PRO:HG3	1.75	0.68
2:B:96:LEU:HD22	2:C:92:VAL:HG23	1.73	0.68
1:A:528:TRP:HB2	1:A:539:TYR:HB2	1.75	0.68
1:A:541:ALA:HB2	1:A:548:ARG:HH12	1.59	0.67
1:A:2065:ARG:NH1	1:A:2066:THR:O	2.27	0.66
1:A:554:CYS:N	1:A:560:CYS:SG	2.66	0.66
1:A:1994:GLU:O	1:A:1998:GLN:NE2	2.29	0.66
1:A:337:MET:HE1	1:A:365:VAL:HG21	1.78	0.65
1:A:707:PRO:HG2	1:A:759:GLU:HA	1.78	0.65
1:A:2558:ILE:HG12	1:A:2573:VAL:HG22	1.78	0.65
1:A:1850:ARG:NH1	1:A:2734:GLY:O	2.30	0.64
2:B:74:PRO:HG2	2:B:81:LEU:HD23	1.79	0.64
1:A:1867:VAL:HG12	1:A:1869:ASN:H	1.61	0.64
2:B:345:ASN:ND2	2:B:382:GLN:OE1	2.30	0.63
2:C:181:ASN:HD21	2:C:189:GLN:HB3	1.63	0.63
2:C:345:ASN:ND2	2:C:382:GLN:OE1	2.30	0.63
1:A:1385:TRP:CD1	1:A:1468:HIS:HB2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:LYS:HB2	1:A:670:VAL:HB	1.81	0.62
1:A:339:TYR:HB2	1:A:2200:PRO:HG2	1.82	0.62
1:A:433:ILE:HB	1:A:445:LYS:HB2	1.82	0.62
1:A:538:VAL:HB	1:A:578:HIS:HB3	1.82	0.62
1:A:2306:LEU:HD12	1:A:2310:THR:HG21	1.80	0.62
1:A:2585:TYR:HE2	1:A:2600:MET:HE2	1.64	0.62
2:B:156:LYS:HE3	2:C:155:MET:HE1	1.83	0.61
1:A:293:ASN:ND2	1:A:297:ASP:O	2.31	0.61
2:B:143:HIS:O	2:B:147:GLN:NE2	2.34	0.61
1:A:957:ASP:OD1	1:A:958:THR:N	2.34	0.60
1:A:279:ARG:HD3	1:A:2672:LEU:HD12	1.83	0.60
1:A:1648:THR:HG22	1:A:1649:GLU:H	1.67	0.60
1:A:2562:TYR:HD1	1:A:2568:ARG:HA	1.67	0.60
1:A:2282:ASP:HB3	1:A:2291:LYS:HB2	1.81	0.60
2:B:347:LEU:HD13	2:B:352:GLN:HB3	1.83	0.60
1:A:1219:ARG:NH1	1:A:1733:ASP:OD1	2.35	0.60
1:A:1271:SER:H	1:A:1280:THR:HG22	1.67	0.59
1:A:21:PRO:HD2	1:A:24:ASN:ND2	2.17	0.59
1:A:1817:ARG:NH2	1:A:1823:GLU:OE2	2.33	0.59
1:A:839:LEU:HD11	1:A:903:LEU:HD11	1.83	0.59
1:A:1853:VAL:HB	1:A:1862:ALA:HB3	1.83	0.59
2:B:232:VAL:HG22	2:B:244:LEU:HD13	1.83	0.59
1:A:613:VAL:HG13	1:A:628:VAL:HG22	1.85	0.59
1:A:1948:ILE:HB	1:A:1957:PHE:HB2	1.85	0.58
2:C:272:ARG:NH2	2:C:321:GLN:OE1	2.36	0.58
1:A:1122:TYR:OH	1:A:1142:SER:HB3	2.02	0.58
1:A:1207:THR:HG22	1:A:1208:LYS:HG3	1.85	0.58
1:A:1317:LEU:HD11	1:A:1323:VAL:HG11	1.86	0.57
1:A:2628:ARG:NH1	1:A:2673:ASP:O	2.37	0.57
2:C:194:TYR:HE1	2:C:203:ILE:HG21	1.69	0.57
2:C:214:VAL:HG22	2:C:224:ARG:HD2	1.86	0.57
1:A:1890:LEU:HD12	1:A:1907:PHE:HZ	1.69	0.57
1:A:2318:ILE:HG23	1:A:2322:LYS:HB3	1.86	0.57
2:B:272:ARG:NH2	2:B:321:GLN:OE1	2.38	0.57
1:A:1601:ARG:NE	1:A:1642:GLU:OE2	2.36	0.57
1:A:1008:ILE:O	1:A:1018:LYS:NZ	2.35	0.57
1:A:699:LEU:HG	1:A:715:LYS:HE3	1.87	0.56
1:A:1569:ILE:HG22	1:A:1574:VAL:HG13	1.87	0.56
1:A:2337:THR:HG23	1:A:2351:GLY:HA2	1.87	0.56
1:A:312:LEU:HB3	1:A:328:PHE:HB2	1.87	0.56
1:A:715:LYS:NZ	1:A:717:PHE:O	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:THR:OG1	2:B:79:ASP:OD1	2.20	0.56
1:A:1605:ASN:HB2	1:A:1687:LYS:HB2	1.87	0.56
2:C:285:TYR:HA	2:C:288:LEU:HD12	1.86	0.56
1:A:1573:GLU:HG2	1:A:1689:ALA:HB2	1.88	0.56
2:C:214:VAL:O	2:C:224:ARG:NH2	2.39	0.56
1:A:2072:GLU:HB3	1:A:2080:SER:HB2	1.87	0.55
1:A:278:LEU:HG	1:A:2672:LEU:HD11	1.89	0.55
1:A:835:PRO:HG2	1:A:838:PHE:HB3	1.88	0.55
1:A:1668:PRO:HB2	1:A:1671:ARG:HB3	1.88	0.55
1:A:562:GLU:HA	1:A:1072:ASP:HA	1.87	0.55
1:A:776:VAL:HB	1:A:788:GLU:HB3	1.88	0.55
1:A:2627:VAL:HG22	1:A:2632:LEU:HD12	1.89	0.55
1:A:1904:THR:HG21	2:B:146:GLN:HG3	1.89	0.55
1:A:581:SER:HB3	1:A:585:ALA:HB3	1.88	0.54
1:A:1712:GLN:NE2	1:A:1726:GLU:OE1	2.40	0.54
1:A:1823:GLU:HB2	1:A:1841:ILE:HD13	1.88	0.54
2:B:237:SER:O	2:B:241:ARG:NE	2.33	0.54
1:A:229:GLU:O	1:A:283:ARG:NH2	2.41	0.54
2:B:245:TYR:O	2:B:267:TYR:OH	2.23	0.54
1:A:1136:ALA:C	1:A:1138:ARG:N	2.61	0.54
1:A:2636:ILE:HB	1:A:2645:LEU:HB2	1.89	0.54
2:C:178:LEU:HD11	2:C:206:LEU:HD21	1.90	0.54
1:A:620:GLN:HG3	1:A:622:LYS:HG3	1.90	0.54
1:A:2574:ARG:NH1	1:A:2578:GLY:O	2.40	0.54
2:B:91:GLN:HB2	5:B:501:NAG:H2	1.90	0.54
1:A:1410:ASN:ND2	1:A:1413:ASN:OD1	2.40	0.54
1:A:89:LYS:NZ	1:A:96:TYR:OH	2.33	0.54
2:B:350:PRO:HB3	2:B:390:ILE:HG12	1.89	0.54
1:A:137:ILE:HB	1:A:152:ALA:HB3	1.91	0.53
1:A:997:LEU:HB3	1:A:1029:PHE:HE1	1.73	0.53
1:A:2097:ASP:HB2	1:A:2106:SER:HB3	1.91	0.53
1:A:93:PHE:HB3	1:A:109:ALA:HB3	1.91	0.53
1:A:1406:VAL:HG13	1:A:1419:LEU:HB2	1.91	0.52
1:A:117:GLY:O	1:A:123:ASN:ND2	2.36	0.52
1:A:949:VAL:HG21	1:A:1076:TRP:HB2	1.92	0.52
2:B:338:ASP:OD1	2:B:378:LYS:NZ	2.34	0.52
1:A:1071:PHE:HB2	1:A:1077:GLN:HG3	1.92	0.52
1:A:1680:LEU:HD23	1:A:1682:PRO:HD3	1.91	0.52
1:A:974:HIS:HB3	1:A:987:LYS:HB2	1.91	0.52
1:A:538:VAL:HG11	1:A:542:TRP:CD1	2.45	0.52
1:A:1589:ARG:NH1	1:A:1590:THR:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:GLY:O	2:B:73:GLN:NE2	2.42	0.52
1:A:437:ASN:HB2	1:A:607:LEU:HD21	1.91	0.51
1:A:963:MET:HG3	1:A:971:PHE:HB2	1.92	0.51
2:C:245:TYR:O	2:C:267:TYR:OH	2.27	0.51
2:C:421:HIS:NE2	2:C:425:GLU:OE2	2.43	0.51
1:A:435:LEU:HB2	1:A:443:VAL:HB	1.93	0.51
2:C:347:LEU:HD13	2:C:352:GLN:HB3	1.91	0.51
1:A:2539:ALA:HB3	1:A:2549:GLU:HB3	1.92	0.51
1:A:727:ARG:HH22	1:A:740:LYS:HA	1.76	0.51
1:A:2249:ASP:OD2	1:A:2391:LYS:NZ	2.30	0.51
2:B:125:ARG:O	2:B:129:GLN:HG2	2.10	0.51
1:A:486:VAL:HG23	1:A:495:LEU:HD11	1.93	0.50
1:A:1737:MET:HE1	1:A:1762:VAL:HG21	1.93	0.50
1:A:974:HIS:HB3	1:A:987:LYS:HD2	1.94	0.50
1:A:2274:PRO:HB3	1:A:2296:HIS:NE2	2.27	0.50
2:B:65:LYS:O	2:B:73:GLN:NE2	2.45	0.50
2:C:187:THR:HG21	2:C:230:ARG:HG3	1.94	0.50
1:A:756:HIS:HB2	1:A:763:VAL:HB	1.93	0.49
1:A:98:TRP:O	1:A:99:ASN:ND2	2.45	0.49
1:A:686:ILE:HG21	1:A:1230:VAL:HG21	1.93	0.49
1:A:924:GLN:HG3	1:A:957:ASP:HB3	1.94	0.49
1:A:530:MET:HB3	1:A:537:PHE:HB2	1.95	0.49
1:A:1651:ARG:NH2	1:A:1719:PRO:O	2.46	0.49
1:A:2306:LEU:HB2	1:A:2455:HIS:HB3	1.95	0.49
2:C:354:LEU:HD13	2:C:402:GLN:HB3	1.94	0.49
1:A:865:GLU:O	1:A:867:GLN:NE2	2.37	0.49
1:A:2661:TYR:CD1	1:A:2726:PRO:HG3	2.47	0.49
1:A:1014:ALA:O	1:A:1018:LYS:N	2.39	0.49
1:A:1880:SER:OG	1:A:1885:HIS:N	2.46	0.49
1:A:1913:THR:OG1	1:A:1916:GLU:OE1	2.30	0.49
1:A:284:ARG:HH11	3:J:1:NAG:H81	1.76	0.49
1:A:164:LEU:HA	2:B:48:PHE:HB3	1.93	0.49
2:B:245:TYR:HD2	2:B:277:VAL:HG11	1.77	0.49
1:A:437:ASN:N	1:A:442:SER:OG	2.36	0.48
1:A:714:ASP:N	1:A:714:ASP:OD1	2.45	0.48
2:B:214:VAL:HG13	2:B:224:ARG:HB3	1.95	0.48
1:A:923:GLY:O	1:A:982:TYR:OH	2.31	0.48
1:A:1212:ARG:NH2	1:A:1215:GLN:O	2.46	0.48
1:A:716:GLU:OE2	1:A:742:LYS:NZ	2.43	0.48
2:C:320:ARG:HA	2:C:323:GLN:HB2	1.95	0.48
2:B:406:LEU:HD23	2:B:409:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2402:ILE:HG13	1:A:2404:LYS:H	1.79	0.48
1:A:396:LEU:O	1:A:1354:ARG:NH2	2.46	0.48
2:C:211:VAL:HG12	2:C:251:GLU:HG3	1.96	0.48
1:A:885:LEU:HD13	1:A:895:SER:HB2	1.96	0.48
1:A:1905:ARG:HH21	1:A:1910:GLY:HA2	1.79	0.48
1:A:2036:ILE:O	1:A:2036:ILE:HG13	2.14	0.48
1:A:2311:PHE:O	1:A:2315:ILE:HG22	2.14	0.48
1:A:2487:ARG:HH22	1:A:2489:ARG:HE	1.62	0.48
1:A:916:ILE:HG23	1:A:931:PHE:HD2	1.79	0.48
1:A:1867:VAL:HG13	1:A:2285:ASP:HB2	1.95	0.48
1:A:1052:GLN:HB3	1:A:1065:GLY:HA2	1.95	0.47
1:A:1411:LEU:HD12	1:A:1448:LYS:HB3	1.95	0.47
1:A:2339:ASP:HB2	2:B:125:ARG:HD3	1.96	0.47
2:C:374:LYS:HG2	2:C:378:LYS:HE3	1.95	0.47
1:A:1914:GLN:HA	1:A:1917:ILE:HD12	1.97	0.47
1:A:505:ASP:OD1	1:A:505:ASP:N	2.47	0.47
1:A:962:ASP:OD1	1:A:972:LYS:HG2	2.14	0.47
1:A:1136:ALA:CB	1:A:1174:THR:HG22	2.45	0.47
1:A:41:ARG:NH2	1:A:70:ASN:O	2.46	0.47
1:A:1567:TRP:CZ3	1:A:1576:TYR:HB2	2.49	0.47
1:A:885:LEU:HD11	1:A:899:ARG:HB3	1.96	0.47
1:A:849:MET:SD	1:A:856:ASP:HB2	2.55	0.47
1:A:2274:PRO:HG2	1:A:2277:TYR:CD1	2.49	0.47
1:A:2584:LYS:NZ	1:A:2597:ASP:OD2	2.38	0.47
2:B:262:TYR:HB2	2:B:311:LEU:HB2	1.97	0.47
1:A:1249:ASN:OD1	1:A:1251:LYS:NZ	2.46	0.47
1:A:1399:ASP:H	1:A:1424:VAL:HG12	1.79	0.46
1:A:2157:ASP:N	1:A:2157:ASP:OD1	2.46	0.46
2:B:137:THR:O	2:B:140:GLU:HG2	2.14	0.46
2:C:227:ASN:HA	2:C:230:ARG:HG2	1.98	0.46
1:A:1603:VAL:HG22	1:A:1690:GLU:HB2	1.98	0.46
1:A:2463:SER:OG	1:A:2464:ALA:N	2.48	0.46
2:C:373:HIS:O	2:C:377:VAL:HG23	2.14	0.46
1:A:557:TRP:HB3	1:A:558:PRO:HD3	1.97	0.46
1:A:74:SER:O	1:A:88:ARG:NH1	2.47	0.46
1:A:1384:PHE:HA	1:A:1468:HIS:O	2.16	0.46
1:A:2266:LYS:O	1:A:2270:THR:OG1	2.28	0.46
2:C:89:PHE:HA	2:C:92:VAL:HG12	1.97	0.46
1:A:1169:VAL:HG12	1:A:1171:ALA:H	1.80	0.46
1:A:1377:LYS:NZ	1:A:1445:ASP:OD1	2.36	0.46
1:A:477:ALA:HB2	1:A:558:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:LEU:HD11	1:A:1707:MET:HB2	1.97	0.46
1:A:858:TRP:CE2	1:A:868:LYS:HD3	2.50	0.46
1:A:1303:TRP:HB3	1:A:1307:LYS:HA	1.97	0.46
1:A:570:LEU:HD12	1:A:571:PRO:HD2	1.97	0.46
1:A:910:TYR:OH	1:A:1061:GLY:HA2	2.16	0.45
1:A:2431:ASN:O	1:A:2434:PHE:HB3	2.16	0.45
2:C:347:LEU:O	2:C:353:ARG:NE	2.42	0.45
1:A:1669:ASP:OD1	1:A:1670:SER:N	2.49	0.45
1:A:179:SER:HB3	1:A:197:LEU:HD11	1.98	0.45
1:A:1648:THR:HG22	1:A:1649:GLU:N	2.31	0.45
1:A:1999:ILE:HA	1:A:2002:THR:HG22	1.98	0.45
1:A:270:TYR:CZ	1:A:272:SER:HB2	2.52	0.45
1:A:2048:ASP:HB3	1:A:2054:ILE:HG13	1.98	0.45
2:B:278:TYR:CZ	2:B:282:ARG:HG3	2.51	0.45
2:C:198:PRO:HG3	2:C:203:ILE:HD13	1.97	0.45
2:C:297:LYS:HE2	2:C:330:GLU:HG3	1.98	0.45
1:A:282:ASN:OD1	1:A:283:ARG:N	2.38	0.45
1:A:1409:VAL:HA	1:A:1415:LYS:O	2.17	0.45
1:A:1703:TYR:OH	1:A:1752:PHE:O	2.33	0.45
1:A:2043:GLU:OE1	1:A:2565:ARG:NH2	2.49	0.45
1:A:1760:THR:HG23	1:A:1771:GLY:HA2	1.98	0.45
2:C:214:VAL:HA	2:C:224:ARG:CZ	2.46	0.45
1:A:2477:ASN:HB3	1:A:2492:TYR:HE2	1.82	0.45
1:A:2657:ASP:HB2	1:A:2666:ARG:HB2	1.99	0.45
1:A:2383:LEU:HD12	1:A:2426:PRO:HB3	1.99	0.45
1:A:812:LYS:HG3	1:A:813:THR:HG22	1.99	0.45
1:A:1132:ILE:H	1:A:1132:ILE:HG13	1.52	0.45
1:A:1486:ASP:OD1	1:A:1487:THR:N	2.45	0.45
1:A:1099:PHE:CZ	1:A:1157:LYS:HG2	2.52	0.44
1:A:1212:ARG:HH11	1:A:1218:LEU:HD21	1.82	0.44
1:A:1341:LYS:NZ	1:A:1370:THR:O	2.39	0.44
1:A:1358:TYR:CD2	1:A:1465:ASP:HB3	2.52	0.44
1:A:2065:ARG:NH2	1:A:2085:MET:O	2.50	0.44
1:A:849:MET:HE1	1:A:858:TRP:CD1	2.52	0.44
1:A:1113:TYR:HE1	1:A:1120:VAL:HG22	1.82	0.44
1:A:1310:LYS:HD2	1:A:1313:ASP:HB2	1.99	0.44
1:A:1986:GLU:HB2	1:A:2012:ILE:HG22	1.98	0.44
2:B:387:GLU:HG3	2:B:403:LEU:HD21	1.99	0.44
1:A:697:VAL:HG11	1:A:1190:VAL:HG23	1.99	0.44
1:A:578:HIS:CD2	1:A:580:GLU:HB2	2.53	0.44
1:A:171:GLU:HG3	1:A:173:ALA:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:GLU:HB3	1:A:1208:LYS:HB2	1.99	0.44
1:A:721:ARG:NE	1:A:746:GLY:O	2.51	0.44
1:A:810:ASP:N	1:A:810:ASP:OD1	2.50	0.44
1:A:1718:ASP:N	1:A:1718:ASP:OD1	2.51	0.44
1:A:2337:THR:OG1	1:A:2350:GLU:O	2.26	0.44
1:A:1244:VAL:HB	1:A:1256:TYR:HB2	2.00	0.44
2:C:331:LEU:HA	2:C:334:TRP:HD1	1.83	0.44
1:A:98:TRP:CZ2	1:A:101:LYS:HA	2.53	0.43
1:A:951:ILE:HD11	1:A:1069:LEU:HD11	2.00	0.43
2:B:145:ALA:O	2:B:149:THR:HG23	2.17	0.43
2:C:214:VAL:HA	2:C:224:ARG:NH1	2.33	0.43
1:A:2213:ASP:OD1	1:A:2213:ASP:N	2.50	0.43
1:A:2579:LYS:HD2	1:A:2579:LYS:HA	1.81	0.43
2:B:54:GLN:HE22	2:C:59:VAL:H	1.65	0.43
1:A:1099:PHE:HZ	1:A:1157:LYS:HG2	1.83	0.43
1:A:1949:TYR:HA	1:A:1955:LEU:HA	1.99	0.43
1:A:162:ARG:NH1	2:B:48:PHE:O	2.52	0.43
1:A:1102:ALA:HB3	1:A:1113:TYR:CE2	2.53	0.43
1:A:793:PHE:CE2	1:A:797:ALA:HB3	2.54	0.43
1:A:1147:LYS:HD3	1:A:1148:GLN:O	2.19	0.43
1:A:1625:PHE:CG	1:A:1637:PRO:HG3	2.53	0.43
1:A:295:ASP:OD2	1:A:314:ARG:NH2	2.52	0.43
1:A:1229:ASP:O	1:A:1239:PHE:HA	2.18	0.43
1:A:72:ASP:OD1	1:A:72:ASP:N	2.50	0.43
1:A:801:VAL:HG12	1:A:806:VAL:HG22	2.00	0.43
1:A:1129:PRO:HA	1:A:1132:ILE:HD11	2.00	0.43
2:C:221:GLN:HA	2:C:224:ARG:HE	1.83	0.43
2:C:91:GLN:O	2:C:94:GLU:HG2	2.19	0.43
2:C:175:ILE:O	2:C:178:LEU:HG	2.19	0.43
1:A:559:LEU:HD12	1:A:912:ASN:HB2	2.00	0.43
1:A:1050:LEU:HD23	1:A:1050:LEU:HA	1.87	0.43
1:A:1575:GLU:HA	1:A:1686:ILE:O	2.19	0.43
2:C:183:ALA:HA	2:C:224:ARG:HD3	1.99	0.43
1:A:697:VAL:HG21	1:A:701:PRO:HB3	2.01	0.42
1:A:1149:LEU:HB3	1:A:1162:GLN:HG3	2.01	0.42
1:A:1990:ASN:HB2	3:G:1:NAG:O5	2.18	0.42
1:A:2333:LYS:HD2	1:A:2333:LYS:HA	1.71	0.42
1:A:183:LEU:HD22	1:A:193:LEU:HD23	2.01	0.42
1:A:503:SER:HB3	1:A:506:CYS:HB2	2.02	0.42
1:A:1197:SER:HA	1:A:1200:LEU:HD13	2.02	0.42
2:C:88:GLN:O	2:C:91:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:323:GLN:NE2	2:C:352:GLN:HA	2.35	0.42
1:A:559:LEU:CD1	1:A:912:ASN:HB2	2.49	0.42
1:A:1978:SER:HB2	1:A:1984:MET:HE3	2.00	0.42
2:B:54:GLN:HE22	2:C:59:VAL:N	2.17	0.42
1:A:1841:ILE:HG23	1:A:1849:ILE:HG23	2.01	0.42
1:A:2034:ARG:HH12	1:A:2543:LEU:HD23	1.83	0.42
1:A:2145:THR:HB	1:A:2154:LYS:HB3	2.02	0.42
1:A:2326:ILE:HD13	1:A:2448:ILE:HD11	2.00	0.42
2:C:143:HIS:HA	2:C:146:GLN:HG2	2.01	0.42
2:C:146:GLN:O	2:C:149:THR:OG1	2.33	0.42
1:A:1406:VAL:HA	1:A:1452:ASN:O	2.19	0.42
1:A:1199:LEU:HD22	1:A:1236:GLY:HA2	2.01	0.42
1:A:1973:VAL:HA	1:A:1987:ALA:O	2.20	0.42
1:A:2060:VAL:HG11	1:A:2063:ILE:HD12	2.01	0.42
2:B:186:GLU:O	2:B:186:GLU:HG2	2.20	0.42
2:C:228:LEU:O	2:C:232:VAL:HG23	2.19	0.42
2:C:387:GLU:OE2	2:C:407:ARG:NH1	2.53	0.42
1:A:407:HIS:CD2	1:A:656:LEU:HD12	2.55	0.41
1:A:1533:VAL:HG12	1:A:1659:HIS:HB2	2.01	0.41
1:A:1383:SER:HB2	1:A:1470:ARG:HG2	2.02	0.41
1:A:2349:ARG:HH12	1:A:2460:LEU:HB2	1.85	0.41
1:A:2377:ILE:O	1:A:2446:PRO:HB3	2.20	0.41
2:C:199:ALA:O	2:C:202:PRO:HD3	2.20	0.41
1:A:221:LYS:HD2	1:A:221:LYS:HA	1.80	0.41
1:A:411:ASP:OD1	1:A:411:ASP:N	2.45	0.41
1:A:1141:GLN:HG2	1:A:1149:LEU:HD11	2.01	0.41
1:A:1343:TRP:HB3	1:A:1367:LEU:HD11	2.02	0.41
1:A:1890:LEU:HD13	1:A:1894:PHE:CE2	2.55	0.41
2:B:110:ASP:OD2	2:B:112:SER:OG	2.34	0.41
1:A:173:ALA:HA	1:A:176:GLN:HG2	2.01	0.41
1:A:522:TYR:O	1:A:526:GLU:N	2.53	0.41
1:A:1157:LYS:HE2	1:A:1157:LYS:HB2	1.79	0.41
1:A:1553:GLU:HB2	1:A:1691:PHE:HB3	2.02	0.41
2:B:228:LEU:O	2:B:232:VAL:HG23	2.20	0.41
2:C:350:PRO:HB3	2:C:390:ILE:HG12	2.03	0.41
1:A:1928:GLU:HB3	1:A:1936:ASP:OD1	2.20	0.41
2:B:202:PRO:HG2	2:B:205:LYS:HB2	2.02	0.41
2:B:315:GLN:HB3	2:B:318:HIS:HB2	2.02	0.41
2:C:267:TYR:O	2:C:271:VAL:HG23	2.20	0.41
1:A:2019:VAL:HG13	1:A:2019:VAL:O	2.20	0.41
1:A:2587:ILE:HB	1:A:2596:MET:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:GLN:NE2	2:B:352:GLN:HA	2.34	0.41
1:A:2522:ASP:OD1	1:A:2523:GLY:N	2.45	0.41
1:A:188:ASP:OD1	1:A:188:ASP:N	2.53	0.41
1:A:888:PHE:CZ	1:A:984:LEU:HB2	2.56	0.41
1:A:340:GLY:HA3	1:A:358:LEU:HD23	2.03	0.41
1:A:503:SER:OG	1:A:504:VAL:N	2.53	0.41
1:A:660:ASP:HB2	1:A:668:LYS:HB3	2.02	0.41
1:A:876:ASN:OD1	1:A:879:THR:OG1	2.37	0.41
1:A:1367:LEU:HB3	1:A:1455:ILE:HG13	2.03	0.41
2:B:210:ILE:O	2:B:214:VAL:HG23	2.20	0.41
1:A:11:GLN:NE2	1:A:370:LYS:HD3	2.36	0.41
1:A:109:ALA:HA	1:A:160:ARG:HD3	2.03	0.41
1:A:2424:ASP:OD1	1:A:2424:ASP:N	2.54	0.41
2:C:89:PHE:O	2:C:92:VAL:HG12	2.21	0.41
1:A:553:VAL:HG11	1:A:570:LEU:HB3	2.02	0.40
1:A:792:ASP:OD1	1:A:792:ASP:N	2.53	0.40
1:A:899:ARG:O	1:A:903:LEU:HB2	2.21	0.40
2:C:313:ALA:HB2	2:C:348:PRO:HG3	2.03	0.40
1:A:1383:SER:OG	1:A:1435:GLU:HG2	2.21	0.40
1:A:1999:ILE:HA	1:A:1999:ILE:HD13	1.96	0.40
1:A:2227:LEU:HD23	1:A:2227:LEU:HA	1.85	0.40
2:B:396:ASP:OD1	2:B:396:ASP:N	2.53	0.40
2:C:245:TYR:HD2	2:C:277:VAL:HG11	1.85	0.40
1:A:62:ARG:HE	1:A:65:PHE:HD1	1.70	0.40
1:A:198:ARG:NH1	1:A:224:LEU:O	2.52	0.40
1:A:1567:TRP:CE2	1:A:1576:TYR:HD1	2.39	0.40
1:A:1181:ARG:HH21	1:A:1191:VAL:HG21	1.87	0.40
1:A:1966:ARG:NH1	1:A:1993:ARG:HH21	2.19	0.40
1:A:2012:ILE:HD11	1:A:2564:VAL:HG12	2.04	0.40
2:C:84:SER:O	2:C:88:GLN:HG2	2.21	0.40
2:C:189:GLN:OE1	2:C:192:SER:OG	2.29	0.40
1:A:437:ASN:H	1:A:442:SER:HG	1.62	0.40
1:A:2377:ILE:HD11	1:A:2426:PRO:HB2	2.04	0.40
2:C:244:LEU:HD23	2:C:244:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	442	SER
1	A	1132	ILE
1	A	1133	GLN
1	A	1134	VAL
1	A	1135	VAL

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Mol	Chain	Res	Type
1	A	1138	ARG

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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 Torsion 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
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.

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	O5-C1-C2	-3.84	105.35	111.29
3	G	1	NAG	C3-C4-C5	3.22	116.07	110.23
3	G	1	NAG	O4-C4-C3	-3.04	103.21	110.38
4	H	3	BMA	C3-C4-C5	2.63	115.00	110.23
4	E	3	BMA	C3-C4-C5	2.58	114.91	110.23
3	D	1	NAG	O5-C1-C2	-2.47	107.46	111.29
4	E	2	NAG	O5-C1-C2	-2.38	107.61	111.29
3	F	1	NAG	O5-C1-C2	-2.36	107.63	111.29
4	E	3	BMA	C2-C3-C4	2.35	114.99	110.86
4	H	3	BMA	C2-C3-C4	2.31	114.92	110.86
3	G	1	NAG	C4-C3-C2	2.12	114.12	111.02
4	E	1	NAG	O5-C1-C2	-2.10	108.03	111.29
3	F	2	NAG	O5-C1-C2	-2.04	108.14	111.29
4	H	2	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

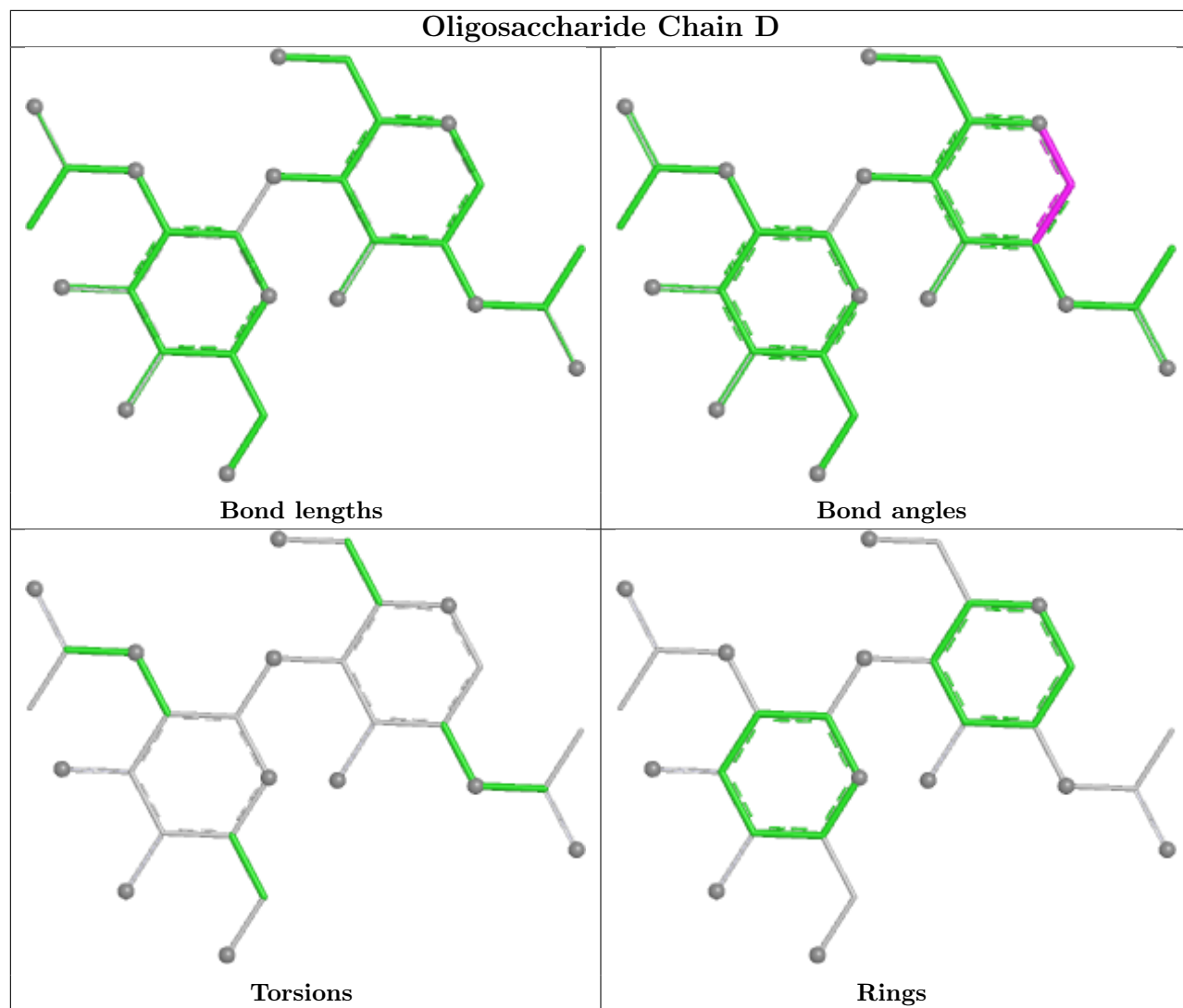
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	J	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C1-C2-N2-C7

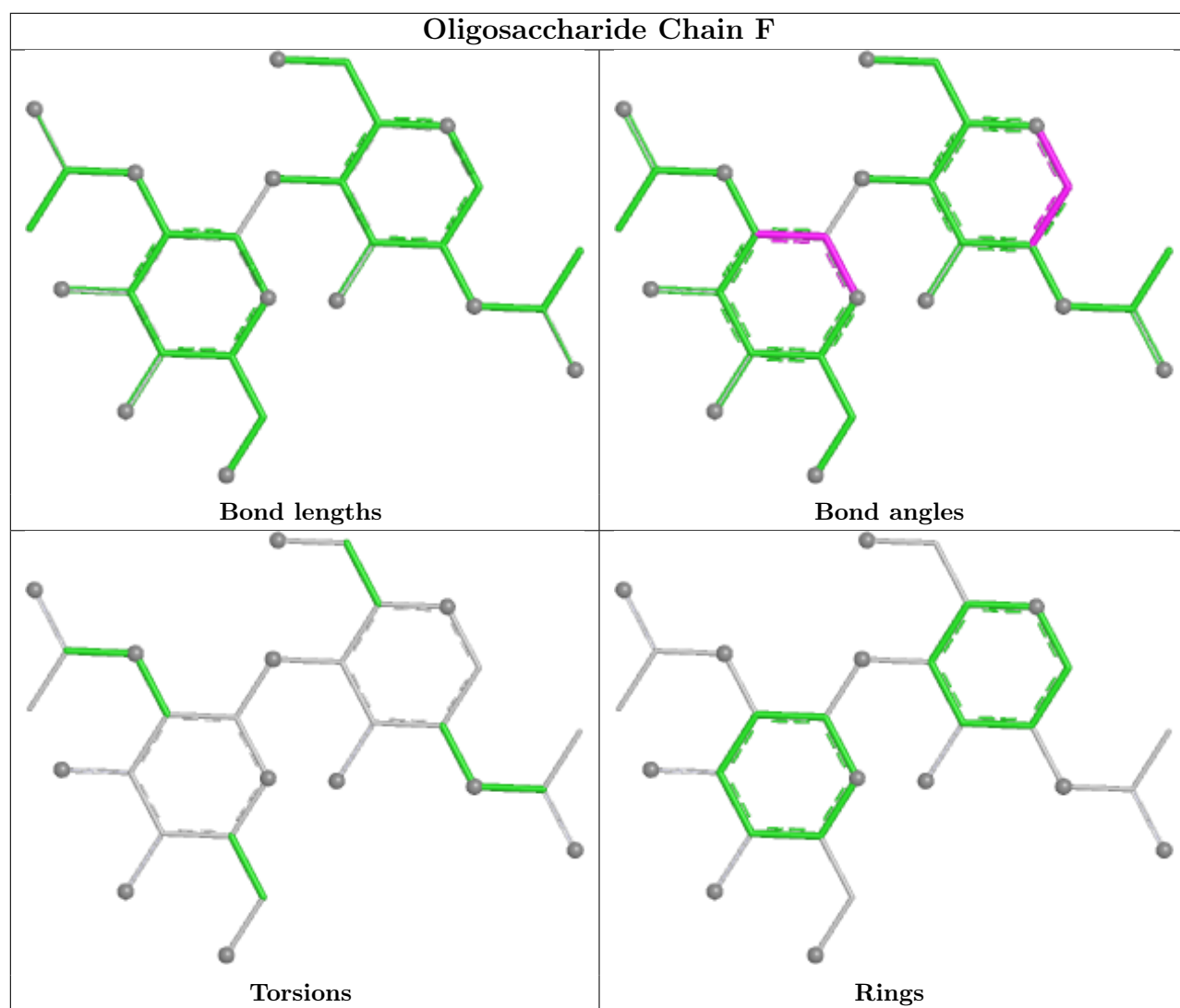
There are no ring outliers.

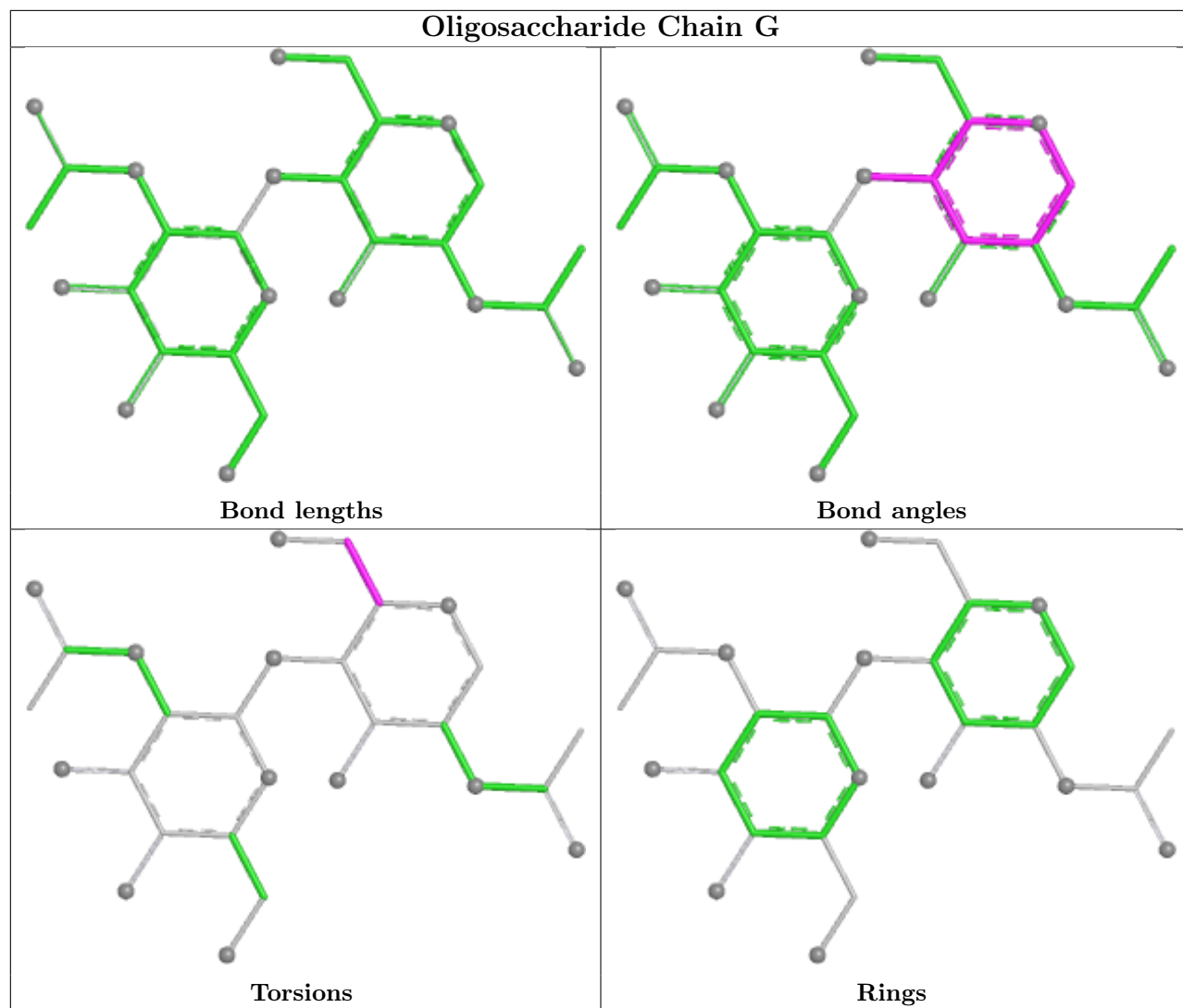
2 monomers are involved in 2 short contacts:

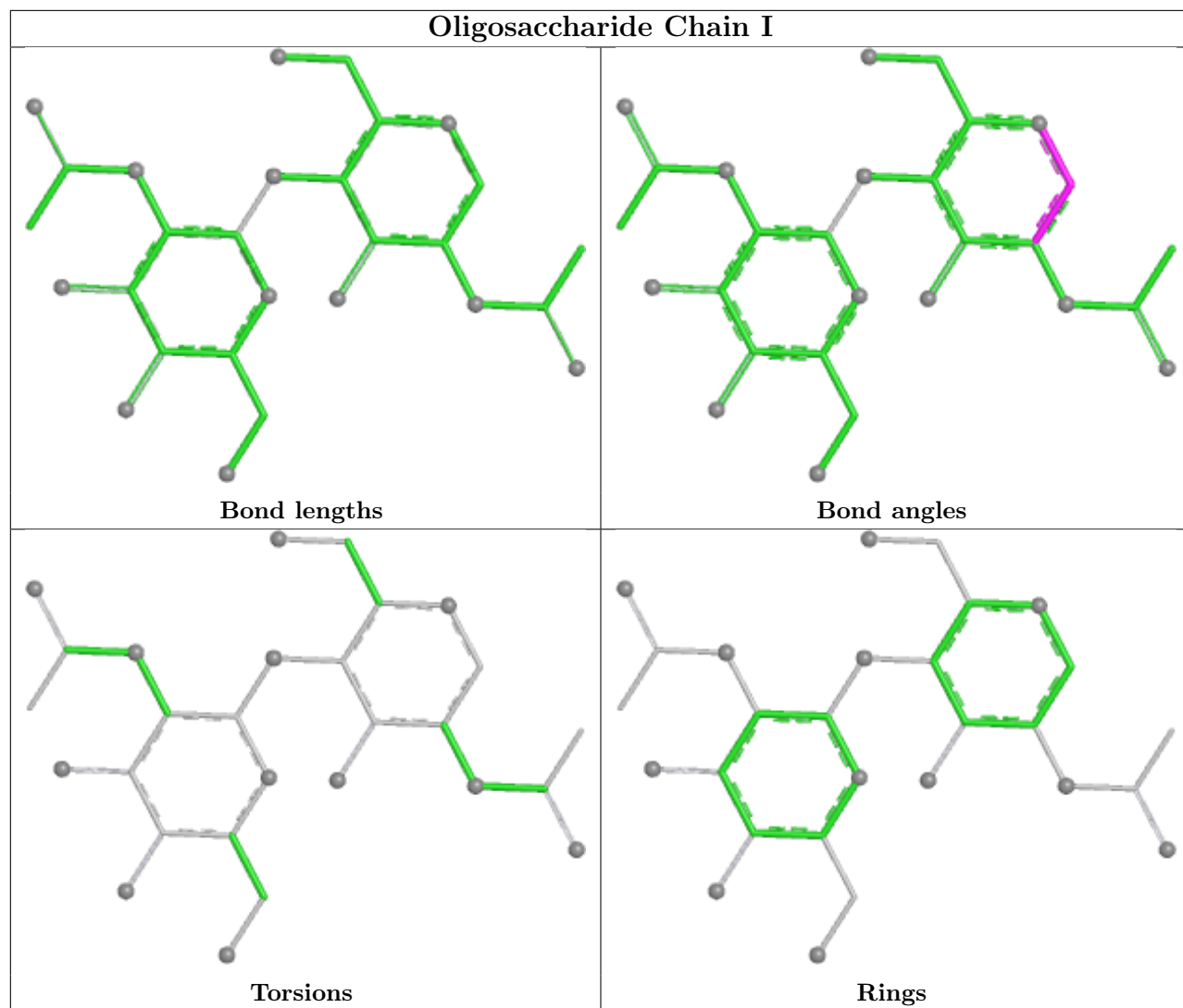
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	J	1	NAG	1	0

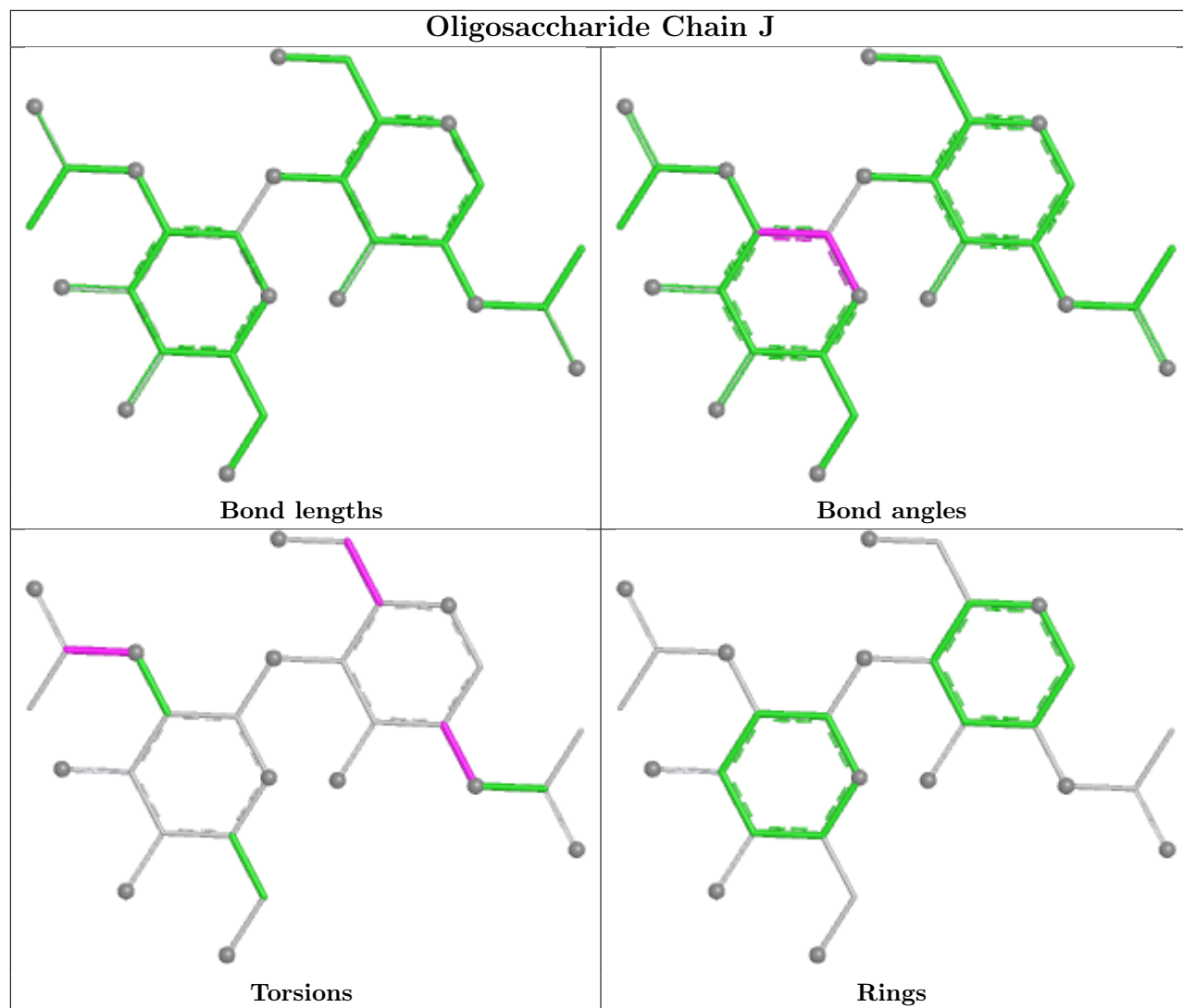
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

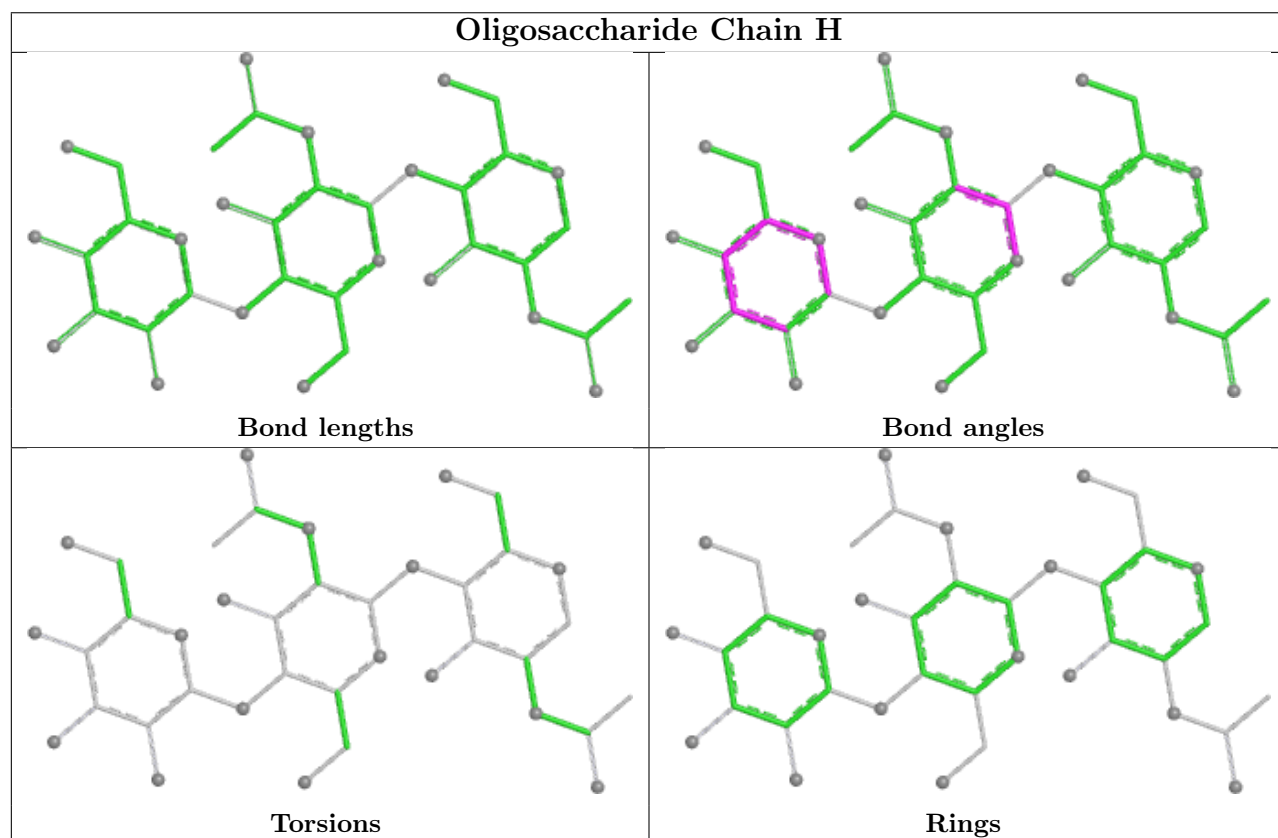
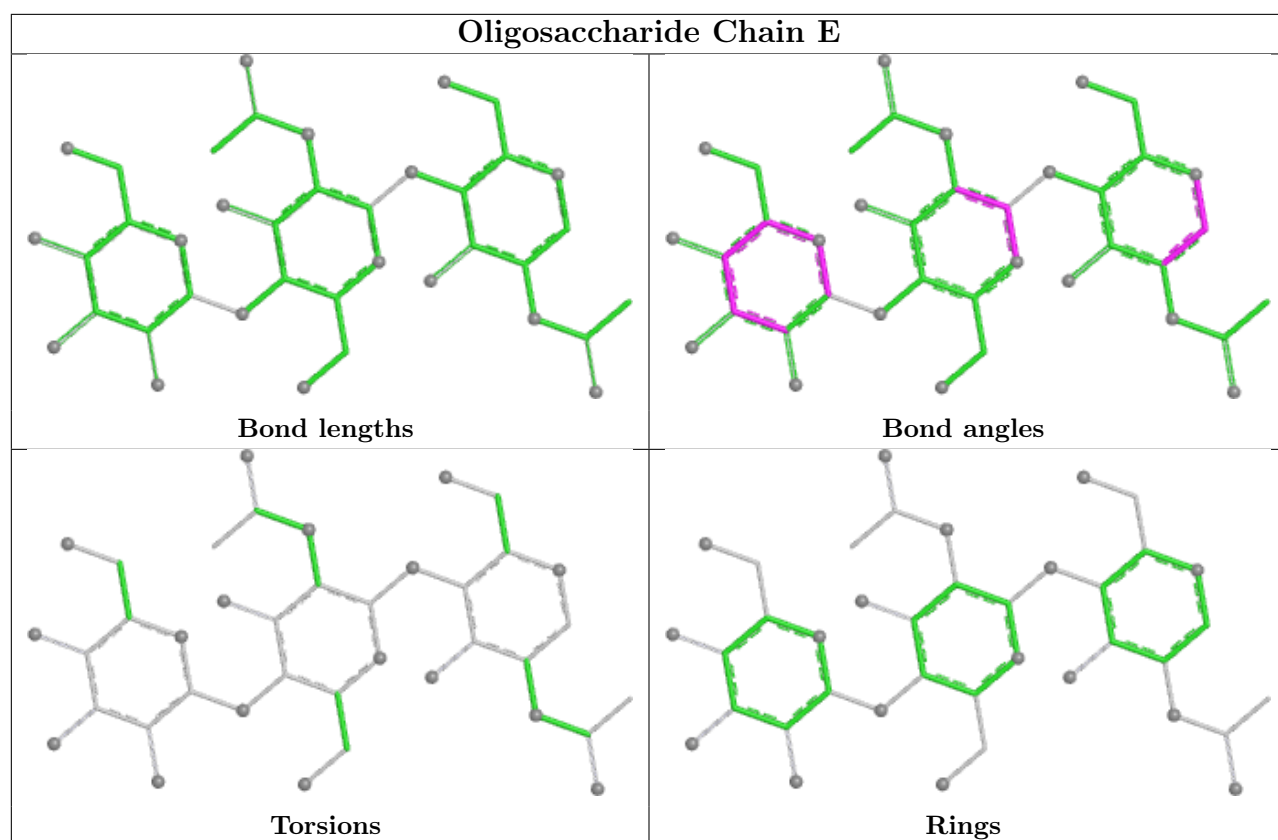












5.6 Ligand geometry

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:

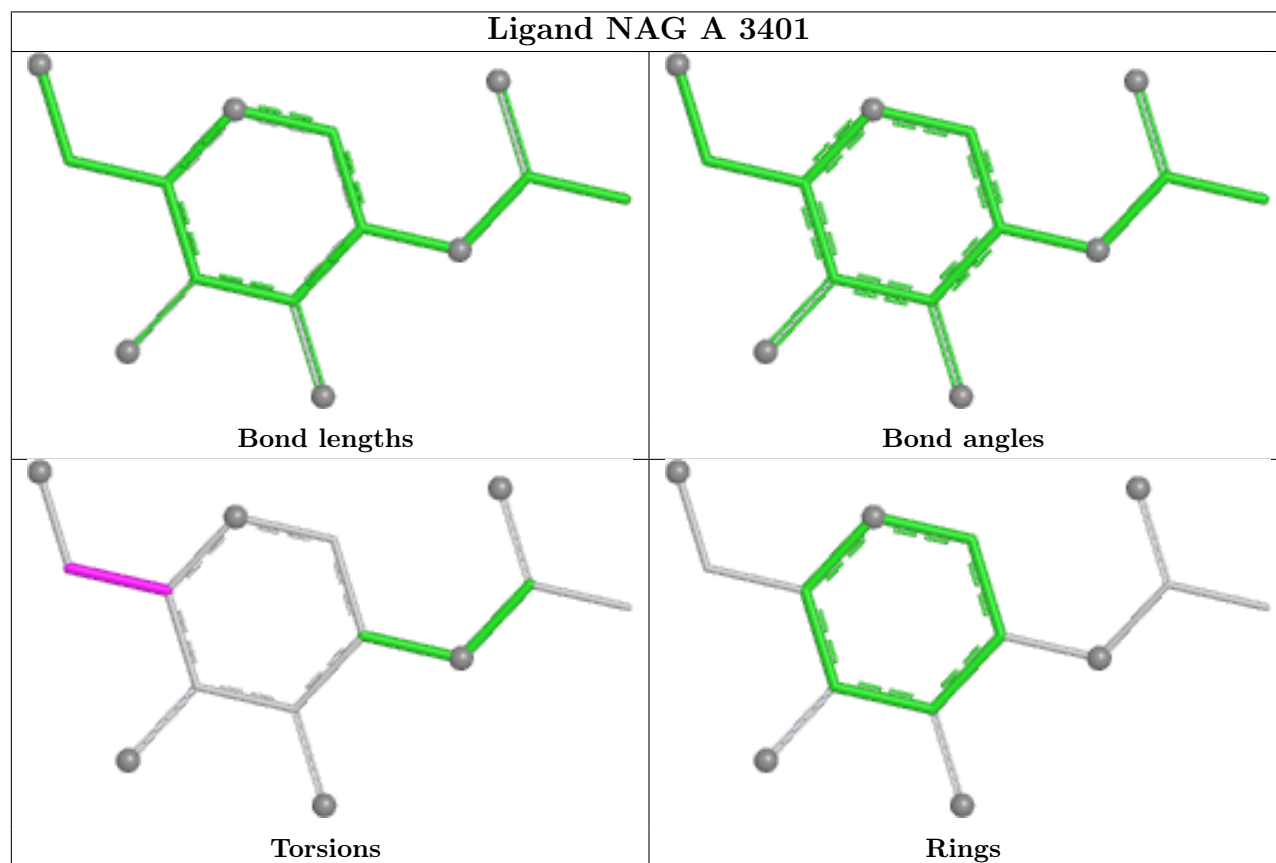
Mol	Chain	Res	Type	Atoms
5	A	3401	NAG	O5-C5-C6-O6
5	A	3402	NAG	O5-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6

There are no ring outliers.

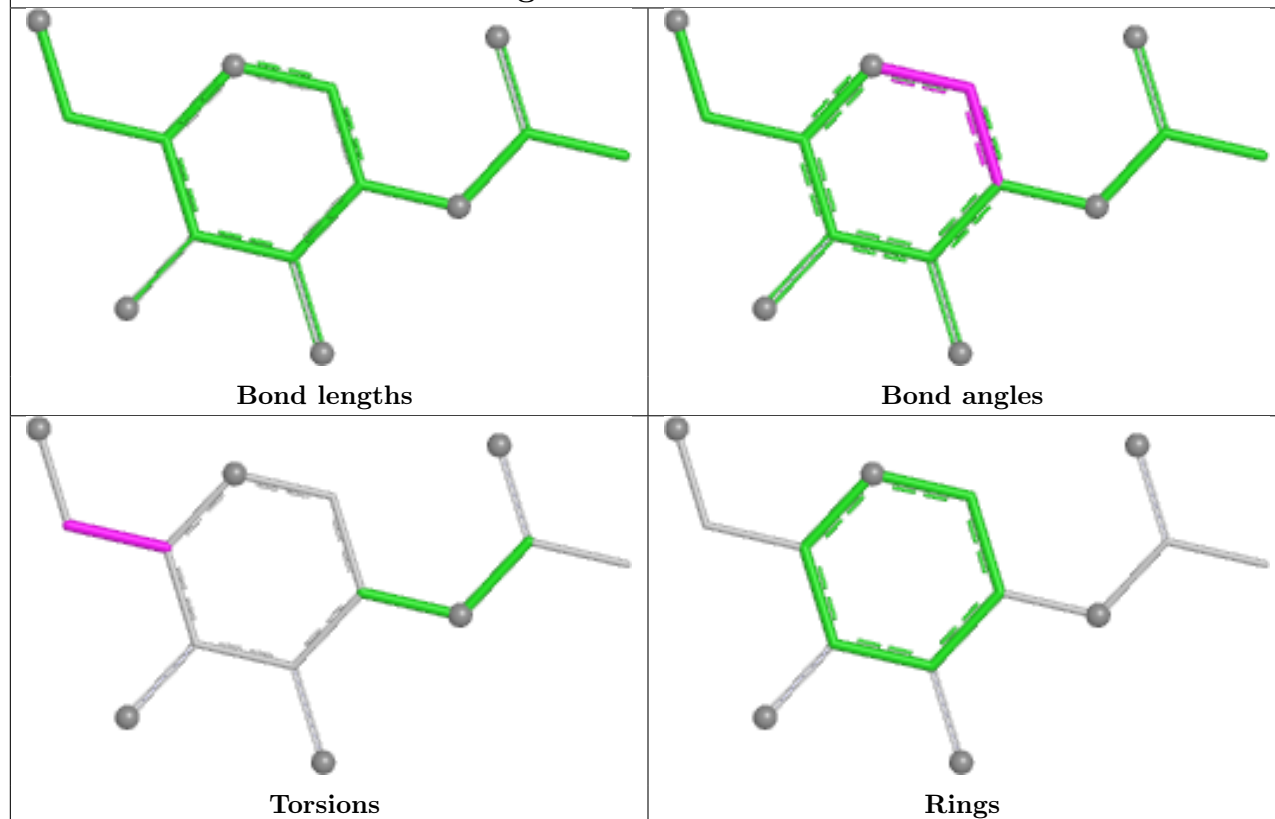
1 monomer is involved in 1 short contact:

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

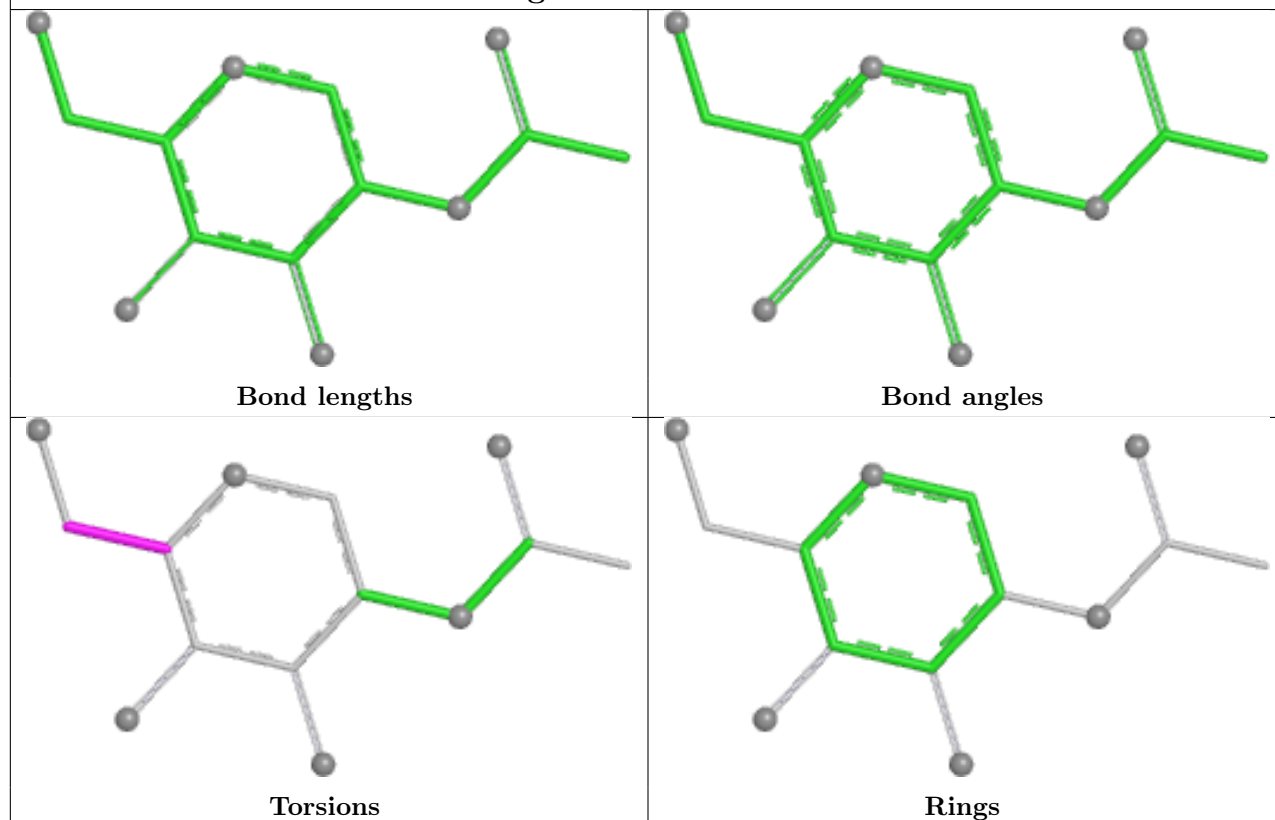
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

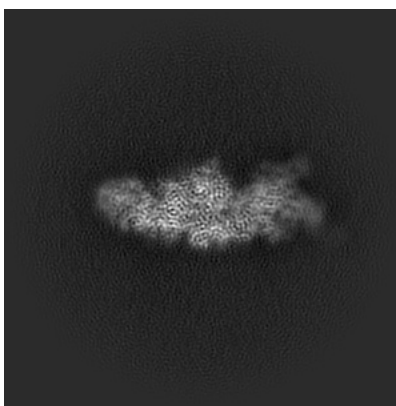
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

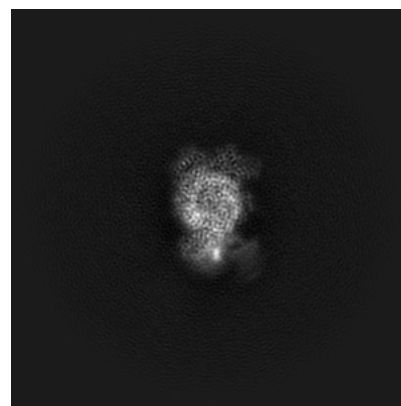
6.1.1 Primary map



X



Y

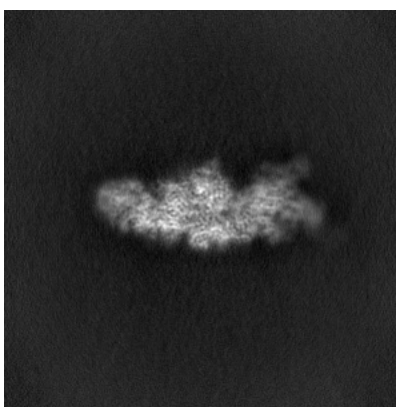


Z

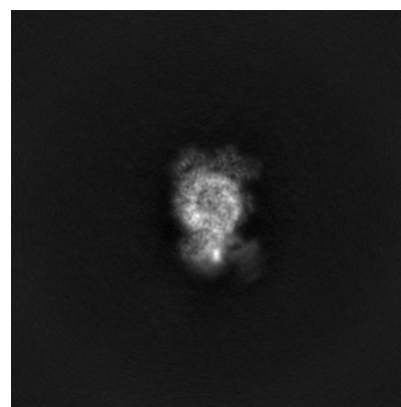
6.1.2 Raw map



X



Y

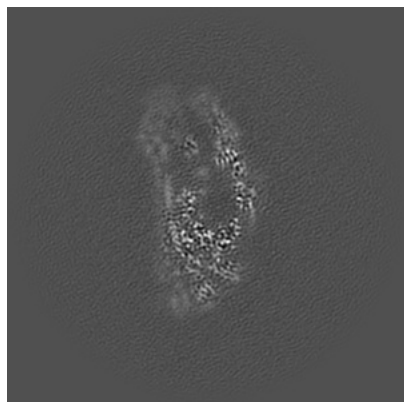


Z

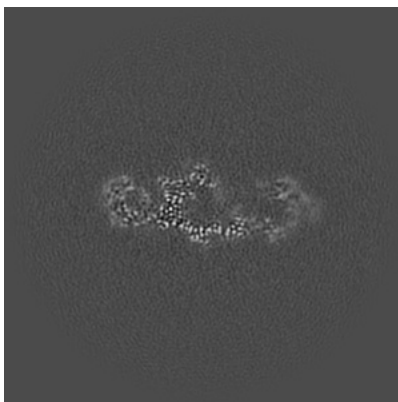
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

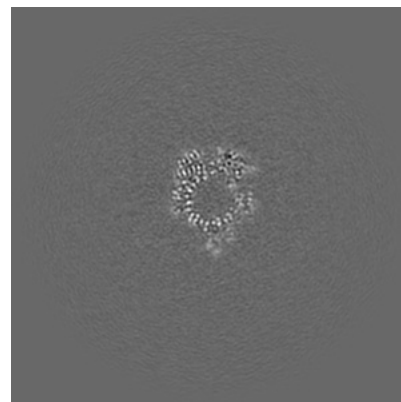
6.2.1 Primary map



X Index: 180

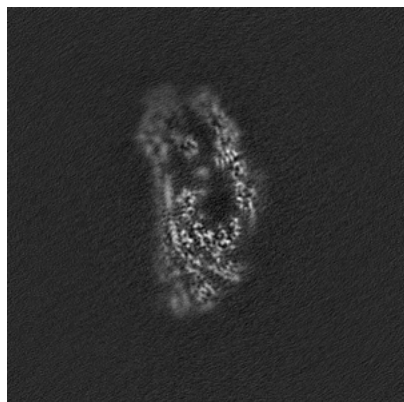


Y Index: 180

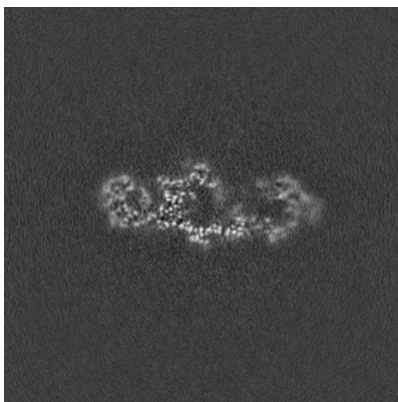


Z Index: 180

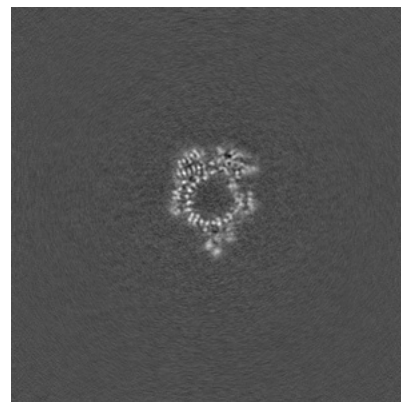
6.2.2 Raw map



X Index: 180



Y Index: 180

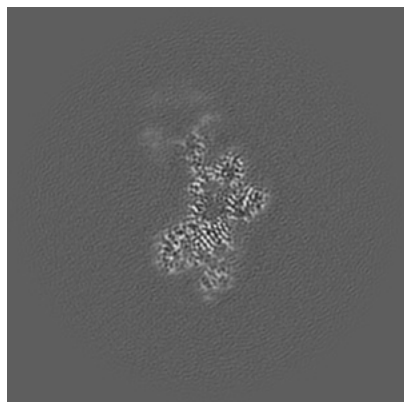


Z Index: 180

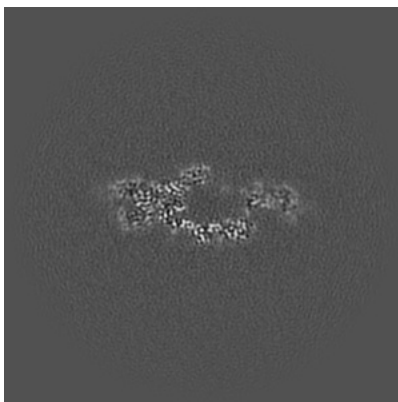
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

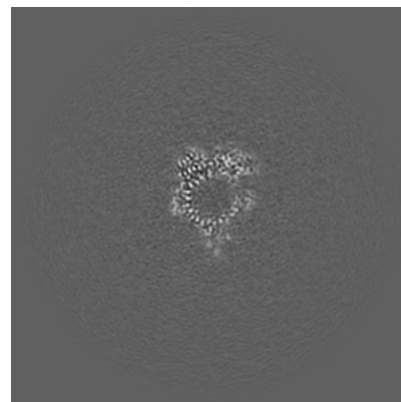
6.3.1 Primary map



X Index: 165

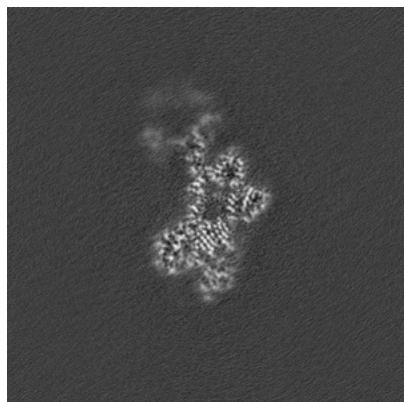


Y Index: 191

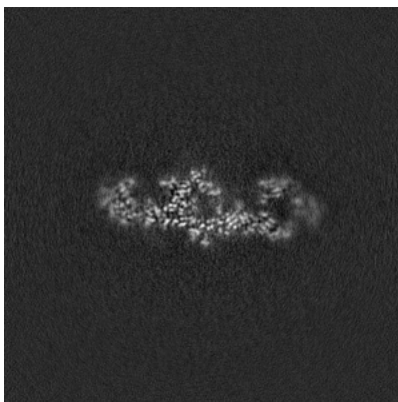


Z Index: 182

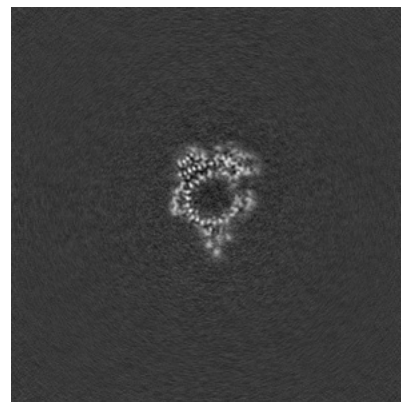
6.3.2 Raw map



X Index: 165



Y Index: 174

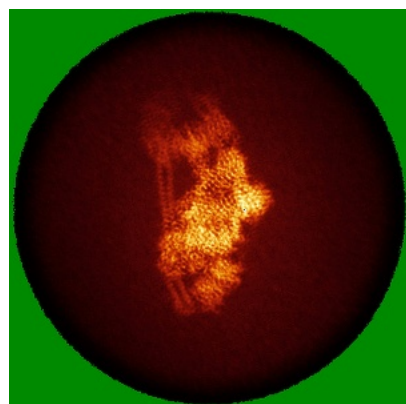


Z Index: 182

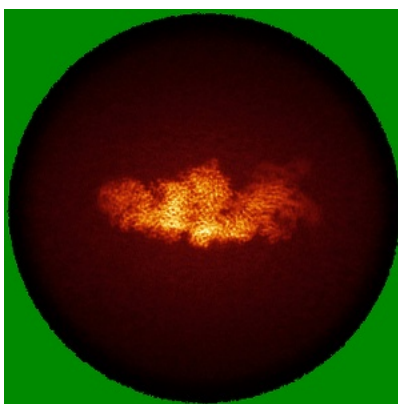
The images above show the largest variance slices of the map in three orthogonal directions.

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

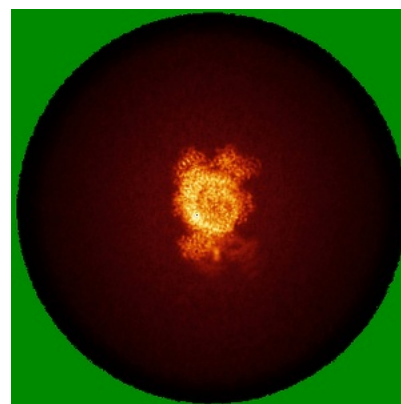
6.4.1 Primary map



X

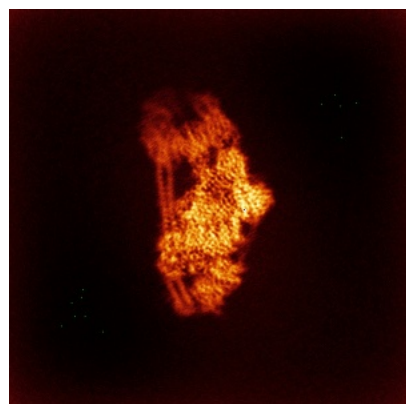


Y

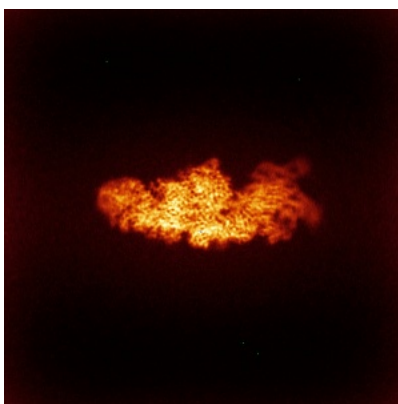


Z

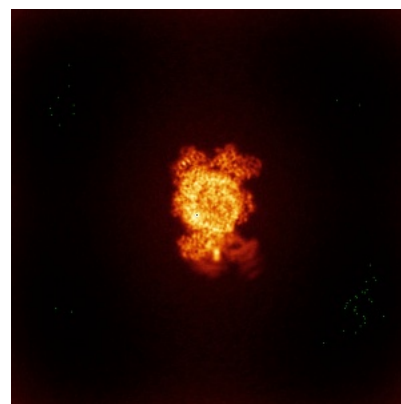
6.4.2 Raw map



X



Y

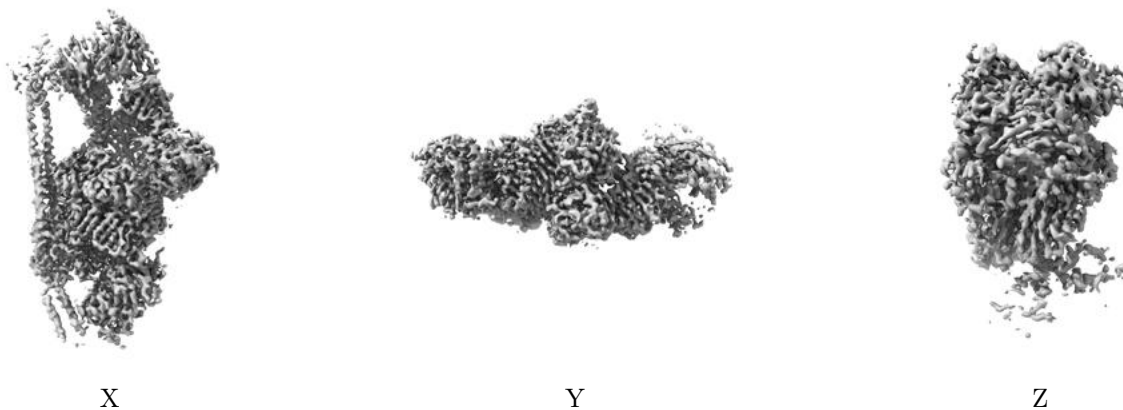


Z

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.

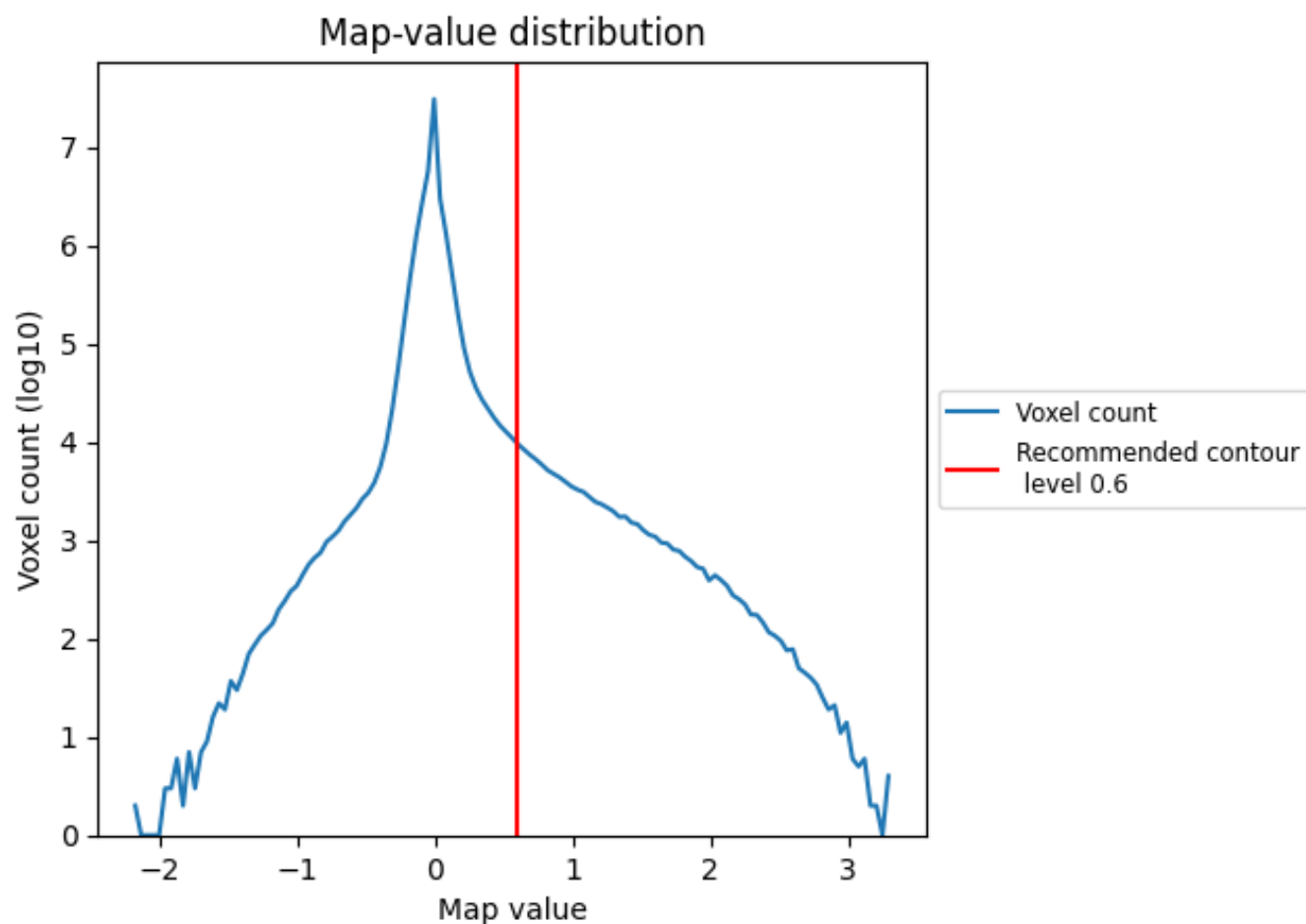
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

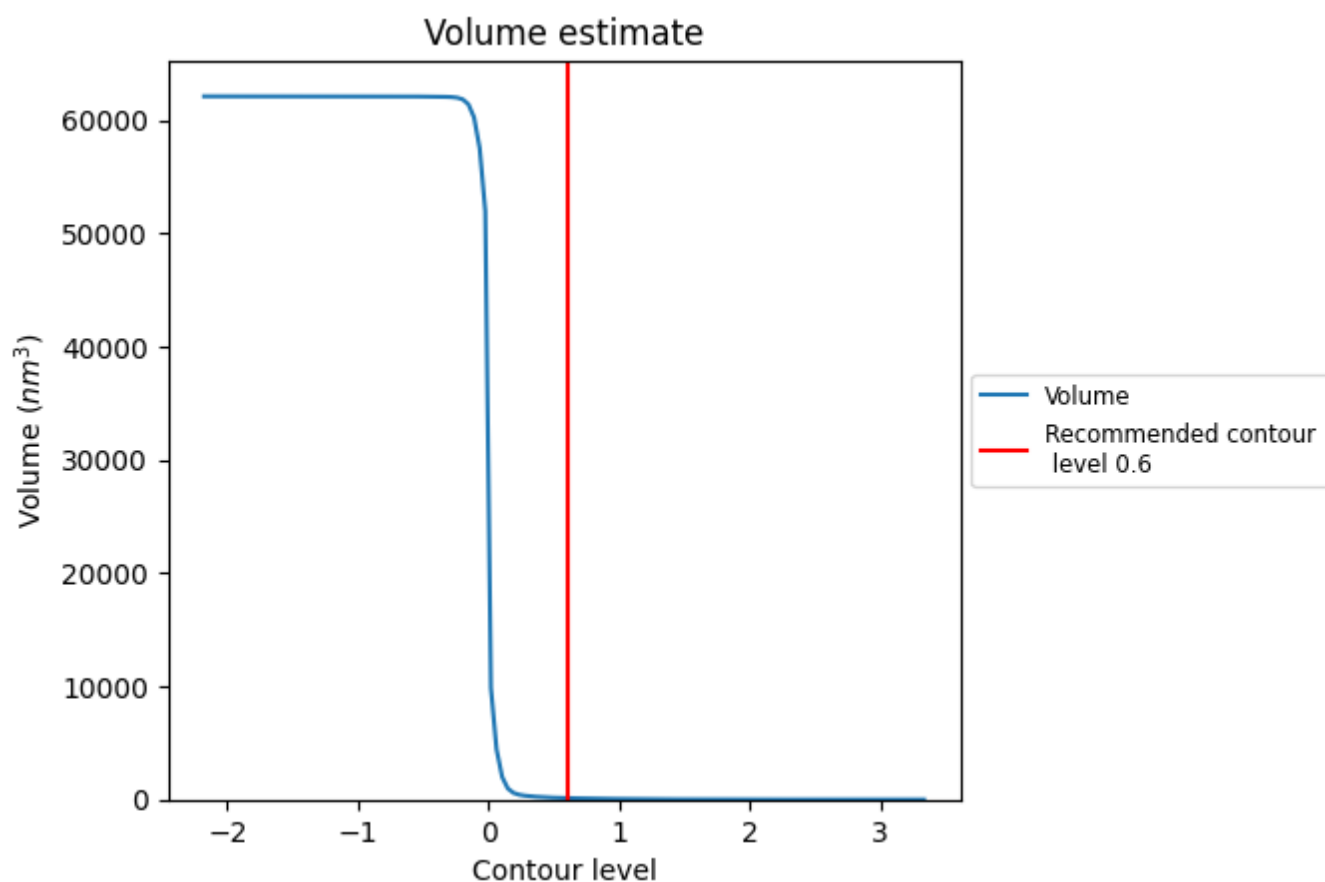
This section contains the results of statistical analysis of the map.

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.

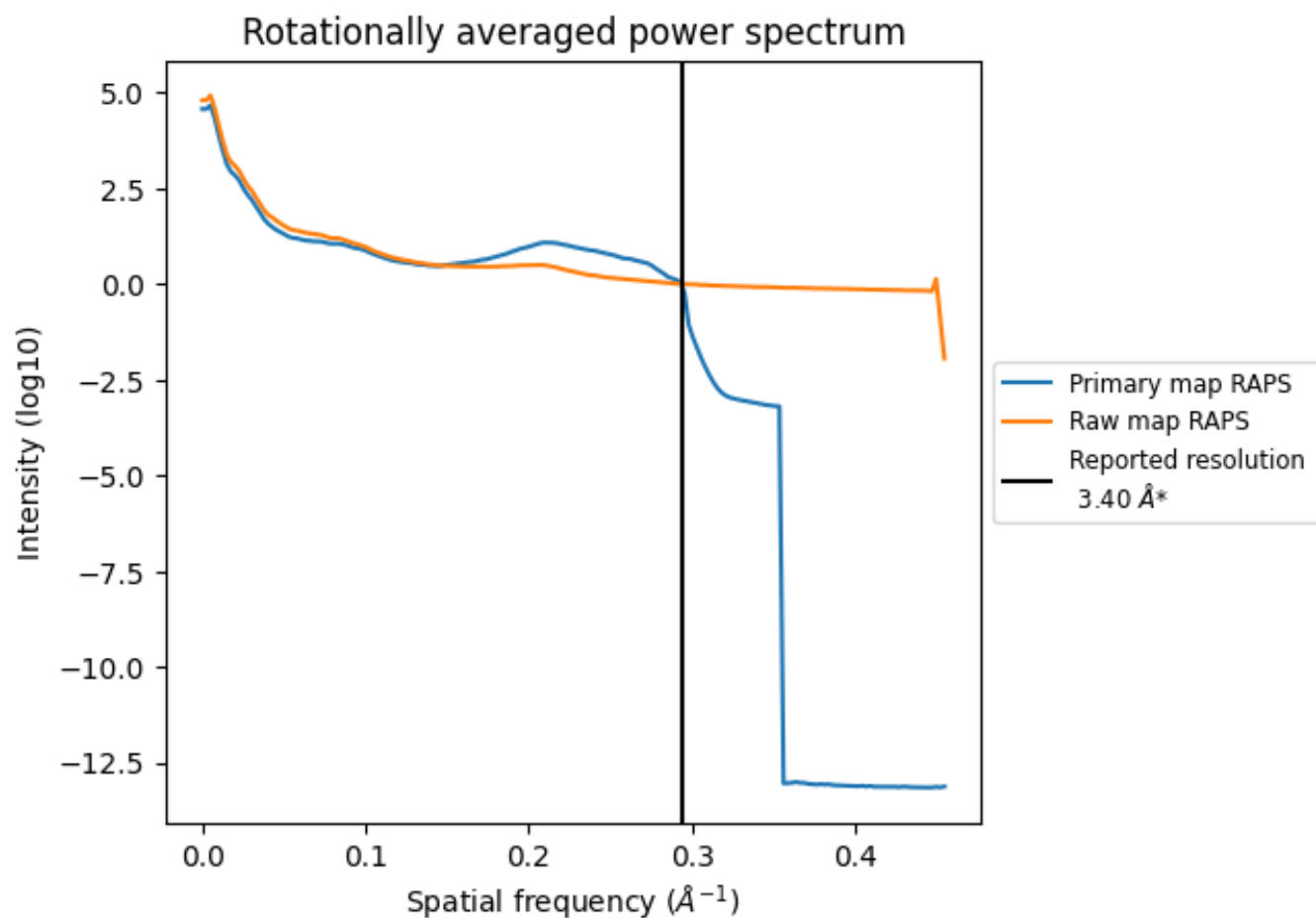
7.2 Volume estimate [i](#)



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 ⓘ

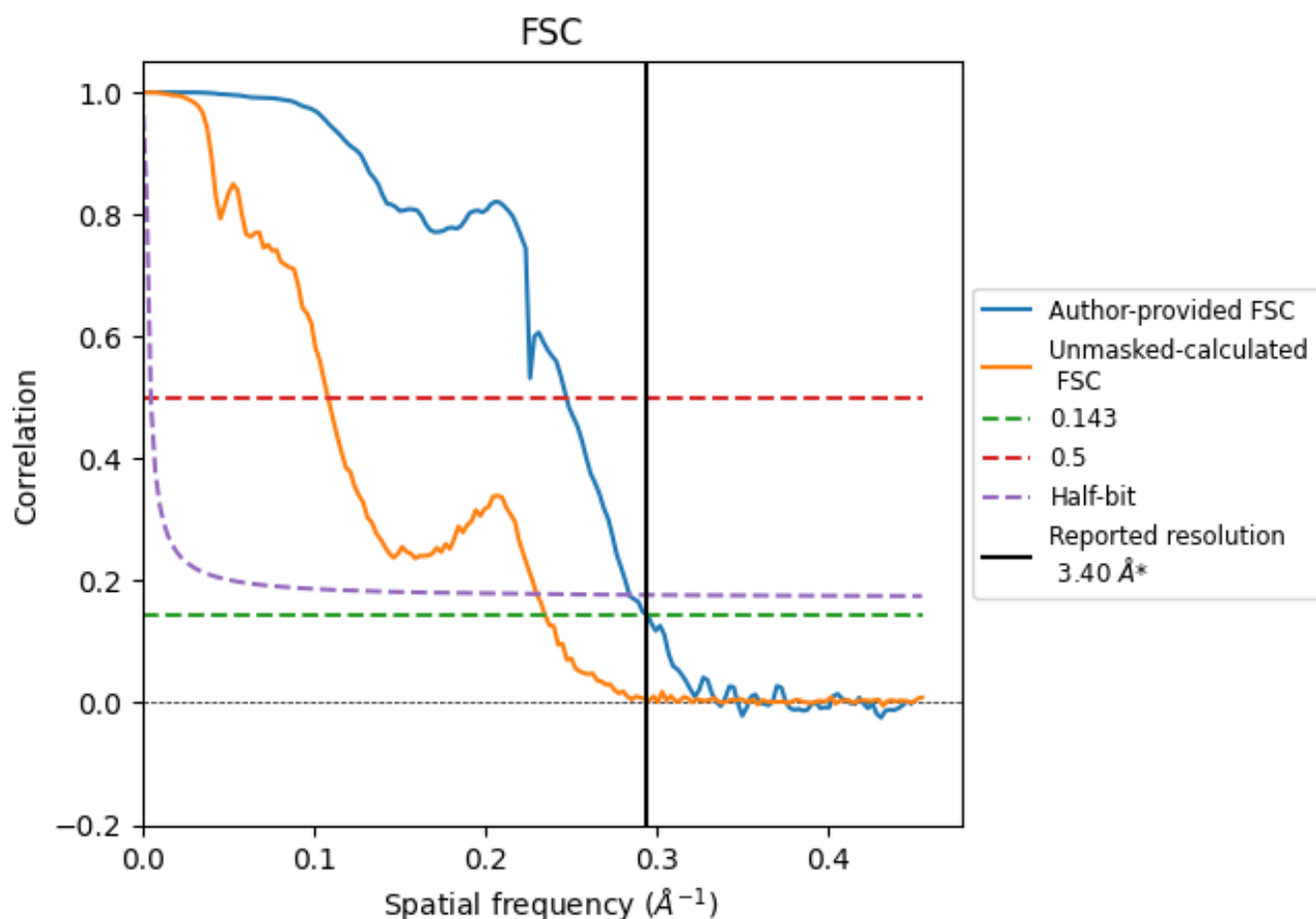


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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](#)

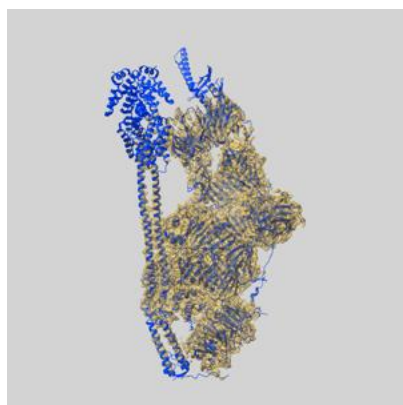
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	4.05	3.52
Unmasked-calculated*	4.26	9.24	4.35

*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 %

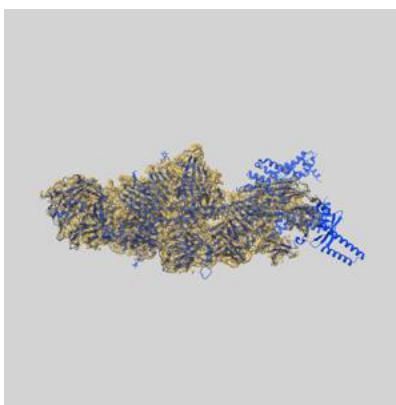
9 Map-model fit [i](#)

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.

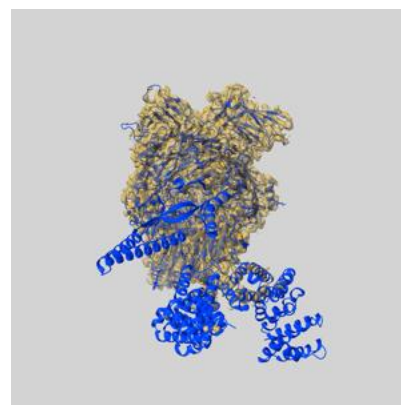
9.1 Map-model overlay [i](#)



X



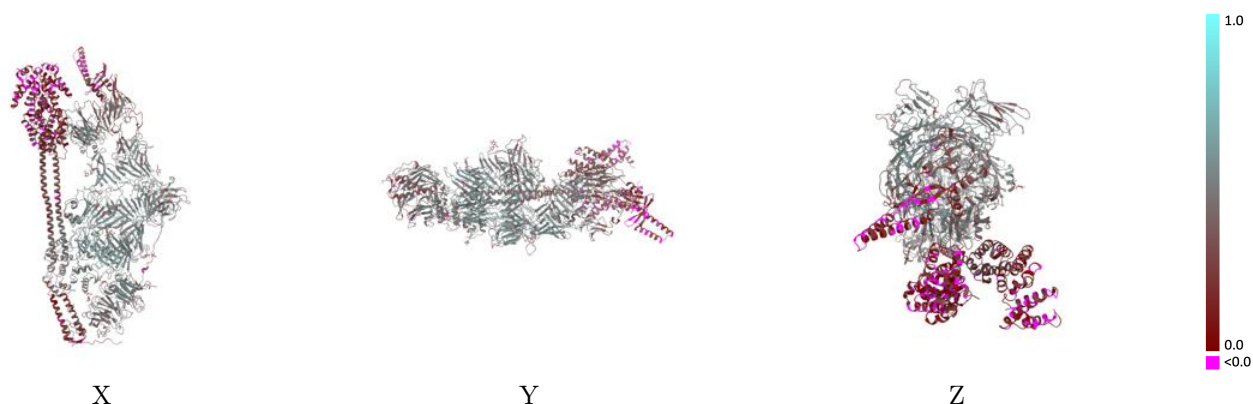
Y



Z

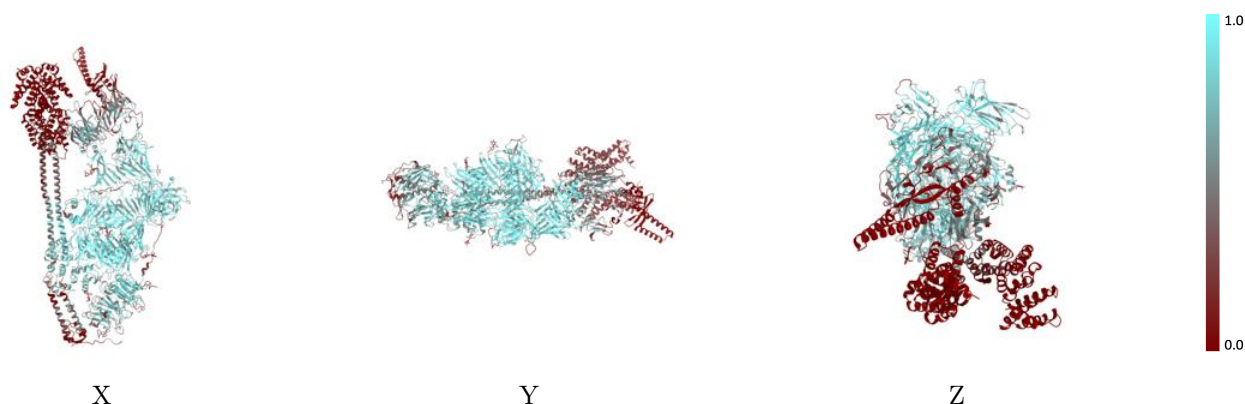
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



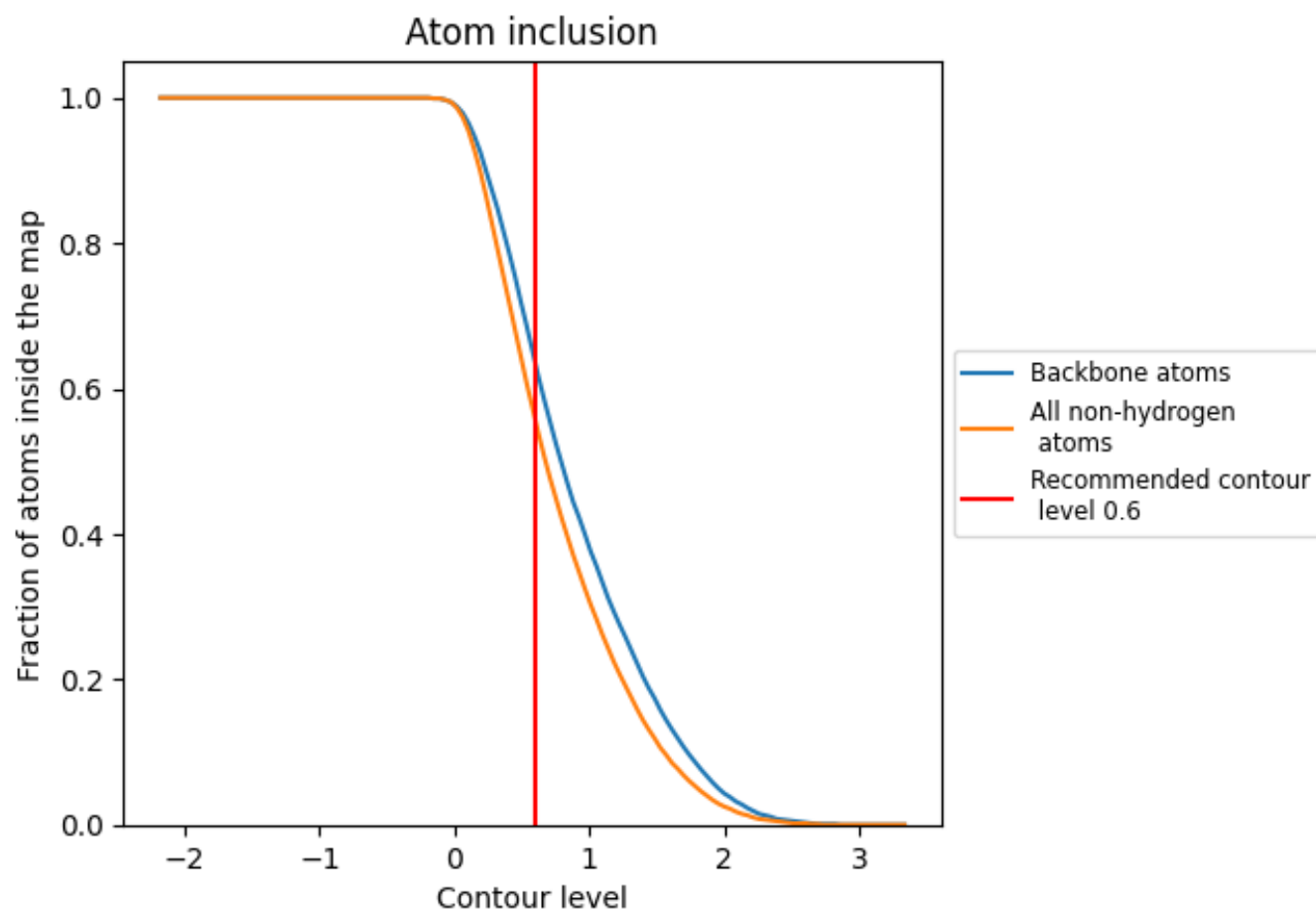
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0

0.0

<0.0