



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 01:59 AM UTC

PDB ID : 7BAN / pdb_00007ban
EMDB ID : EMD-12125
Title : human Teneurin4 Mut C2
Authors : Meijer, D.H.; Janssen, B.J.C.
Deposited on : 2020-12-16
Resolution : 2.70 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

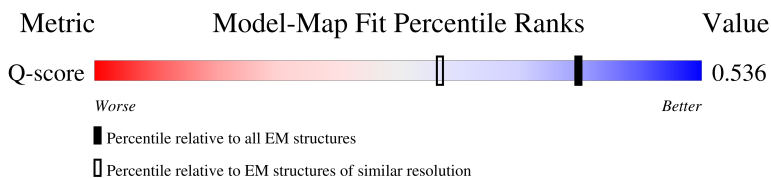
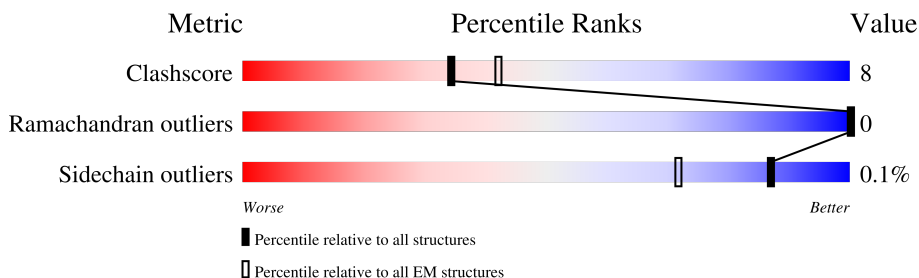
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	1932	21% 79% 20% .
1	B	1932	21% 79% 20% .
2	C	2	100%
2	D	2	100%

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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%
2	J	2	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 30612 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 Teneurin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1904	Total	C	N	O	S	0	0
			15093	9515	2625	2879	74		
1	B	1904	Total	C	N	O	S	0	0
			15093	9515	2625	2879	74		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2585	CYS	SER	engineered mutation	UNP Q6N022
B	2585	CYS	SER	engineered mutation	UNP Q6N022

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



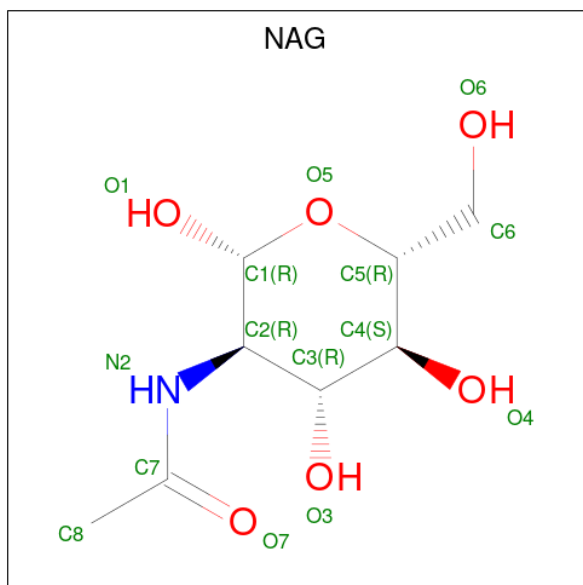
Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 3 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
			Total	C	N	O	
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0

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

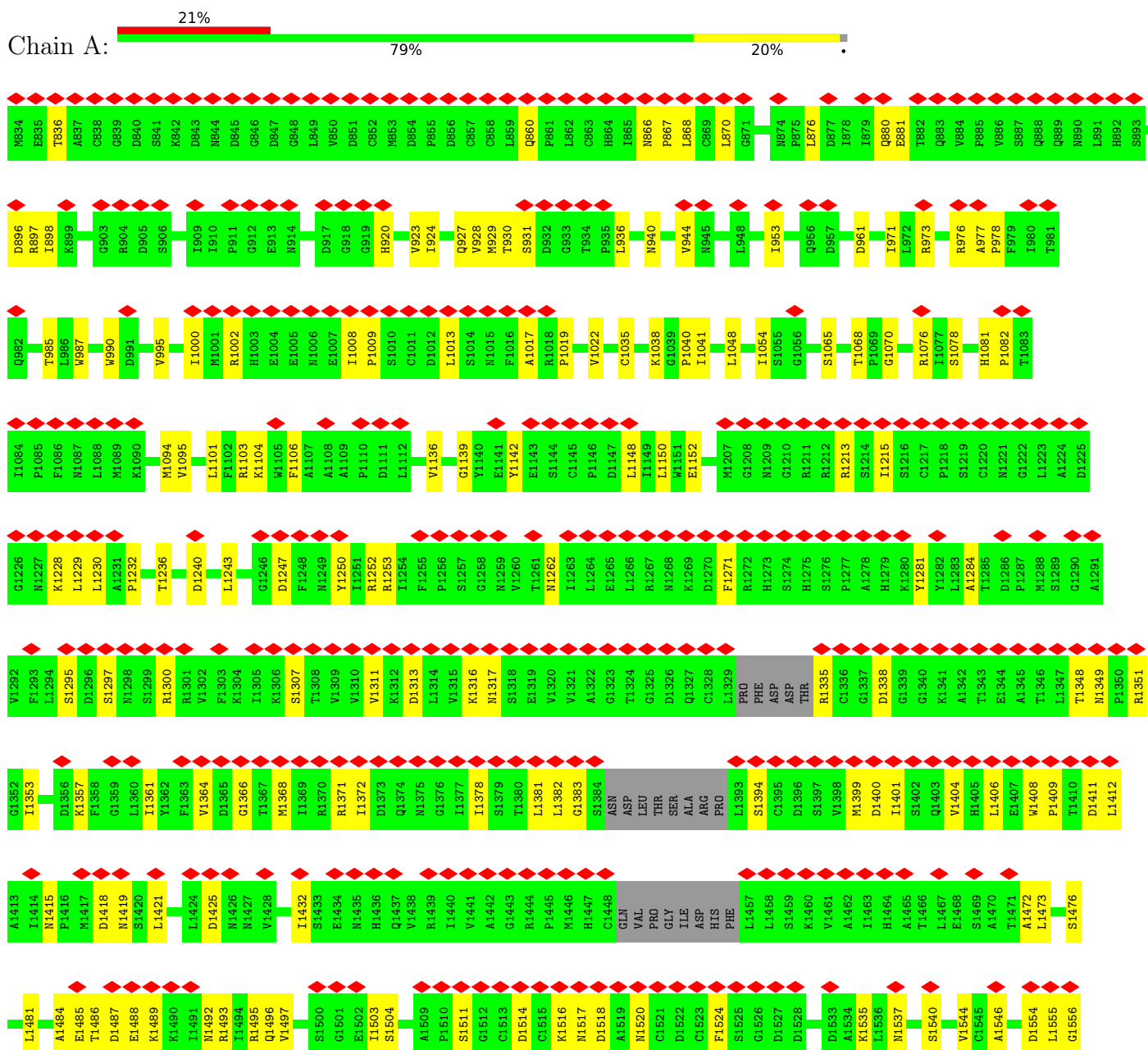
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

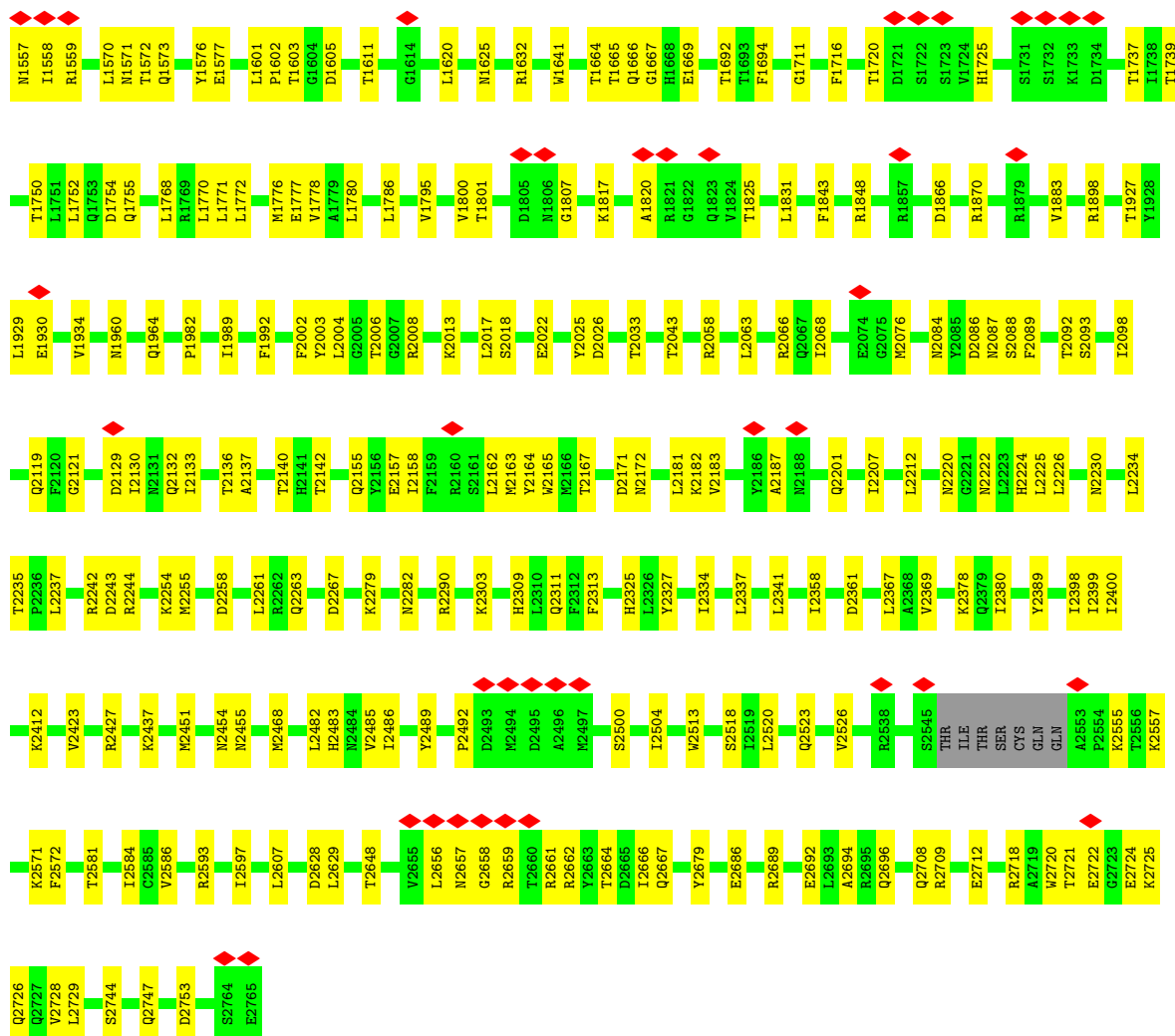
Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	Ca	0
			3	3	
4	B	3	Total	Ca	0
			3	3	

3 Residue-property plots

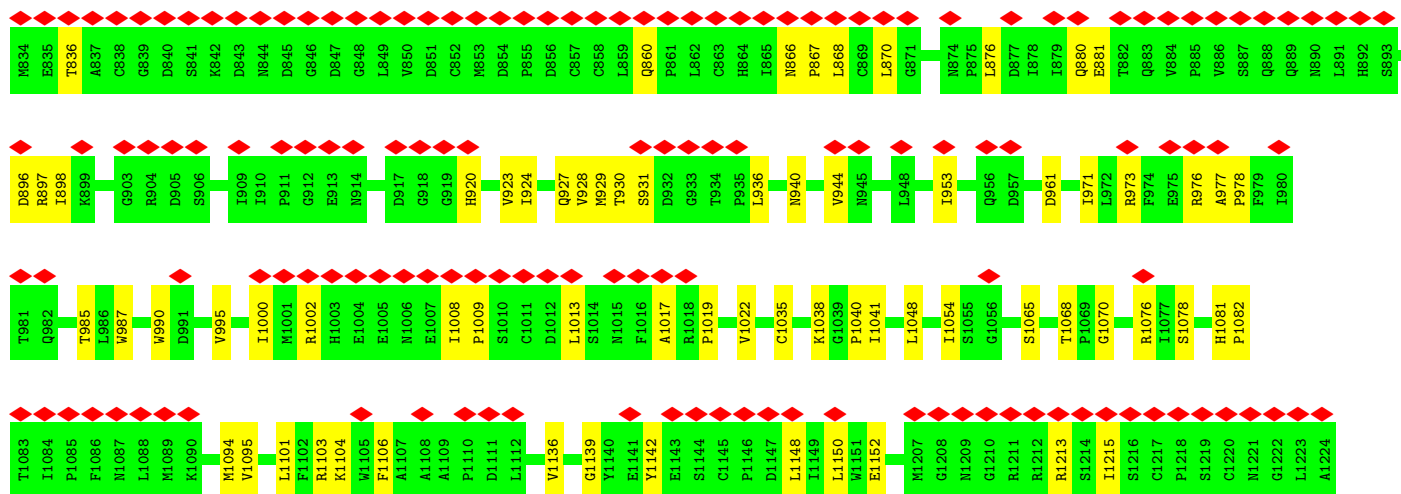
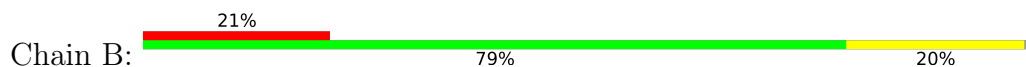
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Teneurin-4





● Molecule 1: Teneurin-4



D1225	G1226	M1227	K1228	L1229	L1230	A1231	P1232	T1236	D1240	L1243	G1246	D1247	F1248	N1249	V1250	I1251	R1252	R1253	I1254	F1255	P1256	S1257	G1258	N1259	V1260	T1261	N1262	I1263	L1264	E1265	L1266	L1267	N1268	K1269	D1270	F1271	R1272	H1273	S1274	H1275	S1276	P1277	A1278	H1279	K1280	Y1281	V1282	L1283	A1284	T1285	D1286	P1287	M1288	S1289	G1290				
A1291	V1292	F1293	L1294	S1295	D1296	K1297	N1298	S1299	R1300	R1301	V1302	F1303	K1304	I1305	K1306	S1307	T1308	V1309	V1310	V1311	K1312	D1313	N1314	V1315	K1316	N1317	S1318	E1319	V1320	V1321	A1322	G1323	L1324	ASP	THR	SER	ALA	ARG	C1328	L1329	PRO	PHE	ASP	THR	R1335	G1336	G1337	D1338	G1339	G1340	K1341	A1342	T1343	E1344	A1345	T1346	L1347	T1348	N1349
R1351	G1352	I1353	D1356	F1357	P1358	G1359	L1360	I1361	Y1362	F1363	V1364	D1365	G1366	T1367	M1368	T1369	R1370	R1371	I1372	D1373	Q1374	N1375	G1376	I1377	I1378	S1379	T1380	L1381	L1382	G1383	S1384	ASN	ASP	LEU	THR	SER	ALA	ARG	PRO	L1393	S1394	C1395	D1396	S1397	V1398	M1399	D1400	I1401	S1402	Q1403	V1404	H1405	L1406	E1407	W1408	P1409	T1410	D1411	
L1412	M1415	P1416	M1417	D1418	N1419	S1420	L1421	L1424	D1425	M1426	T1432	S1433	E1434	M1435	H1436	Q1437	V1438	R1439	I1440	V1441	A1442	G1443	R1444	P1445	K1516	N1517	D1518	A1519	N1520	C1521	D1522	C1523	F1524	S1525	G1526	D1527	D1528	D1533	A1534	K1535	L1536	N1537	S1540	V1544	C1545	A1546	D1554	L1555	G1556	N1557	I1558								
R1559	L1570	M1571	Y1576	E1577	L1601	P1602	T1603	G1604	D1605	T1611	G1614	L1620	M1625	R1632	W1641	T1664	Q1666	G1667	H1668	E1669	T1692	T1693	F1694	G1711	F1716	T1720	D1721	S1722	V1723	V1724	H1725	S1731	S1732	K1733	D1734	T1735	V1736	I1737	I1738	T1739	T1750	L1751																	
L1752	Q1753	D1754	T1755	L1768	E1769	L1770	L1771	L1772	M1776	E1777	V1778	L1780	L1786	V1795	V1800	T1801	D1805	N1806	G1807	K1817	A1820	R1821	G1822	Q1823	V1824	T1825	L1831	L1841	D1842	F1843	R1848	I1852	R1857	D1866	R1870	R1879	V1883	R1898	T1927																				
E1930	V1934	M1960	Q1964	P1982	I1989	F1992	F2002	Y2003	L2004	G2005	T2006	R2008	K2013	L2017	S2018	E2022	Y2025	D2026	T2033	L2041	R2042	T2043	R2058	L2063	R2066	Q2067	T2068	E2074	G2075	N2076	N2084	Y2085	D2086	N2087	S2088	F2089	S2093																						
L2098	L2119	F2120	G2121	D2129	I2130	N2131	Q2132	I2133	T2136	A2137	T2140	H2141	T2142	Q2155	Y2156	E2157	I2158	F2159	R2160	S2161	L2162	N2163	Y2164	W2165	M2166	T2167	D2171	N2172	L2181	K2182	V2183	Y2186	A2187	N2188	Q2201	I2207	L2212	N2220	G2221	N2222	L2223	H2224	L2225	L2226	N2230														
L2234	T2235	P2236	L2237	R2242	D2243	R2244	K2254	M2255	D2258	L2261	R2262	Q2263	D2267	K2279	N2282	R2290	S2305	Q2311	F2312	F2313	H2325	L2326	Y2327	I2334	L2337	L2341	I2358	D2361	L2367	A2368	V2369	K2378	Q2379	I2380	Y2389	L2398	T2399	I2400																					
K2412	V2423	R2427	K2437	M2451	N2454	N2455	M2468	L2482	H2483	N2484	V2485	T2486	Y2489	P2492	D2493	M2494	D2495	A2496	M2497	S2500	L2504	T2510	W2513	S2518	T2519	L2520	Q2523	V2526	R2538	S2545	THR	ILE	THR	SER	CYS	GLN	A2553	P2554	K2555	T2556																			
K2557	K2571	F2572	T2581	L2584	C2585	V2586	R2593	L2597	D2628	L2629	T2648	V2655	N2657	G2658	R2659	T2660	R2661	R2662	Y2663	T2664	D2665	L2666	Q2667	Y2679	E2686	R2689	E2692	L2693	A2694	R2695	Q2696	Q2708	R2709	E2712	R2718	A2719	V2720	T2721	E2722	G2723	E2724	K2725	Q2726																
V2728	L2729	S2744	Q2747	D2753	S2764	E2765																																																					

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

Chain C:  100%



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

Chain D:  100%



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

Chain E:  100%



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

Chain F:  100%
100%



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

Chain G:  100%



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

Chain H:  100%



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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%
 100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242300	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 ($e^-/\text{\AA}^2$)	50.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	303.12, 303.12, 303.12	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.842, 0.842, 0.842	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/15425	0.49	1/20912 (0.0%)
1	B	0.22	0/15425	0.49	1/20912 (0.0%)
All	All	0.22	0/30850	0.49	2/41824 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	870	LEU	O-C-N	-5.40	116.86	122.96
1	B	870	LEU	O-C-N	-5.36	116.90	122.96

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2025	TYR	Peptide
1	B	2025	TYR	Peptide

5.2 Too-close contacts ⓘ

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	15093	0	14709	250	0
1	B	15093	0	14709	248	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
3	A	98	0	91	1	0
3	B	98	0	91	1	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
All	All	30612	0	29800	492	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 8.

The worst 5 of 492 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:B:2242:ARG:HH21	1:B:2244:ARG:HH21	1.25	0.84
1:A:2242:ARG:HH21	1:A:2244:ARG:HH21	1.25	0.83
1:B:1300:ARG:NH1	1:B:1349:ASN:OD1	2.18	0.77
1:B:2119:GLN:NE2	1:B:2121:GLY:O	2.18	0.77
1:B:1300:ARG:NH1	1:B:1348:THR:O	2.19	0.76

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	1894/1932 (98%)	1785 (94%)	109 (6%)	0	100	100
1	B	1894/1932 (98%)	1785 (94%)	109 (6%)	0	100	100
All	All	3788/3864 (98%)	3570 (94%)	218 (6%)	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	1663/1689 (98%)	1662 (100%)	1 (0%)	88	96
1	B	1663/1689 (98%)	1662 (100%)	1 (0%)	88	96
All	All	3326/3378 (98%)	3324 (100%)	2 (0%)	87	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1419	ASN
1	B	1419	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2481	GLN

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Mol	Chain	Res	Type
1	B	2481	GLN
1	B	1003	HIS
1	B	1785	HIS
1	A	2763	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.30	0	17,19,21	0.52	0
2	NAG	C	2	2	14,14,15	0.19	0	17,19,21	0.44	0
2	NAG	D	1	2,1	14,14,15	0.38	0	17,19,21	0.56	0
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	0.47	0
2	NAG	E	1	2,1	14,14,15	0.37	0	17,19,21	0.46	0
2	NAG	E	2	2	14,14,15	0.19	0	17,19,21	0.48	0
2	NAG	F	1	2,1	14,14,15	0.27	0	17,19,21	0.40	0
2	NAG	F	2	2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	G	1	2,1	14,14,15	0.30	0	17,19,21	0.52	0
2	NAG	G	2	2	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	H	1	2,1	14,14,15	0.38	0	17,19,21	0.57	0
2	NAG	H	2	2	14,14,15	0.44	0	17,19,21	0.47	0
2	NAG	I	1	2,1	14,14,15	0.38	0	17,19,21	0.46	0
2	NAG	I	2	2	14,14,15	0.18	0	17,19,21	0.48	0
2	NAG	J	1	2,1	14,14,15	0.27	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	J	2	2	14,14,15	0.24	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

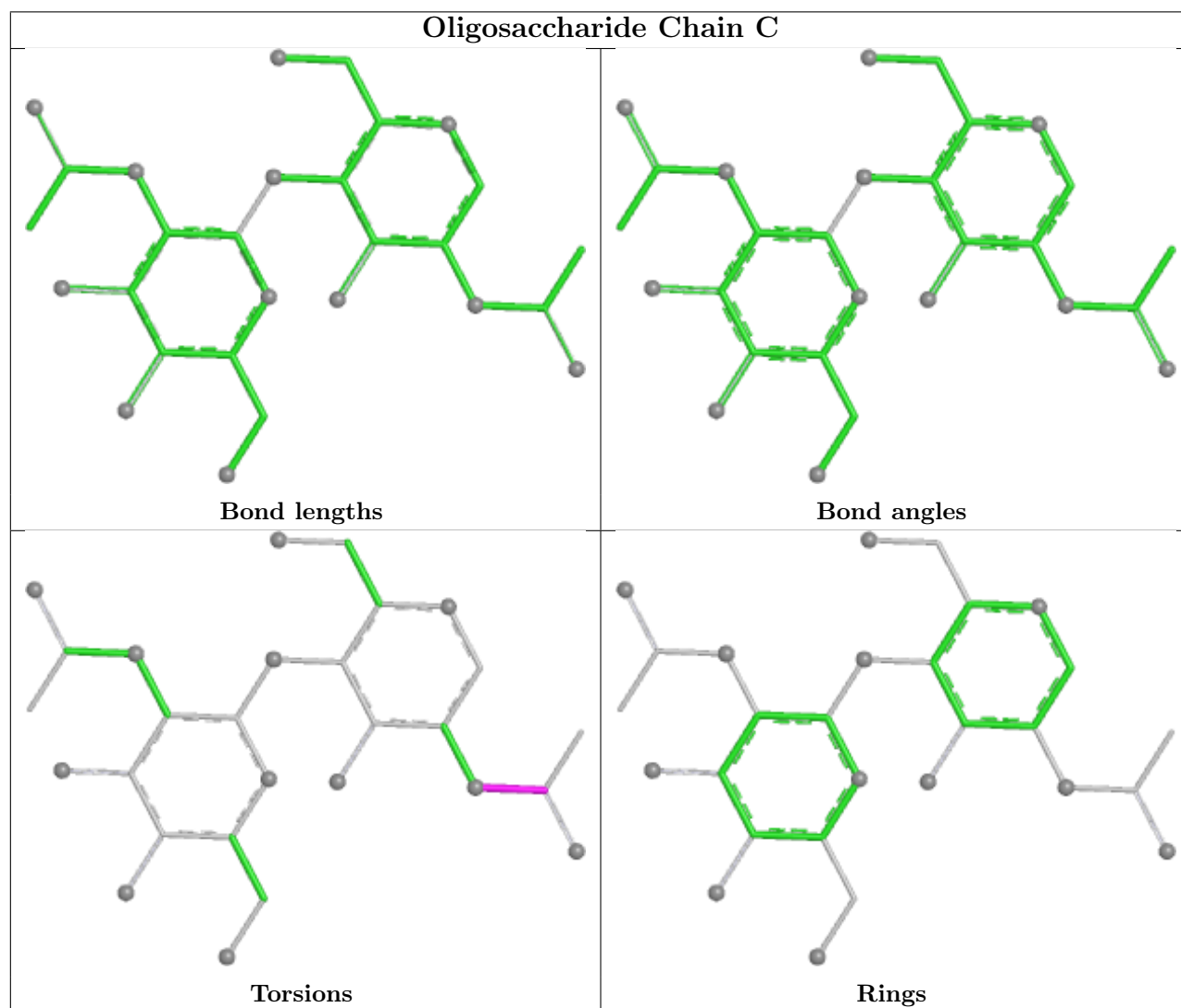
5 of 16 torsion outliers are listed below:

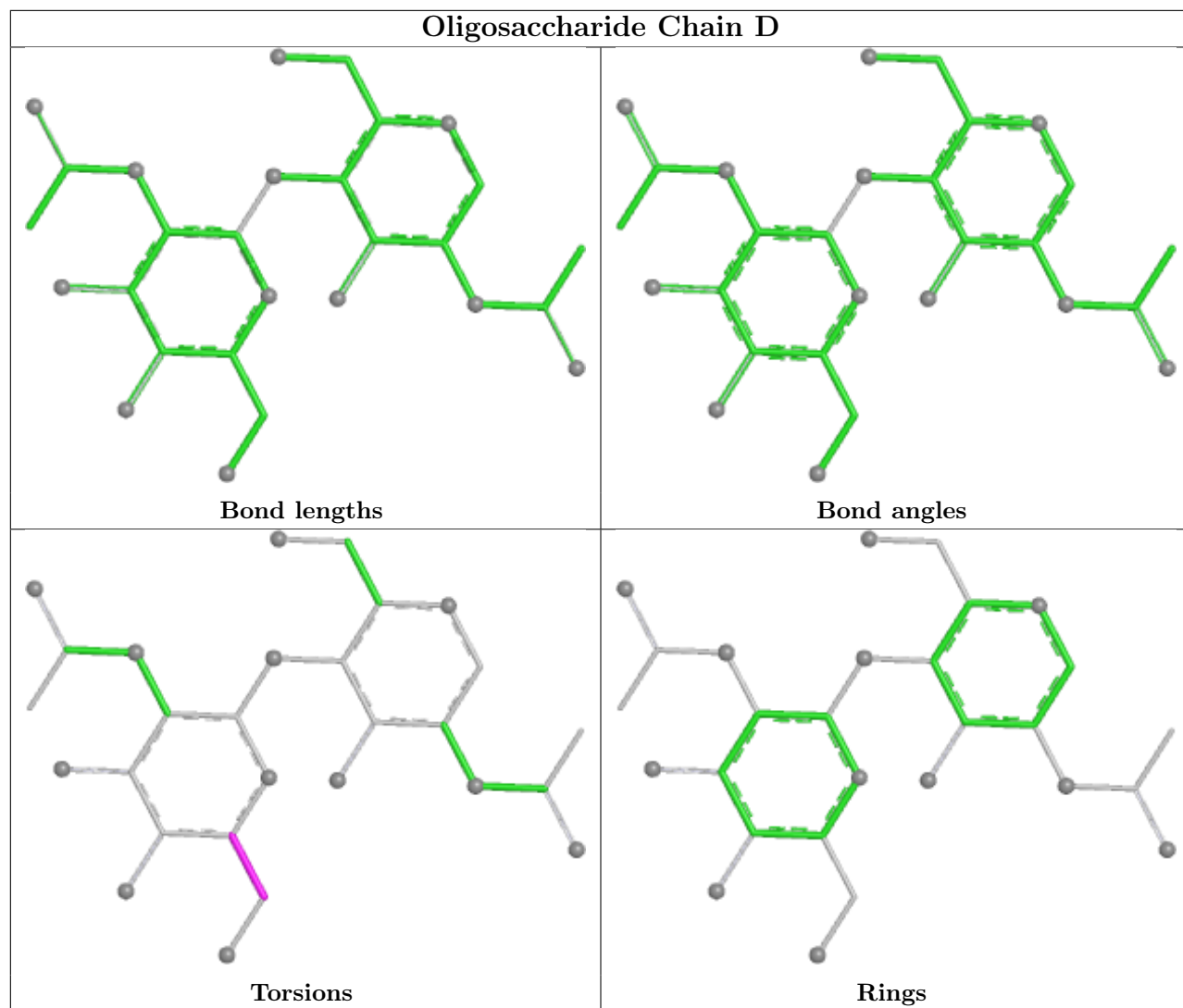
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6

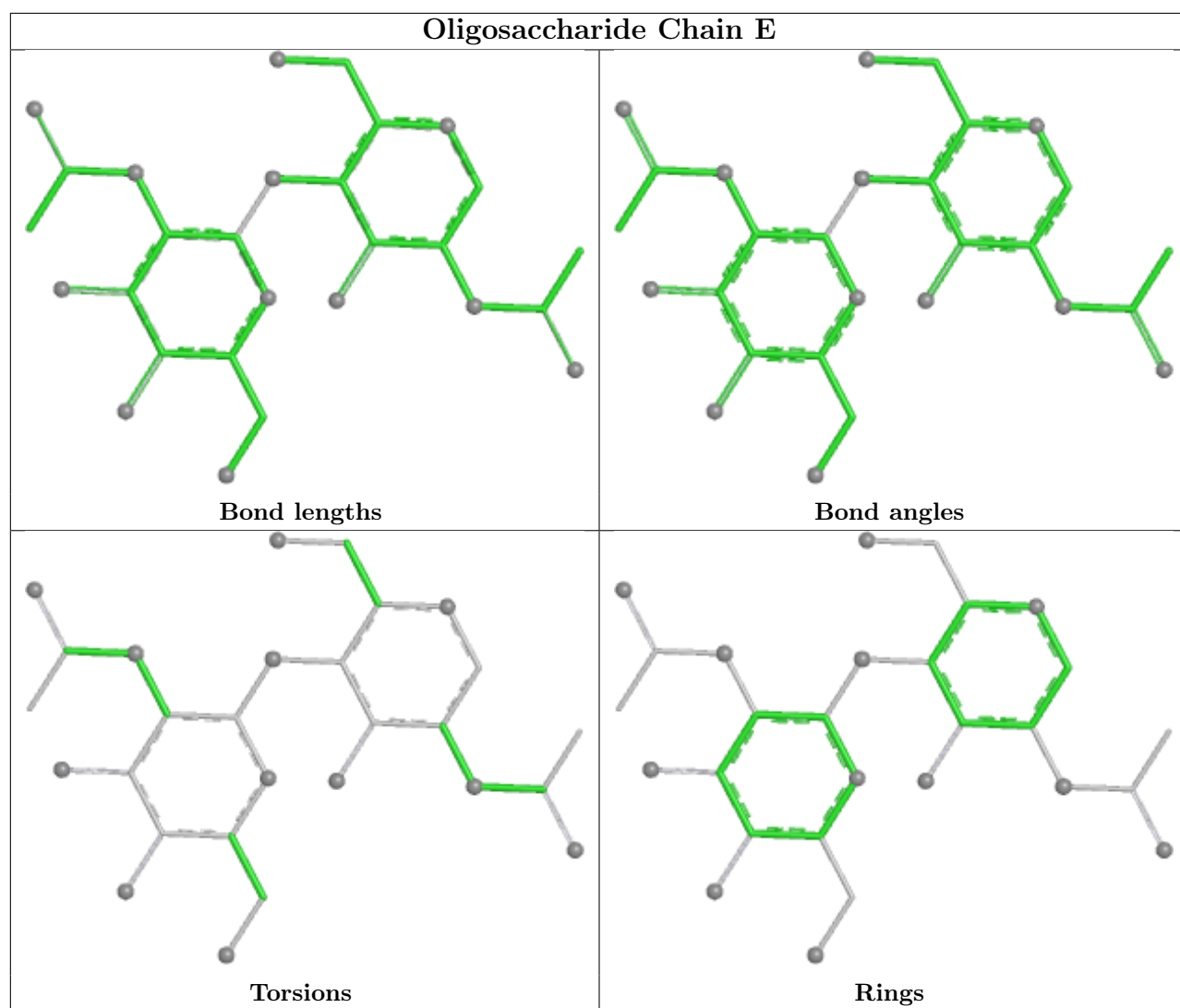
There are no ring outliers.

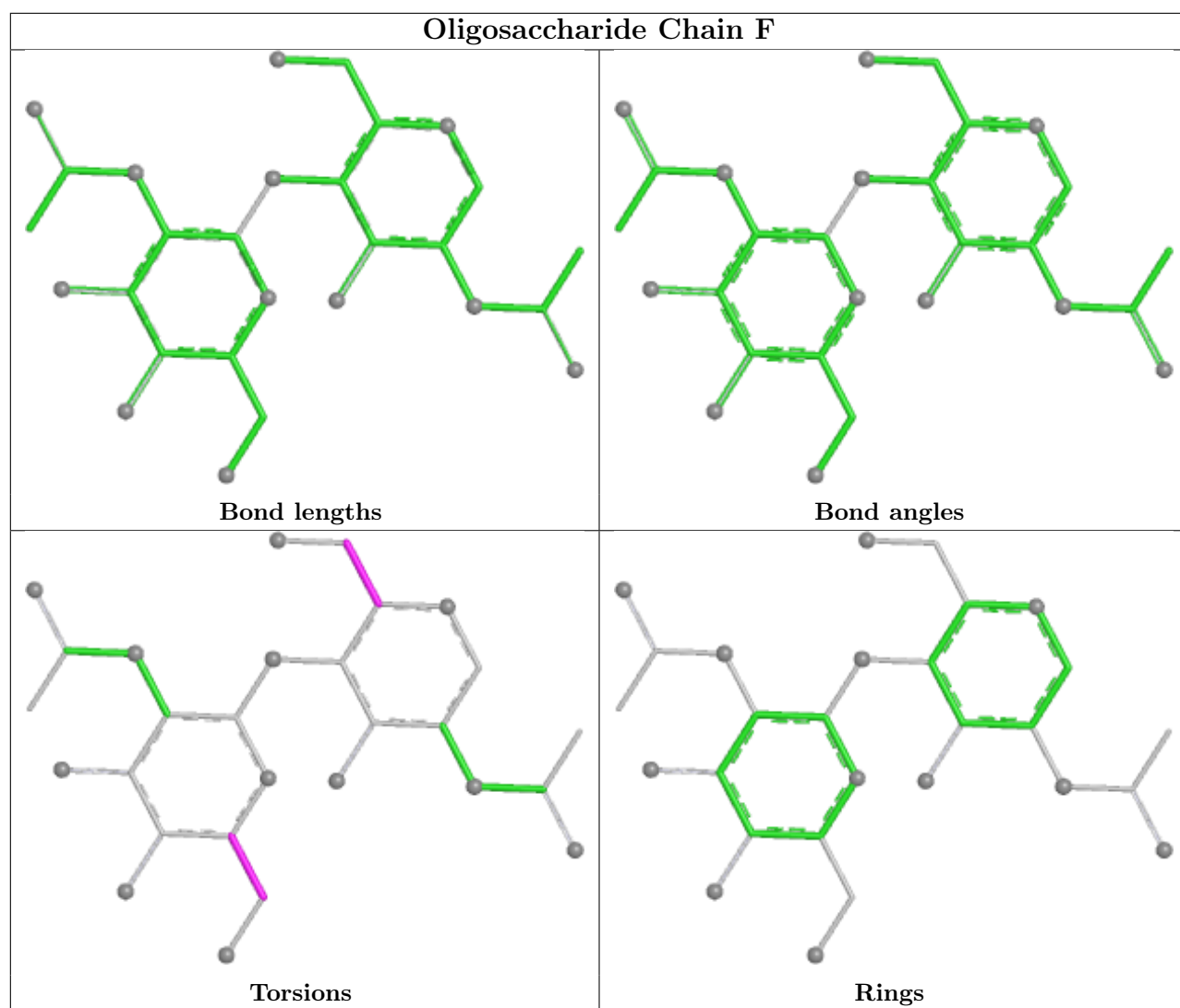
No monomer is involved in short contacts.

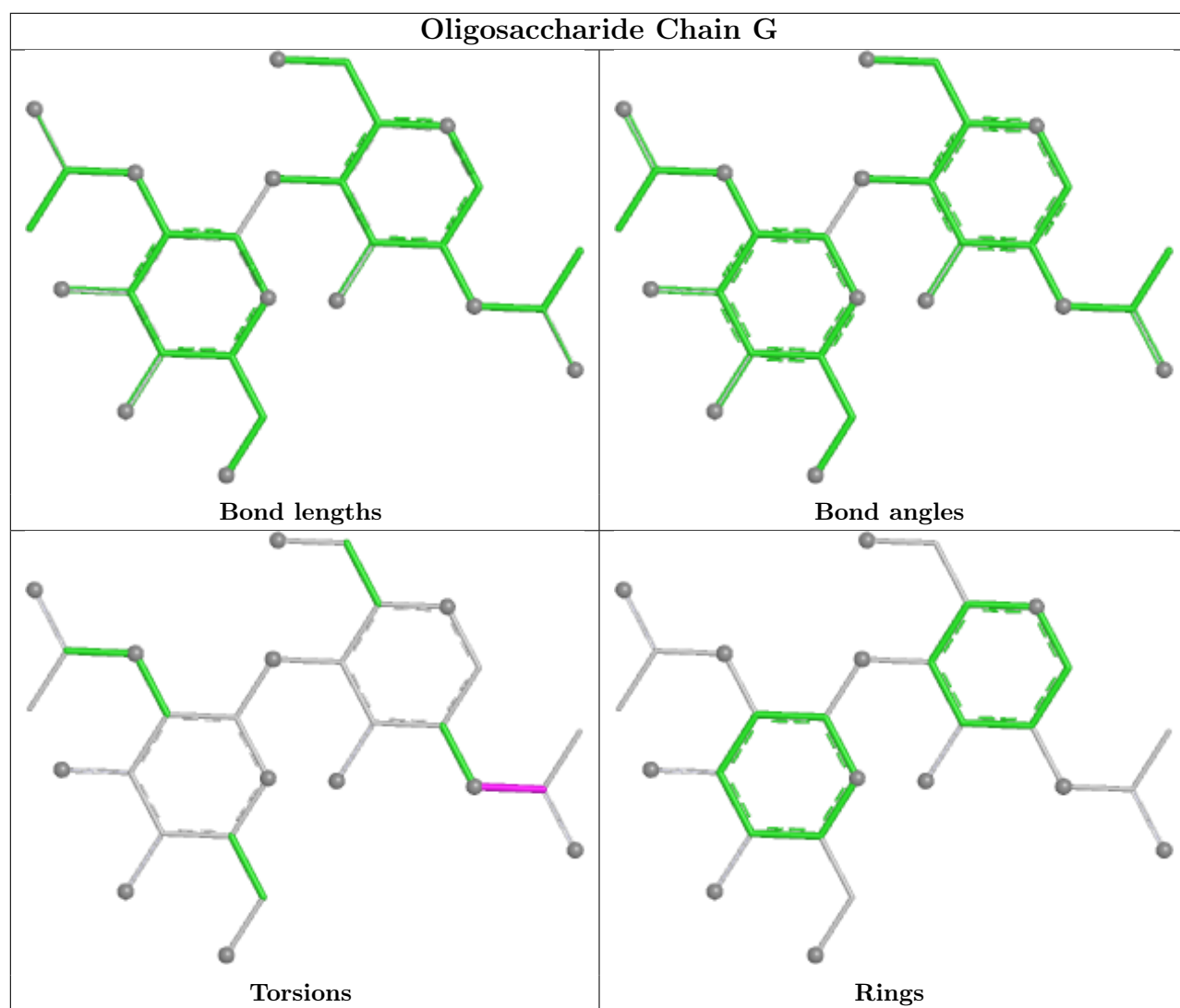
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

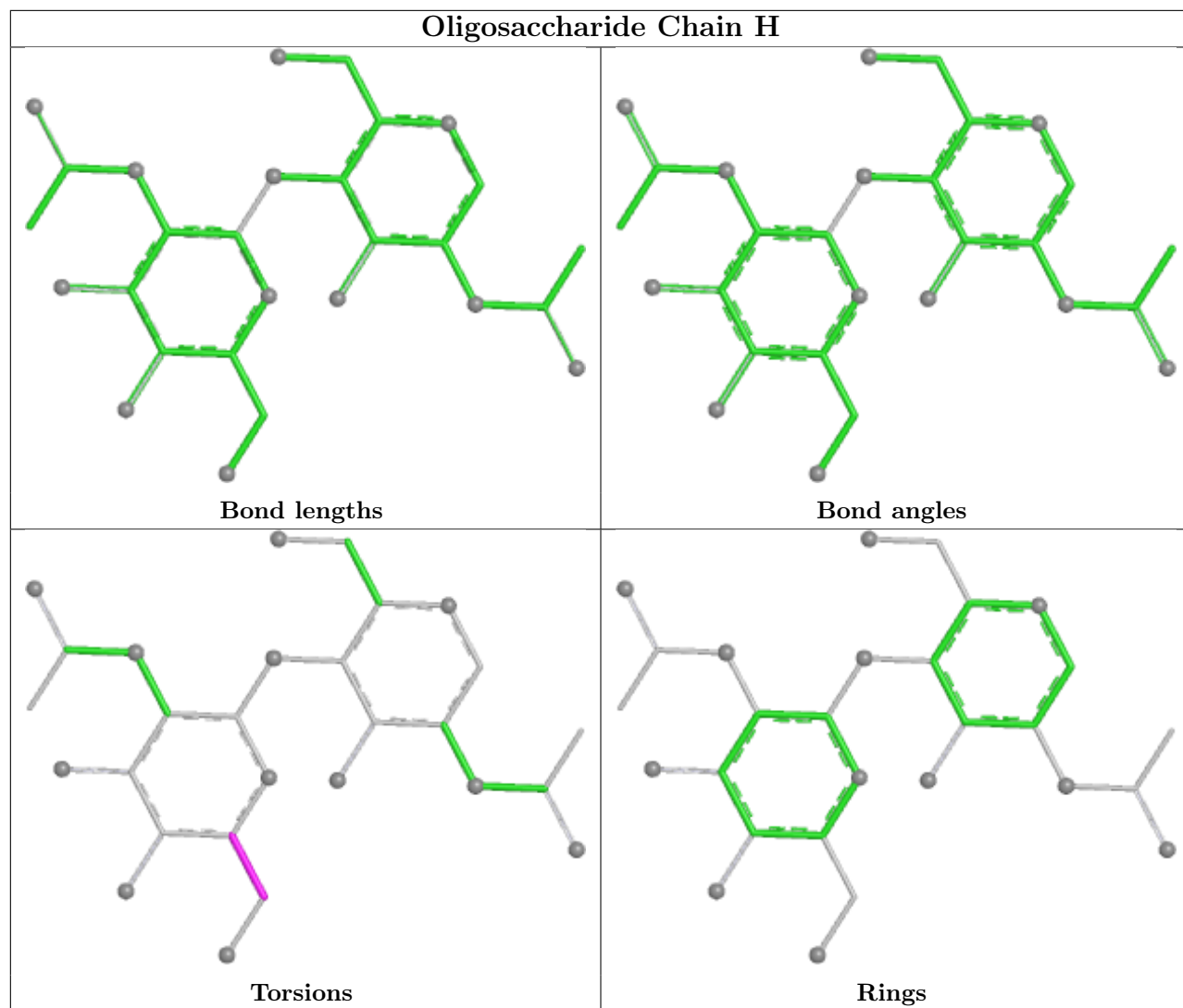


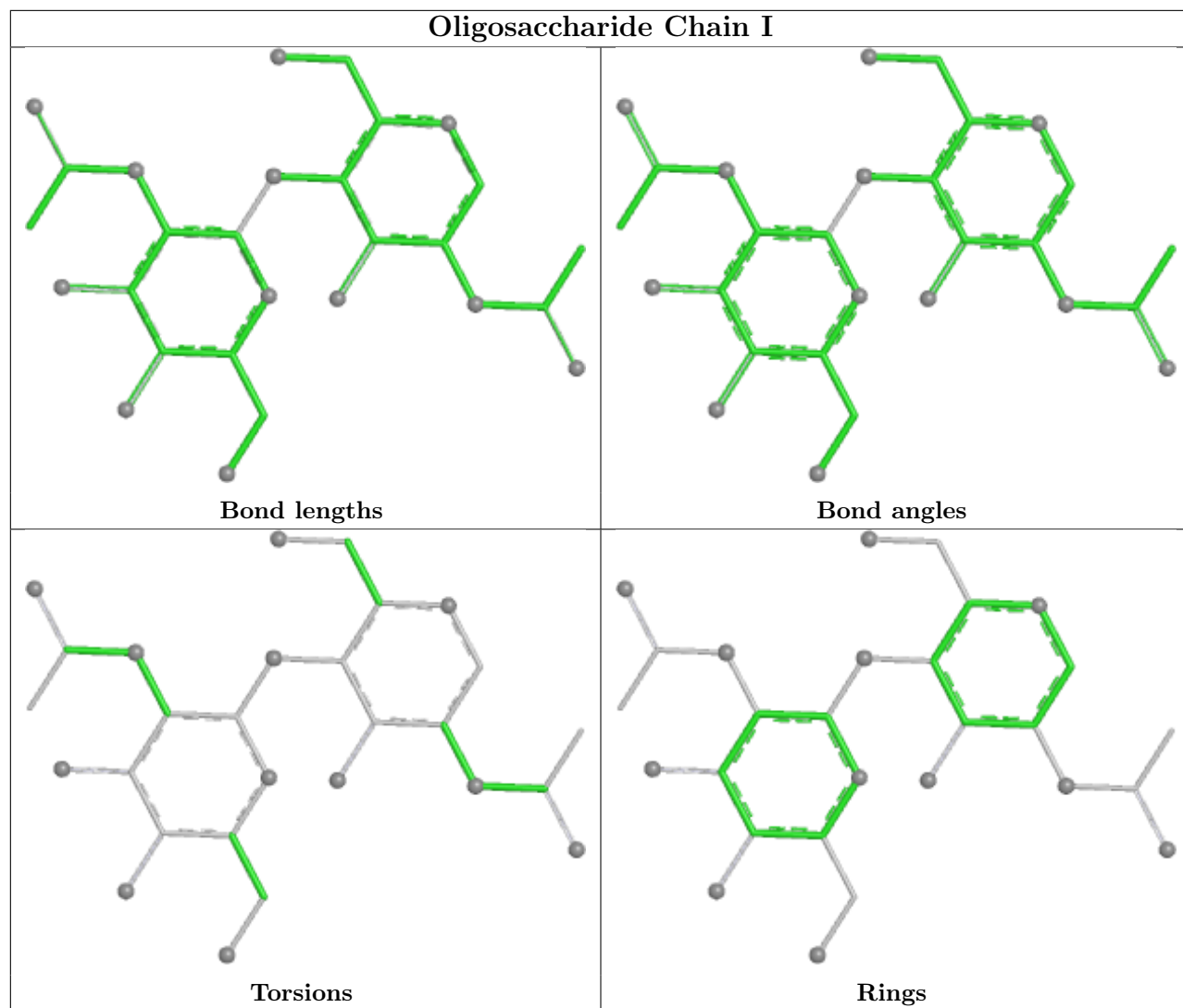


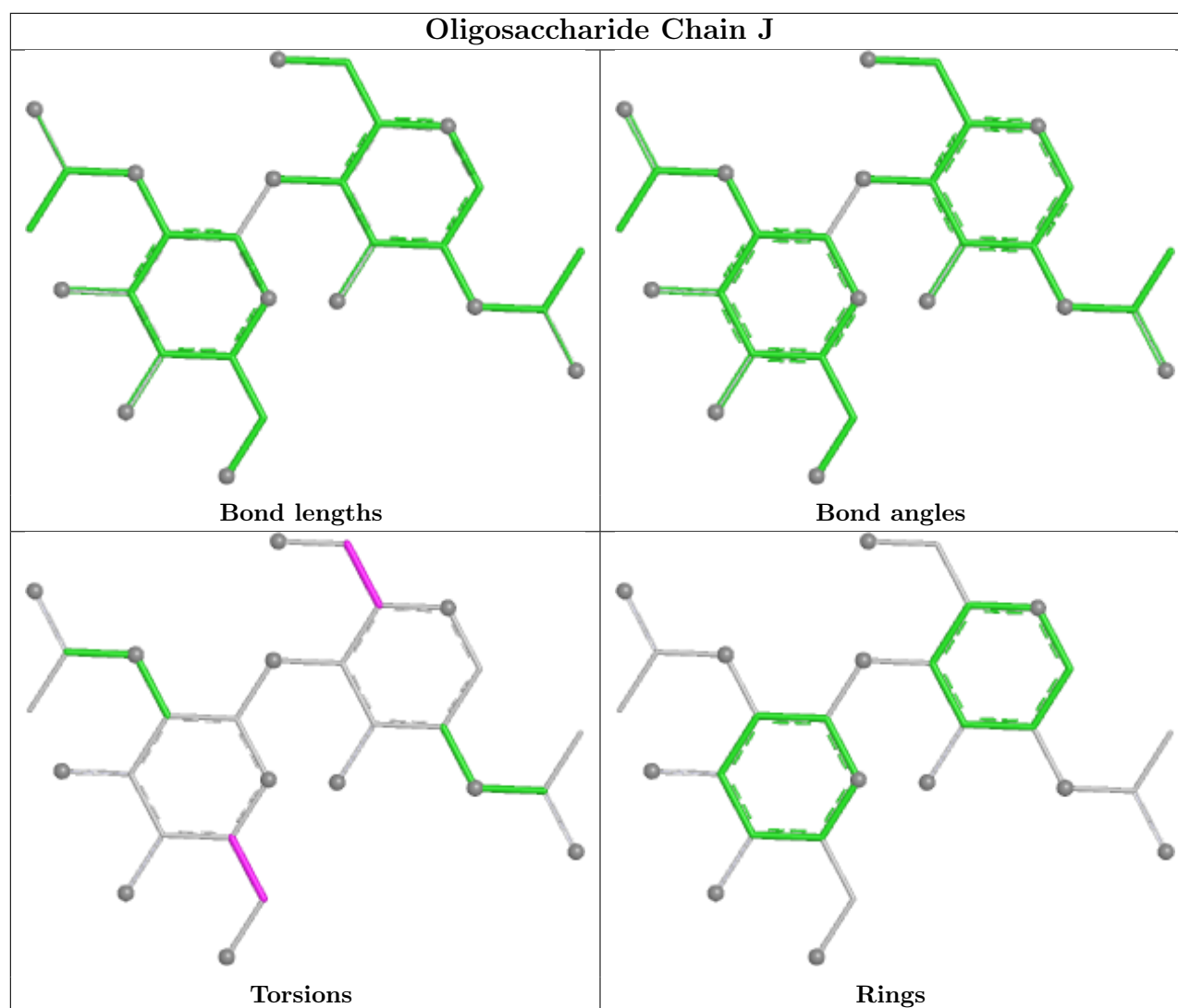












5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	2805	1	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	A	2803	1	14,14,15	0.41	0	17,19,21	1.49	3 (17%)
3	NAG	A	2802	1	14,14,15	0.15	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	2807	1	14,14,15	0.34	0	17,19,21	0.46	0
3	NAG	B	2802	1	14,14,15	0.14	0	17,19,21	0.46	0
3	NAG	B	2805	1	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	B	2807	1	14,14,15	0.34	0	17,19,21	0.47	0
3	NAG	B	2806	1	14,14,15	0.30	0	17,19,21	0.41	0
3	NAG	B	2803	1	14,14,15	0.42	0	17,19,21	1.49	3 (17%)
3	NAG	A	2804	1	14,14,15	0.30	0	17,19,21	0.55	0
3	NAG	B	2804	1	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	A	2806	1	14,14,15	0.29	0	17,19,21	0.41	0
3	NAG	A	2801	1	14,14,15	0.33	0	17,19,21	0.38	0
3	NAG	B	2801	1	14,14,15	0.34	0	17,19,21	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2805	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2803	1	-	6/6/23/26	0/1/1/1
3	NAG	A	2802	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2807	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2802	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2805	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2807	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2806	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2803	1	-	6/6/23/26	0/1/1/1
3	NAG	A	2804	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2804	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2806	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2801	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2803	NAG	C2-N2-C7	4.60	129.07	122.90
3	A	2803	NAG	C2-N2-C7	4.59	129.05	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2803	NAG	C1-O5-C5	2.83	115.98	112.19
3	A	2803	NAG	C1-O5-C5	2.81	115.96	112.19
3	A	2803	NAG	C1-C2-N2	2.06	113.68	110.43

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2803	NAG	O5-C5-C6-O6
3	B	2803	NAG	O5-C5-C6-O6
3	A	2803	NAG	C4-C5-C6-O6
3	B	2803	NAG	C4-C5-C6-O6
3	A	2802	NAG	O5-C5-C6-O6

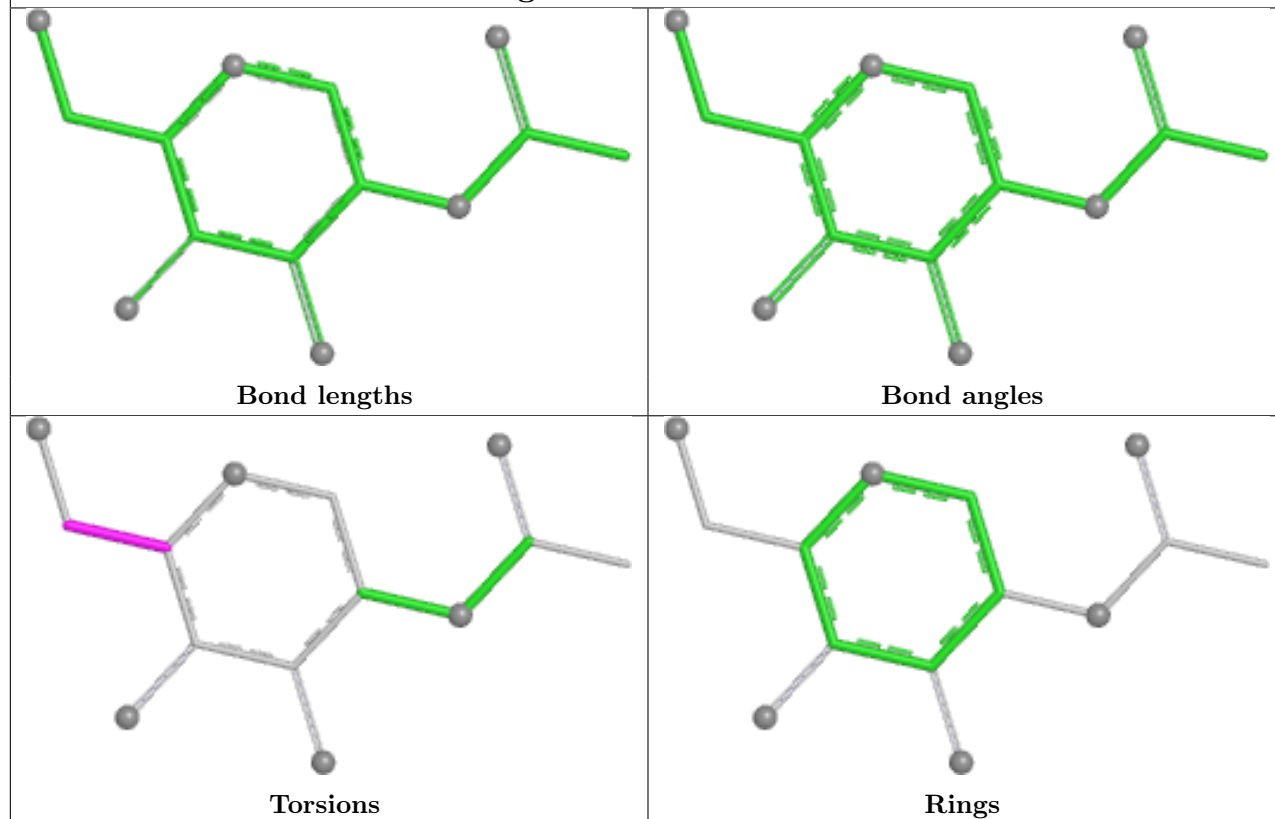
There are no ring outliers.

2 monomers are involved in 2 short contacts:

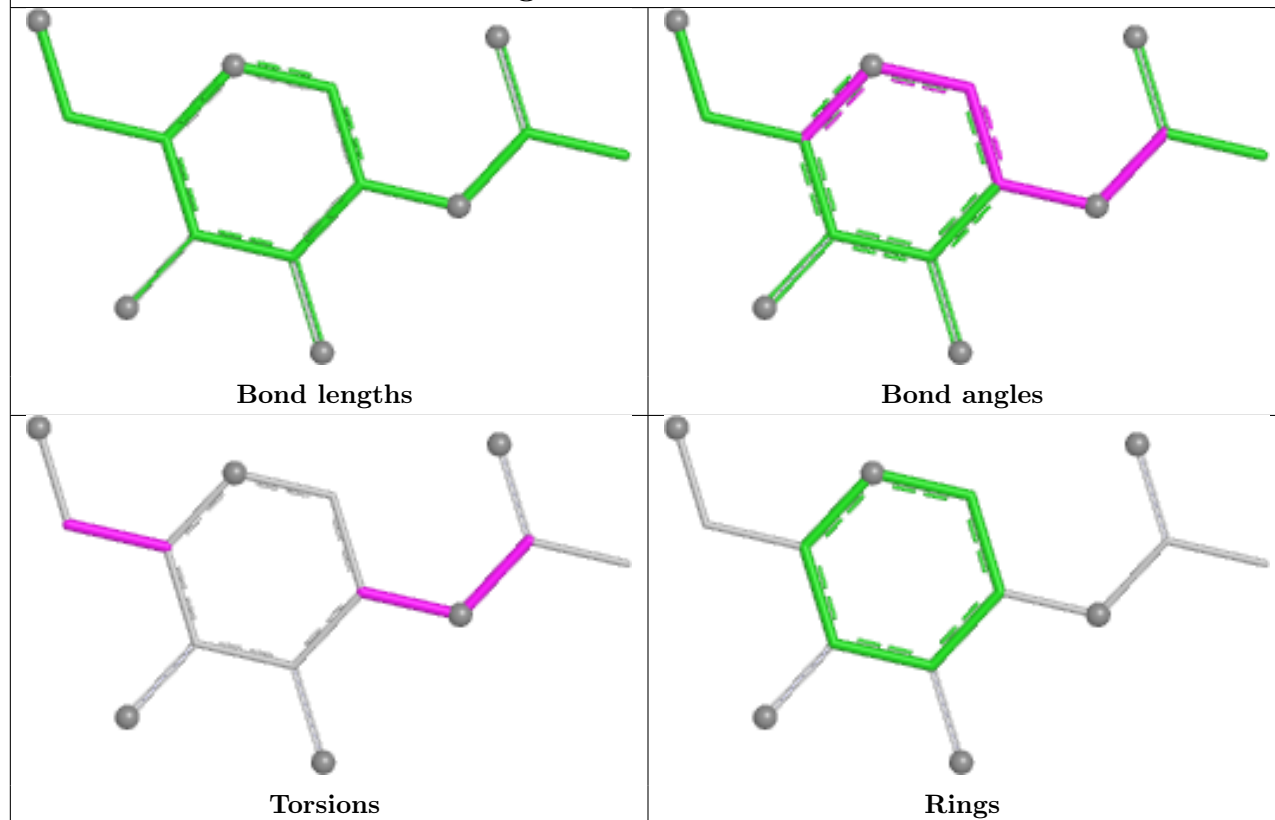
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2803	NAG	1	0
3	B	2803	NAG	1	0

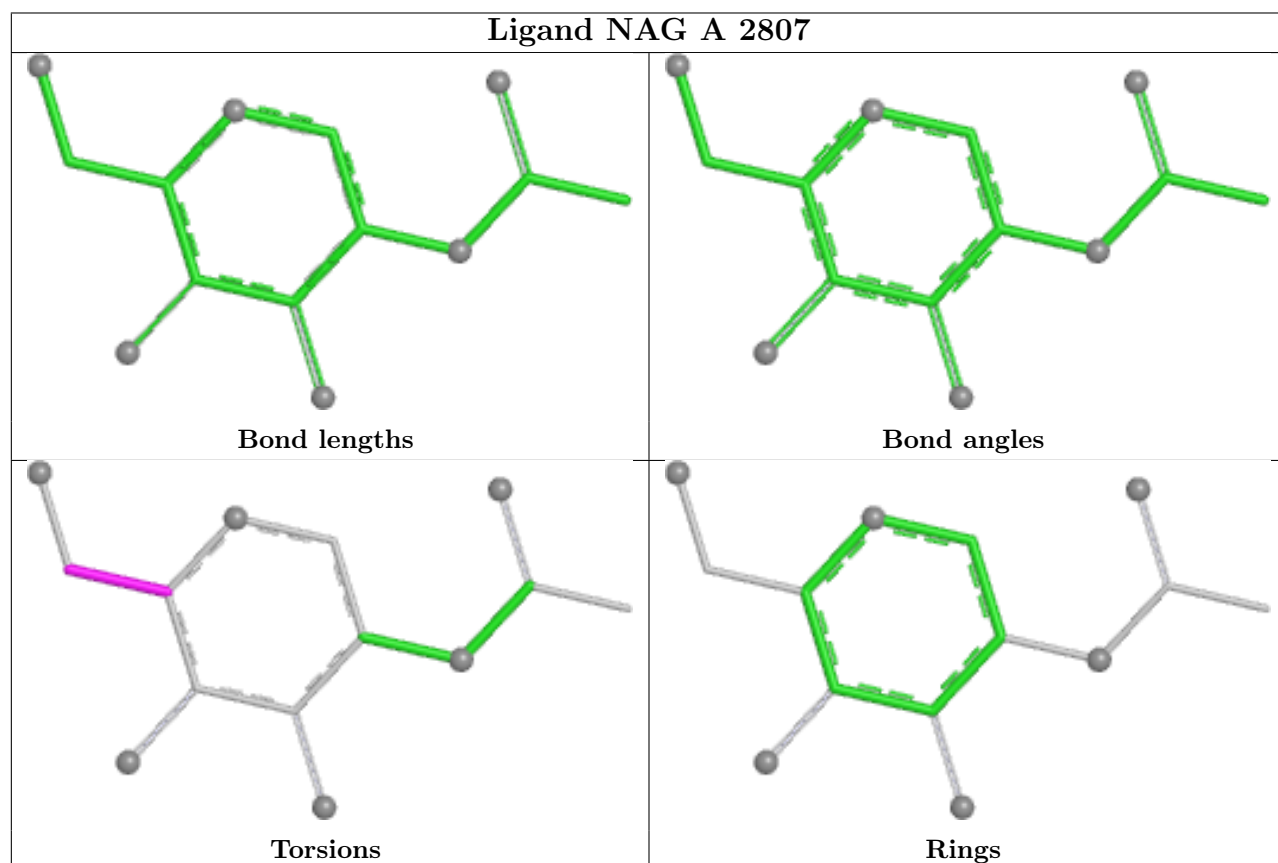
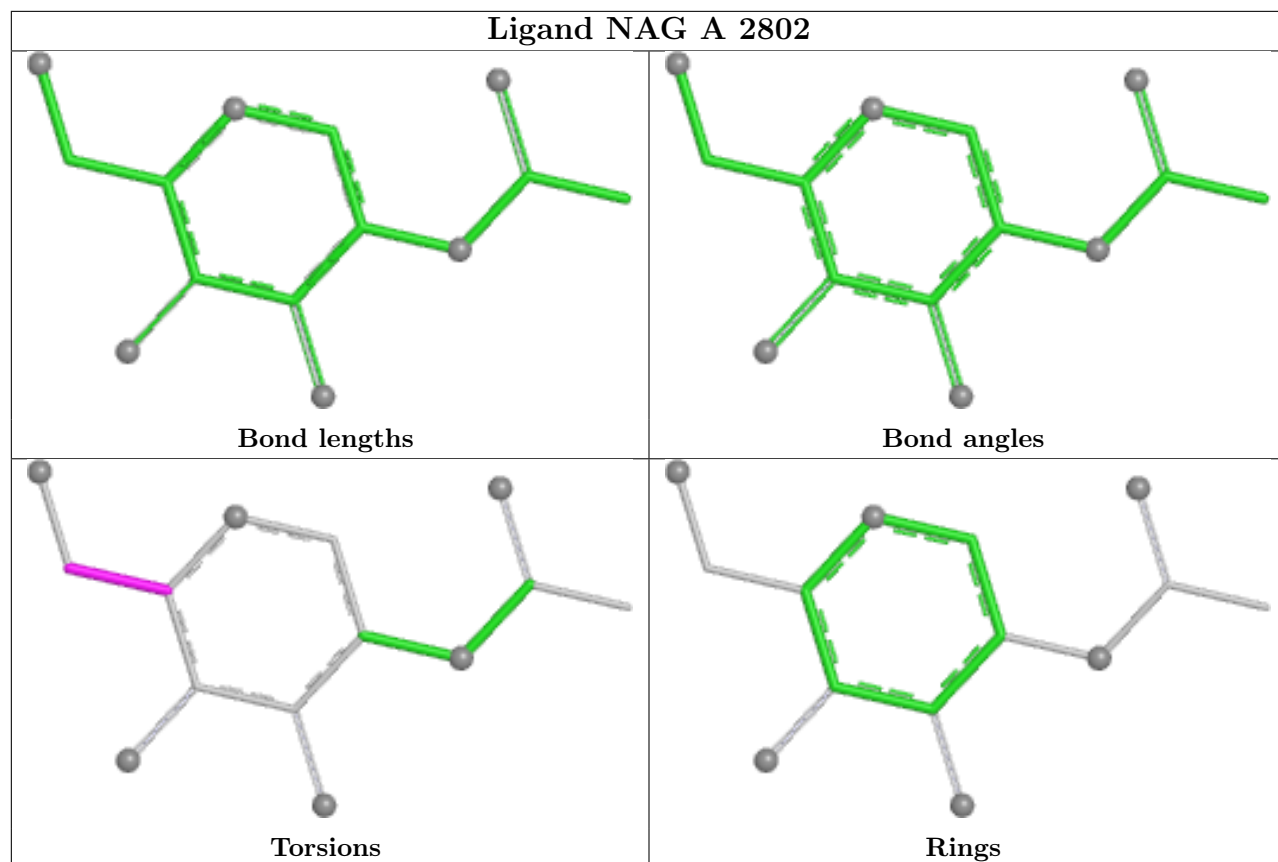
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

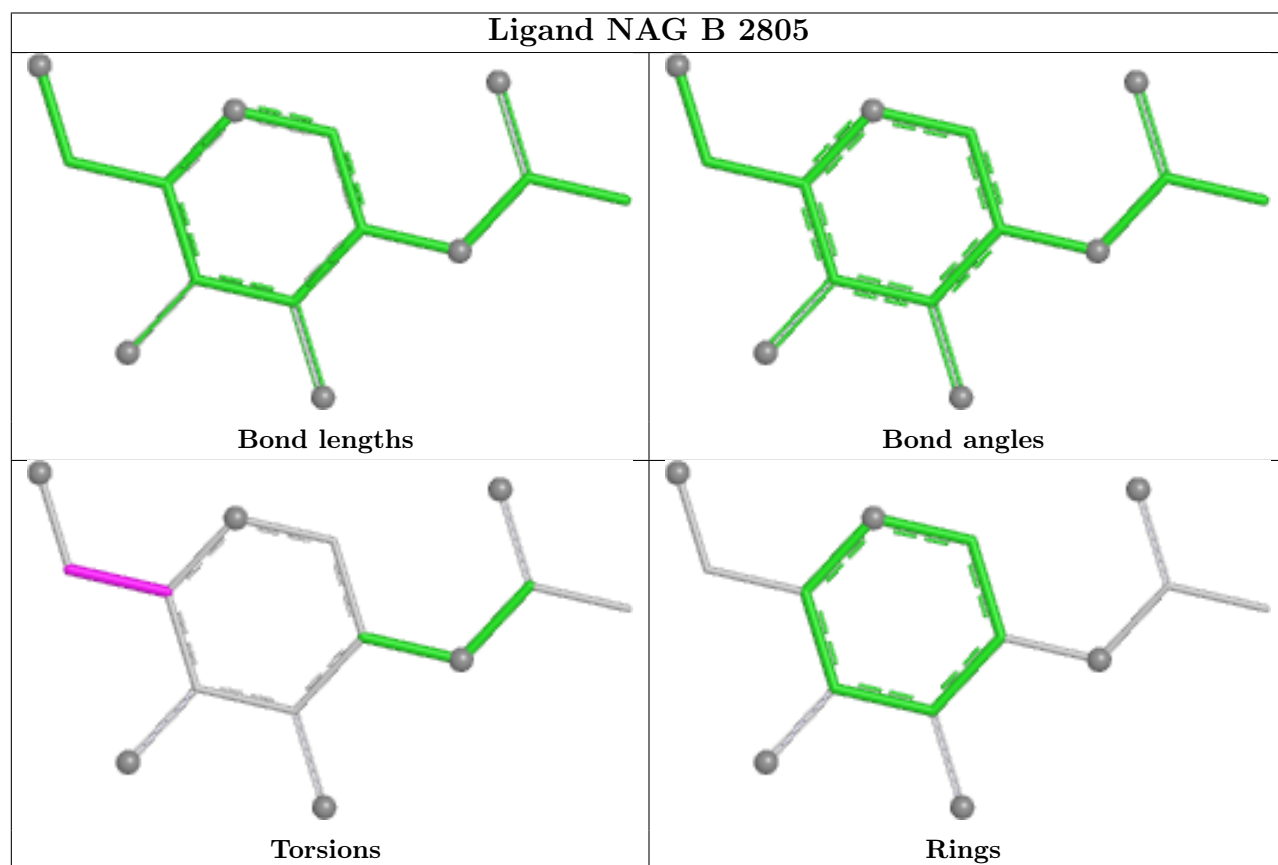
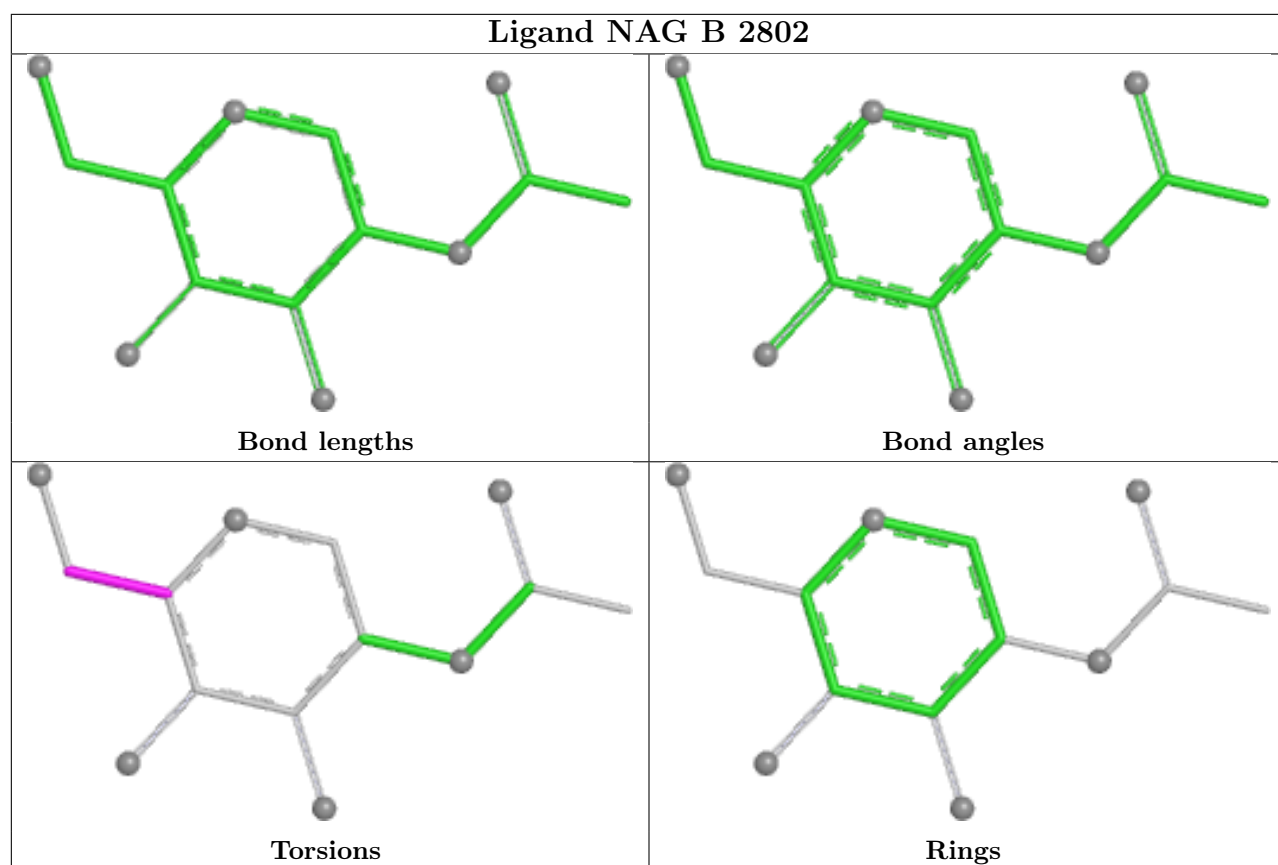
Ligand NAG A 2805

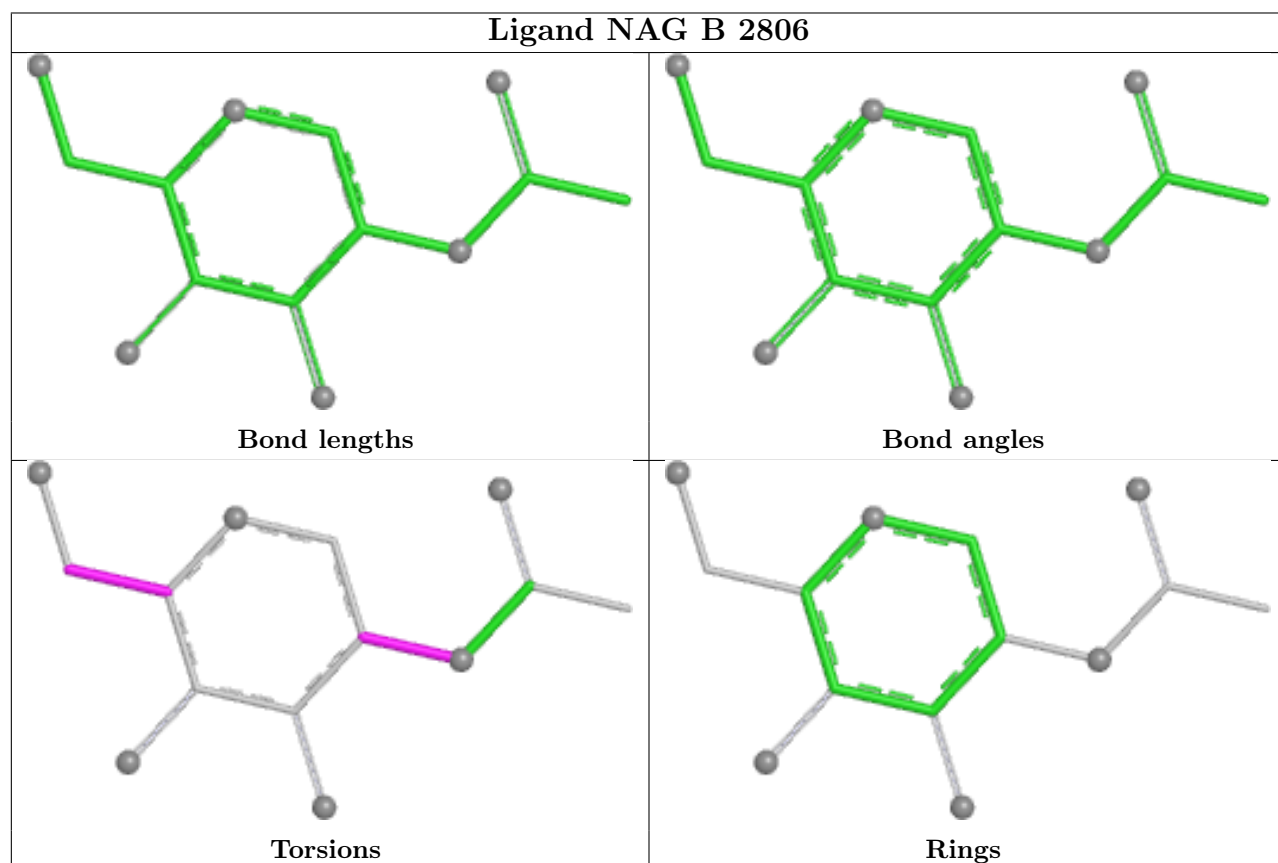
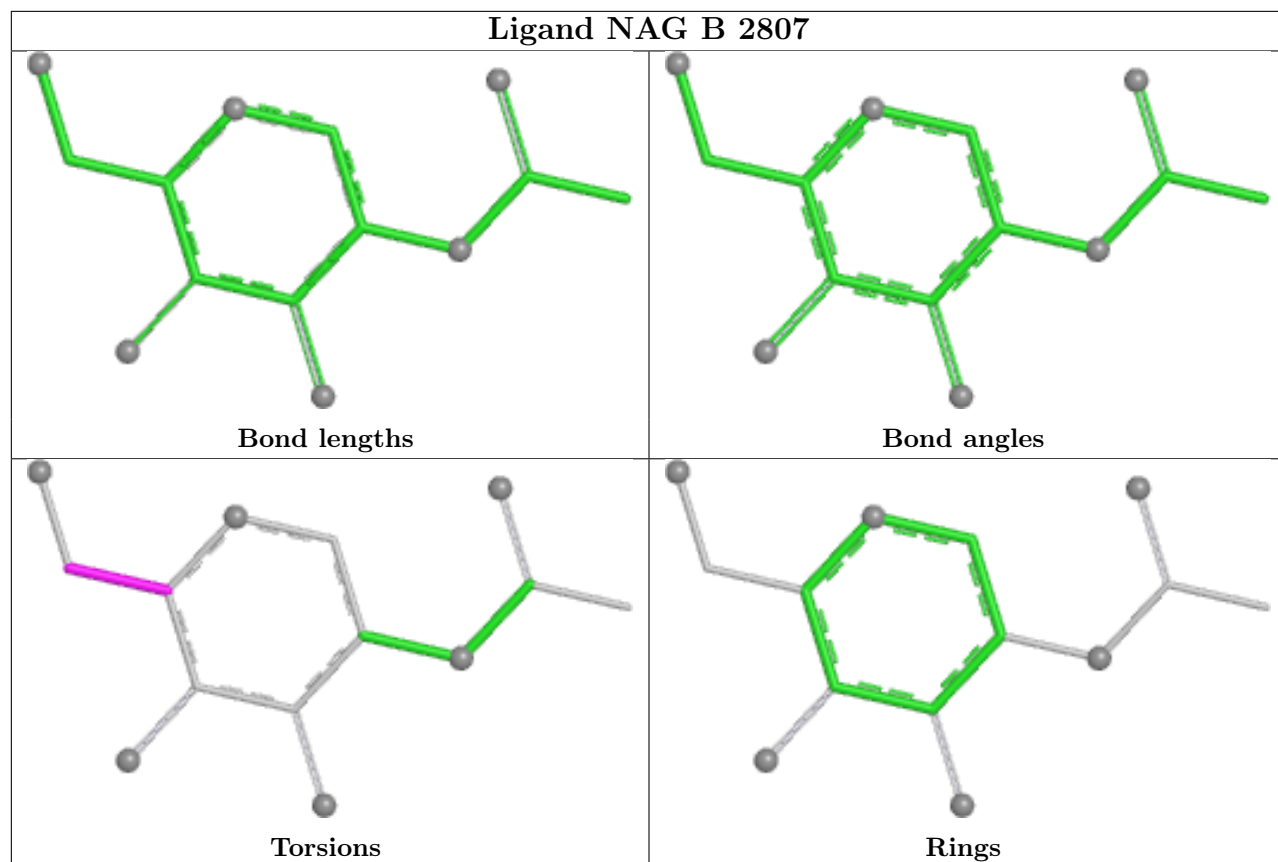


Ligand NAG A 2803

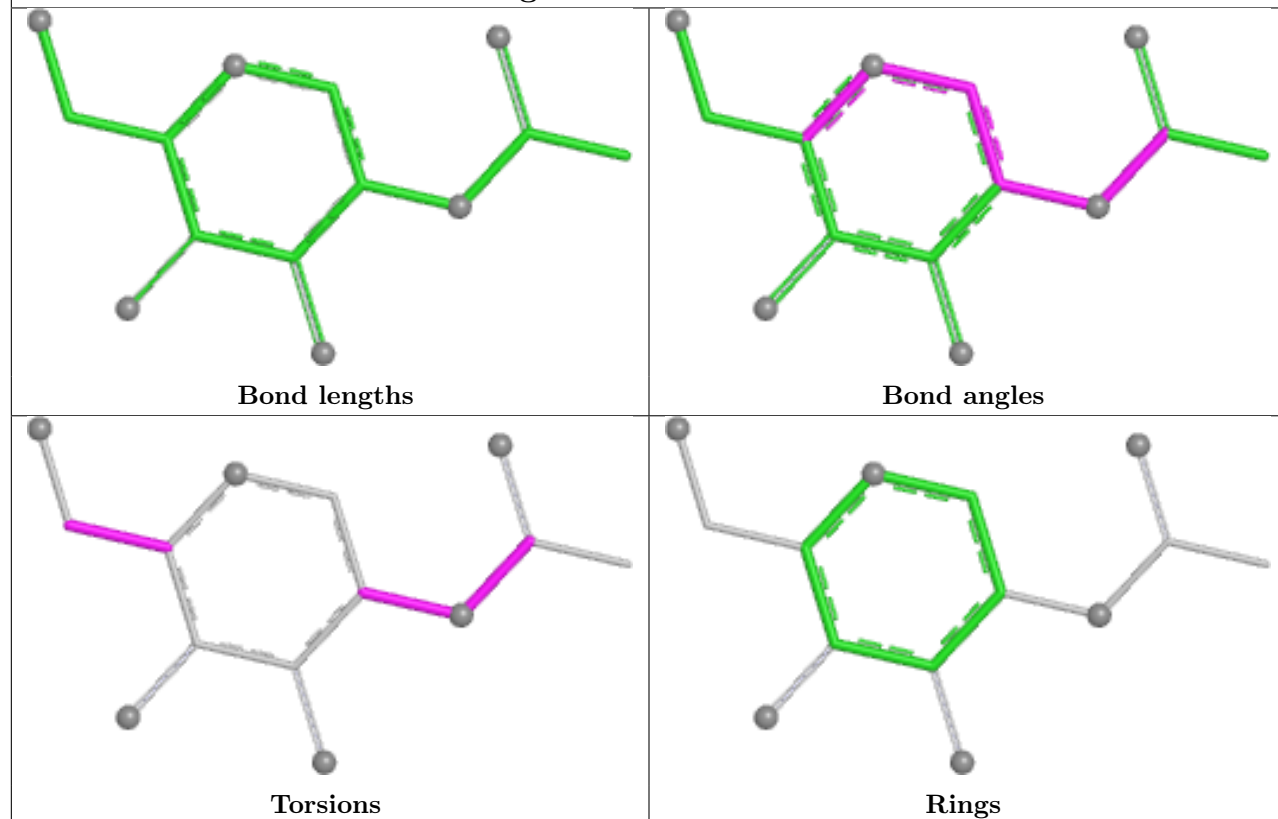




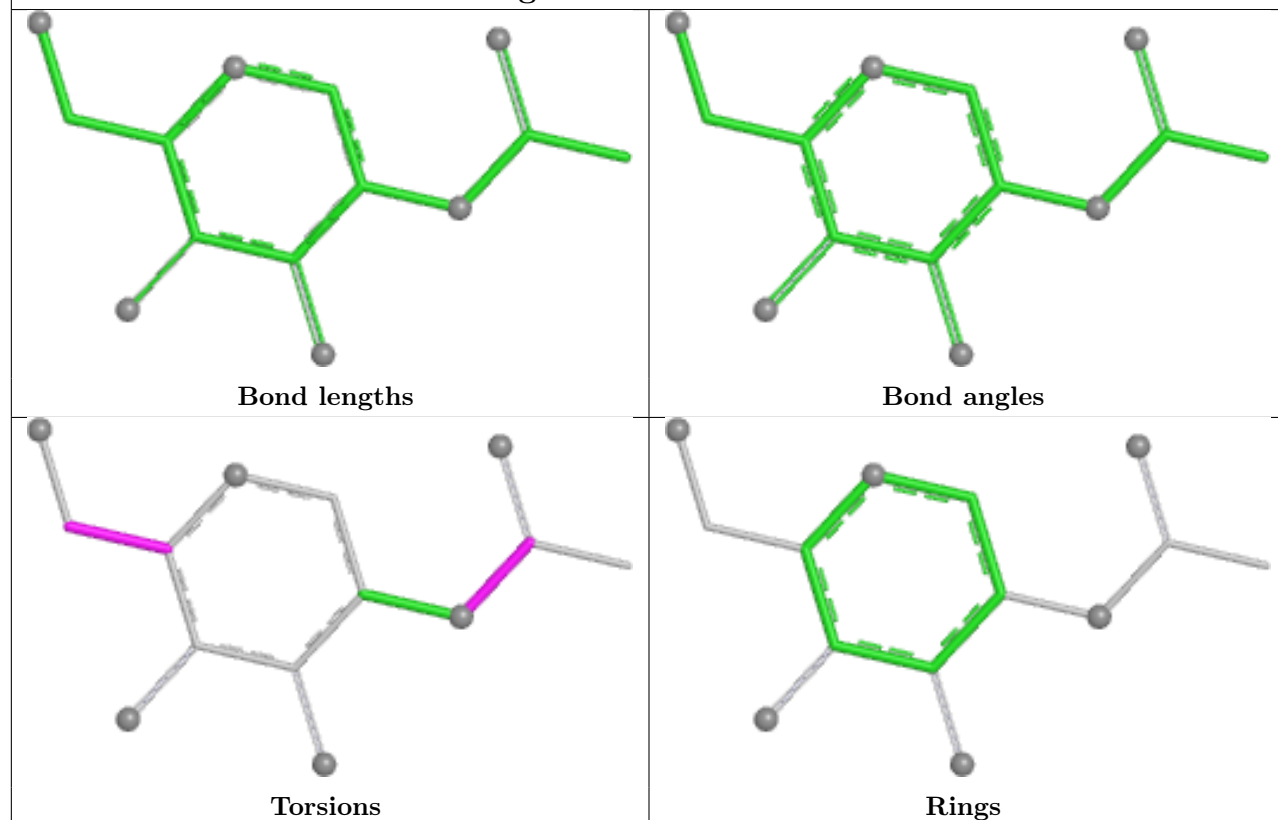


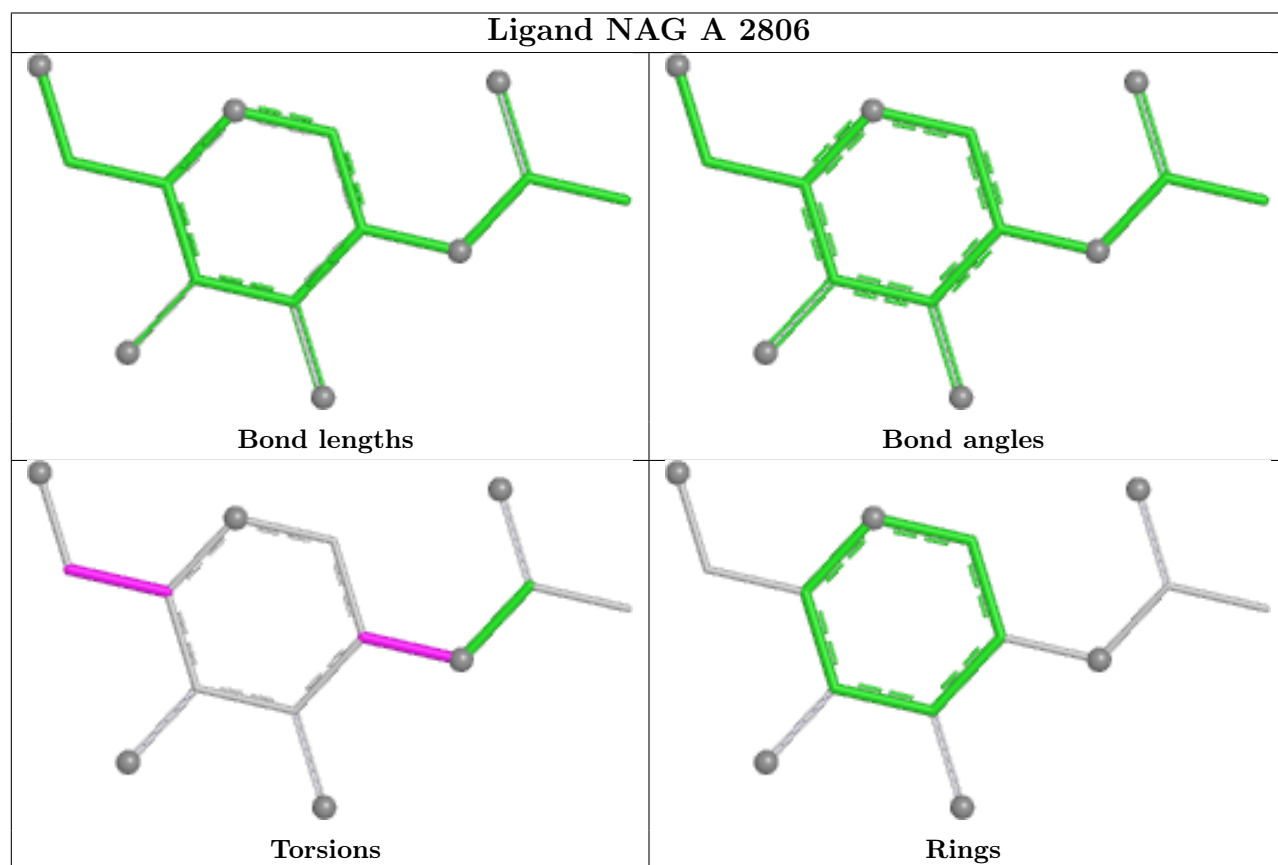
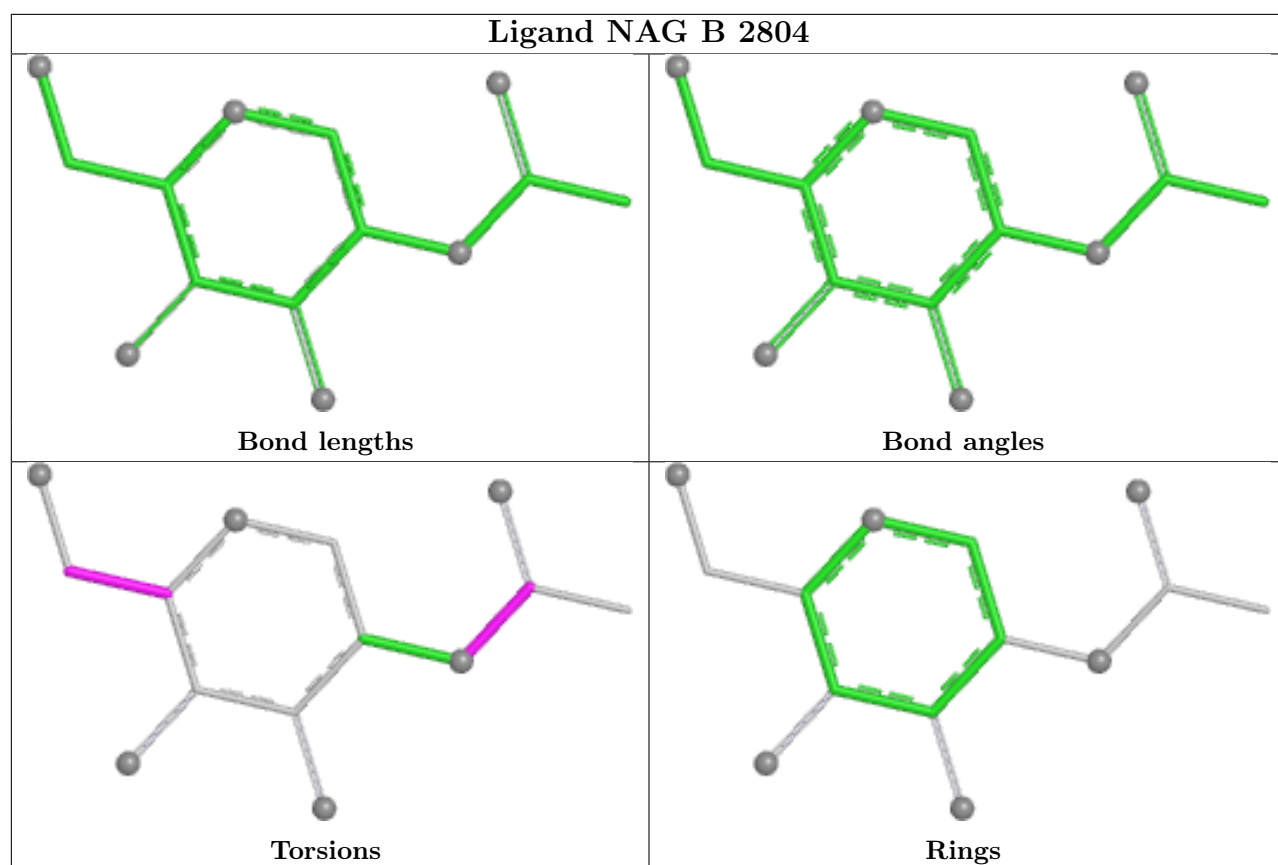


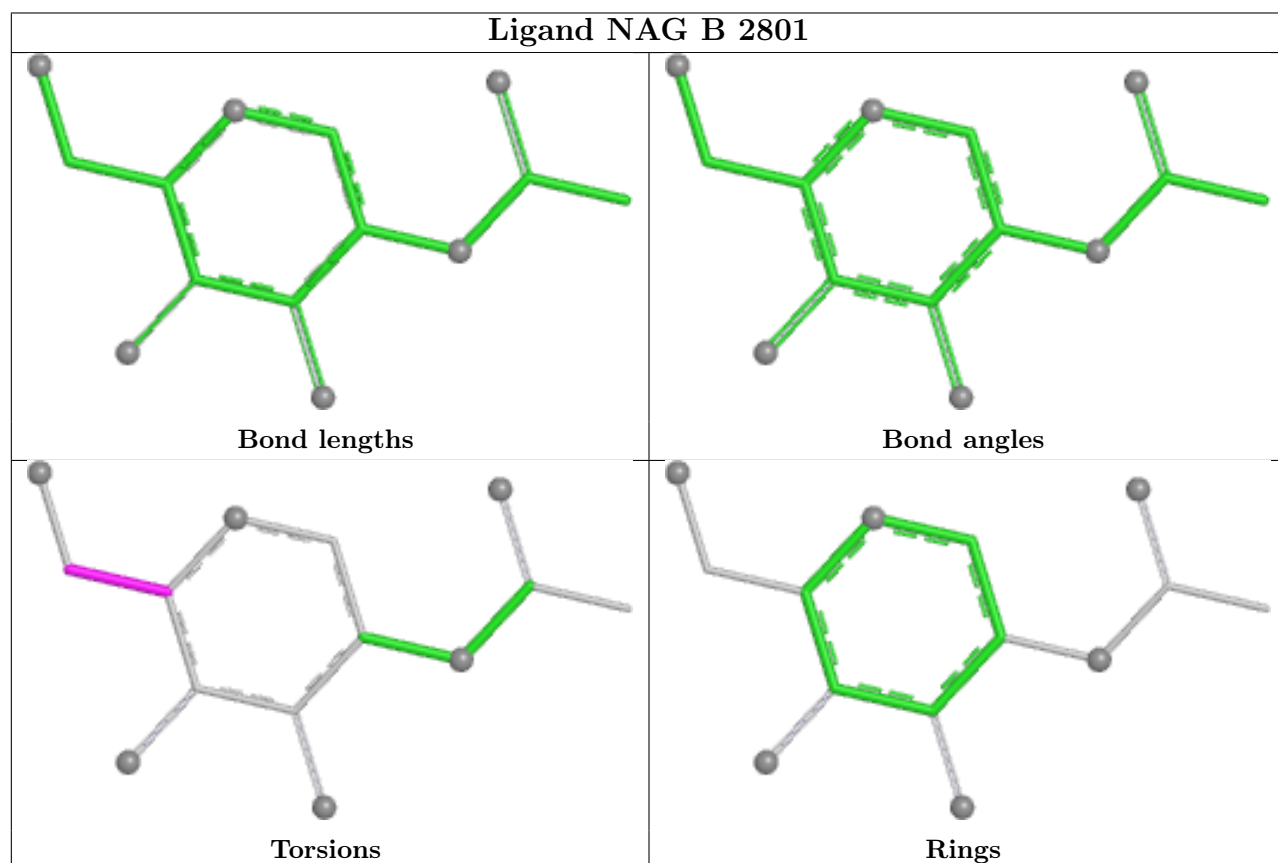
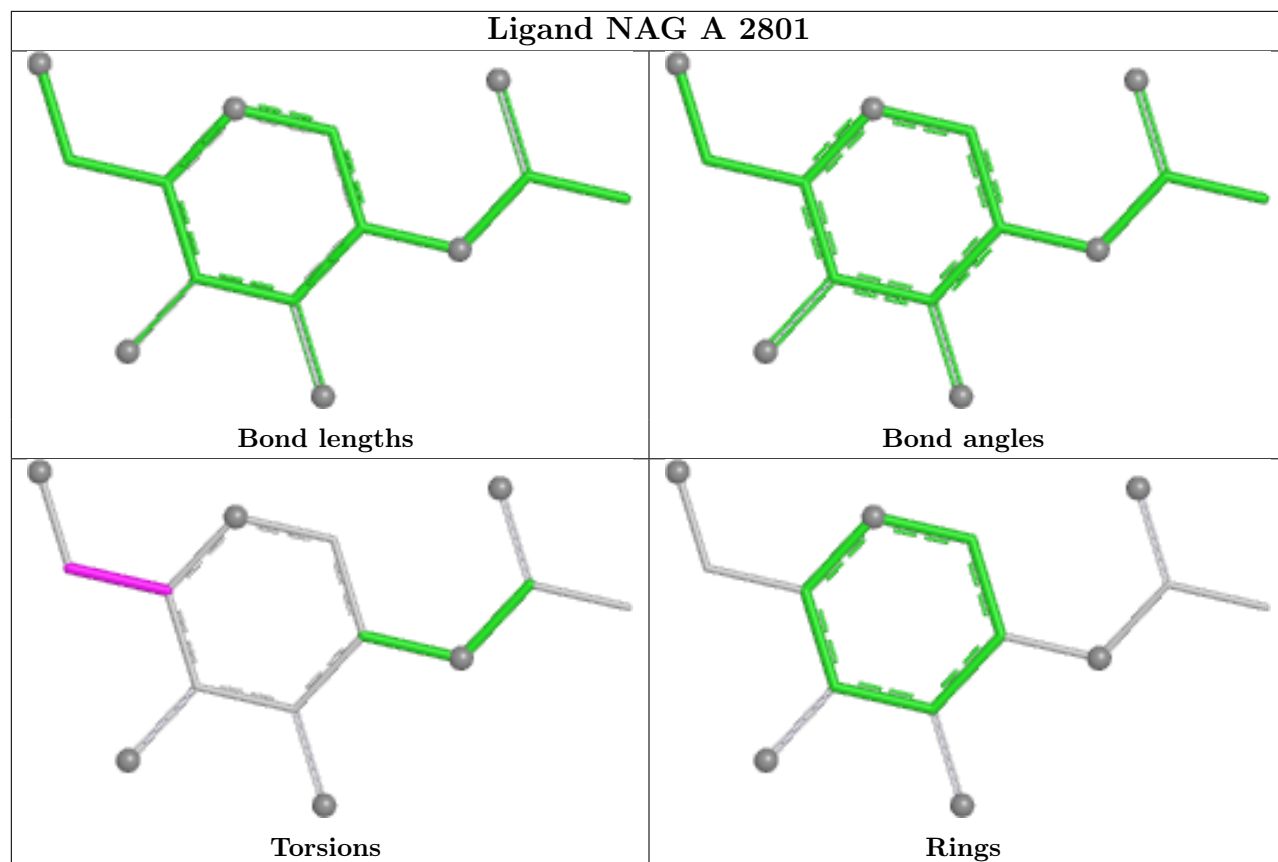
Ligand NAG B 2803



Ligand NAG A 2804







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

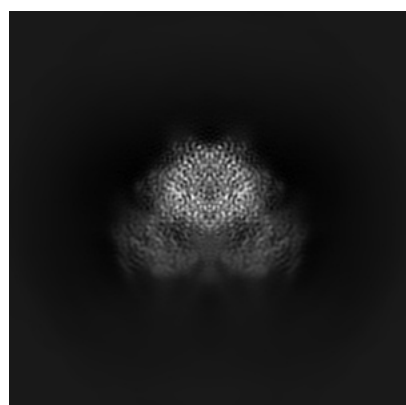
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12125. These allow visual inspection of the internal detail of the map and identification of artifacts.

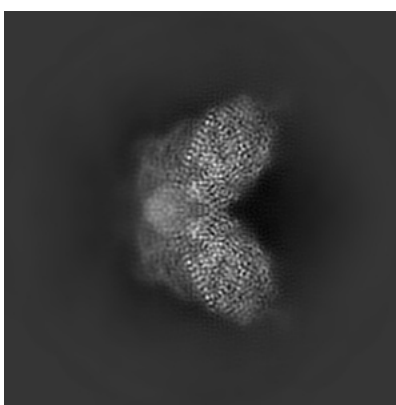
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

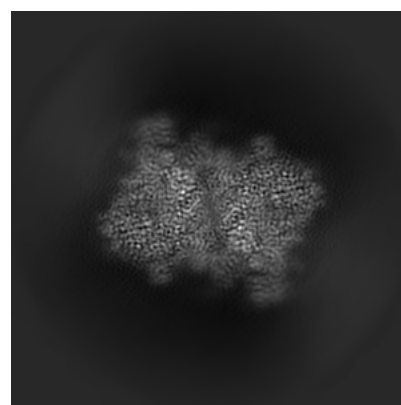
6.1.1 Primary map



X



Y



Z

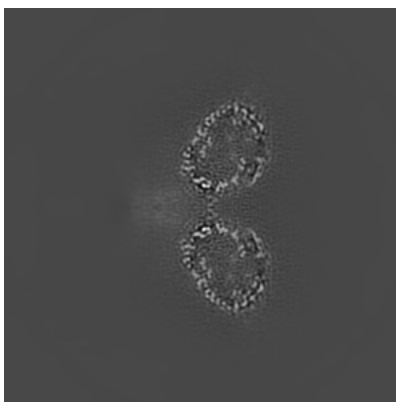
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

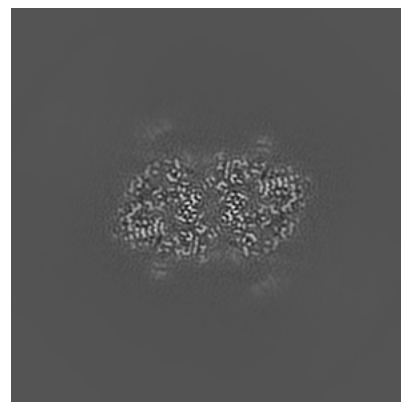
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

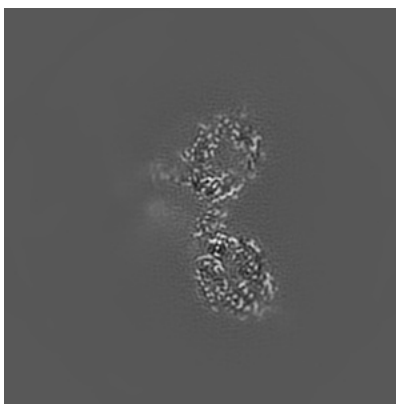
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

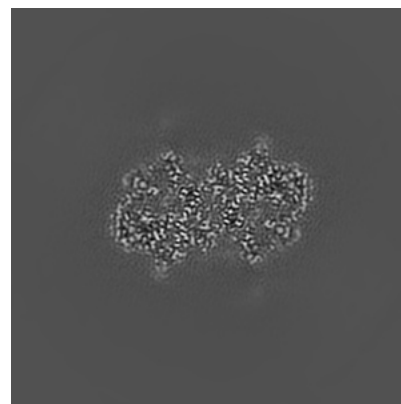
6.3.1 Primary map



X Index: 210



Y Index: 165

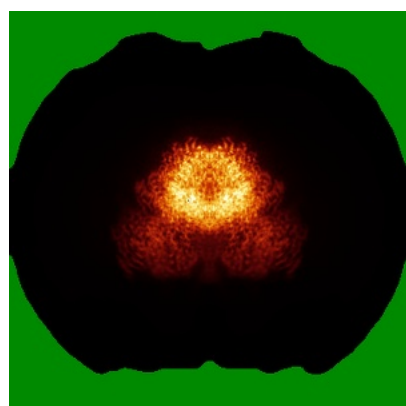


Z Index: 186

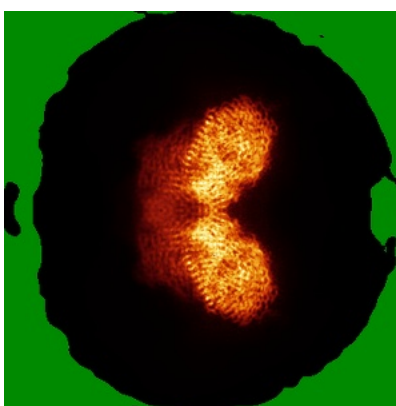
The images above show the largest variance slices of the map in three orthogonal directions.

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

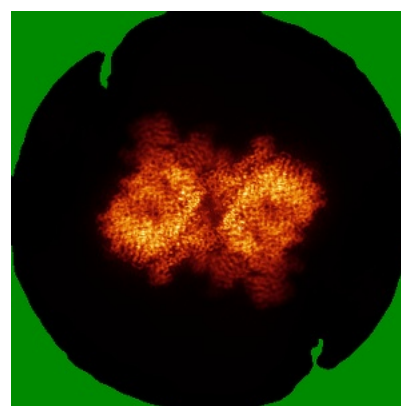
6.4.1 Primary map



X



Y

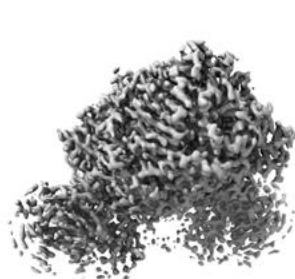


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

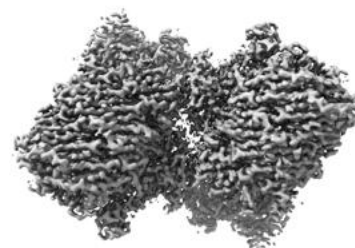
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

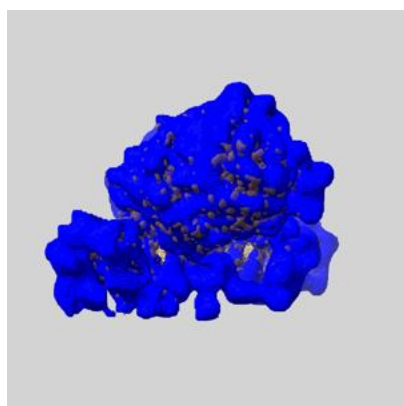
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

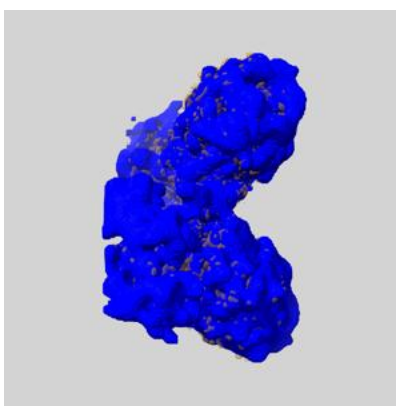
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

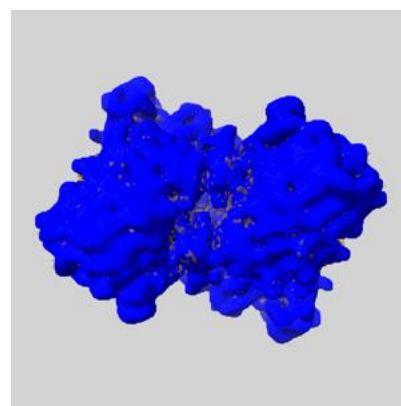
6.6.1 emd_12125_msk_1.map [i](#)



X



Y

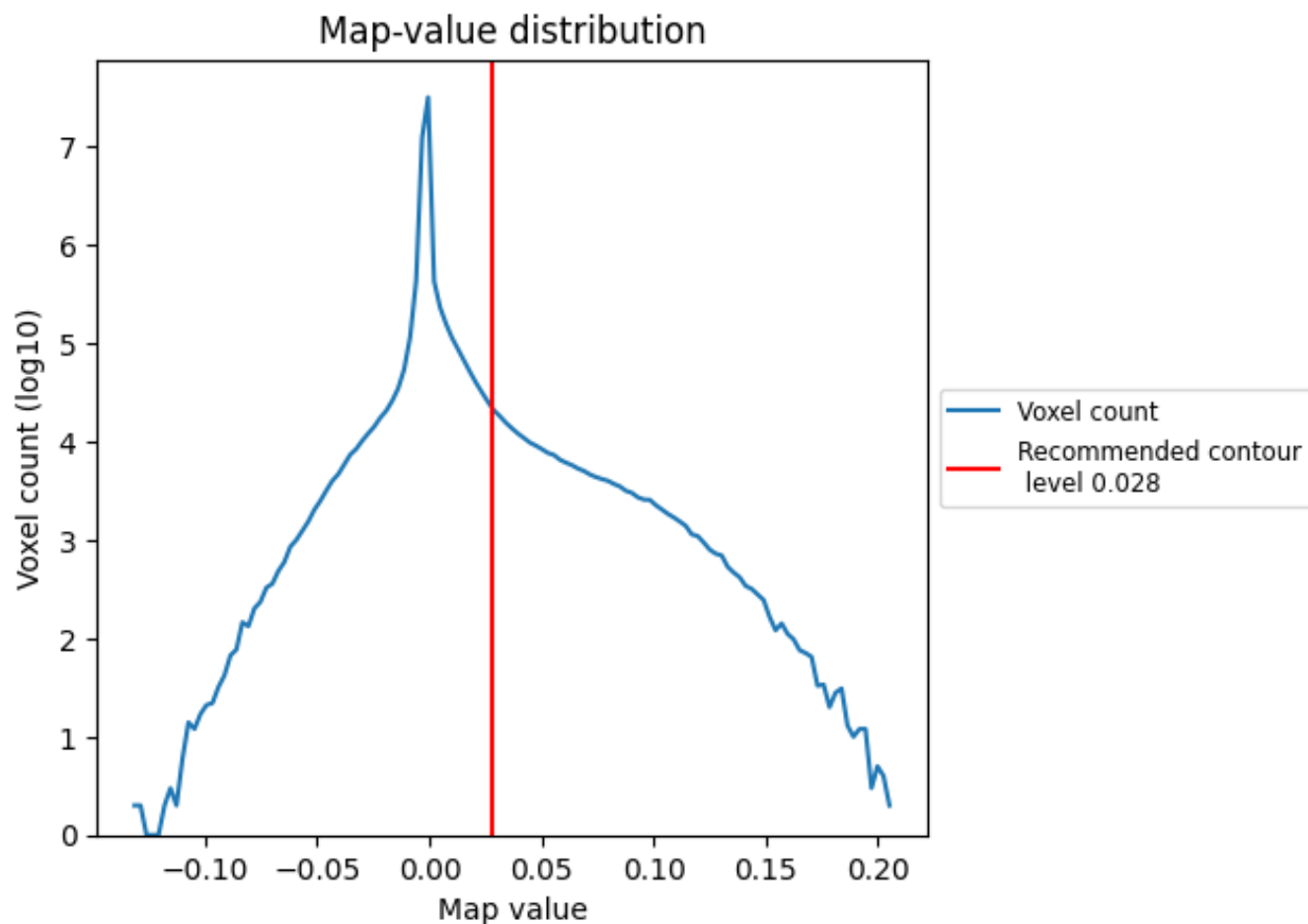


Z

7 Map analysis [i](#)

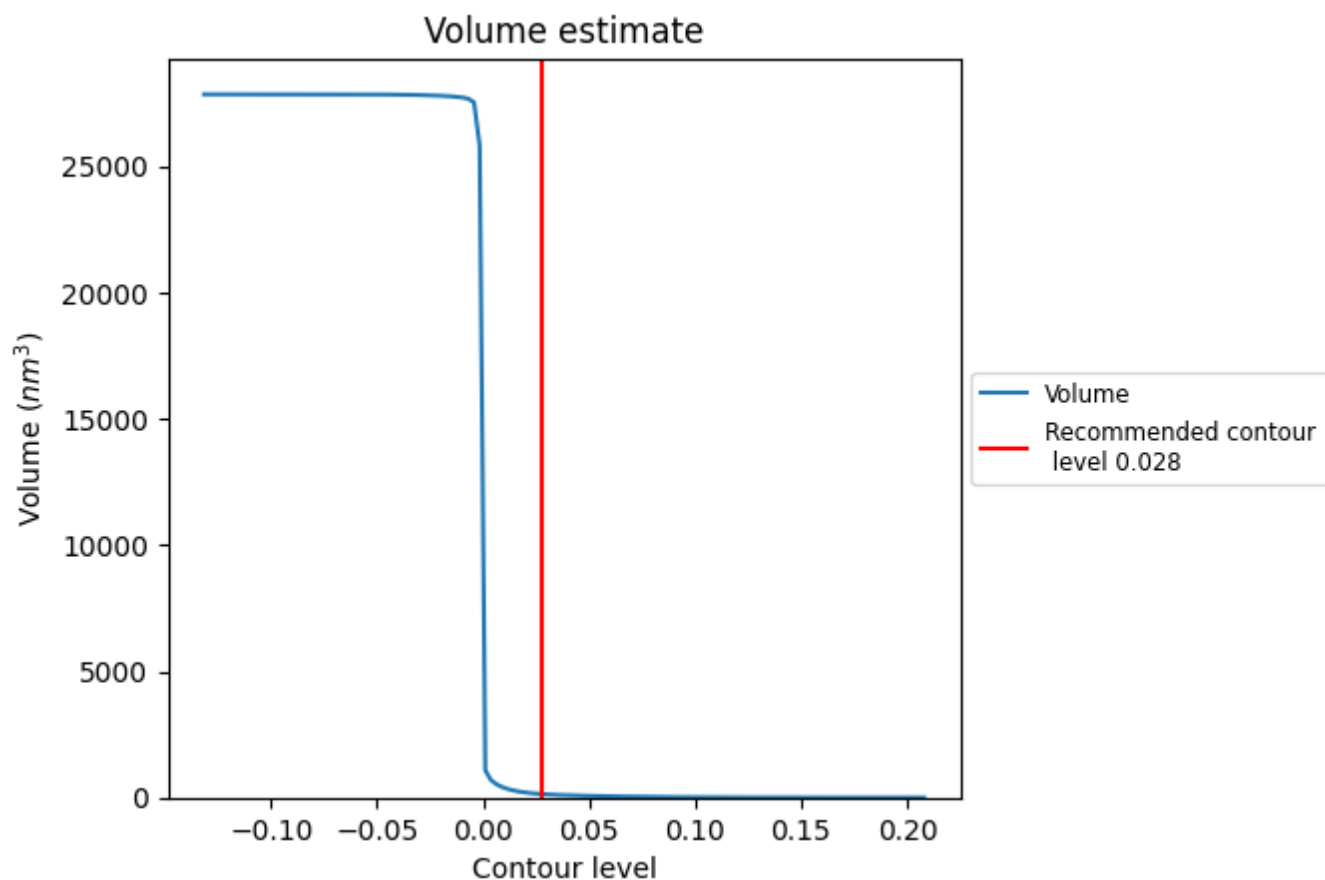
This section contains the results of statistical analysis of the map.

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.

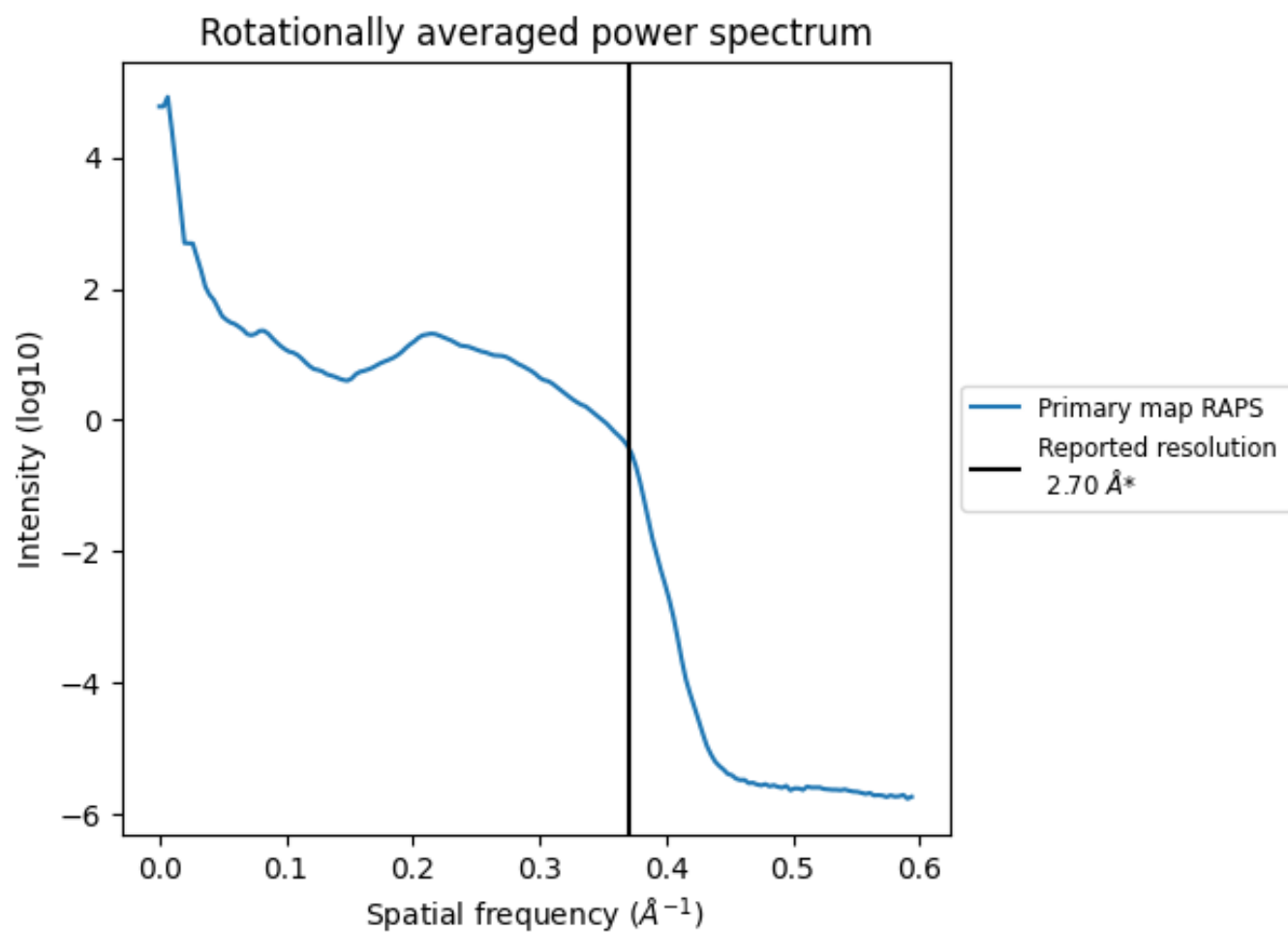
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm^3 ; this corresponds to an approximate mass of 124 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 ⓘ

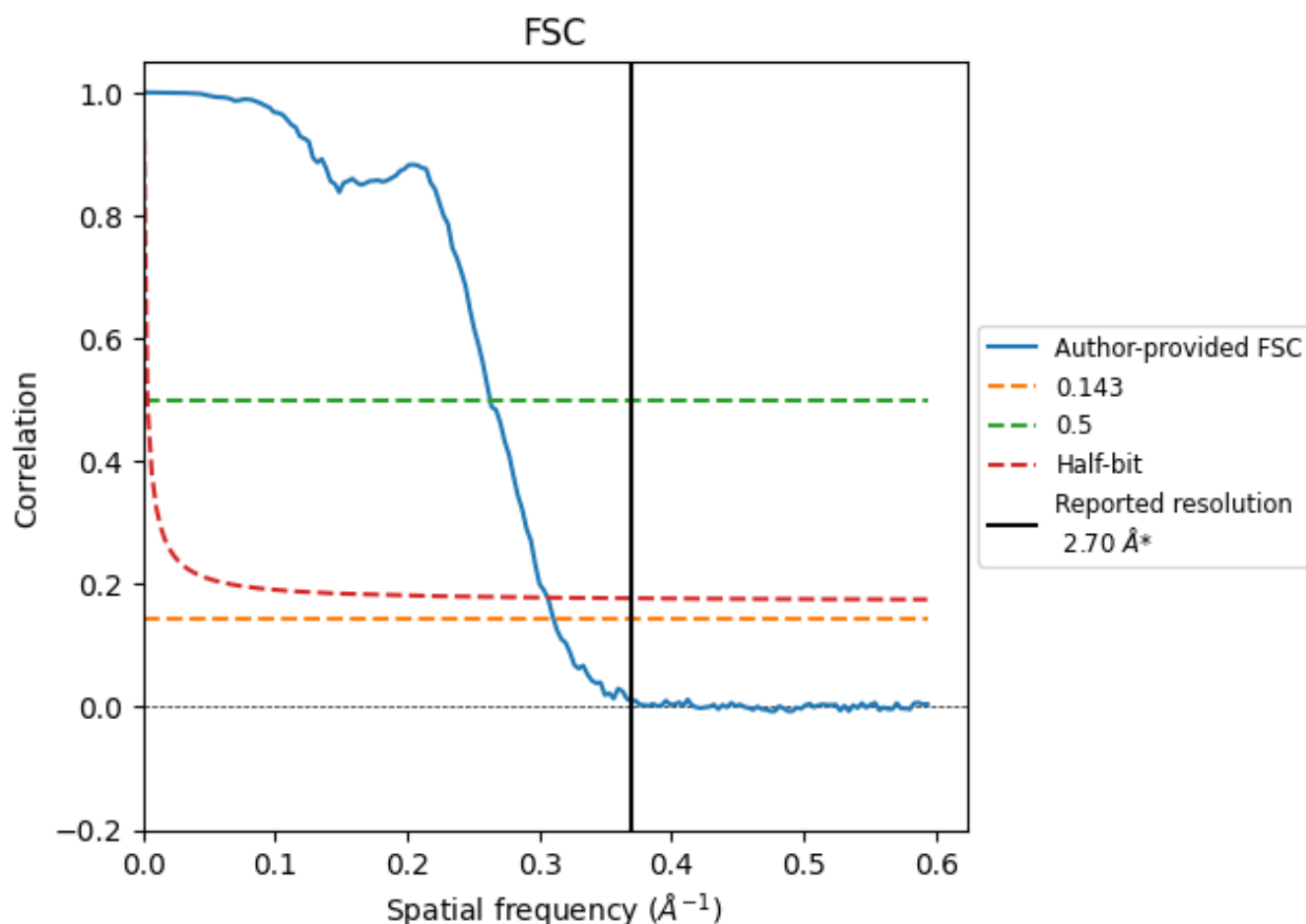


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

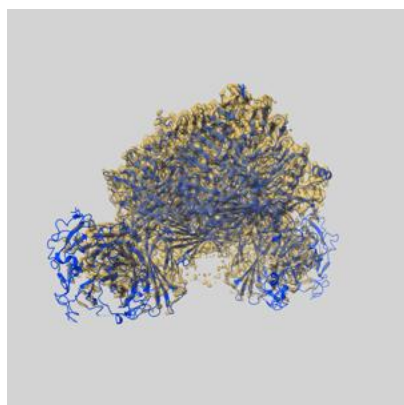
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	3.22	3.81	3.27
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.22 differs from the reported value 2.7 by more than 10 %

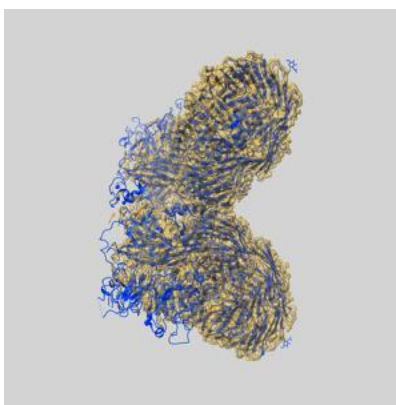
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12125 and PDB model 7BAN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

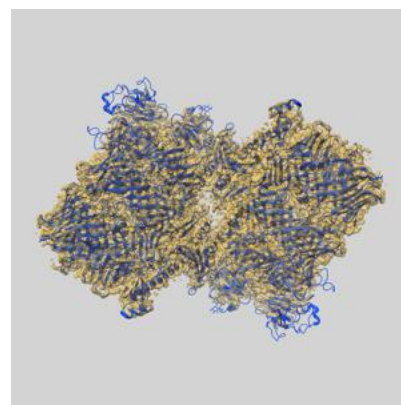
9.1 Map-model overlay [i](#)



X



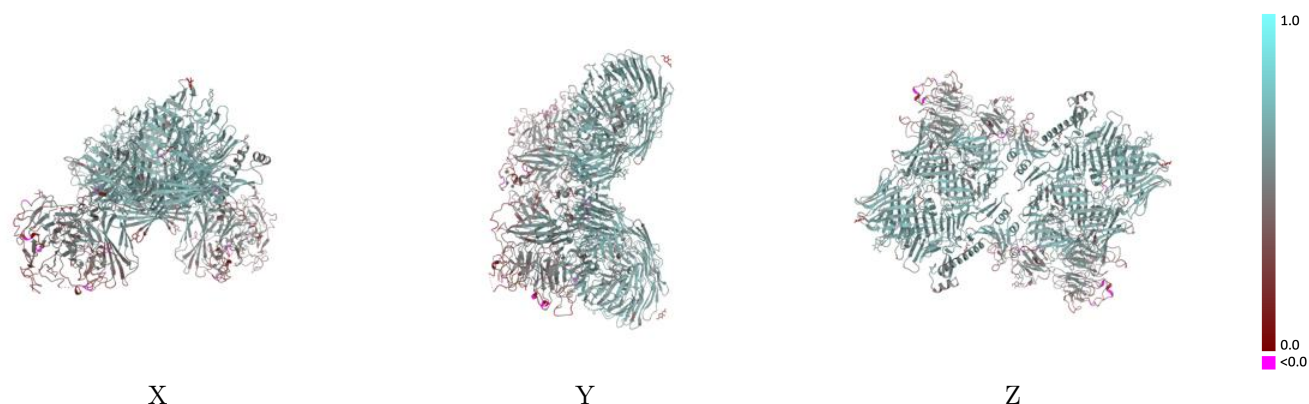
Y



Z

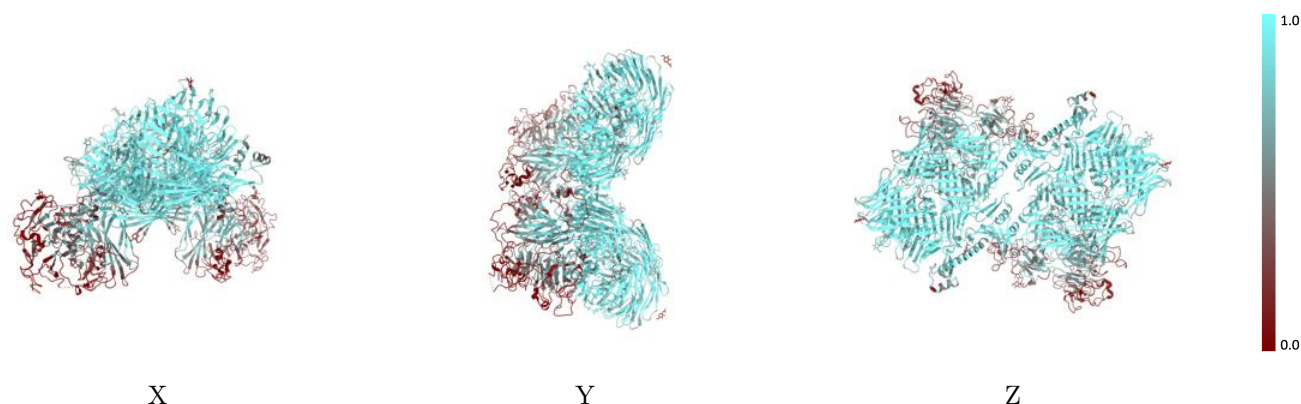
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



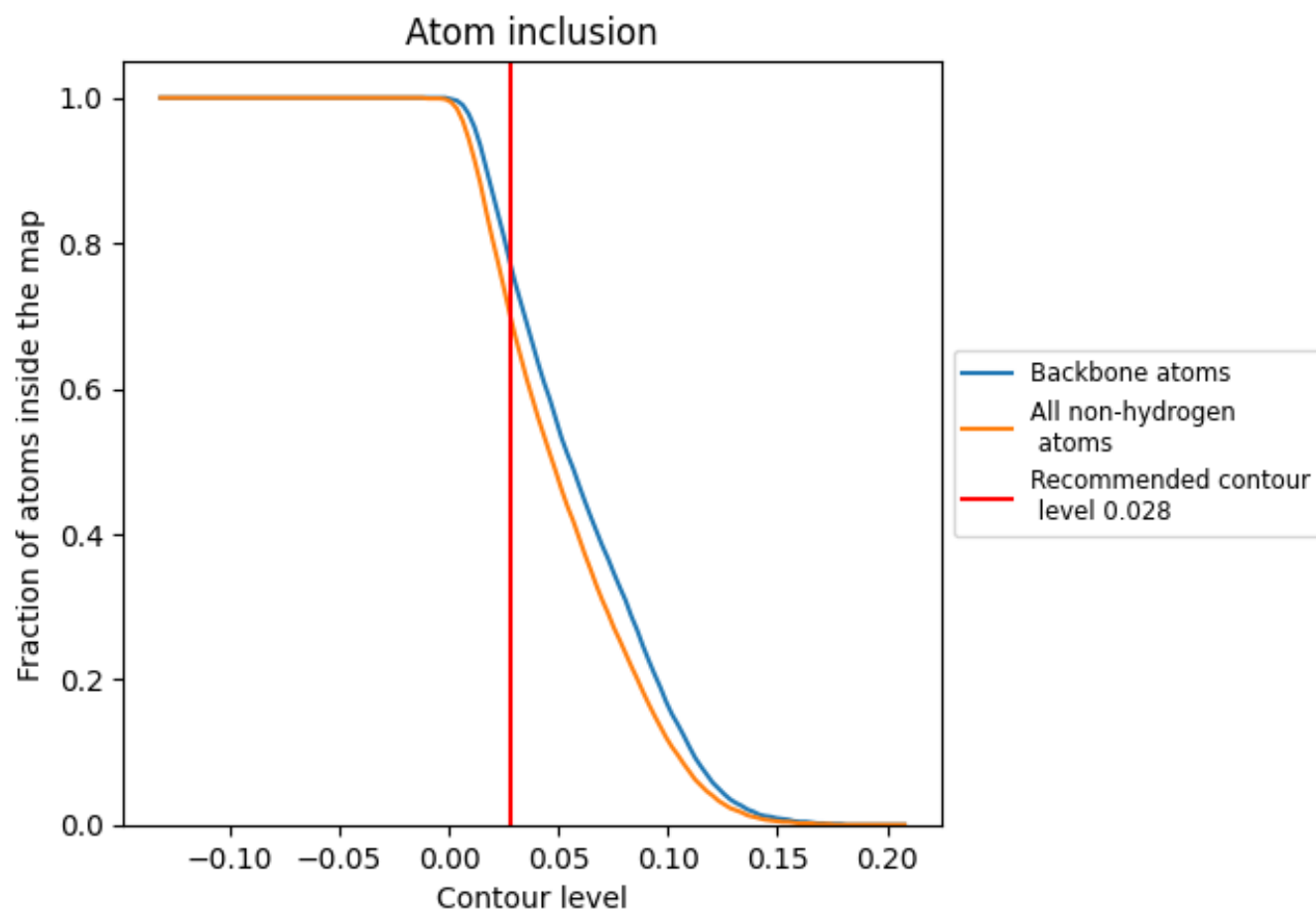
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 70% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7010	0.5360
A	0.7020	0.5360
B	0.7030	0.5370
C	0.7140	0.5510
D	0.7500	0.6100
E	0.7140	0.5620
F	0.1430	0.3530
G	0.7140	0.5450
H	0.7500	0.6030
I	0.7500	0.5530
J	0.1430	0.3670

1.0
0.0
<0.0