



wwPDB EM Validation Summary Report ⓘ

Jun 27, 2024 – 12:10 PM JST

PDB ID : 8XNF
EMDB ID : EMD-38502
Title : Cryo-EM structure of SARS-CoV-2 Omicron BA.2.86 spike protein(6P) in complex with human ACE2
Authors : Li, L.J.; Gu, Y.H.; Shi, K.Y.; Qi, J.X.; Gao, G.F.
Deposited on : 2023-12-29
Resolution : 3.26 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

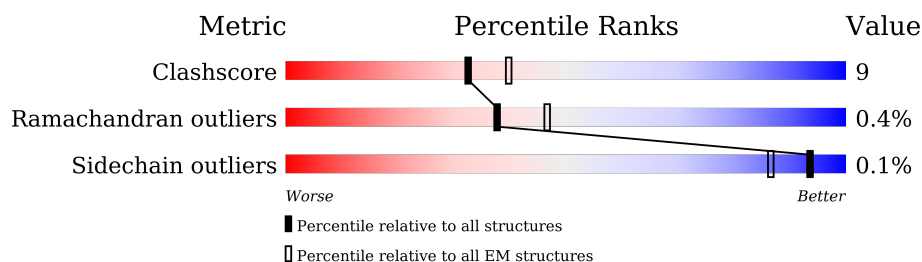
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 Å.

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



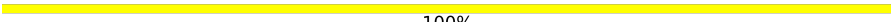

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	603	<div> <div>69%</div> <div>89%</div> <div>9%</div> </div>
2	B	1191	<div> <div>5%</div> <div>68%</div> <div>15%</div> <div>16%</div> </div>
2	C	1191	<div> <div>14%</div> <div>70%</div> <div>15%</div> <div>15%</div> </div>
2	D	1191	<div> <div>14%</div> <div>70%</div> <div>15%</div> <div>15%</div> </div>
3	E	3	<div> <div>100%</div> </div>
4	F	2	<div> <div>100%</div> </div>
4	G	2	<div> <div>100%</div> </div>
4	H	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	I	2	 100%
4	J	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	D	1207	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29301 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	596	Total	C	N	O	S	1	0
			4869	3116	807	917	29		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	HIS	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1001	Total	C	N	O	S	0	0
			7853	5037	1302	1480	34		
2	C	1015	Total	C	N	O	S	0	0
			7965	5107	1318	1504	36		
2	D	1016	Total	C	N	O	S	0	0
			7972	5111	1319	1506	36		

There are 417 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P0DTC2
B	2	PHE	-	expression tag	UNP P0DTC2
B	3	VAL	-	expression tag	UNP P0DTC2
B	4	PHE	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	VAL	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	LEU	-	expression tag	UNP P0DTC2
B	9	PRO	-	expression tag	UNP P0DTC2
B	10	LEU	-	expression tag	UNP P0DTC2
B	11	VAL	-	expression tag	UNP P0DTC2
B	12	SER	-	expression tag	UNP P0DTC2
B	13	SER	-	expression tag	UNP P0DTC2
B	14	GLN	-	expression tag	UNP P0DTC2
B	15	CYS	-	expression tag	UNP P0DTC2
B	16	VAL	-	expression tag	UNP P0DTC2
B	17	MET	-	expression tag	UNP P0DTC2
B	18	PRO	-	expression tag	UNP P0DTC2
B	19	LEU	-	expression tag	UNP P0DTC2
B	20	PHE	-	expression tag	UNP P0DTC2
B	21	ASN	-	expression tag	UNP P0DTC2
B	22	LEU	-	expression tag	UNP P0DTC2
B	23	ILE	-	expression tag	UNP P0DTC2
B	24	THR	-	expression tag	UNP P0DTC2
B	25	THR	-	expression tag	UNP P0DTC2
B	26	THR	-	expression tag	UNP P0DTC2
B	27	GLN	-	expression tag	UNP P0DTC2
B	28	SER	-	expression tag	UNP P0DTC2
B	51	LEU	SER	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	variant	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	variant	UNP P0DTC2
B	158	GLY	ARG	variant	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	variant	UNP P0DTC2
B	245	ASN	HIS	variant	UNP P0DTC2
B	264	ASP	ALA	variant	UNP P0DTC2
B	332	VAL	ILE	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	356	THR	LYS	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	403	LYS	ARG	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	HIS	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	variant	UNP P0DTC2
B	452	TRP	LEU	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	481	LYS	ASN	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	483	LYS	GLU	variant	UNP P0DTC2
B	485	PRO	PHE	variant	UNP P0DTC2
B	497	ARG	GLN	variant	UNP P0DTC2
B	500	TYR	ASN	variant	UNP P0DTC2
B	504	HIS	TYR	variant	UNP P0DTC2
B	553	LYS	GLU	variant	UNP P0DTC2
B	569	VAL	ALA	variant	UNP P0DTC2
B	613	GLY	ASP	variant	UNP P0DTC2
B	620	SER	PRO	variant	UNP P0DTC2
B	654	TYR	HIS	variant	UNP P0DTC2
B	669	VAL	ILE	variant	UNP P0DTC2
B	678	LYS	ASN	variant	UNP P0DTC2
B	680	ARG	PRO	variant	UNP P0DTC2
B	681	GLY	ARG	engineered mutation	UNP P0DTC2
B	682	SER	ARG	engineered mutation	UNP P0DTC2
B	684	SER	ARG	engineered mutation	UNP P0DTC2
B	763	LYS	ASN	variant	UNP P0DTC2
B	795	TYR	ASP	variant	UNP P0DTC2
B	816	PRO	PHE	engineered mutation	UNP P0DTC2
B	891	PRO	ALA	engineered mutation	UNP P0DTC2
B	898	PRO	ALA	engineered mutation	UNP P0DTC2
B	938	PHE	SER	variant	UNP P0DTC2
B	941	PRO	ALA	engineered mutation	UNP P0DTC2
B	953	HIS	GLN	variant	UNP P0DTC2
B	968	LYS	ASN	variant	UNP P0DTC2
B	985	PRO	LYS	engineered mutation	UNP P0DTC2
B	986	PRO	VAL	engineered mutation	UNP P0DTC2
B	1142	LEU	PRO	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1147	GLY	-	expression tag	UNP P0DTC2
B	1148	GLY	-	expression tag	UNP P0DTC2
B	1149	GLY	-	expression tag	UNP P0DTC2
B	1150	SER	-	expression tag	UNP P0DTC2
B	1151	GLY	-	expression tag	UNP P0DTC2
B	1152	GLY	-	expression tag	UNP P0DTC2
B	1153	GLY	-	expression tag	UNP P0DTC2
B	1154	SER	-	expression tag	UNP P0DTC2
B	1155	GLY	-	expression tag	UNP P0DTC2
B	1156	TYR	-	expression tag	UNP P0DTC2
B	1157	ILE	-	expression tag	UNP P0DTC2
B	1158	PRO	-	expression tag	UNP P0DTC2
B	1159	GLU	-	expression tag	UNP P0DTC2
B	1160	ALA	-	expression tag	UNP P0DTC2
B	1161	PRO	-	expression tag	UNP P0DTC2
B	1162	ARG	-	expression tag	UNP P0DTC2
B	1163	ASP	-	expression tag	UNP P0DTC2
B	1164	GLY	-	expression tag	UNP P0DTC2
B	1165	GLN	-	expression tag	UNP P0DTC2
B	1166	ALA	-	expression tag	UNP P0DTC2
B	1167	TYR	-	expression tag	UNP P0DTC2
B	1168	VAL	-	expression tag	UNP P0DTC2
B	1169	ARG	-	expression tag	UNP P0DTC2
B	1170	LYS	-	expression tag	UNP P0DTC2
B	1171	ASP	-	expression tag	UNP P0DTC2
B	1172	GLY	-	expression tag	UNP P0DTC2
B	1173	GLU	-	expression tag	UNP P0DTC2
B	1174	TRP	-	expression tag	UNP P0DTC2
B	1175	VAL	-	expression tag	UNP P0DTC2
B	1176	LEU	-	expression tag	UNP P0DTC2
B	1177	LEU	-	expression tag	UNP P0DTC2
B	1178	SER	-	expression tag	UNP P0DTC2
B	1179	THR	-	expression tag	UNP P0DTC2
B	1180	PHE	-	expression tag	UNP P0DTC2
B	1181	LEU	-	expression tag	UNP P0DTC2
B	1182	GLY	-	expression tag	UNP P0DTC2
B	1183	GLY	-	expression tag	UNP P0DTC2
B	1184	GLY	-	expression tag	UNP P0DTC2
B	1185	SER	-	expression tag	UNP P0DTC2
B	1186	ALA	-	expression tag	UNP P0DTC2
B	1187	TRP	-	expression tag	UNP P0DTC2
B	1188	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1189	HIS	-	expression tag	UNP P0DTC2
B	1190	PRO	-	expression tag	UNP P0DTC2
B	1191	GLN	-	expression tag	UNP P0DTC2
B	1192	PHE	-	expression tag	UNP P0DTC2
B	1193	GLU	-	expression tag	UNP P0DTC2
B	1194	LYS	-	expression tag	UNP P0DTC2
C	1	MET	-	initiating methionine	UNP P0DTC2
C	2	PHE	-	expression tag	UNP P0DTC2
C	3	VAL	-	expression tag	UNP P0DTC2
C	4	PHE	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	VAL	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	LEU	-	expression tag	UNP P0DTC2
C	9	PRO	-	expression tag	UNP P0DTC2
C	10	LEU	-	expression tag	UNP P0DTC2
C	11	VAL	-	expression tag	UNP P0DTC2
C	12	SER	-	expression tag	UNP P0DTC2
C	13	SER	-	expression tag	UNP P0DTC2
C	14	GLN	-	expression tag	UNP P0DTC2
C	15	CYS	-	expression tag	UNP P0DTC2
C	16	VAL	-	expression tag	UNP P0DTC2
C	17	MET	-	expression tag	UNP P0DTC2
C	18	PRO	-	expression tag	UNP P0DTC2
C	19	LEU	-	expression tag	UNP P0DTC2
C	20	PHE	-	expression tag	UNP P0DTC2
C	21	ASN	-	expression tag	UNP P0DTC2
C	22	LEU	-	expression tag	UNP P0DTC2
C	23	ILE	-	expression tag	UNP P0DTC2
C	24	THR	-	expression tag	UNP P0DTC2
C	25	THR	-	expression tag	UNP P0DTC2
C	26	THR	-	expression tag	UNP P0DTC2
C	27	GLN	-	expression tag	UNP P0DTC2
C	28	SER	-	expression tag	UNP P0DTC2
C	51	LEU	SER	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	variant	UNP P0DTC2
C	158	GLY	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	variant	UNP P0DTC2
C	245	ASN	HIS	variant	UNP P0DTC2
C	264	ASP	ALA	variant	UNP P0DTC2
C	332	VAL	ILE	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	356	THR	LYS	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	HIS	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	variant	UNP P0DTC2
C	452	TRP	LEU	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	483	LYS	GLU	variant	UNP P0DTC2
C	485	PRO	PHE	variant	UNP P0DTC2
C	497	ARG	GLN	variant	UNP P0DTC2
C	500	TYR	ASN	variant	UNP P0DTC2
C	504	HIS	TYR	variant	UNP P0DTC2
C	553	LYS	GLU	variant	UNP P0DTC2
C	569	VAL	ALA	variant	UNP P0DTC2
C	613	GLY	ASP	variant	UNP P0DTC2
C	620	SER	PRO	variant	UNP P0DTC2
C	654	TYR	HIS	variant	UNP P0DTC2
C	669	VAL	ILE	variant	UNP P0DTC2
C	678	LYS	ASN	variant	UNP P0DTC2
C	680	ARG	PRO	variant	UNP P0DTC2
C	681	GLY	ARG	engineered mutation	UNP P0DTC2
C	682	SER	ARG	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	684	SER	ARG	engineered mutation	UNP P0DTC2
C	763	LYS	ASN	variant	UNP P0DTC2
C	795	TYR	ASP	variant	UNP P0DTC2
C	816	PRO	PHE	engineered mutation	UNP P0DTC2
C	891	PRO	ALA	engineered mutation	UNP P0DTC2
C	898	PRO	ALA	engineered mutation	UNP P0DTC2
C	938	PHE	SER	variant	UNP P0DTC2
C	941	PRO	ALA	engineered mutation	UNP P0DTC2
C	953	HIS	GLN	variant	UNP P0DTC2
C	968	LYS	ASN	variant	UNP P0DTC2
C	985	PRO	LYS	engineered mutation	UNP P0DTC2
C	986	PRO	VAL	engineered mutation	UNP P0DTC2
C	1142	LEU	PRO	variant	UNP P0DTC2
C	1147	GLY	-	expression tag	UNP P0DTC2
C	1148	GLY	-	expression tag	UNP P0DTC2
C	1149	GLY	-	expression tag	UNP P0DTC2
C	1150	SER	-	expression tag	UNP P0DTC2
C	1151	GLY	-	expression tag	UNP P0DTC2
C	1152	GLY	-	expression tag	UNP P0DTC2
C	1153	GLY	-	expression tag	UNP P0DTC2
C	1154	SER	-	expression tag	UNP P0DTC2
C	1155	GLY	-	expression tag	UNP P0DTC2
C	1156	TYR	-	expression tag	UNP P0DTC2
C	1157	ILE	-	expression tag	UNP P0DTC2
C	1158	PRO	-	expression tag	UNP P0DTC2
C	1159	GLU	-	expression tag	UNP P0DTC2
C	1160	ALA	-	expression tag	UNP P0DTC2
C	1161	PRO	-	expression tag	UNP P0DTC2
C	1162	ARG	-	expression tag	UNP P0DTC2
C	1163	ASP	-	expression tag	UNP P0DTC2
C	1164	GLY	-	expression tag	UNP P0DTC2
C	1165	GLN	-	expression tag	UNP P0DTC2
C	1166	ALA	-	expression tag	UNP P0DTC2
C	1167	TYR	-	expression tag	UNP P0DTC2
C	1168	VAL	-	expression tag	UNP P0DTC2
C	1169	ARG	-	expression tag	UNP P0DTC2
C	1170	LYS	-	expression tag	UNP P0DTC2
C	1171	ASP	-	expression tag	UNP P0DTC2
C	1172	GLY	-	expression tag	UNP P0DTC2
C	1173	GLU	-	expression tag	UNP P0DTC2
C	1174	TRP	-	expression tag	UNP P0DTC2
C	1175	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1176	LEU	-	expression tag	UNP P0DTC2
C	1177	LEU	-	expression tag	UNP P0DTC2
C	1178	SER	-	expression tag	UNP P0DTC2
C	1179	THR	-	expression tag	UNP P0DTC2
C	1180	PHE	-	expression tag	UNP P0DTC2
C	1181	LEU	-	expression tag	UNP P0DTC2
C	1182	GLY	-	expression tag	UNP P0DTC2
C	1183	GLY	-	expression tag	UNP P0DTC2
C	1184	GLY	-	expression tag	UNP P0DTC2
C	1185	SER	-	expression tag	UNP P0DTC2
C	1186	ALA	-	expression tag	UNP P0DTC2
C	1187	TRP	-	expression tag	UNP P0DTC2
C	1188	SER	-	expression tag	UNP P0DTC2
C	1189	HIS	-	expression tag	UNP P0DTC2
C	1190	PRO	-	expression tag	UNP P0DTC2
C	1191	GLN	-	expression tag	UNP P0DTC2
C	1192	PHE	-	expression tag	UNP P0DTC2
C	1193	GLU	-	expression tag	UNP P0DTC2
C	1194	LYS	-	expression tag	UNP P0DTC2
D	1	MET	-	initiating methionine	UNP P0DTC2
D	2	PHE	-	expression tag	UNP P0DTC2
D	3	VAL	-	expression tag	UNP P0DTC2
D	4	PHE	-	expression tag	UNP P0DTC2
D	5	LEU	-	expression tag	UNP P0DTC2
D	6	VAL	-	expression tag	UNP P0DTC2
D	7	LEU	-	expression tag	UNP P0DTC2
D	8	LEU	-	expression tag	UNP P0DTC2
D	9	PRO	-	expression tag	UNP P0DTC2
D	10	LEU	-	expression tag	UNP P0DTC2
D	11	VAL	-	expression tag	UNP P0DTC2
D	12	SER	-	expression tag	UNP P0DTC2
D	13	SER	-	expression tag	UNP P0DTC2
D	14	GLN	-	expression tag	UNP P0DTC2
D	15	CYS	-	expression tag	UNP P0DTC2
D	16	VAL	-	expression tag	UNP P0DTC2
D	17	MET	-	expression tag	UNP P0DTC2
D	18	PRO	-	expression tag	UNP P0DTC2
D	19	LEU	-	expression tag	UNP P0DTC2
D	20	PHE	-	expression tag	UNP P0DTC2
D	21	ASN	-	expression tag	UNP P0DTC2
D	22	LEU	-	expression tag	UNP P0DTC2
D	23	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	24	THR	-	expression tag	UNP P0DTC2
D	25	THR	-	expression tag	UNP P0DTC2
D	26	THR	-	expression tag	UNP P0DTC2
D	27	GLN	-	expression tag	UNP P0DTC2
D	28	SER	-	expression tag	UNP P0DTC2
D	51	LEU	SER	variant	UNP P0DTC2
D	?	-	HIS	deletion	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	127	PHE	VAL	variant	UNP P0DTC2
D	142	ASP	GLY	variant	UNP P0DTC2
D	?	-	TYR	deletion	UNP P0DTC2
D	157	SER	PHE	variant	UNP P0DTC2
D	158	GLY	ARG	variant	UNP P0DTC2
D	?	-	ASN	deletion	UNP P0DTC2
D	212	ILE	LEU	variant	UNP P0DTC2
D	213	GLY	VAL	variant	UNP P0DTC2
D	216	PHE	LEU	variant	UNP P0DTC2
D	245	ASN	HIS	variant	UNP P0DTC2
D	264	ASP	ALA	variant	UNP P0DTC2
D	332	VAL	ILE	variant	UNP P0DTC2
D	339	HIS	GLY	variant	UNP P0DTC2
D	356	THR	LYS	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	403	LYS	ARG	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	445	HIS	VAL	variant	UNP P0DTC2
D	446	SER	GLY	variant	UNP P0DTC2
D	450	ASP	ASN	variant	UNP P0DTC2
D	452	TRP	LEU	variant	UNP P0DTC2
D	460	LYS	ASN	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	481	LYS	ASN	variant	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	483	LYS	GLU	variant	UNP P0DTC2
D	485	PRO	PHE	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	497	ARG	GLN	variant	UNP P0DTC2
D	500	TYR	ASN	variant	UNP P0DTC2
D	504	HIS	TYR	variant	UNP P0DTC2
D	553	LYS	GLU	variant	UNP P0DTC2
D	569	VAL	ALA	variant	UNP P0DTC2
D	613	GLY	ASP	variant	UNP P0DTC2
D	620	SER	PRO	variant	UNP P0DTC2
D	654	TYR	HIS	variant	UNP P0DTC2
D	669	VAL	ILE	variant	UNP P0DTC2
D	678	LYS	ASN	variant	UNP P0DTC2
D	680	ARG	PRO	variant	UNP P0DTC2
D	681	GLY	ARG	engineered mutation	UNP P0DTC2
D	682	SER	ARG	engineered mutation	UNP P0DTC2
D	684	SER	ARG	engineered mutation	UNP P0DTC2
D	763	LYS	ASN	variant	UNP P0DTC2
D	795	TYR	ASP	variant	UNP P0DTC2
D	816	PRO	PHE	engineered mutation	UNP P0DTC2
D	891	PRO	ALA	engineered mutation	UNP P0DTC2
D	898	PRO	ALA	engineered mutation	UNP P0DTC2
D	938	PHE	SER	variant	UNP P0DTC2
D	941	PRO	ALA	engineered mutation	UNP P0DTC2
D	953	HIS	GLN	variant	UNP P0DTC2
D	968	LYS	ASN	variant	UNP P0DTC2
D	985	PRO	LYS	engineered mutation	UNP P0DTC2
D	986	PRO	VAL	engineered mutation	UNP P0DTC2
D	1142	LEU	PRO	variant	UNP P0DTC2
D	1147	GLY	-	expression tag	UNP P0DTC2
D	1148	GLY	-	expression tag	UNP P0DTC2
D	1149	GLY	-	expression tag	UNP P0DTC2
D	1150	SER	-	expression tag	UNP P0DTC2
D	1151	GLY	-	expression tag	UNP P0DTC2
D	1152	GLY	-	expression tag	UNP P0DTC2
D	1153	GLY	-	expression tag	UNP P0DTC2
D	1154	SER	-	expression tag	UNP P0DTC2
D	1155	GLY	-	expression tag	UNP P0DTC2
D	1156	TYR	-	expression tag	UNP P0DTC2
D	1157	ILE	-	expression tag	UNP P0DTC2
D	1158	PRO	-	expression tag	UNP P0DTC2
D	1159	GLU	-	expression tag	UNP P0DTC2
D	1160	ALA	-	expression tag	UNP P0DTC2
D	1161	PRO	-	expression tag	UNP P0DTC2
D	1162	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1163	ASP	-	expression tag	UNP P0DTC2
D	1164	GLY	-	expression tag	UNP P0DTC2
D	1165	GLN	-	expression tag	UNP P0DTC2
D	1166	ALA	-	expression tag	UNP P0DTC2
D	1167	TYR	-	expression tag	UNP P0DTC2
D	1168	VAL	-	expression tag	UNP P0DTC2
D	1169	ARG	-	expression tag	UNP P0DTC2
D	1170	LYS	-	expression tag	UNP P0DTC2
D	1171	ASP	-	expression tag	UNP P0DTC2
D	1172	GLY	-	expression tag	UNP P0DTC2
D	1173	GLU	-	expression tag	UNP P0DTC2
D	1174	TRP	-	expression tag	UNP P0DTC2
D	1175	VAL	-	expression tag	UNP P0DTC2
D	1176	LEU	-	expression tag	UNP P0DTC2
D	1177	LEU	-	expression tag	UNP P0DTC2
D	1178	SER	-	expression tag	UNP P0DTC2
D	1179	THR	-	expression tag	UNP P0DTC2
D	1180	PHE	-	expression tag	UNP P0DTC2
D	1181	LEU	-	expression tag	UNP P0DTC2
D	1182	GLY	-	expression tag	UNP P0DTC2
D	1183	GLY	-	expression tag	UNP P0DTC2
D	1184	GLY	-	expression tag	UNP P0DTC2
D	1185	SER	-	expression tag	UNP P0DTC2
D	1186	ALA	-	expression tag	UNP P0DTC2
D	1187	TRP	-	expression tag	UNP P0DTC2
D	1188	SER	-	expression tag	UNP P0DTC2
D	1189	HIS	-	expression tag	UNP P0DTC2
D	1190	PRO	-	expression tag	UNP P0DTC2
D	1191	GLN	-	expression tag	UNP P0DTC2
D	1192	PHE	-	expression tag	UNP P0DTC2
D	1193	GLU	-	expression tag	UNP P0DTC2
D	1194	LYS	-	expression tag	UNP P0DTC2

- Molecule 3 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
3	E	3	Total	C	N	O	0	0
			39	22	2	15		

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

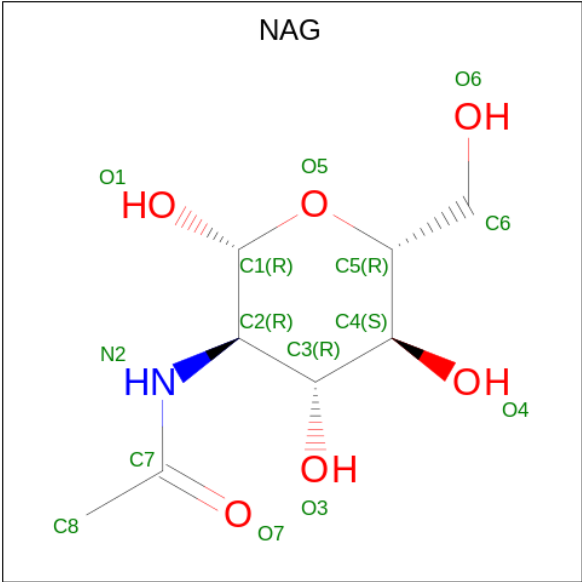


Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

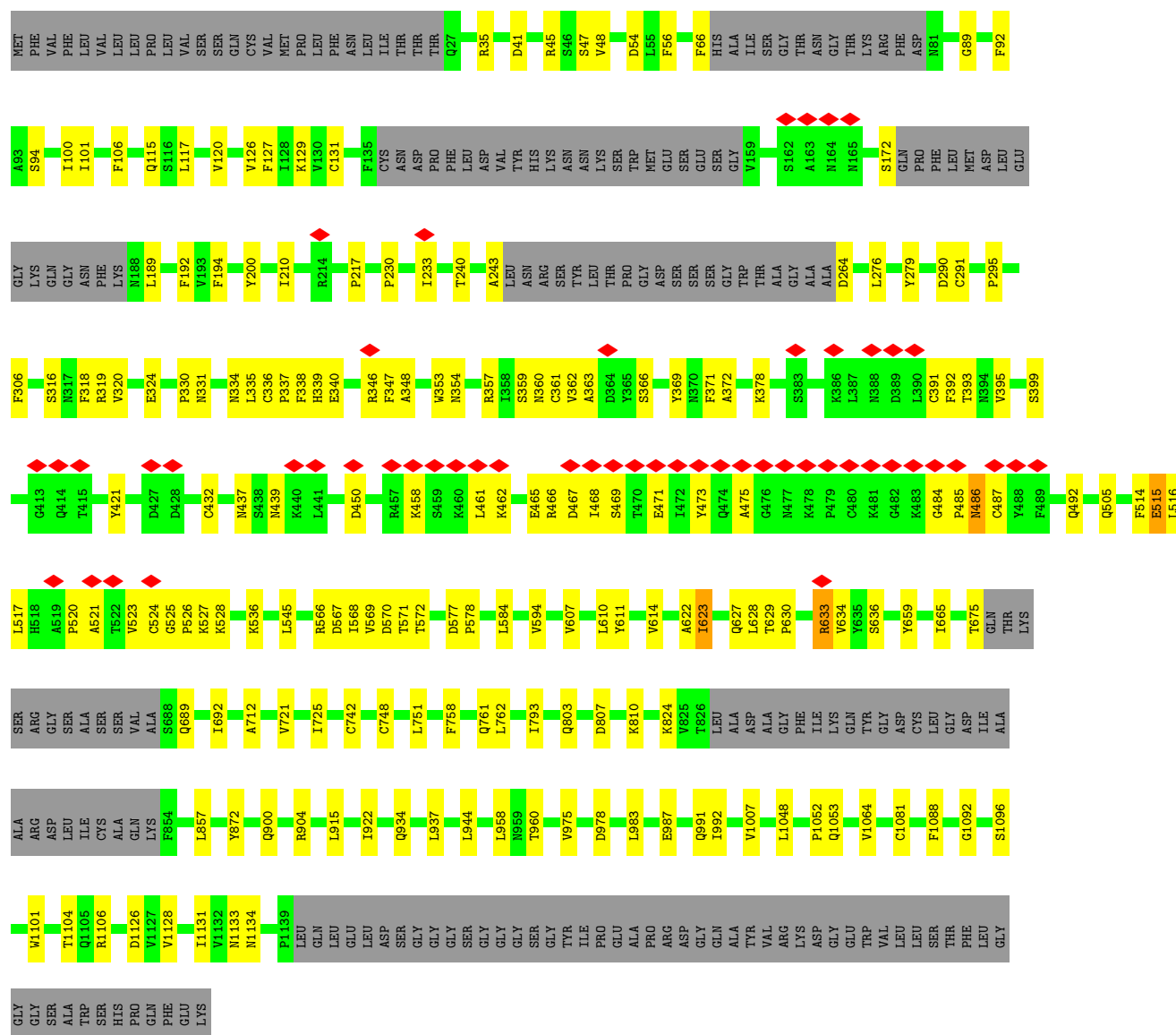


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6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

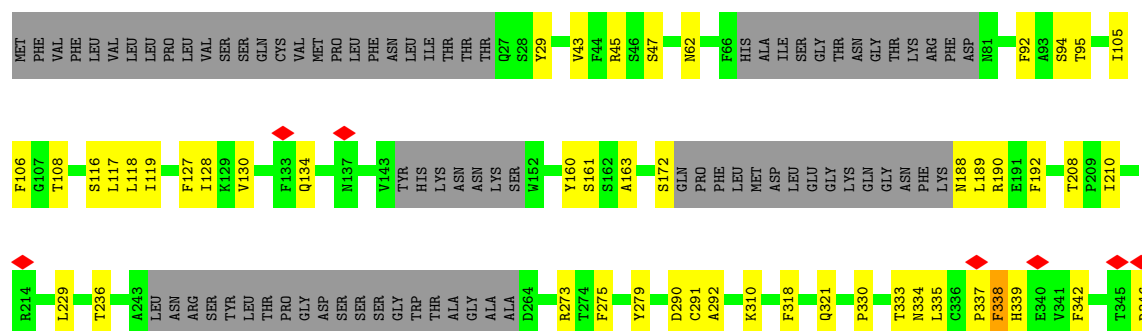
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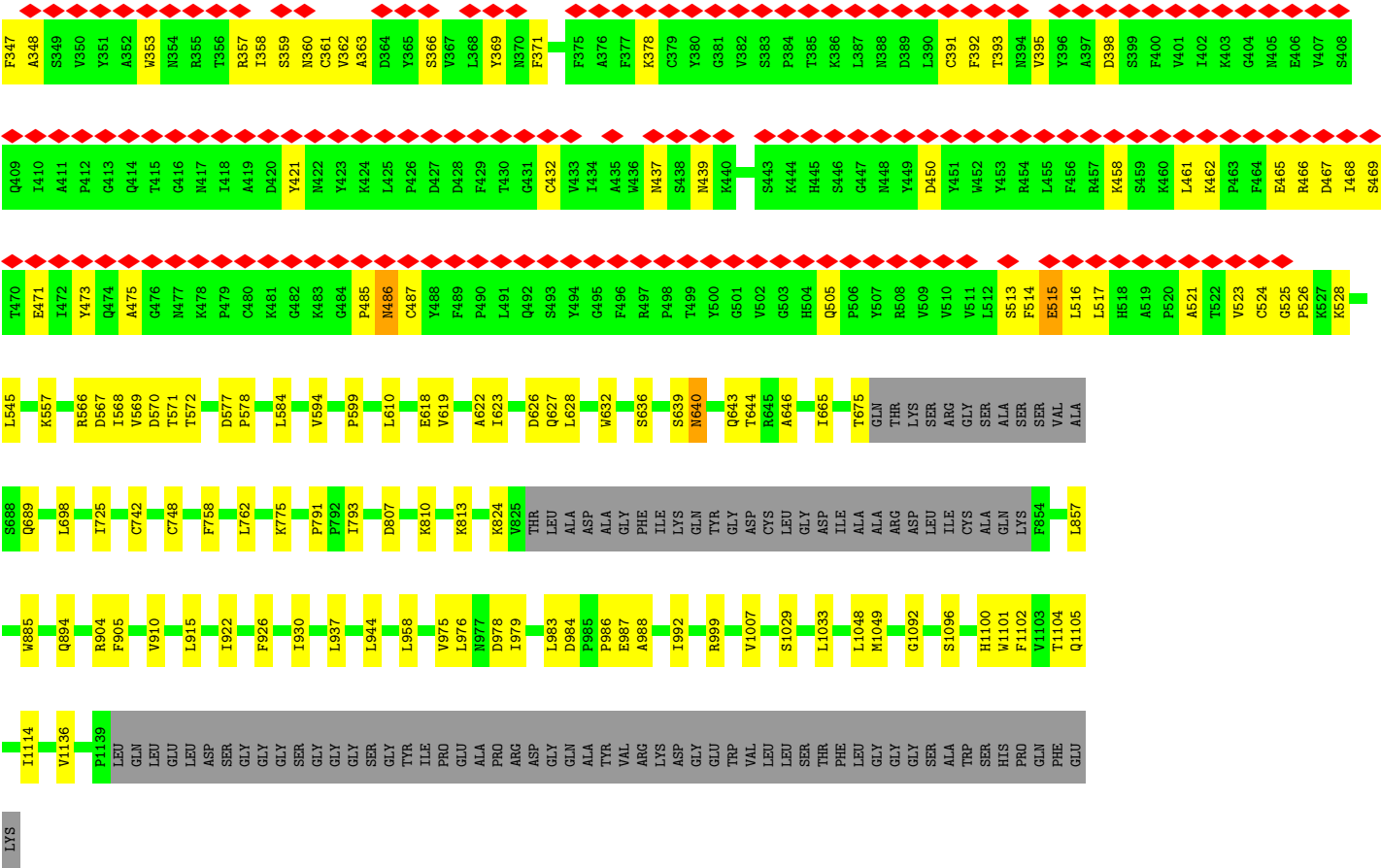
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	D	1	Total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

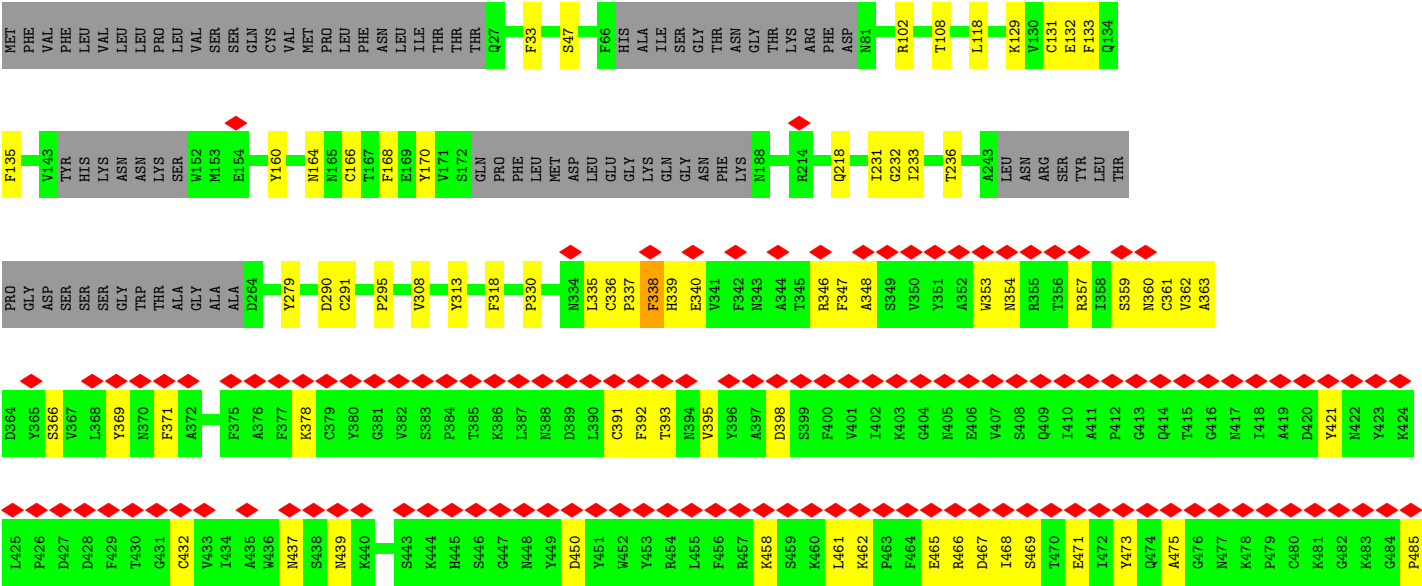


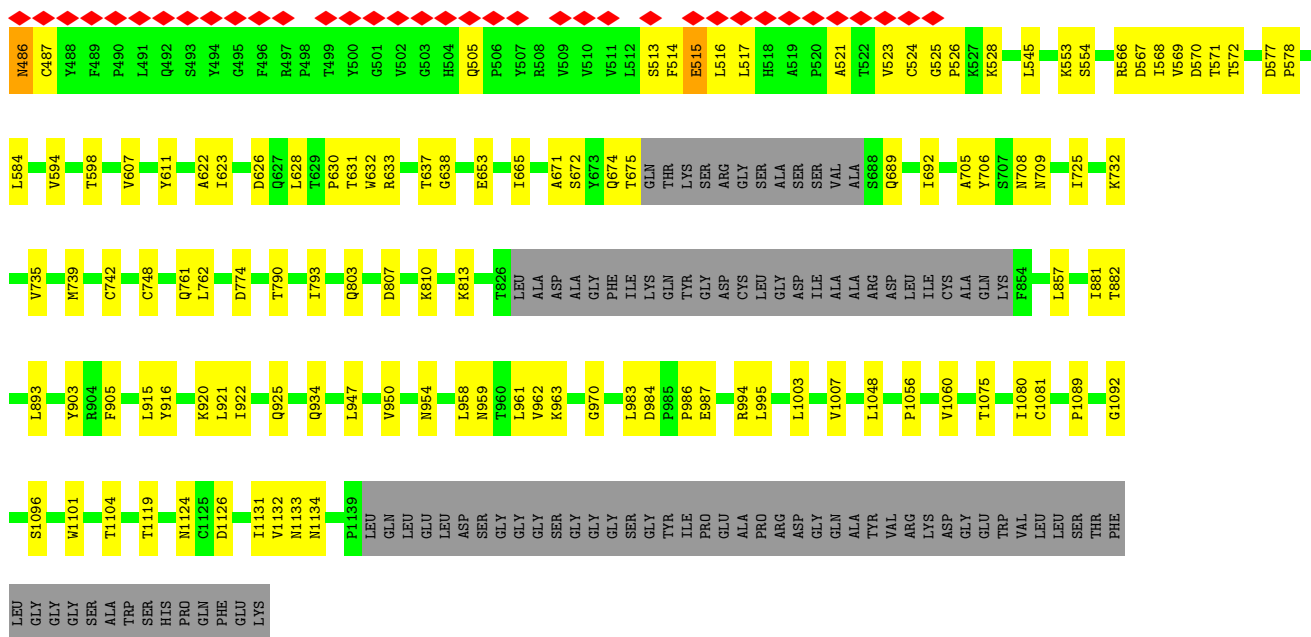
● Molecule 2: Spike glycoprotein





• Molecule 2: Spike glycoprotein





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

Chain E: 100%



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

Chain F:  100%



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

Chain G: 100%



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

Chain H: 100%



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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	313731	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.825	Depositor
Minimum map value	-0.236	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/5010	0.44	0/6807
2	B	0.33	1/8045 (0.0%)	0.52	0/10952
2	C	0.33	1/8161 (0.0%)	0.52	0/11110
2	D	0.34	1/8168 (0.0%)	0.52	0/11120
All	All	0.32	3/29384 (0.0%)	0.51	0/39989

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
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	528	LYS	C-N	-5.06	1.22	1.34
2	B	528	LYS	C-N	-5.03	1.22	1.34
2	D	528	LYS	C-N	-5.03	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	633	ARG	Sidechain

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	4869	0	4640	45	0
2	B	7853	0	7676	174	0
2	C	7965	0	7769	159	0
2	D	7972	0	7772	170	0
3	E	39	0	34	0	0
4	F	28	0	25	1	0
4	G	28	0	25	0	0
4	H	28	0	25	1	0
4	I	28	0	25	1	0
4	J	28	0	25	0	0
5	A	1	0	0	0	0
6	A	84	0	78	0	0
6	B	98	0	91	9	0
6	C	112	0	104	5	0
6	D	168	0	156	14	0
All	All	29301	0	28445	536	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 9.

The worst 5 of 536 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:131:LYS:HB3	1:A:143:LEU:CD2	1.59	1.32
2:B:361:CYS:N	2:B:523:VAL:HG21	1.65	1.11
2:B:623:ILE:HD13	2:B:628:LEU:HD12	1.28	1.11
2:D:361:CYS:N	2:D:523:VAL:HG21	1.65	1.10
2:B:623:ILE:CD1	2:B:628:LEU:HD12	1.81	1.10

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	595/603 (99%)	575 (97%)	20 (3%)	0	100	100
2	B	987/1191 (83%)	895 (91%)	87 (9%)	5 (0%)	29	62
2	C	1001/1191 (84%)	898 (90%)	97 (10%)	6 (1%)	25	59
2	D	1002/1191 (84%)	911 (91%)	88 (9%)	3 (0%)	41	72
All	All	3585/4176 (86%)	3279 (92%)	292 (8%)	14 (0%)	38	67

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	486	ASN
2	C	486	ASN
2	C	640	ASN
2	D	486	ASN
2	B	338	PHE

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	527/533 (99%)	526 (100%)	1 (0%)	93	96
2	B	879/1031 (85%)	877 (100%)	2 (0%)	93	96
2	C	892/1031 (86%)	892 (100%)	0	100	100
2	D	893/1031 (87%)	893 (100%)	0	100	100
All	All	3191/3626 (88%)	3188 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
2	B	623	ILE
2	B	633	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	627	GLN
2	D	1133	ASN
2	C	62	ASN
2	C	134	GLN
2	D	164	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	3,2	14,14,15	0.38	0	17,19,21	0.66	0
3	NAG	E	2	3	14,14,15	0.39	0	17,19,21	0.54	0
3	BMA	E	3	3	11,11,12	0.33	0	15,15,17	0.49	0
4	NAG	F	1	4,2	14,14,15	0.40	0	17,19,21	0.54	0
4	NAG	F	2	4	14,14,15	0.36	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	1	4,2	14,14,15	0.40	0	17,19,21	0.52	0
4	NAG	G	2	4	14,14,15	0.38	0	17,19,21	0.50	0
4	NAG	H	1	4,2	14,14,15	0.43	0	17,19,21	0.69	1 (5%)
4	NAG	H	2	4	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
4	NAG	I	1	4,2	14,14,15	0.19	0	17,19,21	0.51	0
4	NAG	I	2	4	14,14,15	0.22	0	17,19,21	0.37	0
4	NAG	J	1	4,2	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	J	2	4	14,14,15	0.23	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	E	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
4	NAG	F	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	NAG	H	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	5/6/23/26	0/1/1/1
4	NAG	I	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	NAG	C2-N2-C7	2.07	125.86	122.90
4	H	1	NAG	O4-C4-C3	-2.01	105.71	110.35

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

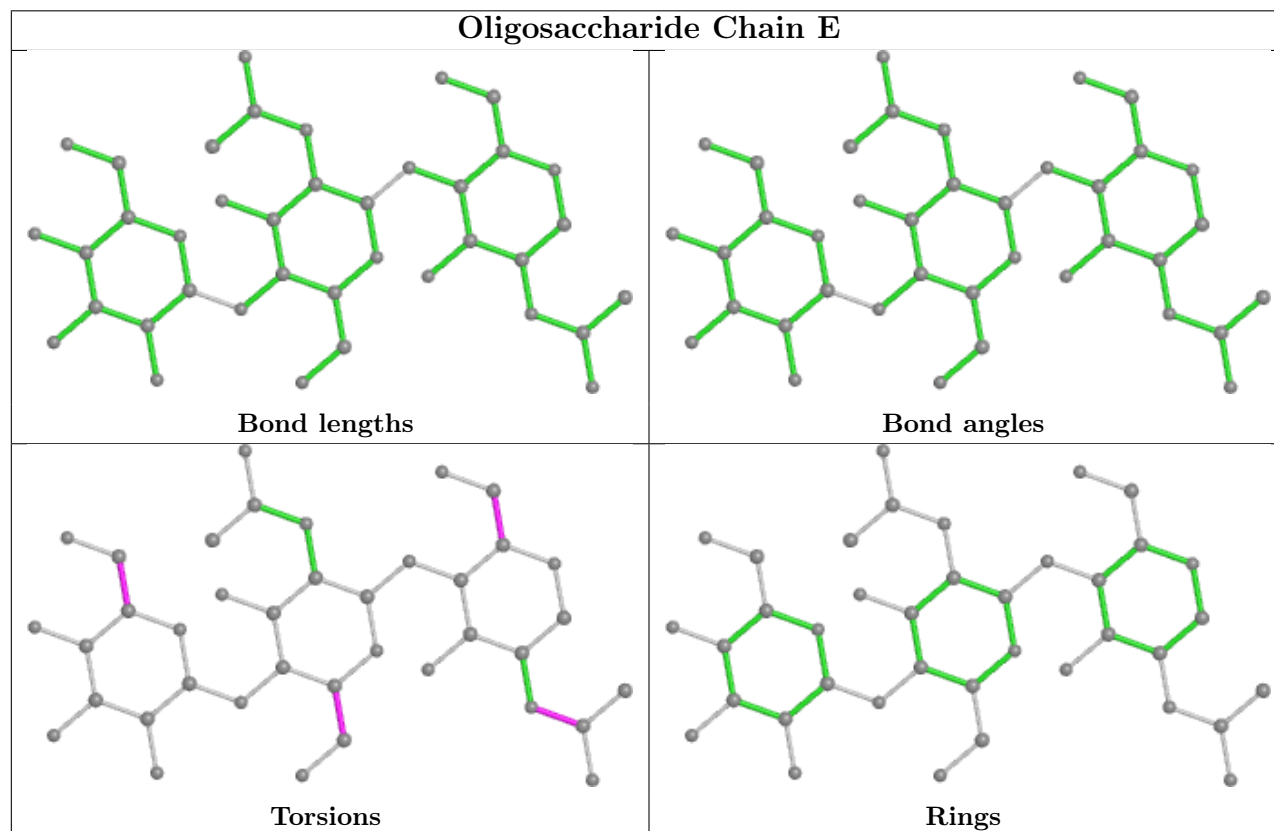
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C3-C2-N2-C7
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2

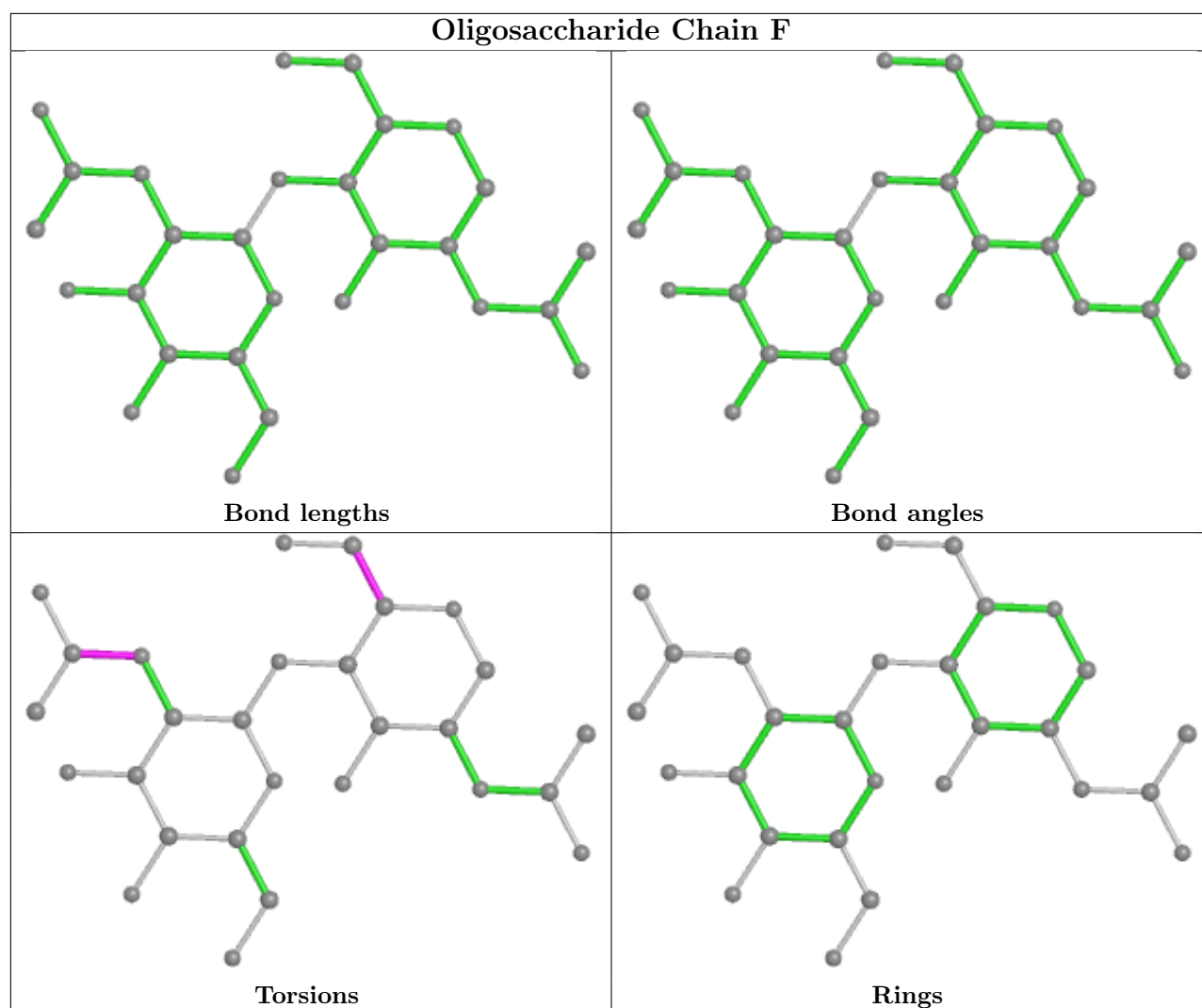
There are no ring outliers.

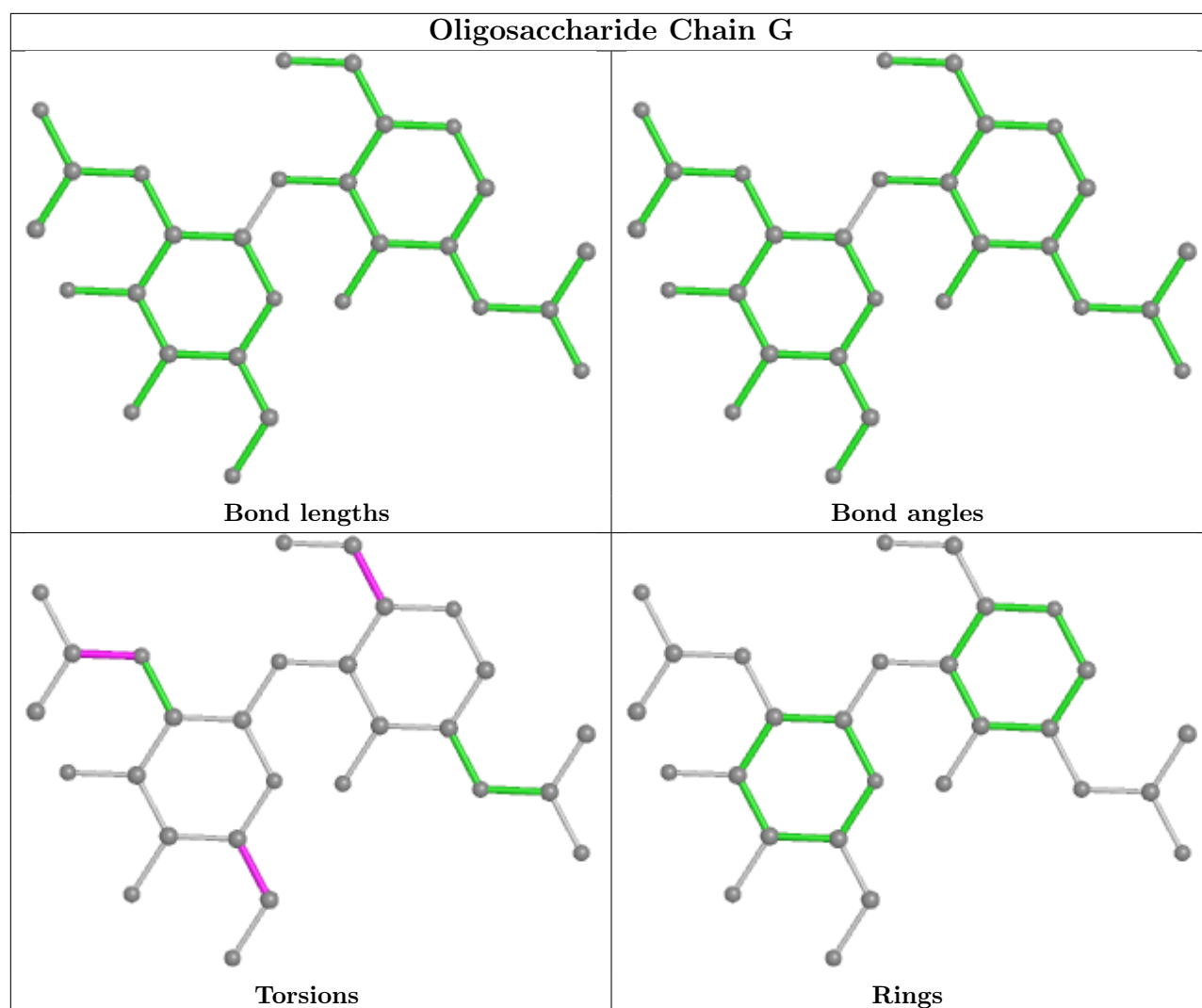
6 monomers are involved in 3 short contacts:

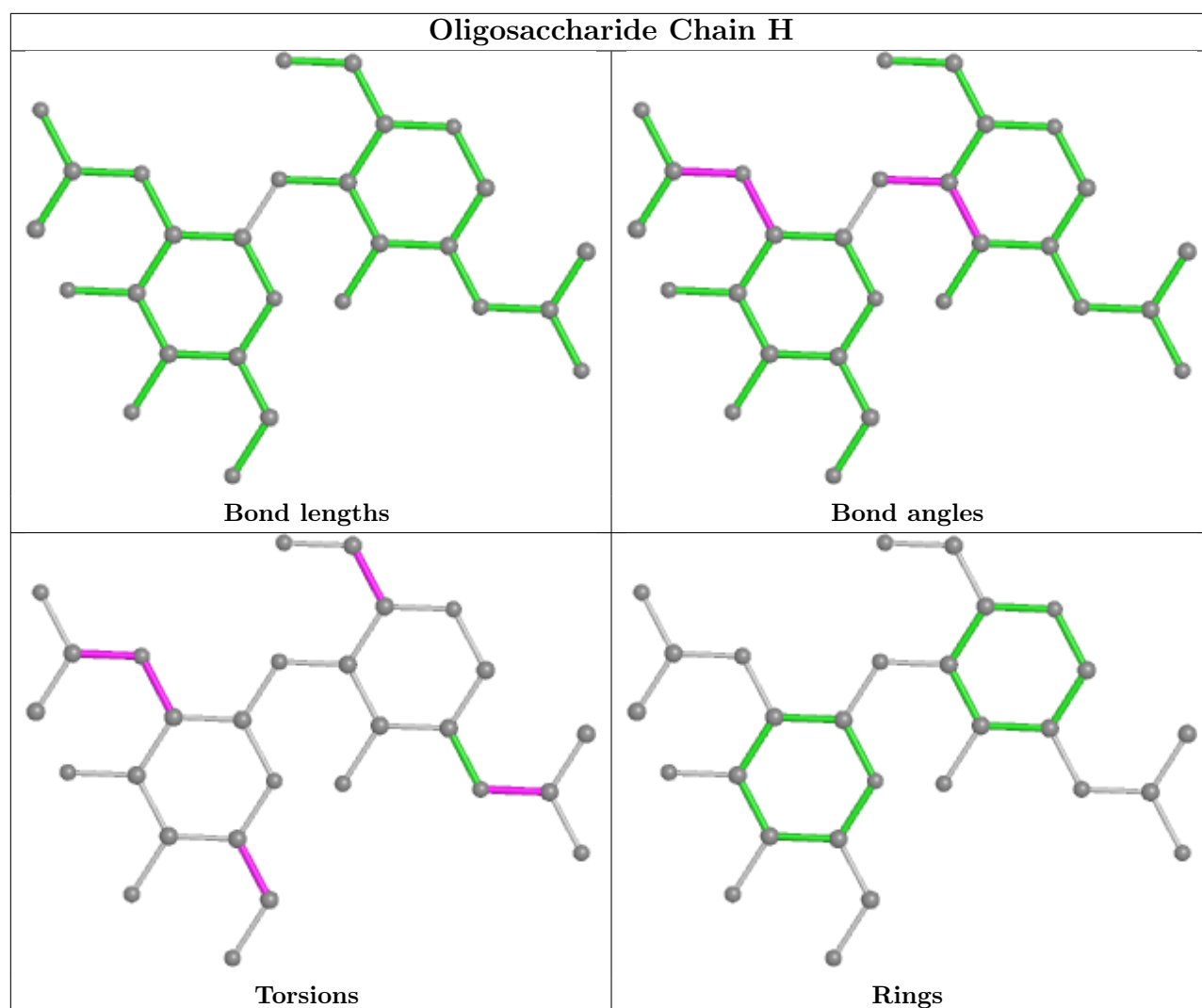
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	NAG	1	0
4	H	1	NAG	1	0
4	I	1	NAG	1	0
4	F	1	NAG	1	0
4	F	2	NAG	1	0
4	H	2	NAG	1	0

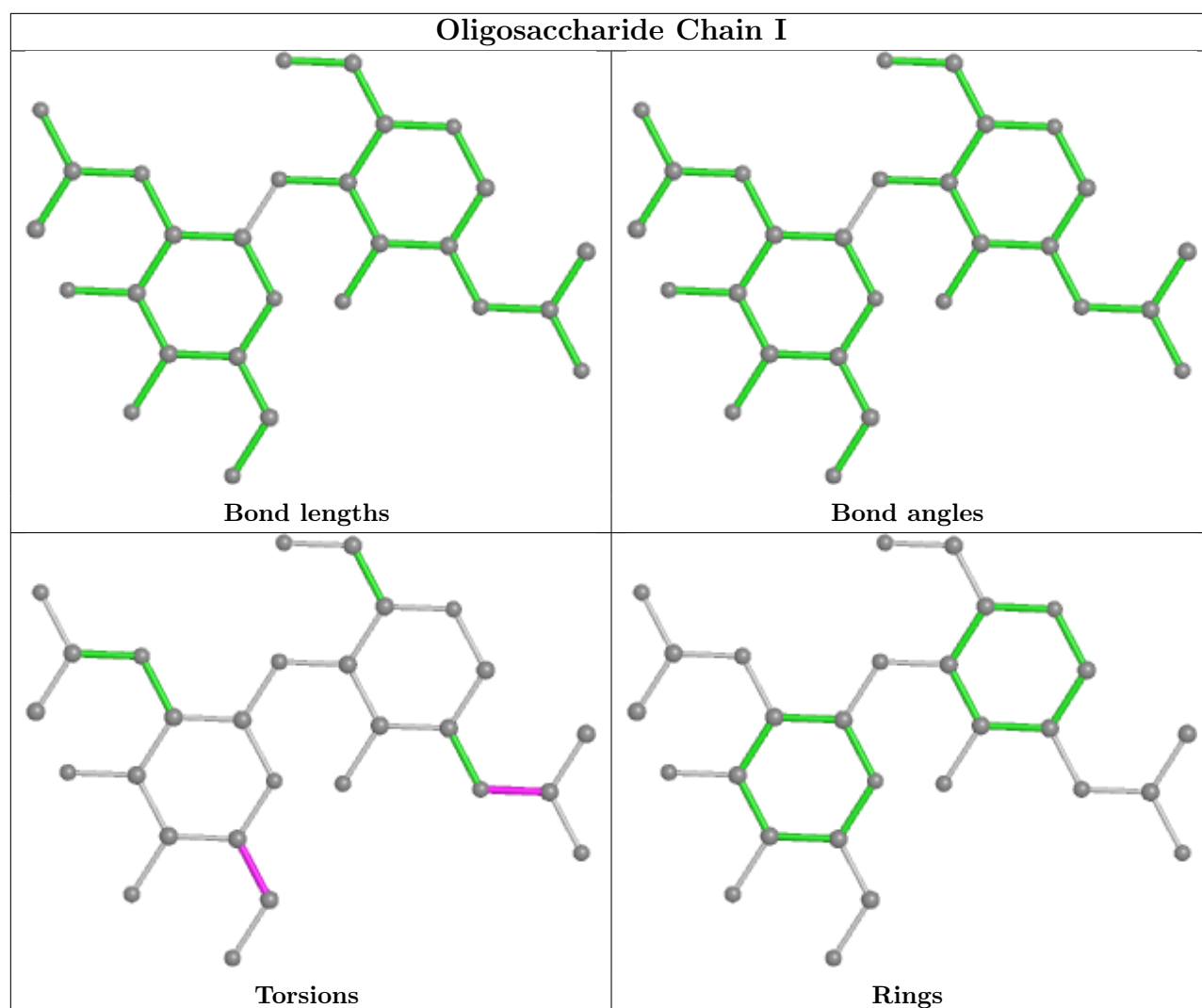
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

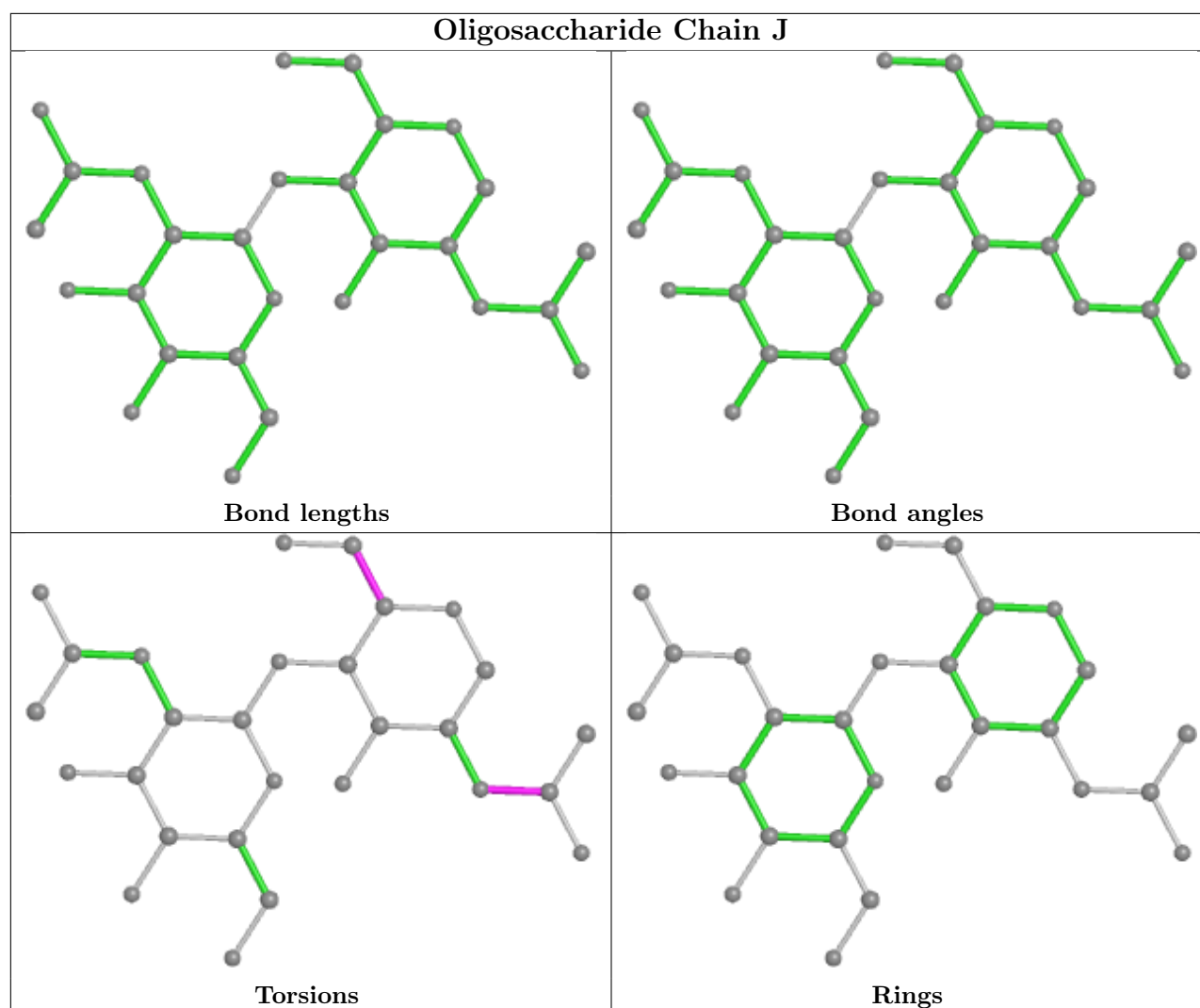












5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 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	$\# Z > 2$
6	NAG	D	1201	2	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	B	1204	2	14,14,15	0.40	0	17,19,21	0.53	0
6	NAG	D	1203	2	14,14,15	0.39	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	1204	2	14,14,15	0.20	0	17,19,21	0.62	0
6	NAG	D	1202	2	14,14,15	0.34	0	17,19,21	0.54	0
6	NAG	D	1205	2	14,14,15	0.37	0	17,19,21	0.69	1 (5%)
6	NAG	C	1205	2	14,14,15	0.39	0	17,19,21	1.14	2 (11%)
6	NAG	D	1208	2	14,14,15	0.39	0	17,19,21	0.82	1 (5%)
6	NAG	D	1211	2	14,14,15	0.38	0	17,19,21	0.85	1 (5%)
6	NAG	B	1201	2	14,14,15	0.38	0	17,19,21	0.65	1 (5%)
6	NAG	B	1202	2	14,14,15	0.39	0	17,19,21	0.62	0
6	NAG	C	1202	2	14,14,15	0.37	0	17,19,21	0.98	2 (11%)
6	NAG	C	1208	2	14,14,15	0.39	0	17,19,21	0.81	0
6	NAG	A	705	1	14,14,15	0.22	0	17,19,21	0.54	0
6	NAG	B	1203	2	14,14,15	0.39	0	17,19,21	0.74	0
6	NAG	A	703	1	14,14,15	0.25	0	17,19,21	0.38	0
6	NAG	B	1205	2	14,14,15	0.37	0	17,19,21	0.80	1 (5%)
6	NAG	D	1209	2	14,14,15	0.38	0	17,19,21	0.54	0
6	NAG	C	1206	2	14,14,15	0.22	0	17,19,21	0.45	0
6	NAG	D	1212	2	14,14,15	0.30	0	17,19,21	0.78	0
6	NAG	C	1201	2	14,14,15	0.41	0	17,19,21	0.48	0
6	NAG	D	1207	-	14,14,15	0.37	0	17,19,21	1.10	2 (11%)
6	NAG	A	706	1	14,14,15	0.25	0	17,19,21	0.48	0
6	NAG	D	1210	2	14,14,15	0.38	0	17,19,21	1.04	2 (11%)
6	NAG	B	1206	2	14,14,15	0.40	0	17,19,21	0.36	0
6	NAG	B	1207	2	14,14,15	0.35	0	17,19,21	0.96	1 (5%)
6	NAG	C	1207	2	14,14,15	0.41	0	17,19,21	0.55	0
6	NAG	D	1206	2	14,14,15	0.25	0	17,19,21	0.57	0
6	NAG	A	702	1	14,14,15	0.23	0	17,19,21	0.55	0
6	NAG	D	1204	2	14,14,15	0.40	0	17,19,21	0.34	0
6	NAG	C	1203	2	14,14,15	0.15	0	17,19,21	0.50	0
6	NAG	A	704	1	14,14,15	0.22	0	17,19,21	0.34	0
6	NAG	A	707	1	14,14,15	0.38	0	17,19,21	0.39	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
6	NAG	D	1201	2	-	4/6/23/26	0/1/1/1
6	NAG	B	1204	2	-	0/6/23/26	0/1/1/1
6	NAG	D	1203	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1204	2	-	3/6/23/26	0/1/1/1
6	NAG	D	1202	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1205	2	-	0/6/23/26	0/1/1/1
6	NAG	C	1205	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1208	2	-	4/6/23/26	0/1/1/1
6	NAG	D	1211	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1201	2	-	4/6/23/26	0/1/1/1
6	NAG	B	1202	2	-	4/6/23/26	0/1/1/1
6	NAG	C	1202	2	-	3/6/23/26	0/1/1/1
6	NAG	C	1208	2	-	0/6/23/26	0/1/1/1
6	NAG	A	705	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1203	2	-	5/6/23/26	0/1/1/1
6	NAG	A	703	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1205	2	-	3/6/23/26	0/1/1/1
6	NAG	D	1209	2	-	3/6/23/26	0/1/1/1
6	NAG	C	1206	2	-	0/6/23/26	0/1/1/1
6	NAG	D	1212	2	-	1/6/23/26	0/1/1/1
6	NAG	C	1201	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1207	-	-	3/6/23/26	0/1/1/1
6	NAG	A	706	1	-	0/6/23/26	0/1/1/1
6	NAG	D	1210	2	-	3/6/23/26	0/1/1/1
6	NAG	B	1206	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1207	2	-	4/6/23/26	0/1/1/1
6	NAG	C	1207	2	-	3/6/23/26	0/1/1/1
6	NAG	D	1206	2	-	3/6/23/26	0/1/1/1
6	NAG	A	702	1	-	2/6/23/26	0/1/1/1
6	NAG	D	1204	2	-	3/6/23/26	0/1/1/1
6	NAG	C	1203	2	-	3/6/23/26	0/1/1/1
6	NAG	A	704	1	-	2/6/23/26	0/1/1/1
6	NAG	A	707	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1205	NAG	C2-N2-C7	3.26	127.54	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1207	NAG	C1-C2-N2	3.05	115.70	110.49
6	D	1203	NAG	C1-O5-C5	2.85	116.06	112.19
6	D	1210	NAG	C2-N2-C7	2.80	126.89	122.90
6	C	1202	NAG	C2-N2-C7	2.79	126.88	122.90

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1201	NAG	C3-C2-N2-C7
6	B	1201	NAG	C8-C7-N2-C2
6	B	1201	NAG	O7-C7-N2-C2
6	B	1203	NAG	C8-C7-N2-C2
6	B	1203	NAG	O7-C7-N2-C2

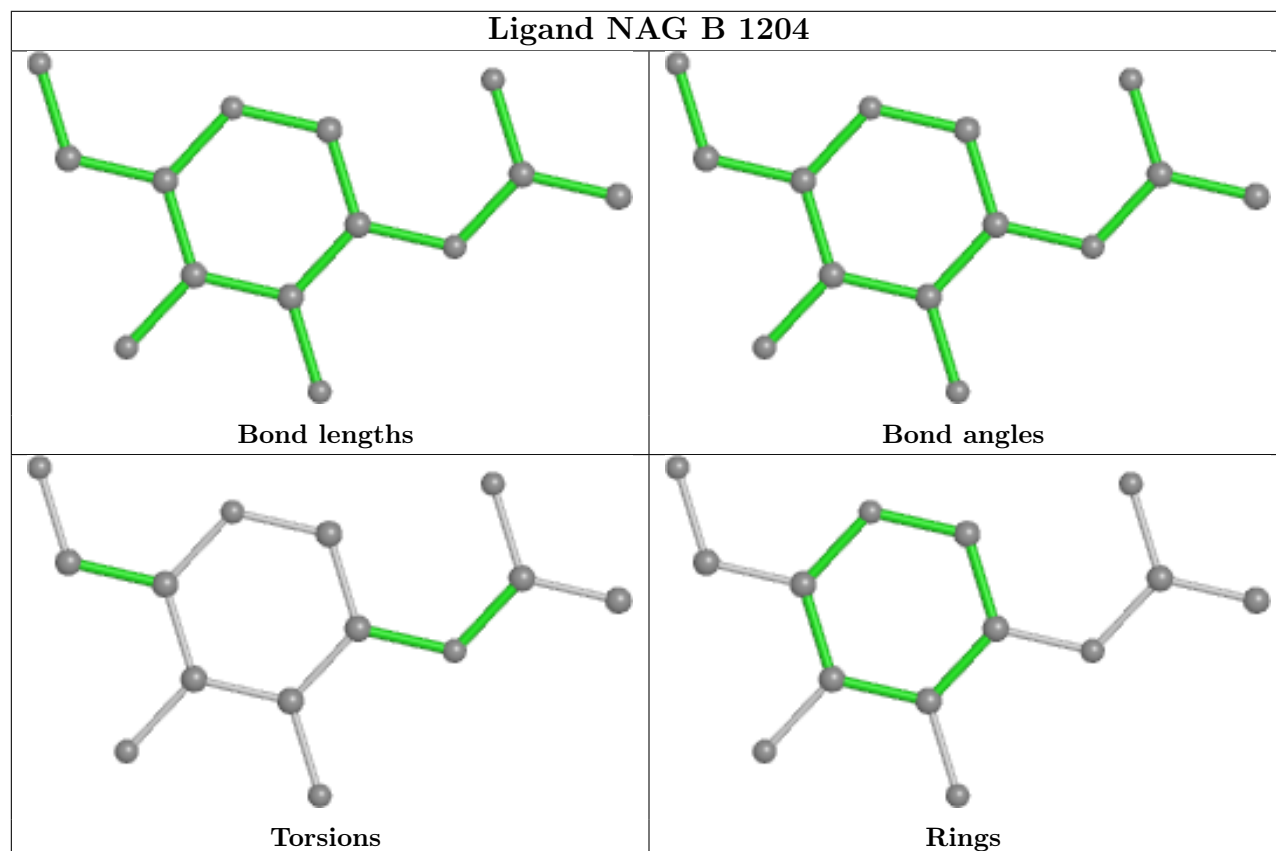
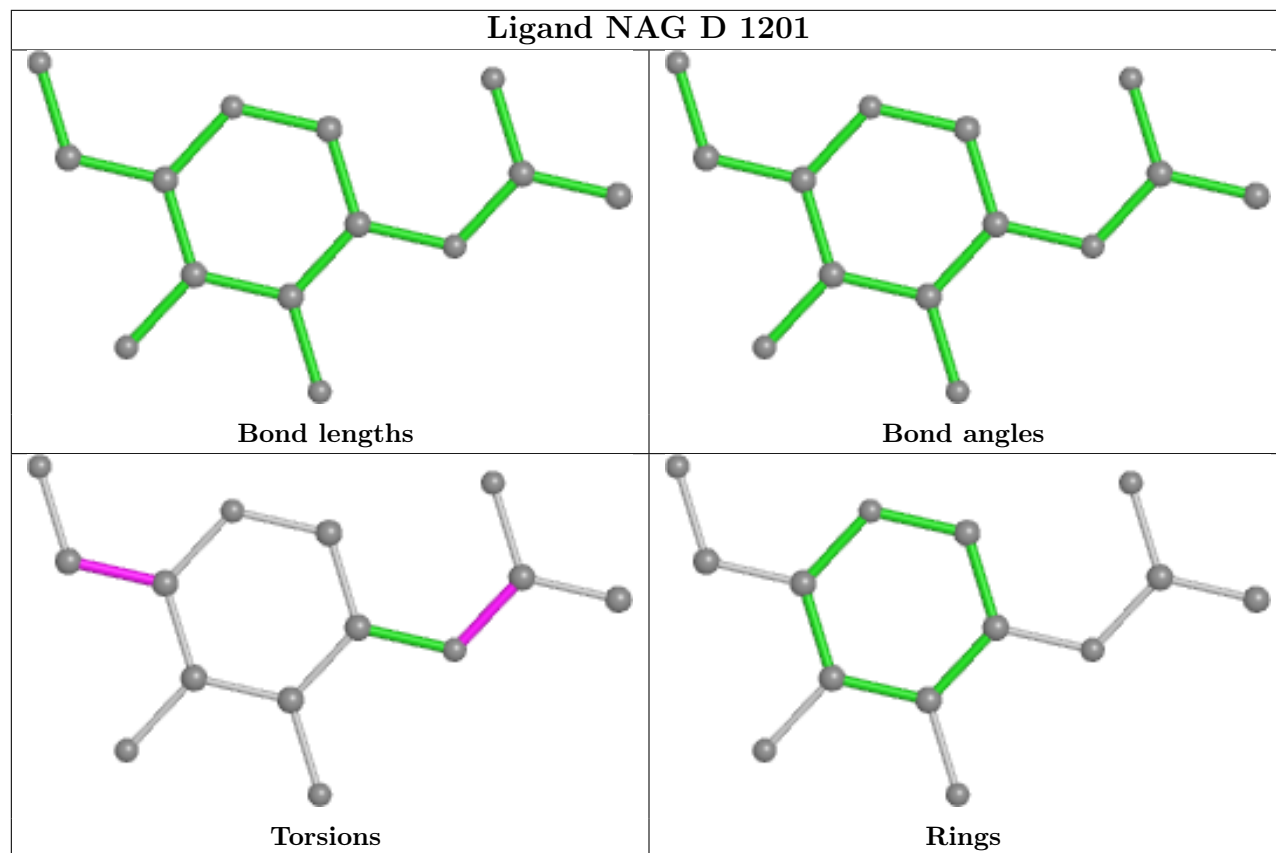
There are no ring outliers.

11 monomers are involved in 28 short contacts:

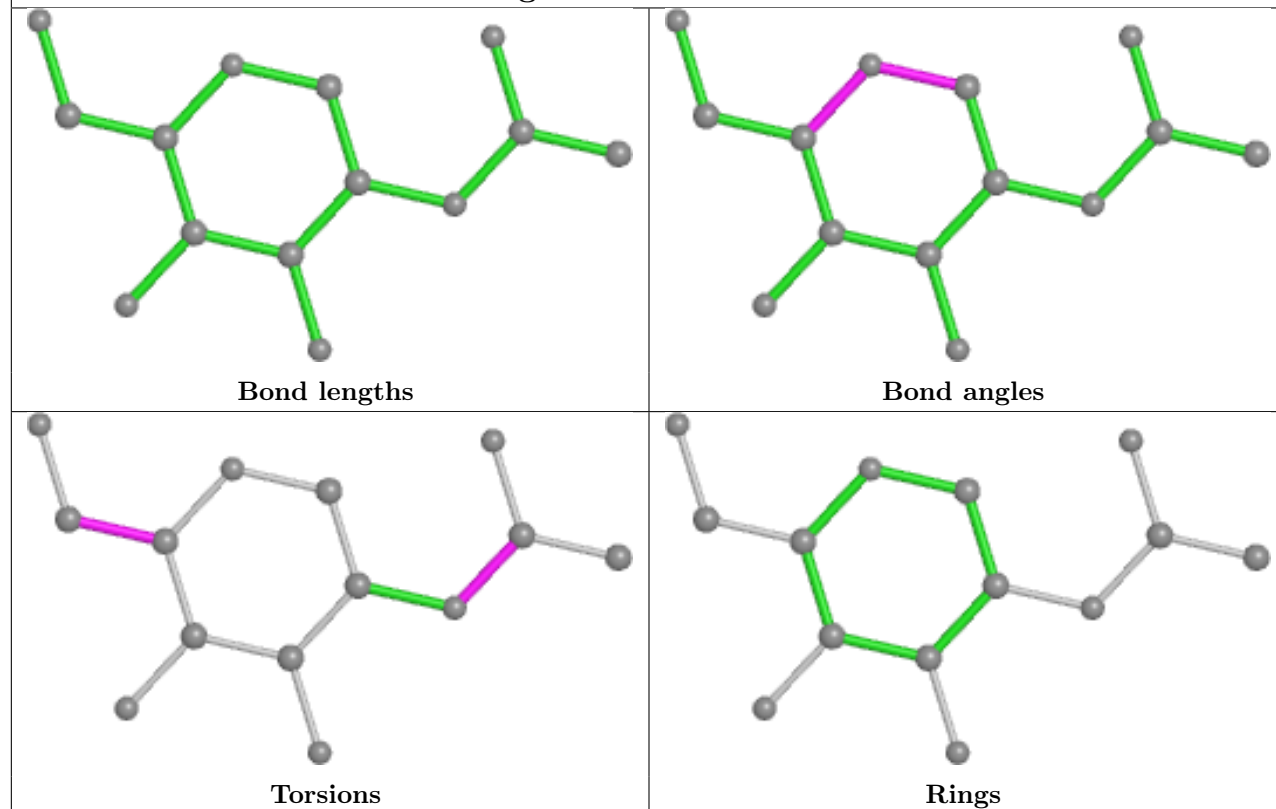
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1205	NAG	1	0
6	C	1205	NAG	2	0
6	D	1211	NAG	4	0
6	B	1201	NAG	1	0
6	C	1208	NAG	1	0
6	D	1209	NAG	1	0
6	D	1212	NAG	1	0
6	D	1207	NAG	7	0
6	B	1206	NAG	6	0
6	B	1207	NAG	2	0
6	C	1207	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

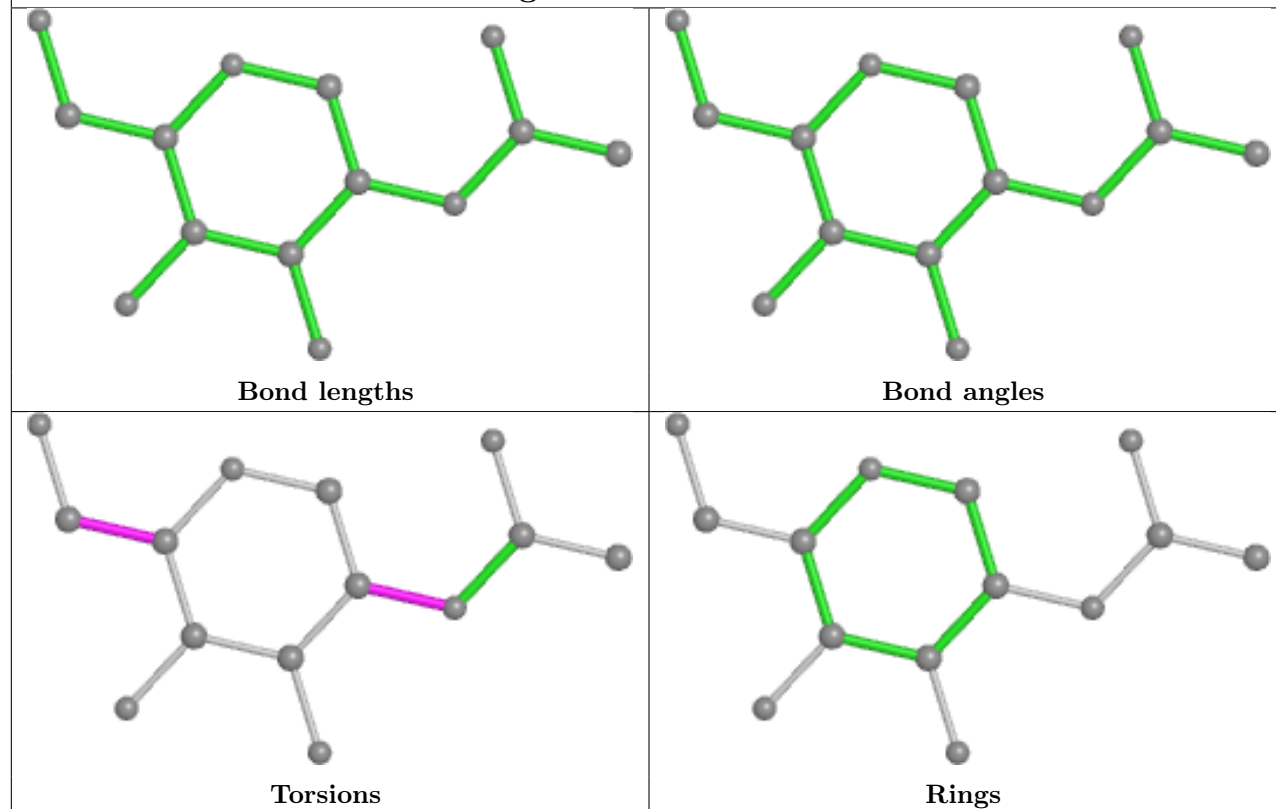
equivalents in the CSD to analyse the geometry.

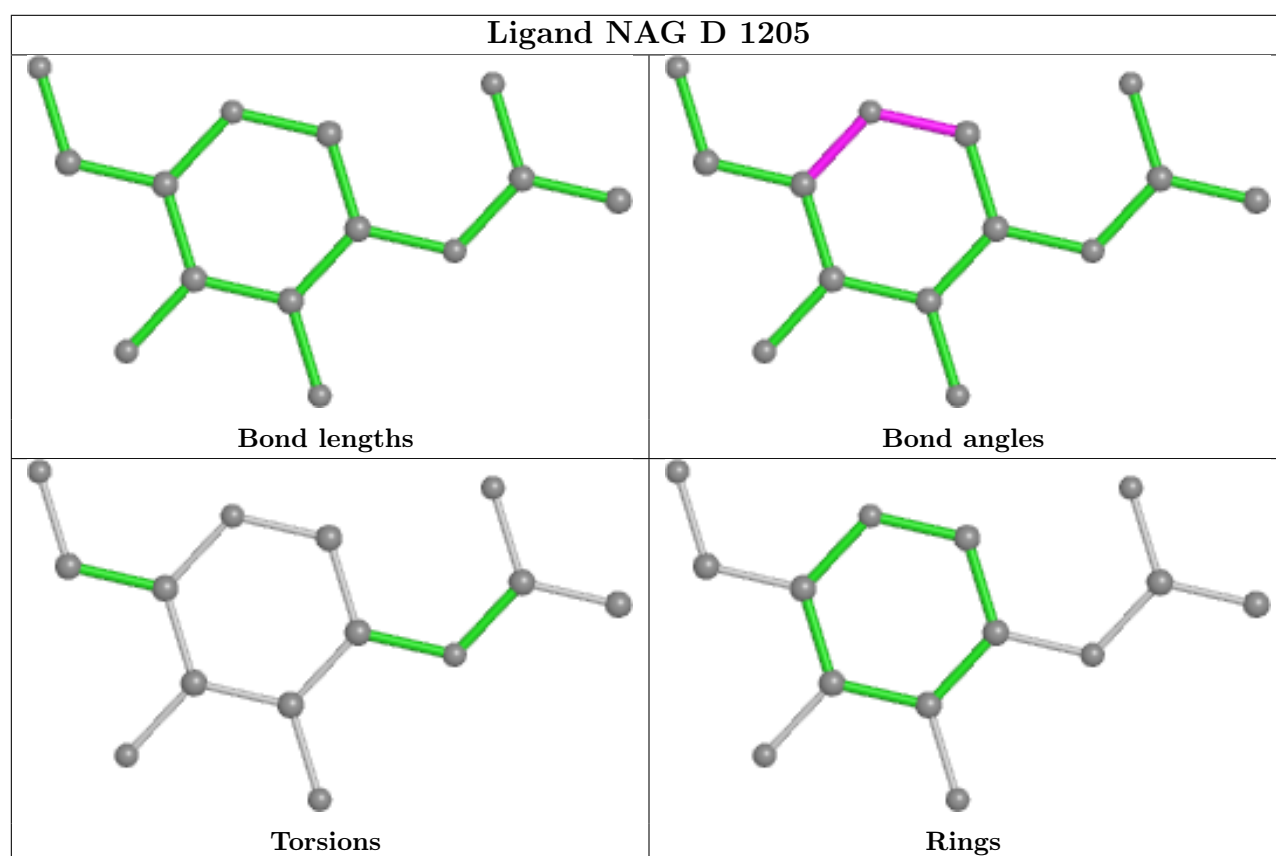
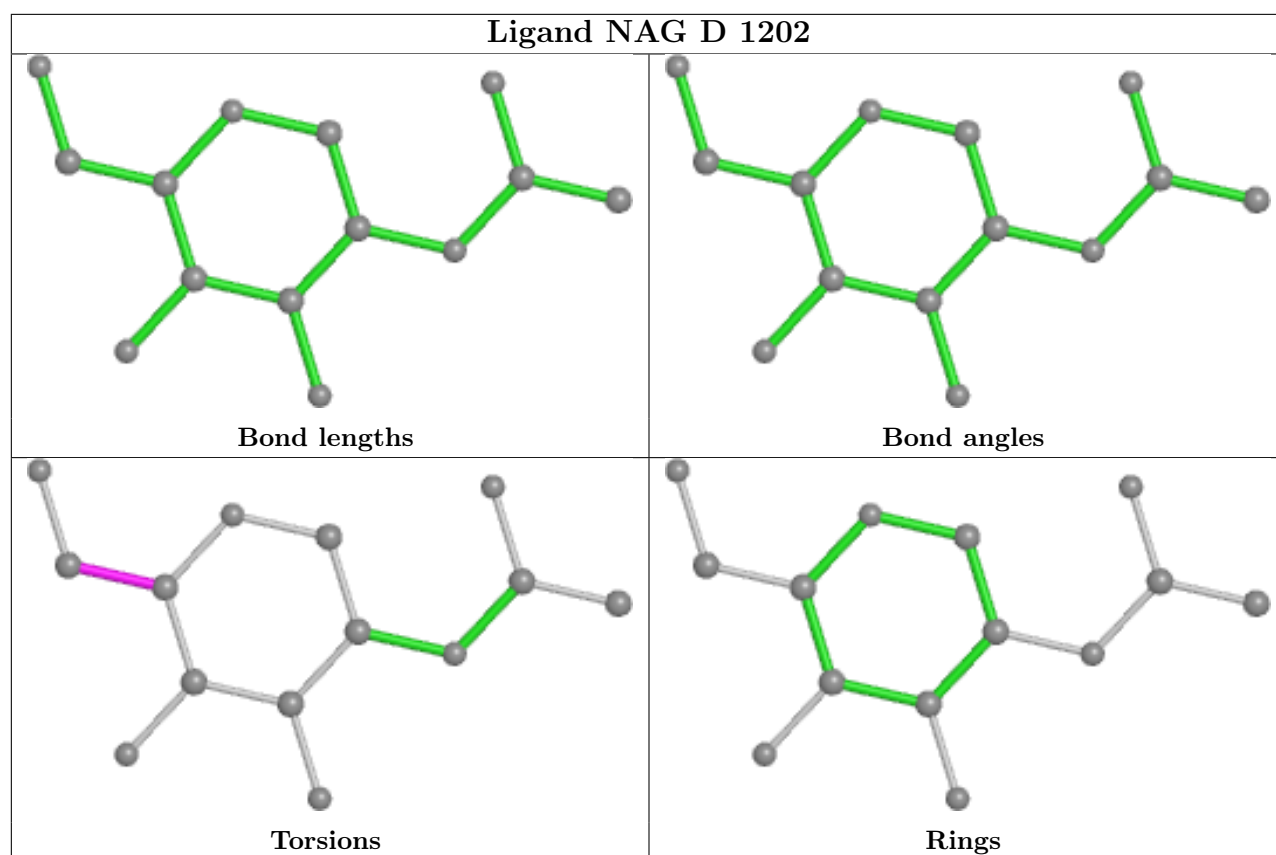


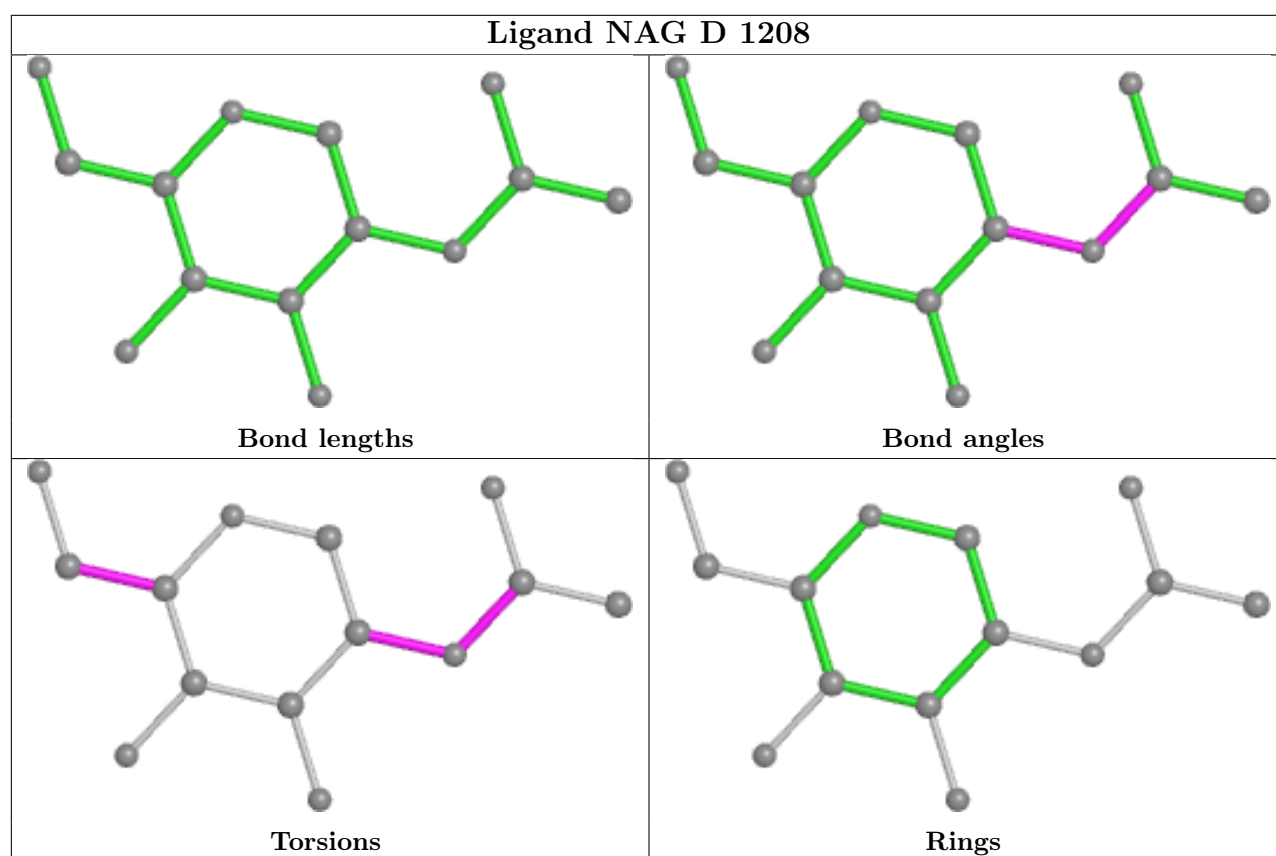
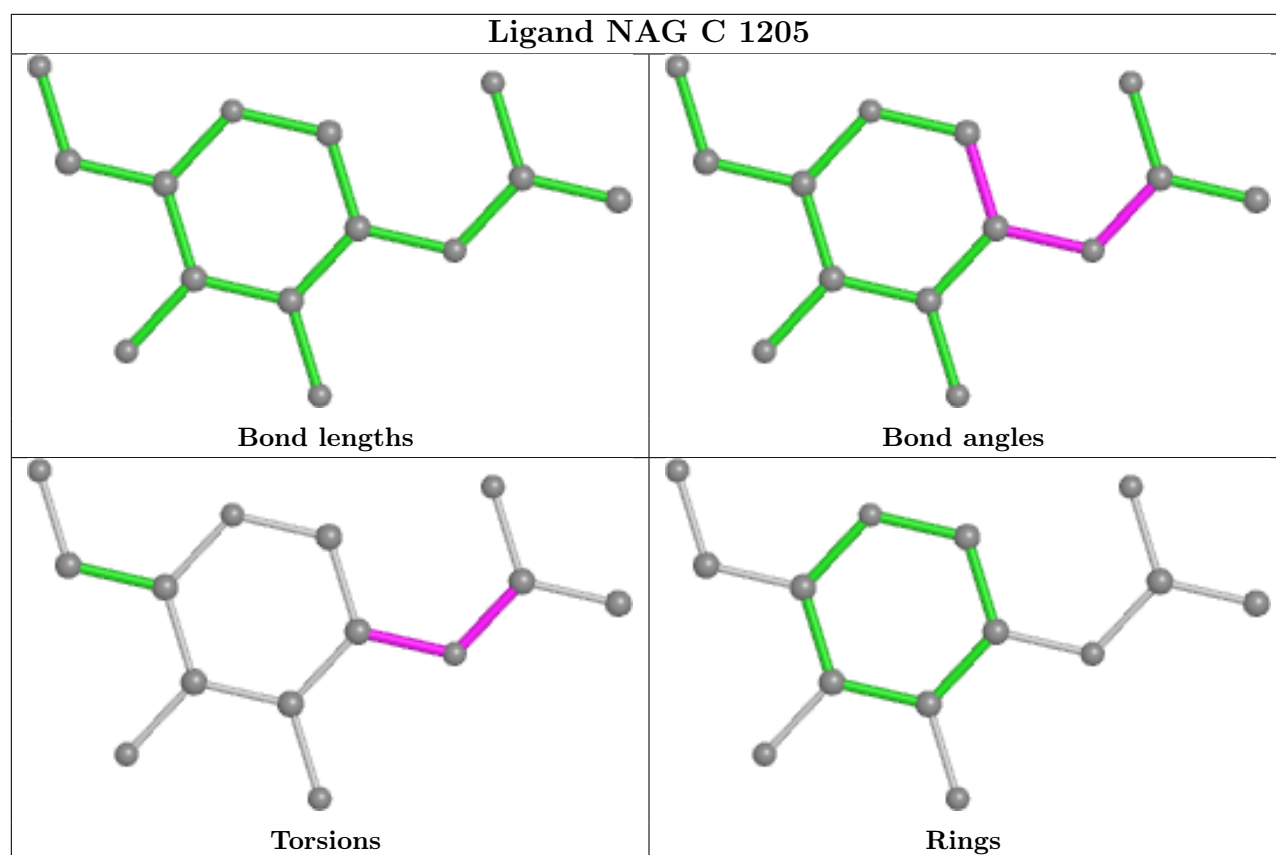
Ligand NAG D 1203

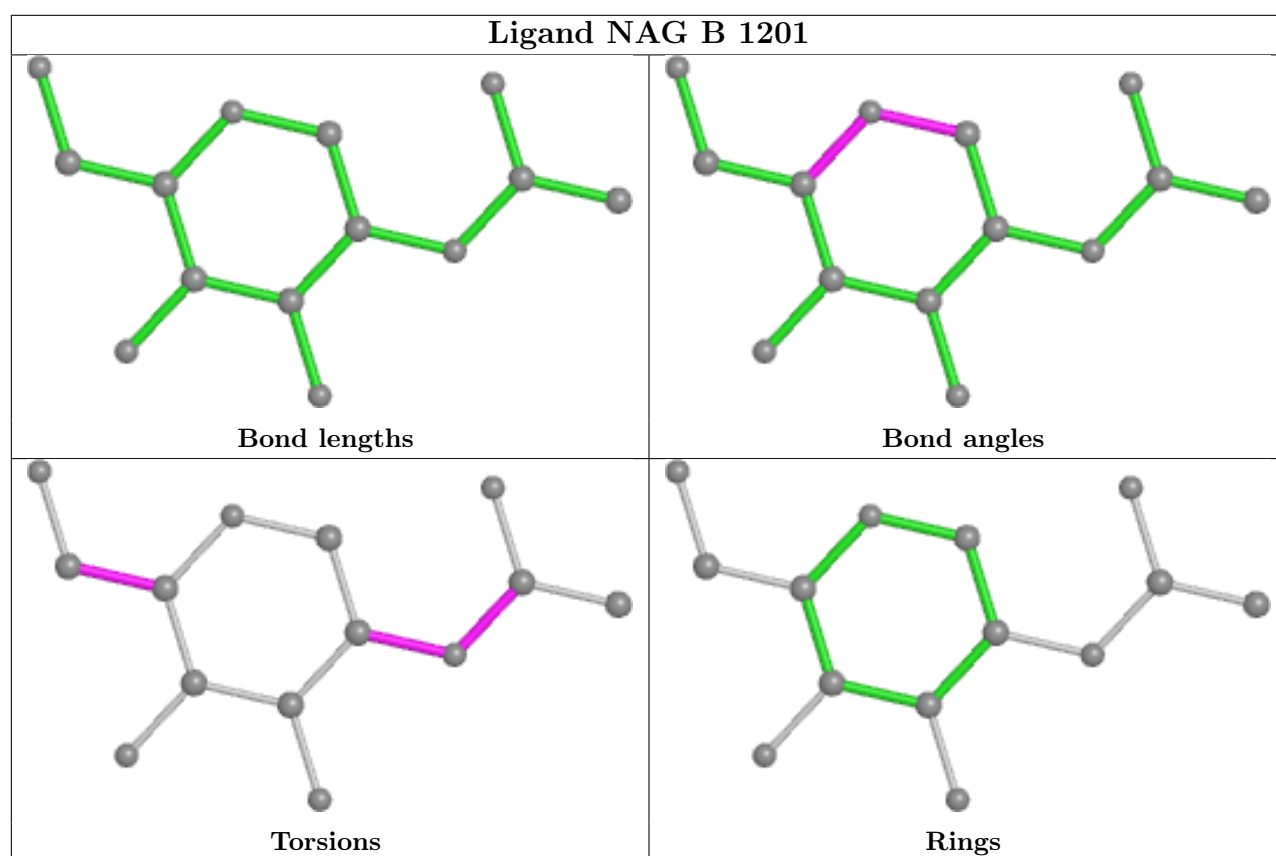
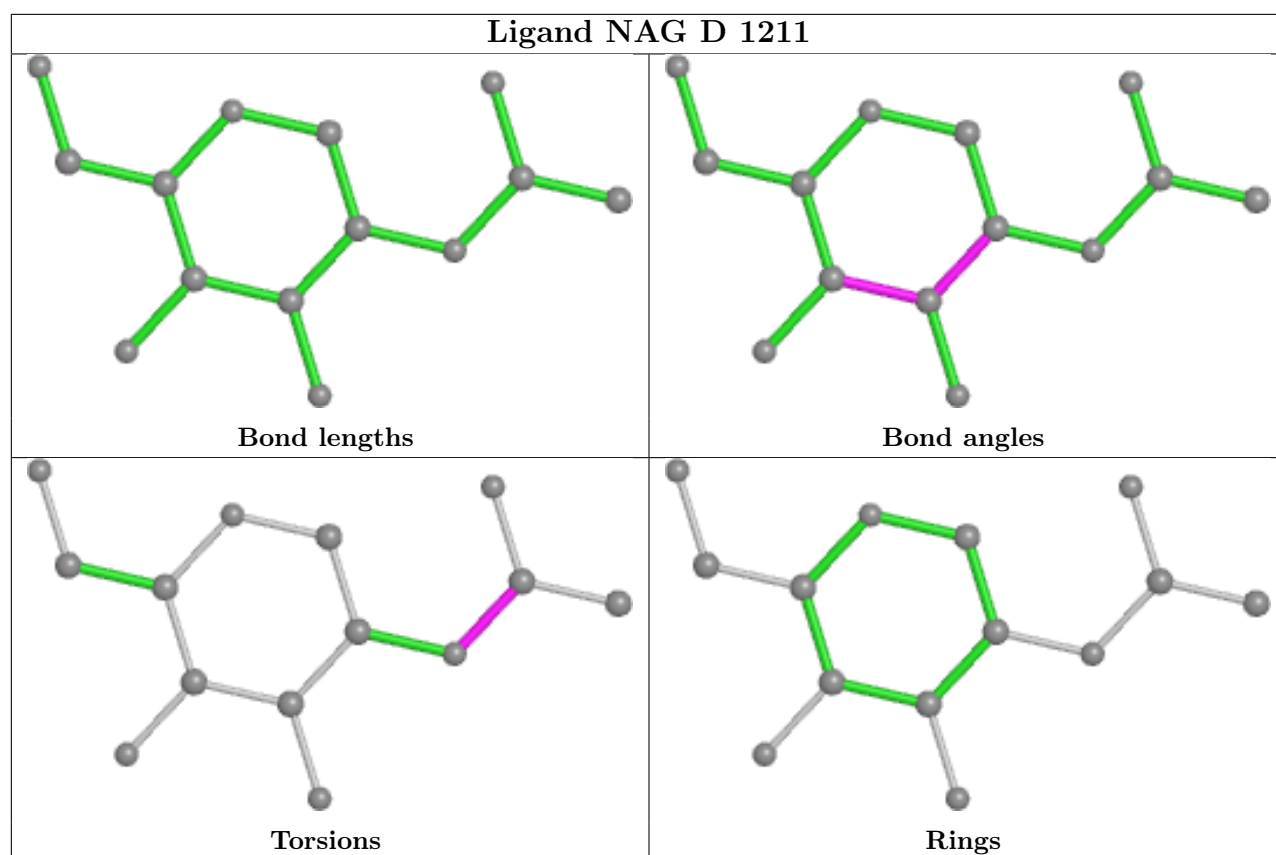


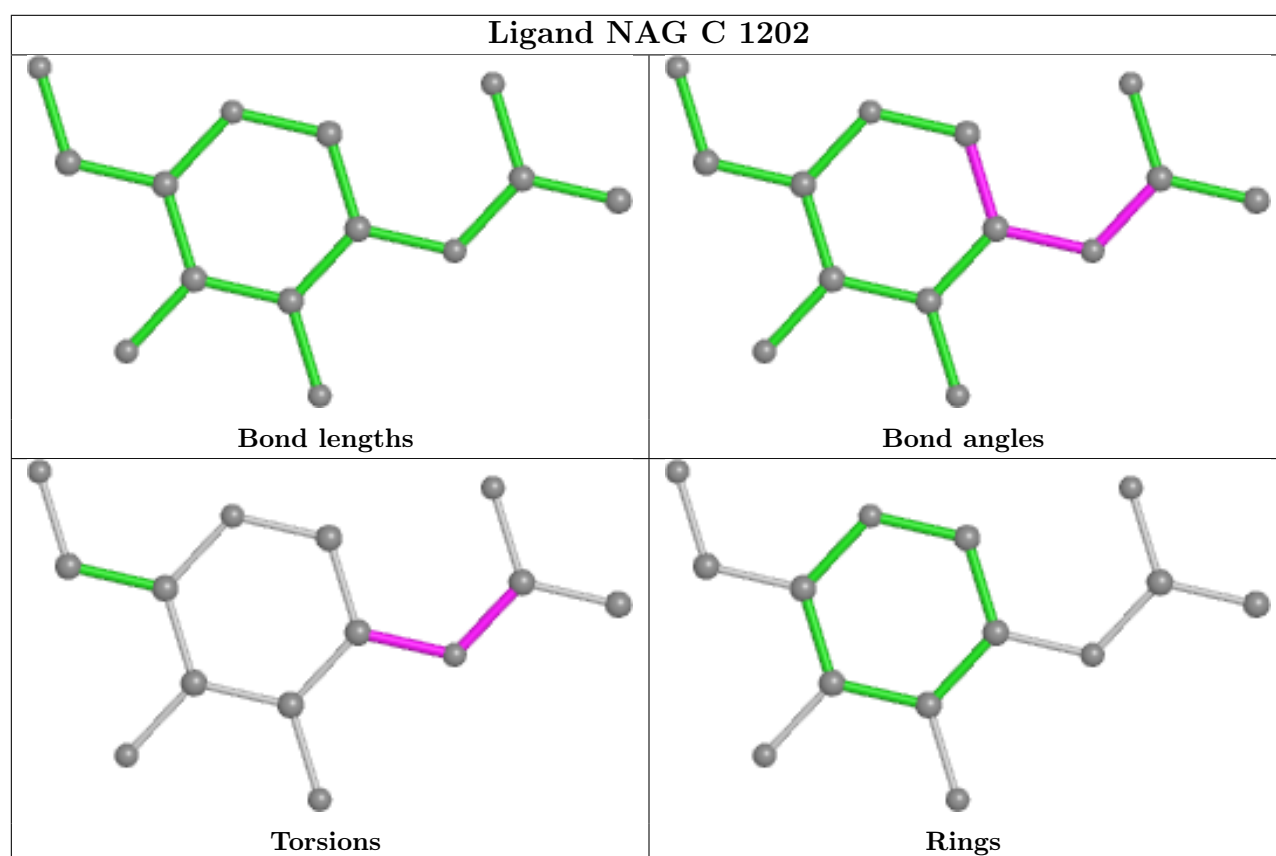
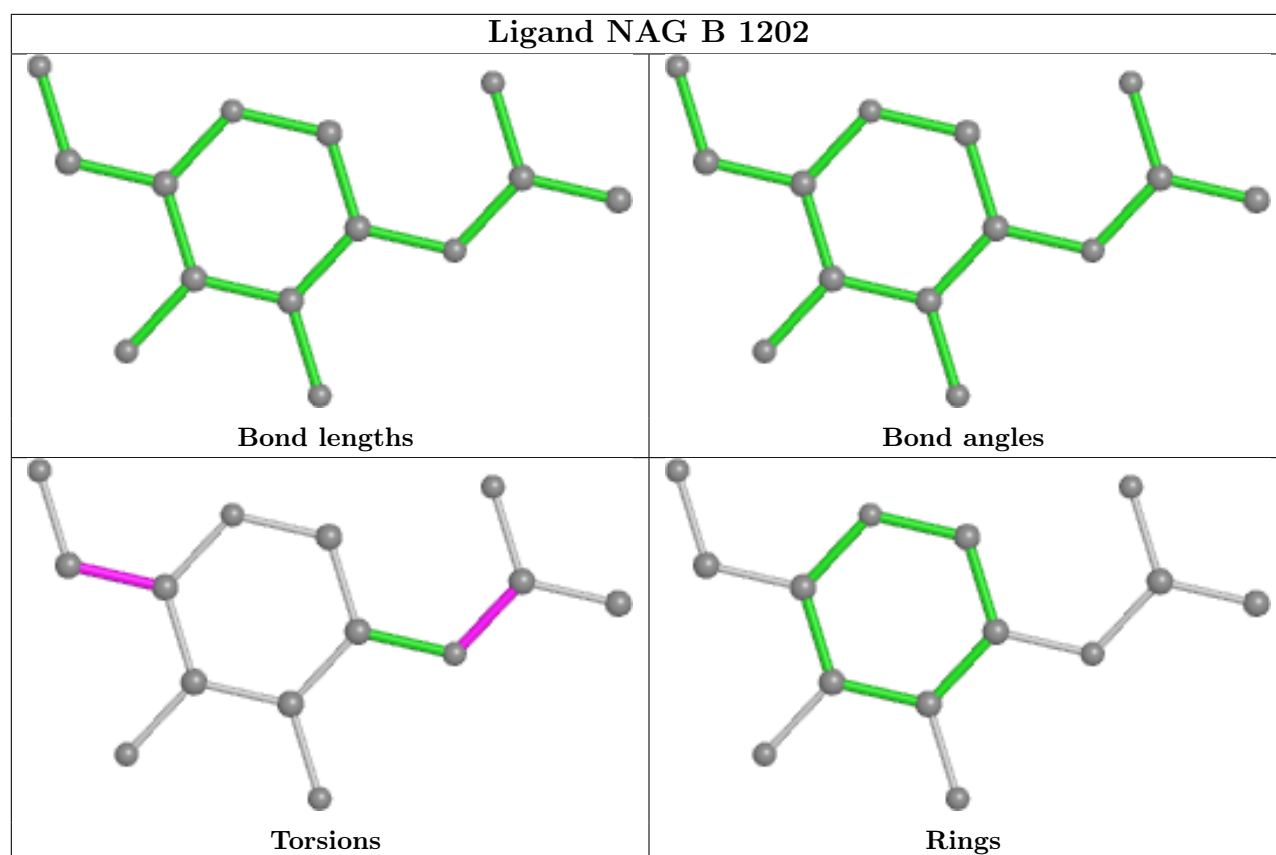
Ligand NAG C 1204

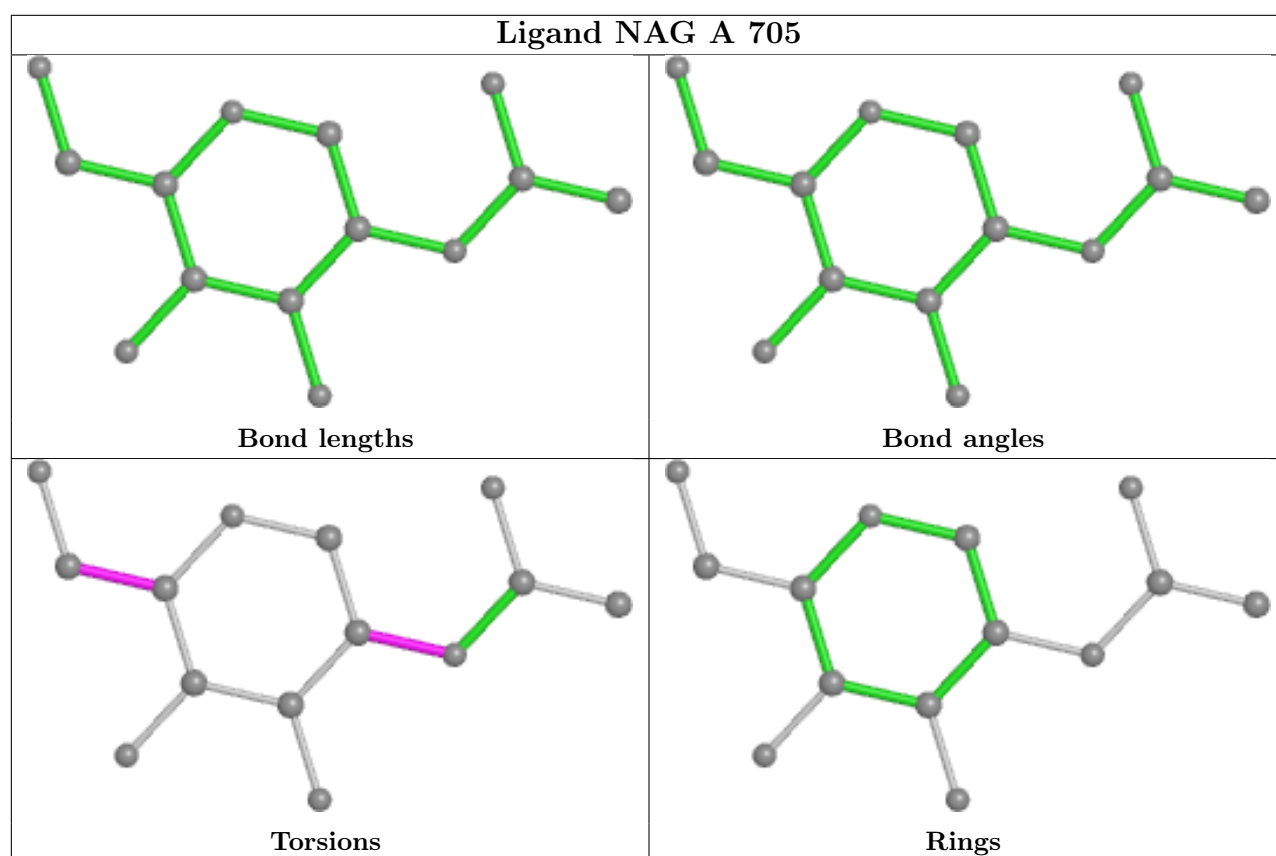
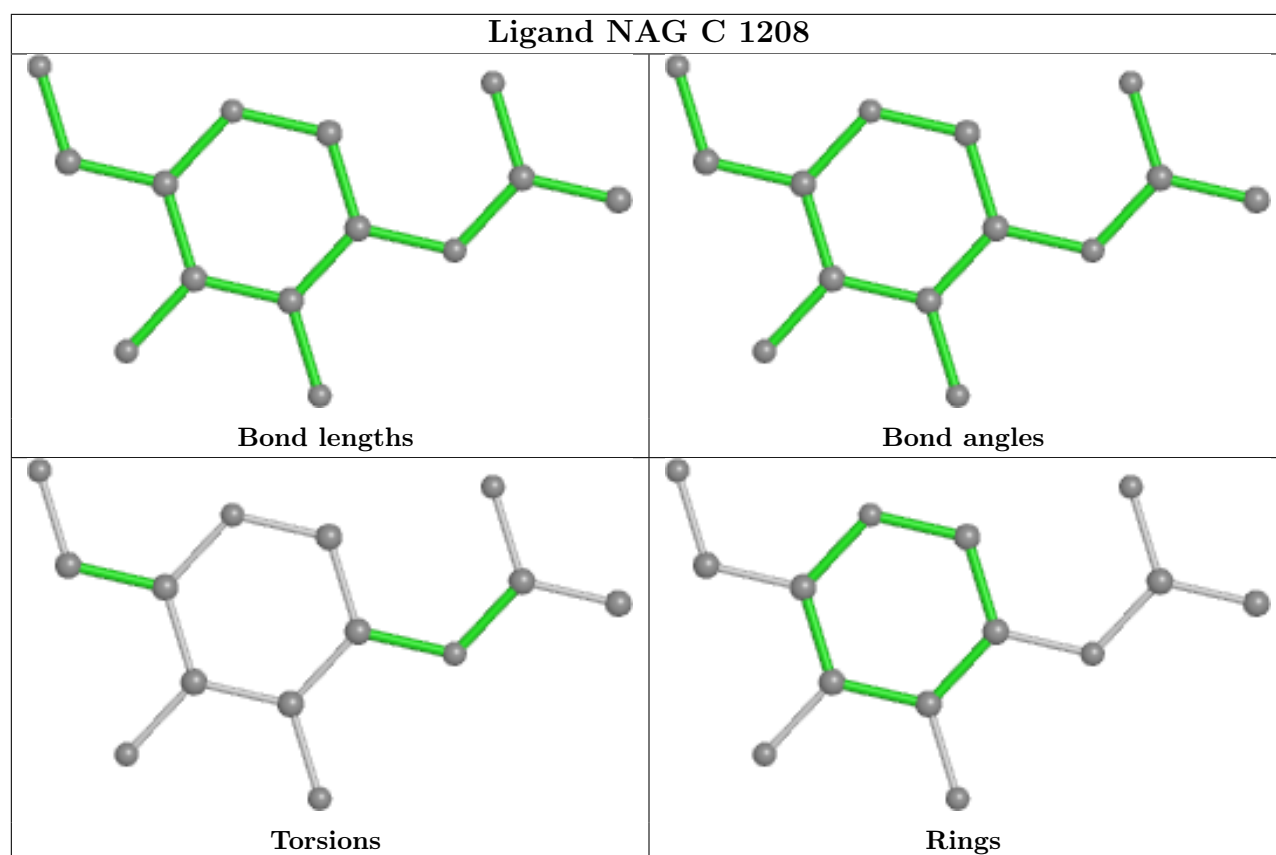


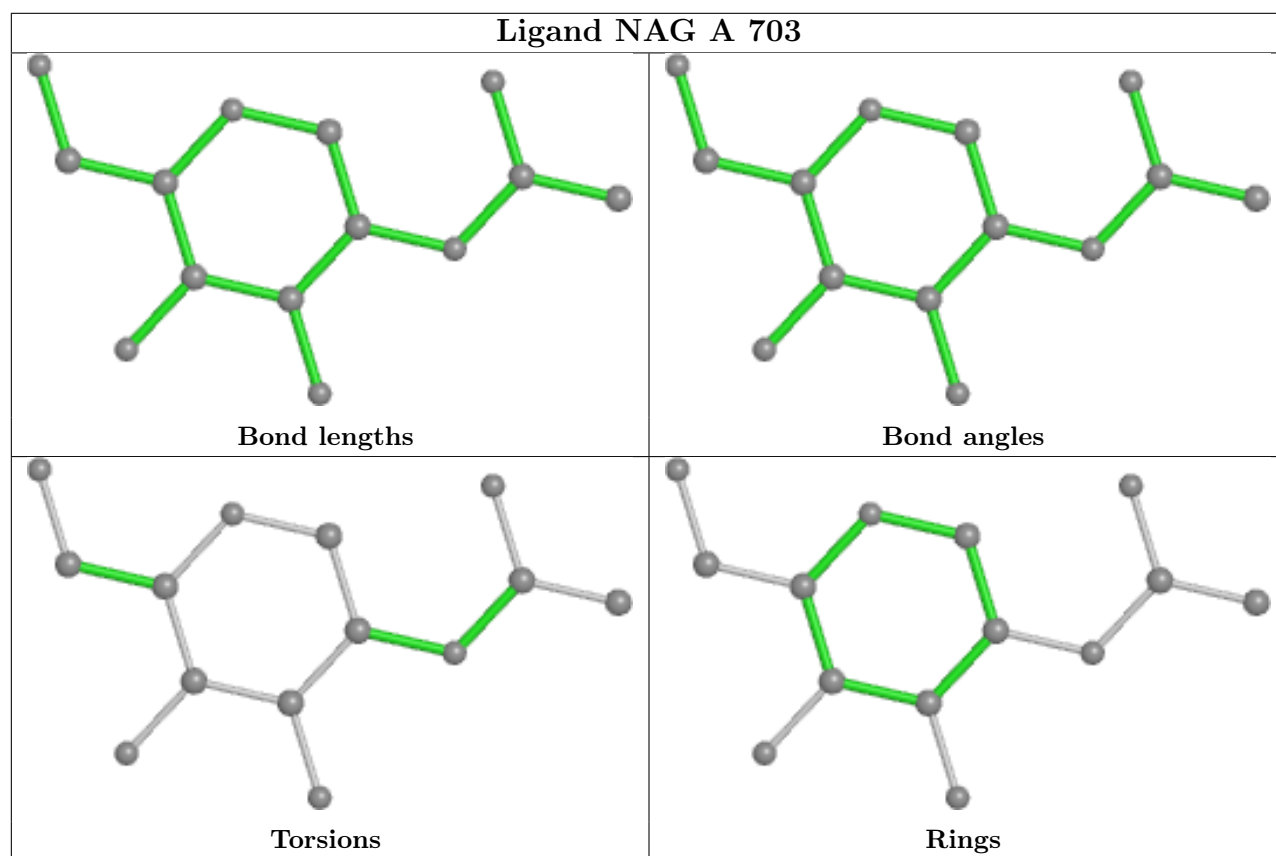
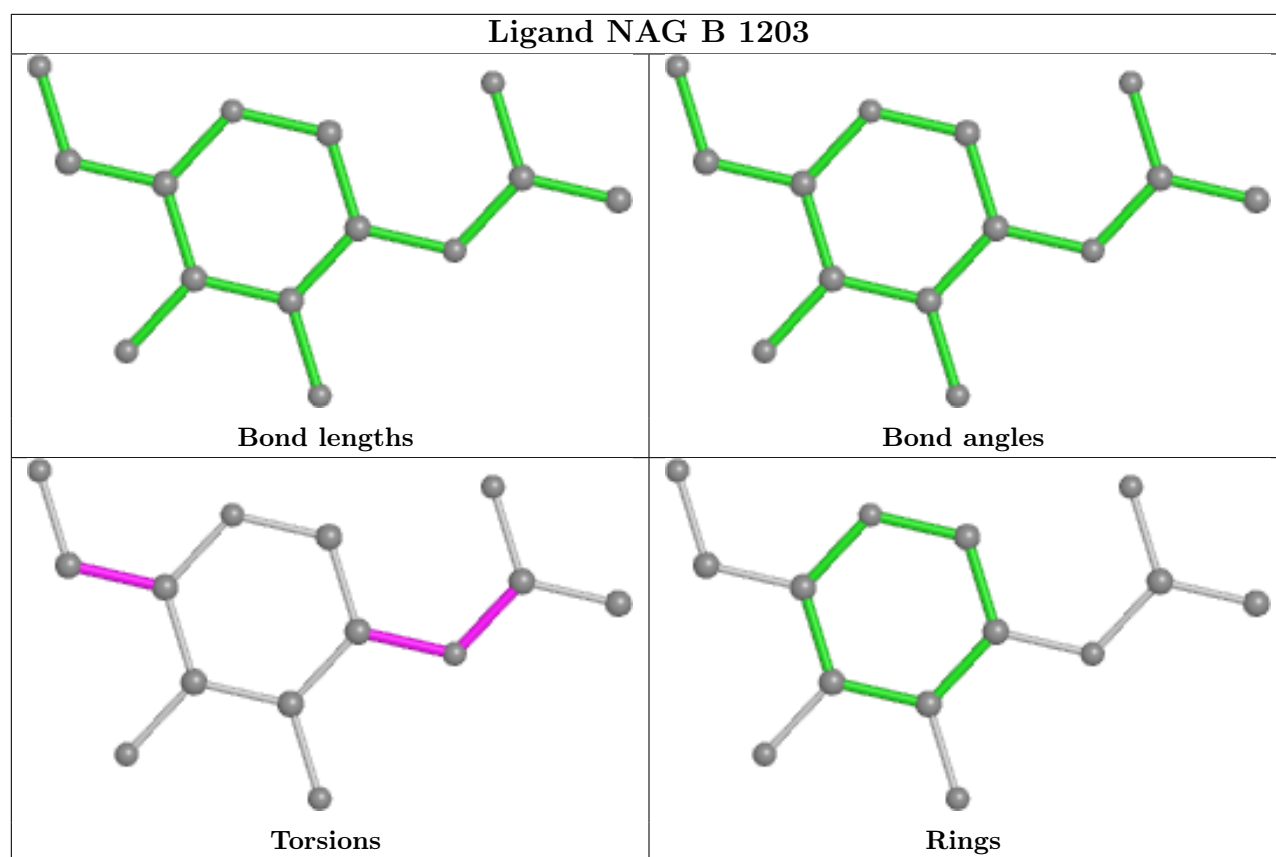


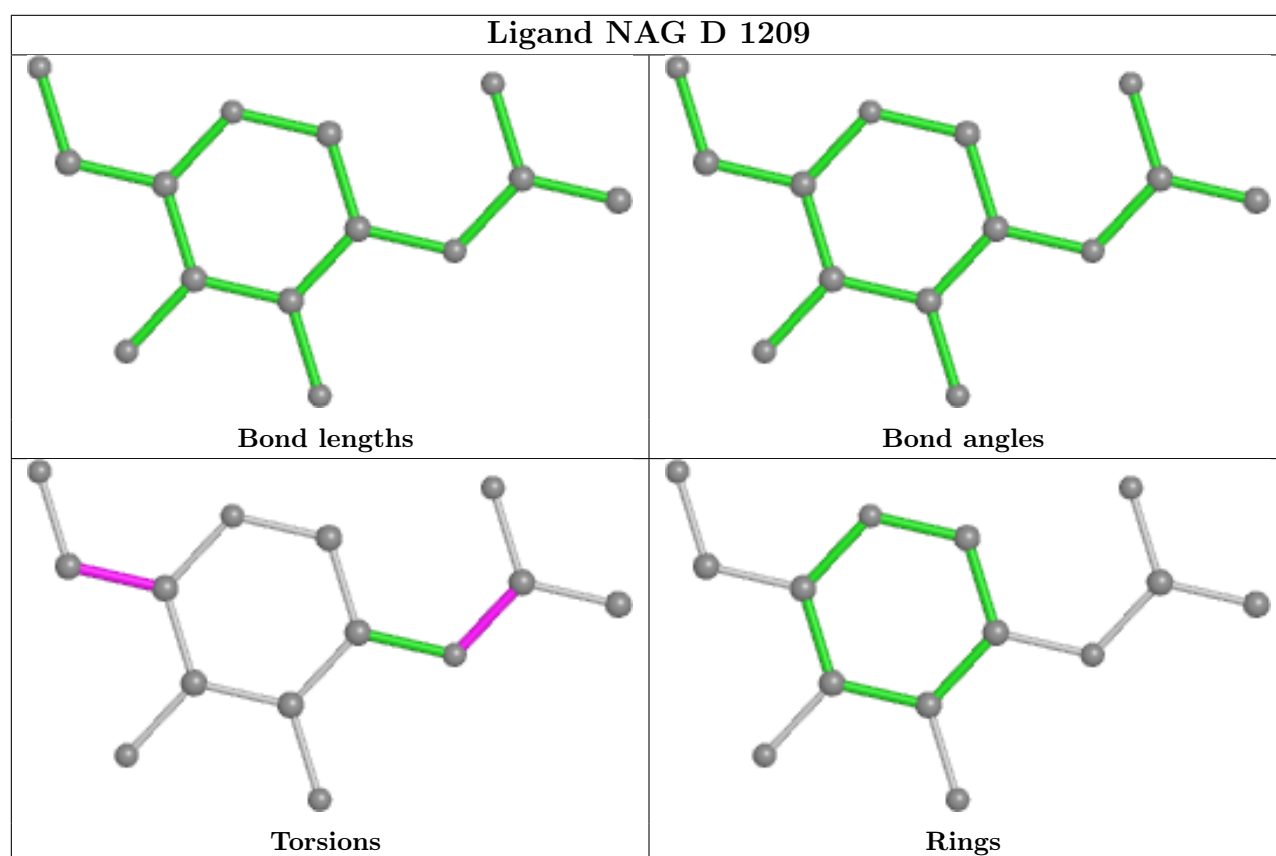
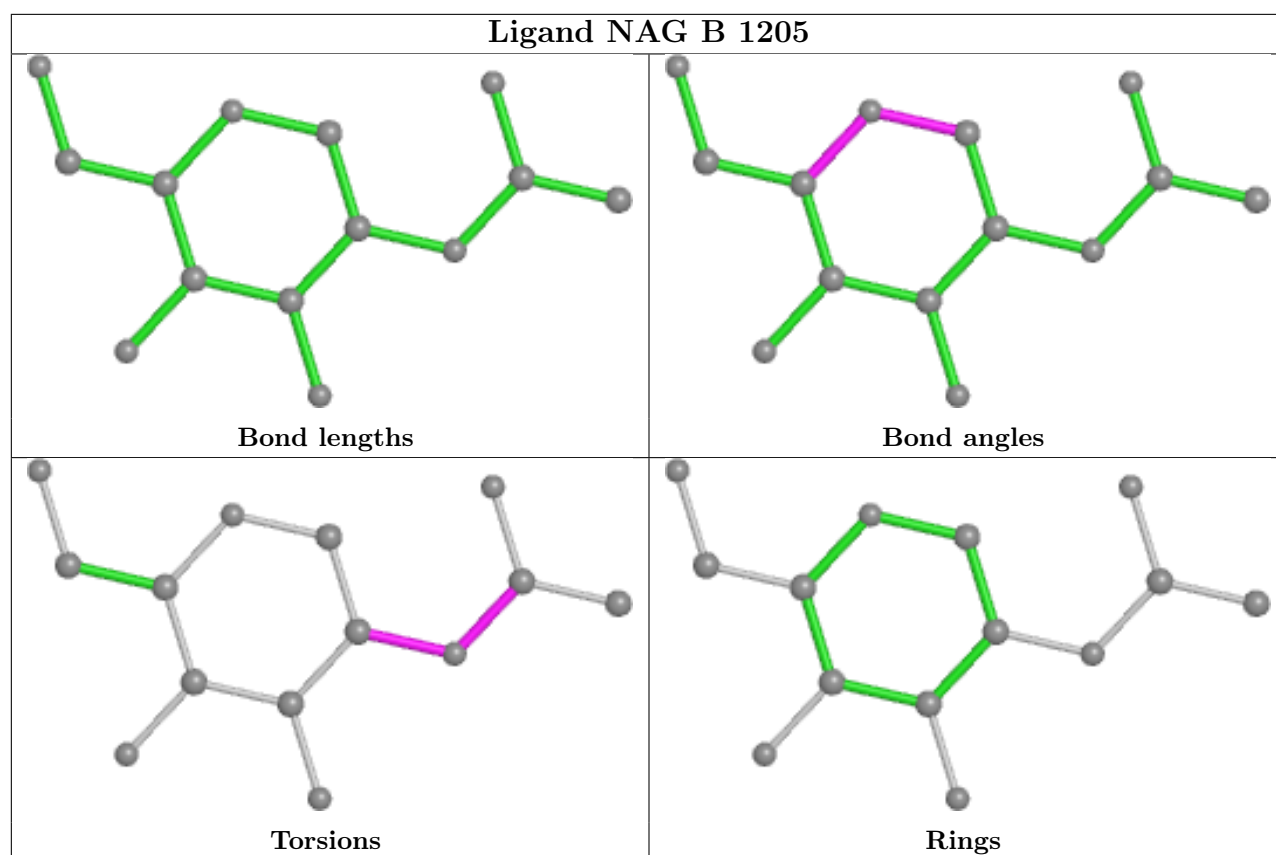


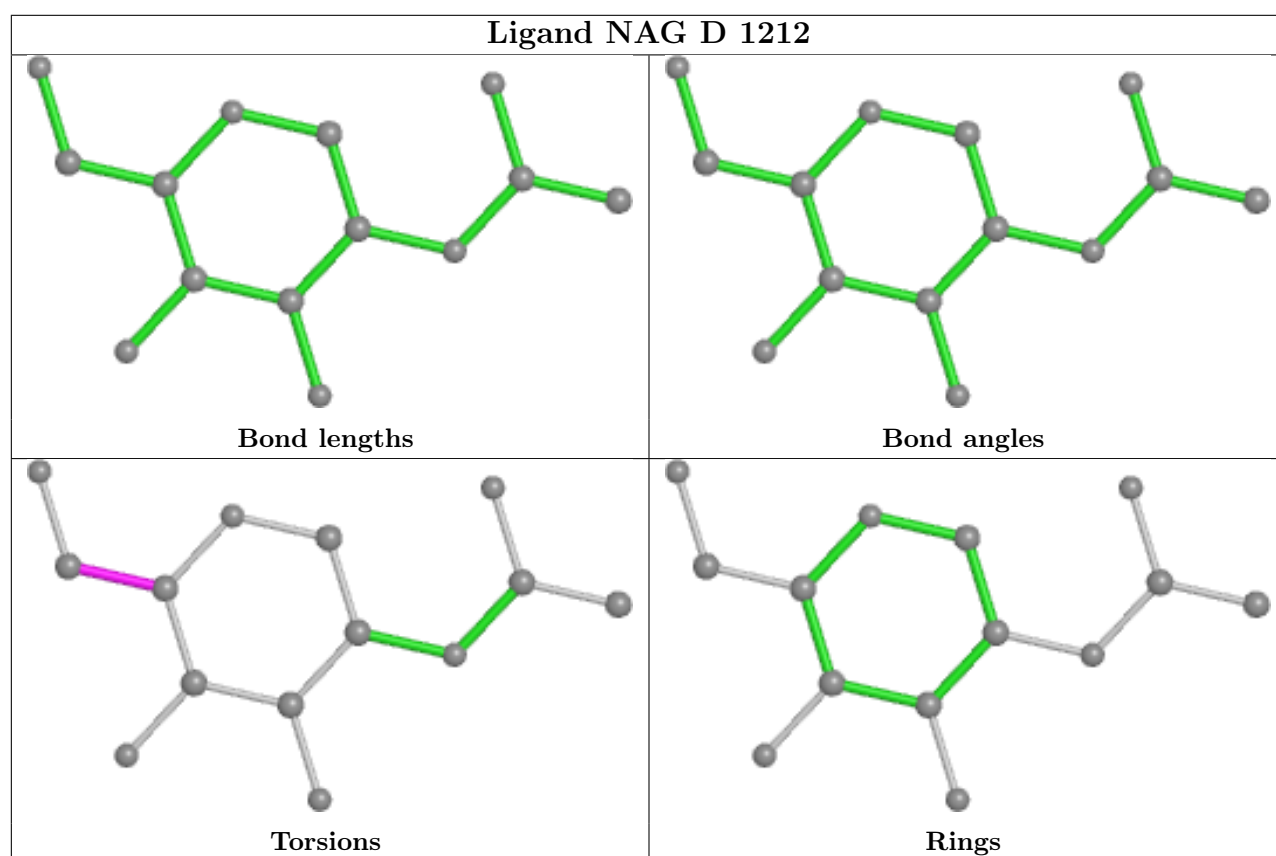
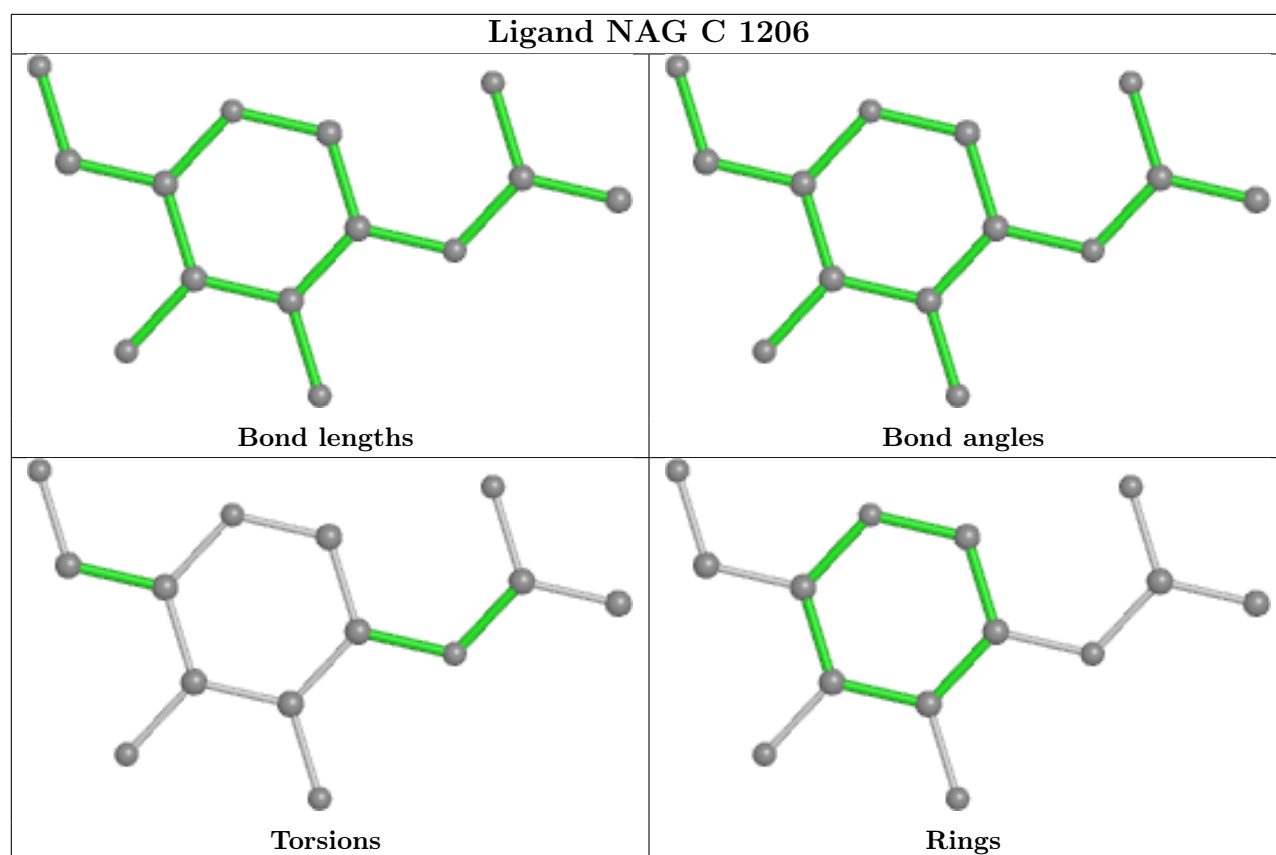


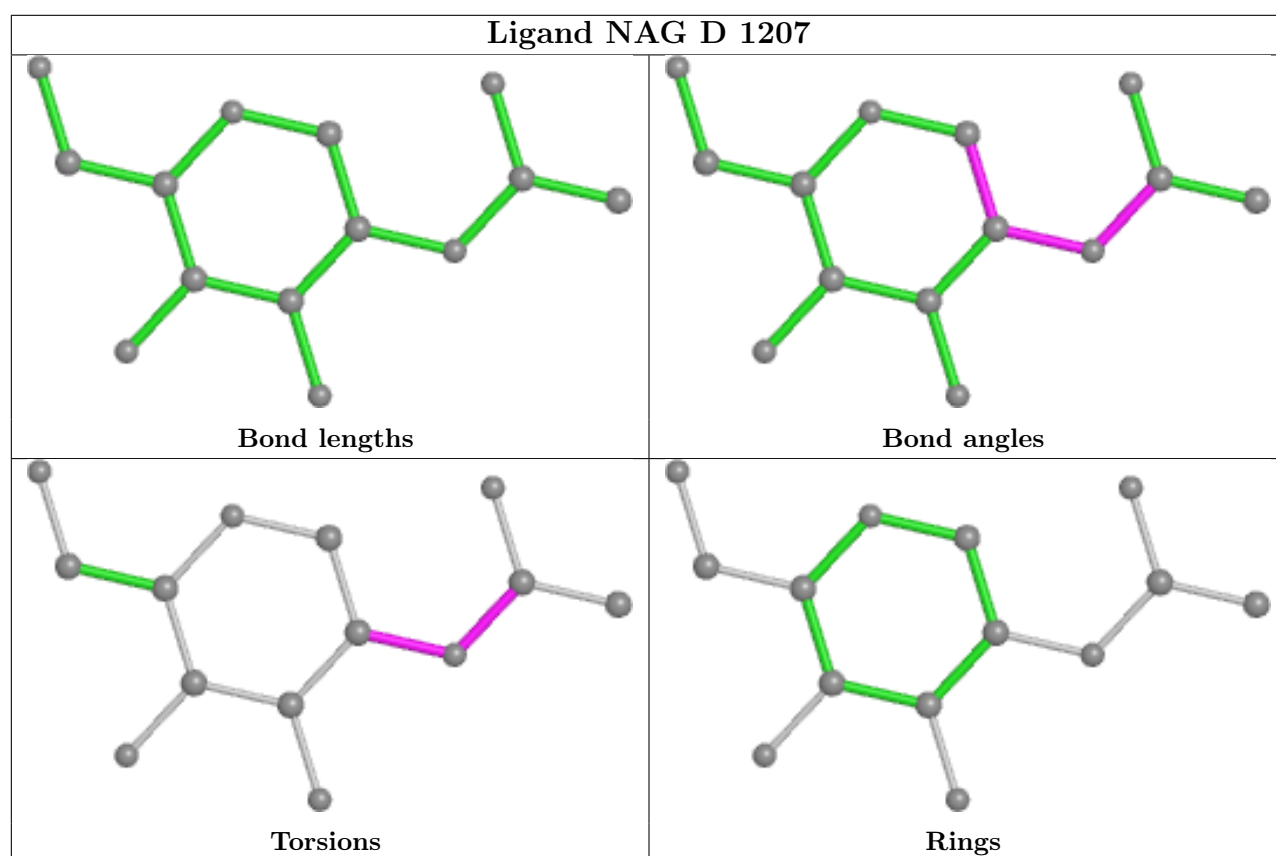
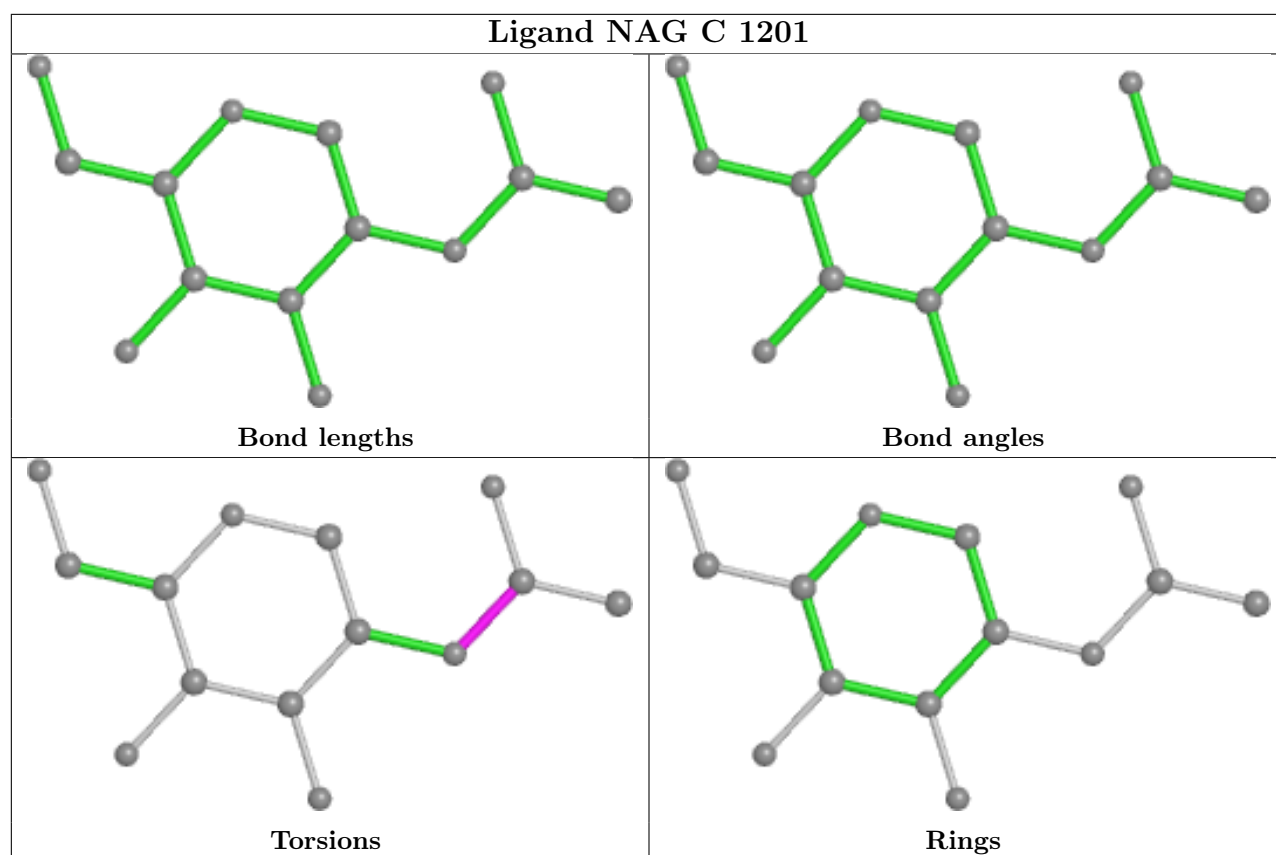


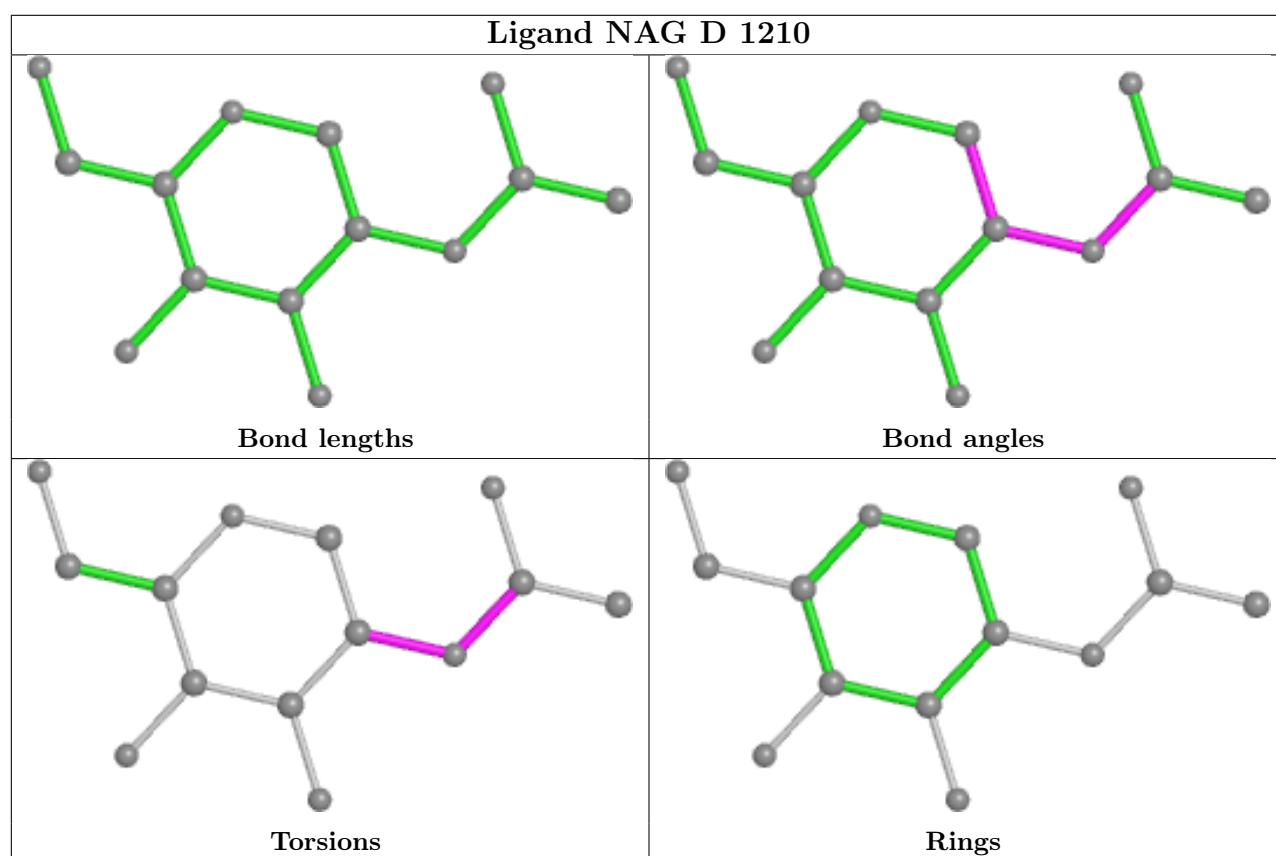
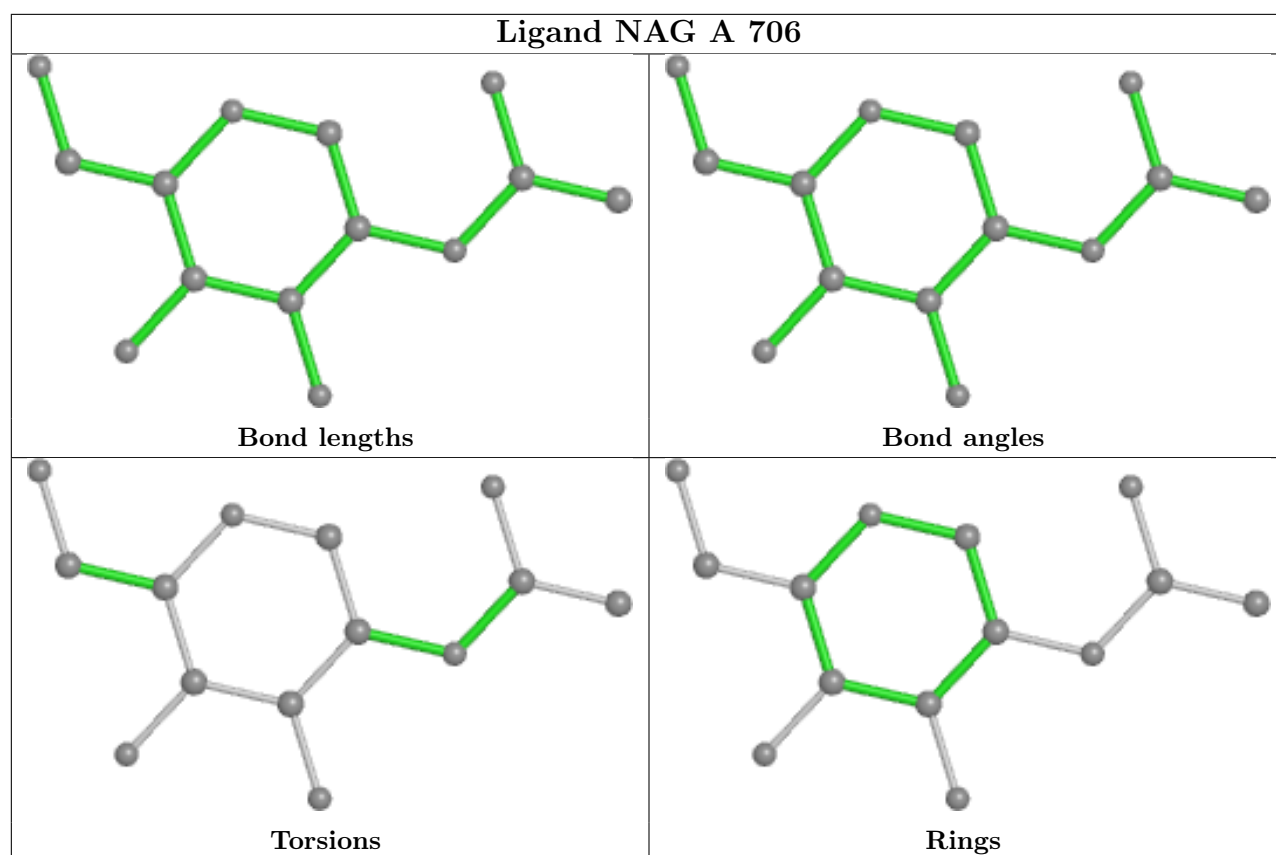


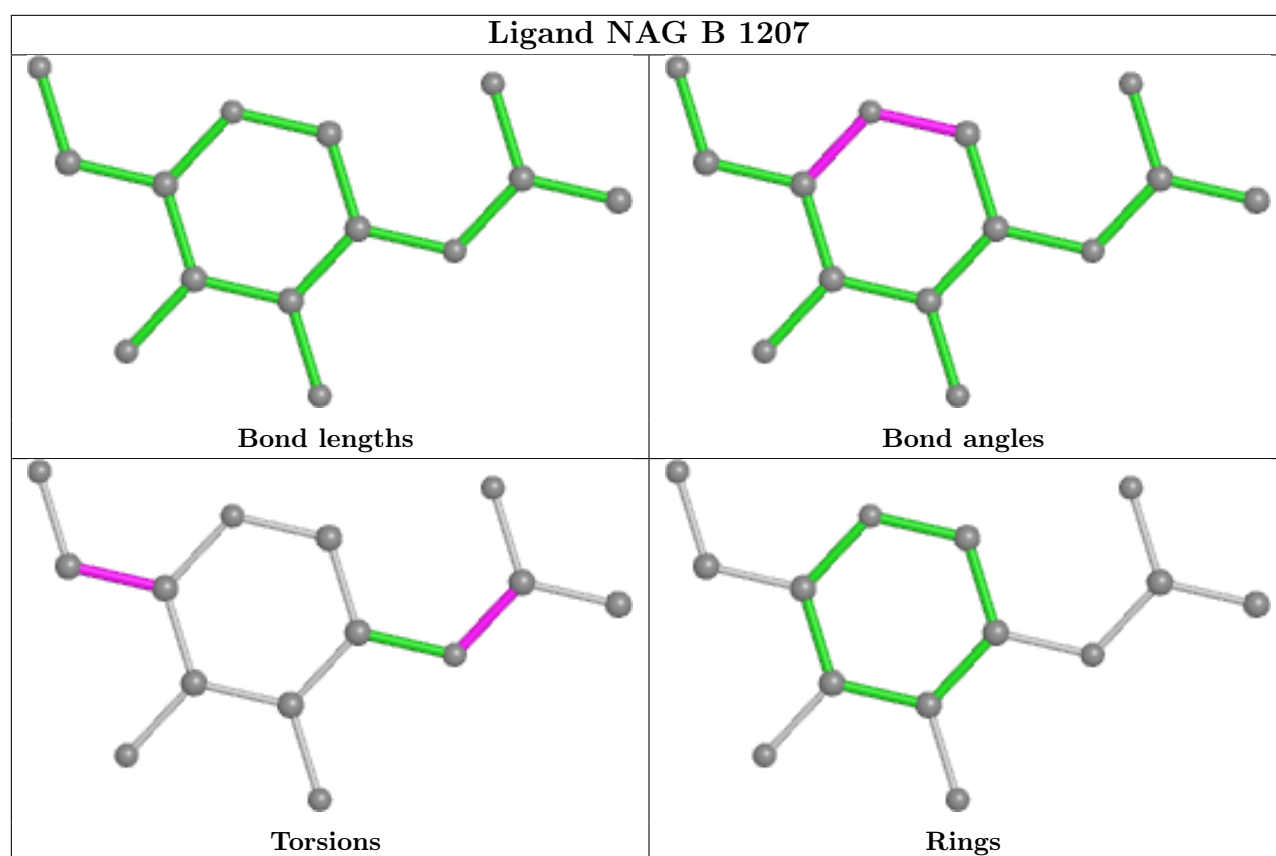
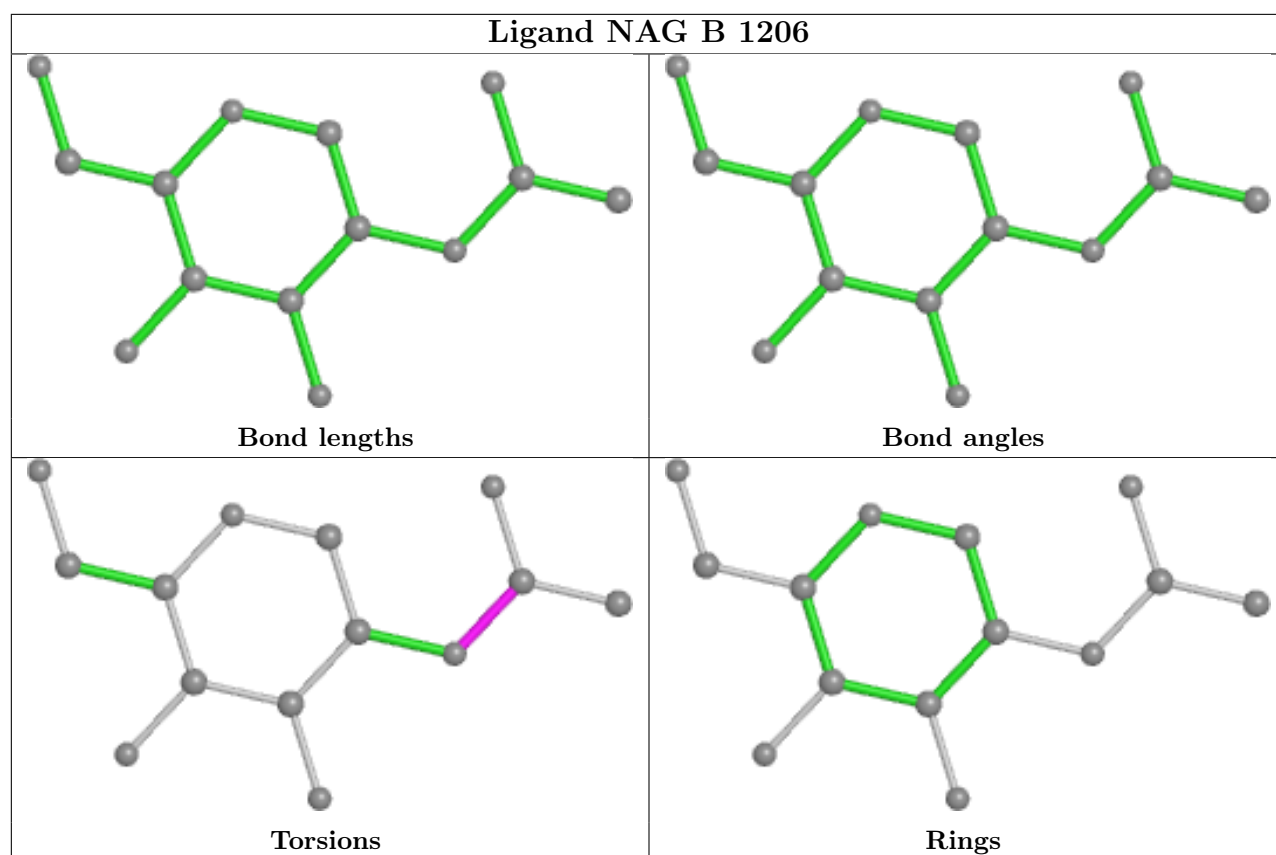


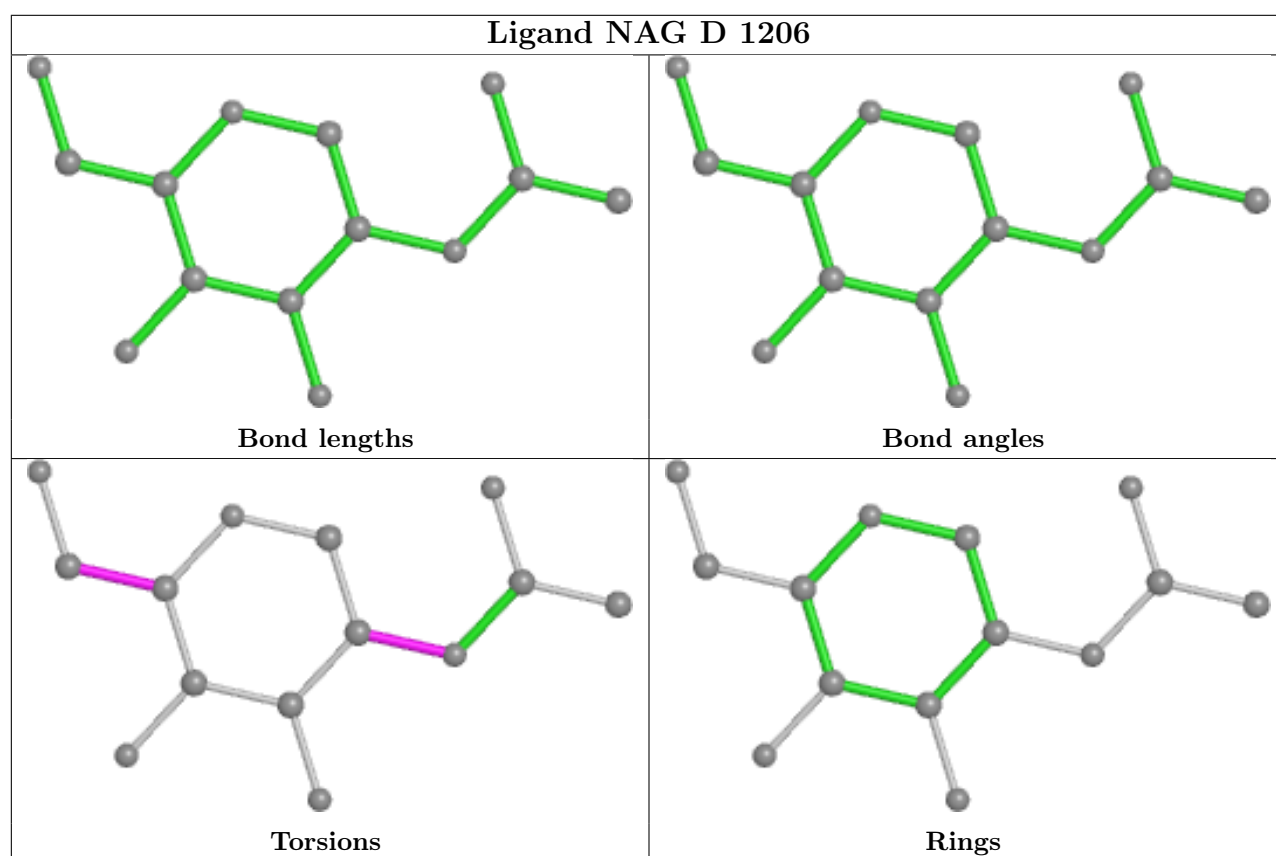
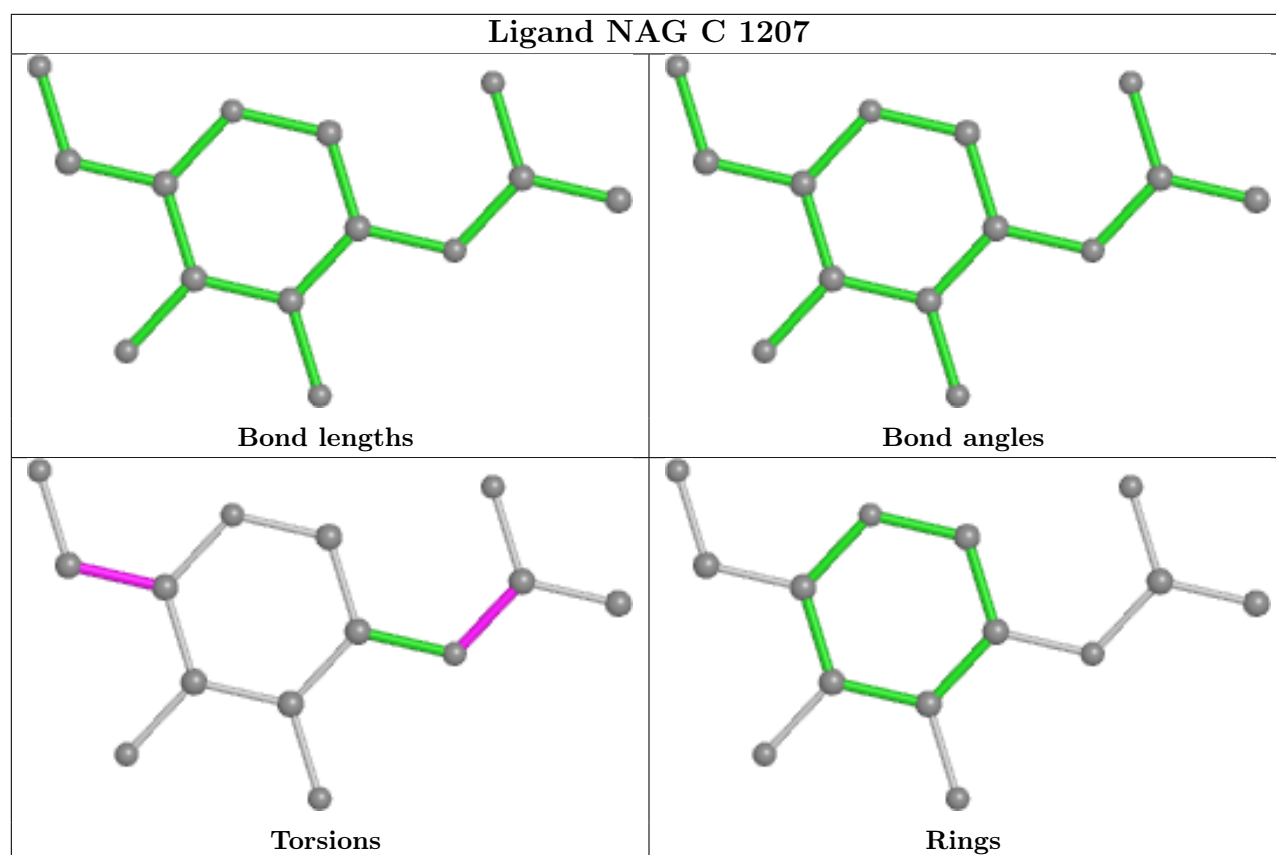


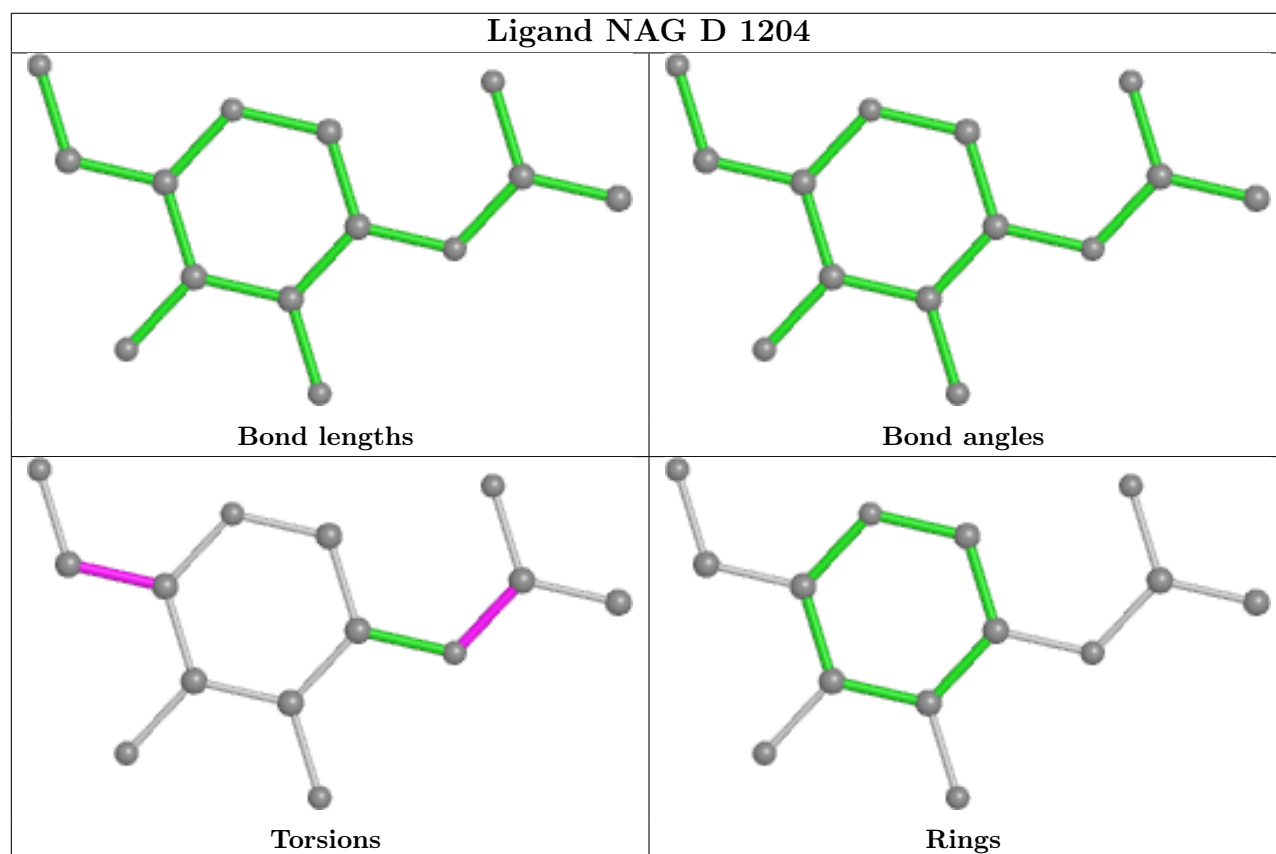
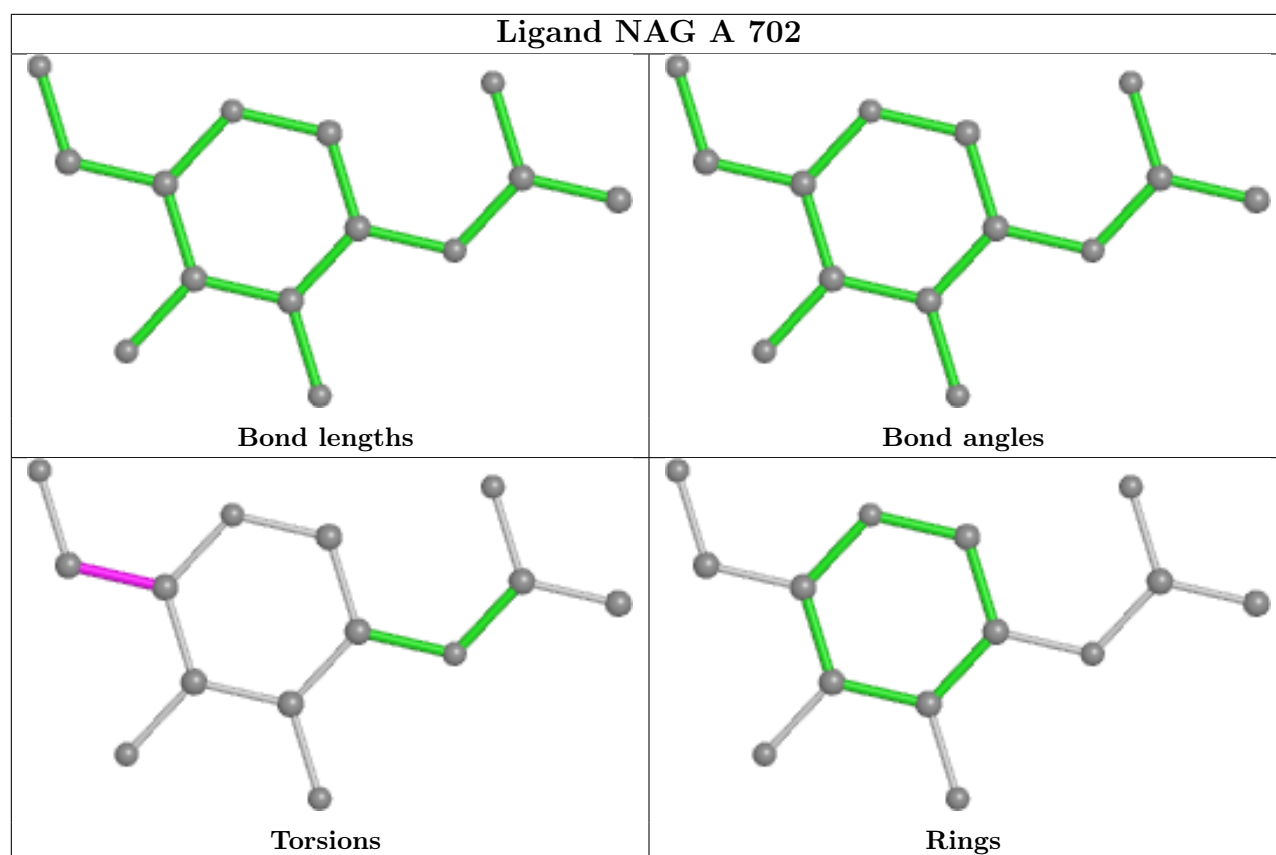




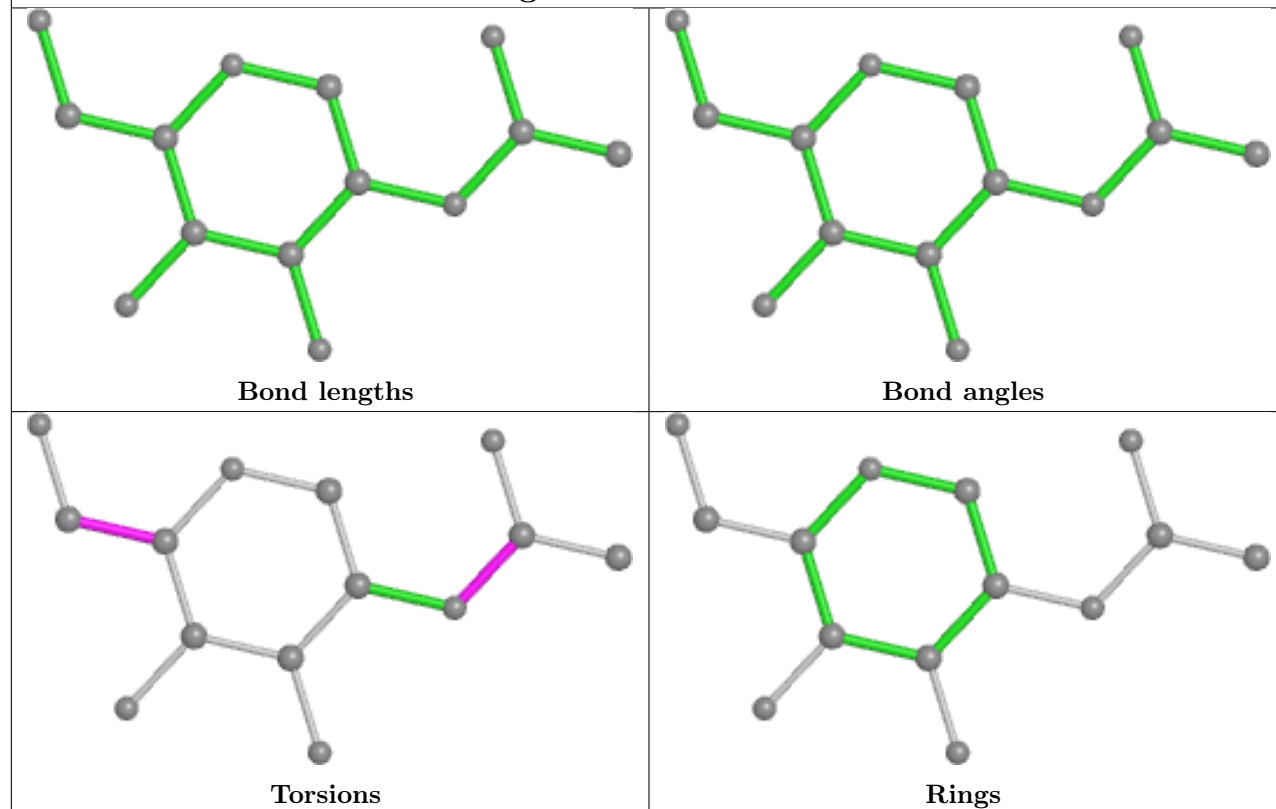




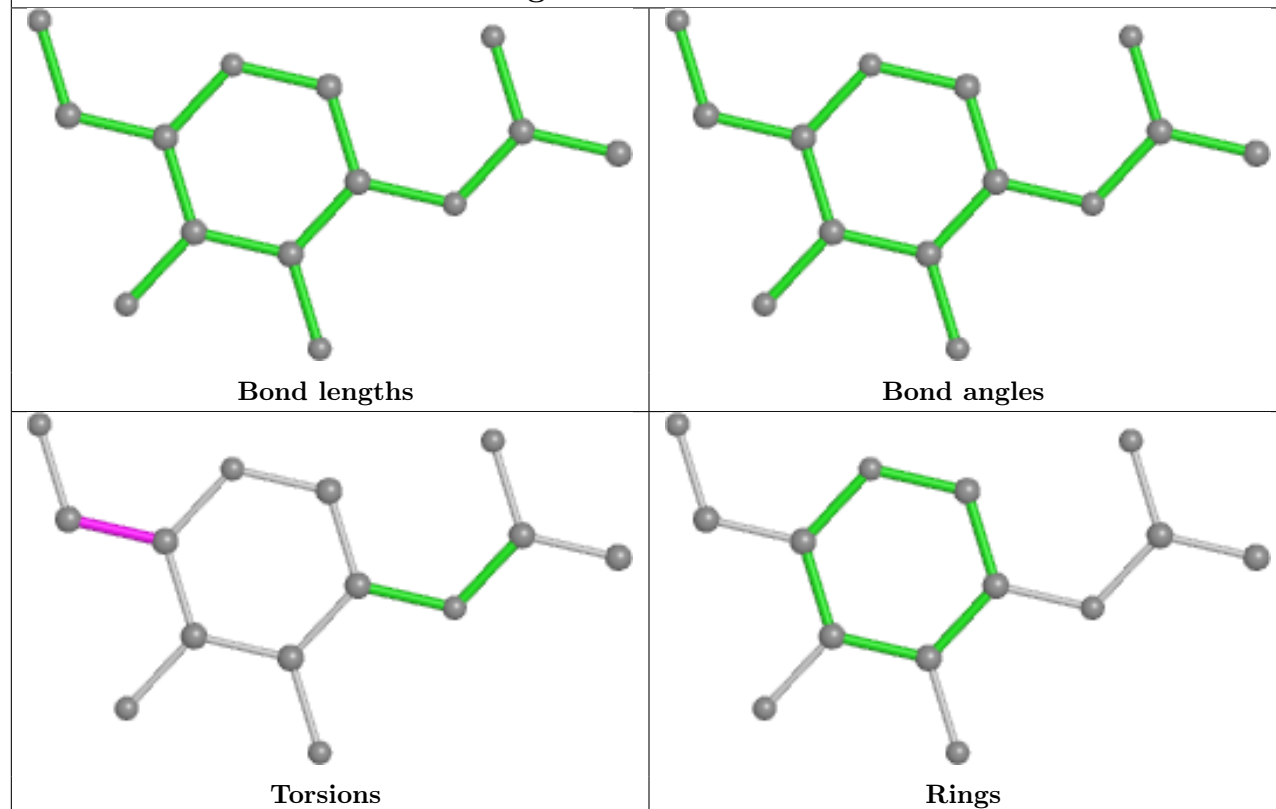


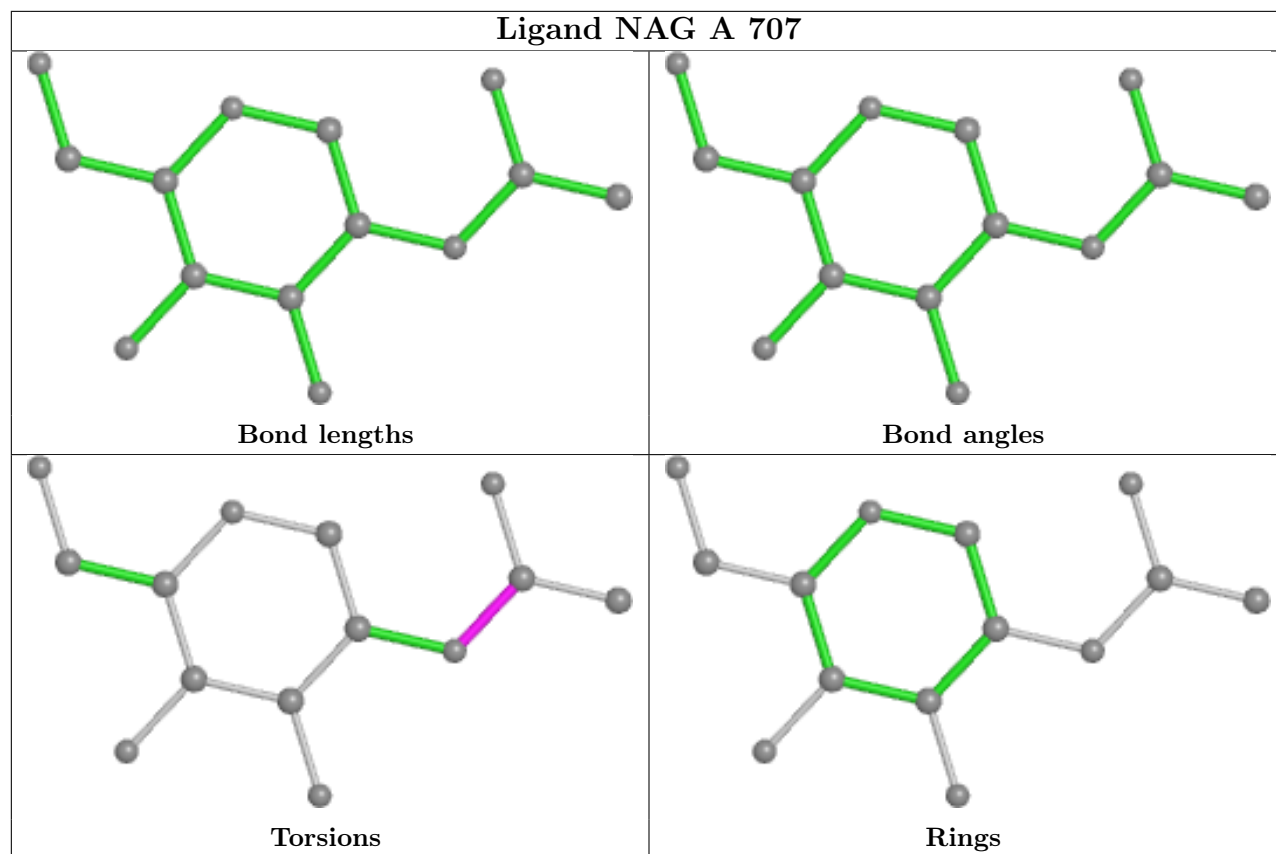


Ligand NAG C 1203



Ligand NAG A 704





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.

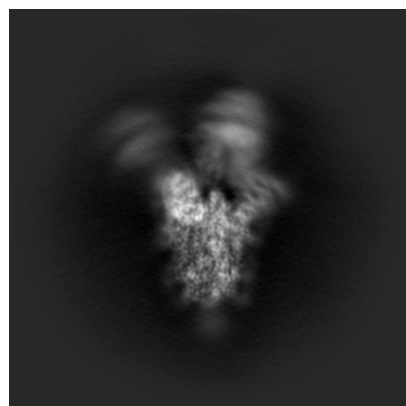
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38502. These allow visual inspection of the internal detail of the map and identification of artifacts.

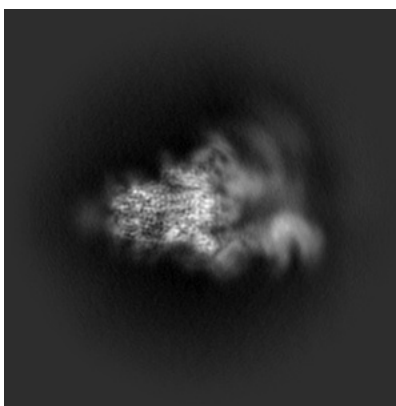
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

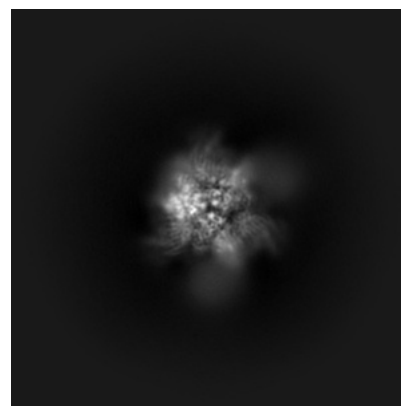
6.1.1 Primary map



X

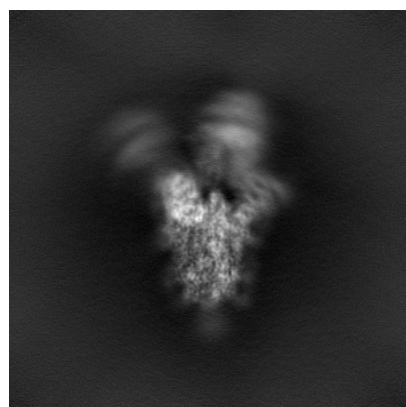


Y

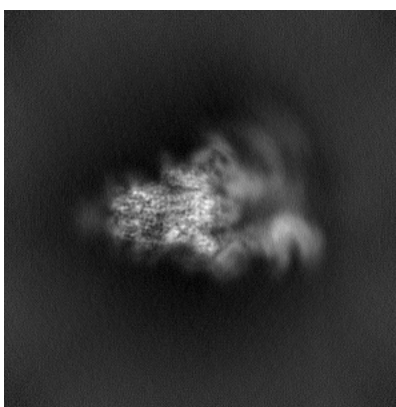


Z

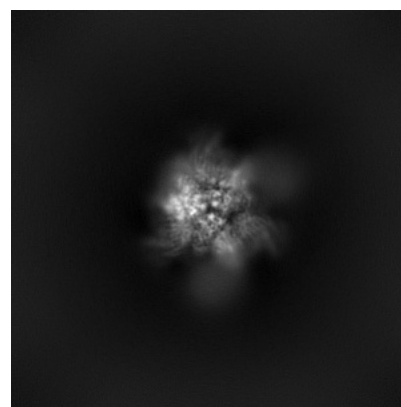
6.1.2 Raw map



X



Y

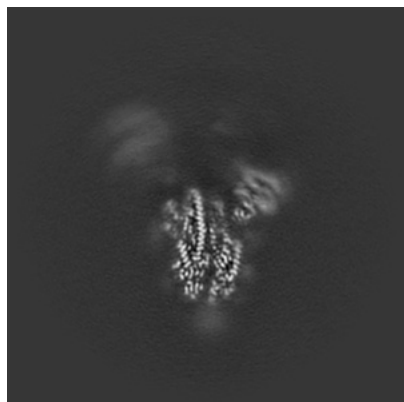


Z

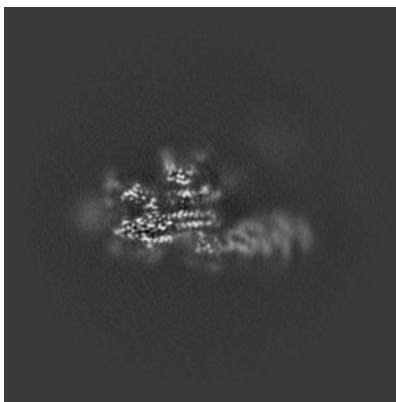
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

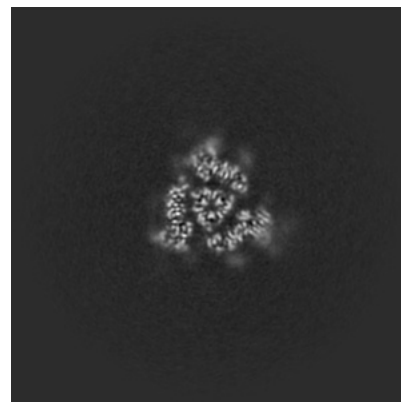
6.2.1 Primary map



X Index: 240

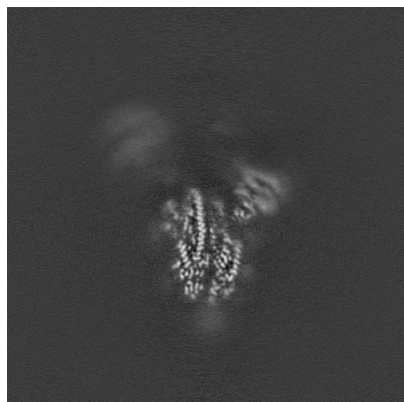


Y Index: 240

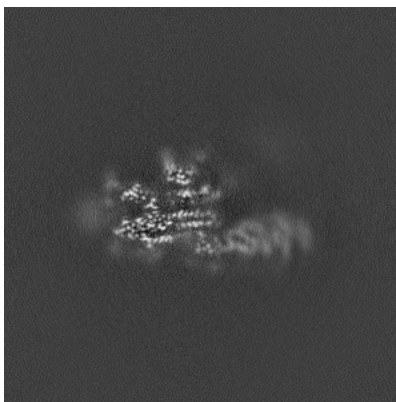


Z Index: 240

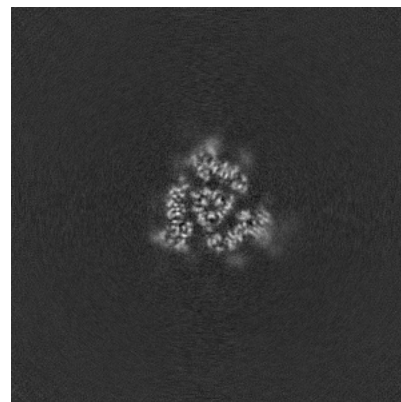
6.2.2 Raw map



X Index: 240



Y Index: 240

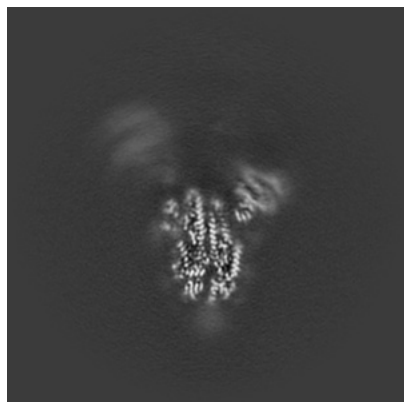


Z Index: 240

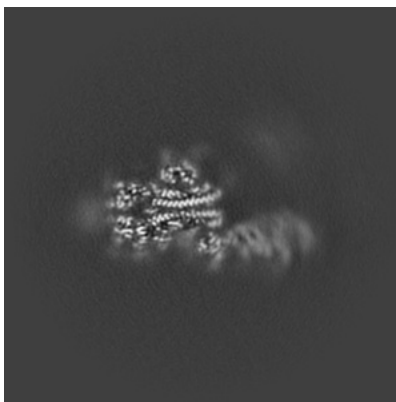
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

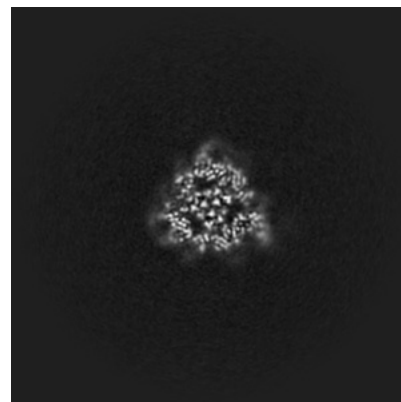
6.3.1 Primary map



X Index: 242

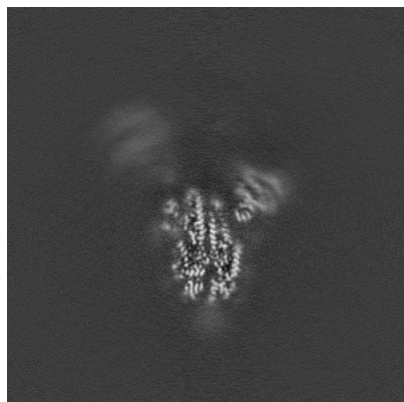


Y Index: 246

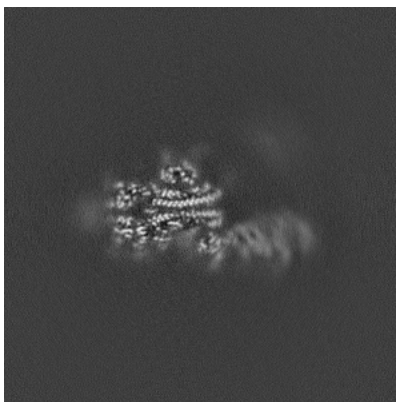


Z Index: 231

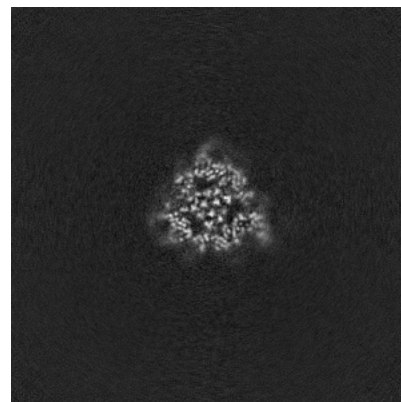
6.3.2 Raw map



X Index: 242



Y Index: 246

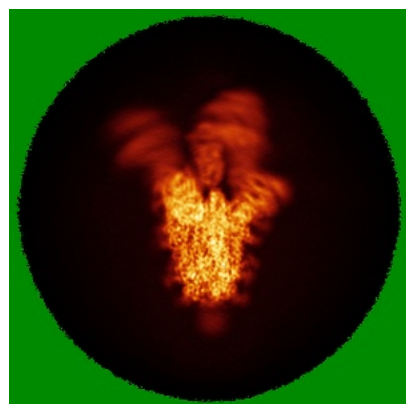


Z Index: 231

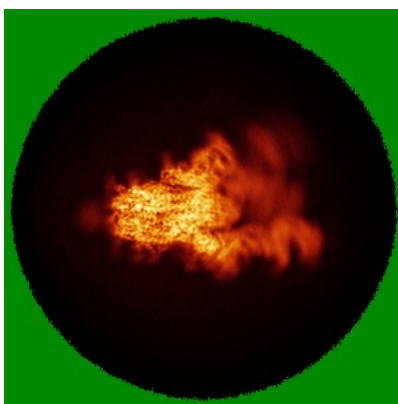
The images above show the largest variance slices of the map in three orthogonal directions.

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

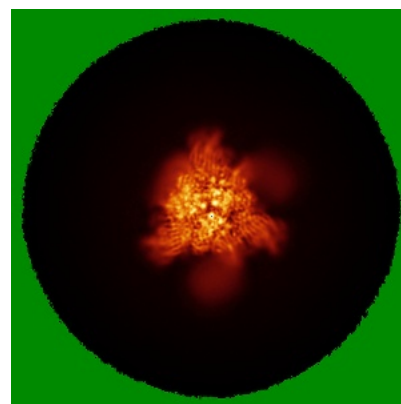
6.4.1 Primary map



X



Y

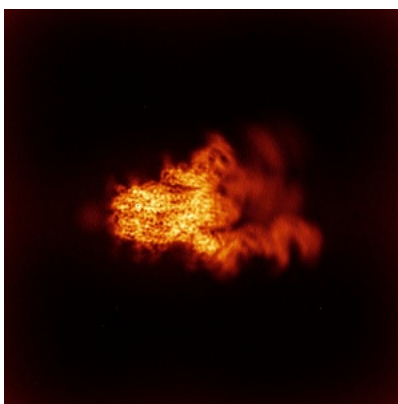


Z

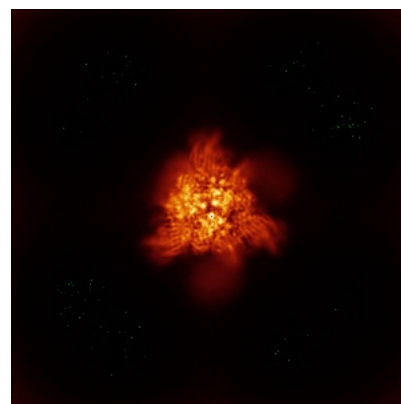
6.4.2 Raw map



X



Y

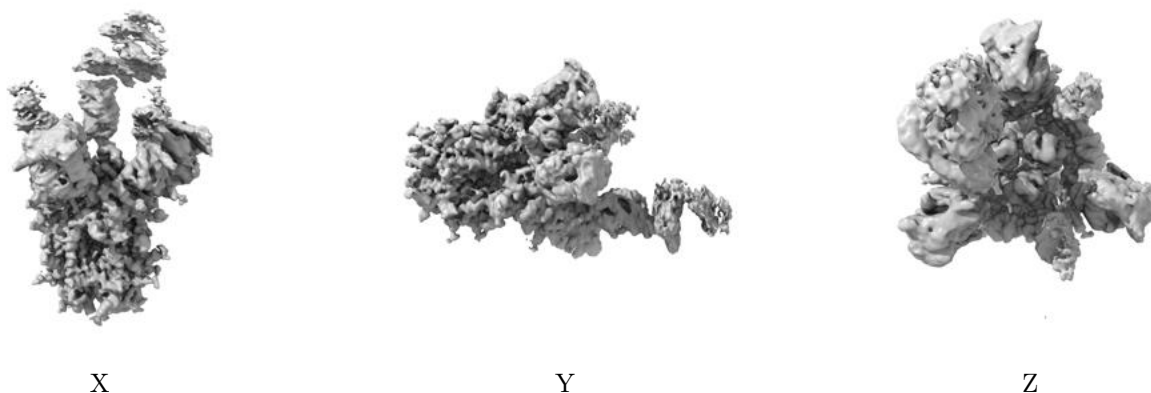


Z

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

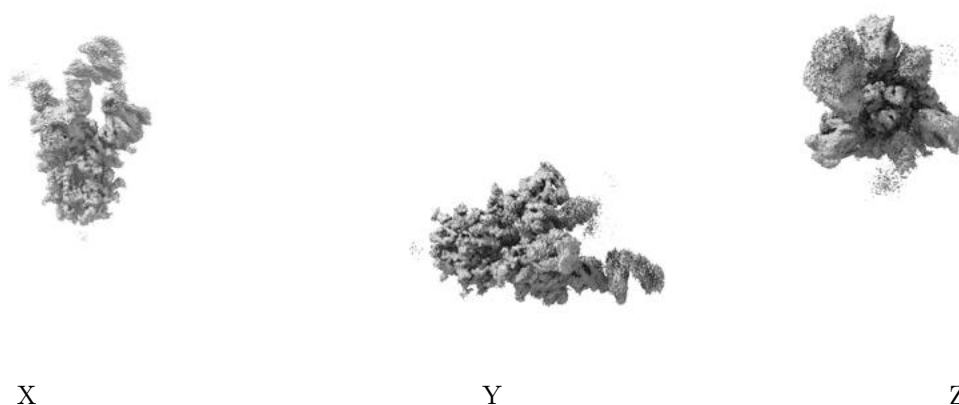
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

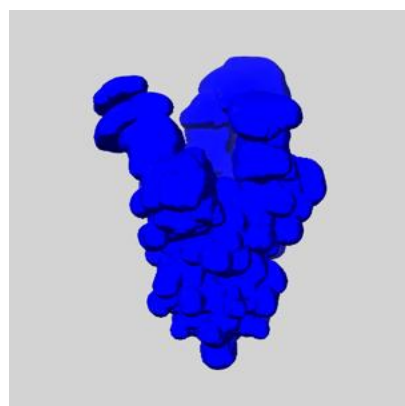
6.6 Mask visualisation [i](#)

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

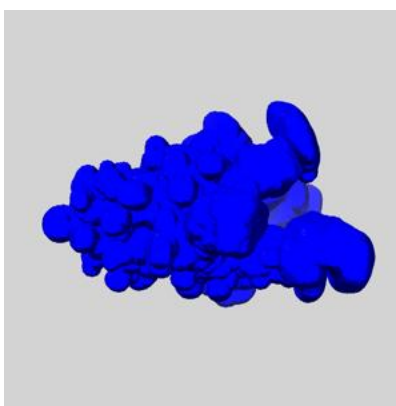
A mask typically either:

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

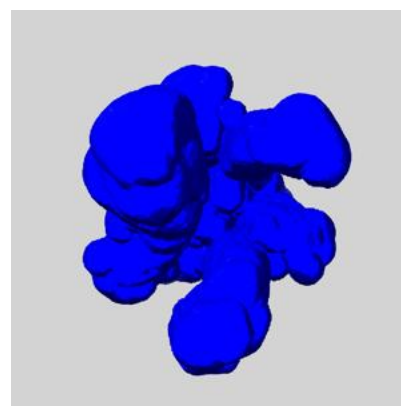
6.6.1 emd_38502_msk_1.map [i](#)



X



Y

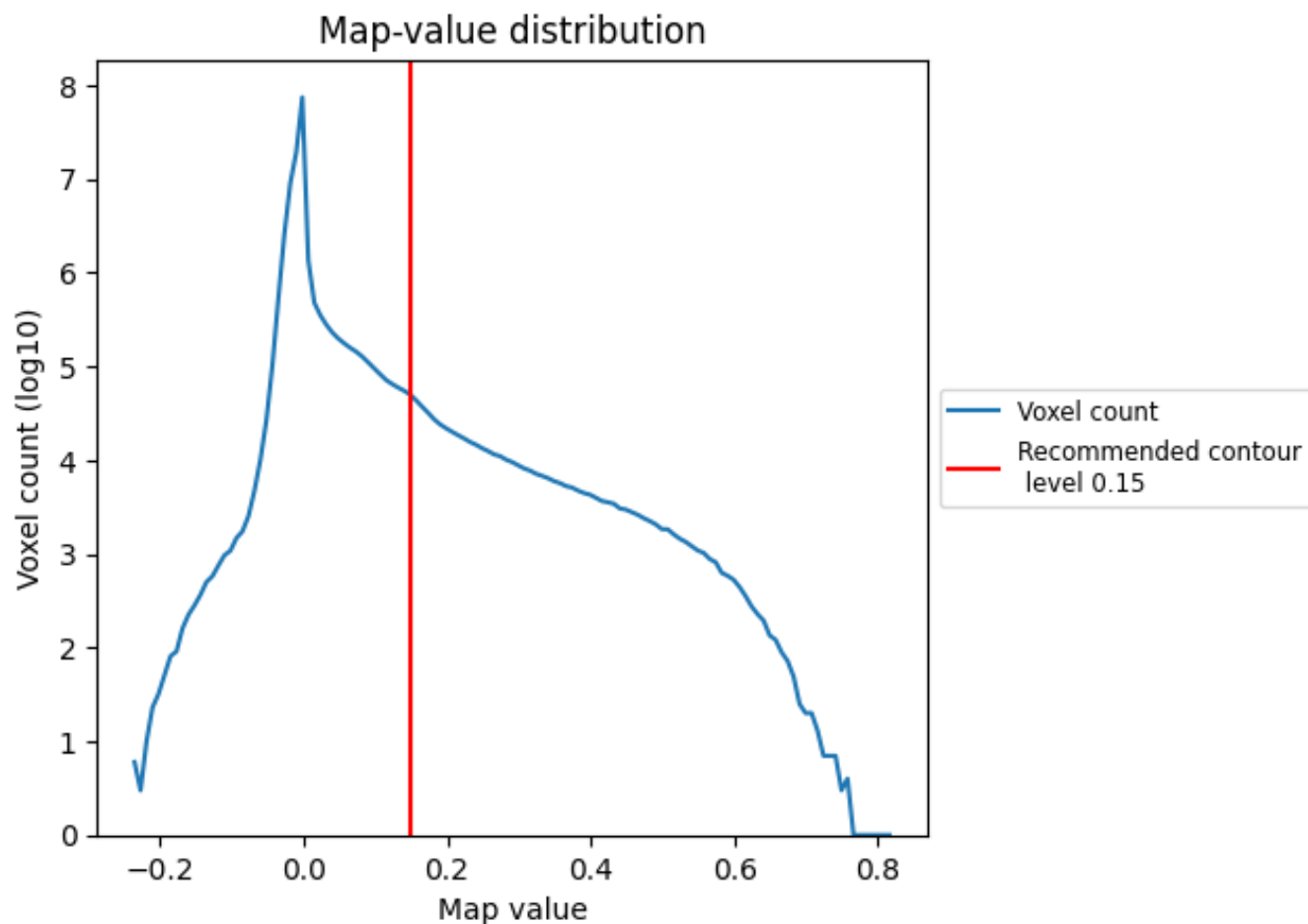


Z

7 Map analysis [i](#)

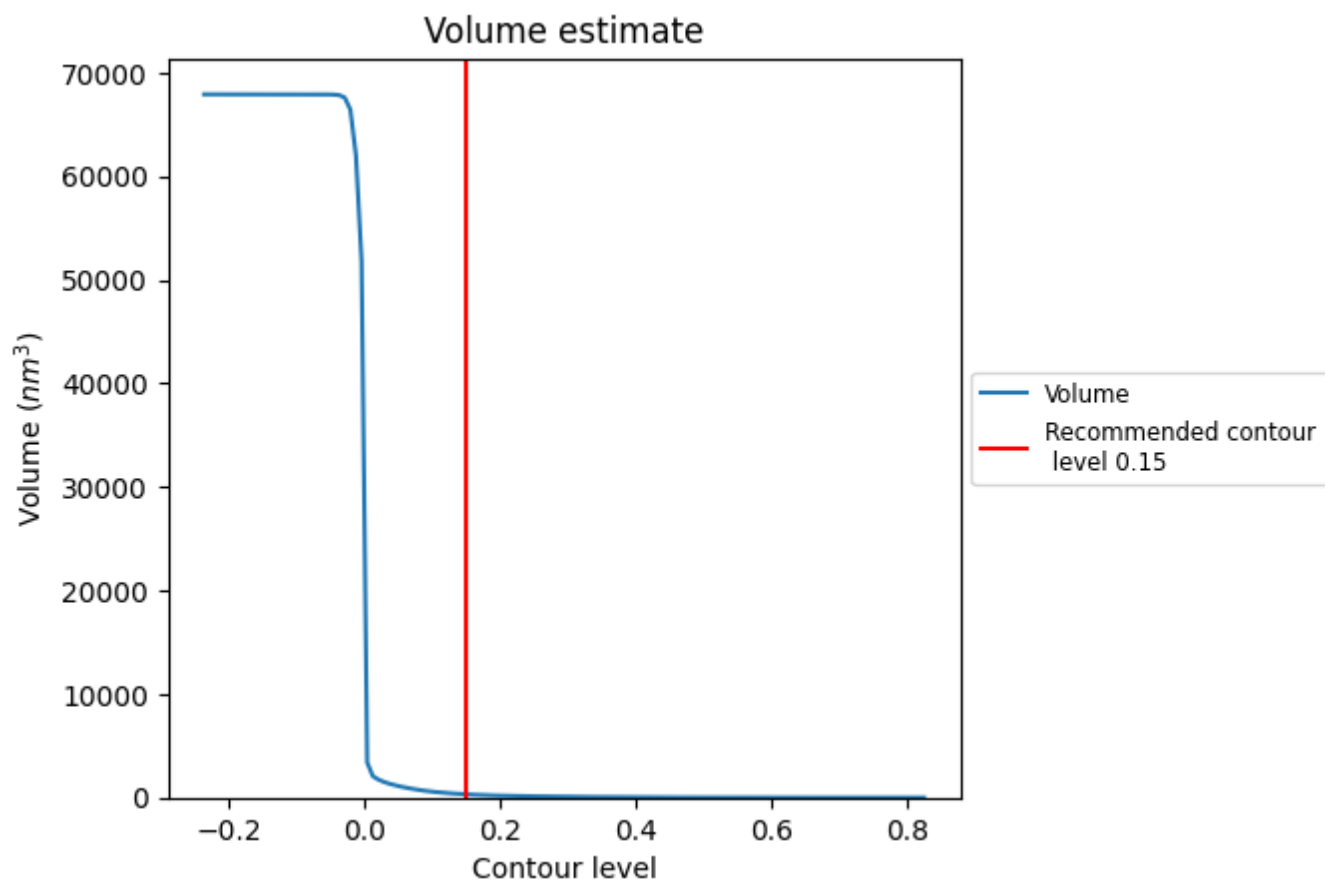
This section contains the results of statistical analysis of the map.

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.

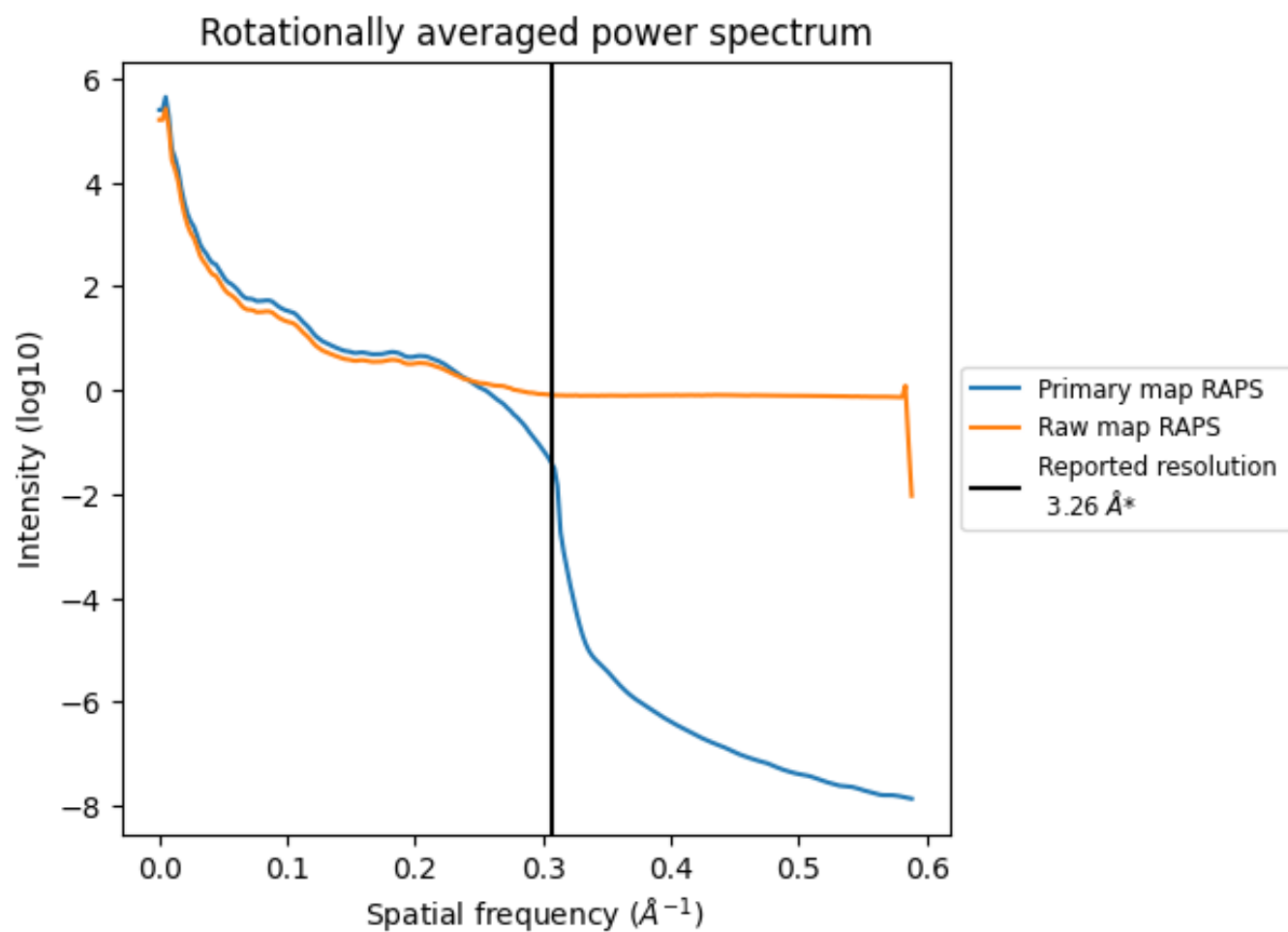
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 314 nm³; this corresponds to an approximate mass of 284 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 ⓘ

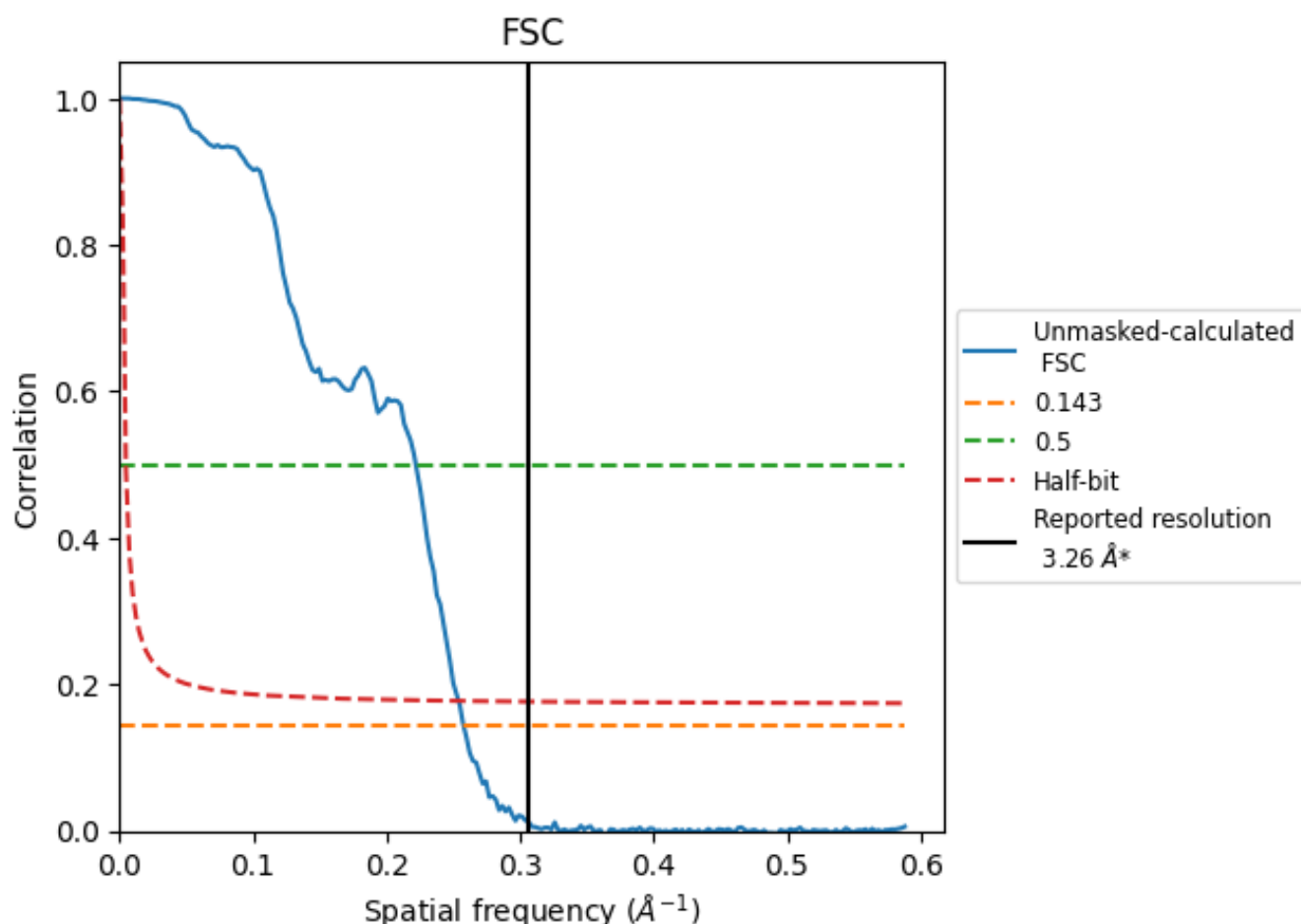


*Reported resolution corresponds to spatial frequency of 0.307 \AA^{-1}

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 0.307 Å⁻¹

8.2 Resolution estimates [i](#)

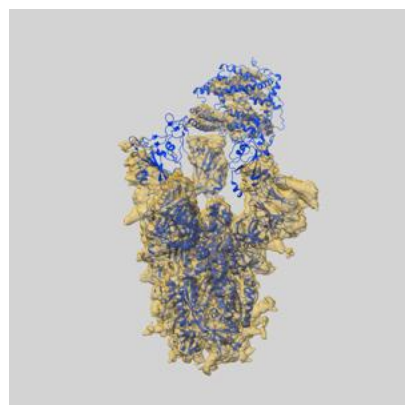
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	4.50	3.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.26 by more than 10 %

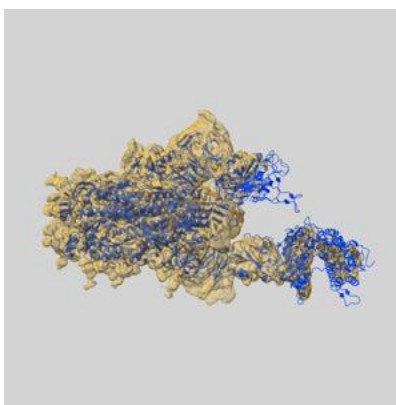
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38502 and PDB model 8XNF. Per-residue inclusion information can be found in section 3 on page 18.

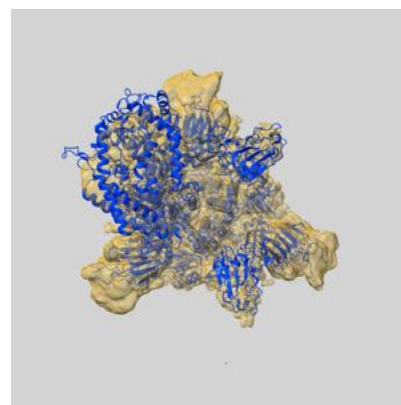
9.1 Map-model overlay [i](#)



X



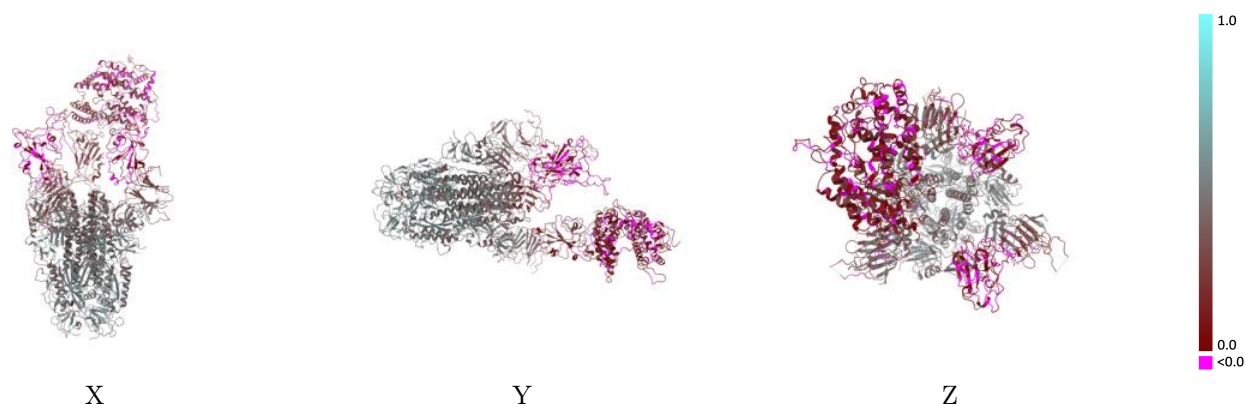
Y



Z

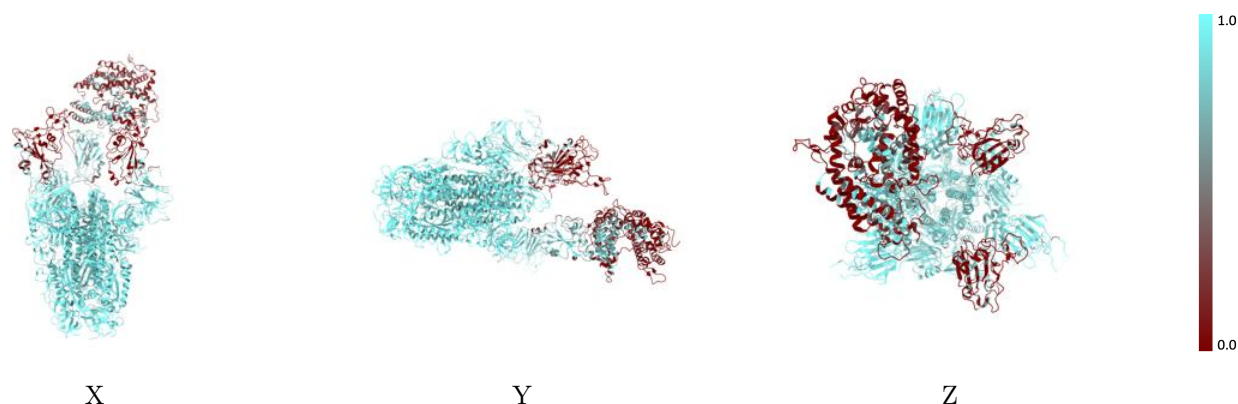
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



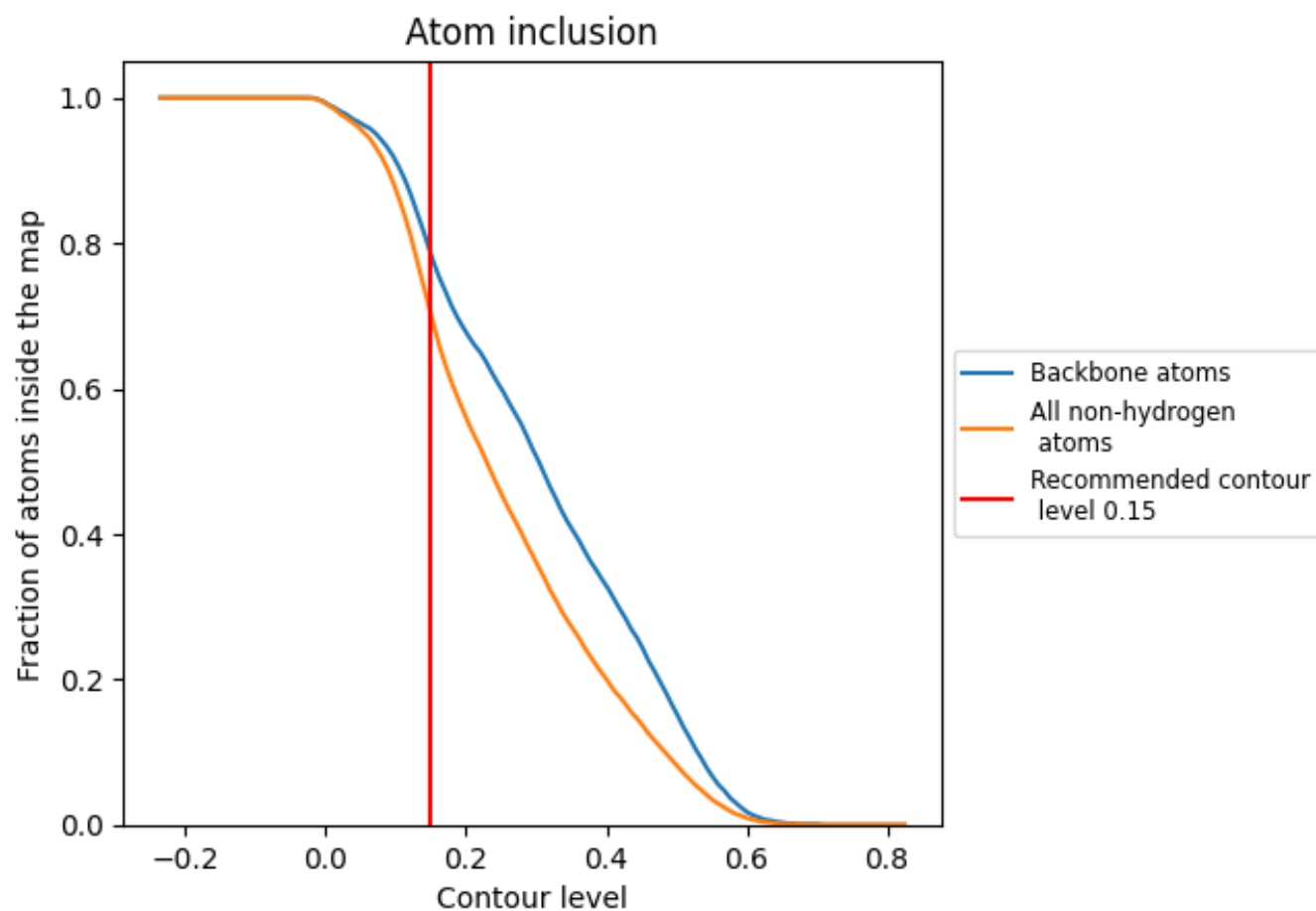
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7010	<div></div> 0.3170
A	<div></div> 0.2710	<div></div> 0.0880
B	<div></div> 0.8450	<div></div> 0.3780
C	<div></div> 0.7540	<div></div> 0.3510
D	<div></div> 0.7620	<div></div> 0.3610
E	<div></div> 0.8970	<div></div> 0.4490
F	<div></div> 0.9640	<div></div> 0.4840
G	<div></div> 0.8210	<div></div> 0.4120
H	<div></div> 0.9290	<div></div> 0.4360
I	<div></div> 0.8930	<div></div> 0.4250
J	<div></div> 0.8570	<div></div> 0.4090

1.0

0.0

<0.0