



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 07:09 PM UTC

PDB ID : 8XMG / pdb_00008xmg
EMDB ID : EMD-38476
Title : Cryo-EM structure of SARS-CoV-2 Omicron HV.1 spike protein(6P), RBD-closed state
Authors : Li, L.J.; Gu, Y.H.; Shi, K.Y.; Qi, J.X.; Gao, G.F.
Deposited on : 2023-12-27
Resolution : 2.90 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

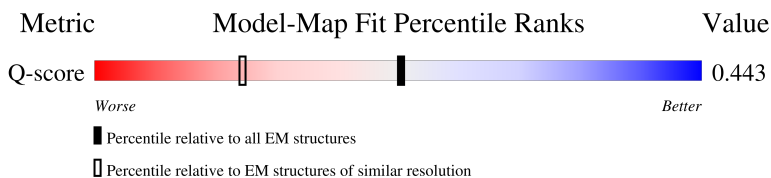
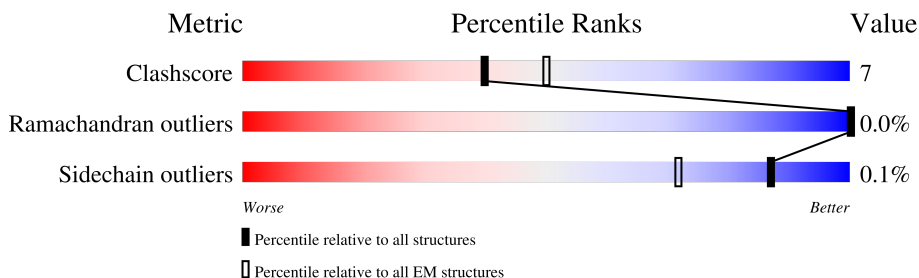
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	1227	 69% 14% 17%
1	B	1227	 69% 14% 17%
1	C	1227	 68% 16% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24476 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1023	Total	C	N	O	S	0	0
			8000	5110	1338	1516	36		
1	B	1016	Total	C	N	O	S	0	0
			7942	5076	1328	1503	35		
1	C	1023	Total	C	N	O	S	0	0
			8002	5112	1339	1515	36		

There are 291 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	VAL	-	expression tag	UNP P0DTC2
A	20	ASN	-	expression tag	UNP P0DTC2
A	21	LEU	-	expression tag	UNP P0DTC2
A	22	ILE	-	expression tag	UNP P0DTC2
A	23	THR	-	expression tag	UNP P0DTC2
A	24	ARG	-	expression tag	UNP P0DTC2
A	25	THR	-	expression tag	UNP P0DTC2
A	26	GLN	-	expression tag	UNP P0DTC2
A	27	SER	-	expression tag	UNP P0DTC2
A	52	HIS	GLN	variant	UNP P0DTC2
A	83	ALA	VAL	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	157	LEU	PHE	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	456	LEU	PHE	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	TYR	-	expression tag	UNP P0DTC2
A	1211	ILE	-	expression tag	UNP P0DTC2
A	1212	PRO	-	expression tag	UNP P0DTC2
A	1213	GLU	-	expression tag	UNP P0DTC2
A	1214	ALA	-	expression tag	UNP P0DTC2
A	1215	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	ASP	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	GLN	-	expression tag	UNP P0DTC2
A	1220	ALA	-	expression tag	UNP P0DTC2
A	1221	TYR	-	expression tag	UNP P0DTC2
A	1222	VAL	-	expression tag	UNP P0DTC2
A	1223	ARG	-	expression tag	UNP P0DTC2
A	1224	LYS	-	expression tag	UNP P0DTC2
A	1225	ASP	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	TRP	-	expression tag	UNP P0DTC2
A	1229	VAL	-	expression tag	UNP P0DTC2
A	1230	LEU	-	expression tag	UNP P0DTC2
A	1231	LEU	-	expression tag	UNP P0DTC2
A	1232	SER	-	expression tag	UNP P0DTC2
A	1233	THR	-	expression tag	UNP P0DTC2
A	1234	PHE	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	ALA	-	expression tag	UNP P0DTC2
A	1237	HIS	-	expression tag	UNP P0DTC2
A	1238	HIS	-	expression tag	UNP P0DTC2
A	1239	HIS	-	expression tag	UNP P0DTC2
A	1240	HIS	-	expression tag	UNP P0DTC2
A	1241	HIS	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
B	19	VAL	-	expression tag	UNP P0DTC2
B	20	ASN	-	expression tag	UNP P0DTC2
B	21	LEU	-	expression tag	UNP P0DTC2
B	22	ILE	-	expression tag	UNP P0DTC2
B	23	THR	-	expression tag	UNP P0DTC2
B	24	ARG	-	expression tag	UNP P0DTC2
B	25	THR	-	expression tag	UNP P0DTC2
B	26	GLN	-	expression tag	UNP P0DTC2
B	27	SER	-	expression tag	UNP P0DTC2
B	52	HIS	GLN	variant	UNP P0DTC2
B	83	ALA	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	157	LEU	PHE	variant	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	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
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	PRO	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	456	LEU	PHE	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	484	ALA	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	490	SER	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	TYR	-	expression tag	UNP P0DTC2
B	1211	ILE	-	expression tag	UNP P0DTC2
B	1212	PRO	-	expression tag	UNP P0DTC2
B	1213	GLU	-	expression tag	UNP P0DTC2
B	1214	ALA	-	expression tag	UNP P0DTC2
B	1215	PRO	-	expression tag	UNP P0DTC2
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	ASP	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	GLN	-	expression tag	UNP P0DTC2
B	1220	ALA	-	expression tag	UNP P0DTC2
B	1221	TYR	-	expression tag	UNP P0DTC2
B	1222	VAL	-	expression tag	UNP P0DTC2
B	1223	ARG	-	expression tag	UNP P0DTC2
B	1224	LYS	-	expression tag	UNP P0DTC2
B	1225	ASP	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	GLU	-	expression tag	UNP P0DTC2
B	1228	TRP	-	expression tag	UNP P0DTC2
B	1229	VAL	-	expression tag	UNP P0DTC2
B	1230	LEU	-	expression tag	UNP P0DTC2
B	1231	LEU	-	expression tag	UNP P0DTC2
B	1232	SER	-	expression tag	UNP P0DTC2
B	1233	THR	-	expression tag	UNP P0DTC2
B	1234	PHE	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	ALA	-	expression tag	UNP P0DTC2
B	1237	HIS	-	expression tag	UNP P0DTC2
B	1238	HIS	-	expression tag	UNP P0DTC2
B	1239	HIS	-	expression tag	UNP P0DTC2
B	1240	HIS	-	expression tag	UNP P0DTC2
B	1241	HIS	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
C	19	VAL	-	expression tag	UNP P0DTC2
C	20	ASN	-	expression tag	UNP P0DTC2
C	21	LEU	-	expression tag	UNP P0DTC2
C	22	ILE	-	expression tag	UNP P0DTC2
C	23	THR	-	expression tag	UNP P0DTC2
C	24	ARG	-	expression tag	UNP P0DTC2
C	25	THR	-	expression tag	UNP P0DTC2
C	26	GLN	-	expression tag	UNP P0DTC2
C	27	SER	-	expression tag	UNP P0DTC2
C	52	HIS	GLN	variant	UNP P0DTC2
C	83	ALA	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	157	LEU	PHE	variant	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	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	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	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	456	LEU	PHE	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	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2

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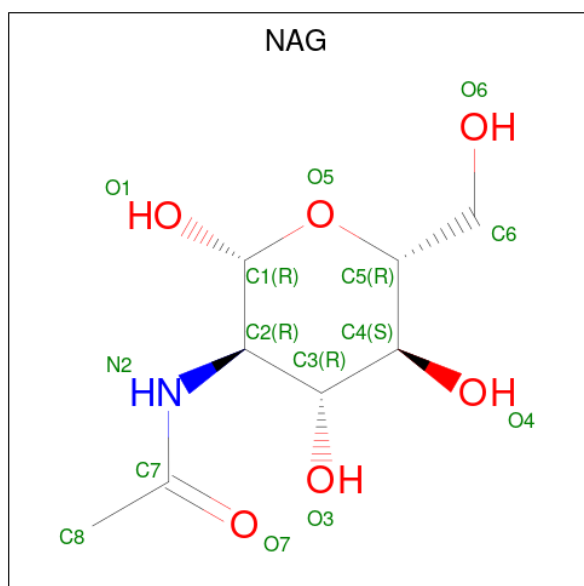
Chain	Residue	Modelled	Actual	Comment	Reference
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	TYR	-	expression tag	UNP P0DTC2
C	1211	ILE	-	expression tag	UNP P0DTC2
C	1212	PRO	-	expression tag	UNP P0DTC2
C	1213	GLU	-	expression tag	UNP P0DTC2
C	1214	ALA	-	expression tag	UNP P0DTC2
C	1215	PRO	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	ASP	-	expression tag	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	GLN	-	expression tag	UNP P0DTC2
C	1220	ALA	-	expression tag	UNP P0DTC2
C	1221	TYR	-	expression tag	UNP P0DTC2
C	1222	VAL	-	expression tag	UNP P0DTC2
C	1223	ARG	-	expression tag	UNP P0DTC2
C	1224	LYS	-	expression tag	UNP P0DTC2
C	1225	ASP	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	GLU	-	expression tag	UNP P0DTC2
C	1228	TRP	-	expression tag	UNP P0DTC2
C	1229	VAL	-	expression tag	UNP P0DTC2
C	1230	LEU	-	expression tag	UNP P0DTC2
C	1231	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1232	SER	-	expression tag	UNP P0DTC2
C	1233	THR	-	expression tag	UNP P0DTC2
C	1234	PHE	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	ALA	-	expression tag	UNP P0DTC2
C	1237	HIS	-	expression tag	UNP P0DTC2
C	1238	HIS	-	expression tag	UNP P0DTC2
C	1239	HIS	-	expression tag	UNP P0DTC2
C	1240	HIS	-	expression tag	UNP P0DTC2
C	1241	HIS	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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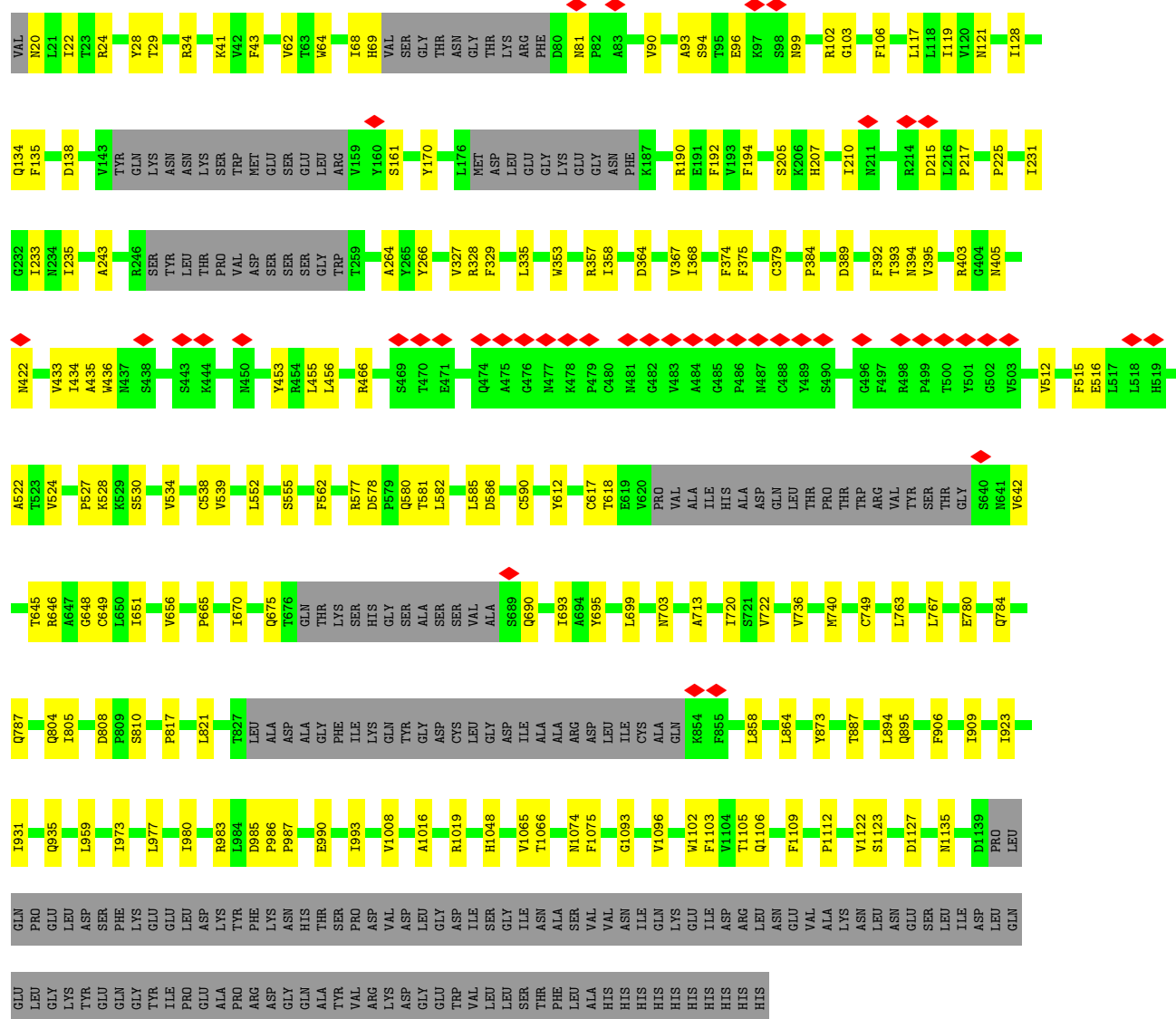
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2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

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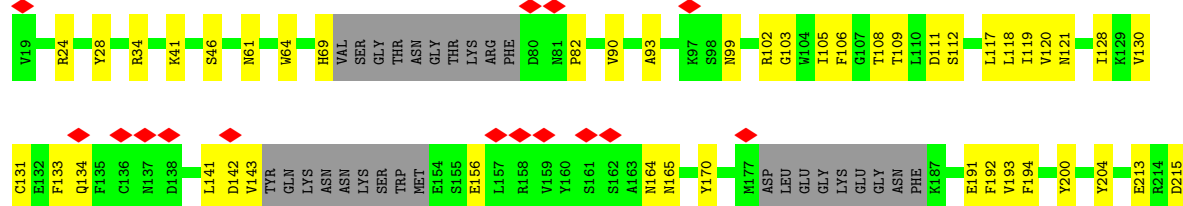
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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C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

Chain B: 69% 14% 17%



Chain C:



L216	P217	L358	S359	D228	V362	L229	P230	I231	G232	I233	F238	L241	L242	A243	R246	SER	TYR	LEU	THR	PRO	VAL	ASP	SER	SER	SER	GLY	TRP	T259	A260	C261	A264	Y265	Y266	L270	Y279	R319	I326	V327	R328	F329	L335	H339	A344	T345	T346	F347	A348	K356	R357					
I358	S359	V362	N370	F375	A376	F377	Y380	G381	V382	S383	P384	D389	F392	V395	R403	G404	M405	E406	A411	P412	Q413	Q414	T415	G416	N417	I418	A419	D420	Y421	M422	L425	P426	D427	D428	V433	S438	D442	S443	N448	R452	Y453	R454	L455	L456										
R457	K458	S459	K460	D467	I468	S469	T470	E471	I472	Y473	Q474	A475	G476	M477	K478	P479	C480	M481	G482	V483	A484	G485	P486	M487	C488	Y489	S490	P491	L492	Q493	S494	Y495	G496	F497	R498	P499	T500	Y501	H505	Q506	P507	V512	F515	E516	L517	H518	H519	A520	P521	A522	T523	G526	P527	K528
L533	V534	K535	V539	N544	L552	S555	N556	K557	L560	P561	F562	Q563	A570	R577	D578	P579	Q580	T581	L582	L585	F592	Y612	V620	PRO	VAL	ALA	ILE	HIS	ALA	ASP	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	S640	N641	V642	R646								
A647	G648	I651	V656	P665	Q677	THR	LYS	SER	HIS	GLY	ALA	SER	SER	VAL	ALA	S689	Q690	Y695	L699	E702	N703	I720	S721	V722	K733	V736	M740	Y741	I742	C743	G744	D745	S746	T747	E748	C749	S750	L763	A771	E780	Q784	Q787												
Q804	P817	F823	V826	THR	ALA	ASP	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	ILE	ALA	ALA	ARG	ASP	LEU	ILE	CYS	ALA	GLN	K854	L858	L864	L865	T866	Y873	L878	Q895	L916	T923	L966	L977	T980	P986											
P987	E988	A989	E990	V991	D992	I993	R1000	V1008	A1016	R1019	F1052	P1057	V1065	M1074	H1088	G1093	M1098	G1099	T1100	H1101	W1102	T1105	Q1106	F1109	P1112	T1116	V1122	S1123	N1135	T1136	Y1137	Y1138	D1139	PRO	LEU	GLN	GLN	PRO	GLY	LEU	LYS	TYR	ASP	SER	PHE									
LYS	GLU	GLU	LEU	ASP	LYS	TYR	PHE	LYS	ASN	THR	SER	PRO	ASP	VAL	LYS	ASP	GLY	GLU	TRP	VAL	ILE	ASP	LEU	GLY	ASN	GLU	VAL	ALA	LYS	ASN	LEU	ASN	GLU	VAL	VAL	LYS	ASN	LEU	GLN	GLU	LEU	PRO	GLY	LEU	LYS	TYR	GLU	GLN						
GLY	TYR	ILE	PRO	GLU	ALA	PRO	ARG	ASP	GLN	ALA	TYR	VAL	LYS	GLY	GLU	SER	LEU	LEU	SER	THR	PHE	LEU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ASN	LEU	ASN	GLU	VAL	VAL	LYS	ASN	LEU	GLN	GLY	LEU	PRO	GLY	LEU	LYS	TYR	GLU	GLN				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135899	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	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.019	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	413.696, 413.696, 413.696	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.808, 0.808, 0.808	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

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	0.20	0/8186	0.36	0/11141
1	B	0.19	0/8128	0.35	0/11063
1	C	0.18	0/8188	0.36	0/11142
All	All	0.19	0/24502	0.36	0/33346

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8000	0	7824	118	0
1	B	7942	0	7768	122	0
1	C	8002	0	7830	135	0
2	A	168	0	156	2	0
2	B	196	0	182	3	0
2	C	168	0	156	3	0
All	All	24476	0	23916	341	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 7.

The worst 5 of 341 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:329:PHE:CE2	1:B:528:LYS:HD3	1.62	1.33
1:C:34:ARG:HD2	1:C:191:GLU:OE2	1.55	1.03
1:B:329:PHE:HE2	1:B:528:LYS:HD3	1.18	0.92
1:A:34:ARG:HD2	1:A:191:GLU:OE2	1.73	0.88
1:B:389:ASP:HA	1:B:528:LYS:HD2	1.55	0.85

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1007/1227 (82%)	969 (96%)	38 (4%)	0	100	100
1	B	1000/1227 (82%)	970 (97%)	30 (3%)	0	100	100
1	C	1007/1227 (82%)	963 (96%)	43 (4%)	1 (0%)	48	77
All	All	3014/3681 (82%)	2902 (96%)	111 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	345	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	896/1070 (84%)	893 (100%)	3 (0%)	86	96
1	B	889/1070 (83%)	889 (100%)	0	100	100
1	C	896/1070 (84%)	896 (100%)	0	100	100
All	All	2681/3210 (84%)	2678 (100%)	3 (0%)	87	97

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

Mol	Chain	Res	Type
1	A	331	ASN
1	A	524	VAL
1	A	528	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	913	GLN
1	C	81	ASN
1	B	1083	HIS
1	C	360	ASN
1	B	121	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

38 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	B	1311	1	14,14,15	0.25	0	17,19,21	0.39	0
2	NAG	B	1305	1	14,14,15	0.37	0	17,19,21	0.48	0
2	NAG	B	1312	1	14,14,15	0.39	0	17,19,21	0.46	0
2	NAG	A	1306	1	14,14,15	0.25	0	17,19,21	0.46	0
2	NAG	C	1310	1	14,14,15	0.37	0	17,19,21	0.54	0
2	NAG	A	1307	1	14,14,15	0.18	0	17,19,21	0.41	0
2	NAG	C	1303	1	14,14,15	0.25	0	17,19,21	0.38	0
2	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.40	0
2	NAG	A	1310	1	14,14,15	0.37	0	17,19,21	0.52	0
2	NAG	A	1302	1	14,14,15	0.37	0	17,19,21	0.78	0
2	NAG	B	1307	1	14,14,15	0.18	0	17,19,21	0.44	0
2	NAG	C	1311	1	14,14,15	0.40	0	17,19,21	0.97	1 (5%)
2	NAG	C	1312	1	14,14,15	0.38	0	17,19,21	0.49	0
2	NAG	B	1308	1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	C	1306	1	14,14,15	0.38	0	17,19,21	1.02	1 (5%)
2	NAG	B	1314	1	14,14,15	0.38	0	17,19,21	0.51	0
2	NAG	C	1302	1	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	A	1303	1	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
2	NAG	A	1305	1	14,14,15	0.39	0	17,19,21	0.49	0
2	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	A	1312	1	14,14,15	0.39	0	17,19,21	0.51	0
2	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.54	0
2	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.58	0
2	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	A	1311	1	14,14,15	0.38	0	17,19,21	0.58	0
2	NAG	B	1306	1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	A	1304	1	14,14,15	0.37	0	17,19,21	0.62	0
2	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	B	1309	1	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	A	1308	1	14,14,15	0.38	0	17,19,21	0.69	1 (5%)
2	NAG	C	1305	1	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	C	1307	1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	B	1310	1	14,14,15	0.24	0	17,19,21	0.50	0
2	NAG	B	1302	1	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	C	1309	1	14,14,15	0.25	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1313	1	14,14,15	0.39	0	17,19,21	1.45	2 (11%)

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	B	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1311	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1311	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1313	1	-	4/6/23/26	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(°)
2	B	1313	NAG	C1-C2-N2	3.99	116.73	110.43
2	B	1313	NAG	C2-N2-C7	3.91	128.13	122.90
2	C	1306	NAG	C2-N2-C7	3.07	127.02	122.90
2	C	1311	NAG	C1-C2-N2	2.96	115.09	110.43
2	A	1308	NAG	C1-O5-C5	2.42	115.43	112.19

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

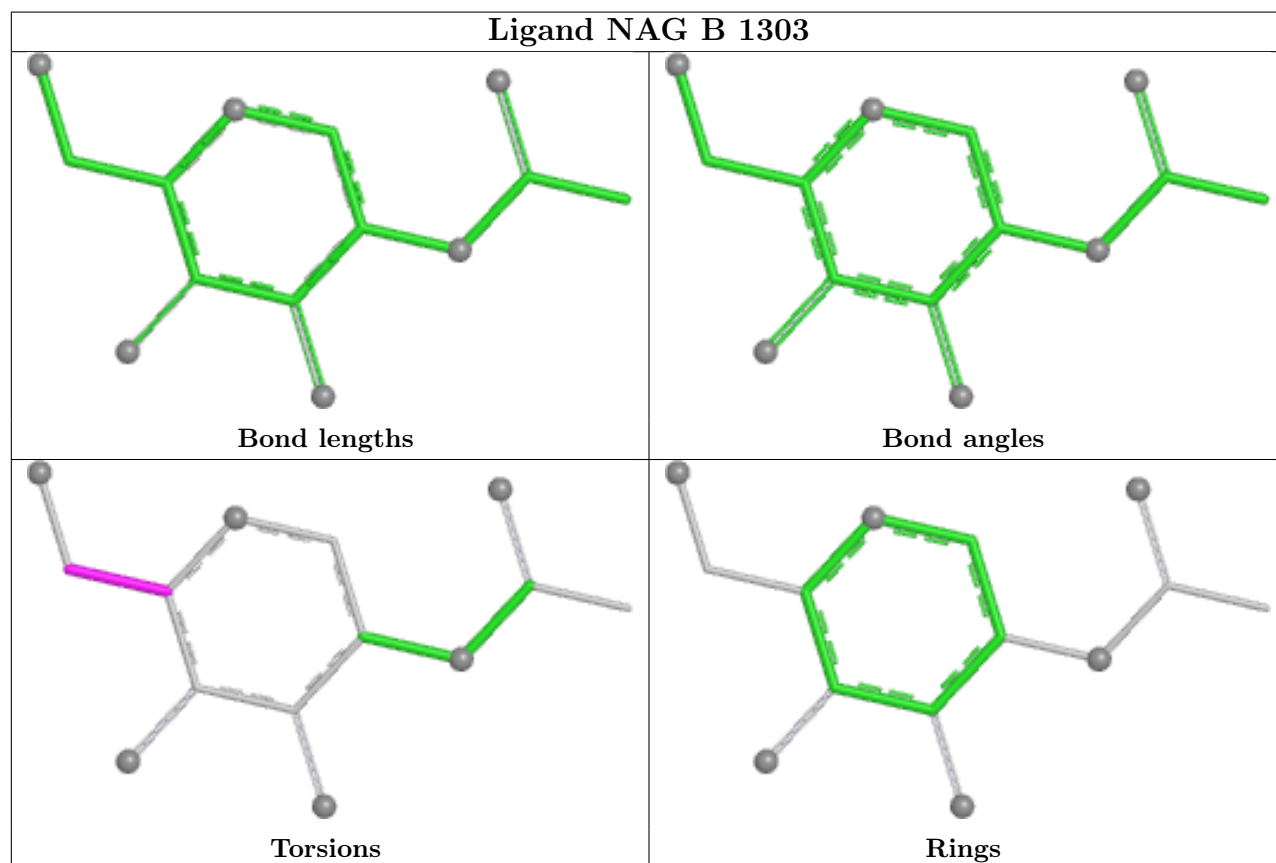
Mol	Chain	Res	Type	Atoms
2	A	1305	NAG	C8-C7-N2-C2
2	A	1305	NAG	O7-C7-N2-C2
2	B	1305	NAG	C8-C7-N2-C2
2	B	1305	NAG	O7-C7-N2-C2
2	B	1313	NAG	C1-C2-N2-C7

There are no ring outliers.

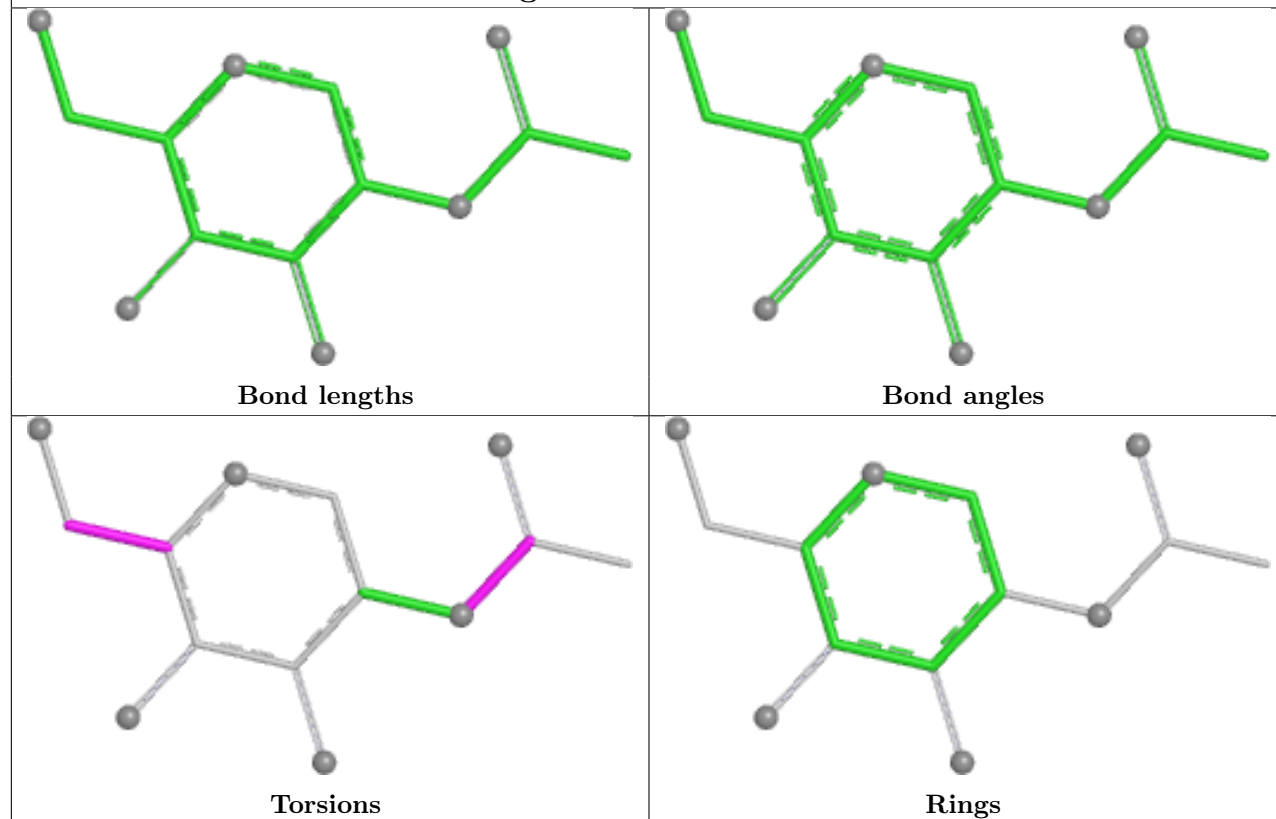
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1305	NAG	1	0
2	C	1303	NAG	1	0
2	A	1302	NAG	1	0
2	C	1312	NAG	2	0
2	B	1314	NAG	1	0
2	A	1311	NAG	1	0
2	B	1313	NAG	1	0

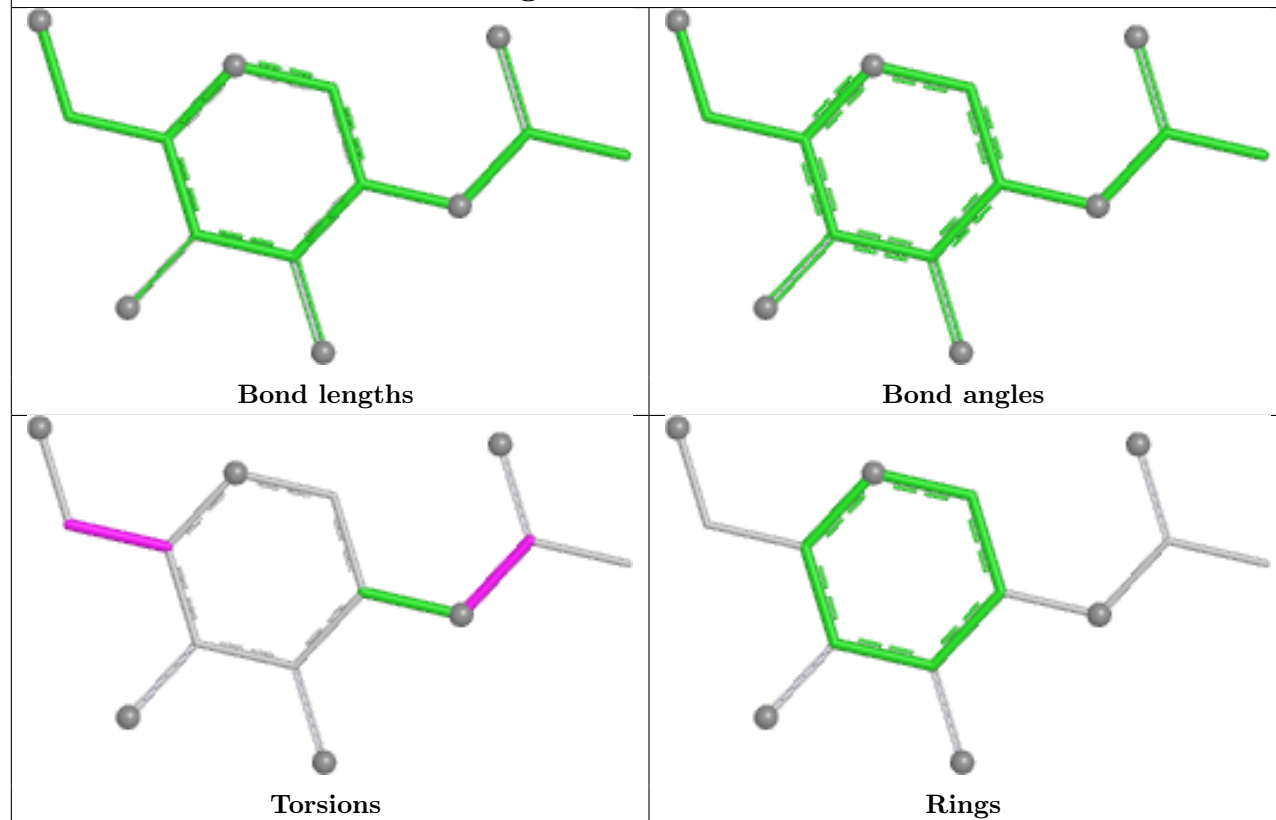
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



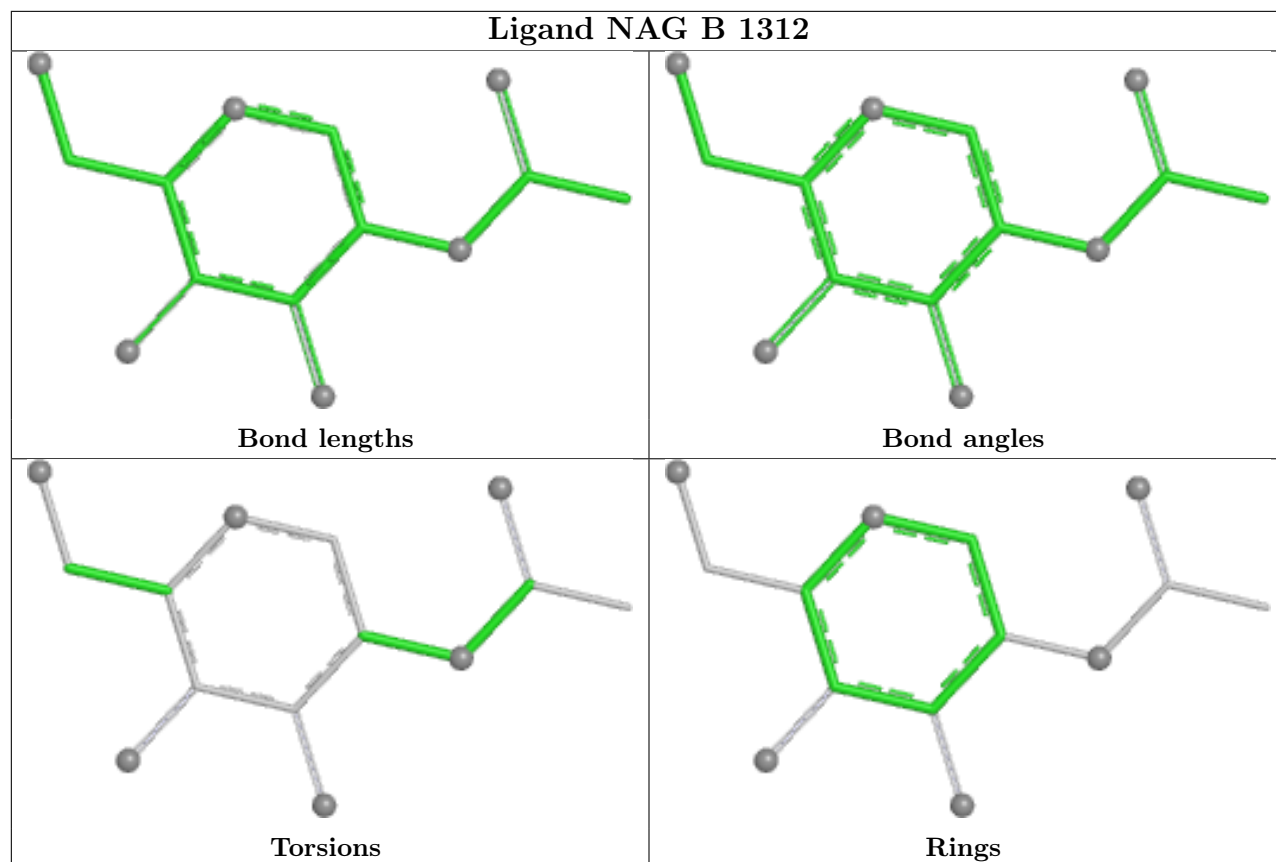
Ligand NAG B 1311



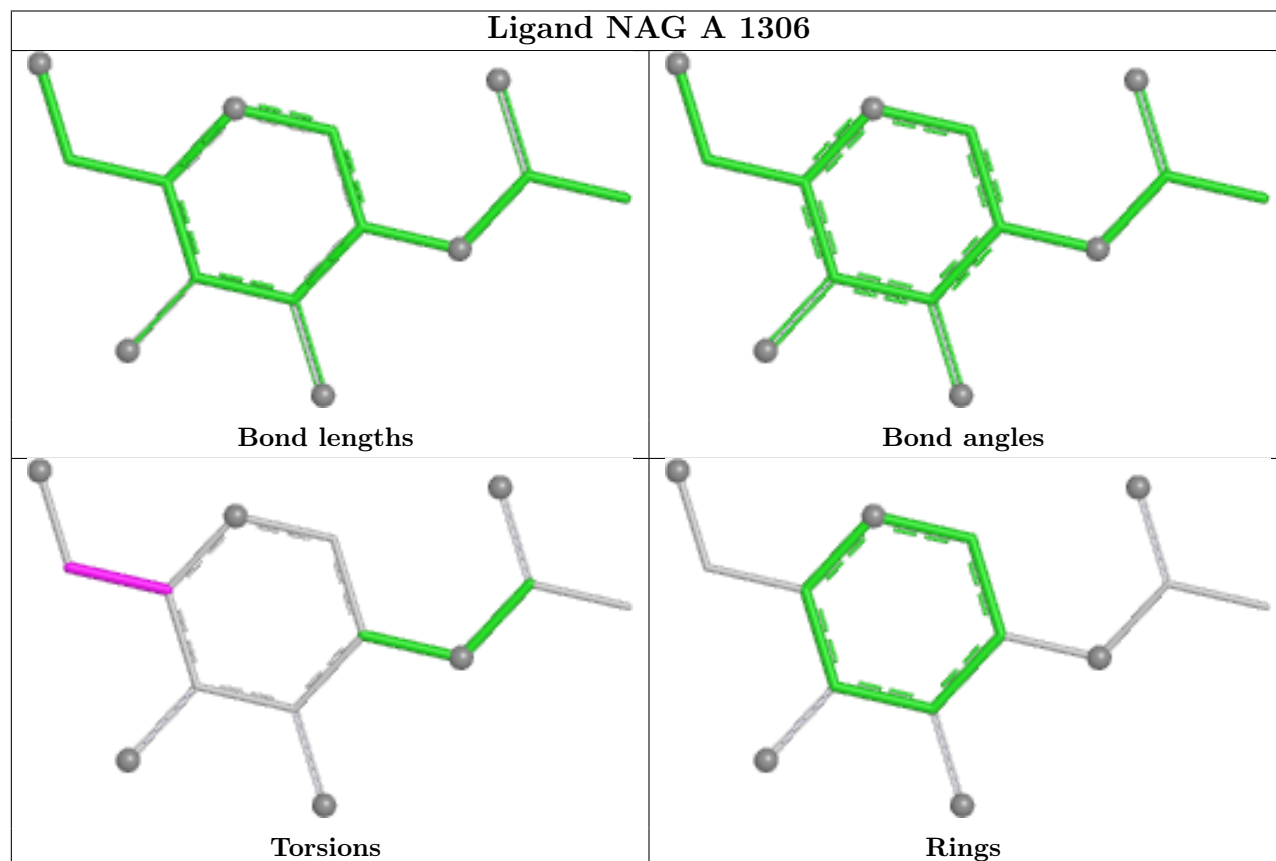
Ligand NAG B 1305



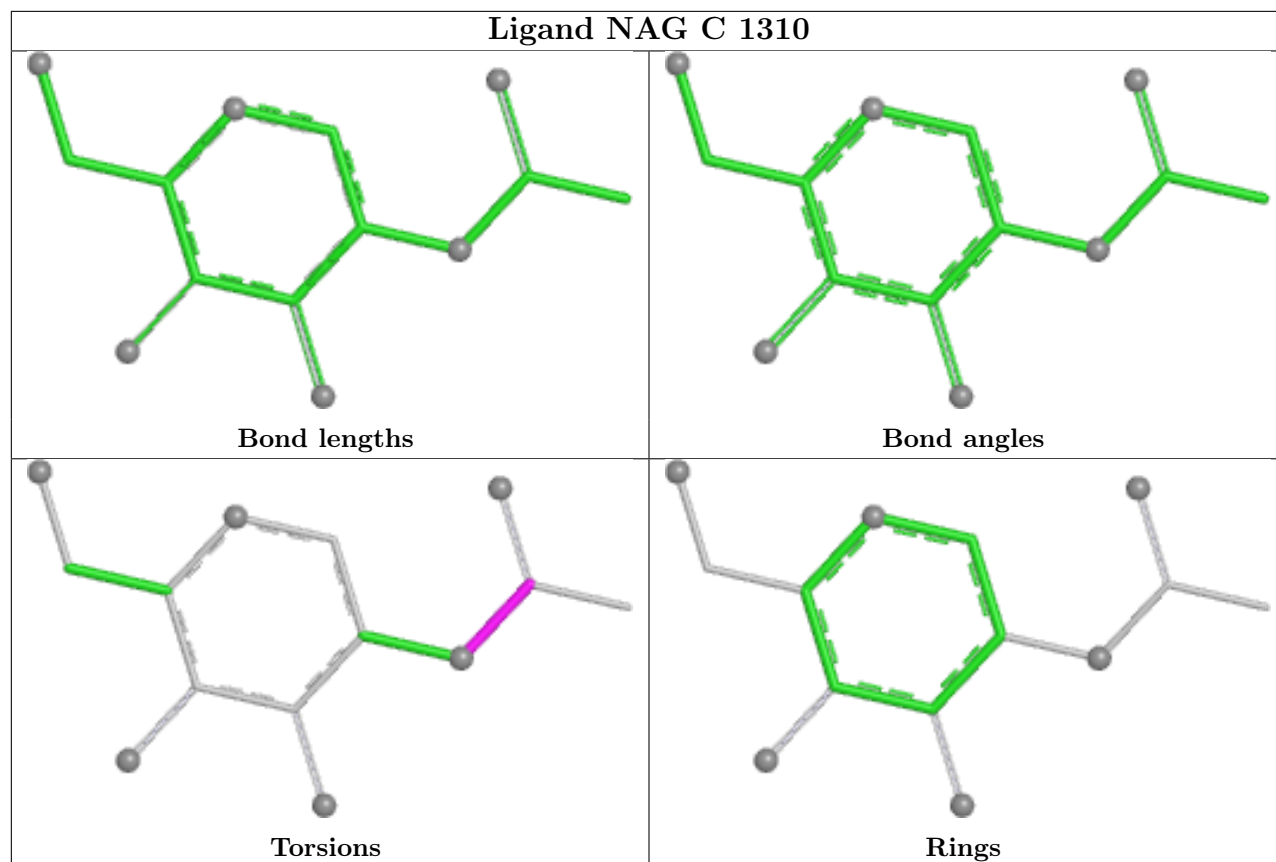
Ligand NAG B 1312



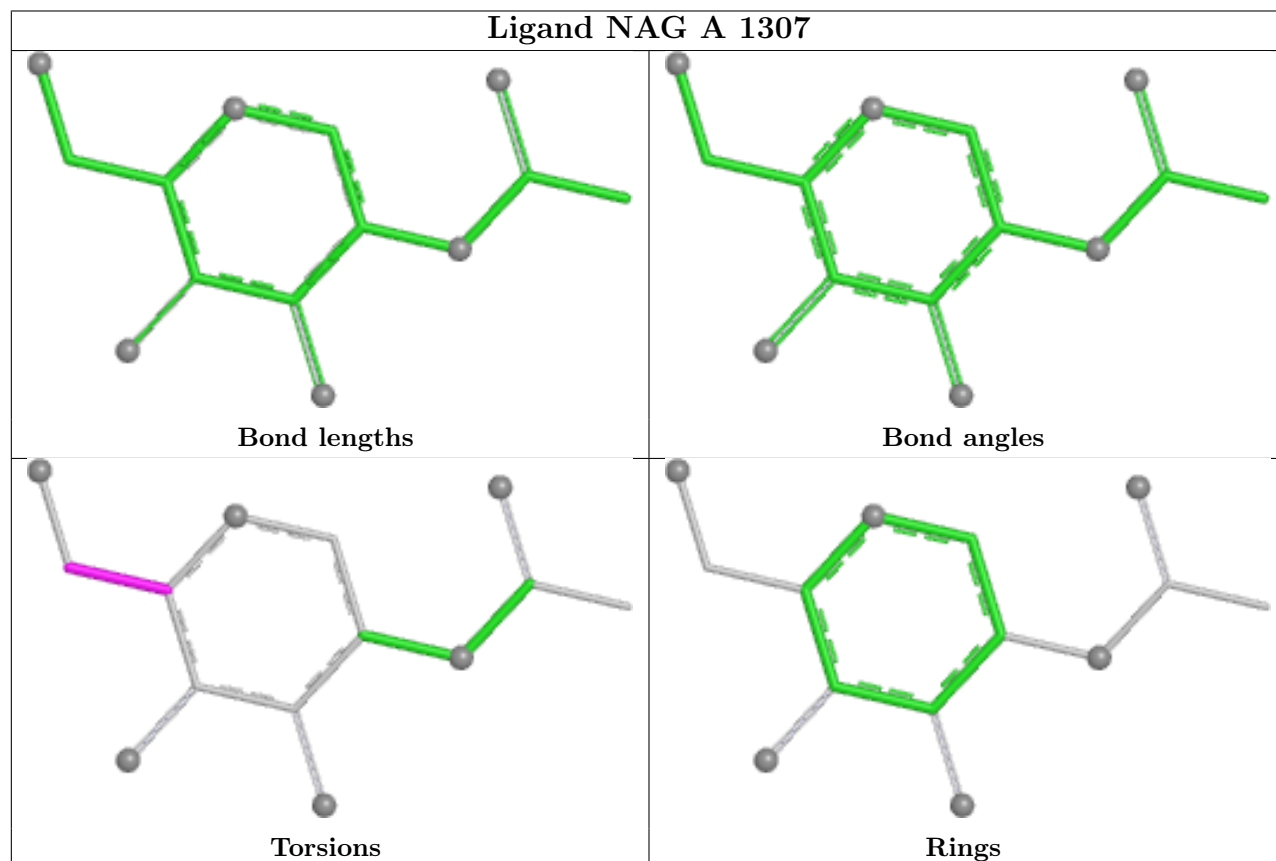
Ligand NAG A 1306



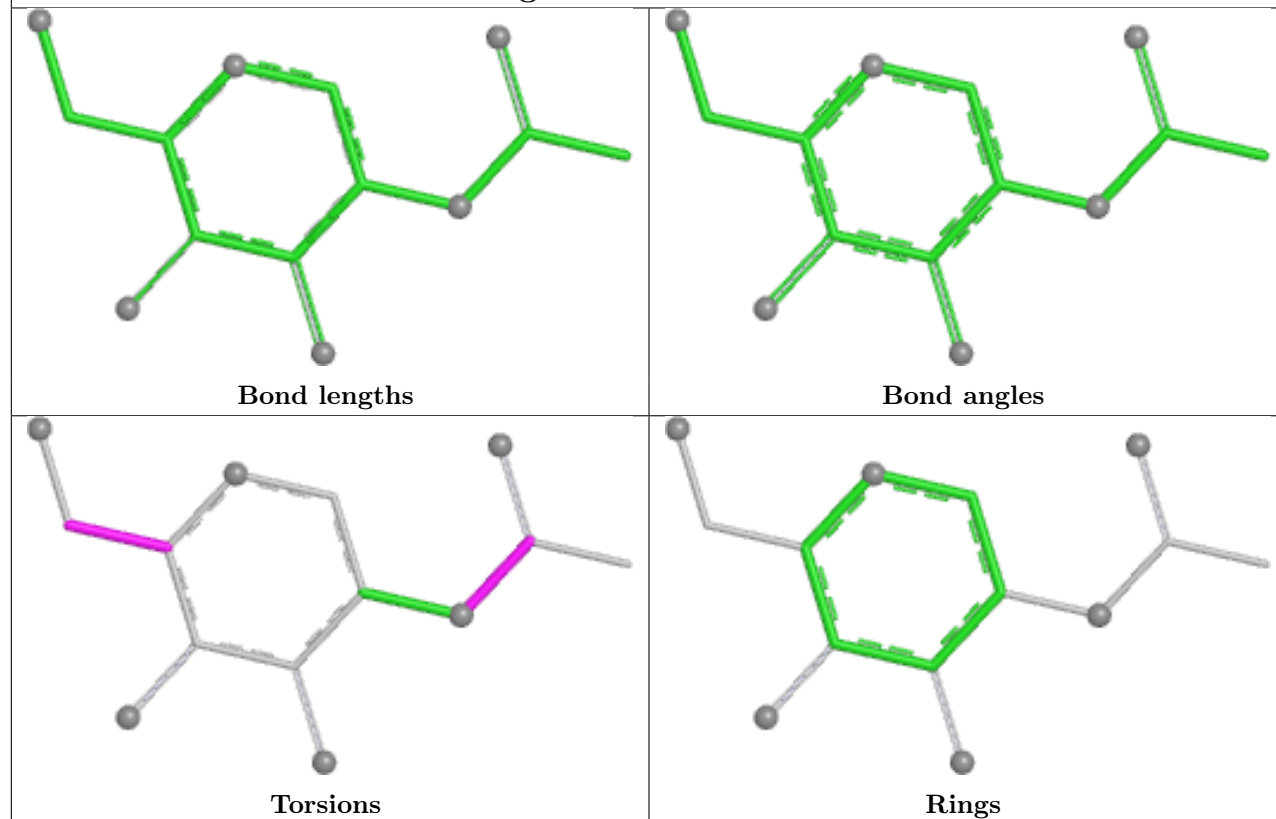
Ligand NAG C 1310



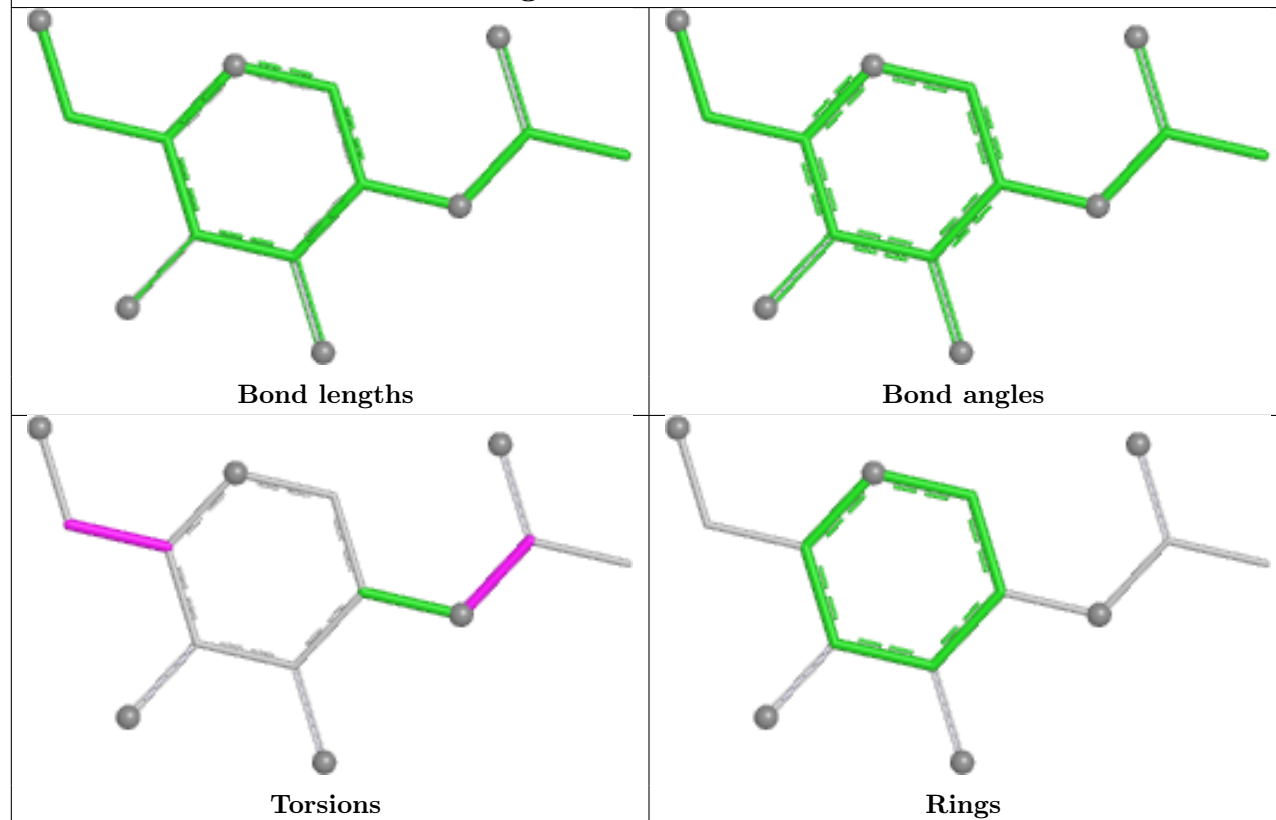
Ligand NAG A 1307



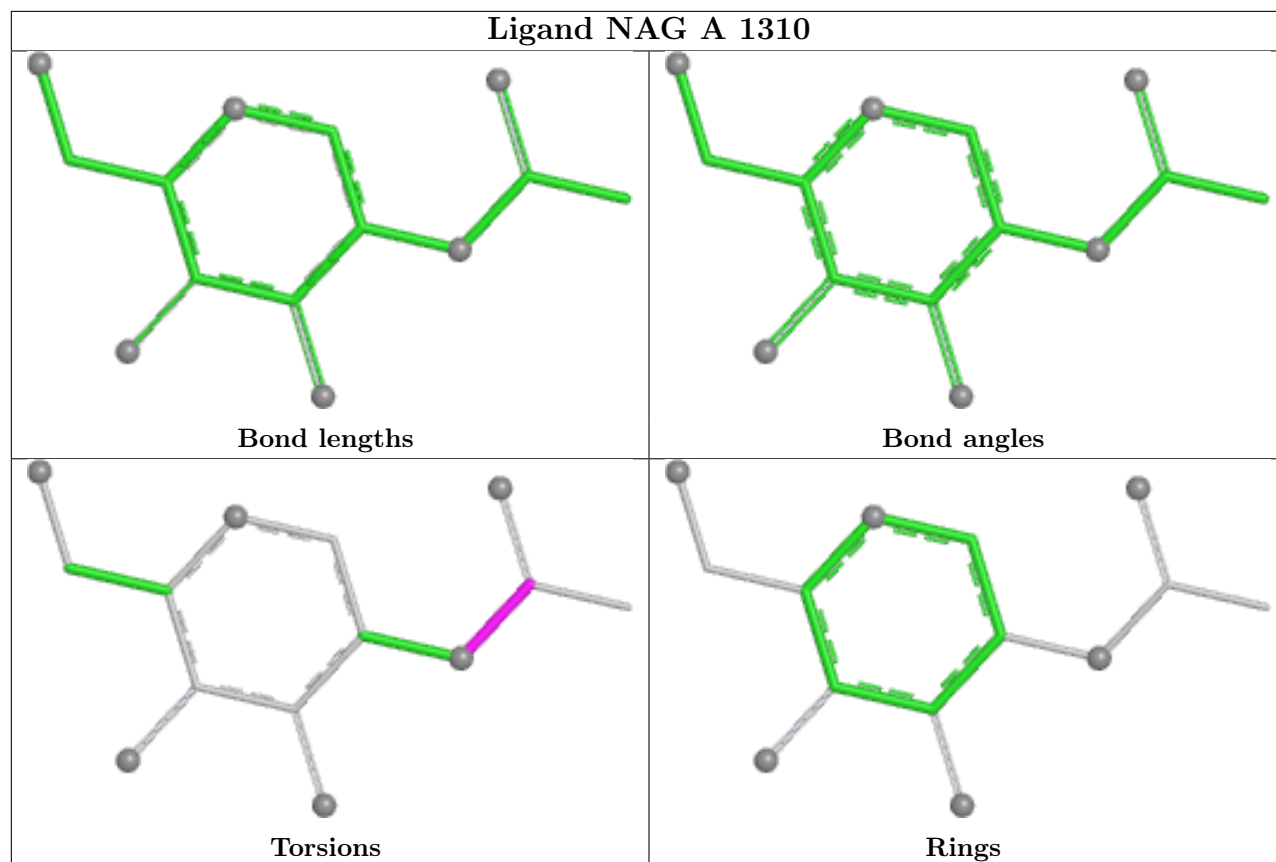
Ligand NAG C 1303



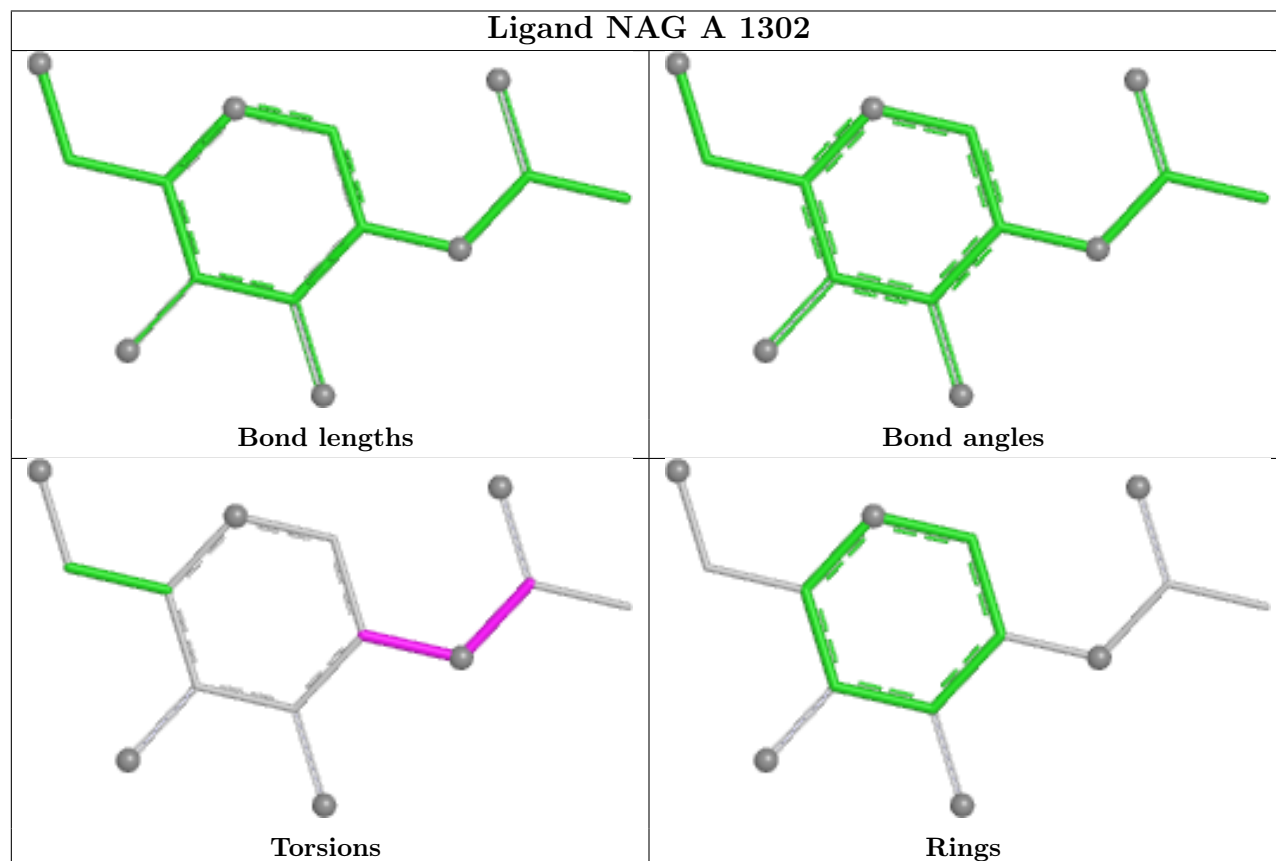
Ligand NAG B 1301



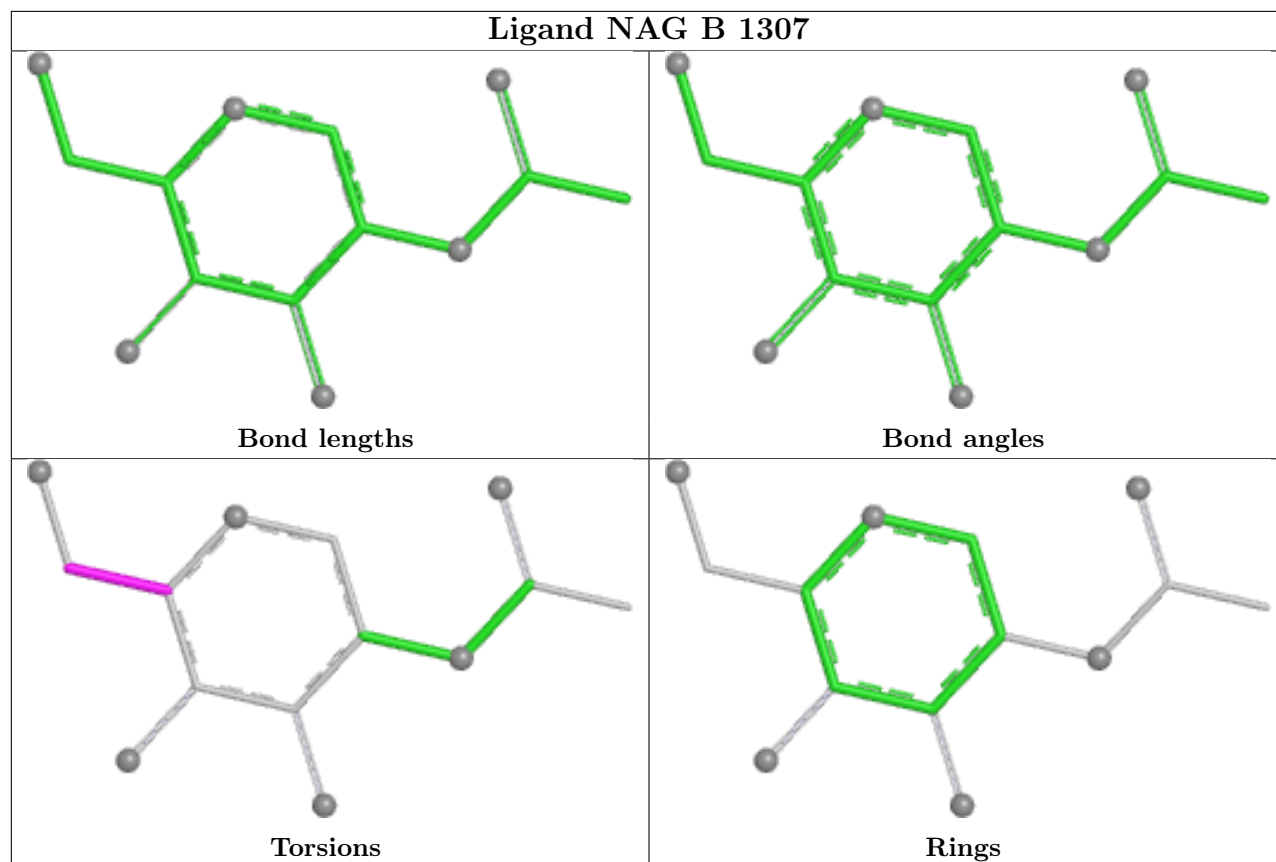
Ligand NAG A 1310



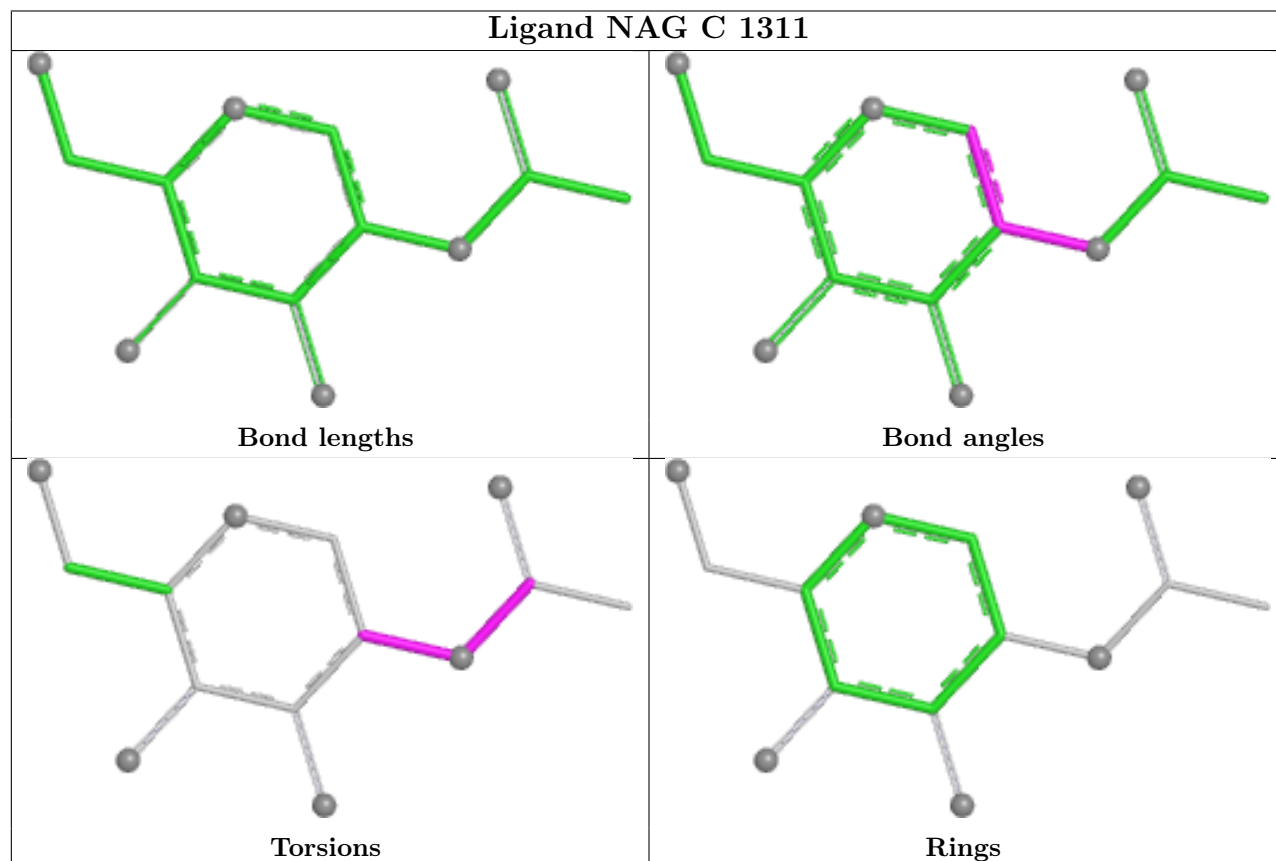
Ligand NAG A 1302



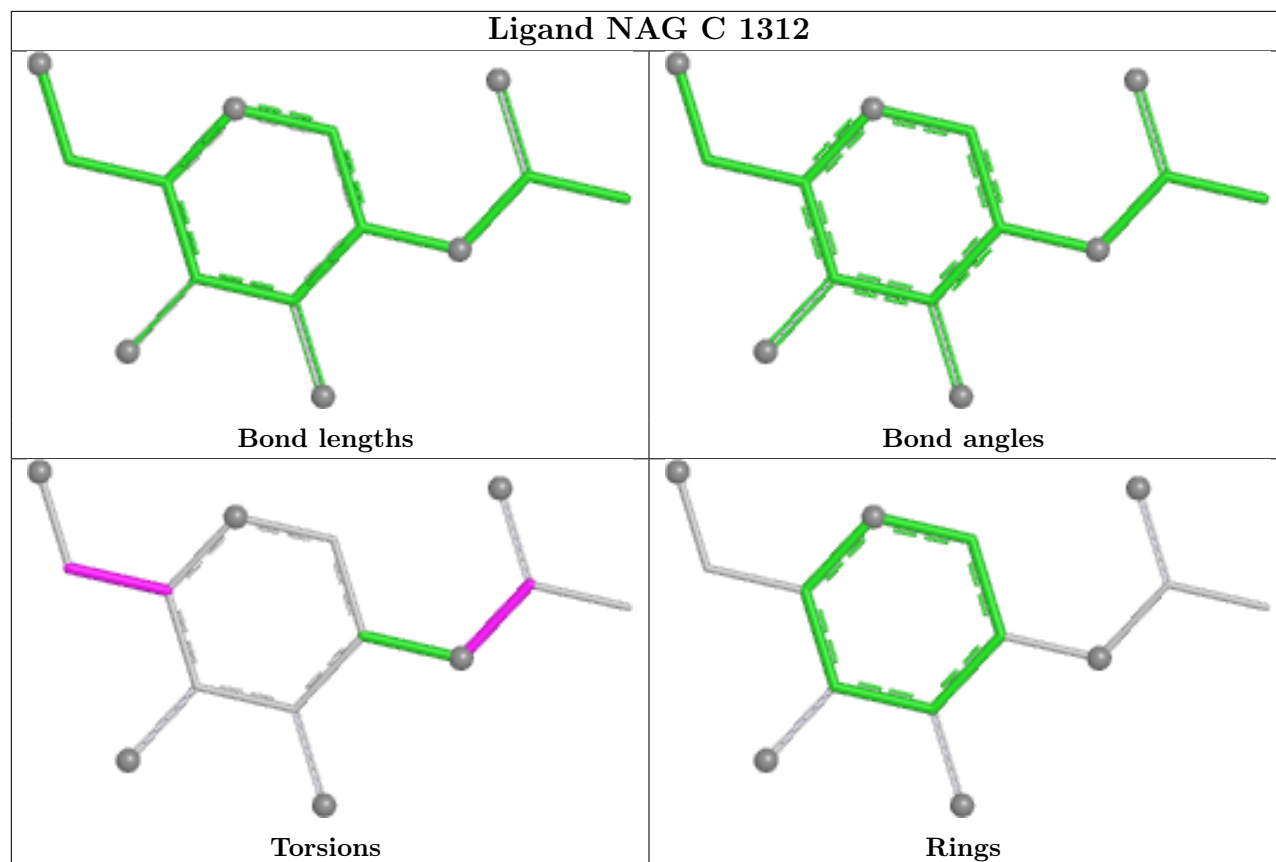
Ligand NAG B 1307



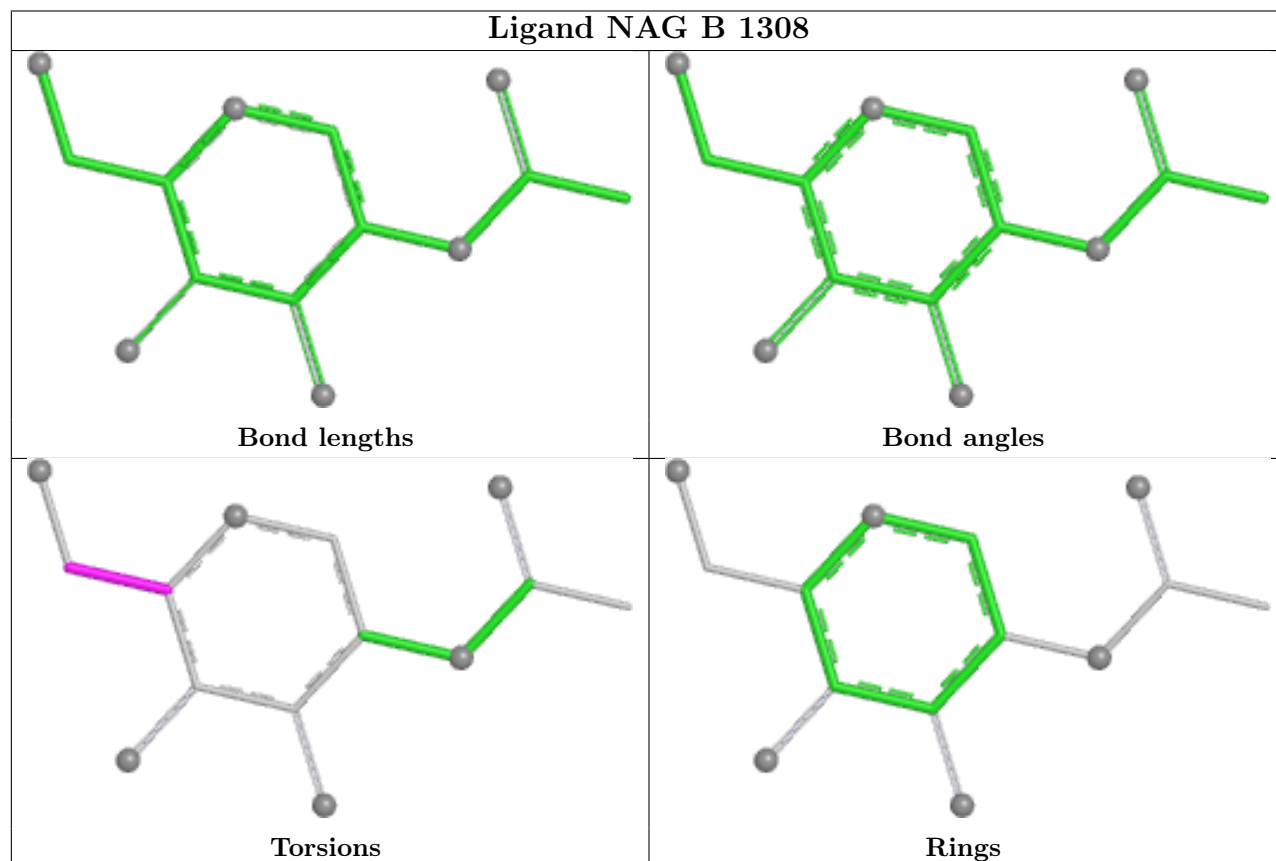
Ligand NAG C 1311

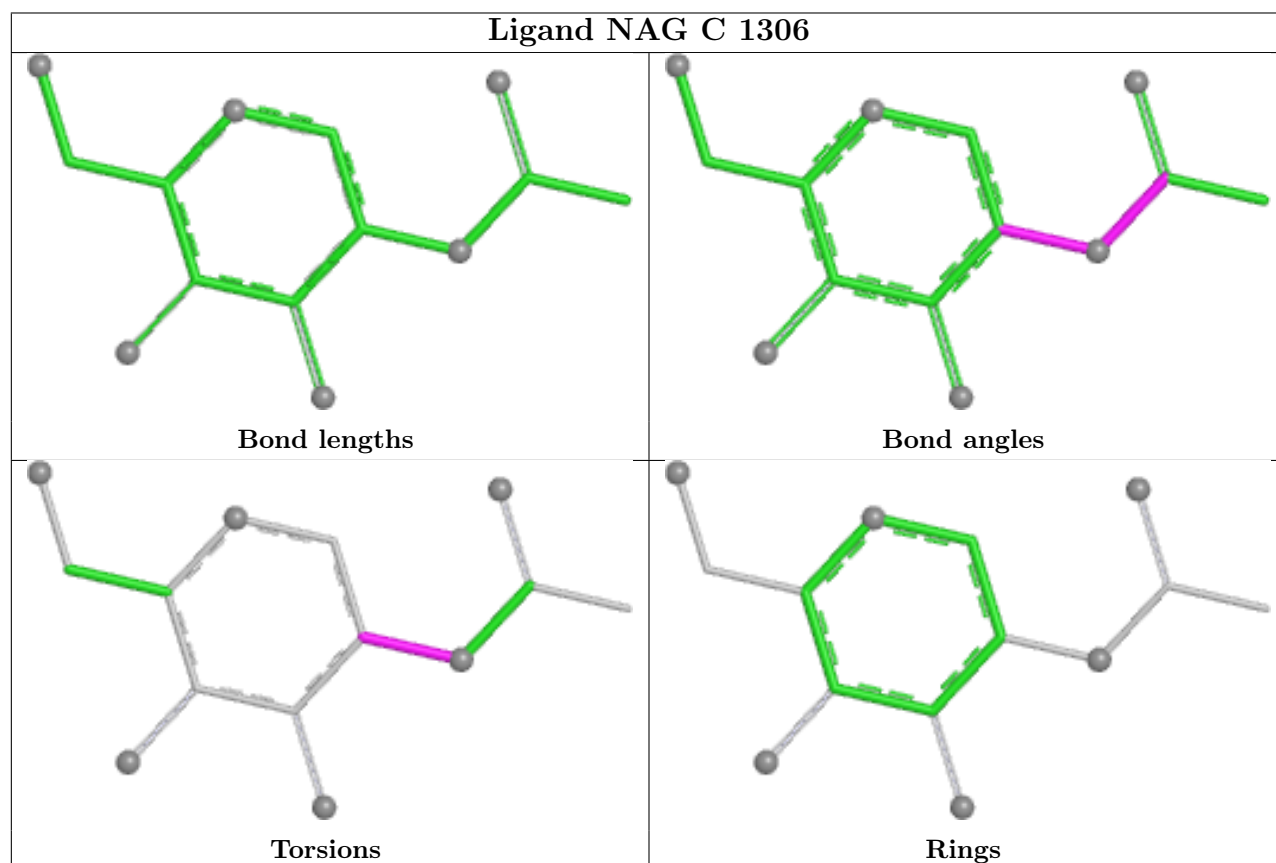
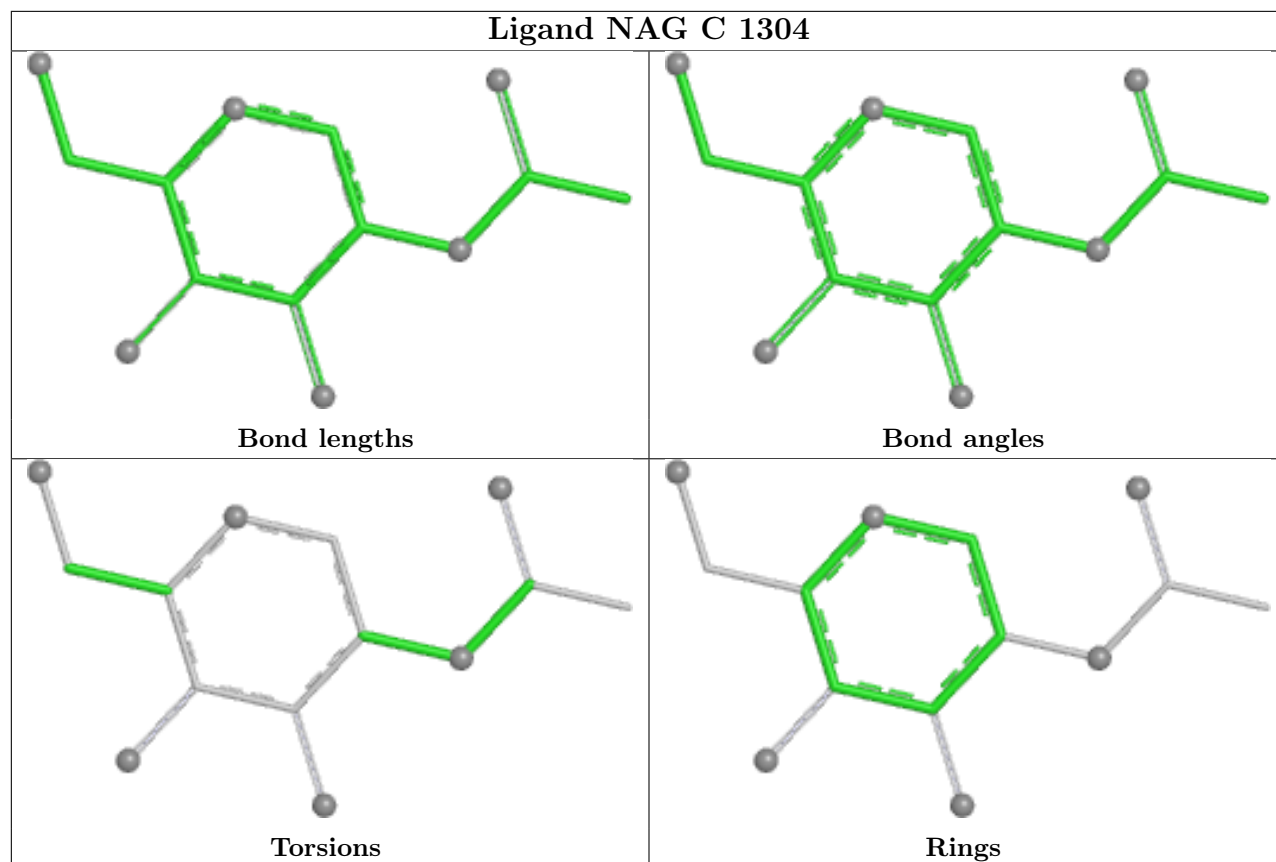


Ligand NAG C 1312

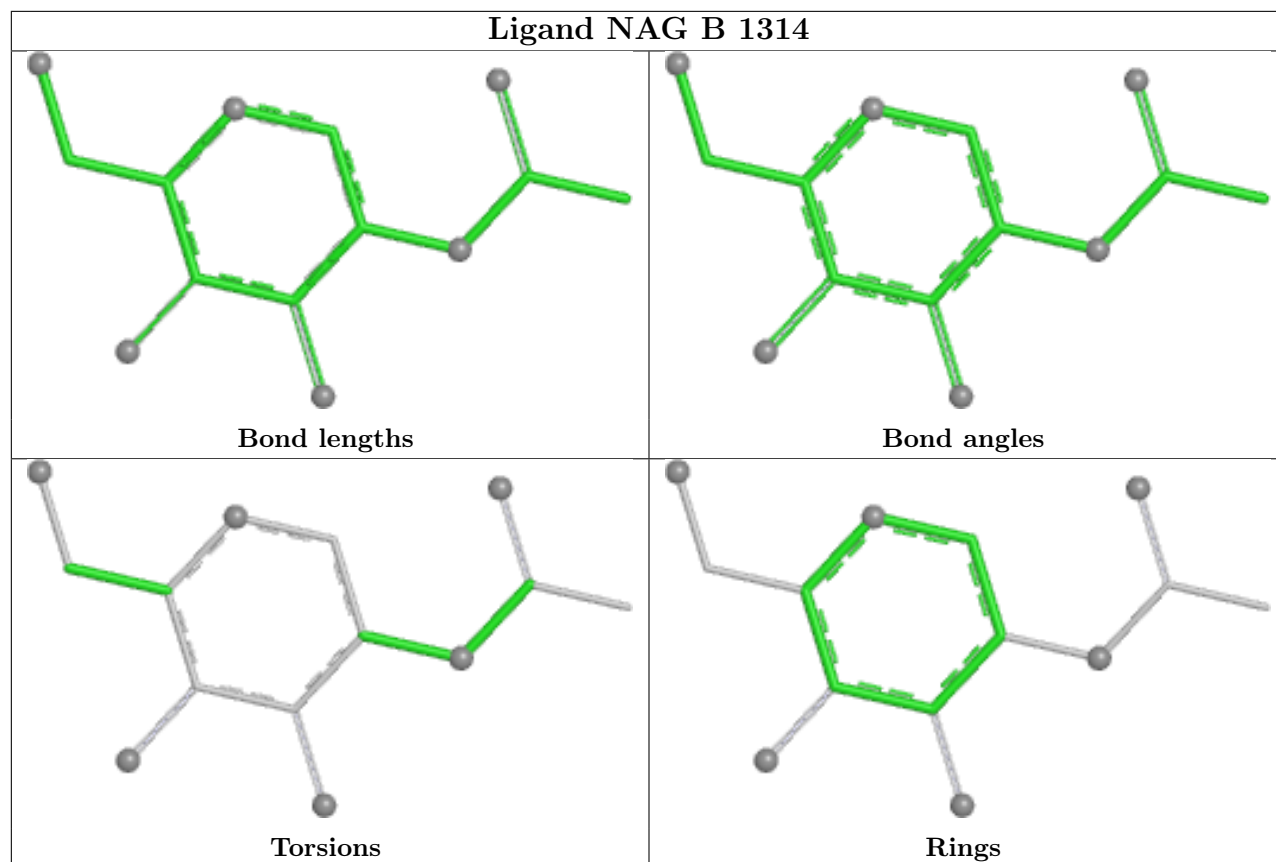


Ligand NAG B 1308

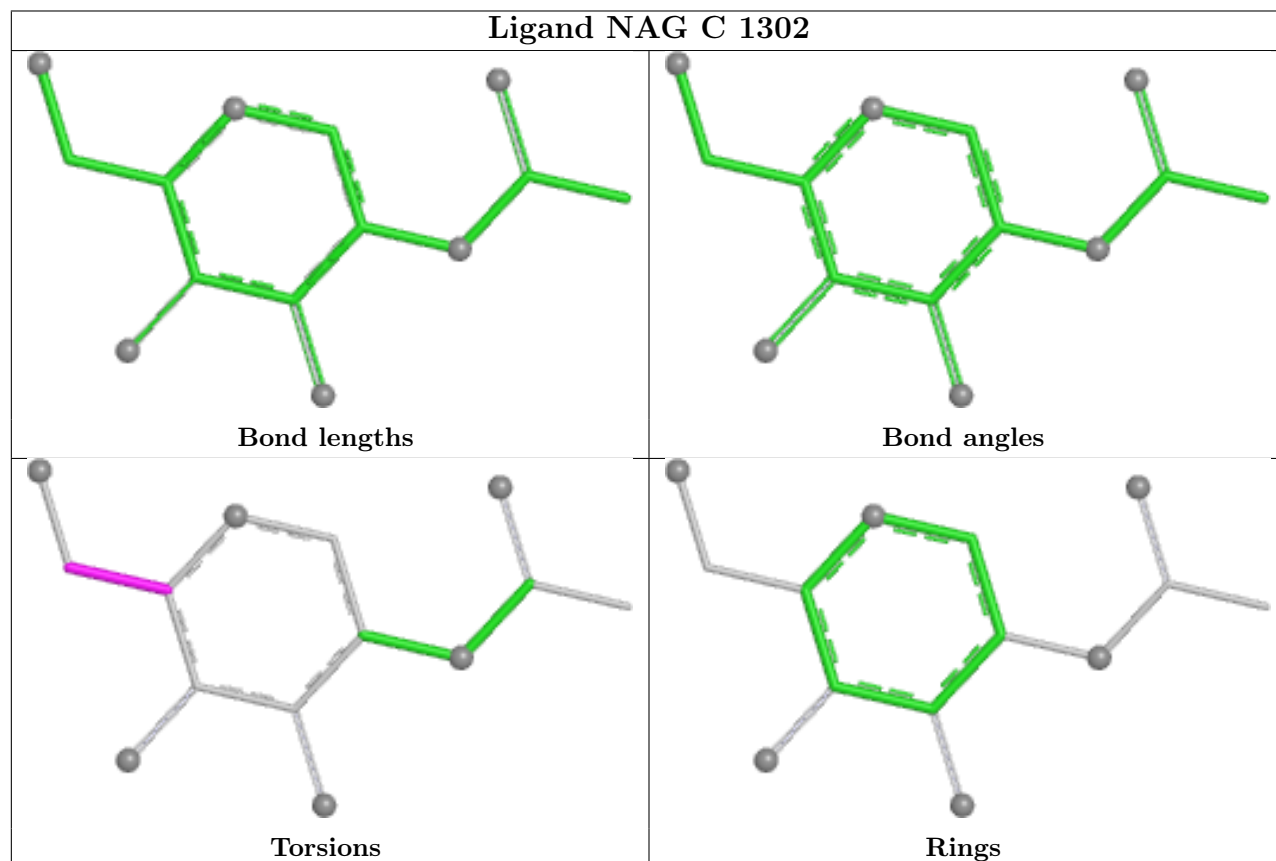


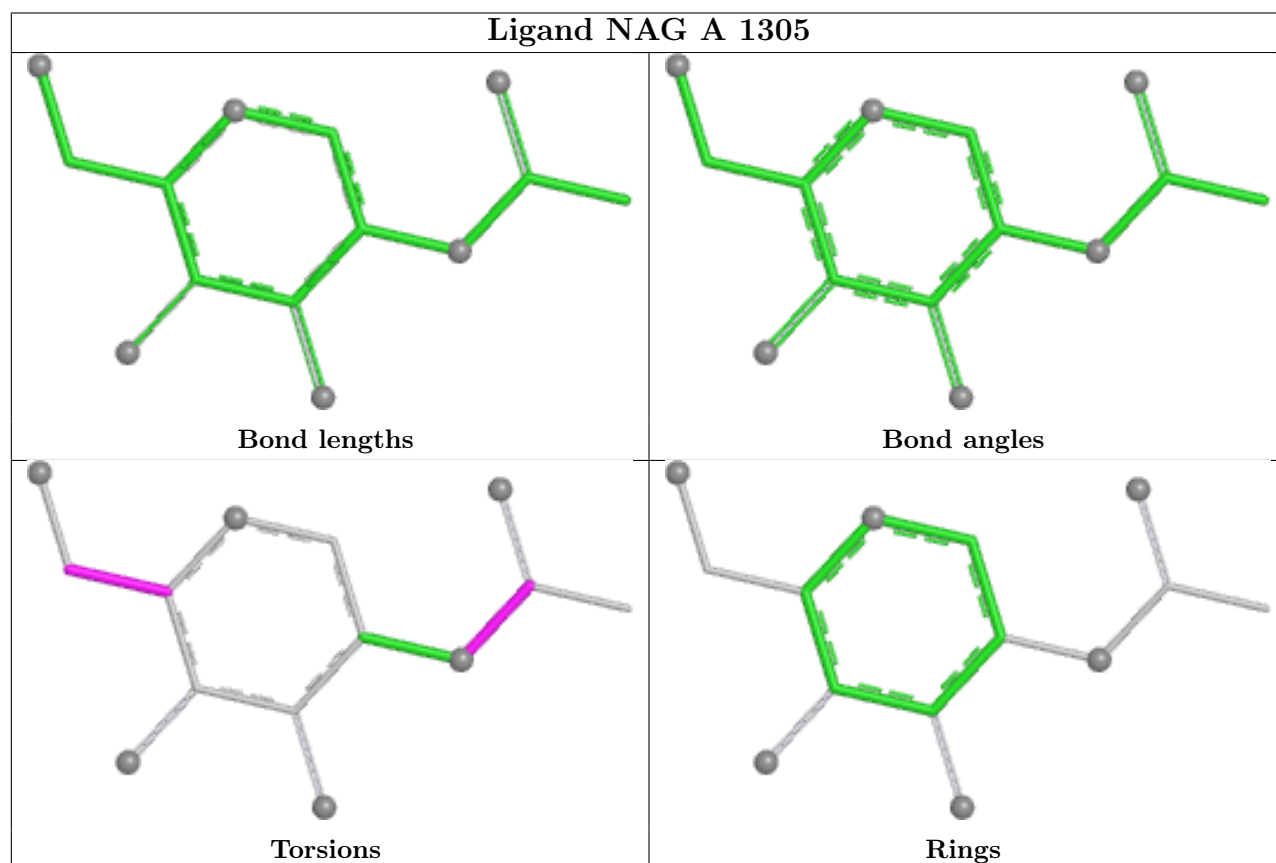
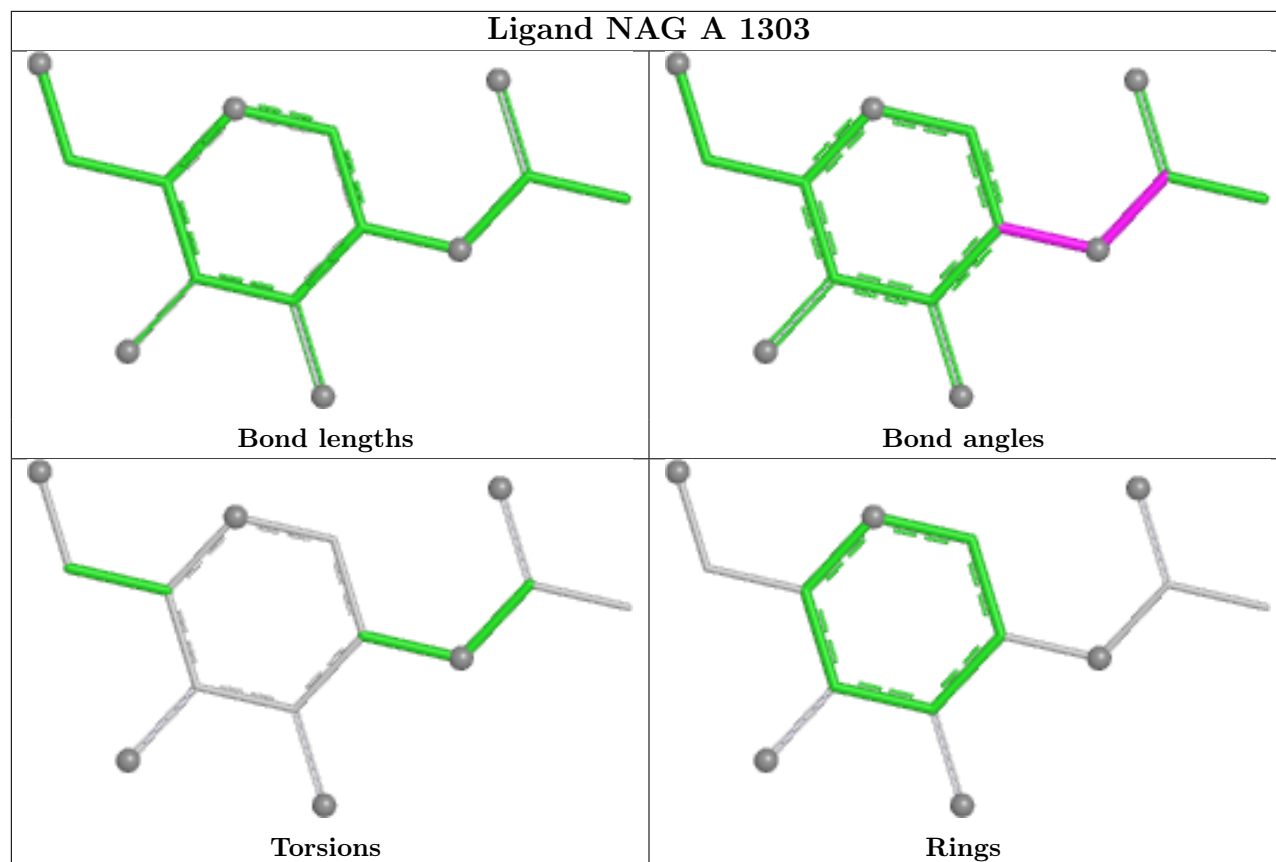


Ligand NAG B 1314

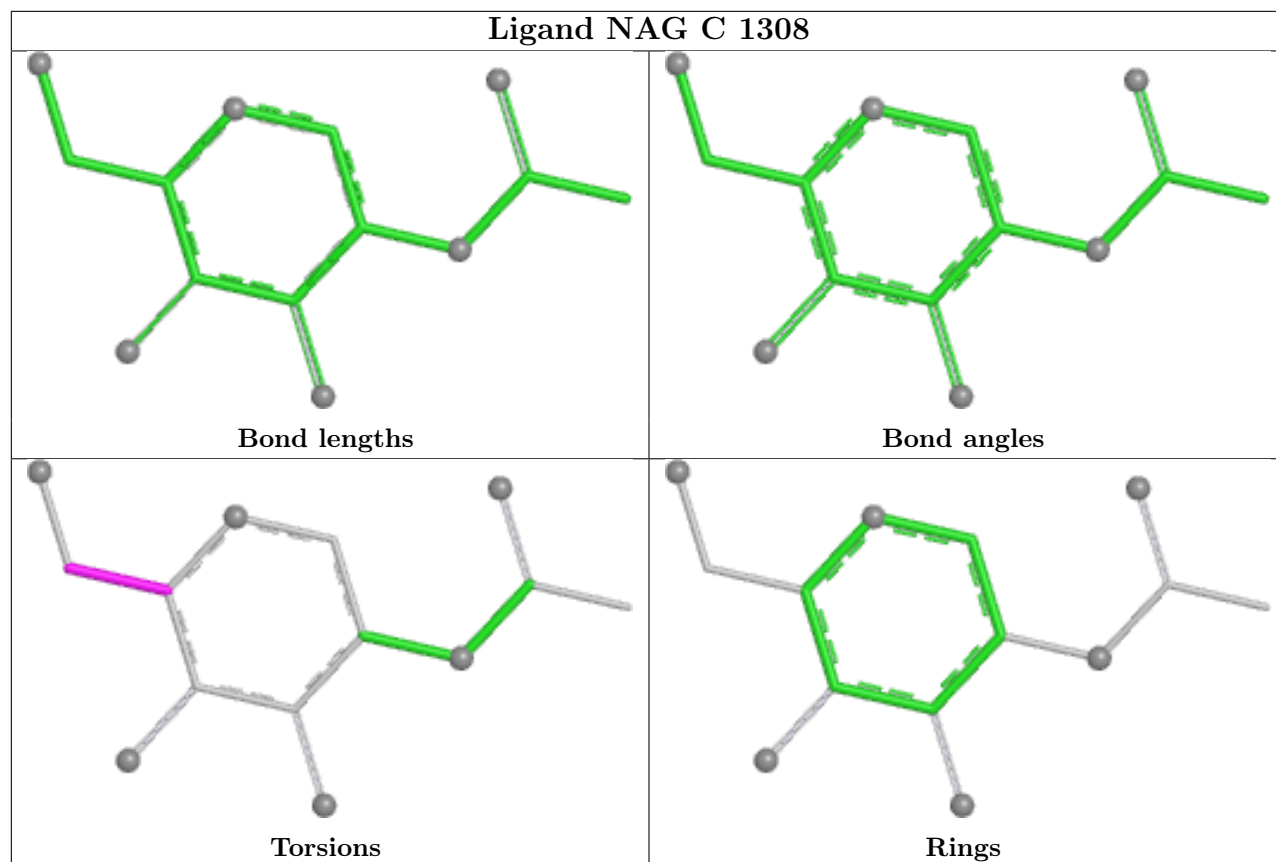


Ligand NAG C 1302

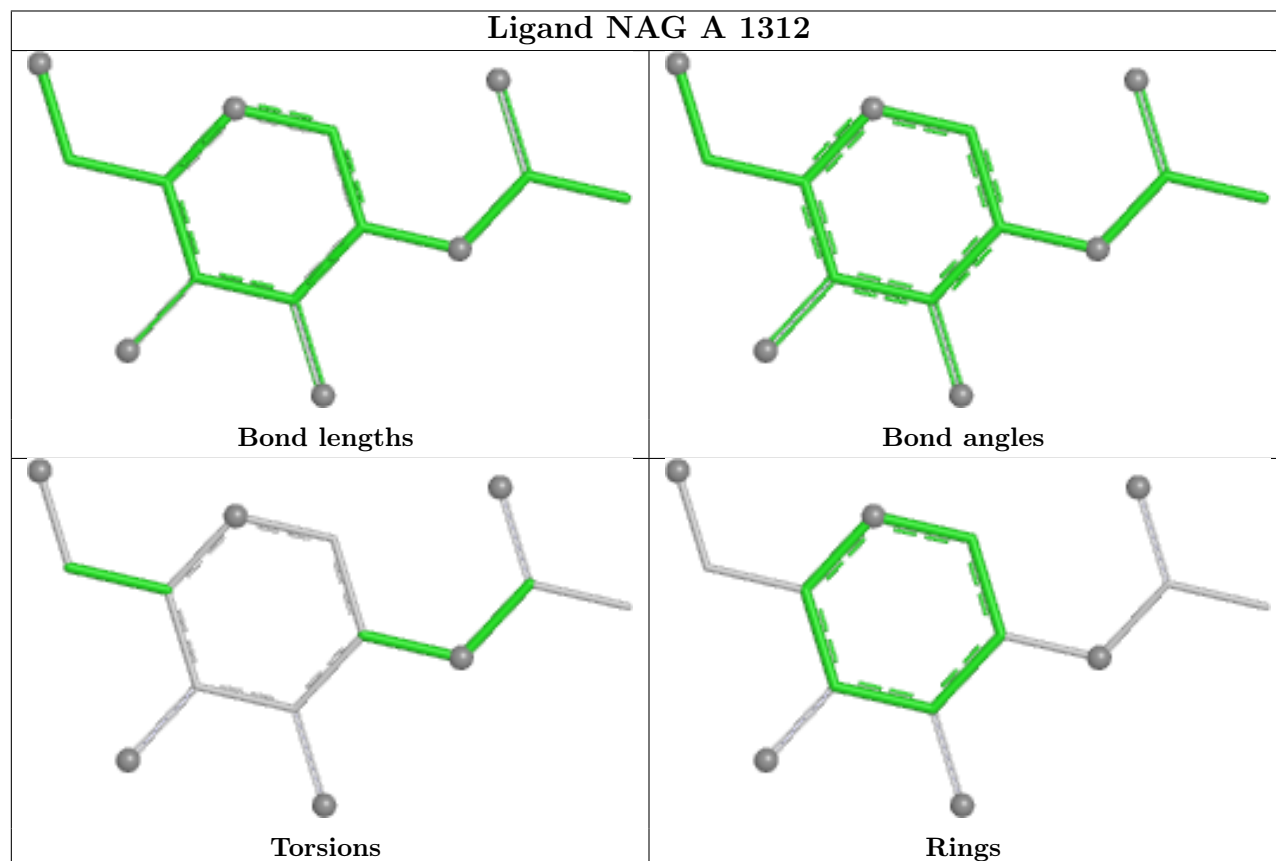




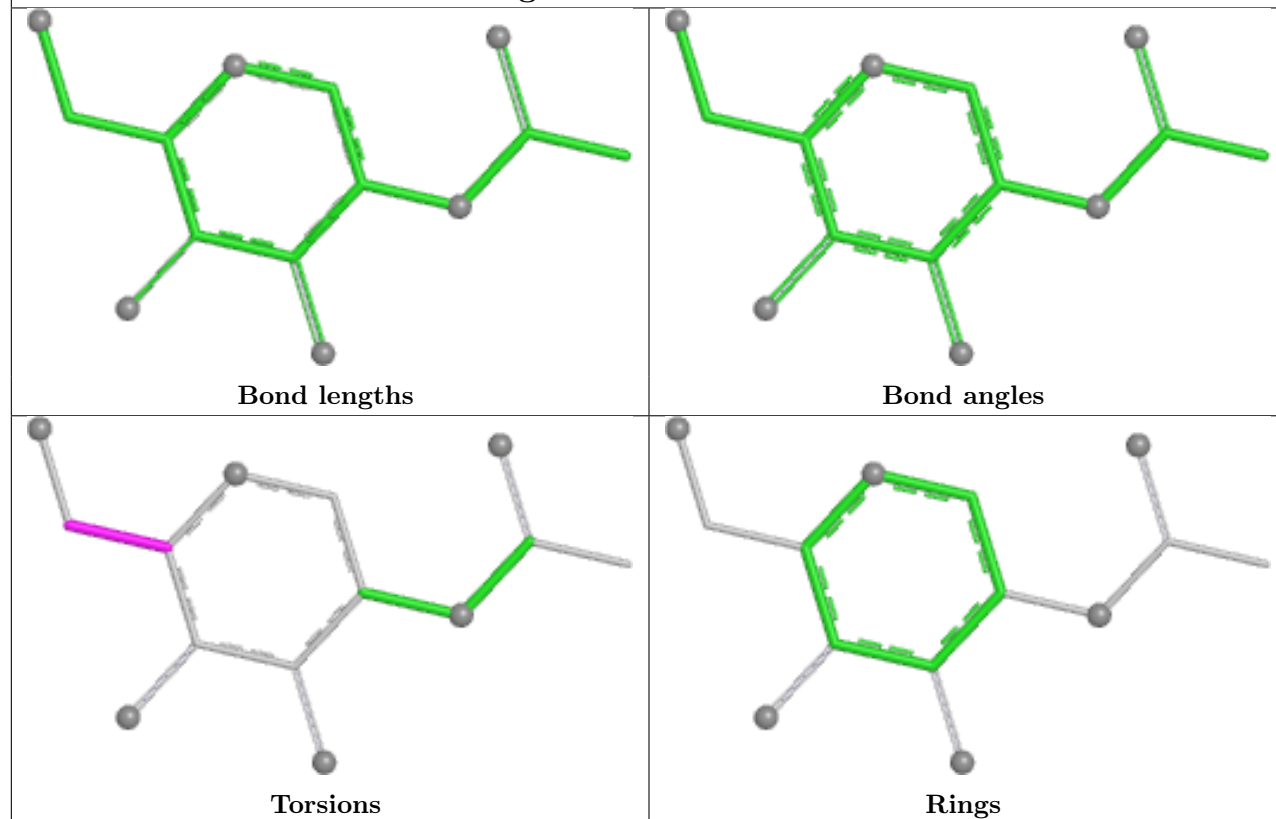
Ligand NAG C 1308



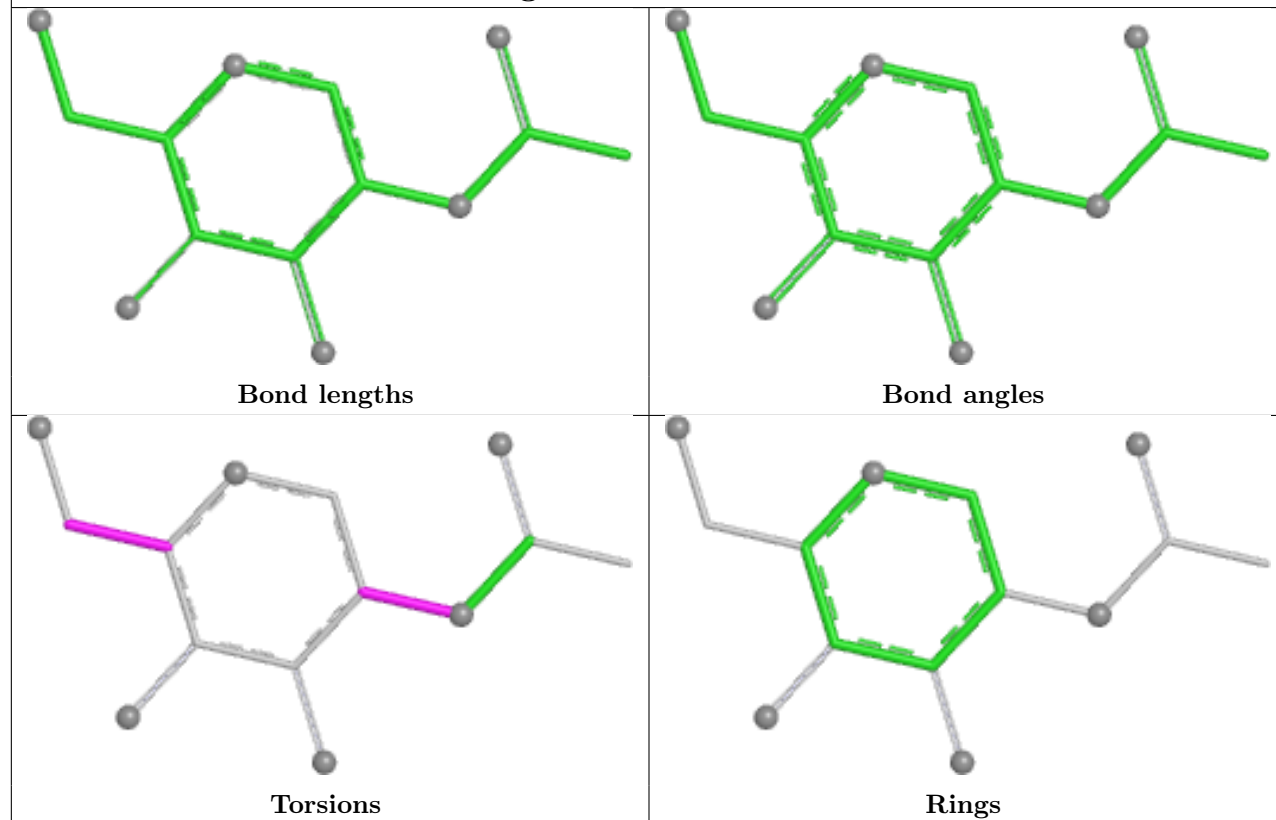
Ligand NAG A 1312



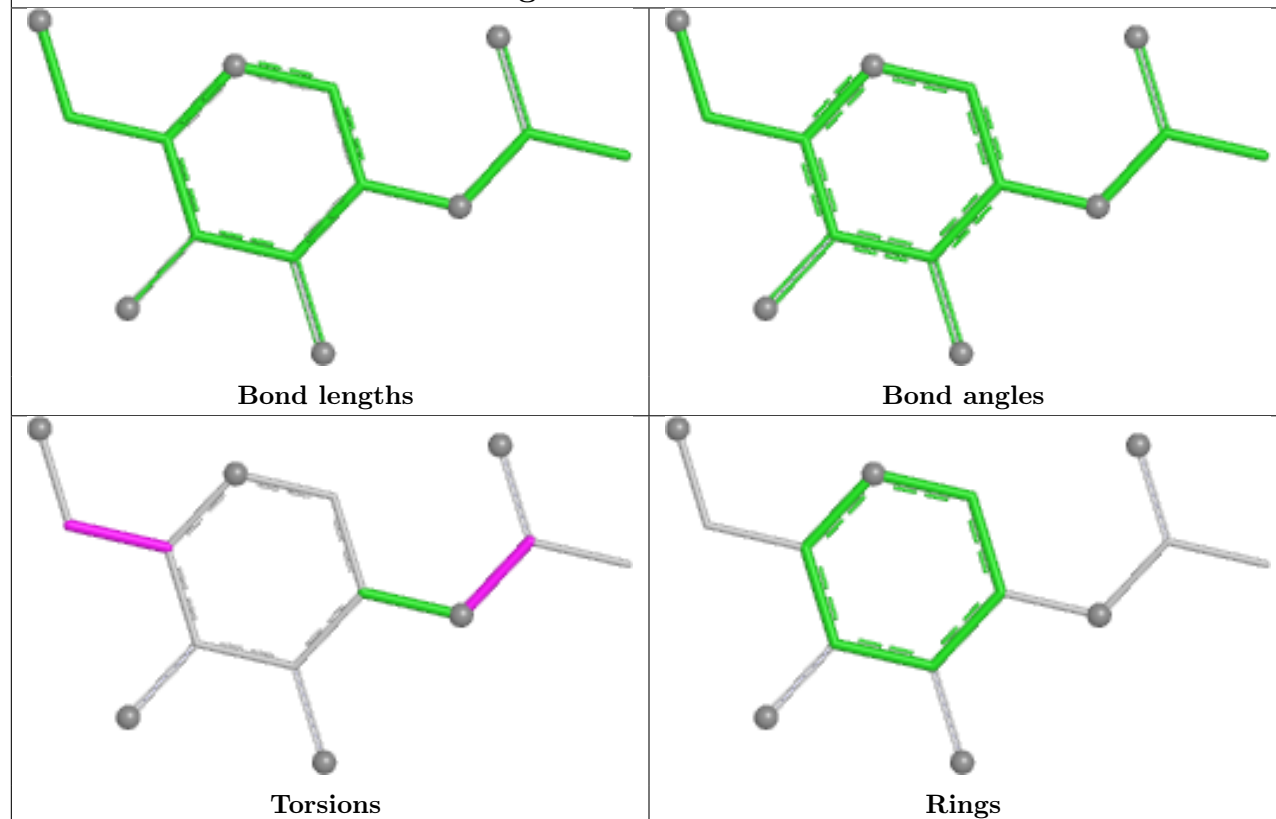
Ligand NAG A 1309



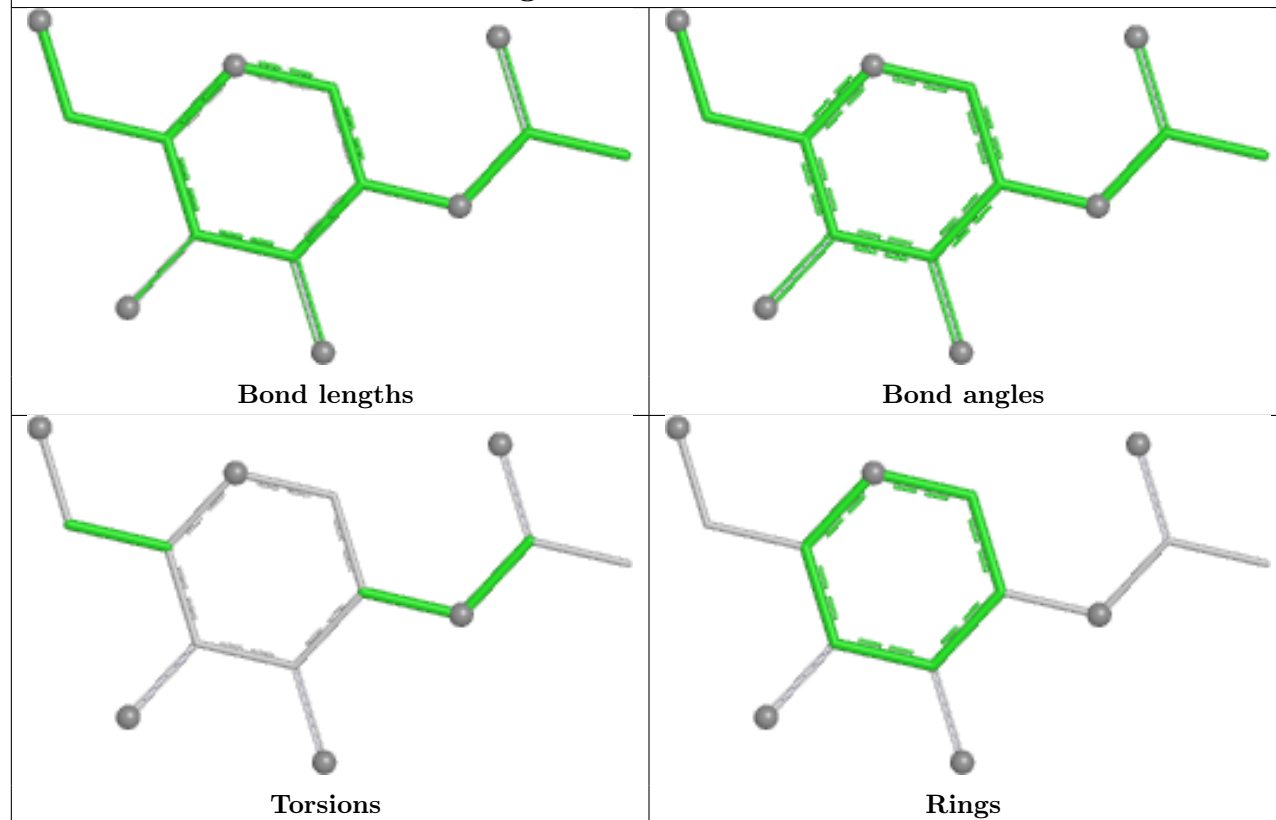
Ligand NAG B 1304



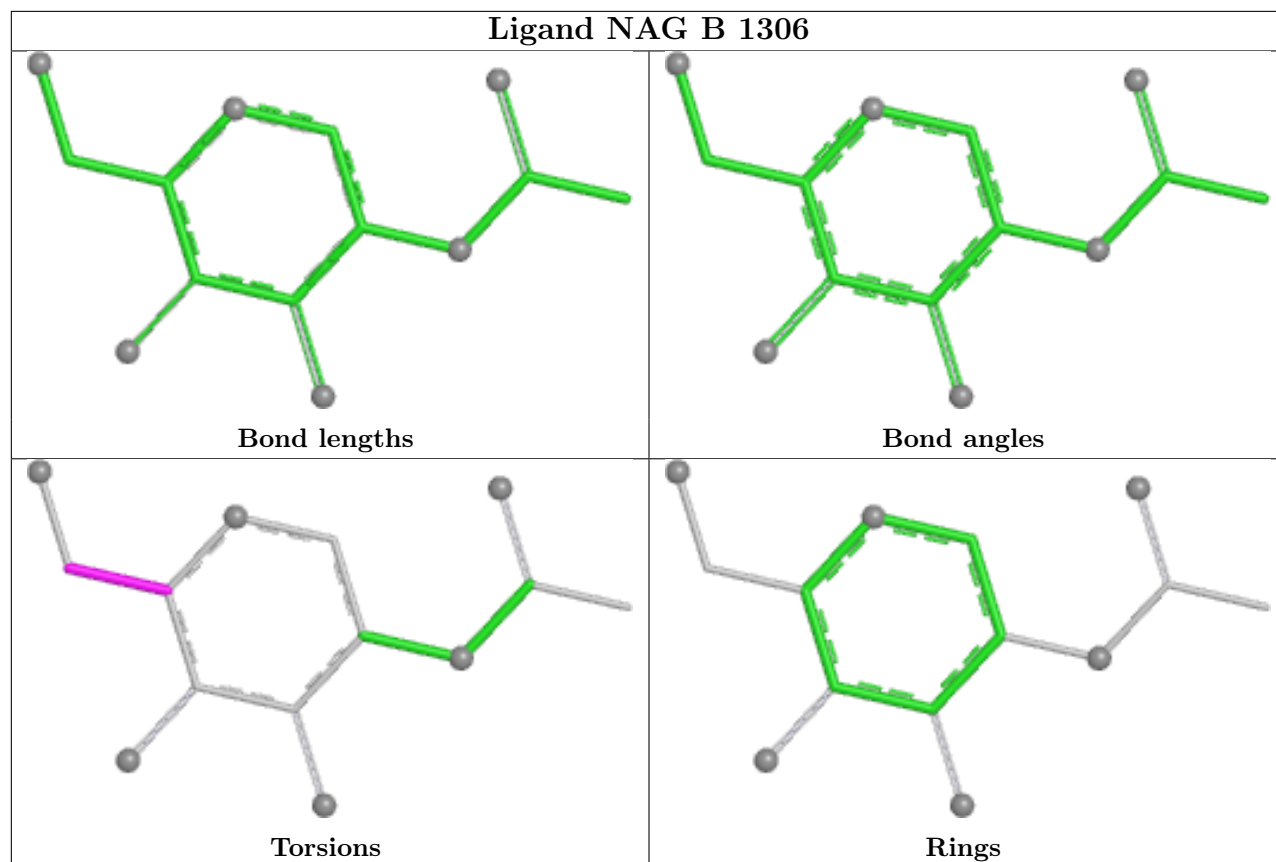
Ligand NAG A 1301



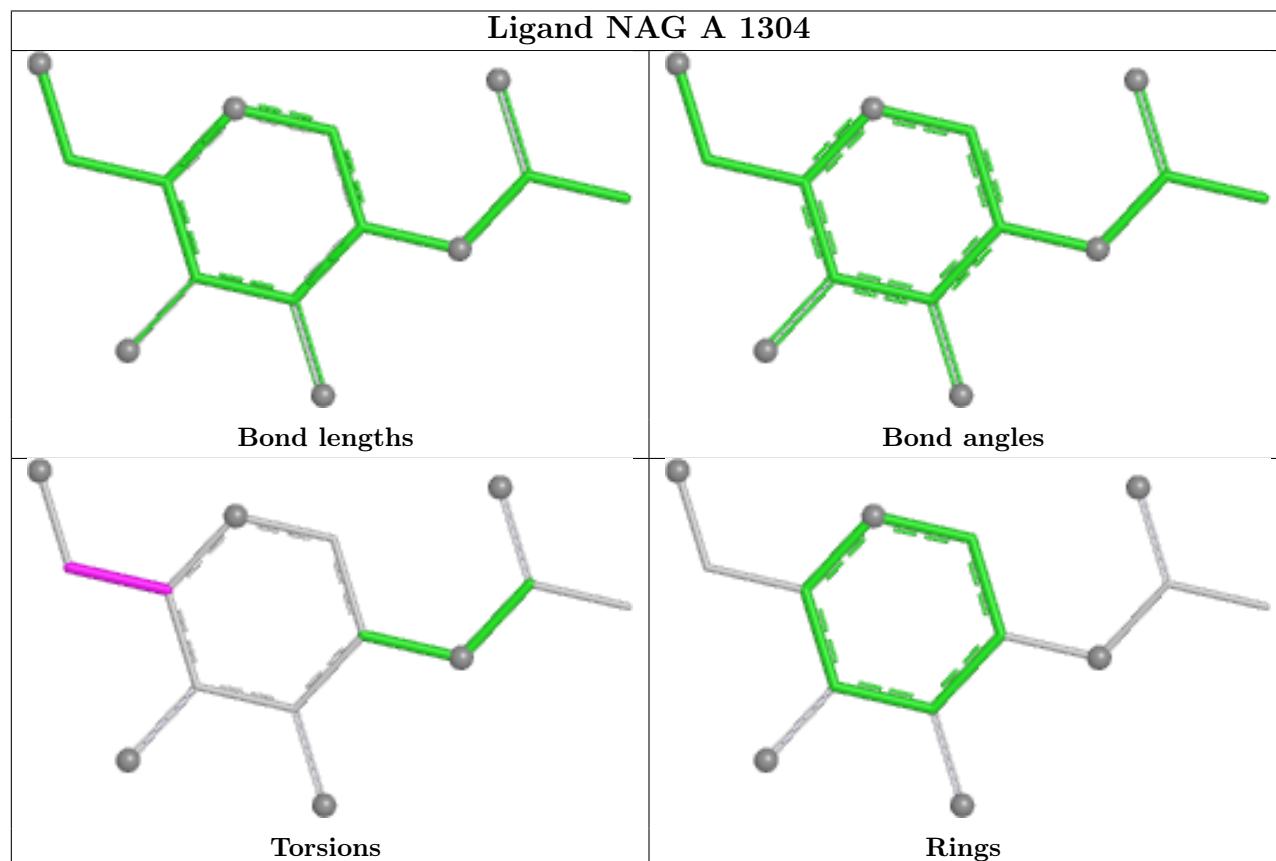
Ligand NAG A 1311



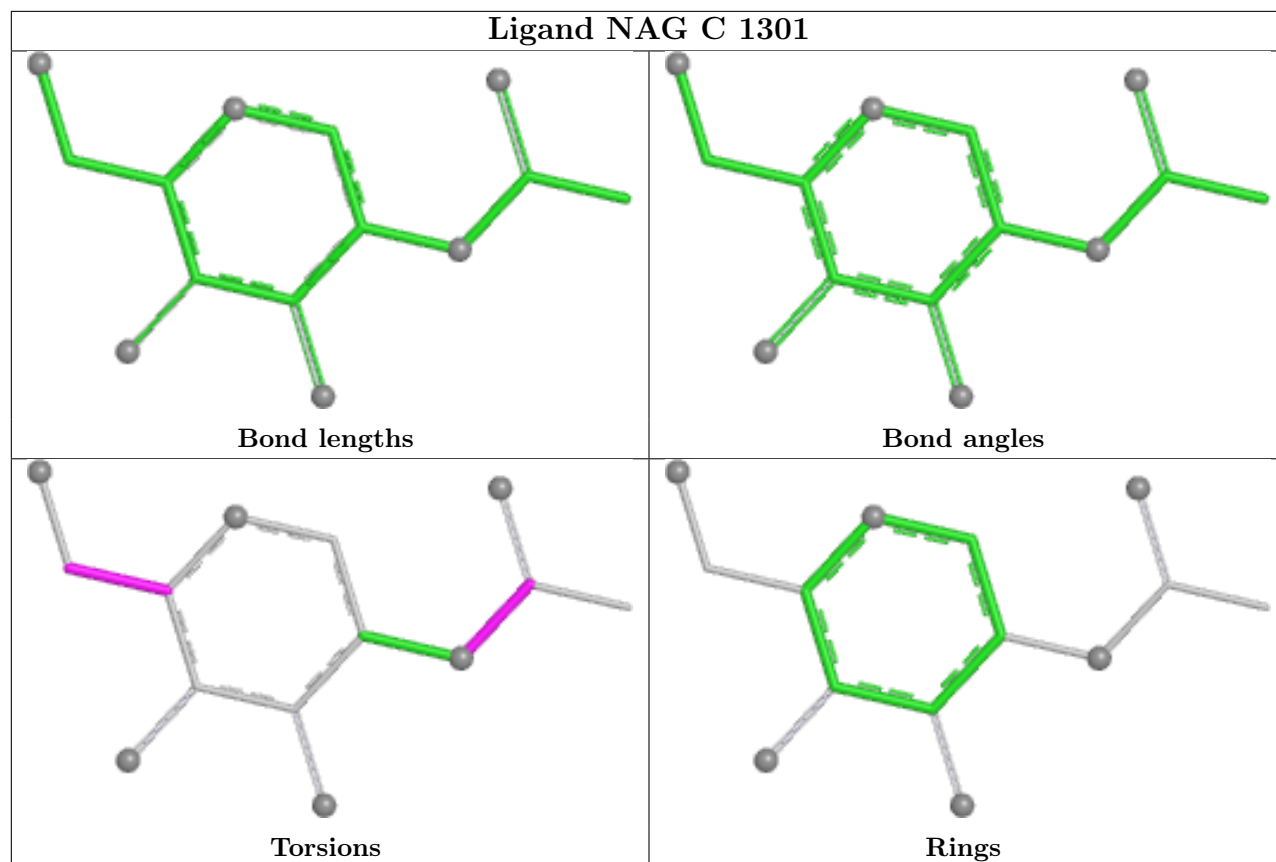
Ligand NAG B 1306



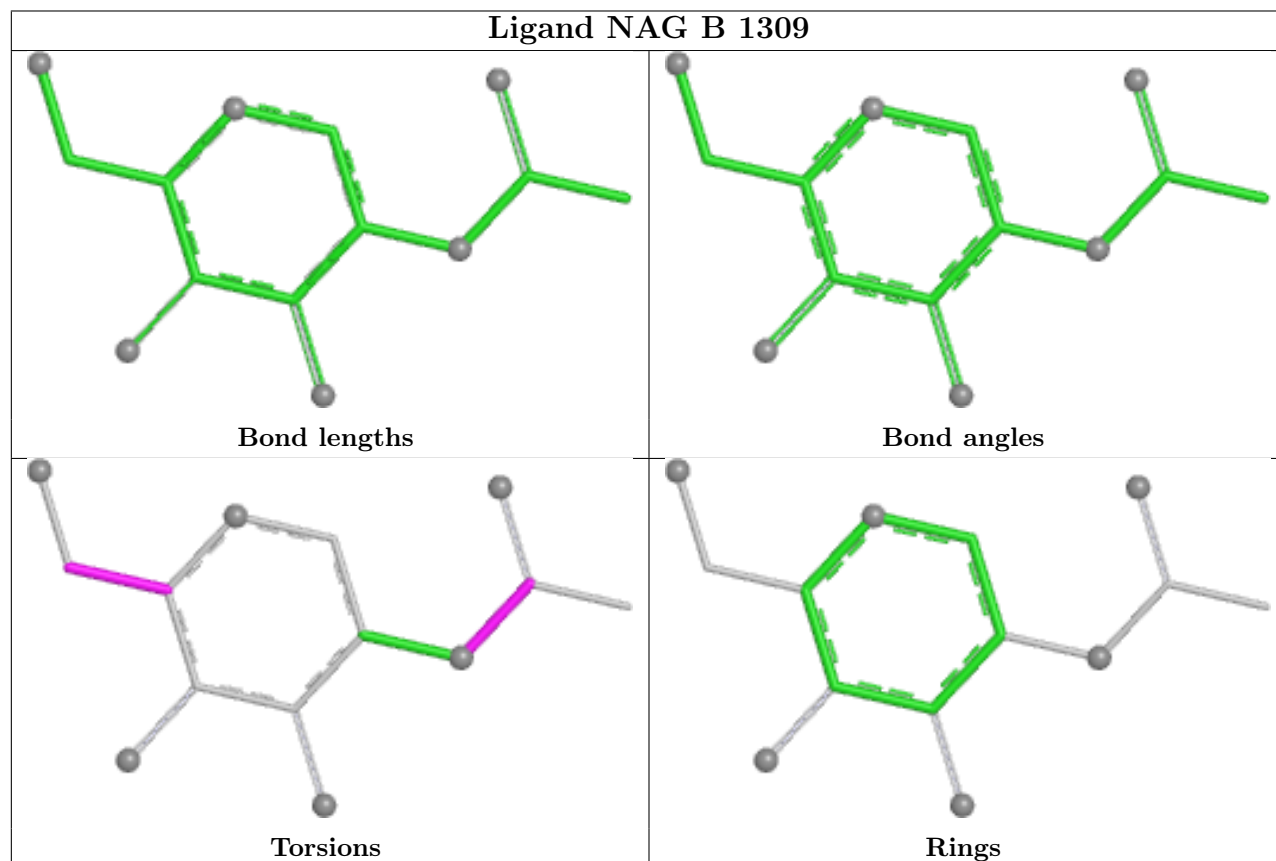
Ligand NAG A 1304



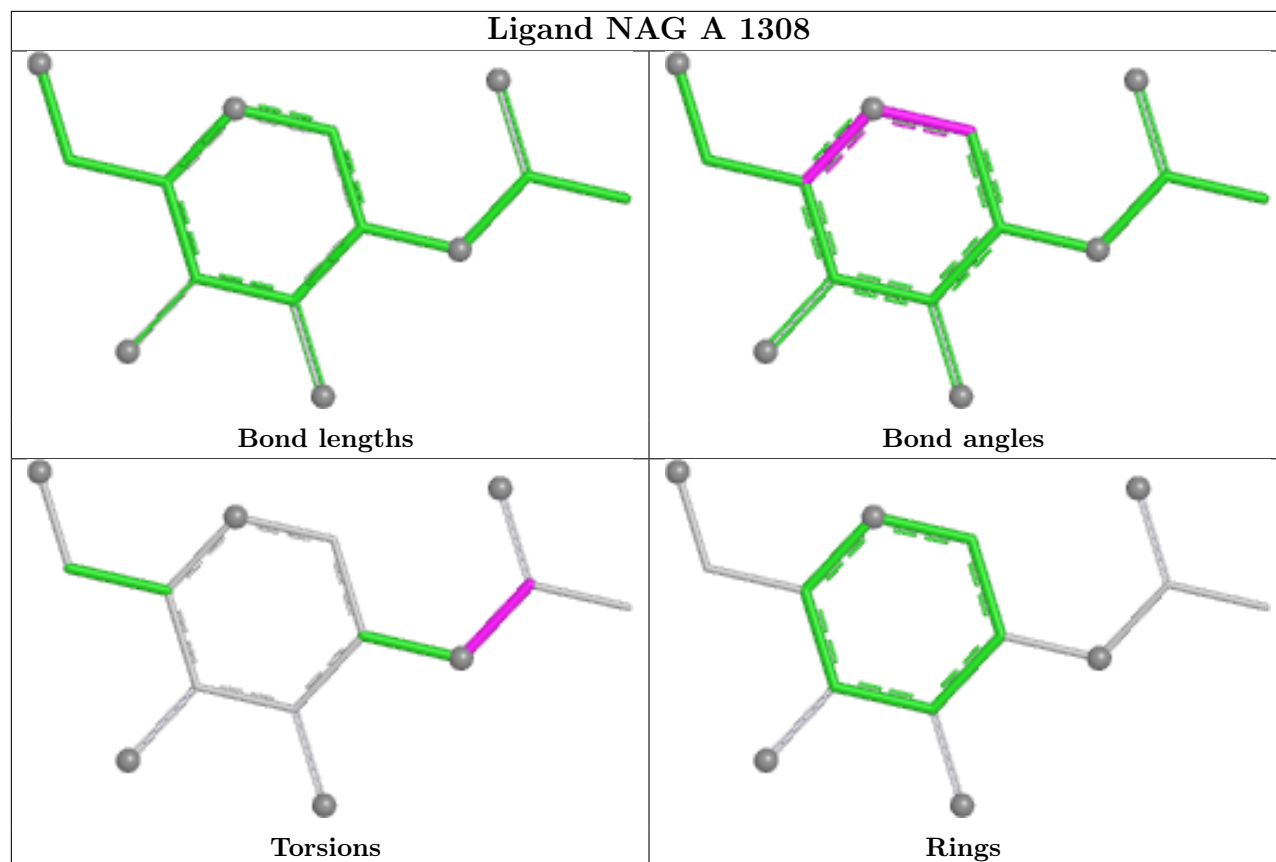
Ligand NAG C 1301



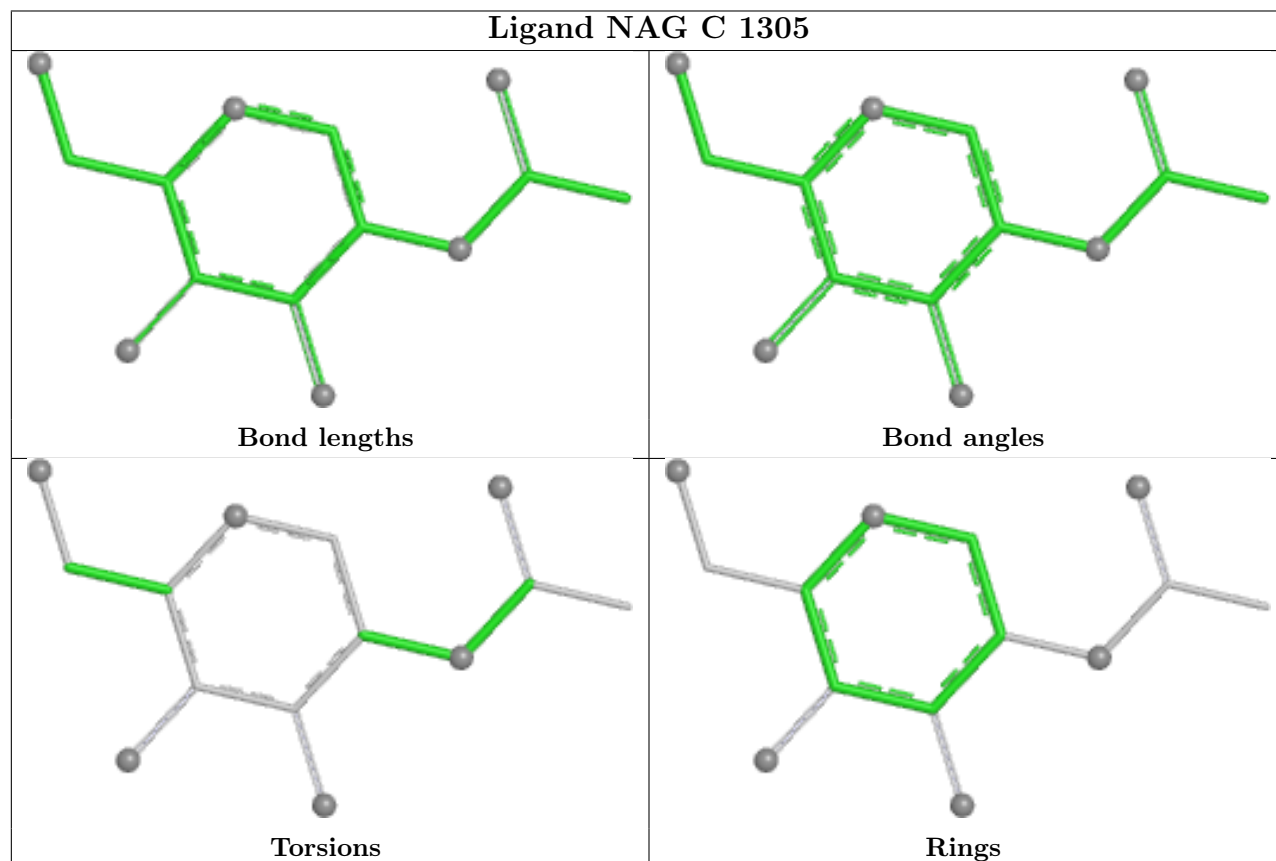
Ligand NAG B 1309



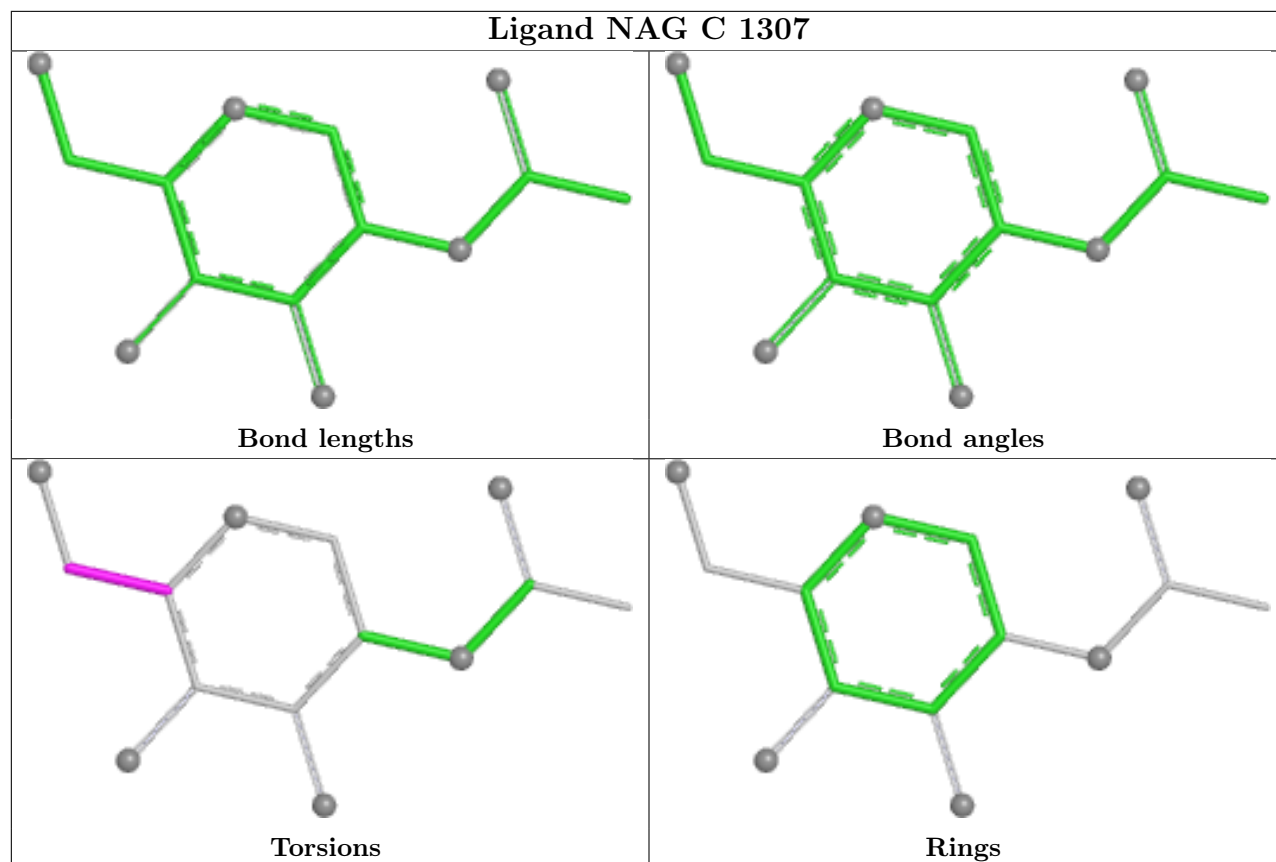
Ligand NAG A 1308



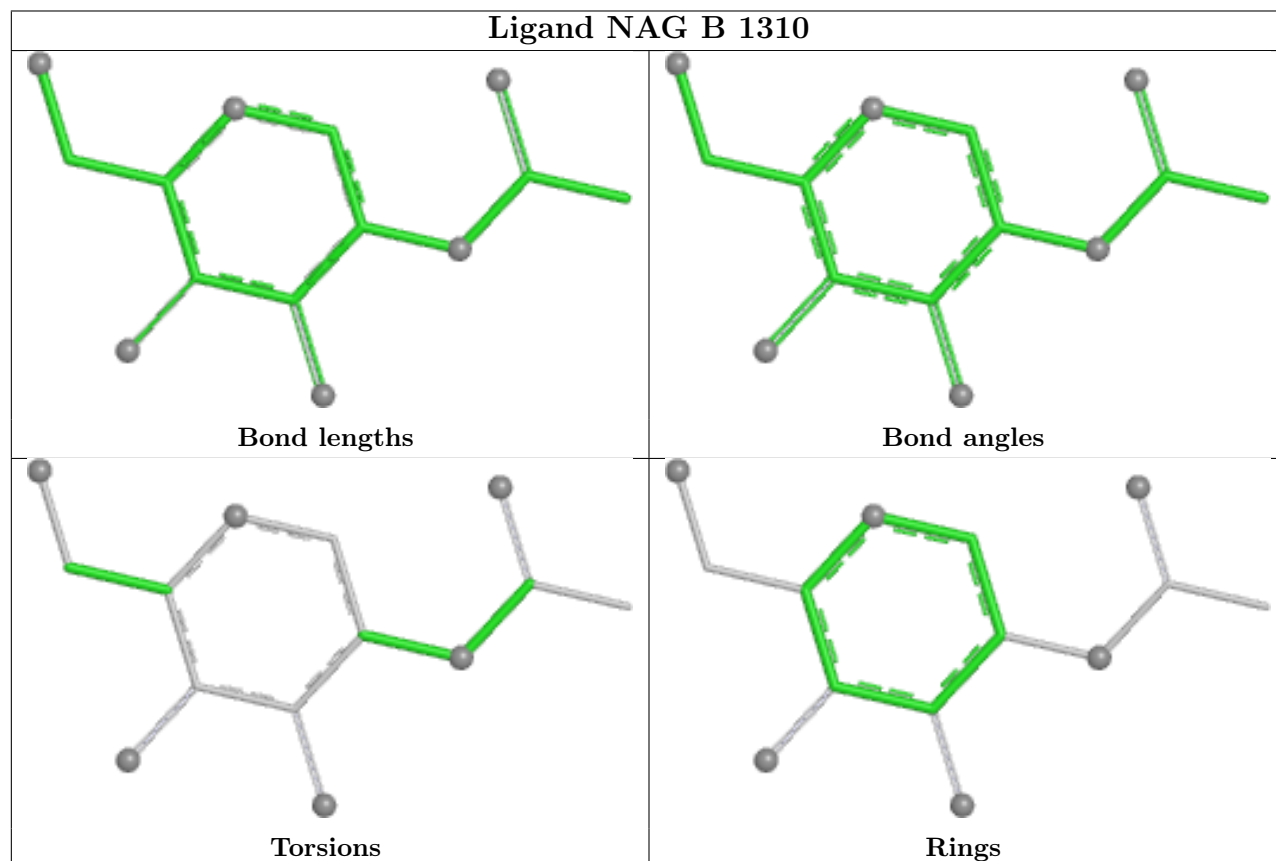
Ligand NAG C 1305



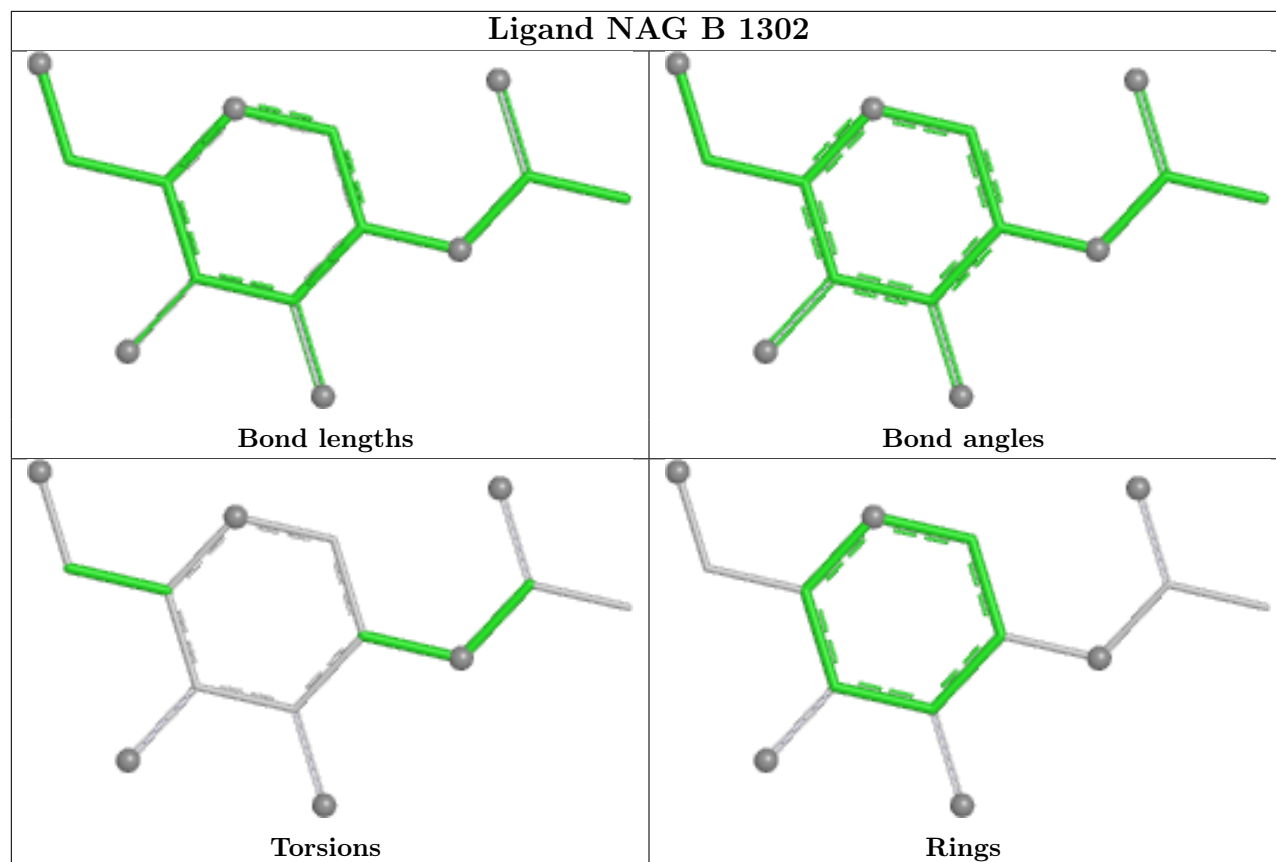
Ligand NAG C 1307



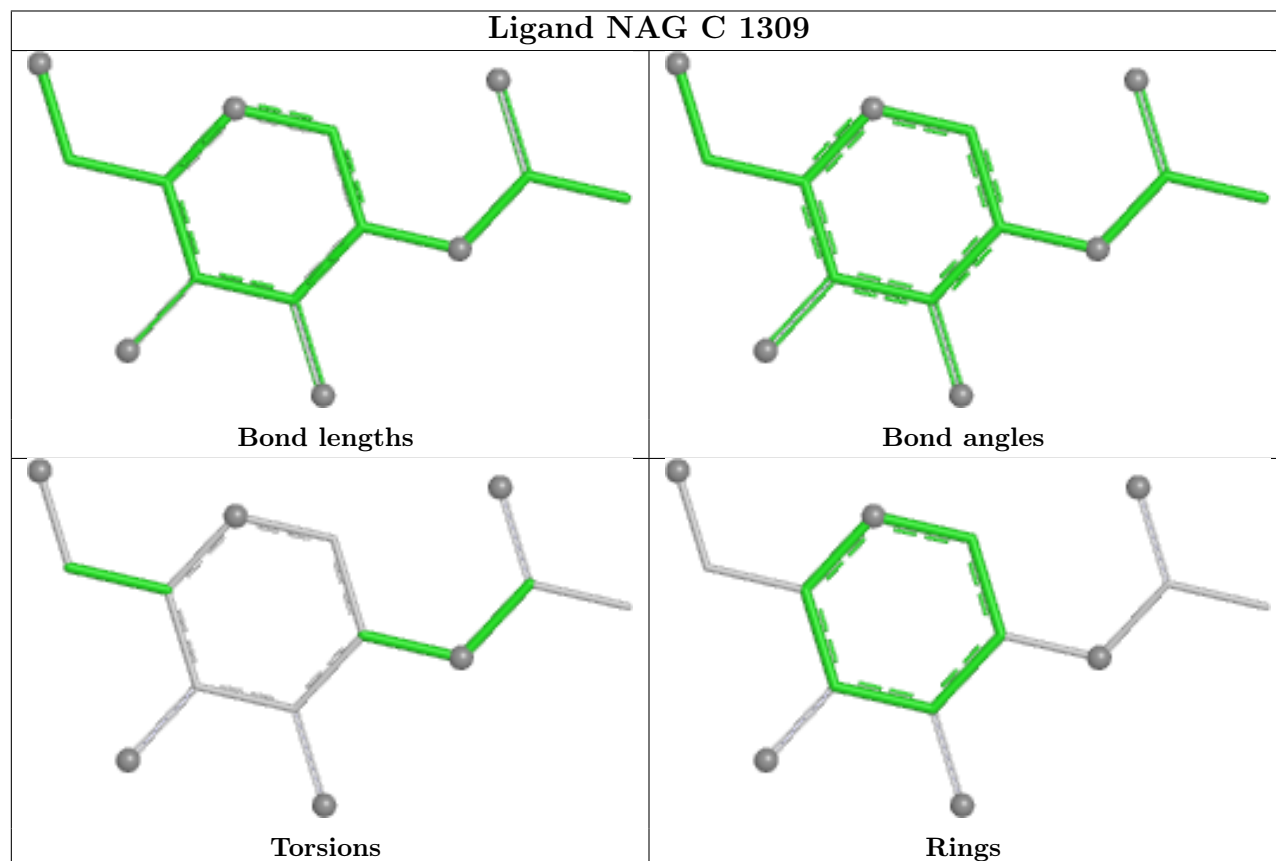
Ligand NAG B 1310

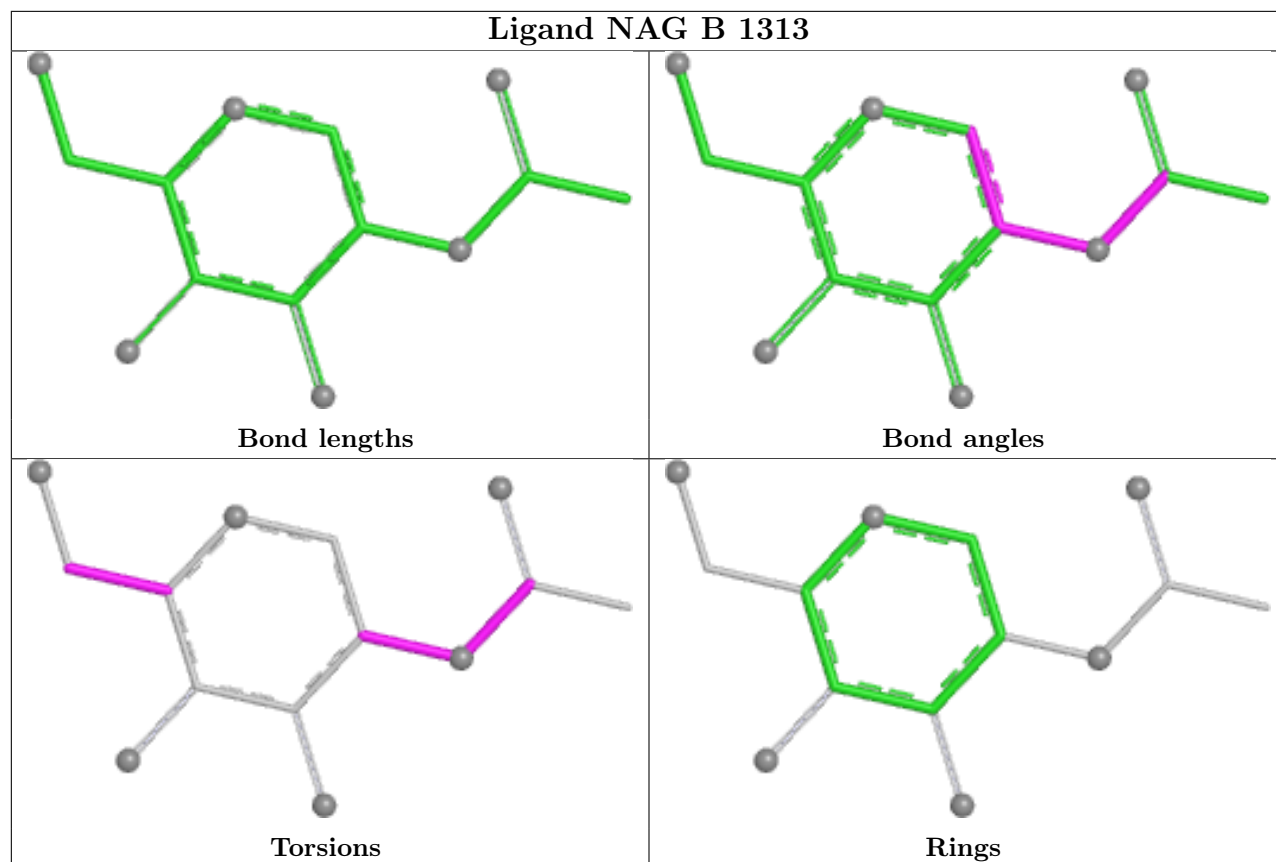


Ligand NAG B 1302



Ligand NAG C 1309





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.

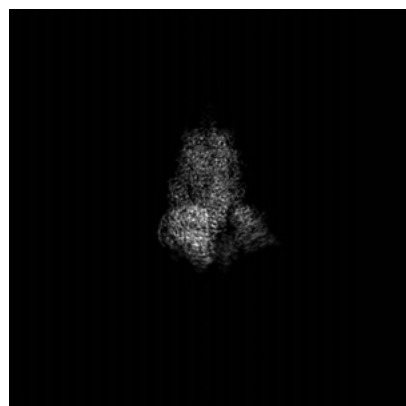
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38476. These allow visual inspection of the internal detail of the map and identification of artifacts.

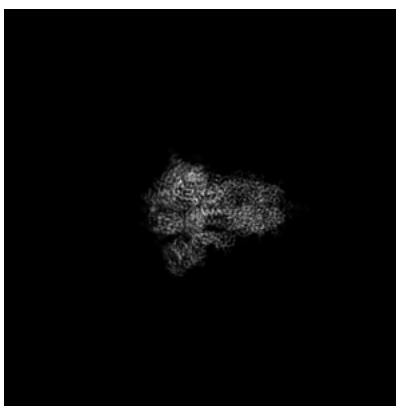
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

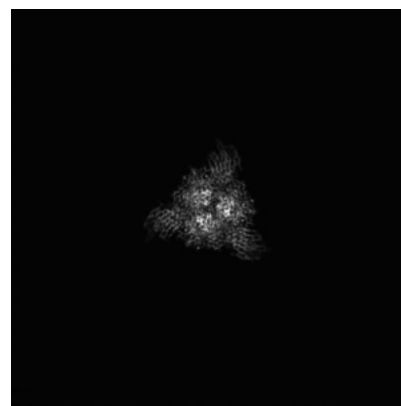
6.1.1 Primary map



X

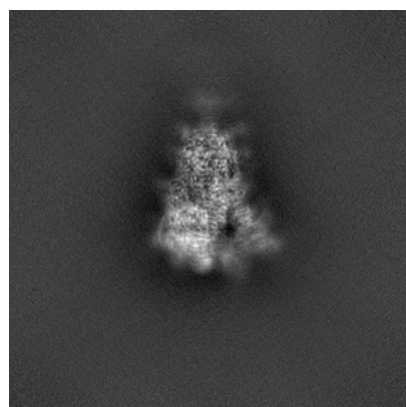


Y

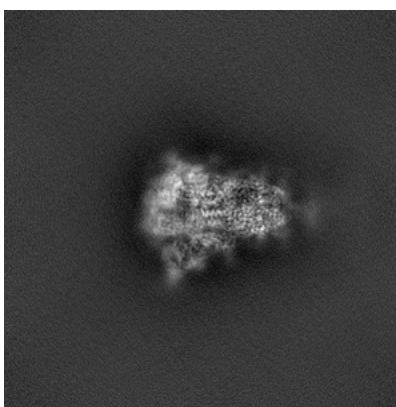


Z

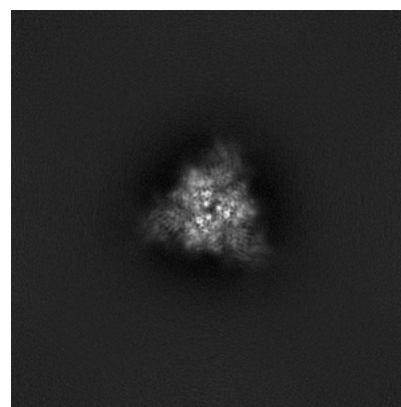
6.1.2 Raw map



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: 256

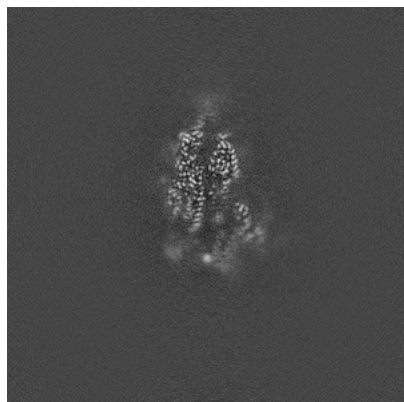


Y Index: 256

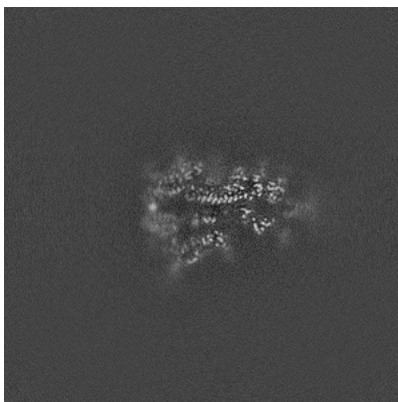


Z Index: 256

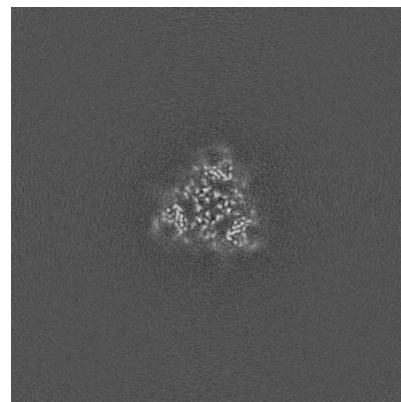
6.2.2 Raw map



X Index: 256



Y Index: 256

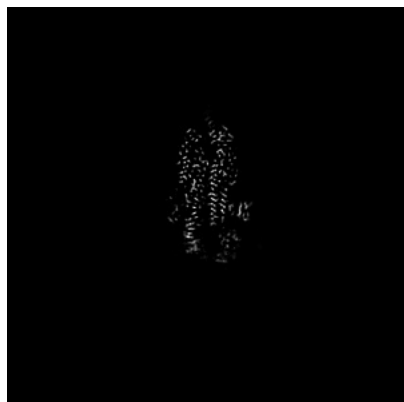


Z Index: 256

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: 249

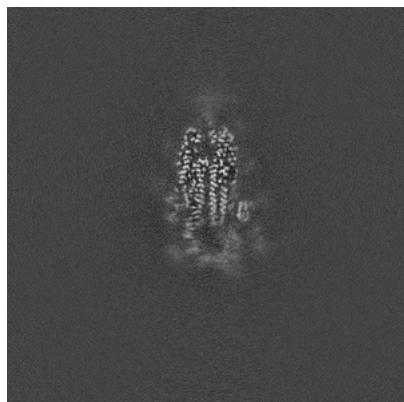


Y Index: 247

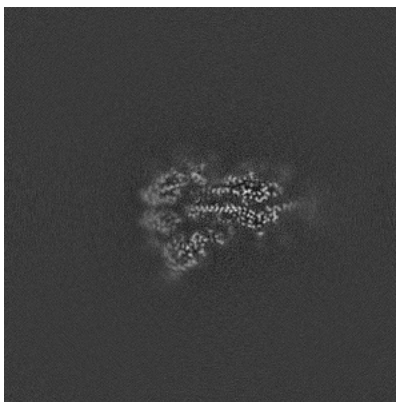


Z Index: 241

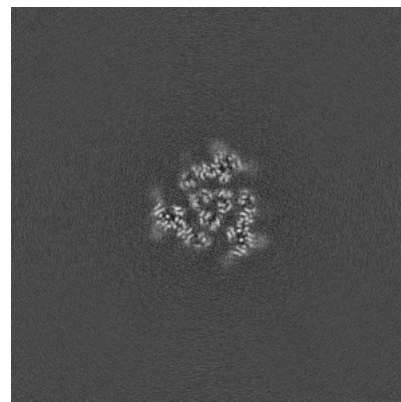
6.3.2 Raw map



X Index: 250



Y Index: 247

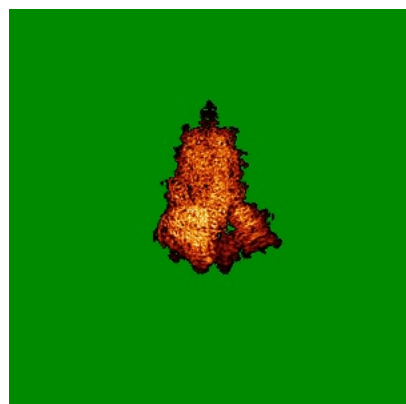


Z Index: 242

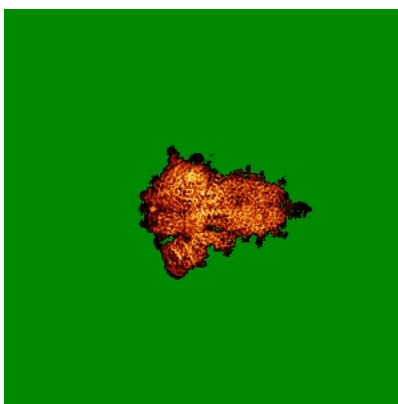
The images above show the largest variance slices of the map in three orthogonal directions.

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

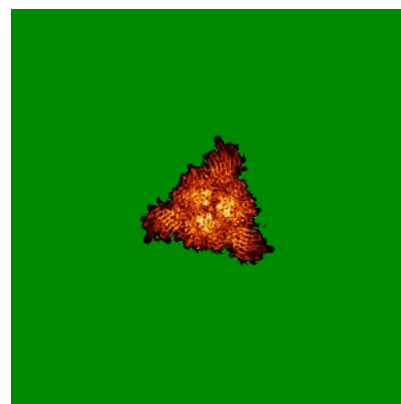
6.4.1 Primary map



X

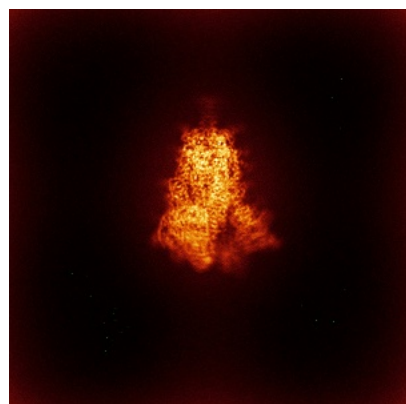


Y

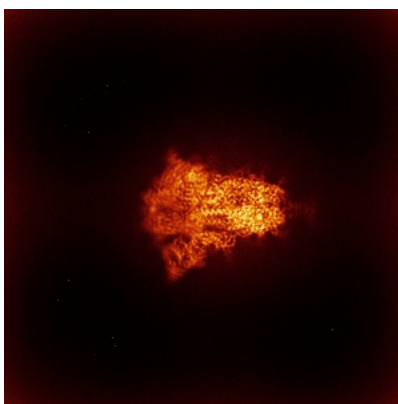


Z

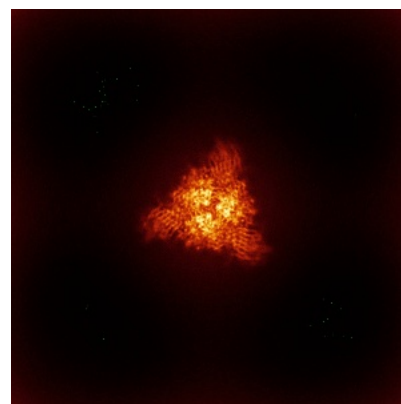
6.4.2 Raw map



X



Y

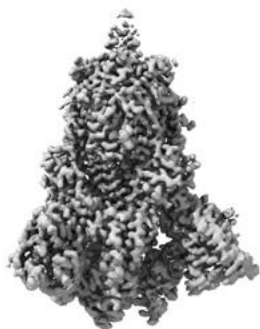


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. 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



X



Y



Z

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.

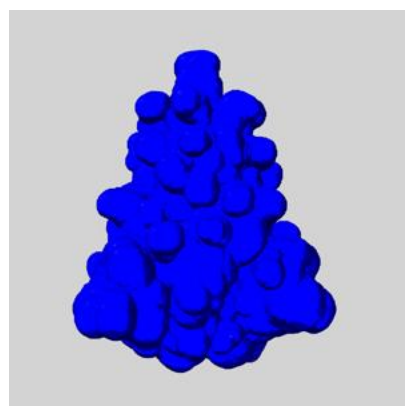
6.6 Mask visualisation [i](#)

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

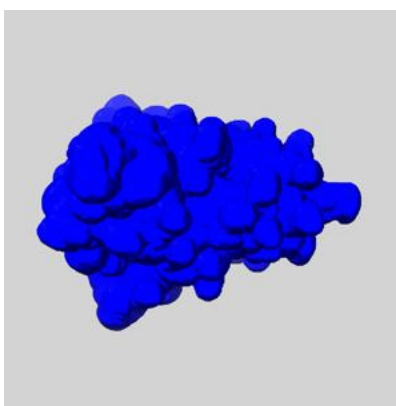
A mask typically either:

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

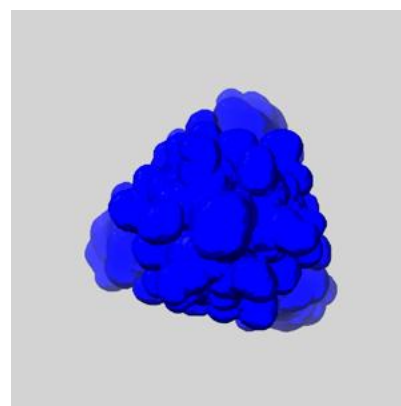
6.6.1 emd_38476_msk_1.map [i](#)



X



Y

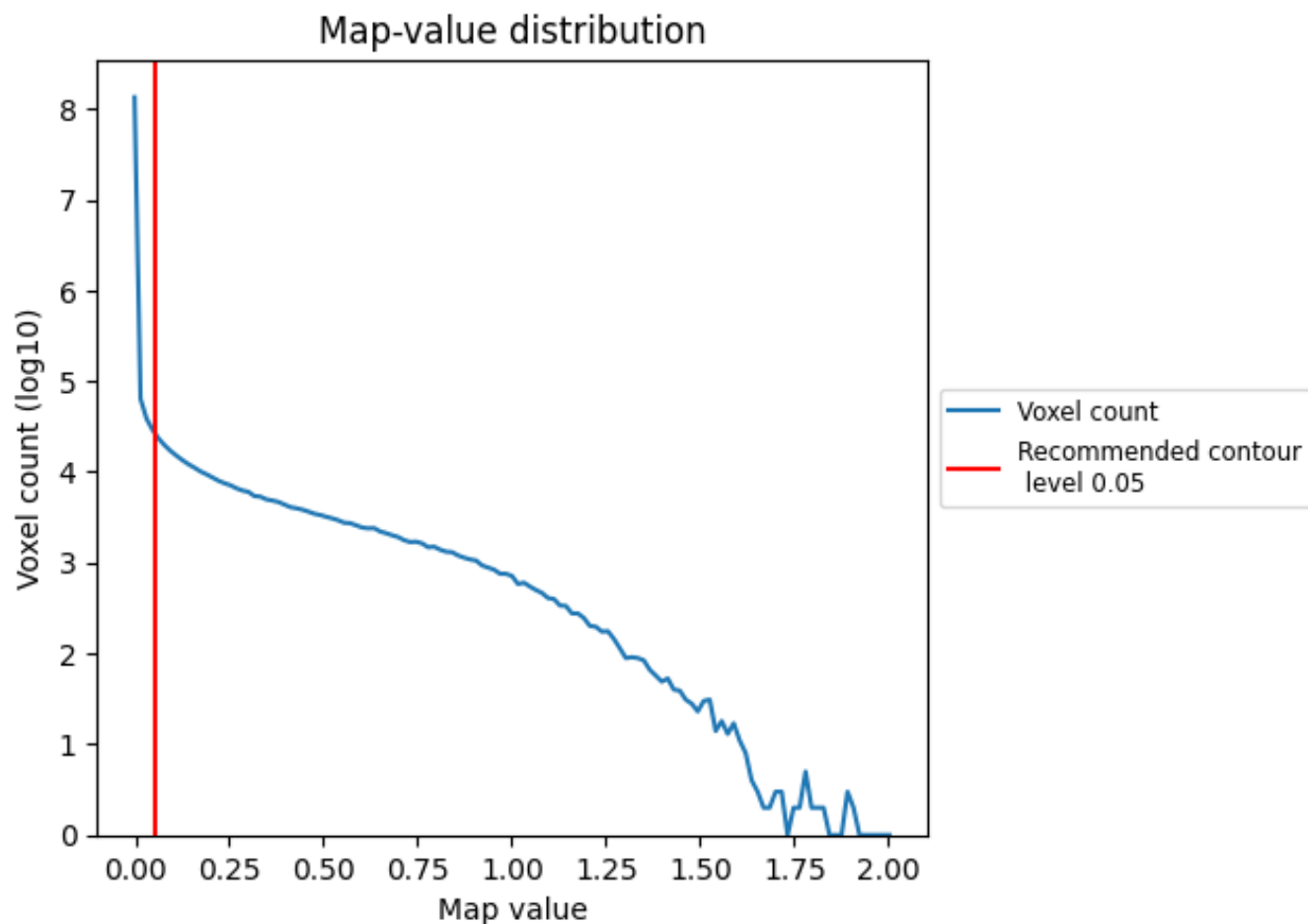


Z

7 Map analysis [i](#)

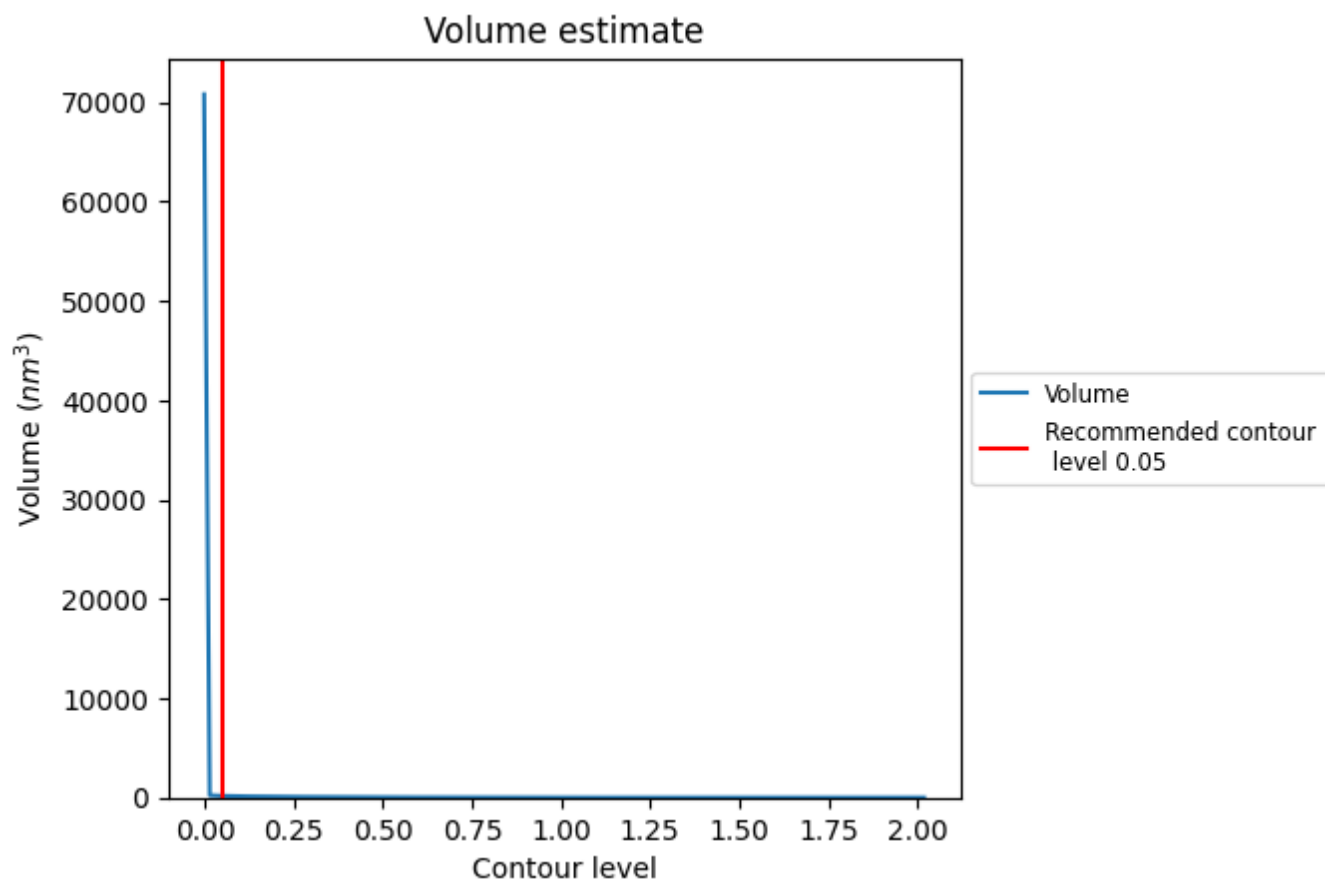
This section contains the results of statistical analysis of the map.

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.

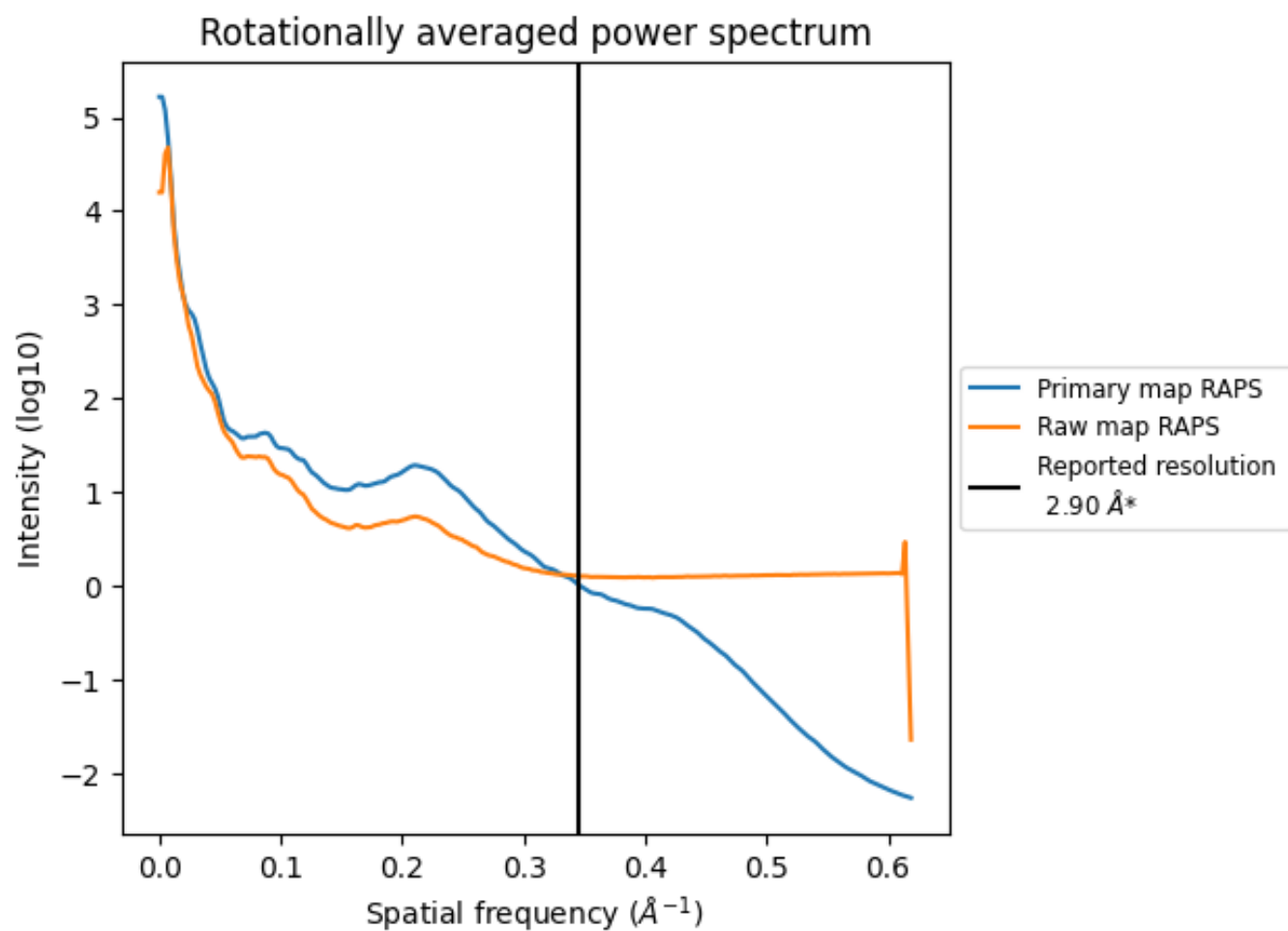
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; this corresponds to an approximate mass of 152 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 ⓘ

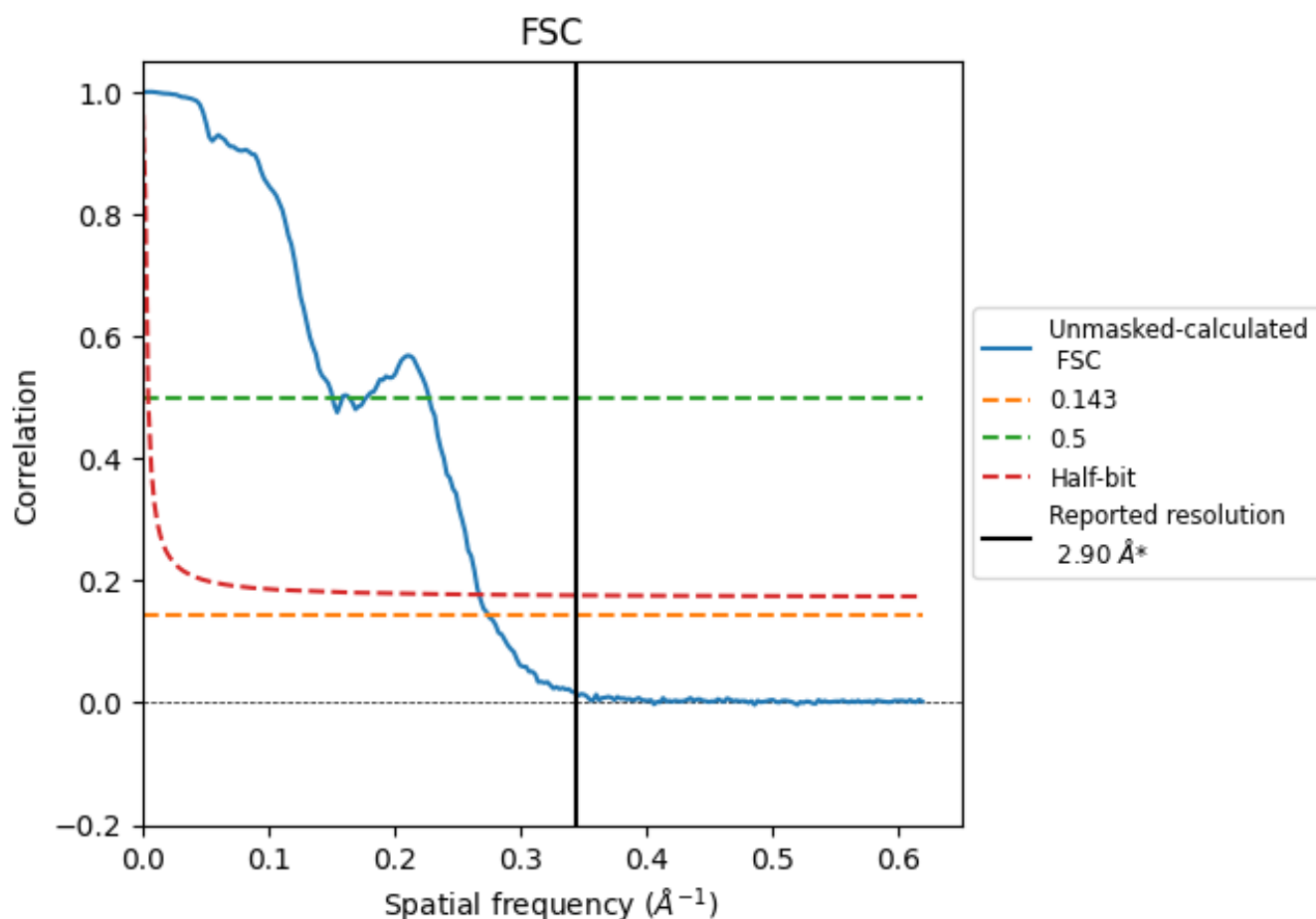


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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 $0.345 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

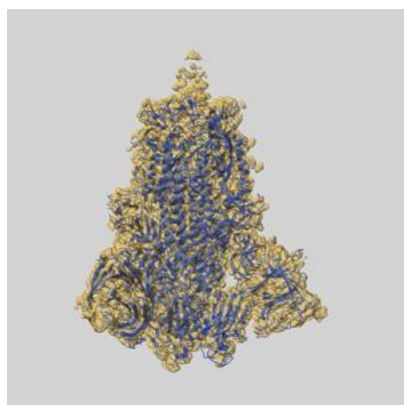
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.64	6.63	3.74

*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 3.64 differs from the reported value 2.9 by more than 10 %

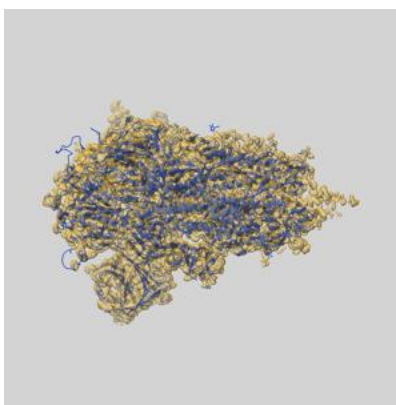
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38476 and PDB model 8XMG. Per-residue inclusion information can be found in section [3](#) on page [13](#).

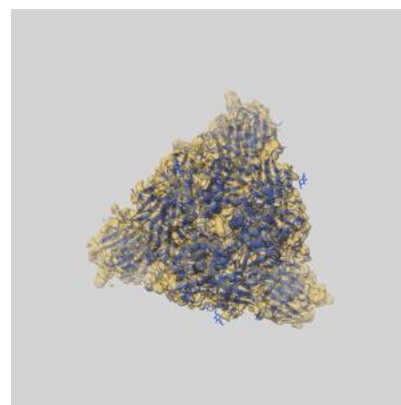
9.1 Map-model overlay [i](#)



X



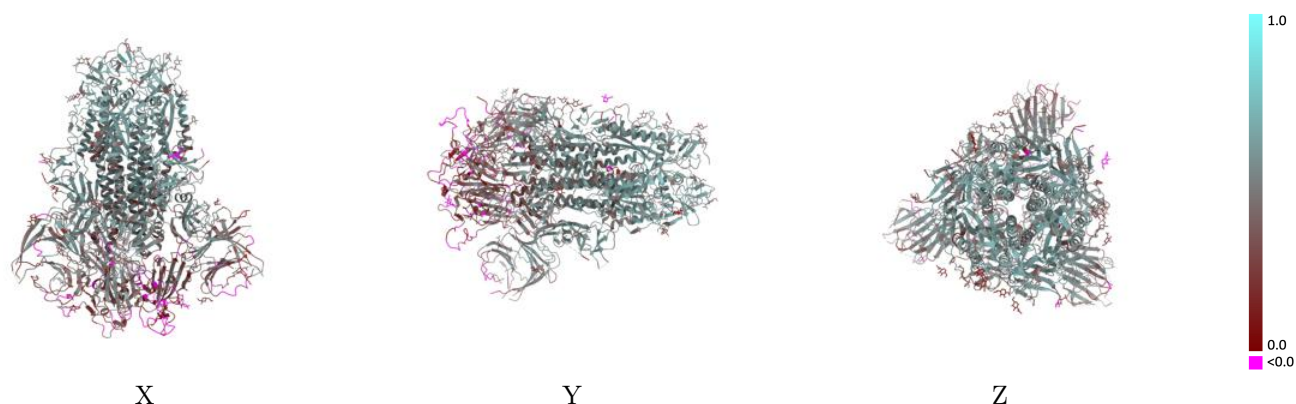
Y



Z

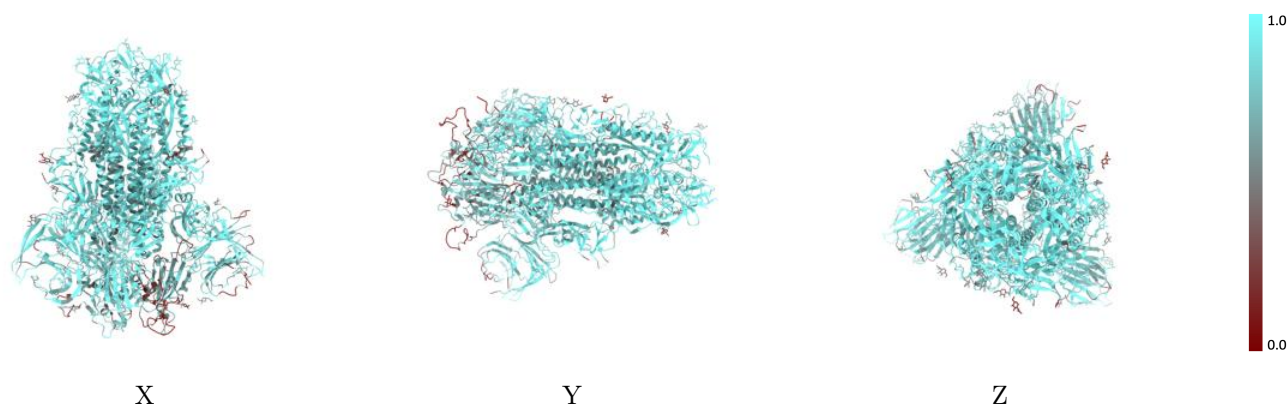
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



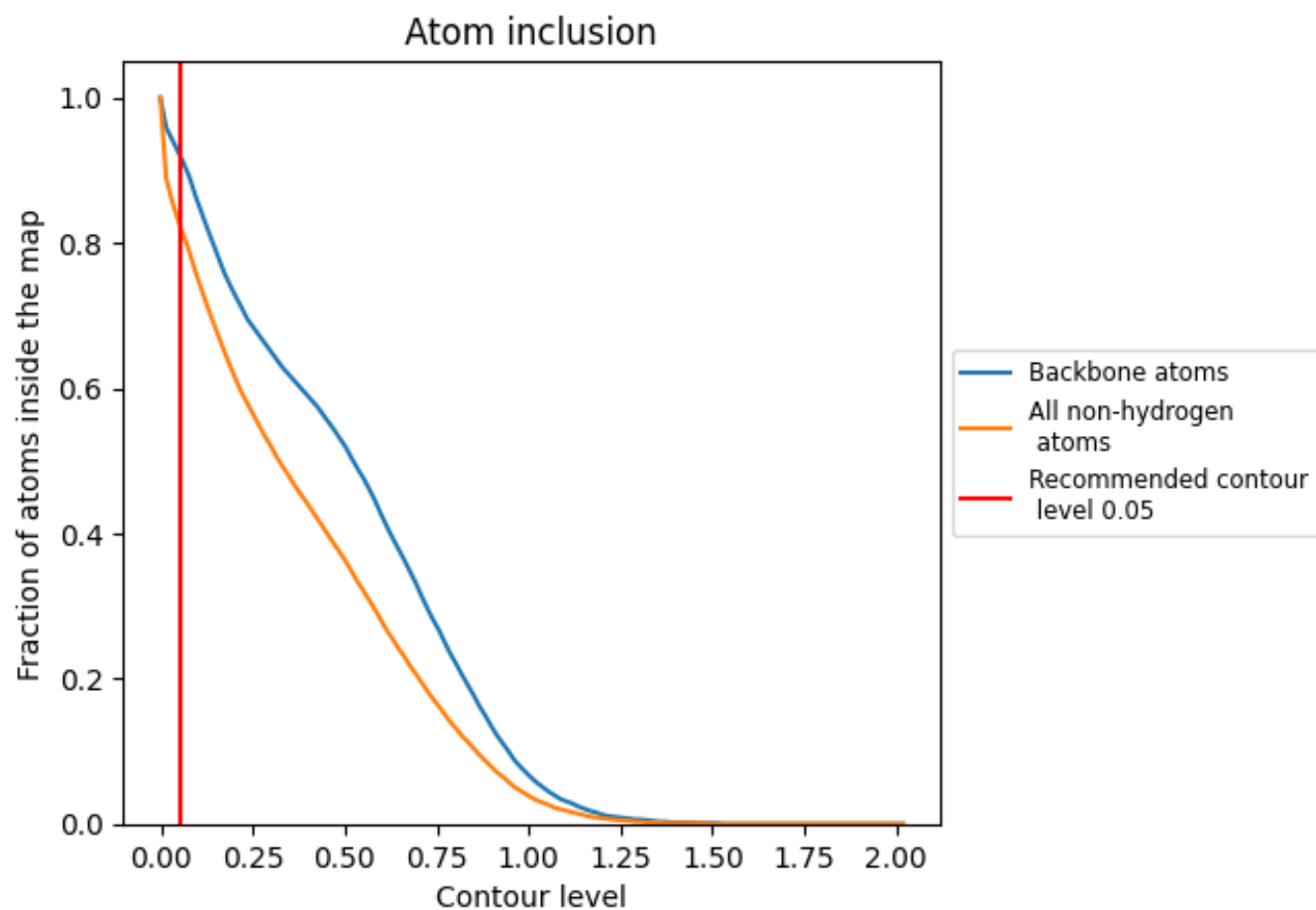
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8260	0.4430
A	0.8380	0.4490
B	0.8360	0.4460
C	0.8030	0.4330

