



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:12 PM UTC

PDB ID : 8XN5 / pdb_00008xn5
EMDB ID : EMD-38498
Title : Cryo-EM structure of SARS-CoV-2 Omicron EG.5.1 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 : 2.87 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

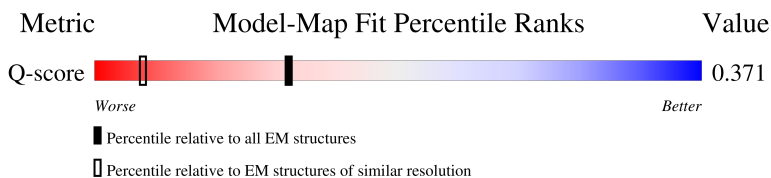
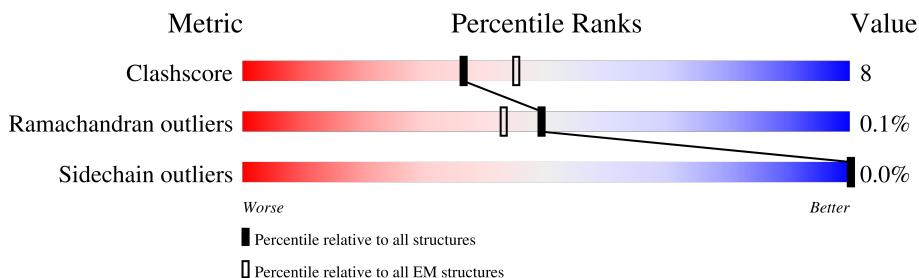
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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	12062 (2.37 - 3.37)

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	
2	B	1227	
2	C	1227	
2	D	1227	

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
3	NAG	C	1301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29149 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
			4872	3117	808	918	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	1011	Total	C	N	O	S	0	0
			7900	5052	1312	1500	36		
2	C	1013	Total	C	N	O	S	0	0
			7924	5066	1322	1500	36		
2	D	1016	Total	C	N	O	S	0	0
			7948	5081	1326	1505	36		

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	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	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	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
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1208	GLN	-	expression tag	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
B	1245	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1246	HIS	-	expression tag	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	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	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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1208	GLN	-	expression tag	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	22	ILE	THR	variant	UNP P0DTC2
D	?	-	LEU	deletion	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	27	SER	ALA	variant	UNP P0DTC2
D	52	HIS	GLN	variant	UNP P0DTC2
D	83	ALA	VAL	variant	UNP P0DTC2
D	142	ASP	GLY	variant	UNP P0DTC2
D	?	-	TYR	deletion	UNP P0DTC2
D	146	GLN	HIS	variant	UNP P0DTC2
D	183	GLU	GLN	variant	UNP P0DTC2
D	213	GLU	VAL	variant	UNP P0DTC2
D	252	VAL	GLY	variant	UNP P0DTC2
D	339	HIS	GLY	variant	UNP P0DTC2
D	346	THR	ARG	variant	UNP P0DTC2
D	368	ILE	LEU	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	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	PRO	VAL	variant	UNP P0DTC2
D	446	SER	GLY	variant	UNP P0DTC2
D	456	LEU	PHE	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	484	ALA	GLU	variant	UNP P0DTC2
D	486	PRO	PHE	variant	UNP P0DTC2
D	490	SER	PHE	variant	UNP P0DTC2

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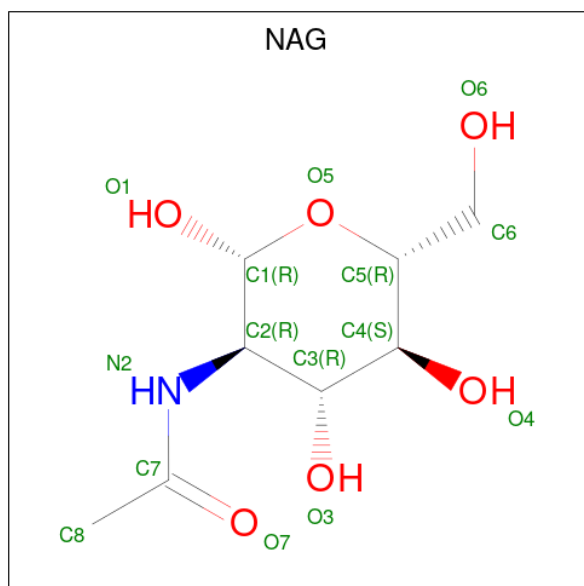
Chain	Residue	Modelled	Actual	Comment	Reference
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	655	TYR	HIS	variant	UNP P0DTC2
D	679	LYS	ASN	variant	UNP P0DTC2
D	681	HIS	PRO	variant	UNP P0DTC2
D	682	GLY	ARG	engineered mutation	UNP P0DTC2
D	683	SER	ARG	engineered mutation	UNP P0DTC2
D	685	SER	ARG	engineered mutation	UNP P0DTC2
D	764	LYS	ASN	variant	UNP P0DTC2
D	796	TYR	ASP	variant	UNP P0DTC2
D	817	PRO	PHE	engineered mutation	UNP P0DTC2
D	892	PRO	ALA	engineered mutation	UNP P0DTC2
D	899	PRO	ALA	engineered mutation	UNP P0DTC2
D	942	PRO	ALA	engineered mutation	UNP P0DTC2
D	954	HIS	GLN	variant	UNP P0DTC2
D	969	LYS	ASN	variant	UNP P0DTC2
D	986	PRO	LYS	engineered mutation	UNP P0DTC2
D	987	PRO	VAL	engineered mutation	UNP P0DTC2
D	1208	GLN	-	expression tag	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	TYR	-	expression tag	UNP P0DTC2
D	1211	ILE	-	expression tag	UNP P0DTC2
D	1212	PRO	-	expression tag	UNP P0DTC2
D	1213	GLU	-	expression tag	UNP P0DTC2
D	1214	ALA	-	expression tag	UNP P0DTC2
D	1215	PRO	-	expression tag	UNP P0DTC2
D	1216	ARG	-	expression tag	UNP P0DTC2
D	1217	ASP	-	expression tag	UNP P0DTC2
D	1218	GLY	-	expression tag	UNP P0DTC2
D	1219	GLN	-	expression tag	UNP P0DTC2
D	1220	ALA	-	expression tag	UNP P0DTC2
D	1221	TYR	-	expression tag	UNP P0DTC2
D	1222	VAL	-	expression tag	UNP P0DTC2
D	1223	ARG	-	expression tag	UNP P0DTC2
D	1224	LYS	-	expression tag	UNP P0DTC2
D	1225	ASP	-	expression tag	UNP P0DTC2
D	1226	GLY	-	expression tag	UNP P0DTC2
D	1227	GLU	-	expression tag	UNP P0DTC2
D	1228	TRP	-	expression tag	UNP P0DTC2
D	1229	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1230	LEU	-	expression tag	UNP P0DTC2
D	1231	LEU	-	expression tag	UNP P0DTC2
D	1232	SER	-	expression tag	UNP P0DTC2
D	1233	THR	-	expression tag	UNP P0DTC2
D	1234	PHE	-	expression tag	UNP P0DTC2
D	1235	LEU	-	expression tag	UNP P0DTC2
D	1236	ALA	-	expression tag	UNP P0DTC2
D	1237	HIS	-	expression tag	UNP P0DTC2
D	1238	HIS	-	expression tag	UNP P0DTC2
D	1239	HIS	-	expression tag	UNP P0DTC2
D	1240	HIS	-	expression tag	UNP P0DTC2
D	1241	HIS	-	expression tag	UNP P0DTC2
D	1242	HIS	-	expression tag	UNP P0DTC2
D	1243	HIS	-	expression tag	UNP P0DTC2
D	1244	HIS	-	expression tag	UNP P0DTC2
D	1245	HIS	-	expression tag	UNP P0DTC2
D	1246	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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

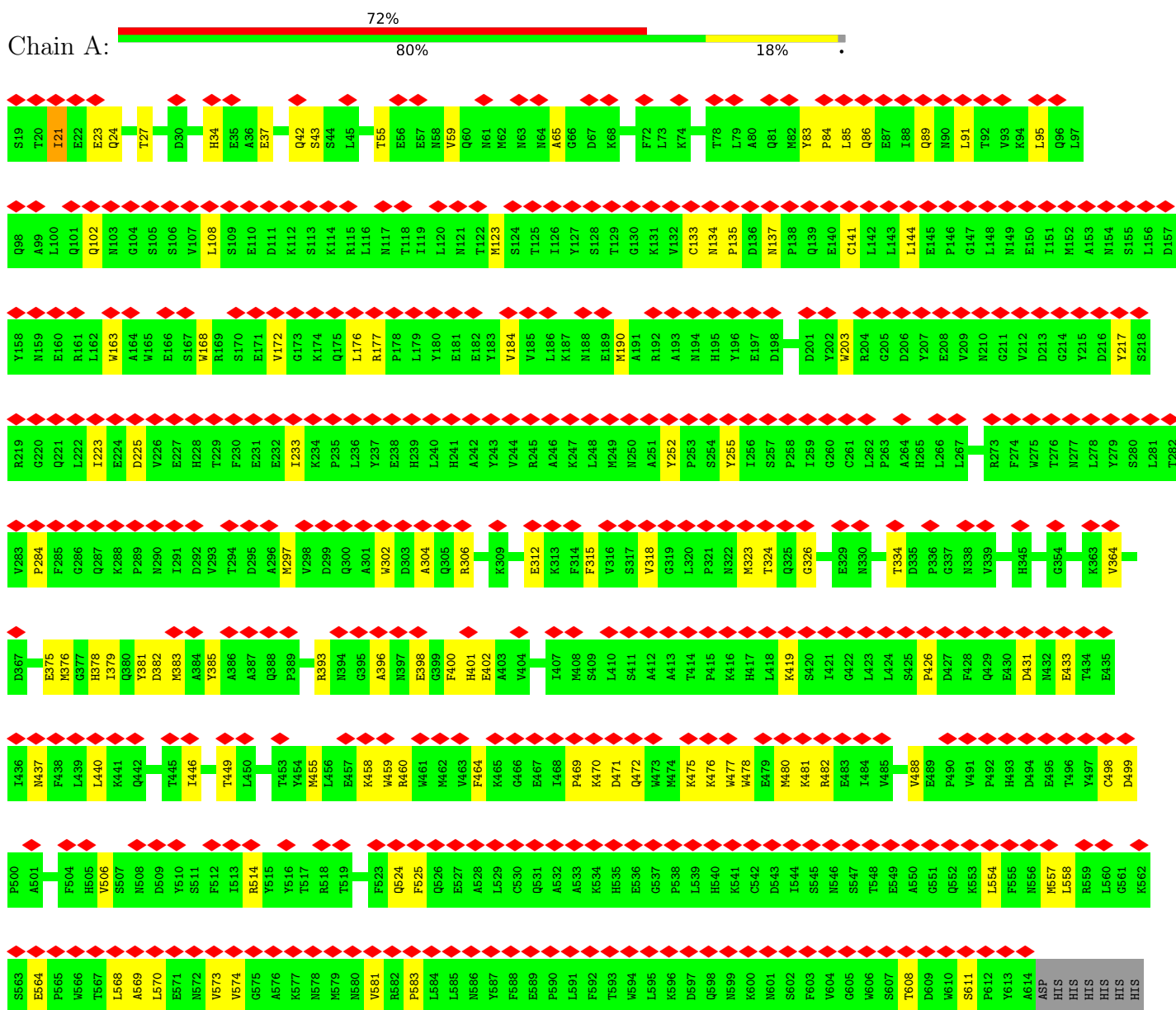
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

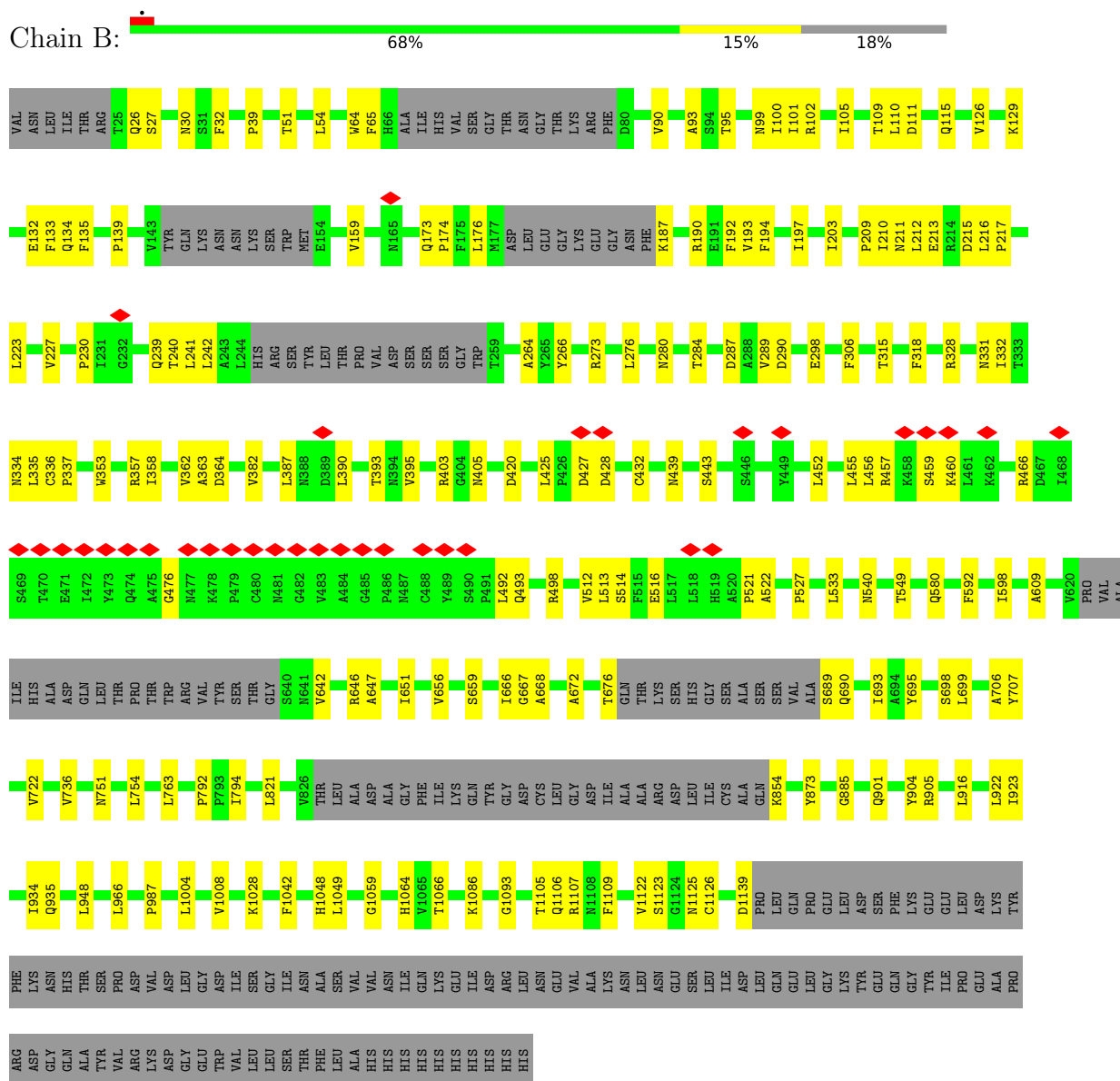
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Angiotensin-converting enzyme 2



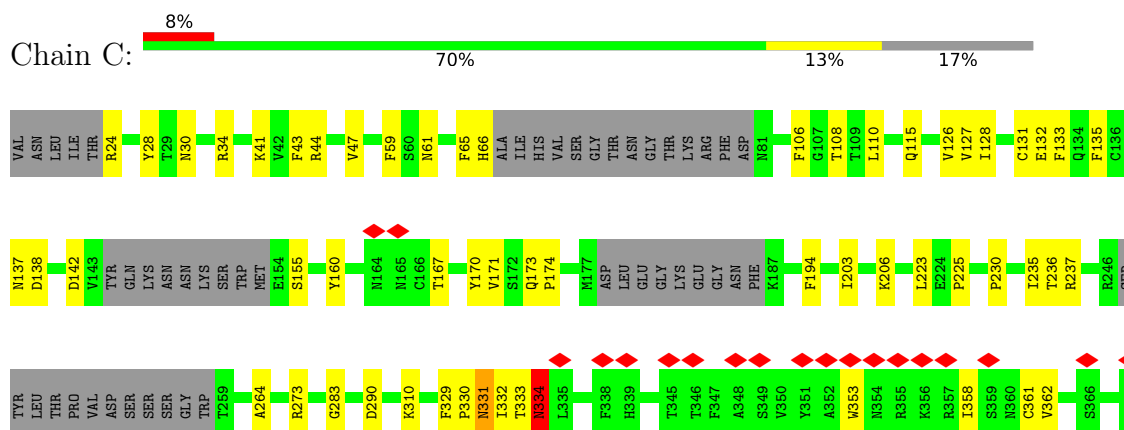
• Molecule 2: Spike glycoprotein

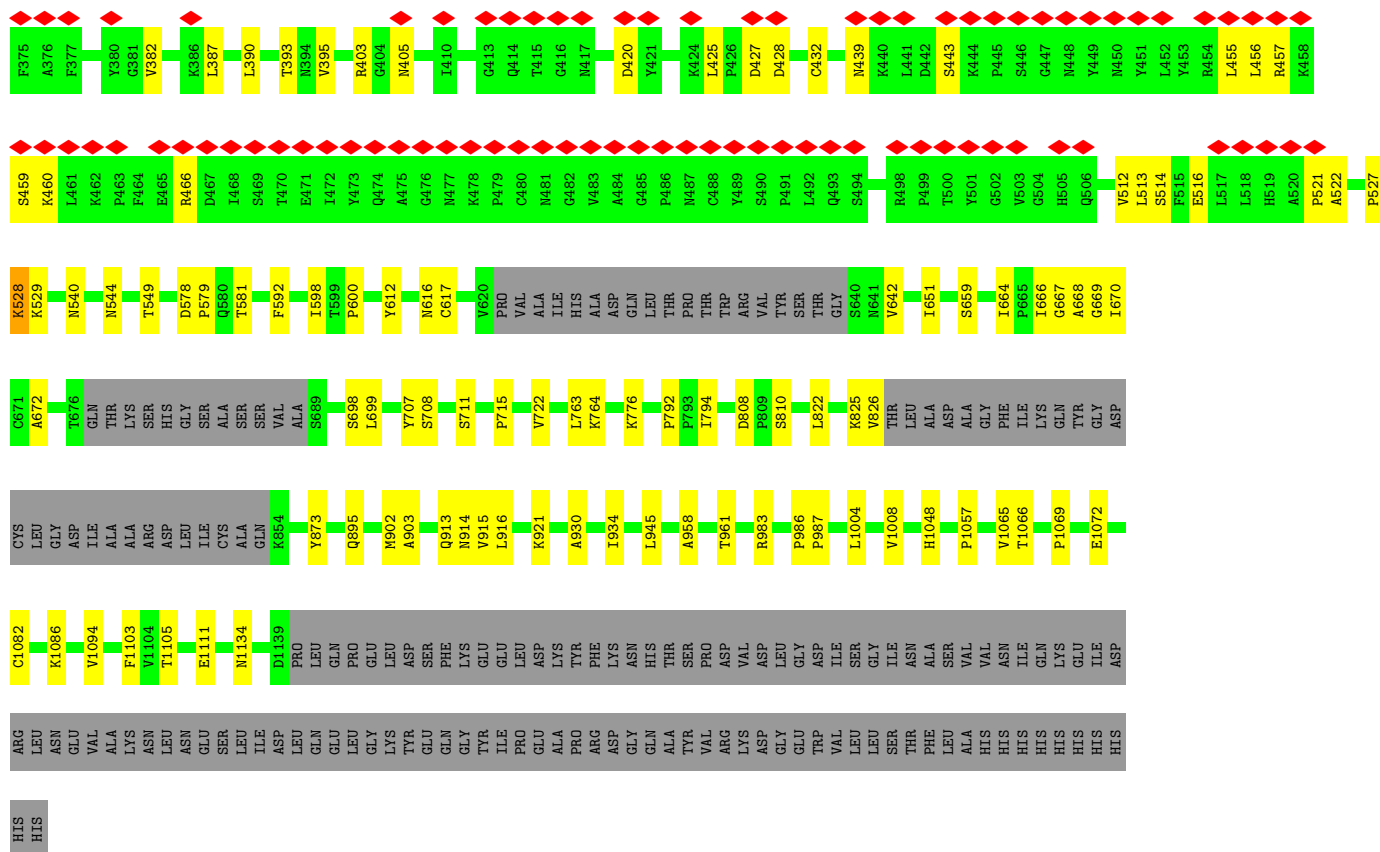
Chain B:



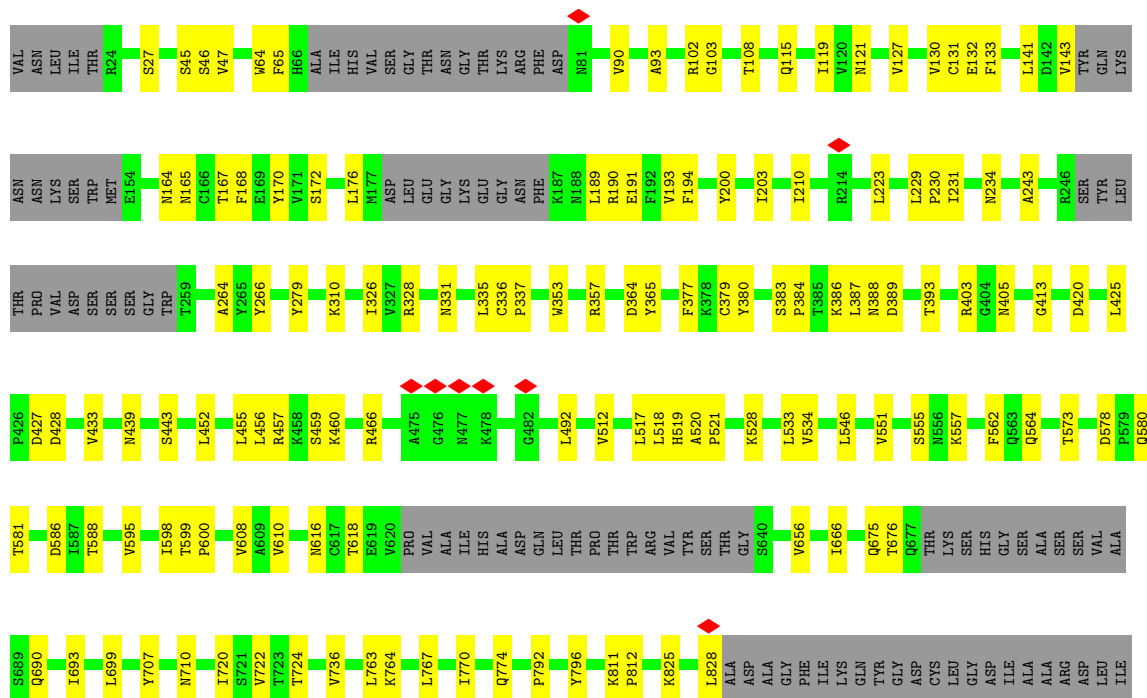
• Molecule 2: Spike glycoprotein

Chain C:





• Molecule 2: Spike glycoprotein



CYS	GLU	GLY
ALA	LEU	LYS
GLN	ASP	TYR
R854	SER	GLU
	PHE	GLN
Y873	LYS	GLY
	GLU	TYR
Q895	GLU	ILE
	LEU	PRO
A903	ASP	GLU
Y904	LYS	ALA
R905	TYR	PRO
F906	PHE	ARG
	LYS	ASP
I909	ASN	GLY
	HIS	GLN
Q913	THR	ALA
N914	SER	TYR
	PRO	VAL
I923	ASP	ARG
	VAL	LYS
A930	ASP	ASP
	LEU	GLY
I934	GLY	GLU
	ASP	TRP
Y952	ILE	VAL
	SER	LEU
P986	GLY	LEU
	ILE	SER
E990	ASN	THR
	ALA	PHE
V1008	SER	LEU
	VAL	ALA
L1049	VAL	HIS
	ASN	HIS
V1061	ILE	HIS
	GLN	HIS
H1064	LYS	HIS
V1065	GLU	HIS
	ILE	HIS
N1074	ASP	HIS
F1075	ARG	HIS
T1076	LEU	HIS
	ASN	
G1093	GLU	
	VAL	
V1096	ALA	
	LYS	
V1104	ASN	
T1105	LEU	
	ASN	
T1115	GLU	
	SER	
S1123	LEU	
	ILE	
D1139	ASP	
	LEU	
PRO	LEU	
GLN	GLN	
	GLU	
PRO	LEU	

GLY
LYS
TYR
GLU
GLN
GLY
TYR
ILE
PRO
GLU
ALA
PRO
ARG
ASP
GLY
GLN
ALA
TYR
VAL
ARG
LYS
ASP
GLY
GLU
TRP
VAL
LEU
LEU
SER
THR
PHE
LEU
ALA
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	403003	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	0.939	Depositor
Minimum map value	-0.279	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	452.48, 452.48, 452.48	wwPDB
Map dimensions	560, 560, 560	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.18	0/5010	0.38	2/6807 (0.0%)
2	B	0.20	0/8085	0.39	2/11003 (0.0%)
2	C	0.19	0/8110	0.39	4/11035 (0.0%)
2	D	0.24	0/8134	0.42	0/11068
All	All	0.21	0/29339	0.40	8/39913 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ILE	CA-C-N	-7.36	109.84	120.29
1	A	21	ILE	C-N-CA	-7.36	109.84	120.29
2	C	668	ALA	N-CA-C	-6.25	98.62	108.63
2	C	528	LYS	N-CA-C	-5.31	99.50	110.80
2	C	334	ASN	CA-C-N	-5.21	113.31	120.71
2	C	334	ASN	C-N-CA	-5.21	113.31	120.71
2	B	334	ASN	CA-C-N	5.20	131.16	122.73
2	B	334	ASN	C-N-CA	5.20	131.16	122.73

There are no chirality outliers.

There are no planarity outliers.

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	4872	0	4640	82	0
2	B	7900	0	7718	159	0
2	C	7924	0	7747	127	0
2	D	7948	0	7775	130	0
3	A	70	0	65	1	0
3	B	154	0	143	4	0
3	C	154	0	143	8	0
3	D	126	0	117	2	0
4	A	1	0	0	0	0
All	All	29149	0	28348	442	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (442) 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)
2:C:983:ARG:HD2	2:D:517:LEU:CD1	1.51	1.38
1:A:34[A]:HIS:CD2	2:B:493:GLN:HG2	1.68	1.27
2:C:983:ARG:CD	2:D:517:LEU:HD13	1.67	1.25
2:C:331:ASN:OD1	3:C:1301:NAG:C1	1.88	1.21
2:B:110:LEU:HD12	2:B:135:PHE:HD2	1.04	1.12
1:A:34[A]:HIS:HD2	2:B:493:GLN:CG	1.62	1.12
1:A:34[A]:HIS:CD2	2:B:493:GLN:CG	2.33	1.12
2:C:983:ARG:HD2	2:D:517:LEU:HD13	1.05	1.04
2:B:110:LEU:HD12	2:B:135:PHE:CD2	1.93	1.04
2:B:110:LEU:CD1	2:B:135:PHE:HD2	1.72	1.02
2:B:230:PRO:CB	2:C:521:PRO:HG2	1.89	1.01
2:B:176:LEU:HB2	2:B:190:ARG:NH2	1.78	0.97
1:A:34[A]:HIS:HD2	2:B:493:GLN:HG2	1.02	0.97
2:C:332:ILE:HG23	2:C:362:VAL:HG21	1.45	0.97
2:B:230:PRO:HB2	2:C:521:PRO:HG2	1.43	0.96
2:B:110:LEU:CD1	2:B:135:PHE:CD2	2.49	0.94
2:C:331:ASN:CG	3:C:1301:NAG:C1	2.40	0.94
2:D:364:ASP:HA	2:D:388:ASN:HD21	1.35	0.91
2:B:362:VAL:CG1	2:B:527:PRO:HG3	2.02	0.90
1:A:21:ILE:HG23	1:A:83:TYR:HD1	1.36	0.89
2:B:362:VAL:HG12	2:B:527:PRO:HG3	1.54	0.88
2:B:987:PRO:HG2	2:D:413:GLY:HA2	1.56	0.87
2:B:230:PRO:HB2	2:C:521:PRO:CG	2.03	0.87
2:C:131:CYS:SG	2:C:167:THR:N	2.50	0.84
2:B:110:LEU:HD11	2:B:135:PHE:HB2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:HIS:HE1	1:A:402:GLU:OE2	1.61	0.84
2:C:332:ILE:HG23	2:C:362:VAL:CG2	2.09	0.82
2:D:64:TRP:HE1	2:D:264:ALA:HB1	1.45	0.80
1:A:21:ILE:HG23	1:A:83:TYR:CD1	2.16	0.80
2:B:987:PRO:HG2	2:D:413:GLY:CA	2.12	0.79
2:C:331:ASN:ND2	3:C:1301:NAG:C1	2.46	0.79
2:C:666:ILE:HD11	2:C:672:ALA:HB2	1.65	0.77
2:B:101:ILE:HD11	2:B:240:THR:HB	1.69	0.75
2:B:332:ILE:O	2:B:335:LEU:HD12	1.87	0.75
2:B:230:PRO:HB2	2:C:521:PRO:CD	2.16	0.74
1:A:21:ILE:CG2	1:A:83:TYR:HD1	2.00	0.74
2:D:130:VAL:HG21	2:D:231:ILE:HG12	1.69	0.74
2:B:357:ARG:NH2	2:D:167:THR:O	2.21	0.73
1:A:34[A]:HIS:CD2	2:B:493:GLN:HG3	2.21	0.73
2:C:331:ASN:HD21	3:C:1301:NAG:C2	2.01	0.72
2:C:895:GLN:NE2	2:D:1074:ASN:OD1	2.21	0.72
2:D:393:THR:HG21	2:D:518:LEU:HD12	1.70	0.72
2:D:102:ARG:HG3	2:D:243:ALA:HB2	1.71	0.72
2:B:357:ARG:NH1	2:D:167:THR:O	2.23	0.72
2:D:1104:VAL:HG23	2:D:1115:ILE:HG12	1.72	0.71
2:C:983:ARG:HD3	2:D:517:LEU:HD13	1.72	0.71
2:B:382:VAL:HG13	2:B:390:LEU:HD12	1.73	0.70
2:D:455:LEU:HD12	2:D:456:LEU:HG	1.74	0.70
2:C:108:THR:HA	2:C:236:THR:HG22	1.74	0.70
2:C:236:THR:HG23	2:C:237:ARG:HG3	1.74	0.69
2:C:382:VAL:HG13	2:C:390:LEU:HD12	1.73	0.69
2:B:230:PRO:HB3	2:C:521:PRO:HG2	1.73	0.69
2:B:455:LEU:HD12	2:B:456:LEU:HG	1.74	0.69
2:C:331:ASN:HD21	3:C:1301:NAG:C1	2.06	0.69
2:C:455:LEU:HD12	2:C:456:LEU:HG	1.74	0.69
2:C:914:ASN:HD22	2:D:1123:SER:HB3	1.57	0.69
2:B:362:VAL:CG1	2:B:527:PRO:CG	2.71	0.68
1:A:34[B]:HIS:ND1	2:B:455:LEU:HD22	2.09	0.68
1:A:525:PHE:HE1	1:A:573:VAL:HG21	1.58	0.68
2:C:142:ASP:HB3	2:C:155:SER:HB2	1.76	0.68
2:D:141:LEU:HD13	2:D:143:VAL:HB	1.76	0.67
2:C:983:ARG:HD2	2:D:517:LEU:HD12	1.72	0.67
2:B:357:ARG:CZ	2:D:167:THR:O	2.43	0.66
1:A:375:GLU:HA	1:A:378:HIS:HD2	1.61	0.66
2:C:763:LEU:HG	2:C:1008:VAL:HG21	1.78	0.66
2:D:389:ASP:HA	2:D:528:LYS:CE	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:128:ILE:HD13	2:C:170:TYR:HD2	1.61	0.65
1:A:252:TYR:HB3	1:A:255:TYR:HD2	1.62	0.65
1:A:419:LYS:HE3	1:A:426:PRO:HA	1.79	0.65
2:B:93:ALA:HB3	2:B:266:TYR:HB2	1.79	0.65
2:B:95:THR:O	2:B:187:LYS:NZ	2.27	0.64
2:B:187:LYS:HB3	2:B:210:ILE:HG22	1.80	0.64
2:B:457:ARG:NH1	2:B:459:SER:O	2.29	0.64
2:C:126:VAL:HB	2:C:174:PRO:HA	1.79	0.63
2:C:983:ARG:HH11	2:D:517:LEU:HD12	1.63	0.63
2:C:331:ASN:O	2:C:332:ILE:HG13	1.97	0.63
2:C:457:ARG:NH1	2:C:459:SER:O	2.29	0.63
2:D:328:ARG:HH21	2:D:580:GLN:HB2	1.61	0.63
2:B:792:PRO:HG2	2:C:707:TYR:HB3	1.79	0.63
1:A:102:GLN:O	1:A:102:GLN:HG3	1.98	0.62
2:C:331:ASN:HD21	3:C:1301:NAG:C7	2.12	0.62
2:B:64:TRP:HE1	2:B:264:ALA:HB1	1.63	0.62
2:D:457:ARG:NH1	2:D:459:SER:O	2.29	0.62
2:D:675:GLN:O	2:D:690:GLN:HA	2.00	0.61
2:B:110:LEU:O	2:B:110:LEU:HG	2.00	0.61
2:C:1048:HIS:HA	2:C:1066:THR:HG22	1.82	0.61
2:D:676:THR:HA	2:D:690:GLN:HG2	1.83	0.60
2:B:362:VAL:HG11	2:B:527:PRO:HG3	1.83	0.60
2:B:176:LEU:HB2	2:B:190:ARG:CZ	2.32	0.60
1:A:431:ASP:HB3	3:A:703:NAG:O7	2.02	0.60
2:C:983:ARG:HD2	2:D:517:LEU:HD11	1.73	0.60
1:A:134:ASN:HB2	1:A:137:ASN:HB3	1.83	0.60
2:B:99:ASN:O	2:B:102:ARG:NH1	2.35	0.60
1:A:478:TRP:NE1	1:A:499:ASP:OD2	2.34	0.60
2:D:102:ARG:NE	2:D:121:ASN:O	2.35	0.60
2:C:527:PRO:O	2:C:528:LYS:C	2.43	0.59
2:B:332:ILE:O	2:B:335:LEU:CD1	2.50	0.59
2:B:105:ILE:HB	2:B:239:GLN:HB3	1.84	0.59
2:B:110:LEU:HD11	2:B:135:PHE:CD2	2.36	0.59
2:D:353:TRP:O	2:D:466:ARG:NH2	2.35	0.59
2:D:389:ASP:HA	2:D:528:LYS:HE3	1.84	0.59
2:D:121:ASN:ND2	2:D:176:LEU:H	2.00	0.59
2:B:353:TRP:O	2:B:466:ARG:NH2	2.35	0.58
2:C:983:ARG:NH1	2:D:517:LEU:HD12	2.17	0.58
1:A:557:MET:HG3	1:A:569:ALA:HB1	1.85	0.58
2:B:276:LEU:HB3	2:B:289:VAL:HG22	1.84	0.58
2:C:41:LYS:HG2	2:D:562:PHE:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:HH21	1:A:488:VAL:HG23	1.69	0.58
2:B:64:TRP:CD2	2:B:266:TYR:HE1	2.22	0.58
2:C:353:TRP:O	2:C:466:ARG:NH2	2.35	0.58
2:B:904:TYR:OH	2:C:1094:VAL:HG12	2.04	0.58
2:C:106:PHE:HB3	2:C:235:ILE:HD13	1.86	0.58
2:B:666:ILE:HD11	2:B:672:ALA:HB2	1.86	0.58
2:B:642:VAL:HG22	2:B:651:ILE:HG12	1.86	0.57
1:A:37:GLU:OE2	1:A:393:ARG:NH2	2.36	0.57
2:D:365:TYR:CE2	2:D:387:LEU:HB3	2.39	0.57
2:C:1105:THR:HG23	2:C:1111:GLU:H	1.69	0.57
2:C:24:ARG:HA	2:C:66:HIS:O	2.05	0.57
2:D:168:PHE:HE2	2:D:229:LEU:HD22	1.70	0.56
2:D:194:PHE:HD1	2:D:203:ILE:HG12	1.69	0.56
1:A:284:PRO:HG3	1:A:440:LEU:HD13	1.87	0.56
1:A:433:GLU:O	1:A:437:ASN:ND2	2.38	0.56
2:D:164:ASN:OD1	2:D:165:ASN:N	2.38	0.56
2:B:65:PHE:O	2:B:264:ALA:HA	2.06	0.56
2:B:139:PRO:HB3	2:B:159:VAL:HA	1.88	0.56
2:D:121:ASN:HD21	2:D:176:LEU:H	1.52	0.56
2:C:763:LEU:HD21	2:C:1004:LEU:HB3	1.87	0.56
2:D:616:ASN:O	2:D:618:THR:N	2.39	0.56
2:B:176:LEU:HB2	2:B:190:ARG:HH22	1.69	0.56
1:A:573:VAL:HG23	1:A:574:VAL:HG13	1.88	0.55
2:D:115:GLN:HA	2:D:132:GLU:HG2	1.87	0.54
2:D:828:LEU:HA	2:D:952:VAL:HG11	1.89	0.54
1:A:233:ILE:HG12	1:A:581:VAL:HG21	1.89	0.54
2:C:792:PRO:HG2	2:D:707:TYR:HB3	1.90	0.54
2:B:328:ARG:NH1	2:B:533:LEU:HB2	2.22	0.54
2:B:646:ARG:NH2	2:B:668:ALA:O	2.40	0.54
2:D:546:LEU:HD21	2:D:573:THR:HG21	1.90	0.54
1:A:381:TYR:HD1	1:A:558:LEU:HD22	1.73	0.54
1:A:476:LYS:HG3	1:A:480:MET:HE2	1.88	0.54
2:D:93:ALA:HB3	2:D:266:TYR:HB2	1.89	0.54
1:A:168:TRP:O	1:A:172:VAL:HG22	2.08	0.54
2:C:642:VAL:HG12	2:C:651:ILE:HG12	1.90	0.54
2:D:310:LYS:HG3	2:D:600:PRO:HA	1.89	0.54
2:B:110:LEU:HD11	2:B:135:PHE:CB	2.35	0.53
2:C:194:PHE:HD1	2:C:203:ILE:HG12	1.71	0.53
2:B:331:ASN:H	3:B:1308:NAG:H82	1.72	0.53
2:B:1048:HIS:HA	2:B:1066:THR:HG22	1.91	0.53
1:A:472:GLN:HB3	1:A:475:LYS:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:GLU:HB3	1:A:568:LEU:HD23	1.90	0.53
2:D:176:LEU:HD22	2:D:190:ARG:HD3	1.90	0.53
2:C:332:ILE:HG22	2:C:334:ASN:H	1.73	0.53
2:D:930:ALA:O	2:D:934:ILE:HG12	2.09	0.53
1:A:378:HIS:HD1	1:A:401:HIS:CD2	2.26	0.53
1:A:460:ARG:HH21	1:A:506:VAL:HG22	1.74	0.53
2:B:298:GLU:HB3	2:B:315:THR:HG21	1.91	0.53
2:B:1028:LYS:NZ	2:B:1042:PHE:O	2.42	0.53
2:B:99:ASN:ND2	2:B:190:ARG:HH22	2.07	0.52
2:C:420:ASP:HB2	2:C:460:LYS:HD2	1.91	0.52
2:D:103:GLY:HA3	2:D:119:ILE:O	2.07	0.52
2:B:854:LYS:NZ	2:C:592:PHE:O	2.42	0.52
2:C:173:GLN:HG2	2:C:174:PRO:HD2	1.90	0.52
2:C:225:PRO:HG2	2:D:562:PHE:CE1	2.44	0.52
2:B:109:THR:HG23	2:B:111:ASP:H	1.73	0.52
2:B:362:VAL:HG12	2:B:527:PRO:CG	2.32	0.52
2:B:280:ASN:ND2	2:B:284:THR:OG1	2.41	0.52
2:B:659:SER:HB3	2:B:698:SER:HB2	1.91	0.52
2:D:420:ASP:HB2	2:D:460:LYS:HD2	1.91	0.52
2:D:722:VAL:HG22	2:D:1065:VAL:HG22	1.92	0.52
2:B:656:VAL:HG23	2:B:695:TYR:HB3	1.92	0.52
2:D:403:ARG:HH12	2:D:405:ASN:HD21	1.58	0.52
2:B:420:ASP:HB2	2:B:460:LYS:HD2	1.91	0.52
2:C:794:ILE:HD12	3:D:1306:NAG:H61	1.92	0.52
2:B:211:ASN:OD1	2:B:212:LEU:N	2.42	0.51
2:D:189:LEU:HB2	2:D:210:ILE:HD13	1.91	0.51
2:B:763:LEU:HD22	2:B:1008:VAL:HG21	1.92	0.51
2:C:334:ASN:O	2:C:361:CYS:HB2	2.10	0.51
1:A:381:TYR:CD1	1:A:558:LEU:HD22	2.45	0.51
2:D:108:THR:OG1	2:D:234:ASN:O	2.29	0.51
2:B:403:ARG:HH12	2:B:405:ASN:HD21	1.58	0.51
2:D:193:VAL:HG23	2:D:223:LEU:HD22	1.92	0.51
2:D:383:SER:HB3	2:D:386:LYS:HG3	1.93	0.51
2:D:736:VAL:HG22	2:D:767:LEU:HD12	1.92	0.51
2:B:105:ILE:HG21	2:B:110:LEU:HD13	1.93	0.50
2:B:328:ARG:HH21	2:B:580:GLN:HB2	1.74	0.50
2:D:328:ARG:NH2	2:D:578:ASP:OD2	2.44	0.50
1:A:323:MET:HE1	1:A:379:ILE:HG21	1.93	0.50
2:B:676:THR:HA	2:B:690:GLN:HA	1.92	0.50
1:A:133:CYS:HA	1:A:141:CYS:HA	1.93	0.50
2:B:425:LEU:HD21	2:B:512:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:403:ARG:HH12	2:C:405:ASN:HD21	1.58	0.50
2:C:332:ILE:CG2	2:C:362:VAL:CG2	2.87	0.50
2:D:425:LEU:HD21	2:D:512:VAL:HG11	1.94	0.50
2:B:230:PRO:HB2	2:C:521:PRO:HD2	1.93	0.50
2:B:514:SER:OG	2:B:516:GLU:OE2	2.27	0.50
2:B:187:LYS:O	2:B:209:PRO:HA	2.12	0.50
2:C:330:PRO:HG3	2:C:579:PRO:HB3	1.93	0.50
2:C:310:LYS:HG3	2:C:600:PRO:HA	1.93	0.50
2:B:287:ASP:HB3	2:B:306:PHE:HE2	1.76	0.49
2:C:41:LYS:HD3	2:D:564:GLN:HE22	1.75	0.49
2:B:126:VAL:HB	2:B:174:PRO:HA	1.93	0.49
2:C:514:SER:OG	2:C:516:GLU:OE2	2.27	0.49
1:A:460:ARG:NH2	1:A:506:VAL:HG22	2.27	0.49
2:B:922:LEU:HD11	3:B:1309:NAG:H5	1.93	0.49
2:C:808:ASP:OD2	2:C:810:SER:OG	2.31	0.49
1:A:396:ALA:HB3	1:A:400:PHE:CD2	2.47	0.49
2:C:425:LEU:HD21	2:C:512:VAL:HG11	1.94	0.49
1:A:482:ARG:HD3	1:A:608:THR:O	2.12	0.49
2:B:215:ASP:OD1	2:B:216:LEU:N	2.44	0.49
2:D:377:PHE:CE2	2:D:384:PRO:HB3	2.48	0.49
2:C:273:ARG:NH1	2:C:290:ASP:OD2	2.46	0.49
2:D:599:THR:HB	2:D:608:VAL:HG12	1.94	0.49
2:B:39:PRO:HG2	2:B:51:THR:HG21	1.94	0.48
2:B:99:ASN:HD21	2:B:176:LEU:HD22	1.77	0.48
1:A:398:GLU:HB2	1:A:514:ARG:HE	1.78	0.48
3:B:1311:NAG:H2	2:D:796:TYR:CD2	2.48	0.48
2:D:986:PRO:O	2:D:990:GLU:HG2	2.13	0.48
2:C:540:ASN:OD1	2:C:549:THR:HG22	2.14	0.48
2:B:210:ILE:HG13	2:B:217:PRO:HB3	1.96	0.48
2:B:364:ASP:HB2	2:B:527:PRO:HG2	1.95	0.48
2:C:65:PHE:O	2:C:264:ALA:HA	2.14	0.48
2:B:111:ASP:OD1	2:B:134:GLN:NE2	2.28	0.48
2:C:578:ASP:HB3	2:C:581:THR:O	2.13	0.48
2:D:65:PHE:O	2:D:264:ALA:HA	2.14	0.48
2:B:699:LEU:HB3	2:D:873:TYR:HE1	1.79	0.48
2:D:127:VAL:HG21	3:D:1303:NAG:H61	1.96	0.48
2:B:318:PHE:O	2:B:592:PHE:HA	2.14	0.47
2:B:358:ILE:HB	2:B:395:VAL:HB	1.96	0.47
2:B:100:ILE:HG22	2:B:242:LEU:HB2	1.95	0.47
2:B:873:TYR:HE1	2:C:699:LEU:HB3	1.77	0.47
2:C:358:ILE:HB	2:C:395:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:ARG:NH1	2:B:290:ASP:OD2	2.47	0.47
2:B:363:ALA:O	2:B:527:PRO:HD3	2.14	0.47
2:C:137:ASN:OD1	2:C:138:ASP:N	2.47	0.47
2:C:331:ASN:ND2	3:C:1301:NAG:C7	2.77	0.47
1:A:203:TRP:HZ3	1:A:460:ARG:HD2	1.79	0.47
1:A:23:GLU:O	1:A:27:THR:HG23	2.14	0.47
2:B:656:VAL:HG21	2:B:693:ILE:HD12	1.96	0.47
2:B:647:ALA:HB2	2:B:667:GLY:HA3	1.96	0.47
2:C:334:ASN:O	2:C:362:VAL:N	2.45	0.47
2:C:794:ILE:HG13	2:C:794:ILE:O	2.15	0.47
2:D:130:VAL:HB	2:D:168:PHE:HB3	1.96	0.47
1:A:135:PRO:HD3	1:A:163:TRP:CZ2	2.50	0.47
1:A:177:ARG:NH2	1:A:470:LYS:O	2.46	0.47
1:A:525:PHE:CE1	1:A:573:VAL:HG21	2.44	0.47
2:B:1123:SER:HB3	2:D:914:ASN:HD22	1.78	0.47
2:D:328:ARG:NH1	2:D:533:LEU:HB2	2.30	0.47
2:B:362:VAL:HG13	2:B:527:PRO:N	2.29	0.47
2:C:983:ARG:CD	2:D:517:LEU:CD1	2.41	0.47
2:D:763:LEU:HD22	2:D:1008:VAL:HG21	1.96	0.47
2:B:173:GLN:HG3	2:B:174:PRO:HD2	1.96	0.47
2:D:1075:PHE:HB3	2:D:1096:VAL:HG13	1.97	0.46
1:A:34[A]:HIS:NE2	2:B:493:GLN:HG3	2.31	0.46
2:B:362:VAL:CG1	2:B:527:PRO:CD	2.92	0.46
2:C:708:SER:HB3	2:C:711:SER:HB2	1.98	0.46
2:C:722:VAL:HG22	2:C:1065:VAL:HG22	1.97	0.46
2:B:27:SER:HB2	2:B:64:TRP:HB3	1.96	0.46
2:B:1107:ARG:HD2	2:D:904:TYR:CE1	2.49	0.46
2:B:115:GLN:HA	2:B:132:GLU:HG2	1.97	0.46
2:B:736:VAL:HG11	2:B:1004:LEU:HD21	1.98	0.46
2:C:826:VAL:HB	2:C:1057:PRO:HG2	1.98	0.46
2:D:656:VAL:HG21	2:D:693:ILE:HD12	1.97	0.46
1:A:21:ILE:CG2	1:A:83:TYR:CD1	2.87	0.46
2:B:54:LEU:HD12	2:B:197:ILE:HD11	1.98	0.46
2:C:439:ASN:O	2:C:443:SER:HB2	2.15	0.46
1:A:86:GLN:O	1:A:89:GLN:NE2	2.49	0.46
2:C:667:GLY:O	2:C:669:GLY:N	2.49	0.46
2:B:439:ASN:O	2:B:443:SER:HB2	2.15	0.46
1:A:233:ILE:CG1	1:A:581:VAL:HG21	2.46	0.45
2:B:1106:GLN:HE21	2:B:1109:PHE:HB3	1.81	0.45
2:D:27:SER:OG	2:D:64:TRP:HB3	2.17	0.45
2:D:720:ILE:HG13	2:D:923:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:ALA:O	2:D:895:GLN:NE2	2.49	0.45
2:C:115:GLN:HG3	2:C:132:GLU:HG2	1.98	0.45
2:C:206:LYS:HB2	2:C:223:LEU:HA	1.98	0.45
2:D:439:ASN:O	2:D:443:SER:HB2	2.15	0.45
2:B:129:LYS:HE2	2:B:133:PHE:HE2	1.82	0.45
2:D:562:PHE:O	2:D:564:GLN:NE2	2.49	0.45
1:A:364:VAL:O	1:A:364:VAL:HG13	2.17	0.45
2:B:521:PRO:CG	2:D:200:TYR:CE1	2.99	0.45
2:C:225:PRO:HG2	2:D:562:PHE:CZ	2.52	0.45
2:C:822:LEU:HD22	2:C:945:LEU:HD21	1.98	0.45
2:C:903:ALA:HB1	2:C:913:GLN:HG2	1.99	0.45
2:D:903:ALA:HB1	2:D:913:GLN:HG2	1.99	0.45
2:D:906:PHE:HA	2:D:909:ILE:HG12	1.99	0.45
1:A:217:TYR:OH	1:A:225:ASP:OD2	2.21	0.45
1:A:304:ALA:HB3	1:A:334:THR:HG22	1.98	0.45
2:B:403:ARG:NH1	2:B:405:ASN:OD1	2.50	0.45
2:B:751:ASN:HA	2:B:754:LEU:HD12	1.98	0.45
2:C:825:LYS:HB2	2:C:825:LYS:HE2	1.71	0.45
2:C:930:ALA:O	2:C:934:ILE:HG12	2.16	0.45
2:D:1093:GLY:HA3	2:D:1105:THR:O	2.17	0.45
2:B:521:PRO:HG2	2:D:230:PRO:CB	2.47	0.45
2:C:616:ASN:OD1	2:C:617:CYS:N	2.49	0.45
1:A:455:MET:HG2	1:A:481:LYS:HG2	1.99	0.44
2:B:1093:GLY:HA3	2:B:1105:THR:O	2.17	0.44
2:D:377:PHE:HE2	2:D:384:PRO:HB3	1.82	0.44
2:D:403:ARG:NH1	2:D:405:ASN:OD1	2.50	0.44
2:B:521:PRO:HG3	2:D:200:TYR:CZ	2.52	0.44
1:A:55:THR:O	1:A:59:VAL:HG23	2.18	0.44
2:B:540:ASN:OD1	2:B:549:THR:HG22	2.17	0.44
2:D:46:SER:HA	2:D:279:TYR:O	2.17	0.44
2:D:598:ILE:HG12	2:D:666:ILE:HD12	1.99	0.44
1:A:123:MET:HG2	1:A:176:LEU:HD22	2.00	0.44
2:B:987:PRO:HG2	2:D:413:GLY:HA3	1.94	0.44
2:D:328:ARG:HH12	2:D:533:LEU:HB2	1.82	0.44
2:D:380:TYR:HE2	2:D:433:VAL:HG23	1.82	0.44
2:B:190:ARG:HB3	2:B:192:PHE:HE1	1.83	0.44
2:B:193:VAL:HG23	2:B:223:LEU:HD22	2.00	0.44
2:C:329:PHE:CD2	2:C:528:LYS:HB3	2.53	0.44
2:C:127:VAL:HG22	2:C:171:VAL:HG22	1.99	0.44
2:D:64:TRP:NE1	2:D:264:ALA:HB1	2.23	0.44
1:A:324:THR:HG22	1:A:326:GLY:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:902:MET:HB3	2:C:916:LEU:HD11	2.00	0.44
2:D:764:LYS:HB3	2:D:764:LYS:HE2	1.88	0.44
1:A:252:TYR:HB3	1:A:255:TYR:CD2	2.48	0.44
2:B:26:GLN:HG2	2:B:65:PHE:CE1	2.53	0.44
2:C:34:ARG:HA	2:C:34:ARG:HD2	1.80	0.44
2:C:403:ARG:NH1	2:C:405:ASN:OD1	2.50	0.43
2:B:213:GLU:HG2	2:B:215:ASP:H	1.82	0.43
2:C:30:ASN:HD21	2:C:59:PHE:HD1	1.66	0.43
2:C:666:ILE:HD12	2:C:670:ILE:HG22	2.01	0.43
2:B:328:ARG:NH2	2:B:580:GLN:HB2	2.33	0.43
2:B:699:LEU:HB3	2:D:873:TYR:CE1	2.53	0.43
2:D:770:ILE:O	2:D:774:GLN:HG2	2.18	0.43
2:D:905:ARG:HD3	2:D:1049:LEU:O	2.18	0.43
2:C:44:ARG:HB3	2:C:47:VAL:HG11	2.00	0.43
2:C:873:TYR:HE1	2:D:699:LEU:HB3	1.82	0.43
2:D:331:ASN:HB3	2:D:580:GLN:HE22	1.82	0.43
2:D:336:CYS:HA	2:D:337:PRO:HD3	1.91	0.43
2:B:203:ILE:HB	2:B:227:VAL:HG12	2.01	0.43
2:C:513:LEU:HD23	2:C:513:LEU:HA	1.91	0.43
2:C:986:PRO:N	2:C:987:PRO:HD2	2.33	0.43
1:A:570:LEU:O	1:A:574:VAL:HG22	2.19	0.43
2:C:28:TYR:HB3	2:C:61:ASN:HD21	1.82	0.43
1:A:144:LEU:HB2	1:A:168:TRP:CH2	2.54	0.43
1:A:554:LEU:O	1:A:558:LEU:HG	2.19	0.43
2:B:722:VAL:HA	2:B:1064:HIS:O	2.19	0.43
2:B:948:LEU:HD21	2:B:1059:GLY:HA3	2.01	0.43
1:A:297:MET:HE2	1:A:364:VAL:HG23	2.01	0.43
2:B:99:ASN:ND2	2:B:176:LEU:HD22	2.33	0.43
2:B:905:ARG:HD3	2:B:1049:LEU:O	2.19	0.43
2:D:131:CYS:HB2	2:D:133:PHE:CD2	2.54	0.43
2:D:379:CYS:HB2	2:D:384:PRO:HD3	2.01	0.43
2:C:764:LYS:HE3	2:C:764:LYS:HB3	1.81	0.42
2:D:326:ILE:HG21	2:D:534:VAL:HG22	2.01	0.42
2:C:612:TYR:HE1	2:C:651:ILE:HD12	1.84	0.42
1:A:315:PHE:HA	1:A:318:VAL:HG22	2.00	0.42
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.86	0.42
2:B:194:PHE:HD1	2:B:203:ILE:HG12	1.84	0.42
2:C:1086:LYS:HE3	2:C:1086:LYS:HB2	1.80	0.42
2:B:689:SER:OG	2:B:690:GLN:N	2.42	0.42
2:B:794:ILE:HG13	2:B:794:ILE:O	2.18	0.42
2:B:1086:LYS:HB3	2:B:1122:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:PHE:HB3	2:C:160:TYR:HB2	2.01	0.42
2:C:332:ILE:O	2:C:333:THR:C	2.63	0.42
2:D:519:HIS:O	2:D:520:ALA:C	2.62	0.42
1:A:184:VAL:HG23	1:A:464:PHE:CD1	2.55	0.42
1:A:524:GLN:HG2	1:A:583:PRO:HG2	2.01	0.42
1:A:91:LEU:O	1:A:95:LEU:HD13	2.20	0.42
2:C:659:SER:HB3	2:C:698:SER:HB2	2.02	0.42
1:A:24:GLN:NE2	2:B:476:GLY:HA2	2.34	0.42
1:A:382:ASP:HA	1:A:385:TYR:CE2	2.55	0.42
2:B:90:VAL:HG12	2:B:194:PHE:HB2	2.02	0.42
2:B:821:LEU:HD22	2:B:935:GLN:OE1	2.19	0.42
2:B:885:GLY:HA2	2:B:901:GLN:NE2	2.34	0.42
2:C:43:PHE:CE1	2:C:283:GLY:HA3	2.55	0.42
2:C:393:THR:HA	2:C:522:ALA:HA	2.01	0.42
2:C:921:LYS:HE3	2:C:921:LYS:HB3	1.89	0.42
1:A:84:PRO:HB2	1:A:86:GLN:HG2	2.02	0.42
2:B:393:THR:HA	2:B:522:ALA:HA	2.01	0.42
2:B:873:TYR:CE1	2:C:699:LEU:HB3	2.53	0.42
1:A:43:SER:HA	1:A:65:ALA:HB1	2.01	0.41
2:B:1139:ASP:N	2:B:1139:ASP:OD1	2.53	0.41
2:C:1103:PHE:HZ	3:C:1308:NAG:H62	1.84	0.41
2:B:30:ASN:HB3	2:B:32:PHE:CE1	2.55	0.41
2:C:914:ASN:OD1	2:C:915:VAL:N	2.54	0.41
2:B:513:LEU:HD23	2:B:513:LEU:HA	1.91	0.41
2:B:707:TYR:HB3	2:D:792:PRO:HG3	2.02	0.41
2:C:715:PRO:HG3	2:C:1069:PRO:HB3	2.02	0.41
2:C:776:LYS:HE2	2:C:776:LYS:HB3	1.80	0.41
2:D:710:ASN:O	2:D:1076:THR:HA	2.20	0.41
1:A:459:TRP:CG	1:A:477:TRP:HE3	2.37	0.41
2:B:105:ILE:HG13	2:B:241:LEU:HD21	2.02	0.41
2:B:190:ARG:HB3	2:B:192:PHE:CE1	2.55	0.41
1:A:102:GLN:O	1:A:102:GLN:CG	2.68	0.41
1:A:108:LEU:HD21	1:A:190:MET:HA	2.02	0.41
2:B:934:ILE:HD13	2:B:934:ILE:HA	1.95	0.41
2:C:1082:CYS:HB3	2:C:1134:ASN:OD1	2.20	0.41
2:D:387:LEU:O	2:D:388:ASN:HB2	2.20	0.41
2:B:362:VAL:HG11	2:B:527:PRO:CG	2.46	0.41
2:B:427:ASP:OD1	2:B:428:ASP:N	2.53	0.41
2:D:191:GLU:HG3	2:D:223:LEU:HD11	2.02	0.41
2:D:393:THR:HG22	2:D:521:PRO:O	2.20	0.41
2:D:452:LEU:HD13	2:D:492:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:722:VAL:HA	2:D:1064:HIS:O	2.20	0.41
2:B:598:ILE:HB	2:B:609:ALA:HB3	2.02	0.41
2:C:353:TRP:CD1	2:C:353:TRP:H	2.39	0.41
2:C:527:PRO:O	2:C:529:LYS:N	2.54	0.41
1:A:42:GLN:HE21	2:B:498:ARG:NH2	2.19	0.41
1:A:223:ILE:HG23	1:A:458:LYS:NZ	2.35	0.41
1:A:469:PRO:HB2	1:A:471:ASP:OD1	2.21	0.41
1:A:488:VAL:HG21	1:A:611:SER:HA	2.02	0.41
2:B:331:ASN:HB2	3:B:1308:NAG:N2	2.36	0.41
2:B:336:CYS:HA	2:B:337:PRO:HD3	1.90	0.41
2:B:966:LEU:HD23	2:B:966:LEU:HA	1.94	0.41
2:C:110:LEU:O	2:C:135:PHE:HB3	2.20	0.41
2:C:427:ASP:OD1	2:C:428:ASP:N	2.53	0.41
2:C:598:ILE:HG23	2:C:664:ILE:HG21	2.02	0.41
2:D:427:ASP:OD1	2:D:428:ASP:N	2.53	0.41
2:D:551:VAL:HG12	2:D:588:THR:O	2.21	0.41
2:D:724:THR:HG23	2:D:1061:VAL:HG13	2.03	0.41
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.88	0.41
1:A:302:TRP:HA	1:A:306:ARG:HD3	2.02	0.41
2:B:332:ILE:O	2:B:332:ILE:HG22	2.21	0.41
2:D:90:VAL:HG12	2:D:194:PHE:HB2	2.02	0.41
2:D:811:LYS:HD2	2:D:812:PRO:HD2	2.02	0.41
1:A:312:GLU:HB2	1:A:376:MET:HE1	2.04	0.40
2:B:328:ARG:HH11	2:B:533:LEU:HB2	1.86	0.40
2:B:387:LEU:HD21	2:B:432:CYS:SG	2.61	0.40
2:B:1125:ASN:OD1	2:B:1126:CYS:N	2.47	0.40
2:C:715:PRO:HA	2:C:1072:GLU:HA	2.03	0.40
2:D:578:ASP:HB3	2:D:581:THR:O	2.21	0.40
2:D:595:VAL:HG13	2:D:610:VAL:HG13	2.03	0.40
1:A:177:ARG:HB2	1:A:498:CYS:HB2	2.02	0.40
2:B:452:LEU:HD13	2:B:492:LEU:HD13	2.03	0.40
2:C:387:LEU:HD21	2:C:432:CYS:SG	2.62	0.40
2:D:170:TYR:CE2	2:D:172:SER:HB2	2.56	0.40
2:B:916:LEU:HD12	2:B:923:ILE:HD12	2.02	0.40
2:C:43:PHE:CE2	2:D:557:LYS:HE2	2.57	0.40
2:C:43:PHE:HE2	2:D:557:LYS:HE2	1.87	0.40
2:C:544:ASN:HB2	2:C:579:PRO:HG3	2.03	0.40
2:C:958:ALA:O	2:C:961:THR:OG1	2.38	0.40
2:D:310:LYS:HB3	2:D:310:LYS:HE2	1.77	0.40
2:D:383:SER:O	2:D:384:PRO:C	2.65	0.40
2:B:521:PRO:HG2	2:D:200:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:PRO:HG3	2:D:357:ARG:NH1	2.37	0.40
2:D:555:SER:HB3	2:D:586:ASP:HB2	2.03	0.40
2:D:825:LYS:HB3	2:D:825:LYS:HE3	1.91	0.40
1:A:379:ILE:HG22	1:A:383:MET:HE3	2.04	0.40
1:A:446:ILE:O	1:A:449:THR:HG22	2.21	0.40
2:B:26:GLN:HG2	2:B:65:PHE:HE1	1.85	0.40
2:D:45:SER:O	2:D:47:VAL:HG23	2.22	0.40

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	595/603 (99%)	579 (97%)	16 (3%)	0	100	100
2	B	995/1227 (81%)	961 (97%)	34 (3%)	0	100	100
2	C	997/1227 (81%)	964 (97%)	31 (3%)	2 (0%)	43	70
2	D	1000/1227 (82%)	965 (96%)	35 (4%)	0	100	100
All	All	3587/4284 (84%)	3469 (97%)	116 (3%)	2 (0%)	49	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	331	ASN
2	C	334	ASN

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	527/533 (99%)	527 (100%)	0	100	100
2	B	885/1070 (83%)	885 (100%)	0	100	100
2	C	887/1070 (83%)	887 (100%)	0	100	100
2	D	890/1070 (83%)	889 (100%)	1 (0%)	88	97
All	All	3189/3743 (85%)	3188 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	335	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	51	ASN
1	A	60	GLN
1	A	102	GLN
1	A	149	ASN
1	A	345	HIS
1	A	472	GLN
1	A	552	GLN
2	B	26	GLN
2	B	99	ASN
2	B	690	GLN
2	B	901	GLN
2	B	928	ASN
2	B	949	GLN
2	B	1002	GLN
2	B	1054	GLN
2	B	1058	HIS
2	C	125	ASN
2	C	245	HIS
2	C	321	GLN
2	C	354	ASN
2	C	675	GLN
2	C	804	GLN
2	C	872	GLN

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Mol	Chain	Res	Type
2	C	949	GLN
2	C	1010	GLN
2	D	134	GLN
2	D	188	ASN
2	D	354	ASN
2	D	388	ASN
2	D	394	ASN
2	D	519	HIS
2	D	564	GLN
2	D	580	GLN
2	D	675	GLN
2	D	804	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	1307	2	14,14,15	0.26	0	17,19,21	0.35	0
3	NAG	D	1307	2	14,14,15	0.20	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	1308	2	14,14,15	0.19	0	17,19,21	0.45	0
3	NAG	D	1309	2	14,14,15	0.37	0	17,19,21	0.97	1 (5%)
3	NAG	C	1303	2	14,14,15	0.21	0	17,19,21	0.49	0
3	NAG	C	1306	2	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	A	704	1	14,14,15	0.40	0	17,19,21	0.55	0
3	NAG	C	1305	2	14,14,15	0.28	0	17,19,21	0.37	0
3	NAG	C	1308	2	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	B	1306	2	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	D	1302	2	14,14,15	0.38	0	17,19,21	0.64	0
3	NAG	B	1308	2	14,14,15	0.39	0	17,19,21	0.51	0
3	NAG	B	1309	2	14,14,15	0.40	0	17,19,21	0.49	0
3	NAG	B	1310	2	14,14,15	0.38	0	17,19,21	1.00	1 (5%)
3	NAG	D	1306	2	14,14,15	0.23	0	17,19,21	0.36	0
3	NAG	C	1301	-	14,14,15	0.26	0	17,19,21	0.50	0
3	NAG	C	1310	2	14,14,15	0.37	0	17,19,21	0.68	0
3	NAG	A	705	1	14,14,15	0.41	0	17,19,21	0.98	1 (5%)
3	NAG	D	1303	2	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	A	701	1	14,14,15	0.35	0	17,19,21	0.58	0
3	NAG	A	702	1	14,14,15	0.40	0	17,19,21	0.43	0
3	NAG	A	703	1	14,14,15	0.44	0	17,19,21	1.24	2 (11%)
3	NAG	D	1305	2	14,14,15	0.39	0	17,19,21	0.78	0
3	NAG	C	1309	2	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	C	1307	2	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	B	1304	2	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	B	1301	2	14,14,15	0.35	0	17,19,21	0.54	0
3	NAG	B	1303	2	14,14,15	0.41	0	17,19,21	0.99	2 (11%)
3	NAG	C	1304	2	14,14,15	0.23	0	17,19,21	0.36	0
3	NAG	B	1302	2	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	D	1304	2	14,14,15	0.32	0	17,19,21	0.33	0
3	NAG	C	1311	2	14,14,15	0.39	0	17,19,21	0.47	0
3	NAG	B	1311	2	14,14,15	0.37	0	17,19,21	0.92	1 (5%)
3	NAG	D	1301	2	14,14,15	0.19	0	17,19,21	0.48	0
3	NAG	B	1305	2	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	C	1302	2	14,14,15	0.20	0	17,19,21	0.49	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	B	1307	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1307	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1308	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1309	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	A	704	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1305	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1302	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1309	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1310	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	2	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1	-	1/6/23/26	0/1/1/1
3	NAG	D	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1
3	NAG	A	702	1	-	2/6/23/26	0/1/1/1
3	NAG	A	703	1	-	2/6/23/26	0/1/1/1
3	NAG	D	1305	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1309	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	2	-	4/6/23/26	0/1/1/1
3	NAG	B	1303	2	-	3/6/23/26	0/1/1/1
3	NAG	C	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1304	2	-	1/6/23/26	0/1/1/1
3	NAG	C	1311	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1301	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	C	1302	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1310	NAG	C2-N2-C7	3.51	127.61	122.90
3	D	1309	NAG	C2-N2-C7	3.39	127.44	122.90
3	A	705	NAG	C2-N2-C7	3.15	127.13	122.90
3	A	703	NAG	O5-C1-C2	-3.02	106.61	111.29
3	B	1303	NAG	C1-O5-C5	2.63	115.71	112.19
3	A	703	NAG	C1-C2-N2	2.39	114.20	110.43
3	B	1303	NAG	O5-C1-C2	2.33	114.89	111.29
3	B	1311	NAG	C1-C2-N2	2.30	114.06	110.43

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	NAG	C8-C7-N2-C2
3	A	703	NAG	O7-C7-N2-C2
3	B	1303	NAG	C8-C7-N2-C2
3	B	1303	NAG	O7-C7-N2-C2
3	B	1310	NAG	C3-C2-N2-C7
3	B	1310	NAG	C8-C7-N2-C2
3	B	1310	NAG	O7-C7-N2-C2
3	B	1311	NAG	C1-C2-N2-C7
3	B	1311	NAG	C8-C7-N2-C2
3	B	1311	NAG	O7-C7-N2-C2
3	D	1308	NAG	C4-C5-C6-O6
3	D	1308	NAG	O5-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	D	1306	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	B	1304	NAG	C8-C7-N2-C2
3	B	1304	NAG	O7-C7-N2-C2
3	D	1302	NAG	C8-C7-N2-C2
3	D	1302	NAG	O7-C7-N2-C2
3	D	1306	NAG	C4-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	1306	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	A	702	NAG	C8-C7-N2-C2
3	B	1305	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	D	1303	NAG	O5-C5-C6-O6
3	D	1309	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6
3	A	704	NAG	O5-C5-C6-O6
3	D	1304	NAG	O5-C5-C6-O6
3	A	702	NAG	O7-C7-N2-C2
3	B	1301	NAG	C1-C2-N2-C7
3	C	1305	NAG	C4-C5-C6-O6
3	A	701	NAG	C3-C2-N2-C7
3	A	705	NAG	C3-C2-N2-C7
3	D	1309	NAG	C3-C2-N2-C7
3	C	1311	NAG	C8-C7-N2-C2
3	D	1301	NAG	C4-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	701	NAG	C1-C2-N2-C7
3	B	1301	NAG	C3-C2-N2-C7
3	B	1303	NAG	C3-C2-N2-C7
3	C	1311	NAG	O7-C7-N2-C2
3	B	1306	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6

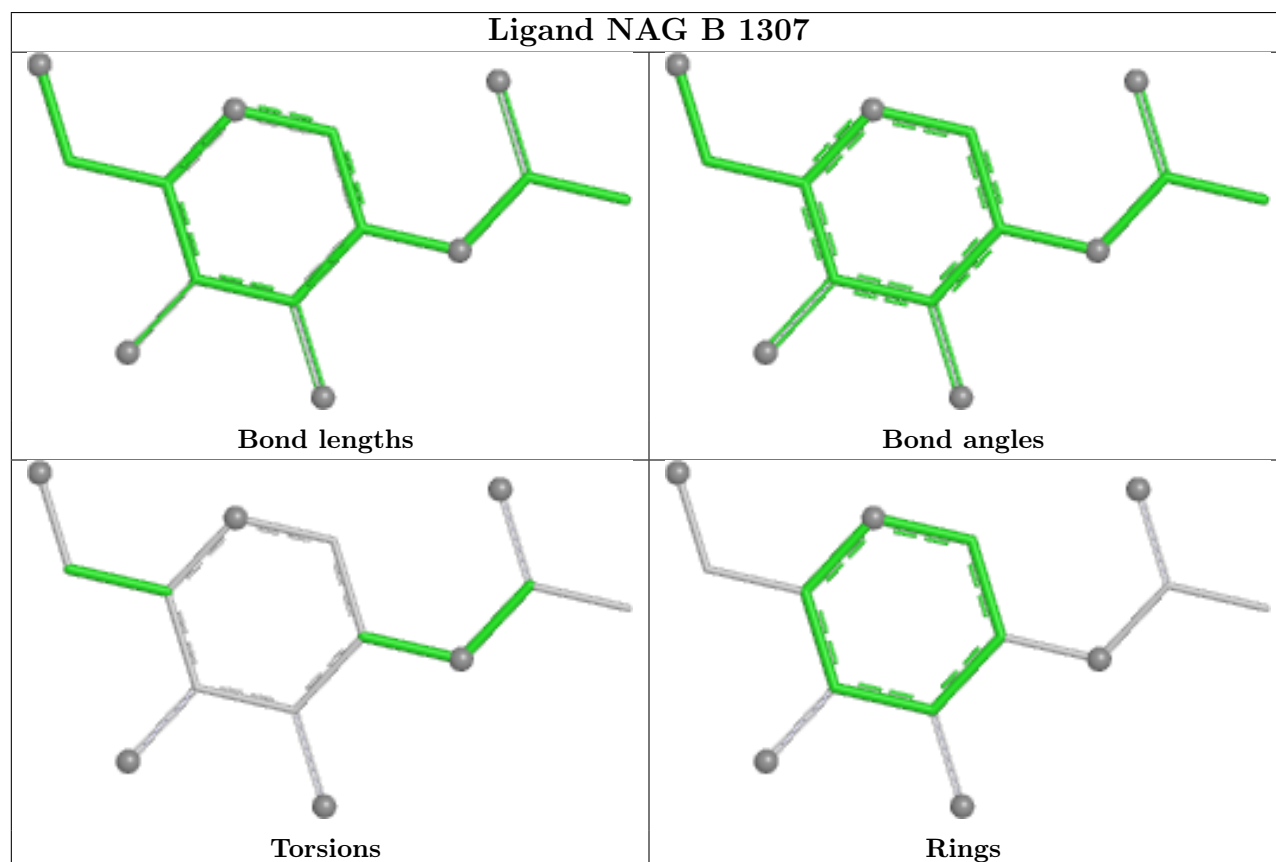
There are no ring outliers.

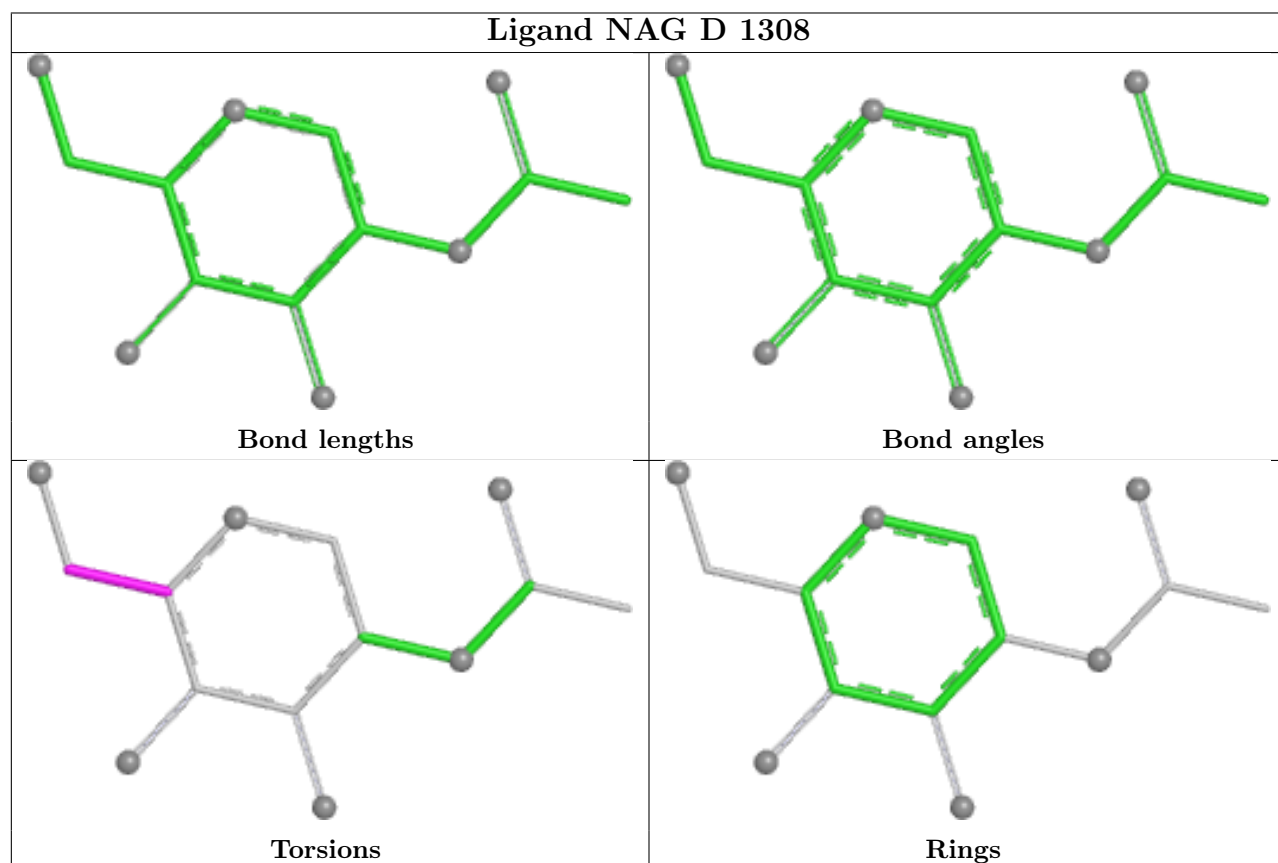
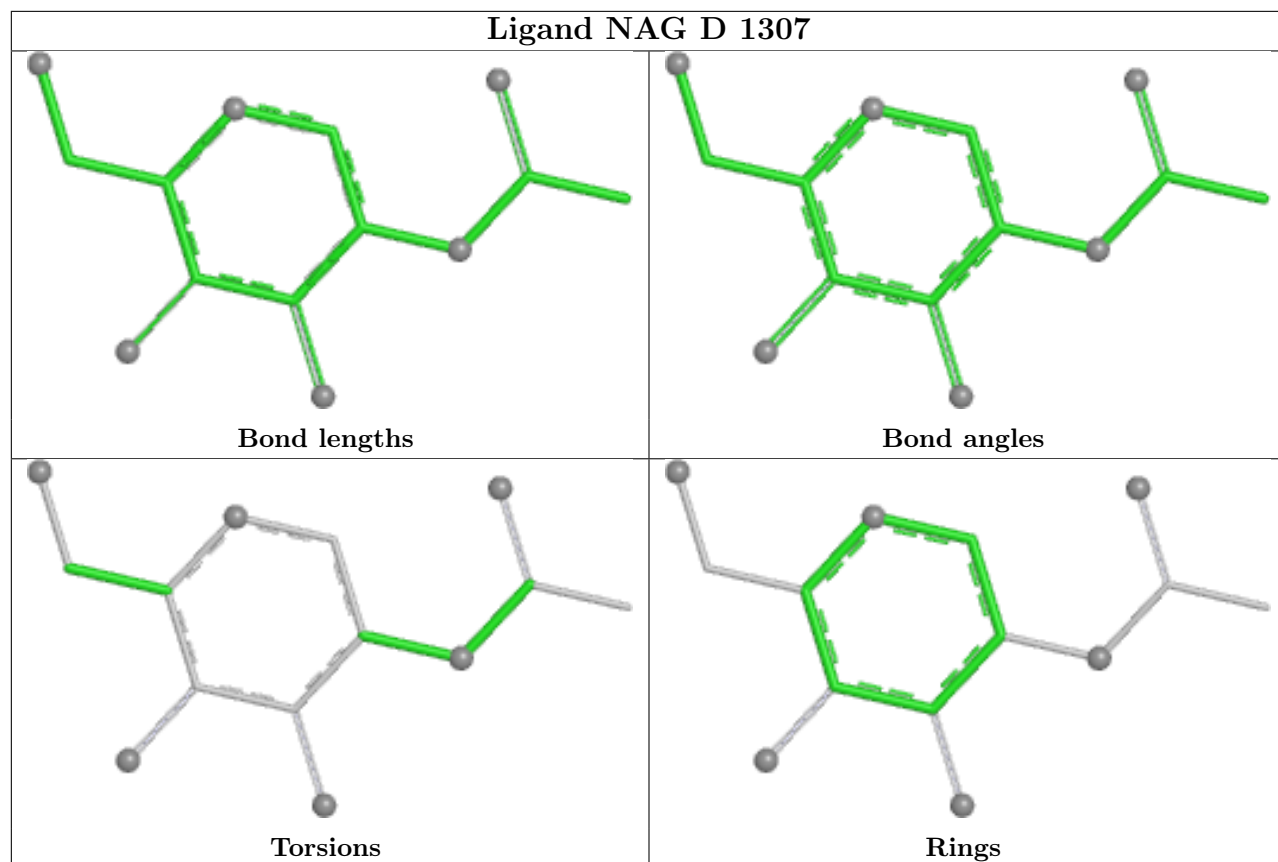
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1308	NAG	1	0
3	B	1308	NAG	2	0
3	B	1309	NAG	1	0
3	D	1306	NAG	1	0
3	C	1301	NAG	7	0
3	D	1303	NAG	1	0
3	A	703	NAG	1	0
3	B	1311	NAG	1	0

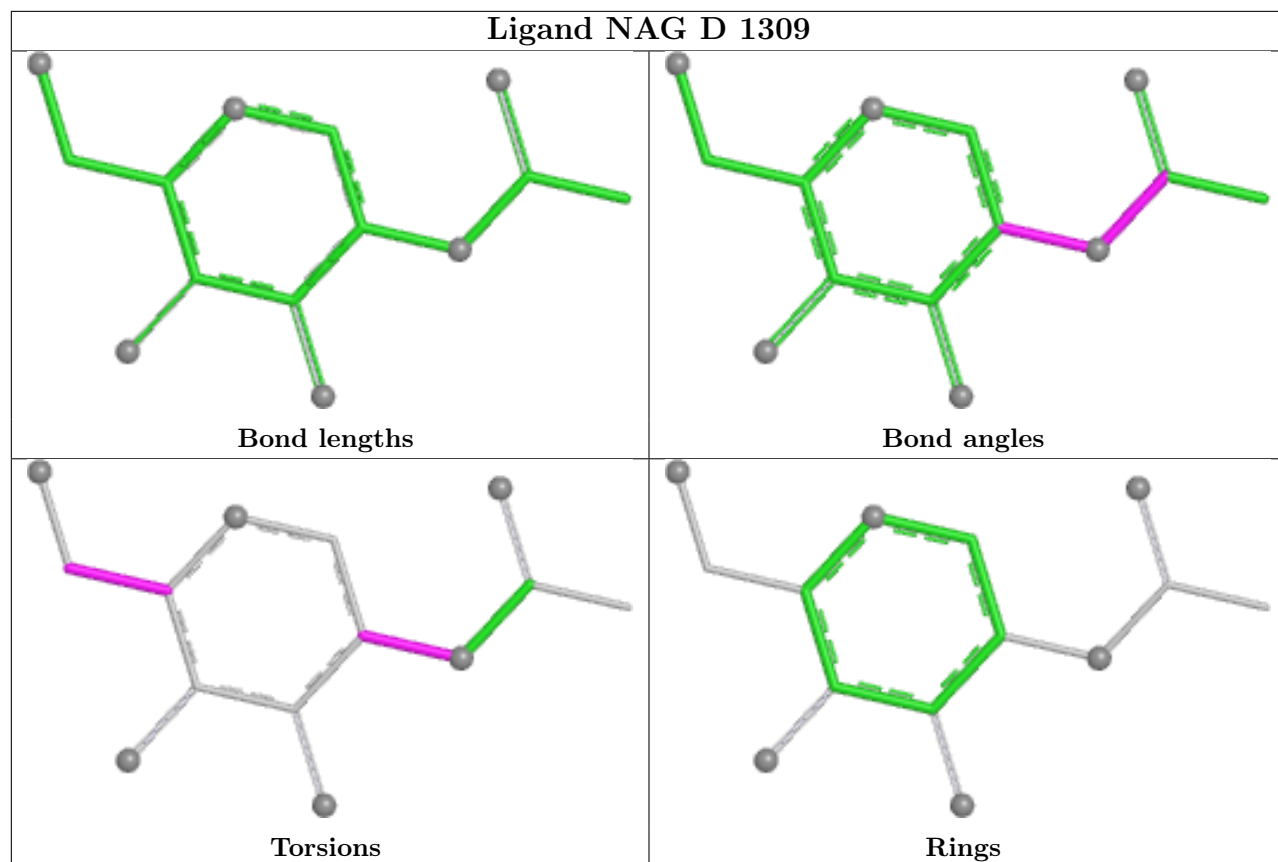
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

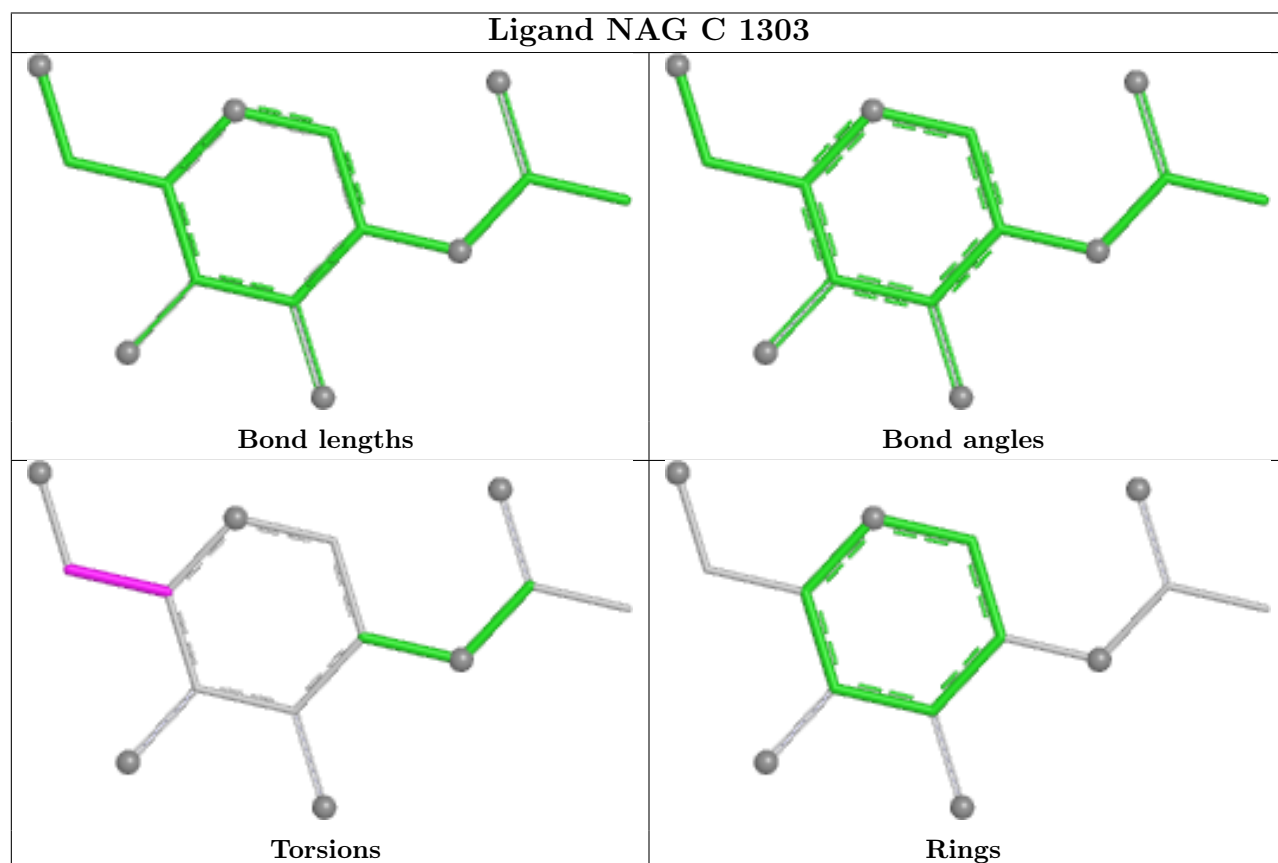




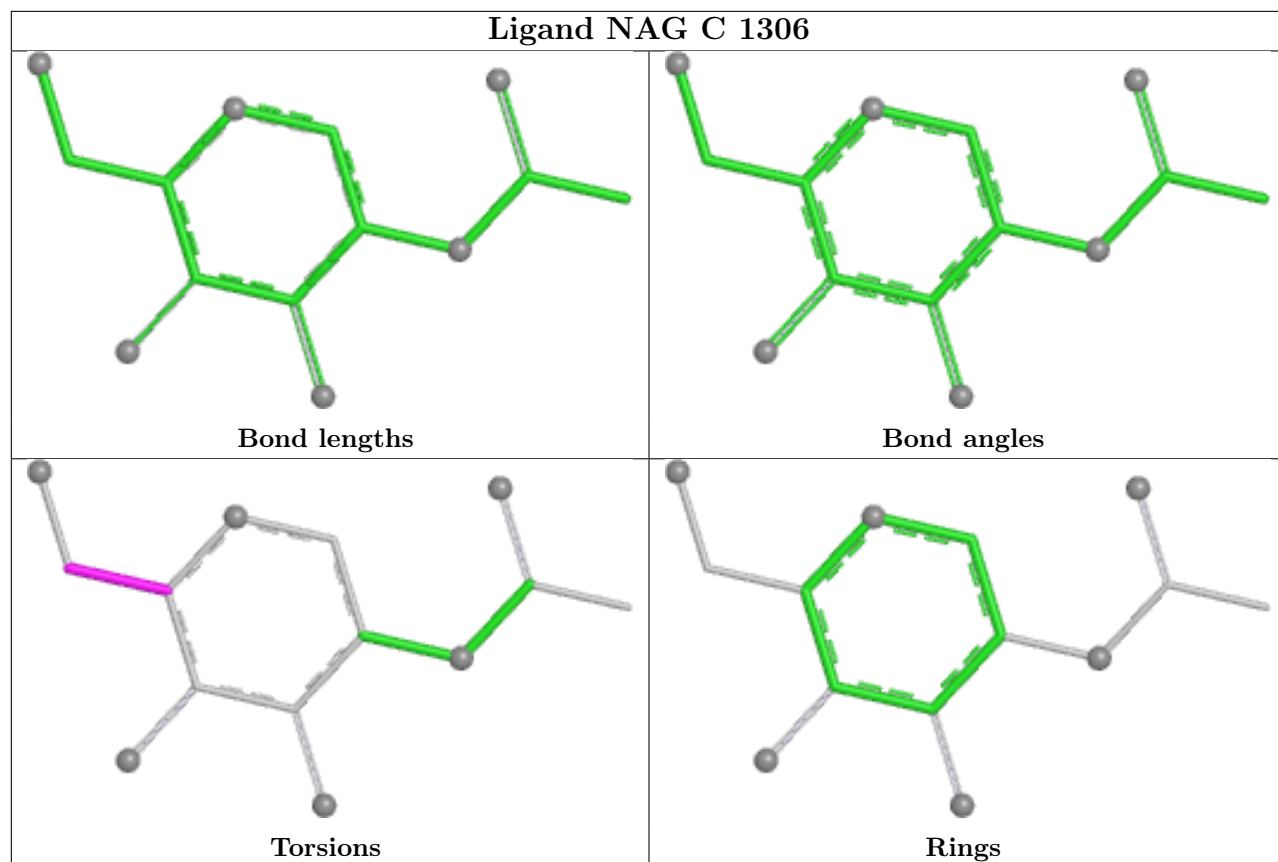
Ligand NAG D 1309



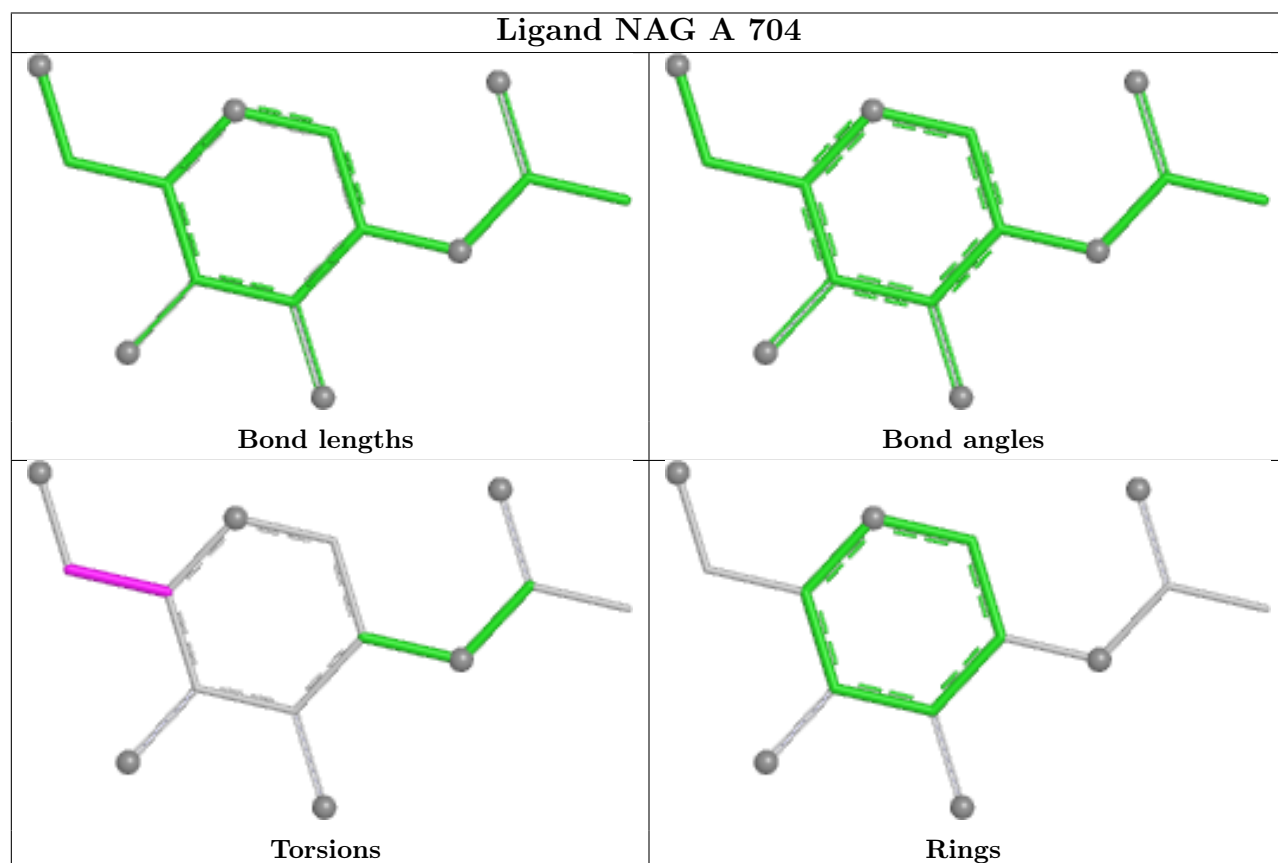
Ligand NAG C 1303



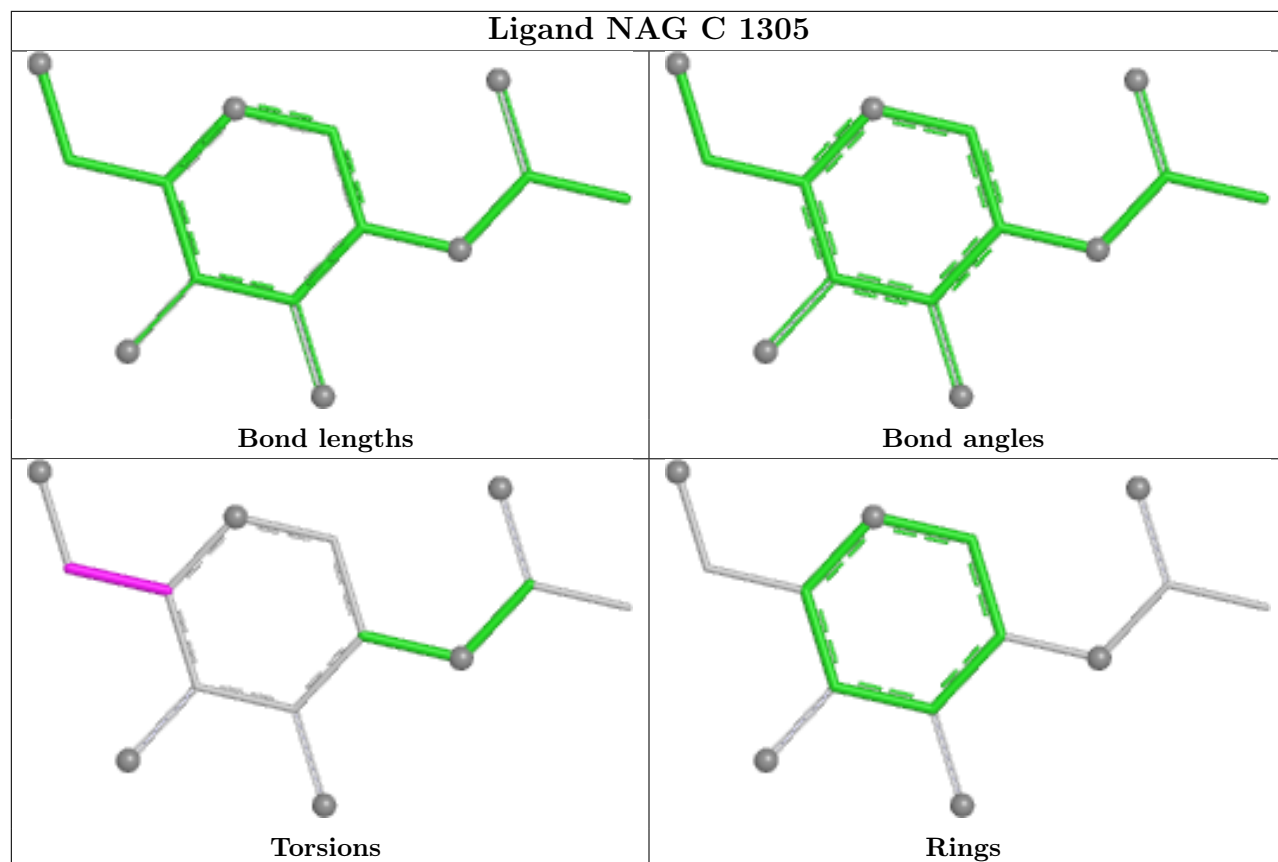
Ligand NAG C 1306



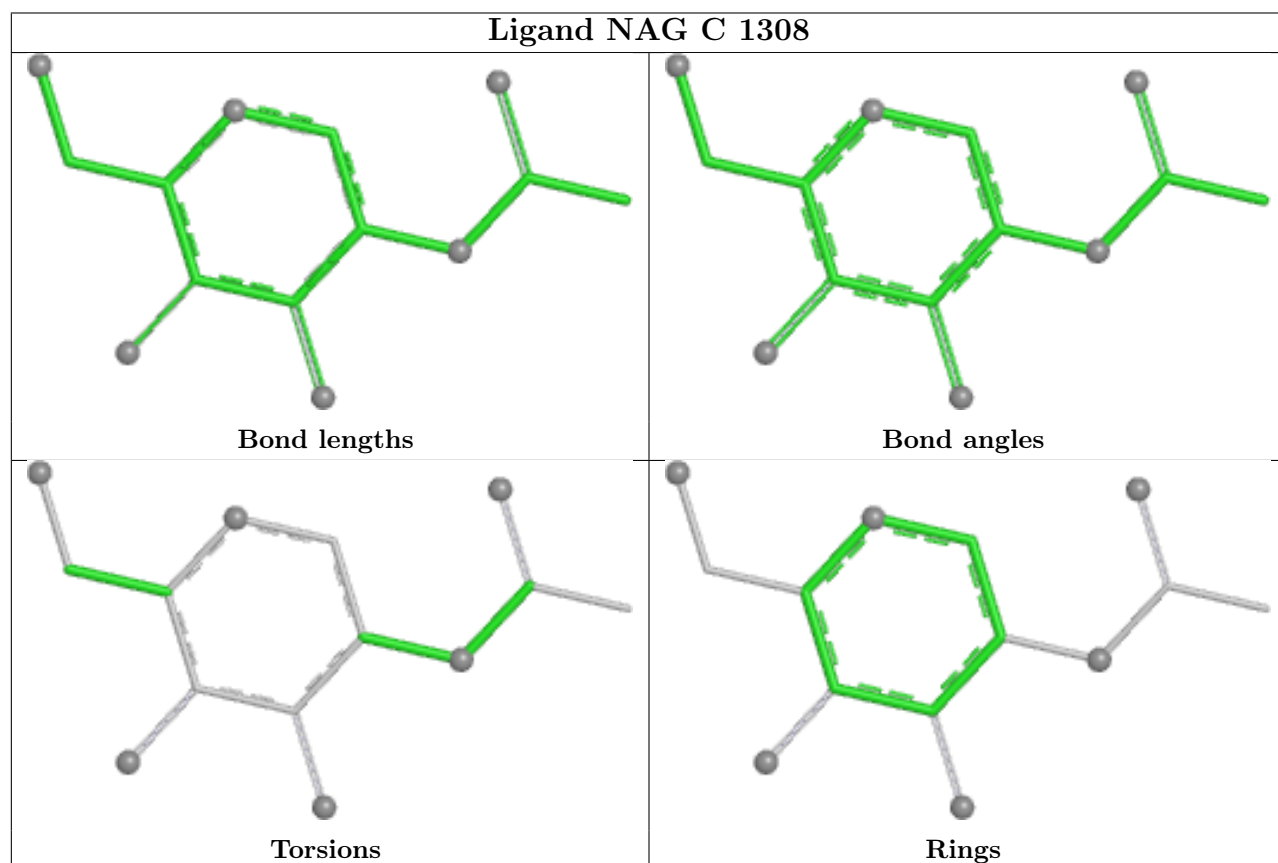
Ligand NAG A 704



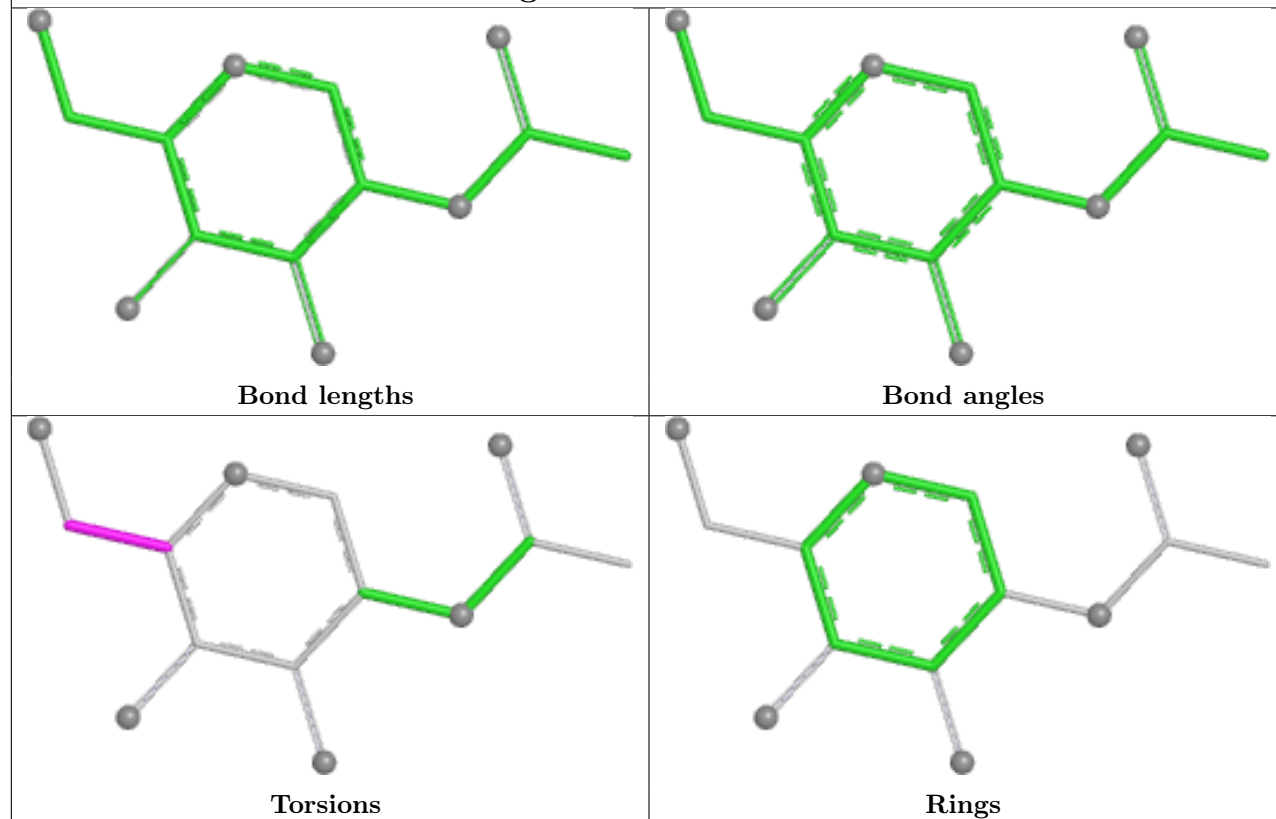
Ligand NAG C 1305



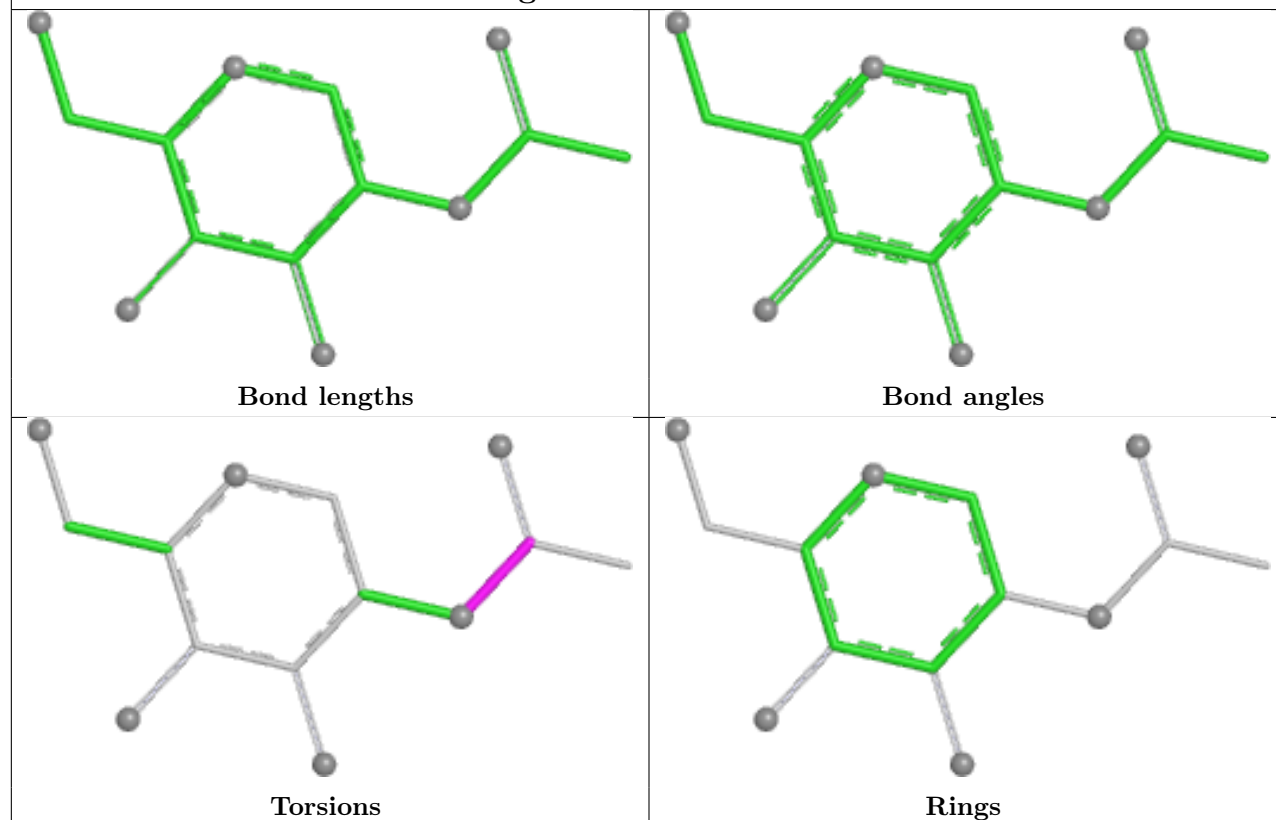
Ligand NAG C 1308

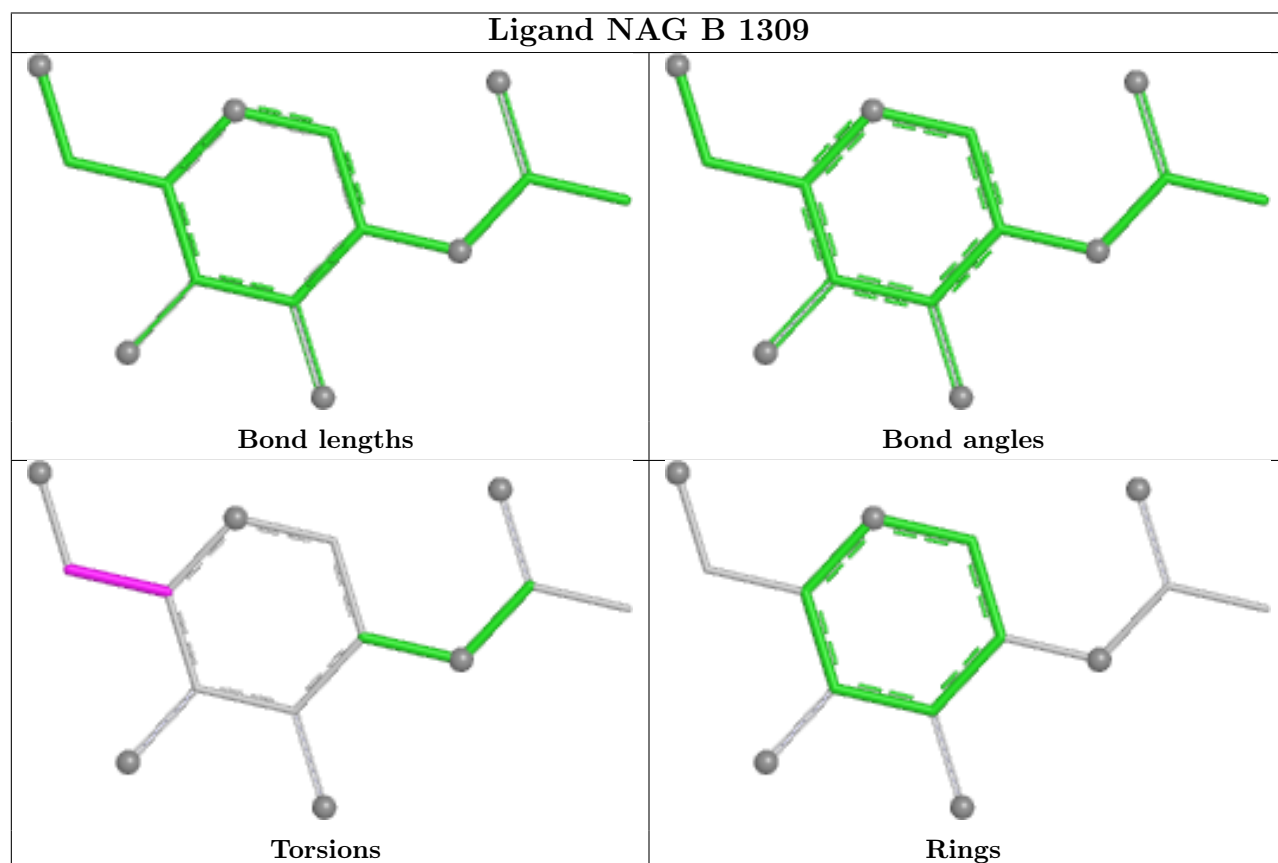
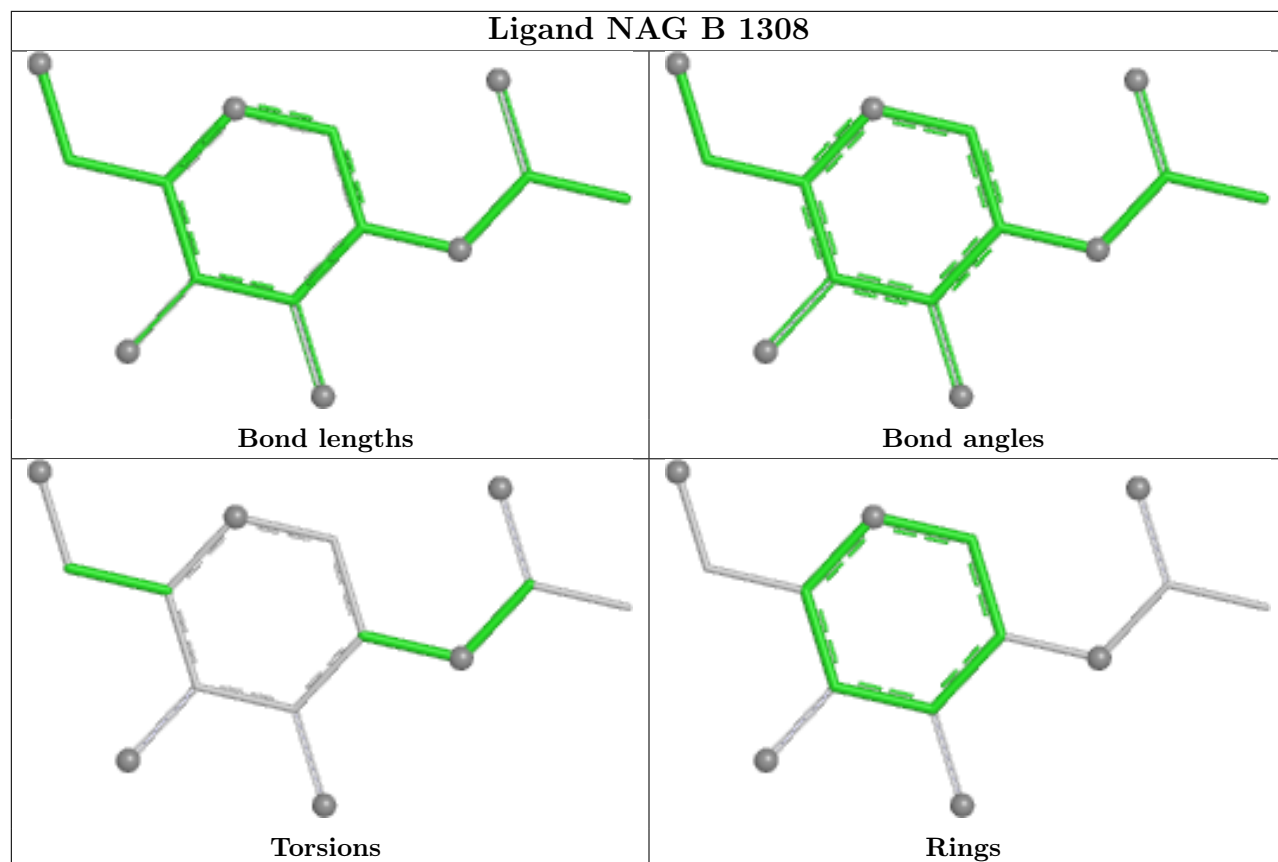


Ligand NAG B 1306

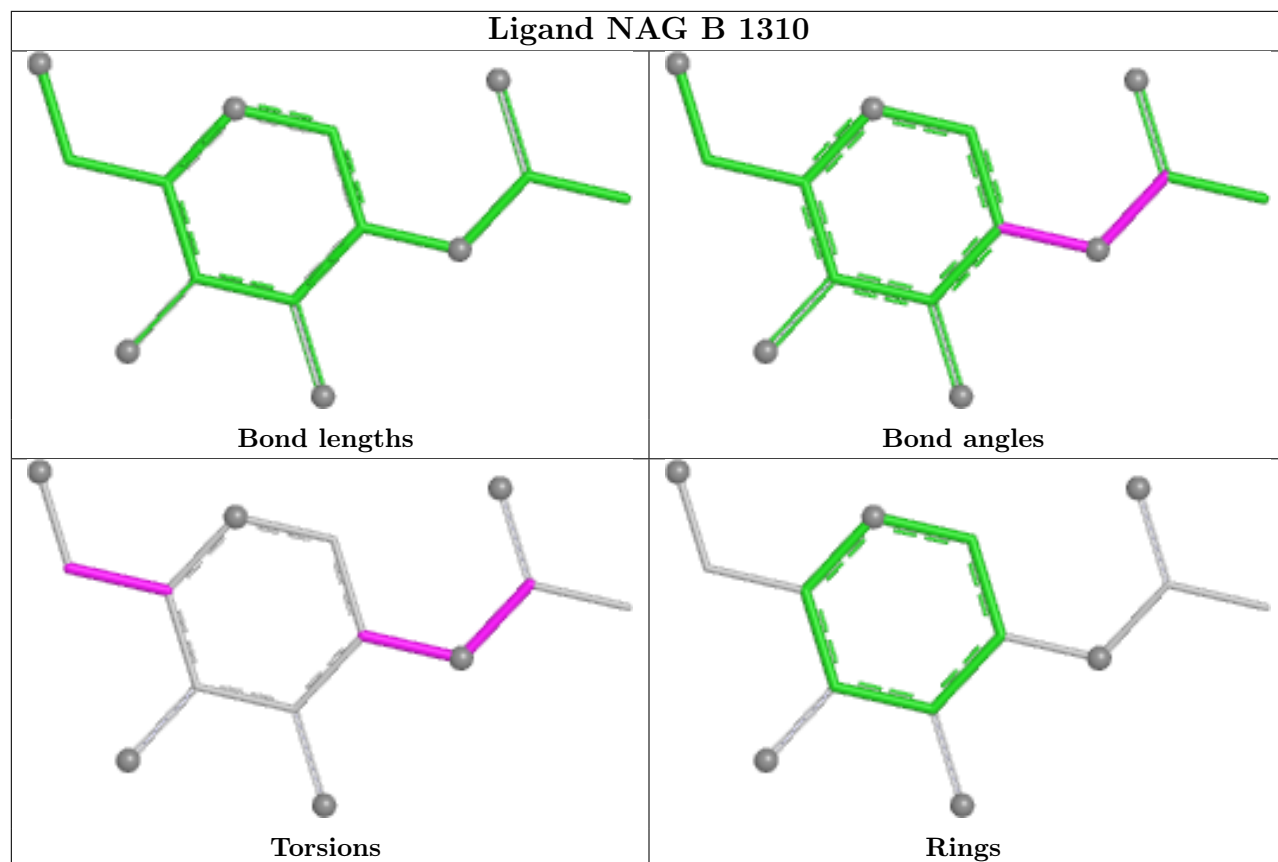


Ligand NAG D 1302

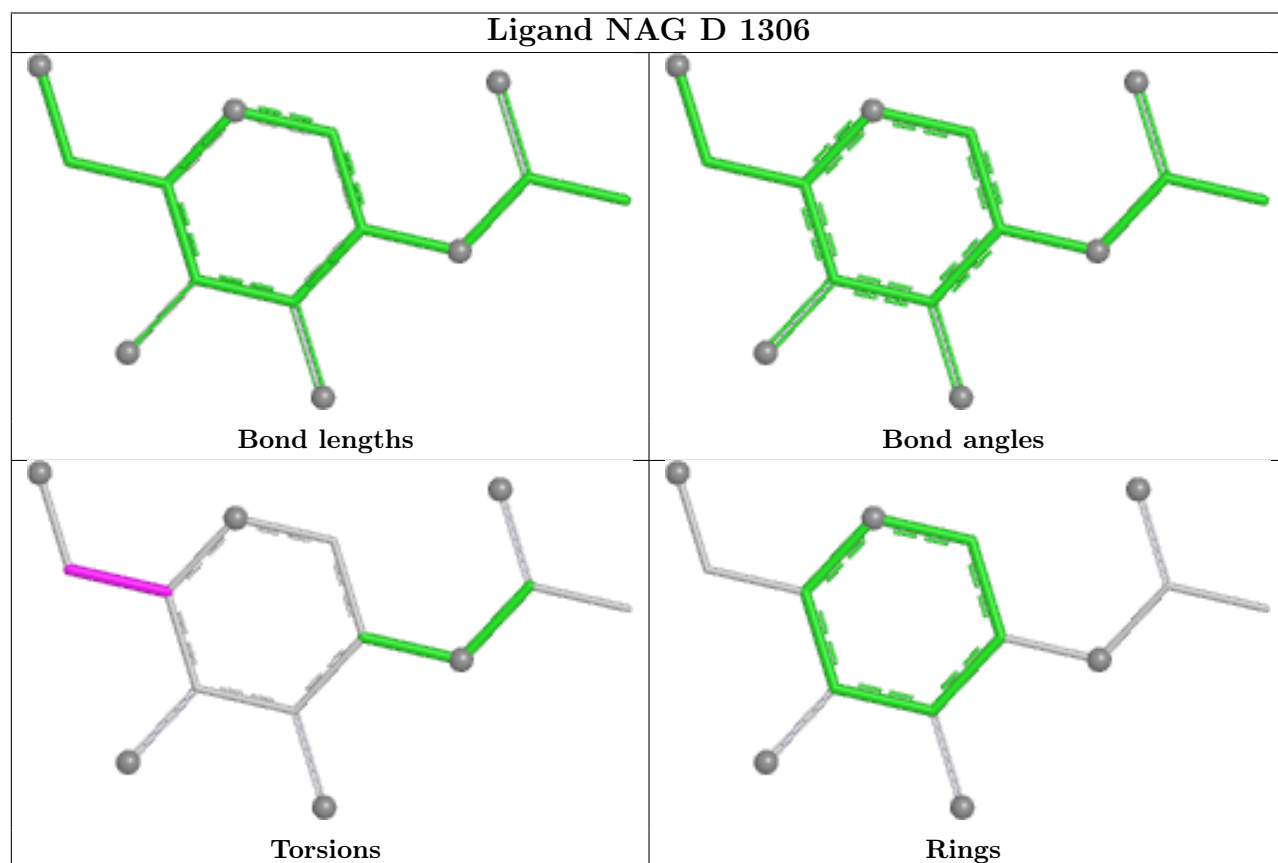


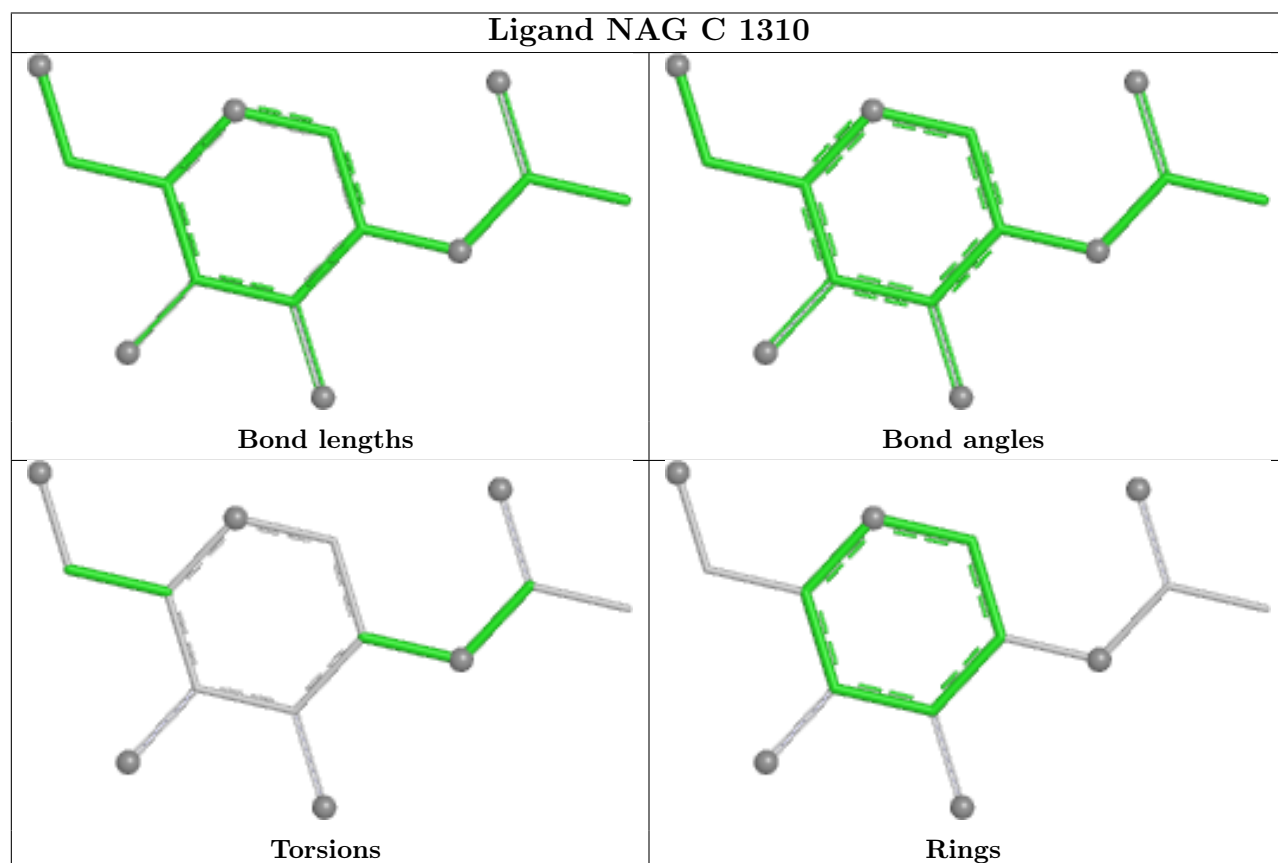
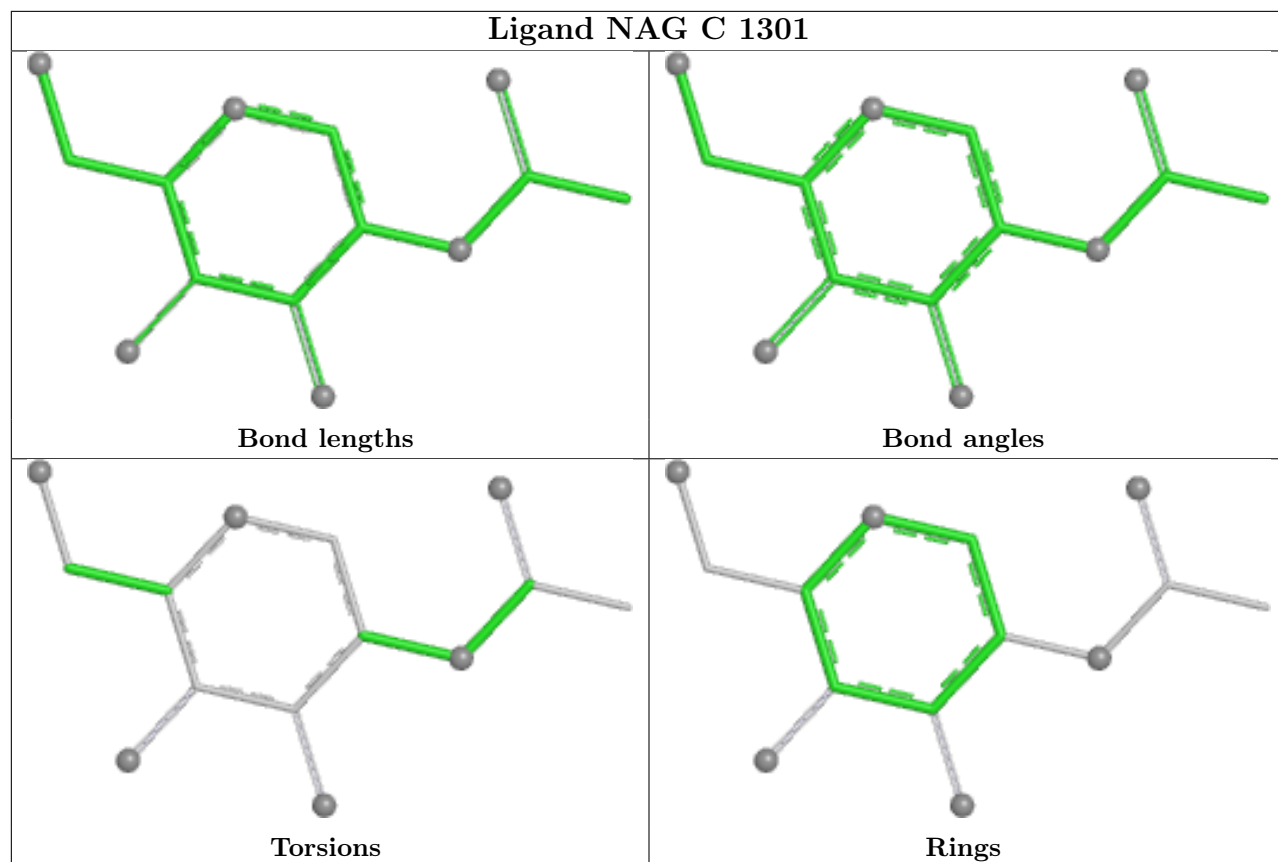


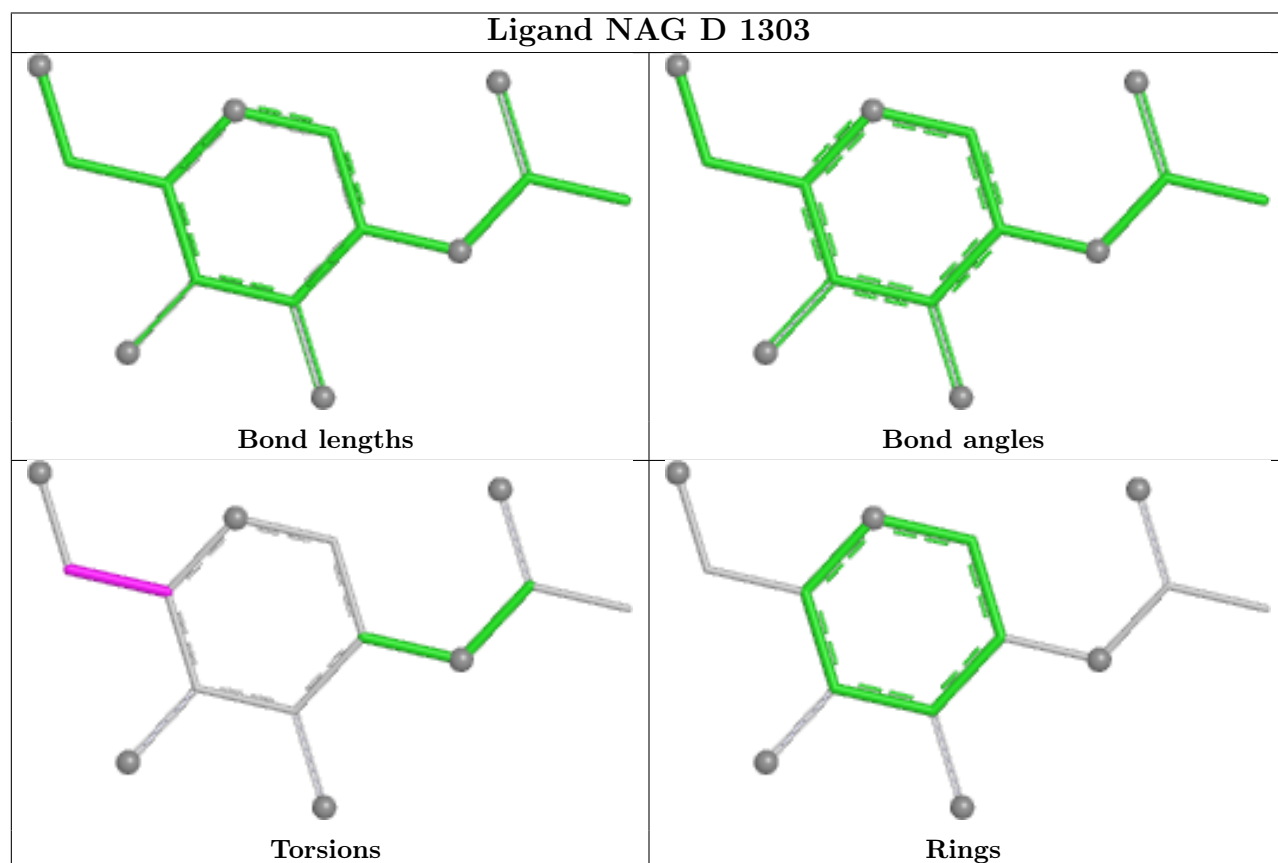
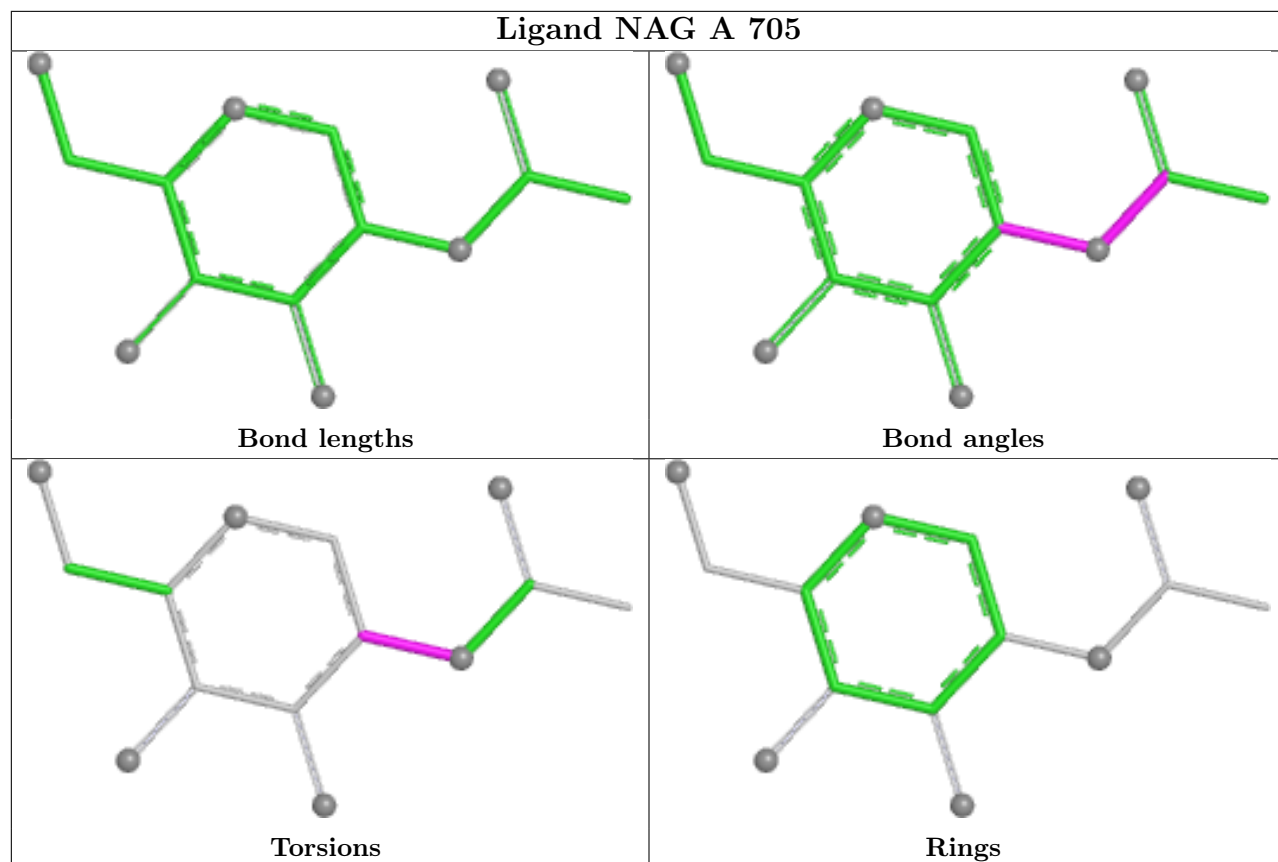
Ligand NAG B 1310

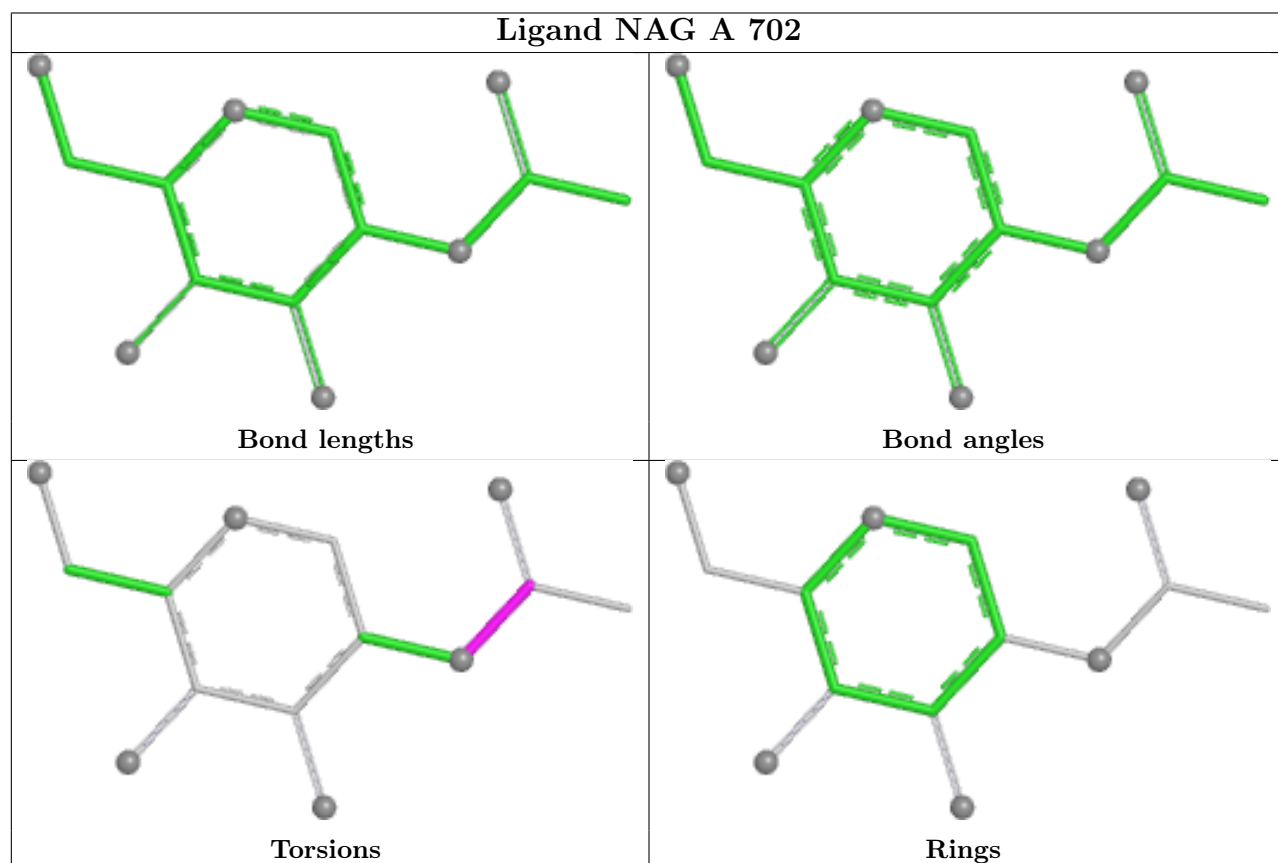
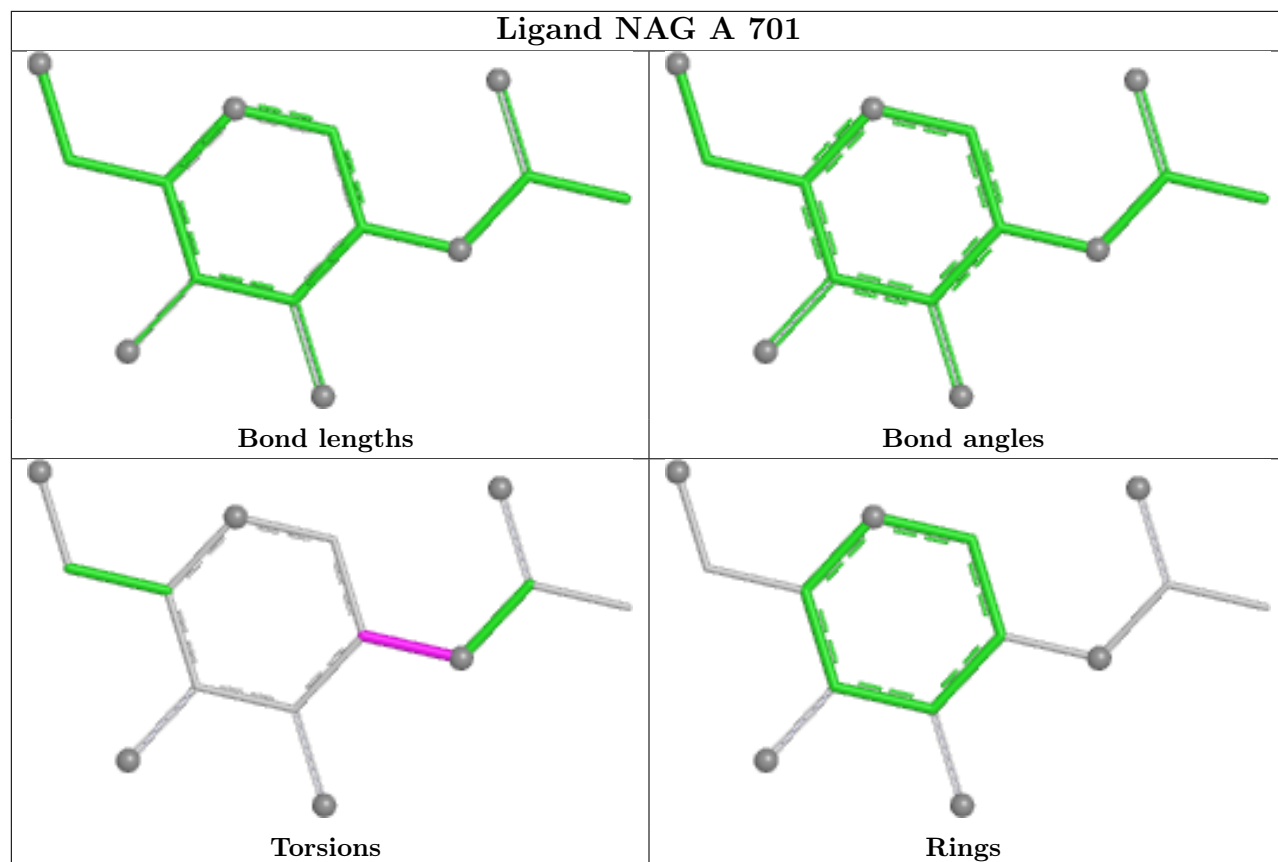


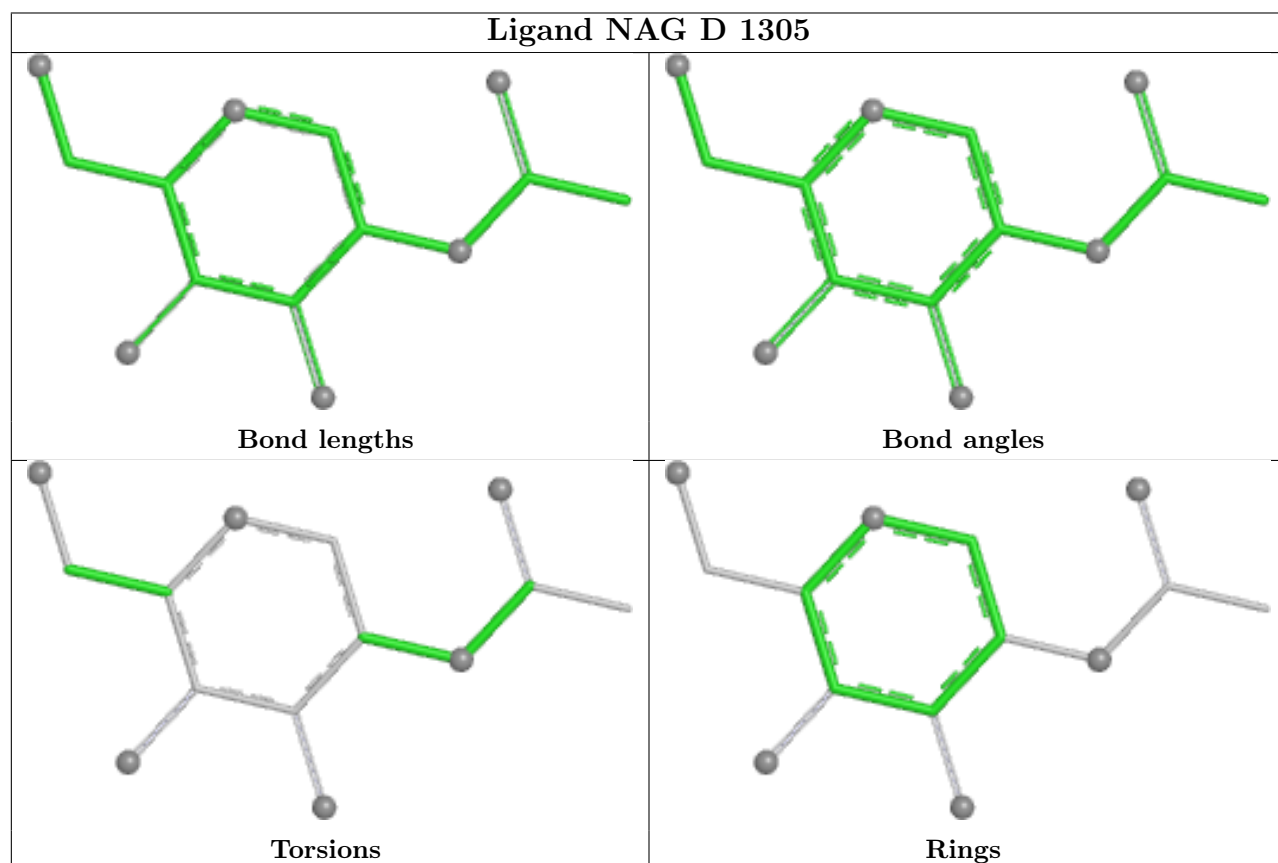
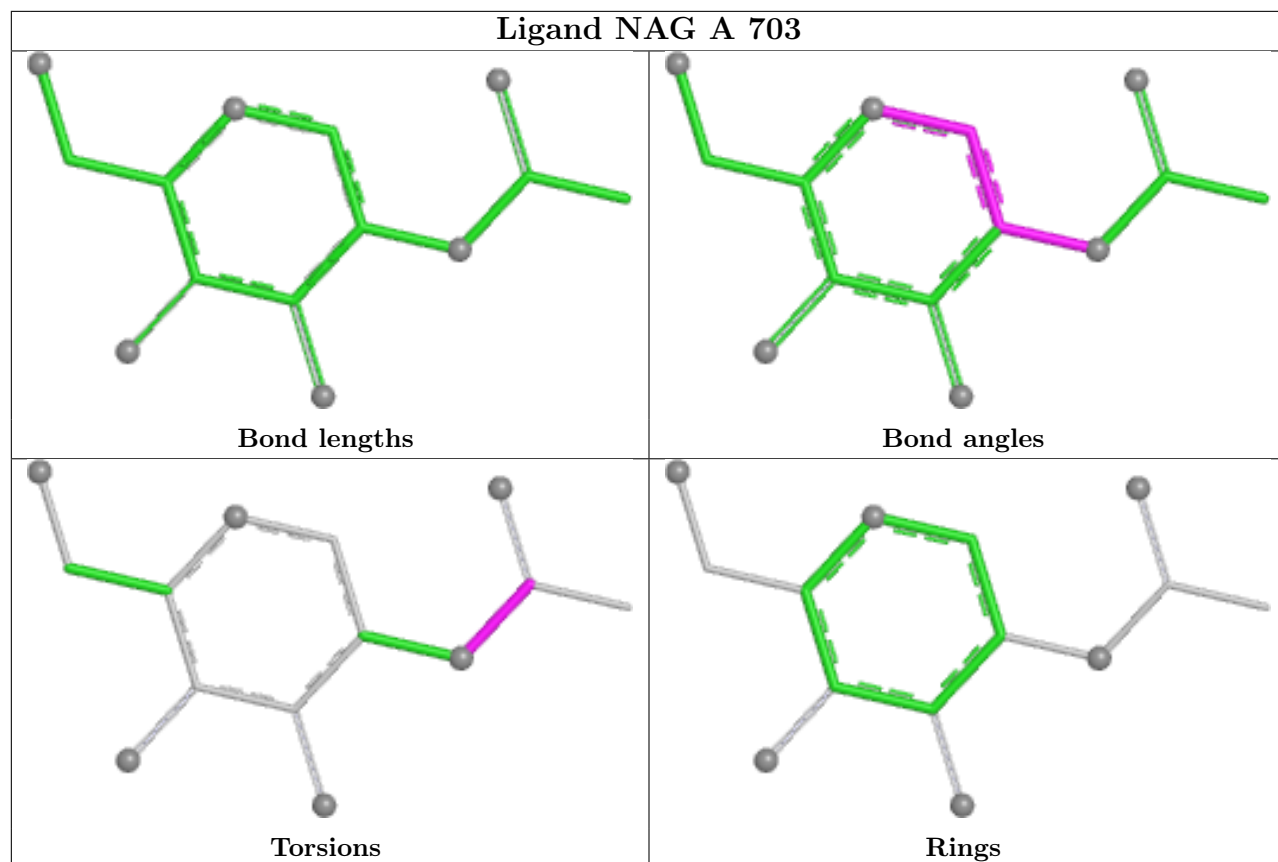
Ligand NAG D 1306

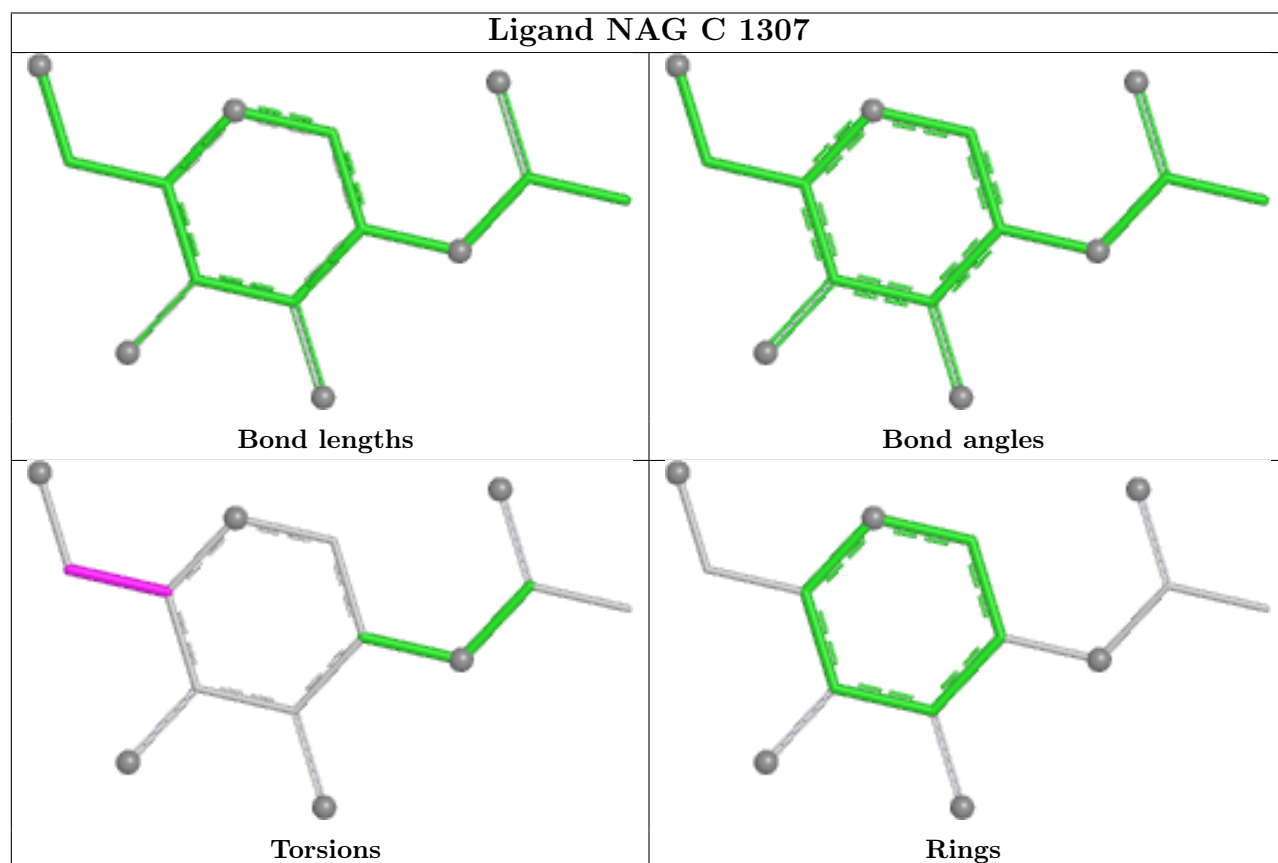
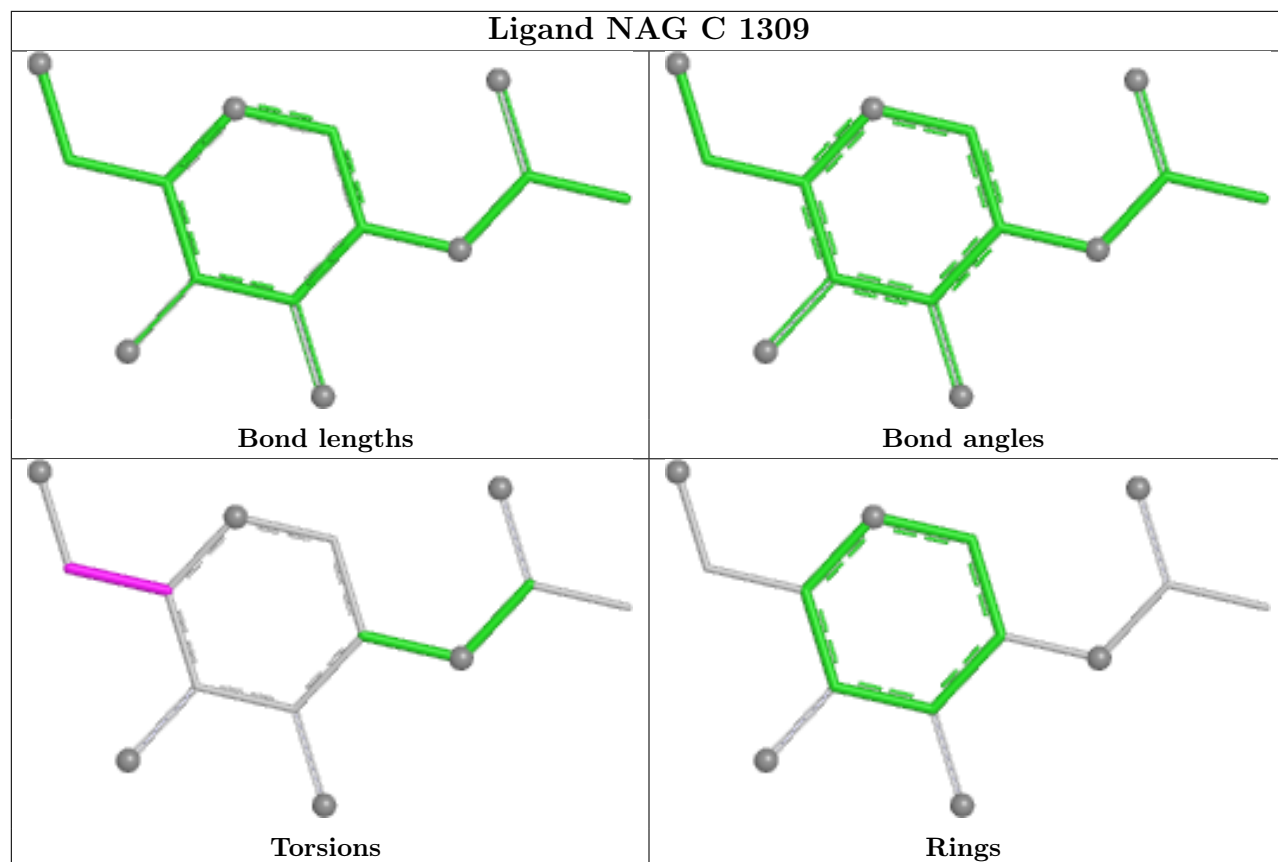


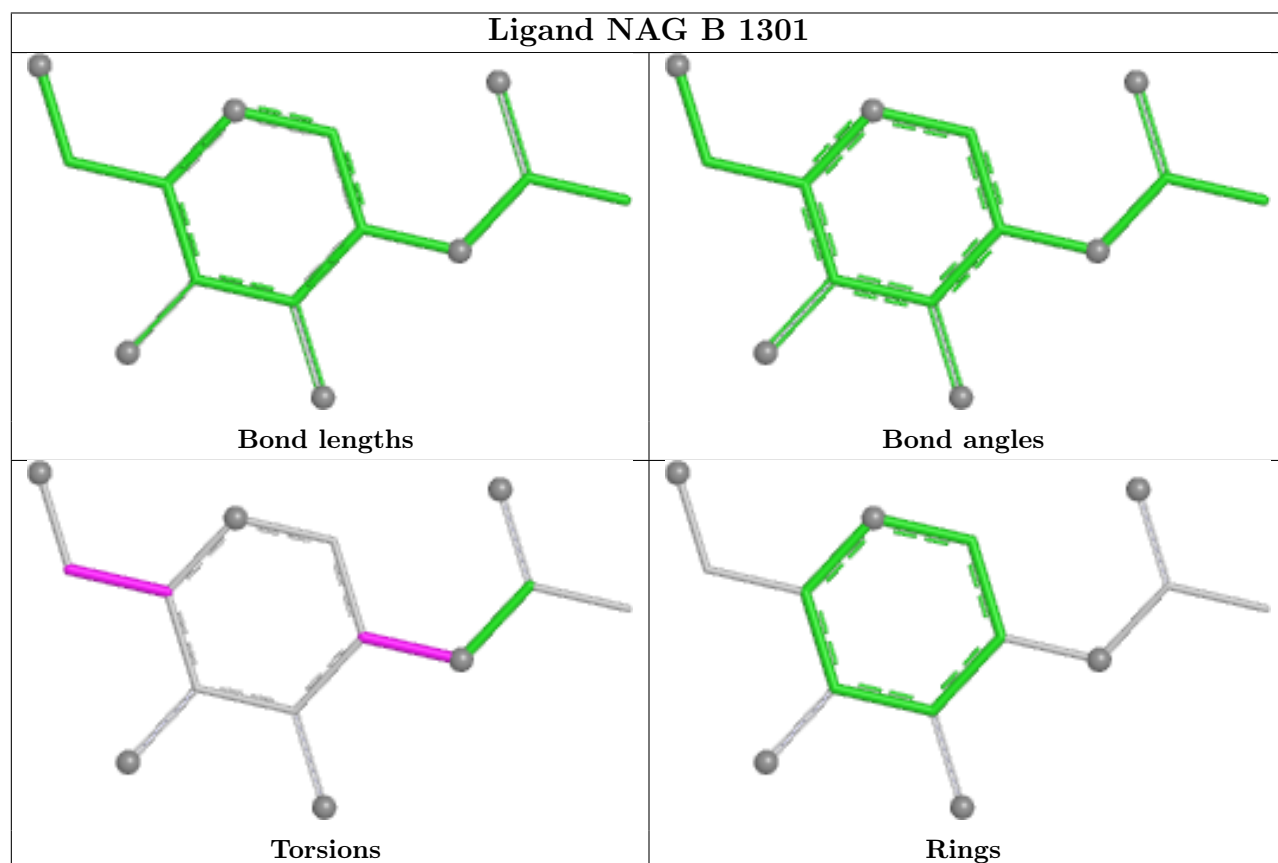
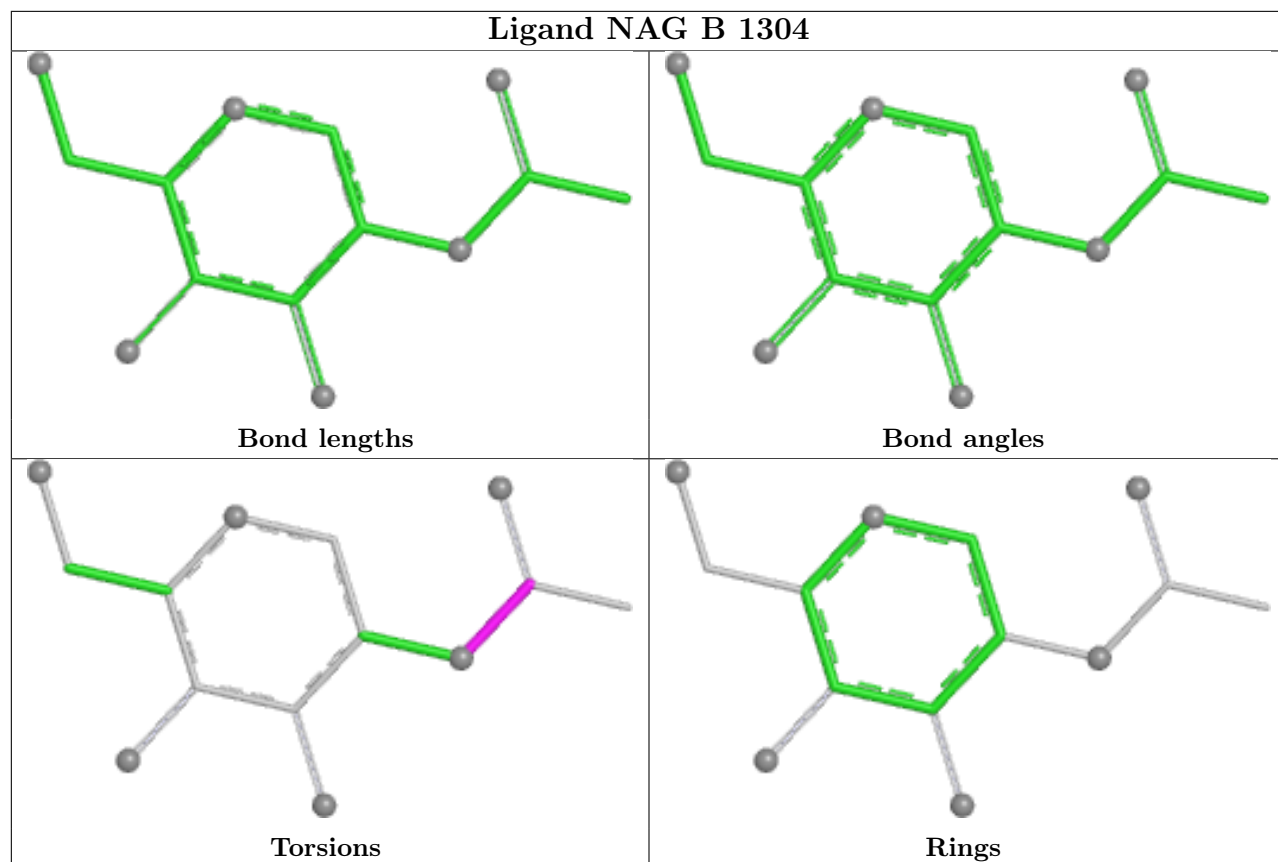




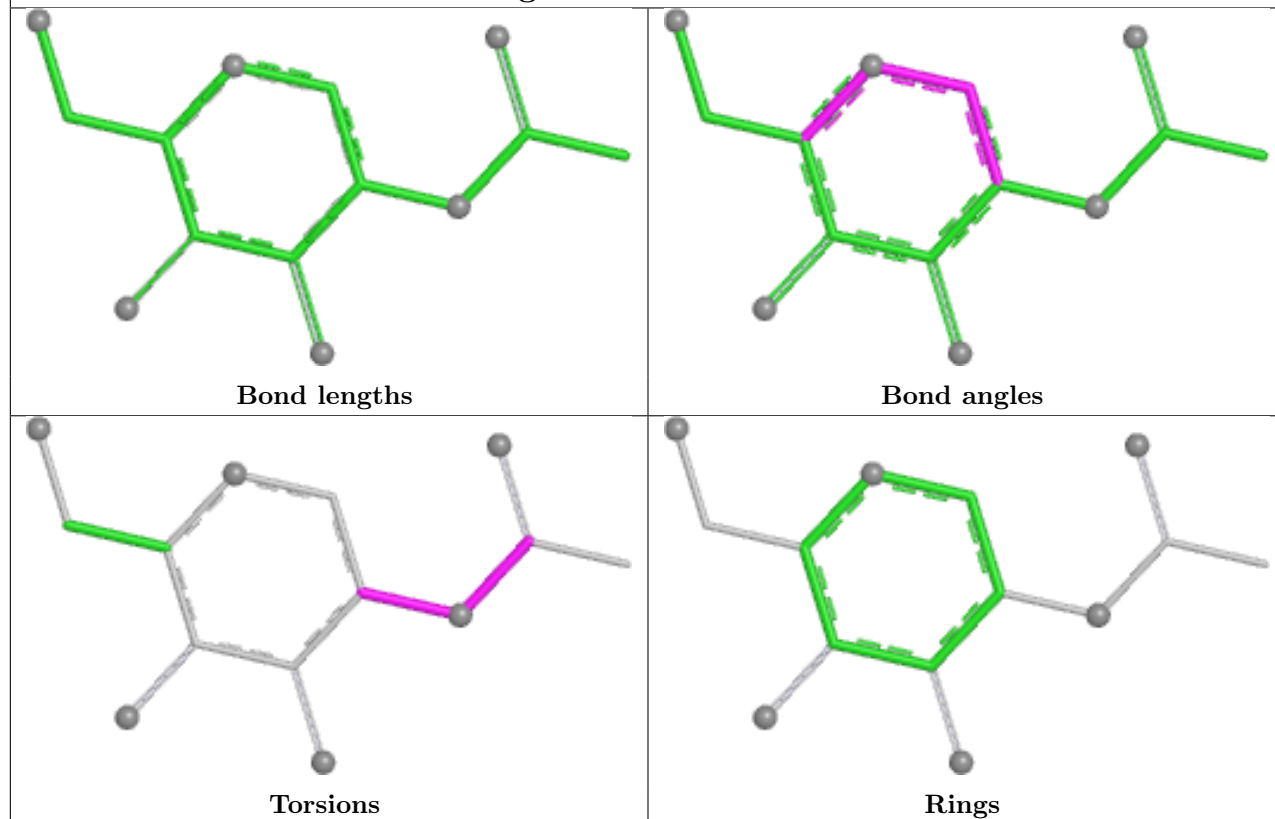




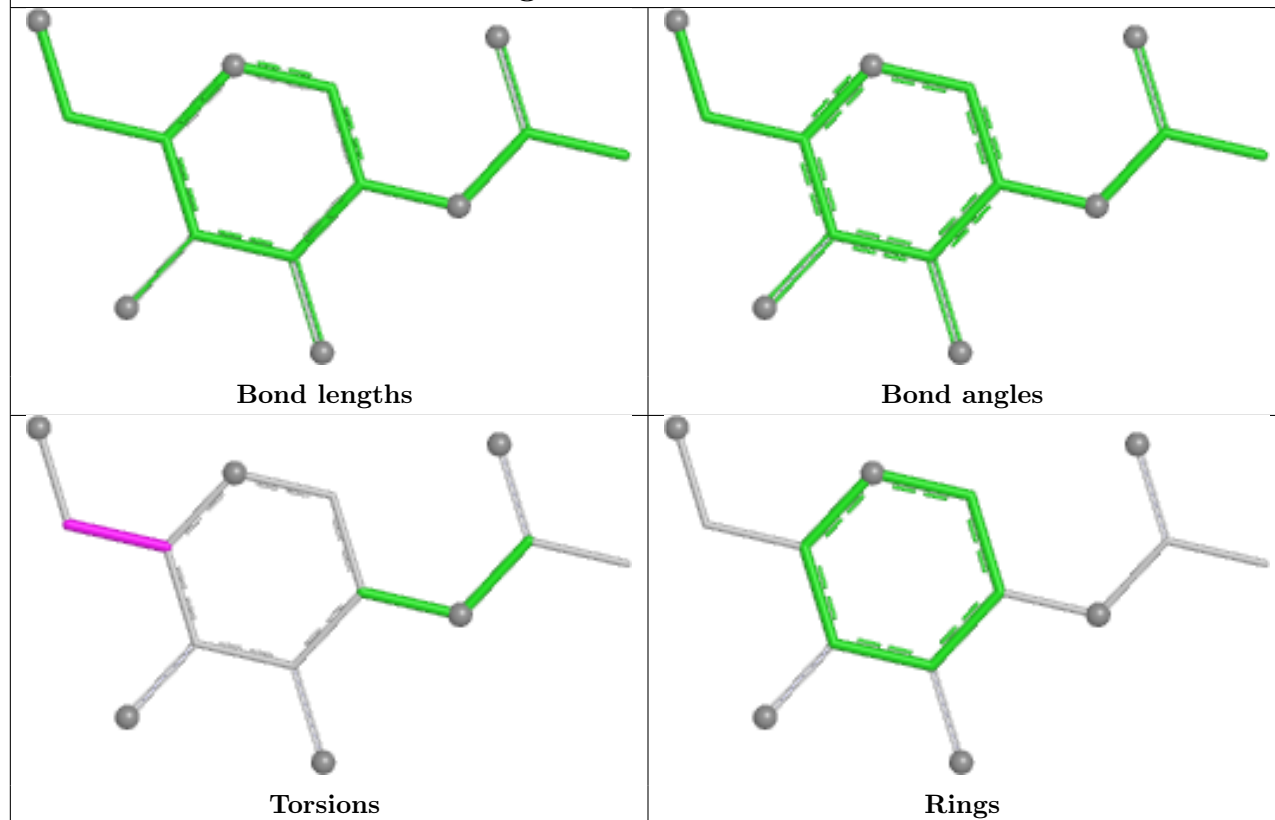




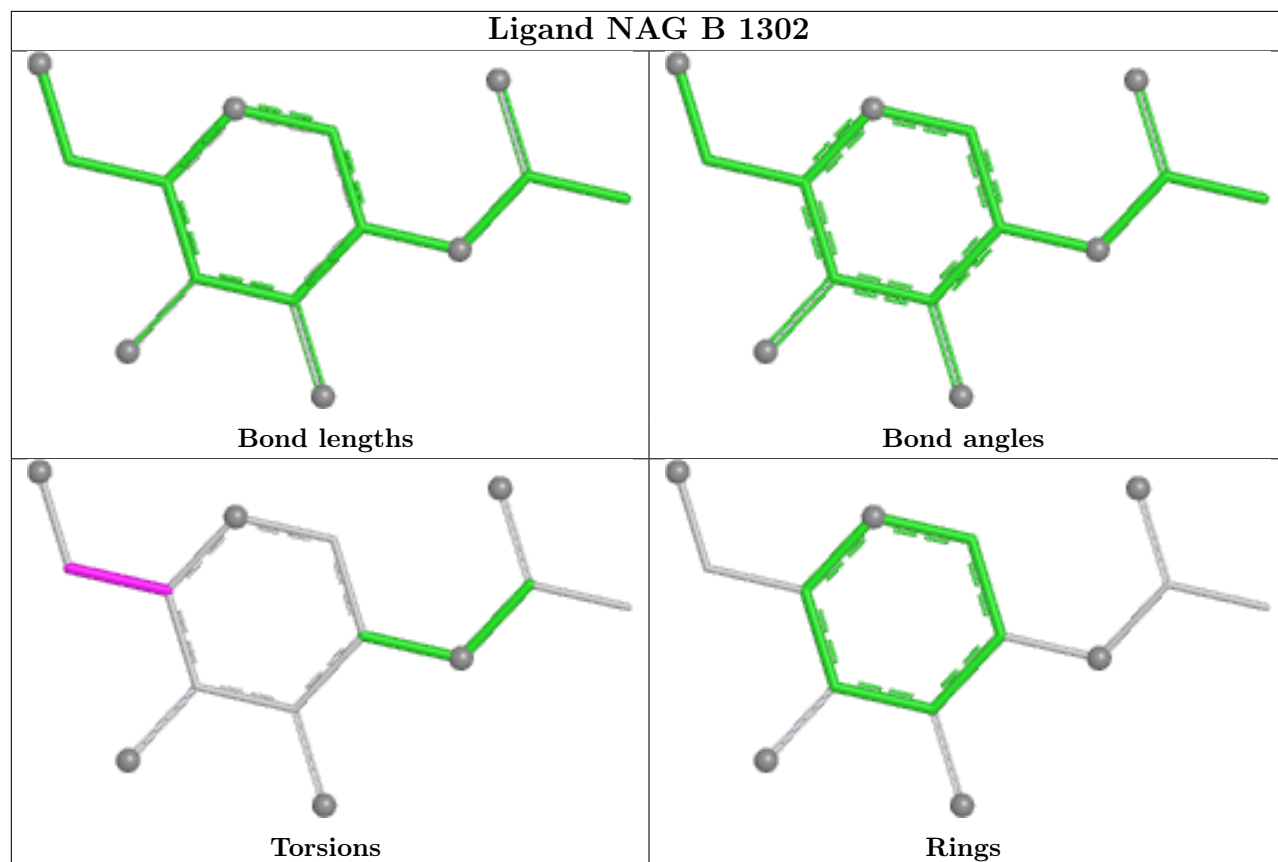
Ligand NAG B 1303



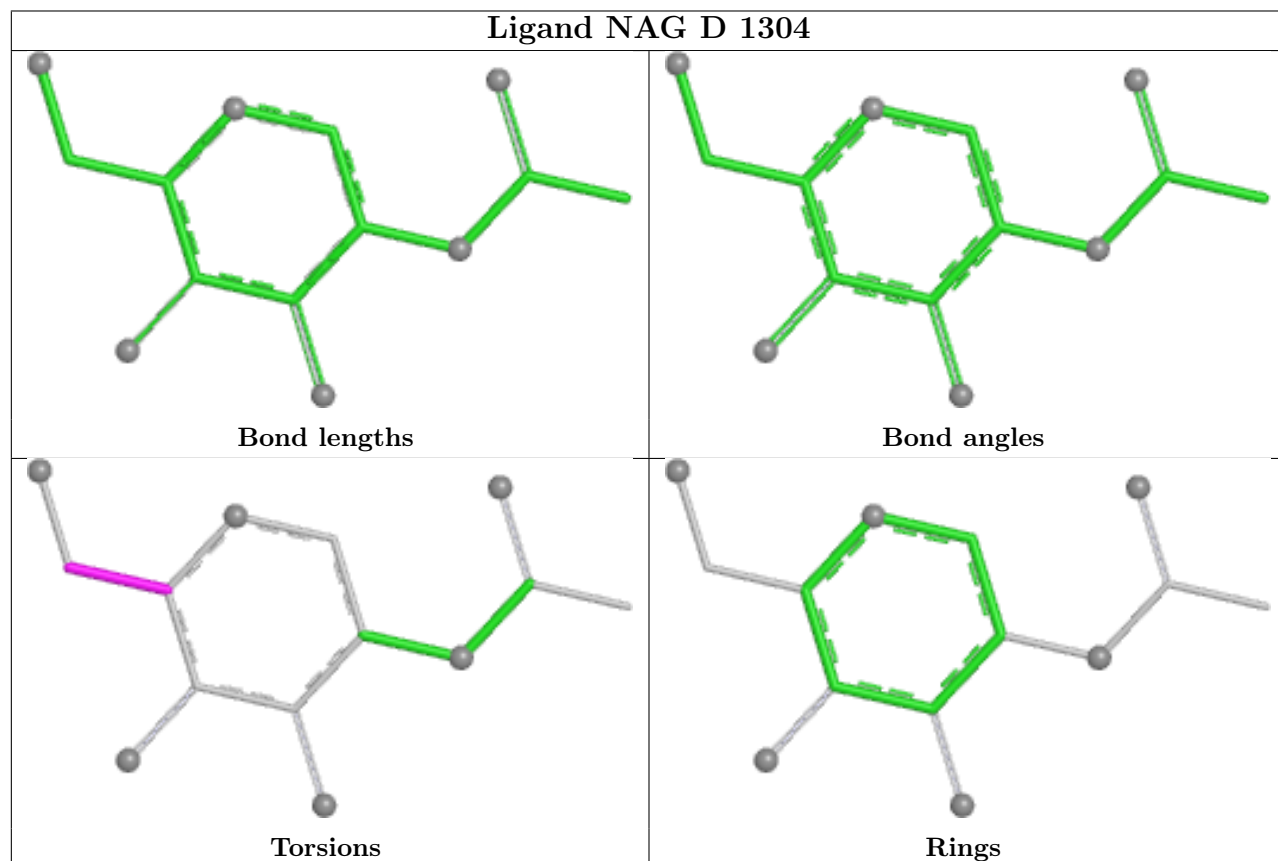
Ligand NAG C 1304



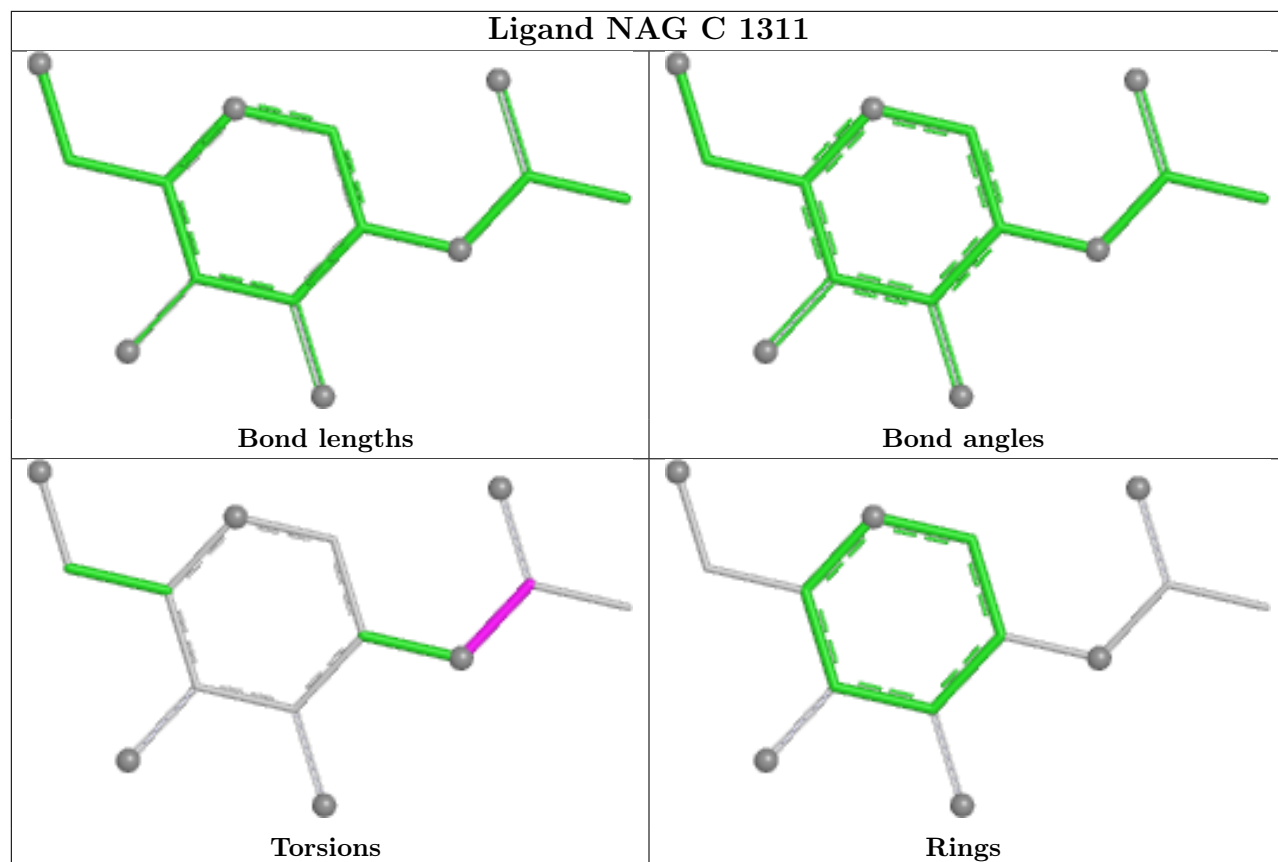
Ligand NAG B 1302



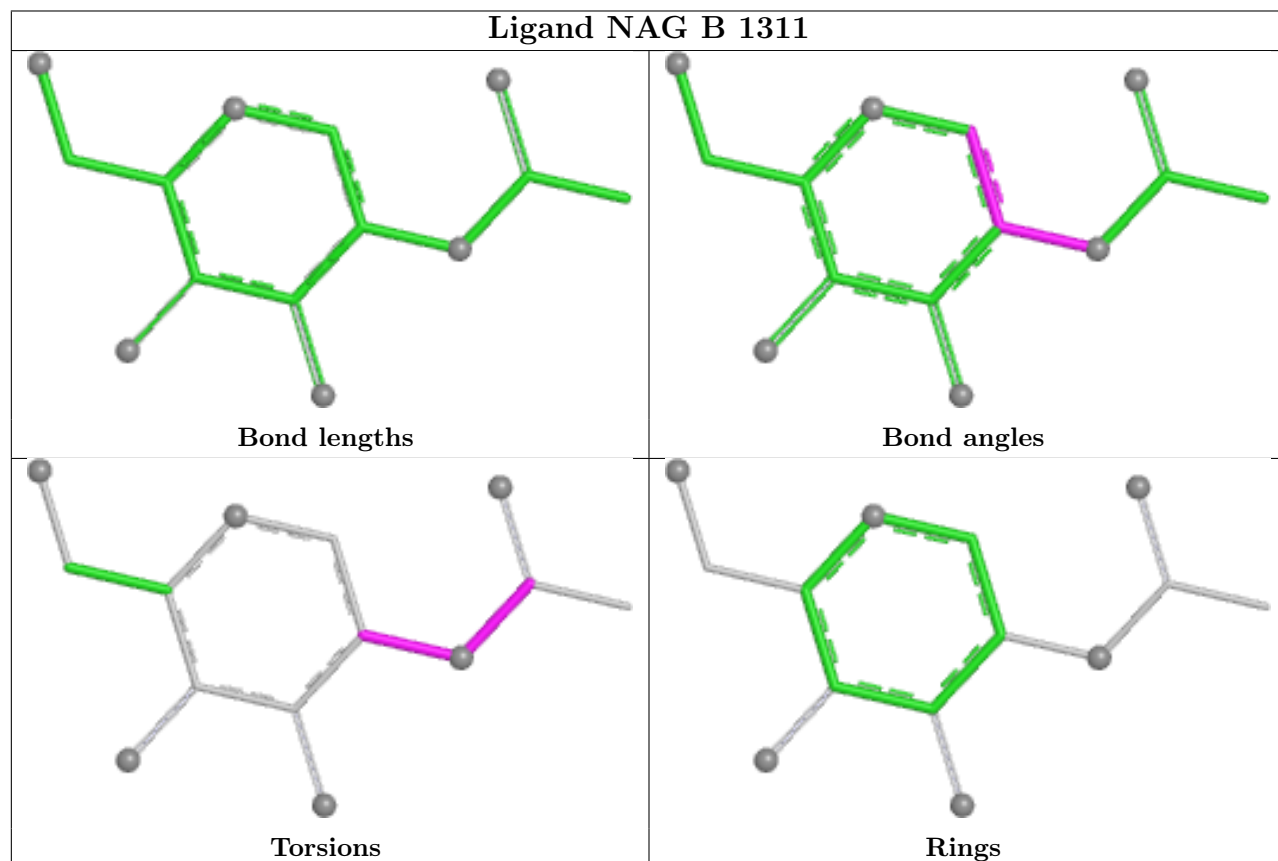
Ligand NAG D 1304



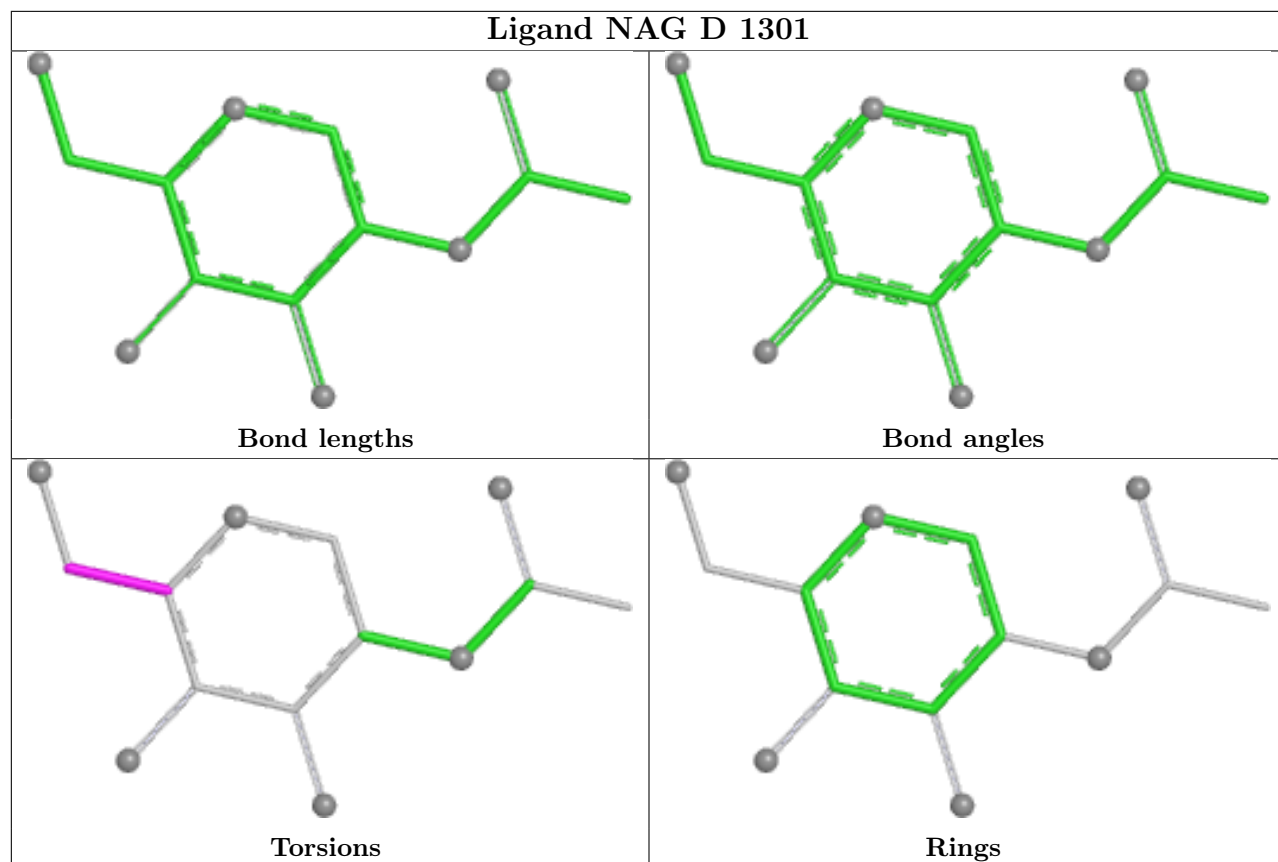
Ligand NAG C 1311



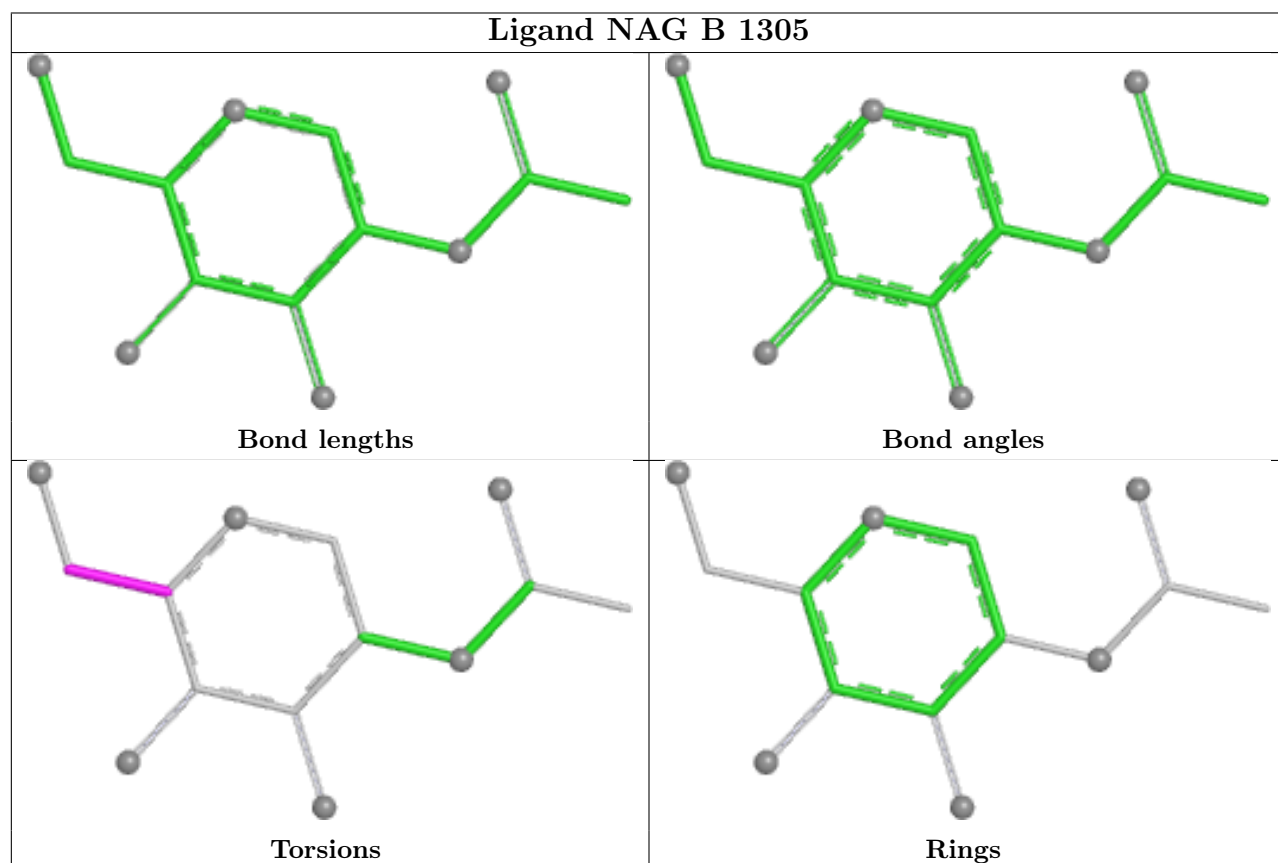
Ligand NAG B 1311

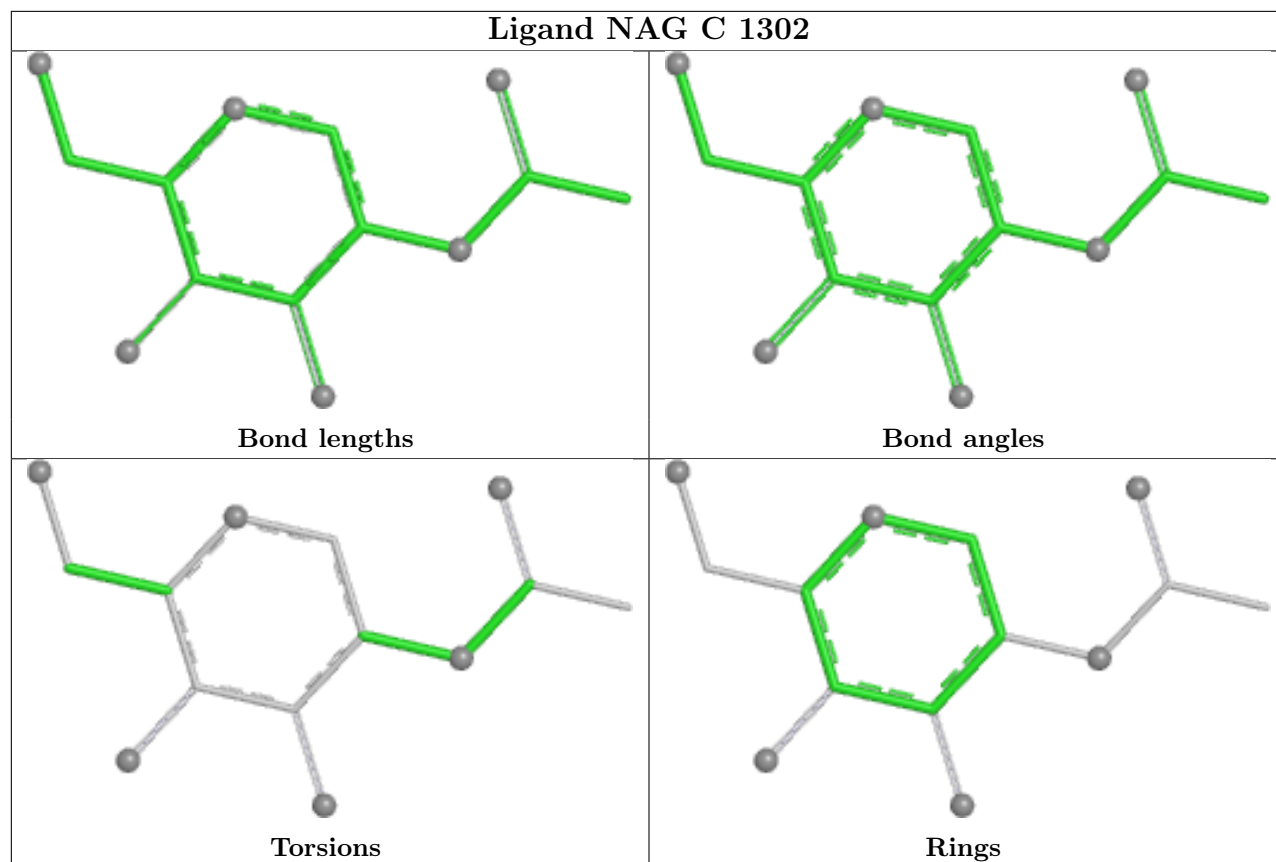


Ligand NAG D 1301



Ligand NAG B 1305





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.

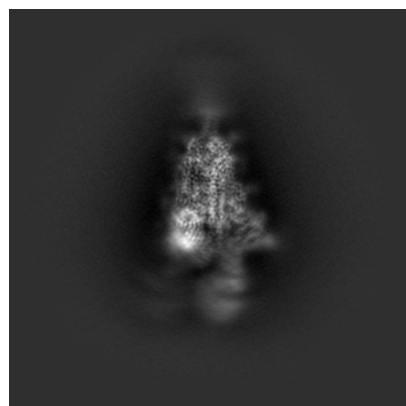
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38498. These allow visual inspection of the internal detail of the map and identification of artifacts.

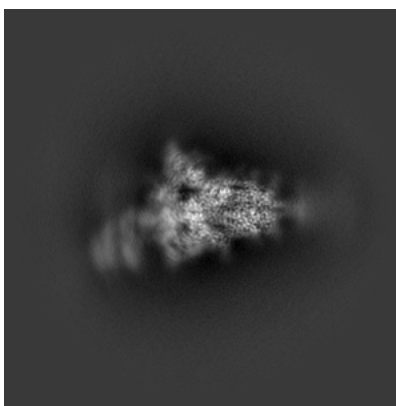
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

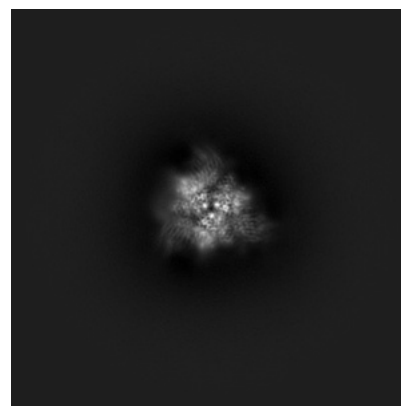
6.1.1 Primary map



X

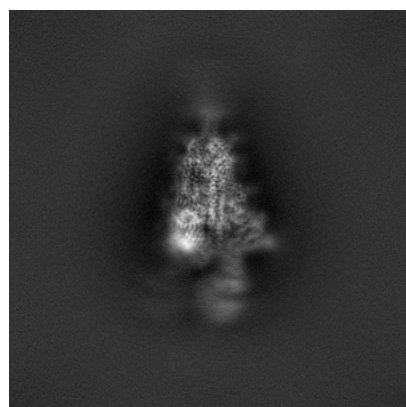


Y

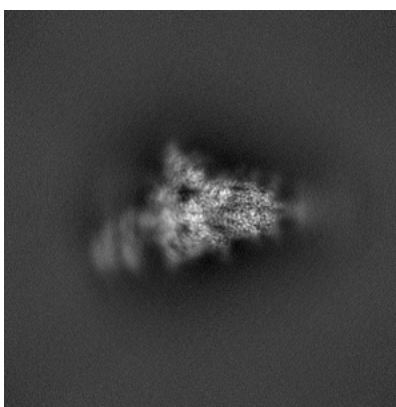


Z

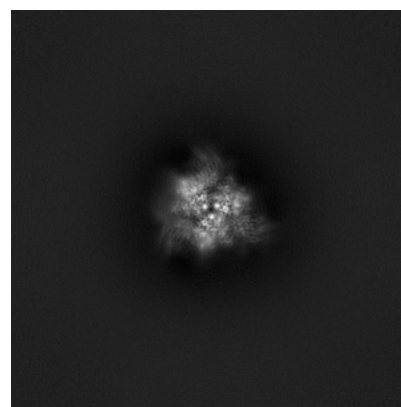
6.1.2 Raw map



X



Y



Z

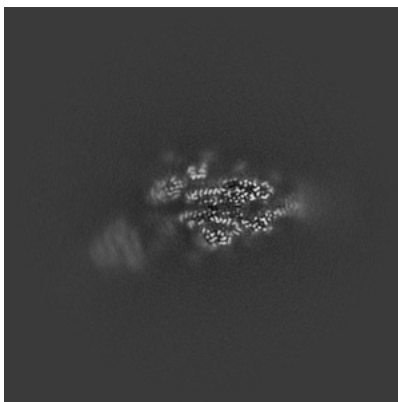
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

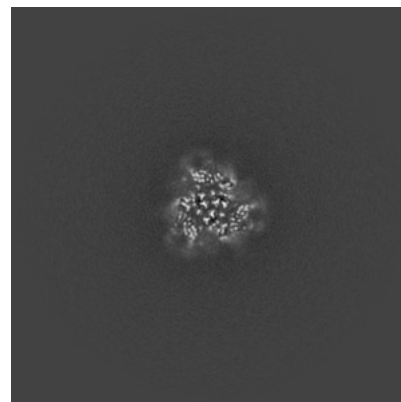
6.2.1 Primary map



X Index: 280



Y Index: 280

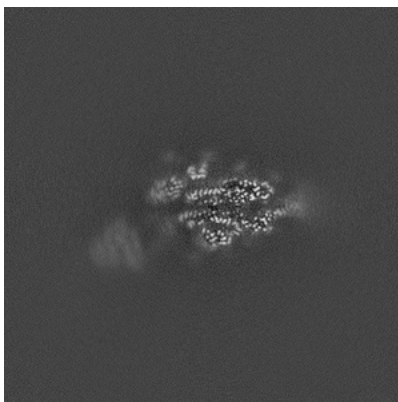


Z Index: 280

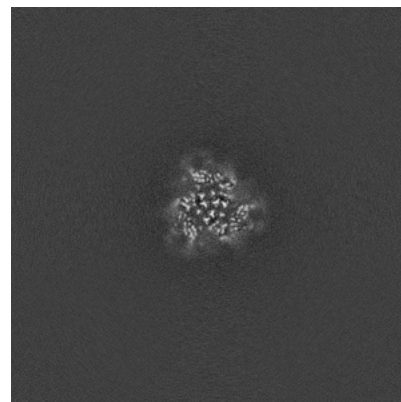
6.2.2 Raw map



X Index: 280



Y Index: 280

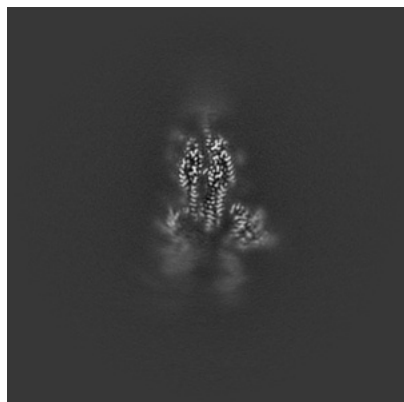


Z Index: 280

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

6.3 Largest variance slices [i](#)

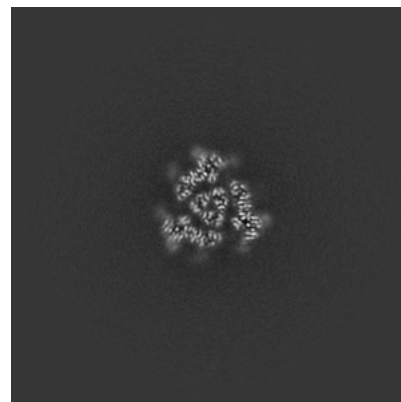
6.3.1 Primary map



X Index: 268



Y Index: 285



Z Index: 263

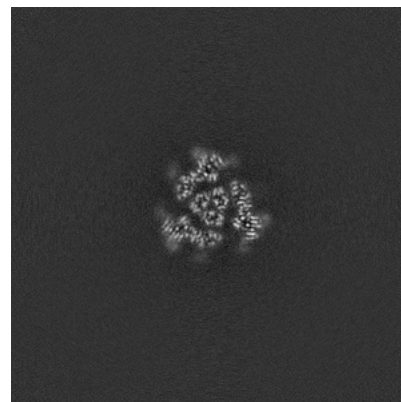
6.3.2 Raw map



X Index: 268



Y Index: 285

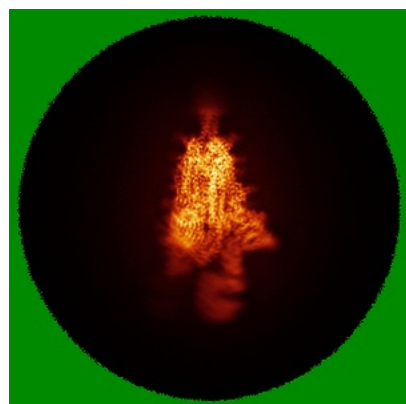


Z Index: 262

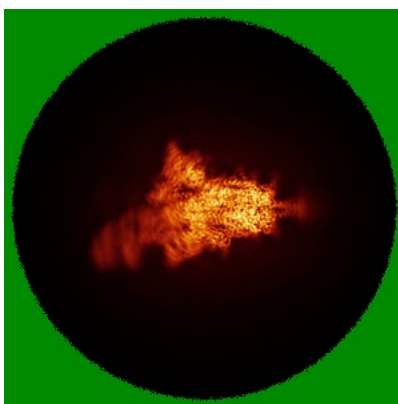
The images above show the largest variance slices of the map in three orthogonal directions.

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

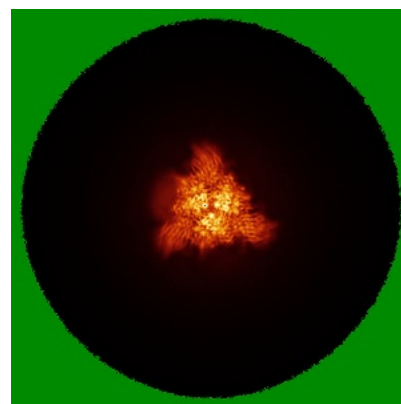
6.4.1 Primary map



X

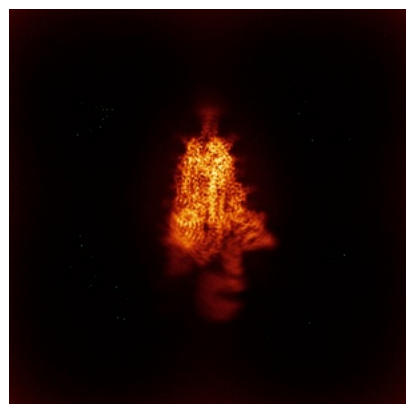


Y

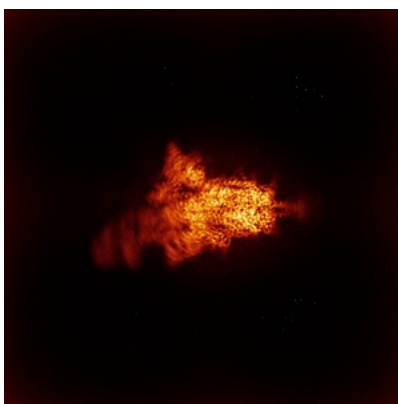


Z

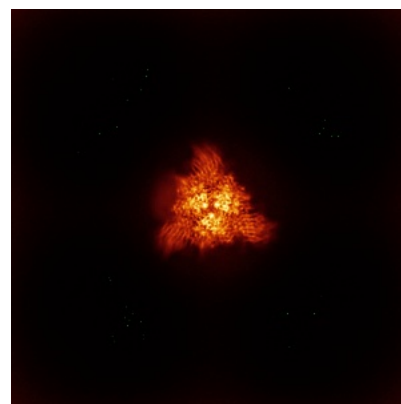
6.4.2 Raw map



X



Y

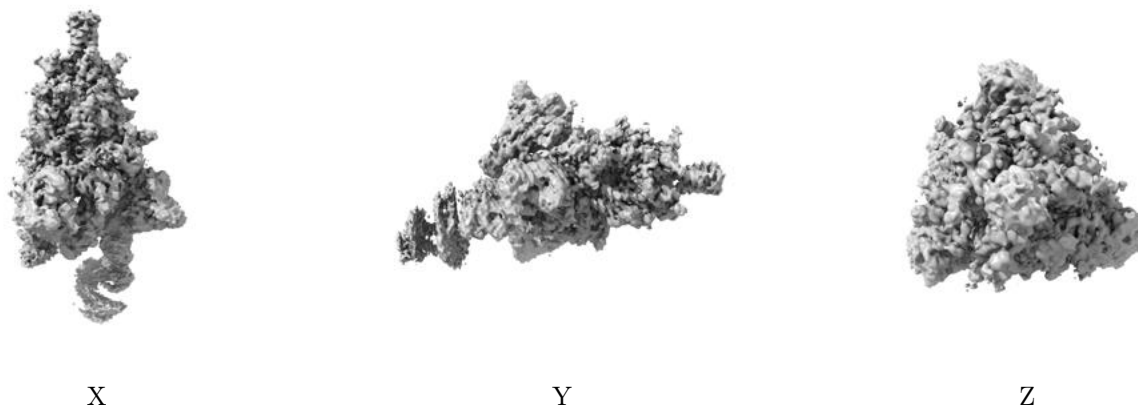


Z

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 0.1. 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.

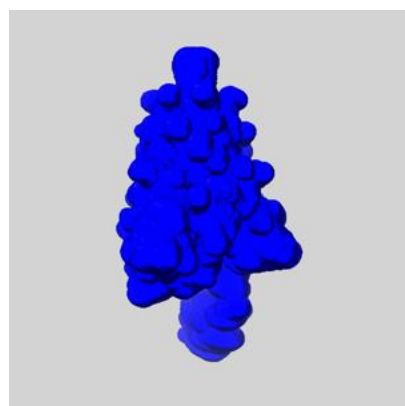
6.6 Mask visualisation [i](#)

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

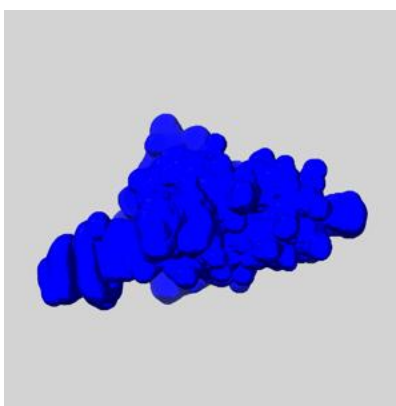
A mask typically either:

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

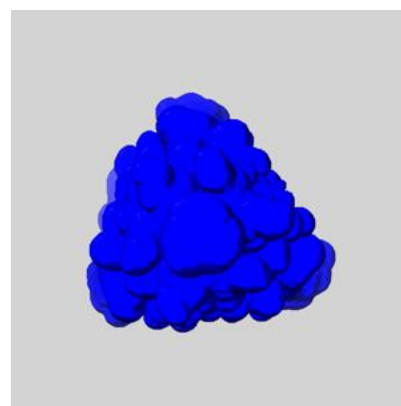
6.6.1 emd_38498_msk_1.map [i](#)



X



Y

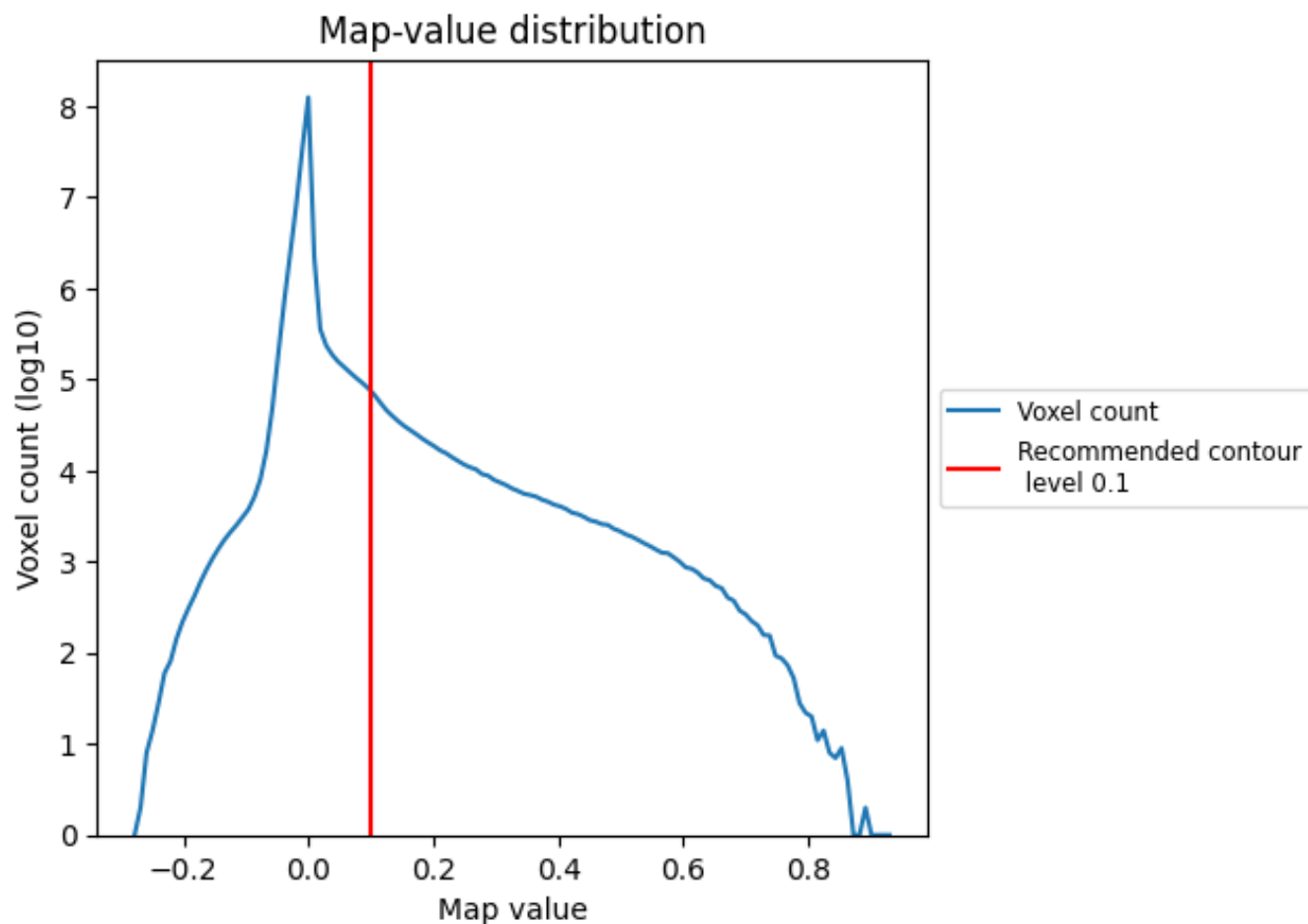


Z

7 Map analysis [i](#)

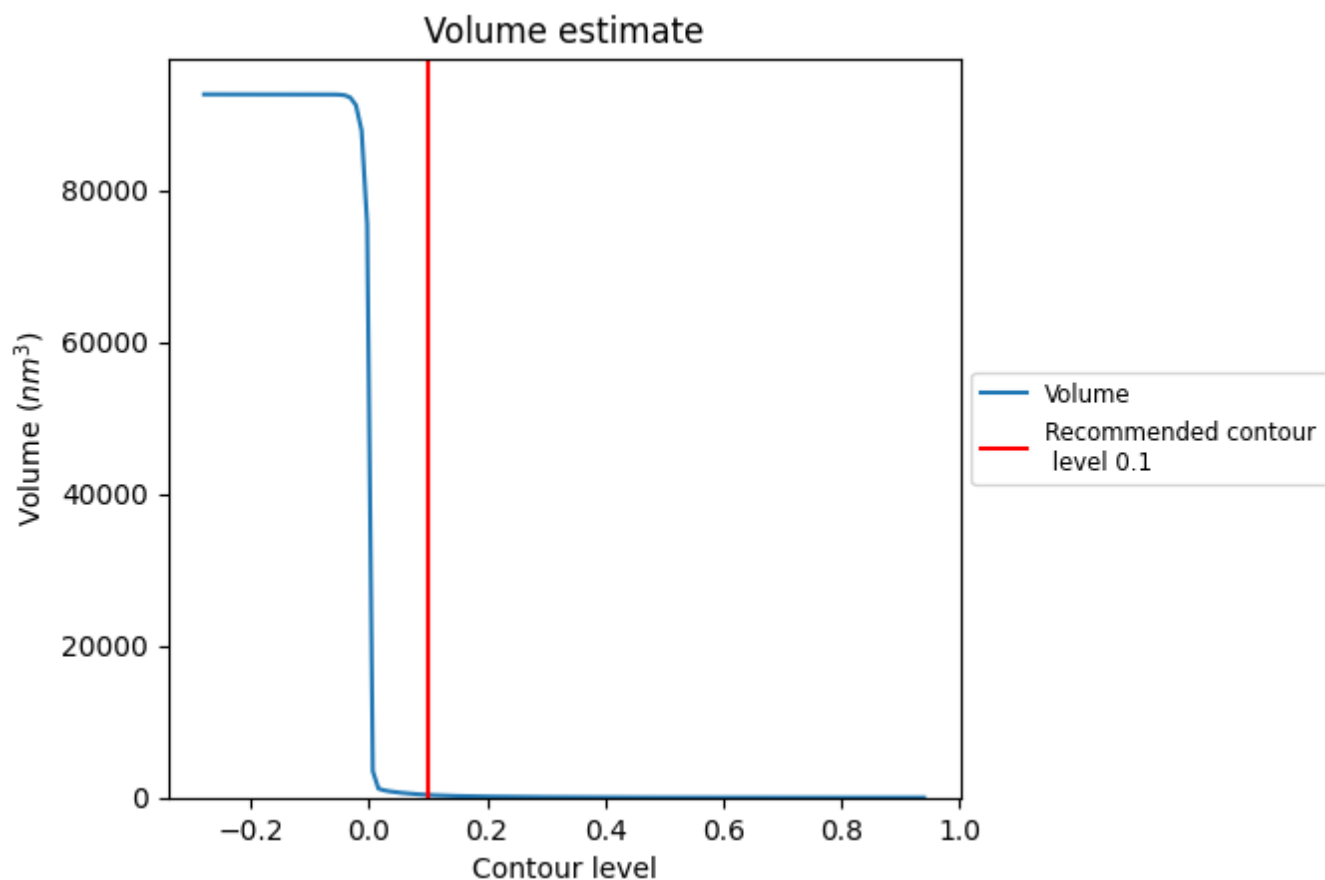
This section contains the results of statistical analysis of the map.

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.

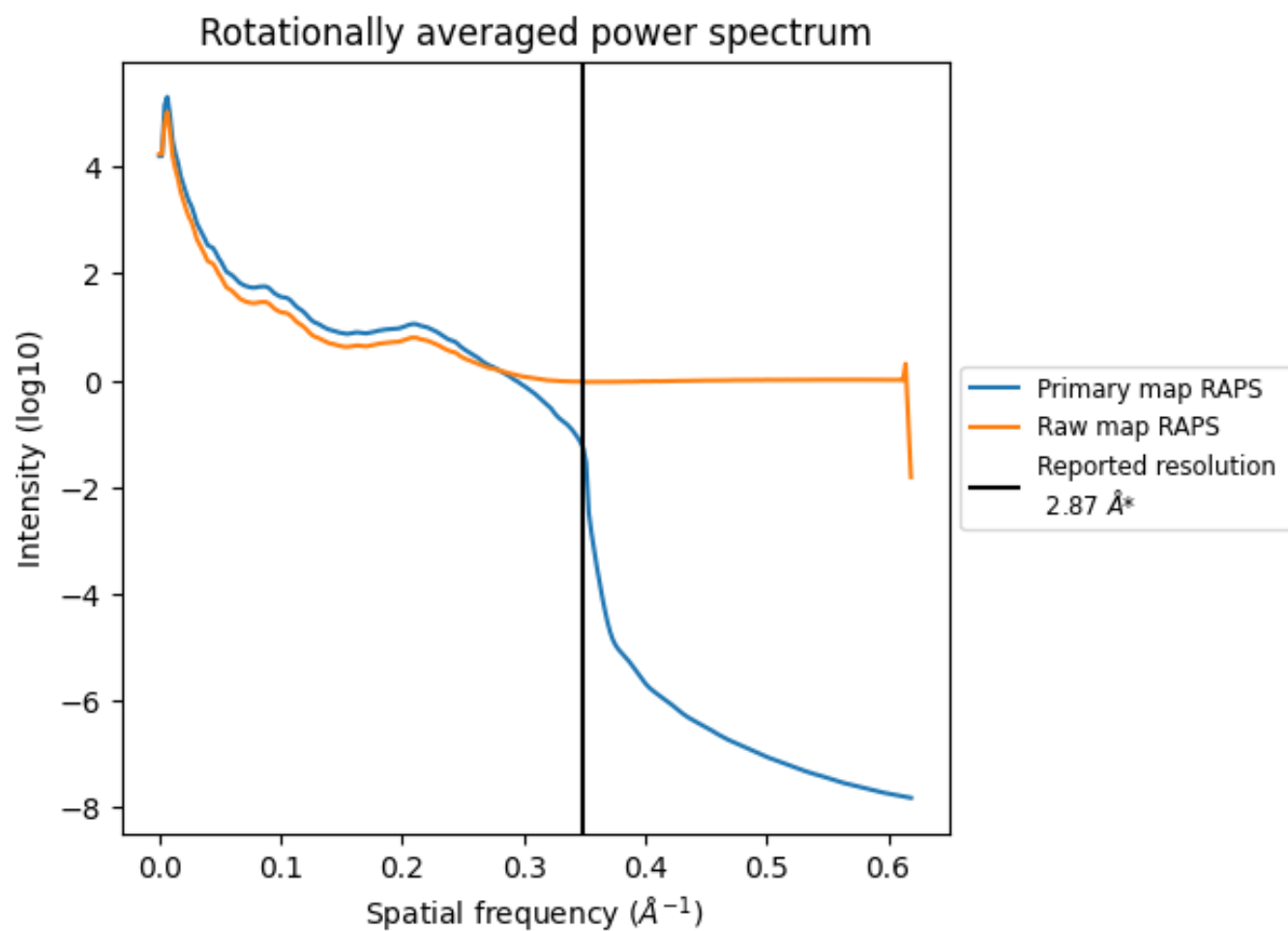
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 349 nm^3 ; this corresponds to an approximate mass of 315 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 ⓘ

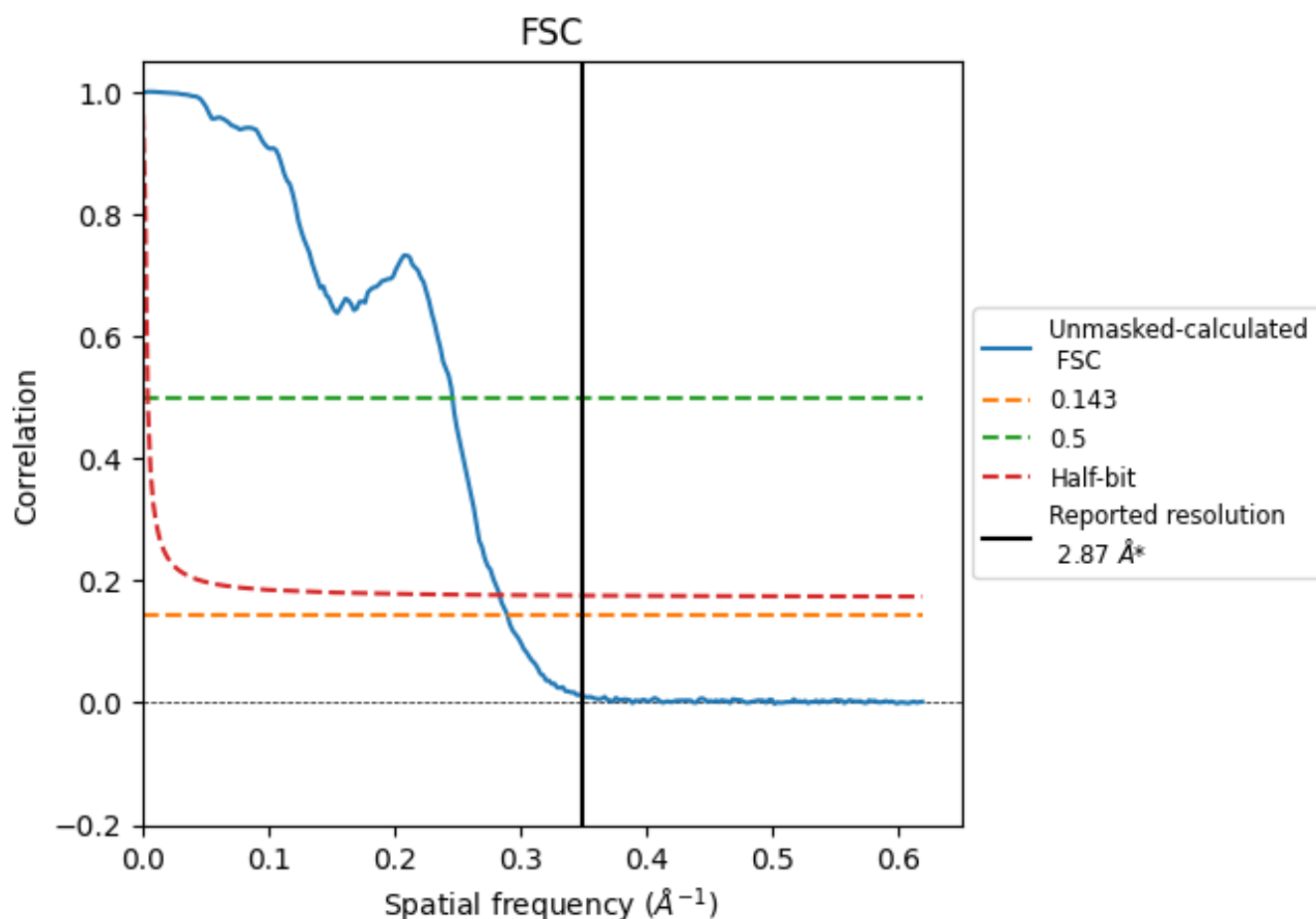


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.348 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

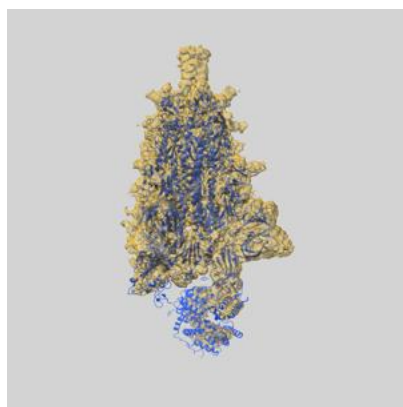
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	4.06	3.53

*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 3.45 differs from the reported value 2.87 by more than 10 %

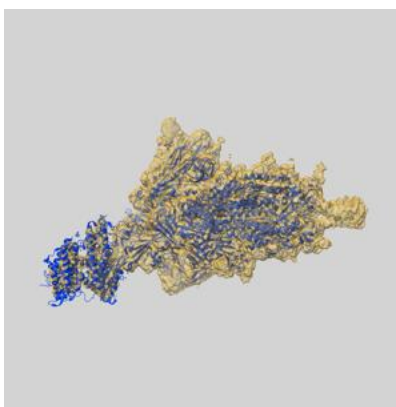
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38498 and PDB model 8XN5. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

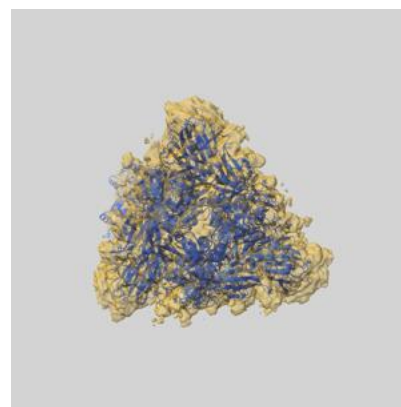
9.1 Map-model overlay [i](#)



X



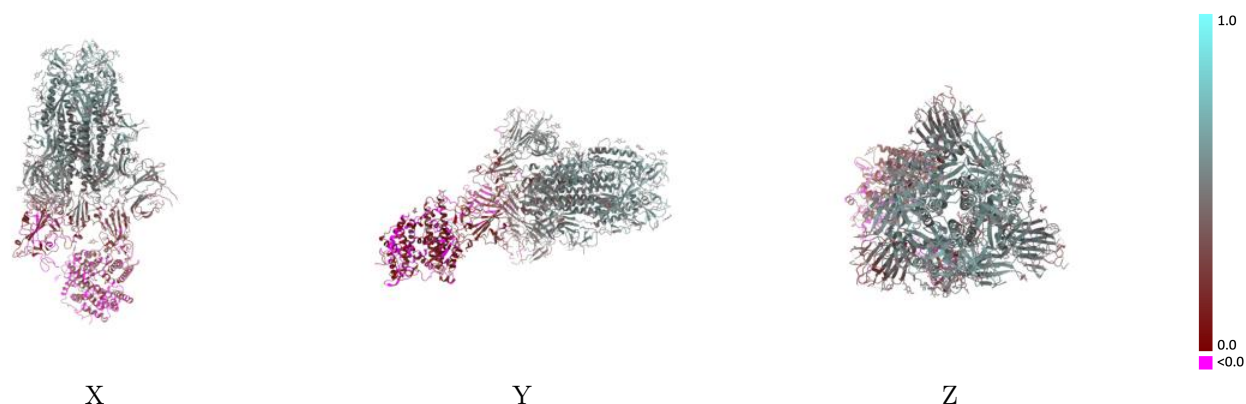
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)

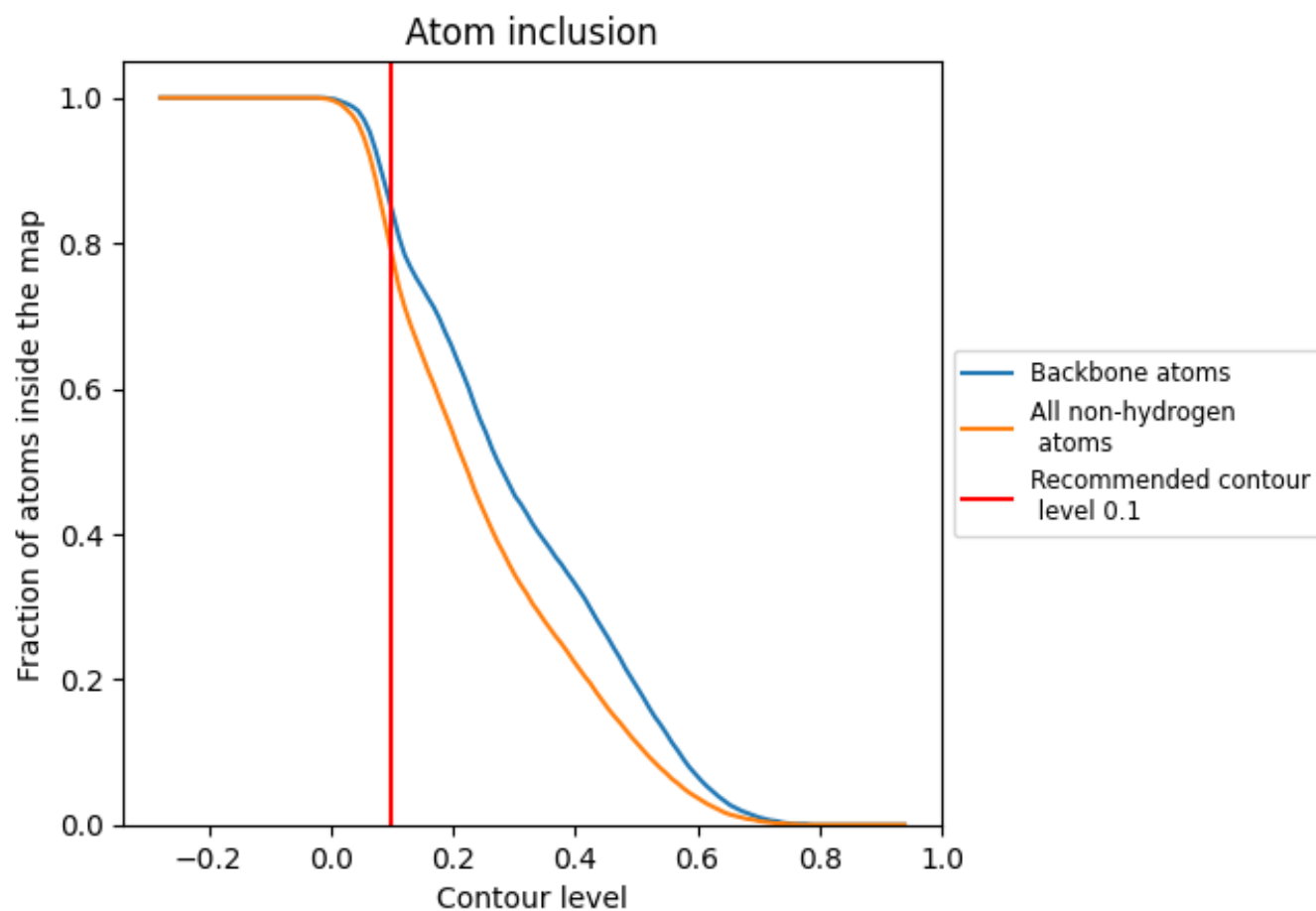


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 78% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7850	0.3710
A	0.2410	0.0710
B	0.9070	0.4190
C	0.8510	0.4210
D	0.9300	0.4550

