



## wwPDB EM Validation Summary Report ⓘ

Jul 7, 2025 – 07:40 PM JST

PDB ID : 8ZC6 / pdb\_00008zc6  
EMDB ID : EMD-39924  
Title : SARS-CoV-2 Omicron BA.4 spike trimer (6P) in complex with D1F6 Fab, head-to-head aggregate  
Authors : Liu, B.; Gao, X.; Li, Z.; Chen, Q.; He, J.; Xiong, X.  
Deposited on : 2024-04-28  
Resolution : 6.85 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](mailto: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>.

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

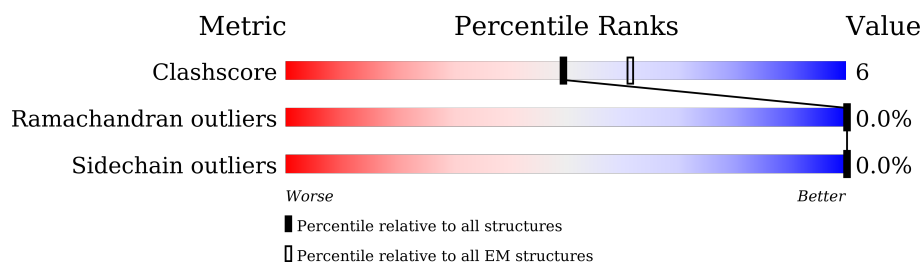
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.85 Å.

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












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1238	
1	B	1238	
1	C	1238	
1	D	1238	
1	E	1238	
1	F	1238	
2	G	223	
2	I	223	
2	K	223	

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Mol	Chain	Length	Quality of chain
2	L	223	 87% 9% .
2	M	223	 80% 16% .
2	N	223	 88% 7% .
3	H	230	 80% 16% .
3	J	230	 83% 12% .
3	O	230	 79% 17% .
3	P	230	 80% 16% .
3	Q	230	 83% 13% .
3	R	230	 85% 11% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 66616 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	994	Total	C	N	O	S	0	0
			7790	4994	1293	1469	34		
1	B	994	Total	C	N	O	S	0	0
			7790	4994	1293	1469	34		
1	C	993	Total	C	N	O	S	0	0
			7778	4988	1288	1468	34		
1	D	994	Total	C	N	O	S	0	0
			7790	4994	1293	1469	34		
1	E	994	Total	C	N	O	S	0	0
			7790	4994	1293	1469	34		
1	F	993	Total	C	N	O	S	0	0
			7778	4988	1288	1468	34		

There are 552 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ARG	LEU	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	VAL	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	683	LYS	ASN	variant	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	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	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
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	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	452	ARG	LEU	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	VAL	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	683	LYS	ASN	variant	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	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
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	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	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	452	ARG	LEU	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	VAL	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	683	LYS	ASN	variant	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	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	1212	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	SER	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	TYR	-	expression tag	UNP P0DTC2
C	1229	ILE	-	expression tag	UNP P0DTC2
C	1230	PRO	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	ALA	-	expression tag	UNP P0DTC2
C	1233	PRO	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	ASP	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	GLN	-	expression tag	UNP P0DTC2
C	1238	ALA	-	expression tag	UNP P0DTC2
C	1239	TYR	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	ARG	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	ASP	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	TRP	-	expression tag	UNP P0DTC2
C	1247	VAL	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	THR	-	expression tag	UNP P0DTC2
C	1252	PHE	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	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	?	-	HIS	deletion	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	142	ASP	GLY	variant	UNP P0DTC2
D	213	GLY	VAL	variant	UNP P0DTC2
D	339	ASP	GLY	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	452	ARG	LEU	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	VAL	PHE	variant	UNP P0DTC2
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	683	LYS	ASN	variant	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	?	-	ARG	deletion	UNP P0DTC2
D	?	-	ARG	deletion	UNP P0DTC2
D	?	-	ALA	deletion	UNP P0DTC2
D	764	LYS	ASN	variant	UNP P0DTC2
D	796	TYR	ASP	variant	UNP P0DTC2
D	817	PRO	PHE	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1212	GLY	-	expression tag	UNP P0DTC2
D	1213	SER	-	expression tag	UNP P0DTC2
D	1214	GLY	-	expression tag	UNP P0DTC2
D	1215	ARG	-	expression tag	UNP P0DTC2
D	1216	GLU	-	expression tag	UNP P0DTC2
D	1217	ASN	-	expression tag	UNP P0DTC2
D	1218	LEU	-	expression tag	UNP P0DTC2
D	1219	TYR	-	expression tag	UNP P0DTC2
D	1220	PHE	-	expression tag	UNP P0DTC2
D	1221	GLN	-	expression tag	UNP P0DTC2
D	1222	GLY	-	expression tag	UNP P0DTC2
D	1223	GLY	-	expression tag	UNP P0DTC2
D	1224	GLY	-	expression tag	UNP P0DTC2
D	1225	GLY	-	expression tag	UNP P0DTC2
D	1226	SER	-	expression tag	UNP P0DTC2
D	1227	GLY	-	expression tag	UNP P0DTC2
D	1228	TYR	-	expression tag	UNP P0DTC2
D	1229	ILE	-	expression tag	UNP P0DTC2
D	1230	PRO	-	expression tag	UNP P0DTC2
D	1231	GLU	-	expression tag	UNP P0DTC2
D	1232	ALA	-	expression tag	UNP P0DTC2
D	1233	PRO	-	expression tag	UNP P0DTC2
D	1234	ARG	-	expression tag	UNP P0DTC2
D	1235	ASP	-	expression tag	UNP P0DTC2
D	1236	GLY	-	expression tag	UNP P0DTC2
D	1237	GLN	-	expression tag	UNP P0DTC2
D	1238	ALA	-	expression tag	UNP P0DTC2
D	1239	TYR	-	expression tag	UNP P0DTC2
D	1240	VAL	-	expression tag	UNP P0DTC2
D	1241	ARG	-	expression tag	UNP P0DTC2
D	1242	LYS	-	expression tag	UNP P0DTC2
D	1243	ASP	-	expression tag	UNP P0DTC2
D	1244	GLY	-	expression tag	UNP P0DTC2
D	1245	GLU	-	expression tag	UNP P0DTC2
D	1246	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1247	VAL	-	expression tag	UNP P0DTC2
D	1248	LEU	-	expression tag	UNP P0DTC2
D	1249	LEU	-	expression tag	UNP P0DTC2
D	1250	SER	-	expression tag	UNP P0DTC2
D	1251	THR	-	expression tag	UNP P0DTC2
D	1252	PHE	-	expression tag	UNP P0DTC2
D	1253	LEU	-	expression tag	UNP P0DTC2
D	1254	GLY	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	HIS	-	expression tag	UNP P0DTC2
D	1259	HIS	-	expression tag	UNP P0DTC2
D	1260	HIS	-	expression tag	UNP P0DTC2
E	22	ILE	THR	variant	UNP P0DTC2
E	?	-	LEU	deletion	UNP P0DTC2
E	?	-	PRO	deletion	UNP P0DTC2
E	?	-	PRO	deletion	UNP P0DTC2
E	27	SER	ALA	variant	UNP P0DTC2
E	?	-	HIS	deletion	UNP P0DTC2
E	?	-	VAL	deletion	UNP P0DTC2
E	142	ASP	GLY	variant	UNP P0DTC2
E	213	GLY	VAL	variant	UNP P0DTC2
E	339	ASP	GLY	variant	UNP P0DTC2
E	371	PHE	SER	variant	UNP P0DTC2
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	376	ALA	THR	variant	UNP P0DTC2
E	405	ASN	ASP	variant	UNP P0DTC2
E	408	SER	ARG	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	440	LYS	ASN	variant	UNP P0DTC2
E	452	ARG	LEU	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2
E	486	VAL	PHE	variant	UNP P0DTC2
E	498	ARG	GLN	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	variant	UNP P0DTC2
E	614	GLY	ASP	variant	UNP P0DTC2
E	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	683	LYS	ASN	variant	UNP P0DTC2
E	?	-	PRO	deletion	UNP P0DTC2
E	?	-	ARG	deletion	UNP P0DTC2
E	?	-	ARG	deletion	UNP P0DTC2
E	?	-	ALA	deletion	UNP P0DTC2
E	764	LYS	ASN	variant	UNP P0DTC2
E	796	TYR	ASP	variant	UNP P0DTC2
E	817	PRO	PHE	engineered mutation	UNP P0DTC2
E	892	PRO	ALA	engineered mutation	UNP P0DTC2
E	899	PRO	ALA	engineered mutation	UNP P0DTC2
E	942	PRO	ALA	engineered mutation	UNP P0DTC2
E	954	HIS	GLN	variant	UNP P0DTC2
E	969	LYS	ASN	variant	UNP P0DTC2
E	986	PRO	LYS	engineered mutation	UNP P0DTC2
E	987	PRO	VAL	engineered mutation	UNP P0DTC2
E	1212	GLY	-	expression tag	UNP P0DTC2
E	1213	SER	-	expression tag	UNP P0DTC2
E	1214	GLY	-	expression tag	UNP P0DTC2
E	1215	ARG	-	expression tag	UNP P0DTC2
E	1216	GLU	-	expression tag	UNP P0DTC2
E	1217	ASN	-	expression tag	UNP P0DTC2
E	1218	LEU	-	expression tag	UNP P0DTC2
E	1219	TYR	-	expression tag	UNP P0DTC2
E	1220	PHE	-	expression tag	UNP P0DTC2
E	1221	GLN	-	expression tag	UNP P0DTC2
E	1222	GLY	-	expression tag	UNP P0DTC2
E	1223	GLY	-	expression tag	UNP P0DTC2
E	1224	GLY	-	expression tag	UNP P0DTC2
E	1225	GLY	-	expression tag	UNP P0DTC2
E	1226	SER	-	expression tag	UNP P0DTC2
E	1227	GLY	-	expression tag	UNP P0DTC2
E	1228	TYR	-	expression tag	UNP P0DTC2
E	1229	ILE	-	expression tag	UNP P0DTC2
E	1230	PRO	-	expression tag	UNP P0DTC2
E	1231	GLU	-	expression tag	UNP P0DTC2
E	1232	ALA	-	expression tag	UNP P0DTC2
E	1233	PRO	-	expression tag	UNP P0DTC2
E	1234	ARG	-	expression tag	UNP P0DTC2
E	1235	ASP	-	expression tag	UNP P0DTC2
E	1236	GLY	-	expression tag	UNP P0DTC2
E	1237	GLN	-	expression tag	UNP P0DTC2
E	1238	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1239	TYR	-	expression tag	UNP P0DTC2
E	1240	VAL	-	expression tag	UNP P0DTC2
E	1241	ARG	-	expression tag	UNP P0DTC2
E	1242	LYS	-	expression tag	UNP P0DTC2
E	1243	ASP	-	expression tag	UNP P0DTC2
E	1244	GLY	-	expression tag	UNP P0DTC2
E	1245	GLU	-	expression tag	UNP P0DTC2
E	1246	TRP	-	expression tag	UNP P0DTC2
E	1247	VAL	-	expression tag	UNP P0DTC2
E	1248	LEU	-	expression tag	UNP P0DTC2
E	1249	LEU	-	expression tag	UNP P0DTC2
E	1250	SER	-	expression tag	UNP P0DTC2
E	1251	THR	-	expression tag	UNP P0DTC2
E	1252	PHE	-	expression tag	UNP P0DTC2
E	1253	LEU	-	expression tag	UNP P0DTC2
E	1254	GLY	-	expression tag	UNP P0DTC2
E	1255	HIS	-	expression tag	UNP P0DTC2
E	1256	HIS	-	expression tag	UNP P0DTC2
E	1257	HIS	-	expression tag	UNP P0DTC2
E	1258	HIS	-	expression tag	UNP P0DTC2
E	1259	HIS	-	expression tag	UNP P0DTC2
E	1260	HIS	-	expression tag	UNP P0DTC2
F	22	ILE	THR	variant	UNP P0DTC2
F	?	-	LEU	deletion	UNP P0DTC2
F	?	-	PRO	deletion	UNP P0DTC2
F	?	-	PRO	deletion	UNP P0DTC2
F	27	SER	ALA	variant	UNP P0DTC2
F	?	-	HIS	deletion	UNP P0DTC2
F	?	-	VAL	deletion	UNP P0DTC2
F	142	ASP	GLY	variant	UNP P0DTC2
F	213	GLY	VAL	variant	UNP P0DTC2
F	339	ASP	GLY	variant	UNP P0DTC2
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	376	ALA	THR	variant	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	452	ARG	LEU	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	478	LYS	THR	variant	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	486	VAL	PHE	variant	UNP P0DTC2
F	498	ARG	GLN	variant	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	variant	UNP P0DTC2
F	614	GLY	ASP	variant	UNP P0DTC2
F	655	TYR	HIS	variant	UNP P0DTC2
F	683	LYS	ASN	variant	UNP P0DTC2
F	?	-	PRO	deletion	UNP P0DTC2
F	?	-	ARG	deletion	UNP P0DTC2
F	?	-	ARG	deletion	UNP P0DTC2
F	?	-	ALA	deletion	UNP P0DTC2
F	764	LYS	ASN	variant	UNP P0DTC2
F	796	TYR	ASP	variant	UNP P0DTC2
F	817	PRO	PHE	engineered mutation	UNP P0DTC2
F	892	PRO	ALA	engineered mutation	UNP P0DTC2
F	899	PRO	ALA	engineered mutation	UNP P0DTC2
F	942	PRO	ALA	engineered mutation	UNP P0DTC2
F	954	HIS	GLN	variant	UNP P0DTC2
F	969	LYS	ASN	variant	UNP P0DTC2
F	986	PRO	LYS	engineered mutation	UNP P0DTC2
F	987	PRO	VAL	engineered mutation	UNP P0DTC2
F	1212	GLY	-	expression tag	UNP P0DTC2
F	1213	SER	-	expression tag	UNP P0DTC2
F	1214	GLY	-	expression tag	UNP P0DTC2
F	1215	ARG	-	expression tag	UNP P0DTC2
F	1216	GLU	-	expression tag	UNP P0DTC2
F	1217	ASN	-	expression tag	UNP P0DTC2
F	1218	LEU	-	expression tag	UNP P0DTC2
F	1219	TYR	-	expression tag	UNP P0DTC2
F	1220	PHE	-	expression tag	UNP P0DTC2
F	1221	GLN	-	expression tag	UNP P0DTC2
F	1222	GLY	-	expression tag	UNP P0DTC2
F	1223	GLY	-	expression tag	UNP P0DTC2
F	1224	GLY	-	expression tag	UNP P0DTC2
F	1225	GLY	-	expression tag	UNP P0DTC2
F	1226	SER	-	expression tag	UNP P0DTC2
F	1227	GLY	-	expression tag	UNP P0DTC2
F	1228	TYR	-	expression tag	UNP P0DTC2
F	1229	ILE	-	expression tag	UNP P0DTC2
F	1230	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1231	GLU	-	expression tag	UNP P0DTC2
F	1232	ALA	-	expression tag	UNP P0DTC2
F	1233	PRO	-	expression tag	UNP P0DTC2
F	1234	ARG	-	expression tag	UNP P0DTC2
F	1235	ASP	-	expression tag	UNP P0DTC2
F	1236	GLY	-	expression tag	UNP P0DTC2
F	1237	GLN	-	expression tag	UNP P0DTC2
F	1238	ALA	-	expression tag	UNP P0DTC2
F	1239	TYR	-	expression tag	UNP P0DTC2
F	1240	VAL	-	expression tag	UNP P0DTC2
F	1241	ARG	-	expression tag	UNP P0DTC2
F	1242	LYS	-	expression tag	UNP P0DTC2
F	1243	ASP	-	expression tag	UNP P0DTC2
F	1244	GLY	-	expression tag	UNP P0DTC2
F	1245	GLU	-	expression tag	UNP P0DTC2
F	1246	TRP	-	expression tag	UNP P0DTC2
F	1247	VAL	-	expression tag	UNP P0DTC2
F	1248	LEU	-	expression tag	UNP P0DTC2
F	1249	LEU	-	expression tag	UNP P0DTC2
F	1250	SER	-	expression tag	UNP P0DTC2
F	1251	THR	-	expression tag	UNP P0DTC2
F	1252	PHE	-	expression tag	UNP P0DTC2
F	1253	LEU	-	expression tag	UNP P0DTC2
F	1254	GLY	-	expression tag	UNP P0DTC2
F	1255	HIS	-	expression tag	UNP P0DTC2
F	1256	HIS	-	expression tag	UNP P0DTC2
F	1257	HIS	-	expression tag	UNP P0DTC2
F	1258	HIS	-	expression tag	UNP P0DTC2
F	1259	HIS	-	expression tag	UNP P0DTC2
F	1260	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Light chain of D1F6 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		
2	M	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		
2	N	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		
2	I	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		

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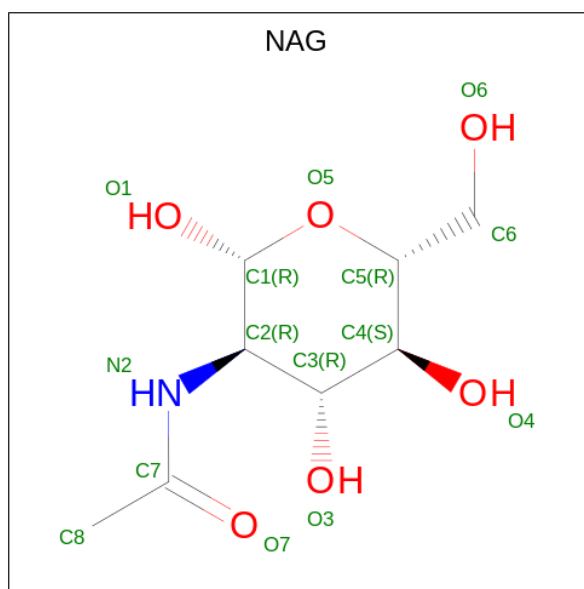
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		
2	L	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		

- Molecule 3 is a protein called Heavy chain of D1F6 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		
3	Q	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		
3	R	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		
3	J	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		
3	O	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		
3	P	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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





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

- Molecule 1: Spike glycoprotein

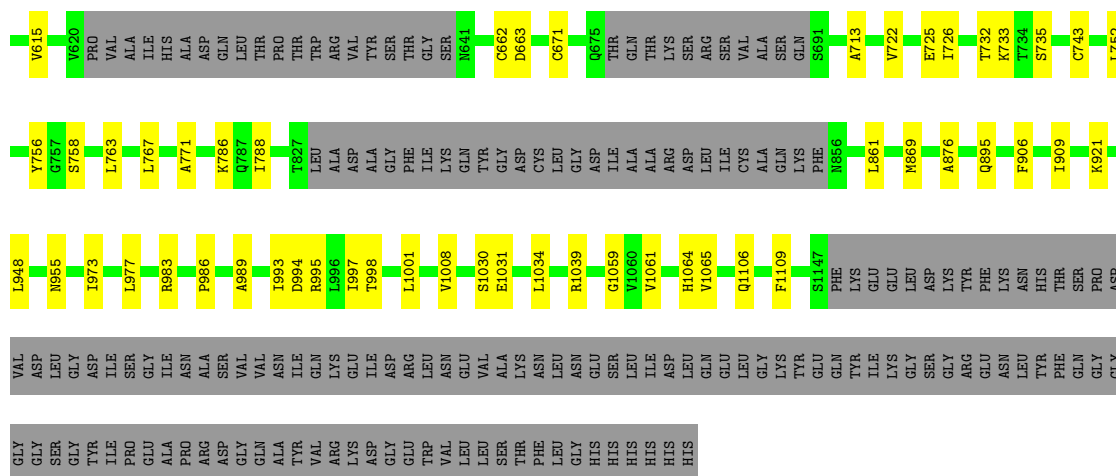
Chain D:  70% 11% 20%

[illegible]

- Molecule 1: Spike glycoprotein

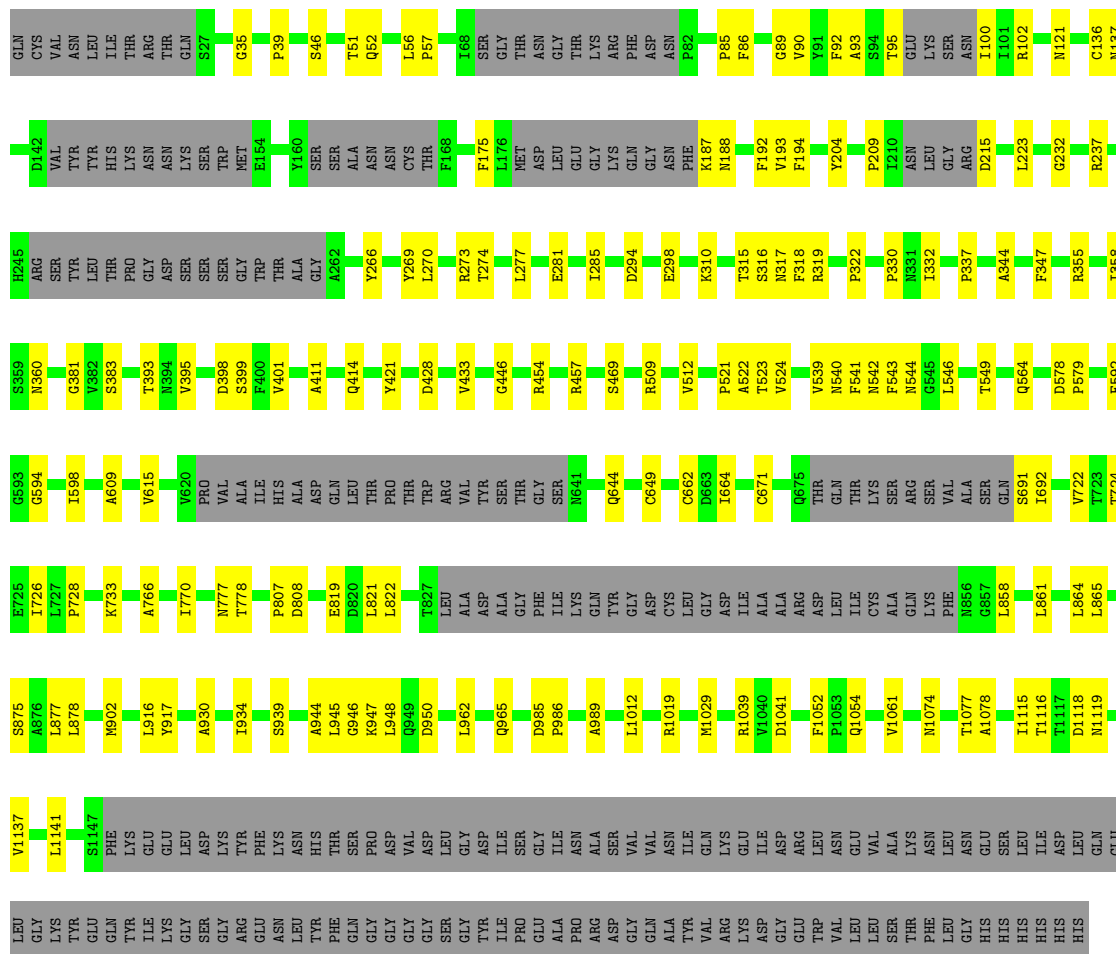
Chain E:  72% 8% 20%

ALA	A263	S316	N317	P330	F338	V341	R346	I358	F377	C391	V395	D398	K424	I434	G447	M450	R452	P463	D467	Q474	C480	L482	T523	V524	C525	T547	G566	D578	P579	I598	A609	V612																		
GLN	CYS	VAL	ASN	LEU	ILE	THR	ARG	THR	GLN	S27	R34	S60	N61	I63	SER	GLY	THR	ASN	GLY	THR	LYS	ARG	PHE	ASP	ASN	P82	E96	LVS	SER	N99	R102	F106	G107	T108	T109	L110	D111	L117	V126	V127	I128	L141	D142	VAL	THR	GLY	HIS	LYS	ASN	ASN
LYS	TRP	MET	GLU	S155	E166	Y160	SER	ALA	ASN	ASN	CYS	THR	F168	P174	F175	L176	MET	ASP	LEU	GLU	GLY	LYS	GLN	GLY	ASN	PHE	R187	F201	L210	ASN	LEU	GLY	ARG	ASP	L216	L229	S247	THR	LEU	THR	PRO	GLY	ASP	SER	SER	SER	GLY	THR	ALA	CYS



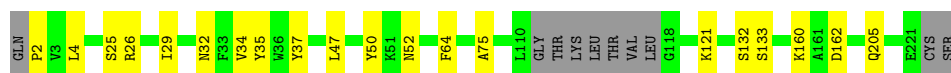
• Molecule 1: Spike glycoprotein

Chain F: 68% 13% 20%



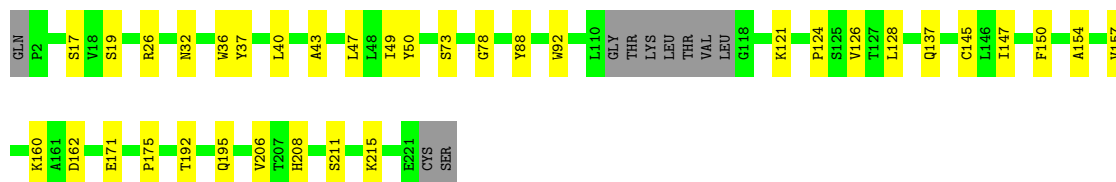
• Molecule 2: Light chain of D1F6 Fab

Chain G: 87% 9%



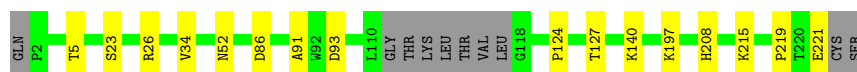
- Molecule 2: Light chain of D1F6 Fab

Chain M: 80% 16% .



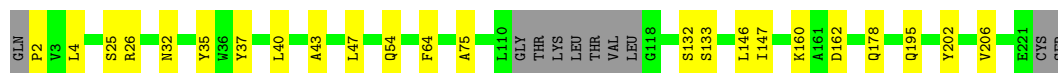
- Molecule 2: Light chain of D1F6 Fab

Chain N: 88% 7% .



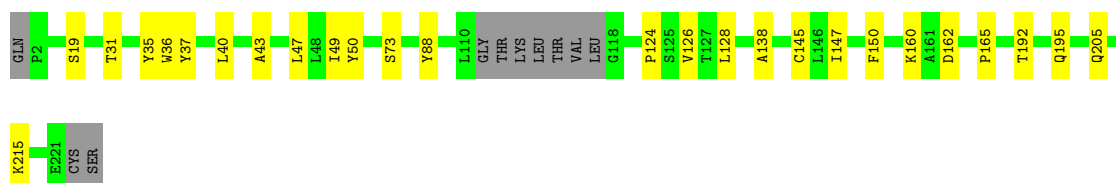
- Molecule 2: Light chain of D1F6 Fab

Chain I: 85% 10% .



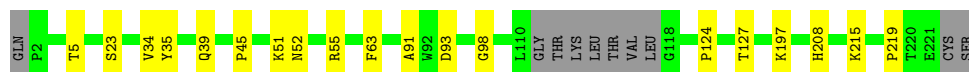
- Molecule 2: Light chain of D1F6 Fab

Chain K: 84% 12% .



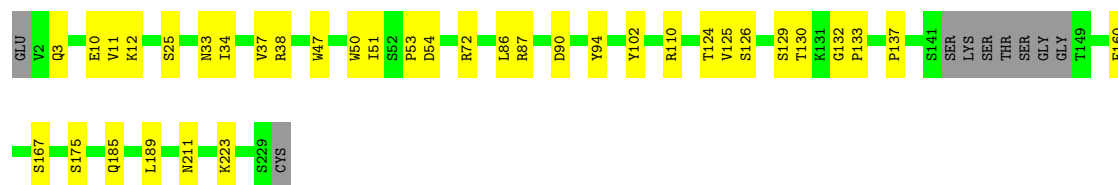
- Molecule 2: Light chain of D1F6 Fab

Chain L: 87% 9% .



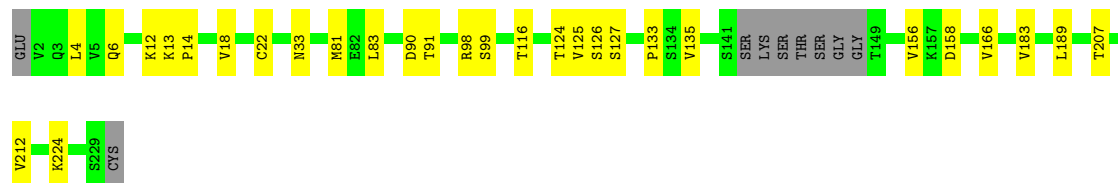
- Molecule 3: Heavy chain of D1F6 Fab

Chain H: 80% 16% .



- Molecule 3: Heavy chain of D1F6 Fab

Chain Q: 83% 13% .



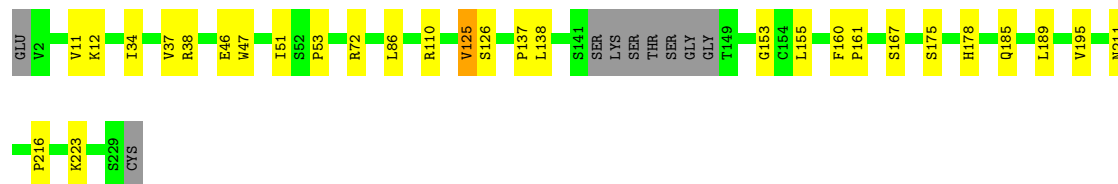
- Molecule 3: Heavy chain of D1F6 Fab

Chain R: 85% 11% .



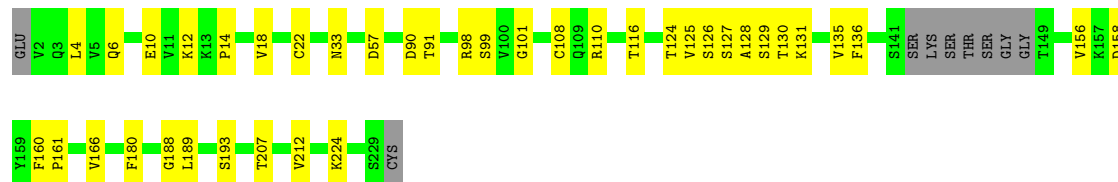
- Molecule 3: Heavy chain of D1F6 Fab

Chain J: 83% 12% .



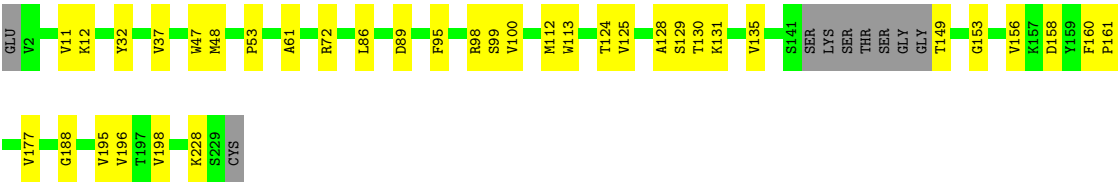
- Molecule 3: Heavy chain of D1F6 Fab

Chain O: 79% 17% .



- Molecule 3: Heavy chain of D1F6 Fab

Chain P: 80% 16% .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30100	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.17	0/7972	0.40	0/10845
1	B	0.19	0/7972	0.40	1/10845 (0.0%)
1	C	0.15	0/7960	0.38	0/10830
1	D	0.13	0/7972	0.35	0/10845
1	E	0.13	0/7972	0.34	0/10845
1	F	0.15	0/7960	0.38	0/10830
2	G	0.12	0/1633	0.31	0/2229
2	I	0.12	0/1633	0.32	0/2229
2	K	0.13	0/1633	0.36	0/2229
2	L	0.12	0/1633	0.33	0/2229
2	M	0.13	0/1633	0.35	0/2229
2	N	0.14	0/1633	0.36	0/2229
3	H	0.14	0/1722	0.39	0/2349
3	J	0.13	0/1722	0.36	0/2349
3	O	0.19	0/1722	0.46	0/2349
3	P	0.16	0/1722	0.44	0/2349
3	Q	0.16	0/1722	0.42	0/2349
3	R	0.15	0/1722	0.42	0/2349
All	All	0.15	0/67938	0.38	1/92508 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1011	GLN	N-CA-C	-7.89	102.63	111.07

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	7790	0	7620	114	0
1	B	7790	0	7622	90	0
1	C	7778	0	7610	88	0
1	D	7790	0	7629	78	0
1	E	7790	0	7629	61	0
1	F	7778	0	7614	97	0
2	G	1591	0	1539	14	0
2	I	1591	0	1539	16	0
2	K	1591	0	1539	18	0
2	L	1591	0	1539	13	0
2	M	1591	0	1539	22	0
2	N	1591	0	1539	14	0
3	H	1679	0	1624	28	0
3	J	1679	0	1624	23	0
3	O	1679	0	1624	30	0
3	P	1679	0	1624	36	0
3	Q	1679	0	1624	18	0
3	R	1679	0	1624	19	0
4	A	126	0	117	22	0
4	B	98	0	91	2	0
4	C	56	0	52	8	0
All	All	66616	0	64962	729	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 729 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:C:710:ASN:HB2	4:C:1301:NAG:O7	1.16	1.30
1:C:710:ASN:CB	4:C:1301:NAG:O7	2.05	1.03
3:O:130:THR:HA	3:O:160:PHE:HB3	1.38	1.01
1:C:710:ASN:HB2	4:C:1301:NAG:C7	1.94	0.98
3:P:130:THR:HA	3:P:160:PHE:HB3	1.51	0.90

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	972/1238 (78%)	928 (96%)	44 (4%)	0	100	100
1	B	972/1238 (78%)	924 (95%)	48 (5%)	0	100	100
1	C	971/1238 (78%)	916 (94%)	55 (6%)	0	100	100
1	D	972/1238 (78%)	942 (97%)	30 (3%)	0	100	100
1	E	972/1238 (78%)	932 (96%)	40 (4%)	0	100	100
1	F	971/1238 (78%)	915 (94%)	55 (6%)	1 (0%)	48	83
2	G	209/223 (94%)	203 (97%)	6 (3%)	0	100	100
2	I	209/223 (94%)	204 (98%)	5 (2%)	0	100	100
2	K	209/223 (94%)	203 (97%)	6 (3%)	0	100	100
2	L	209/223 (94%)	200 (96%)	9 (4%)	0	100	100
2	M	209/223 (94%)	204 (98%)	5 (2%)	0	100	100
2	N	209/223 (94%)	199 (95%)	10 (5%)	0	100	100
3	H	217/230 (94%)	208 (96%)	9 (4%)	0	100	100
3	J	217/230 (94%)	205 (94%)	12 (6%)	0	100	100
3	O	217/230 (94%)	206 (95%)	11 (5%)	0	100	100
3	P	217/230 (94%)	204 (94%)	13 (6%)	0	100	100
3	Q	217/230 (94%)	207 (95%)	10 (5%)	0	100	100
3	R	217/230 (94%)	208 (96%)	9 (4%)	0	100	100
All	All	8386/10146 (83%)	8008 (96%)	377 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	1141	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	871/1075 (81%)	870 (100%)	1 (0%)	92	95
1	B	871/1075 (81%)	871 (100%)	0	100	100
1	C	869/1075 (81%)	869 (100%)	0	100	100
1	D	871/1075 (81%)	871 (100%)	0	100	100
1	E	871/1075 (81%)	871 (100%)	0	100	100
1	F	869/1075 (81%)	869 (100%)	0	100	100
2	G	178/187 (95%)	178 (100%)	0	100	100
2	I	178/187 (95%)	178 (100%)	0	100	100
2	K	178/187 (95%)	178 (100%)	0	100	100
2	L	178/187 (95%)	178 (100%)	0	100	100
2	M	178/187 (95%)	178 (100%)	0	100	100
2	N	178/187 (95%)	178 (100%)	0	100	100
3	H	191/198 (96%)	191 (100%)	0	100	100
3	J	191/198 (96%)	190 (100%)	1 (0%)	86	89
3	O	191/198 (96%)	191 (100%)	0	100	100
3	P	191/198 (96%)	191 (100%)	0	100	100
3	Q	191/198 (96%)	191 (100%)	0	100	100
3	R	191/198 (96%)	191 (100%)	0	100	100
All	All	7436/8760 (85%)	7434 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	709	ASN
3	J	125	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	658	ASN
1	F	644	GLN
1	E	913	GLN
1	F	66	HIS
2	I	52	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](#)

20 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	$\# Z  > 2$
4	NAG	B	1303	1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	A	1309	1	14,14,15	0.34	0	17,19,21	0.68	0
4	NAG	A	1305	1	14,14,15	0.34	0	17,19,21	0.81	1 (5%)
4	NAG	B	1307	1	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	B	1301	1	14,14,15	0.33	0	17,19,21	0.49	0
4	NAG	C	1301	1	14,14,15	0.33	0	17,19,21	0.66	0
4	NAG	A	1303	1	14,14,15	0.35	0	17,19,21	0.74	1 (5%)
4	NAG	C	1304	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	C	1302	1	14,14,15	0.33	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	1305	1	14,14,15	0.32	0	17,19,21	0.63	0
4	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	0.82	0
4	NAG	C	1303	1	14,14,15	0.27	0	17,19,21	0.56	0
4	NAG	B	1302	1	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	A	1306	1	14,14,15	0.31	0	17,19,21	0.63	0
4	NAG	A	1304	1	14,14,15	0.29	0	17,19,21	0.80	0
4	NAG	B	1304	1	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	A	1302	1	14,14,15	0.30	0	17,19,21	0.73	0
4	NAG	A	1308	1	14,14,15	0.29	0	17,19,21	0.67	0
4	NAG	A	1307	1	14,14,15	0.23	0	17,19,21	0.47	0
4	NAG	B	1306	1	14,14,15	0.26	0	17,19,21	0.60	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
4	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1305	NAG	C2-N2-C7	2.43	126.36	122.90
4	A	1303	NAG	C4-C3-C2	-2.09	107.95	111.02

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

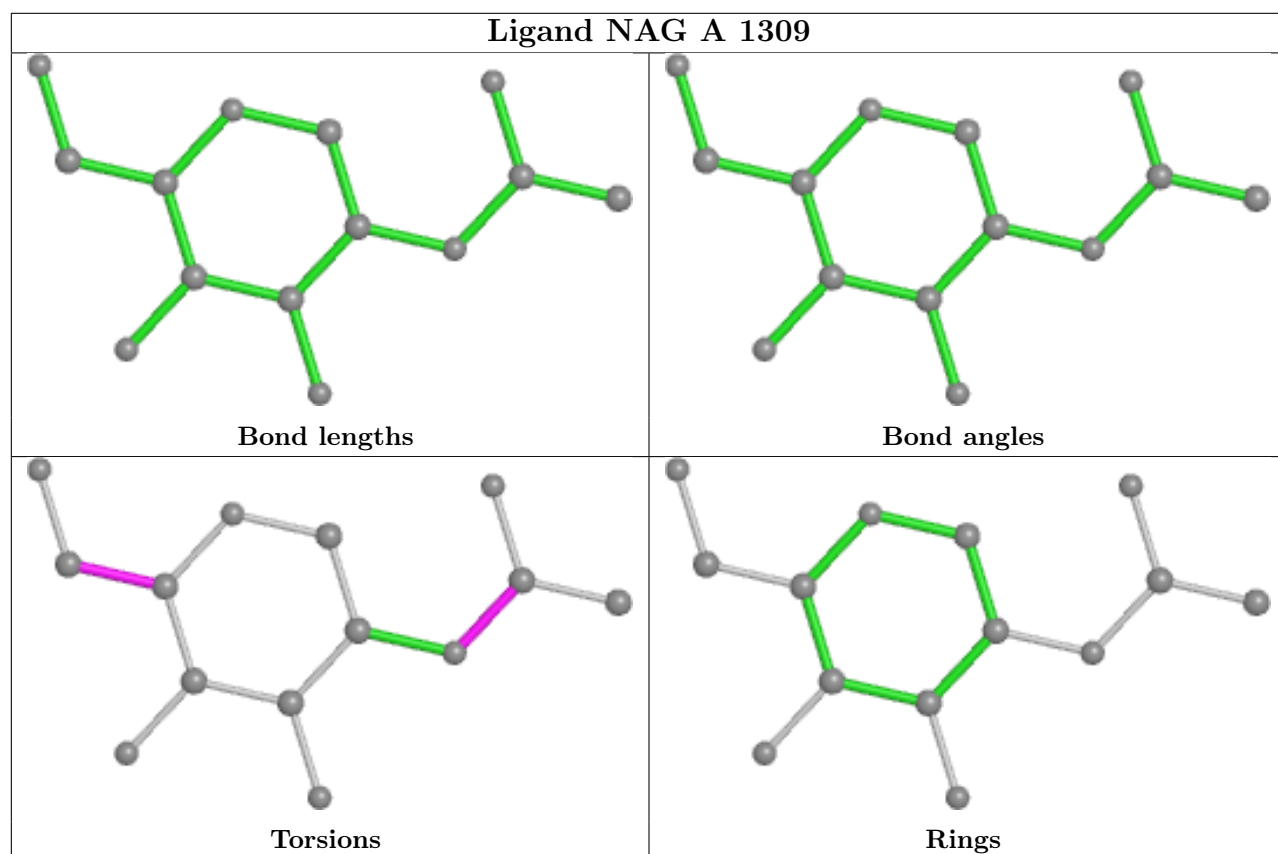
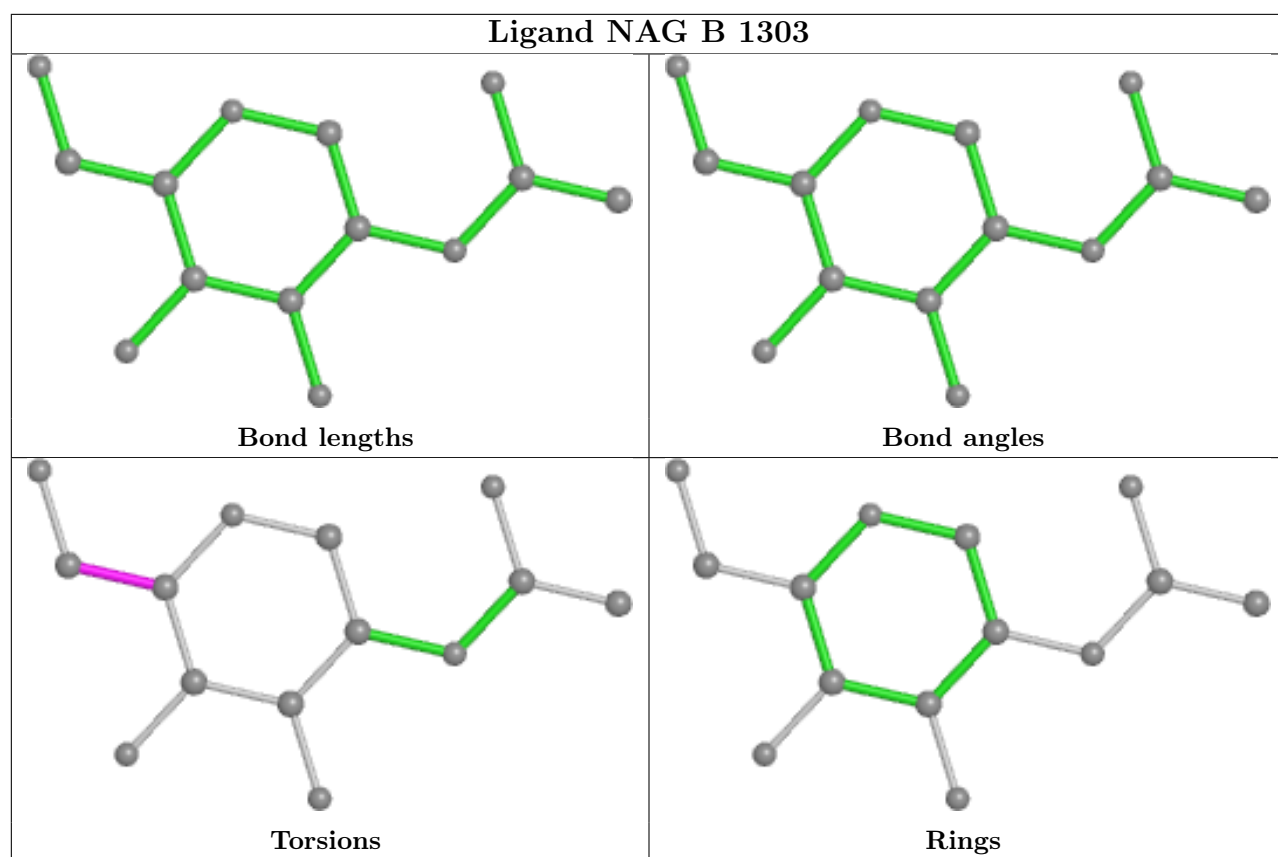
Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	C	1301	NAG	C8-C7-N2-C2
4	C	1301	NAG	O7-C7-N2-C2

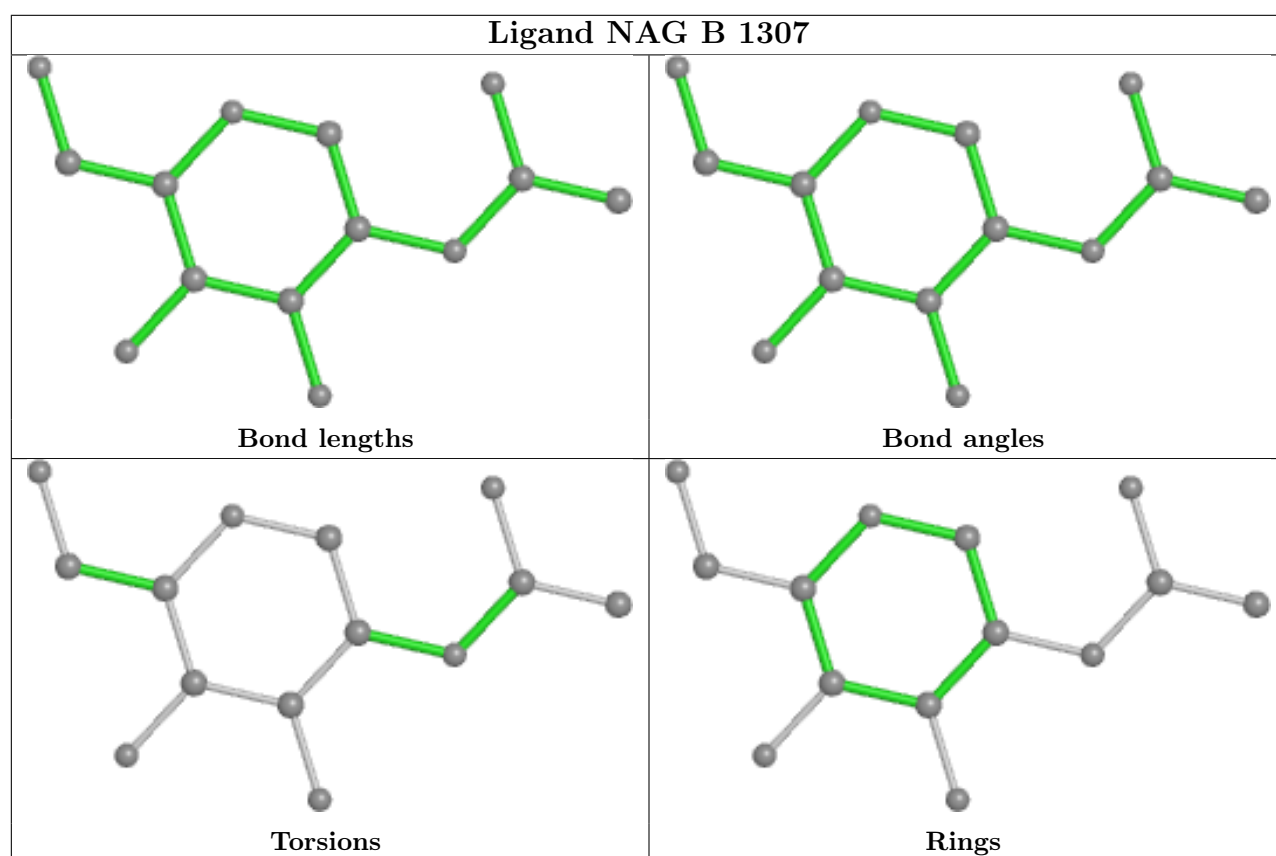
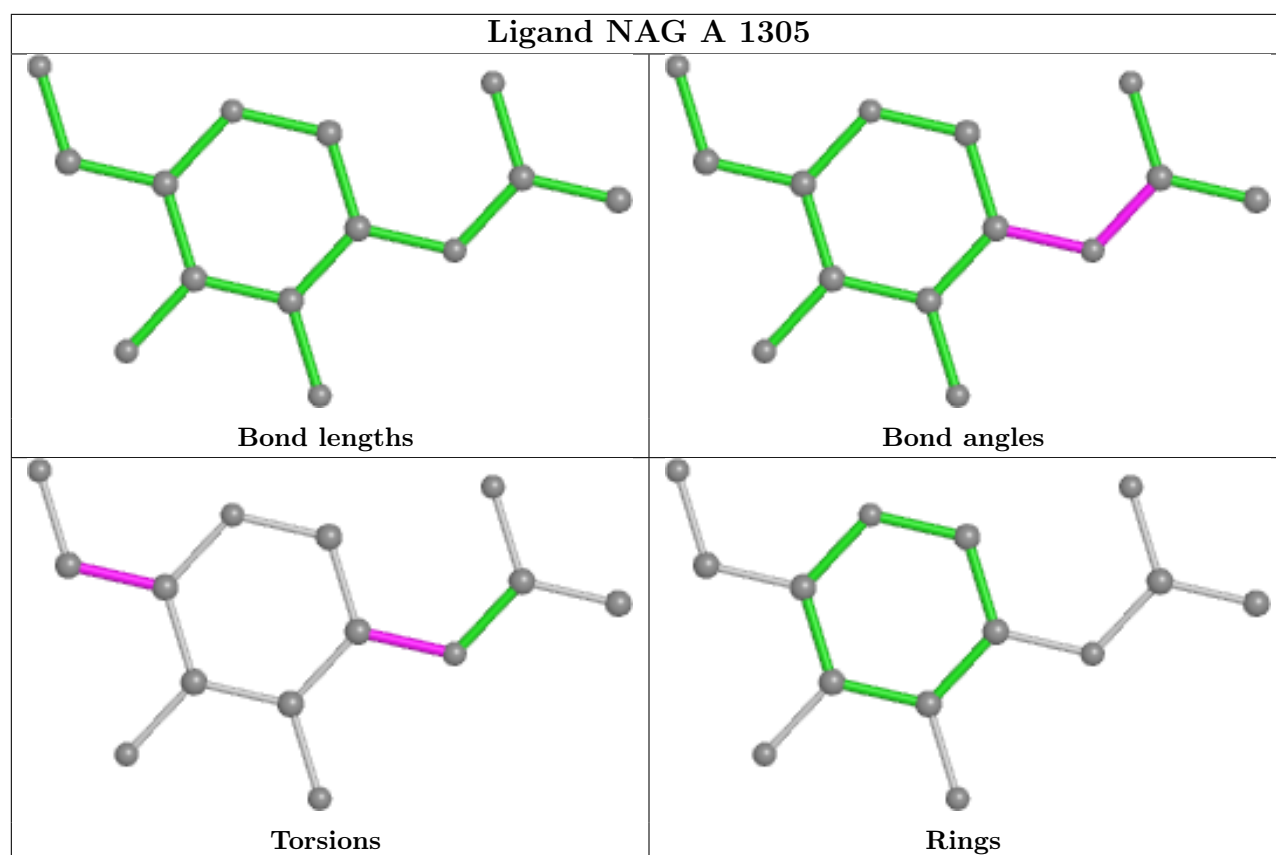
There are no ring outliers.

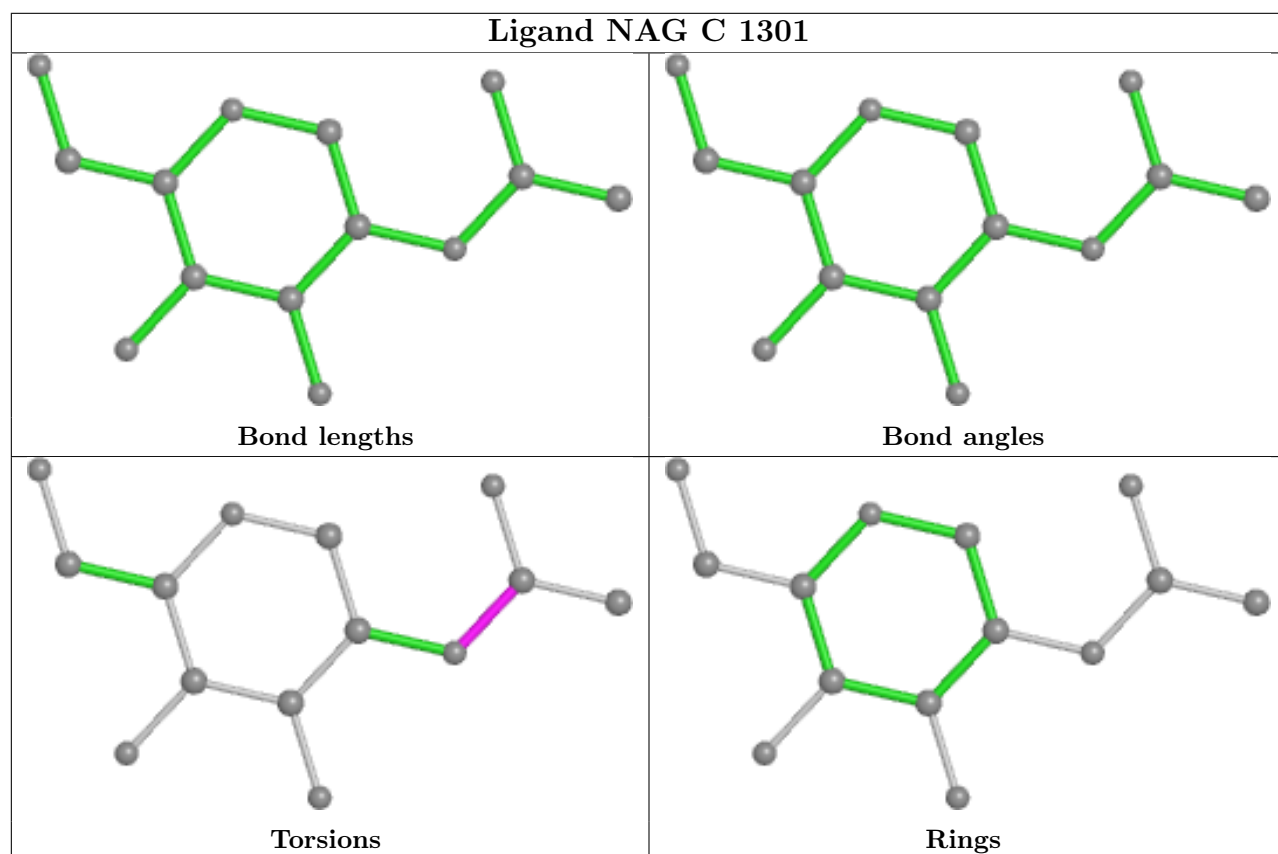
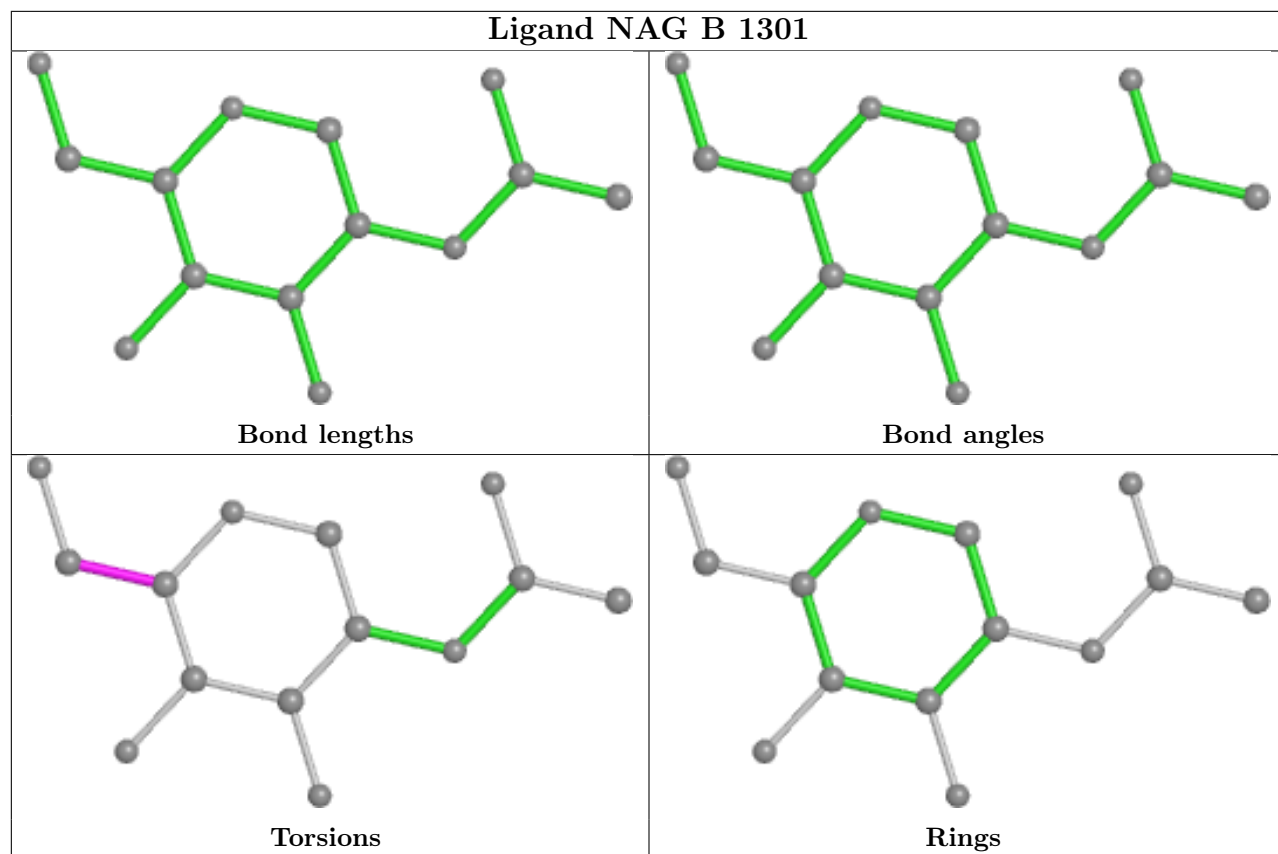
10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1309	NAG	6	0
4	C	1301	NAG	5	0
4	C	1304	NAG	1	0
4	B	1305	NAG	2	0
4	A	1301	NAG	3	0
4	C	1303	NAG	2	0
4	A	1306	NAG	1	0
4	A	1304	NAG	5	0
4	A	1302	NAG	1	0
4	A	1308	NAG	6	0

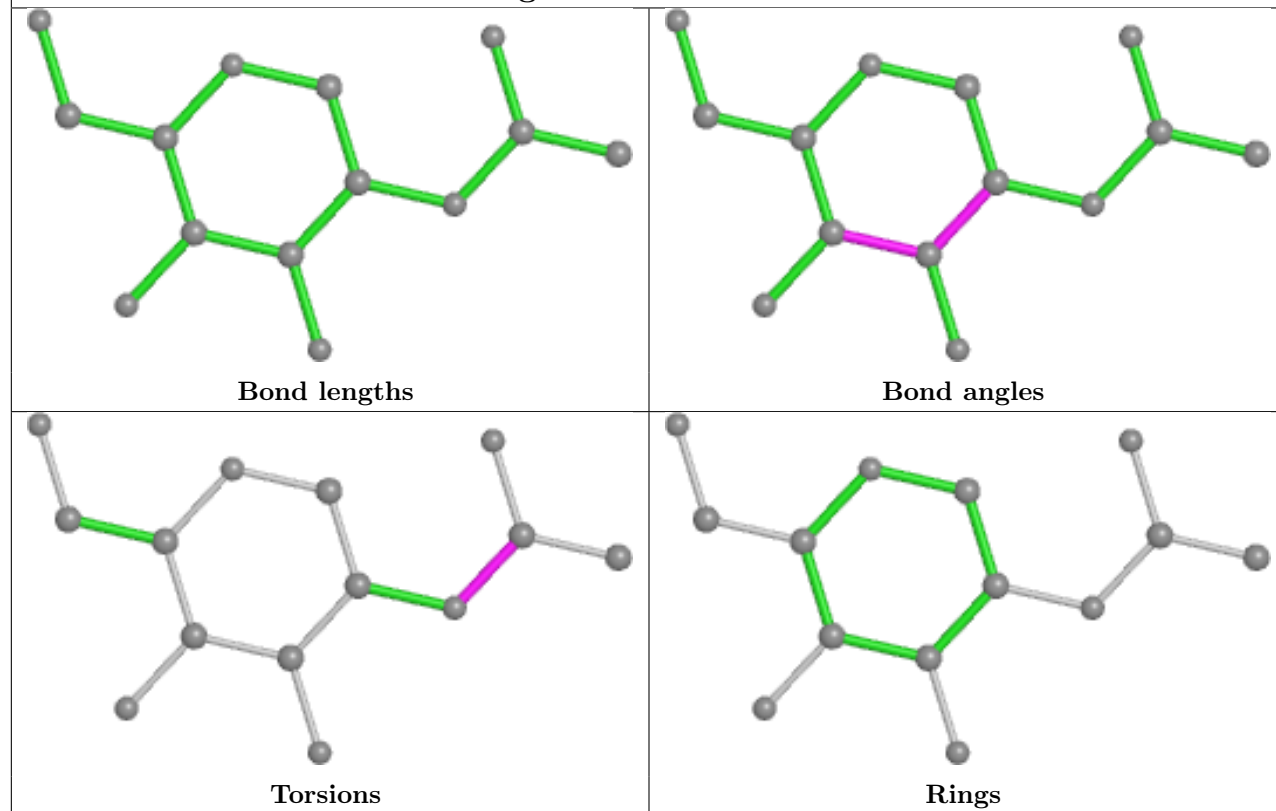
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



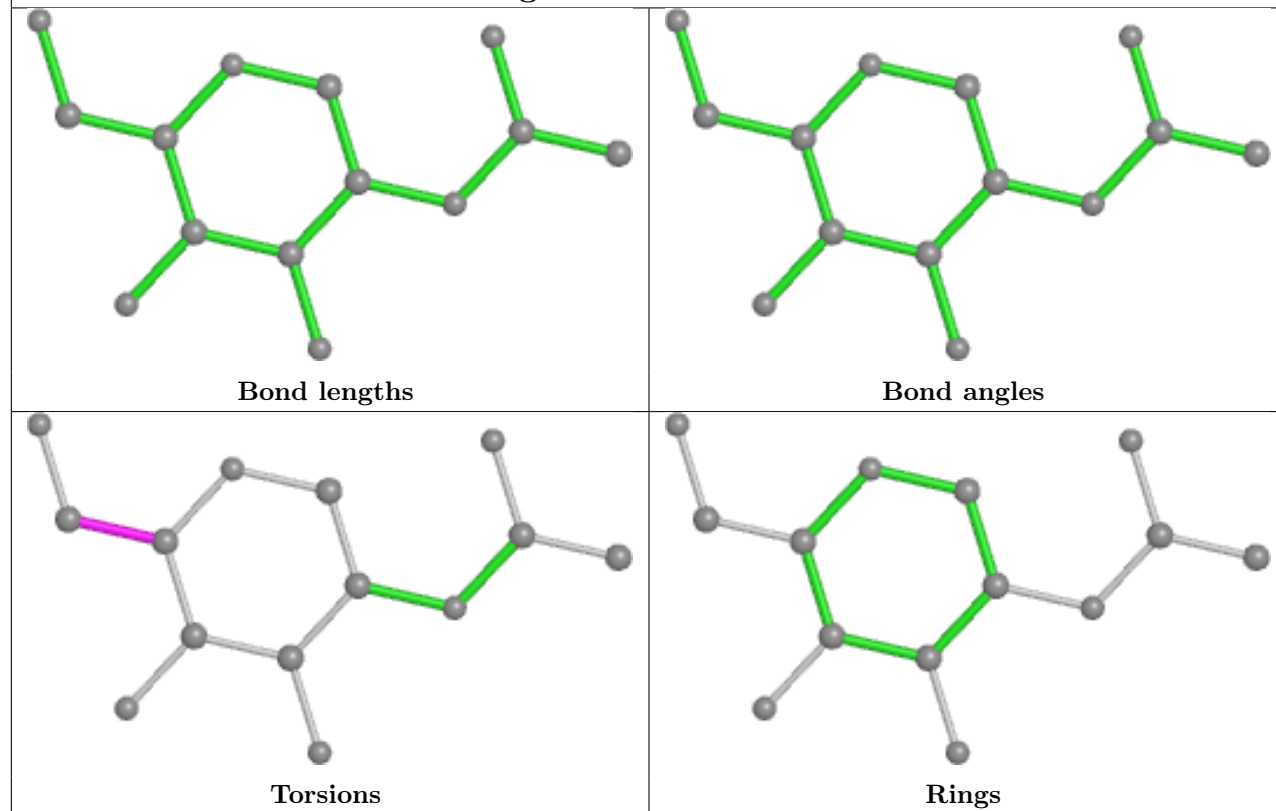




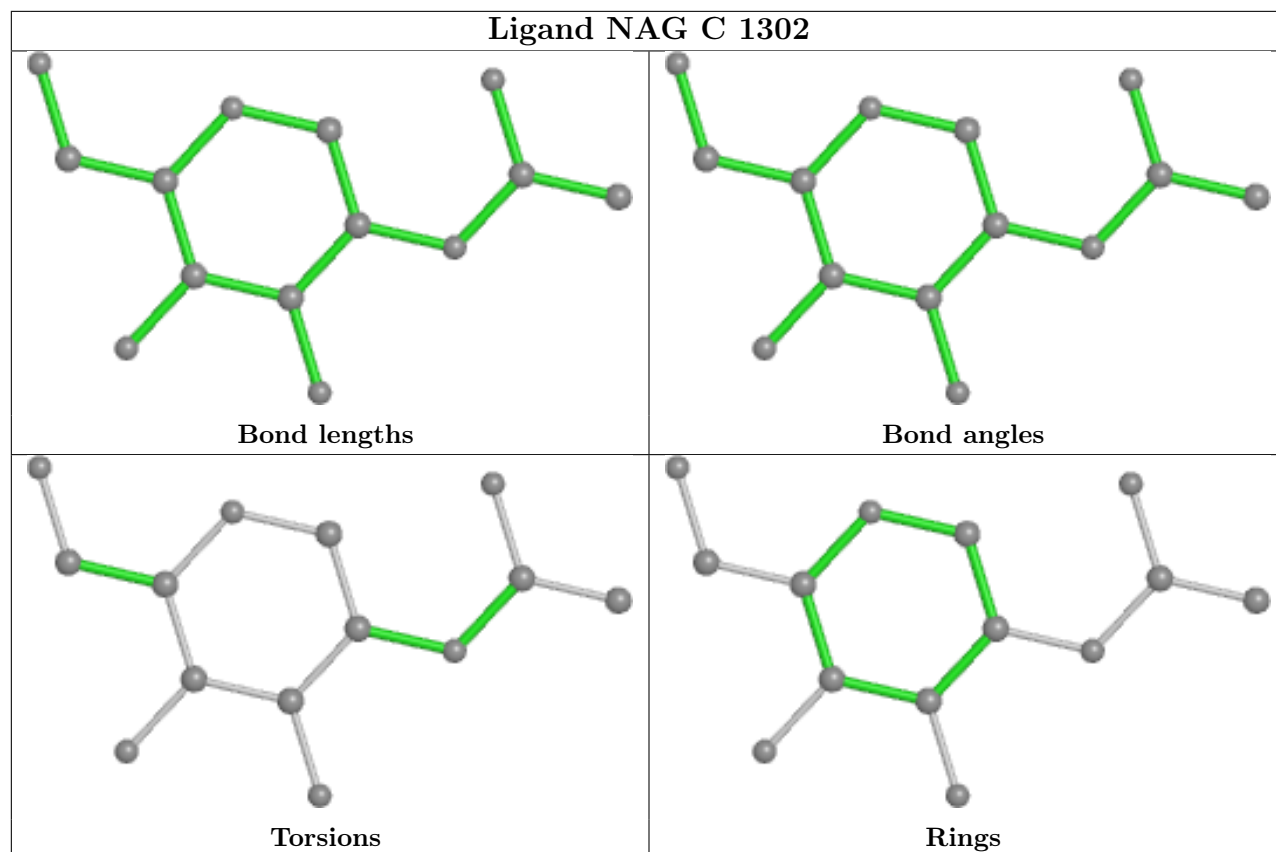
## Ligand NAG A 1303



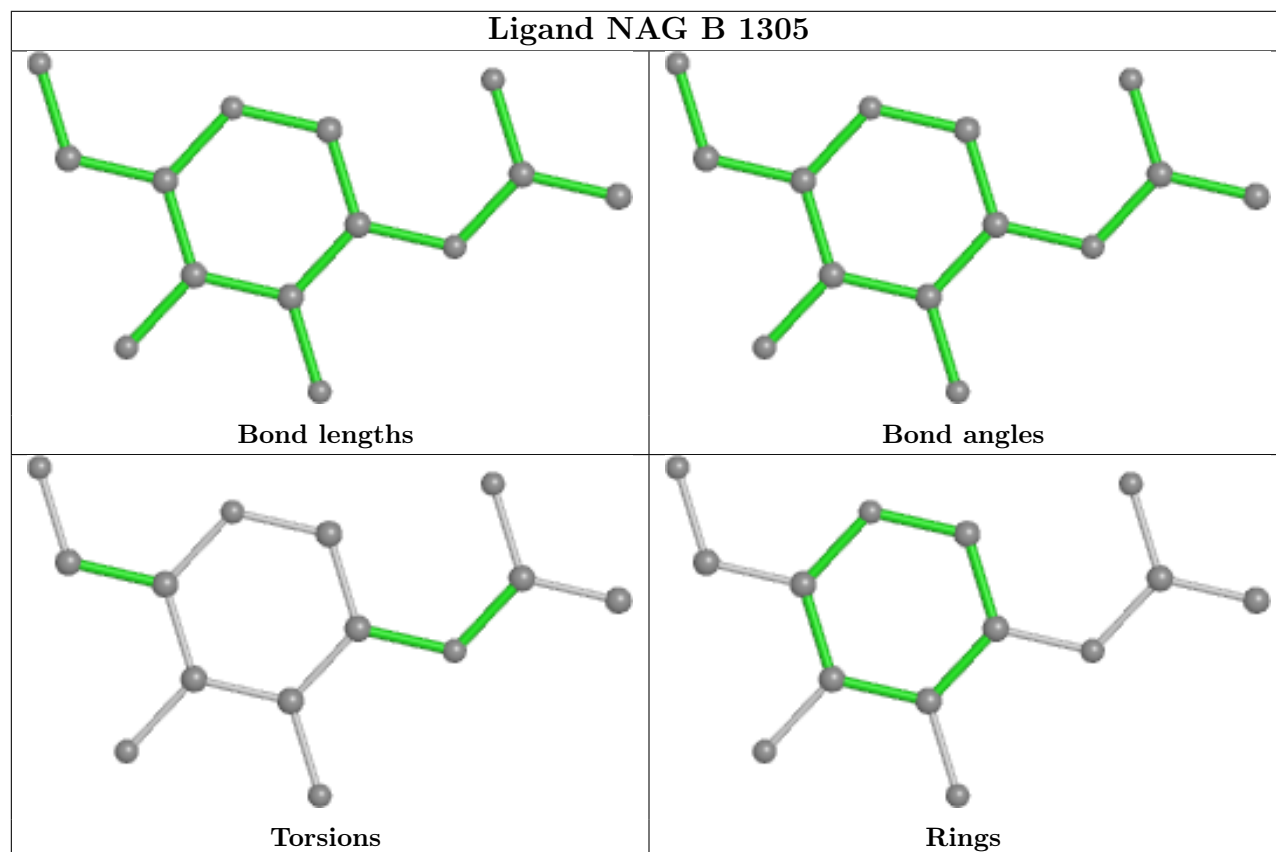
## Ligand NAG C 1304

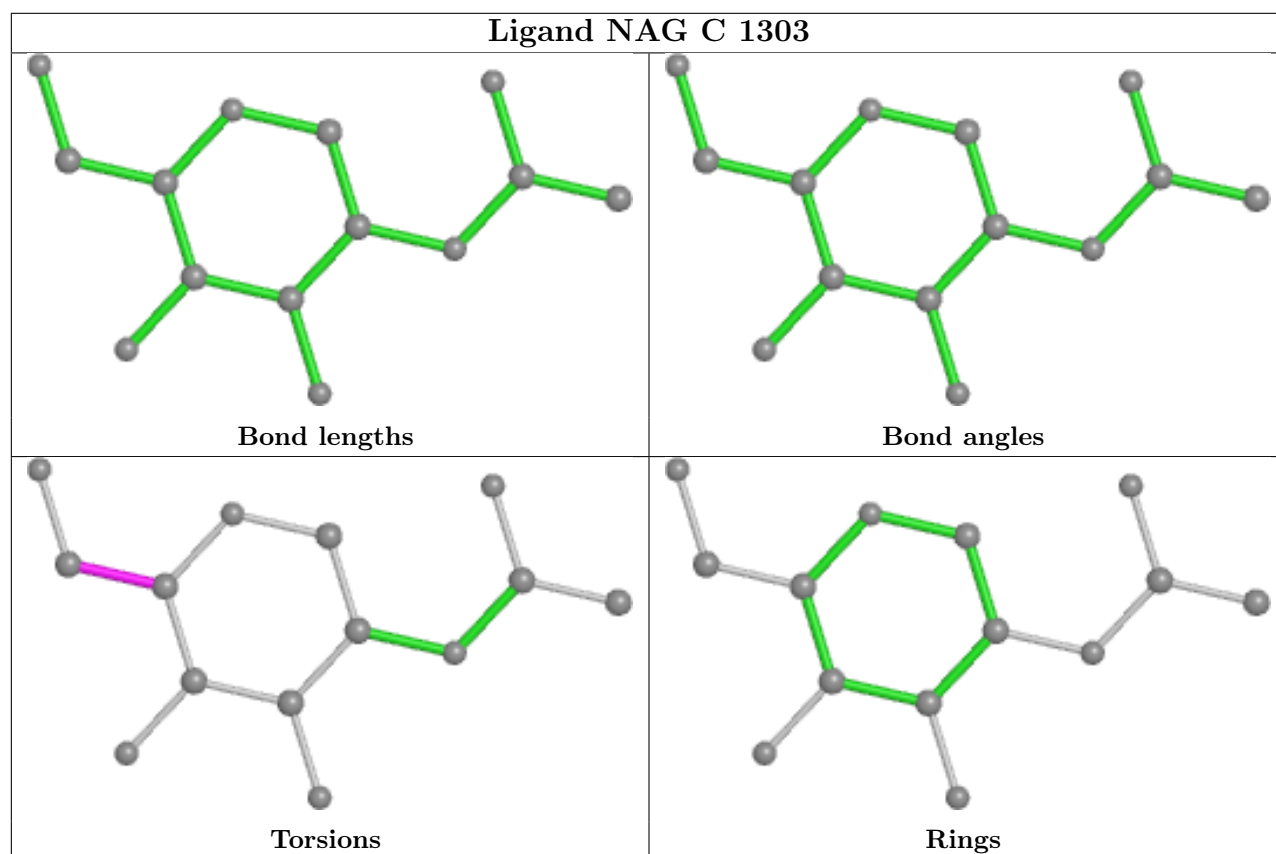
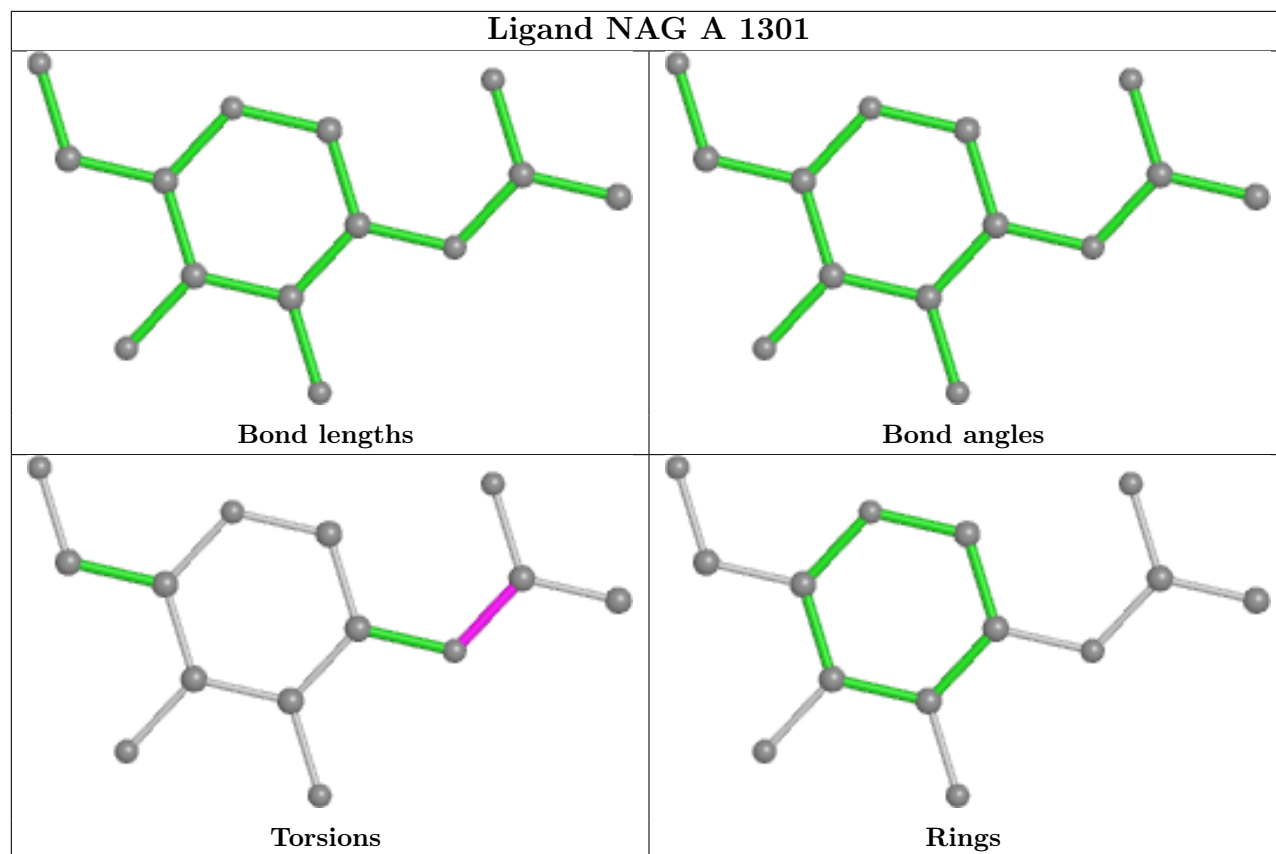


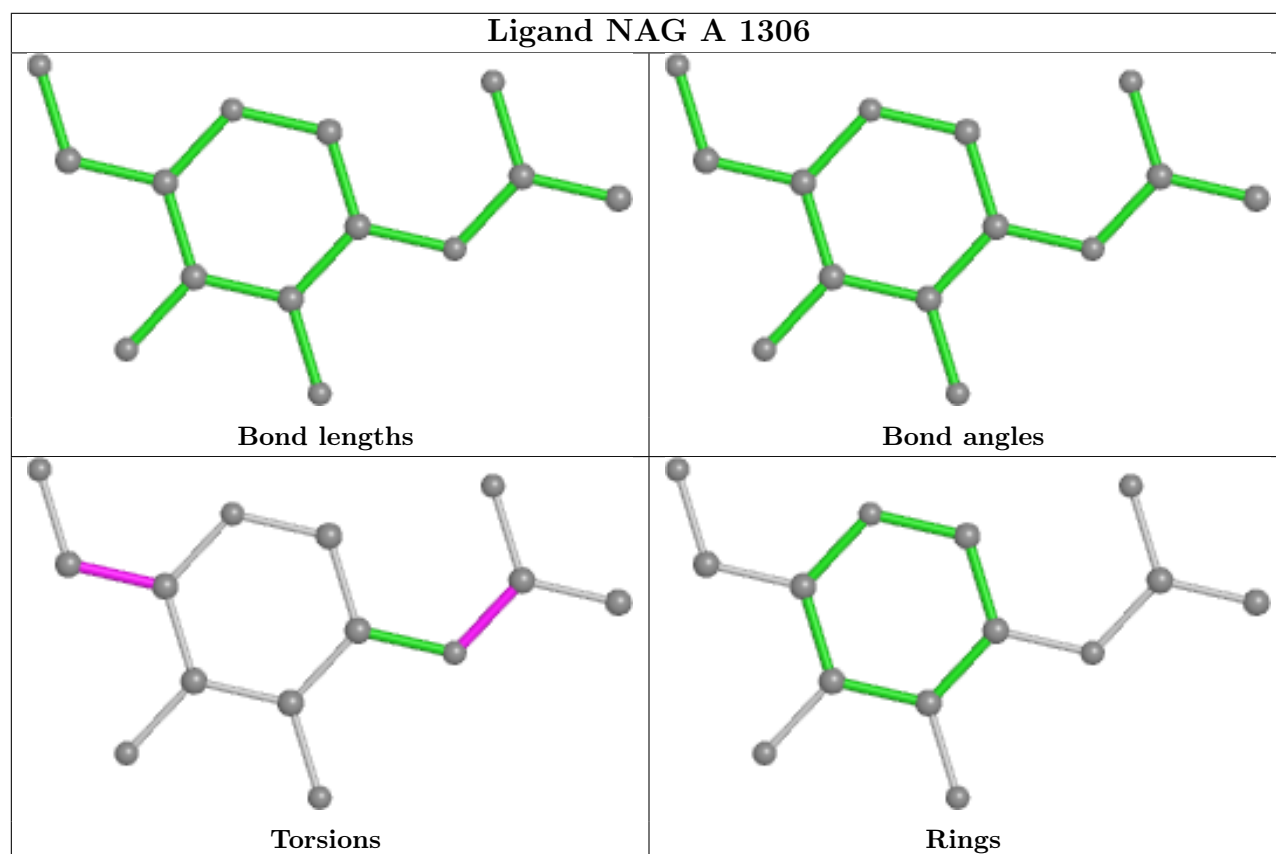
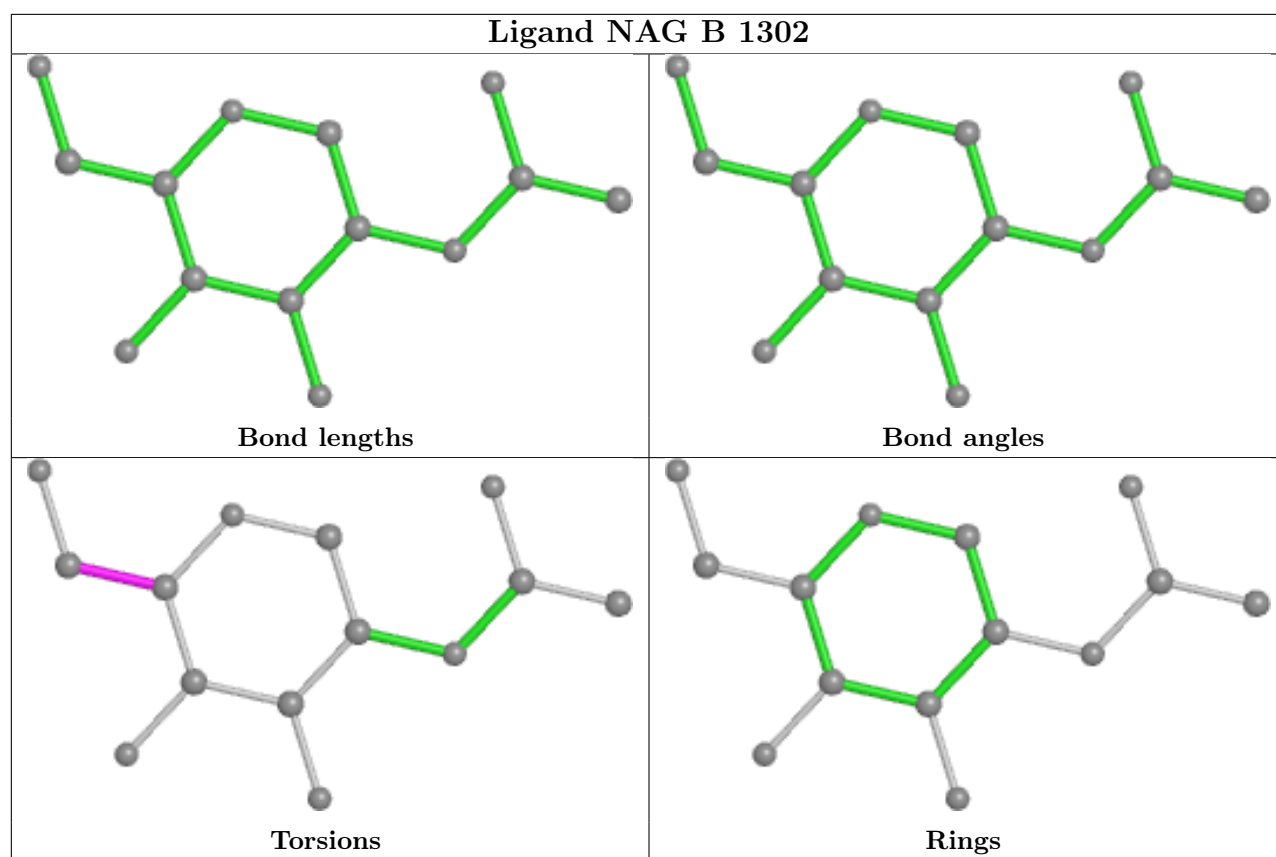
## Ligand NAG C 1302

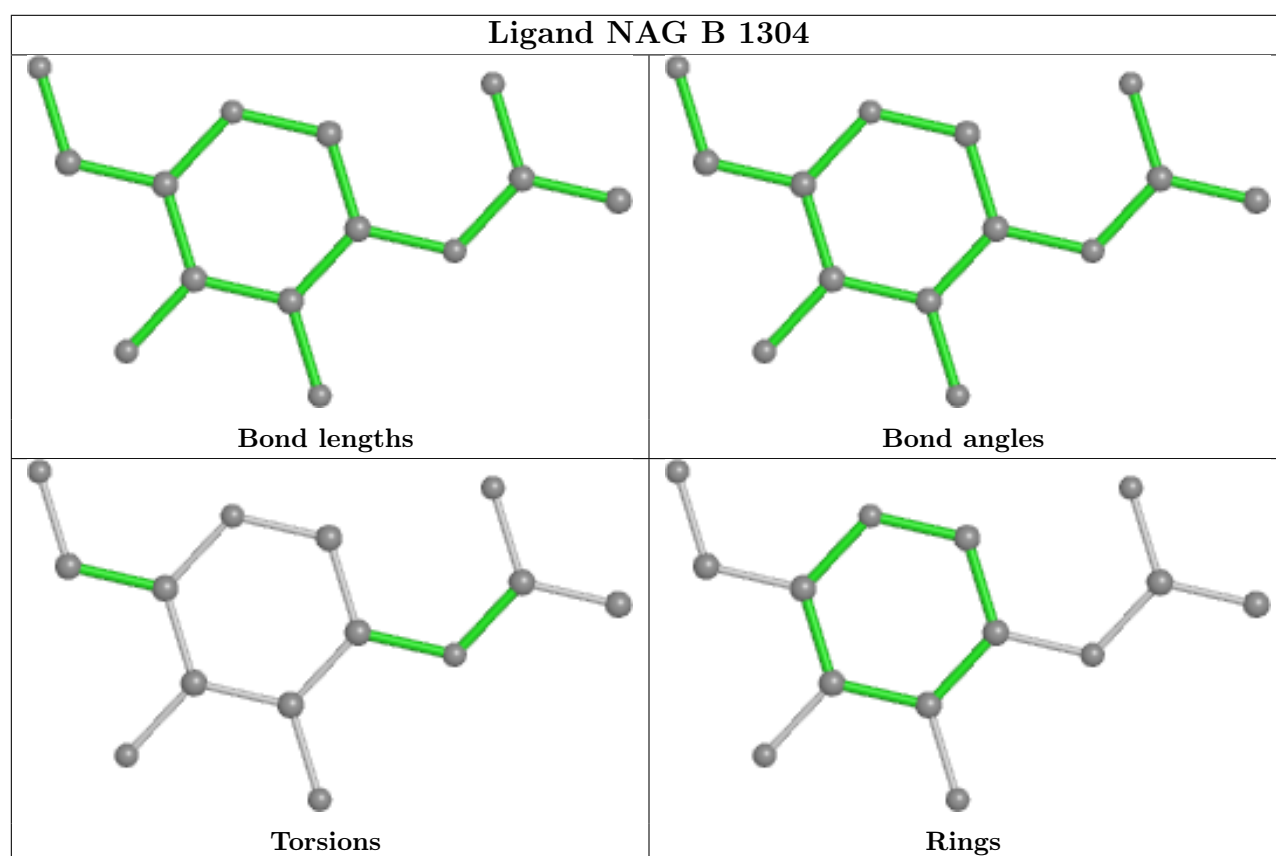
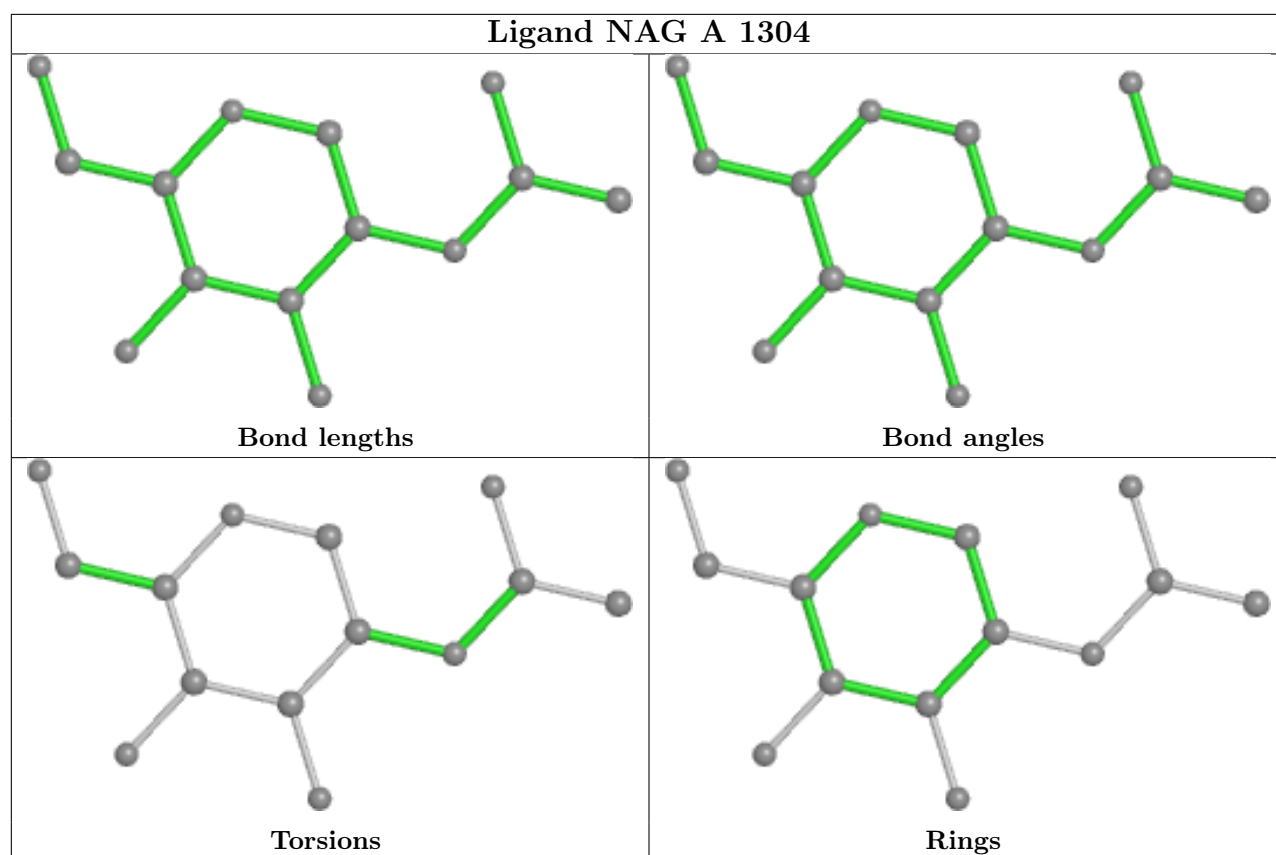


## Ligand NAG B 1305

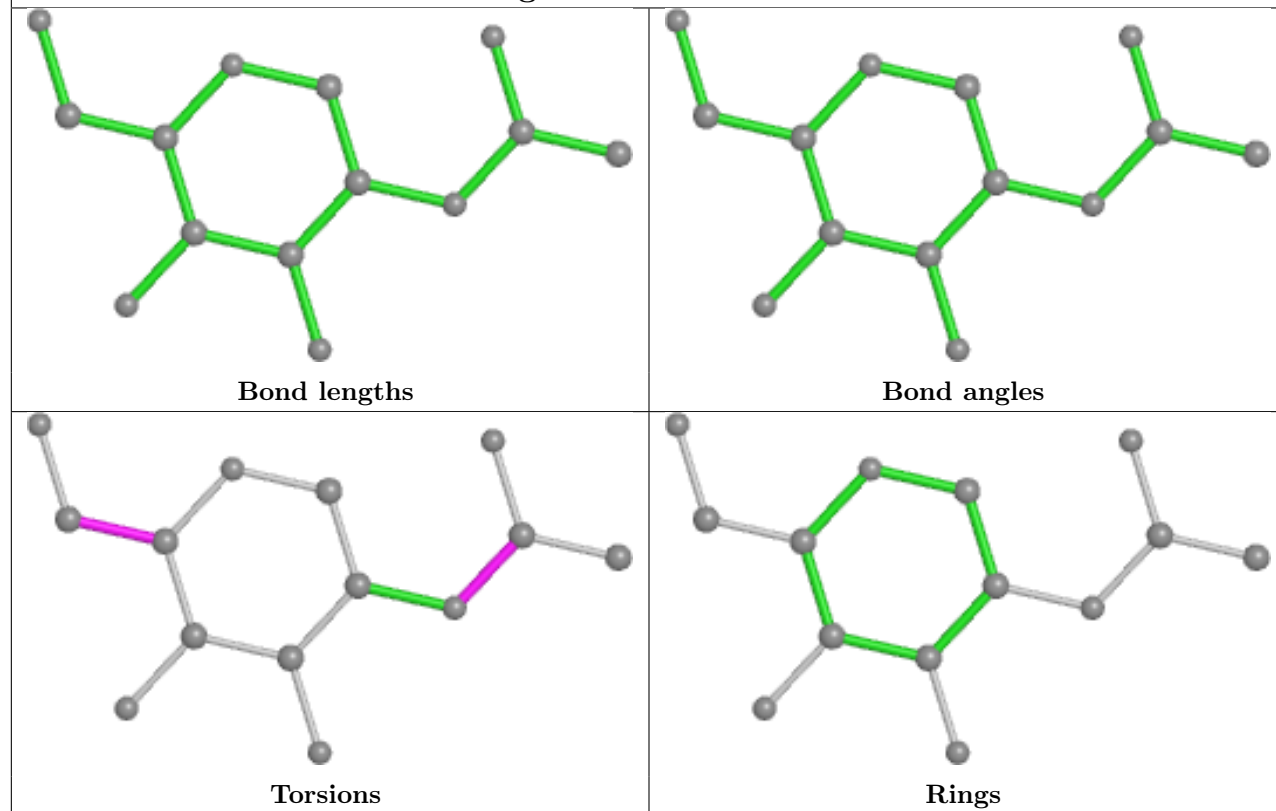




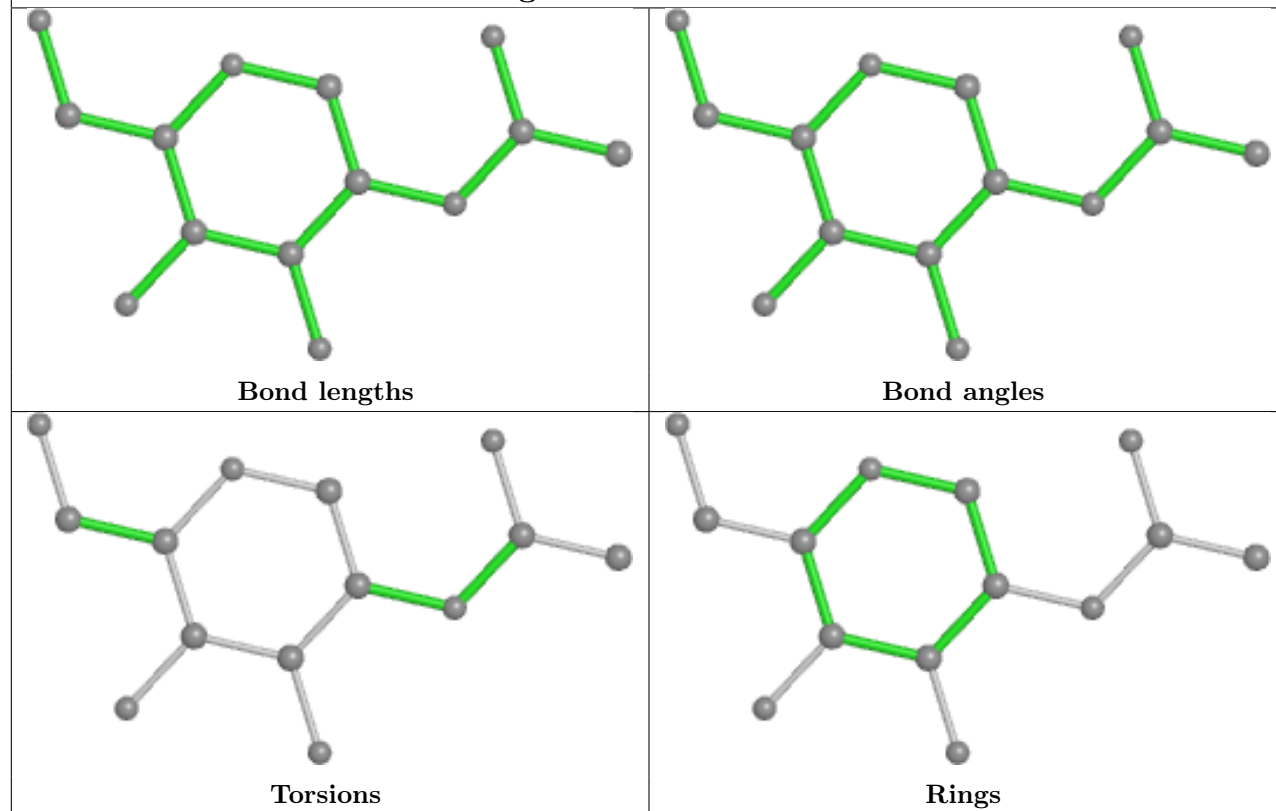


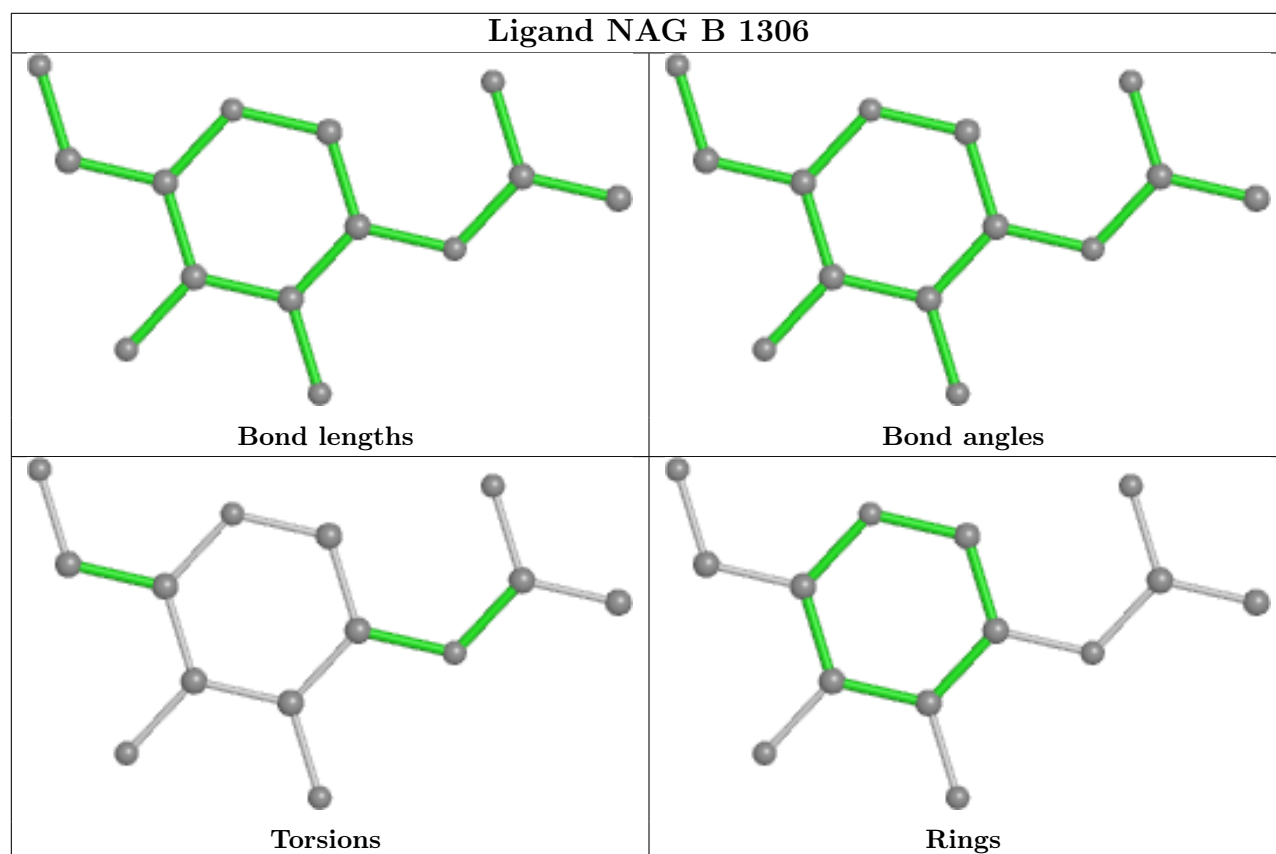
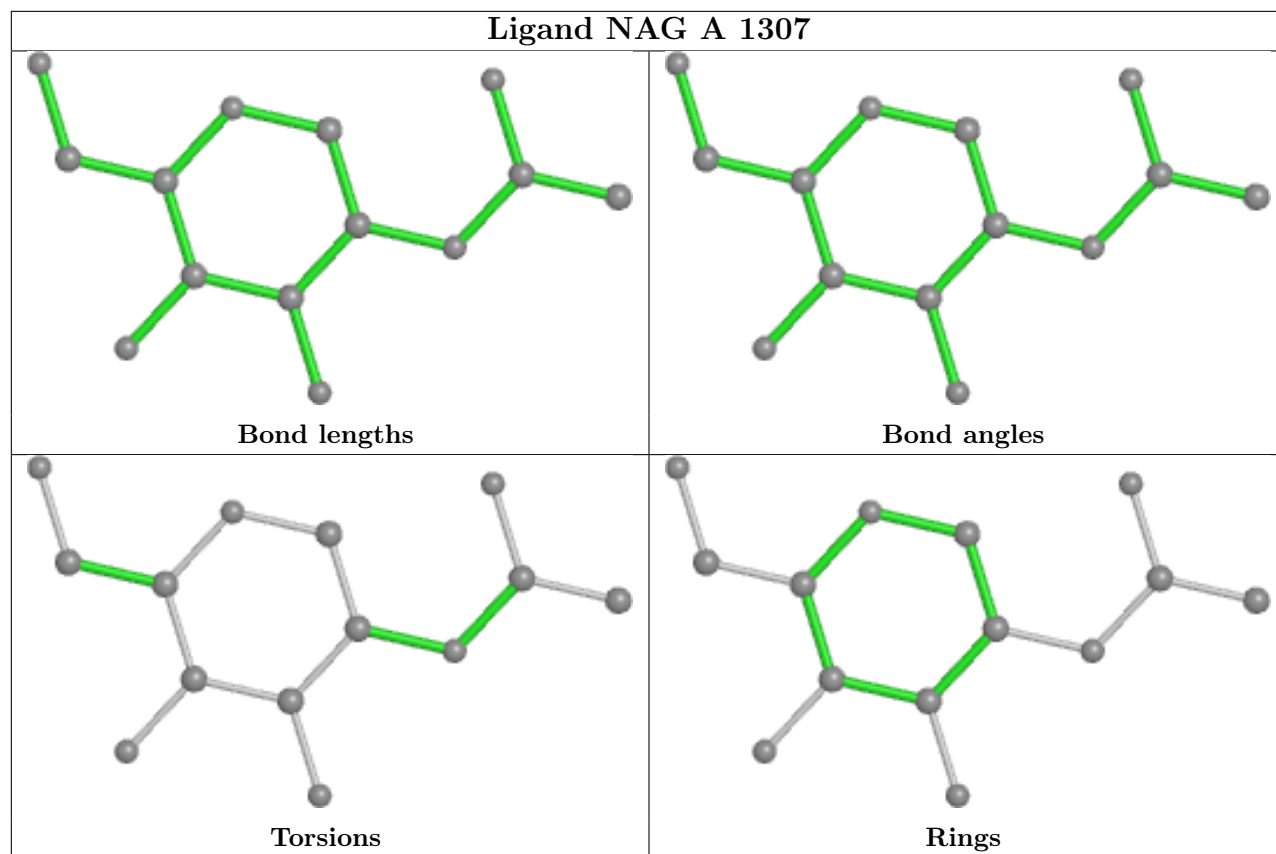


## Ligand NAG A 1302



## Ligand NAG A 1308





## 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.