Full wwPDB EM Validation Report ⓘ

Oct 23, 2023 – 01:36 pm BST

PDB ID	:	8AJL
EMDB ID	:	EMD-15482
Title	:	Structure of the Ancestral Scaffold Antigen-6 of Coronavirus Spike protein
Authors	:	Hueting, D.; Schriever, K.; Wallden, K.; Andrell, J.; Syren, P.O.
Deposited on	:	2022-07-28
Resolution	:	2.77 Å(reported)
Based on initial models	:	6ZOZ, 7BNN

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

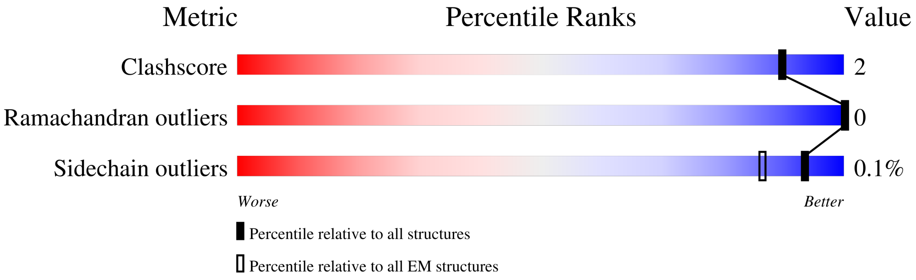
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

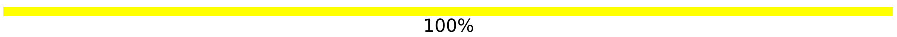
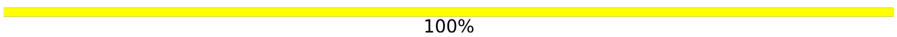
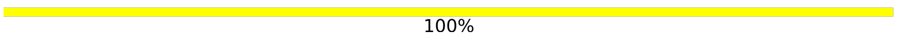
The reported resolution of this entry is 2.77 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1259	
1	B	1259	
1	C	1259	
2	L	2	
2	M	2	
2	N	2	
2	P	2	
2	Q	2	

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Mol	Chain	Length	Quality of chain
2	R	2	🟨 100%
2	U	2	🟩 50% 🟨 50%
2	V	2	🟨 100%
2	W	2	🟨 50% 🟧 50%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 52748 atoms, of which 26003 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,Fibritin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1109	Total 16997	C 5482	H 8376	N 1435	O 1657	S 47	0	0
1	C	1109	Total 16999	C 5482	H 8378	N 1435	O 1657	S 47	0	0
1	B	1109	Total 16997	C 5482	H 8376	N 1435	O 1657	S 47	0	0

There are 933 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	THR	VAL	engineered mutation	UNP P0DTC2
A	20	CYS	ASN	engineered mutation	UNP P0DTC2
A	21	GLY	LEU	engineered mutation	UNP P0DTC2
A	23	LEU	THR	engineered mutation	UNP P0DTC2
A	24	SER	ARG	engineered mutation	UNP P0DTC2
A	25	ASN	THR	engineered mutation	UNP P0DTC2
A	26	LYS	GLN	engineered mutation	UNP P0DTC2
A	27	SER	LEU	engineered mutation	UNP P0DTC2
A	30	ASN	ALA	engineered mutation	UNP P0DTC2
A	31	MET	TYR	engineered mutation	UNP P0DTC2
A	33	GLN	-	insertion	UNP P0DTC2
A	34	PHE	-	insertion	UNP P0DTC2
A	35	SER	ASN	engineered mutation	UNP P0DTC2
A	37	SER	PHE	engineered mutation	UNP P0DTC2
A	38	ARG	THR	engineered mutation	UNP P0DTC2
A	46	ASP	LYS	engineered mutation	UNP P0DTC2
A	47	ILE	VAL	engineered mutation	UNP P0DTC2
A	51	ASP	SER	engineered mutation	UNP P0DTC2
A	55	LEU	SER	engineered mutation	UNP P0DTC2
A	59	TYR	LEU	engineered mutation	UNP P0DTC2
A	64	ASN	PHE	engineered mutation	UNP P0DTC2
A	?	-	TRP	deletion	UNP P0DTC2
A	69	ARG	PHE	engineered mutation	UNP P0DTC2
A	70	TYR	HIS	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	71	LEU	ALA	engineered mutation	UNP P0DTC2
A	72	SER	ILE	engineered mutation	UNP P0DTC2
A	73	LEU	HIS	engineered mutation	UNP P0DTC2
A	74	ASN	VAL	engineered mutation	UNP P0DTC2
A	76	ASP	GLY	engineered mutation	UNP P0DTC2
A	77	SER	THR	engineered mutation	UNP P0DTC2
A	78	ASP	ASN	engineered mutation	UNP P0DTC2
A	79	ARG	GLY	engineered mutation	UNP P0DTC2
A	80	ILE	THR	engineered mutation	UNP P0DTC2
A	81	VAL	LYS	engineered mutation	UNP P0DTC2
A	87	ILE	VAL	engineered mutation	UNP P0DTC2
A	88	ILE	LEU	engineered mutation	UNP P0DTC2
A	91	GLY	ASN	engineered mutation	UNP P0DTC2
A	98	ALA	SER	engineered mutation	UNP P0DTC2
A	104	VAL	ILE	engineered mutation	UNP P0DTC2
A	112	SER	THR	engineered mutation	UNP P0DTC2
A	116	ASN	SER	engineered mutation	UNP P0DTC2
A	117	THR	LYS	engineered mutation	UNP P0DTC2
A	118	SER	THR	engineered mutation	UNP P0DTC2
A	121	ALA	LEU	engineered mutation	UNP P0DTC2
A	122	ILE	LEU	engineered mutation	UNP P0DTC2
A	124	MET	VAL	engineered mutation	UNP P0DTC2
A	127	SER	ALA	engineered mutation	UNP P0DTC2
A	129	HIS	ASN	engineered mutation	UNP P0DTC2
A	130	ILE	VAL	engineered mutation	UNP P0DTC2
A	133	ARG	LYS	engineered mutation	UNP P0DTC2
A	136	ASN	GLU	engineered mutation	UNP P0DTC2
A	139	LEU	PHE	engineered mutation	UNP P0DTC2
A	141	ASP	ASN	engineered mutation	UNP P0DTC2
A	144	MET	PHE	engineered mutation	UNP P0DTC2
A	145	PHE	LEU	engineered mutation	UNP P0DTC2
A	146	ALA	GLY	engineered mutation	UNP P0DTC2
A	148	SER	-	insertion	UNP P0DTC2
A	149	ARG	-	insertion	UNP P0DTC2
A	150	PRO	TYR	engineered mutation	UNP P0DTC2
A	151	THR	TYR	engineered mutation	UNP P0DTC2
A	152	GLY	HIS	engineered mutation	UNP P0DTC2
A	153	GLN	LYS	engineered mutation	UNP P0DTC2
A	154	HIS	ASN	engineered mutation	UNP P0DTC2
A	155	TYR	ASN	engineered mutation	UNP P0DTC2
A	157	THR	SER	engineered mutation	UNP P0DTC2
A	?	-	MET	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P0DTC2
A	?	-	SER	deletion	UNP P0DTC2
A	?	-	GLU	deletion	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	159	ILE	VAL	engineered mutation	UNP P0DTC2
A	161	THR	SER	engineered mutation	UNP P0DTC2
A	162	ASN	SER	engineered mutation	UNP P0DTC2
A	164	ARG	ASN	engineered mutation	UNP P0DTC2
A	168	TYR	PHE	engineered mutation	UNP P0DTC2
A	173	LYS	GLN	engineered mutation	UNP P0DTC2
A	174	SER	PRO	engineered mutation	UNP P0DTC2
A	176	GLN	LEU	engineered mutation	UNP P0DTC2
A	177	LEU	MET	engineered mutation	UNP P0DTC2
A	179	VAL	LEU	engineered mutation	UNP P0DTC2
A	180	SER	GLU	engineered mutation	UNP P0DTC2
A	181	GLU	GLY	engineered mutation	UNP P0DTC2
A	183	PRO	GLN	engineered mutation	UNP P0DTC2
A	188	HIS	ASN	engineered mutation	UNP P0DTC2
A	197	VAL	ILE	engineered mutation	UNP P0DTC2
A	200	PHE	TYR	engineered mutation	UNP P0DTC2
A	201	LEU	PHE	engineered mutation	UNP P0DTC2
A	202	HIS	LYS	engineered mutation	UNP P0DTC2
A	203	VAL	ILE	engineered mutation	UNP P0DTC2
A	206	GLY	LYS	engineered mutation	UNP P0DTC2
A	207	TYR	HIS	engineered mutation	UNP P0DTC2
A	208	GLU	THR	engineered mutation	UNP P0DTC2
A	211	ASP	ASN	engineered mutation	UNP P0DTC2
A	212	VAL	LEU	engineered mutation	UNP P0DTC2
A	213	ALA	VAL	engineered mutation	UNP P0DTC2
A	215	GLY	ASP	engineered mutation	UNP P0DTC2
A	218	SER	GLN	engineered mutation	UNP P0DTC2
A	222	VAL	ALA	engineered mutation	UNP P0DTC2
A	224	LYS	GLU	engineered mutation	UNP P0DTC2
A	226	ILE	LEU	engineered mutation	UNP P0DTC2
A	227	PHE	VAL	engineered mutation	UNP P0DTC2
A	228	LYS	ASP	engineered mutation	UNP P0DTC2
A	231	LEU	ILE	engineered mutation	UNP P0DTC2
A	237	ASN	ARG	engineered mutation	UNP P0DTC2
A	?	-	GLN	deletion	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	240	VAL	SER	engineered mutation	UNP P0DTC2
A	241	ILE	TYR	engineered mutation	UNP P0DTC2
A	242	MET	LEU	engineered mutation	UNP P0DTC2
A	244	MET	-	insertion	UNP P0DTC2
A	245	PHE	PRO	engineered mutation	UNP P0DTC2
A	246	SER	GLY	engineered mutation	UNP P0DTC2
A	247	PRO	ASP	engineered mutation	UNP P0DTC2
A	248	THR	SER	engineered mutation	UNP P0DTC2
A	249	THR	SER	engineered mutation	UNP P0DTC2
A	251	ASN	GLY	engineered mutation	UNP P0DTC2
A	253	GLY	THR	engineered mutation	UNP P0DTC2
A	255	GLU	GLY	engineered mutation	UNP P0DTC2
A	260	PHE	TYR	engineered mutation	UNP P0DTC2
A	265	LYS	GLN	engineered mutation	UNP P0DTC2
A	267	THR	ARG	engineered mutation	UNP P0DTC2
A	270	MET	LEU	engineered mutation	UNP P0DTC2
A	273	PHE	TYR	engineered mutation	UNP P0DTC2
A	274	ASP	ASN	engineered mutation	UNP P0DTC2
A	286	SER	ALA	engineered mutation	UNP P0DTC2
A	287	GLN	LEU	engineered mutation	UNP P0DTC2
A	293	LEU	THR	engineered mutation	UNP P0DTC2
A	297	VAL	LEU	engineered mutation	UNP P0DTC2
A	301	ASN	THR	engineered mutation	UNP P0DTC2
A	315	SER	GLN	engineered mutation	UNP P0DTC2
A	318	LYS	GLU	engineered mutation	UNP P0DTC2
A	319	GLU	SER	engineered mutation	UNP P0DTC2
A	320	VAL	ILE	engineered mutation	UNP P0DTC2
A	340	THR	ARG	engineered mutation	UNP P0DTC2
A	342	PRO	ALA	engineered mutation	UNP P0DTC2
A	348	GLU	ASN	engineered mutation	UNP P0DTC2
A	350	THR	LYS	engineered mutation	UNP P0DTC2
A	354	ASP	ASN	engineered mutation	UNP P0DTC2
A	366	THR	ALA	engineered mutation	UNP P0DTC2
A	387	SER	THR	engineered mutation	UNP P0DTC2
A	388	SER	ASN	engineered mutation	UNP P0DTC2
A	396	VAL	ILE	engineered mutation	UNP P0DTC2
A	397	LYS	ARG	engineered mutation	UNP P0DTC2
A	400	ASP	GLU	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	411	VAL	LYS	engineered mutation	UNP P0DTC2
A	432	THR	SER	engineered mutation	UNP P0DTC2
A	433	ALA	ASN	engineered mutation	UNP P0DTC2
A	437	ALA	SER	engineered mutation	UNP P0DTC2
A	438	THR	LYS	engineered mutation	UNP P0DTC2
A	439	SER	VAL	engineered mutation	UNP P0DTC2
A	440	THR	GLY	engineered mutation	UNP P0DTC2
A	446	TYR	LEU	engineered mutation	UNP P0DTC2
A	449	SER	LEU	engineered mutation	UNP P0DTC2
A	450	LEU	PHE	engineered mutation	UNP P0DTC2
A	452	HIS	LYS	engineered mutation	UNP P0DTC2
A	453	GLY	SER	engineered mutation	UNP P0DTC2
A	454	LYS	ASN	engineered mutation	UNP P0DTC2
A	464	ASN	THR	engineered mutation	UNP P0DTC2
A	465	VAL	GLU	engineered mutation	UNP P0DTC2
A	466	PRO	ILE	engineered mutation	UNP P0DTC2
A	467	PHE	TYR	engineered mutation	UNP P0DTC2
A	468	SER	GLN	engineered mutation	UNP P0DTC2
A	469	PRO	ALA	engineered mutation	UNP P0DTC2
A	470	GLU	GLY	engineered mutation	UNP P0DTC2
A	471	GLY	SER	engineered mutation	UNP P0DTC2
A	472	LYS	THR	engineered mutation	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	475	THR	GLY	engineered mutation	UNP P0DTC2
A	476	PRO	VAL	engineered mutation	UNP P0DTC2
A	477	PRO	GLU	engineered mutation	UNP P0DTC2
A	478	ALA	GLY	engineered mutation	UNP P0DTC2
A	483	ARG	PHE	engineered mutation	UNP P0DTC2
A	486	ASN	GLN	engineered mutation	UNP P0DTC2
A	487	THR	SER	engineered mutation	UNP P0DTC2
A	491	ASN	GLN	engineered mutation	UNP P0DTC2
A	494	VAL	ASN	engineered mutation	UNP P0DTC2
A	496	ILE	VAL	engineered mutation	UNP P0DTC2
A	512	ASN	HIS	engineered mutation	UNP P0DTC2
A	522	LEU	LYS	engineered mutation	UNP P0DTC2
A	525	GLU	ASN	engineered mutation	UNP P0DTC2
A	530	GLN	LYS	engineered mutation	UNP P0DTC2
A	547	ASP	GLU	engineered mutation	UNP P0DTC2
A	549	SER	ASN	engineered mutation	UNP P0DTC2
A	551	ARG	LYS	engineered mutation	UNP P0DTC2
A	553	GLN	LEU	engineered mutation	UNP P0DTC2
A	562	VAL	ILE	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	563	SER	ALA	engineered mutation	UNP P0DTC2
A	565	PHE	THR	engineered mutation	UNP P0DTC2
A	568	SER	ALA	engineered mutation	UNP P0DTC2
A	573	LYS	GLN	engineered mutation	UNP P0DTC2
A	581	SER	THR	engineered mutation	UNP P0DTC2
A	599	SER	ASN	engineered mutation	UNP P0DTC2
A	600	GLU	GLN	engineered mutation	UNP P0DTC2
A	612	ASP	GLU	engineered mutation	UNP P0DTC2
A	615	THR	VAL	engineered mutation	UNP P0DTC2
A	625	ALA	THR	engineered mutation	UNP P0DTC2
A	633	VAL	SER	engineered mutation	UNP P0DTC2
A	639	GLN	ARG	engineered mutation	UNP P0DTC2
A	651	ALA	ASN	engineered mutation	UNP P0DTC2
A	668	HIS	GLN	engineered mutation	UNP P0DTC2
A	670	ALA	-	insertion	UNP P0DTC2
A	671	SER	GLN	engineered mutation	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	?	-	SER	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	673	LEU	ALA	engineered mutation	UNP P0DTC2
A	676	THR	VAL	engineered mutation	UNP P0DTC2
A	677	GLY	ALA	engineered mutation	UNP P0DTC2
A	678	GLN	SER	engineered mutation	UNP P0DTC2
A	679	LYS	GLN	engineered mutation	UNP P0DTC2
A	682	VAL	ILE	engineered mutation	UNP P0DTC2
A	694	ILE	VAL	engineered mutation	UNP P0DTC2
A	700	THR	SER	engineered mutation	UNP P0DTC2
A	708	SER	THR	engineered mutation	UNP P0DTC2
A	715	VAL	ILE	engineered mutation	UNP P0DTC2
A	716	MET	LEU	engineered mutation	UNP P0DTC2
A	721	ALA	THR	engineered mutation	UNP P0DTC2
A	757	SER	THR	engineered mutation	UNP P0DTC2
A	768	ARG	GLN	engineered mutation	UNP P0DTC2
A	777	MET	ILE	engineered mutation	UNP P0DTC2
A	782	ALA	PRO	engineered mutation	UNP P0DTC2
A	802	THR	SER	engineered mutation	UNP P0DTC2
A	823	MET	ILE	engineered mutation	UNP P0DTC2
A	828	GLU	ASP	engineered mutation	UNP P0DTC2
A	834	SER	ALA	engineered mutation	UNP P0DTC2
A	861	ALA	GLN	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	864	ALA	SER	engineered mutation	UNP P0DTC2
A	867	VAL	LEU	engineered mutation	UNP P0DTC2
A	868	SER	ALA	engineered mutation	UNP P0DTC2
A	871	ALA	ILE	engineered mutation	UNP P0DTC2
A	873	ALA	SER	engineered mutation	UNP P0DTC2
A	911	GLN	LEU	engineered mutation	UNP P0DTC2
A	918	LYS	SER	engineered mutation	UNP P0DTC2
A	921	SER	GLY	engineered mutation	UNP P0DTC2
A	922	GLN	LYS	engineered mutation	UNP P0DTC2
A	925	GLU	ASP	engineered mutation	UNP P0DTC2
A	928	THR	SER	engineered mutation	UNP P0DTC2
A	929	THR	SER	engineered mutation	UNP P0DTC2
A	931	SER	ALA	engineered mutation	UNP P0DTC2
A	932	THR	SER	engineered mutation	UNP P0DTC2
A	1044	ALA	SER	engineered mutation	UNP P0DTC2
A	1059	SER	ALA	engineered mutation	UNP P0DTC2
A	1062	ARG	LYS	engineered mutation	UNP P0DTC2
A	1073	GLU	ASP	engineered mutation	UNP P0DTC2
A	1077	TYR	HIS	engineered mutation	UNP P0DTC2
A	1090	SER	HIS	engineered mutation	UNP P0DTC2
A	1093	ILE	VAL	engineered mutation	UNP P0DTC2
A	1100	SER	GLU	engineered mutation	UNP P0DTC2
A	1122	ILE	VAL	engineered mutation	UNP P0DTC2
A	1198	GLY	-	linker	UNP P0DTC2
A	1199	SER	-	linker	UNP P0DTC2
A	1221	LEU	PHE	engineered mutation	UNP P10104
A	1227	GLY	-	expression tag	UNP P10104
A	1228	THR	-	expression tag	UNP P10104
A	1229	SER	-	expression tag	UNP P10104
A	1230	LEU	-	expression tag	UNP P10104
A	1231	GLU	-	expression tag	UNP P10104
A	1232	VAL	-	expression tag	UNP P10104
A	1233	LEU	-	expression tag	UNP P10104
A	1234	PHE	-	expression tag	UNP P10104
A	1235	GLN	-	expression tag	UNP P10104
A	1236	GLY	-	expression tag	UNP P10104
A	1237	PRO	-	expression tag	UNP P10104
A	1238	GLY	-	expression tag	UNP P10104
A	1239	HIS	-	expression tag	UNP P10104
A	1240	HIS	-	expression tag	UNP P10104
A	1241	HIS	-	expression tag	UNP P10104
A	1242	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1243	HIS	-	expression tag	UNP P10104
A	1244	HIS	-	expression tag	UNP P10104
A	1245	HIS	-	expression tag	UNP P10104
A	1246	HIS	-	expression tag	UNP P10104
A	1247	SER	-	expression tag	UNP P10104
A	1248	ALA	-	expression tag	UNP P10104
A	1249	TRP	-	expression tag	UNP P10104
A	1250	SER	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	PRO	-	expression tag	UNP P10104
A	1253	GLN	-	expression tag	UNP P10104
A	1254	PHE	-	expression tag	UNP P10104
A	1255	GLU	-	expression tag	UNP P10104
A	1256	LYS	-	expression tag	UNP P10104
A	1257	GLY	-	expression tag	UNP P10104
A	1258	GLY	-	expression tag	UNP P10104
A	1259	GLY	-	expression tag	UNP P10104
A	1260	SER	-	expression tag	UNP P10104
A	1261	GLY	-	expression tag	UNP P10104
A	1262	GLY	-	expression tag	UNP P10104
A	1263	GLY	-	expression tag	UNP P10104
A	1264	GLY	-	expression tag	UNP P10104
A	1265	SER	-	expression tag	UNP P10104
A	1266	GLY	-	expression tag	UNP P10104
A	1267	GLY	-	expression tag	UNP P10104
A	1268	SER	-	expression tag	UNP P10104
A	1269	ALA	-	expression tag	UNP P10104
A	1270	TRP	-	expression tag	UNP P10104
A	1271	SER	-	expression tag	UNP P10104
A	1272	HIS	-	expression tag	UNP P10104
A	1273	PRO	-	expression tag	UNP P10104
A	1274	GLN	-	expression tag	UNP P10104
A	1275	PHE	-	expression tag	UNP P10104
A	1276	GLU	-	expression tag	UNP P10104
A	1277	LYS	-	expression tag	UNP P10104
C	19	THR	VAL	engineered mutation	UNP P0DTC2
C	20	CYS	ASN	engineered mutation	UNP P0DTC2
C	21	GLY	LEU	engineered mutation	UNP P0DTC2
C	23	LEU	THR	engineered mutation	UNP P0DTC2
C	24	SER	ARG	engineered mutation	UNP P0DTC2
C	25	ASN	THR	engineered mutation	UNP P0DTC2
C	26	LYS	GLN	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	27	SER	LEU	engineered mutation	UNP P0DTC2
C	30	ASN	ALA	engineered mutation	UNP P0DTC2
C	31	MET	TYR	engineered mutation	UNP P0DTC2
C	33	GLN	-	insertion	UNP P0DTC2
C	34	PHE	-	insertion	UNP P0DTC2
C	35	SER	ASN	engineered mutation	UNP P0DTC2
C	37	SER	PHE	engineered mutation	UNP P0DTC2
C	38	ARG	THR	engineered mutation	UNP P0DTC2
C	46	ASP	LYS	engineered mutation	UNP P0DTC2
C	47	ILE	VAL	engineered mutation	UNP P0DTC2
C	51	ASP	SER	engineered mutation	UNP P0DTC2
C	55	LEU	SER	engineered mutation	UNP P0DTC2
C	59	TYR	LEU	engineered mutation	UNP P0DTC2
C	64	ASN	PHE	engineered mutation	UNP P0DTC2
C	?	-	TRP	deletion	UNP P0DTC2
C	69	ARG	PHE	engineered mutation	UNP P0DTC2
C	70	TYR	HIS	engineered mutation	UNP P0DTC2
C	71	LEU	ALA	engineered mutation	UNP P0DTC2
C	72	SER	ILE	engineered mutation	UNP P0DTC2
C	73	LEU	HIS	engineered mutation	UNP P0DTC2
C	74	ASN	VAL	engineered mutation	UNP P0DTC2
C	76	ASP	GLY	engineered mutation	UNP P0DTC2
C	77	SER	THR	engineered mutation	UNP P0DTC2
C	78	ASP	ASN	engineered mutation	UNP P0DTC2
C	79	ARG	GLY	engineered mutation	UNP P0DTC2
C	80	ILE	THR	engineered mutation	UNP P0DTC2
C	81	VAL	LYS	engineered mutation	UNP P0DTC2
C	87	ILE	VAL	engineered mutation	UNP P0DTC2
C	88	ILE	LEU	engineered mutation	UNP P0DTC2
C	91	GLY	ASN	engineered mutation	UNP P0DTC2
C	98	ALA	SER	engineered mutation	UNP P0DTC2
C	104	VAL	ILE	engineered mutation	UNP P0DTC2
C	112	SER	THR	engineered mutation	UNP P0DTC2
C	116	ASN	SER	engineered mutation	UNP P0DTC2
C	117	THR	LYS	engineered mutation	UNP P0DTC2
C	118	SER	THR	engineered mutation	UNP P0DTC2
C	121	ALA	LEU	engineered mutation	UNP P0DTC2
C	122	ILE	LEU	engineered mutation	UNP P0DTC2
C	124	MET	VAL	engineered mutation	UNP P0DTC2
C	127	SER	ALA	engineered mutation	UNP P0DTC2
C	129	HIS	ASN	engineered mutation	UNP P0DTC2
C	130	ILE	VAL	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	133	ARG	LYS	engineered mutation	UNP P0DTC2
C	136	ASN	GLU	engineered mutation	UNP P0DTC2
C	139	LEU	PHE	engineered mutation	UNP P0DTC2
C	141	ASP	ASN	engineered mutation	UNP P0DTC2
C	144	MET	PHE	engineered mutation	UNP P0DTC2
C	145	PHE	LEU	engineered mutation	UNP P0DTC2
C	146	ALA	GLY	engineered mutation	UNP P0DTC2
C	148	SER	-	insertion	UNP P0DTC2
C	149	ARG	-	insertion	UNP P0DTC2
C	150	PRO	TYR	engineered mutation	UNP P0DTC2
C	151	THR	TYR	engineered mutation	UNP P0DTC2
C	152	GLY	HIS	engineered mutation	UNP P0DTC2
C	153	GLN	LYS	engineered mutation	UNP P0DTC2
C	154	HIS	ASN	engineered mutation	UNP P0DTC2
C	155	TYR	ASN	engineered mutation	UNP P0DTC2
C	157	THR	SER	engineered mutation	UNP P0DTC2
C	?	-	MET	deletion	UNP P0DTC2
C	?	-	GLU	deletion	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	?	-	GLU	deletion	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	159	ILE	VAL	engineered mutation	UNP P0DTC2
C	161	THR	SER	engineered mutation	UNP P0DTC2
C	162	ASN	SER	engineered mutation	UNP P0DTC2
C	164	ARG	ASN	engineered mutation	UNP P0DTC2
C	168	TYR	PHE	engineered mutation	UNP P0DTC2
C	173	LYS	GLN	engineered mutation	UNP P0DTC2
C	174	SER	PRO	engineered mutation	UNP P0DTC2
C	176	GLN	LEU	engineered mutation	UNP P0DTC2
C	177	LEU	MET	engineered mutation	UNP P0DTC2
C	179	VAL	LEU	engineered mutation	UNP P0DTC2
C	180	SER	GLU	engineered mutation	UNP P0DTC2
C	181	GLU	GLY	engineered mutation	UNP P0DTC2
C	183	PRO	GLN	engineered mutation	UNP P0DTC2
C	188	HIS	ASN	engineered mutation	UNP P0DTC2
C	197	VAL	ILE	engineered mutation	UNP P0DTC2
C	200	PHE	TYR	engineered mutation	UNP P0DTC2
C	201	LEU	PHE	engineered mutation	UNP P0DTC2
C	202	HIS	LYS	engineered mutation	UNP P0DTC2
C	203	VAL	ILE	engineered mutation	UNP P0DTC2
C	206	GLY	LYS	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	207	TYR	HIS	engineered mutation	UNP P0DTC2
C	208	GLU	THR	engineered mutation	UNP P0DTC2
C	211	ASP	ASN	engineered mutation	UNP P0DTC2
C	212	VAL	LEU	engineered mutation	UNP P0DTC2
C	213	ALA	VAL	engineered mutation	UNP P0DTC2
C	215	GLY	ASP	engineered mutation	UNP P0DTC2
C	218	SER	GLN	engineered mutation	UNP P0DTC2
C	222	VAL	ALA	engineered mutation	UNP P0DTC2
C	224	LYS	GLU	engineered mutation	UNP P0DTC2
C	226	ILE	LEU	engineered mutation	UNP P0DTC2
C	227	PHE	VAL	engineered mutation	UNP P0DTC2
C	228	LYS	ASP	engineered mutation	UNP P0DTC2
C	231	LEU	ILE	engineered mutation	UNP P0DTC2
C	237	ASN	ARG	engineered mutation	UNP P0DTC2
C	?	-	GLN	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	240	VAL	SER	engineered mutation	UNP P0DTC2
C	241	ILE	TYR	engineered mutation	UNP P0DTC2
C	242	MET	LEU	engineered mutation	UNP P0DTC2
C	244	MET	-	insertion	UNP P0DTC2
C	245	PHE	PRO	engineered mutation	UNP P0DTC2
C	246	SER	GLY	engineered mutation	UNP P0DTC2
C	247	PRO	ASP	engineered mutation	UNP P0DTC2
C	248	THR	SER	engineered mutation	UNP P0DTC2
C	249	THR	SER	engineered mutation	UNP P0DTC2
C	251	ASN	GLY	engineered mutation	UNP P0DTC2
C	253	GLY	THR	engineered mutation	UNP P0DTC2
C	255	GLU	GLY	engineered mutation	UNP P0DTC2
C	260	PHE	TYR	engineered mutation	UNP P0DTC2
C	265	LYS	GLN	engineered mutation	UNP P0DTC2
C	267	THR	ARG	engineered mutation	UNP P0DTC2
C	270	MET	LEU	engineered mutation	UNP P0DTC2
C	273	PHE	TYR	engineered mutation	UNP P0DTC2
C	274	ASP	ASN	engineered mutation	UNP P0DTC2
C	286	SER	ALA	engineered mutation	UNP P0DTC2
C	287	GLN	LEU	engineered mutation	UNP P0DTC2
C	293	LEU	THR	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	297	VAL	LEU	engineered mutation	UNP P0DTC2
C	301	ASN	THR	engineered mutation	UNP P0DTC2
C	315	SER	GLN	engineered mutation	UNP P0DTC2
C	318	LYS	GLU	engineered mutation	UNP P0DTC2
C	319	GLU	SER	engineered mutation	UNP P0DTC2
C	320	VAL	ILE	engineered mutation	UNP P0DTC2
C	340	THR	ARG	engineered mutation	UNP P0DTC2
C	342	PRO	ALA	engineered mutation	UNP P0DTC2
C	348	GLU	ASN	engineered mutation	UNP P0DTC2
C	350	THR	LYS	engineered mutation	UNP P0DTC2
C	354	ASP	ASN	engineered mutation	UNP P0DTC2
C	366	THR	ALA	engineered mutation	UNP P0DTC2
C	387	SER	THR	engineered mutation	UNP P0DTC2
C	388	SER	ASN	engineered mutation	UNP P0DTC2
C	396	VAL	ILE	engineered mutation	UNP P0DTC2
C	397	LYS	ARG	engineered mutation	UNP P0DTC2
C	400	ASP	GLU	engineered mutation	UNP P0DTC2
C	411	VAL	LYS	engineered mutation	UNP P0DTC2
C	432	THR	SER	engineered mutation	UNP P0DTC2
C	433	ALA	ASN	engineered mutation	UNP P0DTC2
C	437	ALA	SER	engineered mutation	UNP P0DTC2
C	438	THR	LYS	engineered mutation	UNP P0DTC2
C	439	SER	VAL	engineered mutation	UNP P0DTC2
C	440	THR	GLY	engineered mutation	UNP P0DTC2
C	446	TYR	LEU	engineered mutation	UNP P0DTC2
C	449	SER	LEU	engineered mutation	UNP P0DTC2
C	450	LEU	PHE	engineered mutation	UNP P0DTC2
C	452	HIS	LYS	engineered mutation	UNP P0DTC2
C	453	GLY	SER	engineered mutation	UNP P0DTC2
C	454	LYS	ASN	engineered mutation	UNP P0DTC2
C	464	ASN	THR	engineered mutation	UNP P0DTC2
C	465	VAL	GLU	engineered mutation	UNP P0DTC2
C	466	PRO	ILE	engineered mutation	UNP P0DTC2
C	467	PHE	TYR	engineered mutation	UNP P0DTC2
C	468	SER	GLN	engineered mutation	UNP P0DTC2
C	469	PRO	ALA	engineered mutation	UNP P0DTC2
C	470	GLU	GLY	engineered mutation	UNP P0DTC2
C	471	GLY	SER	engineered mutation	UNP P0DTC2
C	472	LYS	THR	engineered mutation	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	475	THR	GLY	engineered mutation	UNP P0DTC2
C	476	PRO	VAL	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	477	PRO	GLU	engineered mutation	UNP P0DTC2
C	478	ALA	GLY	engineered mutation	UNP P0DTC2
C	483	ARG	PHE	engineered mutation	UNP P0DTC2
C	486	ASN	GLN	engineered mutation	UNP P0DTC2
C	487	THR	SER	engineered mutation	UNP P0DTC2
C	491	ASN	GLN	engineered mutation	UNP P0DTC2
C	494	VAL	ASN	engineered mutation	UNP P0DTC2
C	496	ILE	VAL	engineered mutation	UNP P0DTC2
C	512	ASN	HIS	engineered mutation	UNP P0DTC2
C	522	LEU	LYS	engineered mutation	UNP P0DTC2
C	525	GLU	ASN	engineered mutation	UNP P0DTC2
C	530	GLN	LYS	engineered mutation	UNP P0DTC2
C	547	ASP	GLU	engineered mutation	UNP P0DTC2
C	549	SER	ASN	engineered mutation	UNP P0DTC2
C	551	ARG	LYS	engineered mutation	UNP P0DTC2
C	553	GLN	LEU	engineered mutation	UNP P0DTC2
C	562	VAL	ILE	engineered mutation	UNP P0DTC2
C	563	SER	ALA	engineered mutation	UNP P0DTC2
C	565	PHE	THR	engineered mutation	UNP P0DTC2
C	568	SER	ALA	engineered mutation	UNP P0DTC2
C	573	LYS	GLN	engineered mutation	UNP P0DTC2
C	581	SER	THR	engineered mutation	UNP P0DTC2
C	599	SER	ASN	engineered mutation	UNP P0DTC2
C	600	GLU	GLN	engineered mutation	UNP P0DTC2
C	612	ASP	GLU	engineered mutation	UNP P0DTC2
C	615	THR	VAL	engineered mutation	UNP P0DTC2
C	625	ALA	THR	engineered mutation	UNP P0DTC2
C	633	VAL	SER	engineered mutation	UNP P0DTC2
C	639	GLN	ARG	engineered mutation	UNP P0DTC2
C	651	ALA	ASN	engineered mutation	UNP P0DTC2
C	668	HIS	GLN	engineered mutation	UNP P0DTC2
C	670	ALA	-	insertion	UNP P0DTC2
C	671	SER	GLN	engineered mutation	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	673	LEU	ALA	engineered mutation	UNP P0DTC2
C	676	THR	VAL	engineered mutation	UNP P0DTC2
C	677	GLY	ALA	engineered mutation	UNP P0DTC2
C	678	GLN	SER	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	679	LYS	GLN	engineered mutation	UNP P0DTC2
C	682	VAL	ILE	engineered mutation	UNP P0DTC2
C	694	ILE	VAL	engineered mutation	UNP P0DTC2
C	700	THR	SER	engineered mutation	UNP P0DTC2
C	708	SER	THR	engineered mutation	UNP P0DTC2
C	715	VAL	ILE	engineered mutation	UNP P0DTC2
C	716	MET	LEU	engineered mutation	UNP P0DTC2
C	721	ALA	THR	engineered mutation	UNP P0DTC2
C	757	SER	THR	engineered mutation	UNP P0DTC2
C	768	ARG	GLN	engineered mutation	UNP P0DTC2
C	777	MET	ILE	engineered mutation	UNP P0DTC2
C	782	ALA	PRO	engineered mutation	UNP P0DTC2
C	802	THR	SER	engineered mutation	UNP P0DTC2
C	823	MET	ILE	engineered mutation	UNP P0DTC2
C	828	GLU	ASP	engineered mutation	UNP P0DTC2
C	834	SER	ALA	engineered mutation	UNP P0DTC2
C	861	ALA	GLN	engineered mutation	UNP P0DTC2
C	864	ALA	SER	engineered mutation	UNP P0DTC2
C	867	VAL	LEU	engineered mutation	UNP P0DTC2
C	868	SER	ALA	engineered mutation	UNP P0DTC2
C	871	ALA	ILE	engineered mutation	UNP P0DTC2
C	873	ALA	SER	engineered mutation	UNP P0DTC2
C	911	GLN	LEU	engineered mutation	UNP P0DTC2
C	918	LYS	SER	engineered mutation	UNP P0DTC2
C	921	SER	GLY	engineered mutation	UNP P0DTC2
C	922	GLN	LYS	engineered mutation	UNP P0DTC2
C	925	GLU	ASP	engineered mutation	UNP P0DTC2
C	928	THR	SER	engineered mutation	UNP P0DTC2
C	929	THR	SER	engineered mutation	UNP P0DTC2
C	931	SER	ALA	engineered mutation	UNP P0DTC2
C	932	THR	SER	engineered mutation	UNP P0DTC2
C	1044	ALA	SER	engineered mutation	UNP P0DTC2
C	1059	SER	ALA	engineered mutation	UNP P0DTC2
C	1062	ARG	LYS	engineered mutation	UNP P0DTC2
C	1073	GLU	ASP	engineered mutation	UNP P0DTC2
C	1077	TYR	HIS	engineered mutation	UNP P0DTC2
C	1090	SER	HIS	engineered mutation	UNP P0DTC2
C	1093	ILE	VAL	engineered mutation	UNP P0DTC2
C	1100	SER	GLU	engineered mutation	UNP P0DTC2
C	1122	ILE	VAL	engineered mutation	UNP P0DTC2
C	1198	GLY	-	linker	UNP P0DTC2
C	1199	SER	-	linker	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1221	LEU	PHE	engineered mutation	UNP P10104
C	1227	GLY	-	expression tag	UNP P10104
C	1228	THR	-	expression tag	UNP P10104
C	1229	SER	-	expression tag	UNP P10104
C	1230	LEU	-	expression tag	UNP P10104
C	1231	GLU	-	expression tag	UNP P10104
C	1232	VAL	-	expression tag	UNP P10104
C	1233	LEU	-	expression tag	UNP P10104
C	1234	PHE	-	expression tag	UNP P10104
C	1235	GLN	-	expression tag	UNP P10104
C	1236	GLY	-	expression tag	UNP P10104
C	1237	PRO	-	expression tag	UNP P10104
C	1238	GLY	-	expression tag	UNP P10104
C	1239	HIS	-	expression tag	UNP P10104
C	1240	HIS	-	expression tag	UNP P10104
C	1241	HIS	-	expression tag	UNP P10104
C	1242	HIS	-	expression tag	UNP P10104
C	1243	HIS	-	expression tag	UNP P10104
C	1244	HIS	-	expression tag	UNP P10104
C	1245	HIS	-	expression tag	UNP P10104
C	1246	HIS	-	expression tag	UNP P10104
C	1247	SER	-	expression tag	UNP P10104
C	1248	ALA	-	expression tag	UNP P10104
C	1249	TRP	-	expression tag	UNP P10104
C	1250	SER	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104
C	1252	PRO	-	expression tag	UNP P10104
C	1253	GLN	-	expression tag	UNP P10104
C	1254	PHE	-	expression tag	UNP P10104
C	1255	GLU	-	expression tag	UNP P10104
C	1256	LYS	-	expression tag	UNP P10104
C	1257	GLY	-	expression tag	UNP P10104
C	1258	GLY	-	expression tag	UNP P10104
C	1259	GLY	-	expression tag	UNP P10104
C	1260	SER	-	expression tag	UNP P10104
C	1261	GLY	-	expression tag	UNP P10104
C	1262	GLY	-	expression tag	UNP P10104
C	1263	GLY	-	expression tag	UNP P10104
C	1264	GLY	-	expression tag	UNP P10104
C	1265	SER	-	expression tag	UNP P10104
C	1266	GLY	-	expression tag	UNP P10104
C	1267	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1268	SER	-	expression tag	UNP P10104
C	1269	ALA	-	expression tag	UNP P10104
C	1270	TRP	-	expression tag	UNP P10104
C	1271	SER	-	expression tag	UNP P10104
C	1272	HIS	-	expression tag	UNP P10104
C	1273	PRO	-	expression tag	UNP P10104
C	1274	GLN	-	expression tag	UNP P10104
C	1275	PHE	-	expression tag	UNP P10104
C	1276	GLU	-	expression tag	UNP P10104
C	1277	LYS	-	expression tag	UNP P10104
B	19	THR	VAL	engineered mutation	UNP P0DTC2
B	20	CYS	ASN	engineered mutation	UNP P0DTC2
B	21	GLY	LEU	engineered mutation	UNP P0DTC2
B	23	LEU	THR	engineered mutation	UNP P0DTC2
B	24	SER	ARG	engineered mutation	UNP P0DTC2
B	25	ASN	THR	engineered mutation	UNP P0DTC2
B	26	LYS	GLN	engineered mutation	UNP P0DTC2
B	27	SER	LEU	engineered mutation	UNP P0DTC2
B	30	ASN	ALA	engineered mutation	UNP P0DTC2
B	31	MET	TYR	engineered mutation	UNP P0DTC2
B	33	GLN	-	insertion	UNP P0DTC2
B	34	PHE	-	insertion	UNP P0DTC2
B	35	SER	ASN	engineered mutation	UNP P0DTC2
B	37	SER	PHE	engineered mutation	UNP P0DTC2
B	38	ARG	THR	engineered mutation	UNP P0DTC2
B	46	ASP	LYS	engineered mutation	UNP P0DTC2
B	47	ILE	VAL	engineered mutation	UNP P0DTC2
B	51	ASP	SER	engineered mutation	UNP P0DTC2
B	55	LEU	SER	engineered mutation	UNP P0DTC2
B	59	TYR	LEU	engineered mutation	UNP P0DTC2
B	64	ASN	PHE	engineered mutation	UNP P0DTC2
B	?	-	TRP	deletion	UNP P0DTC2
B	69	ARG	PHE	engineered mutation	UNP P0DTC2
B	70	TYR	HIS	engineered mutation	UNP P0DTC2
B	71	LEU	ALA	engineered mutation	UNP P0DTC2
B	72	SER	ILE	engineered mutation	UNP P0DTC2
B	73	LEU	HIS	engineered mutation	UNP P0DTC2
B	74	ASN	VAL	engineered mutation	UNP P0DTC2
B	76	ASP	GLY	engineered mutation	UNP P0DTC2
B	77	SER	THR	engineered mutation	UNP P0DTC2
B	78	ASP	ASN	engineered mutation	UNP P0DTC2
B	79	ARG	GLY	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	80	ILE	THR	engineered mutation	UNP P0DTC2
B	81	VAL	LYS	engineered mutation	UNP P0DTC2
B	87	ILE	VAL	engineered mutation	UNP P0DTC2
B	88	ILE	LEU	engineered mutation	UNP P0DTC2
B	91	GLY	ASN	engineered mutation	UNP P0DTC2
B	98	ALA	SER	engineered mutation	UNP P0DTC2
B	104	VAL	ILE	engineered mutation	UNP P0DTC2
B	112	SER	THR	engineered mutation	UNP P0DTC2
B	116	ASN	SER	engineered mutation	UNP P0DTC2
B	117	THR	LYS	engineered mutation	UNP P0DTC2
B	118	SER	THR	engineered mutation	UNP P0DTC2
B	121	ALA	LEU	engineered mutation	UNP P0DTC2
B	122	ILE	LEU	engineered mutation	UNP P0DTC2
B	124	MET	VAL	engineered mutation	UNP P0DTC2
B	127	SER	ALA	engineered mutation	UNP P0DTC2
B	129	HIS	ASN	engineered mutation	UNP P0DTC2
B	130	ILE	VAL	engineered mutation	UNP P0DTC2
B	133	ARG	LYS	engineered mutation	UNP P0DTC2
B	136	ASN	GLU	engineered mutation	UNP P0DTC2
B	139	LEU	PHE	engineered mutation	UNP P0DTC2
B	141	ASP	ASN	engineered mutation	UNP P0DTC2
B	144	MET	PHE	engineered mutation	UNP P0DTC2
B	145	PHE	LEU	engineered mutation	UNP P0DTC2
B	146	ALA	GLY	engineered mutation	UNP P0DTC2
B	148	SER	-	insertion	UNP P0DTC2
B	149	ARG	-	insertion	UNP P0DTC2
B	150	PRO	TYR	engineered mutation	UNP P0DTC2
B	151	THR	TYR	engineered mutation	UNP P0DTC2
B	152	GLY	HIS	engineered mutation	UNP P0DTC2
B	153	GLN	LYS	engineered mutation	UNP P0DTC2
B	154	HIS	ASN	engineered mutation	UNP P0DTC2
B	155	TYR	ASN	engineered mutation	UNP P0DTC2
B	157	THR	SER	engineered mutation	UNP P0DTC2
B	?	-	MET	deletion	UNP P0DTC2
B	?	-	GLU	deletion	UNP P0DTC2
B	?	-	SER	deletion	UNP P0DTC2
B	?	-	GLU	deletion	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	159	ILE	VAL	engineered mutation	UNP P0DTC2
B	161	THR	SER	engineered mutation	UNP P0DTC2
B	162	ASN	SER	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	164	ARG	ASN	engineered mutation	UNP P0DTC2
B	168	TYR	PHE	engineered mutation	UNP P0DTC2
B	173	LYS	GLN	engineered mutation	UNP P0DTC2
B	174	SER	PRO	engineered mutation	UNP P0DTC2
B	176	GLN	LEU	engineered mutation	UNP P0DTC2
B	177	LEU	MET	engineered mutation	UNP P0DTC2
B	179	VAL	LEU	engineered mutation	UNP P0DTC2
B	180	SER	GLU	engineered mutation	UNP P0DTC2
B	181	GLU	GLY	engineered mutation	UNP P0DTC2
B	183	PRO	GLN	engineered mutation	UNP P0DTC2
B	188	HIS	ASN	engineered mutation	UNP P0DTC2
B	197	VAL	ILE	engineered mutation	UNP P0DTC2
B	200	PHE	TYR	engineered mutation	UNP P0DTC2
B	201	LEU	PHE	engineered mutation	UNP P0DTC2
B	202	HIS	LYS	engineered mutation	UNP P0DTC2
B	203	VAL	ILE	engineered mutation	UNP P0DTC2
B	206	GLY	LYS	engineered mutation	UNP P0DTC2
B	207	TYR	HIS	engineered mutation	UNP P0DTC2
B	208	GLU	THR	engineered mutation	UNP P0DTC2
B	211	ASP	ASN	engineered mutation	UNP P0DTC2
B	212	VAL	LEU	engineered mutation	UNP P0DTC2
B	213	ALA	VAL	engineered mutation	UNP P0DTC2
B	215	GLY	ASP	engineered mutation	UNP P0DTC2
B	218	SER	GLN	engineered mutation	UNP P0DTC2
B	222	VAL	ALA	engineered mutation	UNP P0DTC2
B	224	LYS	GLU	engineered mutation	UNP P0DTC2
B	226	ILE	LEU	engineered mutation	UNP P0DTC2
B	227	PHE	VAL	engineered mutation	UNP P0DTC2
B	228	LYS	ASP	engineered mutation	UNP P0DTC2
B	231	LEU	ILE	engineered mutation	UNP P0DTC2
B	237	ASN	ARG	engineered mutation	UNP P0DTC2
B	?	-	GLN	deletion	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	240	VAL	SER	engineered mutation	UNP P0DTC2
B	241	ILE	TYR	engineered mutation	UNP P0DTC2
B	242	MET	LEU	engineered mutation	UNP P0DTC2
B	244	MET	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	245	PHE	PRO	engineered mutation	UNP P0DTC2
B	246	SER	GLY	engineered mutation	UNP P0DTC2
B	247	PRO	ASP	engineered mutation	UNP P0DTC2
B	248	THR	SER	engineered mutation	UNP P0DTC2
B	249	THR	SER	engineered mutation	UNP P0DTC2
B	251	ASN	GLY	engineered mutation	UNP P0DTC2
B	253	GLY	THR	engineered mutation	UNP P0DTC2
B	255	GLU	GLY	engineered mutation	UNP P0DTC2
B	260	PHE	TYR	engineered mutation	UNP P0DTC2
B	265	LYS	GLN	engineered mutation	UNP P0DTC2
B	267	THR	ARG	engineered mutation	UNP P0DTC2
B	270	MET	LEU	engineered mutation	UNP P0DTC2
B	273	PHE	TYR	engineered mutation	UNP P0DTC2
B	274	ASP	ASN	engineered mutation	UNP P0DTC2
B	286	SER	ALA	engineered mutation	UNP P0DTC2
B	287	GLN	LEU	engineered mutation	UNP P0DTC2
B	293	LEU	THR	engineered mutation	UNP P0DTC2
B	297	VAL	LEU	engineered mutation	UNP P0DTC2
B	301	ASN	THR	engineered mutation	UNP P0DTC2
B	315	SER	GLN	engineered mutation	UNP P0DTC2
B	318	LYS	GLU	engineered mutation	UNP P0DTC2
B	319	GLU	SER	engineered mutation	UNP P0DTC2
B	320	VAL	ILE	engineered mutation	UNP P0DTC2
B	340	THR	ARG	engineered mutation	UNP P0DTC2
B	342	PRO	ALA	engineered mutation	UNP P0DTC2
B	348	GLU	ASN	engineered mutation	UNP P0DTC2
B	350	THR	LYS	engineered mutation	UNP P0DTC2
B	354	ASP	ASN	engineered mutation	UNP P0DTC2
B	366	THR	ALA	engineered mutation	UNP P0DTC2
B	387	SER	THR	engineered mutation	UNP P0DTC2
B	388	SER	ASN	engineered mutation	UNP P0DTC2
B	396	VAL	ILE	engineered mutation	UNP P0DTC2
B	397	LYS	ARG	engineered mutation	UNP P0DTC2
B	400	ASP	GLU	engineered mutation	UNP P0DTC2
B	411	VAL	LYS	engineered mutation	UNP P0DTC2
B	432	THR	SER	engineered mutation	UNP P0DTC2
B	433	ALA	ASN	engineered mutation	UNP P0DTC2
B	437	ALA	SER	engineered mutation	UNP P0DTC2
B	438	THR	LYS	engineered mutation	UNP P0DTC2
B	439	SER	VAL	engineered mutation	UNP P0DTC2
B	440	THR	GLY	engineered mutation	UNP P0DTC2
B	446	TYR	LEU	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	449	SER	LEU	engineered mutation	UNP P0DTC2
B	450	LEU	PHE	engineered mutation	UNP P0DTC2
B	452	HIS	LYS	engineered mutation	UNP P0DTC2
B	453	GLY	SER	engineered mutation	UNP P0DTC2
B	454	LYS	ASN	engineered mutation	UNP P0DTC2
B	464	ASN	THR	engineered mutation	UNP P0DTC2
B	465	VAL	GLU	engineered mutation	UNP P0DTC2
B	466	PRO	ILE	engineered mutation	UNP P0DTC2
B	467	PHE	TYR	engineered mutation	UNP P0DTC2
B	468	SER	GLN	engineered mutation	UNP P0DTC2
B	469	PRO	ALA	engineered mutation	UNP P0DTC2
B	470	GLU	GLY	engineered mutation	UNP P0DTC2
B	471	GLY	SER	engineered mutation	UNP P0DTC2
B	472	LYS	THR	engineered mutation	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	475	THR	GLY	engineered mutation	UNP P0DTC2
B	476	PRO	VAL	engineered mutation	UNP P0DTC2
B	477	PRO	GLU	engineered mutation	UNP P0DTC2
B	478	ALA	GLY	engineered mutation	UNP P0DTC2
B	483	ARG	PHE	engineered mutation	UNP P0DTC2
B	486	ASN	GLN	engineered mutation	UNP P0DTC2
B	487	THR	SER	engineered mutation	UNP P0DTC2
B	491	ASN	GLN	engineered mutation	UNP P0DTC2
B	494	VAL	ASN	engineered mutation	UNP P0DTC2
B	496	ILE	VAL	engineered mutation	UNP P0DTC2
B	512	ASN	HIS	engineered mutation	UNP P0DTC2
B	522	LEU	LYS	engineered mutation	UNP P0DTC2
B	525	GLU	ASN	engineered mutation	UNP P0DTC2
B	530	GLN	LYS	engineered mutation	UNP P0DTC2
B	547	ASP	GLU	engineered mutation	UNP P0DTC2
B	549	SER	ASN	engineered mutation	UNP P0DTC2
B	551	ARG	LYS	engineered mutation	UNP P0DTC2
B	553	GLN	LEU	engineered mutation	UNP P0DTC2
B	562	VAL	ILE	engineered mutation	UNP P0DTC2
B	563	SER	ALA	engineered mutation	UNP P0DTC2
B	565	PHE	THR	engineered mutation	UNP P0DTC2
B	568	SER	ALA	engineered mutation	UNP P0DTC2
B	573	LYS	GLN	engineered mutation	UNP P0DTC2
B	581	SER	THR	engineered mutation	UNP P0DTC2
B	599	SER	ASN	engineered mutation	UNP P0DTC2
B	600	GLU	GLN	engineered mutation	UNP P0DTC2
B	612	ASP	GLU	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	615	THR	VAL	engineered mutation	UNP P0DTC2
B	625	ALA	THR	engineered mutation	UNP P0DTC2
B	633	VAL	SER	engineered mutation	UNP P0DTC2
B	639	GLN	ARG	engineered mutation	UNP P0DTC2
B	651	ALA	ASN	engineered mutation	UNP P0DTC2
B	668	HIS	GLN	engineered mutation	UNP P0DTC2
B	670	ALA	-	insertion	UNP P0DTC2
B	671	SER	GLN	engineered mutation	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	?	-	SER	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	673	LEU	ALA	engineered mutation	UNP P0DTC2
B	676	THR	VAL	engineered mutation	UNP P0DTC2
B	677	GLY	ALA	engineered mutation	UNP P0DTC2
B	678	GLN	SER	engineered mutation	UNP P0DTC2
B	679	LYS	GLN	engineered mutation	UNP P0DTC2
B	682	VAL	ILE	engineered mutation	UNP P0DTC2
B	694	ILE	VAL	engineered mutation	UNP P0DTC2
B	700	THR	SER	engineered mutation	UNP P0DTC2
B	708	SER	THR	engineered mutation	UNP P0DTC2
B	715	VAL	ILE	engineered mutation	UNP P0DTC2
B	716	MET	LEU	engineered mutation	UNP P0DTC2
B	721	ALA	THR	engineered mutation	UNP P0DTC2
B	757	SER	THR	engineered mutation	UNP P0DTC2
B	768	ARG	GLN	engineered mutation	UNP P0DTC2
B	777	MET	ILE	engineered mutation	UNP P0DTC2
B	782	ALA	PRO	engineered mutation	UNP P0DTC2
B	802	THR	SER	engineered mutation	UNP P0DTC2
B	823	MET	ILE	engineered mutation	UNP P0DTC2
B	828	GLU	ASP	engineered mutation	UNP P0DTC2
B	834	SER	ALA	engineered mutation	UNP P0DTC2
B	861	ALA	GLN	engineered mutation	UNP P0DTC2
B	864	ALA	SER	engineered mutation	UNP P0DTC2
B	867	VAL	LEU	engineered mutation	UNP P0DTC2
B	868	SER	ALA	engineered mutation	UNP P0DTC2
B	871	ALA	ILE	engineered mutation	UNP P0DTC2
B	873	ALA	SER	engineered mutation	UNP P0DTC2
B	911	GLN	LEU	engineered mutation	UNP P0DTC2
B	918	LYS	SER	engineered mutation	UNP P0DTC2
B	921	SER	GLY	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	922	GLN	LYS	engineered mutation	UNP P0DTC2
B	925	GLU	ASP	engineered mutation	UNP P0DTC2
B	928	THR	SER	engineered mutation	UNP P0DTC2
B	929	THR	SER	engineered mutation	UNP P0DTC2
B	931	SER	ALA	engineered mutation	UNP P0DTC2
B	932	THR	SER	engineered mutation	UNP P0DTC2
B	1044	ALA	SER	engineered mutation	UNP P0DTC2
B	1059	SER	ALA	engineered mutation	UNP P0DTC2
B	1062	ARG	LYS	engineered mutation	UNP P0DTC2
B	1073	GLU	ASP	engineered mutation	UNP P0DTC2
B	1077	TYR	HIS	engineered mutation	UNP P0DTC2
B	1090	SER	HIS	engineered mutation	UNP P0DTC2
B	1093	ILE	VAL	engineered mutation	UNP P0DTC2
B	1100	SER	GLU	engineered mutation	UNP P0DTC2
B	1122	ILE	VAL	engineered mutation	UNP P0DTC2
B	1198	GLY	-	linker	UNP P0DTC2
B	1199	SER	-	linker	UNP P0DTC2
B	1221	LEU	PHE	engineered mutation	UNP P10104
B	1227	GLY	-	expression tag	UNP P10104
B	1228	THR	-	expression tag	UNP P10104
B	1229	SER	-	expression tag	UNP P10104
B	1230	LEU	-	expression tag	UNP P10104
B	1231	GLU	-	expression tag	UNP P10104
B	1232	VAL	-	expression tag	UNP P10104
B	1233	LEU	-	expression tag	UNP P10104
B	1234	PHE	-	expression tag	UNP P10104
B	1235	GLN	-	expression tag	UNP P10104
B	1236	GLY	-	expression tag	UNP P10104
B	1237	PRO	-	expression tag	UNP P10104
B	1238	GLY	-	expression tag	UNP P10104
B	1239	HIS	-	expression tag	UNP P10104
B	1240	HIS	-	expression tag	UNP P10104
B	1241	HIS	-	expression tag	UNP P10104
B	1242	HIS	-	expression tag	UNP P10104
B	1243	HIS	-	expression tag	UNP P10104
B	1244	HIS	-	expression tag	UNP P10104
B	1245	HIS	-	expression tag	UNP P10104
B	1246	HIS	-	expression tag	UNP P10104
B	1247	SER	-	expression tag	UNP P10104
B	1248	ALA	-	expression tag	UNP P10104
B	1249	TRP	-	expression tag	UNP P10104
B	1250	SER	-	expression tag	UNP P10104

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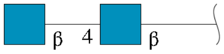
Chain	Residue	Modelled	Actual	Comment	Reference
B	1251	HIS	-	expression tag	UNP P10104
B	1252	PRO	-	expression tag	UNP P10104
B	1253	GLN	-	expression tag	UNP P10104
B	1254	PHE	-	expression tag	UNP P10104
B	1255	GLU	-	expression tag	UNP P10104
B	1256	LYS	-	expression tag	UNP P10104
B	1257	GLY	-	expression tag	UNP P10104
B	1258	GLY	-	expression tag	UNP P10104
B	1259	GLY	-	expression tag	UNP P10104
B	1260	SER	-	expression tag	UNP P10104
B	1261	GLY	-	expression tag	UNP P10104
B	1262	GLY	-	expression tag	UNP P10104
B	1263	GLY	-	expression tag	UNP P10104
B	1264	GLY	-	expression tag	UNP P10104
B	1265	SER	-	expression tag	UNP P10104
B	1266	GLY	-	expression tag	UNP P10104
B	1267	GLY	-	expression tag	UNP P10104
B	1268	SER	-	expression tag	UNP P10104
B	1269	ALA	-	expression tag	UNP P10104
B	1270	TRP	-	expression tag	UNP P10104
B	1271	SER	-	expression tag	UNP P10104
B	1272	HIS	-	expression tag	UNP P10104
B	1273	PRO	-	expression tag	UNP P10104
B	1274	GLN	-	expression tag	UNP P10104
B	1275	PHE	-	expression tag	UNP P10104
B	1276	GLU	-	expression tag	UNP P10104
B	1277	LYS	-	expression tag	UNP P10104

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



Mol	Chain	Residues	Atoms	AltConf	Trace
2	L	2	Total C H N O 55 16 27 2 10	0	0
2	M	2	Total C H N O 55 16 27 2 10	0	0
2	N	2	Total C H N O 55 16 27 2 10	0	0

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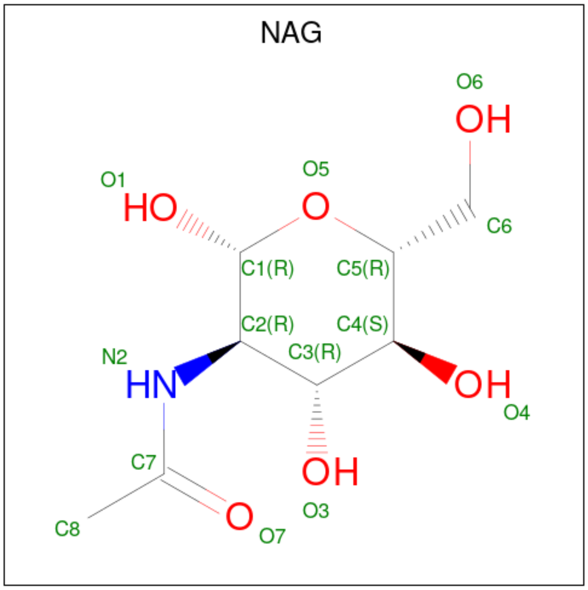
Mol	Chain	Residues	Atoms	AltConf	Trace
2	P	2	Total C H N O 55 16 27 2 10	0	0
2	Q	2	Total C H N O 55 16 27 2 10	0	0
2	R	2	Total C H N O 55 16 27 2 10	0	0
2	U	2	Total C H N O 55 16 27 2 10	0	0
2	V	2	Total C H N O 55 16 27 2 10	0	0
2	W	2	Total C H N O 55 16 27 2 10	0	0

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



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0

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Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	A	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0

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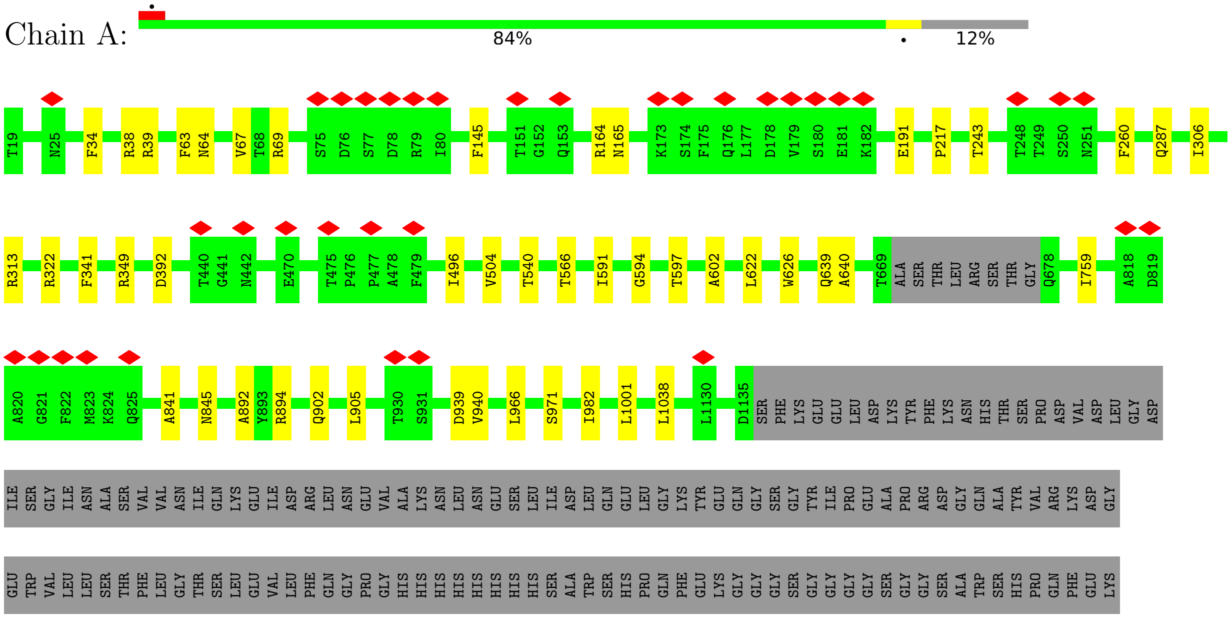
Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	C	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0
3	B	1	Total C H N O 28 8 14 1 5	0

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.

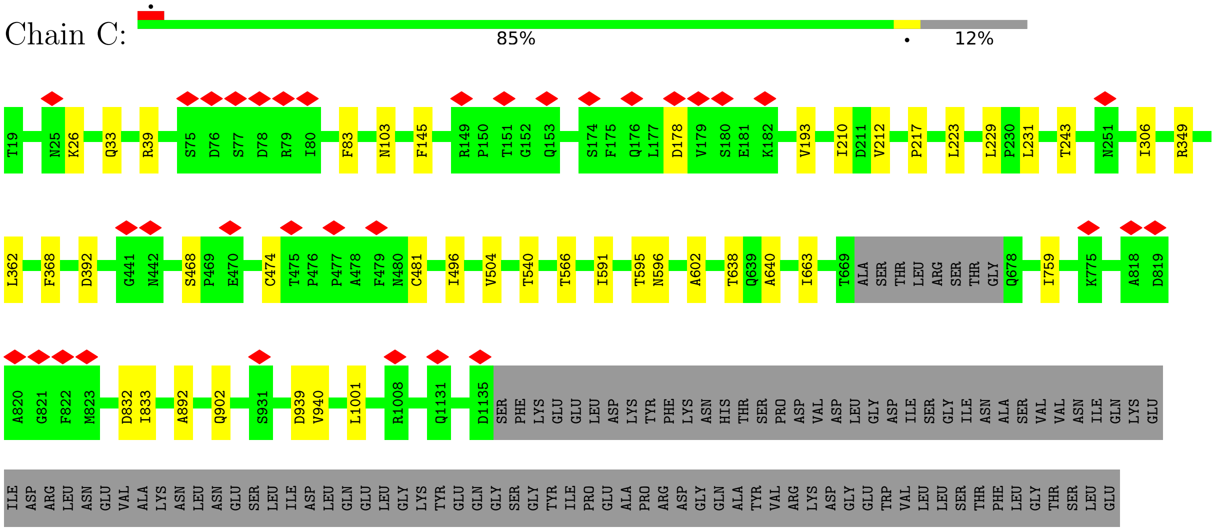
- Molecule 1: Spike glycoprotein,Fibritin

Chain A:



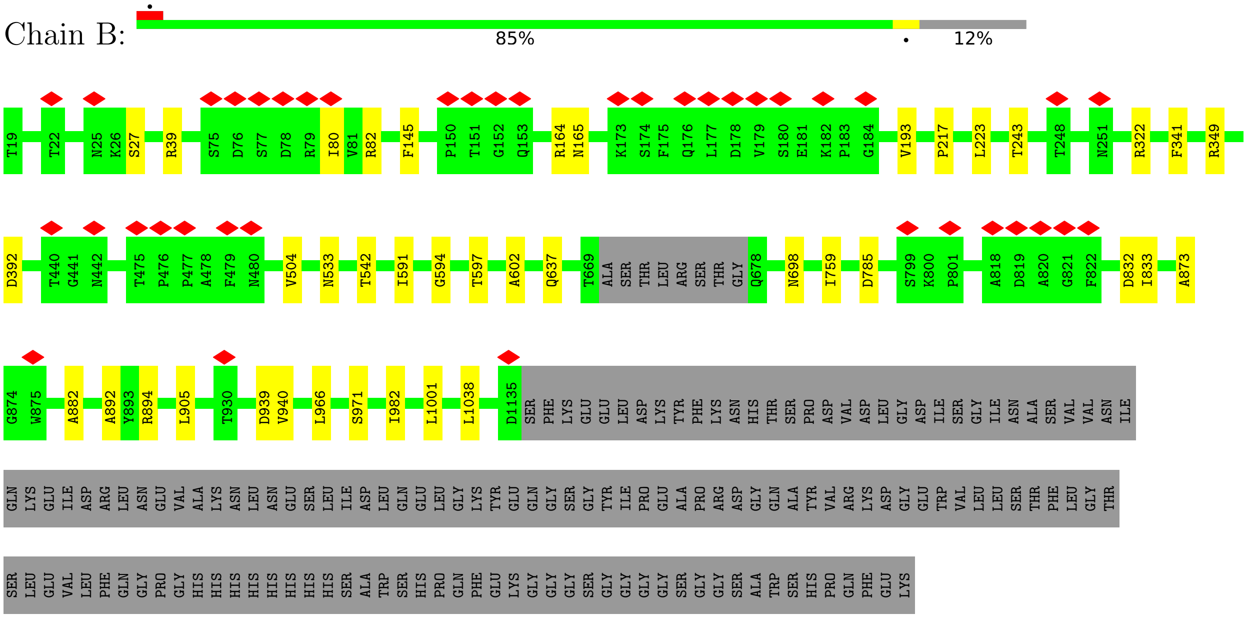
- Molecule 1: Spike glycoprotein,Fibritin

Chain C:



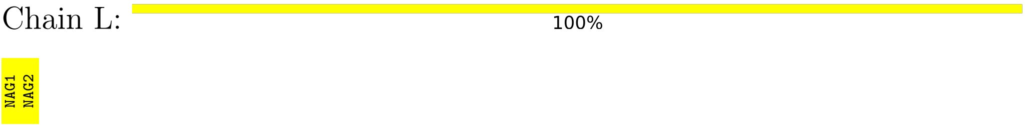
- Molecule 1: Spike glycoprotein,Fibritin

Chain B:



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

Chain L:

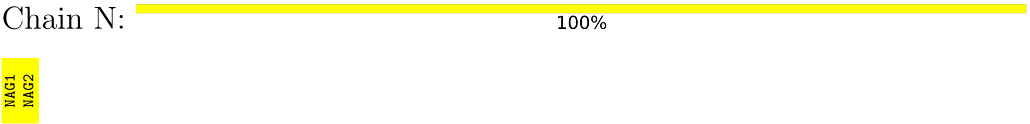


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

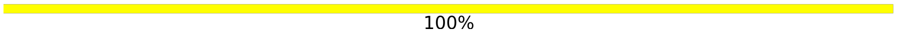
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain P:

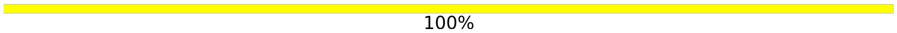


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

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

Chain R:

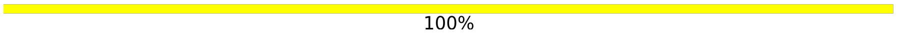


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

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

Chain V:



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

Chain W:

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	253429	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.11	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.341	Depositor
Minimum map value	-2.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.36	0/8824	0.52	0/12017
1	B	0.35	0/8824	0.51	0/12017
1	C	0.36	0/8824	0.52	0/12017
All	All	0.36	0/26472	0.52	0/36051

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ARG	Sidechain
1	A	322	ARG	Sidechain
1	A	349	ARG	Sidechain
1	B	322	ARG	Sidechain
1	B	349	ARG	Sidechain
1	C	349	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8621	8376	8368	29	0
1	B	8621	8376	8368	22	0
1	C	8621	8378	8370	25	0
2	L	28	27	25	0	0
2	M	28	27	25	0	0
2	N	28	27	25	0	0
2	P	28	27	25	0	0
2	Q	28	27	25	0	0
2	R	28	27	25	0	0
2	U	28	27	25	0	0
2	V	28	27	25	0	0
2	W	28	27	25	1	0
3	A	210	210	195	4	0
3	B	210	210	195	8	0
3	C	210	210	195	6	0
All	All	26745	26003	25916	88	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 2.

All (88) 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)
3:C:1304:NAG:O7	3:C:1304:NAG:O3	1.96	0.81
3:B:1302:NAG:O7	3:B:1302:NAG:O3	2.03	0.75
3:B:1301:NAG:O7	3:B:1301:NAG:O3	2.05	0.75
3:C:1302:NAG:O3	3:C:1302:NAG:O7	2.07	0.73
3:A:1302:NAG:O3	3:A:1302:NAG:O7	2.07	0.70
3:A:1301:NAG:O7	3:A:1301:NAG:O3	2.09	0.69
3:B:1304:NAG:HO3	3:B:1304:NAG:C7	2.06	0.67
1:B:39:ARG:NH2	1:B:217:PRO:O	2.31	0.63
1:A:39:ARG:NH2	1:A:217:PRO:O	2.34	0.58
1:A:287:GLN:NE2	1:A:287:GLN:HA	2.19	0.57
3:B:1304:NAG:O7	3:B:1304:NAG:O3	2.03	0.57
1:C:103:ASN:ND2	1:C:178:ASP:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1301:NAG:HO3	3:B:1301:NAG:C7	2.14	0.56
3:B:1302:NAG:HO3	3:B:1302:NAG:C7	2.15	0.56
1:A:287:GLN:HA	1:A:287:GLN:HE21	1.69	0.55
3:A:1304:NAG:O7	3:A:1304:NAG:O3	2.23	0.55
1:C:892:ALA:HB1	1:C:902:GLN:HG3	1.89	0.54
1:B:637:GLN:HG2	3:B:1304:NAG:H82	1.89	0.54
1:B:594:GLY:O	1:B:597:THR:HG22	2.08	0.52
1:A:164:ARG:HG3	1:A:165:ASN:H	1.75	0.51
1:B:145:PHE:HB2	1:B:243:THR:HG22	1.92	0.51
1:A:594:GLY:O	1:A:597:THR:HG22	2.11	0.51
1:A:894:ARG:NH1	1:A:1038:LEU:O	2.41	0.51
1:C:595:THR:O	1:C:596:ASN:ND2	2.41	0.50
1:C:638:THR:HG22	1:C:640:ALA:H	1.76	0.50
1:B:164:ARG:HG3	1:B:165:ASN:H	1.76	0.50
1:C:145:PHE:HB2	1:C:243:THR:HG22	1.93	0.50
1:A:64:ASN:ND2	1:A:287:GLN:OE1	2.40	0.49
1:C:39:ARG:NH2	1:C:217:PRO:O	2.34	0.49
1:C:306:ILE:HD12	1:C:591:ILE:CD1	2.42	0.49
1:A:639:GLN:O	1:A:640:ALA:HB3	2.11	0.49
1:A:939:ASP:OD1	1:A:940:VAL:N	2.46	0.49
1:B:392:ASP:O	1:B:504:VAL:HA	2.13	0.49
1:C:638:THR:HG23	1:C:663:ILE:HG13	1.94	0.49
1:C:468:SER:OG	1:C:474:CYS:SG	2.70	0.48
1:C:759:ILE:HD11	1:C:1001:LEU:HD23	1.95	0.48
3:C:1301:NAG:O7	3:C:1301:NAG:O3	2.28	0.47
1:A:892:ALA:HB1	1:A:902:GLN:HG3	1.95	0.47
1:C:229:LEU:HB3	1:C:231:LEU:HD21	1.98	0.46
1:B:939:ASP:OD1	1:B:940:VAL:N	2.48	0.46
1:B:832:ASP:OD1	1:B:833:ILE:N	2.46	0.46
3:A:1301:NAG:HO3	3:A:1301:NAG:C7	2.20	0.46
1:C:362:LEU:HD13	1:C:368:PHE:HZ	1.80	0.46
1:A:622:LEU:HD23	1:A:626:TRP:CD1	2.51	0.46
1:B:966:LEU:HD11	1:B:982:ILE:HD12	1.97	0.46
1:A:566:THR:O	1:A:566:THR:HG23	2.16	0.45
1:B:894:ARG:NH1	1:B:1038:LEU:O	2.47	0.45
1:A:306:ILE:HD12	1:A:591:ILE:CD1	2.46	0.45
3:C:1313:NAG:O7	3:C:1313:NAG:O3	2.29	0.45
1:B:80:ILE:HG22	1:B:80:ILE:O	2.16	0.44
1:C:939:ASP:OD1	1:C:940:VAL:N	2.51	0.44
1:B:80:ILE:O	1:B:80:ILE:CG2	2.65	0.44
1:B:193:VAL:HG23	1:B:223:LEU:HD12	1.99	0.43

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:C:26:LYS:HE3	1:C:83:PHE:O	2.19	0.43
1:B:698:ASN:ND2	3:B:1306:NAG:O7	2.52	0.43
1:B:759:ILE:HD11	1:B:1001:LEU:HD23	2.00	0.43
1:A:145:PHE:HB2	1:A:243:THR:HG22	2.00	0.43
1:A:34:PHE:CE1	1:A:69:ARG:HD2	2.54	0.43
1:C:33:GLN:HB2	3:C:1301:NAG:H82	1.99	0.43
1:B:785:ASP:HB2	2:W:1:NAG:H82	2.01	0.43
1:C:468:SER:OG	1:C:481:CYS:SG	2.76	0.43
1:B:533:ASN:OD1	1:B:542:THR:HG22	2.19	0.43
1:B:27:SER:HB2	1:B:82:ARG:HG2	2.00	0.43
1:C:392:ASP:O	1:C:504:VAL:HA	2.19	0.42
1:A:841:ALA:O	1:A:845:ASN:ND2	2.52	0.42
1:B:873:ALA:CB	1:B:882:ALA:HB1	2.50	0.42
1:A:966:LEU:HD11	1:A:982:ILE:HD12	2.01	0.42
1:C:193:VAL:HG23	1:C:223:LEU:HD12	2.02	0.42
1:A:971:SER:HB2	1:C:540:THR:HG22	2.03	0.41
3:C:1304:NAG:HO3	3:C:1304:NAG:C7	2.15	0.41
1:A:939:ASP:OD1	1:A:939:ASP:C	2.58	0.41
1:C:832:ASP:OD1	1:C:833:ILE:N	2.47	0.41
1:C:566:THR:HG23	1:C:566:THR:O	2.20	0.41
1:A:287:GLN:NE2	1:A:287:GLN:CA	2.82	0.41
1:C:210:ILE:HD11	1:C:212:VAL:HB	2.02	0.41
1:C:591:ILE:N	1:C:602:ALA:O	2.47	0.41
1:B:892:ALA:HB2	1:B:905:LEU:HD23	2.03	0.41
1:A:39:ARG:HD2	1:A:191:GLU:CD	2.41	0.41
1:A:496:ILE:HD13	1:C:496:ILE:HG22	2.02	0.41
1:A:759:ILE:HD11	1:A:1001:LEU:HD23	2.02	0.41
1:A:892:ALA:HB2	1:A:905:LEU:HD23	2.02	0.41
1:A:38:ARG:HA	1:A:63:PHE:CD1	2.56	0.40
1:A:67:VAL:CG1	1:A:260:PHE:HB3	2.51	0.40
1:A:591:ILE:N	1:A:602:ALA:O	2.47	0.40
1:A:392:ASP:O	1:A:504:VAL:HA	2.22	0.40
1:A:540:THR:HG22	1:B:971:SER:HB2	2.04	0.40
1:C:306:ILE:HD12	1:C:591:ILE:HD11	2.04	0.40
1:B:591:ILE:N	1:B:602:ALA:O	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1105/1259 (88%)	1054 (95%)	51 (5%)	0	100	100
1	B	1105/1259 (88%)	1047 (95%)	58 (5%)	0	100	100
1	C	1105/1259 (88%)	1057 (96%)	48 (4%)	0	100	100
All	All	3315/3777 (88%)	3158 (95%)	157 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	965/1088 (89%)	964 (100%)	1 (0%)	93	98
1	B	965/1088 (89%)	964 (100%)	1 (0%)	93	98
1	C	965/1088 (89%)	965 (100%)	0	100	100
All	All	2895/3264 (89%)	2893 (100%)	2 (0%)	93	98

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

Mol	Chain	Res	Type
1	A	341	PHE
1	B	341	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	202	HIS
1	B	202	HIS
1	B	648	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	L	1	1,2	14,14,15	0.19	0	17,19,21	0.86	1 (5%)
2	NAG	L	2	2	14,14,15	0.22	0	17,19,21	0.92	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.45	0	17,19,21	0.50	0
2	NAG	M	2	2	14,14,15	0.21	0	17,19,21	0.71	1 (5%)
2	NAG	N	1	1,2	14,14,15	0.88	1 (7%)	17,19,21	1.41	1 (5%)
2	NAG	N	2	2	14,14,15	0.29	0	17,19,21	0.88	1 (5%)
2	NAG	P	1	1,2	14,14,15	0.28	0	17,19,21	0.75	1 (5%)
2	NAG	P	2	2	14,14,15	0.18	0	17,19,21	0.88	1 (5%)
2	NAG	Q	1	1,2	14,14,15	0.43	0	17,19,21	0.54	0
2	NAG	Q	2	2	14,14,15	0.18	0	17,19,21	0.61	1 (5%)
2	NAG	R	1	1,2	14,14,15	0.87	1 (7%)	17,19,21	1.29	1 (5%)
2	NAG	R	2	2	14,14,15	0.26	0	17,19,21	0.79	1 (5%)
2	NAG	U	1	1,2	14,14,15	0.27	0	17,19,21	0.61	0
2	NAG	U	2	2	14,14,15	0.18	0	17,19,21	0.66	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
2	NAG	V	1	1,2	14,14,15	0.73	1 (7%)	17,19,21	0.59	0
2	NAG	V	2	2	14,14,15	0.21	0	17,19,21	0.75	1 (5%)
2	NAG	W	1	1,2	14,14,15	0.80	1 (7%)	17,19,21	1.28	1 (5%)
2	NAG	W	2	2	14,14,15	0.17	0	17,19,21	0.74	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1	NAG	O5-C1	3.11	1.48	1.43
2	R	1	NAG	O5-C1	2.85	1.48	1.43
2	W	1	NAG	O5-C1	2.81	1.48	1.43
2	V	1	NAG	O5-C1	-2.63	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1	NAG	C1-O5-C5	5.08	119.07	112.19
2	R	1	NAG	C1-O5-C5	4.86	118.78	112.19
2	W	1	NAG	C1-O5-C5	4.71	118.58	112.19
2	L	2	NAG	C1-O5-C5	3.51	116.95	112.19
2	P	2	NAG	C1-O5-C5	3.41	116.81	112.19
2	N	2	NAG	C1-O5-C5	3.40	116.79	112.19
2	L	1	NAG	C1-O5-C5	2.98	116.23	112.19
2	R	2	NAG	C1-O5-C5	2.96	116.20	112.19
2	V	2	NAG	C1-O5-C5	2.81	116.01	112.19
2	W	2	NAG	C1-O5-C5	2.68	115.82	112.19
2	M	2	NAG	C1-O5-C5	2.66	115.80	112.19
2	U	2	NAG	C1-O5-C5	2.38	115.41	112.19
2	P	1	NAG	C1-O5-C5	2.35	115.37	112.19
2	Q	2	NAG	C1-O5-C5	2.07	114.99	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	P	1	NAG	C1-C2-N2-C7
2	W	2	NAG	O5-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	U	1	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	R	1	NAG	C4-C5-C6-O6

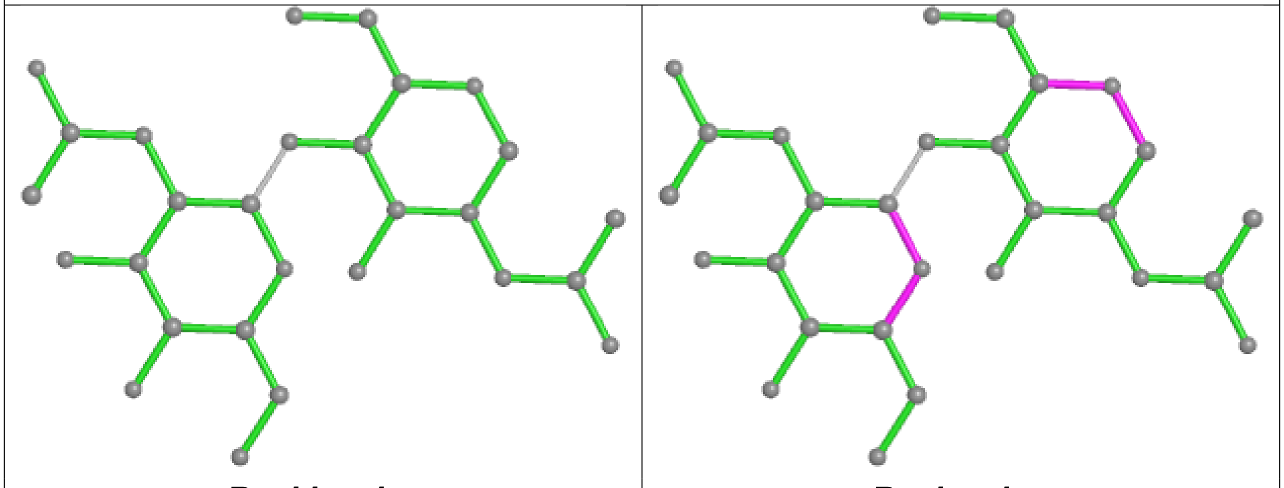
There are no ring outliers.

1 monomer is involved in 1 short contact:

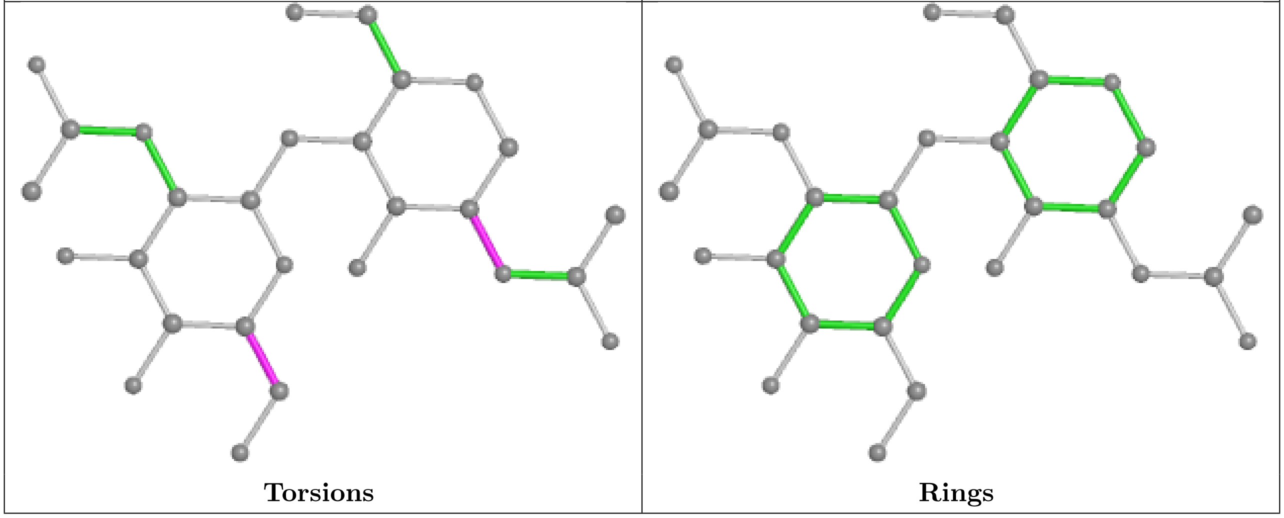
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	1	NAG	1	0

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

Oligosaccharide Chain L

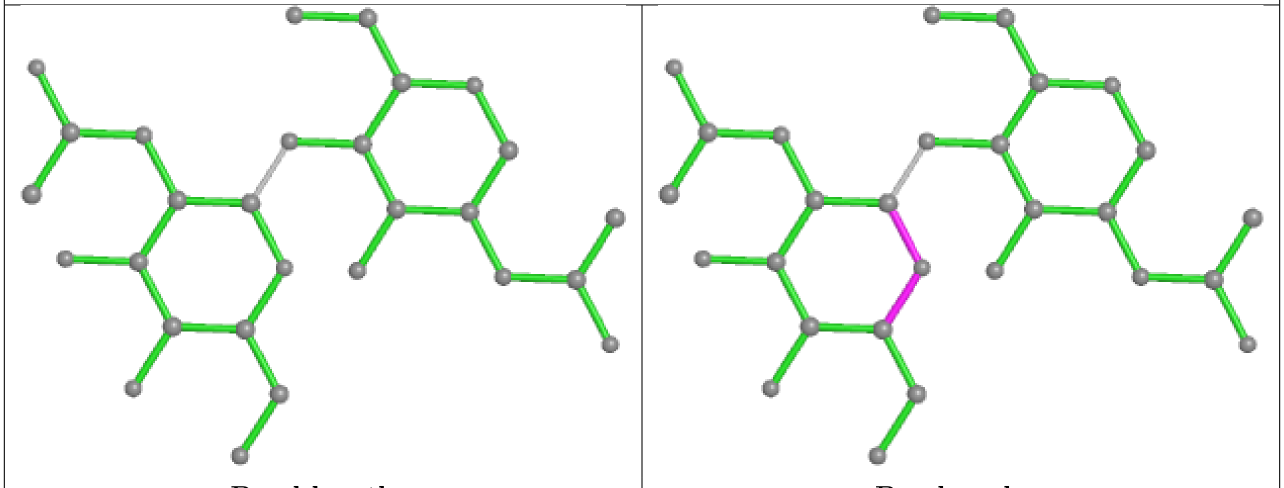


Bond lengths **Bond angles**

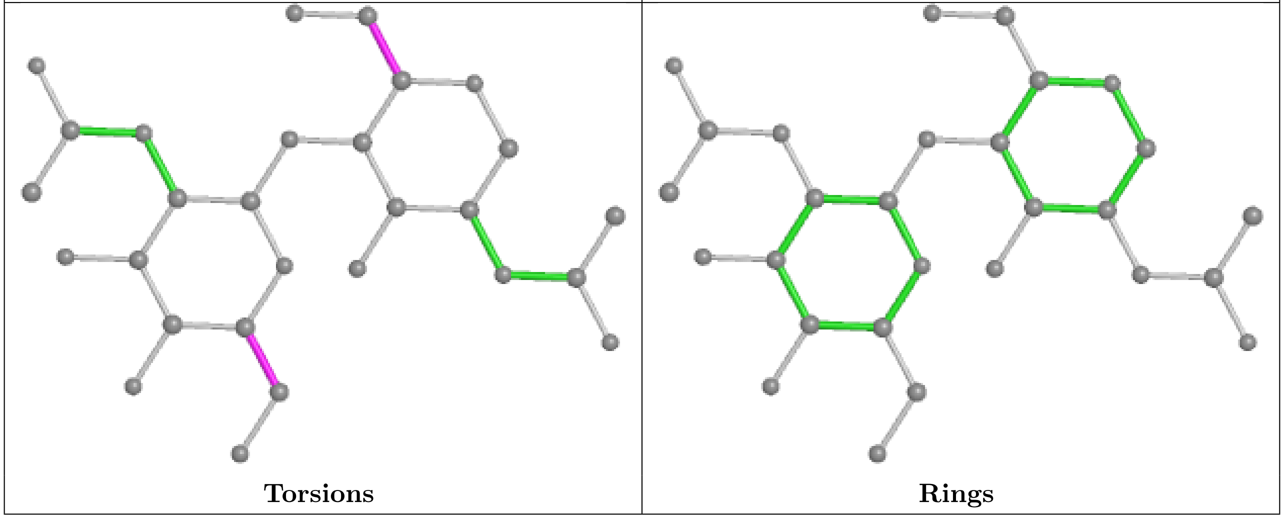


Torsions **Rings**

Oligosaccharide Chain M

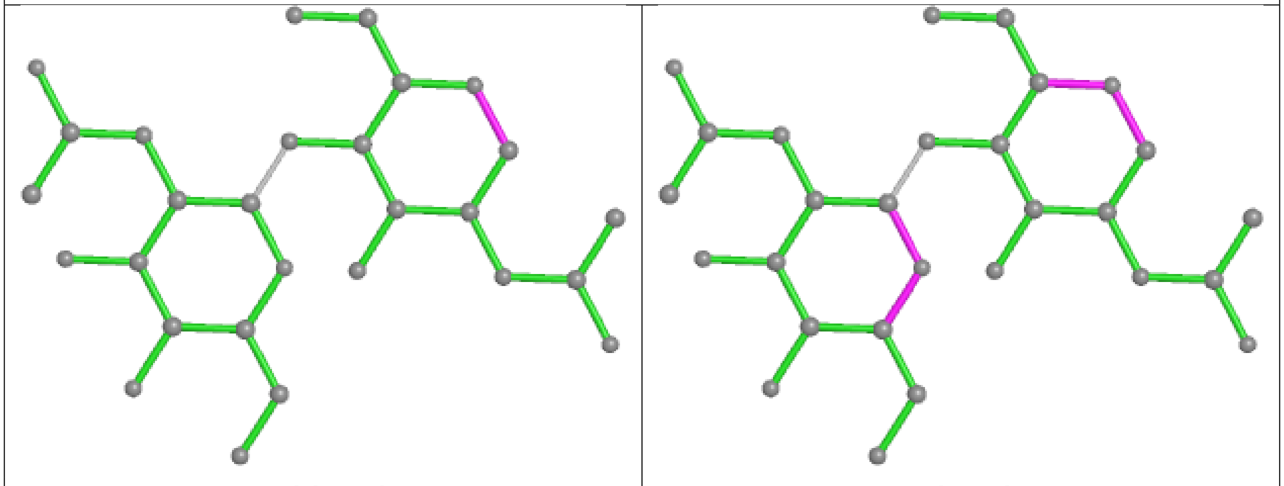


Bond lengths **Bond angles**

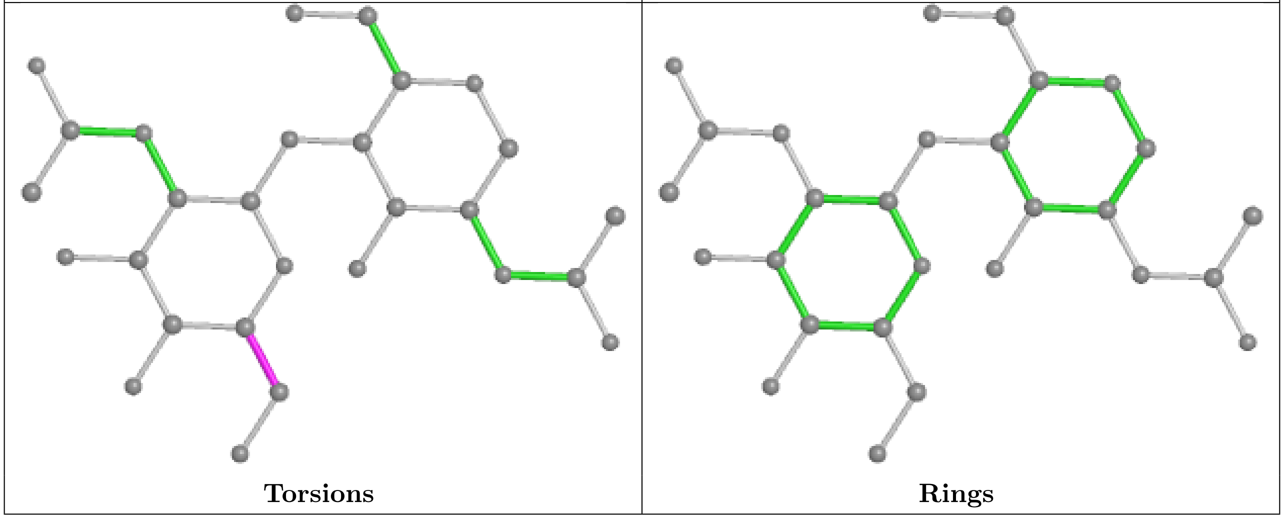


Torsions **Rings**

Oligosaccharide Chain N

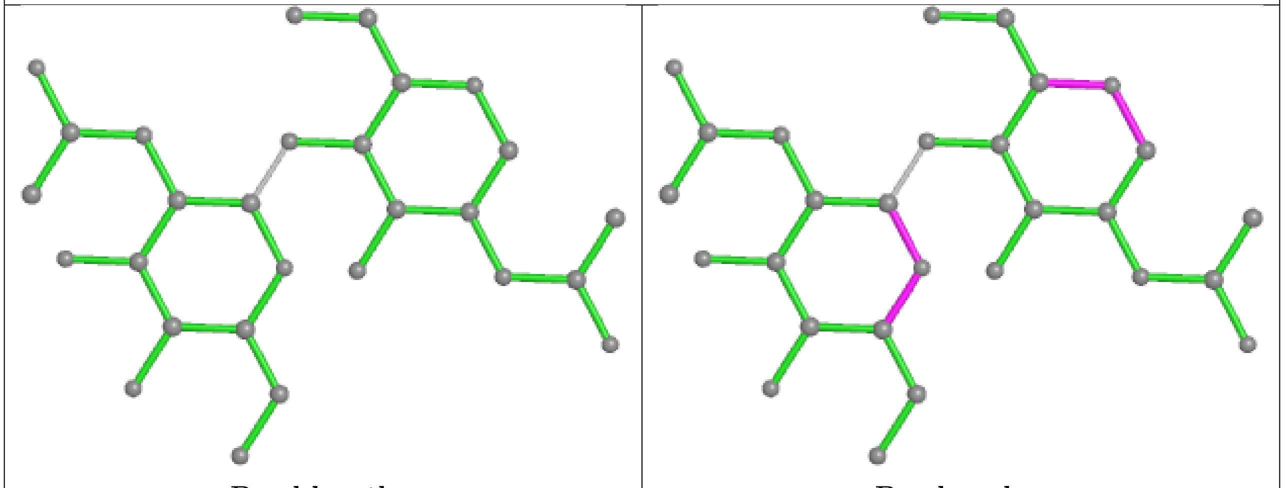


Bond lengths **Bond angles**



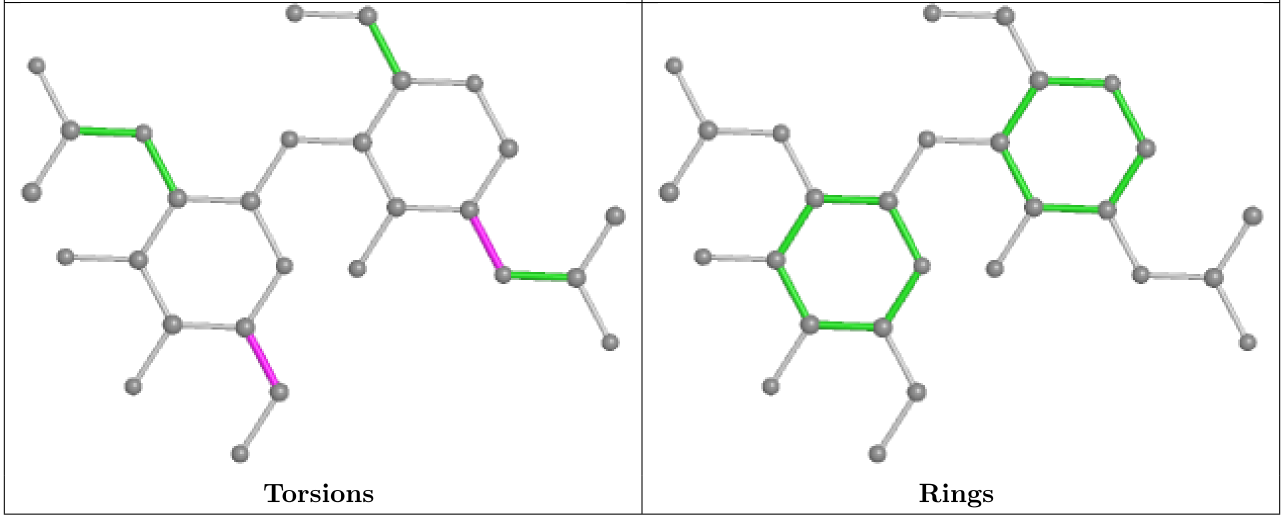
Torsions **Rings**

Oligosaccharide Chain P



Bond lengths

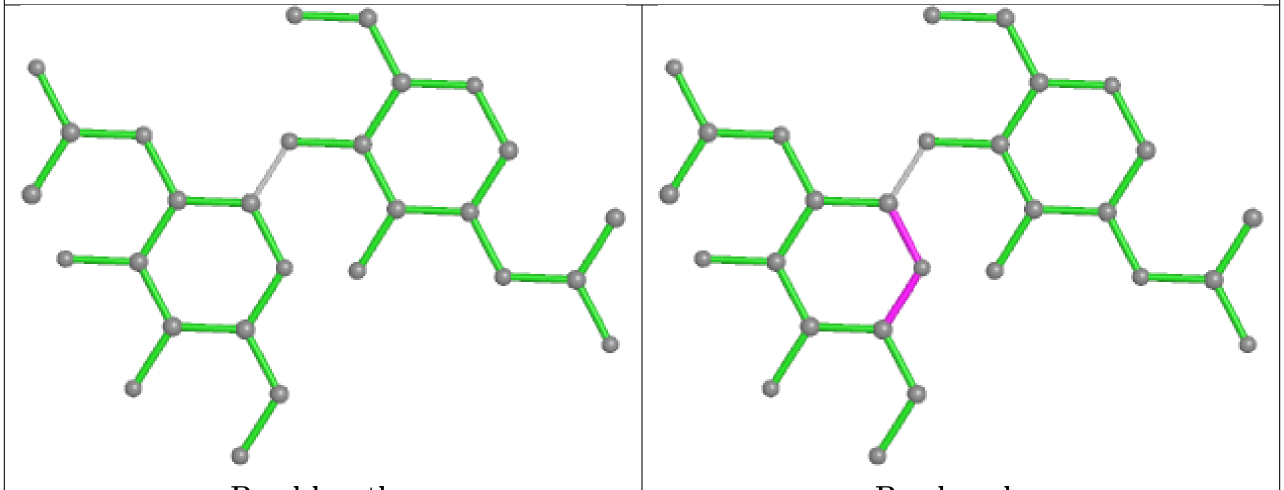
Bond angles



Torsions

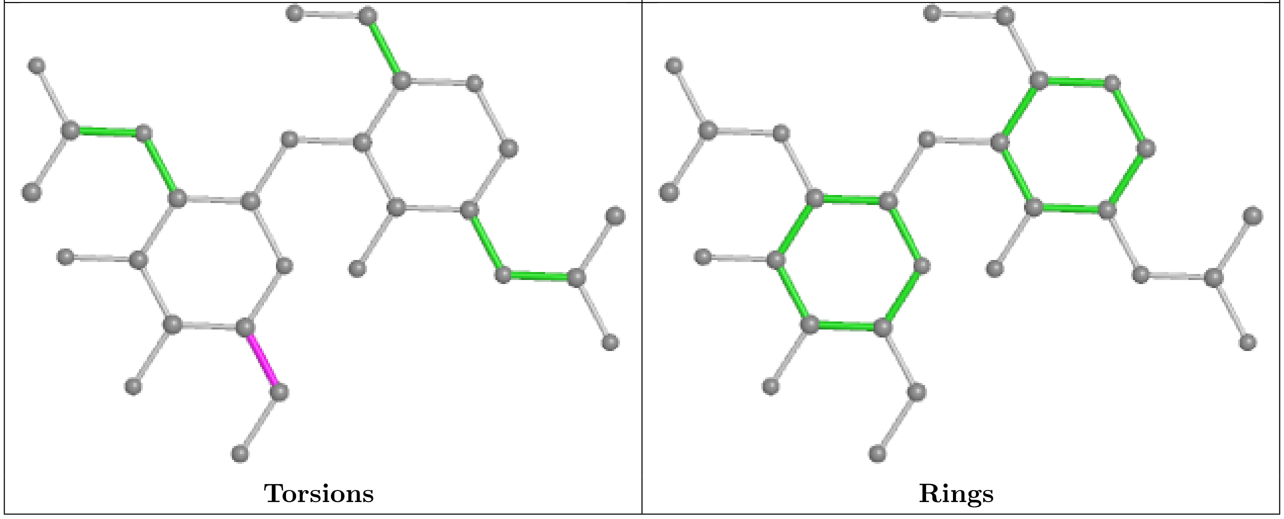
Rings

Oligosaccharide Chain Q



Bond lengths

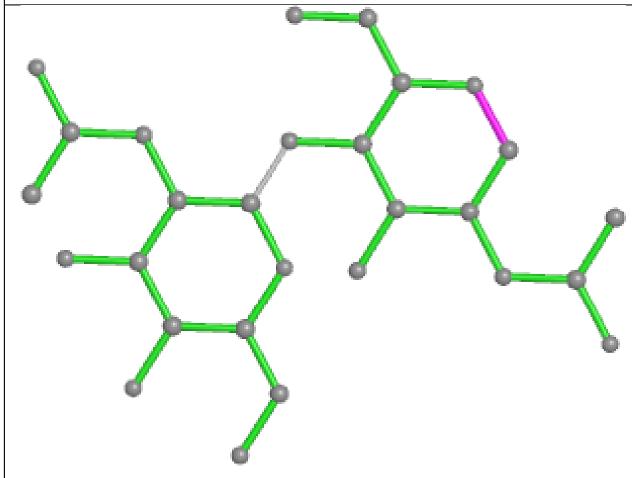
Bond angles



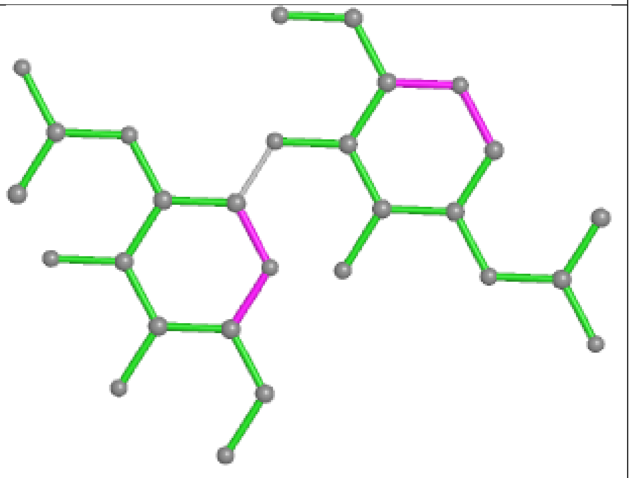
Torsions

Rings

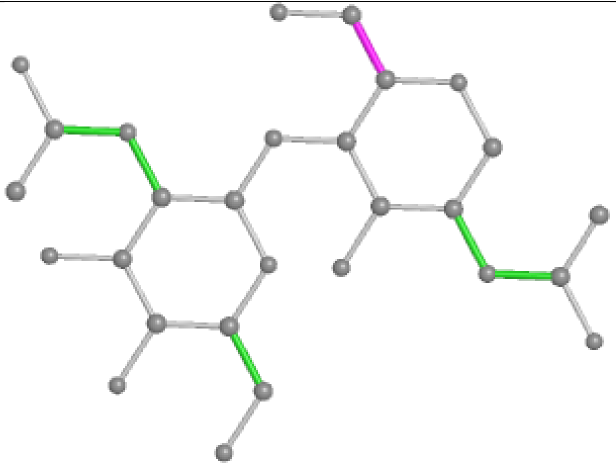
Oligosaccharide Chain R



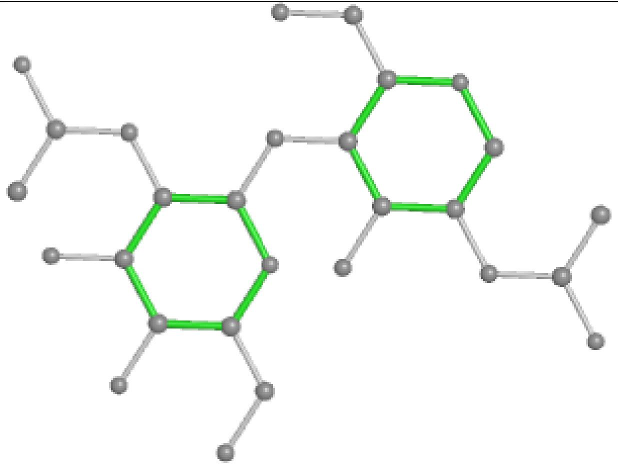
Bond lengths



Bond angles

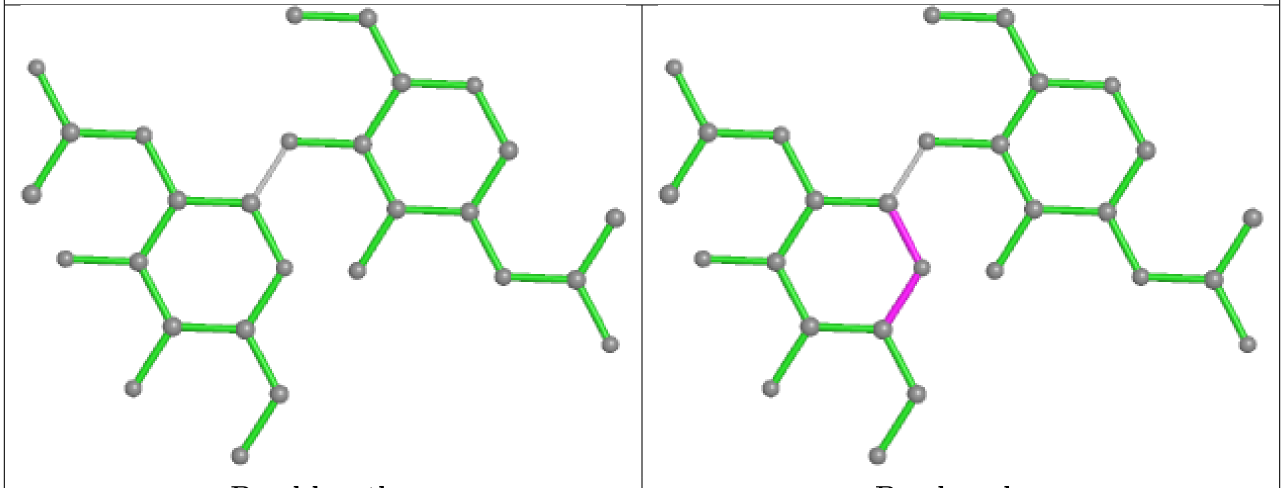


Torsions



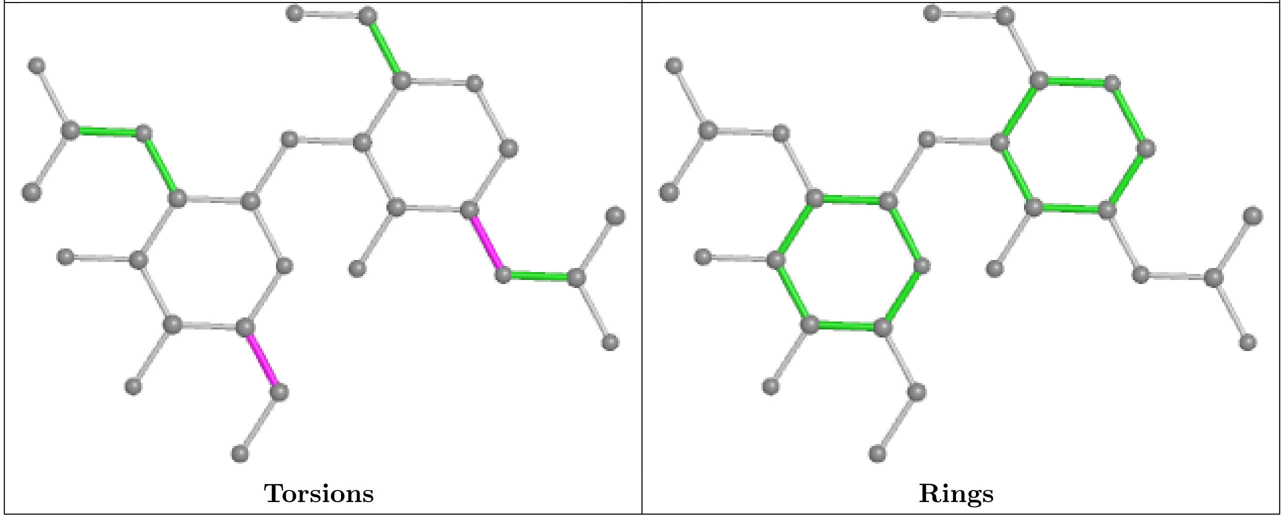
Rings

Oligosaccharide Chain U



Bond lengths

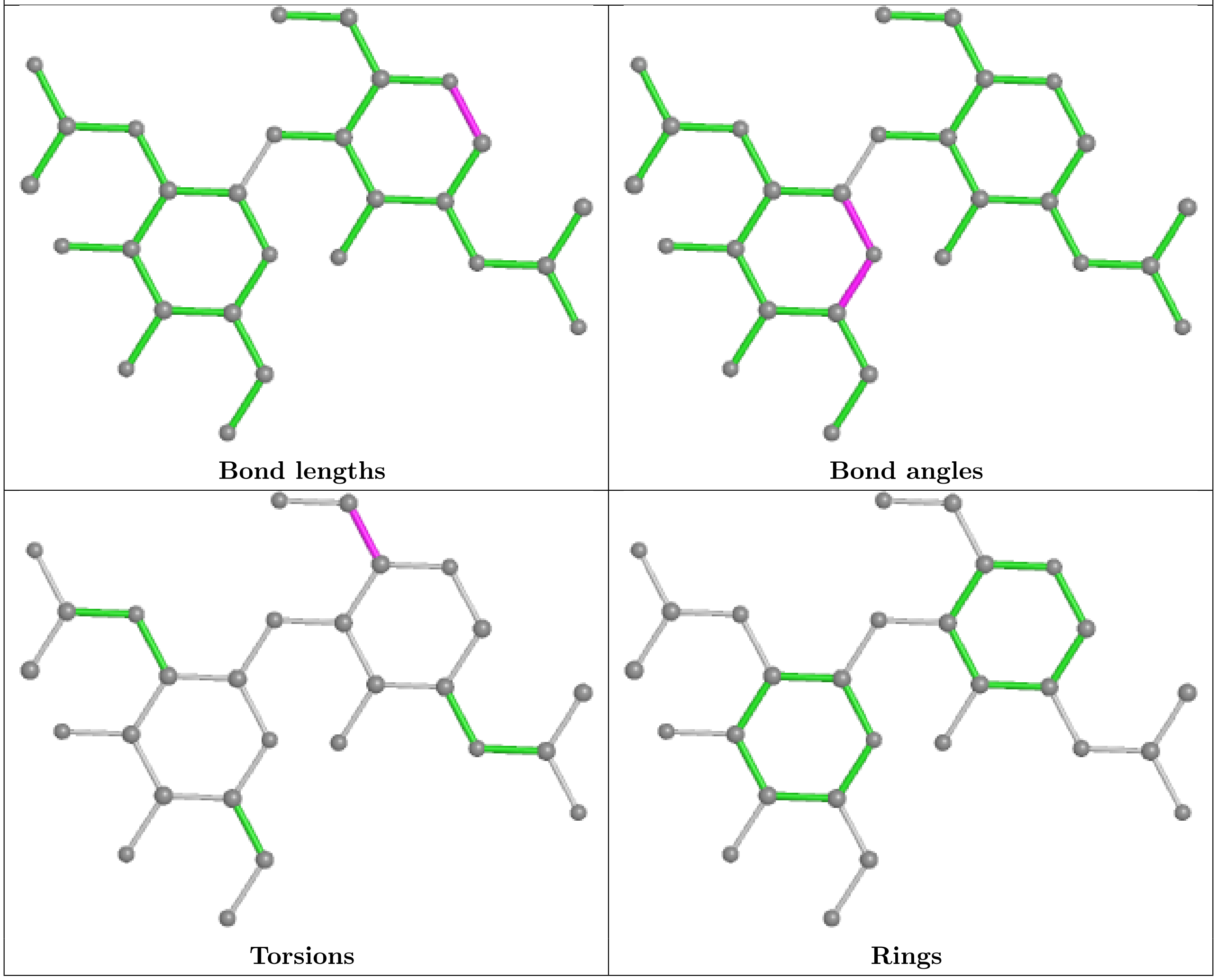
Bond angles



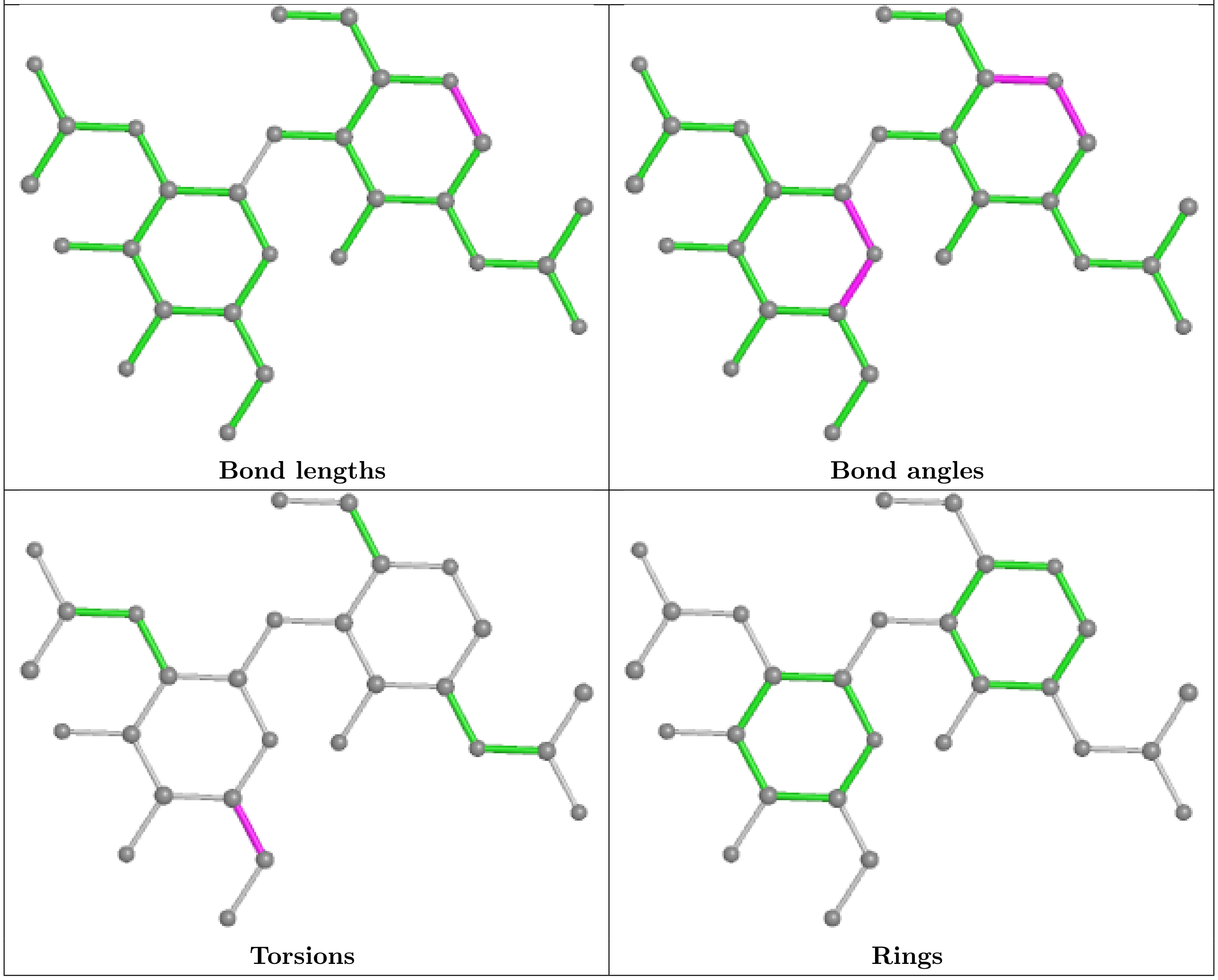
Torsions

Rings

Oligosaccharide Chain V



Oligosaccharide Chain W



Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

45 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	$\#\|Z\| > 2$
3	NAG	C	1304	1	14,14,15	0.53	0	17,19,21	0.95	1 (5%)
3	NAG	C	1305	1	14,14,15	0.51	0	17,19,21	1.00	1 (5%)
3	NAG	B	1302	1	14,14,15	0.45	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
3	NAG	A	1309	1	14,14,15	0.34	0	17,19,21	0.64	0
3	NAG	C	1303	1	14,14,15	0.42	0	17,19,21	0.48	0
3	NAG	B	1315	1	14,14,15	0.18	0	17,19,21	0.91	1 (5%)
3	NAG	C	1308	1	14,14,15	0.32	0	17,19,21	0.88	1 (5%)
3	NAG	A	1312	1	14,14,15	0.21	0	17,19,21	0.65	1 (5%)
3	NAG	A	1303	1	14,14,15	0.44	0	17,19,21	0.51	0
3	NAG	A	1313	1	14,14,15	0.47	0	17,19,21	0.43	0
3	NAG	C	1307	1	14,14,15	0.41	0	17,19,21	0.92	1 (5%)
3	NAG	B	1310	1	14,14,15	0.37	0	17,19,21	0.82	1 (5%)
3	NAG	C	1310	1	14,14,15	0.26	0	17,19,21	0.81	1 (5%)
3	NAG	A	1305	1	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	A	1301	1	14,14,15	0.48	0	17,19,21	1.14	1 (5%)
3	NAG	B	1313	1	14,14,15	0.84	1 (7%)	17,19,21	1.29	1 (5%)
3	NAG	A	1302	1	14,14,15	0.61	1 (7%)	17,19,21	0.37	0
3	NAG	A	1314	1	14,14,15	0.21	0	17,19,21	0.50	0
3	NAG	B	1301	1	14,14,15	0.17	0	17,19,21	0.86	1 (5%)
3	NAG	C	1306	1	14,14,15	0.16	0	17,19,21	0.55	0
3	NAG	C	1315	1	14,14,15	0.19	0	17,19,21	0.80	1 (5%)
3	NAG	B	1311	1	14,14,15	0.20	0	17,19,21	0.66	1 (5%)
3	NAG	C	1311	1	14,14,15	0.26	0	17,19,21	0.70	1 (5%)
3	NAG	B	1308	1	14,14,15	0.17	0	17,19,21	0.66	1 (5%)
3	NAG	B	1314	1	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	A	1307	1	14,14,15	0.19	0	17,19,21	0.71	1 (5%)
3	NAG	A	1311	1	14,14,15	0.30	0	17,19,21	0.81	1 (5%)
3	NAG	B	1309	1	14,14,15	0.19	0	17,19,21	0.60	0
3	NAG	A	1304	1	14,14,15	0.28	0	17,19,21	0.43	0
3	NAG	C	1309	1	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
3	NAG	B	1307	1	14,14,15	0.41	0	17,19,21	0.95	1 (5%)
3	NAG	A	1308	1	14,14,15	0.25	0	17,19,21	0.86	1 (5%)
3	NAG	C	1301	1	14,14,15	0.29	0	17,19,21	0.95	1 (5%)
3	NAG	A	1306	1	14,14,15	0.26	0	17,19,21	0.54	0
3	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.63	0
3	NAG	A	1310	1	14,14,15	0.16	0	17,19,21	0.70	1 (5%)
3	NAG	C	1302	1	14,14,15	0.58	0	17,19,21	0.40	0
3	NAG	C	1314	1	14,14,15	0.20	0	17,19,21	0.49	0
3	NAG	B	1304	1	14,14,15	0.64	1 (7%)	17,19,21	1.05	1 (5%)
3	NAG	C	1312	1	14,14,15	1.14	2 (14%)	17,19,21	1.06	1 (5%)
3	NAG	C	1313	1	14,14,15	0.21	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	B	1303	1	14,14,15	0.54	0	17,19,21	0.49	0
3	NAG	B	1312	1	14,14,15	0.51	0	17,19,21	0.74	1 (5%)
3	NAG	A	1315	1	14,14,15	0.25	0	17,19,21	0.68	1 (5%)
3	NAG	B	1306	1	14,14,15	0.33	0	17,19,21	0.54	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	C	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1315	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1313	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1314	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1315	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1314	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1313	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1315	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1312	NAG	O5-C1	3.02	1.48	1.43
3	C	1312	NAG	C1-C2	2.88	1.56	1.52
3	B	1313	NAG	O5-C1	2.80	1.48	1.43
3	A	1302	NAG	O5-C1	-2.09	1.40	1.43
3	B	1304	NAG	C1-C2	2.03	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1313	NAG	C1-O5-C5	5.20	119.24	112.19
3	A	1301	NAG	C1-O5-C5	4.51	118.31	112.19
3	C	1312	NAG	C1-O5-C5	4.23	117.93	112.19
3	B	1304	NAG	C1-O5-C5	4.09	117.74	112.19
3	C	1305	NAG	C1-O5-C5	3.97	117.57	112.19
3	B	1307	NAG	C1-O5-C5	3.76	117.28	112.19
3	C	1301	NAG	C1-O5-C5	3.63	117.12	112.19
3	C	1304	NAG	C1-O5-C5	3.59	117.06	112.19
3	B	1315	NAG	C1-O5-C5	3.50	116.93	112.19
3	C	1307	NAG	C1-O5-C5	3.35	116.72	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1301	NAG	C1-O5-C5	3.11	116.41	112.19
3	C	1308	NAG	C1-O5-C5	3.11	116.40	112.19
3	B	1310	NAG	C1-O5-C5	3.09	116.38	112.19
3	C	1315	NAG	C1-O5-C5	3.07	116.36	112.19
3	A	1311	NAG	C1-O5-C5	3.06	116.33	112.19
3	A	1308	NAG	C1-O5-C5	2.97	116.21	112.19
3	C	1310	NAG	C1-O5-C5	2.94	116.18	112.19
3	C	1309	NAG	C1-O5-C5	2.86	116.06	112.19
3	B	1312	NAG	C1-O5-C5	2.81	116.00	112.19
3	C	1311	NAG	C1-O5-C5	2.59	115.70	112.19
3	A	1310	NAG	C1-O5-C5	2.57	115.68	112.19
3	A	1307	NAG	C1-O5-C5	2.48	115.55	112.19
3	A	1315	NAG	C1-O5-C5	2.45	115.51	112.19
3	B	1311	NAG	C1-O5-C5	2.41	115.46	112.19
3	B	1308	NAG	C1-O5-C5	2.33	115.35	112.19
3	A	1312	NAG	C1-O5-C5	2.32	115.33	112.19

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1301	NAG	C1-C2-N2-C7
3	C	1304	NAG	C3-C2-N2-C7
3	B	1301	NAG	O5-C5-C6-O6
3	A	1304	NAG	C1-C2-N2-C7
3	A	1308	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1315	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6
3	C	1315	NAG	O5-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1302	NAG	C1-C2-N2-C7
3	C	1302	NAG	C1-C2-N2-C7
3	B	1301	NAG	C1-C2-N2-C7
3	B	1302	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	1303	NAG	O5-C5-C6-O6
3	C	1313	NAG	C4-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6
3	B	1310	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	C	1315	NAG	C4-C5-C6-O6
3	A	1315	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	C	1311	NAG	C4-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	C	1313	NAG	C1-C2-N2-C7
3	B	1304	NAG	C1-C2-N2-C7
3	B	1313	NAG	C4-C5-C6-O6
3	A	1311	NAG	O5-C5-C6-O6
3	B	1313	NAG	O5-C5-C6-O6
3	C	1301	NAG	C1-C2-N2-C7
3	A	1311	NAG	C4-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	C	1313	NAG	O5-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	B	1315	NAG	C4-C5-C6-O6
3	A	1312	NAG	O5-C5-C6-O6
3	B	1315	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	A	1302	NAG	C3-C2-N2-C7
3	C	1302	NAG	C3-C2-N2-C7
3	B	1302	NAG	C3-C2-N2-C7
3	B	1304	NAG	C3-C2-N2-C7
3	B	1312	NAG	O5-C5-C6-O6
3	B	1311	NAG	C4-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	C	1304	NAG	C1-C2-N2-C7
3	A	1304	NAG	C4-C5-C6-O6
3	A	1301	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	A	1303	NAG	C3-C2-N2-C7
3	A	1304	NAG	C3-C2-N2-C7
3	C	1301	NAG	C3-C2-N2-C7
3	C	1303	NAG	C3-C2-N2-C7
3	B	1301	NAG	C3-C2-N2-C7
3	B	1303	NAG	C3-C2-N2-C7
3	C	1310	NAG	O5-C5-C6-O6
3	C	1313	NAG	C3-C2-N2-C7
3	A	1313	NAG	C4-C5-C6-O6

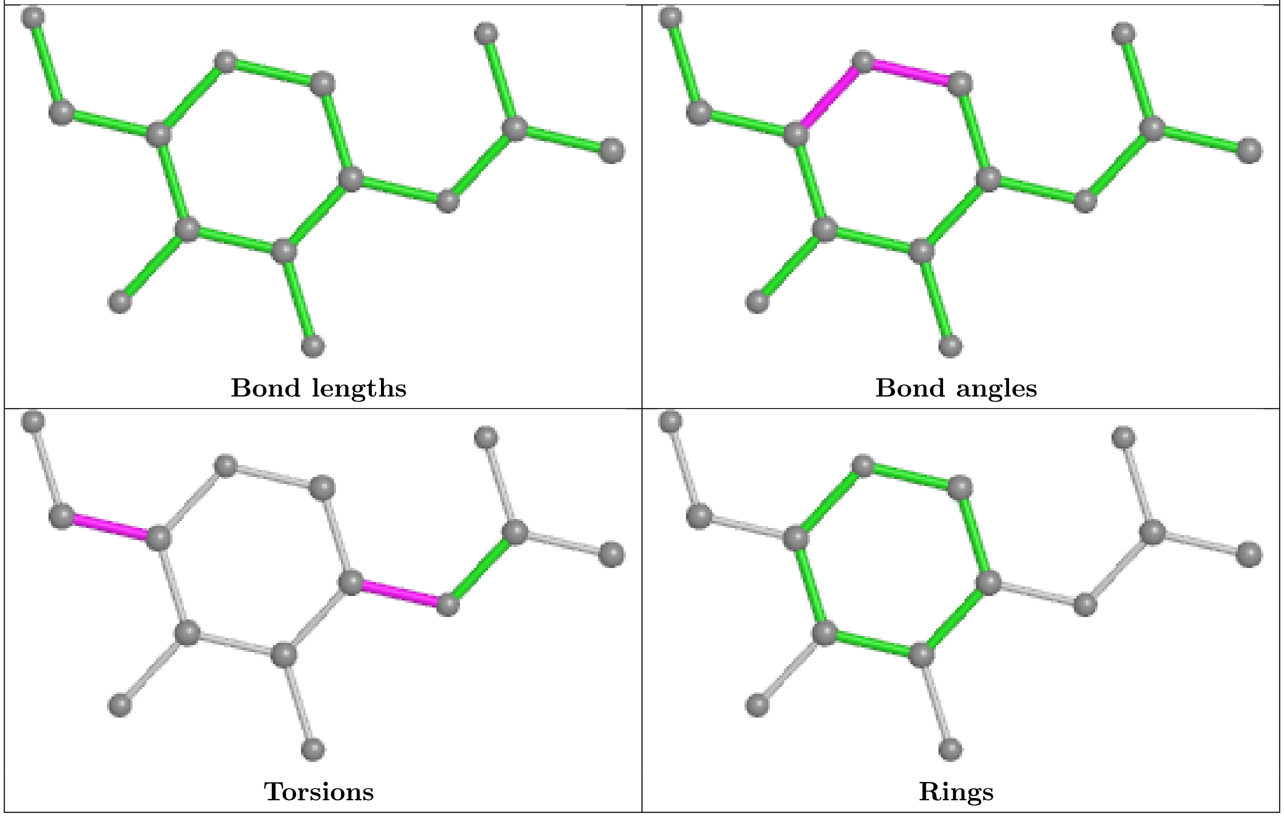
There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1304	NAG	2	0
3	B	1302	NAG	2	0
3	A	1301	NAG	2	0
3	A	1302	NAG	1	0
3	B	1301	NAG	2	0
3	A	1304	NAG	1	0
3	C	1301	NAG	2	0
3	C	1302	NAG	1	0
3	B	1304	NAG	3	0
3	C	1313	NAG	1	0
3	B	1306	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 then 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 C 1304



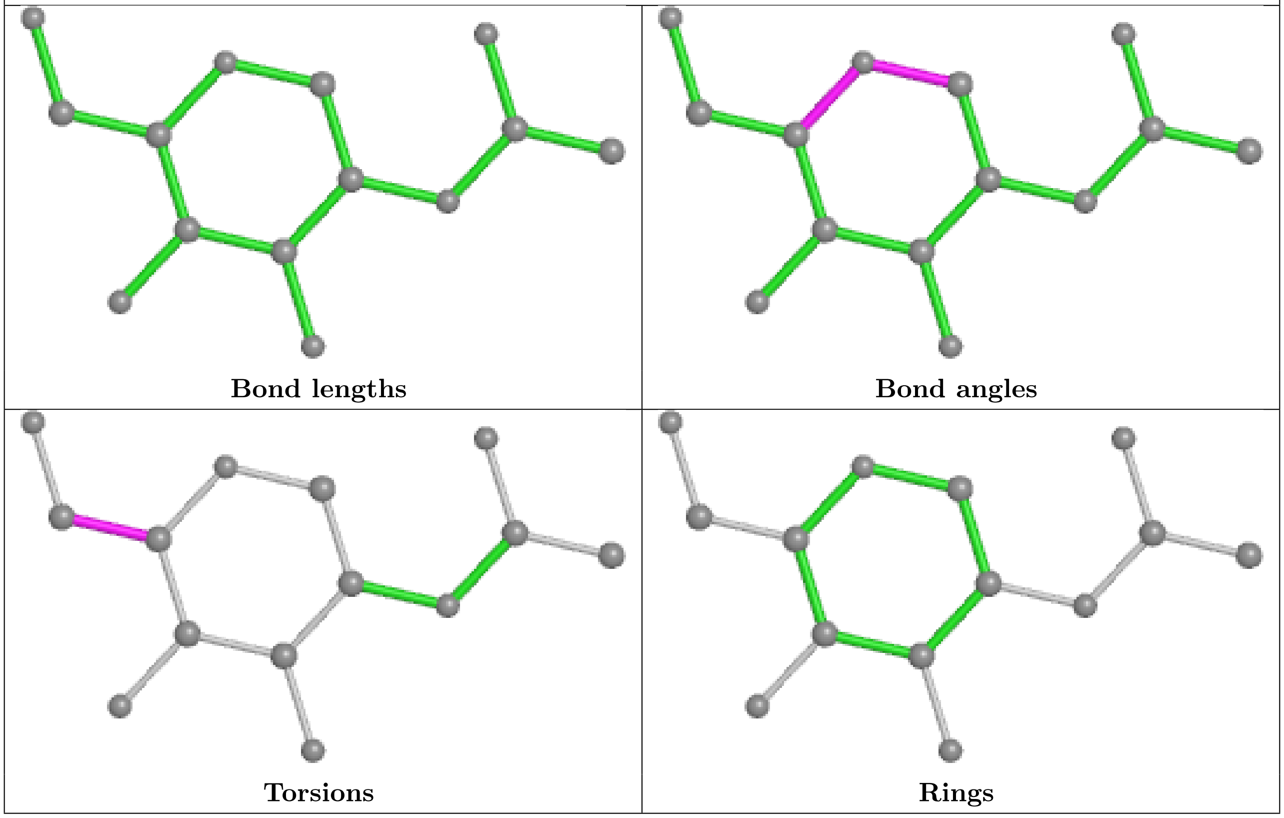
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 1305



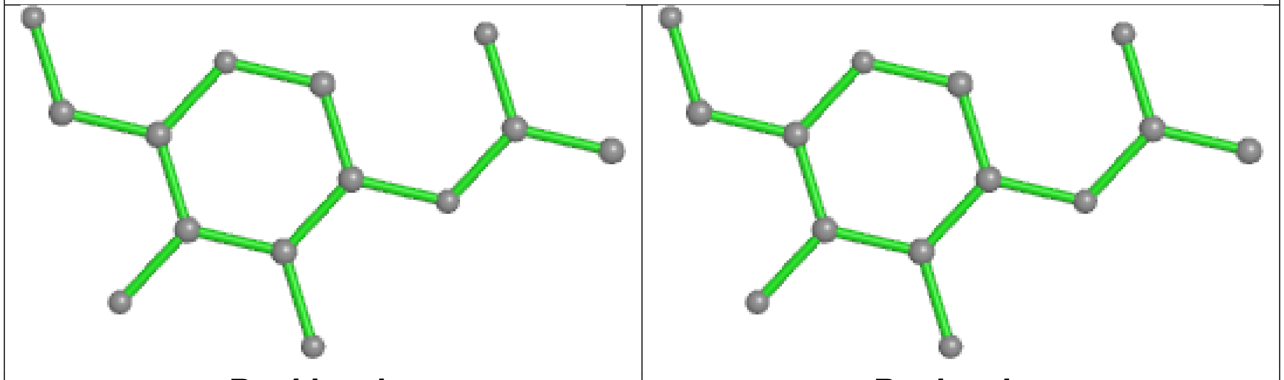
Bond lengths

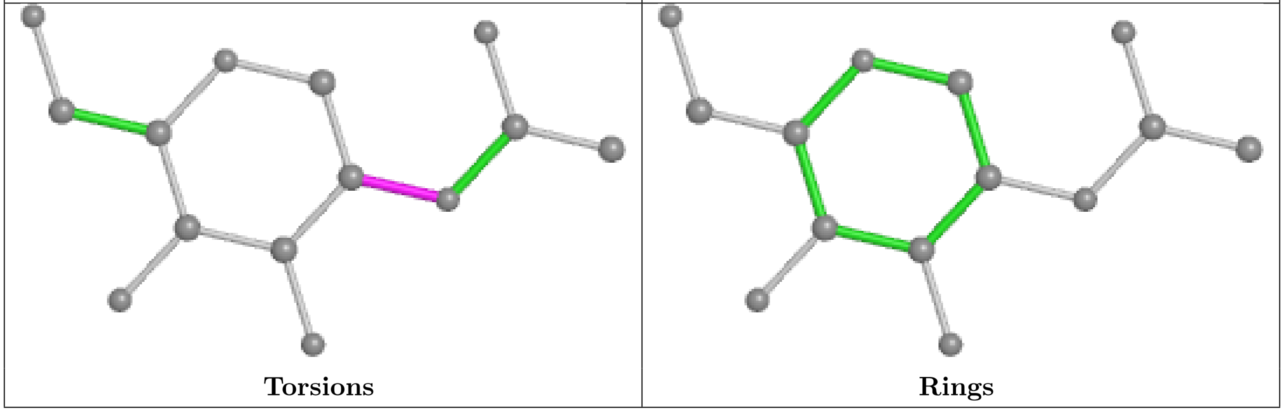
Bond angles

Torsions

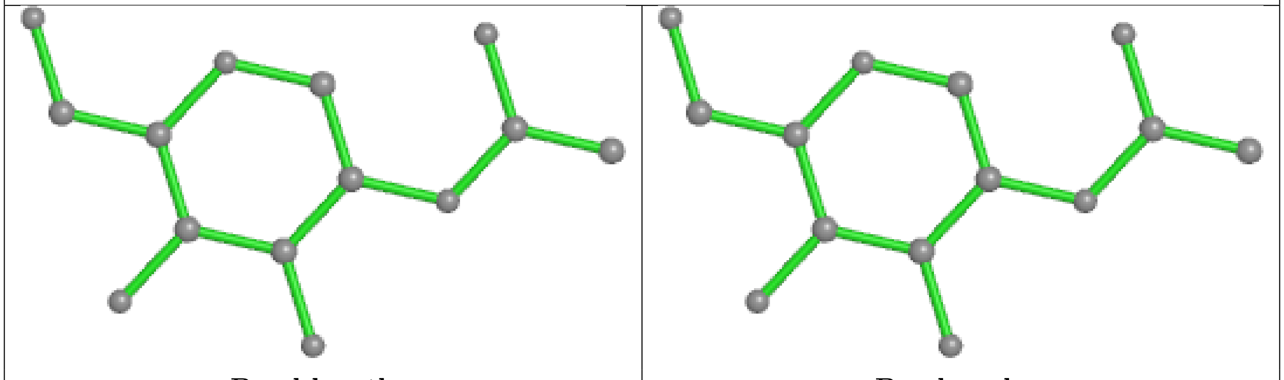
Rings

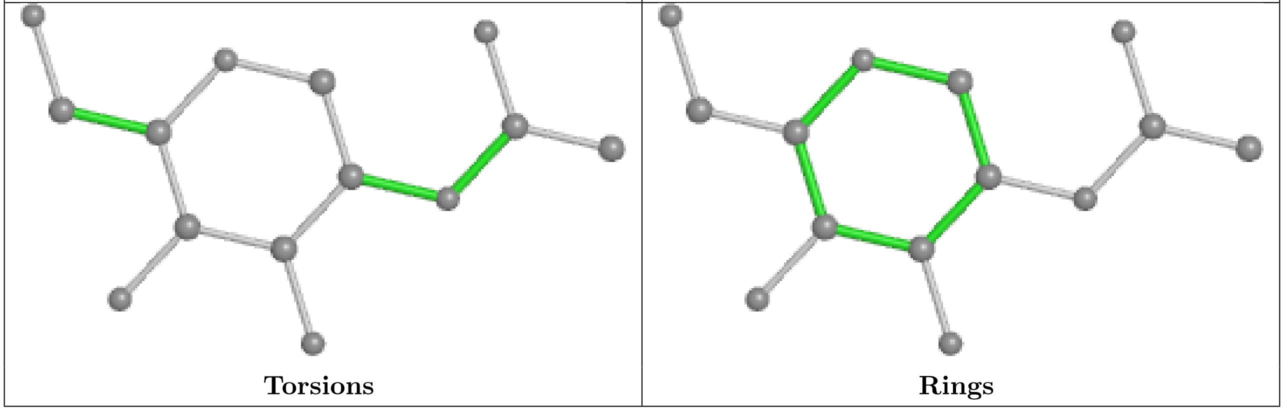
Ligand NAG B 1302


Bond lengths Bond angles

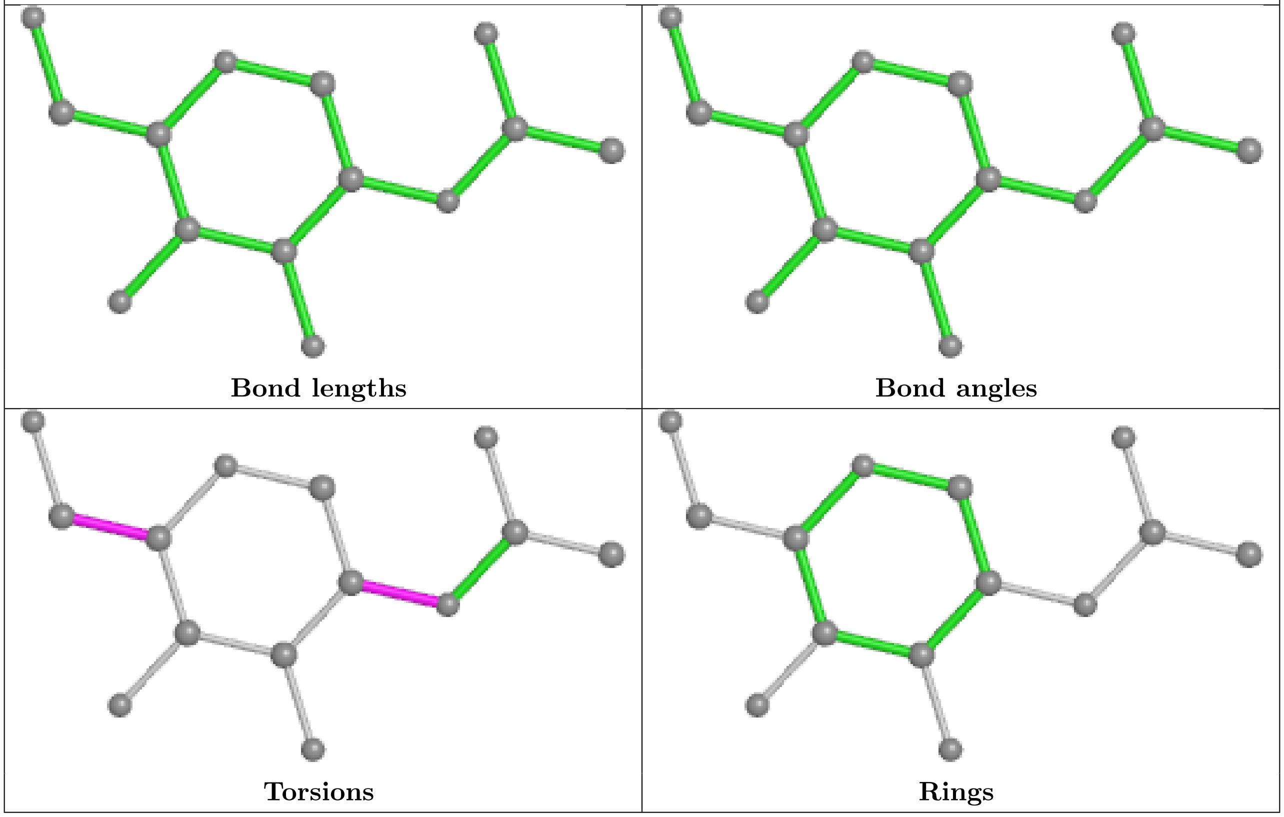

Torsions Rings

Ligand NAG A 1309

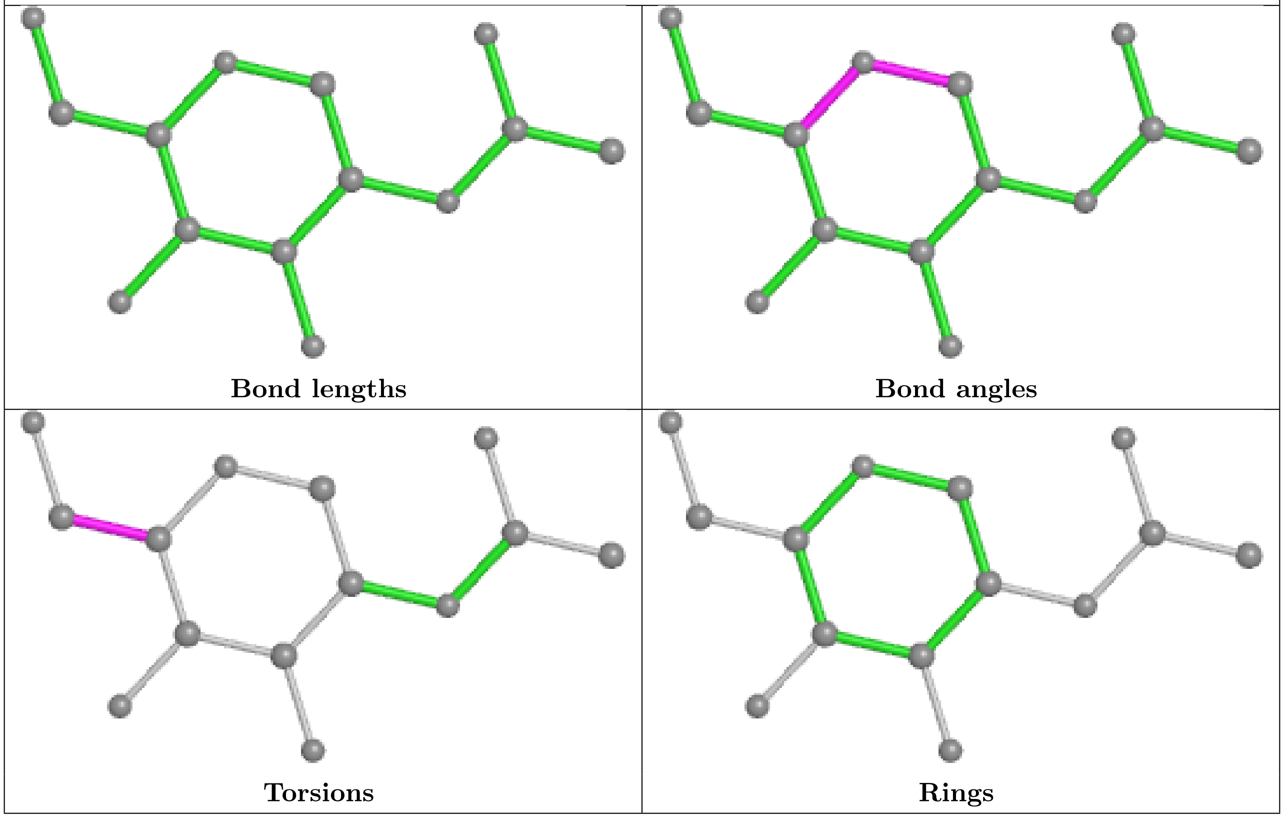

Bond lengths Bond angles


Torsions Rings

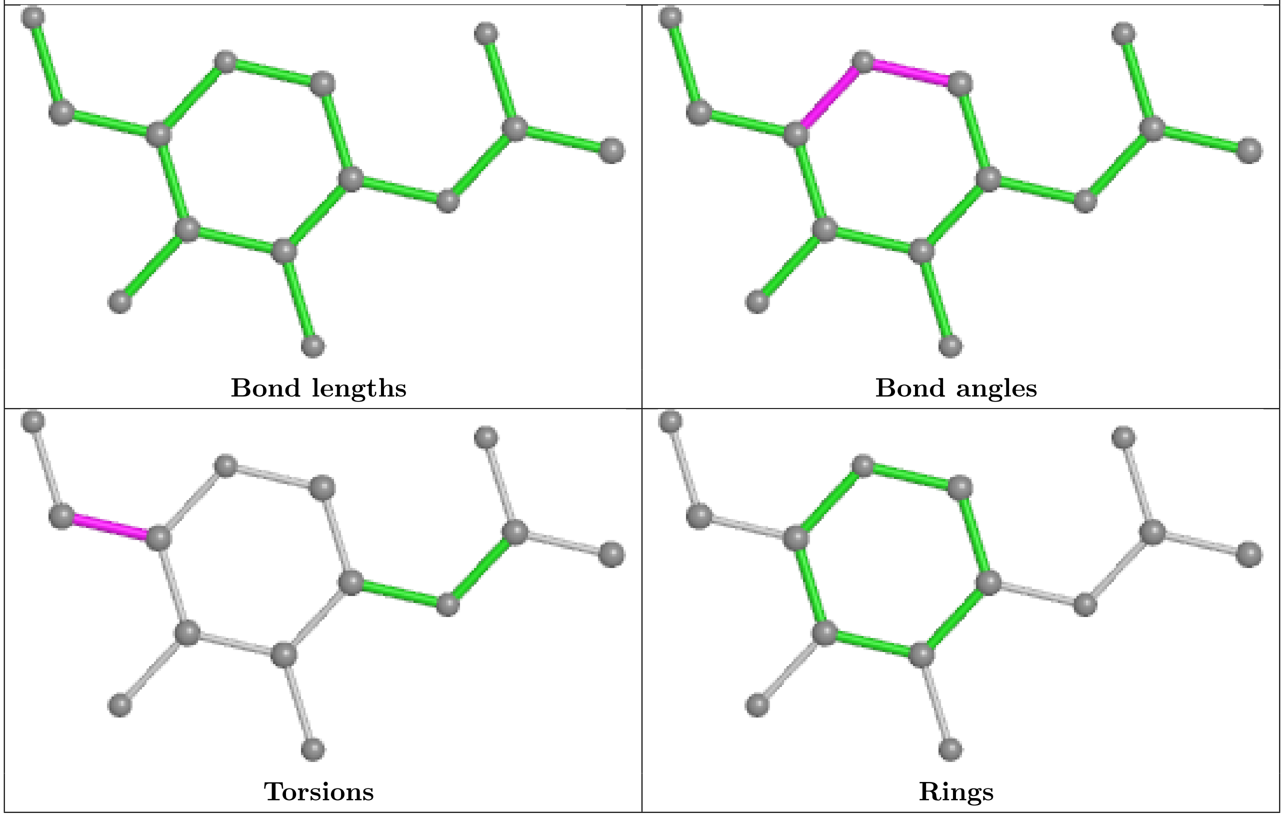
Ligand NAG C 1303


Bond lengths
Bond angles
Torsions
Rings

Ligand NAG B 1315


Bond lengths
Bond angles
Torsions
Rings

Ligand NAG C 1308



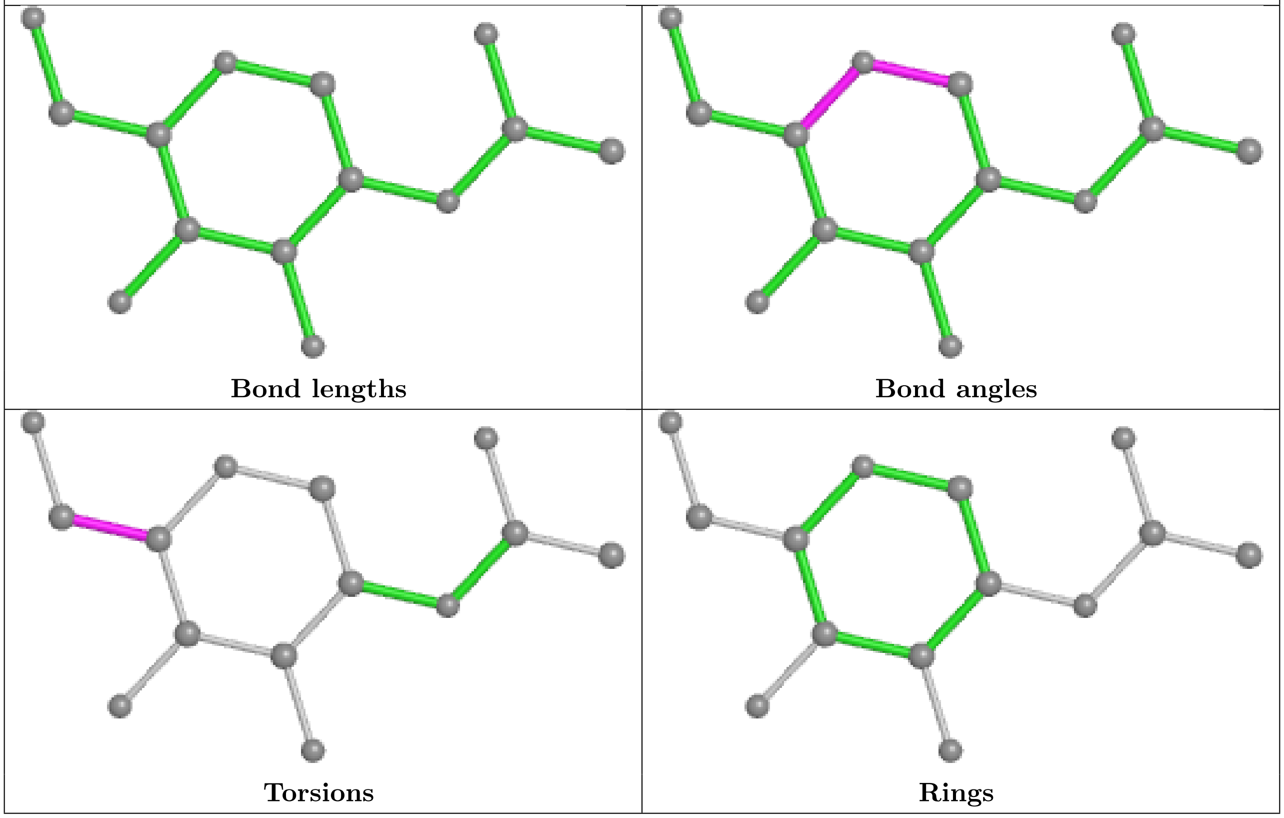
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 1312



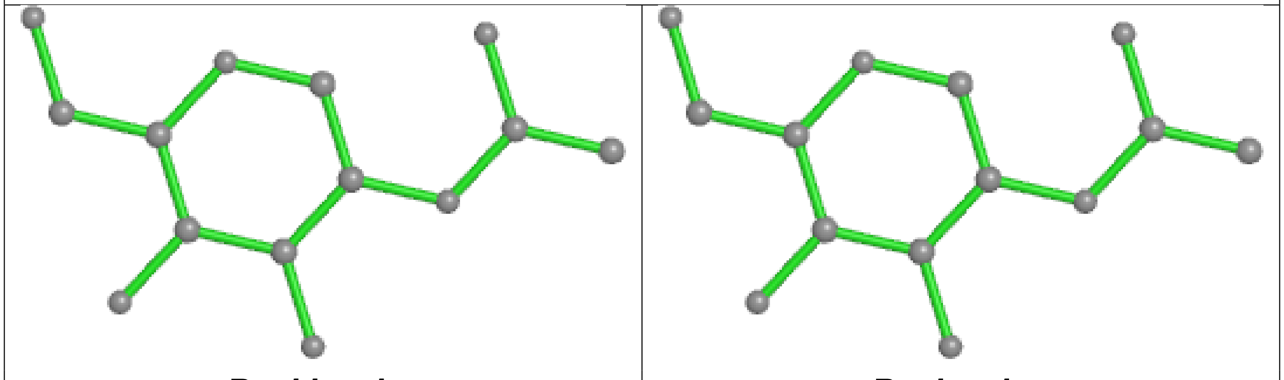
Bond lengths

Bond angles

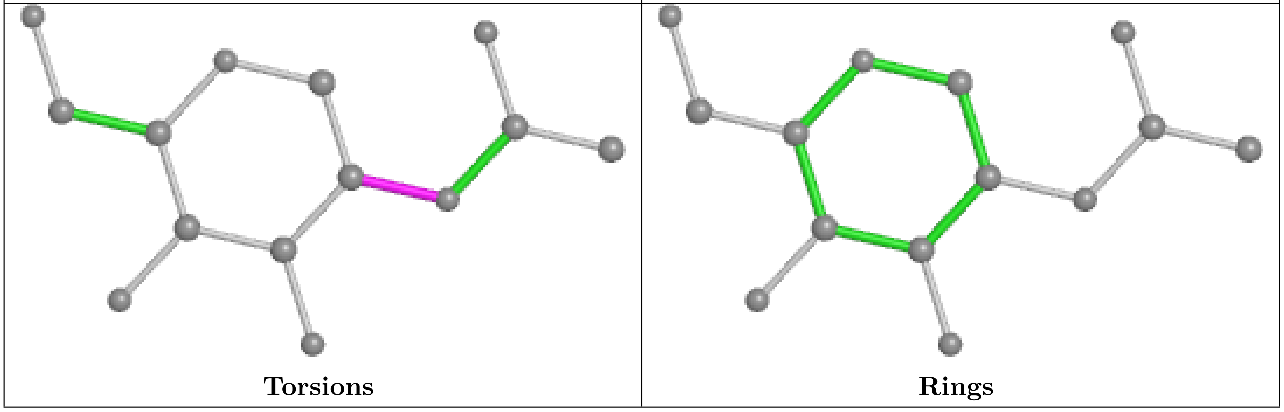
Torsions

Rings

Ligand NAG A 1303

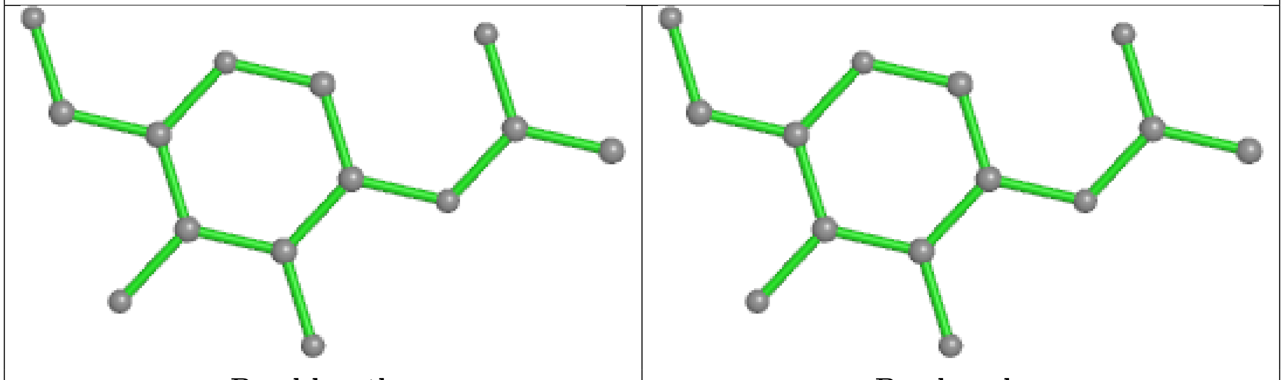


Bond lengths Bond angles

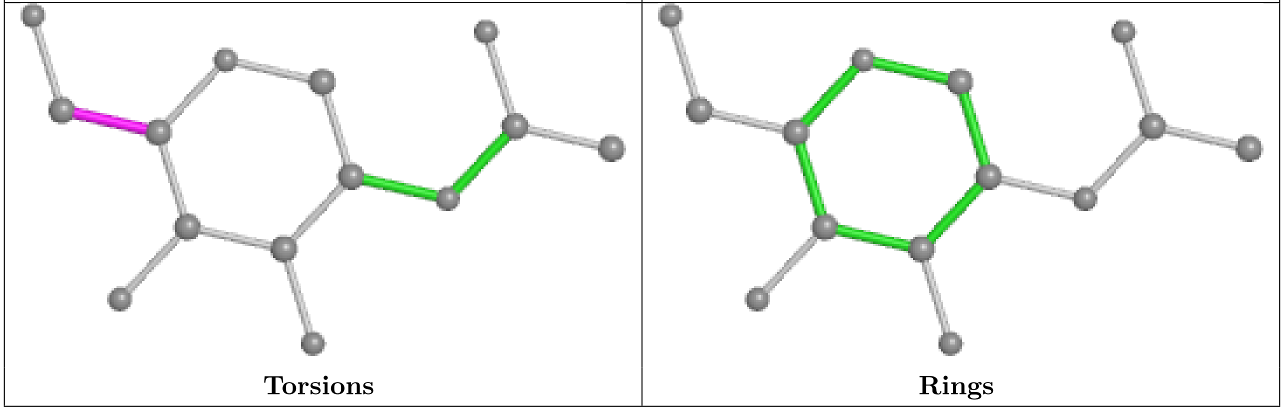


Torsions Rings

Ligand NAG A 1313

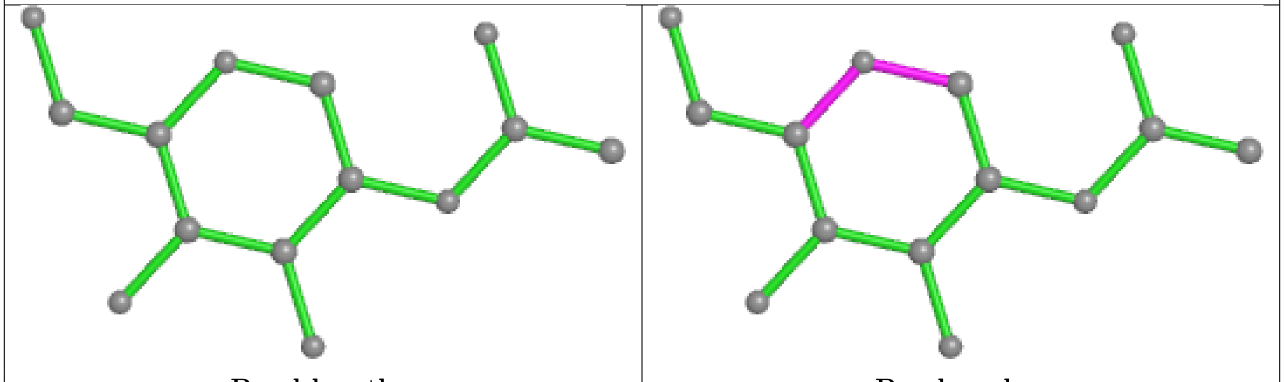


Bond lengths Bond angles



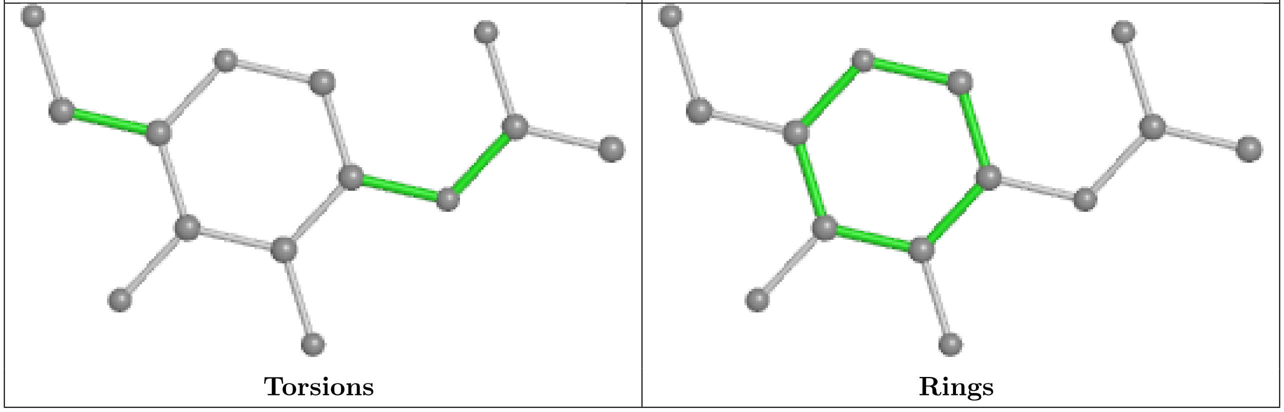
Torsions Rings

Ligand NAG C 1307



Bond lengths

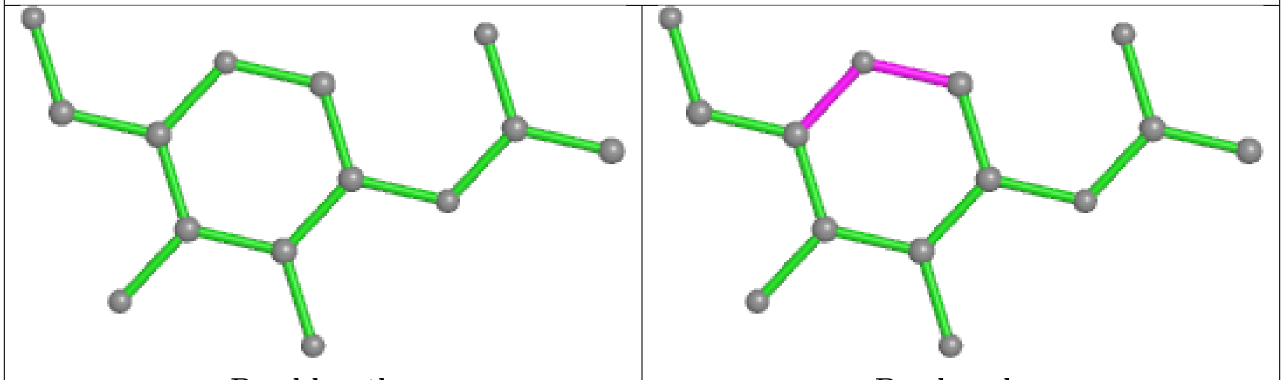
Bond angles



Torsions

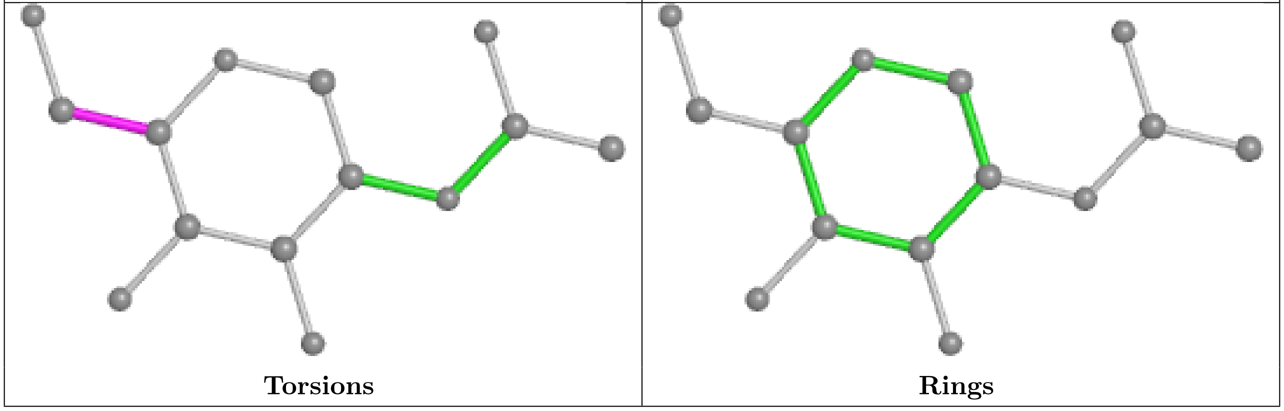
Rings

Ligand NAG B 1310



Bond lengths

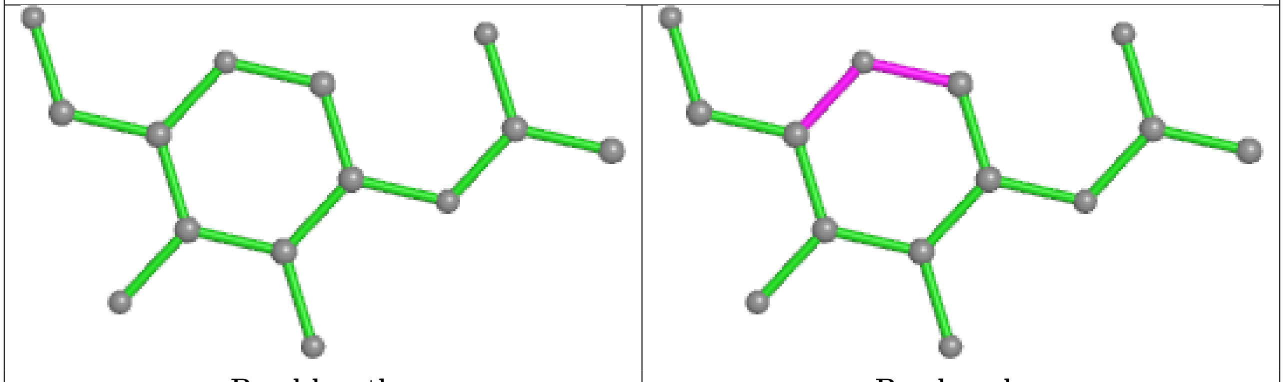
Bond angles



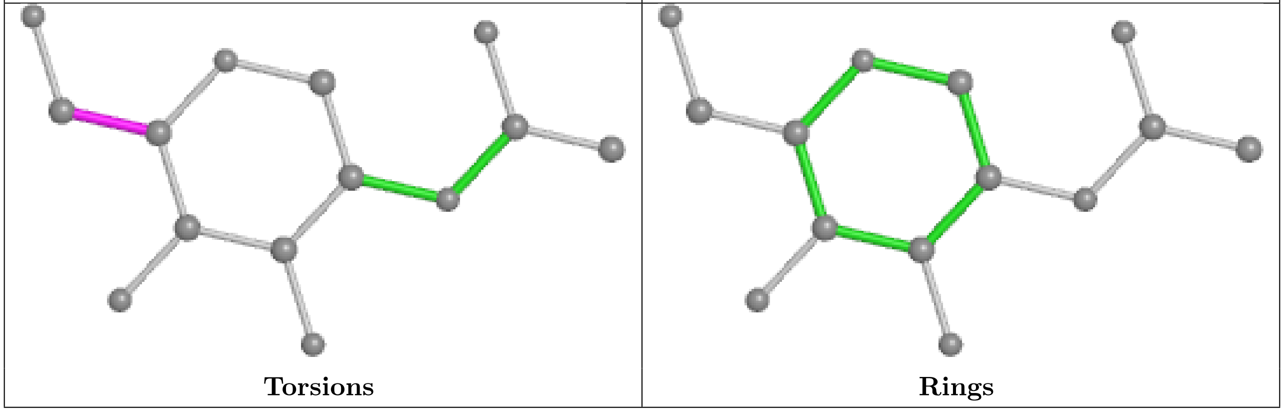
Torsions

Rings

Ligand NAG C 1310



Bond lengths Bond angles



Torsions Rings

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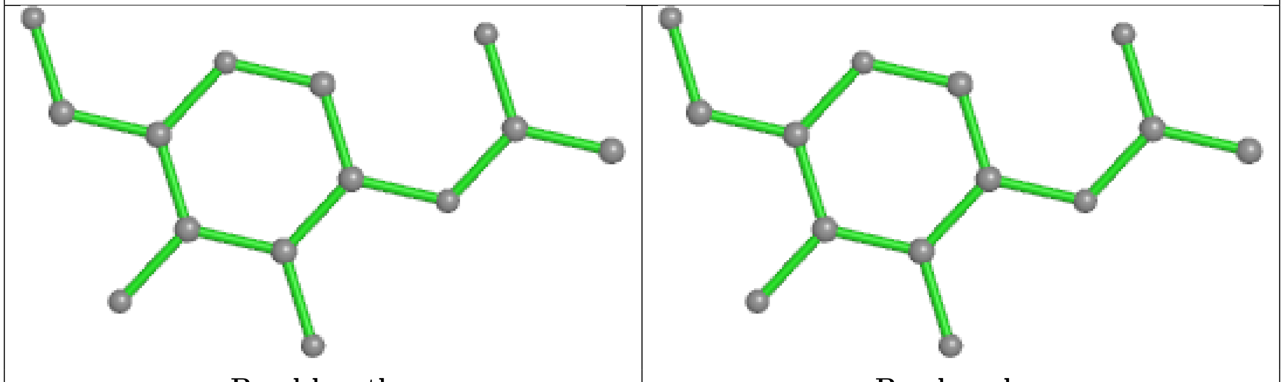
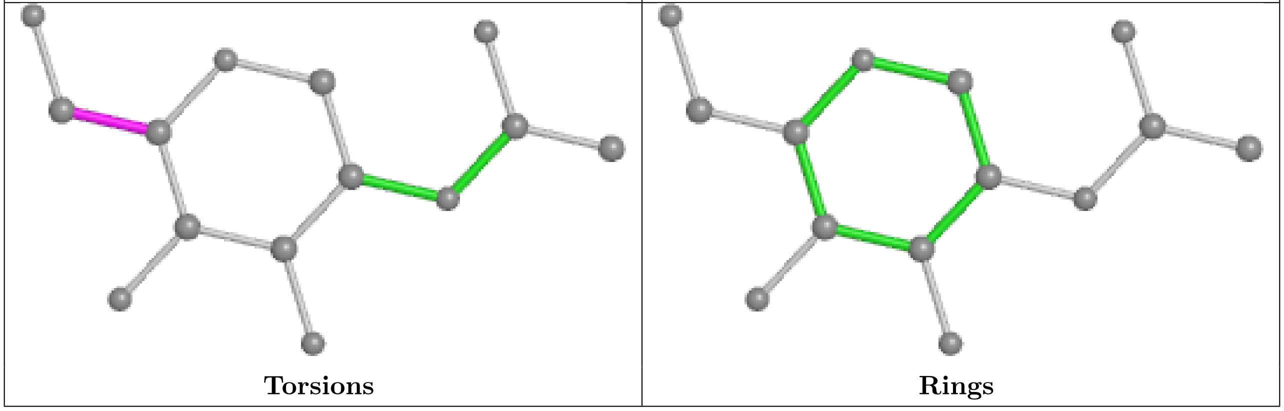
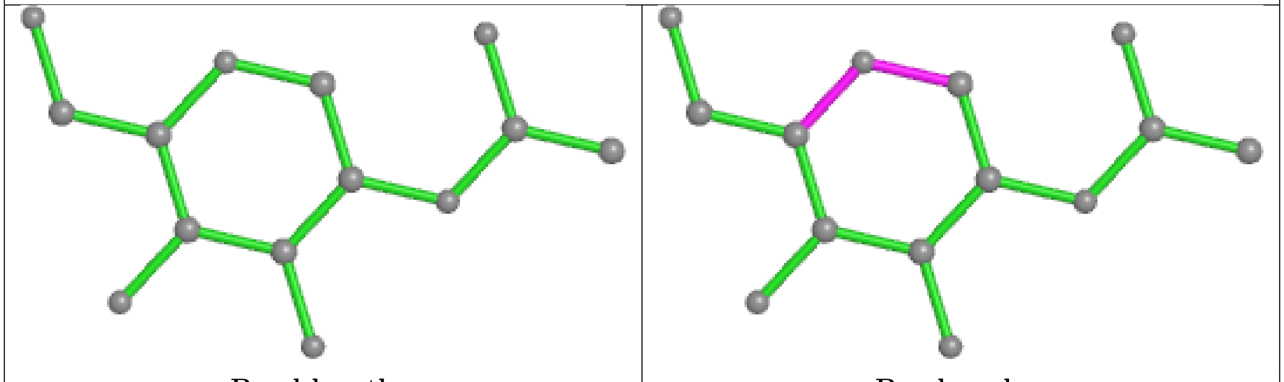


Bond lengths Bond angles

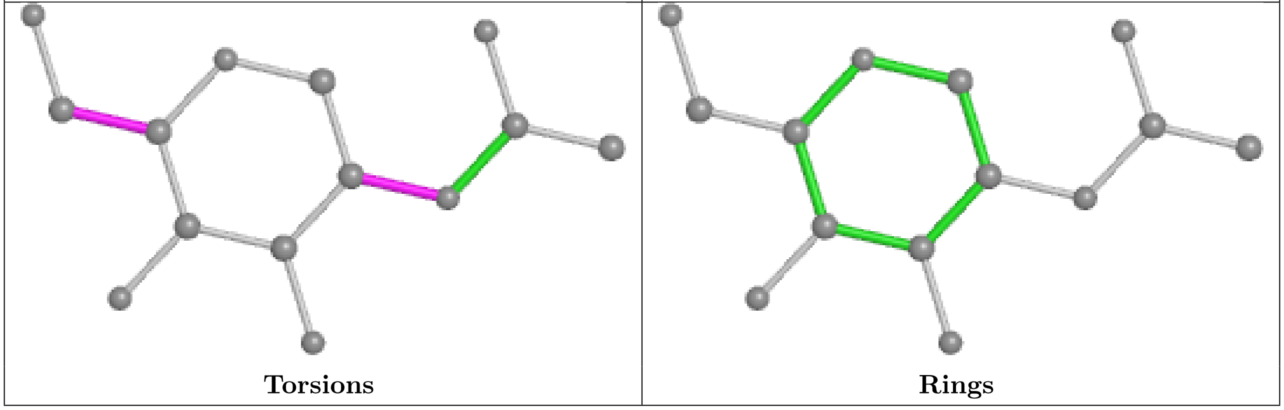


Torsions Rings

Ligand NAG A 1301

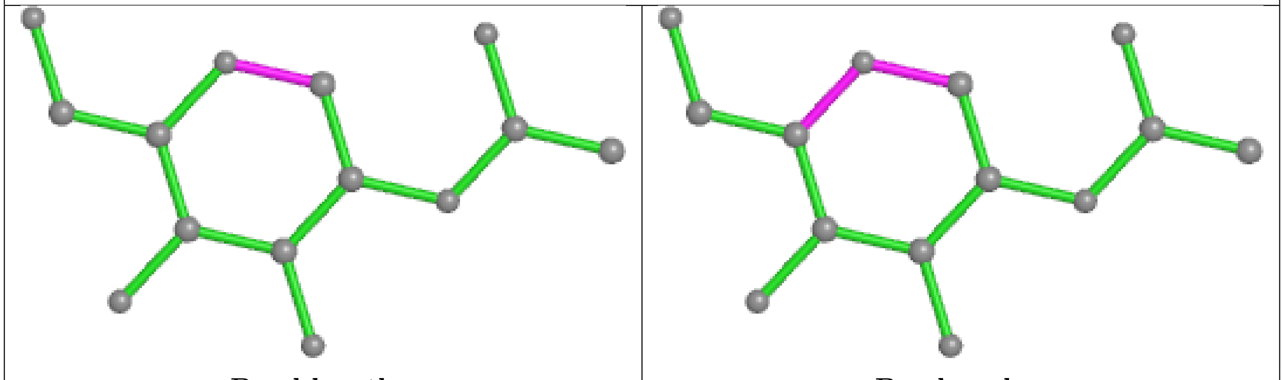


Bond lengths Bond angles

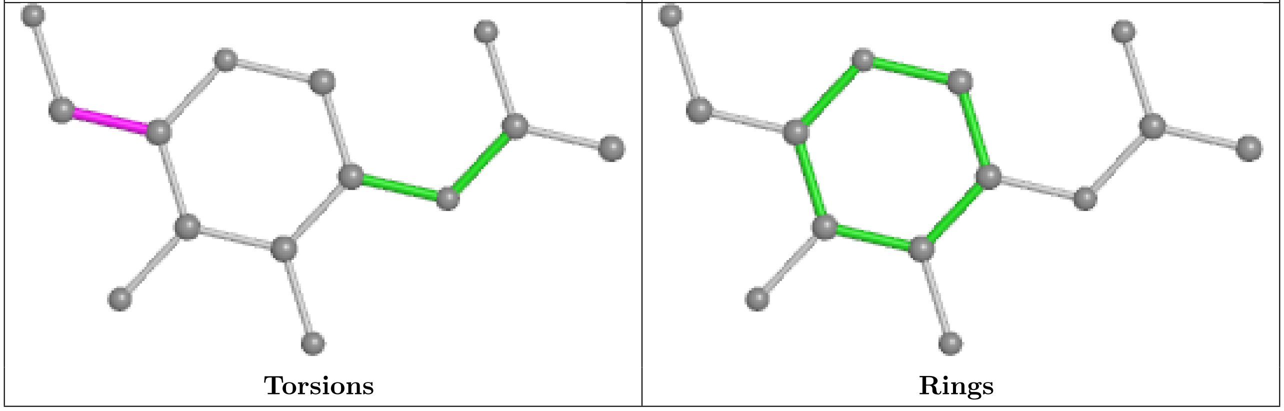


Torsions Rings

Ligand NAG B 1313

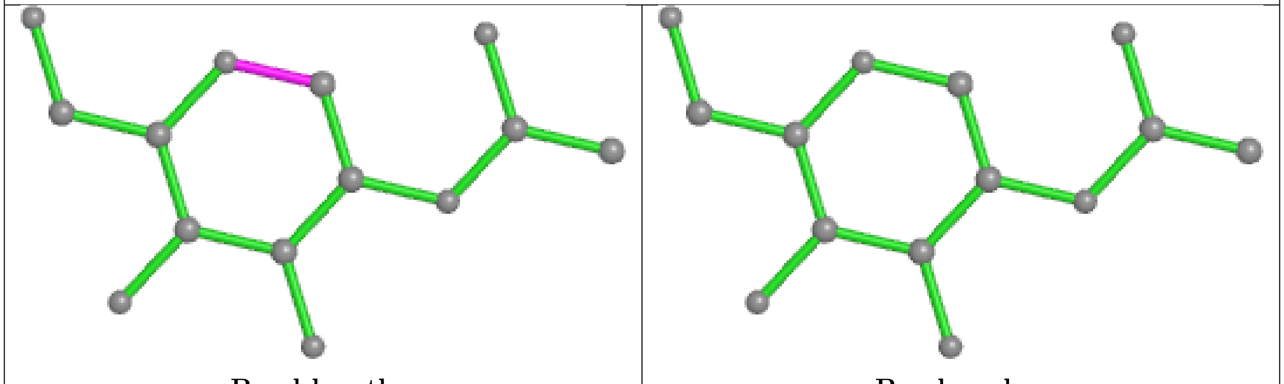


Bond lengths Bond angles

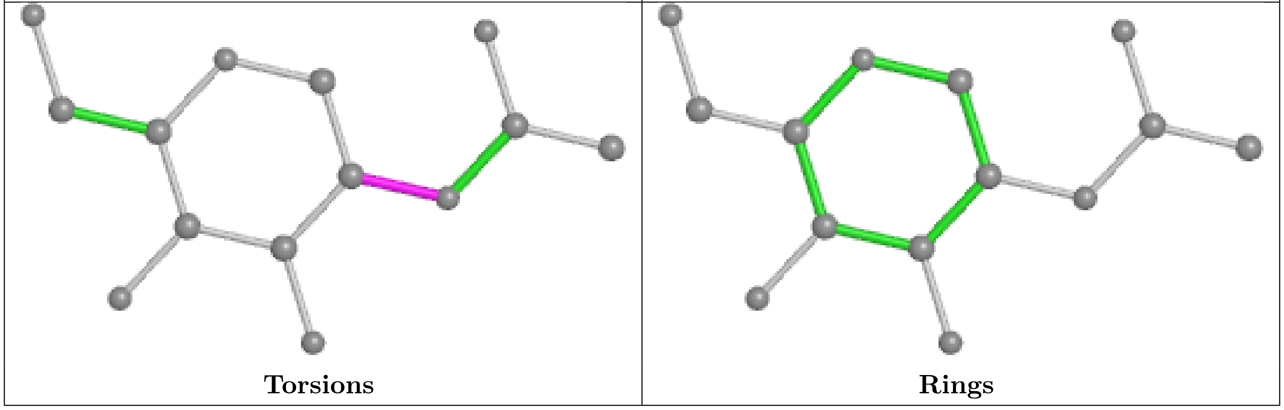


Torsions Rings

Ligand NAG A 1302

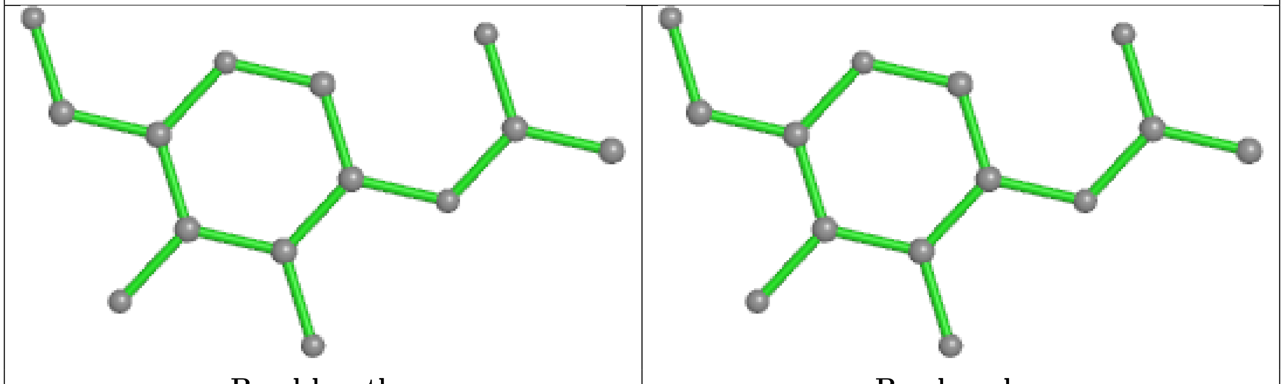


Bond lengths Bond angles

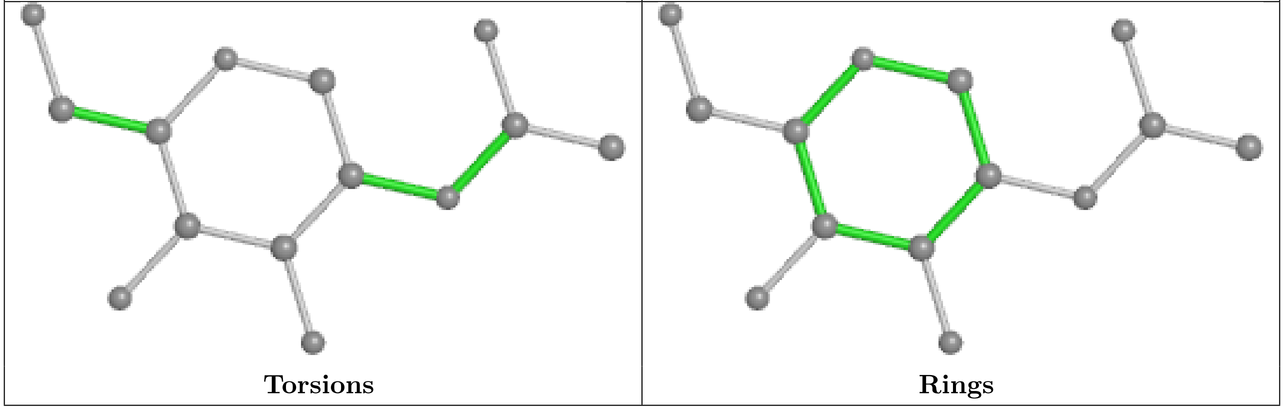


Torsions Rings

Ligand NAG A 1314

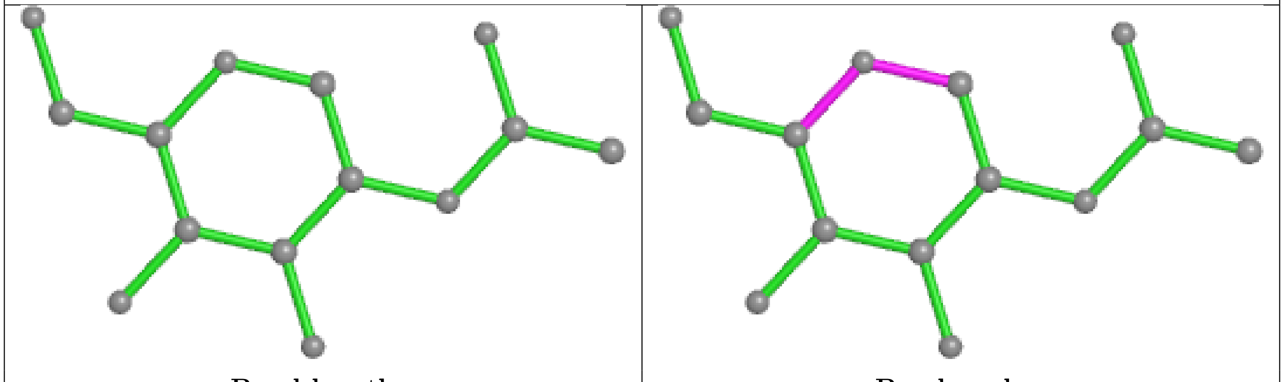


Bond lengths Bond angles

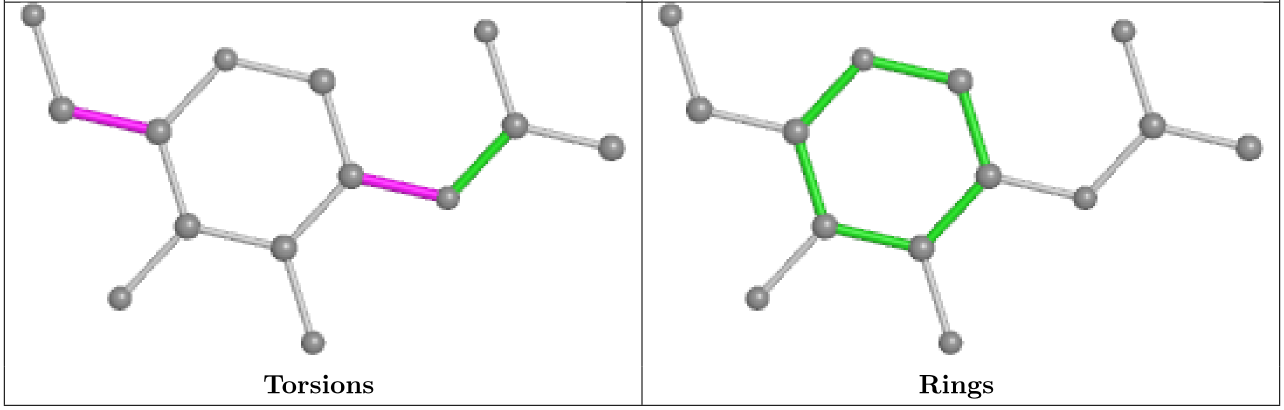


Torsions Rings

Ligand NAG B 1301

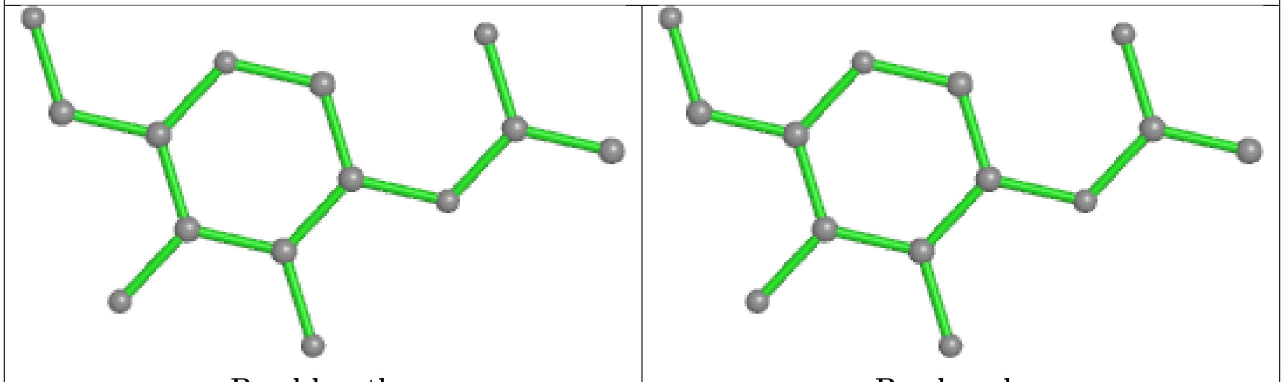


Bond lengths Bond angles

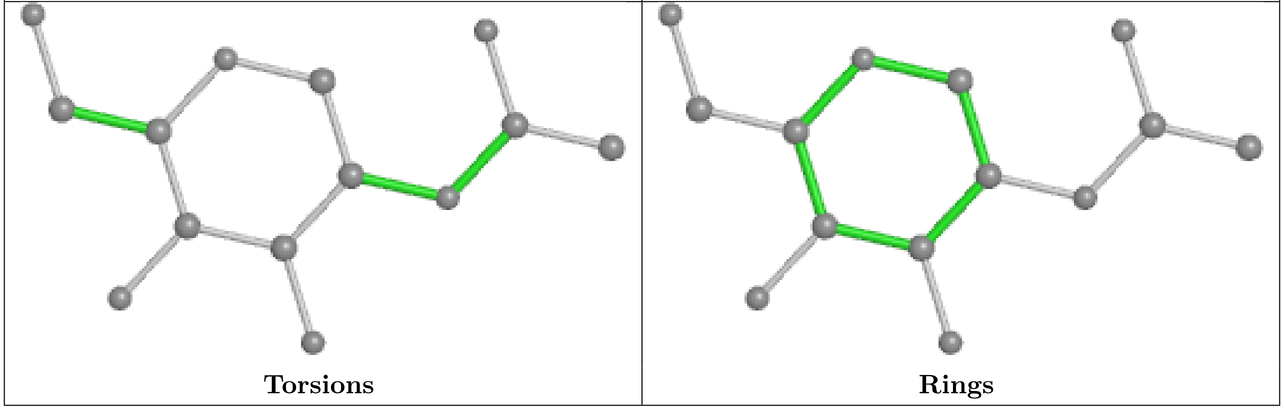


Torsions Rings

Ligand NAG C 1306



Bond lengths Bond angles



Torsions Rings

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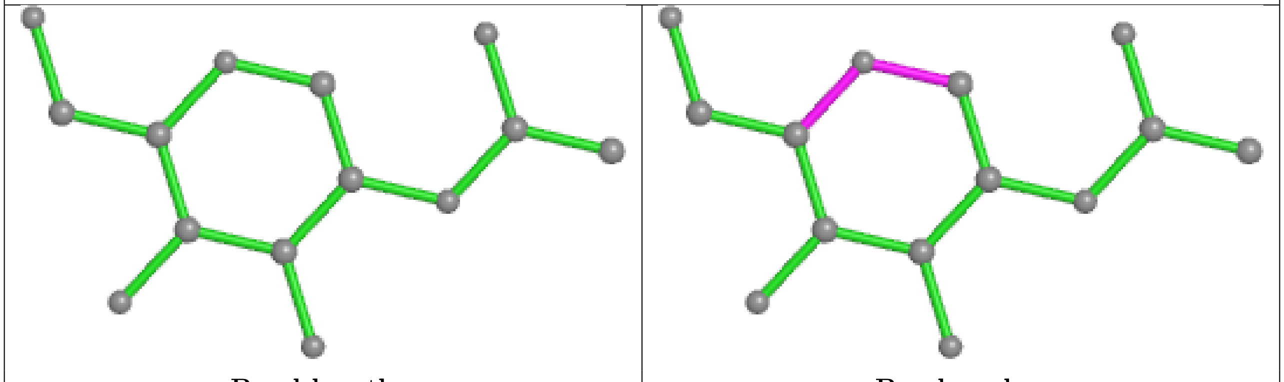
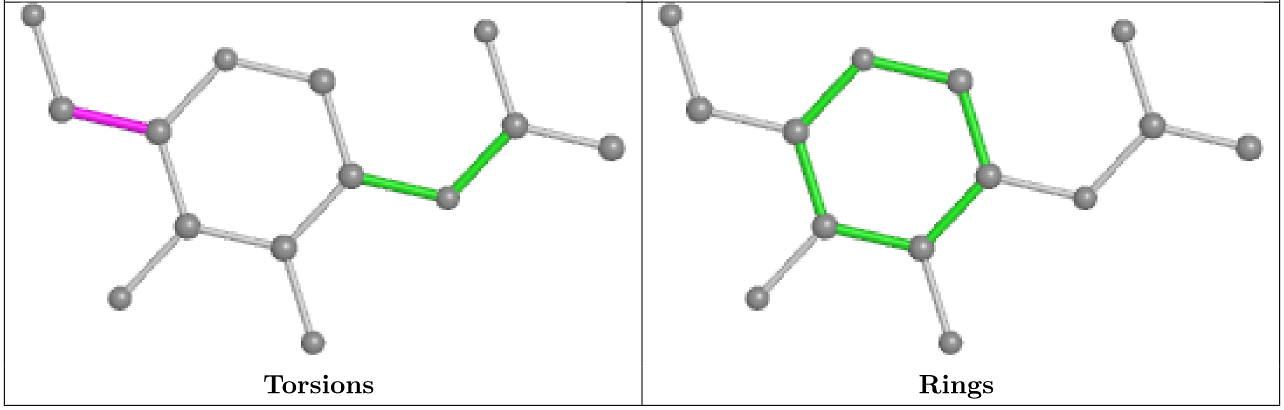


Bond lengths

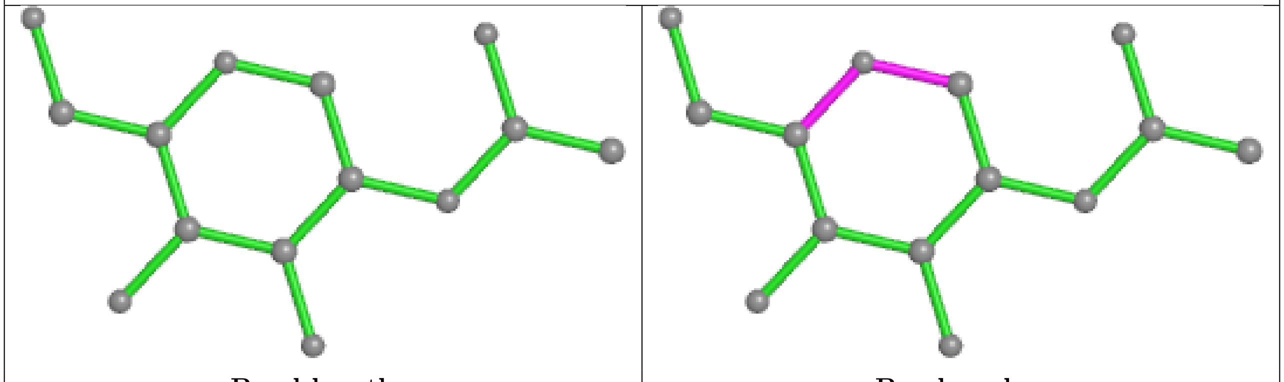
Bond angles



Torsions

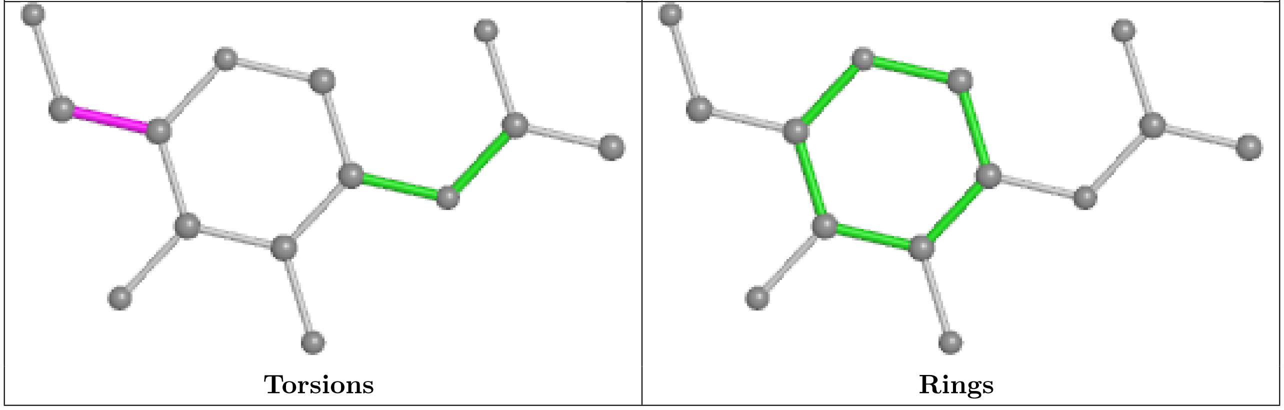
Rings

Ligand NAG B 1311



Bond lengths

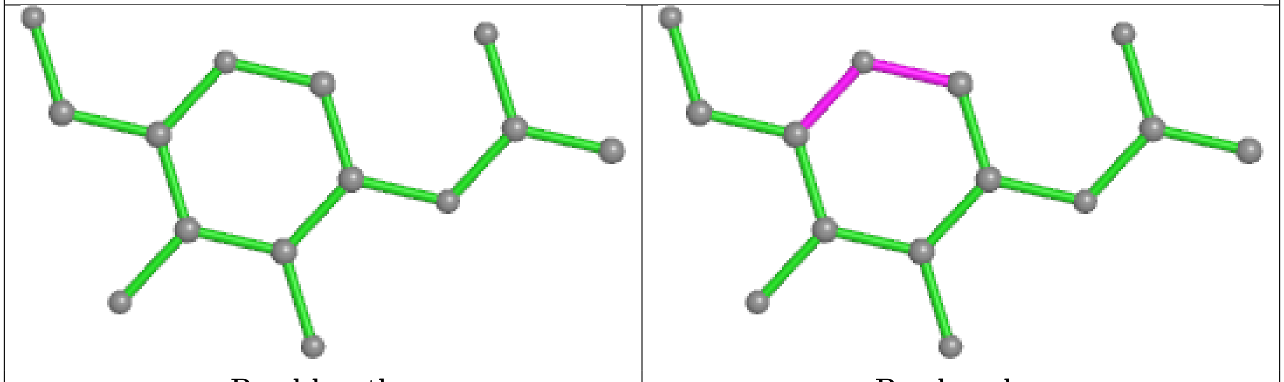
Bond angles



Torsions

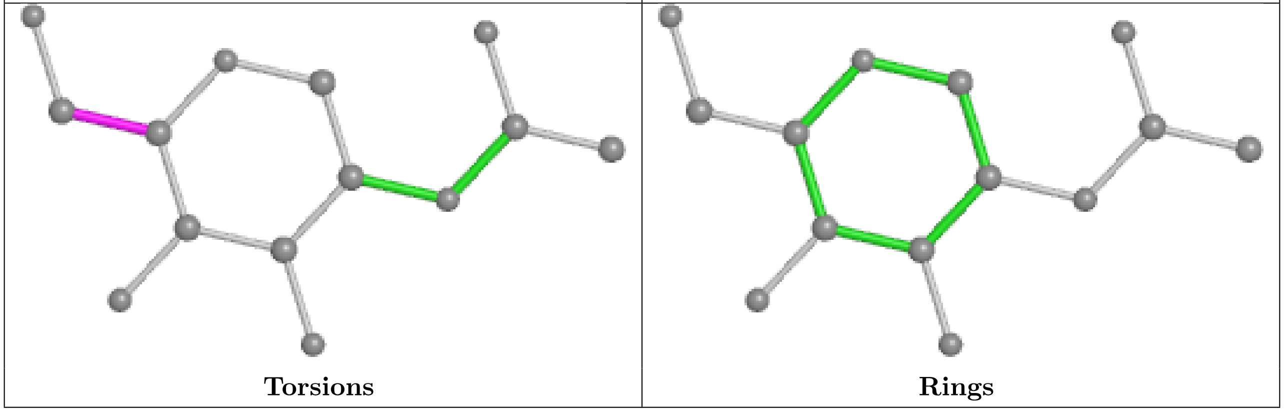
Rings

Ligand NAG C 1311



Bond lengths

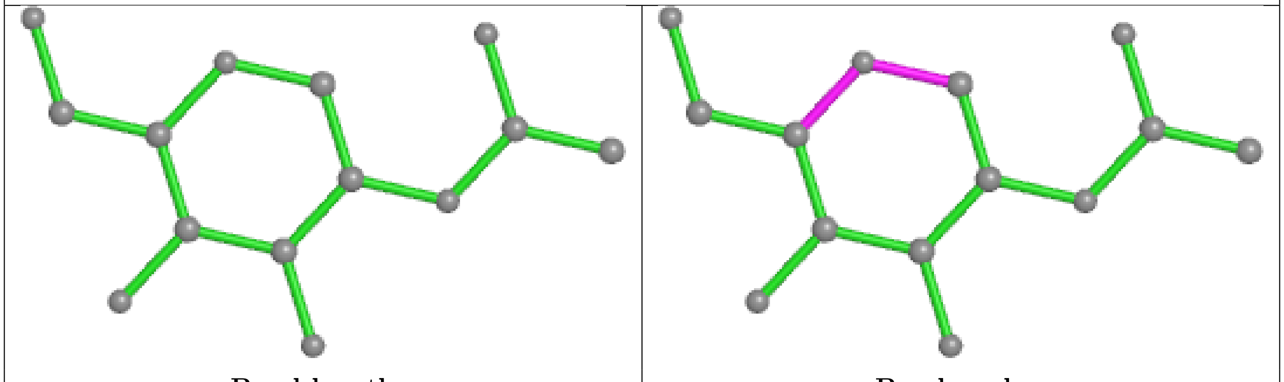
Bond angles



Torsions

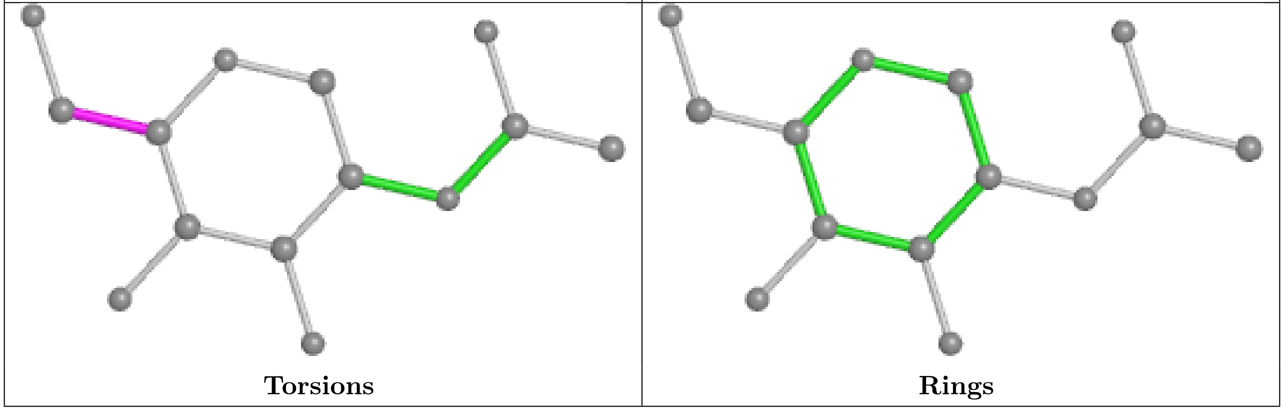
Rings

Ligand NAG B 1308



Bond lengths

Bond angles



Torsions

Rings

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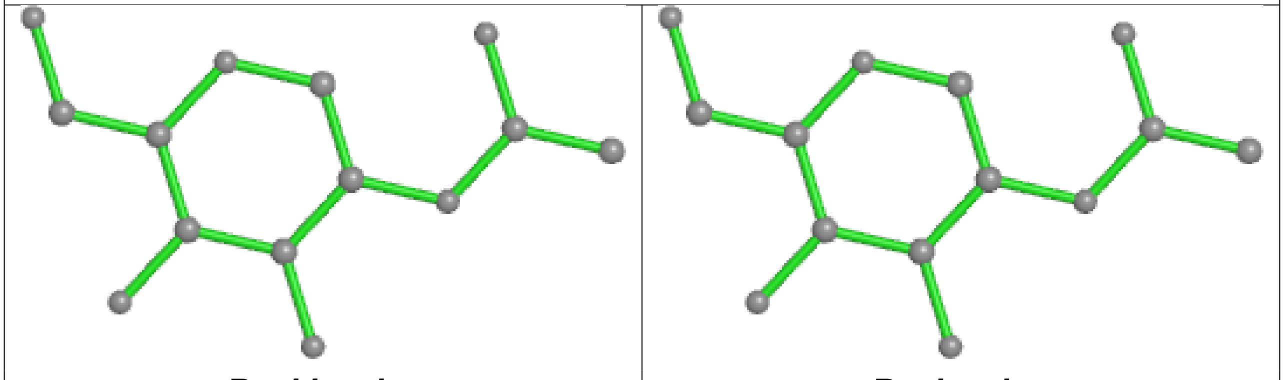
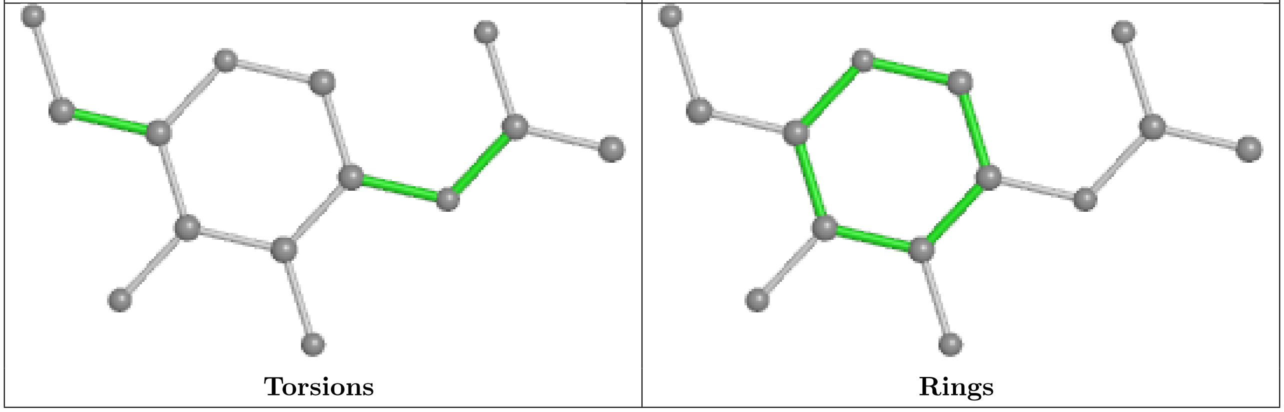


Bond lengths Bond angles



Torsions Rings

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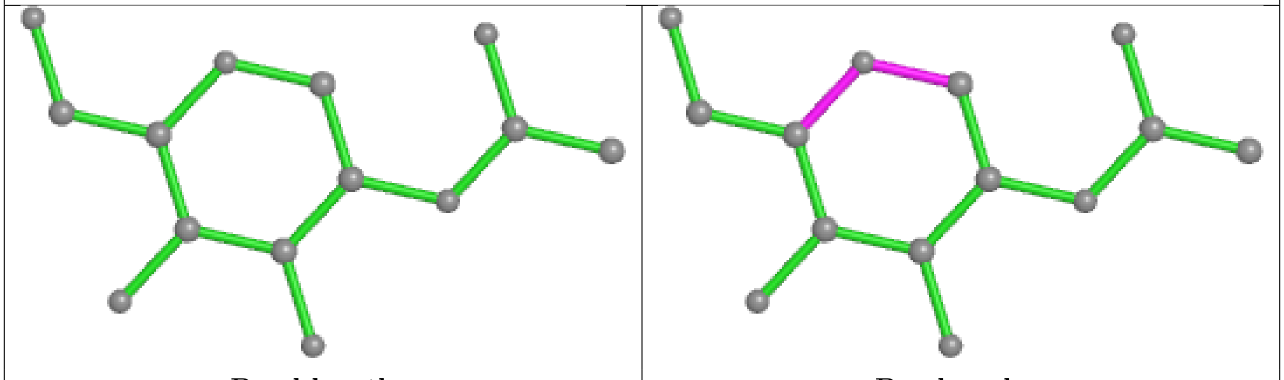
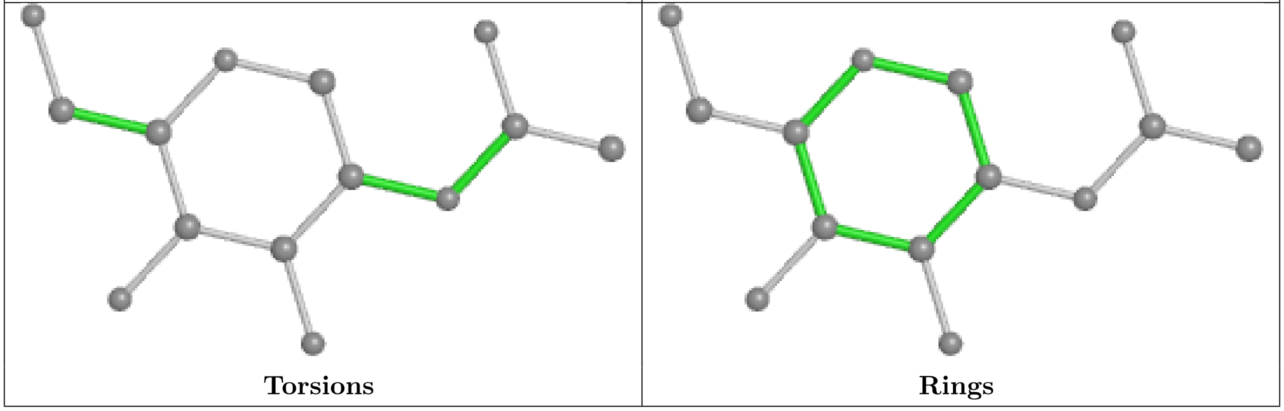
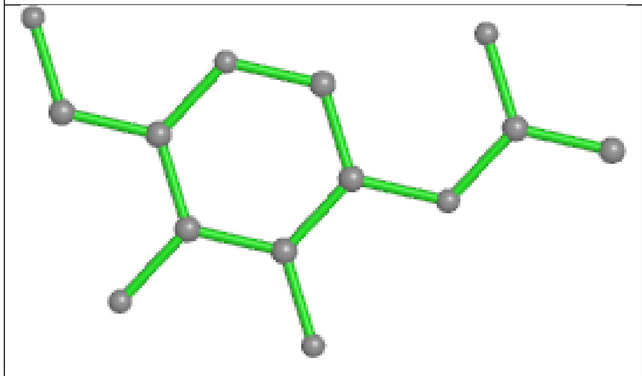


Bond lengths Bond angles

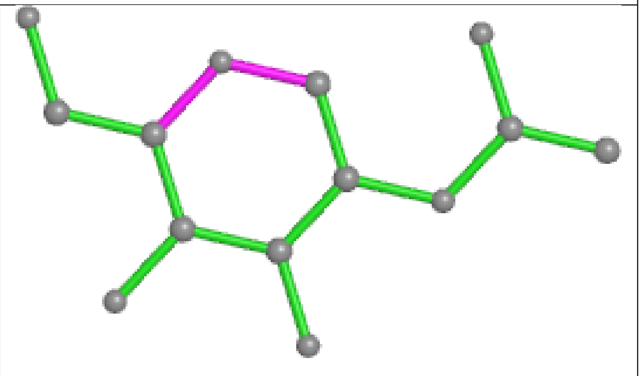


Torsions Rings

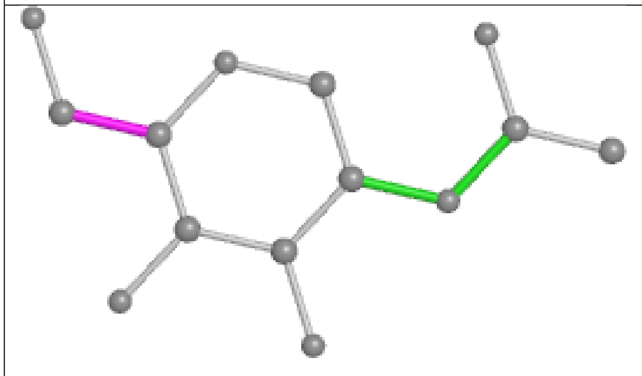
Ligand NAG A 1311



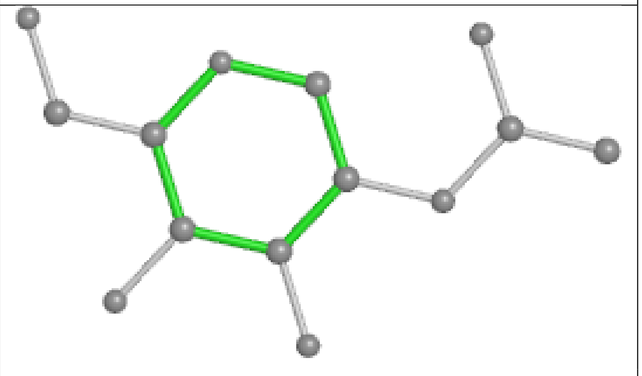
Bond lengths



Bond angles

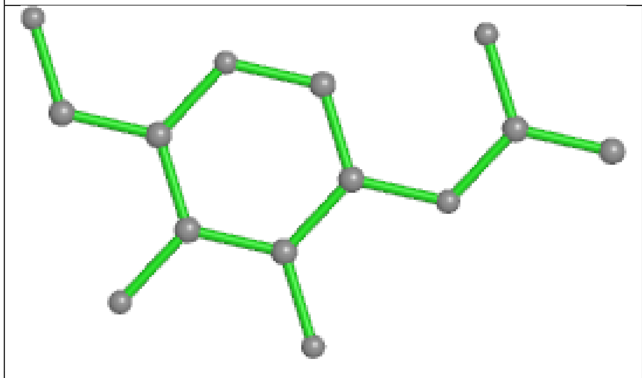


Torsions

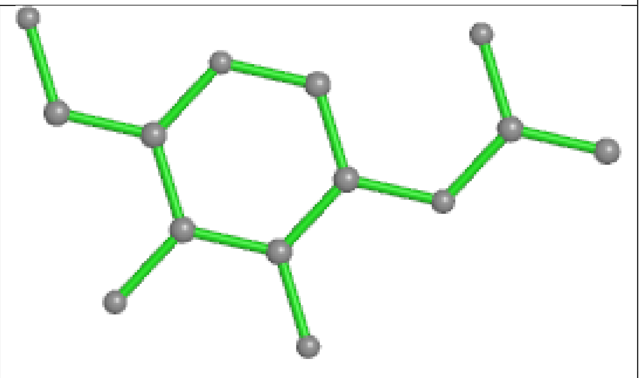


Rings

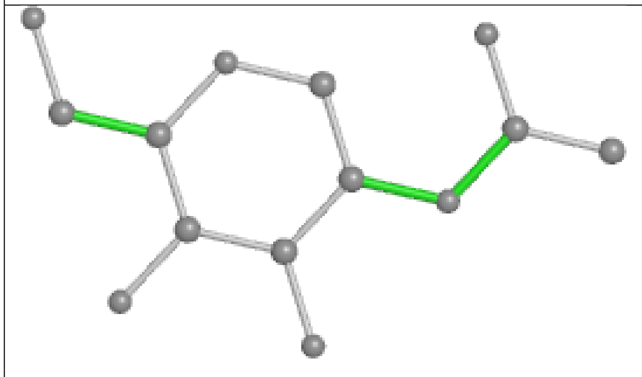
Ligand NAG B 1309



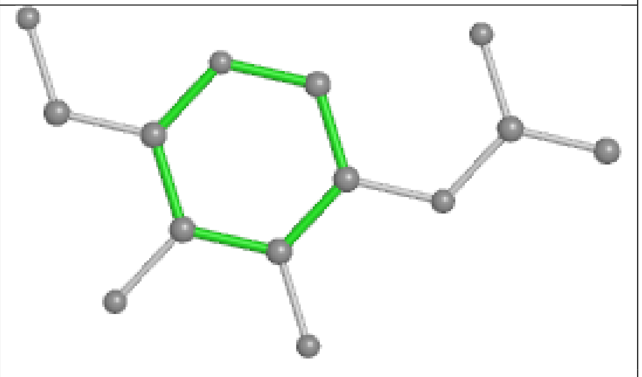
Bond lengths



Bond angles

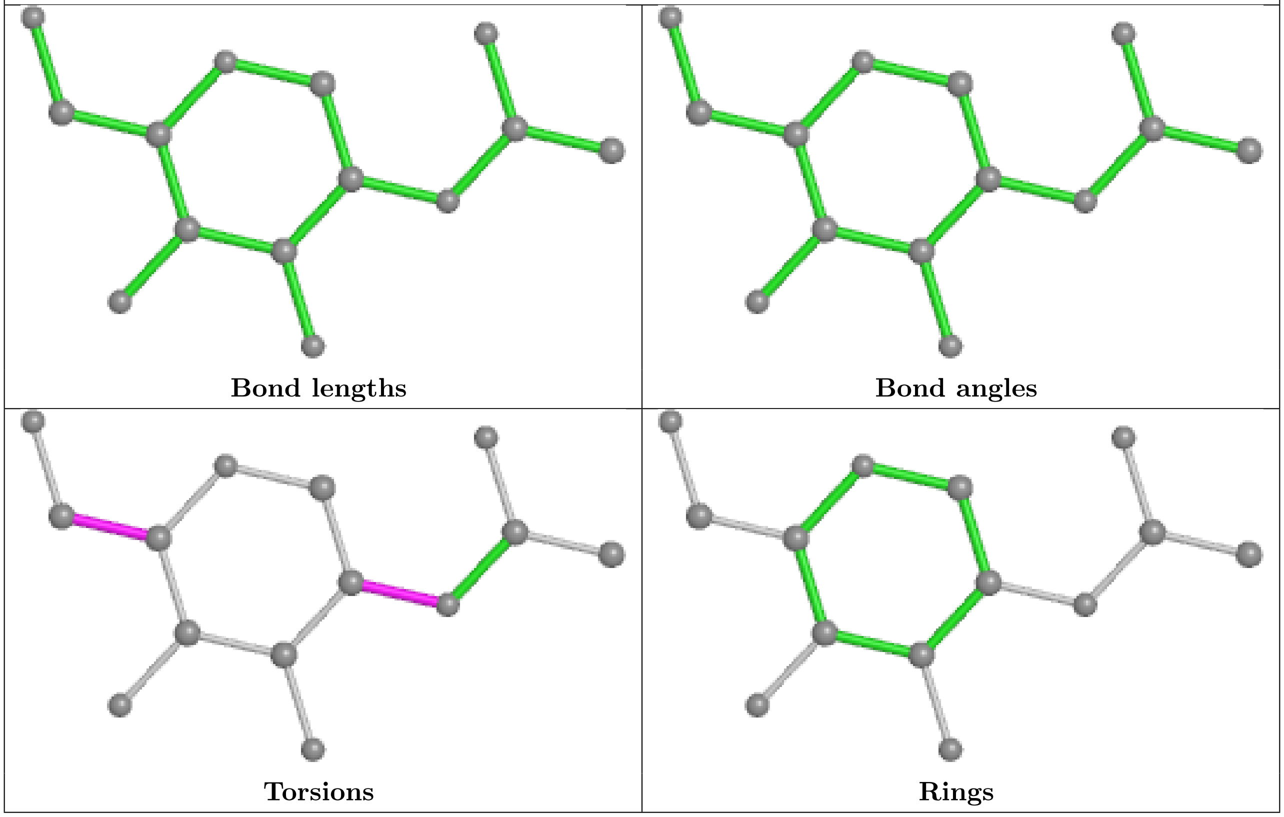


Torsions



Rings

Ligand NAG A 1304



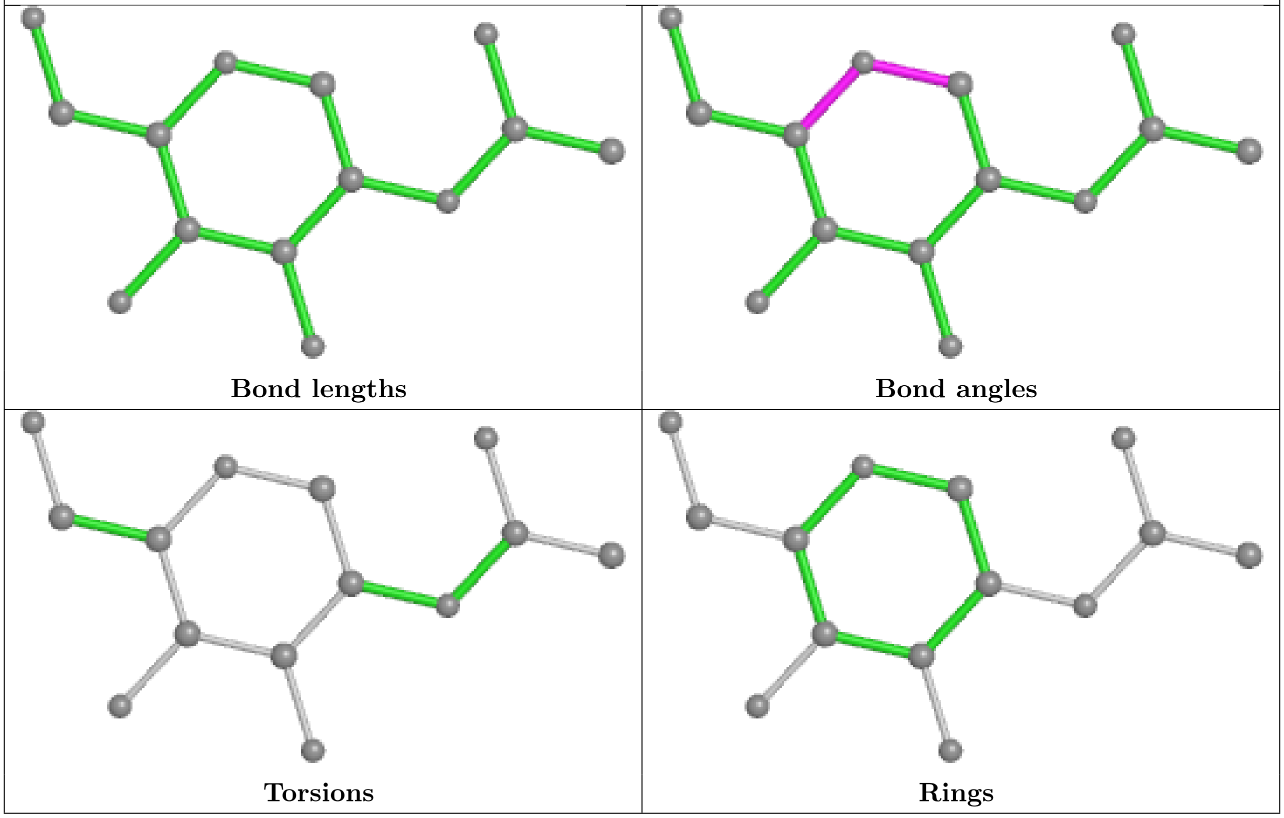
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 1309



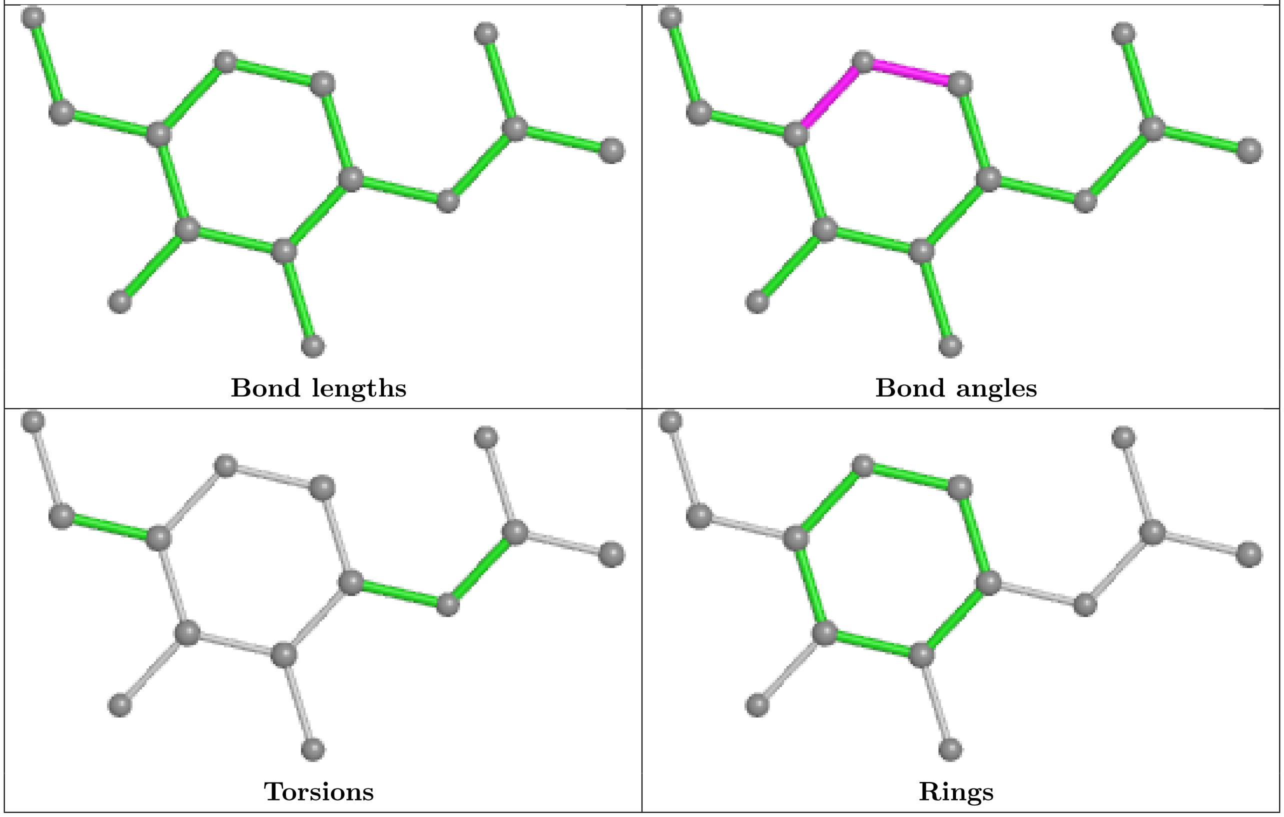
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1307



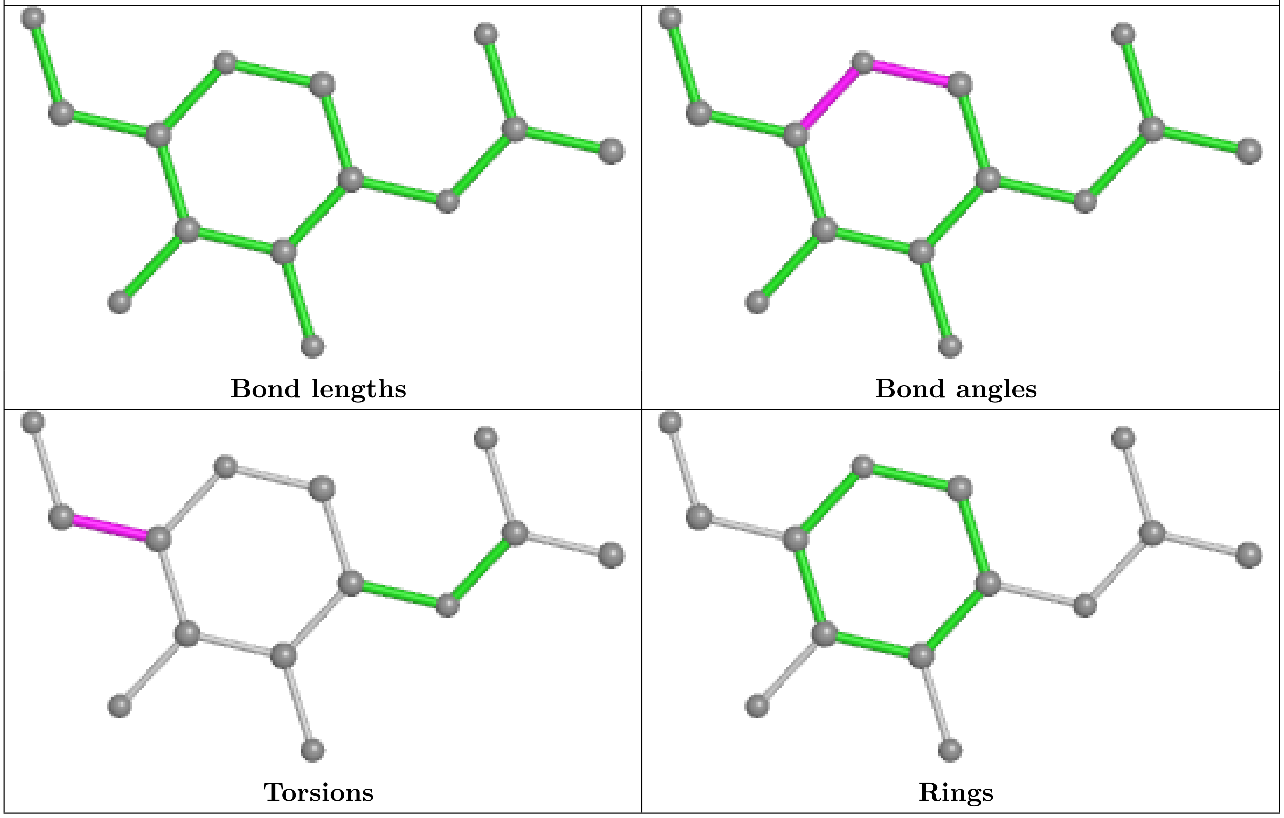
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 1308



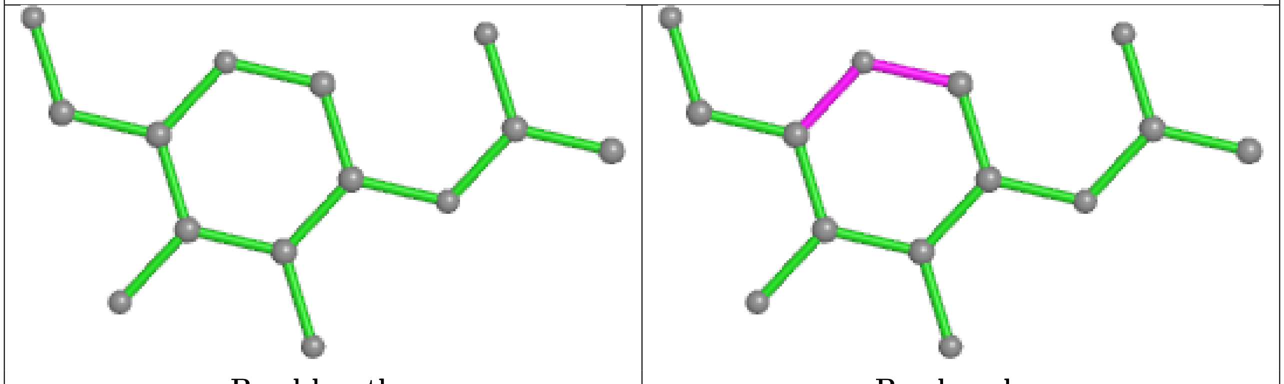
Bond lengths

Bond angles

Torsions

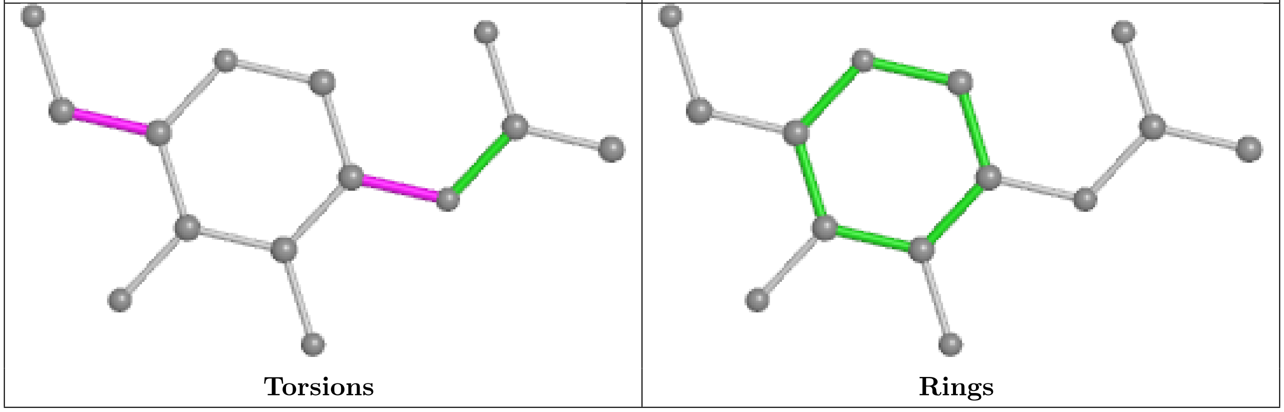
Rings

Ligand NAG C 1301



Bond lengths

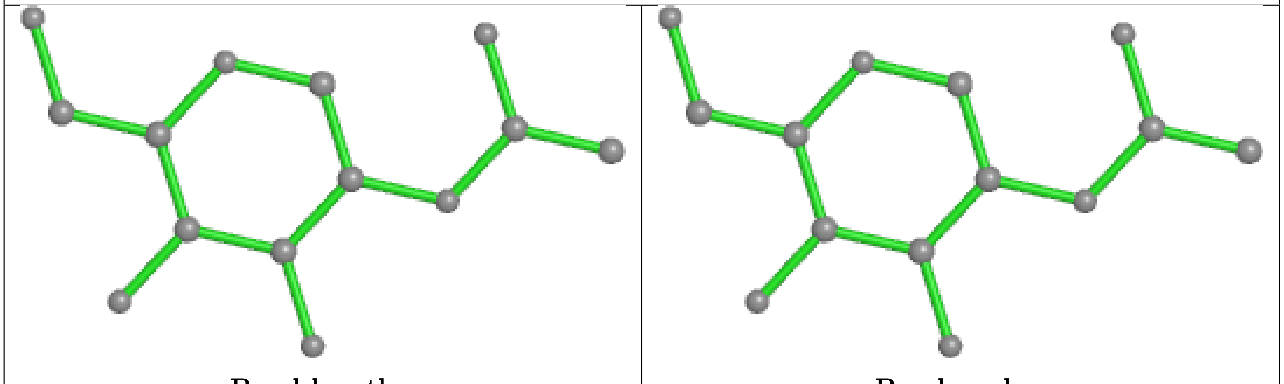
Bond angles



Torsions

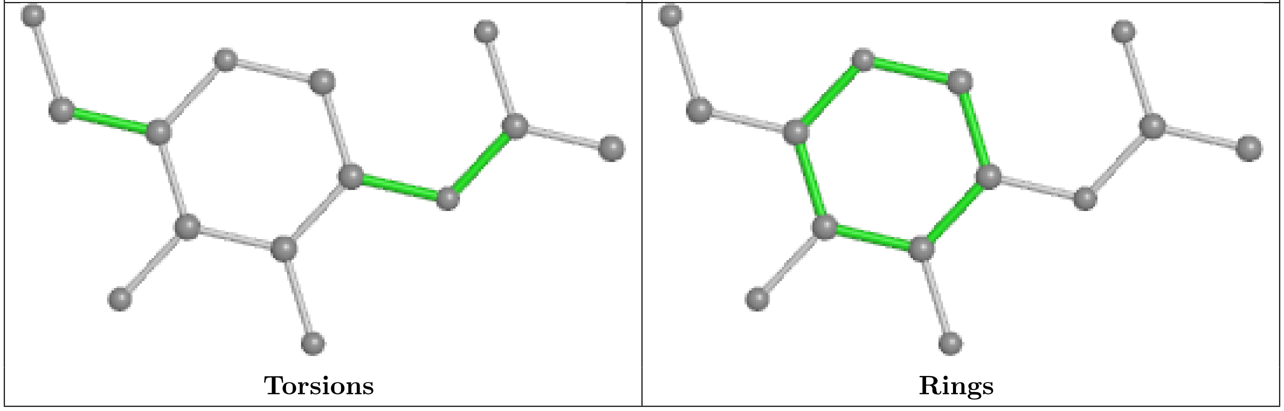
Rings

Ligand NAG A 1306



Bond lengths

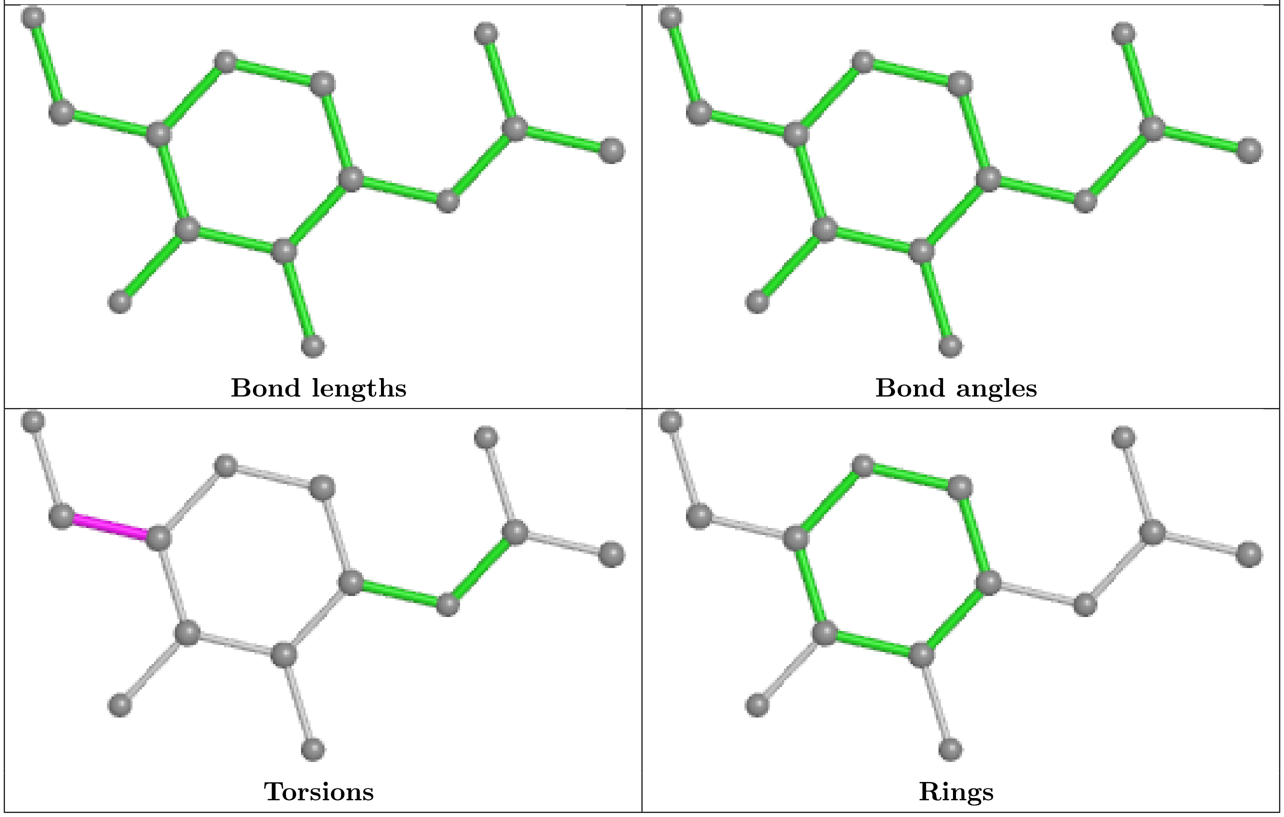
Bond angles



Torsions

Rings

Ligand NAG B 1305



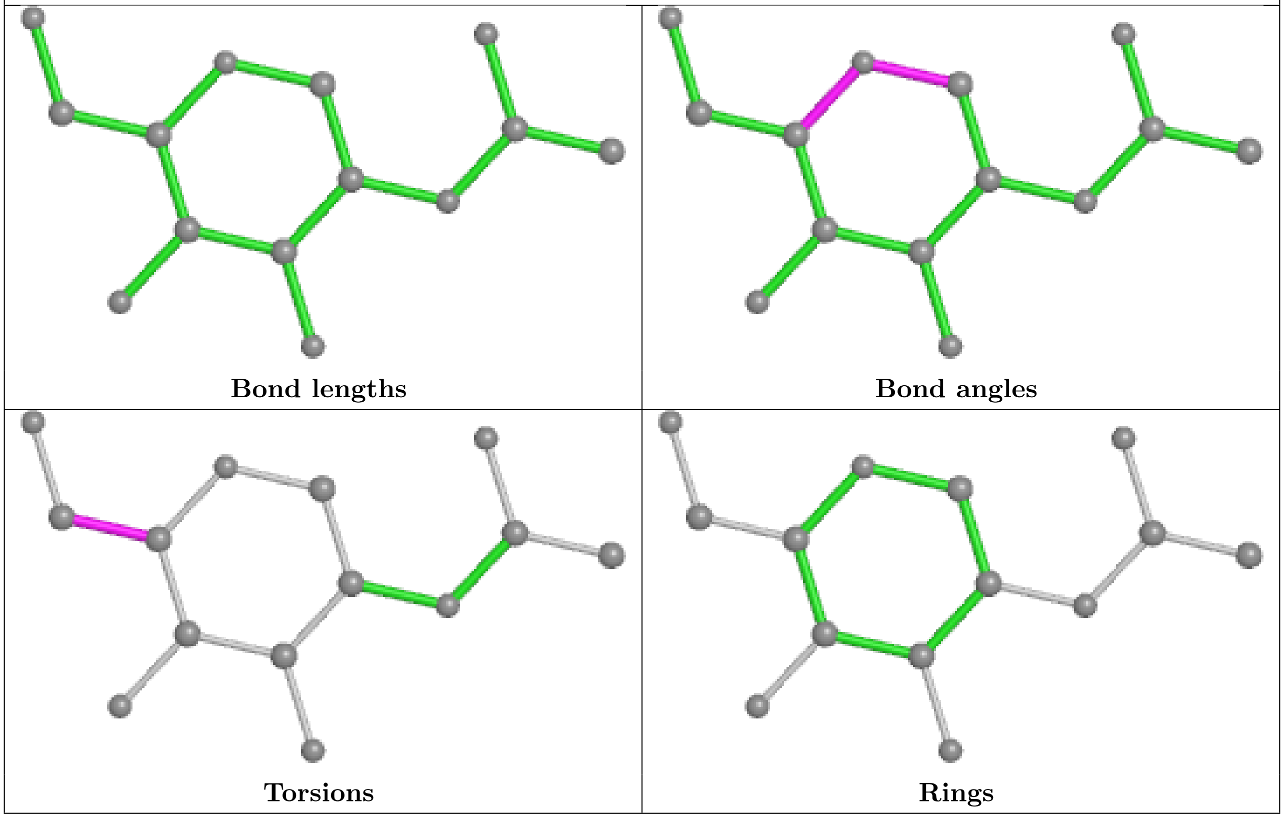
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 1310



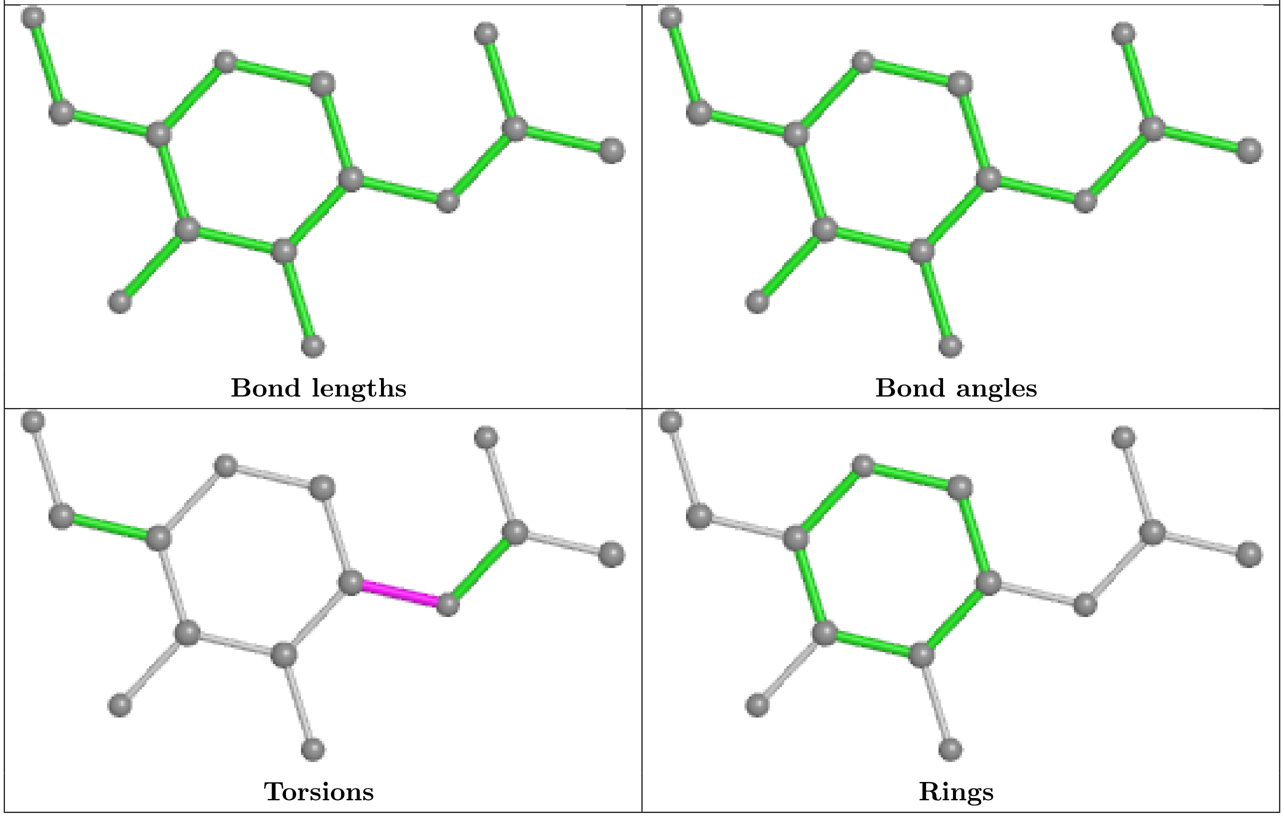
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 1302



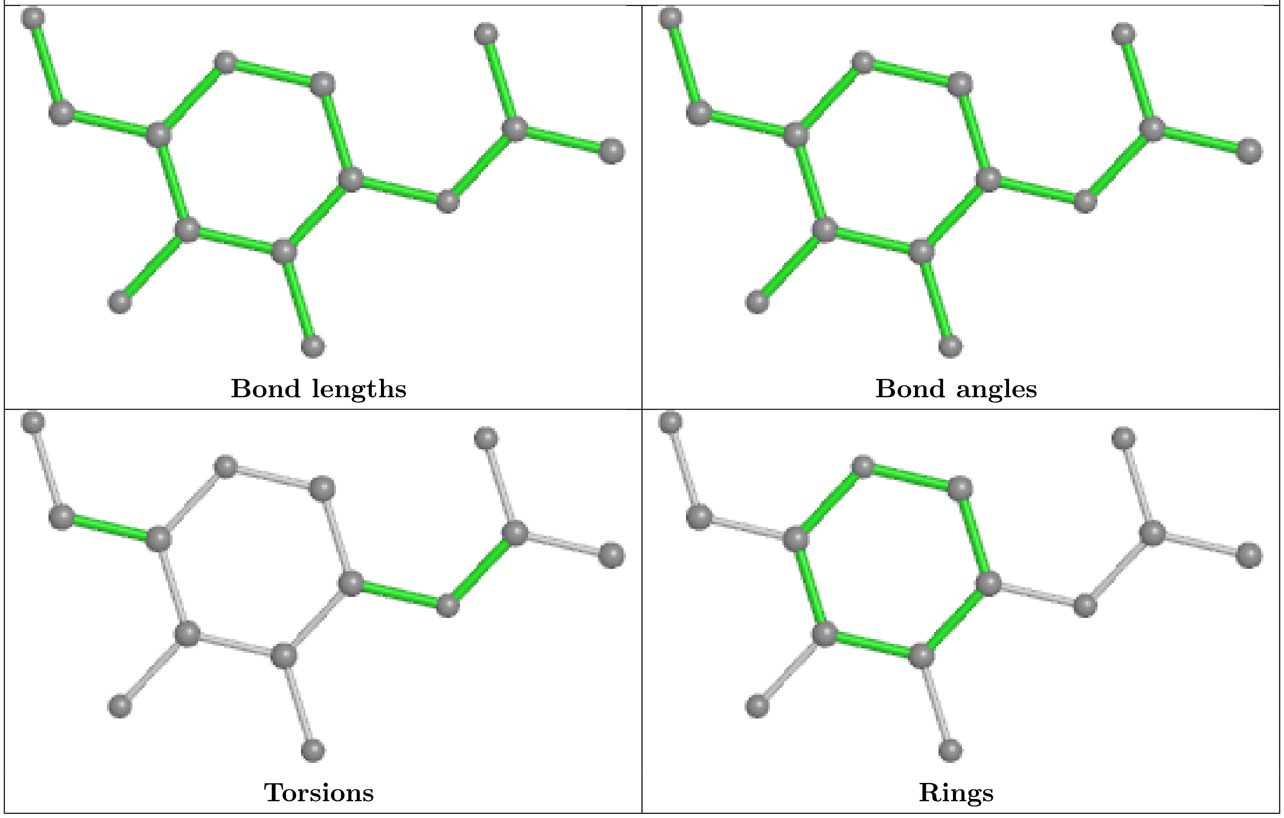
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 1314



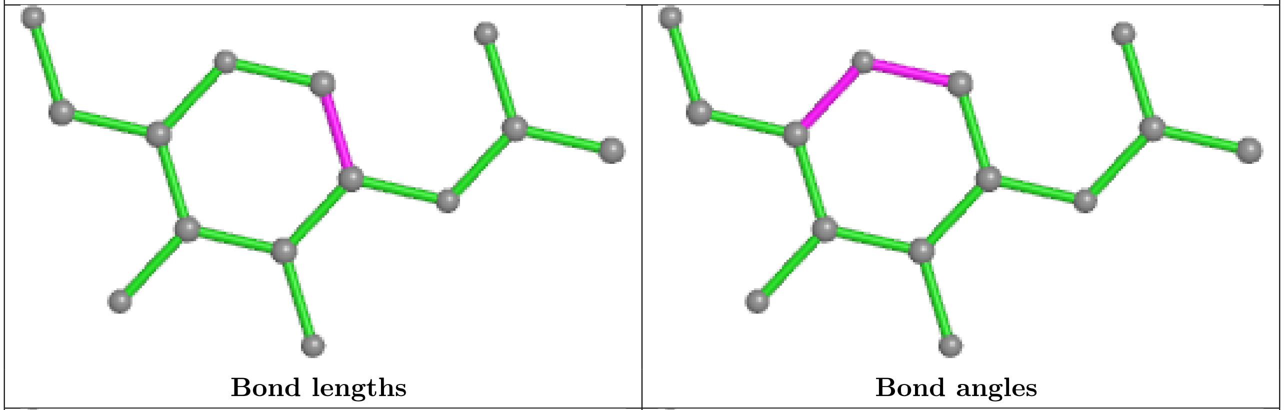
Bond lengths

Bond angles

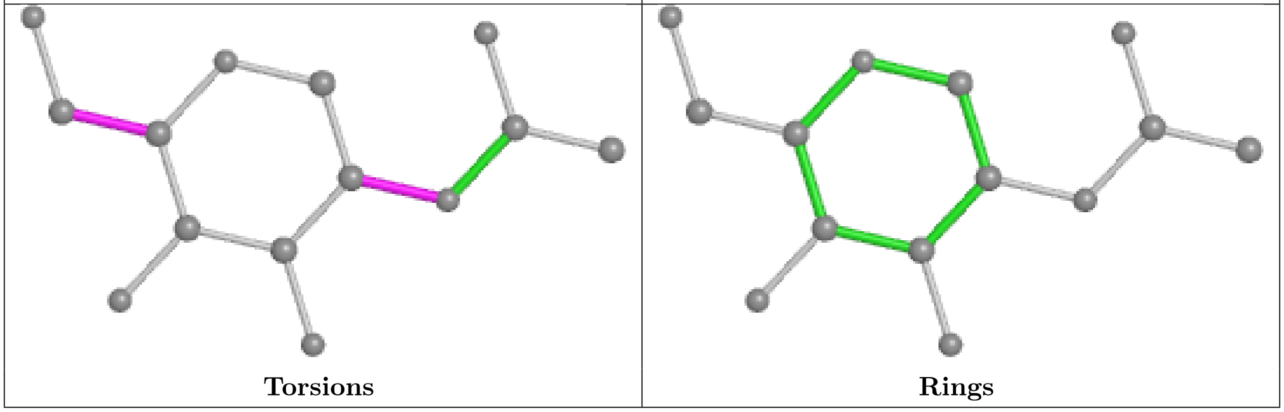
Torsions

Rings

Ligand NAG B 1304

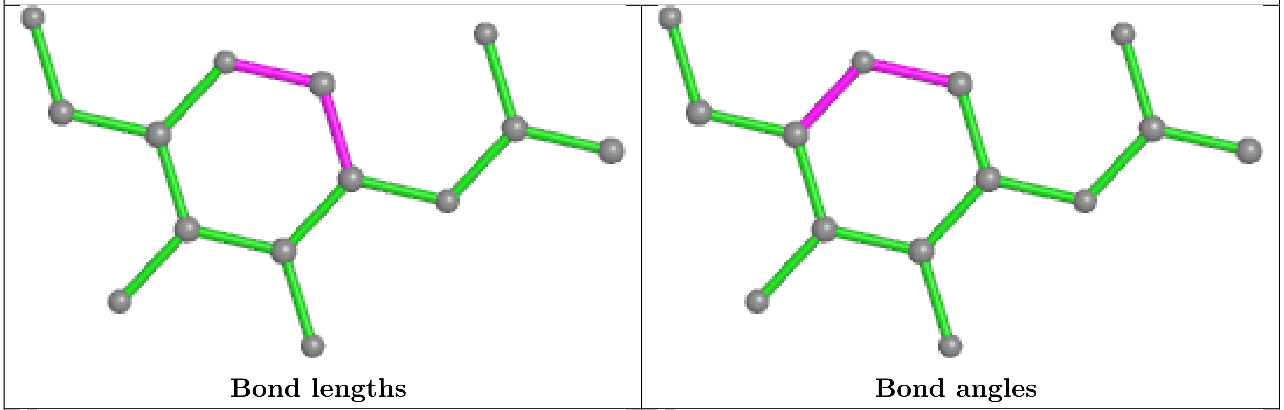


Bond lengths Bond angles

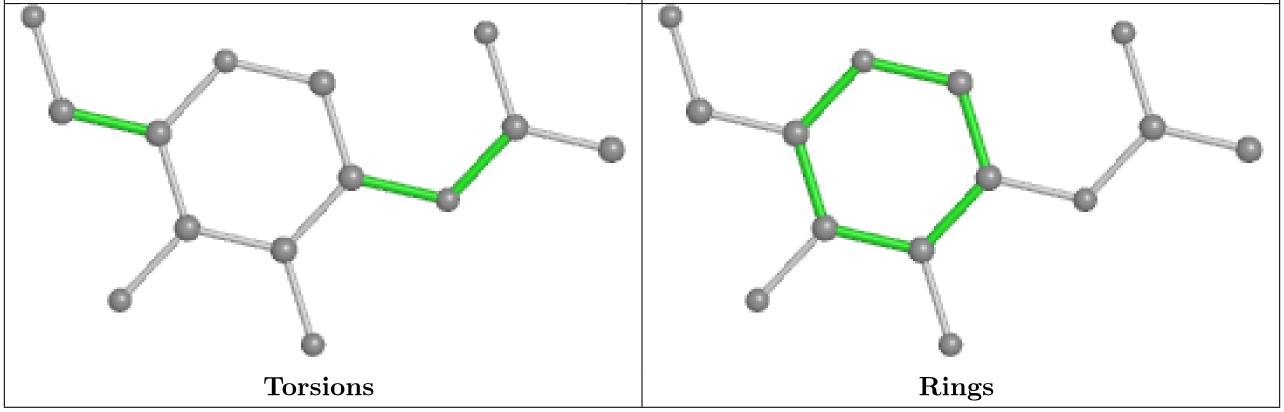


Torsions Rings

Ligand NAG C 1312

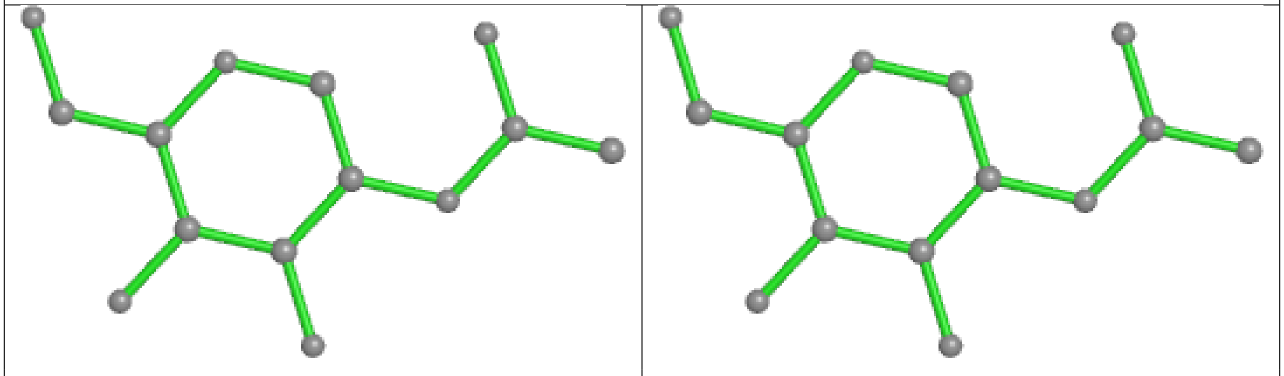


Bond lengths Bond angles



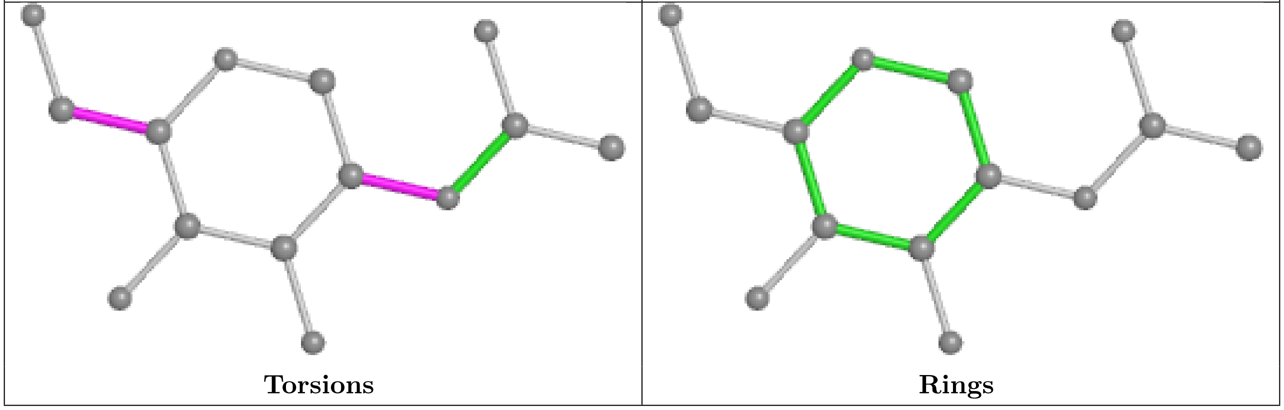
Torsions Rings

Ligand NAG C 1313



Bond lengths

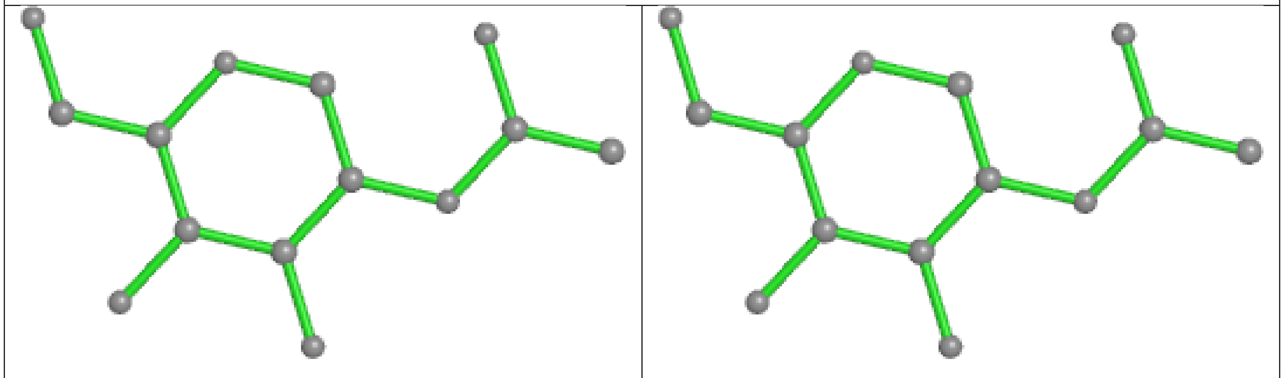
Bond angles



Torsions

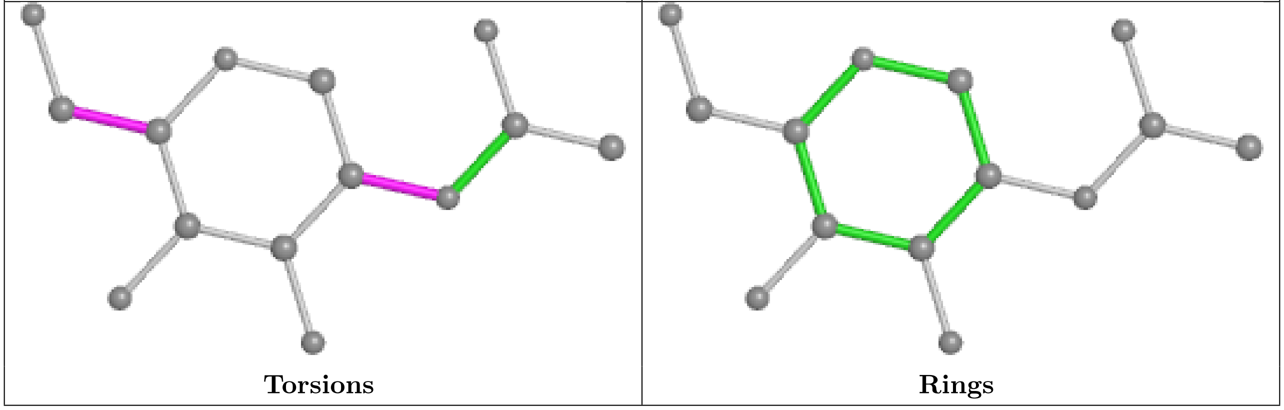
Rings

Ligand NAG B 1303



Bond lengths

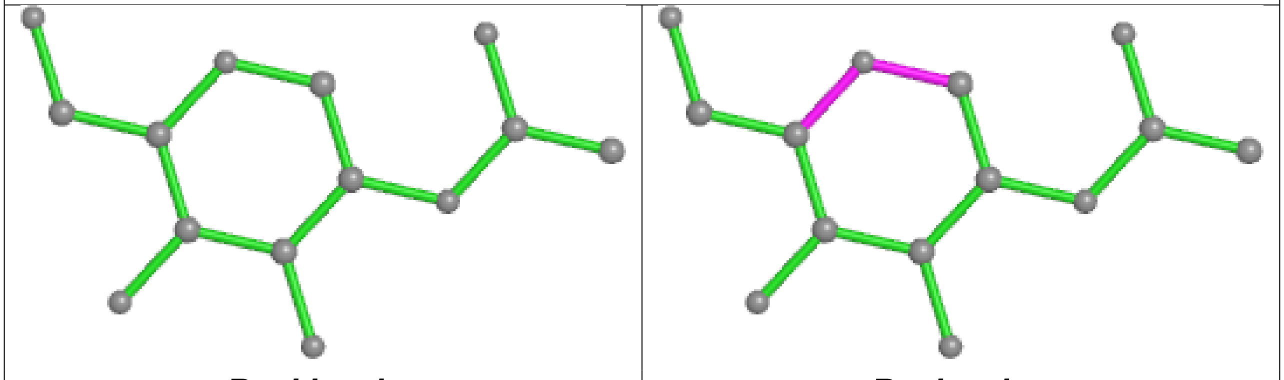
Bond angles



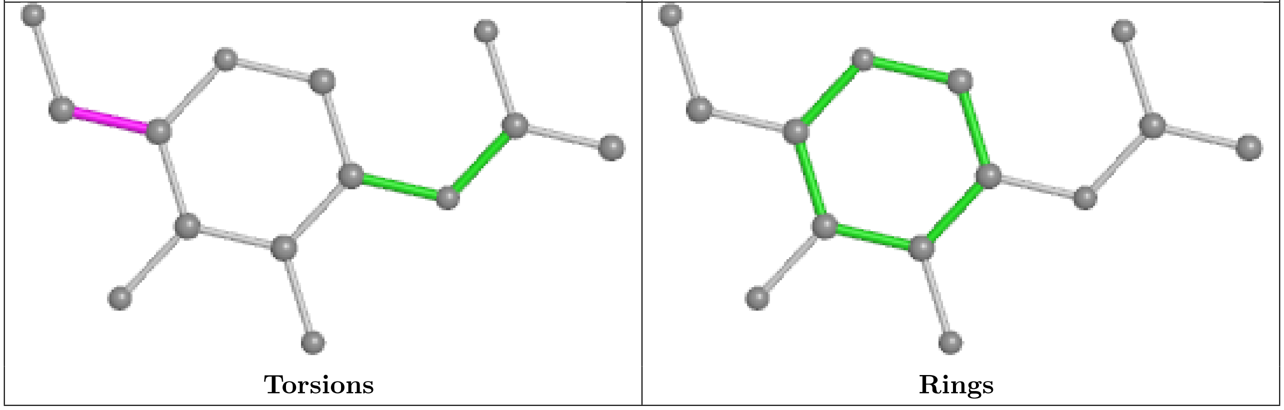
Torsions

Rings

Ligand NAG B 1312

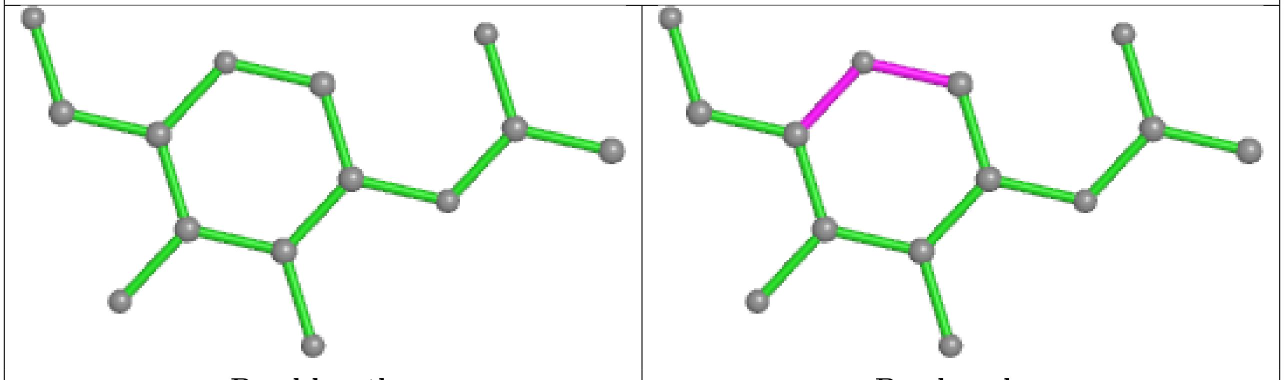


Bond lengths **Bond angles**

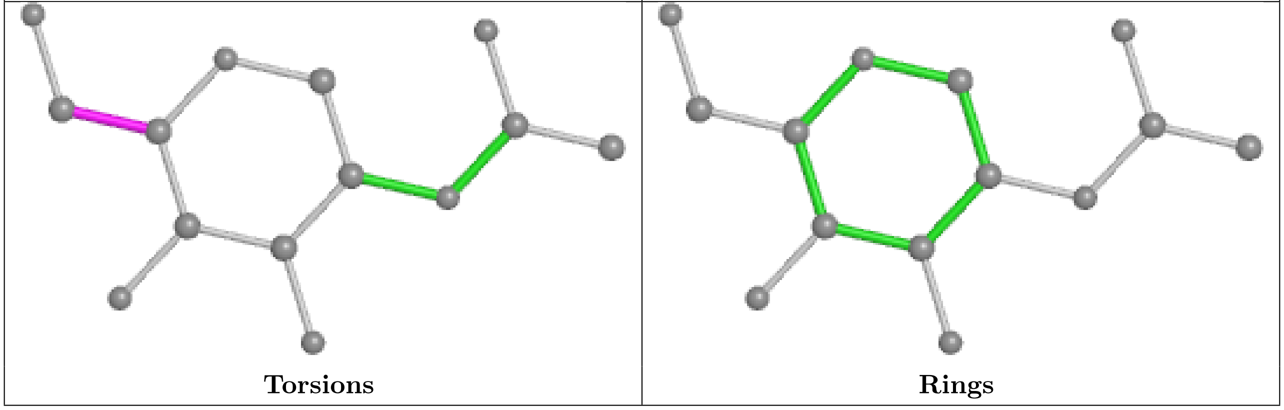


Torsions **Rings**

Ligand NAG A 1315

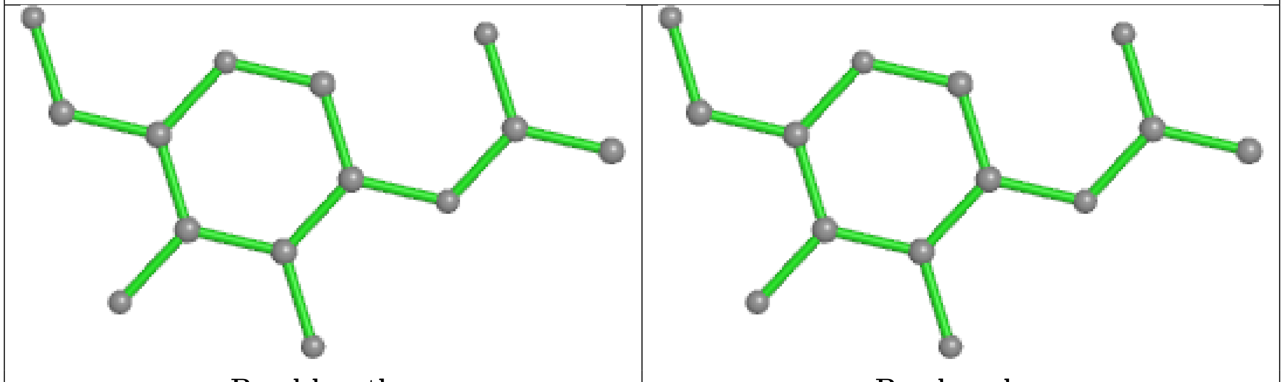


Bond lengths **Bond angles**

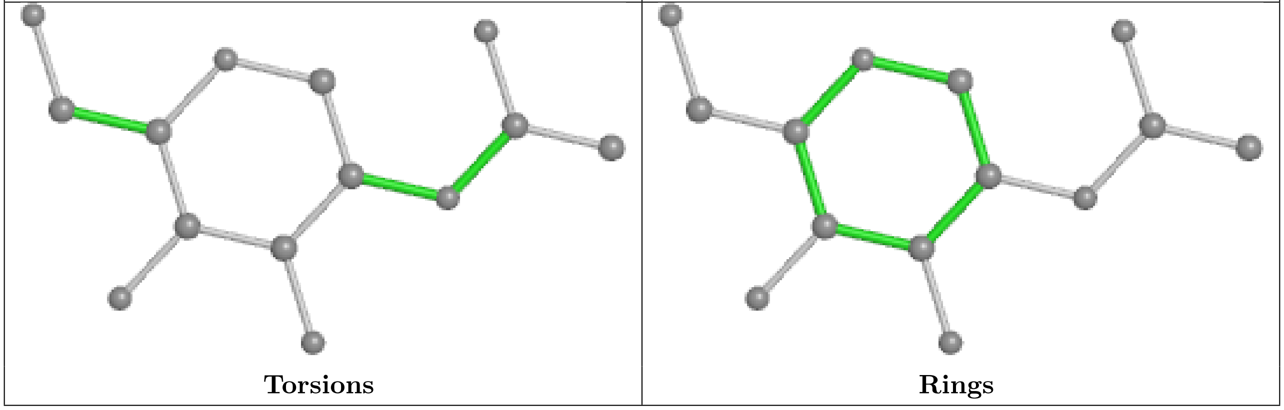


Torsions **Rings**

Ligand NAG B 1306



Bond lengths Bond angles



Torsions Rings

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

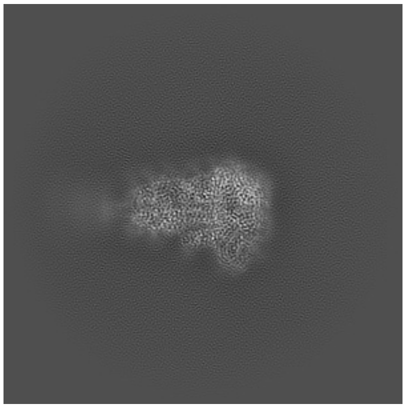
This section contains visualisations of the EMDB entry EMD-15482. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

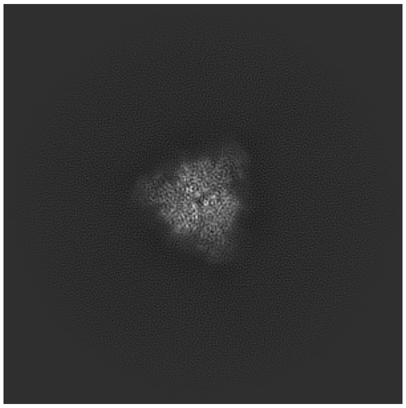
6.1 Orthogonal projections

6.1.1 Primary map

X

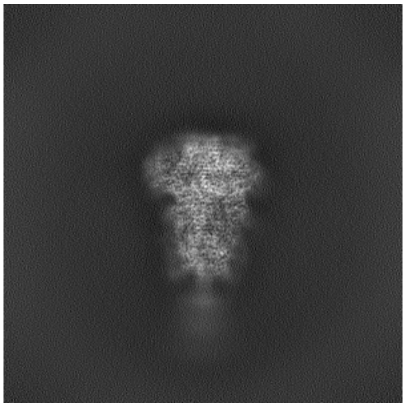


Y

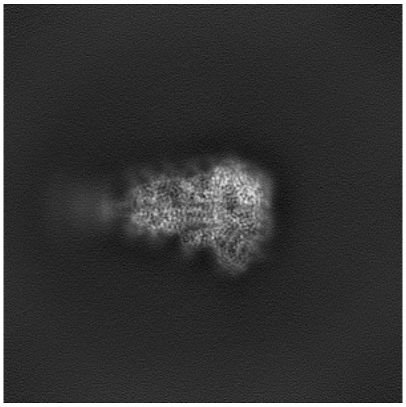


Z

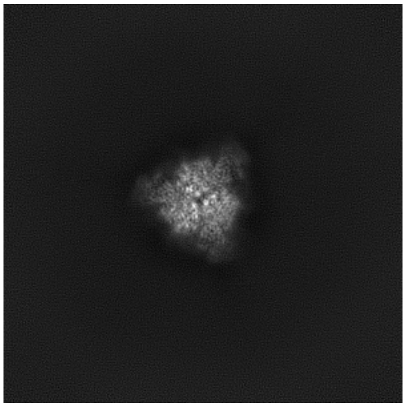
6.1.2 Raw map



X



Y

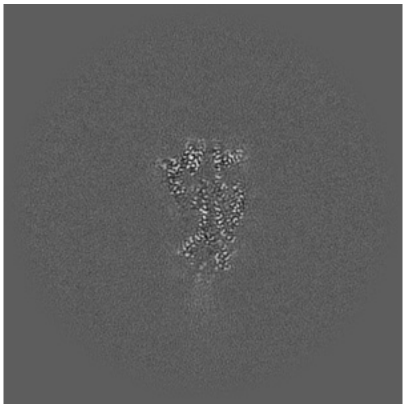


Z

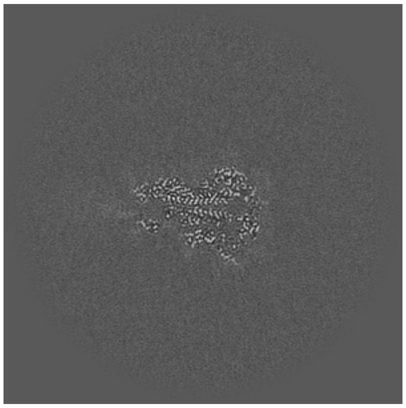
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

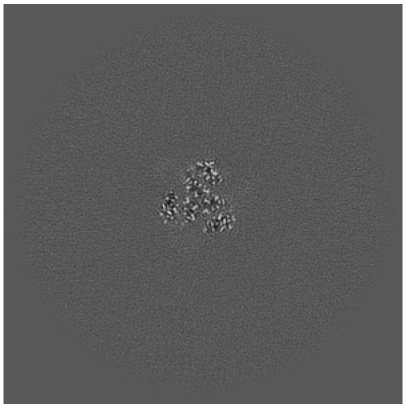
6.2.1 Primary map



X Index: 192

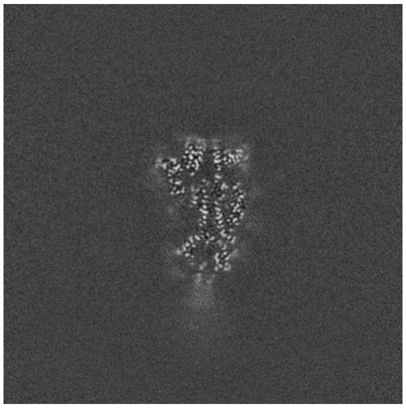


Y Index: 192

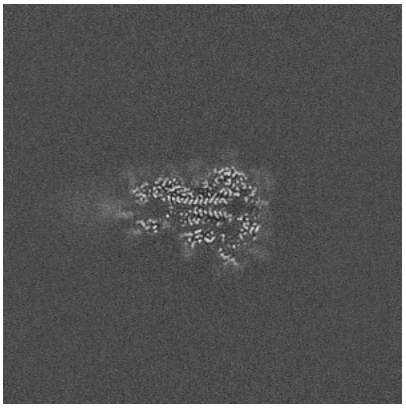


Z Index: 192

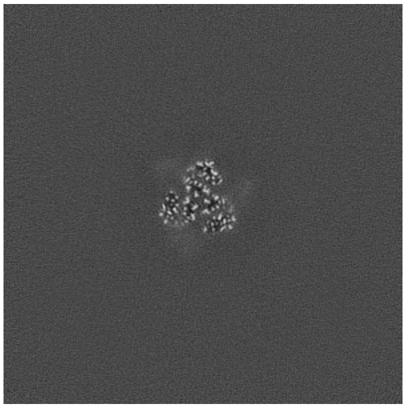
6.2.2 Raw map



X Index: 192



Y Index: 192

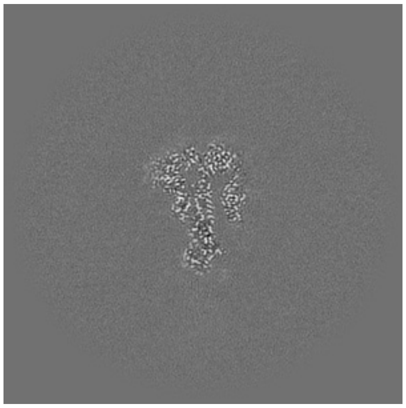


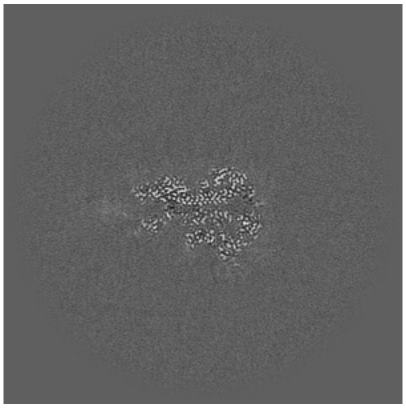
Z Index: 192

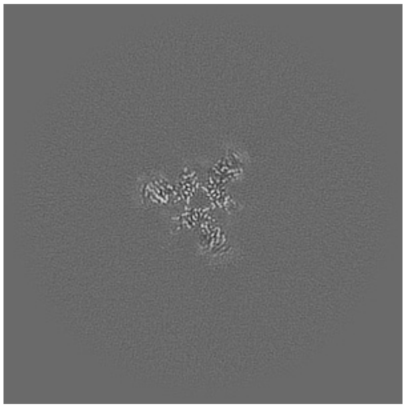
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

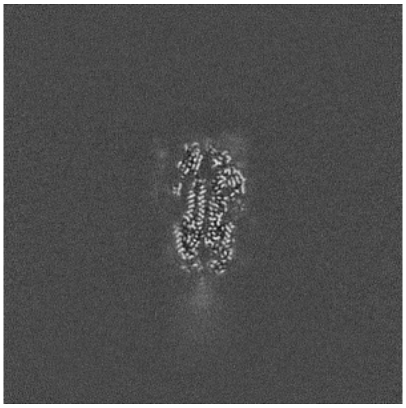
6.3.1 Primary map

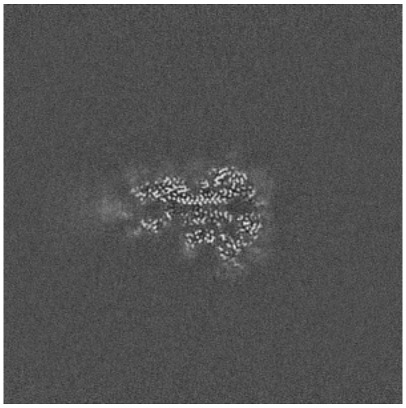

X Index: 202

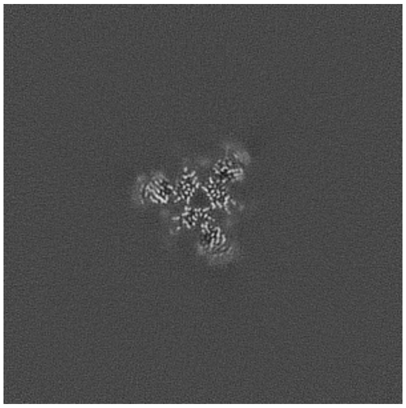

Y Index: 193


Z Index: 225

6.3.2 Raw map


X Index: 184

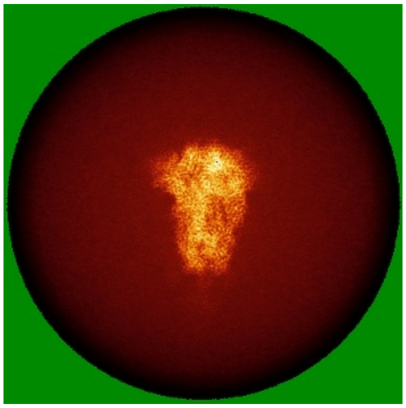

Y Index: 193

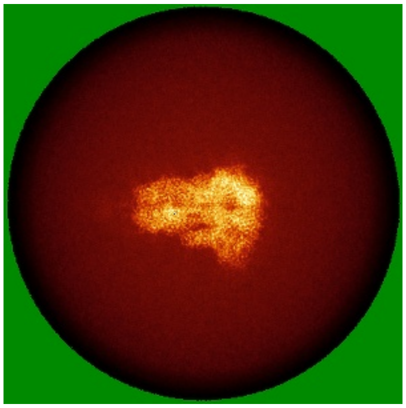

Z Index: 225

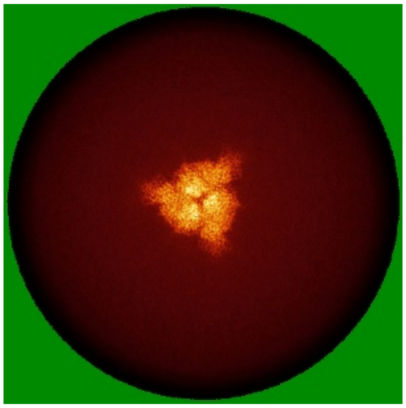
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

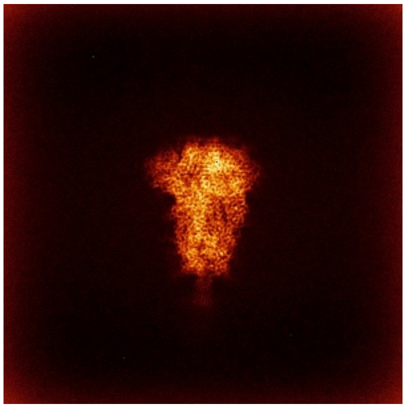
6.4.1 Primary map

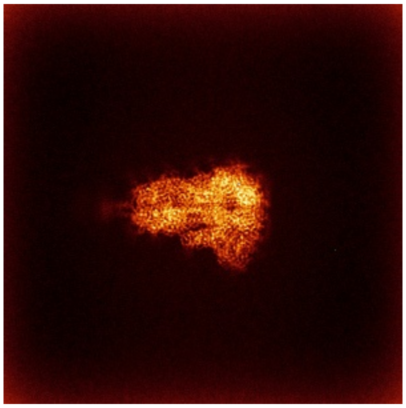

X

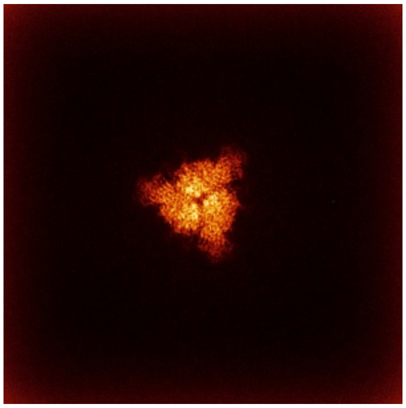

Y


Z

6.4.2 Raw map


X

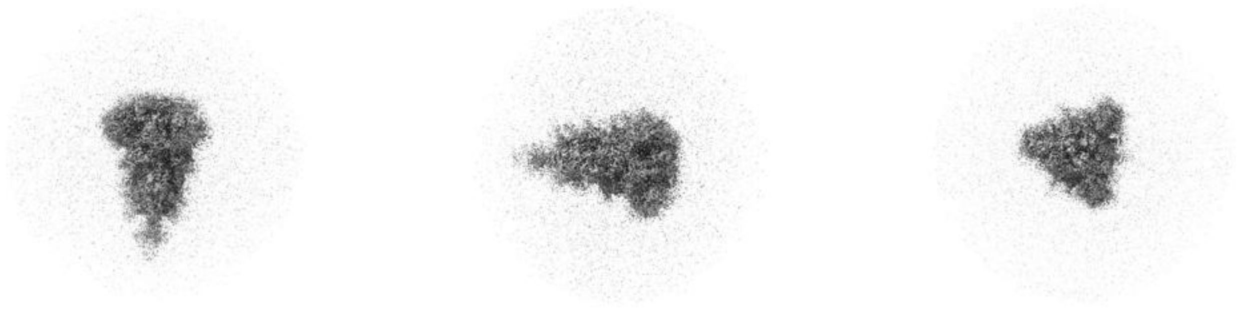

Y


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

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

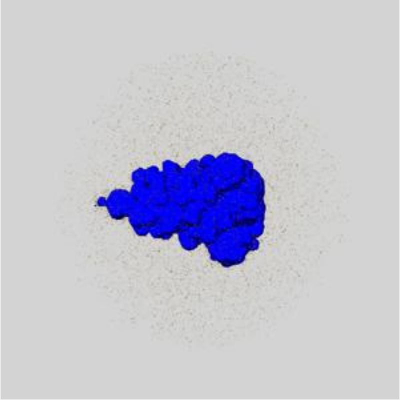
This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

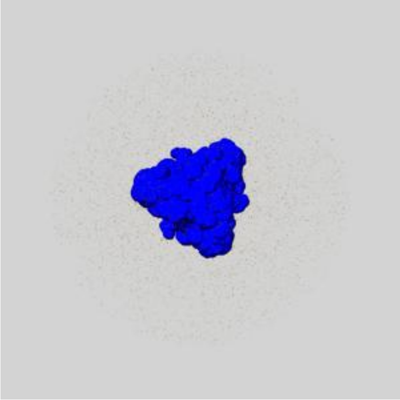
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_15482_msk_1.map ⓘ

X



Y

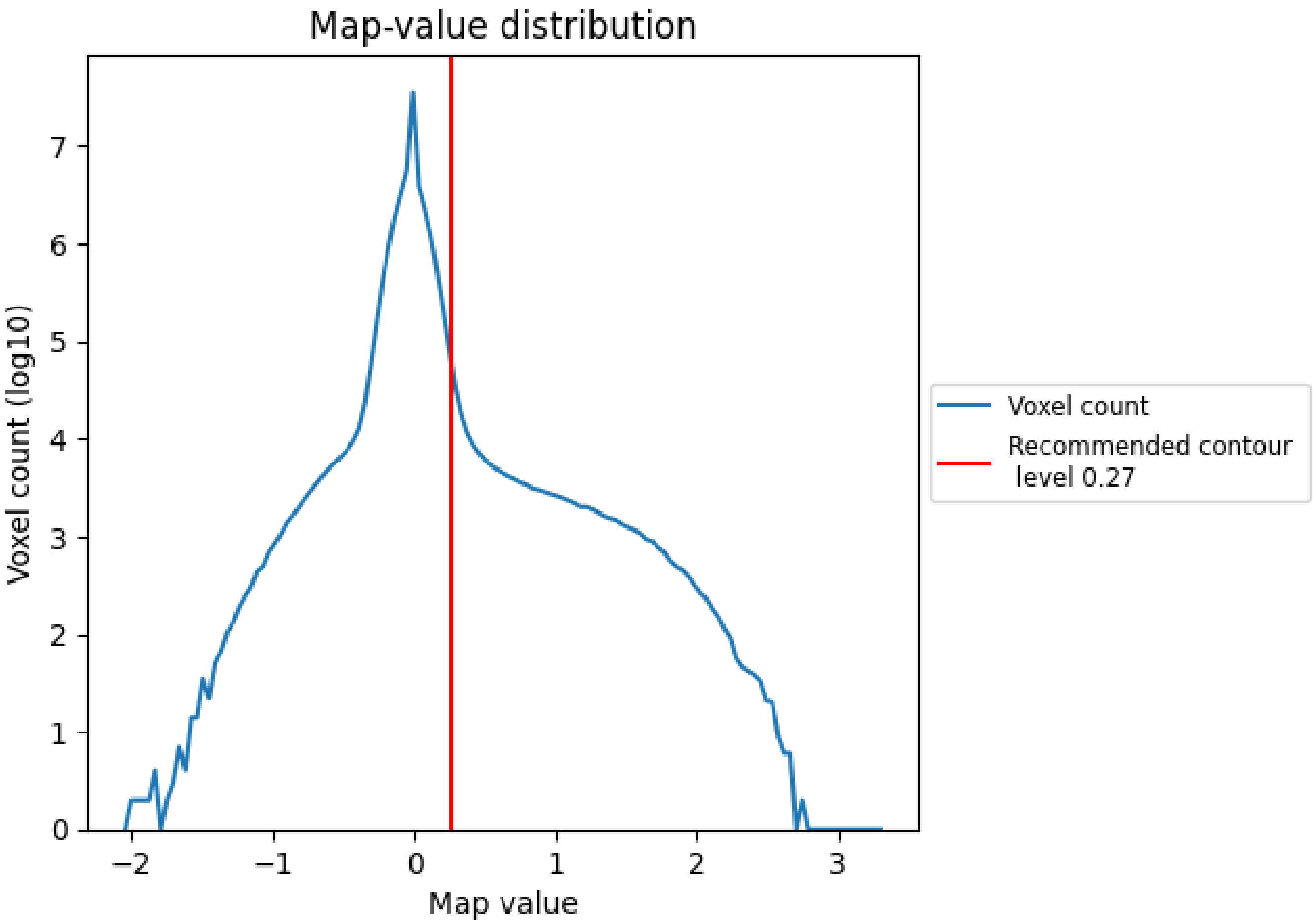


Z

7 Map analysis ⓘ

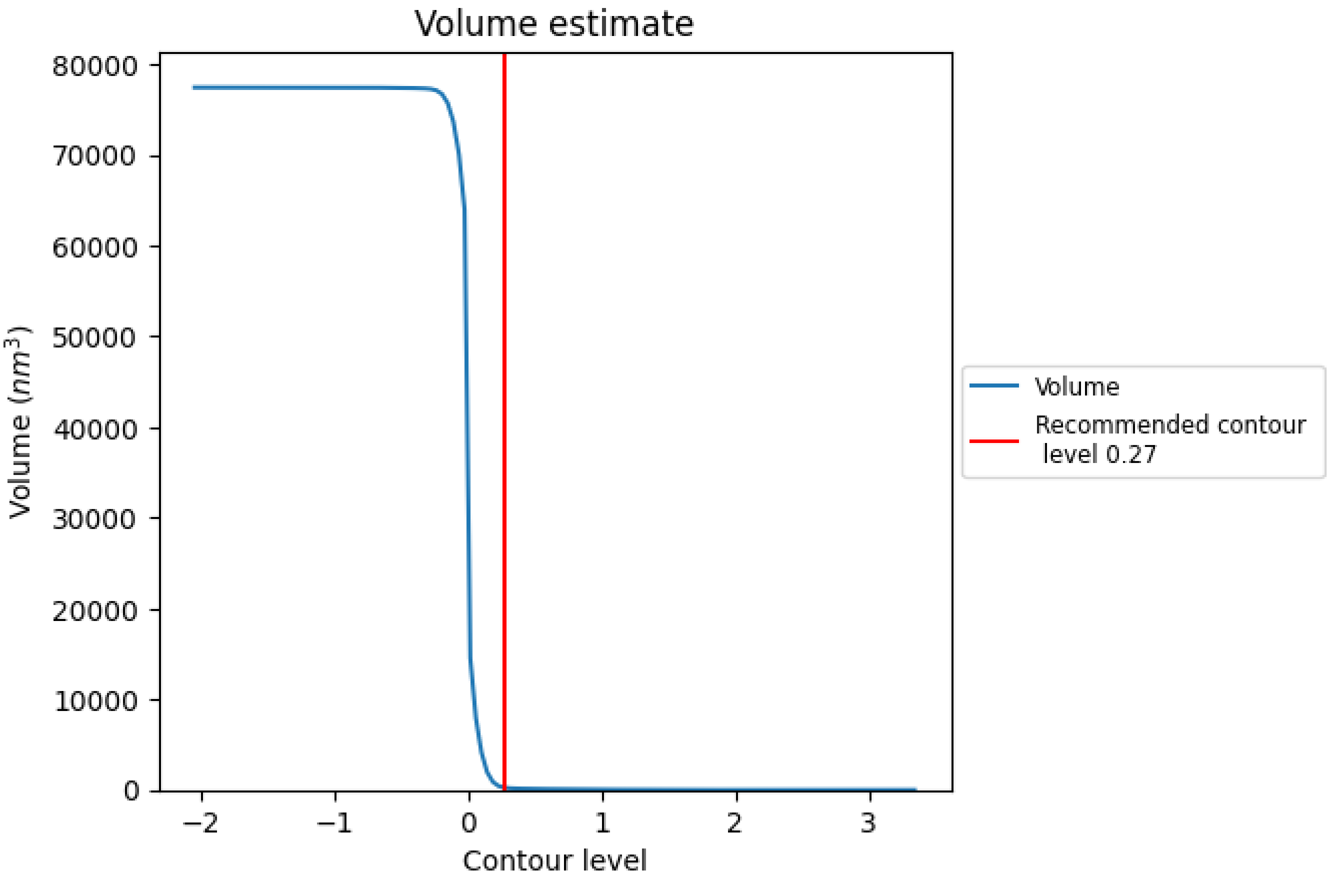
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

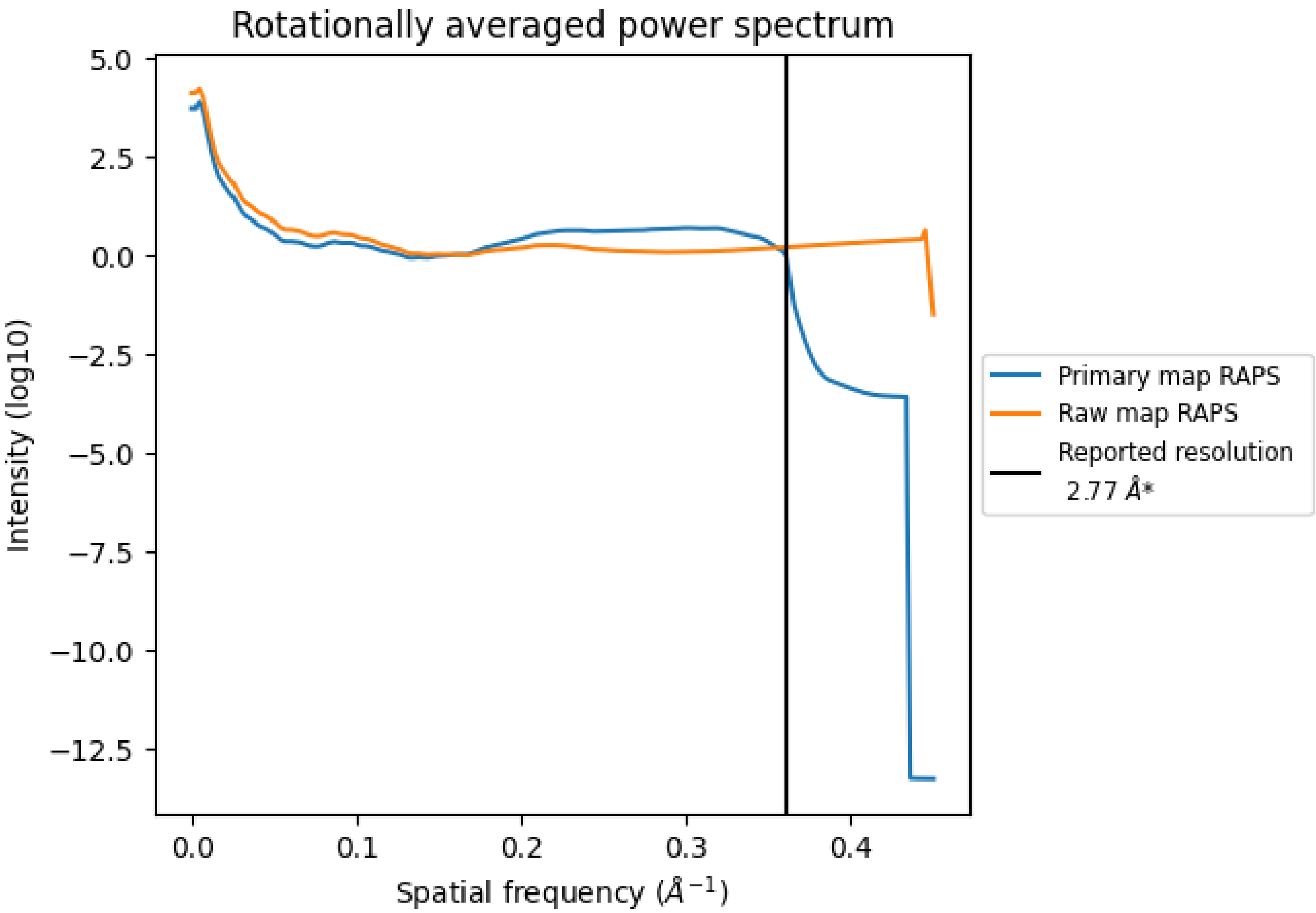
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 261 nm^3; this corresponds to an approximate mass of 235 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 ⓘ

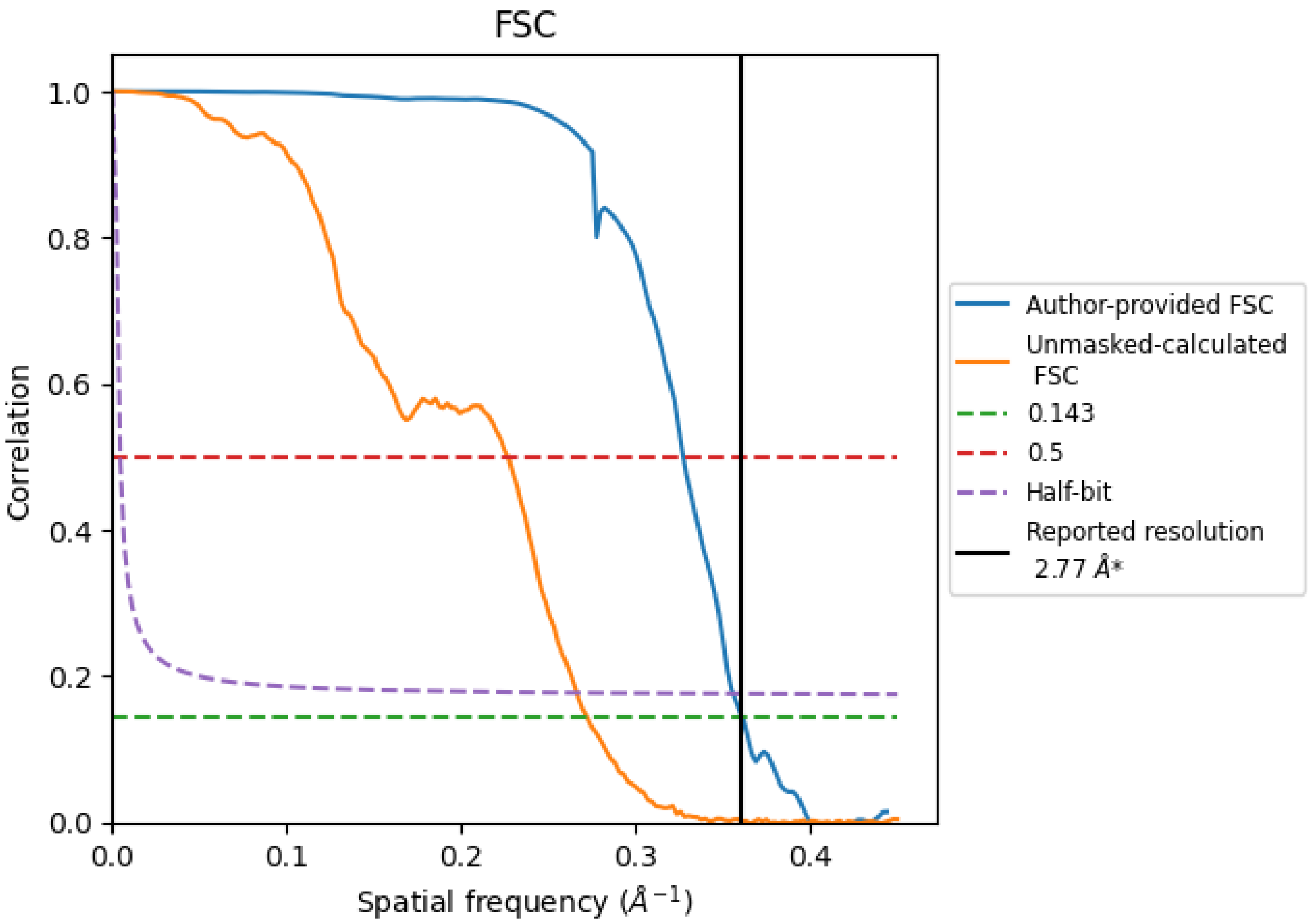


*Reported resolution corresponds to spatial frequency of 0.361 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.361 $Å^{-1}$

8.2 Resolution estimates ⓘ

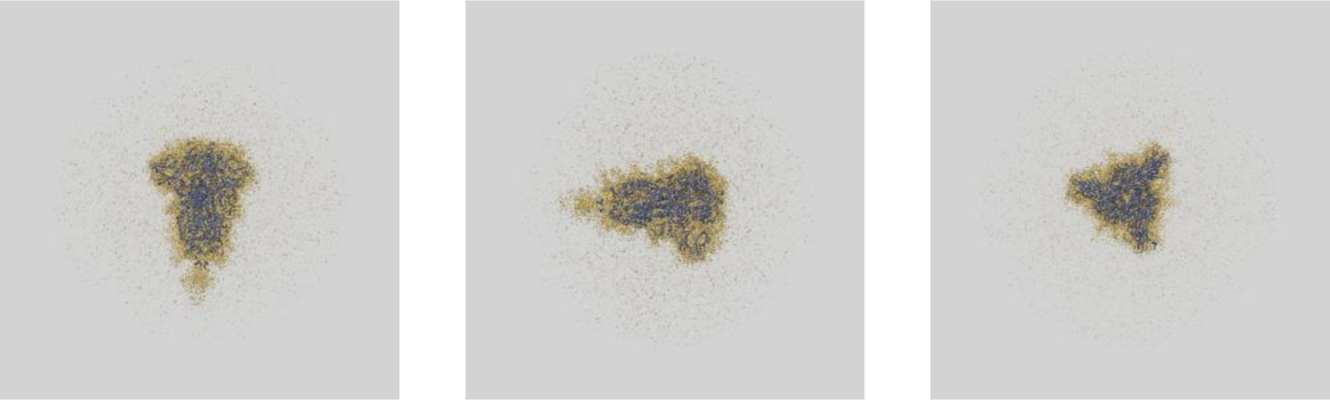
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.05	2.81
Unmasked-calculated*	3.67	4.40	3.75

*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 3.67 differs from the reported value 2.77 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-15482 and PDB model 8AJL. Per-residue inclusion information can be found in section 3 on page 30.

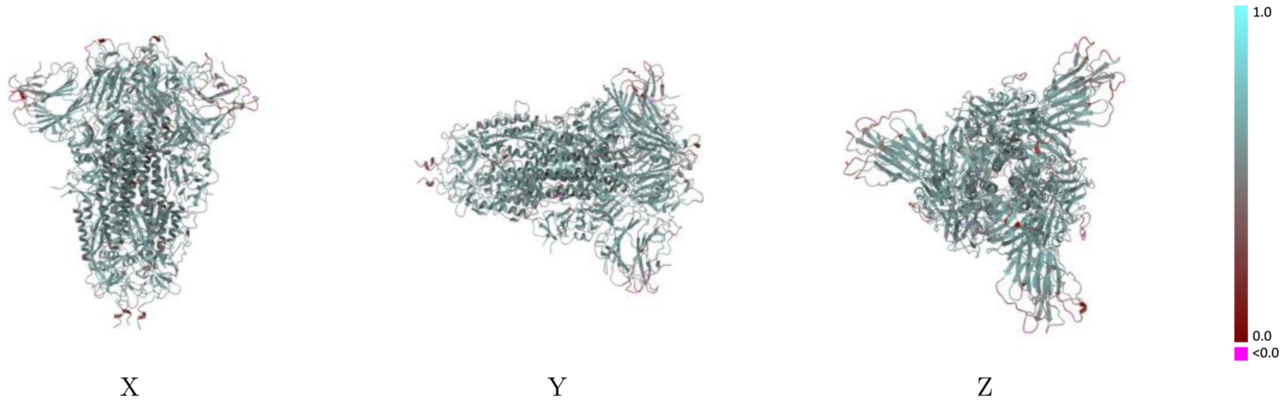
9.1 Map-model overlay ⓘ



X Y Z

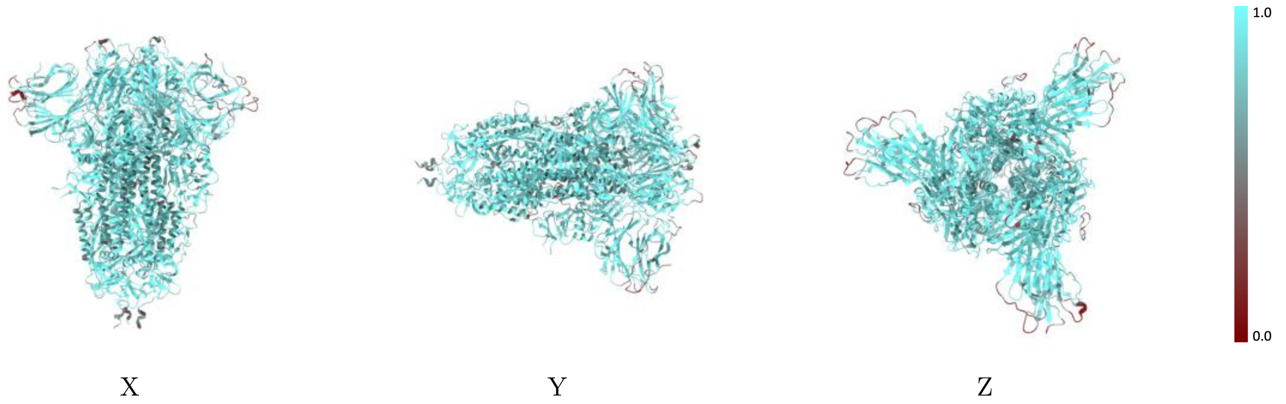
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



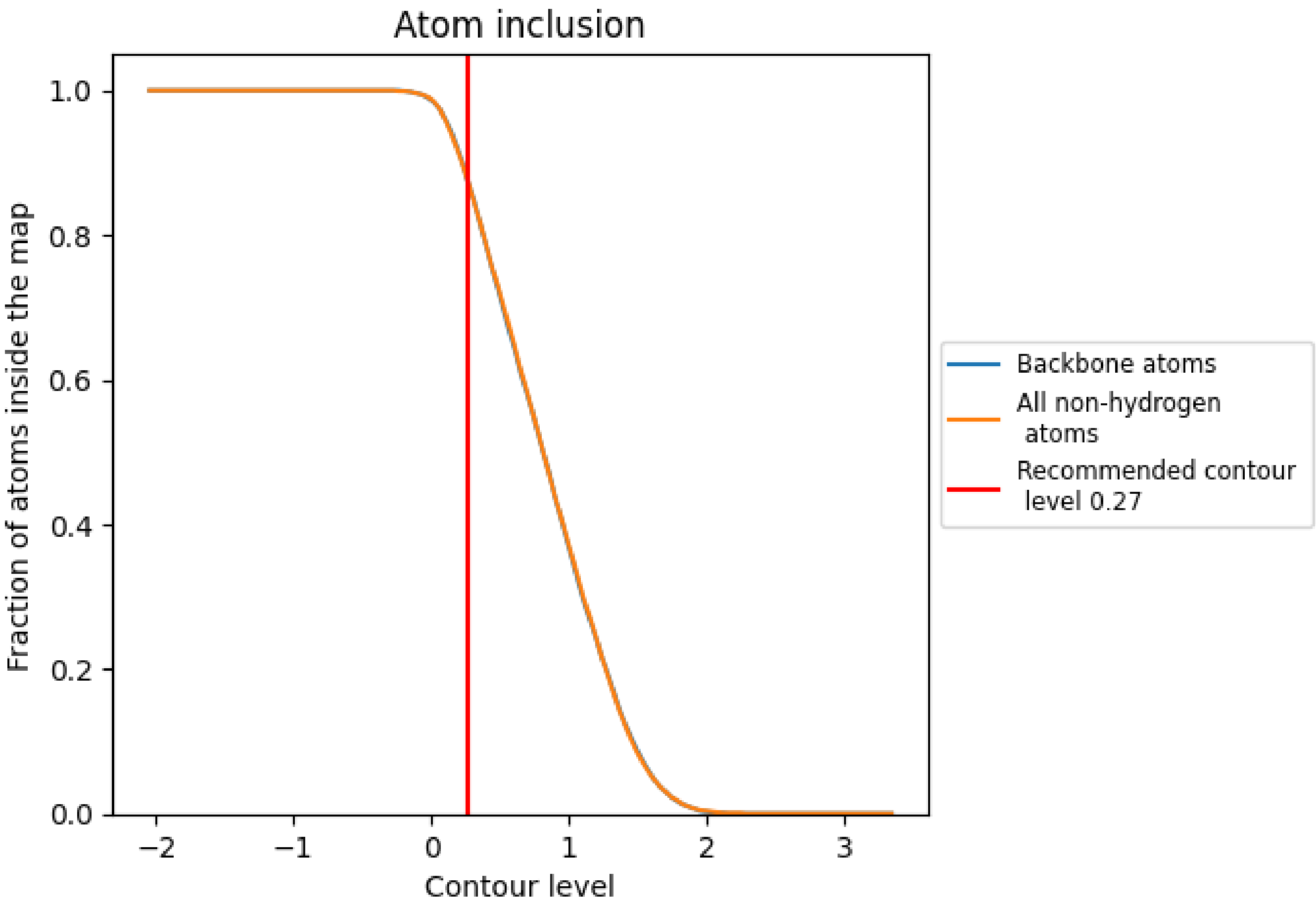
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.27).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8720	0.5550
A	0.8760	0.5590
B	0.8740	0.5560
C	0.8720	0.5530
L	0.9290	0.5650
M	0.5710	0.3940
N	0.6790	0.3490
P	0.9290	0.5560
Q	0.5360	0.3730
R	0.6070	0.3810
U	0.9640	0.5500
V	0.6070	0.3670
W	0.7860	0.4090