



Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 09:28 pm BST

PDB ID : 8AJA
EMDB ID : EMD-15475
Title : Structure of the Ancestral Scaffold Antigen-5 of Coronavirus Spike protein
Authors : Hueting, D.; Schriever, K.; Wallden, K.; Andrell, J.; Syren, P.O.
Deposited on : 2022-07-27
Resolution : 2.59 Å(reported)
Based on initial models : 7BNN, 6ZOZ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

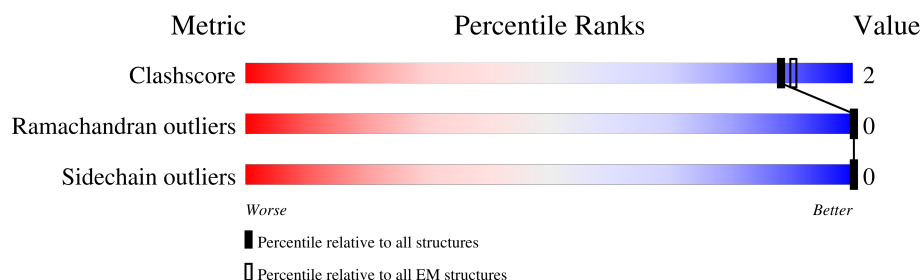
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.59 Å.

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



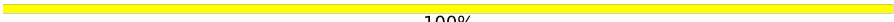



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1240	
1	B	1240	
1	C	1240	
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	T	2	 50%50%
2	U	2	 50%50%
2	V	2	 50%50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51942 atoms, of which 25659 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	1090	Total	C	H	N	O	S	0	0
			16785	5395	8290	1421	1635	44		
1	B	1090	Total	C	H	N	O	S	0	0
			16785	5395	8290	1421	1635	44		
1	C	1090	Total	C	H	N	O	S	0	0
			16785	5395	8290	1421	1635	44		

There are 996 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	ILE	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	THR	LEU	engineered mutation	UNP P0DTC2
A	30	ASN	-	insertion	UNP P0DTC2
A	31	MET	-	insertion	UNP P0DTC2
A	32	ASN	ALA	engineered mutation	UNP P0DTC2
A	33	GLN	TYR	engineered mutation	UNP P0DTC2
A	34	PHE	THR	engineered mutation	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	69	ARG	-	insertion	UNP P0DTC2
A	70	TYR	TRP	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	71	LEU	PHE	engineered mutation	UNP P0DTC2
A	72	SER	HIS	engineered mutation	UNP P0DTC2
A	73	LEU	ALA	engineered mutation	UNP P0DTC2
A	74	ASN	ILE	engineered mutation	UNP P0DTC2
A	75	ALA	HIS	engineered mutation	UNP P0DTC2
A	76	ASP	VAL	engineered mutation	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	THR	deletion	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	91	GLY	ASN	engineered mutation	UNP P0DTC2
A	94	ILE	VAL	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	127	SER	ALA	engineered mutation	UNP P0DTC2
A	129	HIS	ASN	engineered mutation	UNP P0DTC2
A	130	ILE	VAL	engineered mutation	UNP P0DTC2
A	131	ILE	VAL	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	THR	GLY	engineered mutation	UNP P0DTC2
A	148	SER	TYR	engineered mutation	UNP P0DTC2
A	149	ARG	TYR	engineered mutation	UNP P0DTC2
A	150	GLY	HIS	engineered mutation	UNP P0DTC2
A	151	GLN	LYS	engineered mutation	UNP P0DTC2
A	152	HIS	ASN	engineered mutation	UNP P0DTC2
A	153	TYR	ASN	engineered mutation	UNP P0DTC2
A	155	THR	SER	engineered mutation	UNP P0DTC2
A	?	-	MET	deletion	UNP P0DTC2
A	?	-	GLU	deletion	UNP P0DTC2
A	?	-	SER	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	159	THR	SER	engineered mutation	UNP P0DTC2
A	160	ASN	SER	engineered mutation	UNP P0DTC2
A	162	ARG	ASN	engineered mutation	UNP P0DTC2
A	166	TYR	PHE	engineered mutation	UNP P0DTC2
A	171	LYS	GLN	engineered mutation	UNP P0DTC2
A	172	SER	PRO	engineered mutation	UNP P0DTC2
A	174	GLN	LEU	engineered mutation	UNP P0DTC2
A	175	LEU	MET	engineered mutation	UNP P0DTC2
A	177	VAL	LEU	engineered mutation	UNP P0DTC2
A	178	SER	GLU	engineered mutation	UNP P0DTC2
A	179	GLU	GLY	engineered mutation	UNP P0DTC2
A	181	ASN	GLN	engineered mutation	UNP P0DTC2
A	186	HIS	ASN	engineered mutation	UNP P0DTC2
A	195	VAL	ILE	engineered mutation	UNP P0DTC2
A	198	PHE	TYR	engineered mutation	UNP P0DTC2
A	199	LEU	PHE	engineered mutation	UNP P0DTC2
A	200	HIS	LYS	engineered mutation	UNP P0DTC2
A	201	VAL	ILE	engineered mutation	UNP P0DTC2
A	204	ALA	LYS	engineered mutation	UNP P0DTC2
A	205	TYR	HIS	engineered mutation	UNP P0DTC2
A	206	GLU	THR	engineered mutation	UNP P0DTC2
A	209	ASP	ASN	engineered mutation	UNP P0DTC2
A	211	ALA	VAL	engineered mutation	UNP P0DTC2
A	213	GLY	ASP	engineered mutation	UNP P0DTC2
A	216	SER	GLN	engineered mutation	UNP P0DTC2
A	220	VAL	ALA	engineered mutation	UNP P0DTC2
A	222	LYS	GLU	engineered mutation	UNP P0DTC2
A	224	ILE	LEU	engineered mutation	UNP P0DTC2
A	225	LEU	VAL	engineered mutation	UNP P0DTC2
A	226	LYS	ASP	engineered mutation	UNP P0DTC2
A	229	LEU	ILE	engineered mutation	UNP P0DTC2
A	235	SER	ARG	engineered mutation	UNP P0DTC2
A	?	-	GLN	deletion	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	238	VAL	SER	engineered mutation	UNP P0DTC2
A	239	VAL	TYR	engineered mutation	UNP P0DTC2
A	240	MET	LEU	engineered mutation	UNP P0DTC2
A	242	MET	-	insertion	UNP P0DTC2
A	243	PHE	PRO	engineered mutation	UNP P0DTC2
A	244	SER	GLY	engineered mutation	UNP P0DTC2
A	245	PRO	ASP	engineered mutation	UNP P0DTC2
A	246	THR	SER	engineered mutation	UNP P0DTC2
A	247	THR	SER	engineered mutation	UNP P0DTC2
A	249	ASN	GLY	engineered mutation	UNP P0DTC2
A	251	LEU	THR	engineered mutation	UNP P0DTC2
A	253	GLU	GLY	engineered mutation	UNP P0DTC2
A	254	SER	ALA	engineered mutation	UNP P0DTC2
A	258	PHE	TYR	engineered mutation	UNP P0DTC2
A	263	LYS	GLN	engineered mutation	UNP P0DTC2
A	265	THR	ARG	engineered mutation	UNP P0DTC2
A	268	MET	LEU	engineered mutation	UNP P0DTC2
A	271	PHE	TYR	engineered mutation	UNP P0DTC2
A	284	SER	ALA	engineered mutation	UNP P0DTC2
A	285	GLN	LEU	engineered mutation	UNP P0DTC2
A	291	LEU	THR	engineered mutation	UNP P0DTC2
A	299	ASN	THR	engineered mutation	UNP P0DTC2
A	313	SER	GLN	engineered mutation	UNP P0DTC2
A	316	GLN	GLU	engineered mutation	UNP P0DTC2
A	317	GLU	SER	engineered mutation	UNP P0DTC2
A	318	VAL	ILE	engineered mutation	UNP P0DTC2
A	331	ASP	GLY	engineered mutation	UNP P0DTC2
A	332	LYS	GLU	engineered mutation	UNP P0DTC2
A	340	PRO	ALA	engineered mutation	UNP P0DTC2
A	346	GLU	ASN	engineered mutation	UNP P0DTC2
A	348	THR	LYS	engineered mutation	UNP P0DTC2
A	349	LYS	ARG	engineered mutation	UNP P0DTC2
A	352	ASP	ASN	engineered mutation	UNP P0DTC2
A	358	THR	SER	engineered mutation	UNP P0DTC2
A	364	THR	ALA	engineered mutation	UNP P0DTC2
A	377	SER	THR	engineered mutation	UNP P0DTC2
A	380	ILE	ASN	engineered mutation	UNP P0DTC2
A	386	SER	ASN	engineered mutation	UNP P0DTC2
A	391	THR	SER	engineered mutation	UNP P0DTC2
A	393	LEU	VAL	engineered mutation	UNP P0DTC2
A	396	SER	GLY	engineered mutation	UNP P0DTC2
A	397	SER	ASP	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	402	VAL	ILE	engineered mutation	UNP P0DTC2
A	409	VAL	LYS	engineered mutation	UNP P0DTC2
A	430	THR	SER	engineered mutation	UNP P0DTC2
A	431	ALA	ASN	engineered mutation	UNP P0DTC2
A	432	LYS	ASN	engineered mutation	UNP P0DTC2
A	433	GLN	LEU	engineered mutation	UNP P0DTC2
A	?	-	SER	deletion	UNP P0DTC2
A	?	-	LYS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	435	ALA	ASN	engineered mutation	UNP P0DTC2
A	436	GLY	TYR	engineered mutation	UNP P0DTC2
A	439	TYR	LEU	engineered mutation	UNP P0DTC2
A	442	SER	LEU	engineered mutation	UNP P0DTC2
A	443	HIS	PHE	engineered mutation	UNP P0DTC2
A	446	THR	SER	engineered mutation	UNP P0DTC2
A	447	LYS	ASN	engineered mutation	UNP P0DTC2
A	455	LEU	ILE	engineered mutation	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	GLU	deletion	UNP P0DTC2
A	?	-	ILE	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	GLN	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	SER	deletion	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	CYS	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	457	ASN	VAL	engineered mutation	UNP P0DTC2
A	458	SER	GLU	engineered mutation	UNP P0DTC2
A	459	ASP	GLY	engineered mutation	UNP P0DTC2
A	460	GLU	PHE	engineered mutation	UNP P0DTC2
A	462	GLY	CYS	engineered mutation	UNP P0DTC2
A	463	VAL	TYR	engineered mutation	UNP P0DTC2
A	464	ARG	PHE	engineered mutation	UNP P0DTC2
A	465	THR	PRO	engineered mutation	UNP P0DTC2
A	467	SER	GLN	engineered mutation	UNP P0DTC2
A	468	THR	SER	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	470	ASP	GLY	engineered mutation	UNP P0DTC2
A	472	ASN	GLN	engineered mutation	UNP P0DTC2
A	474	ASN	THR	engineered mutation	UNP P0DTC2
A	475	VAL	ASN	engineered mutation	UNP P0DTC2
A	476	PRO	GLY	engineered mutation	UNP P0DTC2
A	477	ILE	VAL	engineered mutation	UNP P0DTC2
A	478	GLU	GLY	engineered mutation	UNP P0DTC2
A	481	ALA	PRO	engineered mutation	UNP P0DTC2
A	482	THR	TYR	engineered mutation	UNP P0DTC2
A	493	ASN	HIS	engineered mutation	UNP P0DTC2
A	503	LEU	LYS	engineered mutation	UNP P0DTC2
A	506	GLN	ASN	engineered mutation	UNP P0DTC2
A	511	GLN	LYS	engineered mutation	UNP P0DTC2
A	521	LYS	THR	engineered mutation	UNP P0DTC2
A	528	ASP	GLU	engineered mutation	UNP P0DTC2
A	530	SER	ASN	engineered mutation	UNP P0DTC2
A	532	ARG	LYS	engineered mutation	UNP P0DTC2
A	534	GLN	LEU	engineered mutation	UNP P0DTC2
A	535	SER	PRO	engineered mutation	UNP P0DTC2
A	543	ALA	ILE	engineered mutation	UNP P0DTC2
A	544	SER	ALA	engineered mutation	UNP P0DTC2
A	546	PHE	THR	engineered mutation	UNP P0DTC2
A	549	SER	ALA	engineered mutation	UNP P0DTC2
A	562	SER	THR	engineered mutation	UNP P0DTC2
A	578	ALA	THR	engineered mutation	UNP P0DTC2
A	580	SER	ASN	engineered mutation	UNP P0DTC2
A	581	GLU	GLN	engineered mutation	UNP P0DTC2
A	593	ASP	GLU	engineered mutation	UNP P0DTC2
A	596	THR	VAL	engineered mutation	UNP P0DTC2
A	606	ALA	THR	engineered mutation	UNP P0DTC2
A	614	VAL	SER	engineered mutation	UNP P0DTC2
A	620	GLN	ARG	engineered mutation	UNP P0DTC2
A	632	ALA	ASN	engineered mutation	UNP P0DTC2
A	649	HIS	GLN	engineered mutation	UNP P0DTC2
A	651	ALA	-	insertion	UNP P0DTC2
A	652	SER	GLN	conflict	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	654	LEU	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	657	THR	VAL	engineered mutation	UNP P0DTC2
A	658	GLY	ALA	engineered mutation	UNP P0DTC2
A	659	GLN	SER	engineered mutation	UNP P0DTC2
A	660	LYS	GLN	engineered mutation	UNP P0DTC2
A	663	VAL	ILE	engineered mutation	UNP P0DTC2
A	675	ILE	VAL	engineered mutation	UNP P0DTC2
A	678	ALA	SER	engineered mutation	UNP P0DTC2
A	689	SER	THR	engineered mutation	UNP P0DTC2
A	696	VAL	ILE	engineered mutation	UNP P0DTC2
A	697	MET	LEU	engineered mutation	UNP P0DTC2
A	702	ALA	THR	engineered mutation	UNP P0DTC2
A	717	GLN	THR	engineered mutation	UNP P0DTC2
A	742	ILE	VAL	engineered mutation	UNP P0DTC2
A	758	MET	ILE	engineered mutation	UNP P0DTC2
A	763	ALA	PRO	engineered mutation	UNP P0DTC2
A	783	THR	SER	engineered mutation	UNP P0DTC2
A	804	MET	ILE	engineered mutation	UNP P0DTC2
A	809	GLU	ASP	engineered mutation	UNP P0DTC2
A	815	SER	ALA	engineered mutation	UNP P0DTC2
A	842	ALA	GLN	engineered mutation	UNP P0DTC2
A	845	ALA	SER	engineered mutation	UNP P0DTC2
A	848	VAL	LEU	engineered mutation	UNP P0DTC2
A	849	SER	ALA	engineered mutation	UNP P0DTC2
A	852	ALA	ILE	engineered mutation	UNP P0DTC2
A	854	ALA	SER	engineered mutation	UNP P0DTC2
A	892	GLN	LEU	engineered mutation	UNP P0DTC2
A	899	LYS	SER	engineered mutation	UNP P0DTC2
A	902	SER	GLY	engineered mutation	UNP P0DTC2
A	903	GLN	LYS	engineered mutation	UNP P0DTC2
A	906	GLU	ASP	engineered mutation	UNP P0DTC2
A	909	THR	SER	engineered mutation	UNP P0DTC2
A	910	THR	SER	engineered mutation	UNP P0DTC2
A	912	SER	ALA	engineered mutation	UNP P0DTC2
A	913	THR	SER	engineered mutation	UNP P0DTC2
A	1025	ALA	SER	engineered mutation	UNP P0DTC2
A	1040	SER	ALA	engineered mutation	UNP P0DTC2
A	1043	ARG	LYS	engineered mutation	UNP P0DTC2
A	1054	GLU	ASP	engineered mutation	UNP P0DTC2
A	1058	TYR	HIS	engineered mutation	UNP P0DTC2
A	1071	SER	HIS	engineered mutation	UNP P0DTC2
A	1074	ILE	VAL	engineered mutation	UNP P0DTC2
A	1081	SER	GLU	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1093	ALA	SER	engineered mutation	UNP P0DTC2
A	1103	ILE	VAL	engineered mutation	UNP P0DTC2
A	1179	GLY	-	linker	UNP P0DTC2
A	1180	SER	-	linker	UNP P0DTC2
A	1202	LEU	PHE	engineered mutation	UNP P10104
A	1208	GLY	-	expression tag	UNP P10104
A	1209	THR	-	expression tag	UNP P10104
A	1210	SER	-	expression tag	UNP P10104
A	1211	LEU	-	expression tag	UNP P10104
A	1212	GLU	-	expression tag	UNP P10104
A	1213	VAL	-	expression tag	UNP P10104
A	1214	LEU	-	expression tag	UNP P10104
A	1215	PHE	-	expression tag	UNP P10104
A	1216	GLN	-	expression tag	UNP P10104
A	1217	GLY	-	expression tag	UNP P10104
A	1218	PRO	-	expression tag	UNP P10104
A	1219	GLY	-	expression tag	UNP P10104
A	1220	HIS	-	expression tag	UNP P10104
A	1221	HIS	-	expression tag	UNP P10104
A	1222	HIS	-	expression tag	UNP P10104
A	1223	HIS	-	expression tag	UNP P10104
A	1224	HIS	-	expression tag	UNP P10104
A	1225	HIS	-	expression tag	UNP P10104
A	1226	HIS	-	expression tag	UNP P10104
A	1227	HIS	-	expression tag	UNP P10104
A	1228	SER	-	expression tag	UNP P10104
A	1229	ALA	-	expression tag	UNP P10104
A	1230	TRP	-	expression tag	UNP P10104
A	1231	SER	-	expression tag	UNP P10104
A	1232	HIS	-	expression tag	UNP P10104
A	1233	PRO	-	expression tag	UNP P10104
A	1234	GLN	-	expression tag	UNP P10104
A	1235	PHE	-	expression tag	UNP P10104
A	1236	GLU	-	expression tag	UNP P10104
A	1237	LYS	-	expression tag	UNP P10104
A	1238	GLY	-	expression tag	UNP P10104
A	1239	GLY	-	expression tag	UNP P10104
A	1240	GLY	-	expression tag	UNP P10104
A	1241	SER	-	expression tag	UNP P10104
A	1242	GLY	-	expression tag	UNP P10104
A	1243	GLY	-	expression tag	UNP P10104
A	1244	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1245	GLY	-	expression tag	UNP P10104
A	1246	SER	-	expression tag	UNP P10104
A	1247	GLY	-	expression tag	UNP P10104
A	1248	GLY	-	expression tag	UNP P10104
A	1249	SER	-	expression tag	UNP P10104
A	1250	ALA	-	expression tag	UNP P10104
A	1251	TRP	-	expression tag	UNP P10104
A	1252	SER	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104
A	1254	PRO	-	expression tag	UNP P10104
A	1255	GLN	-	expression tag	UNP P10104
A	1256	PHE	-	expression tag	UNP P10104
A	1257	GLU	-	expression tag	UNP P10104
A	1258	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	ILE	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	THR	LEU	engineered mutation	UNP P0DTC2
B	30	ASN	-	insertion	UNP P0DTC2
B	31	MET	-	insertion	UNP P0DTC2
B	32	ASN	ALA	engineered mutation	UNP P0DTC2
B	33	GLN	TYR	engineered mutation	UNP P0DTC2
B	34	PHE	THR	engineered mutation	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	69	ARG	-	insertion	UNP P0DTC2
B	70	TYR	TRP	engineered mutation	UNP P0DTC2
B	71	LEU	PHE	engineered mutation	UNP P0DTC2
B	72	SER	HIS	engineered mutation	UNP P0DTC2
B	73	LEU	ALA	engineered mutation	UNP P0DTC2
B	74	ASN	ILE	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	75	ALA	HIS	engineered mutation	UNP P0DTC2
B	76	ASP	VAL	engineered mutation	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	79	ARG	GLY	engineered mutation	UNP P0DTC2
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	91	GLY	ASN	engineered mutation	UNP P0DTC2
B	94	ILE	VAL	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	127	SER	ALA	engineered mutation	UNP P0DTC2
B	129	HIS	ASN	engineered mutation	UNP P0DTC2
B	130	ILE	VAL	engineered mutation	UNP P0DTC2
B	131	ILE	VAL	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	THR	GLY	engineered mutation	UNP P0DTC2
B	148	SER	TYR	engineered mutation	UNP P0DTC2
B	149	ARG	TYR	engineered mutation	UNP P0DTC2
B	150	GLY	HIS	engineered mutation	UNP P0DTC2
B	151	GLN	LYS	engineered mutation	UNP P0DTC2
B	152	HIS	ASN	engineered mutation	UNP P0DTC2
B	153	TYR	ASN	engineered mutation	UNP P0DTC2
B	155	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	THR	SER	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	160	ASN	SER	engineered mutation	UNP P0DTC2
B	162	ARG	ASN	engineered mutation	UNP P0DTC2
B	166	TYR	PHE	engineered mutation	UNP P0DTC2
B	171	LYS	GLN	engineered mutation	UNP P0DTC2
B	172	SER	PRO	engineered mutation	UNP P0DTC2
B	174	GLN	LEU	engineered mutation	UNP P0DTC2
B	175	LEU	MET	engineered mutation	UNP P0DTC2
B	177	VAL	LEU	engineered mutation	UNP P0DTC2
B	178	SER	GLU	engineered mutation	UNP P0DTC2
B	179	GLU	GLY	engineered mutation	UNP P0DTC2
B	181	ASN	GLN	engineered mutation	UNP P0DTC2
B	186	HIS	ASN	engineered mutation	UNP P0DTC2
B	195	VAL	ILE	engineered mutation	UNP P0DTC2
B	198	PHE	TYR	engineered mutation	UNP P0DTC2
B	199	LEU	PHE	engineered mutation	UNP P0DTC2
B	200	HIS	LYS	engineered mutation	UNP P0DTC2
B	201	VAL	ILE	engineered mutation	UNP P0DTC2
B	204	ALA	LYS	engineered mutation	UNP P0DTC2
B	205	TYR	HIS	engineered mutation	UNP P0DTC2
B	206	GLU	THR	engineered mutation	UNP P0DTC2
B	209	ASP	ASN	engineered mutation	UNP P0DTC2
B	211	ALA	VAL	engineered mutation	UNP P0DTC2
B	213	GLY	ASP	engineered mutation	UNP P0DTC2
B	216	SER	GLN	engineered mutation	UNP P0DTC2
B	220	VAL	ALA	engineered mutation	UNP P0DTC2
B	222	LYS	GLU	engineered mutation	UNP P0DTC2
B	224	ILE	LEU	engineered mutation	UNP P0DTC2
B	225	LEU	VAL	engineered mutation	UNP P0DTC2
B	226	LYS	ASP	engineered mutation	UNP P0DTC2
B	229	LEU	ILE	engineered mutation	UNP P0DTC2
B	235	SER	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	238	VAL	SER	engineered mutation	UNP P0DTC2
B	239	VAL	TYR	engineered mutation	UNP P0DTC2
B	240	MET	LEU	engineered mutation	UNP P0DTC2
B	242	MET	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	243	PHE	PRO	engineered mutation	UNP P0DTC2
B	244	SER	GLY	engineered mutation	UNP P0DTC2
B	245	PRO	ASP	engineered mutation	UNP P0DTC2
B	246	THR	SER	engineered mutation	UNP P0DTC2
B	247	THR	SER	engineered mutation	UNP P0DTC2
B	249	ASN	GLY	engineered mutation	UNP P0DTC2
B	251	LEU	THR	engineered mutation	UNP P0DTC2
B	253	GLU	GLY	engineered mutation	UNP P0DTC2
B	254	SER	ALA	engineered mutation	UNP P0DTC2
B	258	PHE	TYR	engineered mutation	UNP P0DTC2
B	263	LYS	GLN	engineered mutation	UNP P0DTC2
B	265	THR	ARG	engineered mutation	UNP P0DTC2
B	268	MET	LEU	engineered mutation	UNP P0DTC2
B	271	PHE	TYR	engineered mutation	UNP P0DTC2
B	284	SER	ALA	engineered mutation	UNP P0DTC2
B	285	GLN	LEU	engineered mutation	UNP P0DTC2
B	291	LEU	THR	engineered mutation	UNP P0DTC2
B	299	ASN	THR	engineered mutation	UNP P0DTC2
B	313	SER	GLN	engineered mutation	UNP P0DTC2
B	316	GLN	GLU	engineered mutation	UNP P0DTC2
B	317	GLU	SER	engineered mutation	UNP P0DTC2
B	318	VAL	ILE	engineered mutation	UNP P0DTC2
B	331	ASP	GLY	engineered mutation	UNP P0DTC2
B	332	LYS	GLU	engineered mutation	UNP P0DTC2
B	340	PRO	ALA	engineered mutation	UNP P0DTC2
B	346	GLU	ASN	engineered mutation	UNP P0DTC2
B	348	THR	LYS	engineered mutation	UNP P0DTC2
B	349	LYS	ARG	engineered mutation	UNP P0DTC2
B	352	ASP	ASN	engineered mutation	UNP P0DTC2
B	358	THR	SER	engineered mutation	UNP P0DTC2
B	364	THR	ALA	engineered mutation	UNP P0DTC2
B	377	SER	THR	engineered mutation	UNP P0DTC2
B	380	ILE	ASN	engineered mutation	UNP P0DTC2
B	386	SER	ASN	engineered mutation	UNP P0DTC2
B	391	THR	SER	engineered mutation	UNP P0DTC2
B	393	LEU	VAL	engineered mutation	UNP P0DTC2
B	396	SER	GLY	engineered mutation	UNP P0DTC2
B	397	SER	ASP	engineered mutation	UNP P0DTC2
B	402	VAL	ILE	engineered mutation	UNP P0DTC2
B	409	VAL	LYS	engineered mutation	UNP P0DTC2
B	430	THR	SER	engineered mutation	UNP P0DTC2
B	431	ALA	ASN	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	432	LYS	ASN	engineered mutation	UNP P0DTC2
B	433	GLN	LEU	engineered mutation	UNP P0DTC2
B	?	-	SER	deletion	UNP P0DTC2
B	?	-	LYS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	435	ALA	ASN	engineered mutation	UNP P0DTC2
B	436	GLY	TYR	engineered mutation	UNP P0DTC2
B	439	TYR	LEU	engineered mutation	UNP P0DTC2
B	442	SER	LEU	engineered mutation	UNP P0DTC2
B	443	HIS	PHE	engineered mutation	UNP P0DTC2
B	446	THR	SER	engineered mutation	UNP P0DTC2
B	447	LYS	ASN	engineered mutation	UNP P0DTC2
B	455	LEU	ILE	engineered mutation	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	?	-	GLU	deletion	UNP P0DTC2
B	?	-	ILE	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	GLN	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	SER	deletion	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	CYS	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	457	ASN	VAL	engineered mutation	UNP P0DTC2
B	458	SER	GLU	engineered mutation	UNP P0DTC2
B	459	ASP	GLY	engineered mutation	UNP P0DTC2
B	460	GLU	PHE	engineered mutation	UNP P0DTC2
B	462	GLY	CYS	engineered mutation	UNP P0DTC2
B	463	VAL	TYR	engineered mutation	UNP P0DTC2
B	464	ARG	PHE	engineered mutation	UNP P0DTC2
B	465	THR	PRO	engineered mutation	UNP P0DTC2
B	467	SER	GLN	engineered mutation	UNP P0DTC2
B	468	THR	SER	engineered mutation	UNP P0DTC2
B	470	ASP	GLY	engineered mutation	UNP P0DTC2
B	472	ASN	GLN	engineered mutation	UNP P0DTC2
B	474	ASN	THR	engineered mutation	UNP P0DTC2
B	475	VAL	ASN	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	476	PRO	GLY	engineered mutation	UNP P0DTC2
B	477	ILE	VAL	engineered mutation	UNP P0DTC2
B	478	GLU	GLY	engineered mutation	UNP P0DTC2
B	481	ALA	PRO	engineered mutation	UNP P0DTC2
B	482	THR	TYR	engineered mutation	UNP P0DTC2
B	493	ASN	HIS	engineered mutation	UNP P0DTC2
B	503	LEU	LYS	engineered mutation	UNP P0DTC2
B	506	GLN	ASN	engineered mutation	UNP P0DTC2
B	511	GLN	LYS	engineered mutation	UNP P0DTC2
B	521	LYS	THR	engineered mutation	UNP P0DTC2
B	528	ASP	GLU	engineered mutation	UNP P0DTC2
B	530	SER	ASN	engineered mutation	UNP P0DTC2
B	532	ARG	LYS	engineered mutation	UNP P0DTC2
B	534	GLN	LEU	engineered mutation	UNP P0DTC2
B	535	SER	PRO	engineered mutation	UNP P0DTC2
B	543	ALA	ILE	engineered mutation	UNP P0DTC2
B	544	SER	ALA	engineered mutation	UNP P0DTC2
B	546	PHE	THR	engineered mutation	UNP P0DTC2
B	549	SER	ALA	engineered mutation	UNP P0DTC2
B	562	SER	THR	engineered mutation	UNP P0DTC2
B	578	ALA	THR	engineered mutation	UNP P0DTC2
B	580	SER	ASN	engineered mutation	UNP P0DTC2
B	581	GLU	GLN	engineered mutation	UNP P0DTC2
B	593	ASP	GLU	engineered mutation	UNP P0DTC2
B	596	THR	VAL	engineered mutation	UNP P0DTC2
B	606	ALA	THR	engineered mutation	UNP P0DTC2
B	614	VAL	SER	engineered mutation	UNP P0DTC2
B	620	GLN	ARG	engineered mutation	UNP P0DTC2
B	632	ALA	ASN	engineered mutation	UNP P0DTC2
B	649	HIS	GLN	engineered mutation	UNP P0DTC2
B	651	ALA	-	insertion	UNP P0DTC2
B	652	SER	GLN	conflict	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	654	LEU	ALA	engineered mutation	UNP P0DTC2
B	657	THR	VAL	engineered mutation	UNP P0DTC2
B	658	GLY	ALA	engineered mutation	UNP P0DTC2
B	659	GLN	SER	engineered mutation	UNP P0DTC2
B	660	LYS	GLN	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	663	VAL	ILE	engineered mutation	UNP P0DTC2
B	675	ILE	VAL	engineered mutation	UNP P0DTC2
B	678	ALA	SER	engineered mutation	UNP P0DTC2
B	689	SER	THR	engineered mutation	UNP P0DTC2
B	696	VAL	ILE	engineered mutation	UNP P0DTC2
B	697	MET	LEU	engineered mutation	UNP P0DTC2
B	702	ALA	THR	engineered mutation	UNP P0DTC2
B	717	GLN	THR	engineered mutation	UNP P0DTC2
B	742	ILE	VAL	engineered mutation	UNP P0DTC2
B	758	MET	ILE	engineered mutation	UNP P0DTC2
B	763	ALA	PRO	engineered mutation	UNP P0DTC2
B	783	THR	SER	engineered mutation	UNP P0DTC2
B	804	MET	ILE	engineered mutation	UNP P0DTC2
B	809	GLU	ASP	engineered mutation	UNP P0DTC2
B	815	SER	ALA	engineered mutation	UNP P0DTC2
B	842	ALA	GLN	engineered mutation	UNP P0DTC2
B	845	ALA	SER	engineered mutation	UNP P0DTC2
B	848	VAL	LEU	engineered mutation	UNP P0DTC2
B	849	SER	ALA	engineered mutation	UNP P0DTC2
B	852	ALA	ILE	engineered mutation	UNP P0DTC2
B	854	ALA	SER	engineered mutation	UNP P0DTC2
B	892	GLN	LEU	engineered mutation	UNP P0DTC2
B	899	LYS	SER	engineered mutation	UNP P0DTC2
B	902	SER	GLY	engineered mutation	UNP P0DTC2
B	903	GLN	LYS	engineered mutation	UNP P0DTC2
B	906	GLU	ASP	engineered mutation	UNP P0DTC2
B	909	THR	SER	engineered mutation	UNP P0DTC2
B	910	THR	SER	engineered mutation	UNP P0DTC2
B	912	SER	ALA	engineered mutation	UNP P0DTC2
B	913	THR	SER	engineered mutation	UNP P0DTC2
B	1025	ALA	SER	engineered mutation	UNP P0DTC2
B	1040	SER	ALA	engineered mutation	UNP P0DTC2
B	1043	ARG	LYS	engineered mutation	UNP P0DTC2
B	1054	GLU	ASP	engineered mutation	UNP P0DTC2
B	1058	TYR	HIS	engineered mutation	UNP P0DTC2
B	1071	SER	HIS	engineered mutation	UNP P0DTC2
B	1074	ILE	VAL	engineered mutation	UNP P0DTC2
B	1081	SER	GLU	engineered mutation	UNP P0DTC2
B	1093	ALA	SER	engineered mutation	UNP P0DTC2
B	1103	ILE	VAL	engineered mutation	UNP P0DTC2
B	1179	GLY	-	linker	UNP P0DTC2
B	1180	SER	-	linker	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1202	LEU	PHE	engineered mutation	UNP P10104
B	1208	GLY	-	expression tag	UNP P10104
B	1209	THR	-	expression tag	UNP P10104
B	1210	SER	-	expression tag	UNP P10104
B	1211	LEU	-	expression tag	UNP P10104
B	1212	GLU	-	expression tag	UNP P10104
B	1213	VAL	-	expression tag	UNP P10104
B	1214	LEU	-	expression tag	UNP P10104
B	1215	PHE	-	expression tag	UNP P10104
B	1216	GLN	-	expression tag	UNP P10104
B	1217	GLY	-	expression tag	UNP P10104
B	1218	PRO	-	expression tag	UNP P10104
B	1219	GLY	-	expression tag	UNP P10104
B	1220	HIS	-	expression tag	UNP P10104
B	1221	HIS	-	expression tag	UNP P10104
B	1222	HIS	-	expression tag	UNP P10104
B	1223	HIS	-	expression tag	UNP P10104
B	1224	HIS	-	expression tag	UNP P10104
B	1225	HIS	-	expression tag	UNP P10104
B	1226	HIS	-	expression tag	UNP P10104
B	1227	HIS	-	expression tag	UNP P10104
B	1228	SER	-	expression tag	UNP P10104
B	1229	ALA	-	expression tag	UNP P10104
B	1230	TRP	-	expression tag	UNP P10104
B	1231	SER	-	expression tag	UNP P10104
B	1232	HIS	-	expression tag	UNP P10104
B	1233	PRO	-	expression tag	UNP P10104
B	1234	GLN	-	expression tag	UNP P10104
B	1235	PHE	-	expression tag	UNP P10104
B	1236	GLU	-	expression tag	UNP P10104
B	1237	LYS	-	expression tag	UNP P10104
B	1238	GLY	-	expression tag	UNP P10104
B	1239	GLY	-	expression tag	UNP P10104
B	1240	GLY	-	expression tag	UNP P10104
B	1241	SER	-	expression tag	UNP P10104
B	1242	GLY	-	expression tag	UNP P10104
B	1243	GLY	-	expression tag	UNP P10104
B	1244	GLY	-	expression tag	UNP P10104
B	1245	GLY	-	expression tag	UNP P10104
B	1246	SER	-	expression tag	UNP P10104
B	1247	GLY	-	expression tag	UNP P10104
B	1248	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1249	SER	-	expression tag	UNP P10104
B	1250	ALA	-	expression tag	UNP P10104
B	1251	TRP	-	expression tag	UNP P10104
B	1252	SER	-	expression tag	UNP P10104
B	1253	HIS	-	expression tag	UNP P10104
B	1254	PRO	-	expression tag	UNP P10104
B	1255	GLN	-	expression tag	UNP P10104
B	1256	PHE	-	expression tag	UNP P10104
B	1257	GLU	-	expression tag	UNP P10104
B	1258	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	ILE	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
C	27	THR	LEU	engineered mutation	UNP P0DTC2
C	30	ASN	-	insertion	UNP P0DTC2
C	31	MET	-	insertion	UNP P0DTC2
C	32	ASN	ALA	engineered mutation	UNP P0DTC2
C	33	GLN	TYR	engineered mutation	UNP P0DTC2
C	34	PHE	THR	engineered mutation	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	69	ARG	-	insertion	UNP P0DTC2
C	70	TYR	TRP	engineered mutation	UNP P0DTC2
C	71	LEU	PHE	engineered mutation	UNP P0DTC2
C	72	SER	HIS	engineered mutation	UNP P0DTC2
C	73	LEU	ALA	engineered mutation	UNP P0DTC2
C	74	ASN	ILE	engineered mutation	UNP P0DTC2
C	75	ALA	HIS	engineered mutation	UNP P0DTC2
C	76	ASP	VAL	engineered mutation	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	91	GLY	ASN	engineered mutation	UNP P0DTC2
C	94	ILE	VAL	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	127	SER	ALA	engineered mutation	UNP P0DTC2
C	129	HIS	ASN	engineered mutation	UNP P0DTC2
C	130	ILE	VAL	engineered mutation	UNP P0DTC2
C	131	ILE	VAL	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	THR	GLY	engineered mutation	UNP P0DTC2
C	148	SER	TYR	engineered mutation	UNP P0DTC2
C	149	ARG	TYR	engineered mutation	UNP P0DTC2
C	150	GLY	HIS	engineered mutation	UNP P0DTC2
C	151	GLN	LYS	engineered mutation	UNP P0DTC2
C	152	HIS	ASN	engineered mutation	UNP P0DTC2
C	153	TYR	ASN	engineered mutation	UNP P0DTC2
C	155	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	THR	SER	engineered mutation	UNP P0DTC2
C	160	ASN	SER	engineered mutation	UNP P0DTC2
C	162	ARG	ASN	engineered mutation	UNP P0DTC2
C	166	TYR	PHE	engineered mutation	UNP P0DTC2
C	171	LYS	GLN	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	172	SER	PRO	engineered mutation	UNP P0DTC2
C	174	GLN	LEU	engineered mutation	UNP P0DTC2
C	175	LEU	MET	engineered mutation	UNP P0DTC2
C	177	VAL	LEU	engineered mutation	UNP P0DTC2
C	178	SER	GLU	engineered mutation	UNP P0DTC2
C	179	GLU	GLY	engineered mutation	UNP P0DTC2
C	181	ASN	GLN	engineered mutation	UNP P0DTC2
C	186	HIS	ASN	engineered mutation	UNP P0DTC2
C	195	VAL	ILE	engineered mutation	UNP P0DTC2
C	198	PHE	TYR	engineered mutation	UNP P0DTC2
C	199	LEU	PHE	engineered mutation	UNP P0DTC2
C	200	HIS	LYS	engineered mutation	UNP P0DTC2
C	201	VAL	ILE	engineered mutation	UNP P0DTC2
C	204	ALA	LYS	engineered mutation	UNP P0DTC2
C	205	TYR	HIS	engineered mutation	UNP P0DTC2
C	206	GLU	THR	engineered mutation	UNP P0DTC2
C	209	ASP	ASN	engineered mutation	UNP P0DTC2
C	211	ALA	VAL	engineered mutation	UNP P0DTC2
C	213	GLY	ASP	engineered mutation	UNP P0DTC2
C	216	SER	GLN	engineered mutation	UNP P0DTC2
C	220	VAL	ALA	engineered mutation	UNP P0DTC2
C	222	LYS	GLU	engineered mutation	UNP P0DTC2
C	224	ILE	LEU	engineered mutation	UNP P0DTC2
C	225	LEU	VAL	engineered mutation	UNP P0DTC2
C	226	LYS	ASP	engineered mutation	UNP P0DTC2
C	229	LEU	ILE	engineered mutation	UNP P0DTC2
C	235	SER	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	238	VAL	SER	engineered mutation	UNP P0DTC2
C	239	VAL	TYR	engineered mutation	UNP P0DTC2
C	240	MET	LEU	engineered mutation	UNP P0DTC2
C	242	MET	-	insertion	UNP P0DTC2
C	243	PHE	PRO	engineered mutation	UNP P0DTC2
C	244	SER	GLY	engineered mutation	UNP P0DTC2
C	245	PRO	ASP	engineered mutation	UNP P0DTC2
C	246	THR	SER	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	247	THR	SER	engineered mutation	UNP P0DTC2
C	249	ASN	GLY	engineered mutation	UNP P0DTC2
C	251	LEU	THR	engineered mutation	UNP P0DTC2
C	253	GLU	GLY	engineered mutation	UNP P0DTC2
C	254	SER	ALA	engineered mutation	UNP P0DTC2
C	258	PHE	TYR	engineered mutation	UNP P0DTC2
C	263	LYS	GLN	engineered mutation	UNP P0DTC2
C	265	THR	ARG	engineered mutation	UNP P0DTC2
C	268	MET	LEU	engineered mutation	UNP P0DTC2
C	271	PHE	TYR	engineered mutation	UNP P0DTC2
C	284	SER	ALA	engineered mutation	UNP P0DTC2
C	285	GLN	LEU	engineered mutation	UNP P0DTC2
C	291	LEU	THR	engineered mutation	UNP P0DTC2
C	299	ASN	THR	engineered mutation	UNP P0DTC2
C	313	SER	GLN	engineered mutation	UNP P0DTC2
C	316	GLN	GLU	engineered mutation	UNP P0DTC2
C	317	GLU	SER	engineered mutation	UNP P0DTC2
C	318	VAL	ILE	engineered mutation	UNP P0DTC2
C	331	ASP	GLY	engineered mutation	UNP P0DTC2
C	332	LYS	GLU	engineered mutation	UNP P0DTC2
C	340	PRO	ALA	engineered mutation	UNP P0DTC2
C	346	GLU	ASN	engineered mutation	UNP P0DTC2
C	348	THR	LYS	engineered mutation	UNP P0DTC2
C	349	LYS	ARG	engineered mutation	UNP P0DTC2
C	352	ASP	ASN	engineered mutation	UNP P0DTC2
C	358	THR	SER	engineered mutation	UNP P0DTC2
C	364	THR	ALA	engineered mutation	UNP P0DTC2
C	377	SER	THR	engineered mutation	UNP P0DTC2
C	380	ILE	ASN	engineered mutation	UNP P0DTC2
C	386	SER	ASN	engineered mutation	UNP P0DTC2
C	391	THR	SER	engineered mutation	UNP P0DTC2
C	393	LEU	VAL	engineered mutation	UNP P0DTC2
C	396	SER	GLY	engineered mutation	UNP P0DTC2
C	397	SER	ASP	engineered mutation	UNP P0DTC2
C	402	VAL	ILE	engineered mutation	UNP P0DTC2
C	409	VAL	LYS	engineered mutation	UNP P0DTC2
C	430	THR	SER	engineered mutation	UNP P0DTC2
C	431	ALA	ASN	engineered mutation	UNP P0DTC2
C	432	LYS	ASN	engineered mutation	UNP P0DTC2
C	433	GLN	LEU	engineered mutation	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	?	-	LYS	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	435	ALA	ASN	engineered mutation	UNP P0DTC2
C	436	GLY	TYR	engineered mutation	UNP P0DTC2
C	439	TYR	LEU	engineered mutation	UNP P0DTC2
C	442	SER	LEU	engineered mutation	UNP P0DTC2
C	443	HIS	PHE	engineered mutation	UNP P0DTC2
C	446	THR	SER	engineered mutation	UNP P0DTC2
C	447	LYS	ASN	engineered mutation	UNP P0DTC2
C	455	LEU	ILE	engineered mutation	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	GLU	deletion	UNP P0DTC2
C	?	-	ILE	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	GLN	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	CYS	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	457	ASN	VAL	engineered mutation	UNP P0DTC2
C	458	SER	GLU	engineered mutation	UNP P0DTC2
C	459	ASP	GLY	engineered mutation	UNP P0DTC2
C	460	GLU	PHE	engineered mutation	UNP P0DTC2
C	462	GLY	CYS	engineered mutation	UNP P0DTC2
C	463	VAL	TYR	engineered mutation	UNP P0DTC2
C	464	ARG	PHE	engineered mutation	UNP P0DTC2
C	465	THR	PRO	engineered mutation	UNP P0DTC2
C	467	SER	GLN	engineered mutation	UNP P0DTC2
C	468	THR	SER	engineered mutation	UNP P0DTC2
C	470	ASP	GLY	engineered mutation	UNP P0DTC2
C	472	ASN	GLN	engineered mutation	UNP P0DTC2
C	474	ASN	THR	engineered mutation	UNP P0DTC2
C	475	VAL	ASN	engineered mutation	UNP P0DTC2
C	476	PRO	GLY	engineered mutation	UNP P0DTC2
C	477	ILE	VAL	engineered mutation	UNP P0DTC2
C	478	GLU	GLY	engineered mutation	UNP P0DTC2
C	481	ALA	PRO	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	482	THR	TYR	engineered mutation	UNP P0DTC2
C	493	ASN	HIS	engineered mutation	UNP P0DTC2
C	503	LEU	LYS	engineered mutation	UNP P0DTC2
C	506	GLN	ASN	engineered mutation	UNP P0DTC2
C	511	GLN	LYS	engineered mutation	UNP P0DTC2
C	521	LYS	THR	engineered mutation	UNP P0DTC2
C	528	ASP	GLU	engineered mutation	UNP P0DTC2
C	530	SER	ASN	engineered mutation	UNP P0DTC2
C	532	ARG	LYS	engineered mutation	UNP P0DTC2
C	534	GLN	LEU	engineered mutation	UNP P0DTC2
C	535	SER	PRO	engineered mutation	UNP P0DTC2
C	543	ALA	ILE	engineered mutation	UNP P0DTC2
C	544	SER	ALA	engineered mutation	UNP P0DTC2
C	546	PHE	THR	engineered mutation	UNP P0DTC2
C	549	SER	ALA	engineered mutation	UNP P0DTC2
C	562	SER	THR	engineered mutation	UNP P0DTC2
C	578	ALA	THR	engineered mutation	UNP P0DTC2
C	580	SER	ASN	engineered mutation	UNP P0DTC2
C	581	GLU	GLN	engineered mutation	UNP P0DTC2
C	593	ASP	GLU	engineered mutation	UNP P0DTC2
C	596	THR	VAL	engineered mutation	UNP P0DTC2
C	606	ALA	THR	engineered mutation	UNP P0DTC2
C	614	VAL	SER	engineered mutation	UNP P0DTC2
C	620	GLN	ARG	engineered mutation	UNP P0DTC2
C	632	ALA	ASN	engineered mutation	UNP P0DTC2
C	649	HIS	GLN	engineered mutation	UNP P0DTC2
C	651	ALA	-	insertion	UNP P0DTC2
C	652	SER	GLN	conflict	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	654	LEU	ALA	engineered mutation	UNP P0DTC2
C	657	THR	VAL	engineered mutation	UNP P0DTC2
C	658	GLY	ALA	engineered mutation	UNP P0DTC2
C	659	GLN	SER	engineered mutation	UNP P0DTC2
C	660	LYS	GLN	engineered mutation	UNP P0DTC2
C	663	VAL	ILE	engineered mutation	UNP P0DTC2
C	675	ILE	VAL	engineered mutation	UNP P0DTC2
C	678	ALA	SER	engineered mutation	UNP P0DTC2
C	689	SER	THR	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	696	VAL	ILE	engineered mutation	UNP P0DTC2
C	697	MET	LEU	engineered mutation	UNP P0DTC2
C	702	ALA	THR	engineered mutation	UNP P0DTC2
C	717	GLN	THR	engineered mutation	UNP P0DTC2
C	742	ILE	VAL	engineered mutation	UNP P0DTC2
C	758	MET	ILE	engineered mutation	UNP P0DTC2
C	763	ALA	PRO	engineered mutation	UNP P0DTC2
C	783	THR	SER	engineered mutation	UNP P0DTC2
C	804	MET	ILE	engineered mutation	UNP P0DTC2
C	809	GLU	ASP	engineered mutation	UNP P0DTC2
C	815	SER	ALA	engineered mutation	UNP P0DTC2
C	842	ALA	GLN	engineered mutation	UNP P0DTC2
C	845	ALA	SER	engineered mutation	UNP P0DTC2
C	848	VAL	LEU	engineered mutation	UNP P0DTC2
C	849	SER	ALA	engineered mutation	UNP P0DTC2
C	852	ALA	ILE	engineered mutation	UNP P0DTC2
C	854	ALA	SER	engineered mutation	UNP P0DTC2
C	892	GLN	LEU	engineered mutation	UNP P0DTC2
C	899	LYS	SER	engineered mutation	UNP P0DTC2
C	902	SER	GLY	engineered mutation	UNP P0DTC2
C	903	GLN	LYS	engineered mutation	UNP P0DTC2
C	906	GLU	ASP	engineered mutation	UNP P0DTC2
C	909	THR	SER	engineered mutation	UNP P0DTC2
C	910	THR	SER	engineered mutation	UNP P0DTC2
C	912	SER	ALA	engineered mutation	UNP P0DTC2
C	913	THR	SER	engineered mutation	UNP P0DTC2
C	1025	ALA	SER	engineered mutation	UNP P0DTC2
C	1040	SER	ALA	engineered mutation	UNP P0DTC2
C	1043	ARG	LYS	engineered mutation	UNP P0DTC2
C	1054	GLU	ASP	engineered mutation	UNP P0DTC2
C	1058	TYR	HIS	engineered mutation	UNP P0DTC2
C	1071	SER	HIS	engineered mutation	UNP P0DTC2
C	1074	ILE	VAL	engineered mutation	UNP P0DTC2
C	1081	SER	GLU	engineered mutation	UNP P0DTC2
C	1093	ALA	SER	engineered mutation	UNP P0DTC2
C	1103	ILE	VAL	engineered mutation	UNP P0DTC2
C	1179	GLY	-	linker	UNP P0DTC2
C	1180	SER	-	linker	UNP P0DTC2
C	1202	LEU	PHE	engineered mutation	UNP P10104
C	1208	GLY	-	expression tag	UNP P10104
C	1209	THR	-	expression tag	UNP P10104
C	1210	SER	-	expression tag	UNP P10104

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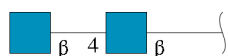
Chain	Residue	Modelled	Actual	Comment	Reference
C	1211	LEU	-	expression tag	UNP P10104
C	1212	GLU	-	expression tag	UNP P10104
C	1213	VAL	-	expression tag	UNP P10104
C	1214	LEU	-	expression tag	UNP P10104
C	1215	PHE	-	expression tag	UNP P10104
C	1216	GLN	-	expression tag	UNP P10104
C	1217	GLY	-	expression tag	UNP P10104
C	1218	PRO	-	expression tag	UNP P10104
C	1219	GLY	-	expression tag	UNP P10104
C	1220	HIS	-	expression tag	UNP P10104
C	1221	HIS	-	expression tag	UNP P10104
C	1222	HIS	-	expression tag	UNP P10104
C	1223	HIS	-	expression tag	UNP P10104
C	1224	HIS	-	expression tag	UNP P10104
C	1225	HIS	-	expression tag	UNP P10104
C	1226	HIS	-	expression tag	UNP P10104
C	1227	HIS	-	expression tag	UNP P10104
C	1228	SER	-	expression tag	UNP P10104
C	1229	ALA	-	expression tag	UNP P10104
C	1230	TRP	-	expression tag	UNP P10104
C	1231	SER	-	expression tag	UNP P10104
C	1232	HIS	-	expression tag	UNP P10104
C	1233	PRO	-	expression tag	UNP P10104
C	1234	GLN	-	expression tag	UNP P10104
C	1235	PHE	-	expression tag	UNP P10104
C	1236	GLU	-	expression tag	UNP P10104
C	1237	LYS	-	expression tag	UNP P10104
C	1238	GLY	-	expression tag	UNP P10104
C	1239	GLY	-	expression tag	UNP P10104
C	1240	GLY	-	expression tag	UNP P10104
C	1241	SER	-	expression tag	UNP P10104
C	1242	GLY	-	expression tag	UNP P10104
C	1243	GLY	-	expression tag	UNP P10104
C	1244	GLY	-	expression tag	UNP P10104
C	1245	GLY	-	expression tag	UNP P10104
C	1246	SER	-	expression tag	UNP P10104
C	1247	GLY	-	expression tag	UNP P10104
C	1248	GLY	-	expression tag	UNP P10104
C	1249	SER	-	expression tag	UNP P10104
C	1250	ALA	-	expression tag	UNP P10104
C	1251	TRP	-	expression tag	UNP P10104
C	1252	SER	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1253	HIS	-	expression tag	UNP P10104
C	1254	PRO	-	expression tag	UNP P10104
C	1255	GLN	-	expression tag	UNP P10104
C	1256	PHE	-	expression tag	UNP P10104
C	1257	GLU	-	expression tag	UNP P10104
C	1258	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	0	0
			55	16	27	2	10		
2	M	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	N	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	P	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	Q	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	R	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	T	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	U	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
2	V	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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


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

GLY THR SER LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS SER SER TRP SER HIS PRO PHE PHE GLU LYS GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 1: Spike glycoprotein,Fibritin

Chain C:  85% 12%

T19 N25 R39 R49 V67 N78 R79 V134 C135 F145 T155 N163 I208 D209 P215 L229 T241 T247 F258 G275 R320 R347 F366 K531 Q537 R551 T612 G613 T619 Q620 A621 T644 T650 ALA

SER THR ARG THR GLY Q639 L733 L740 Q774 F782 K795 A799 D800 A801 R875 S912 D920 V921 V978 L982 L1019 D1116 SER PHE LYS GLU LEU LEU ASP TYR PHE LYS ASN THR THR SER PRO ASP VAL ASP LEU ASP ILE

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

TRP VAL LEU LEU SER THR PHE LEU GLY THR SER LEU GLU VAL LEU PHE GLY GLN PRO GLY HIS HIS HIS HIS HIS HIS SER LEU TRP SER HIS PRO PHE PHE GLU LYS

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

Chain L:  50% 50%

MAG1
MAG2

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

Chain M:  50% 50%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain P:  50% 50%

MAG1
MAG2

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

Chain Q:  50% 50%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

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

Chain U:  50% 50%

MAG1
MAG2

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

Chain V:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	959111	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 ($e^-/\text{\AA}^2$)	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	5.736	Depositor
Minimum map value	-3.350	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.27	Depositor
Map size (\AA)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/8683	0.55	0/11815
1	B	0.33	0/8683	0.55	0/11815
1	C	0.33	0/8683	0.54	0/11815
All	All	0.33	0/26049	0.55	0/35445

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	3
1	C	0	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ARG	Sidechain
1	A	347	ARG	Sidechain
1	A	586	TYR	Peptide
1	B	320	ARG	Sidechain
1	B	347	ARG	Sidechain
1	B	400	ARG	Sidechain
1	C	320	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	347	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	8495	8290	8282	32	0
1	B	8495	8290	8282	34	0
1	C	8495	8290	8282	26	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	T	28	27	25	0	0
2	U	28	27	25	0	0
2	V	28	27	25	1	0
3	A	182	182	169	3	0
3	B	182	182	169	2	0
3	C	182	182	169	2	0
All	All	26283	25659	25578	95	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 (95) 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:A:1302:NAG:O3	3:A:1302:NAG:O7	2.04	0.75
1:B:732:GLN:OE1	1:B:735:ARG:NH1	2.28	0.66
1:B:726:TYR:OH	1:B:964:ASP:OD1	2.14	0.65
1:B:400:ARG:NH1	1:C:366:PHE:O	2.28	0.65
1:A:103:ASN:ND2	1:A:176:ASP:O	2.30	0.62
1:A:732:GLN:OE1	1:A:735:ARG:NH1	2.33	0.61
1:B:76:ASP:O	1:B:79:ARG:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:HB2	3:A:1302:NAG:H82	1.82	0.61
1:C:39:ARG:NH2	1:C:215:PRO:O	2.33	0.56
1:C:134:VAL:CG2	1:C:229:LEU:HD22	2.36	0.55
1:C:537:GLN:O	1:C:551:ARG:NH1	2.40	0.55
1:A:537:GLN:O	1:A:551:ARG:NH1	2.40	0.54
1:A:740:ILE:HD11	1:A:982:LEU:HD23	1.89	0.54
1:A:145:PHE:HB2	1:A:241:THR:HG22	1.89	0.54
1:A:1084:ILE:O	1:A:1089:ASN:ND2	2.41	0.54
1:C:619:THR:HG22	1:C:621:ALA:H	1.74	0.53
1:B:39:ARG:NH2	1:B:215:PRO:O	2.40	0.53
1:C:145:PHE:HB2	1:C:241:THR:HG22	1.90	0.52
1:A:619:THR:HG23	1:A:644:ILE:HG13	1.90	0.52
1:C:875:ARG:NH1	1:C:1019:LEU:O	2.40	0.52
1:B:619:THR:HG22	1:B:621:ALA:H	1.75	0.52
1:B:246:THR:O	1:B:246:THR:HG22	2.09	0.51
1:B:619:THR:HG23	1:B:644:ILE:HG13	1.92	0.51
1:A:177:VAL:O	1:A:177:VAL:HG12	2.11	0.51
1:C:619:THR:HG23	1:C:644:ILE:HG13	1.93	0.50
1:B:34:PHE:CE1	1:B:69:ARG:HD2	2.47	0.50
1:C:135:CYS:HA	1:C:163:ASN:O	2.12	0.50
1:C:740:ILE:HD11	1:C:982:LEU:HD23	1.95	0.49
1:A:38:ARG:HA	1:A:63:PHE:CD1	2.47	0.49
3:C:1302:NAG:O7	3:C:1302:NAG:O3	2.24	0.49
1:A:814:ILE:HD13	1:C:531:LYS:HD2	1.95	0.48
1:C:920:ASP:OD1	1:C:921:VAL:N	2.46	0.48
1:B:49:ARG:O	1:B:275:GLY:HA2	2.14	0.48
1:A:39:ARG:NH2	1:A:215:PRO:O	2.41	0.48
1:B:740:ILE:HD11	1:B:982:LEU:HD23	1.95	0.48
1:A:920:ASP:OD1	1:A:921:VAL:N	2.47	0.47
1:A:34:PHE:CE1	1:A:69:ARG:HD2	2.49	0.47
1:A:873:ALA:HB2	1:A:886:LEU:HD23	1.96	0.47
1:B:145:PHE:HB2	1:B:241:THR:HG22	1.97	0.47
1:A:247:THR:HG22	1:A:247:THR:O	2.14	0.47
1:B:38:ARG:HA	1:B:63:PHE:CD1	2.50	0.46
1:C:134:VAL:CG2	1:C:229:LEU:CD2	2.93	0.46
1:B:750:GLU:OE2	1:B:993:ASN:ND2	2.48	0.46
1:B:949:ASP:OD1	1:B:953:ARG:NH2	2.45	0.46
1:C:612:THR:HG22	1:C:613:GLY:N	2.30	0.46
1:C:247:THR:HG22	1:C:247:THR:O	2.15	0.46
1:A:509:LYS:NZ	1:A:528:ASP:OD1	2.42	0.46
1:A:619:THR:HG22	1:A:621:ALA:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:THR:O	1:A:547:THR:HG23	2.16	0.45
3:B:1302:NAG:O7	3:B:1302:NAG:O3	2.31	0.45
1:C:134:VAL:HG21	1:C:229:LEU:CD2	2.46	0.45
1:B:828:LEU:HD12	1:B:933:VAL:CG1	2.46	0.45
1:B:475:VAL:HG13	1:B:476:PRO:HD2	1.99	0.45
1:A:191:VAL:HG23	1:A:221:LEU:HD12	1.99	0.44
3:B:1303:NAG:O7	3:B:1303:NAG:O3	2.31	0.44
1:C:134:VAL:HG21	1:C:229:LEU:HD22	1.98	0.44
1:A:208:ILE:HG12	1:A:209:ASP:N	2.33	0.44
1:B:103:ASN:ND2	1:B:176:ASP:O	2.50	0.44
1:B:429:ASN:HA	1:B:482:THR:HG22	2.00	0.44
1:A:135:CYS:HB3	1:A:161:ALA:O	2.18	0.43
1:B:145:PHE:CE2	1:B:155:THR:HG22	2.52	0.43
1:C:145:PHE:CE2	1:C:155:THR:HG22	2.54	0.43
1:A:875:ARG:NH1	1:A:1019:LEU:O	2.49	0.43
1:A:694:THR:HG23	1:A:1031:VAL:CG1	2.49	0.43
1:A:873:ALA:HB1	1:A:883:GLN:HG3	2.00	0.43
1:B:453:ARG:HD3	1:B:455:LEU:HD21	2.00	0.43
1:A:376:PRO:HA	1:A:379:LEU:HD13	2.00	0.42
1:A:1072:TRP:CZ2	1:A:1103:ILE:HD13	2.54	0.42
1:B:191:VAL:HG23	1:B:221:LEU:HD12	1.99	0.42
1:A:475:VAL:HG13	1:A:476:PRO:HD2	2.00	0.42
1:A:679:ASN:ND2	3:A:1307:NAG:O7	2.52	0.42
1:C:774:GLN:OE1	2:V:1:NAG:O6	2.30	0.42
1:B:761:THR:HG21	1:B:777:PRO:HD2	2.01	0.42
1:C:67:VAL:CG1	1:C:258:PHE:HB3	2.49	0.42
1:C:208:ILE:HG12	1:C:209:ASP:N	2.35	0.42
1:A:357:TYR:HE2	1:A:361:TYR:HH	1.63	0.42
1:B:135:CYS:HA	1:B:163:ASN:O	2.19	0.42
1:B:873:ALA:HB1	1:B:883:GLN:HG3	2.01	0.41
1:C:733:LEU:HD22	1:C:978:VAL:HG21	2.03	0.41
1:B:875:ARG:NH1	1:B:1019:LEU:O	2.50	0.41
1:B:694:THR:HG23	1:B:1031:VAL:CG1	2.51	0.41
1:B:1057:ALA:HB2	1:B:1096:CYS:HA	2.03	0.41
1:B:351:SER:HA	1:B:497:THR:HG22	2.02	0.41
1:B:109:ILE:HD13	1:B:139:LEU:HD22	2.03	0.41
1:B:795:LYS:HE3	1:B:908:LEU:O	2.21	0.41
1:B:920:ASP:OD1	1:B:921:VAL:N	2.54	0.41
1:C:795:LYS:HD2	1:C:912:SER:HA	2.03	0.41
1:C:145:PHE:CD2	1:C:155:THR:HG22	2.56	0.41
1:A:67:VAL:CG1	1:A:258:PHE:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1072:TRP:CZ2	1:B:1103:ILE:HD13	2.56	0.41
1:C:67:VAL:HG11	1:C:258:PHE:HB3	2.03	0.41
1:B:1112:GLN:HB3	1:B:1113:PRO:HD3	2.04	0.40
1:C:49:ARG:O	1:C:275:GLY:HA2	2.21	0.40
3:C:1304:NAG:H3	3:C:1304:NAG:O7	2.20	0.40
1:A:36:SER:CB	1:A:61:LEU:HD21	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1086/1240 (88%)	1039 (96%)	47 (4%)	0	100	100
1	B	1086/1240 (88%)	1040 (96%)	46 (4%)	0	100	100
1	C	1086/1240 (88%)	1047 (96%)	39 (4%)	0	100	100
All	All	3258/3720 (88%)	3126 (96%)	132 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	950/1073 (88%)	950 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	950/1073 (88%)	950 (100%)	0	100	100
1	C	950/1073 (88%)	950 (100%)	0	100	100
All	All	2850/3219 (88%)	2850 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	2,1	14,14,15	0.19	0	17,19,21	0.71	0
2	NAG	L	2	2	14,14,15	0.30	0	17,19,21	1.18	1 (5%)
2	NAG	M	1	2,1	14,14,15	0.37	0	17,19,21	0.54	0
2	NAG	M	2	2	14,14,15	0.15	0	17,19,21	0.67	1 (5%)
2	NAG	N	1	2,1	14,14,15	0.81	1 (7%)	17,19,21	1.43	2 (11%)
2	NAG	N	2	2	14,14,15	0.21	0	17,19,21	0.90	1 (5%)
2	NAG	P	1	2,1	14,14,15	0.32	0	17,19,21	0.68	0
2	NAG	P	2	2	14,14,15	0.26	0	17,19,21	0.97	1 (5%)
2	NAG	Q	1	2,1	14,14,15	0.43	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Q	2	2	14,14,15	0.26	0	17,19,21	0.78	1 (5%)
2	NAG	R	1	2,1	14,14,15	0.91	1 (7%)	17,19,21	1.33	1 (5%)
2	NAG	R	2	2	14,14,15	0.18	0	17,19,21	0.70	1 (5%)
2	NAG	T	1	2,1	14,14,15	0.20	0	17,19,21	0.60	0
2	NAG	T	2	2	14,14,15	0.17	0	17,19,21	1.03	1 (5%)
2	NAG	U	1	2,1	14,14,15	0.51	0	17,19,21	0.57	0
2	NAG	U	2	2	14,14,15	0.23	0	17,19,21	0.78	1 (5%)
2	NAG	V	1	2,1	14,14,15	0.84	1 (7%)	17,19,21	1.37	1 (5%)
2	NAG	V	2	2	14,14,15	0.15	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	2,1	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	NAG	V	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	1	NAG	O5-C1	3.18	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	1	NAG	O5-C1	2.84	1.48	1.43
2	N	1	NAG	O5-C1	2.82	1.48	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	1	NAG	C1-O5-C5	5.13	119.15	112.19
2	R	1	NAG	C1-O5-C5	4.99	118.95	112.19
2	N	1	NAG	C1-O5-C5	4.97	118.93	112.19
2	L	2	NAG	C1-O5-C5	4.61	118.44	112.19
2	T	2	NAG	C1-O5-C5	3.92	117.50	112.19
2	P	2	NAG	C1-O5-C5	3.50	116.93	112.19
2	N	2	NAG	C1-O5-C5	3.42	116.82	112.19
2	U	2	NAG	C1-O5-C5	2.96	116.20	112.19
2	Q	2	NAG	C1-O5-C5	2.94	116.18	112.19
2	V	2	NAG	C1-O5-C5	2.75	115.92	112.19
2	R	2	NAG	C1-O5-C5	2.49	115.56	112.19
2	M	2	NAG	C1-O5-C5	2.44	115.50	112.19
2	N	1	NAG	O4-C4-C5	2.04	114.36	109.30

There are no chirality outliers.

All (18) torsion outliers are listed below:

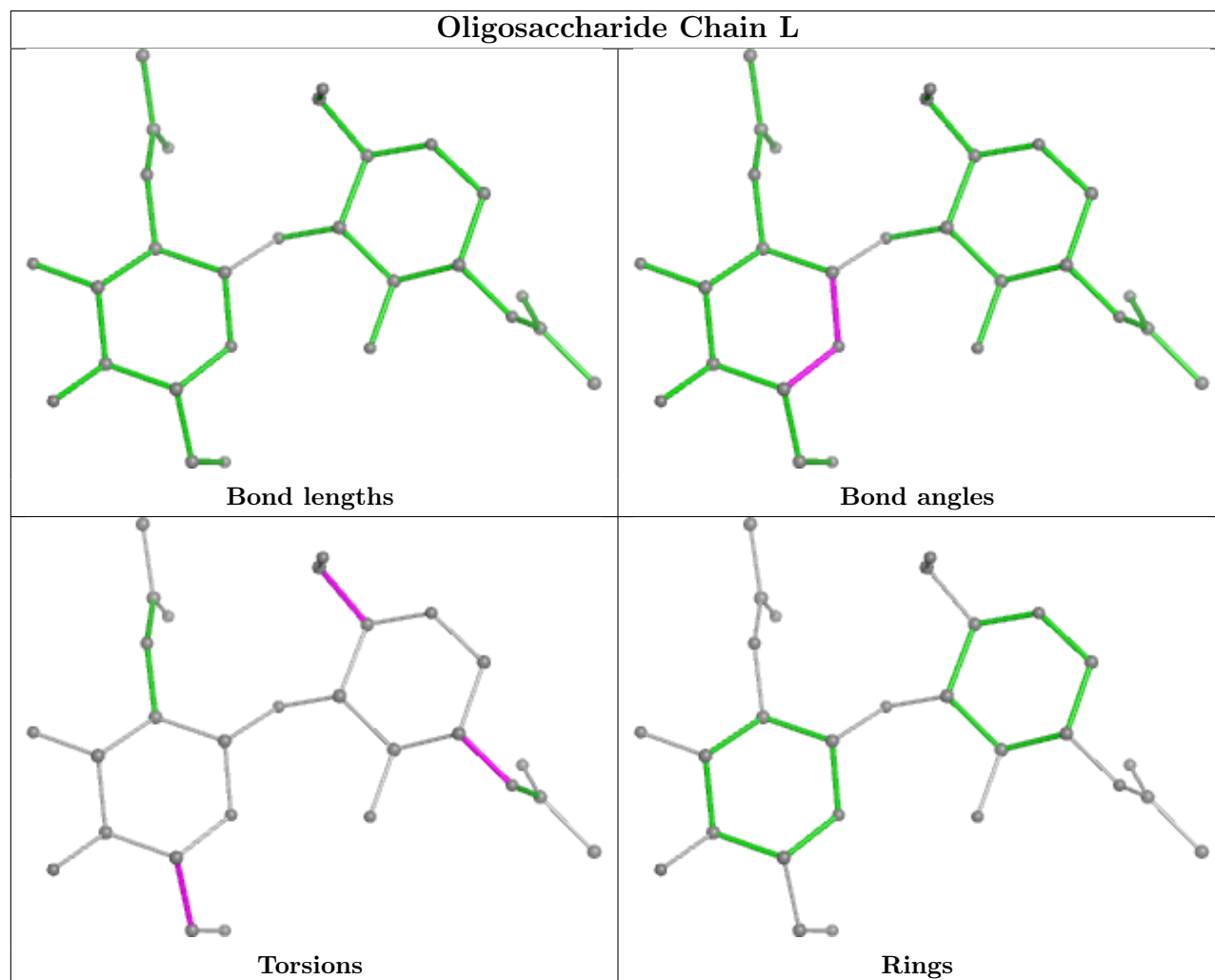
Mol	Chain	Res	Type	Atoms
2	M	2	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	L	1	NAG	C3-C2-N2-C7
2	T	1	NAG	C3-C2-N2-C7
2	P	1	NAG	C1-C2-N2-C7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

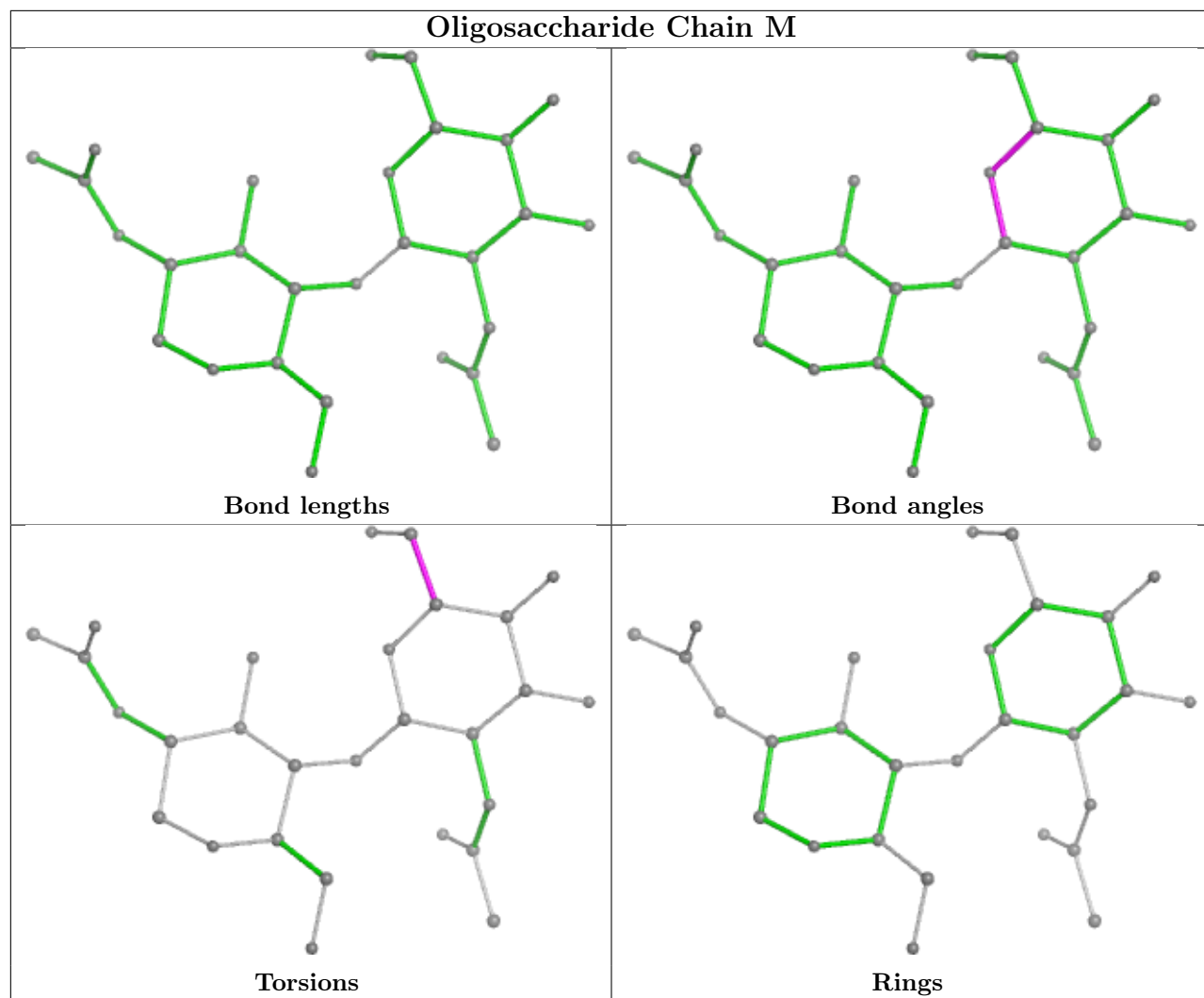
There are no ring outliers.

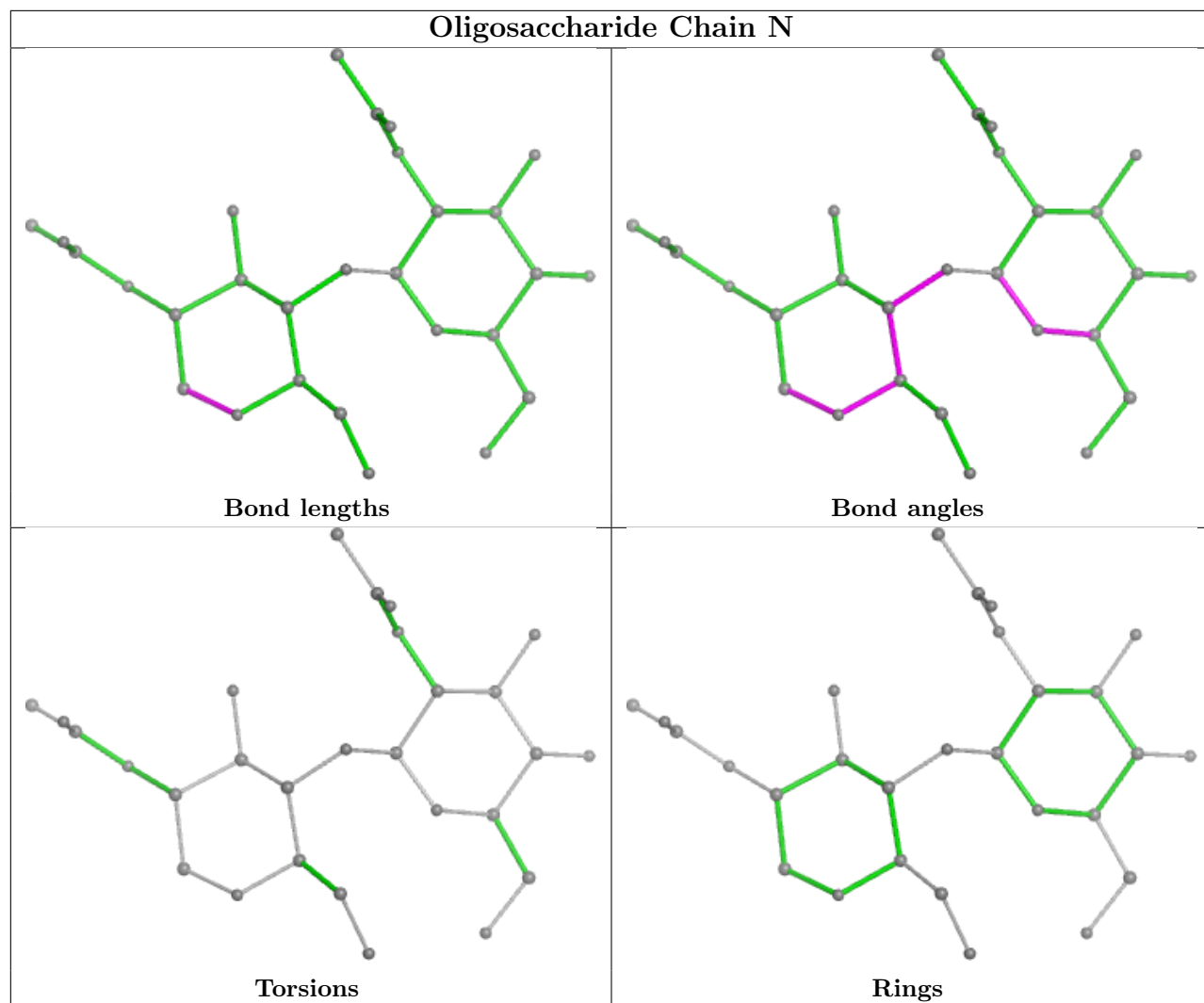
1 monomer is involved in 1 short contact:

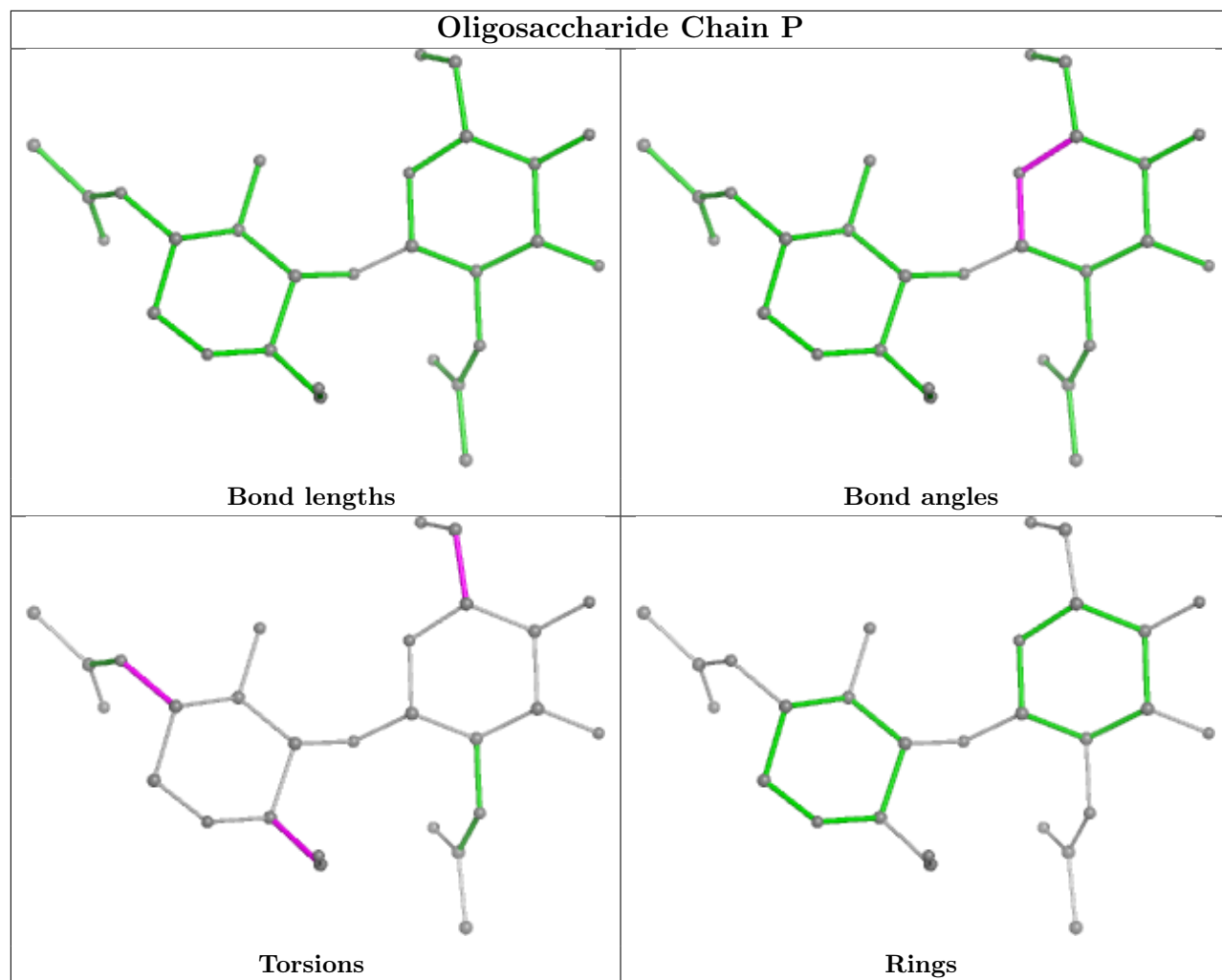
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	1	NAG	1	0

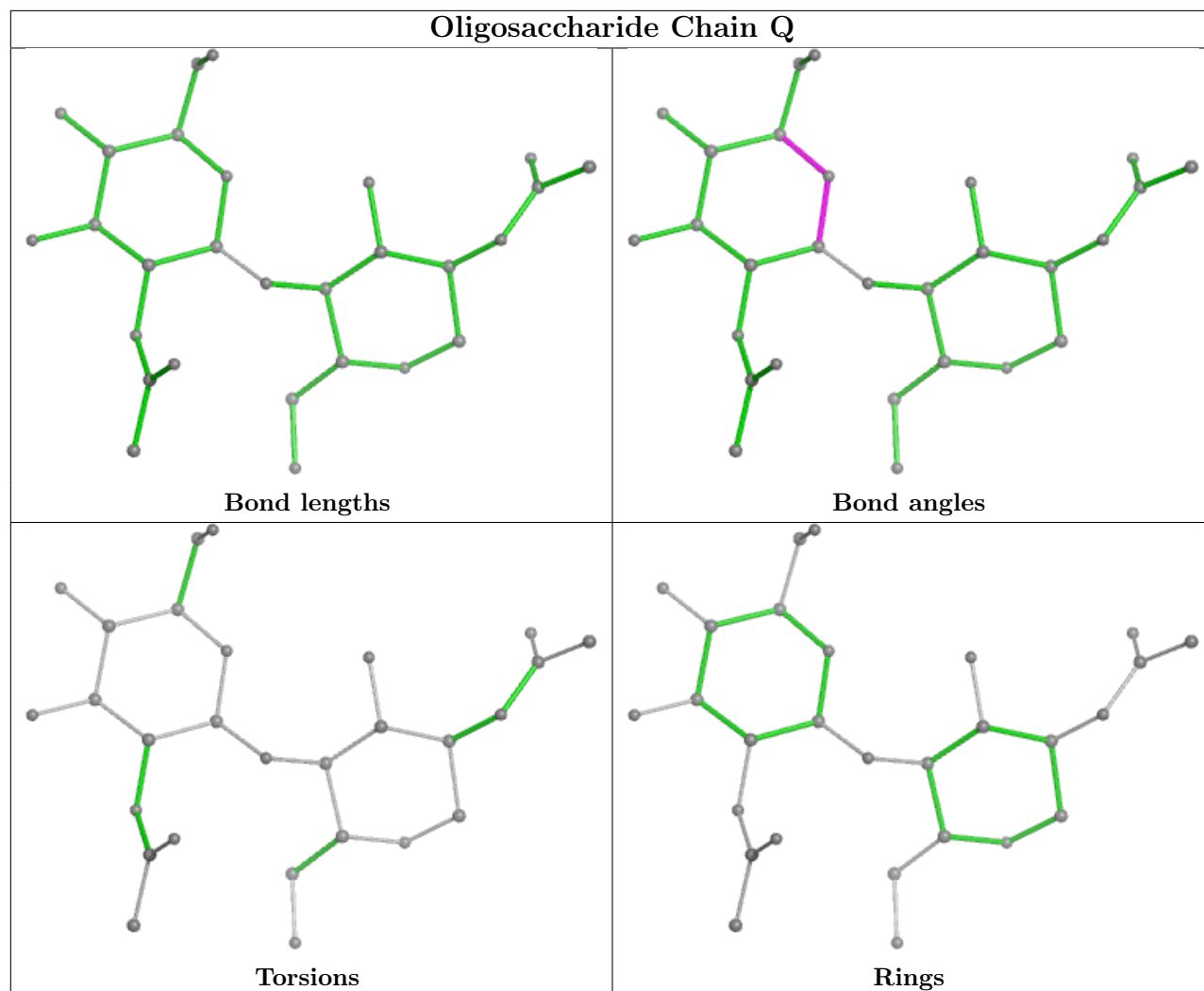
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

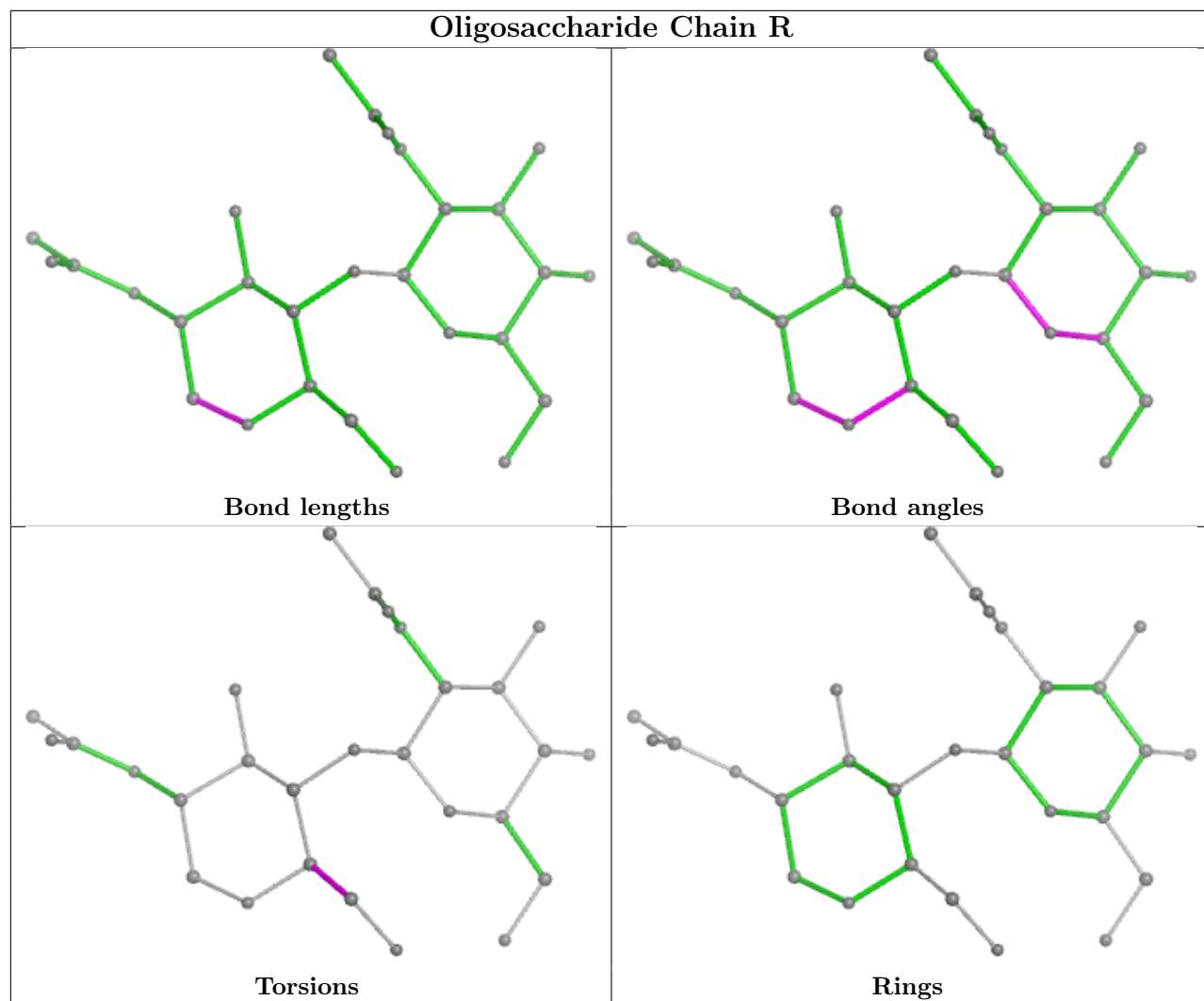


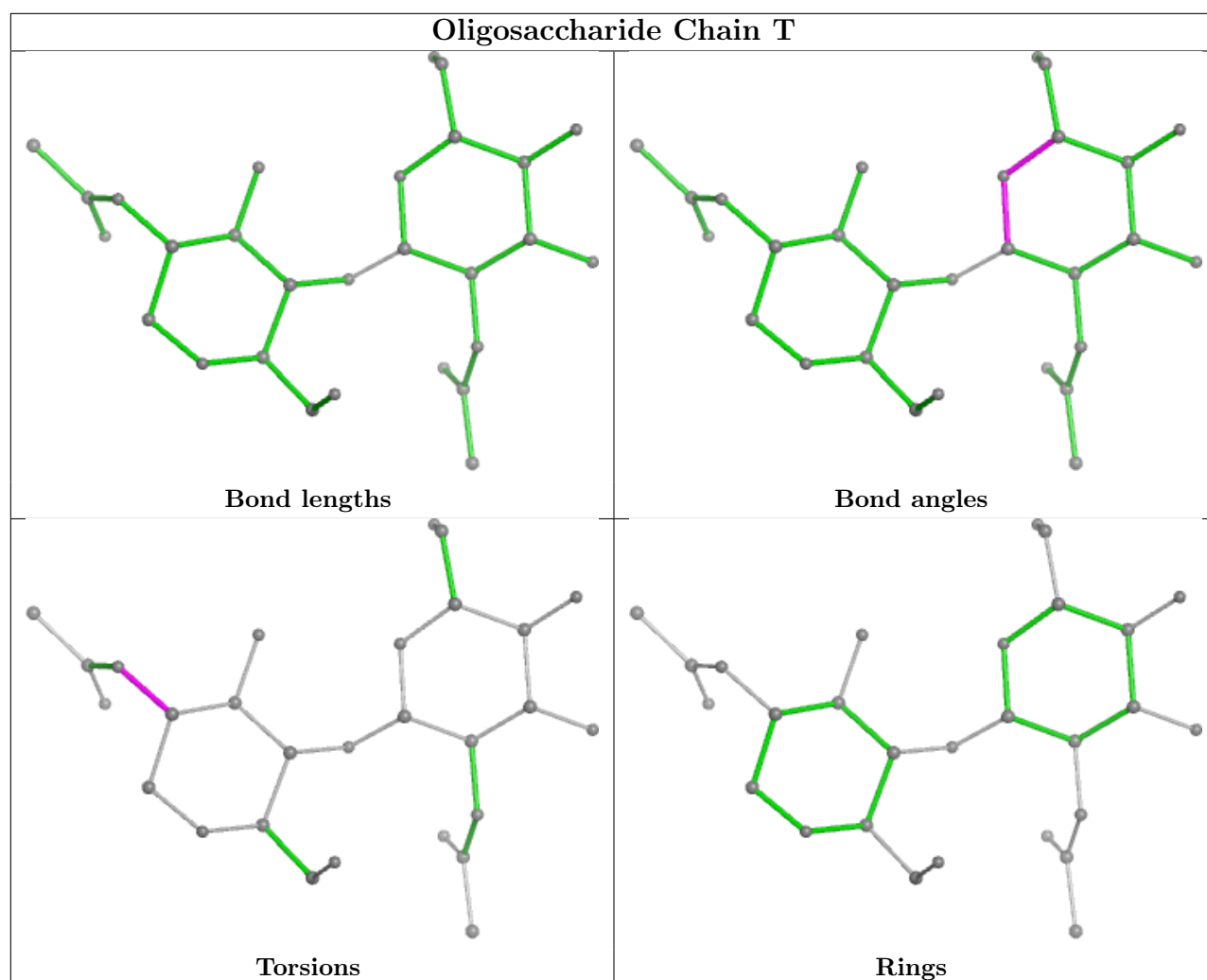


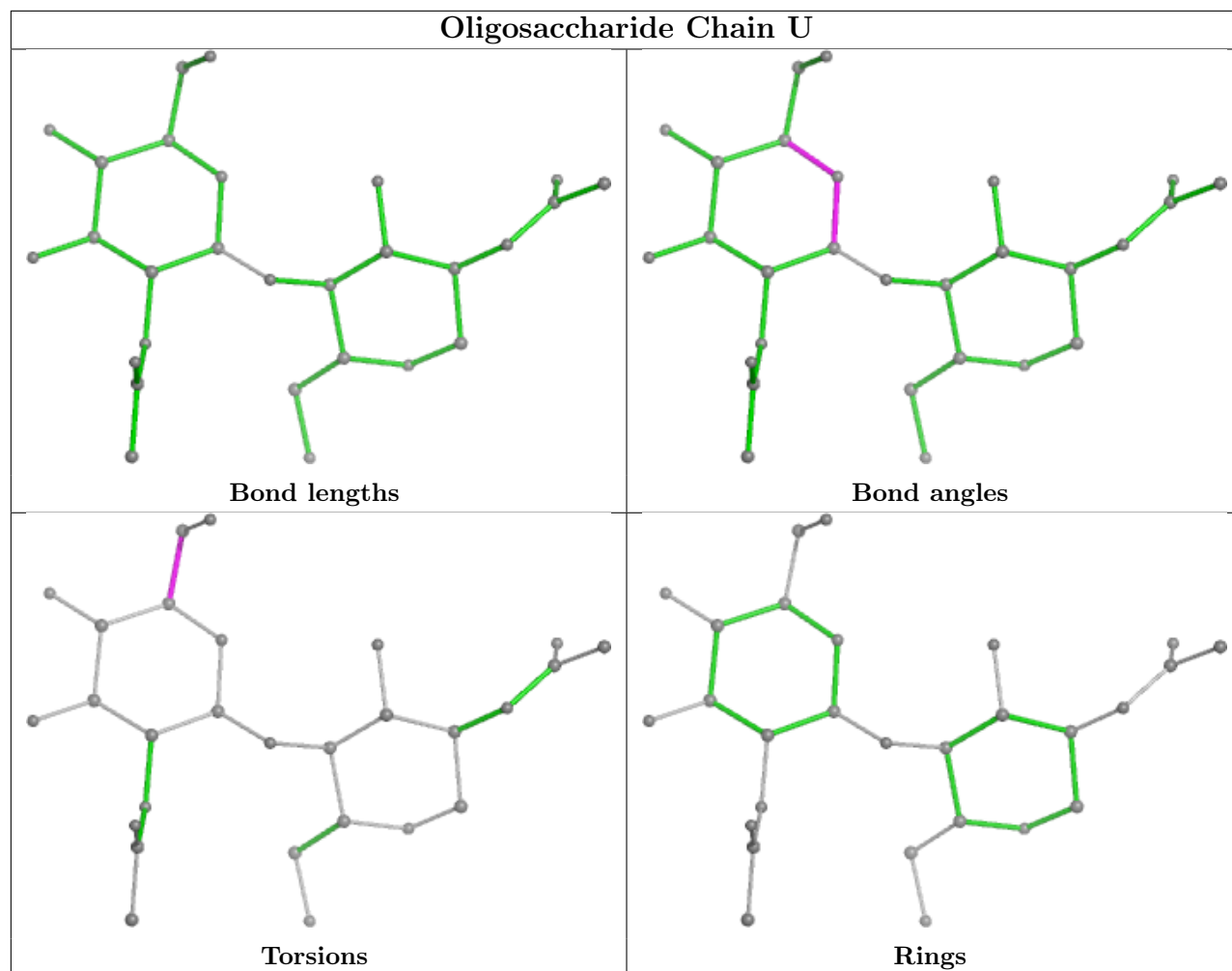


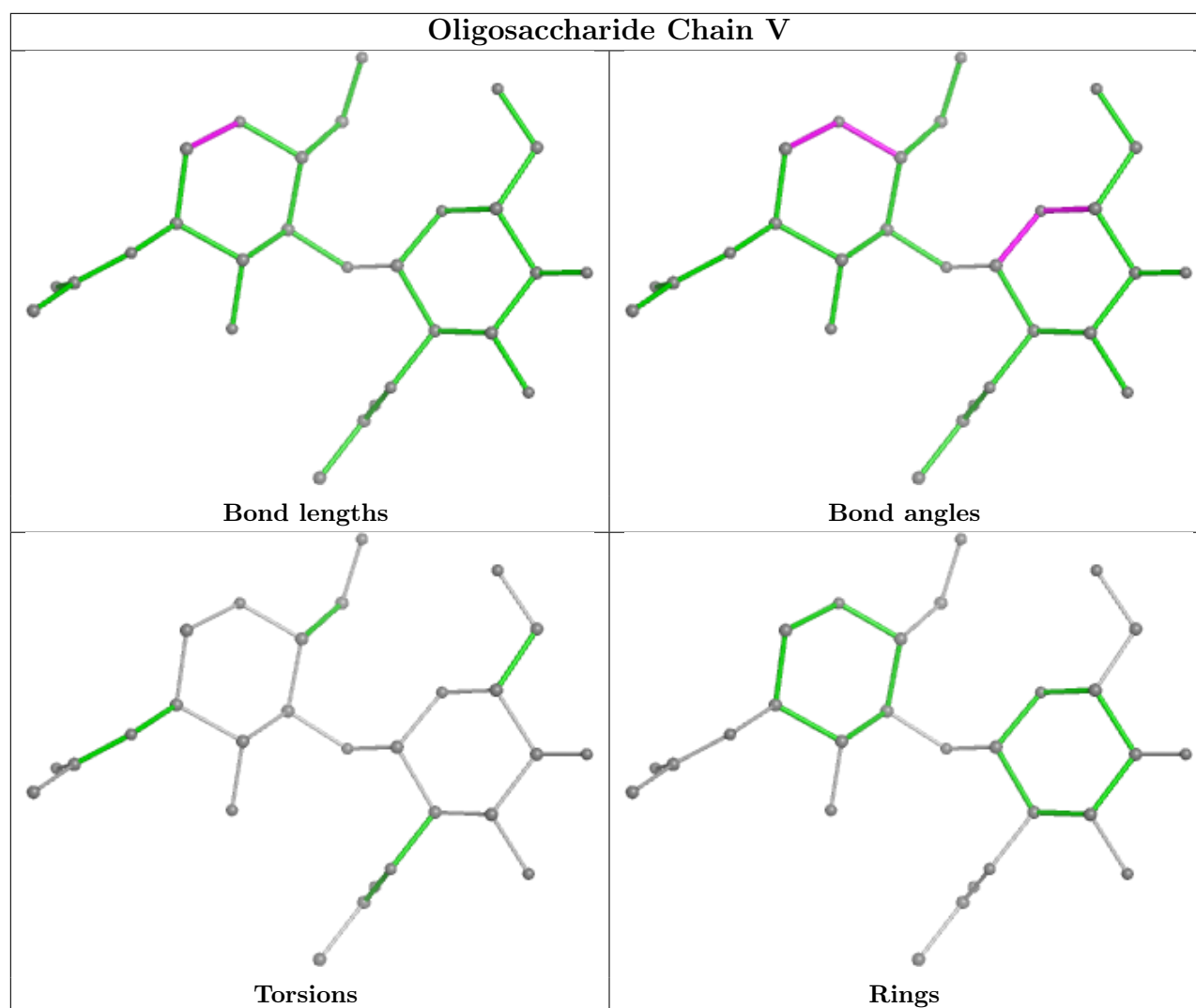












5.6 Ligand geometry [i](#)

39 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	1310	1	14,14,15	0.22	0	17,19,21	0.57	0
3	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.58	1 (5%)
3	NAG	C	1303	1	14,14,15	0.35	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1309	1	14,14,15	0.25	0	17,19,21	0.80	1 (5%)
3	NAG	A	1311	1	14,14,15	0.35	0	17,19,21	0.86	1 (5%)
3	NAG	B	1311	1	14,14,15	0.18	0	17,19,21	0.73	1 (5%)
3	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.65	1 (5%)
3	NAG	B	1302	1	14,14,15	0.18	0	17,19,21	0.96	1 (5%)
3	NAG	B	1312	1	14,14,15	0.16	0	17,19,21	0.64	1 (5%)
3	NAG	C	1307	1	14,14,15	0.19	0	17,19,21	0.56	0
3	NAG	C	1308	1	14,14,15	0.45	0	17,19,21	1.13	1 (5%)
3	NAG	C	1313	1	14,14,15	0.28	0	17,19,21	0.35	0
3	NAG	A	1302	1	14,14,15	0.38	0	17,19,21	0.67	1 (5%)
3	NAG	A	1308	1	14,14,15	0.47	0	17,19,21	1.02	1 (5%)
3	NAG	A	1307	1	14,14,15	0.17	0	17,19,21	0.52	0
3	NAG	A	1303	1	14,14,15	0.55	0	17,19,21	0.39	0
3	NAG	A	1310	1	14,14,15	0.15	0	17,19,21	0.66	1 (5%)
3	NAG	B	1310	1	14,14,15	0.17	0	17,19,21	0.54	0
3	NAG	B	1306	1	14,14,15	0.19	0	17,19,21	0.61	1 (5%)
3	NAG	C	1312	1	14,14,15	0.20	0	17,19,21	0.61	1 (5%)
3	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.66	1 (5%)
3	NAG	C	1311	1	14,14,15	0.37	0	17,19,21	0.83	1 (5%)
3	NAG	C	1304	1	14,14,15	0.45	0	17,19,21	0.62	0
3	NAG	C	1309	1	14,14,15	0.29	0	17,19,21	0.85	1 (5%)
3	NAG	A	1305	1	14,14,15	0.39	0	17,19,21	0.40	0
3	NAG	A	1312	1	14,14,15	0.35	0	17,19,21	0.58	0
3	NAG	C	1301	1	14,14,15	0.47	0	17,19,21	0.89	1 (5%)
3	NAG	C	1302	1	14,14,15	0.50	0	17,19,21	0.95	1 (5%)
3	NAG	A	1309	1	14,14,15	0.29	0	17,19,21	1.03	1 (5%)
3	NAG	A	1304	1	14,14,15	0.38	0	17,19,21	0.56	0
3	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.63	0
3	NAG	B	1301	1	14,14,15	0.16	0	17,19,21	0.66	1 (5%)
3	NAG	B	1307	1	14,14,15	0.15	0	17,19,21	0.59	0
3	NAG	C	1305	1	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	A	1313	1	14,14,15	0.30	0	17,19,21	0.40	0
3	NAG	B	1303	1	14,14,15	0.61	1 (7%)	17,19,21	0.37	0
3	NAG	B	1313	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	B	1308	1	14,14,15	0.57	0	17,19,21	1.00	1 (5%)
3	NAG	C	1306	1	14,14,15	0.18	0	17,19,21	0.64	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
3	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1309	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	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1313	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1303	NAG	O5-C1	-2.22	1.40	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1308	NAG	C1-O5-C5	4.52	118.32	112.19
3	A	1308	NAG	C1-O5-C5	4.06	117.69	112.19
3	B	1308	NAG	C1-O5-C5	3.97	117.57	112.19
3	A	1309	NAG	C1-O5-C5	3.90	117.48	112.19
3	C	1302	NAG	C1-O5-C5	3.68	117.18	112.19
3	B	1302	NAG	C1-O5-C5	3.65	117.14	112.19
3	C	1301	NAG	C1-O5-C5	3.43	116.84	112.19
3	A	1311	NAG	C1-O5-C5	3.34	116.72	112.19
3	C	1311	NAG	C1-O5-C5	3.23	116.57	112.19
3	C	1309	NAG	C1-O5-C5	2.94	116.18	112.19
3	B	1309	NAG	C1-O5-C5	2.75	115.92	112.19
3	B	1311	NAG	C1-O5-C5	2.69	115.84	112.19
3	A	1302	NAG	C1-O5-C5	2.41	115.45	112.19
3	B	1301	NAG	C1-O5-C5	2.39	115.43	112.19
3	C	1306	NAG	C1-O5-C5	2.31	115.33	112.19
3	A	1310	NAG	C1-O5-C5	2.29	115.29	112.19
3	B	1305	NAG	C1-O5-C5	2.26	115.26	112.19
3	A	1301	NAG	C1-O5-C5	2.21	115.19	112.19
3	B	1306	NAG	C1-O5-C5	2.12	115.07	112.19
3	B	1312	NAG	C1-O5-C5	2.11	115.05	112.19
3	A	1306	NAG	C1-O5-C5	2.05	114.97	112.19
3	C	1312	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1312	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	A	1311	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	B	1313	NAG	O5-C5-C6-O6
3	A	1311	NAG	C4-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	B	1312	NAG	C4-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1302	NAG	C1-C2-N2-C7
3	C	1302	NAG	C1-C2-N2-C7
3	B	1313	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	B	1303	NAG	C1-C2-N2-C7
3	C	1301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1304	NAG	C4-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6
3	B	1302	NAG	C1-C2-N2-C7
3	C	1313	NAG	O5-C5-C6-O6
3	C	1303	NAG	C1-C2-N2-C7
3	B	1311	NAG	C4-C5-C6-O6
3	C	1311	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	C	1304	NAG	C3-C2-N2-C7
3	A	1309	NAG	C4-C5-C6-O6
3	A	1303	NAG	C1-C2-N2-C7
3	B	1305	NAG	O5-C5-C6-O6
3	A	1305	NAG	C1-C2-N2-C7
3	A	1302	NAG	C3-C2-N2-C7
3	A	1304	NAG	C3-C2-N2-C7
3	B	1302	NAG	C3-C2-N2-C7
3	B	1304	NAG	C3-C2-N2-C7
3	C	1302	NAG	C3-C2-N2-C7
3	C	1313	NAG	C4-C5-C6-O6
3	B	1303	NAG	C3-C2-N2-C7
3	C	1303	NAG	C3-C2-N2-C7

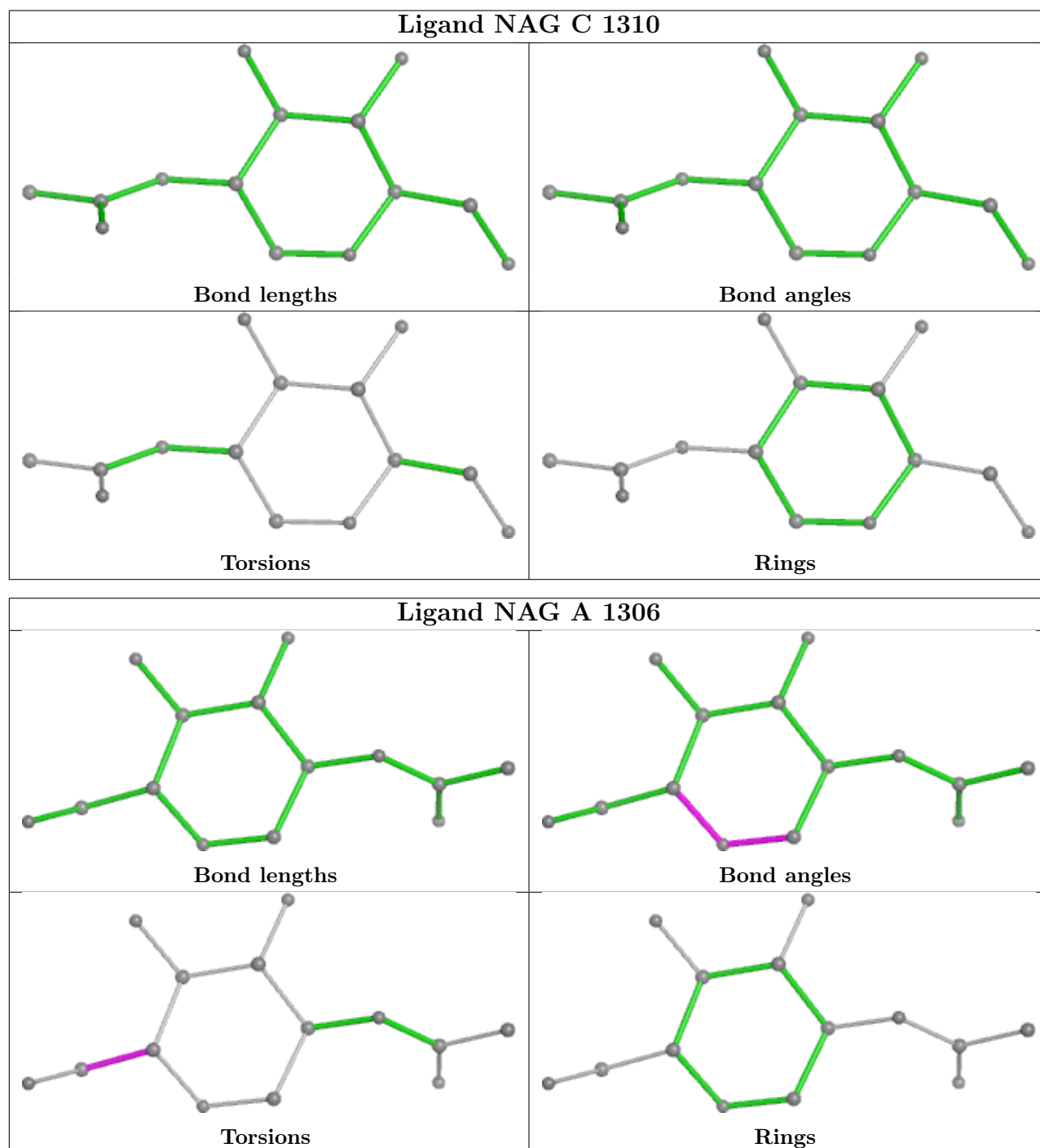
There are no ring outliers.

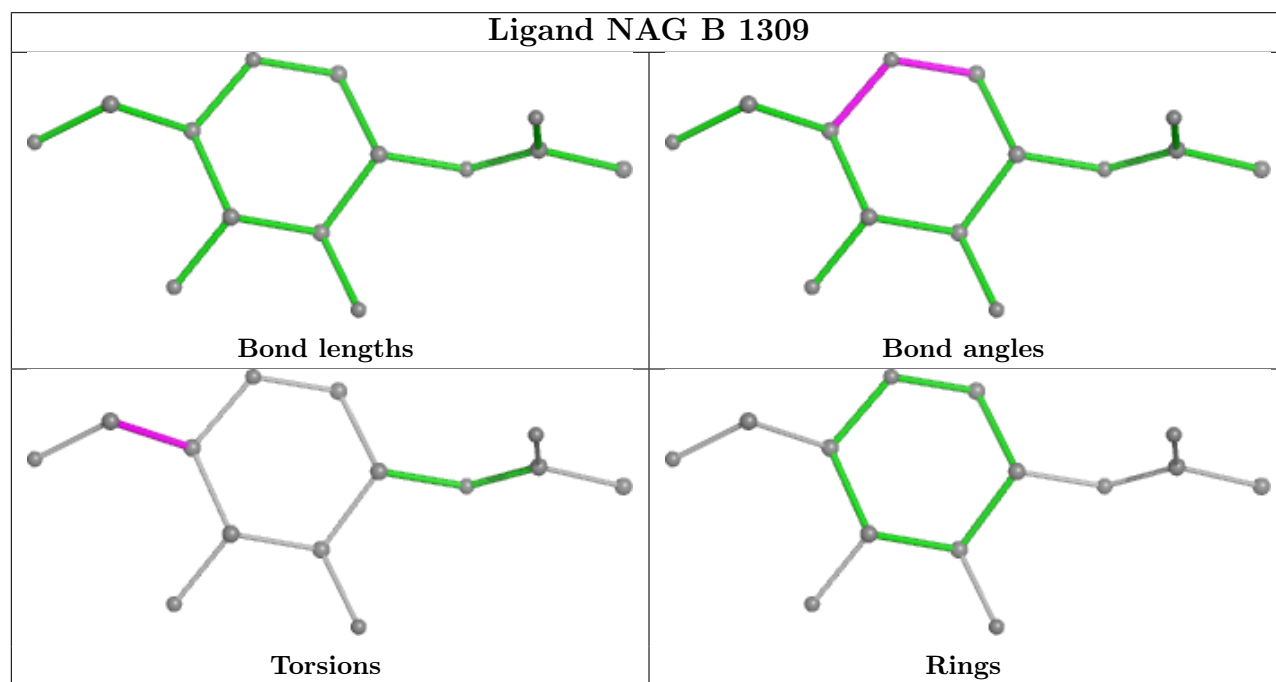
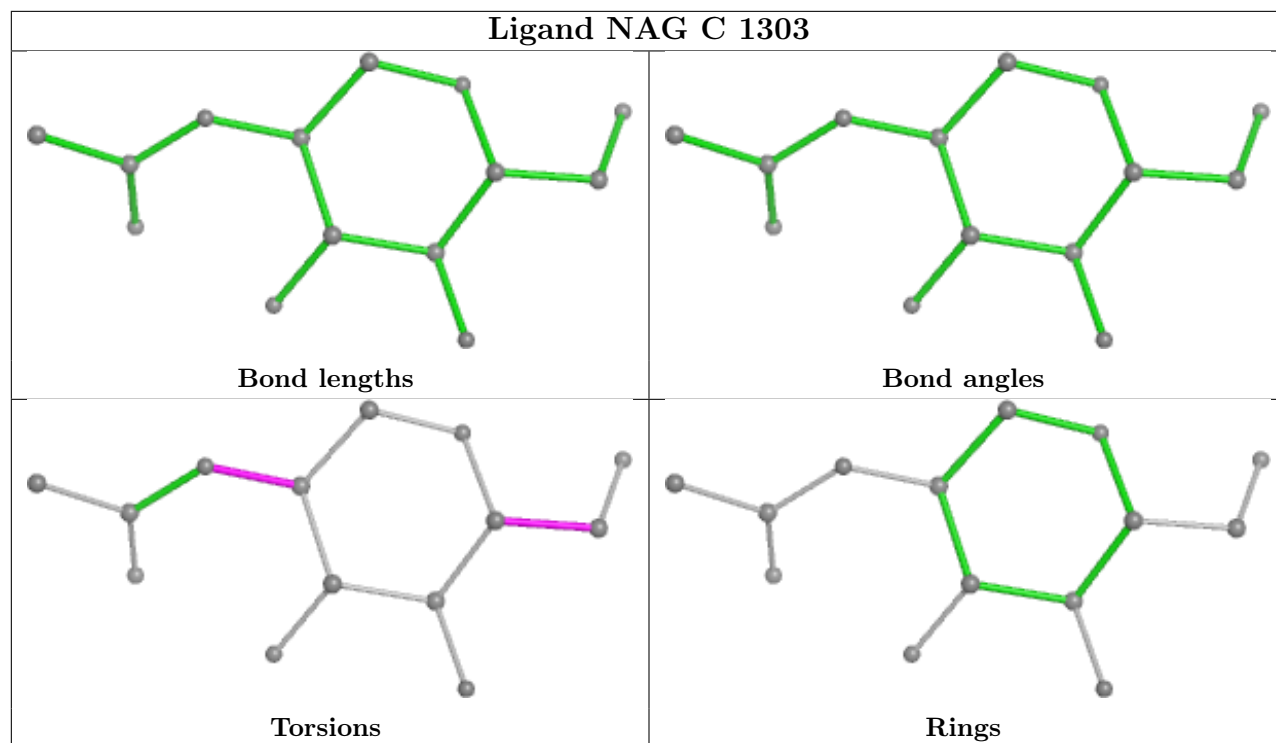
6 monomers are involved in 7 short contacts:

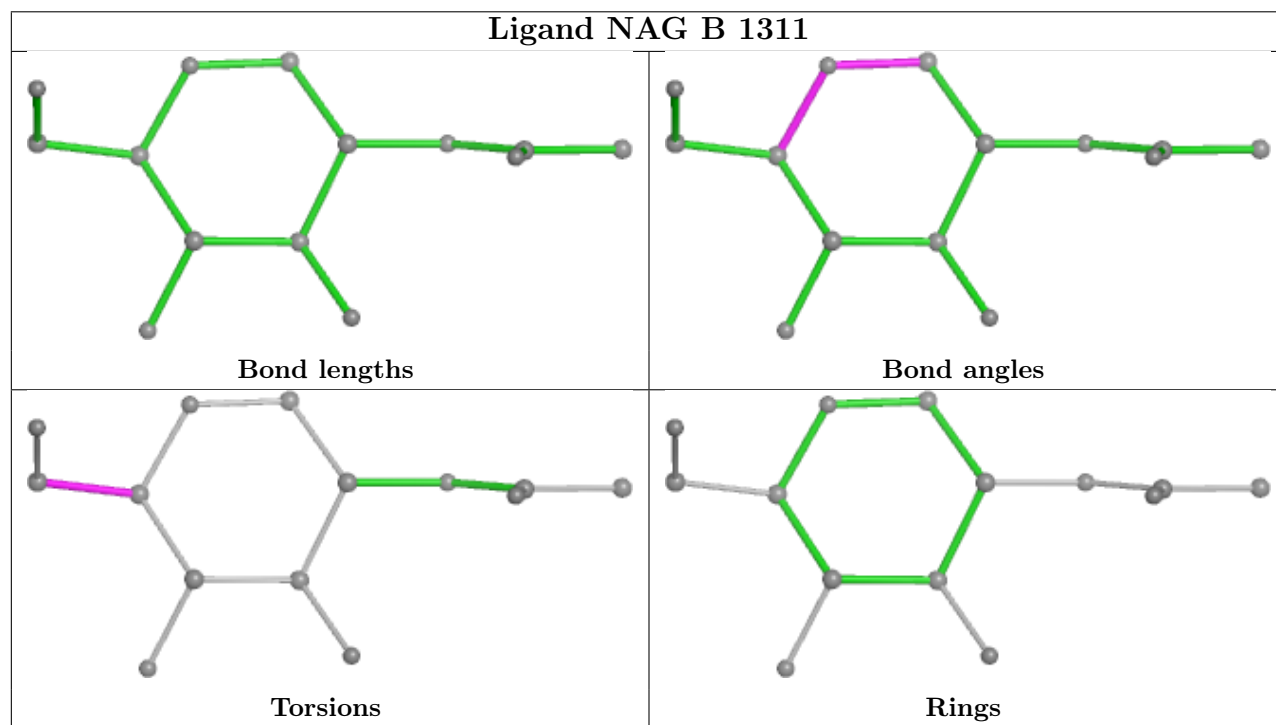
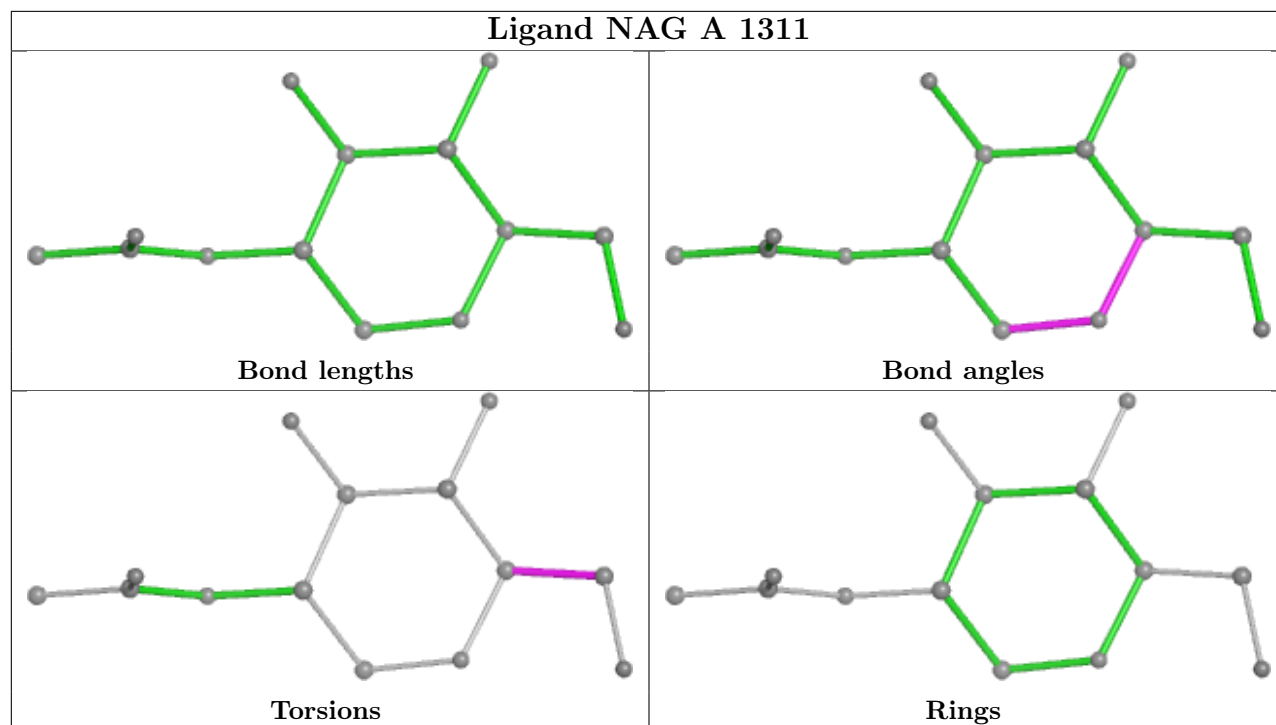
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1302	NAG	1	0
3	A	1302	NAG	2	0
3	A	1307	NAG	1	0
3	C	1304	NAG	1	0
3	C	1302	NAG	1	0
3	B	1303	NAG	1	0

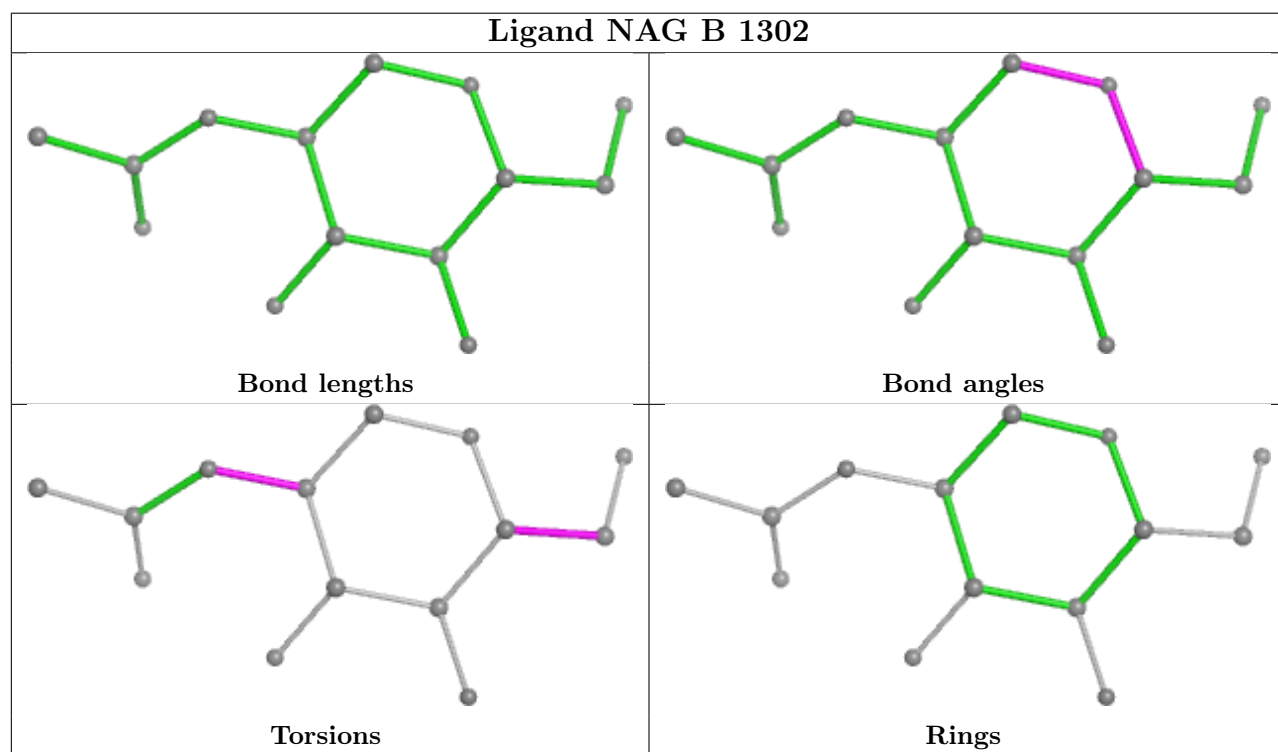
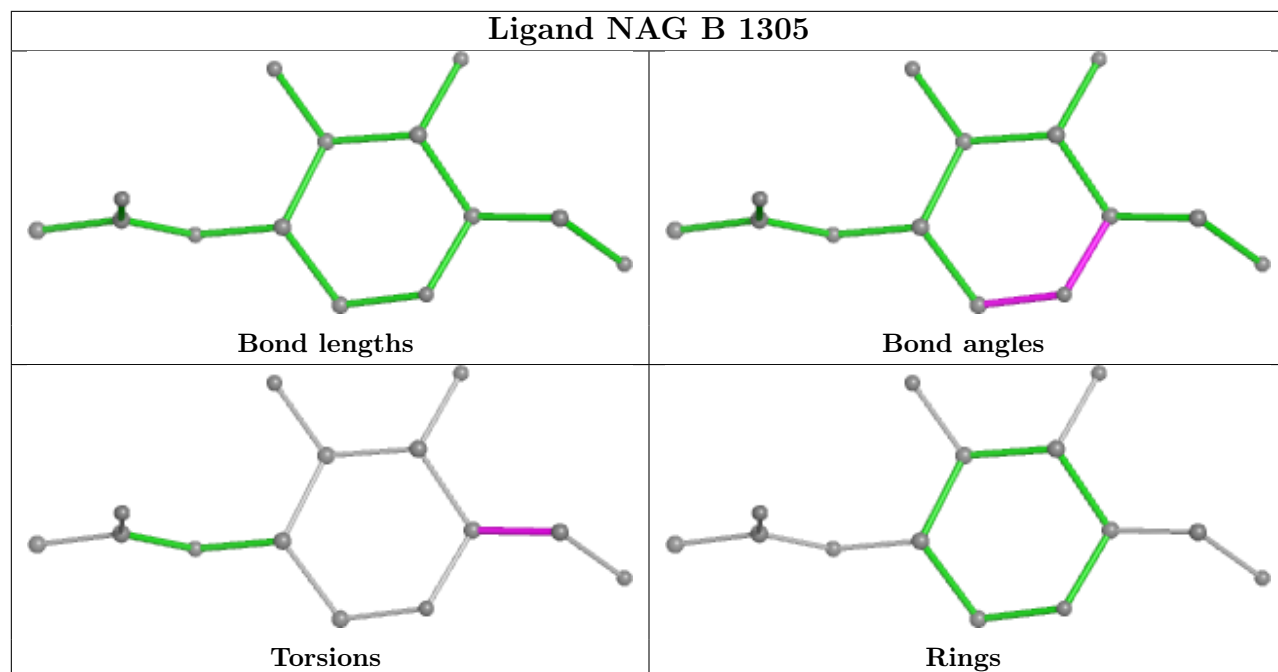
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

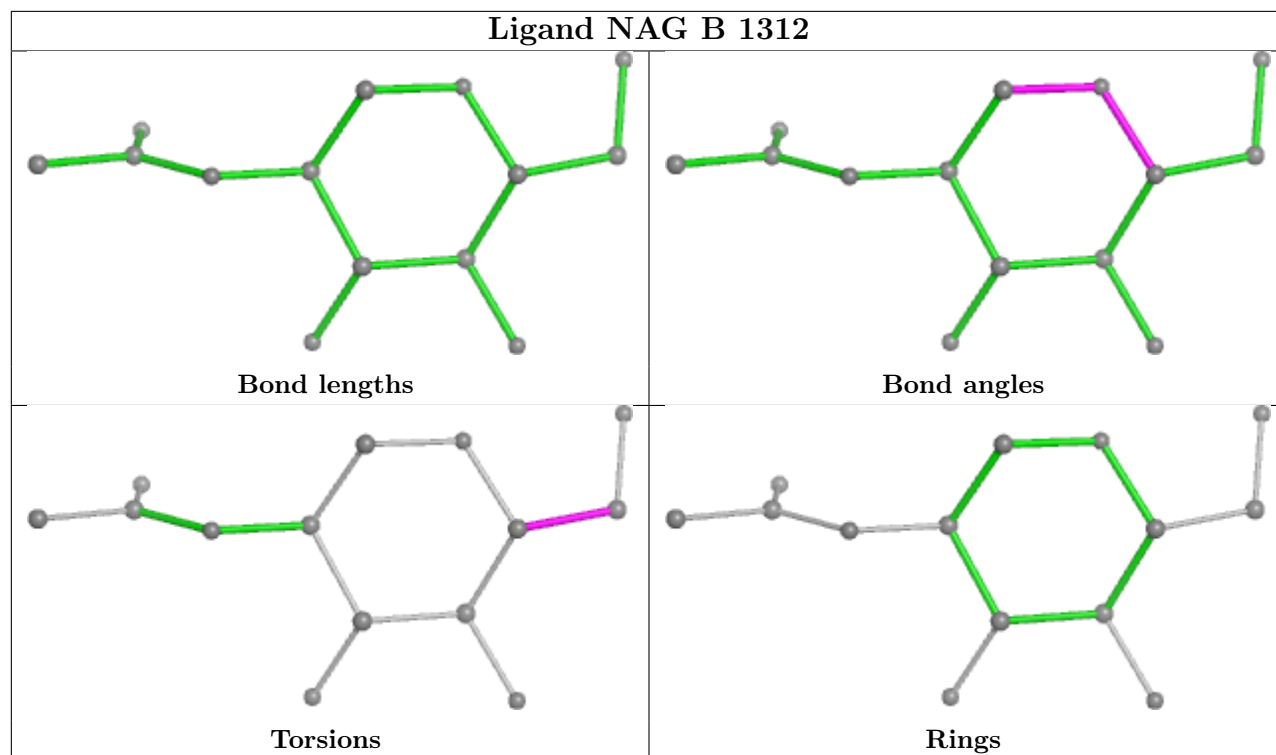




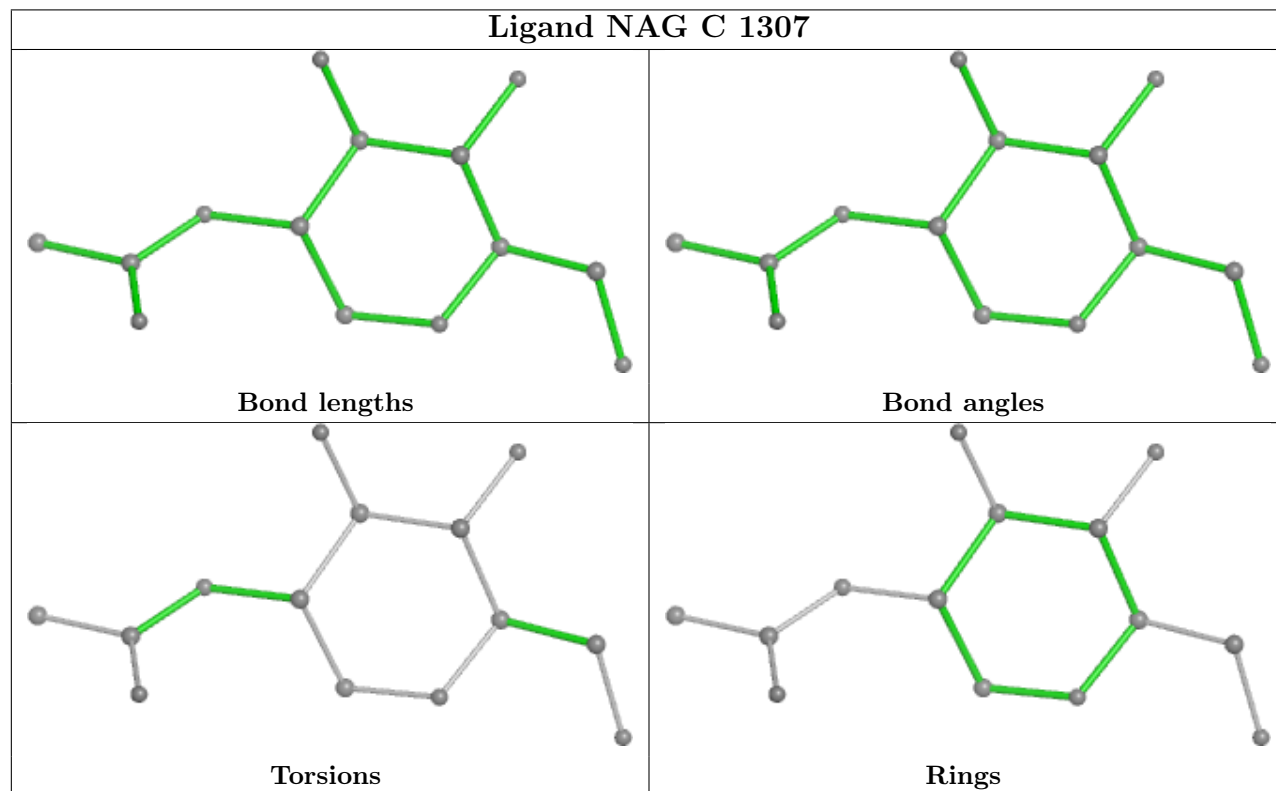


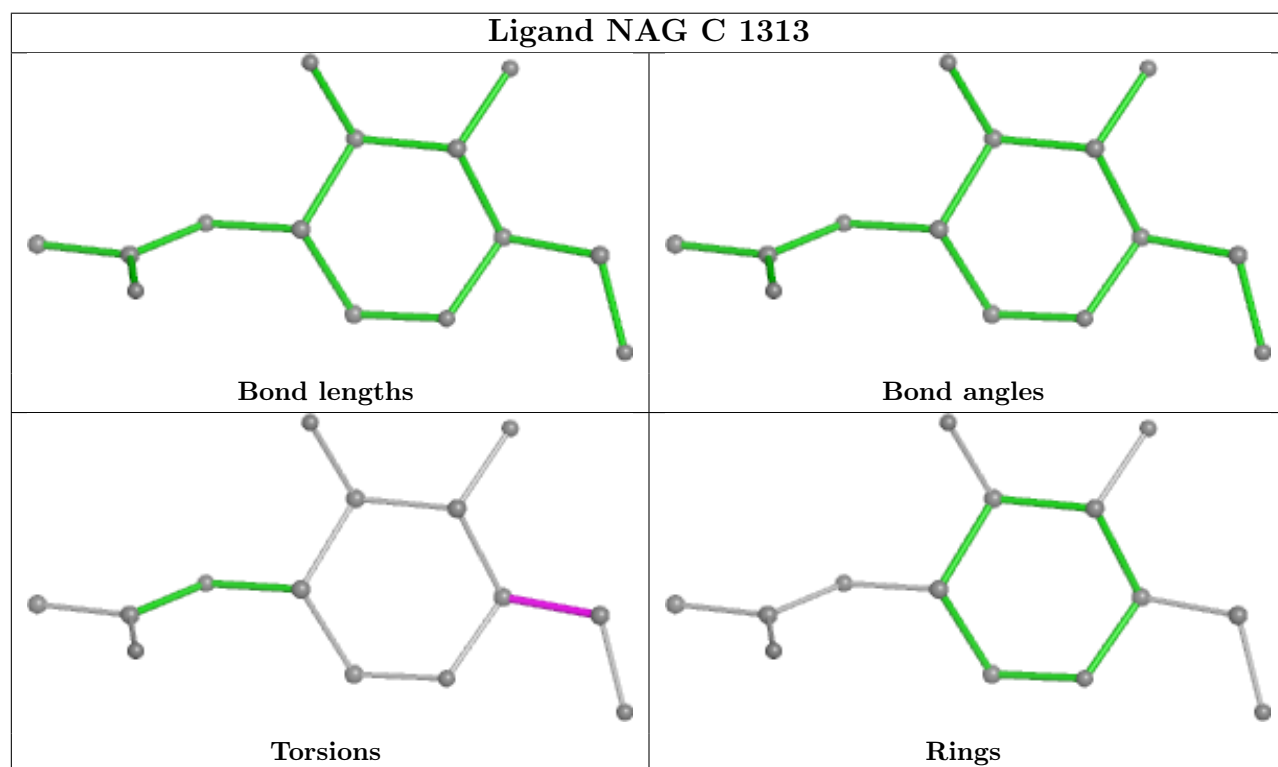
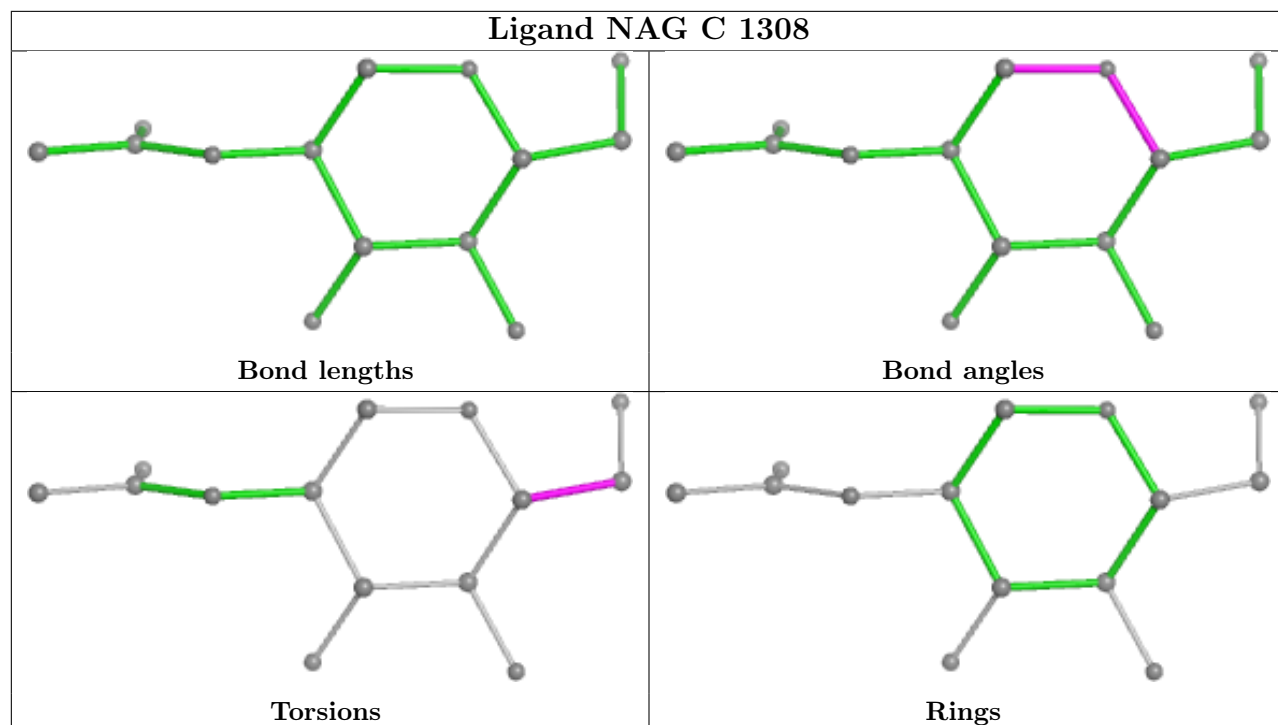


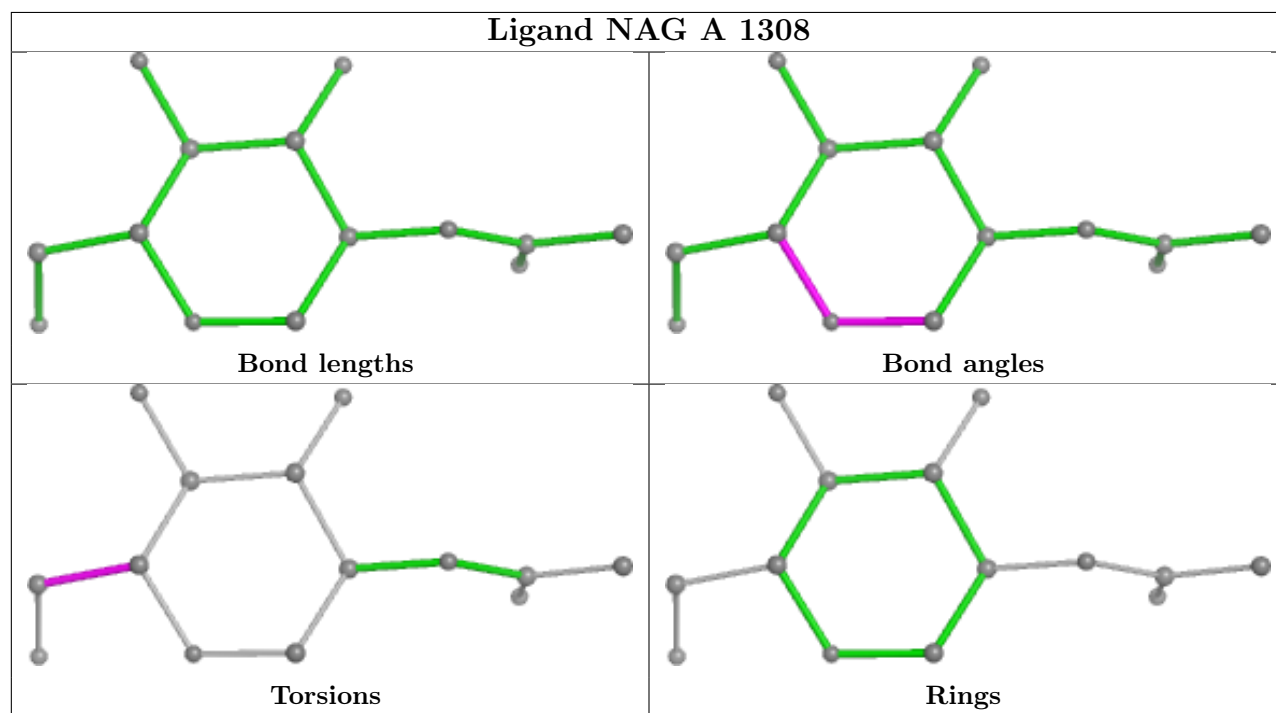
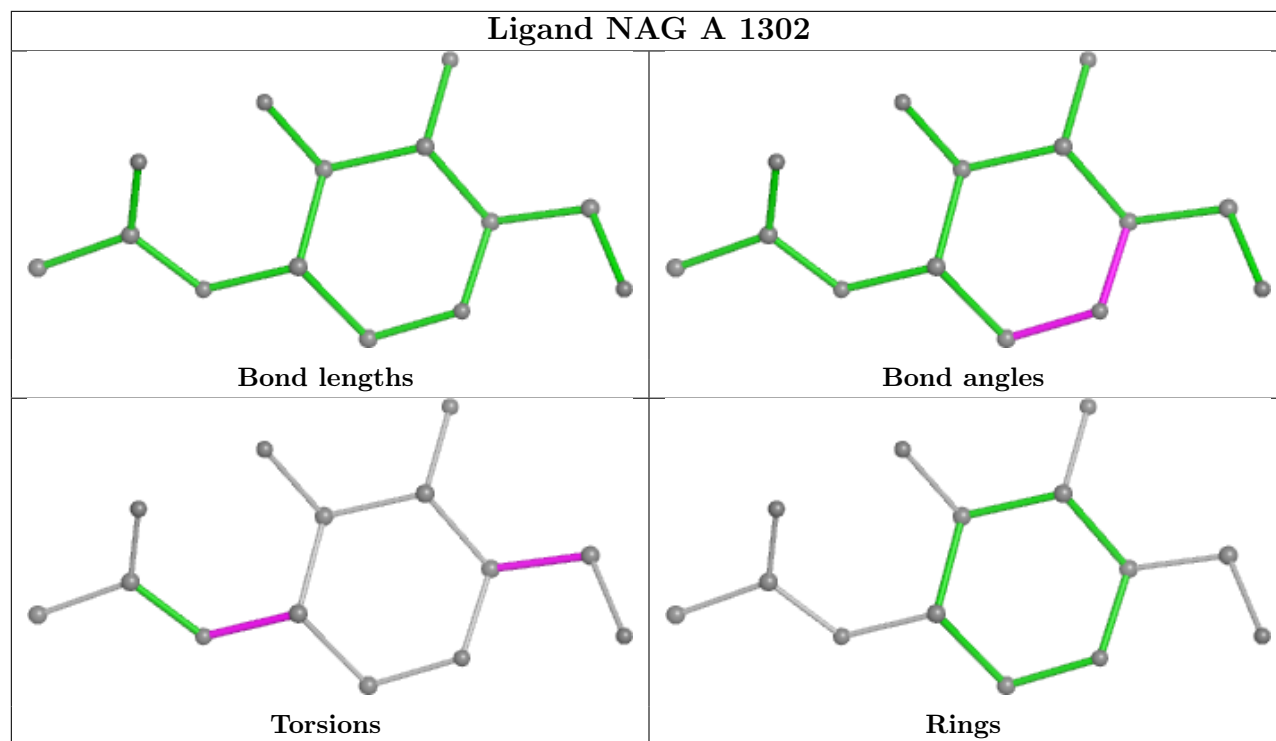
Ligand NAG B 1312

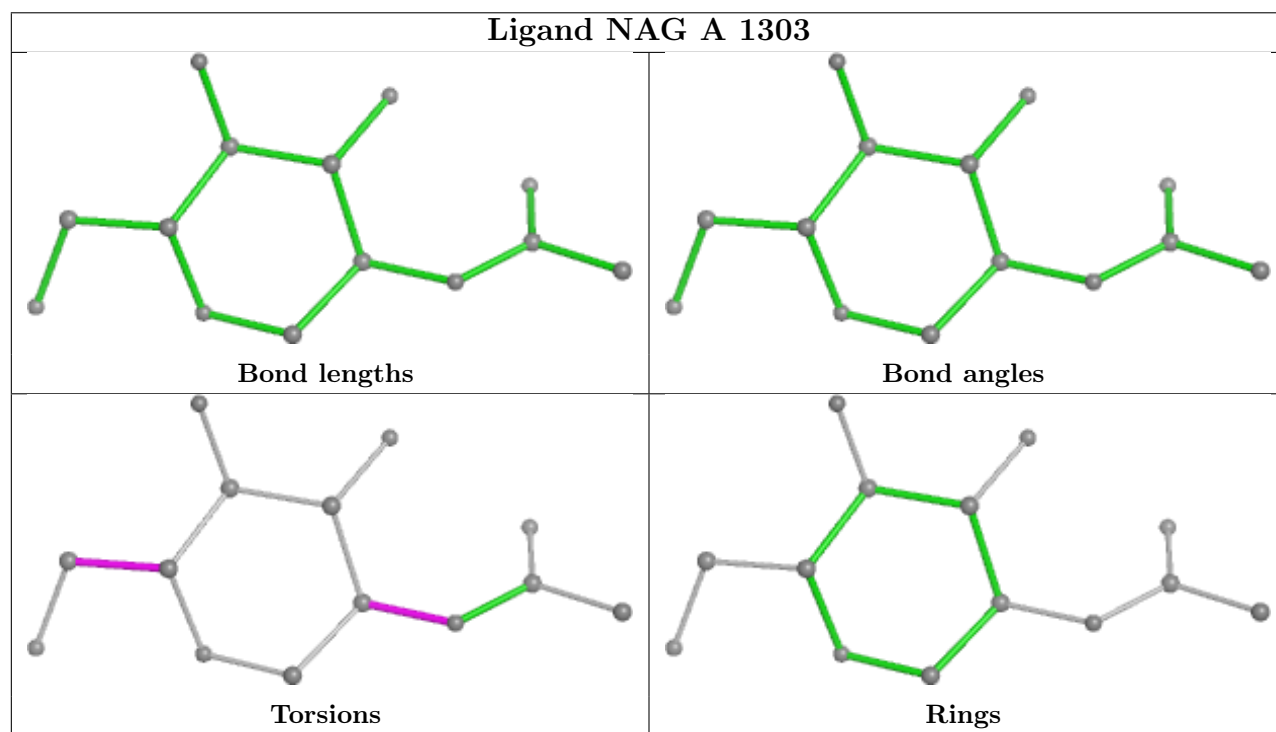
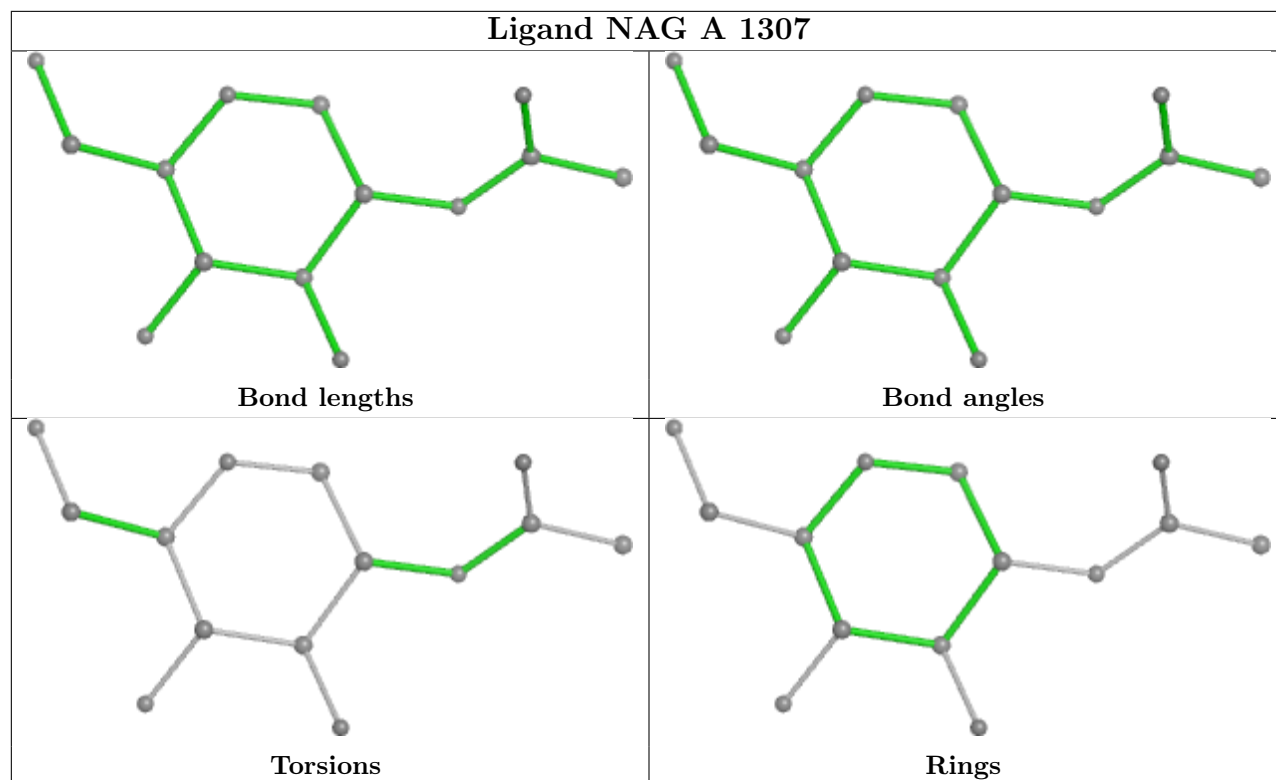


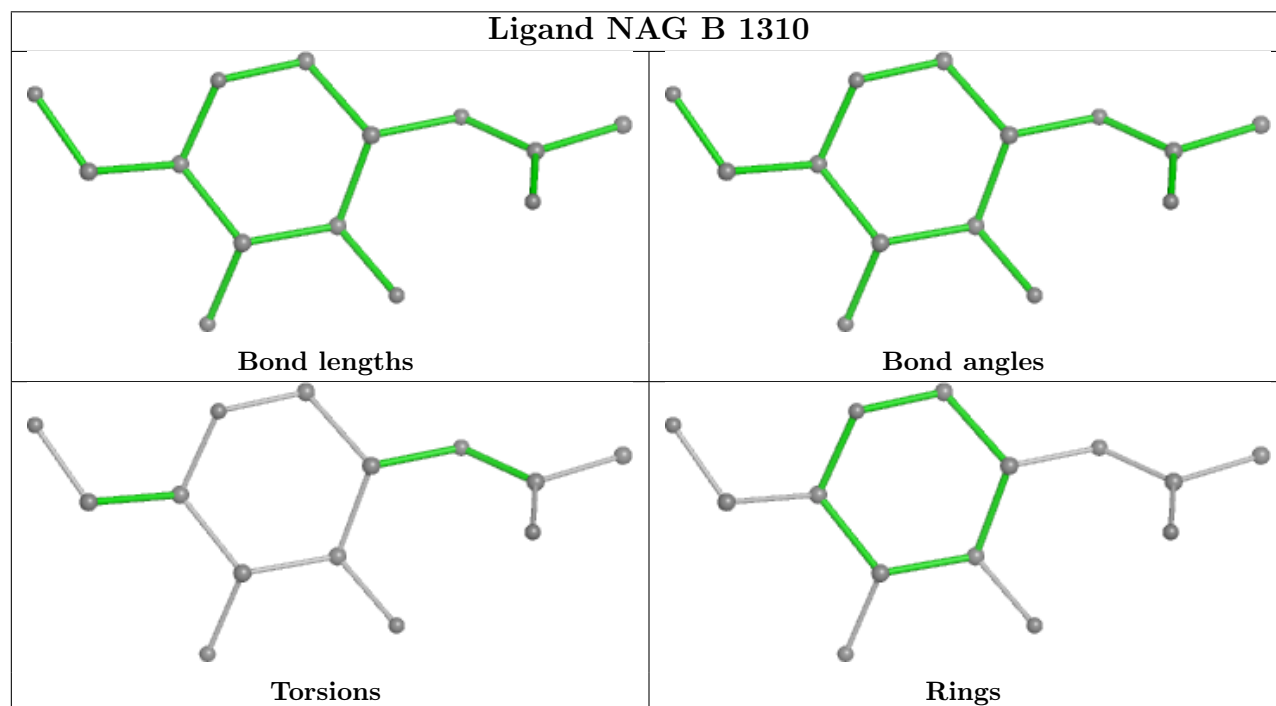
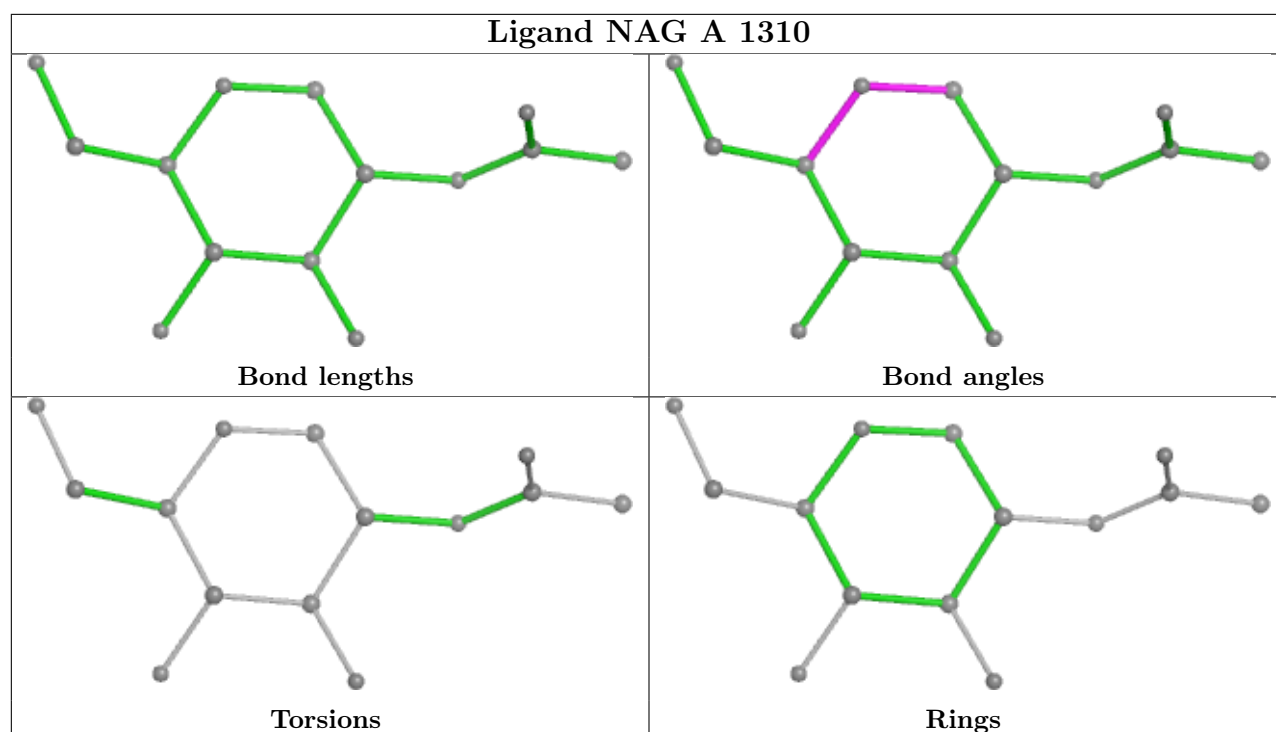
Ligand NAG C 1307

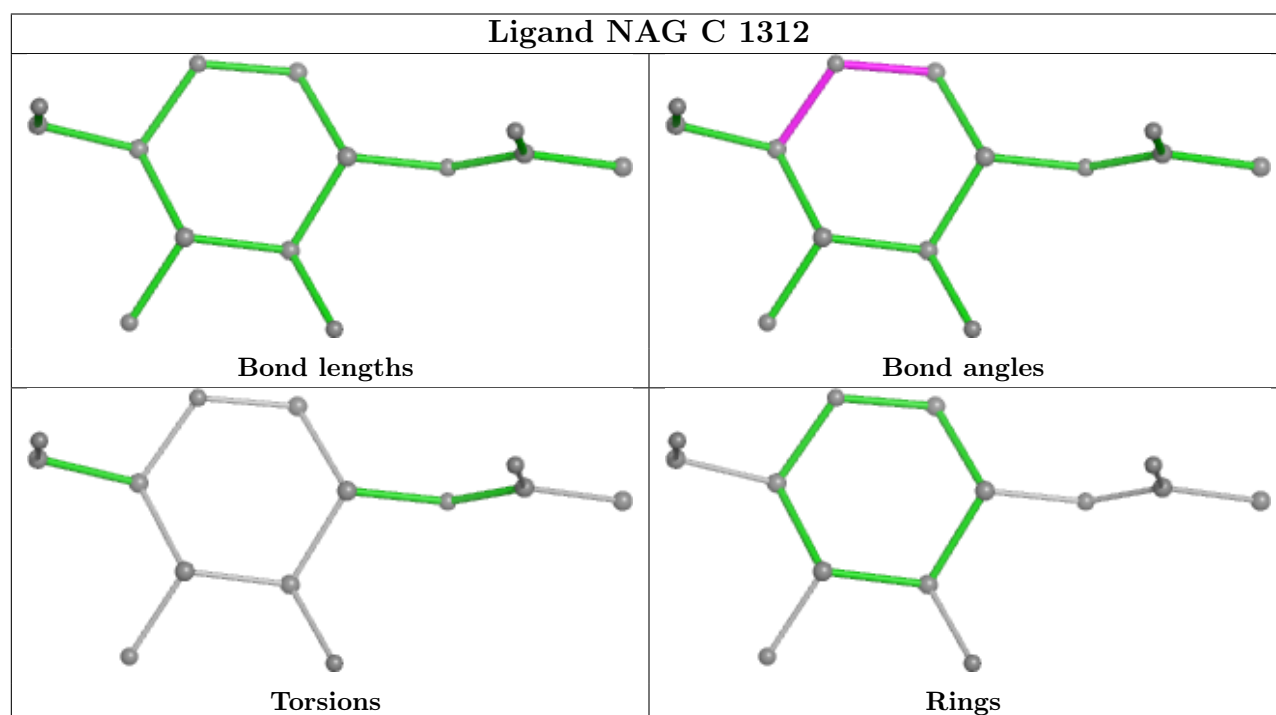
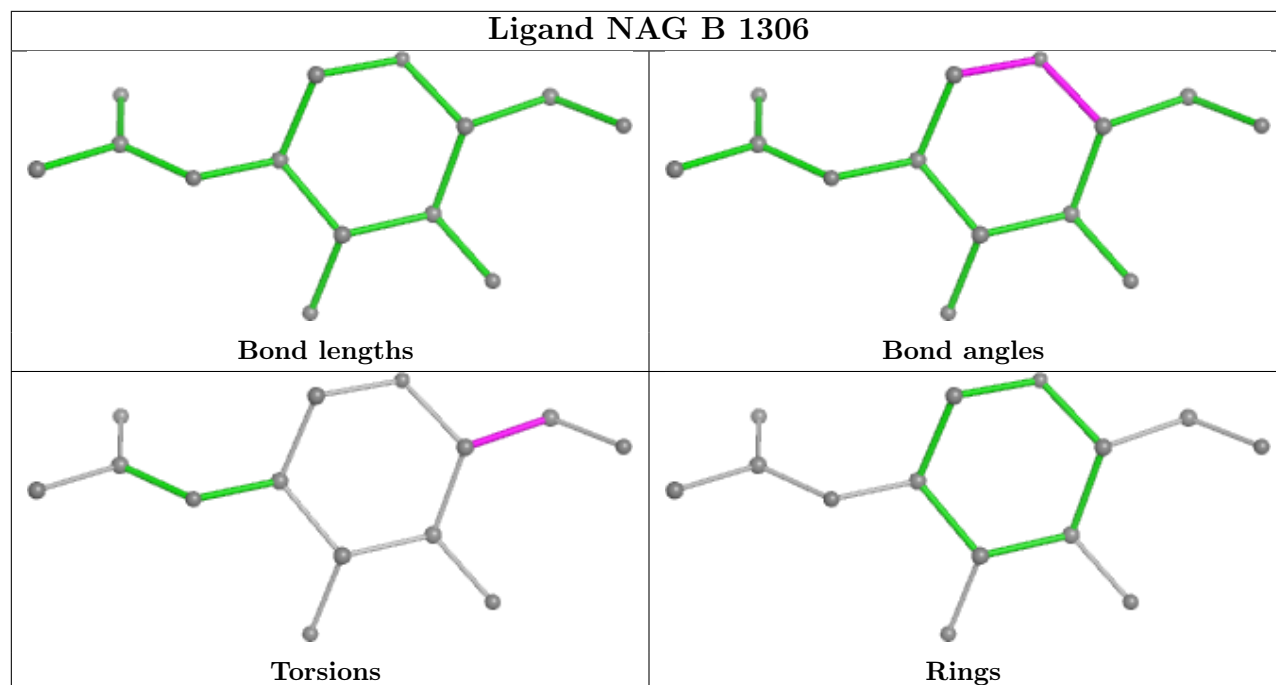


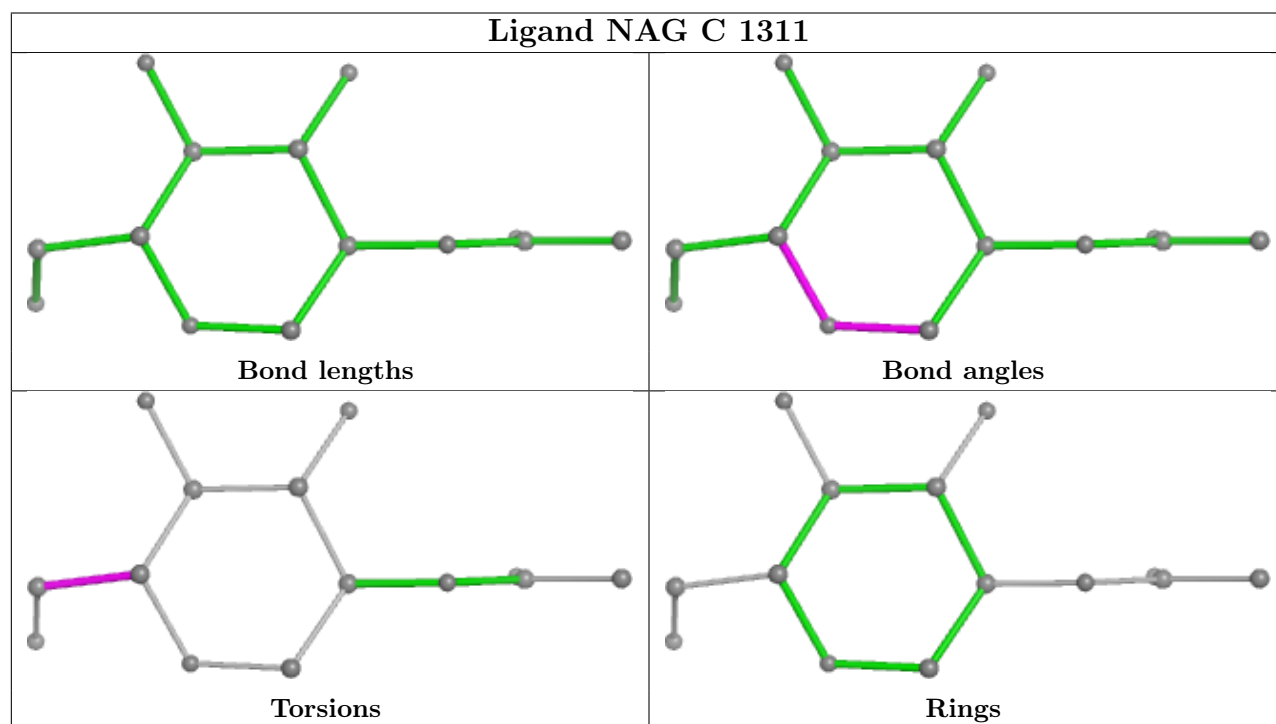
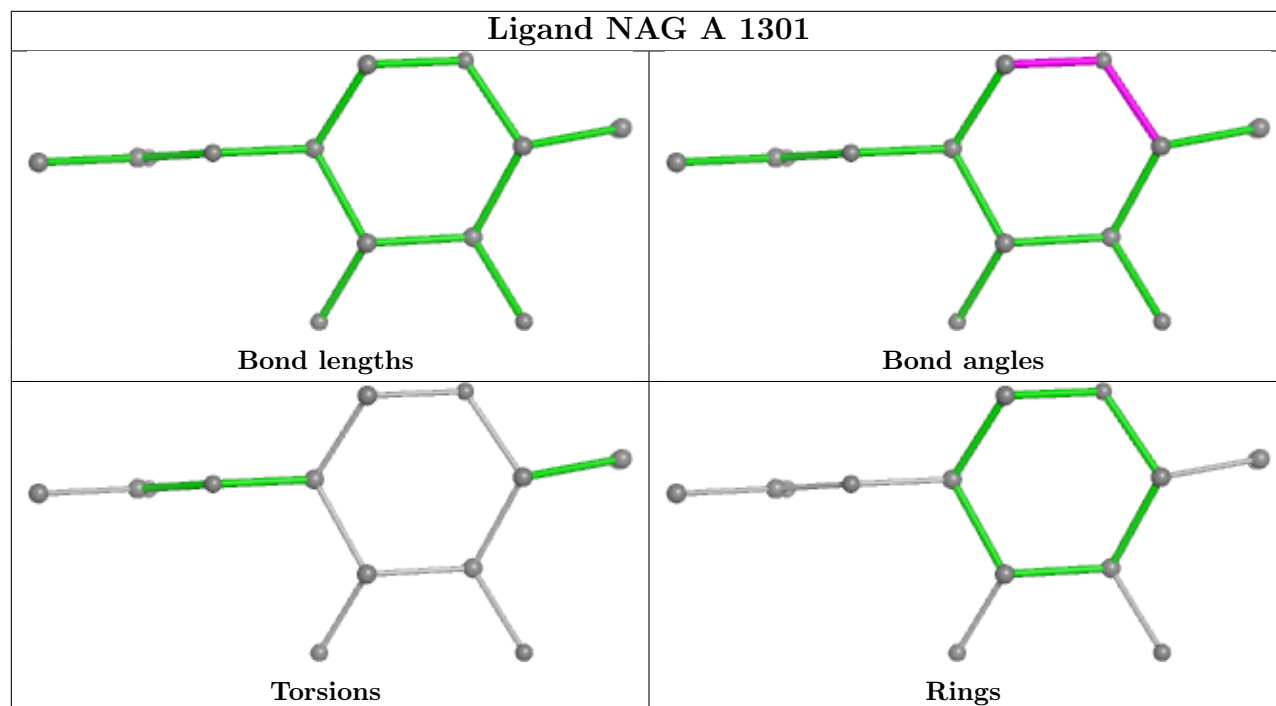


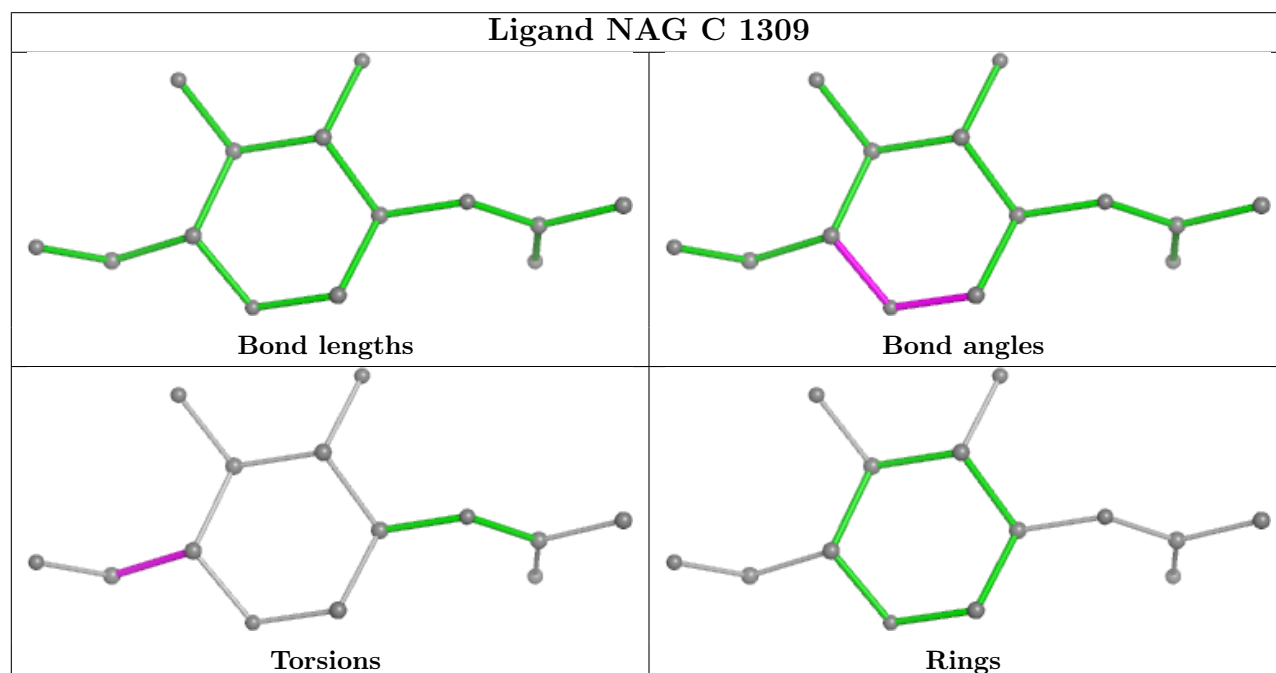
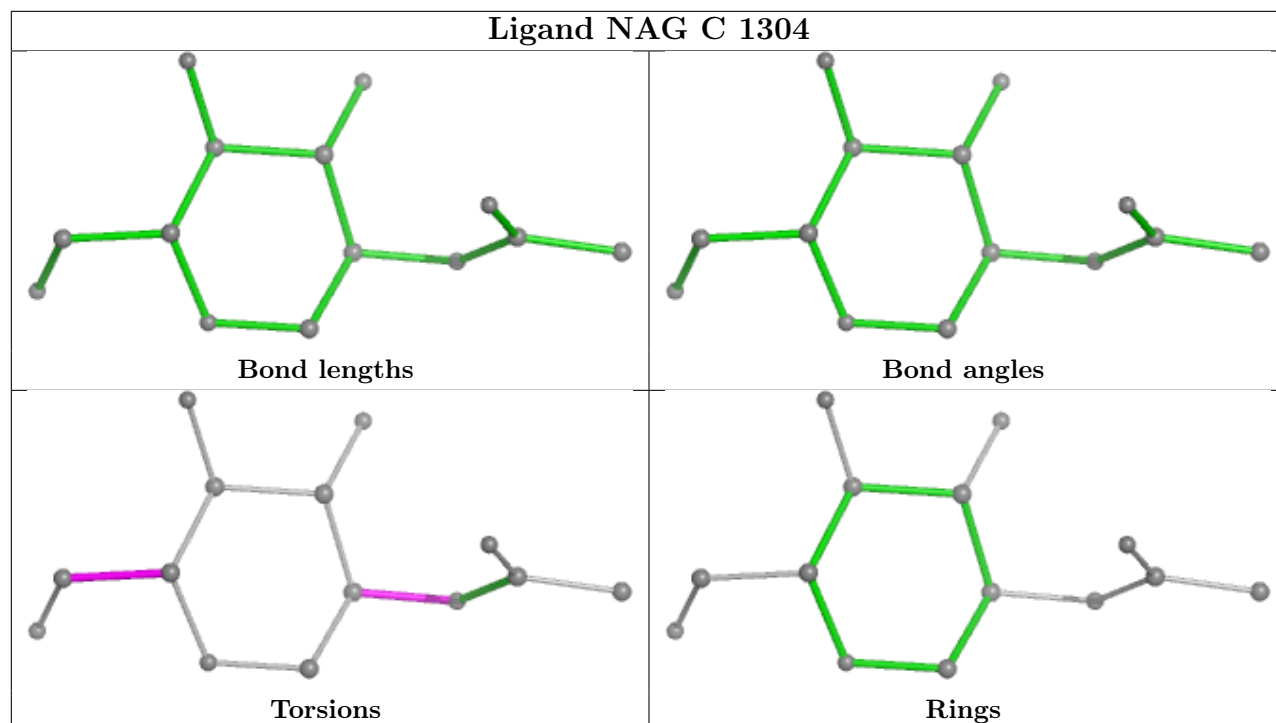


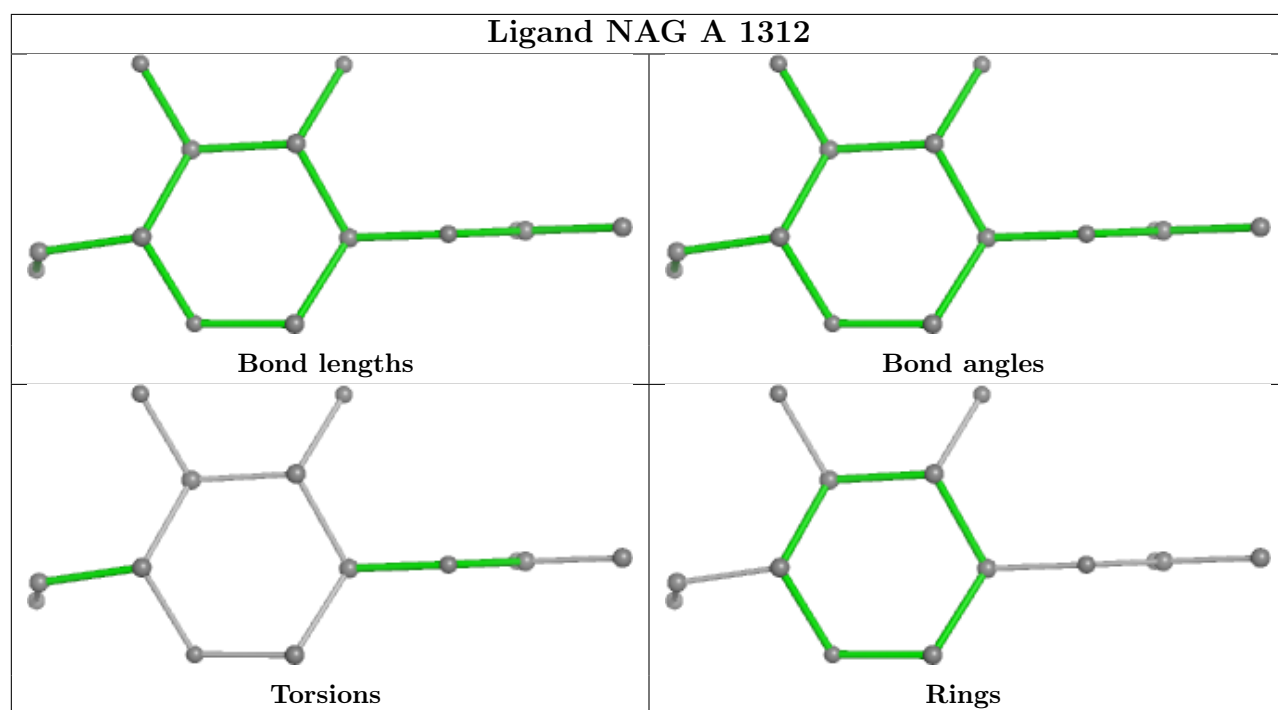
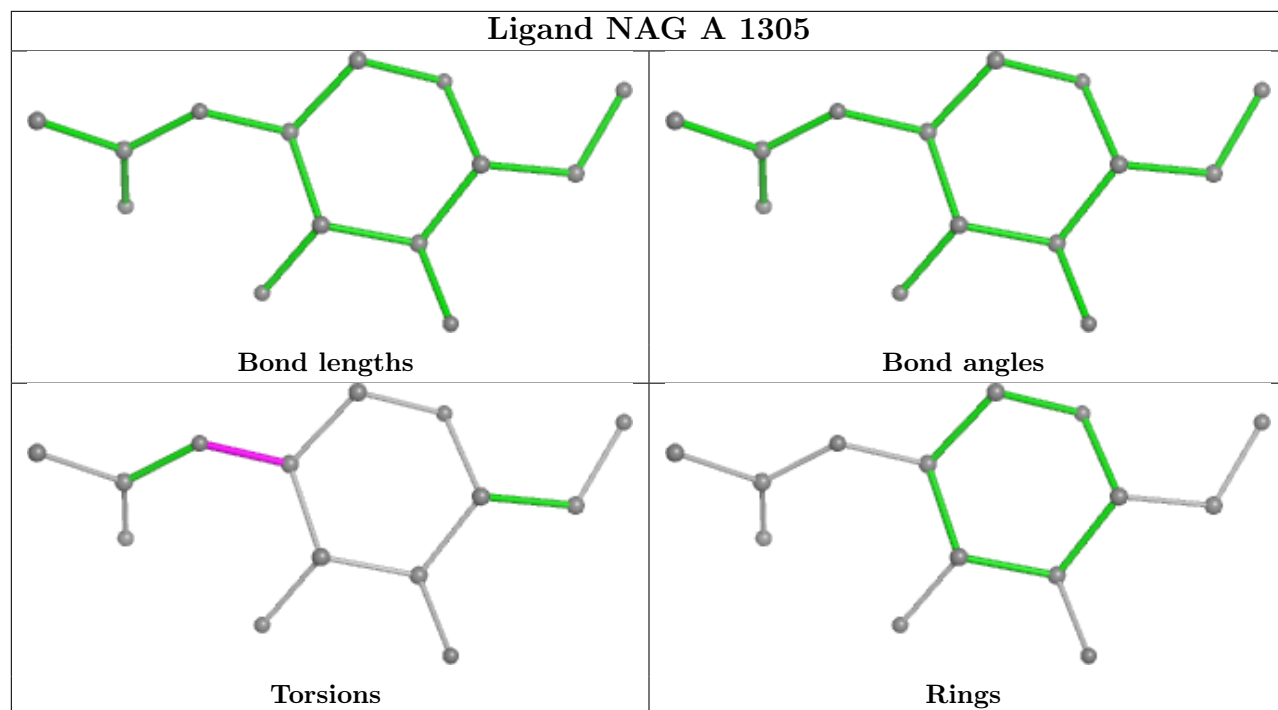


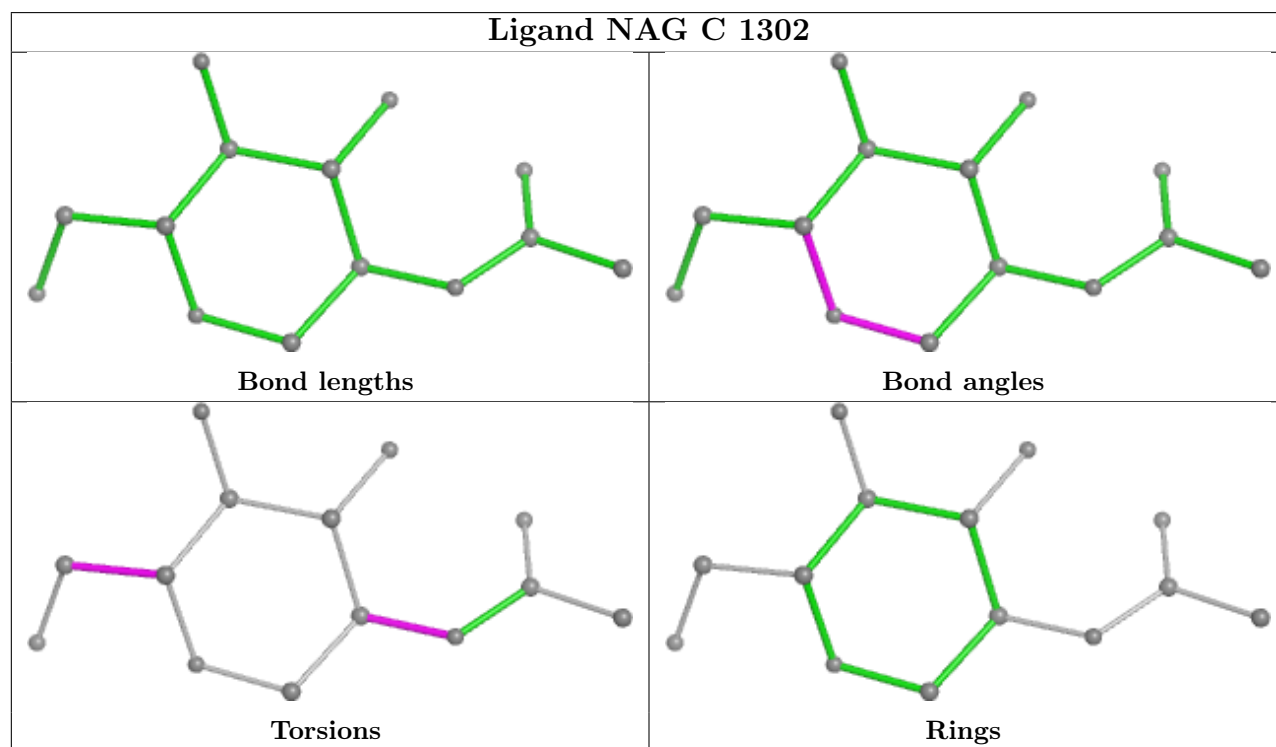
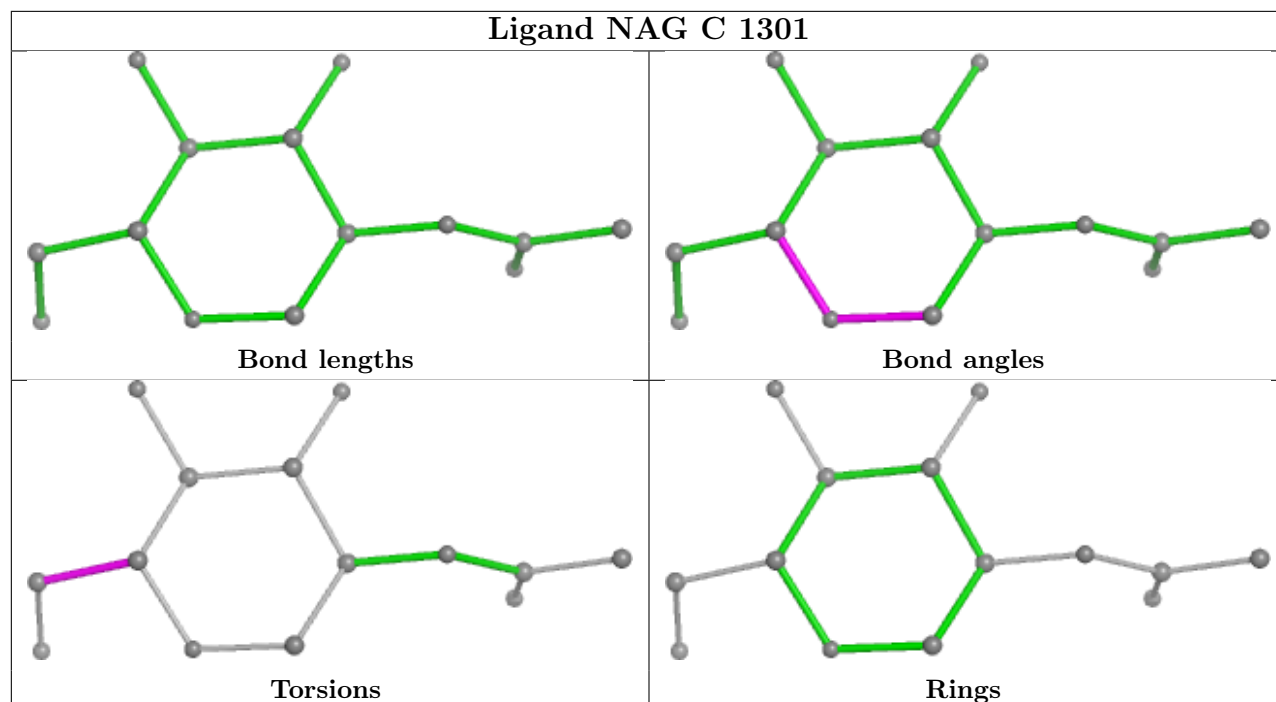


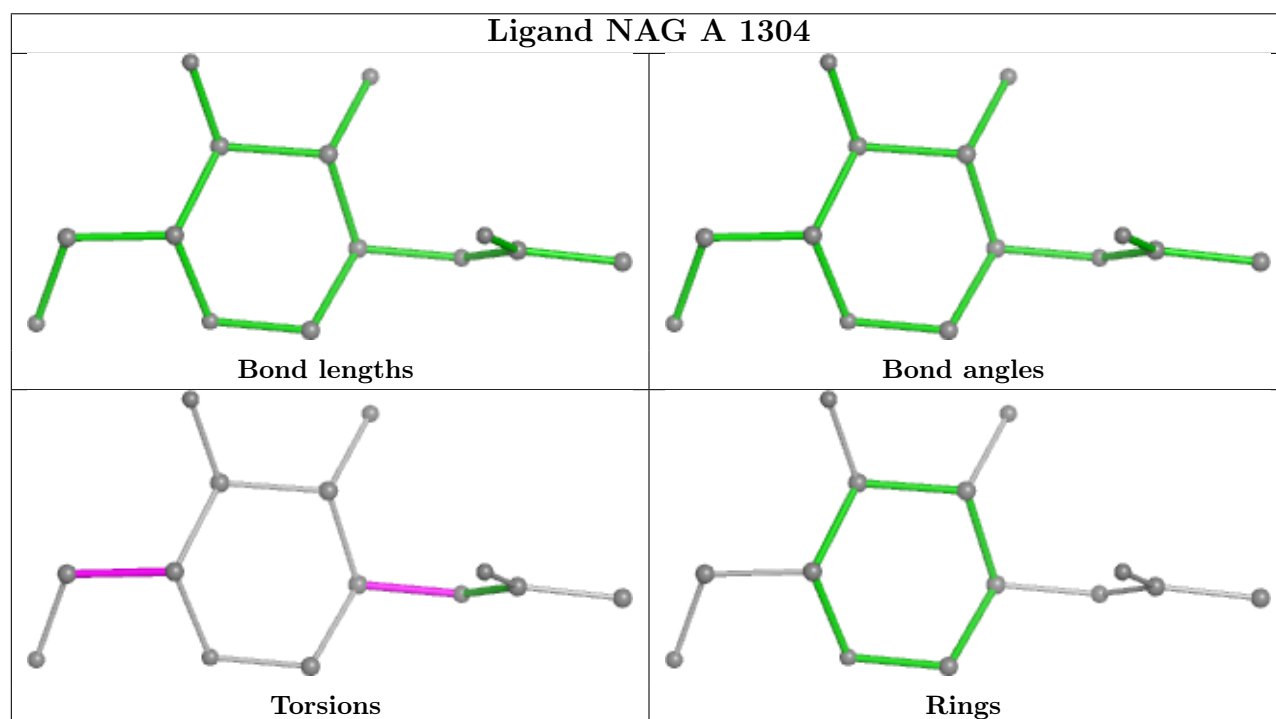
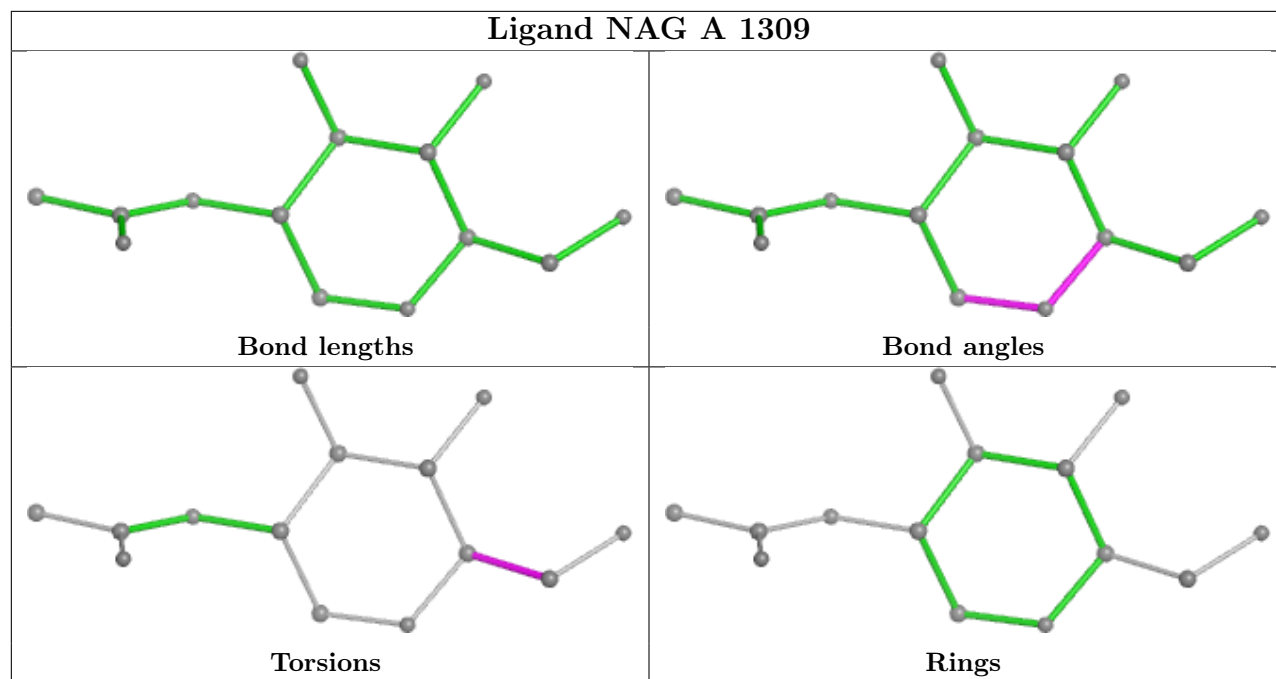


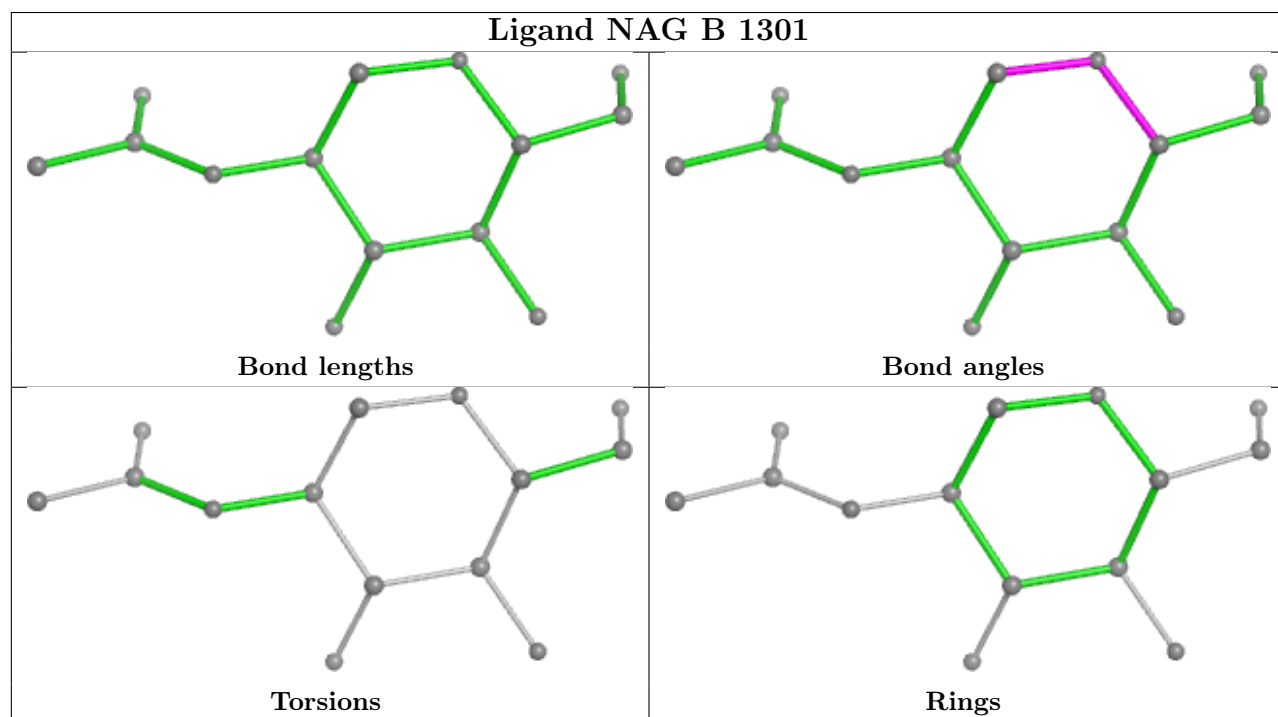
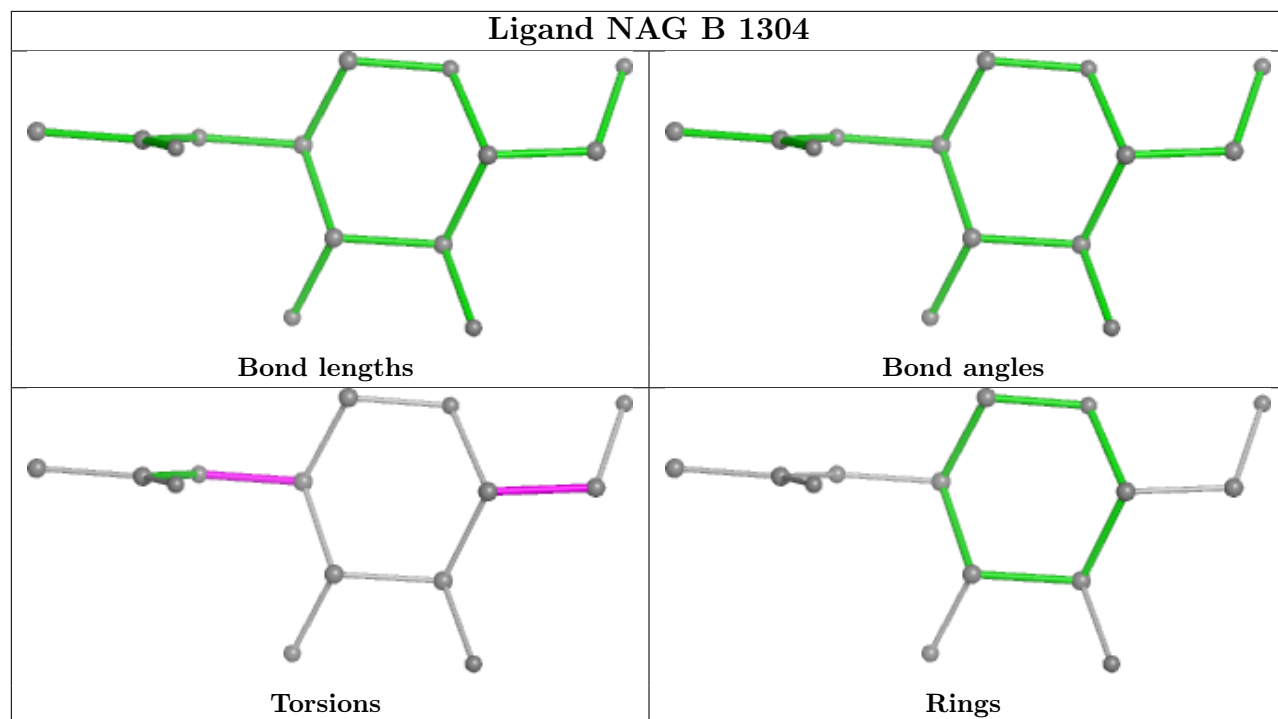


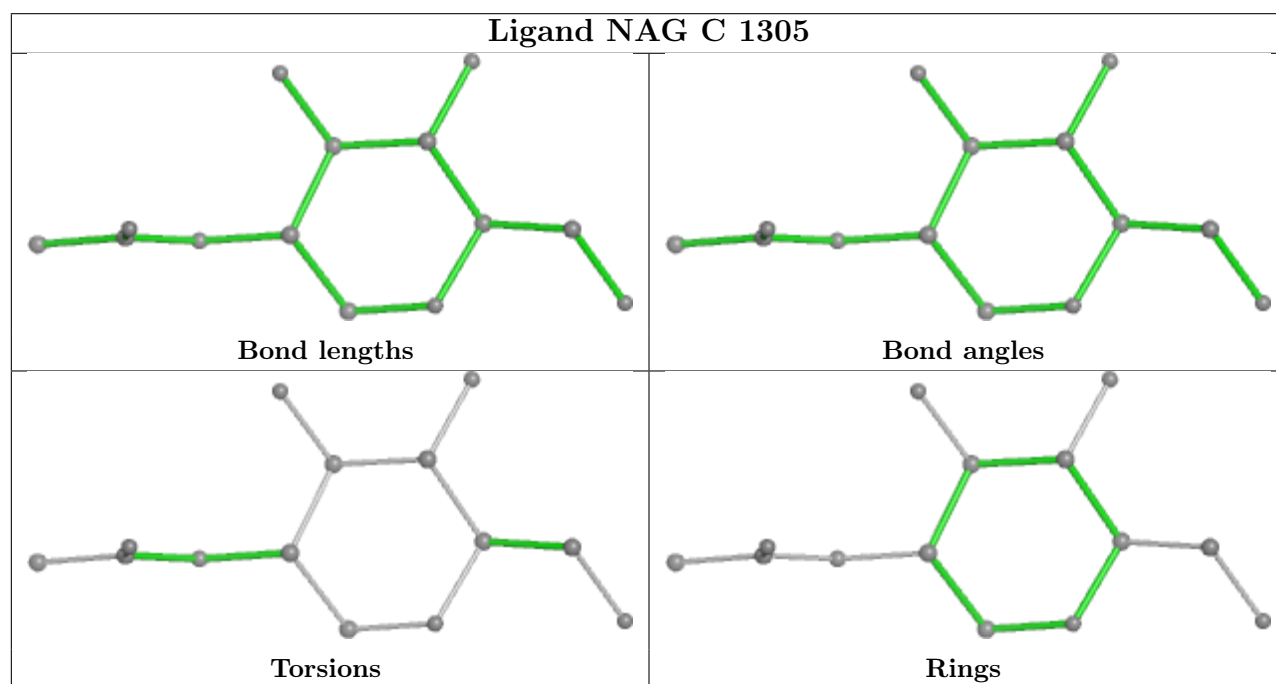
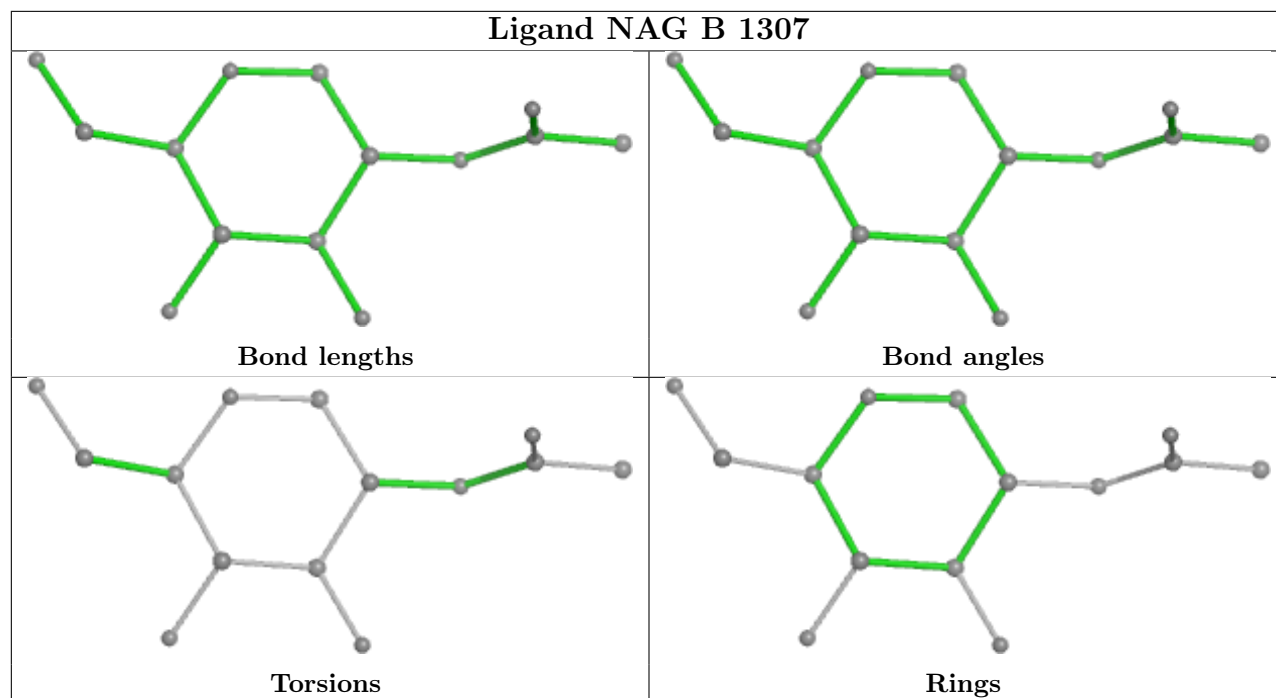


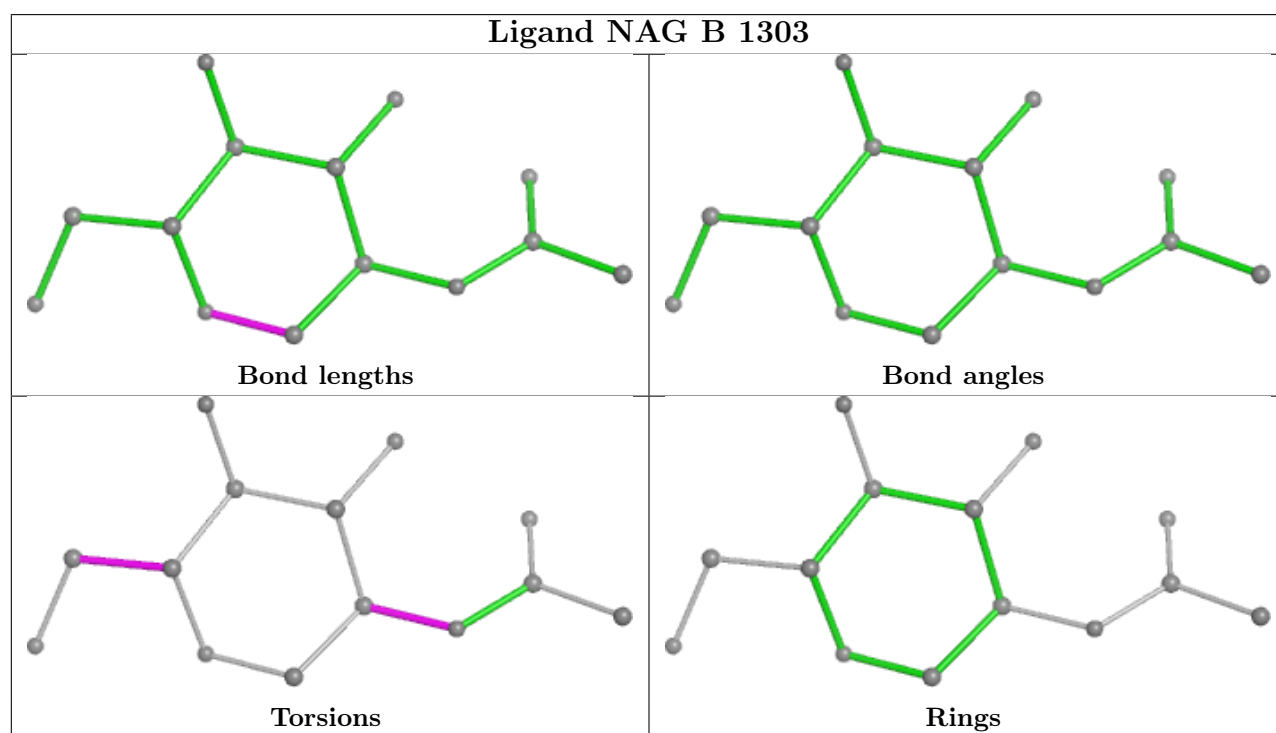
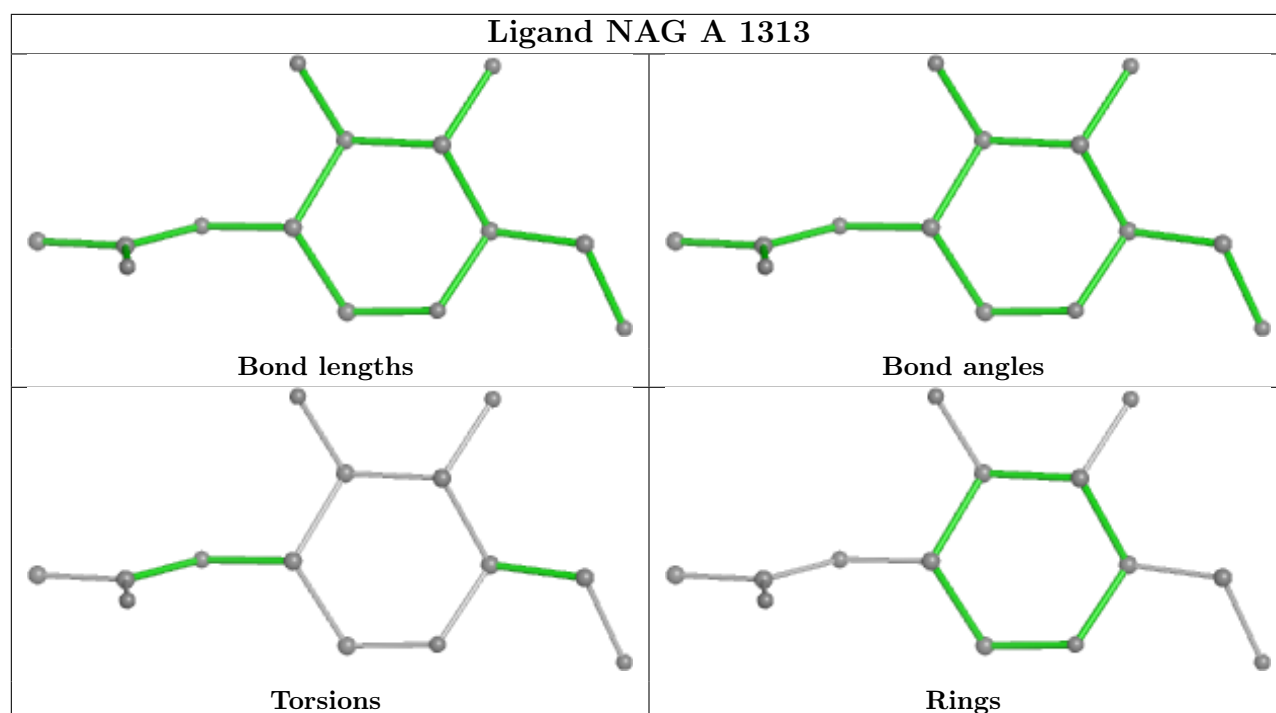


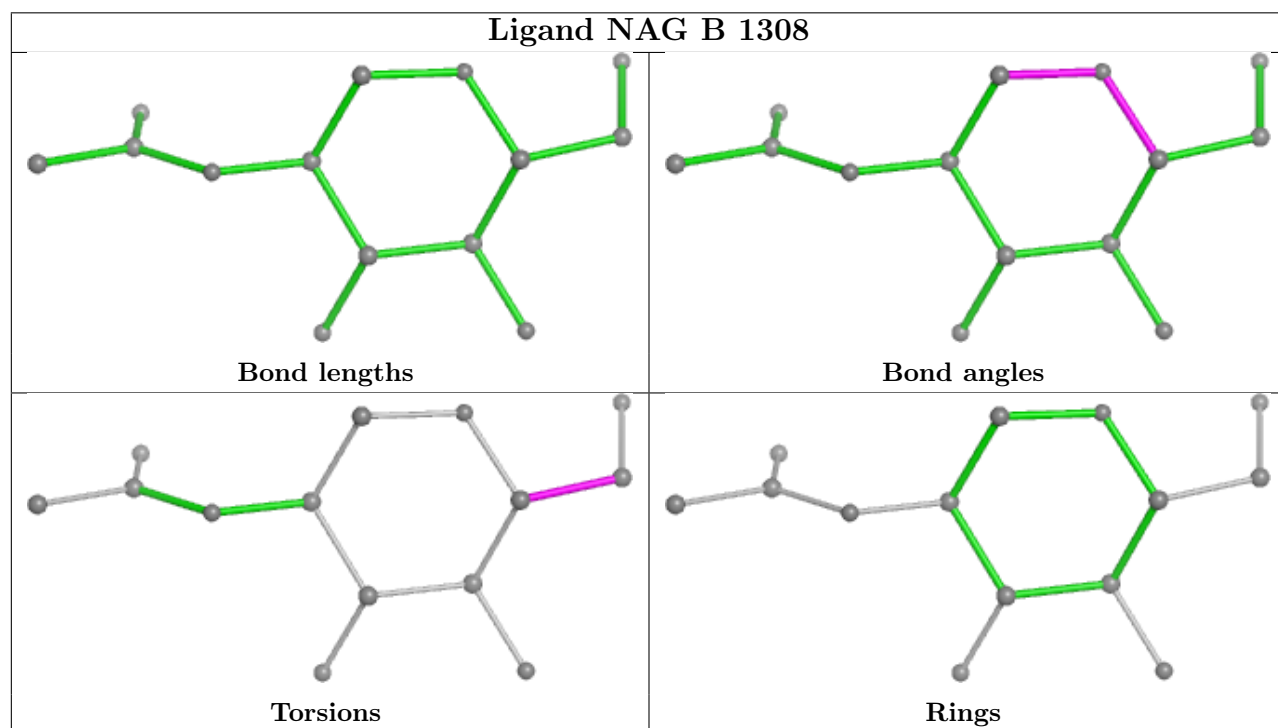
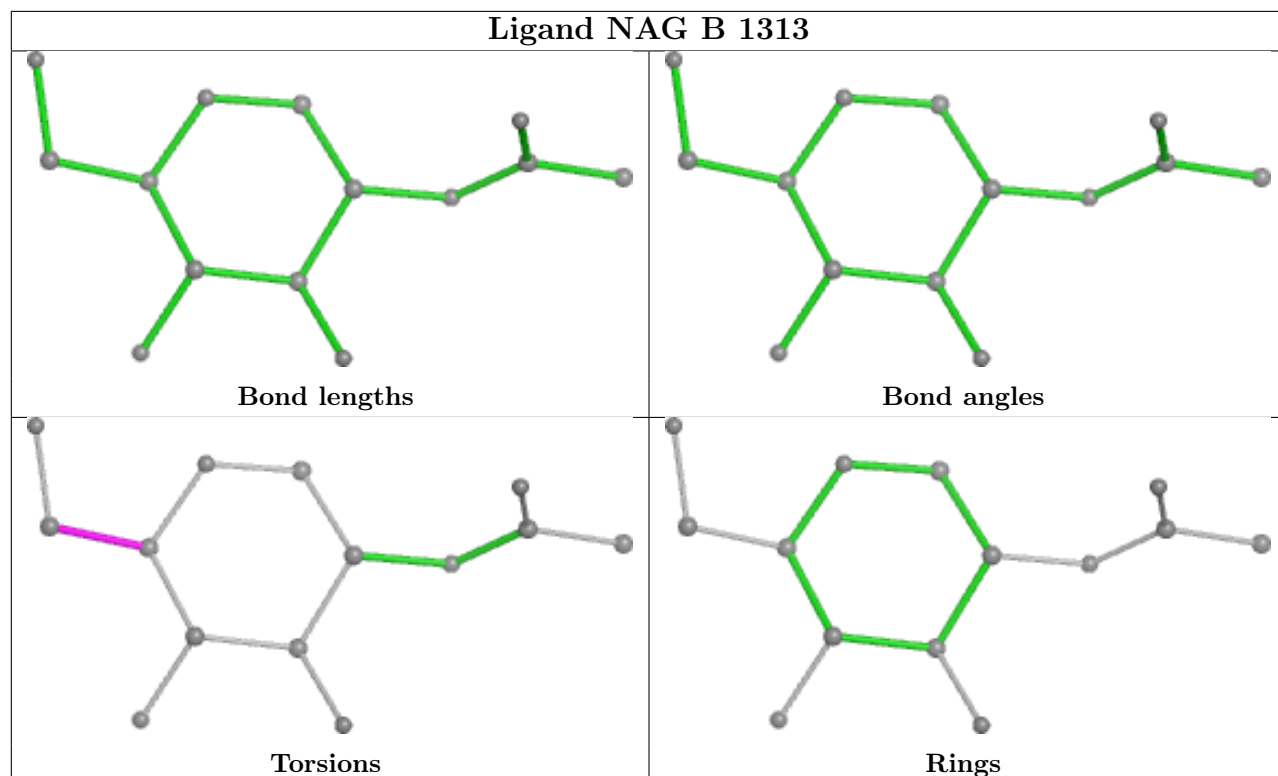


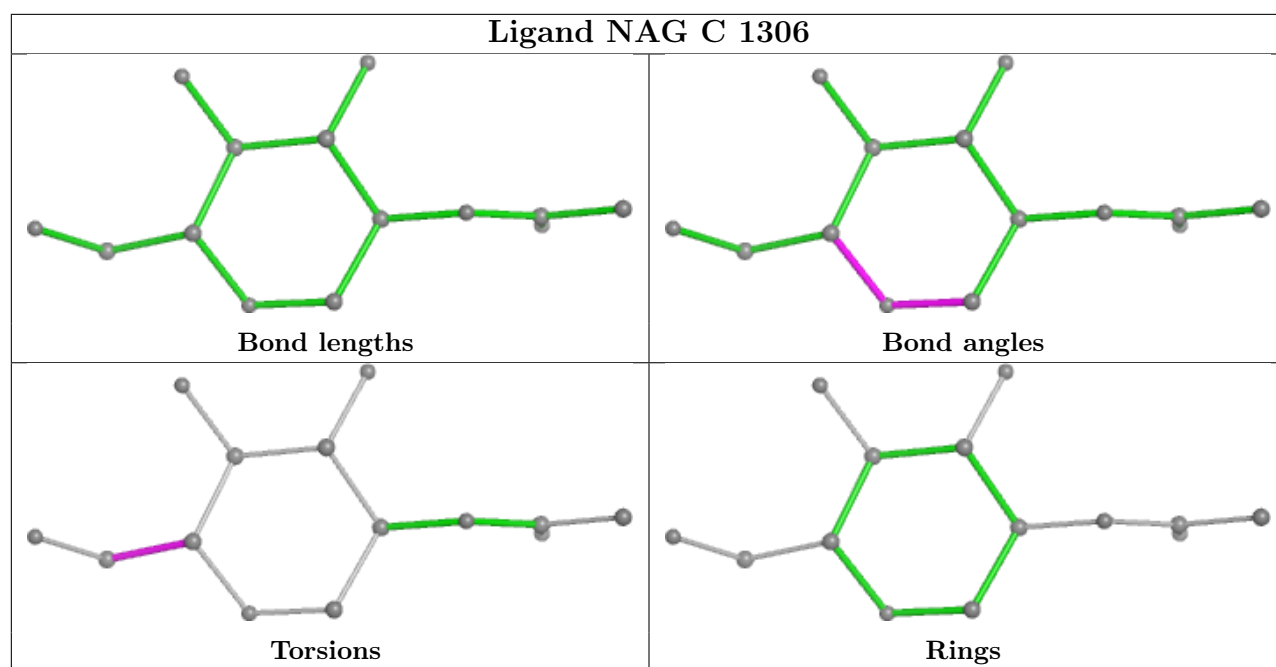












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

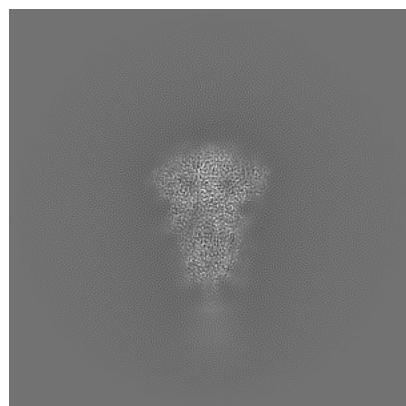
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15475. These allow visual inspection of the internal detail of the map and identification of artifacts.

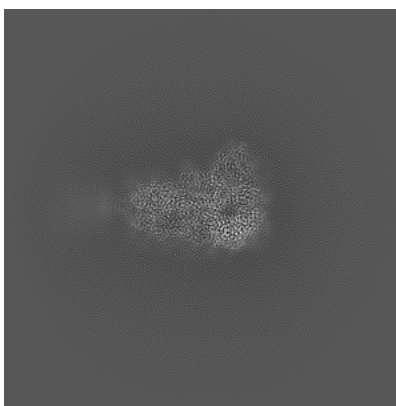
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

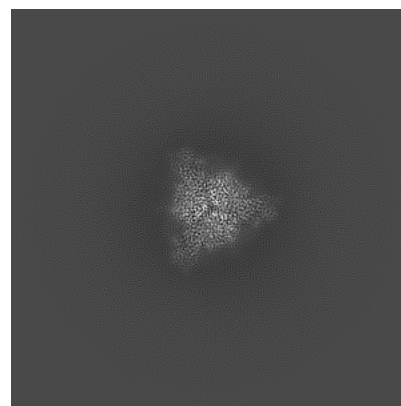
6.1.1 Primary map



X

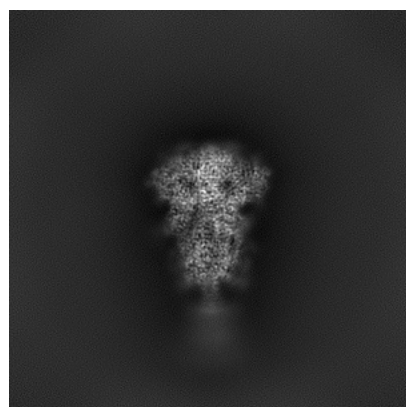


Y

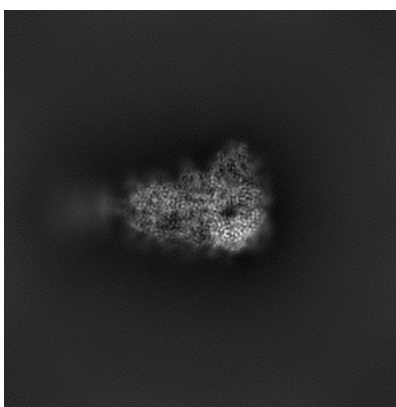


Z

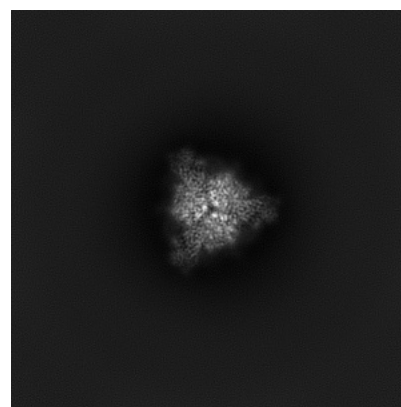
6.1.2 Raw map



X



Y

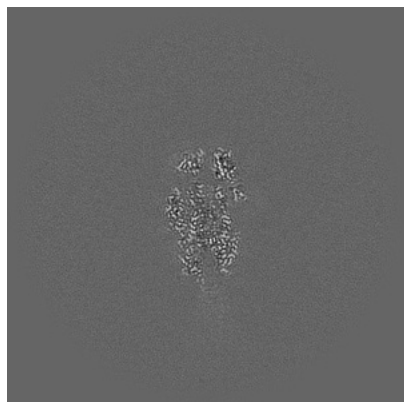


Z

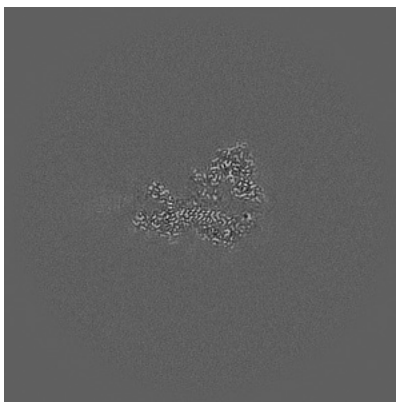
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

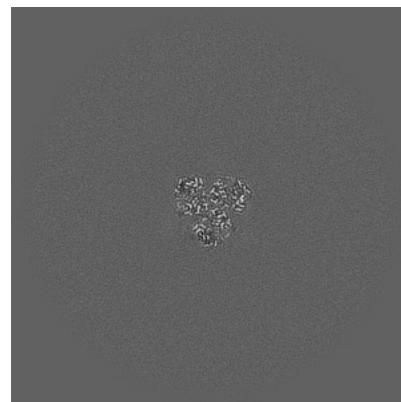
6.2.1 Primary map



X Index: 192

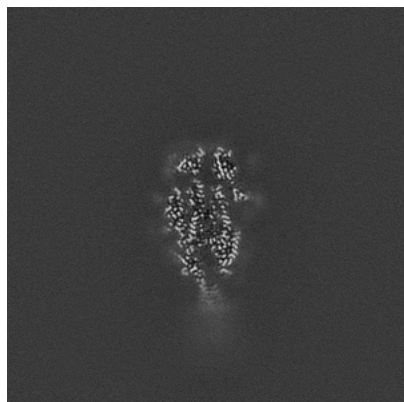


Y Index: 192

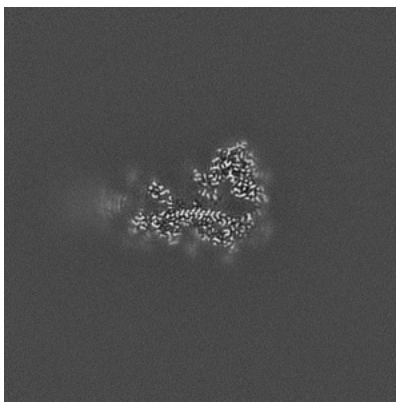


Z Index: 192

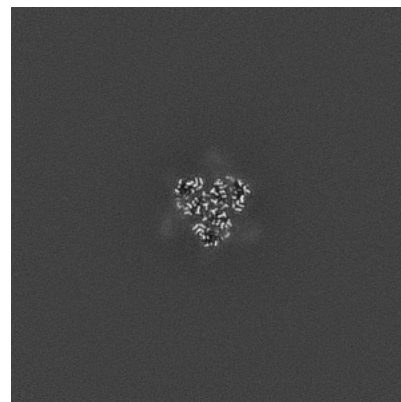
6.2.2 Raw map



X Index: 192



Y Index: 192

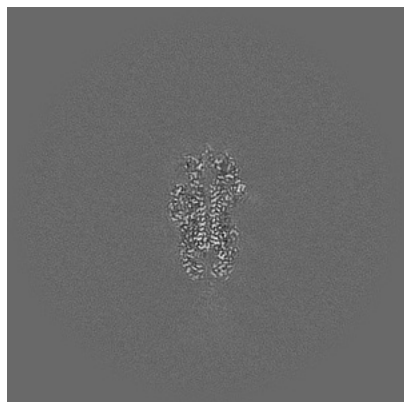


Z Index: 192

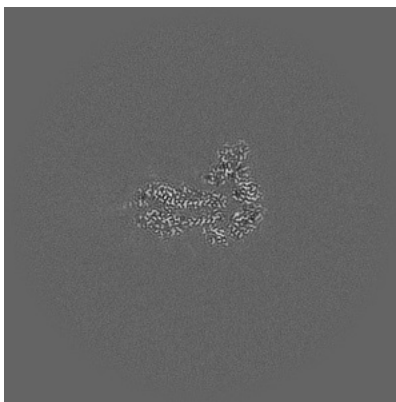
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

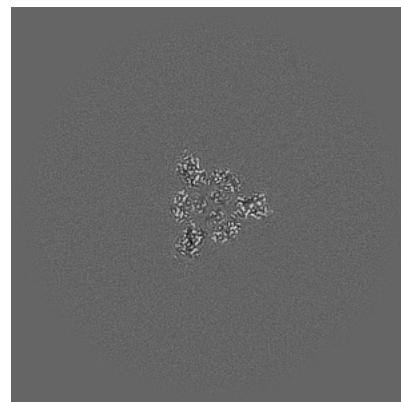
6.3.1 Primary map



X Index: 197



Y Index: 186

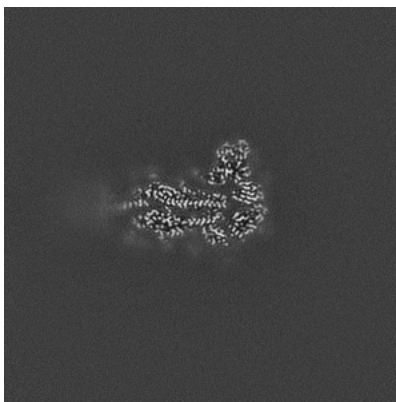


Z Index: 210

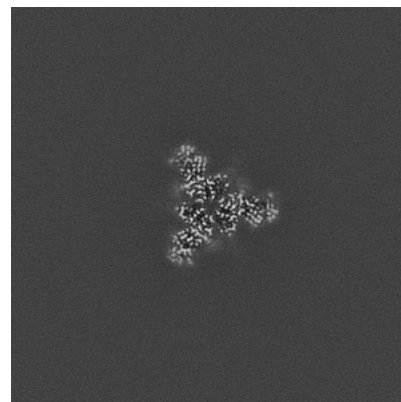
6.3.2 Raw map



X Index: 197



Y Index: 186

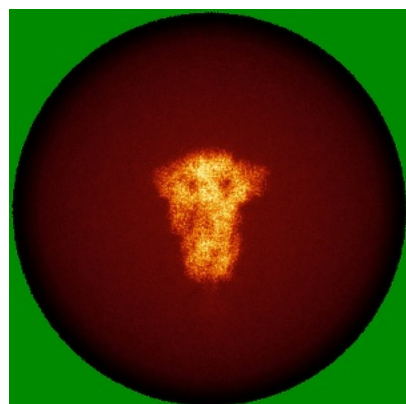


Z Index: 226

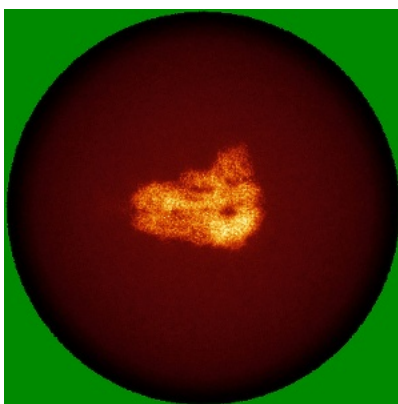
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

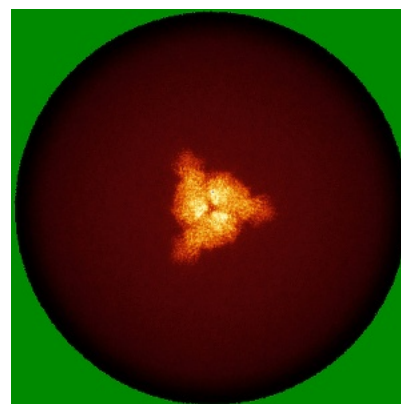
6.4.1 Primary map



X

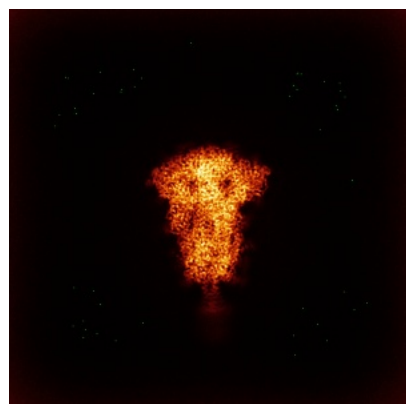


Y

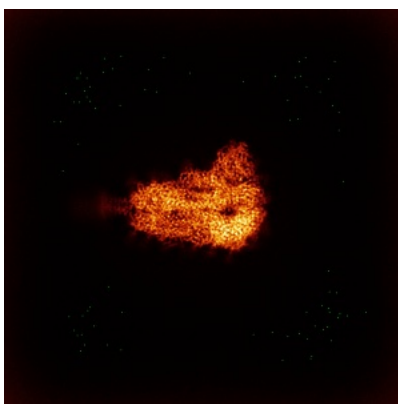


Z

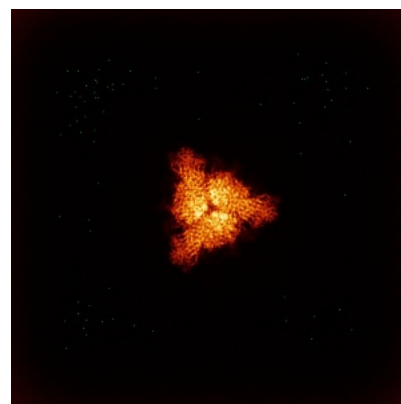
6.4.2 Raw map



X



Y

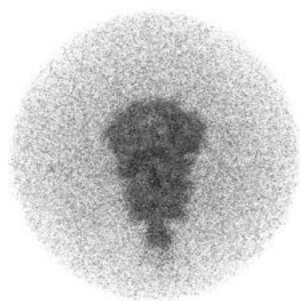


Z

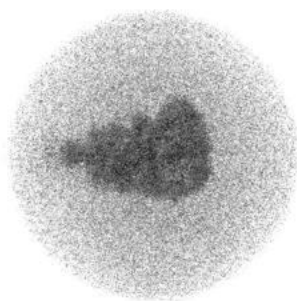
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

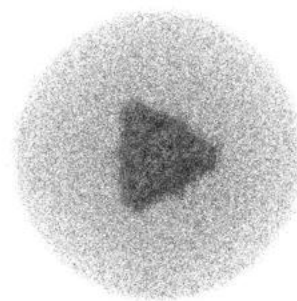
6.5.1 Primary map



X



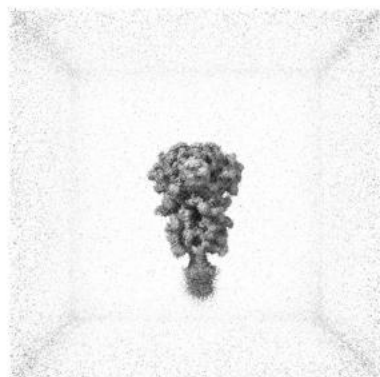
Y



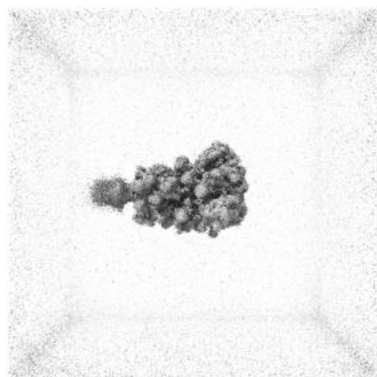
Z

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

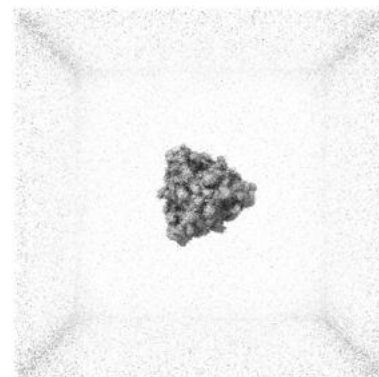
6.5.2 Raw map



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.

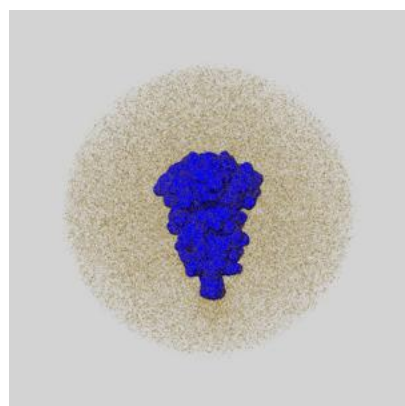
6.6 Mask visualisation [i](#)

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

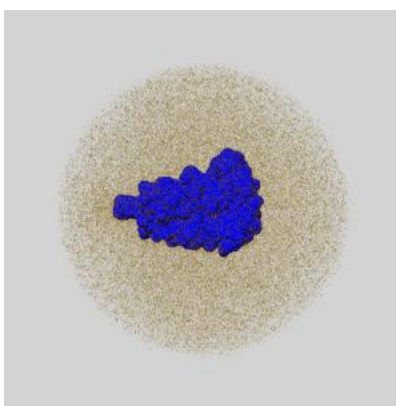
A mask typically either:

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

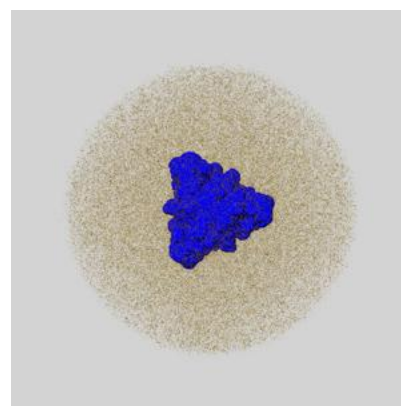
6.6.1 emd_15475_msk_1.map [i](#)



X



Y

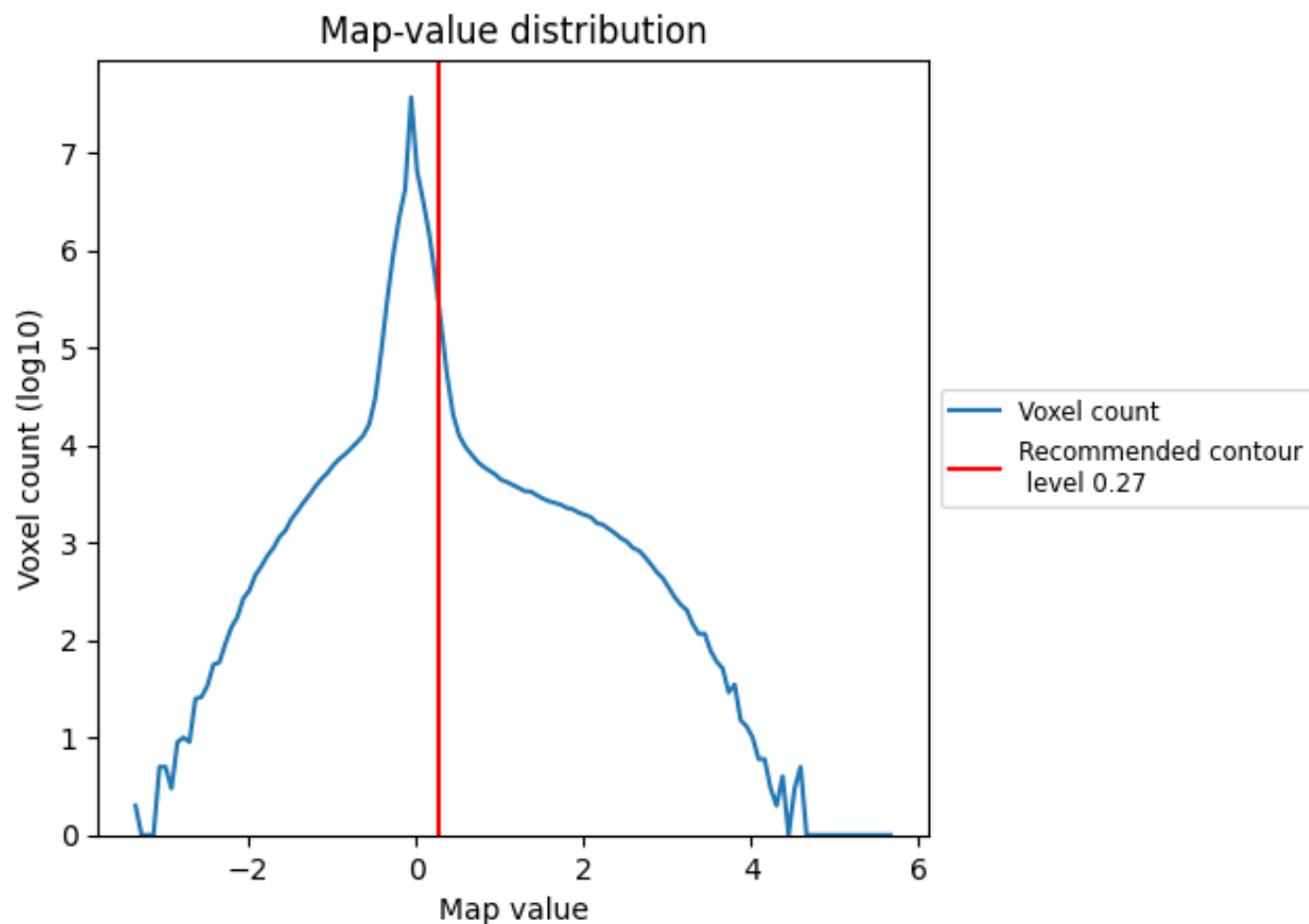


Z

7 Map analysis [i](#)

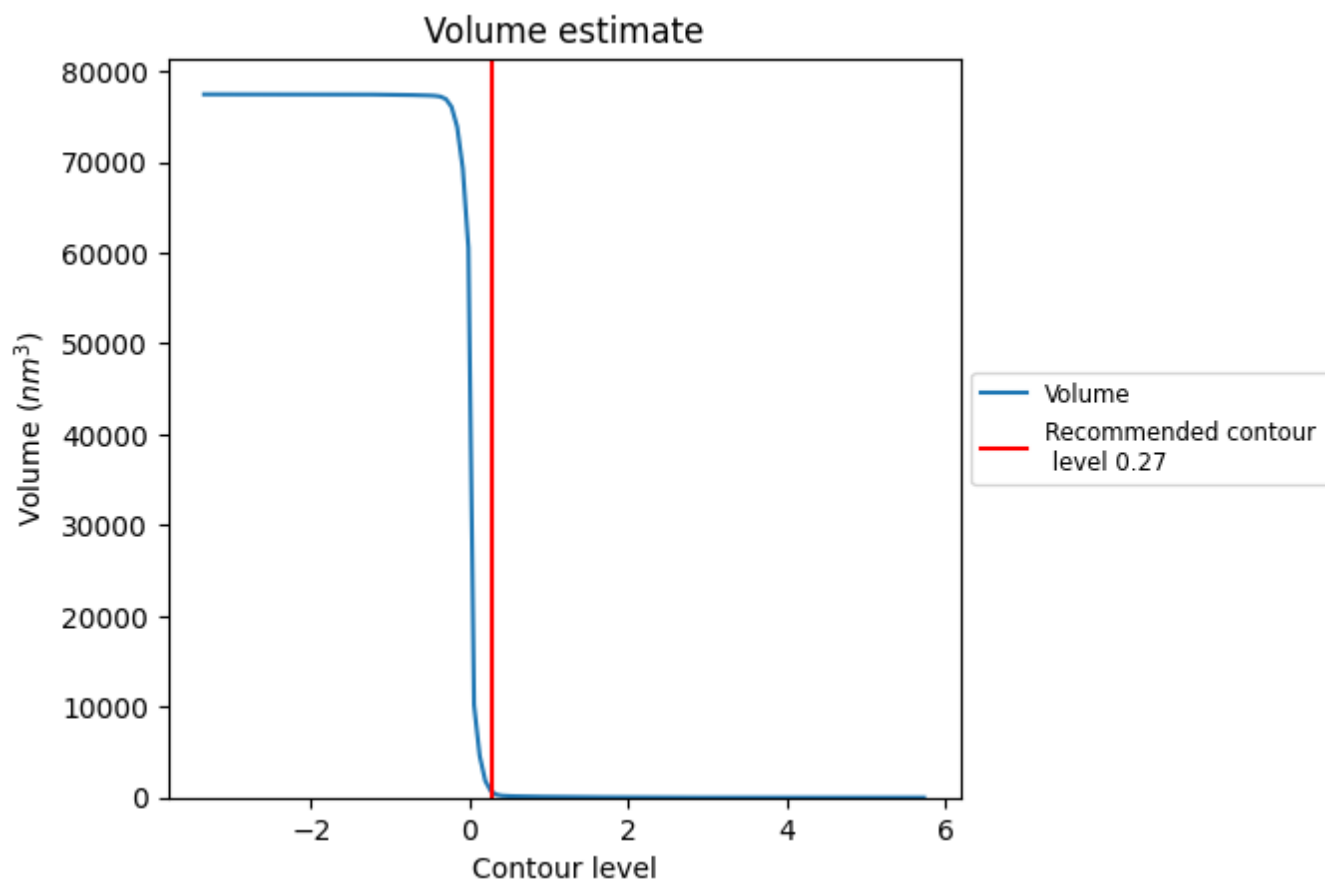
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

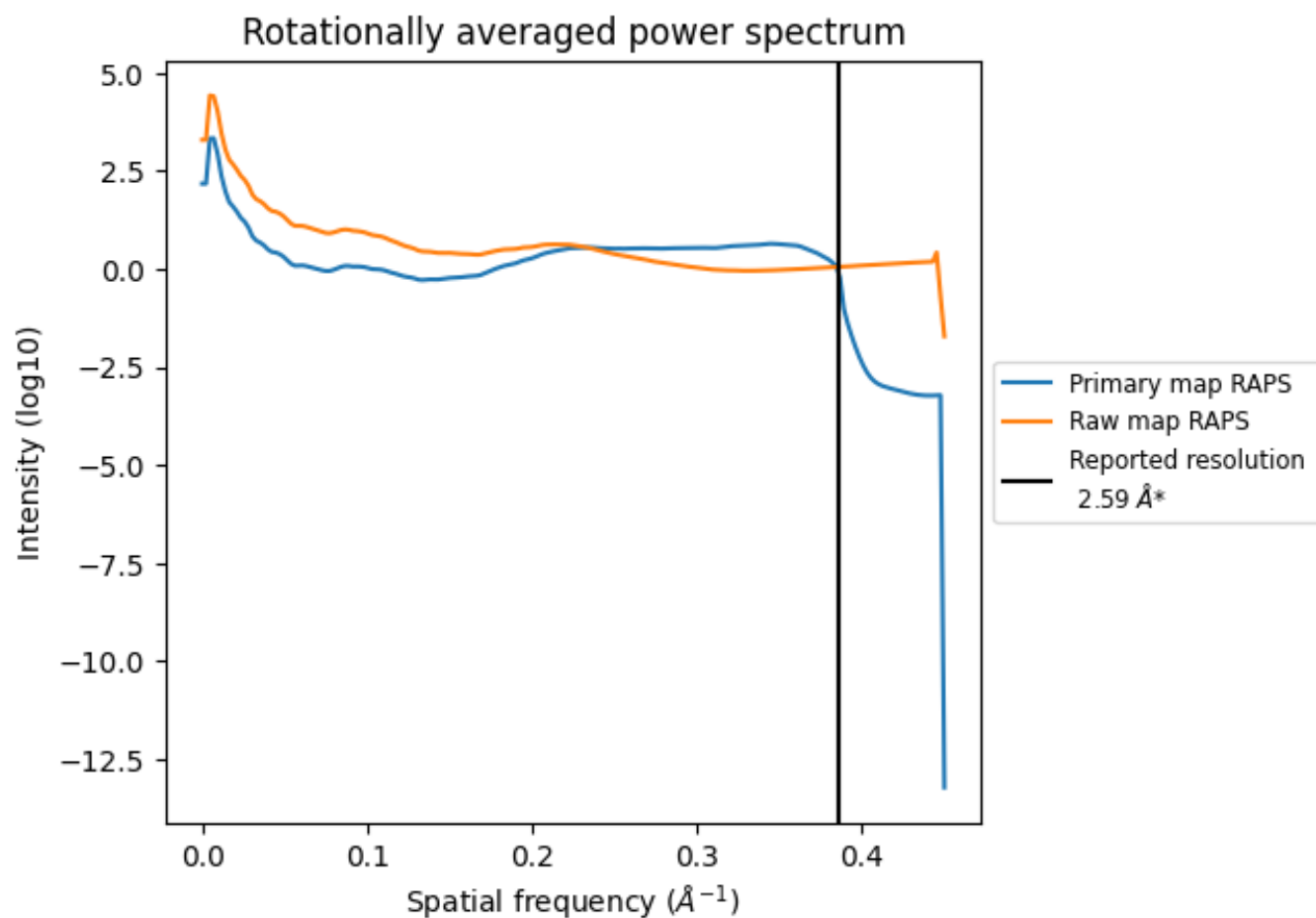
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 698 nm^3 ; this corresponds to an approximate mass of 631 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 ⓘ

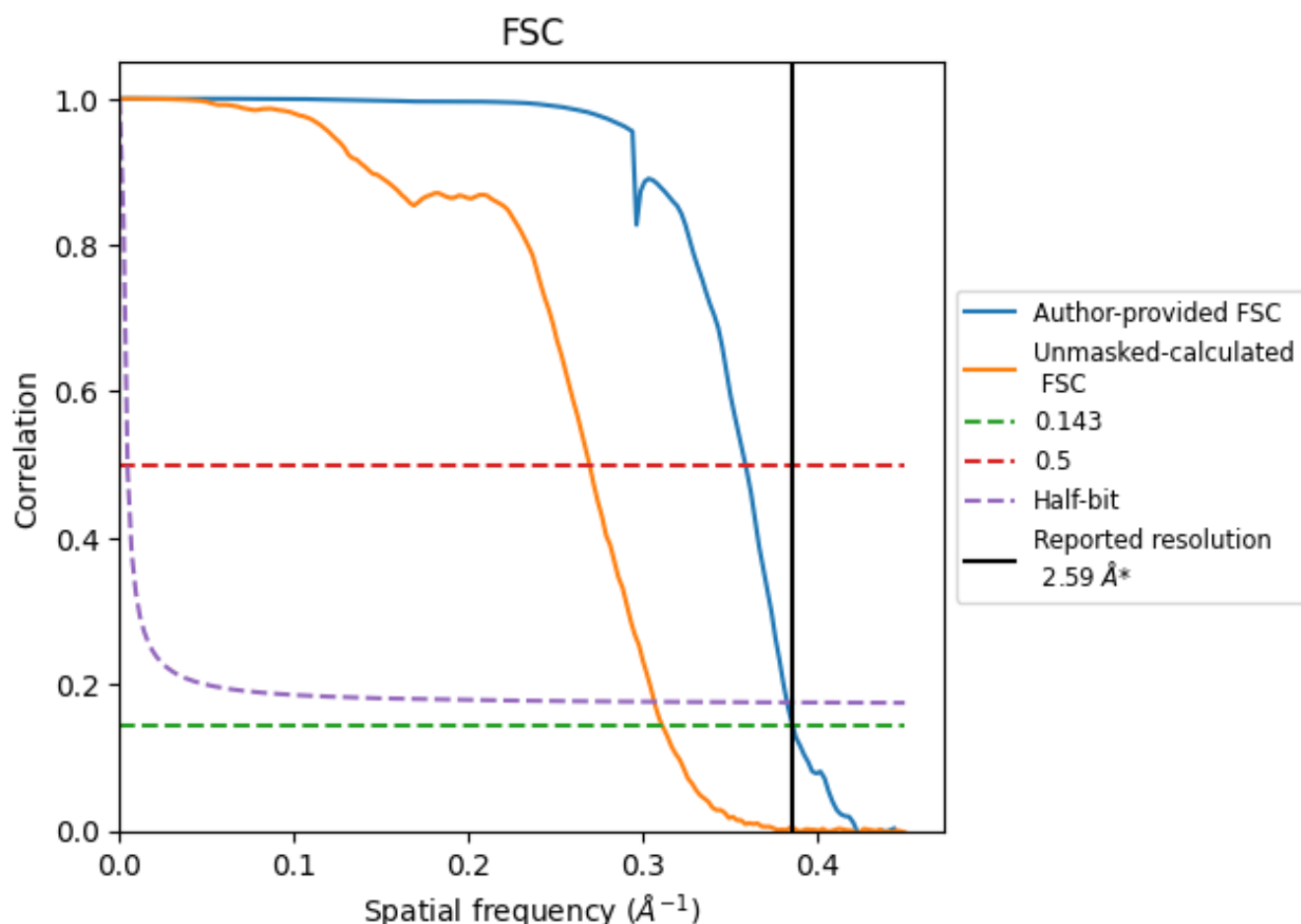


*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

8.2 Resolution estimates [i](#)

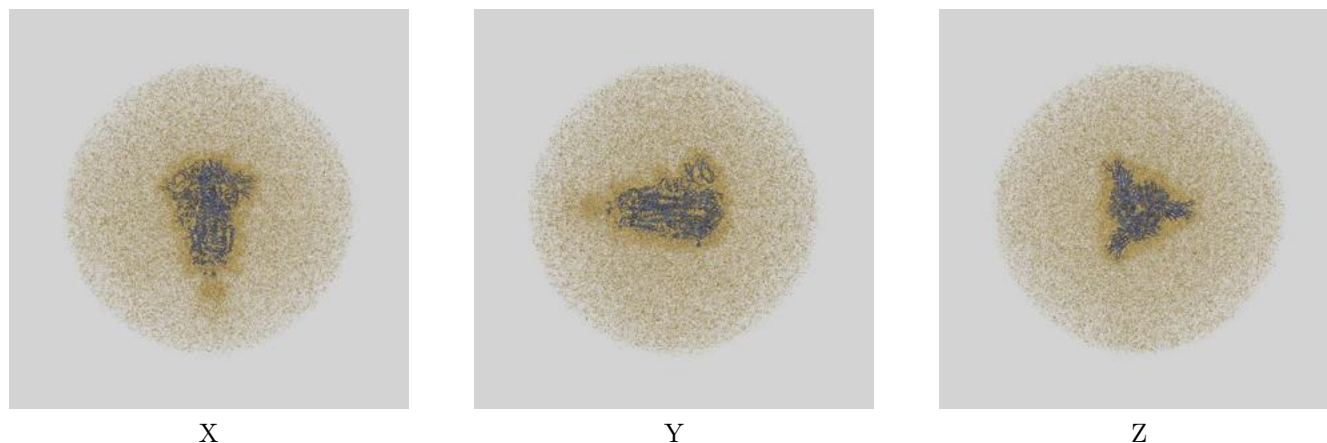
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	2.78	2.61
Unmasked-calculated*	3.21	3.71	3.26

*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 3.21 differs from the reported value 2.59 by more than 10 %

9 Map-model fit [i](#)

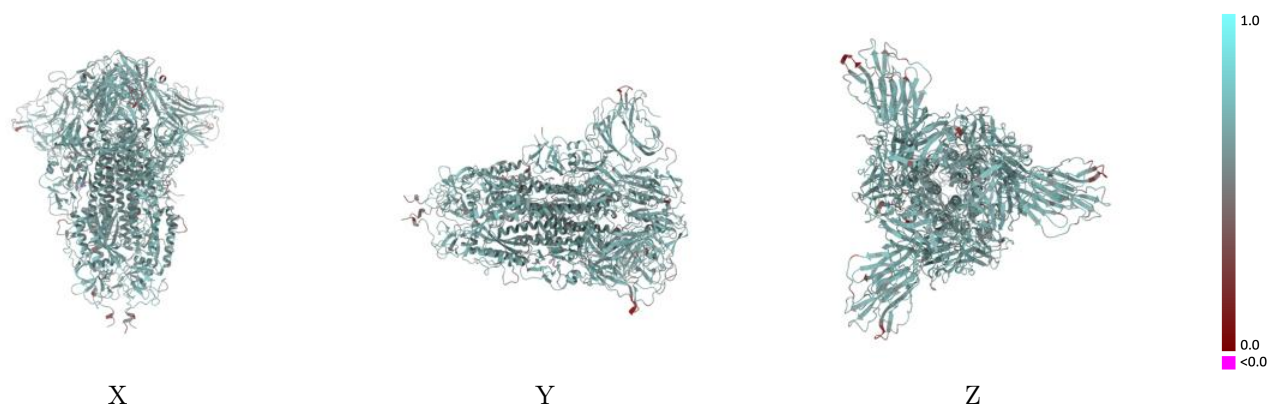
This section contains information regarding the fit between EMDB map EMD-15475 and PDB model 8AJA. Per-residue inclusion information can be found in [section 3](#) on [page 32](#).

9.1 Map-model overlay [i](#)



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 [i](#)



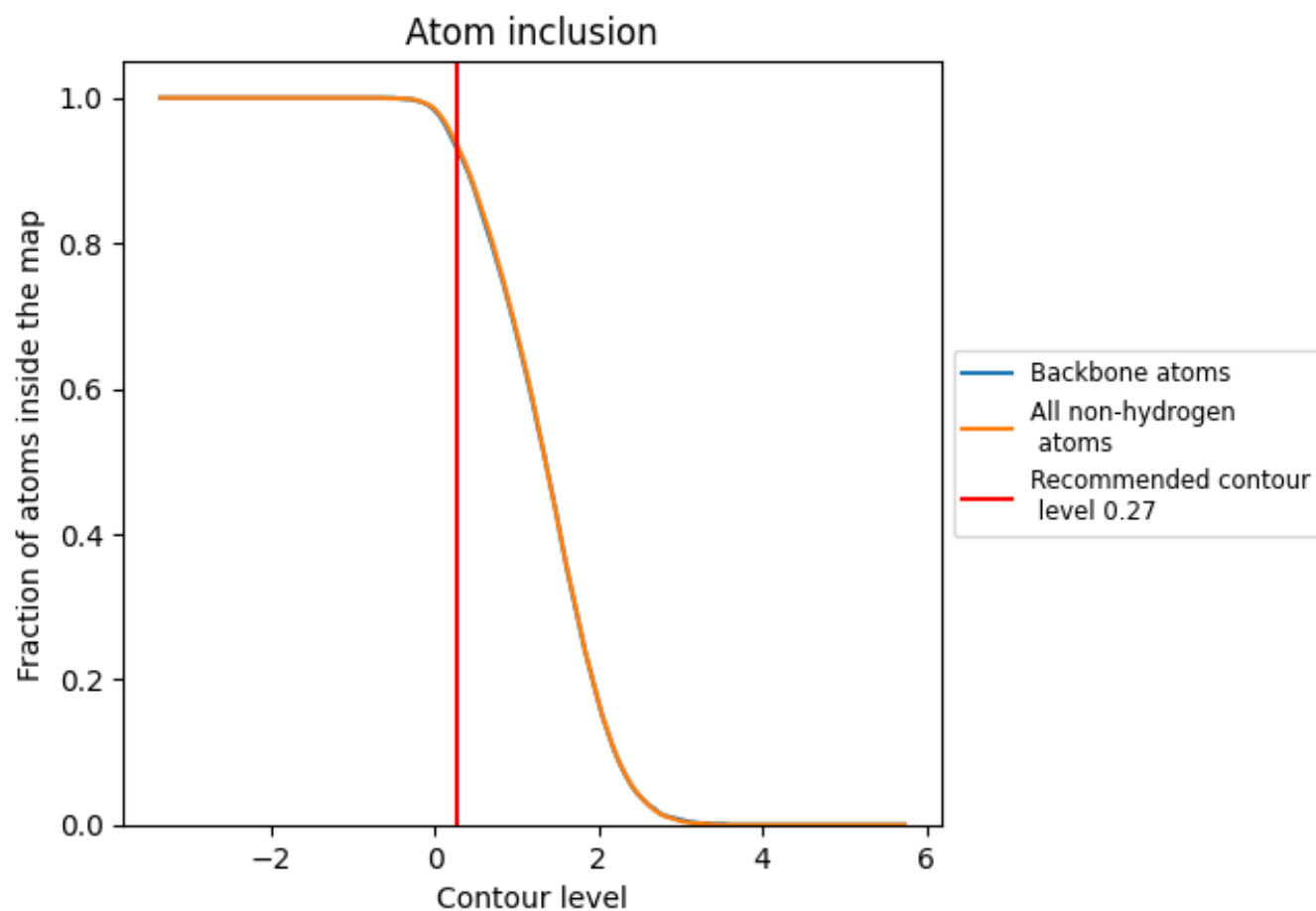
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 94% 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	<div></div> 0.9350	<div></div> 0.6040
A	<div></div> 0.9370	<div></div> 0.6050
B	<div></div> 0.9390	<div></div> 0.6080
C	<div></div> 0.9370	<div></div> 0.6060
L	<div></div> 0.8570	<div></div> 0.5210
M	<div></div> 0.7140	<div></div> 0.3740
N	<div></div> 0.7500	<div></div> 0.3920
P	<div></div> 0.7860	<div></div> 0.4520
Q	<div></div> 0.6790	<div></div> 0.4010
R	<div></div> 0.7140	<div></div> 0.3880
T	<div></div> 0.7500	<div></div> 0.4810
U	<div></div> 0.7500	<div></div> 0.4430
V	<div></div> 0.7860	<div></div> 0.4490

