



wwPDB EM Validation Summary Report ⓘ

Apr 25, 2023 – 02:19 PM JST

PDB ID : 7YE9
EMDB ID : EMD-33766
Title : SARS-CoV-2 Spike (6P) in complex with 3 R1-32 Fabs
Authors : Liu, B.; Gao, X.; Li, Z.; Chen, X.; He, J.; Chen, L.; Xiong, X.
Deposited on : 2022-07-05
Resolution : 4.17 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

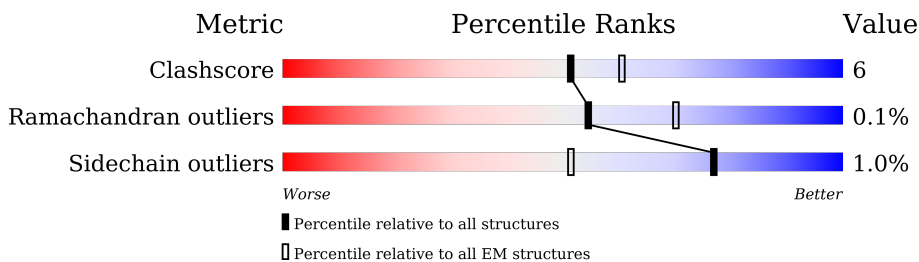
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.17 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1208	
1	B	1208	
1	C	1208	
2	G	228	
2	H	228	
2	N	228	
3	I	214	
3	L	214	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	O	214	<p>84% 79% 20%</p>
4	D	2	<p>50% 50%</p>
4	E	2	<p>50% 100%</p>
4	F	2	<p>50% 50%</p>
4	J	2	<p>50% 100%</p>
4	K	2	<p>50% 50%</p>
4	M	2	<p>50% 100%</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35208 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1066	8344	5324	1394	1588	38	0	0
1	B	1066	8344	5324	1394	1588	38	0	0
1	C	1066	8344	5324	1394	1588	38	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of R1-32 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	227	Total	C	N	O	S	2	0
			1667	1049	277	332	9		
2	G	227	Total	C	N	O	S	2	0
			1667	1049	277	332	9		
2	N	227	Total	C	N	O	S	2	0
			1667	1049	277	332	9		

- Molecule 3 is a protein called Light chain of R1-32 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	213	Total	C	N	O	S	0	0
			1557	971	261	321	4		
3	I	213	Total	C	N	O	S	0	0
			1557	971	261	321	4		
3	O	213	Total	C	N	O	S	0	0
			1557	971	261	321	4		

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



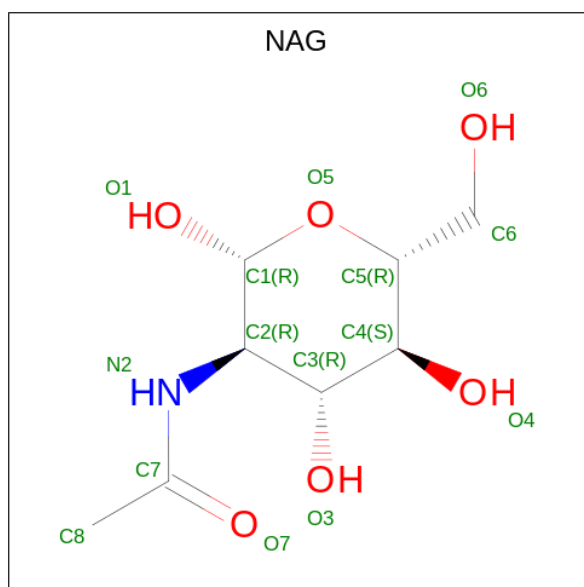
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	M	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

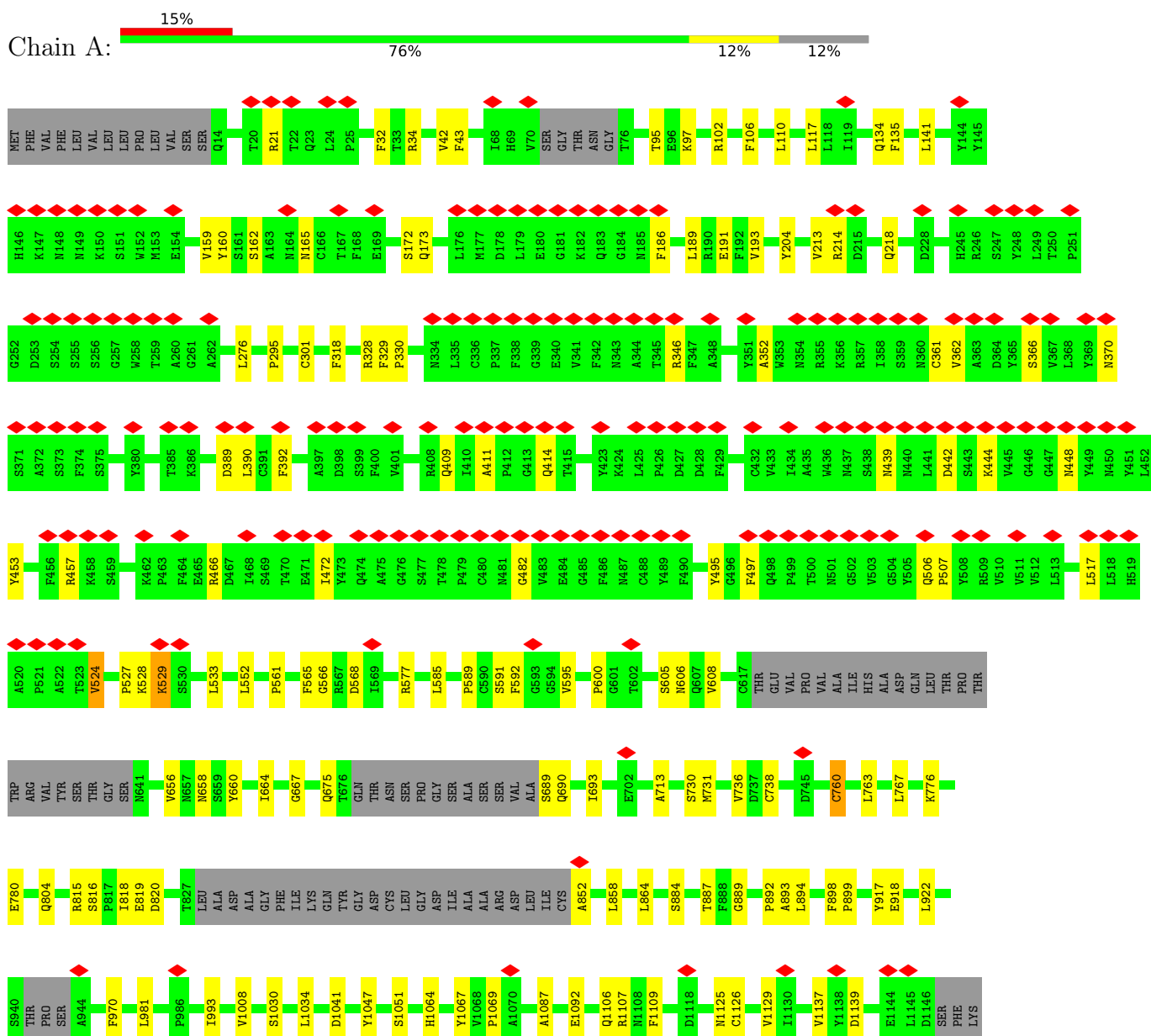
Continued from previous page...

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

3 Residue-property plots

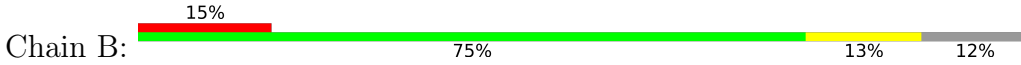
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein



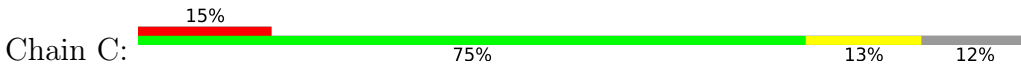
GLU	GLU	PHE	ASP	LYS	TYR	PHE	LYS	ASN	HIS	THR	SER	SER	PRO	ASP	VAL	ASP	LEU	GLY	ASP	ILE	SER	GLY	ILE	ASN	ALA	SER	VAL	VAL	VAL	ASN	ILE	ILE	GLN	LYS	GLU	ILE	ASP	ARG	LEU	ASN	GLY	VAL	VAL	ALA	LYS	ASN	LEU	ASN	GLU	SER	SER	LEU	LEU	LEU	GLY	LYS	TYR	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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

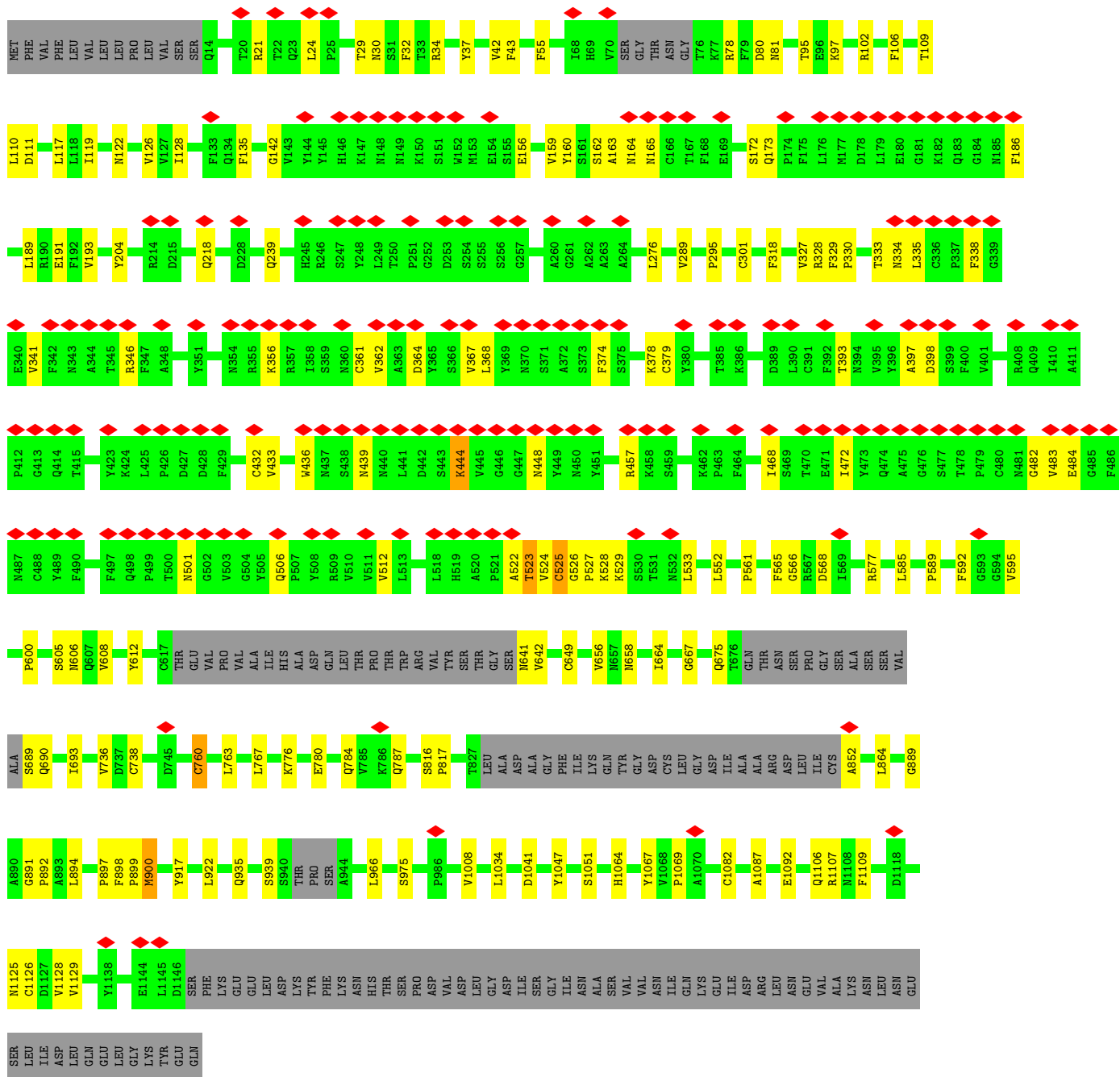
● Molecule 1: Spike glycoprotein



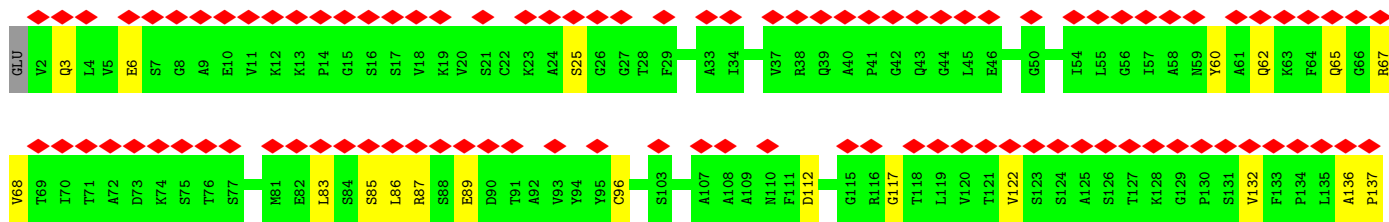
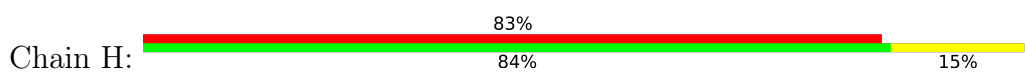
MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	VAL	THR	SER	SER	PRO	SER	ASP	VAL	ASP	LEU	GLY	ASP	ILE	SER	GLY	ILE	ASN	ALA	SER	VAL	VAL	VAL	ASN	ILE	ILE	GLN	LYS	GLU	ILE	ASP	ARG	LEU	ASN	GLY	VAL	VAL	ALA	LYS	ASN	LEU	ASN	GLU	SER	SER	LEU	LEU	LEU	GLY	LYS	TYR	GLN	
L118	I119	M122	V126	F135	G142	Y144	Y145	H146	K147	N148	N149	K150	S151	W152	M153	E154	S155	E156	V159	Y160	M164	N165	C166	T167	H69	V70	SER	GLY	THR	ASN	ALA	LYS	GLY	S172	Q173	L176	M177	D178	L179	E180	G181	K182	Q183	G184	N185	F186	L189	R190	E191	F192	V193	Y204	R214	D215						
L216	P217	Q218	D228	Q239	L242	S247	Y248	L249	T250	P251	G252	D253	S254	S255	S256	Q257	A260	Q261	A262	A263	A264	L276	V289	P295	C301	R319	T323	E324	V327	R328	F329	P330	N331	N334	L335	C336	F337	F338	G339	E340	A411	P412	G413	Q414	A344	T415	G416	Y423	K424	L425										
F347	A348	S349	V350	Y351	A352	N354	R355	K356	R357	S359	N360	C361	V362	A363	D364	Y365	S366	V367	L368	Y369	N370	S371	A372	S373	F374	S375	Y380	T385	K386	L387	N388	D389	L390	F392	T393	N394	A397	D398	V407	R408	Q409	I410	A411	P412	G413	Q414	T415	G416	Y423	K424	L425									
P426	D427	D428	F429	T430	G431	C432	V433	A435	W436	N437	S438	N439	N440	L441	D442	S443	K444	V445	G446	G447	N448	V449	N450	Y451	R457	K458	S459	N460	L461	K462	P463	F464	E465	R466	D467	I468	S469	T470	E471	I472	Y473	Q474	A475	G476	S477	T478	P479	C480	N481	G482	V483	E484	G485	F486	N487	C488	Y489			
F490	F497	Q498	P499	T500	H501	G502	V503	G504	Y505	Q506	P507	Y508	R509	V510	W511	Y512	L513	L517	L518	H519	A520	P521	A522	T523	Y524	C525	K528	K529	S530	T531	N532	V539	N542	L552	P561	F565	G566	R567	D568	I569	R577	L585	S591	S605	N606	I607	Y608													
C617	THR	VAL	PRO	VAL	ALA	HIS	ALA	ASP	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	N641	V656	N657	N658	S659	Y660	O667	S673	Y674	Q675	T676	GLN	THR	ASN	ASN	PRO	GLY	ALA	SER	ALA	ALA	ARG	ASP	LEU	LEU	ILE	CYS	A852	L864	S884	G889	P892								
I726	V736	D745	S746	T747	N751	F759	C760	L767	K776	E780	Q784	R814	S816	F817	T827	LEU	ALA	ASP	ALA	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	ILE	ALA	ALA	LYS	R1107	N1108	F1109	D1118	N1125	C1126	V1129	Y1138	E1144	L1145														
A893	L894	F898	P899	Y917	L922	S940	THR	P80	SER	A944	K947	V976	L977	N978	P986	S1030	L1034	Y1047	S1051	H1064	Y1067	V1068	P1069	C1082	A1087	E1082	Q1106	R1107	N1108	F1109	D1118	N1125	C1126	V1129	Y1138	E1144	L1145																							
B1146	SER	PHE	LYS	GLU	GLU	LEU	ASP	TYR	PHE	LYS	ASN	HIS	THR	SER	PRO	ASP	VAL	ASP	LEU	GLY	ASP	ILE	SER	GLY	ILE	ASN	ALA	SER	VAL	VAL	VAL	ASN	ILE	LYS	GLU	ILE	ASP	ARG	LEU	ASN	ASN	GLU	VAL	ALA	LYS	ASN	LEU	ASN	ASN	GLU	SER	LEU	ILE	ASP	LEU	GLN	GLU	LEU	GLY	LYS
TYR	GLU	GLN																																																										

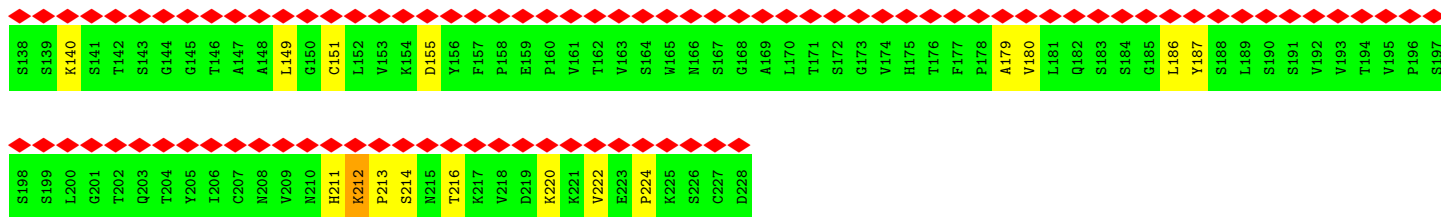
● Molecule 1: Spike glycoprotein



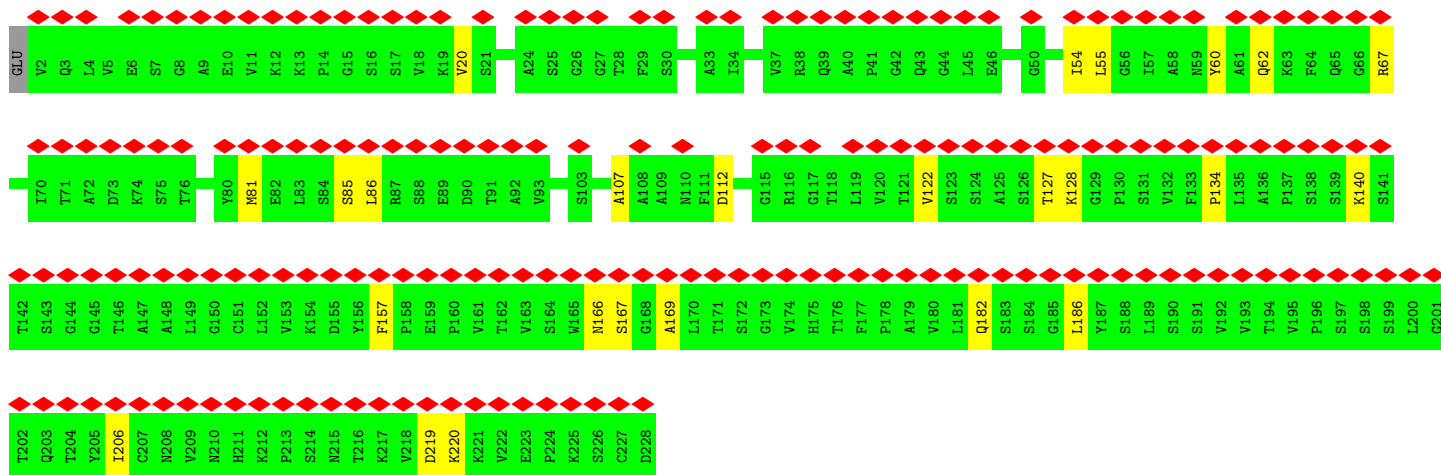
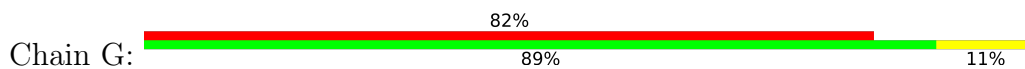


• Molecule 2: Heavy chain of R1-32 Fab

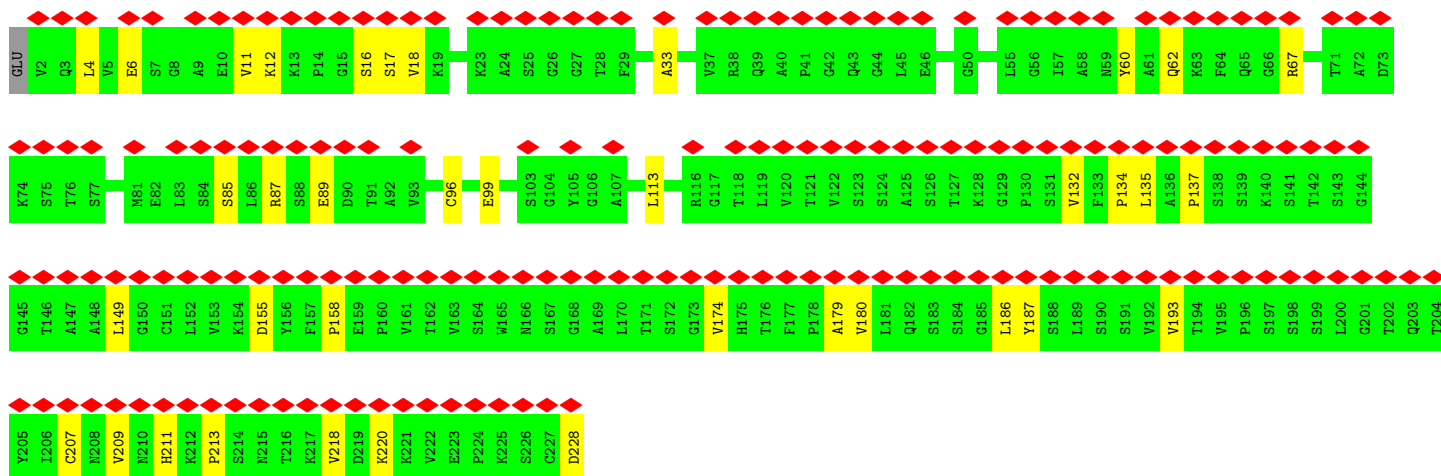
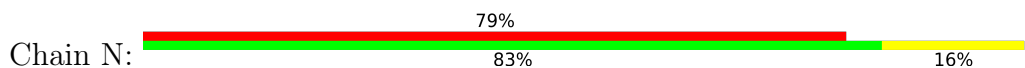




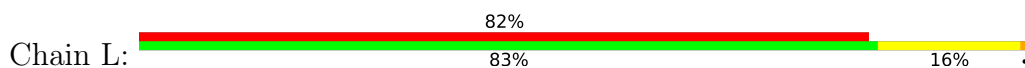
• Molecule 2: Heavy chain of R1-32 Fab



• Molecule 2: Heavy chain of R1-32 Fab

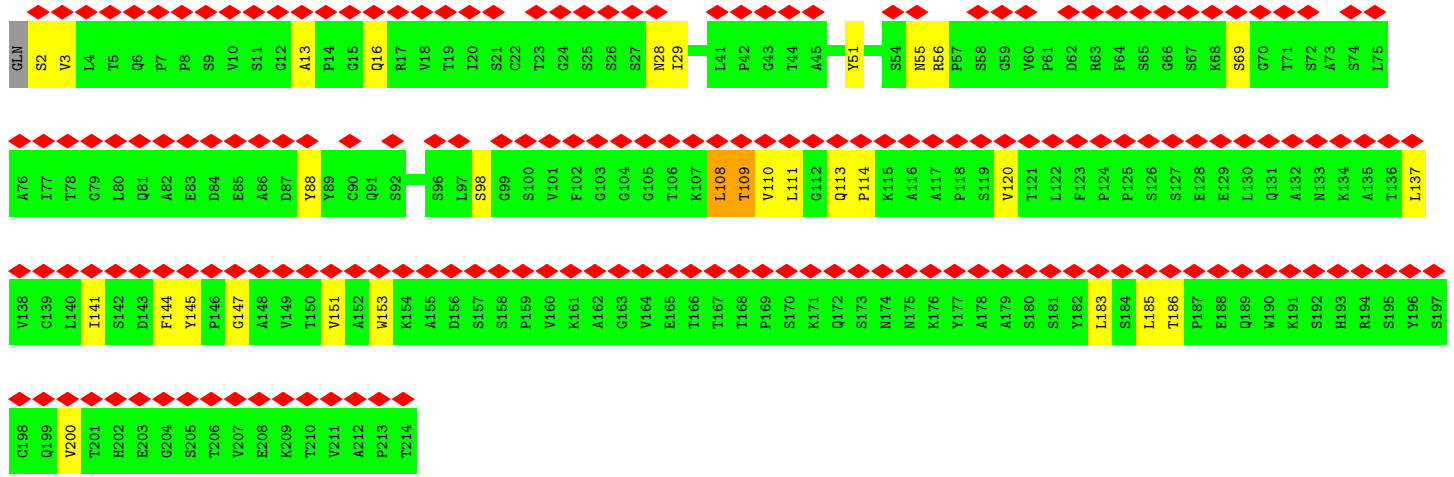
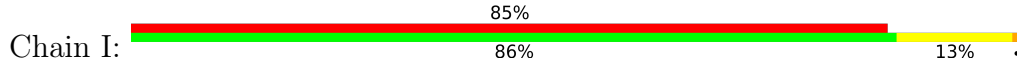


• Molecule 3: Light chain of R1-32 Fab

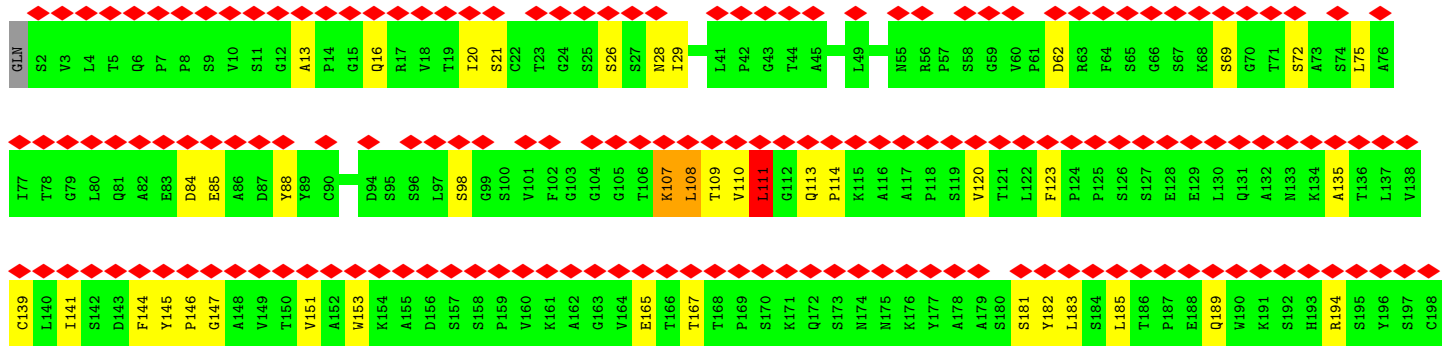
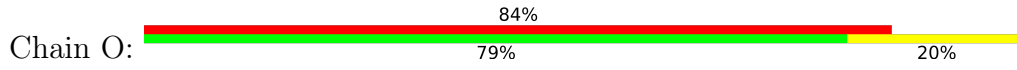




• Molecule 3: Light chain of R1-32 Fab



• Molecule 3: Light chain of R1-32 Fab





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



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



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



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



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



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56902	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	337.91998, 337.91998, 337.91998	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7599999, 1.7599999, 1.7599999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/8540	0.42	0/11624
1	B	0.25	0/8540	0.42	0/11624
1	C	0.25	0/8540	0.42	0/11624
2	G	0.25	0/1710	0.47	0/2328
2	H	0.25	0/1710	0.47	0/2328
2	N	0.25	0/1710	0.45	0/2328
3	I	0.25	0/1595	0.45	0/2181
3	L	0.25	0/1595	0.44	0/2181
3	O	0.25	0/1595	0.45	0/2181
All	All	0.25	0/35535	0.43	0/48399

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8344	0	8128	93	0
1	B	8344	0	8128	103	0
1	C	8344	0	8128	114	0
2	G	1667	0	1639	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1667	0	1639	26	0
2	N	1667	0	1639	21	0
3	I	1557	0	1498	22	0
3	L	1557	0	1498	28	0
3	O	1557	0	1498	36	0
4	D	28	0	25	1	0
4	E	28	0	25	0	0
4	F	28	0	25	1	0
4	J	28	0	25	0	0
4	K	28	0	25	1	0
4	M	28	0	25	0	0
5	A	112	0	104	0	0
5	B	112	0	104	0	0
5	C	112	0	104	0	0
All	All	35208	0	34257	404	0

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

The worst 5 of 404 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1069:PRO:HG2	1:C:892:PRO:HD2	1.52	0.90
1:A:1069:PRO:HG2	1:B:892:PRO:HD2	1.52	0.89
3:I:113:GLN:HA	3:I:145:TYR:HE1	1.39	0.86
1:B:328:ARG:HG2	1:B:530:SER:HA	1.60	0.82
1:C:816:SER:HB3	1:C:817:PRO:HD2	1.64	0.78

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	1054/1208 (87%)	1017 (96%)	35 (3%)	2 (0%)	47	80
1	B	1054/1208 (87%)	1026 (97%)	28 (3%)	0	100	100
1	C	1054/1208 (87%)	1021 (97%)	32 (3%)	1 (0%)	51	85
2	G	227/228 (100%)	220 (97%)	7 (3%)	0	100	100
2	H	227/228 (100%)	223 (98%)	4 (2%)	0	100	100
2	N	227/228 (100%)	221 (97%)	6 (3%)	0	100	100
3	I	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
3	L	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
3	O	211/214 (99%)	201 (95%)	9 (4%)	1 (0%)	29	68
All	All	4476/4950 (90%)	4333 (97%)	139 (3%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	529	LYS
3	O	111	LEU
1	C	522	ALA
1	A	527	PRO

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	934/1056 (88%)	927 (99%)	7 (1%)	84	90
1	B	934/1056 (88%)	924 (99%)	10 (1%)	73	84
1	C	934/1056 (88%)	928 (99%)	6 (1%)	86	92
2	G	186/186 (100%)	185 (100%)	1 (0%)	88	93
2	H	186/186 (100%)	184 (99%)	2 (1%)	73	84
2	N	186/186 (100%)	184 (99%)	2 (1%)	73	84
3	I	174/177 (98%)	170 (98%)	4 (2%)	50	69
3	L	174/177 (98%)	171 (98%)	3 (2%)	60	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	O	174/177 (98%)	168 (97%)	6 (3%)	37 60
All	All	3882/4257 (91%)	3841 (99%)	41 (1%)	77 84

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	140	LYS
3	O	107	LYS
3	I	108	LEU
3	I	111	LEU
3	O	109	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	613	GLN
2	G	39	GLN
1	C	137	ASN
3	L	189	GLN
3	O	199	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

12 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
4	NAG	D	1	4,1	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	D	2	4	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	E	1	4,1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	E	2	4	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	F	1	4,1	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	F	2	4	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	J	1	4,1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	J	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	K	1	4,1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	K	2	4	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	M	1	4,1	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	M	2	4	14,14,15	0.24	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

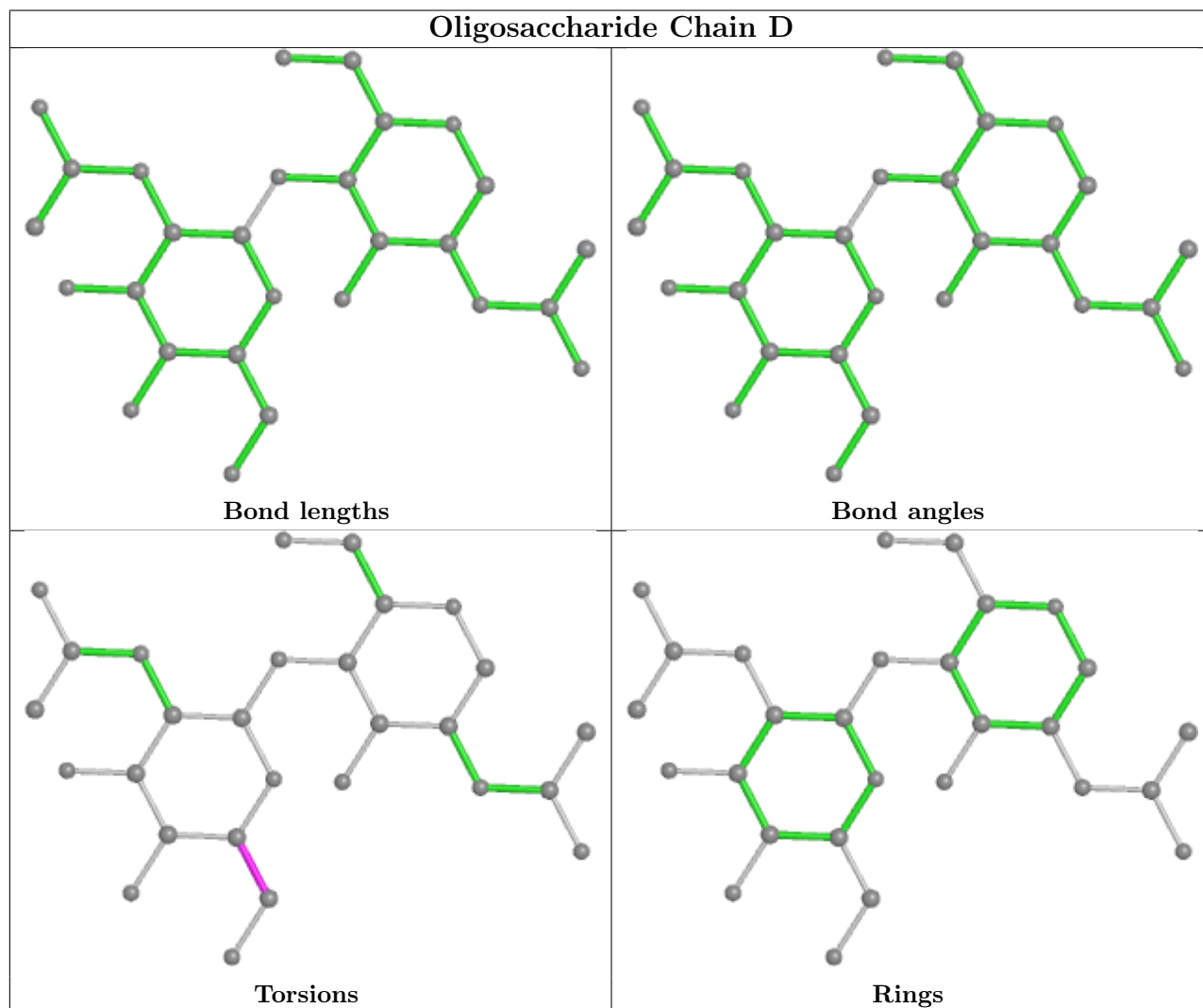
Mol	Chain	Res	Type	Atoms
4	M	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6

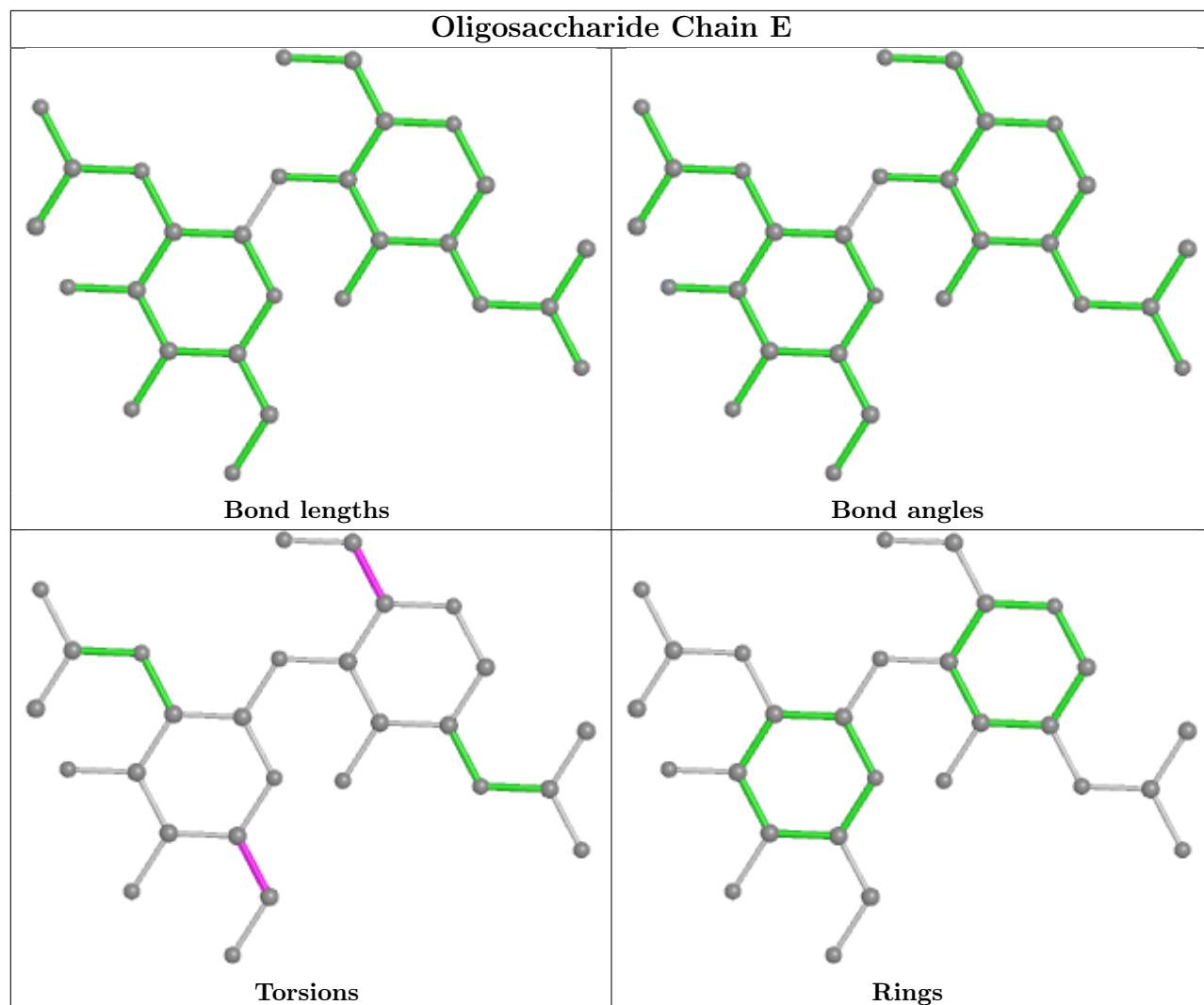
There are no ring outliers.

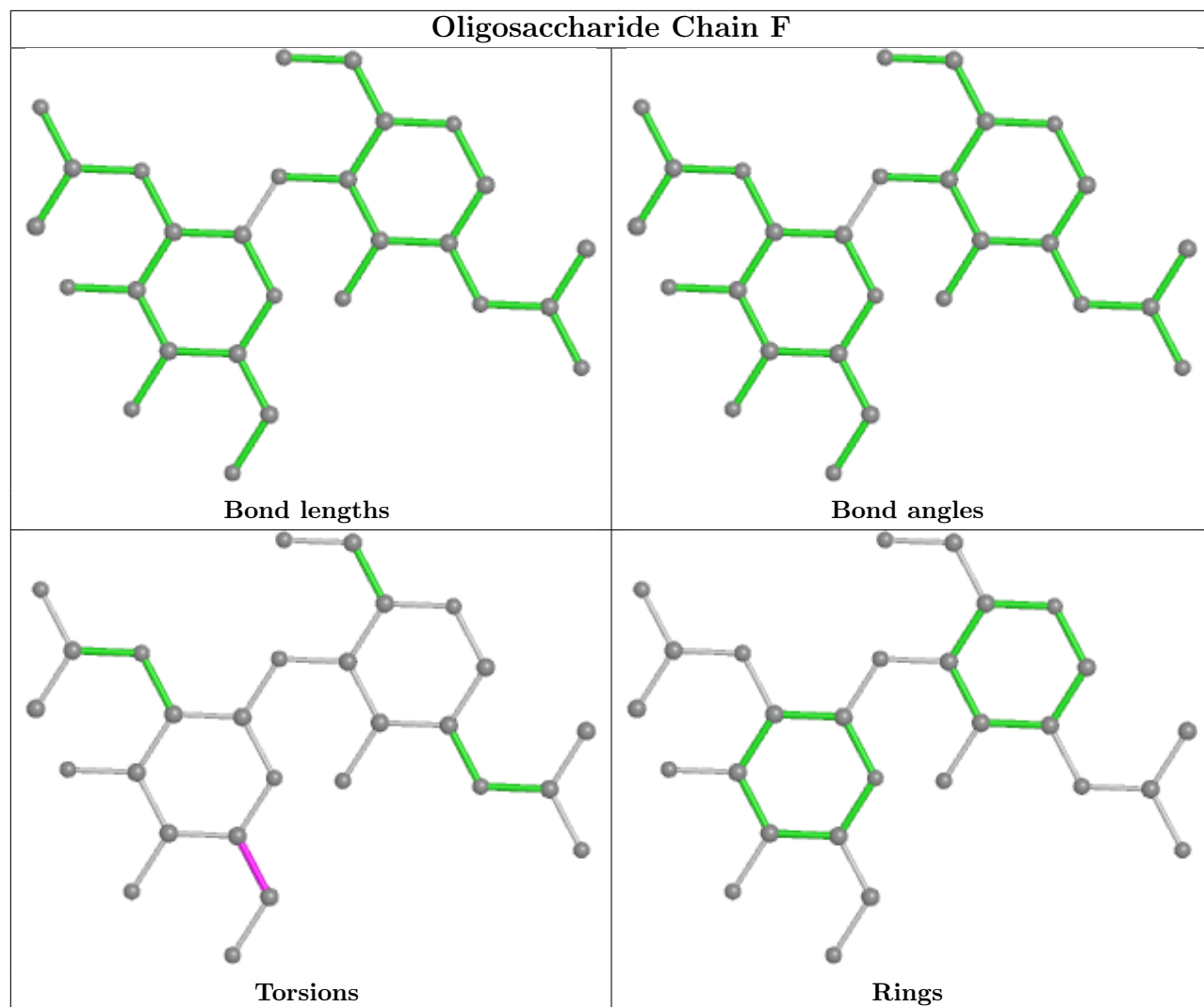
3 monomers are involved in 3 short contacts:

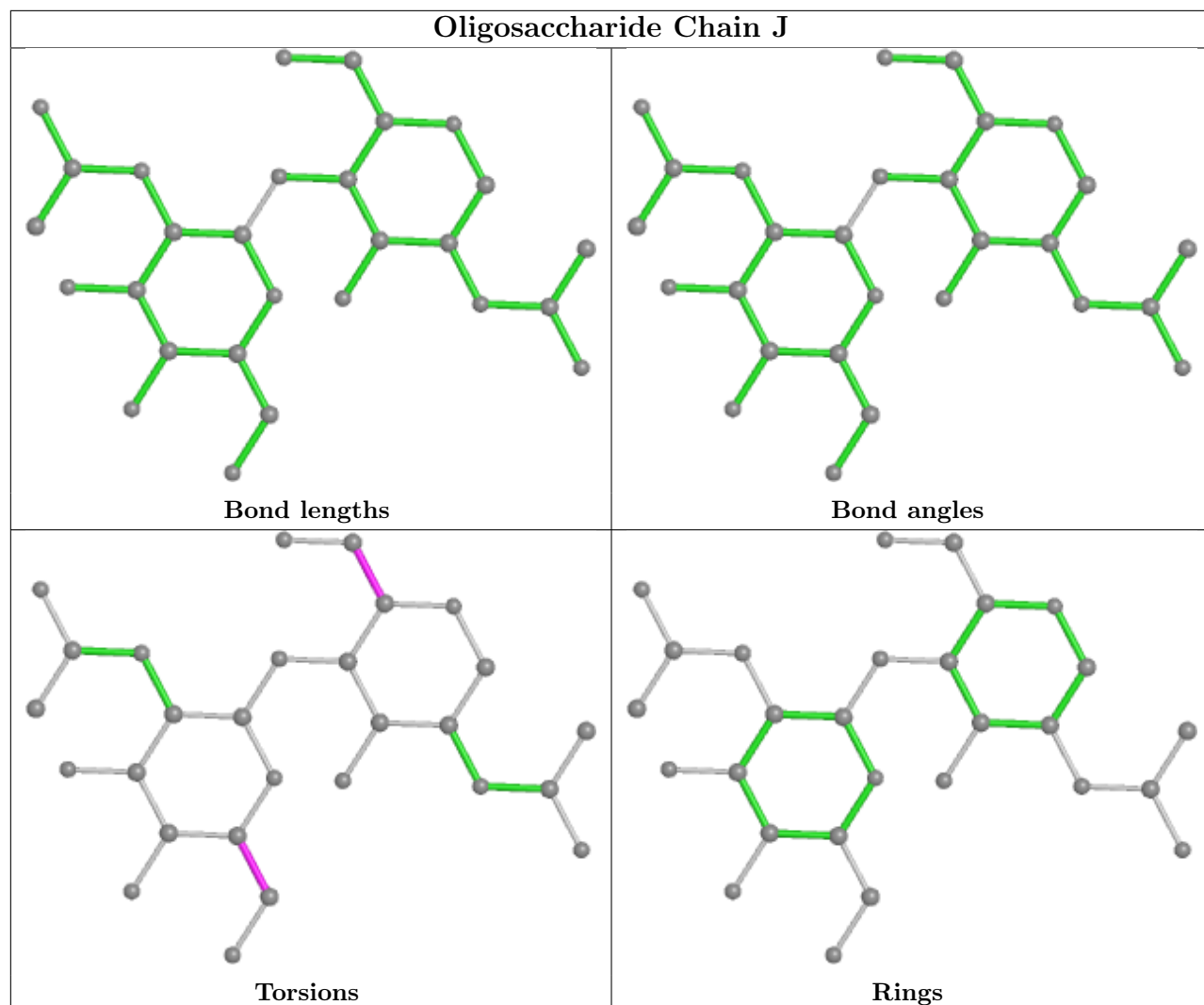
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0
4	K	1	NAG	1	0
4	D	1	NAG	1	0

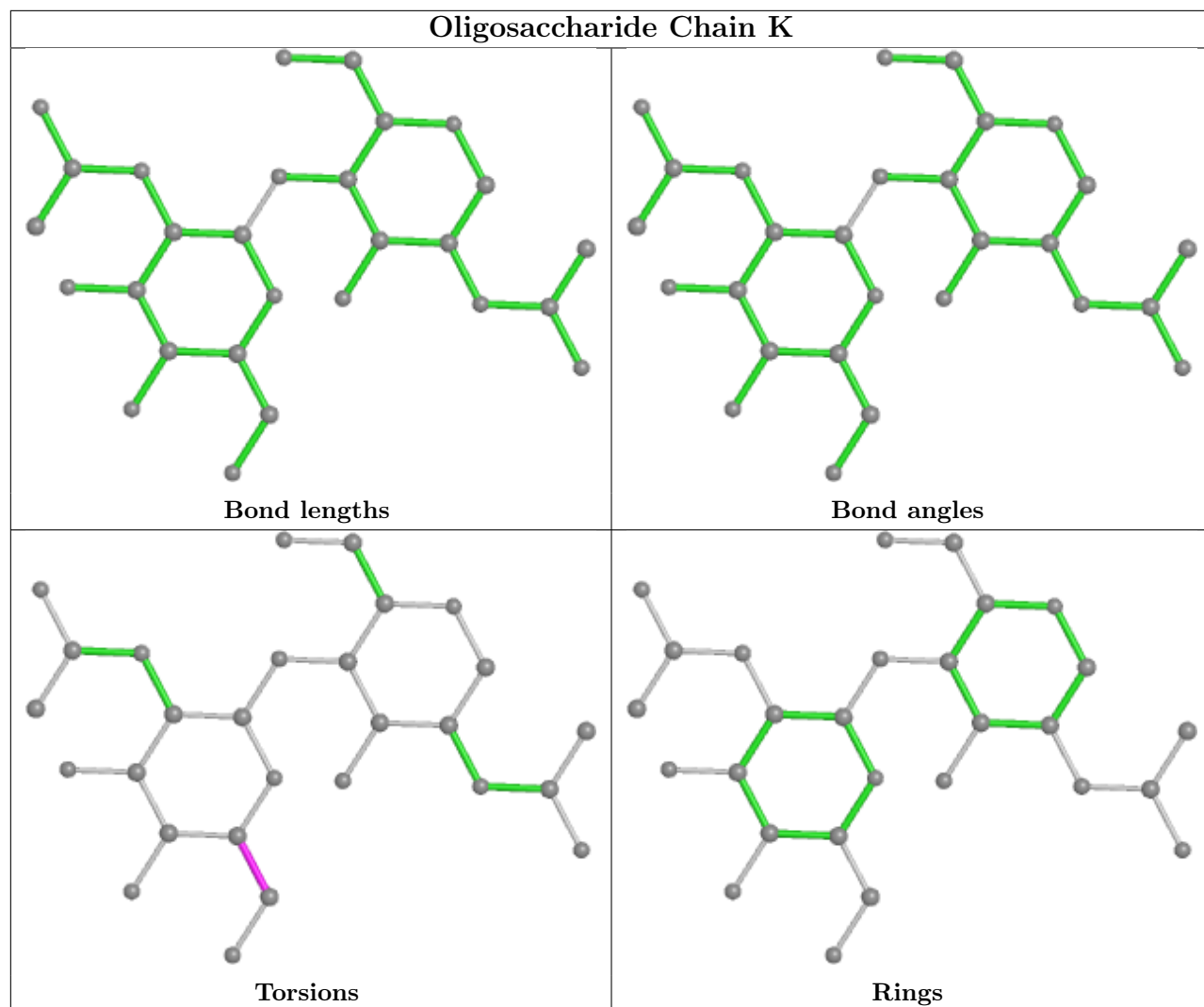
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

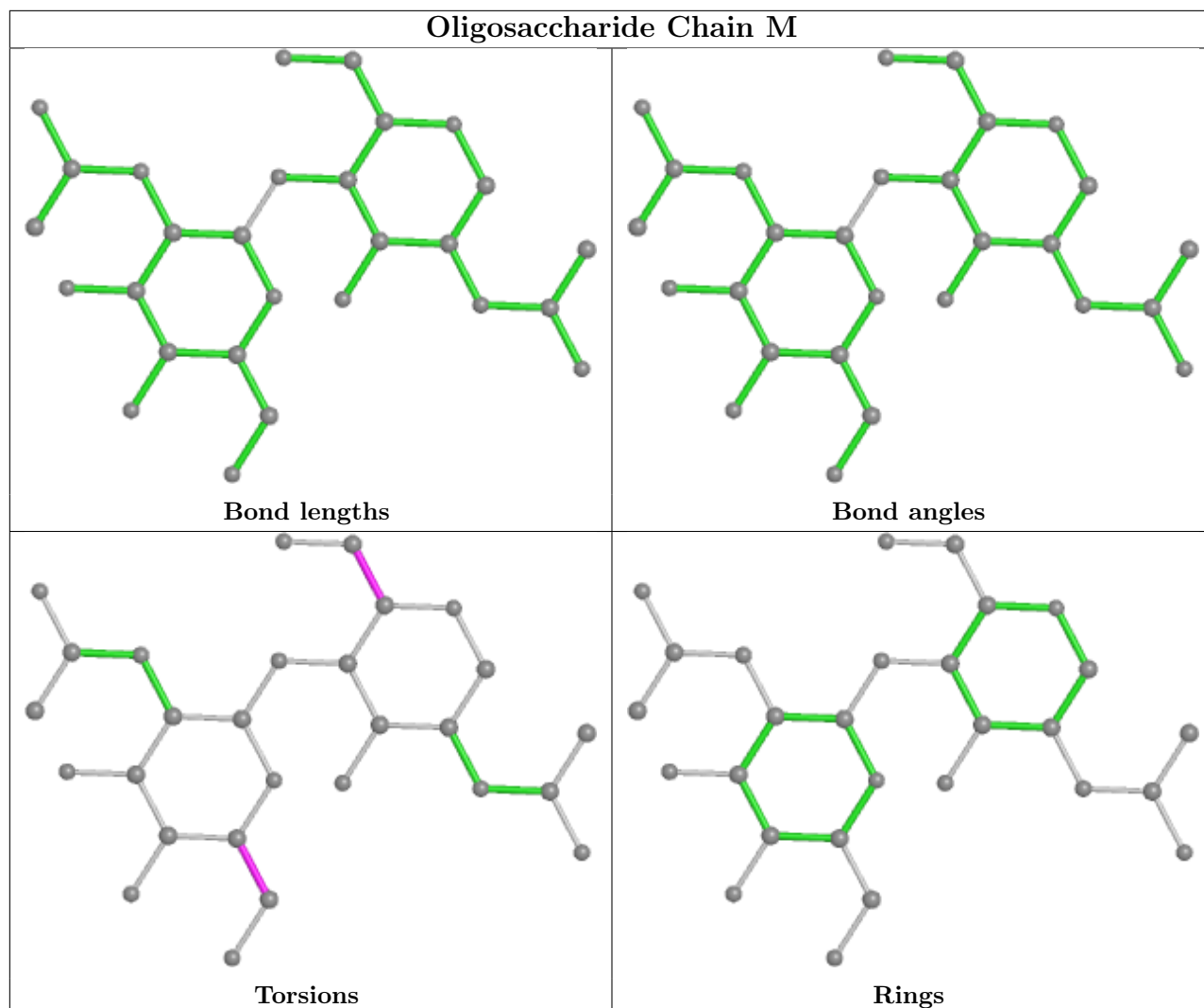












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
5	NAG	A	1307	1	14,14,15	0.25	0	17,19,21	0.34	0
5	NAG	C	1306	1	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1304	1	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	B	1308	1	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	C	1301	1	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	C	1302	1	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	C	1305	1	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	B	1302	1	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	A	1308	1	14,14,15	0.23	0	17,19,21	0.39	0
5	NAG	A	1304	1	14,14,15	0.26	0	17,19,21	0.41	0
5	NAG	B	1305	1	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	A	1303	1	14,14,15	0.28	0	17,19,21	0.36	0
5	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	B	1303	1	14,14,15	0.28	0	17,19,21	0.37	0
5	NAG	C	1303	1	14,14,15	0.26	0	17,19,21	0.37	0
5	NAG	C	1307	1	14,14,15	0.24	0	17,19,21	0.35	0
5	NAG	A	1305	1	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	A	1306	1	14,14,15	0.22	0	17,19,21	0.39	0
5	NAG	B	1307	1	14,14,15	0.25	0	17,19,21	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

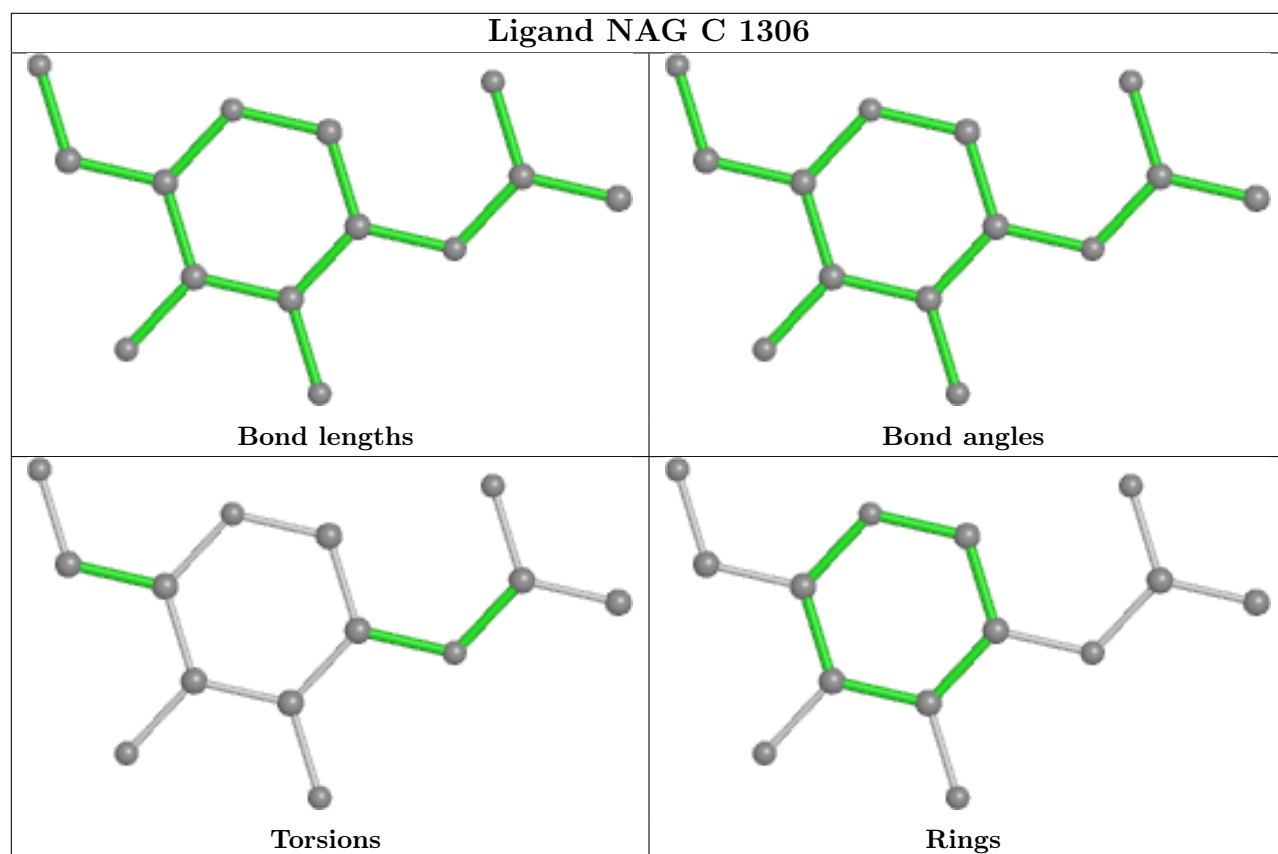
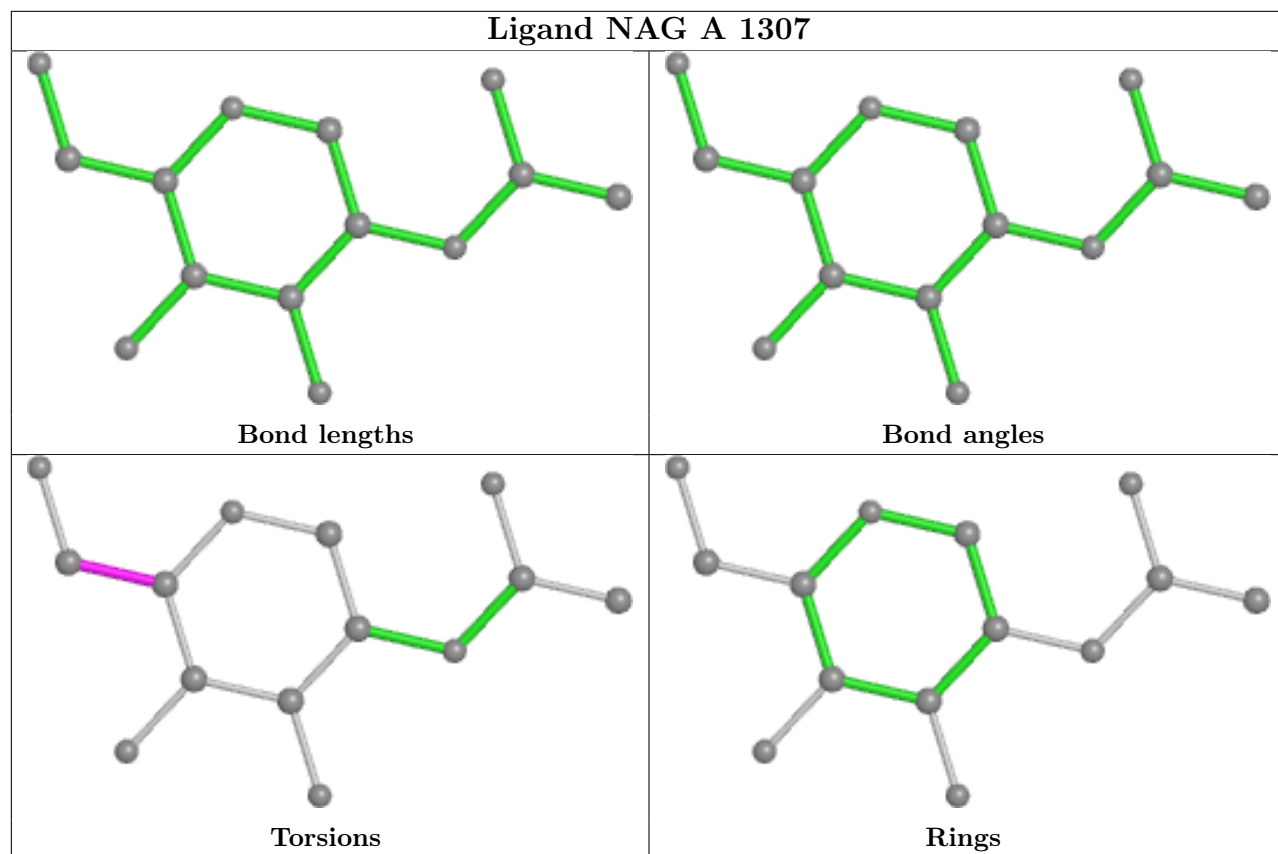
5 of 43 torsion outliers are listed below:

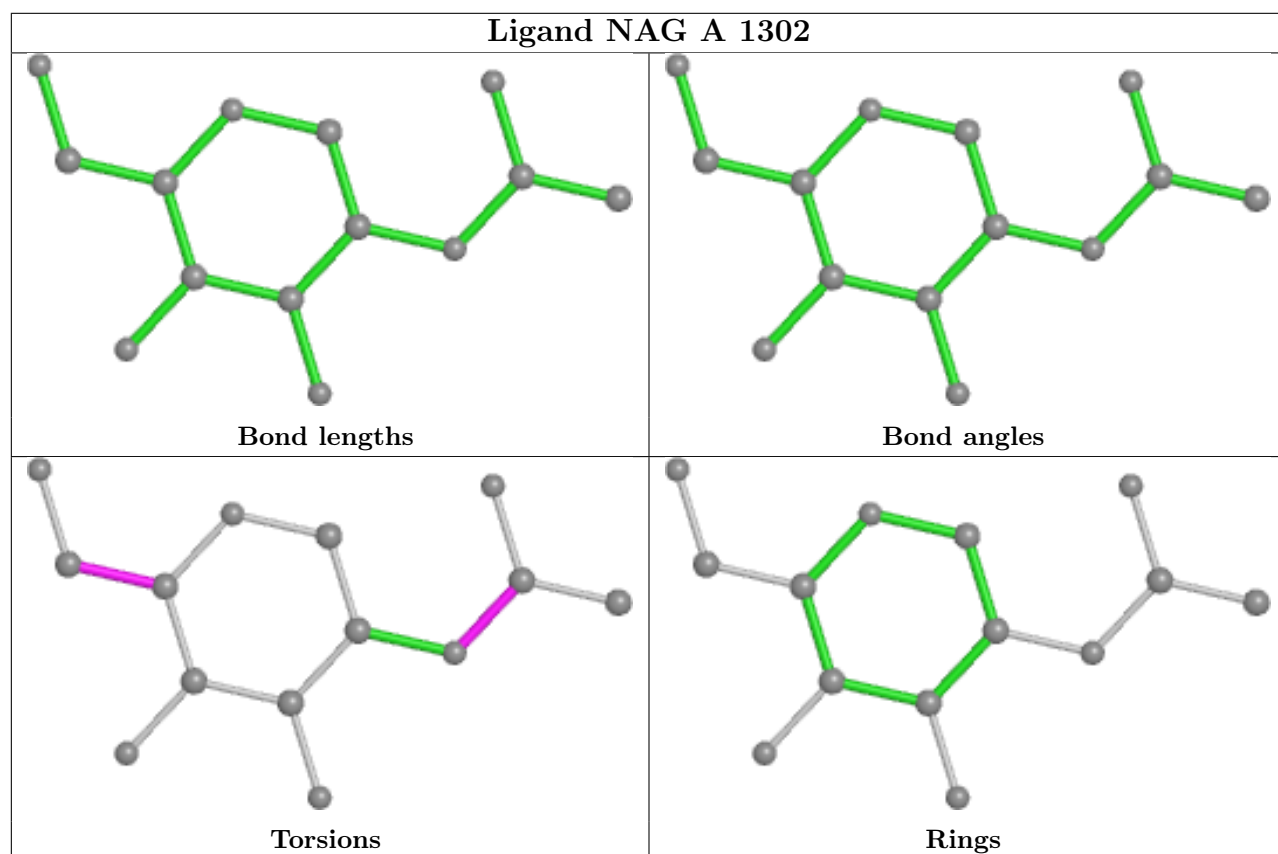
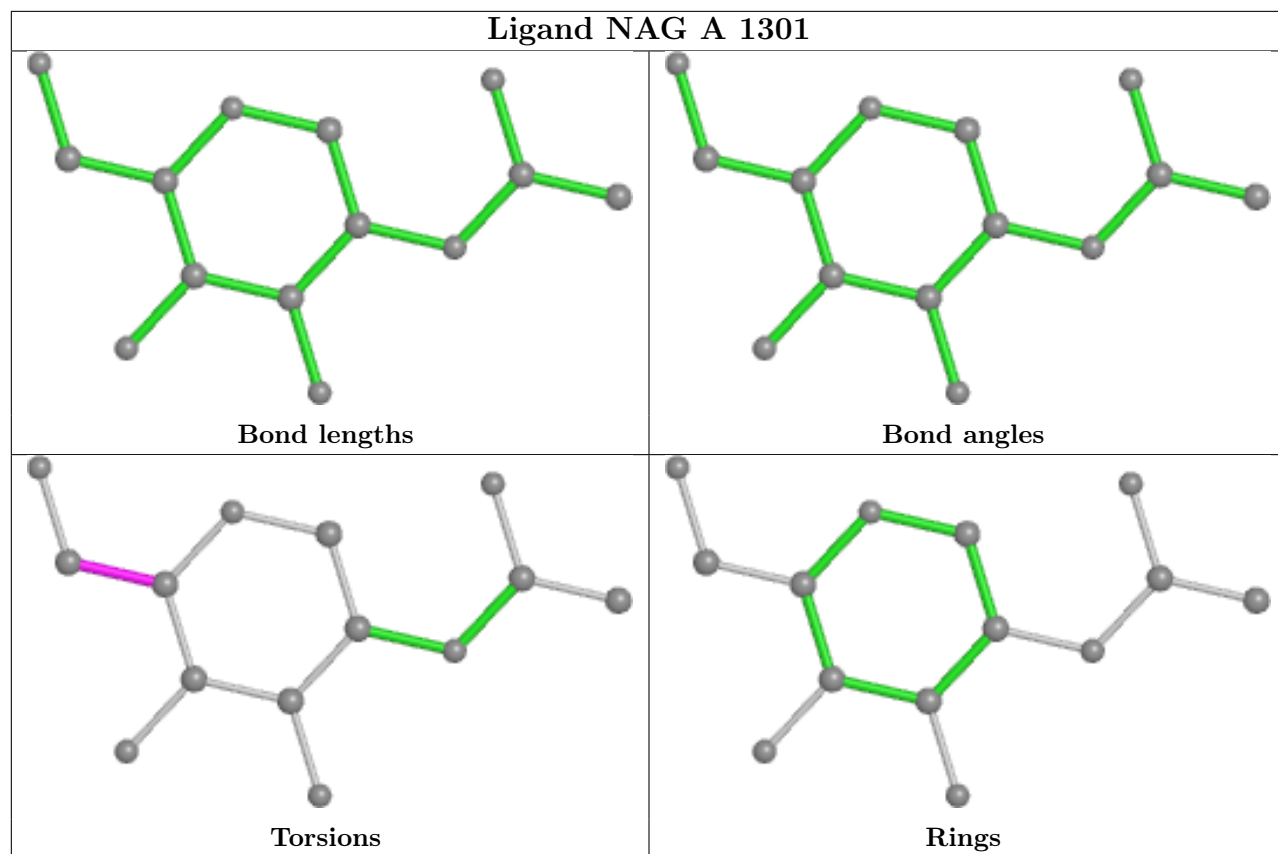
Mol	Chain	Res	Type	Atoms
5	A	1302	NAG	O5-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6

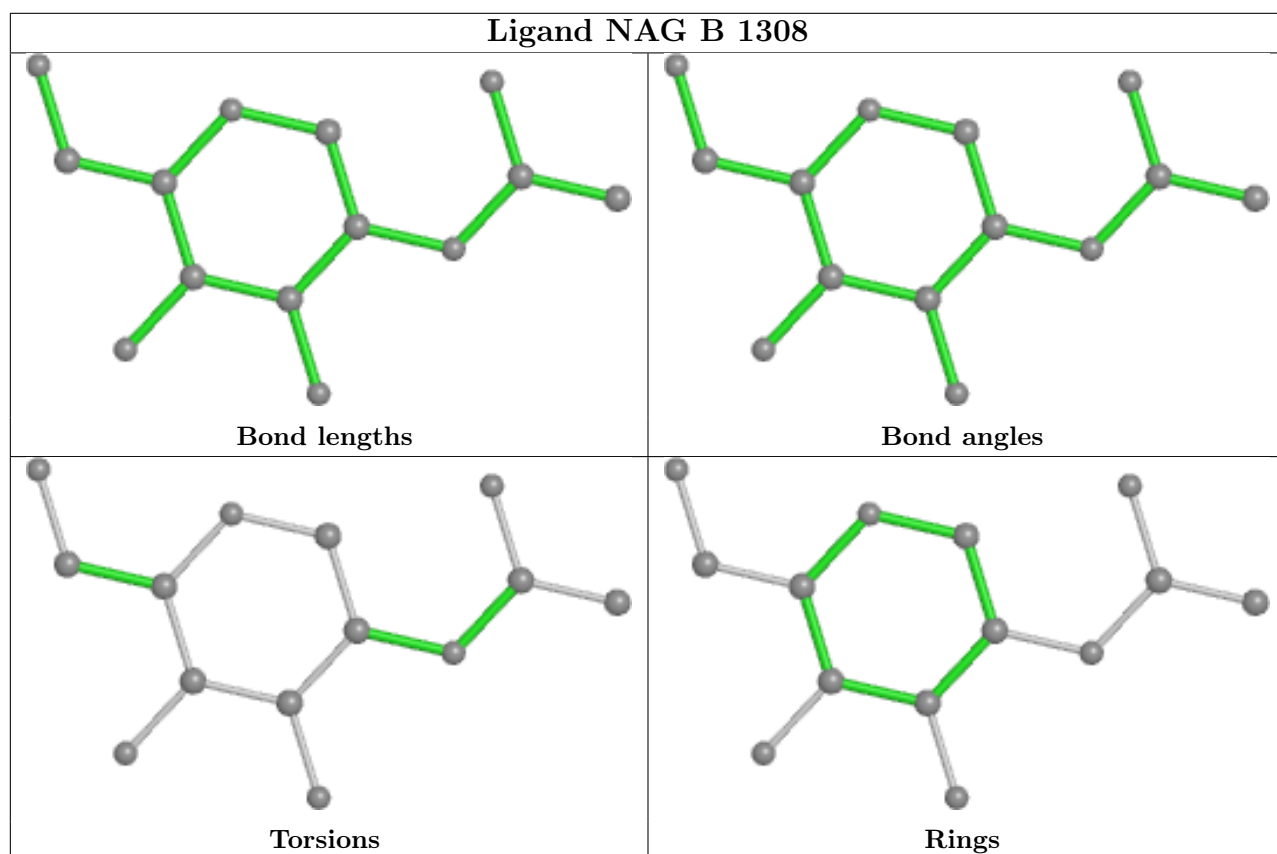
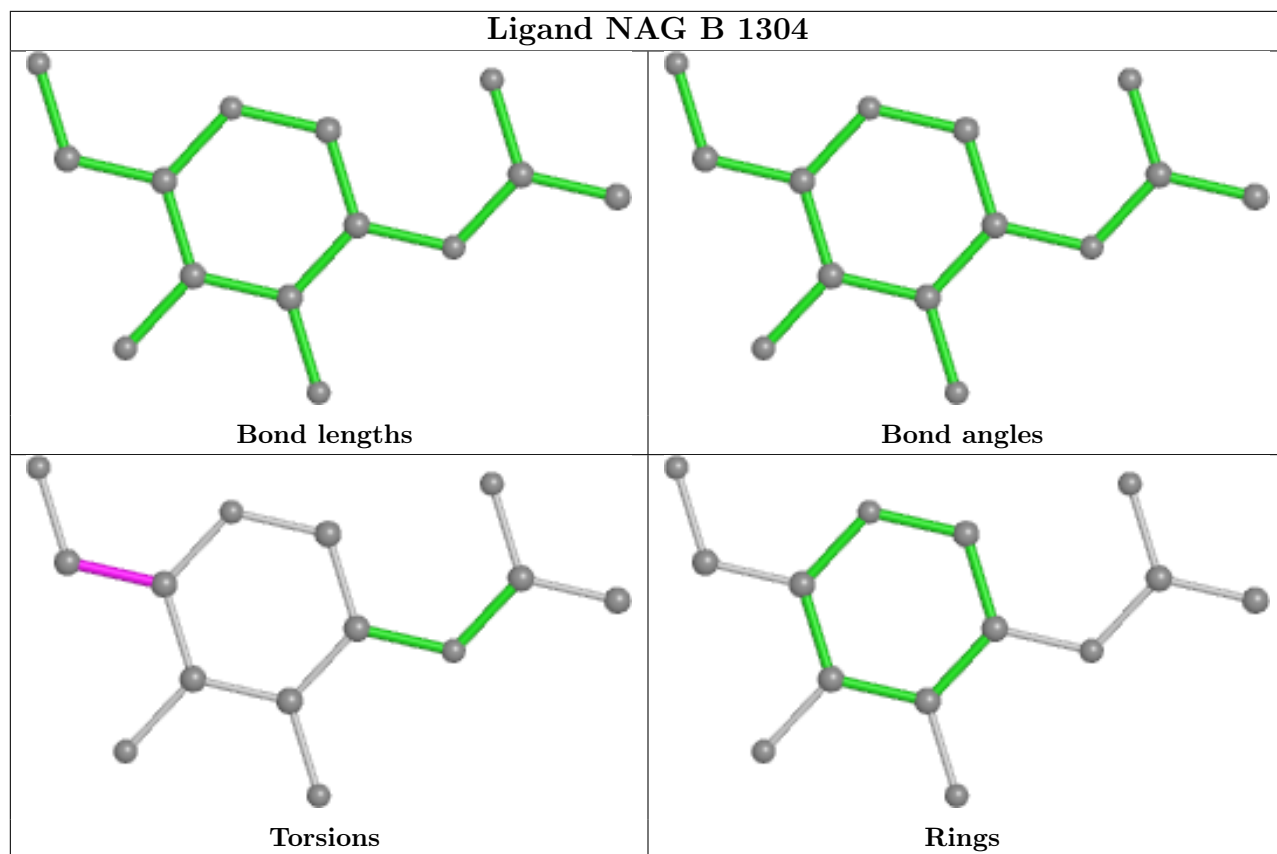
There are no ring outliers.

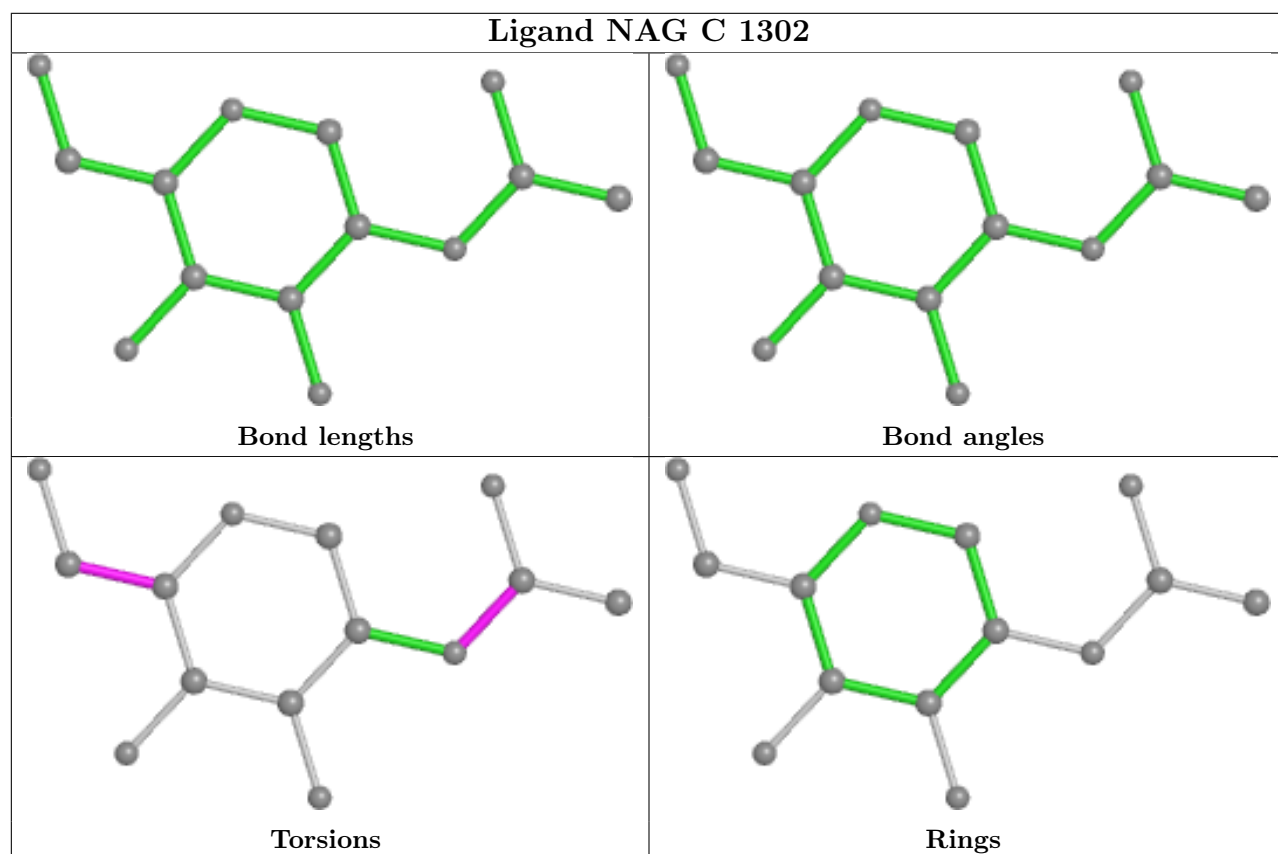
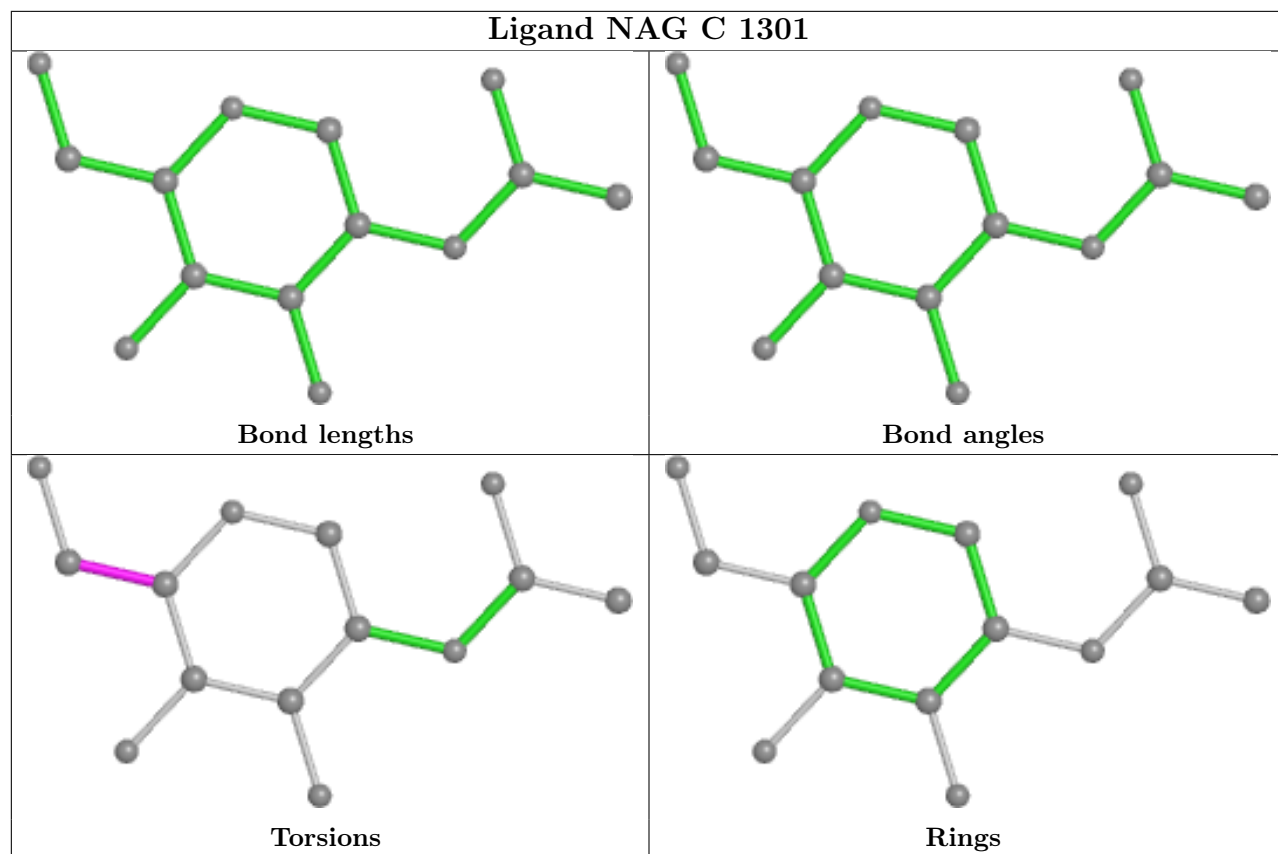
No monomer is involved in short contacts.

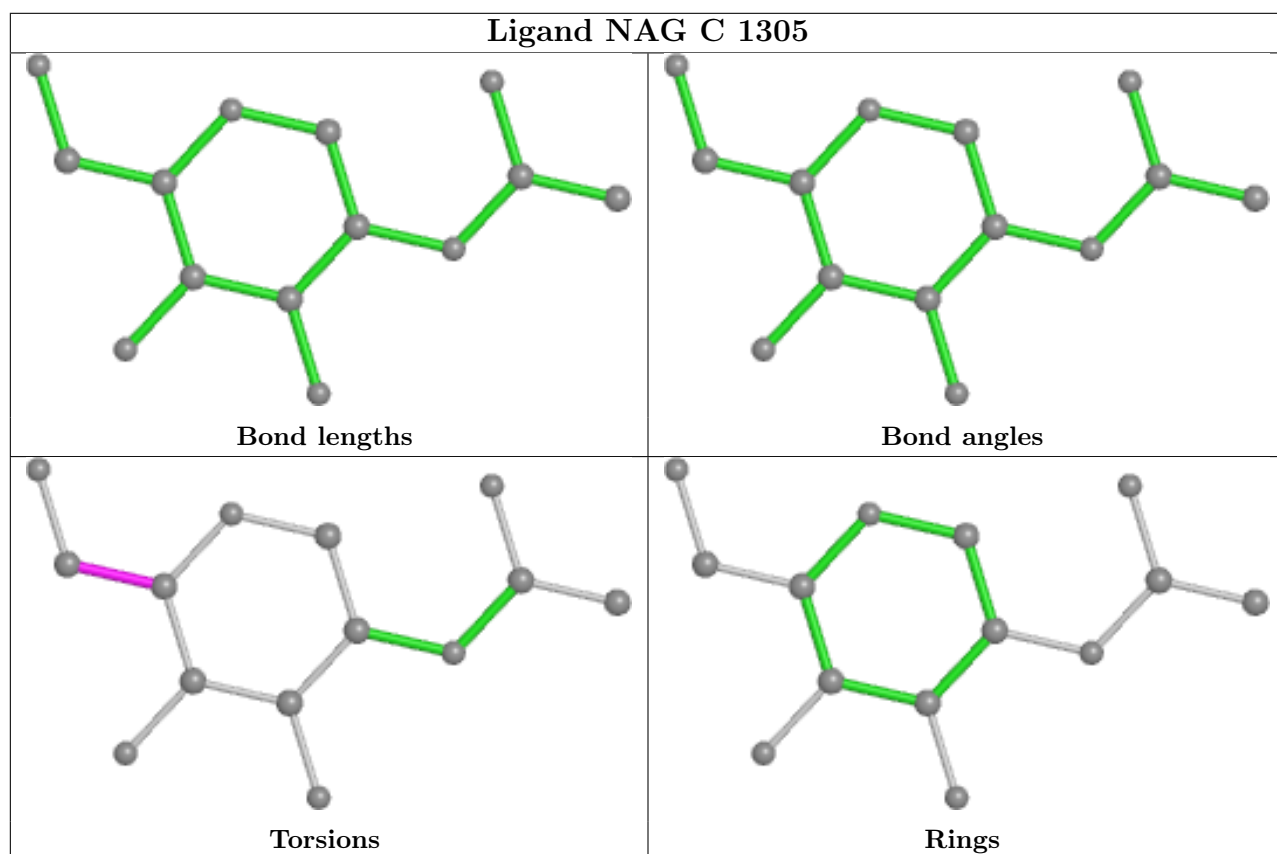
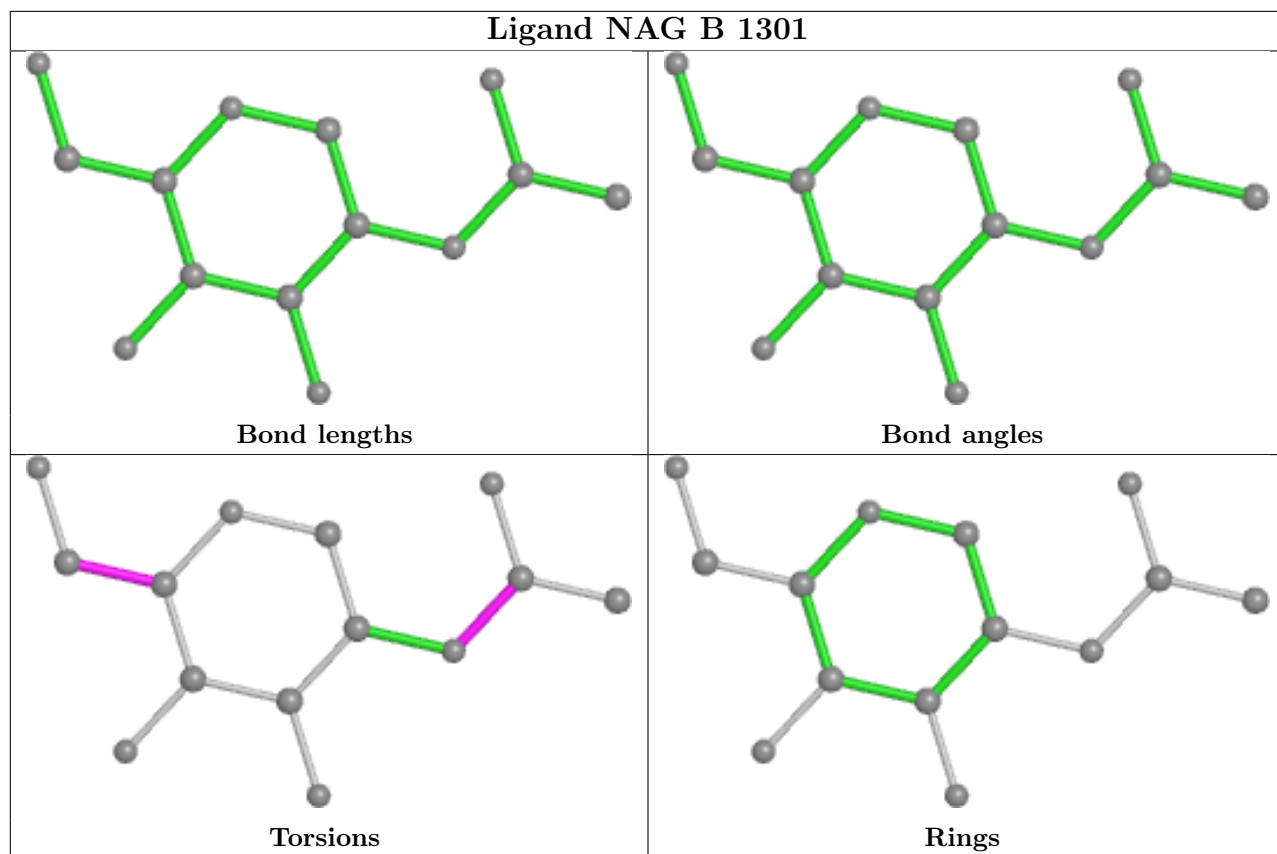
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

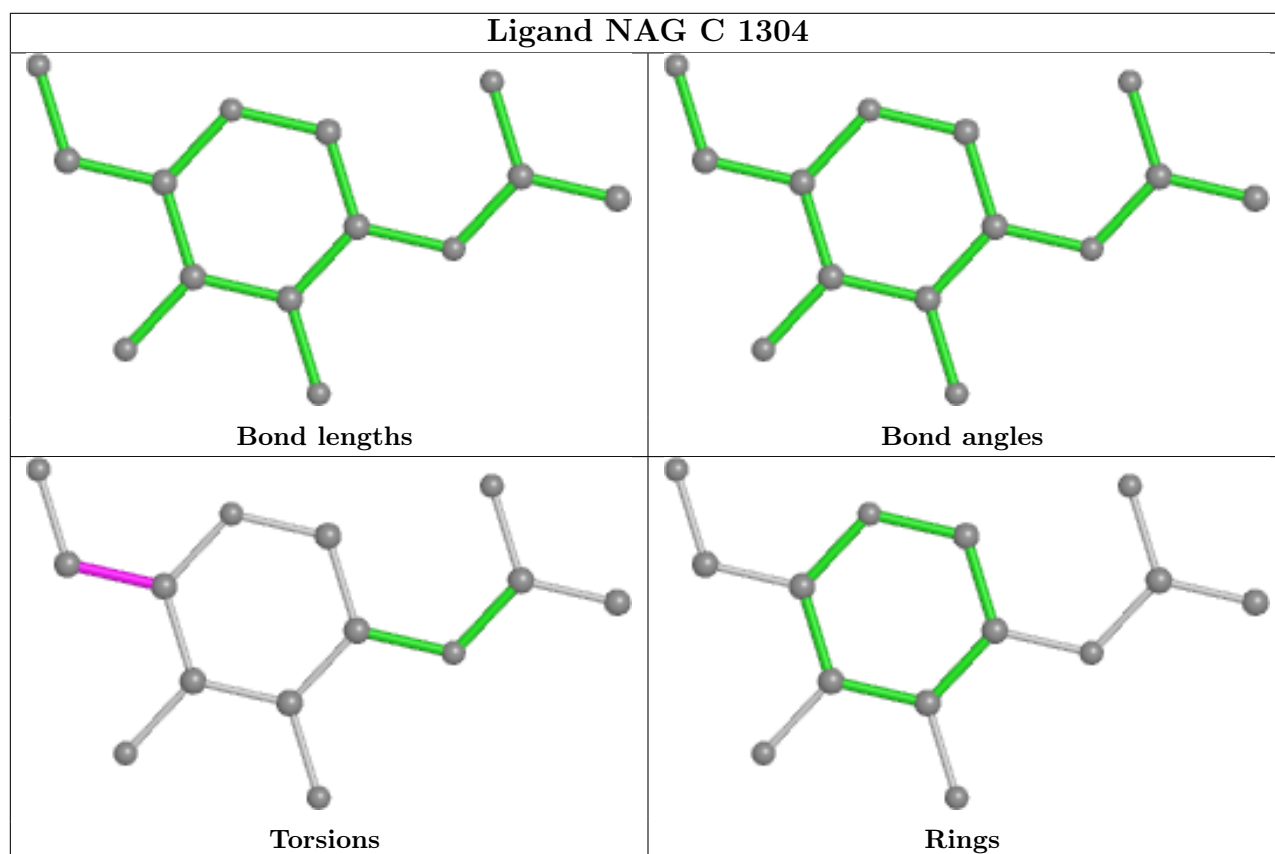
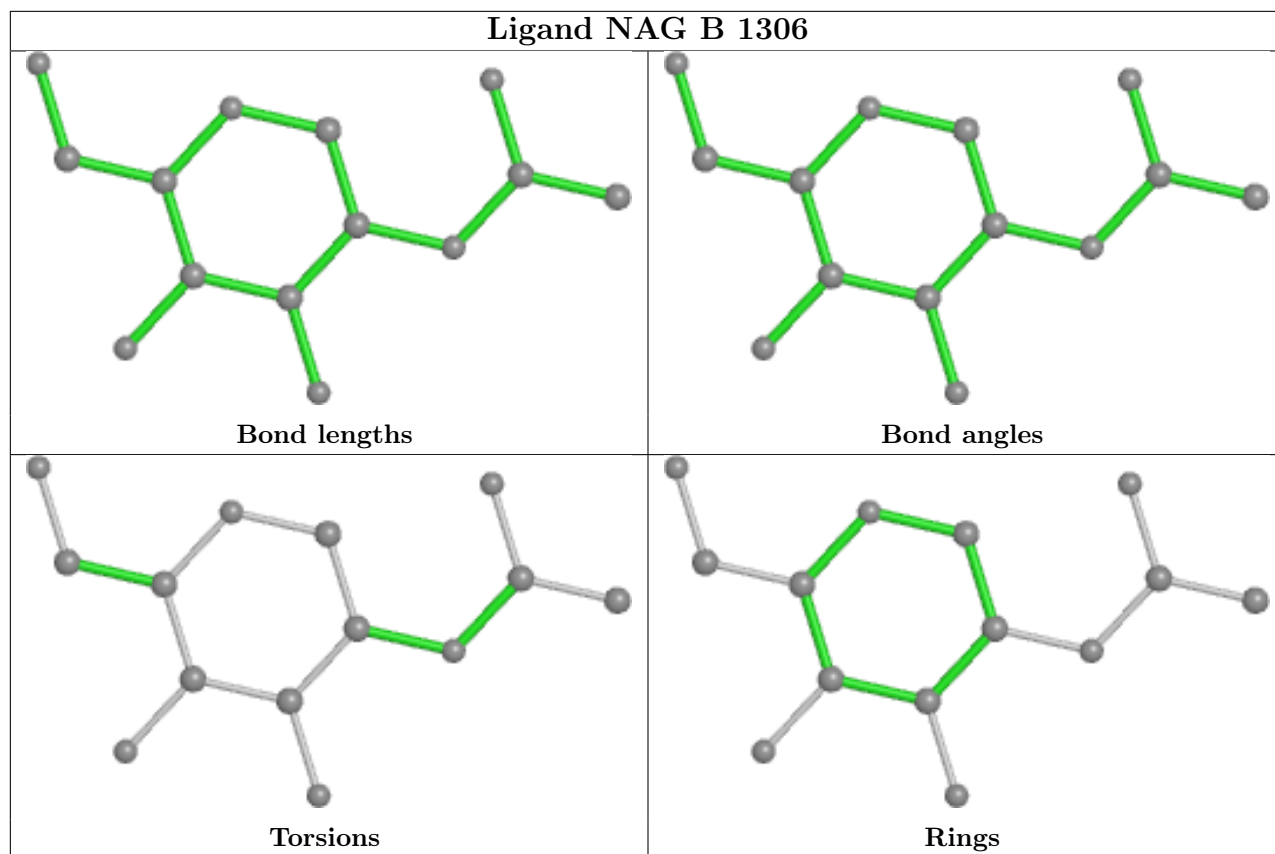


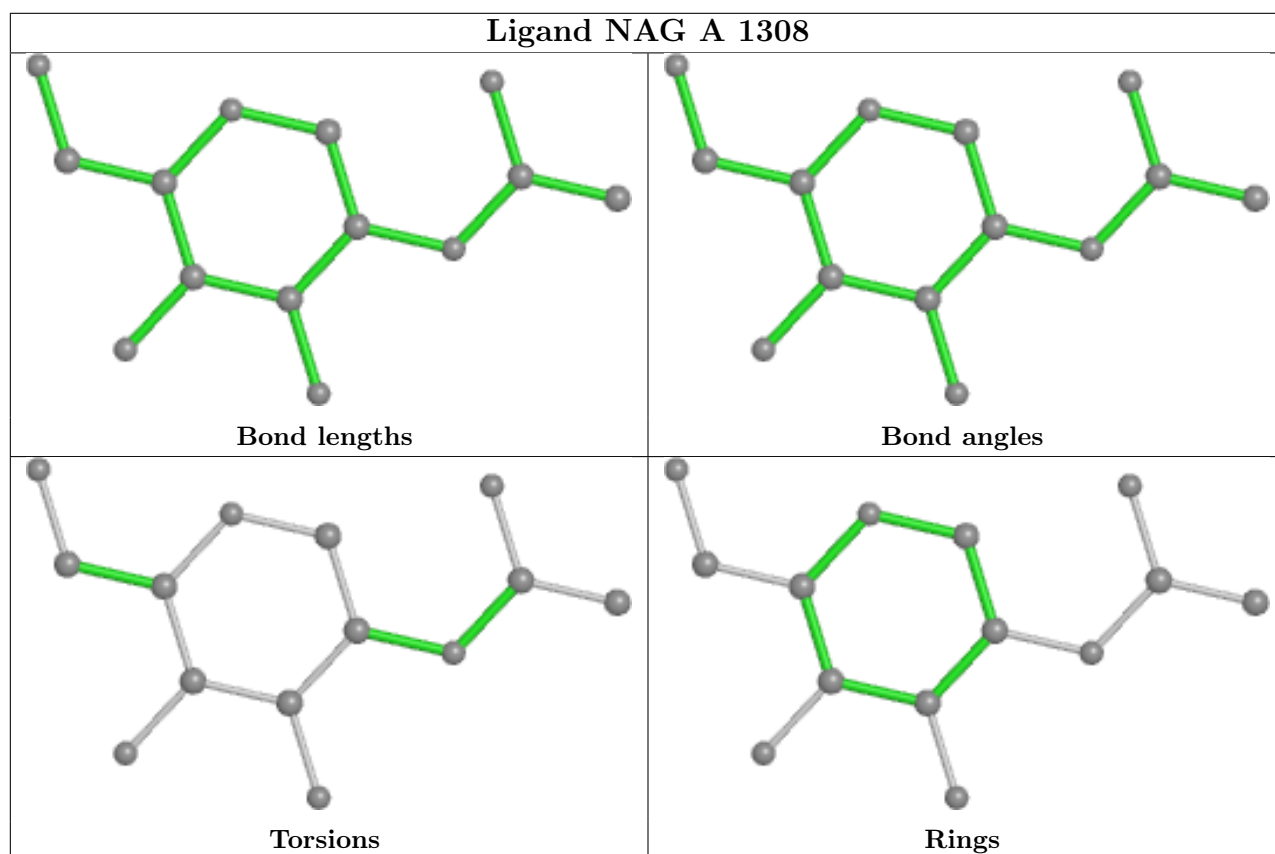
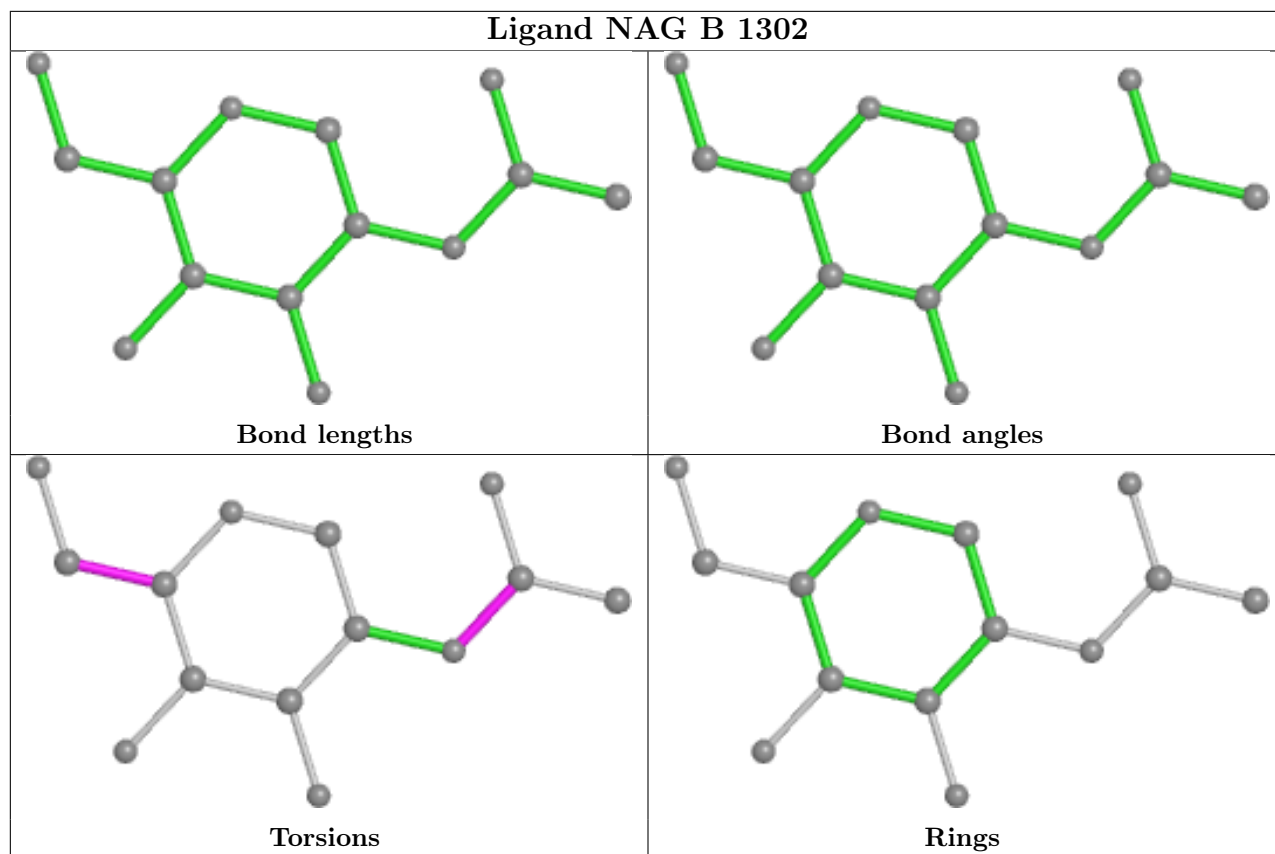


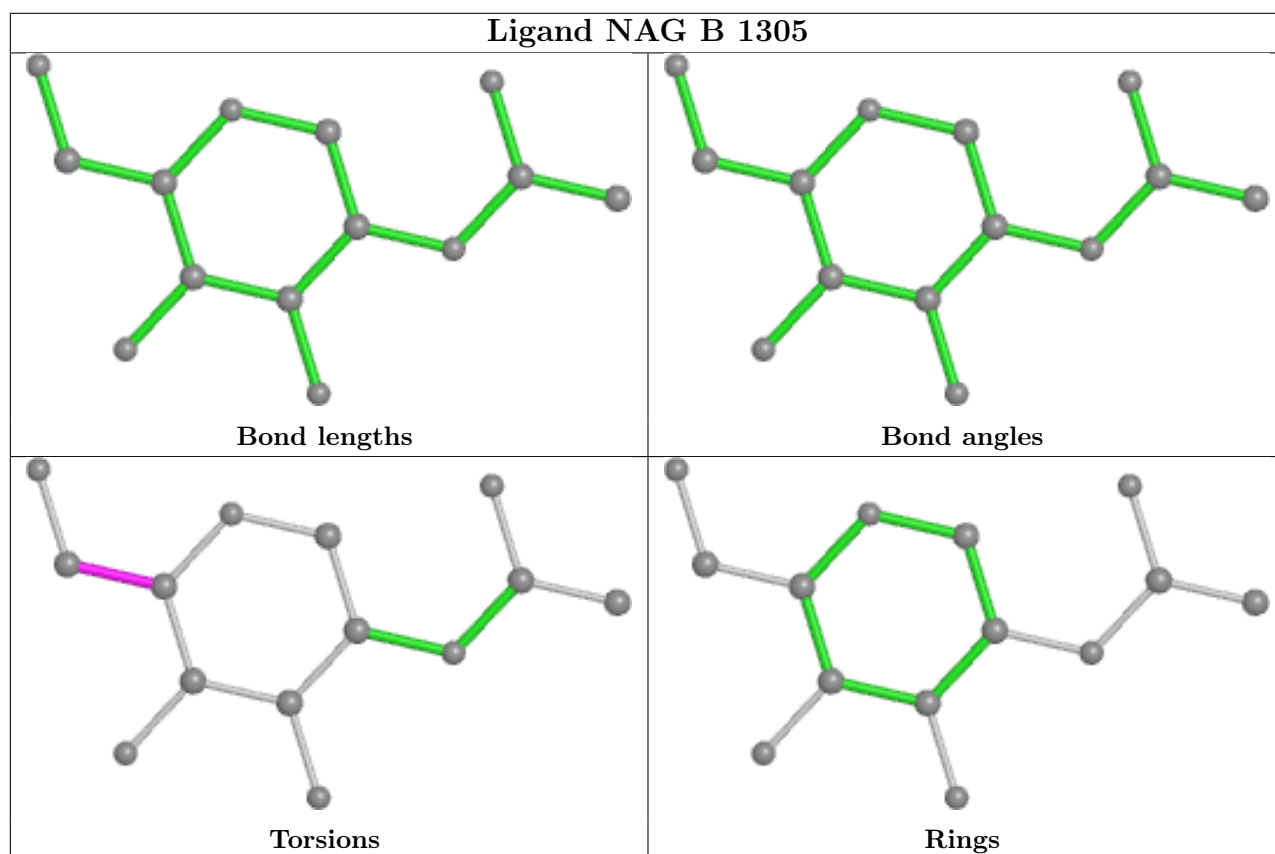
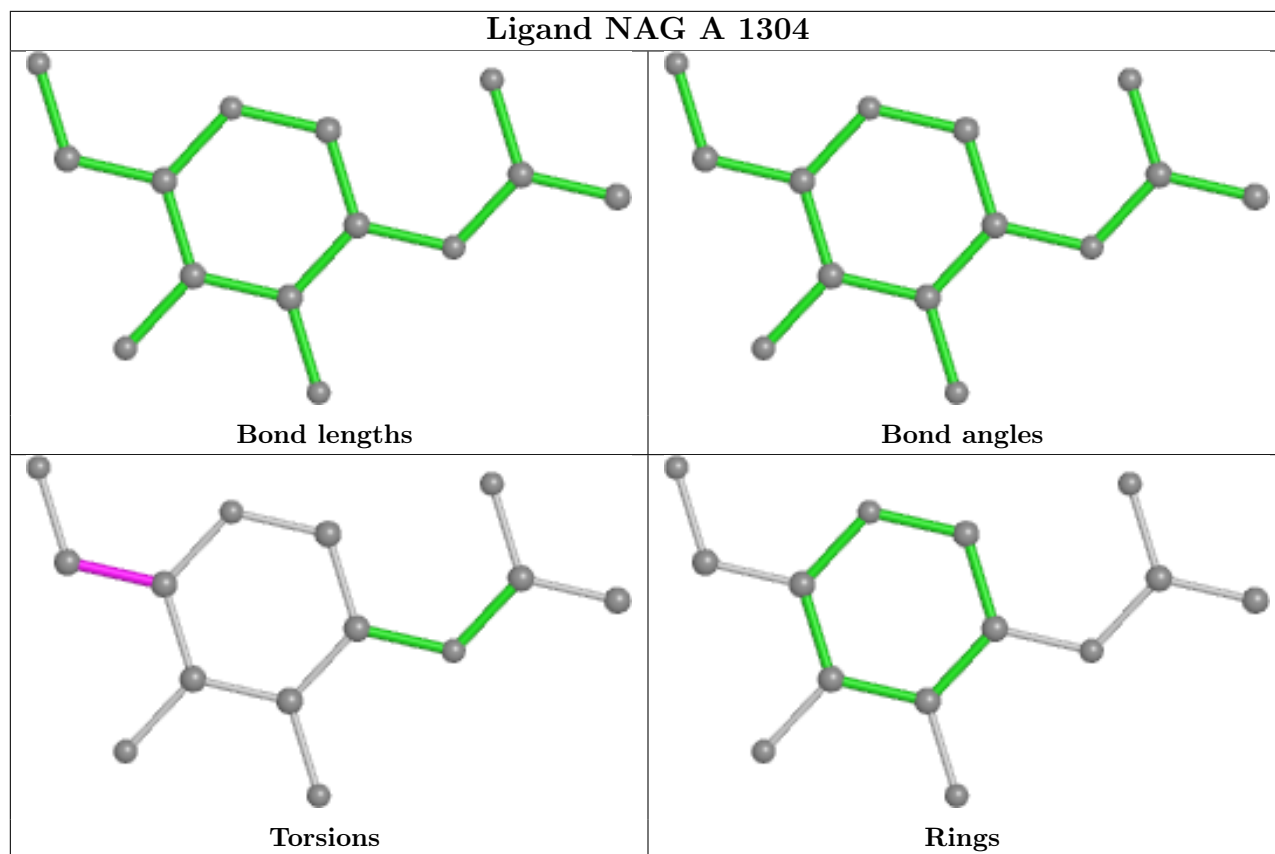


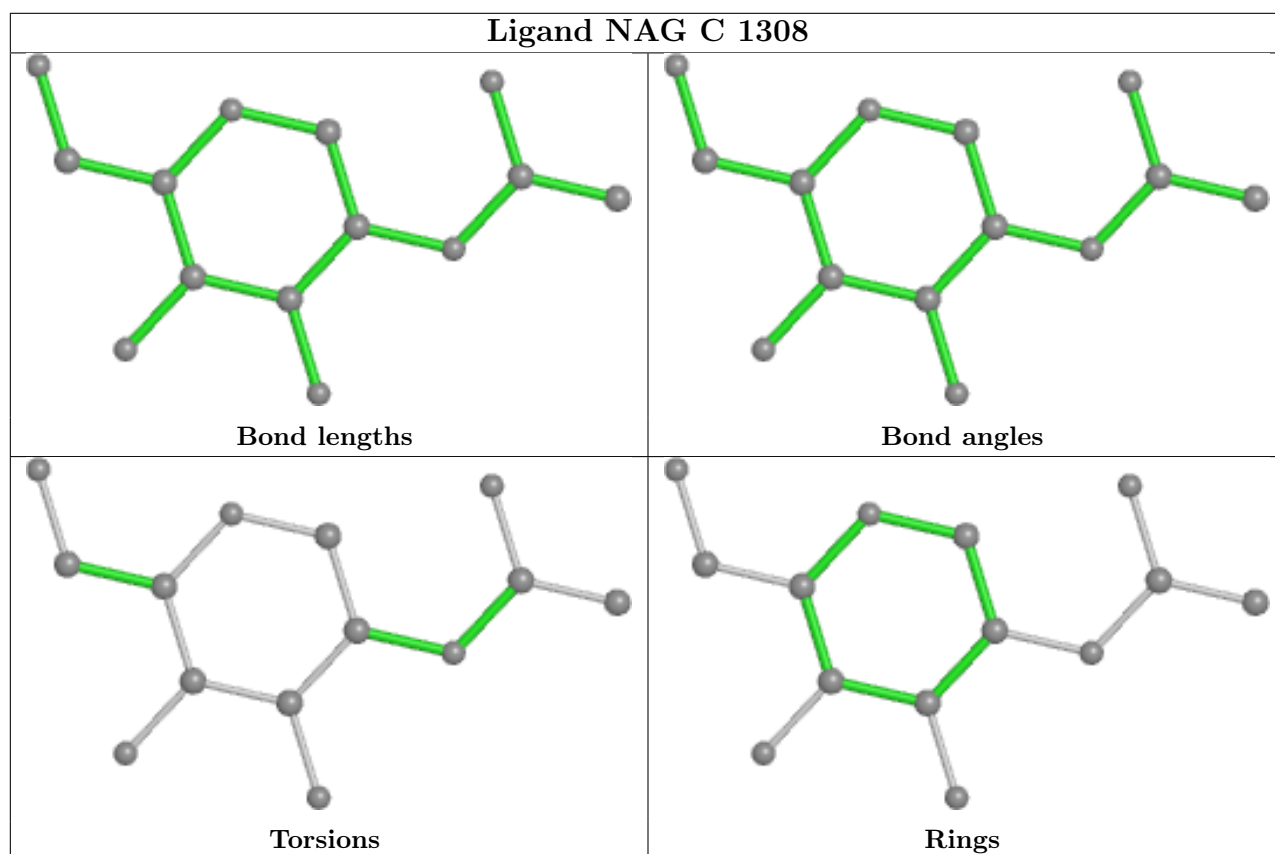
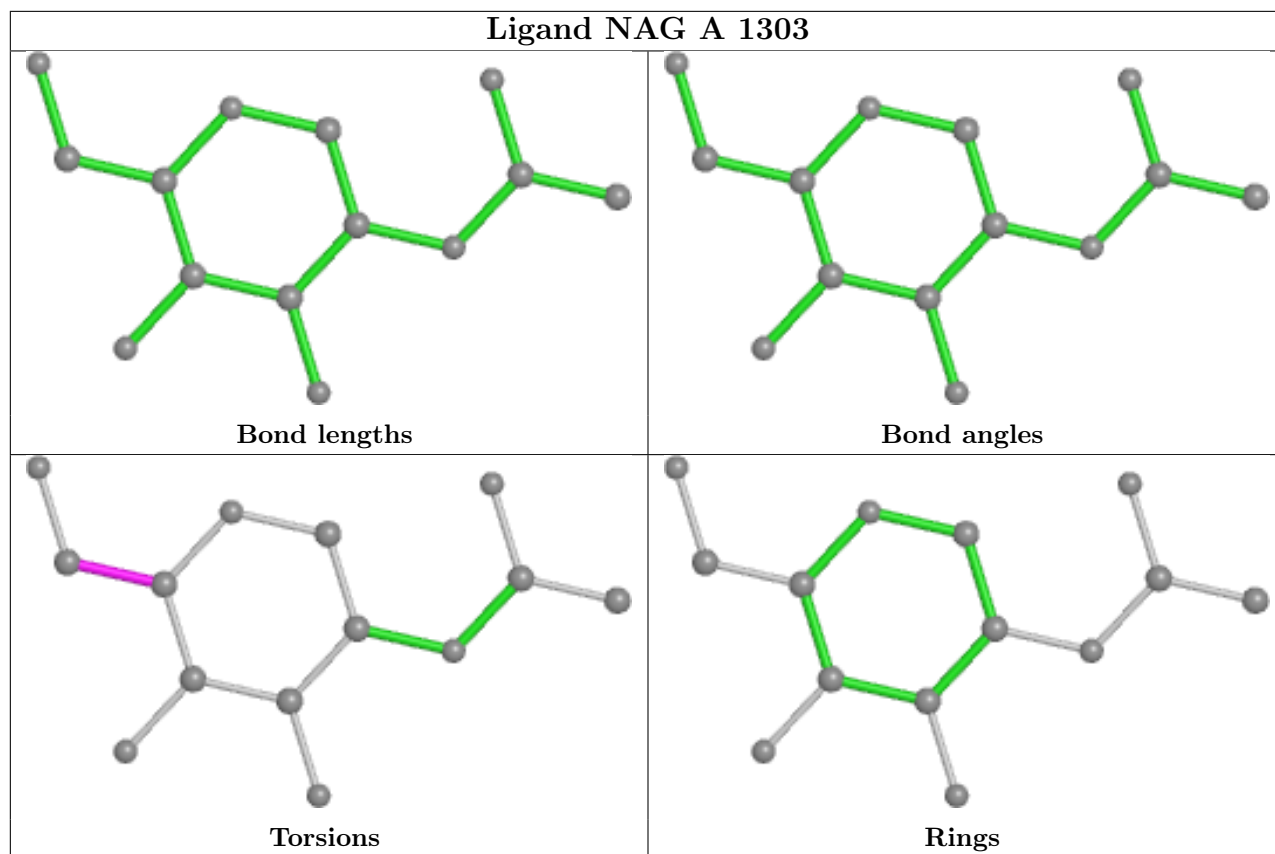


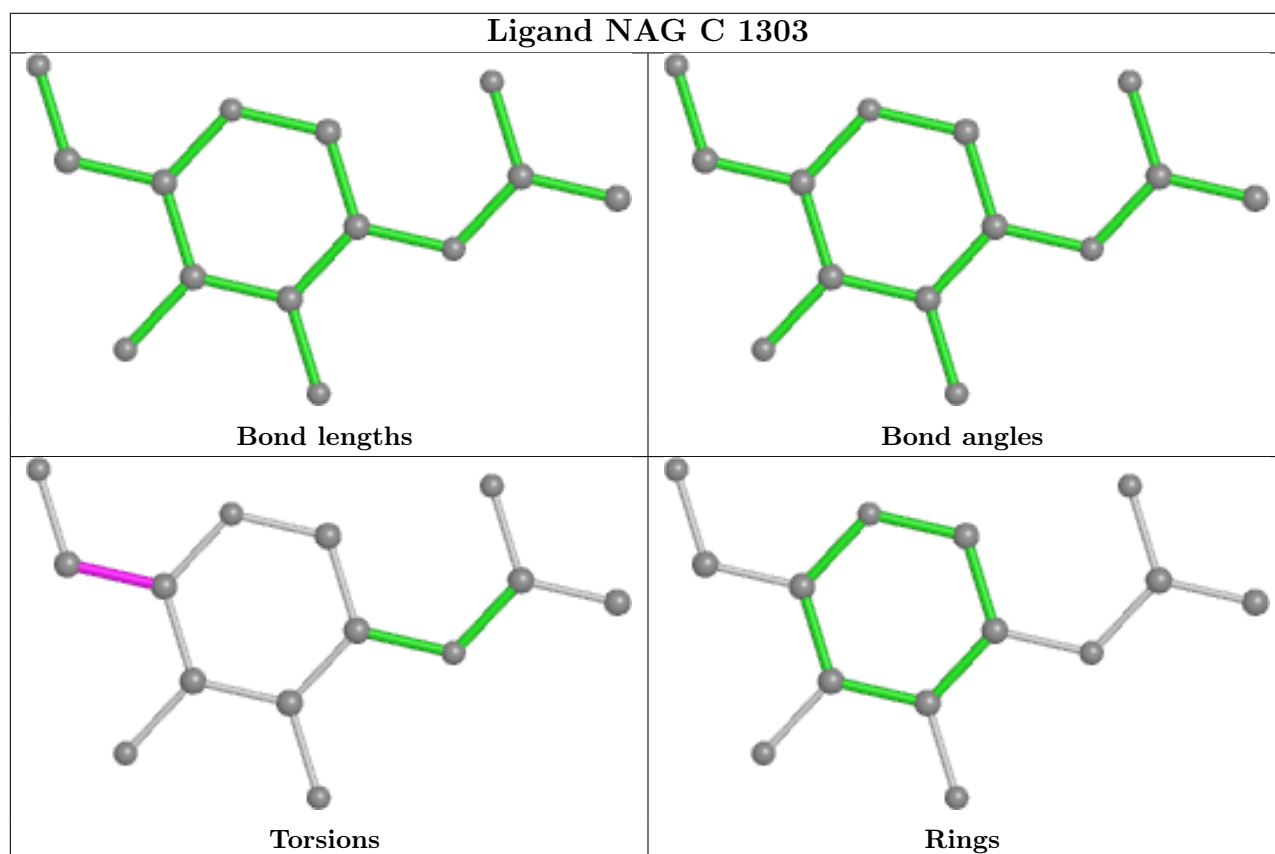
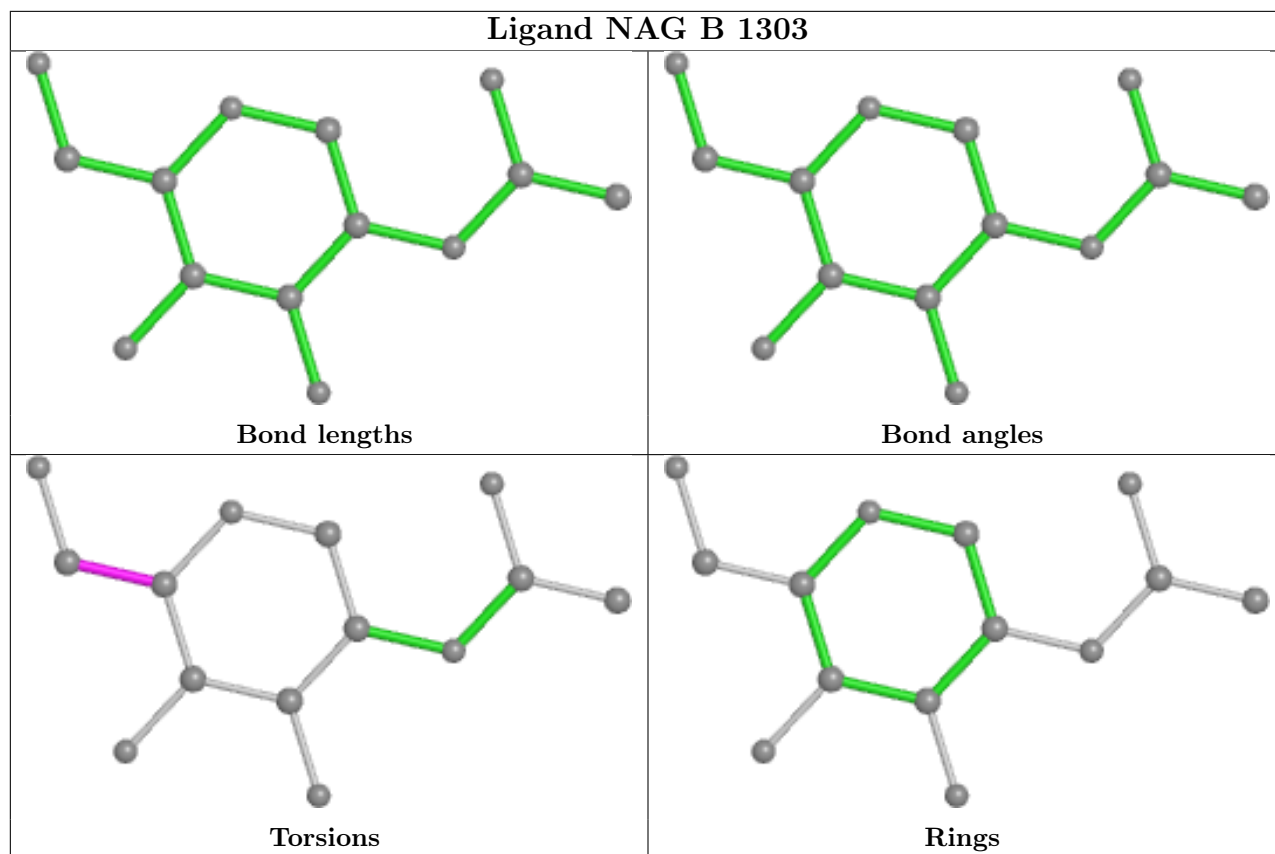


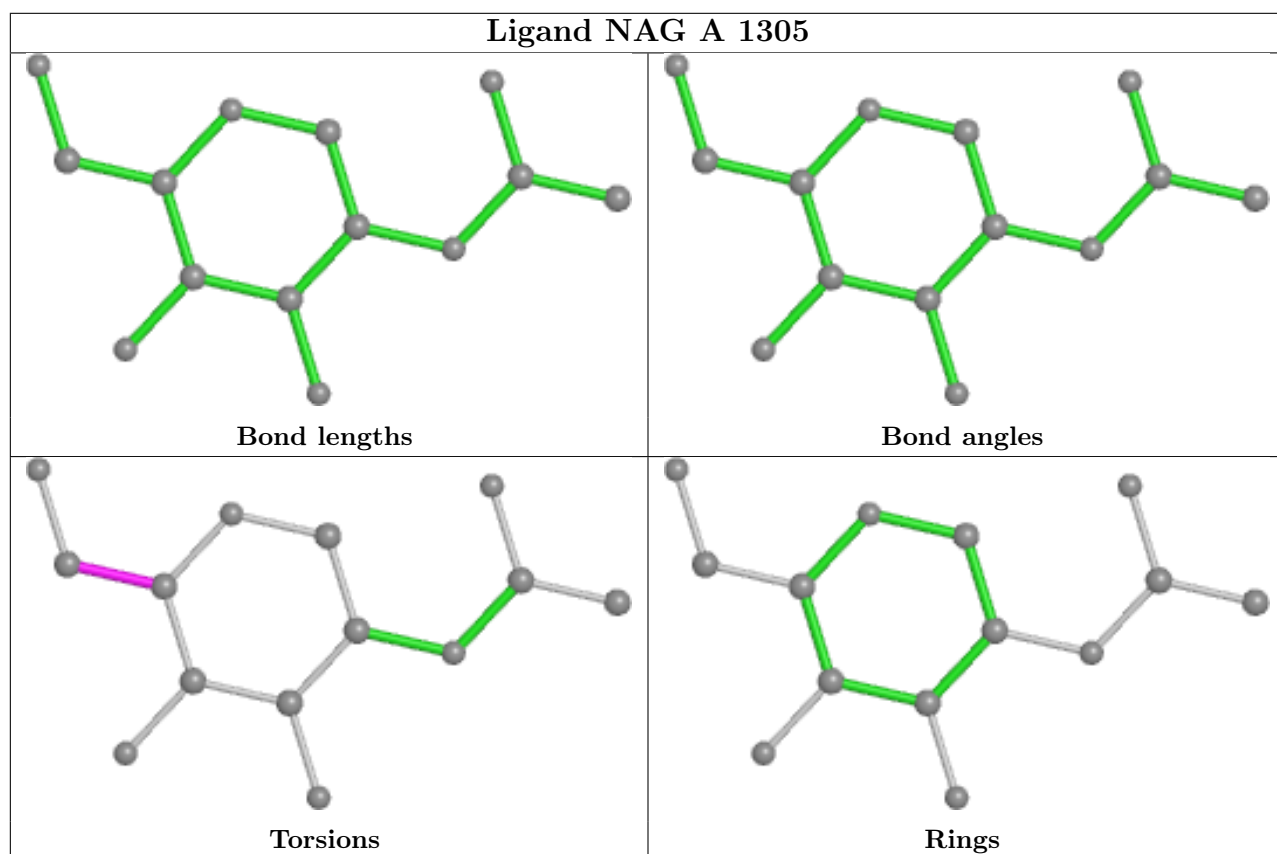
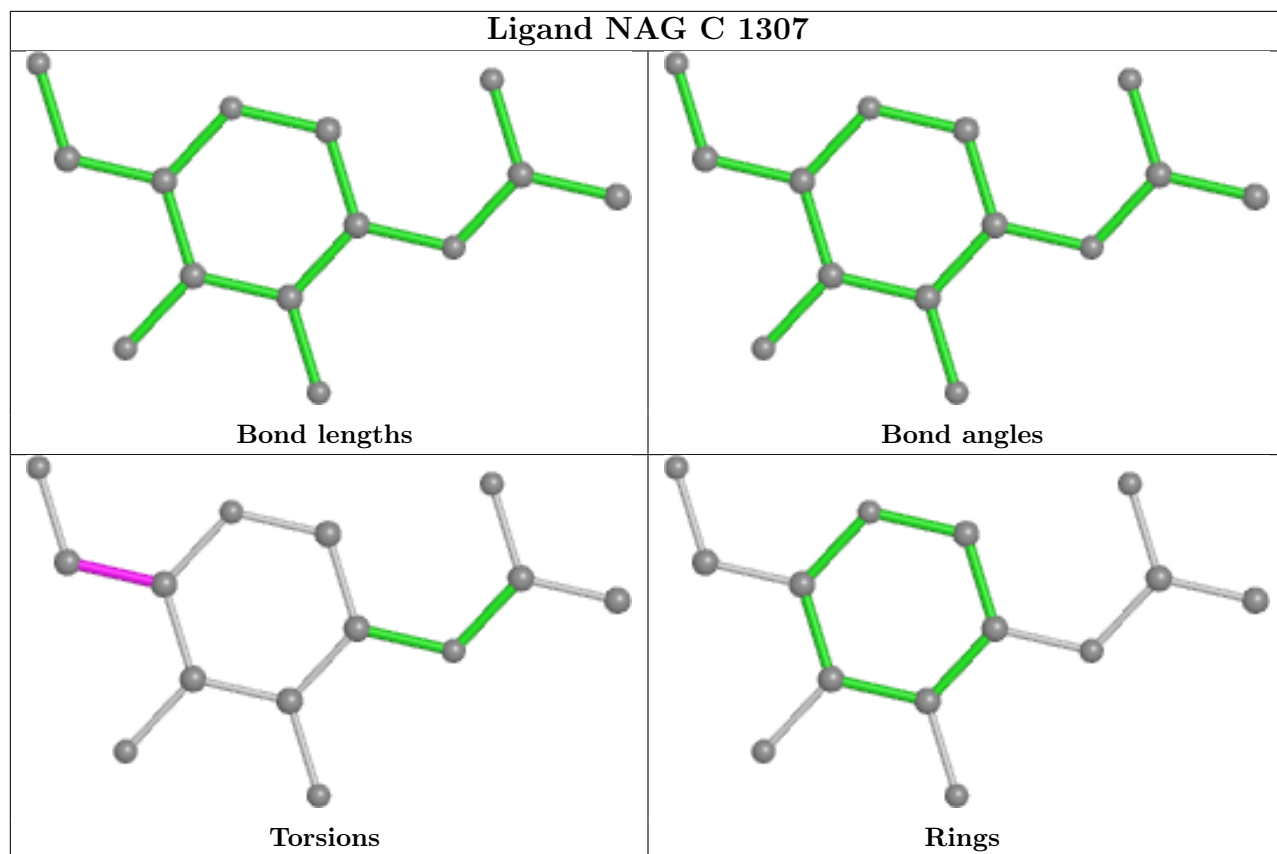


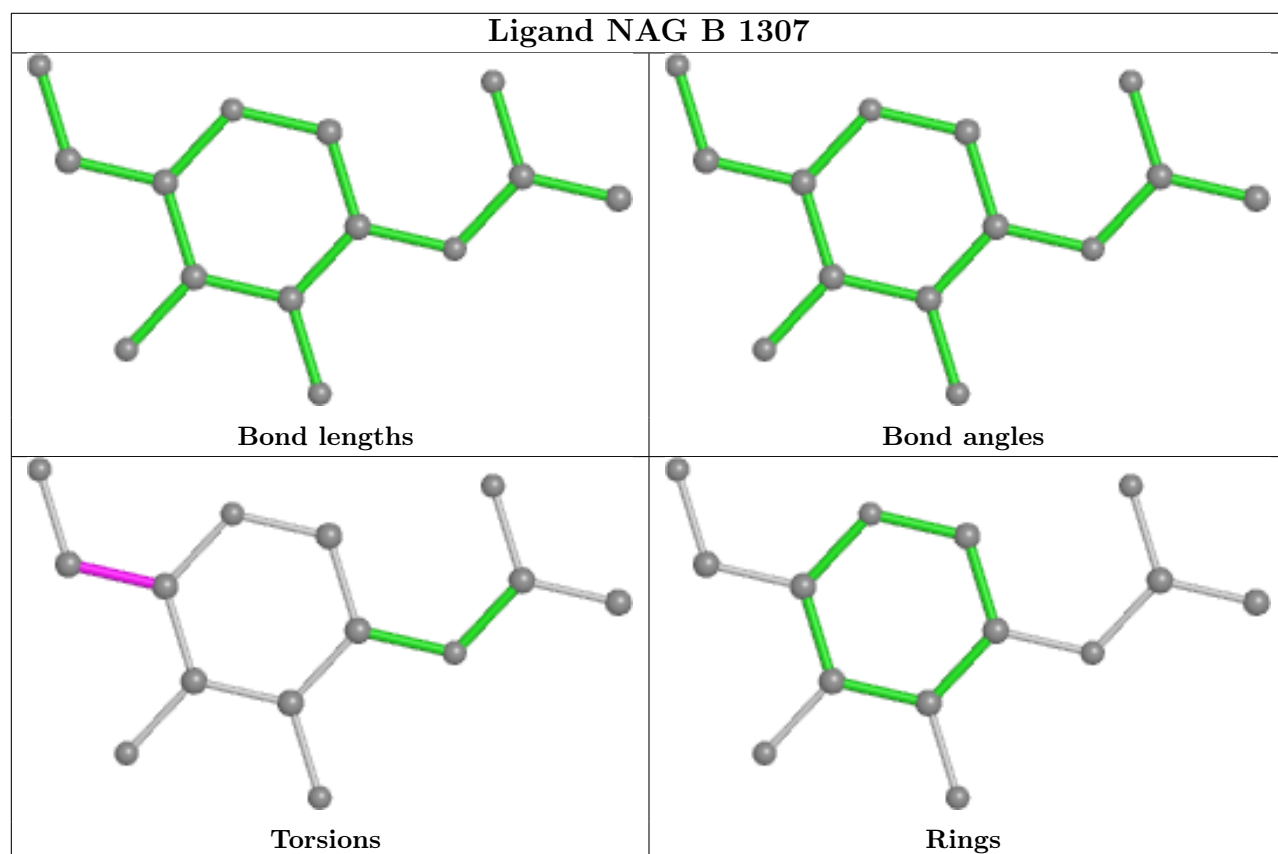
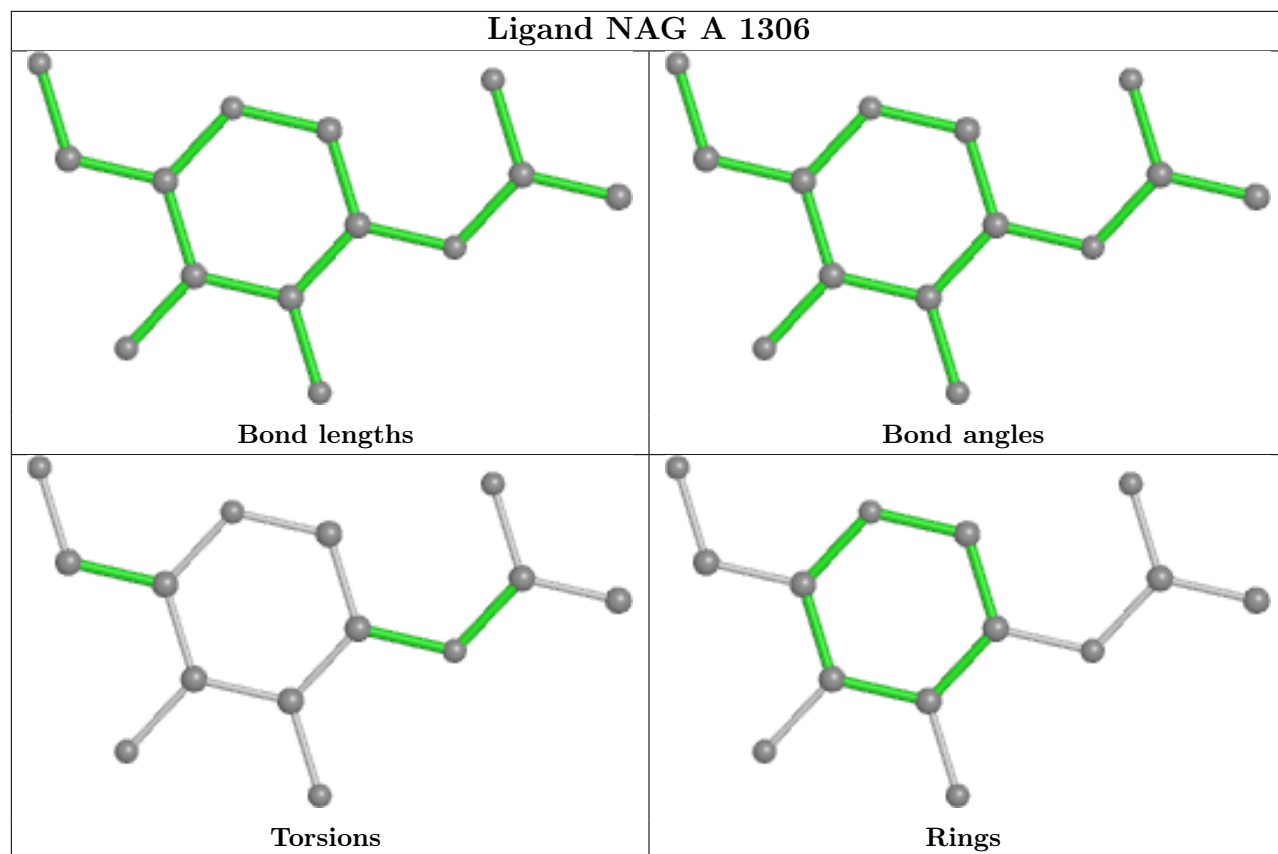












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

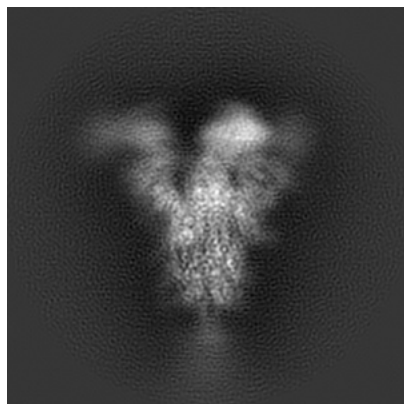
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33766. These allow visual inspection of the internal detail of the map and identification of artifacts.

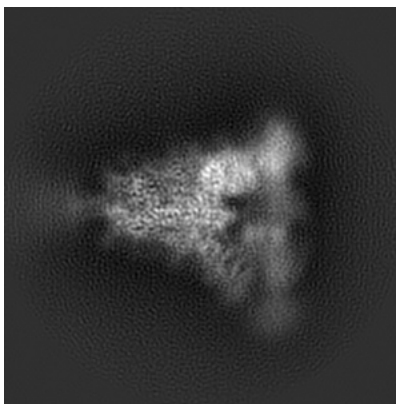
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

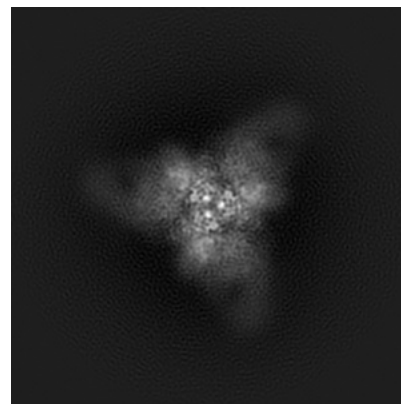
6.1.1 Primary map



X

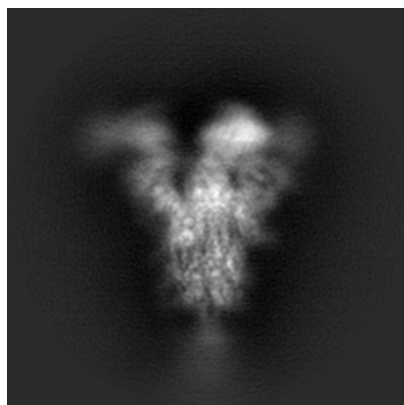


Y

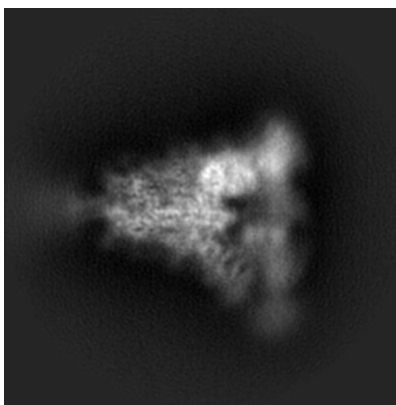


Z

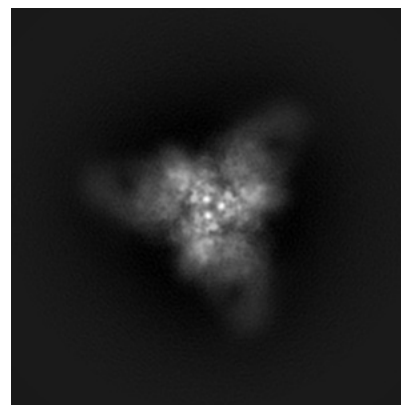
6.1.2 Raw map



X



Y

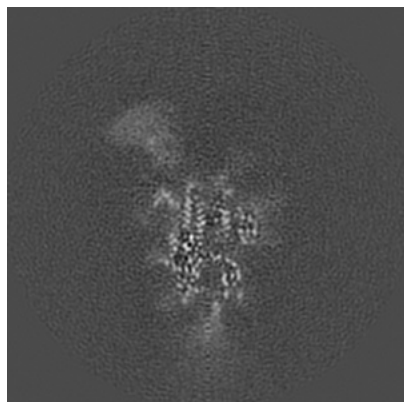


Z

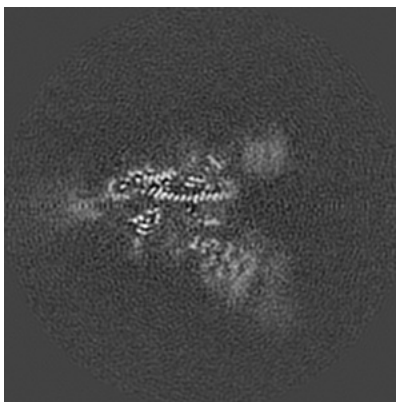
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

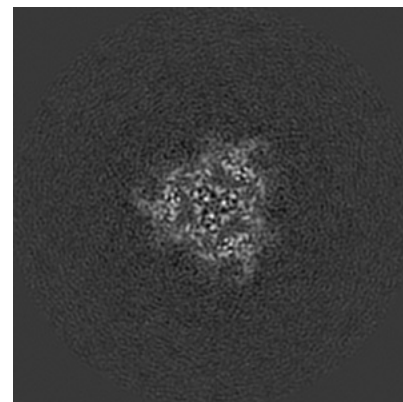
6.2.1 Primary map



X Index: 96

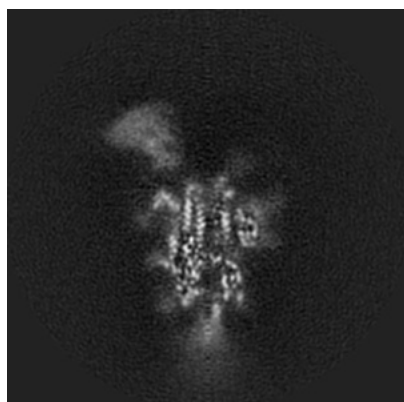


Y Index: 96

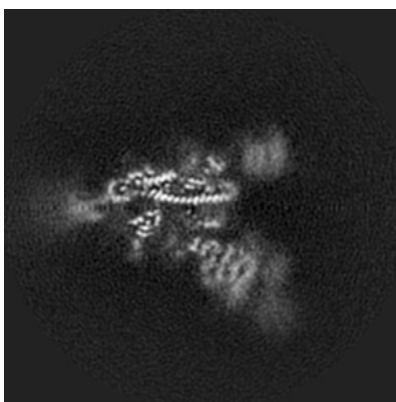


Z Index: 96

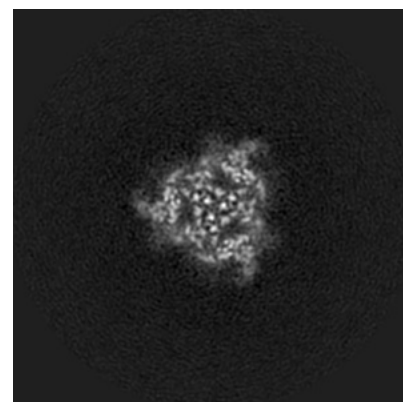
6.2.2 Raw map



X Index: 96



Y Index: 96

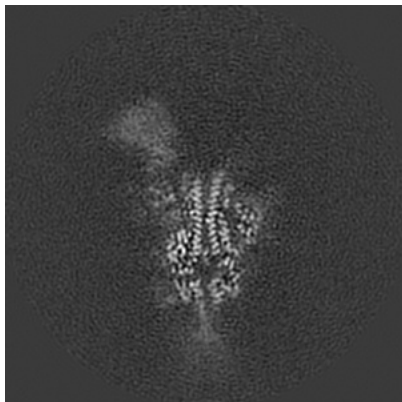


Z Index: 96

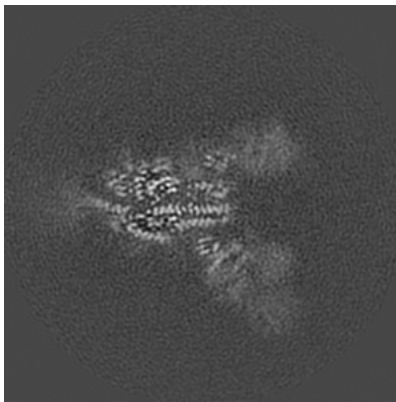
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

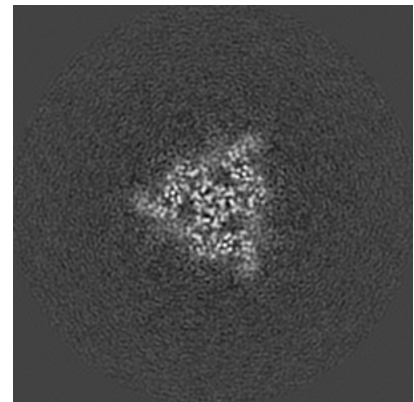
6.3.1 Primary map



X Index: 94

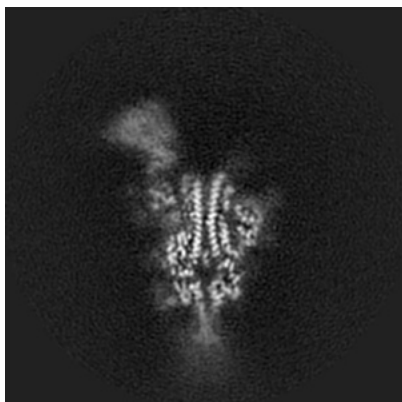


Y Index: 100

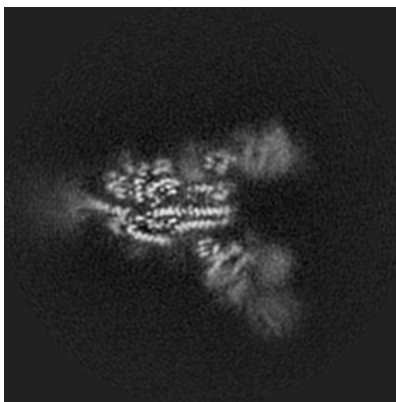


Z Index: 97

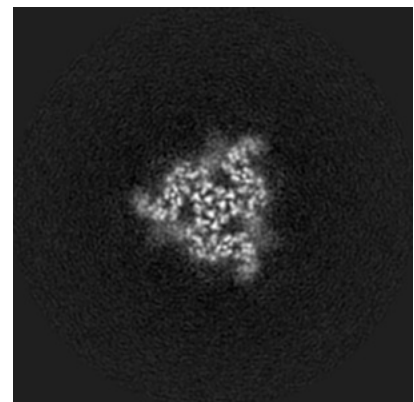
6.3.2 Raw map



X Index: 94



Y Index: 100

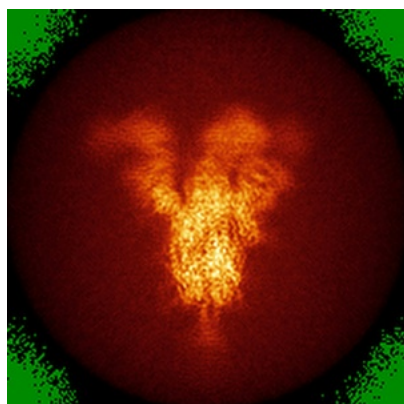


Z Index: 97

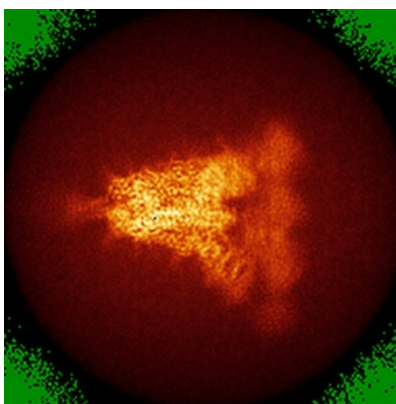
The images above show the largest variance slices of the map in three orthogonal directions.

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

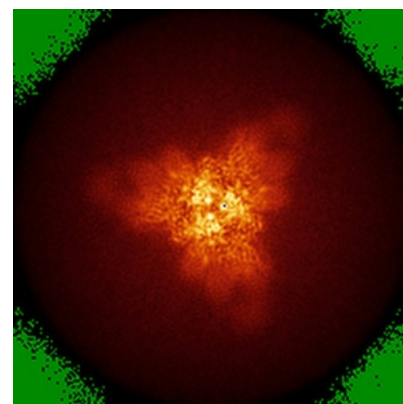
6.4.1 Primary map



X



Y

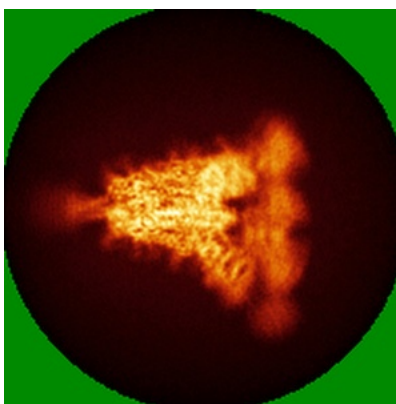


Z

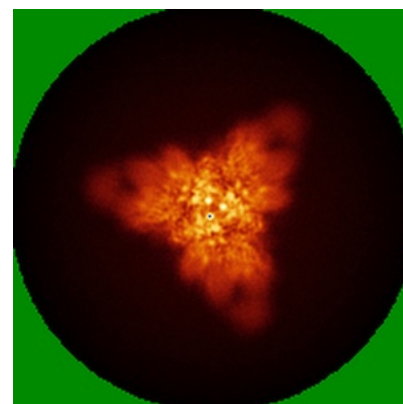
6.4.2 Raw map



X



Y

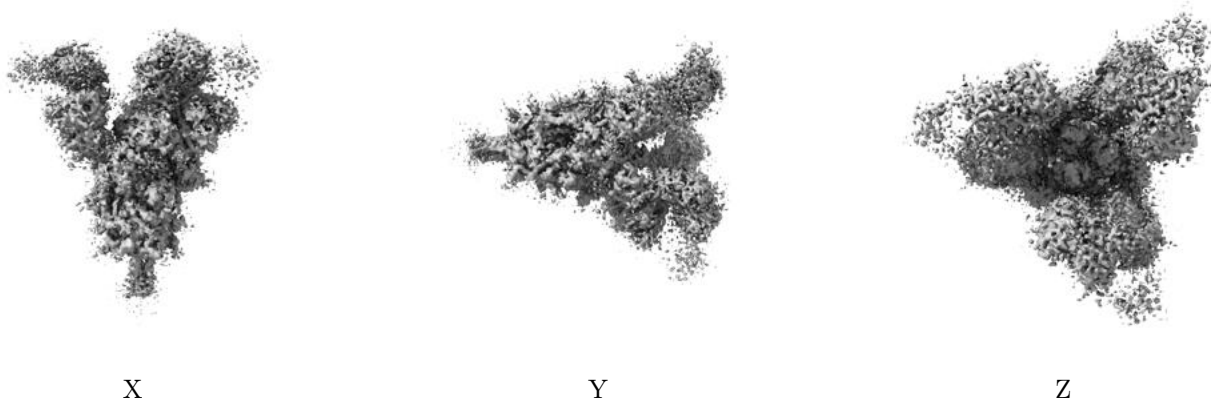


Z

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

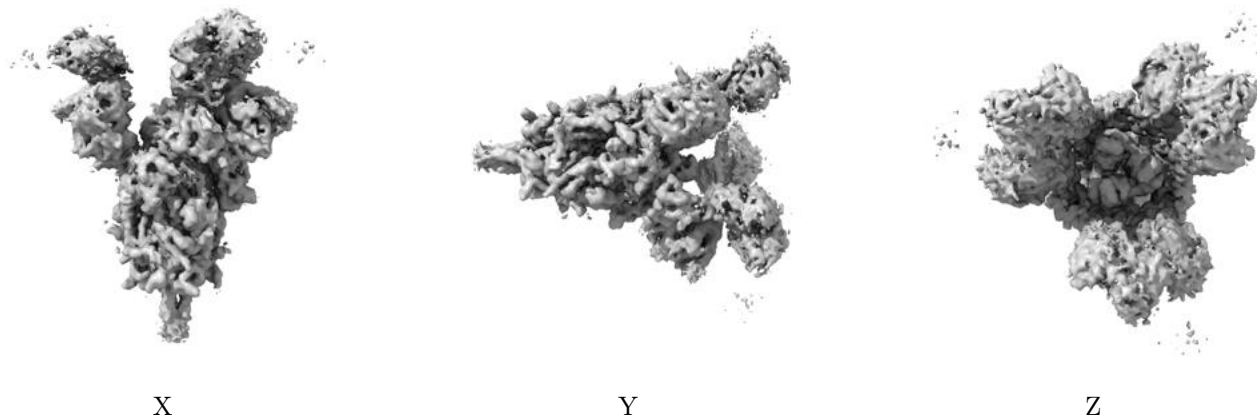
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

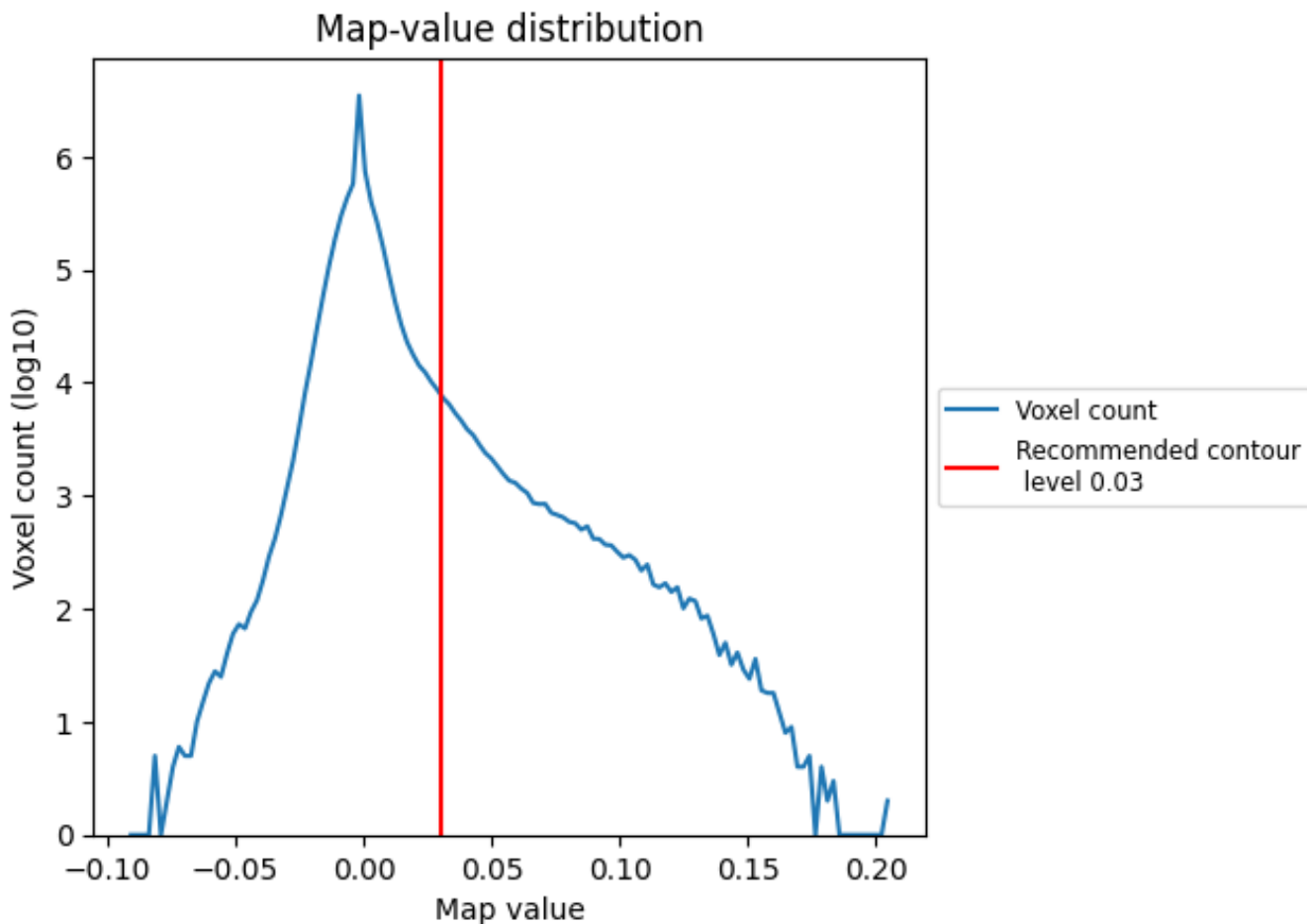
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

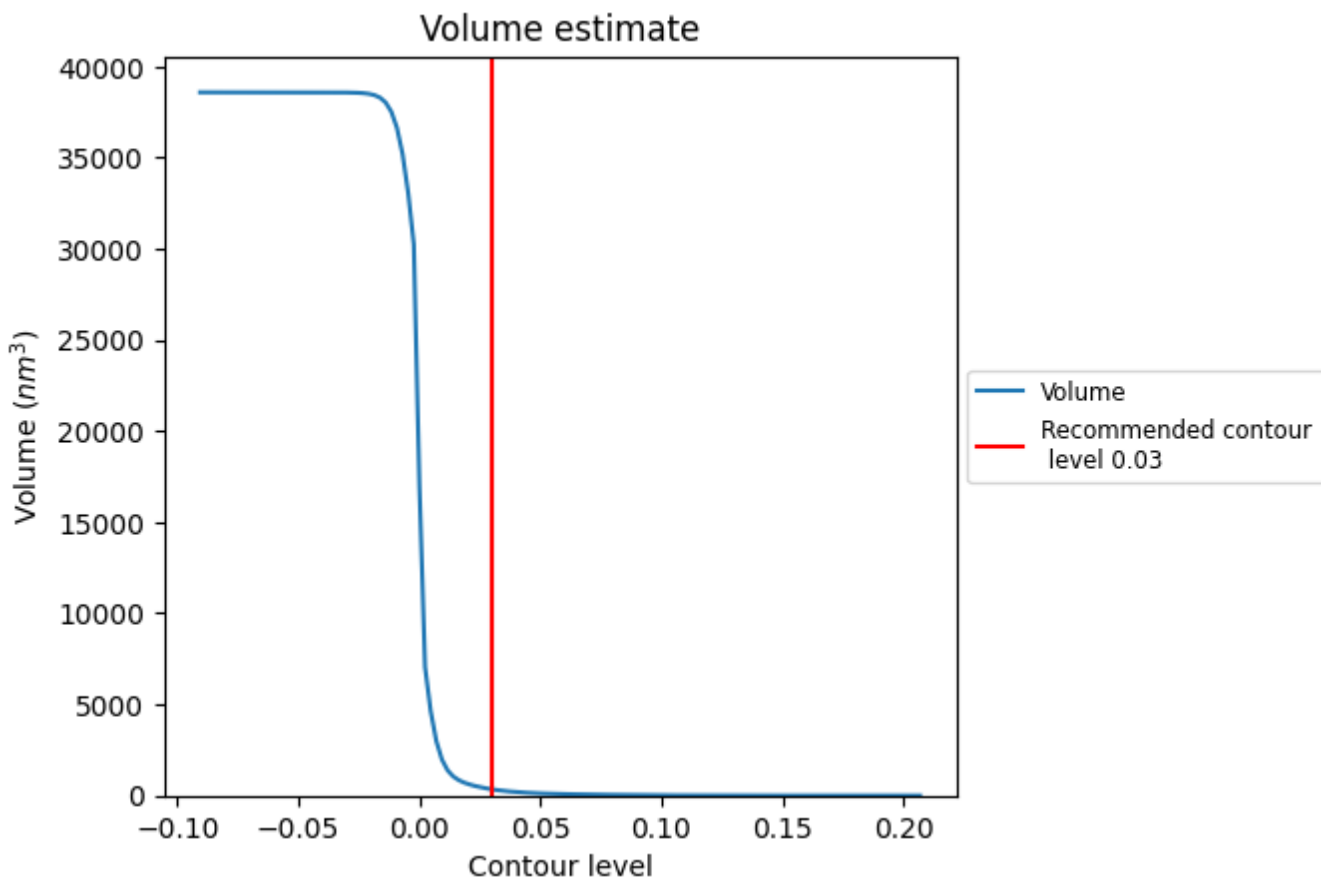
This section contains the results of statistical analysis of the map.

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.

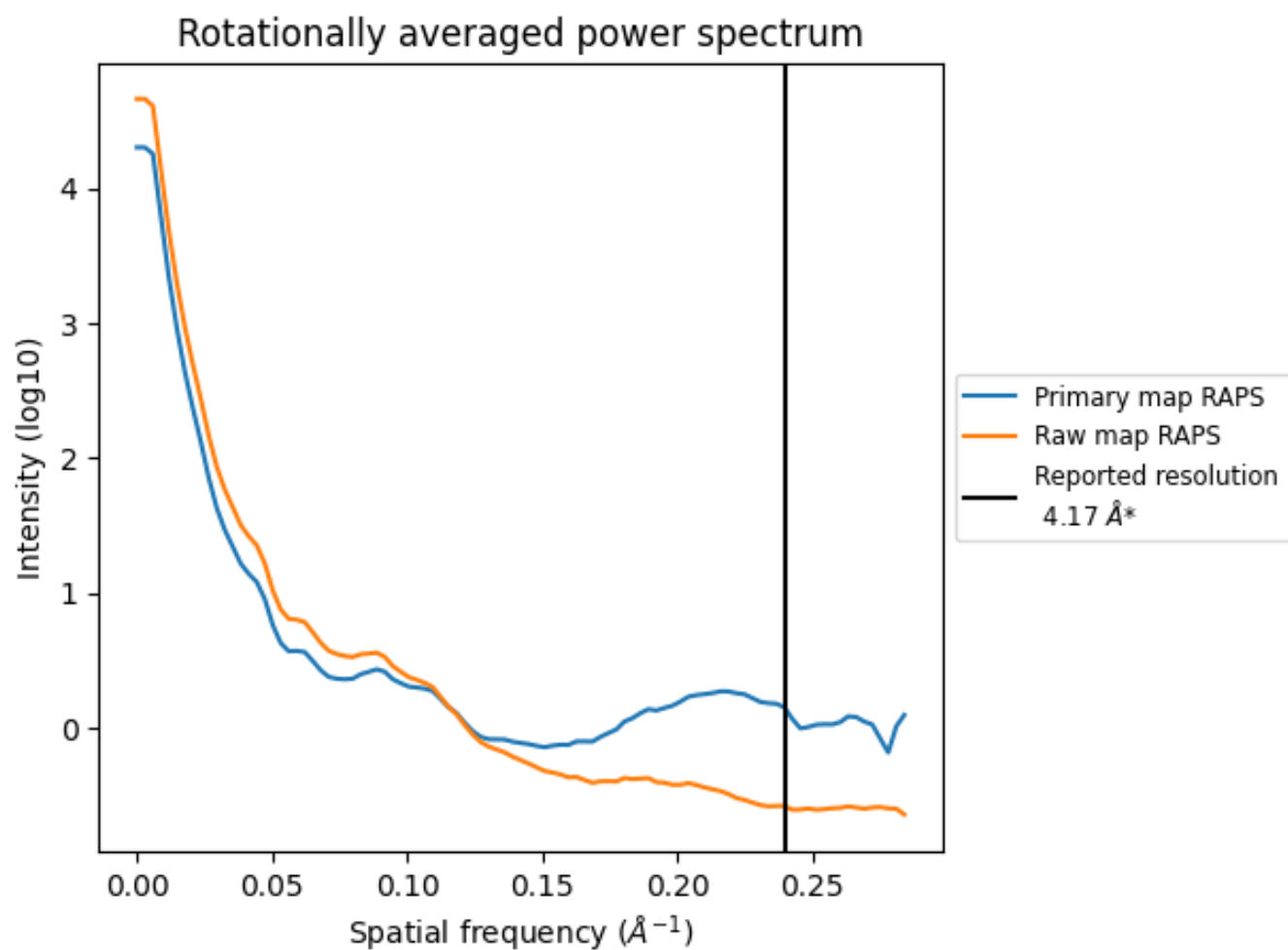
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 342 nm³; this corresponds to an approximate mass of 309 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 i

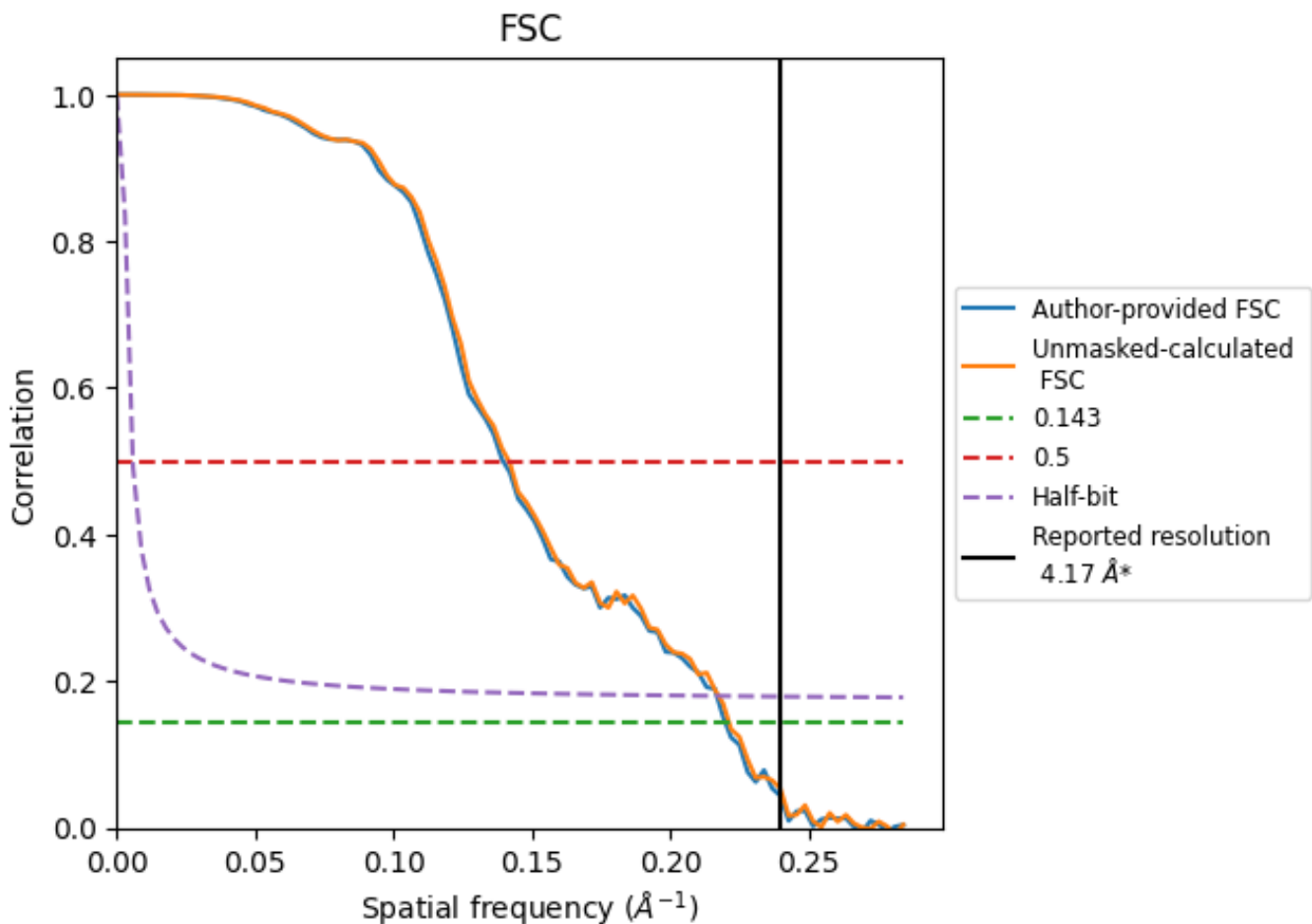


*Reported resolution corresponds to spatial frequency of 0.240 Å⁻¹

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 0.240 Å⁻¹

8.2 Resolution estimates [i](#)

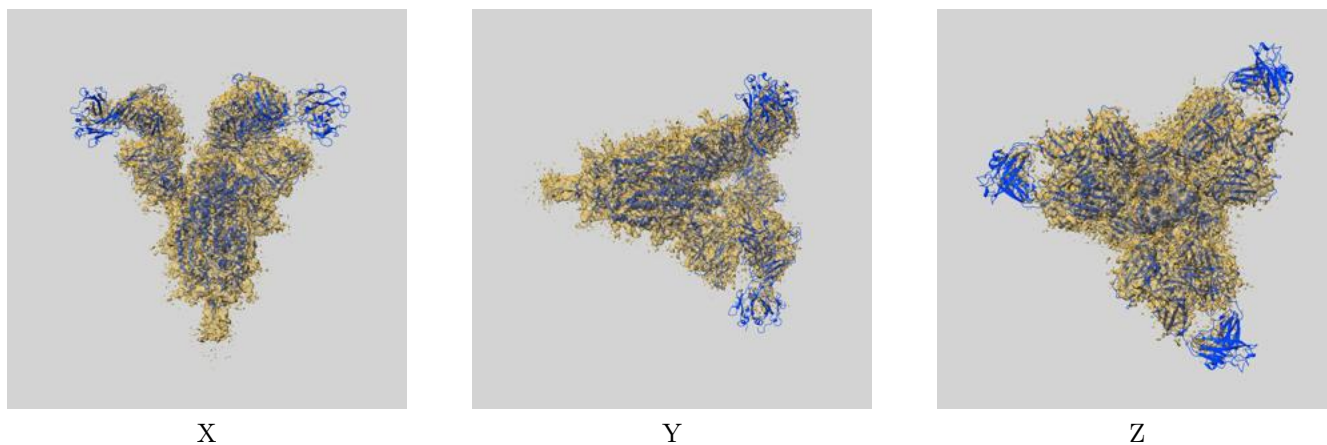
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.17	-	-
Author-provided FSC curve	4.55	7.16	4.61
Unmasked-calculated*	4.52	7.06	4.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

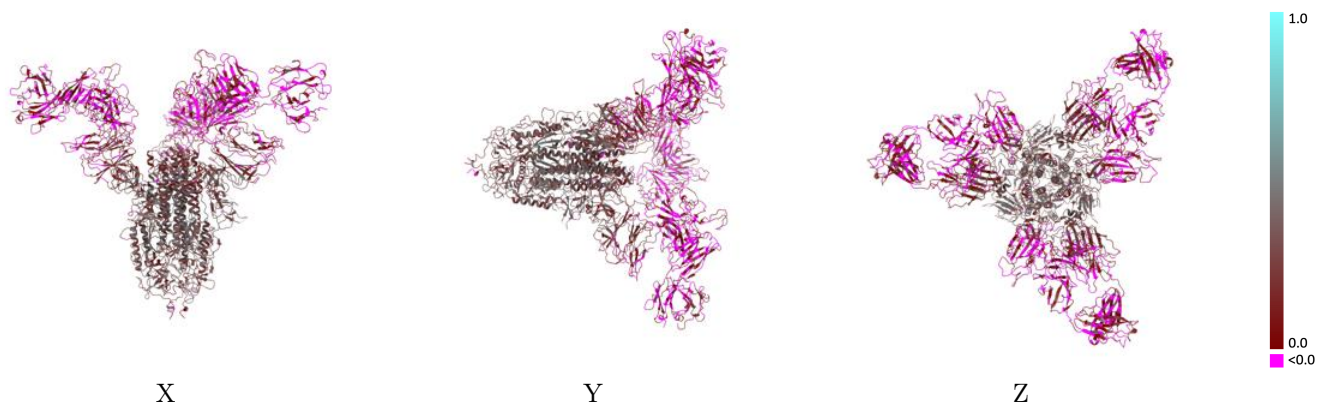
This section contains information regarding the fit between EMDB map EMD-33766 and PDB model 7YE9. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



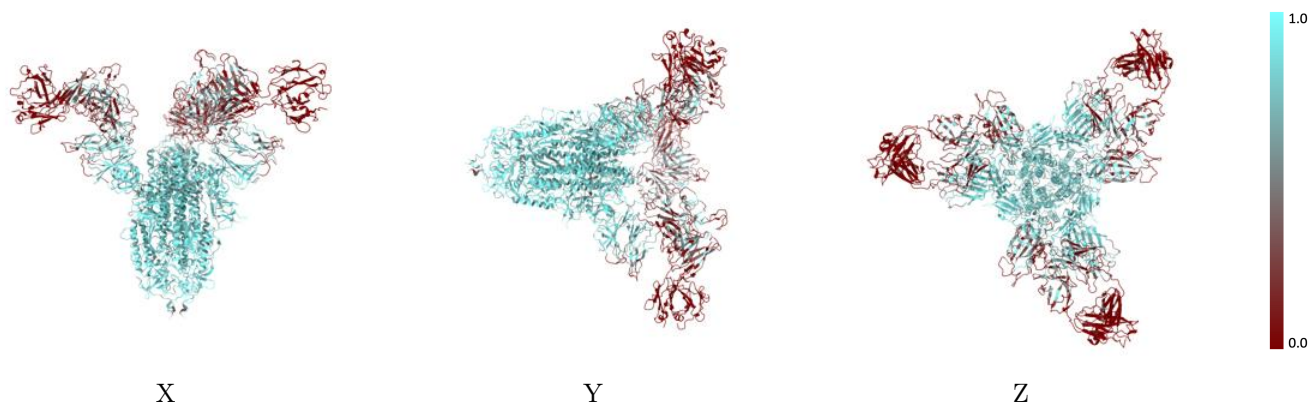
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



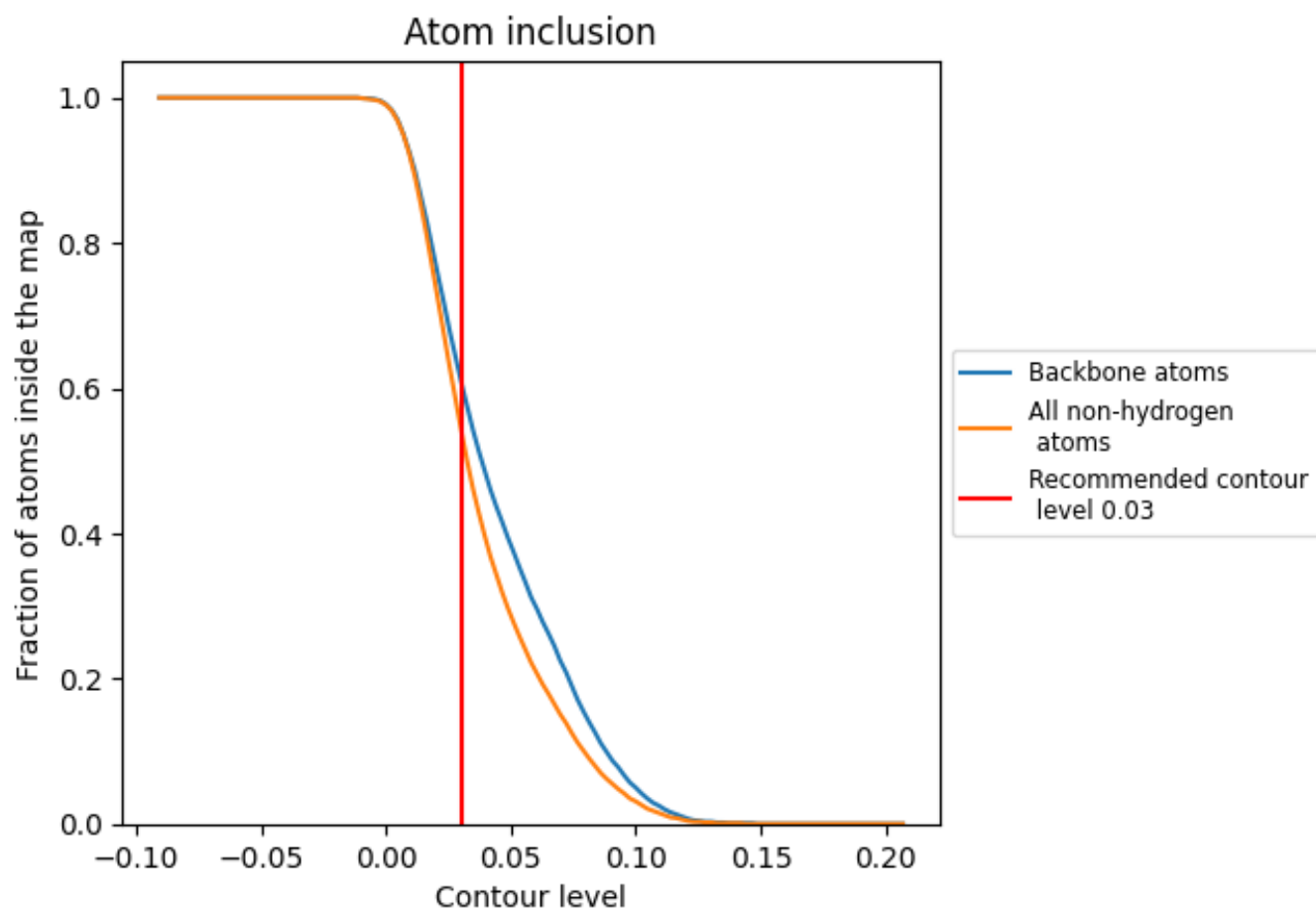
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 54% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5440	 0.1700
A	 0.6860	 0.2230
B	 0.6900	 0.2200
C	 0.6910	 0.2230
D	 0.6790	 0.2690
E	 0.6070	 0.2190
F	 0.7860	 0.3110
G	 0.1660	 0.0130
H	 0.1740	 0.0280
I	 0.1480	 0.0310
J	 0.5360	 0.2070
K	 0.7860	 0.3030
L	 0.1480	 0.0370
M	 0.5360	 0.2160
N	 0.1870	 0.0360
O	 0.1440	 0.0410

