



wwPDB EM Validation Summary Report ⓘ

Oct 20, 2024 – 09:00 PM EDT

PDB ID : 8EYH
EMDB ID : EMD-28688
Title : SARS-CoV-2 spike protein bound with a nanobody
Authors : Laughlin, Z.T.; Patel, A.; Ortlund, E.A.
Deposited on : 2022-10-27
Resolution : 3.75 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.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
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

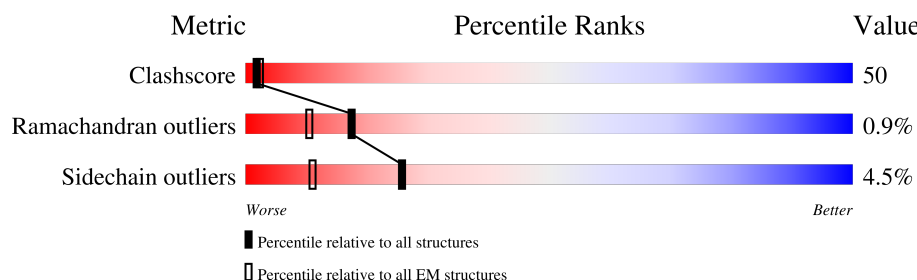
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.75 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	D	118	<div> <div>59%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	A	1136	<div> <div>37%</div> <div>54%</div> <div>6%</div> <div>.</div> </div>
2	B	1136	<div> <div>36%</div> <div>57%</div> <div>.</div> <div>.</div> </div>
2	C	1136	<div> <div>42%</div> <div>54%</div> <div>6%</div> <div>.</div> <div>.</div> </div>
3	E	2	<div> <div>50%</div> <div>100%</div> </div>
3	F	2	<div> <div>50%</div> <div>50%</div> </div>
3	G	2	<div> <div>50%</div> <div>50%</div> </div>
3	H	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	2	<div> <div>100%</div> <div>  </div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	I	1	-	-	X	-
4	NAG	C	1201	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26575 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 Nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	118	Total	C	N	O	S	0	0
			868	543	147	174	4		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1088	Total	C	N	O	S	0	0
			8515	5436	1421	1620	38		
2	C	1067	Total	C	N	O	S	0	0
			8350	5327	1395	1589	39		
2	A	1069	Total	C	N	O	S	0	0
			8366	5339	1397	1591	39		

There are 18 discrepancies between the modelled and reference sequences:

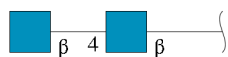
Chain	Residue	Modelled	Actual	Comment	Reference
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2

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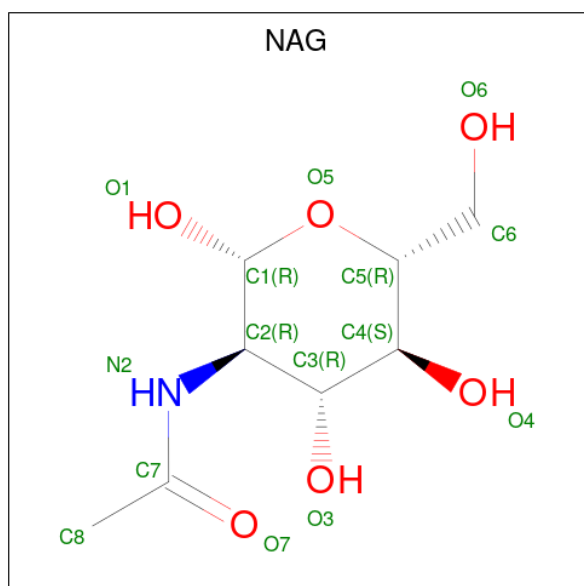
Chain	Residue	Modelled	Actual	Comment	Reference
A	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 3 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
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

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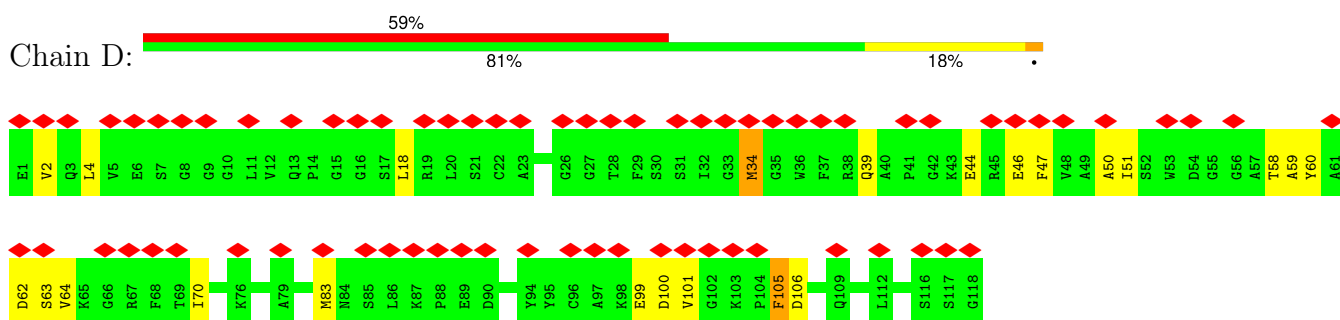
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

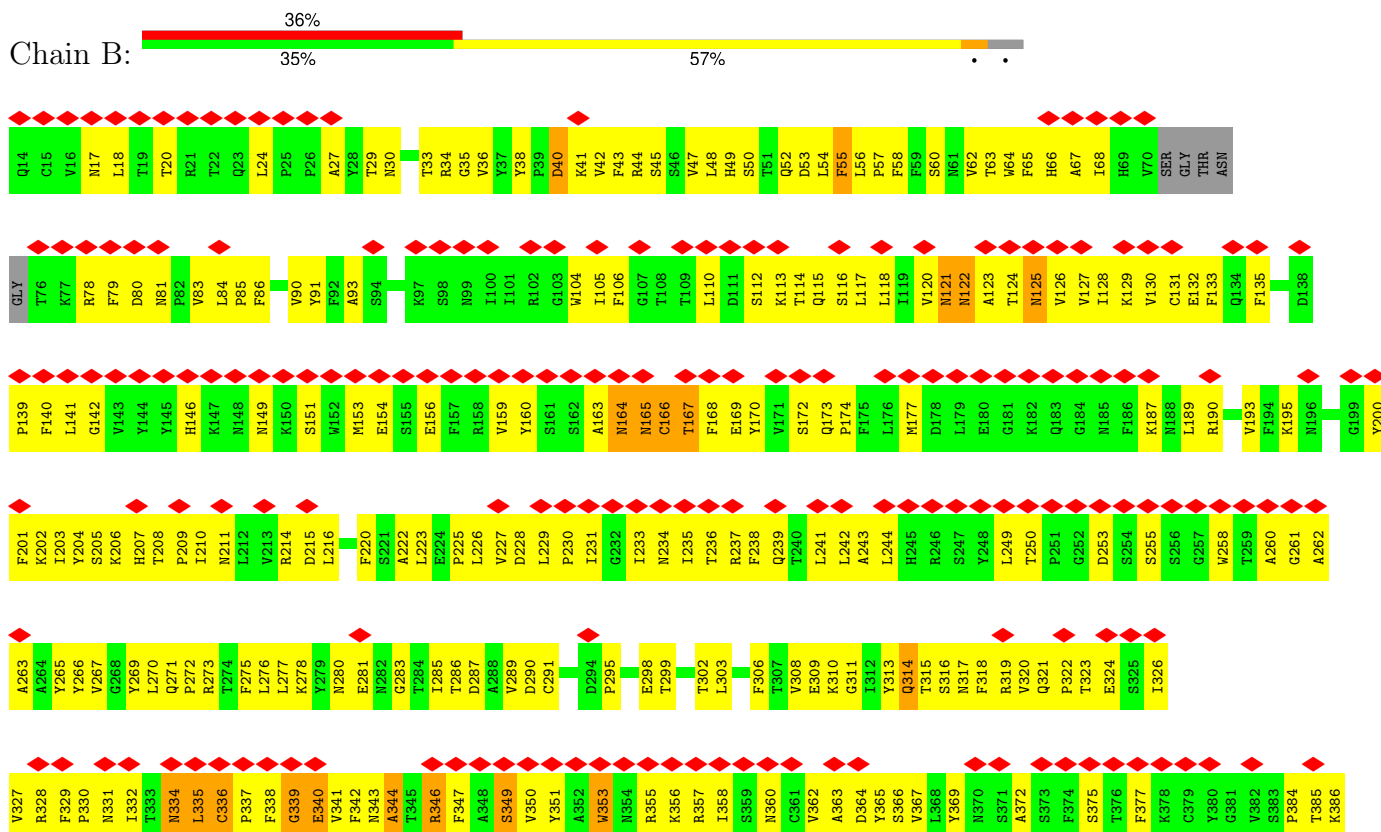
3 Residue-property plots [i](#)

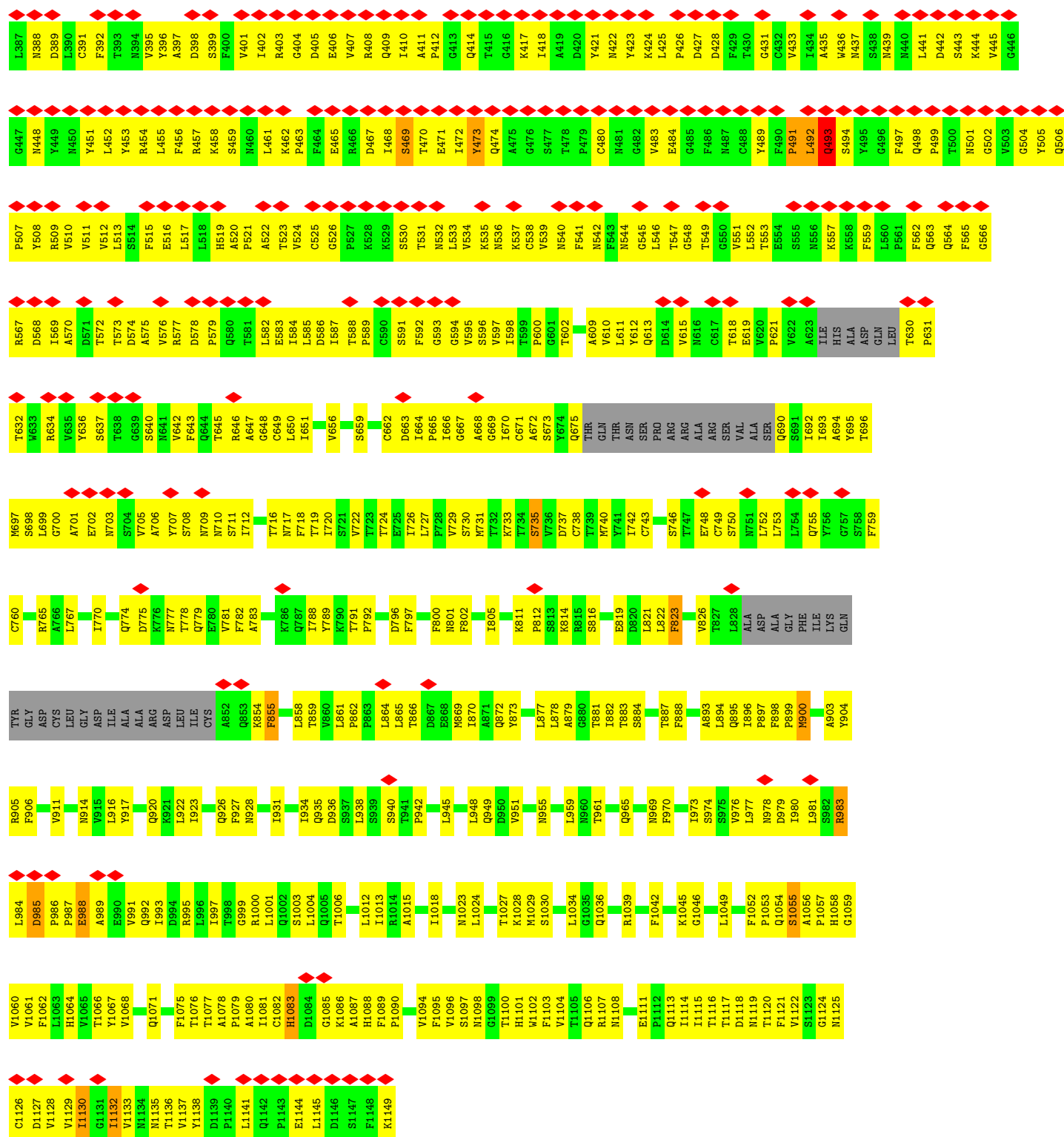
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Nanobody

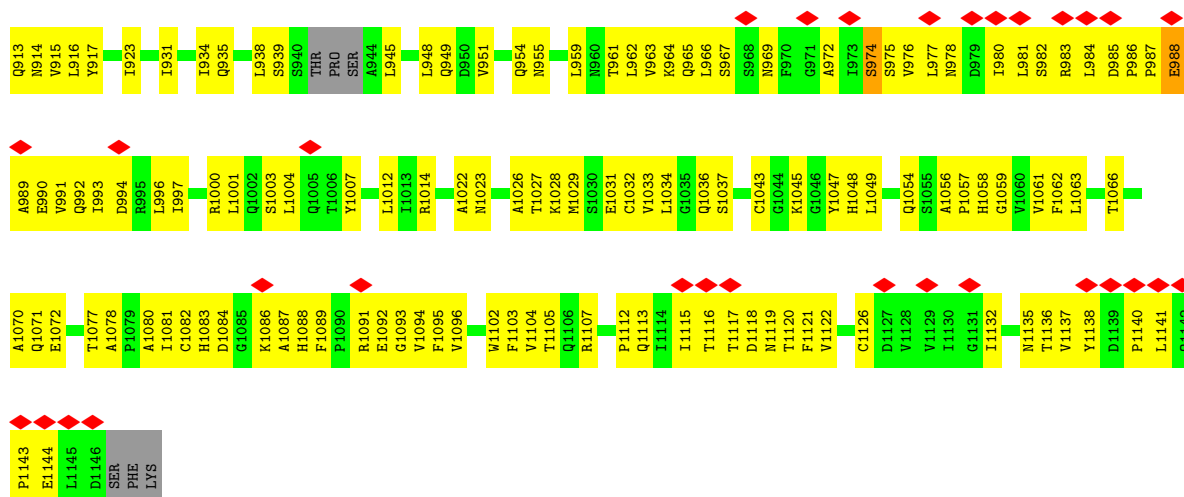


• Molecule 2: Spike glycoprotein

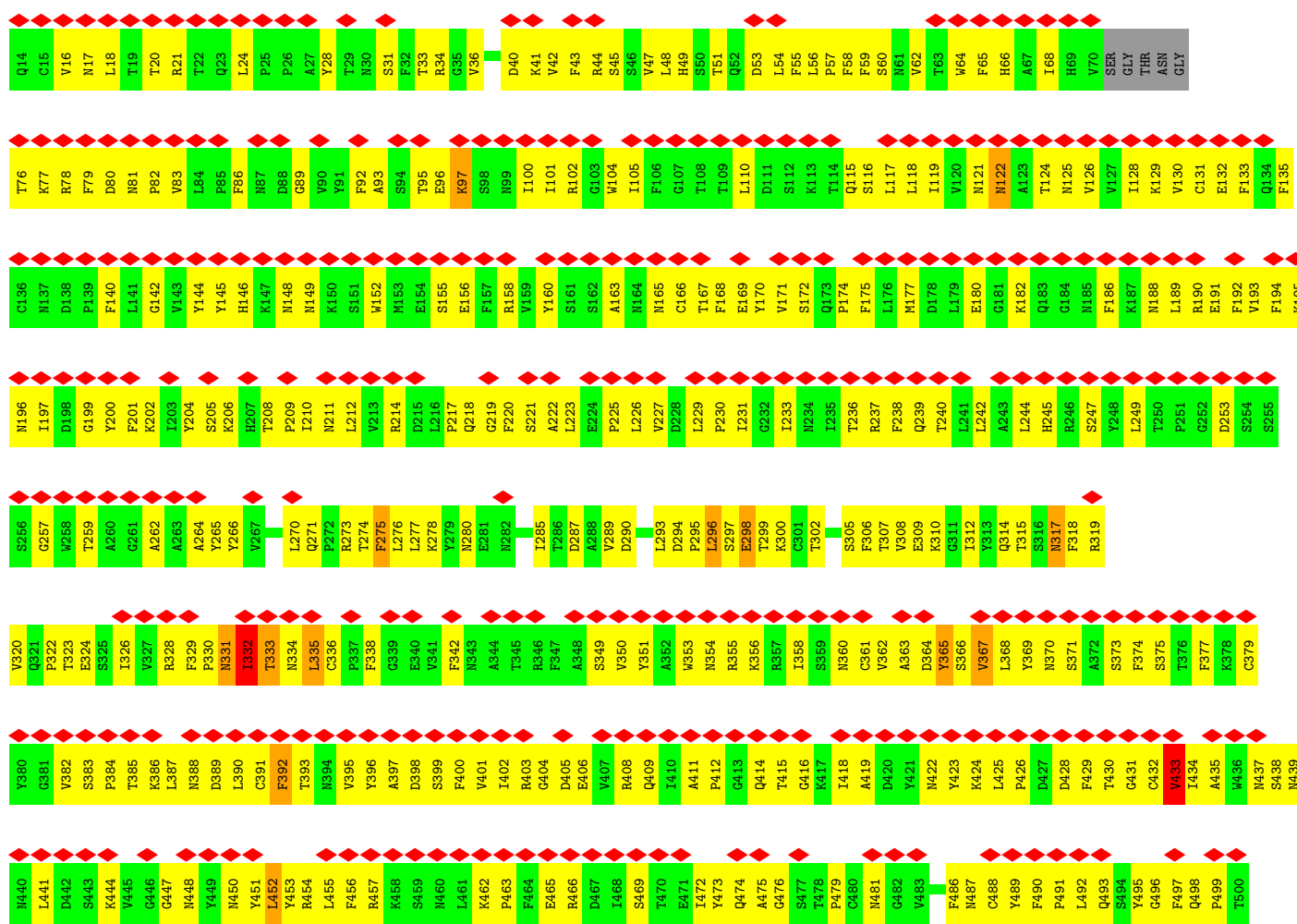


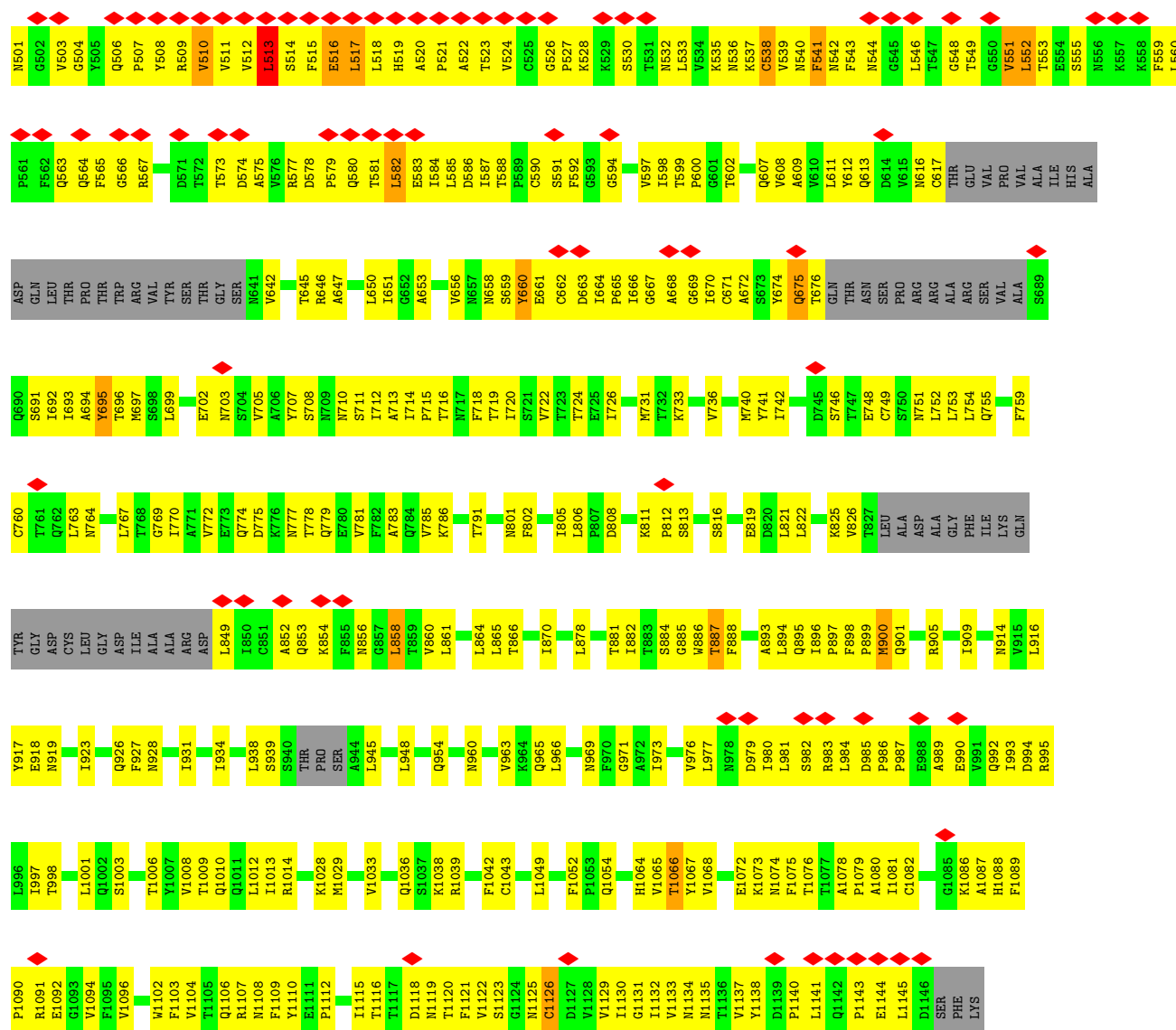


ALA	ALA	ARG	ASP	LEU	ILE	C851	A852	K853	K854	F855	N856	G857	L858	F859	V860	L861	P862	P863	L864	L865	Y873	L877	L878	A879	P880	P881	L882	L883	T884	S885	S886	W887	L888	F889	G890	D891	P892	L894	K895	L896	P897	F898	P899	M900	Q901	T902	A903	Y904	R905	F906	N907	G908	I909	G910	V911	T912					
A771	V772	E773	Q774	D775	K776	N777	T778	Q779	E780	V781	F782	A783	Q784	V785	K786	Q787	T788	Y789	K790	P791	P792	F802	S803	Q804	L805	L806	P807	P808	K811	T883	S884	G885	W886	L887	L821	L822	L823	N824	K825	V826	T827	LEU	L894	K895	L896	P897	F898	P899	M900	Q901	T902	A903	Y904	R905	F906	N907	G908	I909	G910	V911	T912
THR	PRO	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	SER	N641	V642	T645	V646	A647	L650	L651	L652	A653	E654	H655	V656	C662	D663	T664	P665	P666	C667	A668	G669	I670	C671	A672	T676	GLN	THR	ASN	PRO	ARG	ARG	ALA	ALA	ARG	ARG	SER	VAL	ALA	S689	T692	I693	A694	M697	S704								
G566	R567	D568	I569	A570	D571	T572	T573	D574	A575	V576	R577	D578	P579	Q580	L582	E583	I584	L585	D586	I587	T588	P589	C590	S591	F592	G593	G594	V595	S596	V597	I598	T599	P600	G601	T602	S605	V608	A609	V610	L611	V612	Q613	C617	THR	GLU	VAL	PRO	VAL	ALA	ILE	HIS	ALA	ASP	GLN	LEU						
Q506	P507	Y508	R509	V510	V511	V512	L513	S514	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	P527	K528	K529	S530	T531	N532	L533	V534	K535	N536	K537	C538	V539	F541	N542	F543	N544	G545	L546	T547	G548	T549	G550	V551	L552	T553	E554	S555	N556	K557	K558	F559	L560	P561	F562	Q563	Q564	F565			
G446	G447	N448	Y449	N450	N451	L452	Y453	R454	L455	F456	R457	K458	S459	N460	L461	K462	F463	F464	E465	R466	D467	I468	S469	T470	E471	I472	Y473	Q474	A475	G476	S477	T478	P479	C480	N481	G482	V483	E484	G485	F486	C488	Y489	F490	P491	L492	Q493	S494	Y495	G496	F497	Q498	P499	T500	N501	G502	V503	G504	Y505			
K386	L387	N388	D389	L390	C391	F392	T393	N394	V395	Y396	D397	D398	S399	F400	V401	I402	R403	G404	D405	E406	V407	R408	Q409	I410	A411	P412	G413	Q414	T415	G416	K417	I418	A419	D420	Y421	N422	Y423	K424	L425	P426	D427	D428	F429	T430	G431	C432	V433	I434	A435	W436	N437	S438	N439	N440	L441	D442	S443	K444	V445		
I326	V327	R328	F329	P330	N331	L332	T333	N334	L335	C336	P337	F338	G339	E340	V341	F342	K343	A344	T345	R346	F347	A348	S349	V350	Y351	A352	L353	N354	R355	K356	R357	T358	S359	N360	C361	V362	A363	D364	Y365	S366	V367	L368	Y369	N370	S371	A372	S373	F374	S375	T376	F377	K378	C379	Y380	G381	V382	S383	P384	T385		
K77	R78	F79	D80	N81	P82	V83	L84	P85	F86	N87	D88	G89	V90	Y91	F92	E96	K97	S98	N99	I100	I101	R102	G103	W104	I105	R106	G107	T108	T109	L110	D111	S112	K113	T114	Q115	S116	L117	L118	I119	V120	N121	N122	W123	A123	G124	H125	Q126	G127	K128	V129	K129	V130	C131	E132	F133	Q134	F135	C136	N137	D138	
P139	F140	L141	G142	V143	Y144	Y145	H146	K147	N148	N149	K150	S151	W152	M153	E154	S155	E156	F157	R158	V159	Y160	G161	S162	A163	N164	N165	C166	T167	F168	E169	S170	V171	K172	Q173	P174	F175	L176	M177	D178	L179	A180	G181	K182	Q183	G184	N185	F186	V187	K187	N188	L189	R190	E191	F192	V193	F194	K195	N196	I197	D198	
G199	Y200	F201	K202	I203	Y204	S205	K206	H207	T210	N211	L212	V213	R214	D215	L216	F217	Q218	Q219	F220	S221	A222	L223	E224	P225	L226	V227	D228	L229	P230	T231	G232	S233	N234	I235	T236	R237	F238	Q239	T240	L241	A242	A243	L244	H245	R246	S247	Y248	L249	T250	P251	G252	D253	S254	S255	S256	G257	W258	T259			
A260	G261	A262	A263	A264	Y265	Y266	G267	G268	Y269	L270	Q271	P272	R273	T274	F275	L276	L277	K278	Y279	E281	N282	G283	T284	L285	T286	D287	D290	C291	A292	L293	D294	P295	L296	E297	E298	T299	L303	K304	S305	F306	T307	V308	E309	K310	G311	I312	S316	N317	F318	R319	P322	T323	E324	S325							
T326	V327	R328	F329	P330	N331	L332	T333	N334	L335	C336	P337	F338	G339	E340	V341	F342	K343	A344	T345	R346	F347	A348	S349	V350	Y351	A352	L353	N354	R355	K356	R357	T358	S359	N360	C361	V362	A363	D364	Y365	S366	V367	L368	Y369	N370	S371	A372	S373	F374	S375	T376	F377	K378	C379	Y380	G381	V382	S383	P384	T385		
K386	L387	N388	D389	L390	C391	F392	T393	N394	V395	Y396	D397	D398	S399	F400	V401	I402	R403	G404	D405	E406	V407	R408	Q409	I410	A411	P412	G413	Q414	T415	G416	K417	I418	A419	D420	Y421	N422	Y423	K424	L425	P426	D427	D428	F429	T430	G431	C432	V433	I434	A435	W436	N437	S438	N439	N440	L441	D442	S443	K444	V445		
G446	G447	N448	Y449	N450	N451	L452	Y453	R454	L455	F456	R457	K458	S459	N460	L461	K462	F463	F464	E465	R466	D467	I468	S469	T470	E471	I472	Y473	Q474	A475	G476	S477	T478	P479	C480	N481	G482	V483	E484	G485	F486	C488	Y489	F490	P491	L492	Q493	S494	Y495	G496	F497	Q498	P499	T500	N501	G502	V503	G504	Y505			
Q506	P507	Y508	R509	V510	V511	V512	L513	S514	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	P527	K528	K529	S530	T531	N532	L533	V534	K535	N536	K537	C538	V539	F541	N542	F543	N544	G545	L546	T547	G548	T549	G550	V551	L552	T553	E554	S555	N556	K557	K558	F559	L560	P561	F562	Q563	Q564	F565			
G566	R567	D568	I569	A570	D571	T572	T573	D574	A575	V576	R577	D578	P579	Q580	L582	E583	I584	L585	D586	I587	T588	P589	C590	S591	F592	G593	G594	V595	S596	V597	I598	T599	P600	G601	T602	S605	V608	A609	V610	L611	V612	Q613	C617	THR	GLU	VAL	PRO	VAL	ALA	ILE	HIS	ALA	ASP	GLN	LEU						
THR	PRO	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	SER	N641	V642	T645	V646	A647	L650	L651	L652	A653	E654	H655	V656	C662	D663	T664	P665	P666	C667	A668	G669	I670	C671	A672	T676	GLN	THR	ASN	PRO	ARG	ARG	ALA	ALA	ARG	ARG	SER	VAL	ALA	S689	T692	I693	A694	M697	S704								
V705	A706	Y707	S708	N709	N710	S711	I712	A713	V714	F715	T716	N717	F718	T719	T724	E725	V726	L727	P728	V729	S730	T732	K733	T734	S735	V736	D737	C738	T739	M740	Y741	I742	C743	G744	D745	S746	T747	E748	C749	S750	N751	L752	L753	L754	Q755	S758	F759	C760	T761	R765	A766	L767	T768	G769	I770						
A771	V772	E773	Q774	D775	K776	N777	T778	Q779	E780	V781	F782	A783	Q784	V785	K786	Q787	T788	Y789	K790	P791	P792	F802	S803	Q804	L805	L806	P807	P808	K811	T883	S884	G885	W886	L887	L821	L822	L823	N824	K825	V826	T827	LEU	L894	K895	L896	P897	F898	P899	M900	Q901	T902	A903	Y904	R905	F906	N907	G908	I909	G910	V911	T912
ALA	ALA	ARG	ASP	LEU	ILE	C851	A852	K853	K854	F855	N856	G857	L858	F859	V860	L861	P862	P863	L864	L865	Y873	L877	L878	A879	P880	P881	L882	L883	T884	S885	S886	W887	L888	F889	G890	D891	P892	L894	K895	L896	P897	F898	P899	M900	Q901	T902	A903	Y904	R905	F906	N907	G908	I909	G910	V911	T912					



• Molecule 2: Spike glycoprotein





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	615492	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.81	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	66.367	Depositor
Minimum map value	-45.933	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.755	Depositor
Recommended contour level	5	Depositor
Map size (Å)	444.7456, 444.7456, 444.7456	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0691, 1.0691, 1.0691	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	D	0.25	0/886	0.47	0/1198
2	A	0.29	0/8562	0.48	0/11654
2	B	0.29	0/8719	0.47	0/11874
2	C	0.30	0/8546	0.48	0/11632
All	All	0.29	0/26713	0.47	0/36358

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	D	868	0	831	18	0
2	A	8366	0	8167	880	0
2	B	8515	0	8324	1084	0
2	C	8350	0	8147	964	0
3	E	28	0	25	0	0
3	F	28	0	25	6	0
3	G	28	0	25	4	0
3	H	28	0	25	4	0
3	I	28	0	25	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	126	0	116	9	0
4	B	98	0	91	6	0
4	C	112	0	104	19	0
All	All	26575	0	25905	2628	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 50.

The worst 5 of 2628 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ASN:HD21	3:I:1:NAG:C1	1.07	1.63
2:C:331:ASN:ND2	4:C:1201:NAG:C1	1.77	1.47
2:C:331:ASN:HD21	4:C:1201:NAG:C1	1.31	1.41
2:B:343:ASN:ND2	3:I:1:NAG:C1	1.93	1.30
2:A:334:ASN:HA	2:A:362:VAL:HG13	1.18	1.16

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	D	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
2	A	1057/1136 (93%)	957 (90%)	90 (8%)	10 (1%)	14	47
2	B	1078/1136 (95%)	963 (89%)	110 (10%)	5 (0%)	25	58
2	C	1055/1136 (93%)	933 (88%)	107 (10%)	15 (1%)	9	39
All	All	3306/3526 (94%)	2963 (90%)	313 (10%)	30 (1%)	17	47

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	329	PHE
2	C	330	PRO
2	C	450	ASN
2	A	332	ILE
2	A	367	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	89/89 (100%)	85 (96%)	4 (4%)	23	49
2	A	937/990 (95%)	897 (96%)	40 (4%)	25	50
2	B	954/990 (96%)	912 (96%)	42 (4%)	24	50
2	C	935/990 (94%)	889 (95%)	46 (5%)	21	47
All	All	2915/3059 (95%)	2783 (96%)	132 (4%)	26	49

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	551	VAL
2	A	582	LEU
2	A	1126	CYS
2	C	64	TRP
2	C	58	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	804	GLN
2	A	926	GLN
2	A	1119	ASN
2	C	149	ASN
2	C	66	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 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$
3	NAG	E	1	3,2	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	F	1	3,2	14,14,15	0.67	1 (7%)	17,19,21	0.98	1 (5%)
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	G	1	3,2	14,14,15	0.39	0	17,19,21	0.49	0
3	NAG	G	2	3	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	H	1	3,2	14,14,15	0.64	1 (7%)	17,19,21	0.64	0
3	NAG	H	2	3	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	I	1	3	14,14,15	0.48	0	17,19,21	0.37	0
3	NAG	I	2	3	14,14,15	0.36	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	NAG	I	1	3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-2.22	1.40	1.43
3	F	1	NAG	O5-C1	2.14	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-O5-C5	3.73	117.18	112.19

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C1-C2-N2-C7
3	F	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6

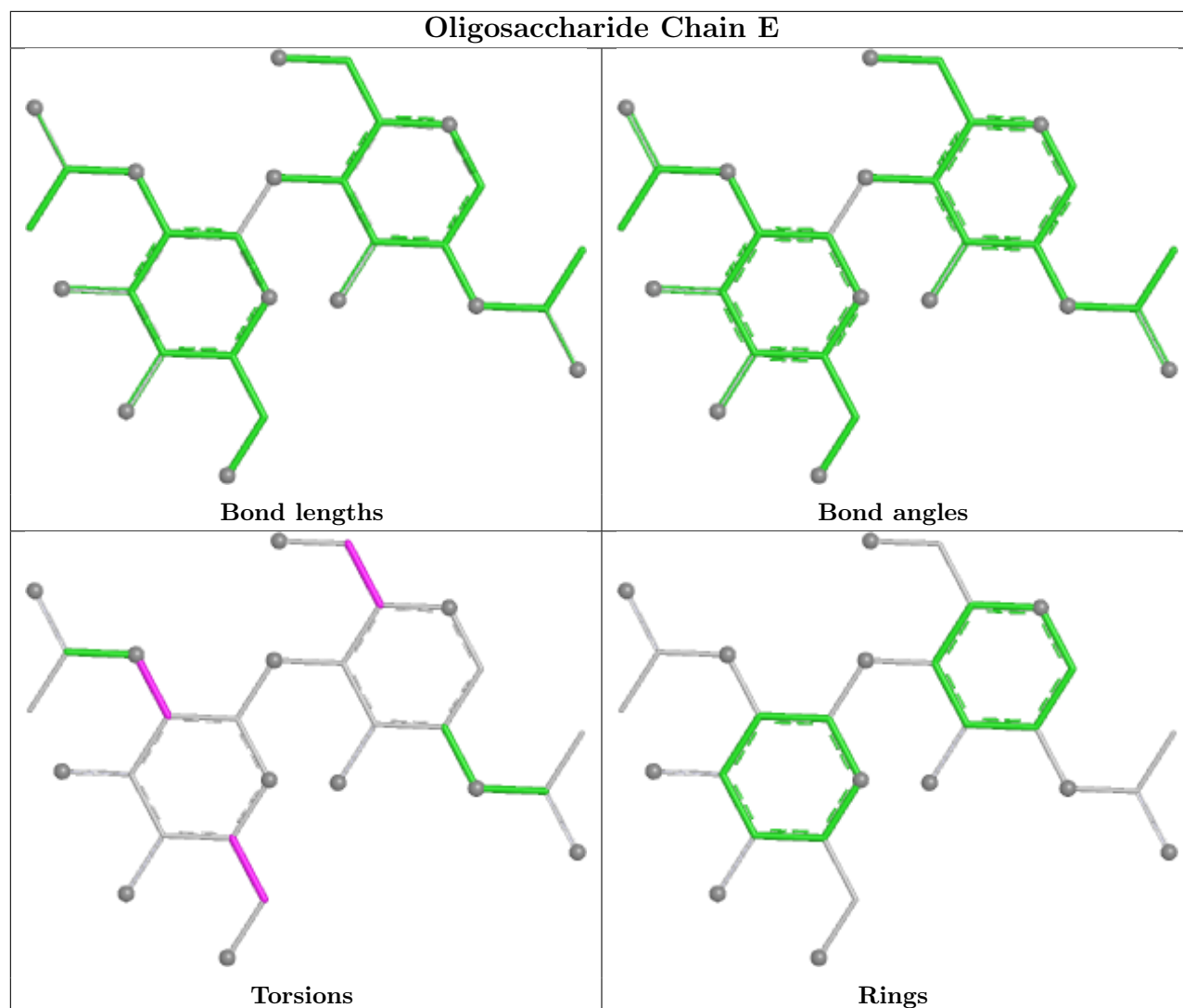
There are no ring outliers.

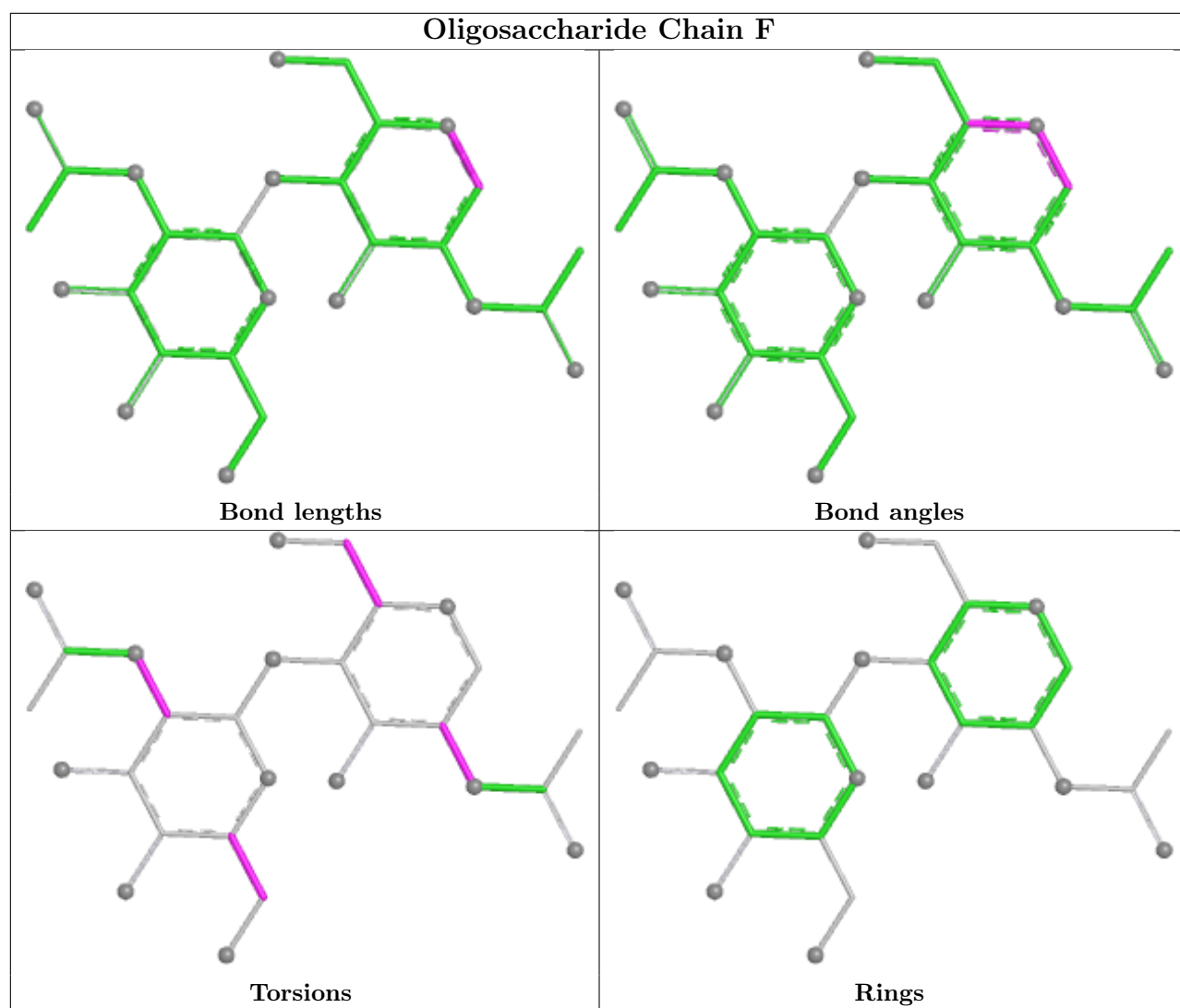
6 monomers are involved in 23 short contacts:

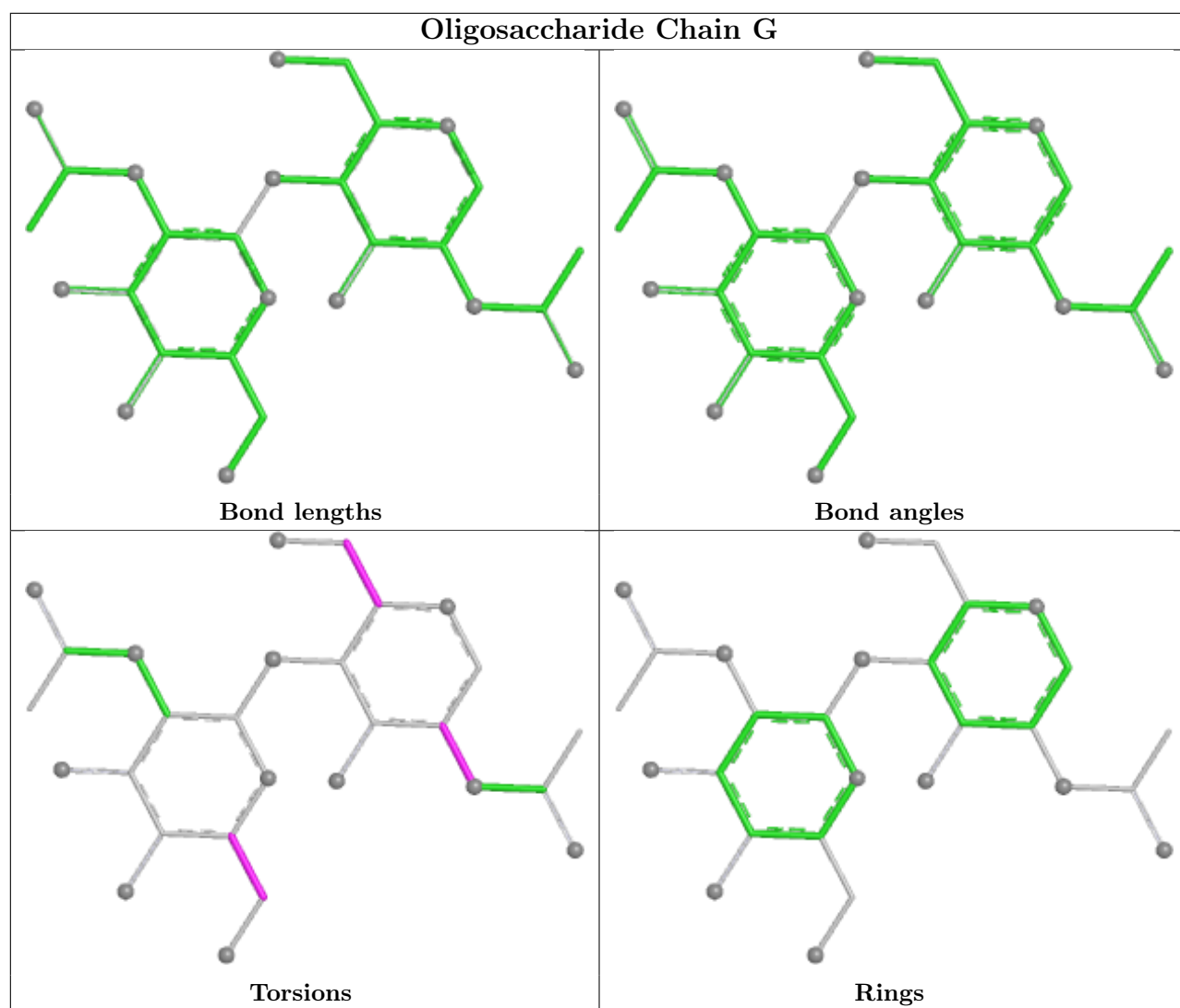
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2	NAG	1	0
3	G	1	NAG	4	0
3	I	1	NAG	9	0
3	I	2	NAG	1	0
3	H	1	NAG	3	0
3	F	1	NAG	6	0

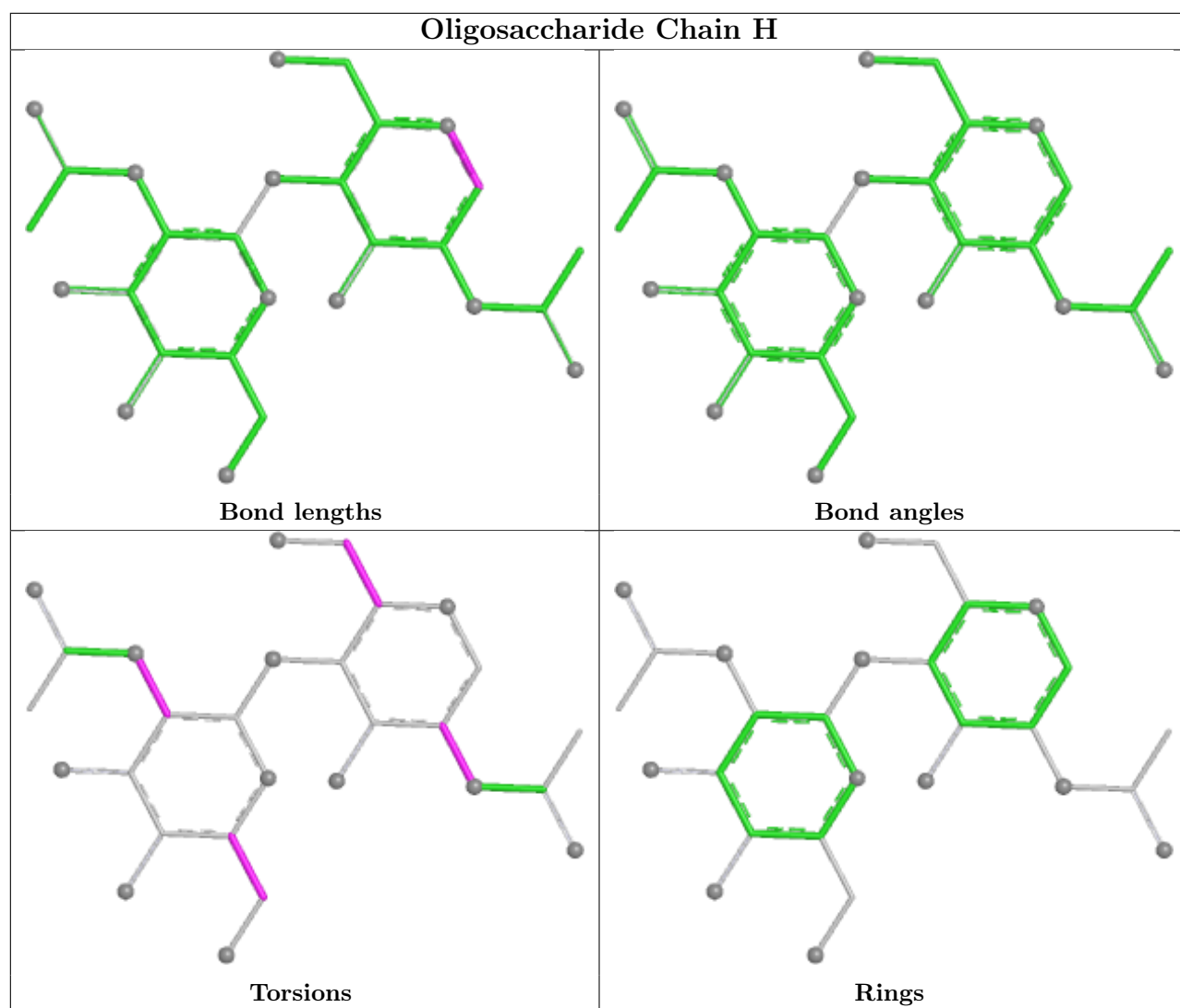
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

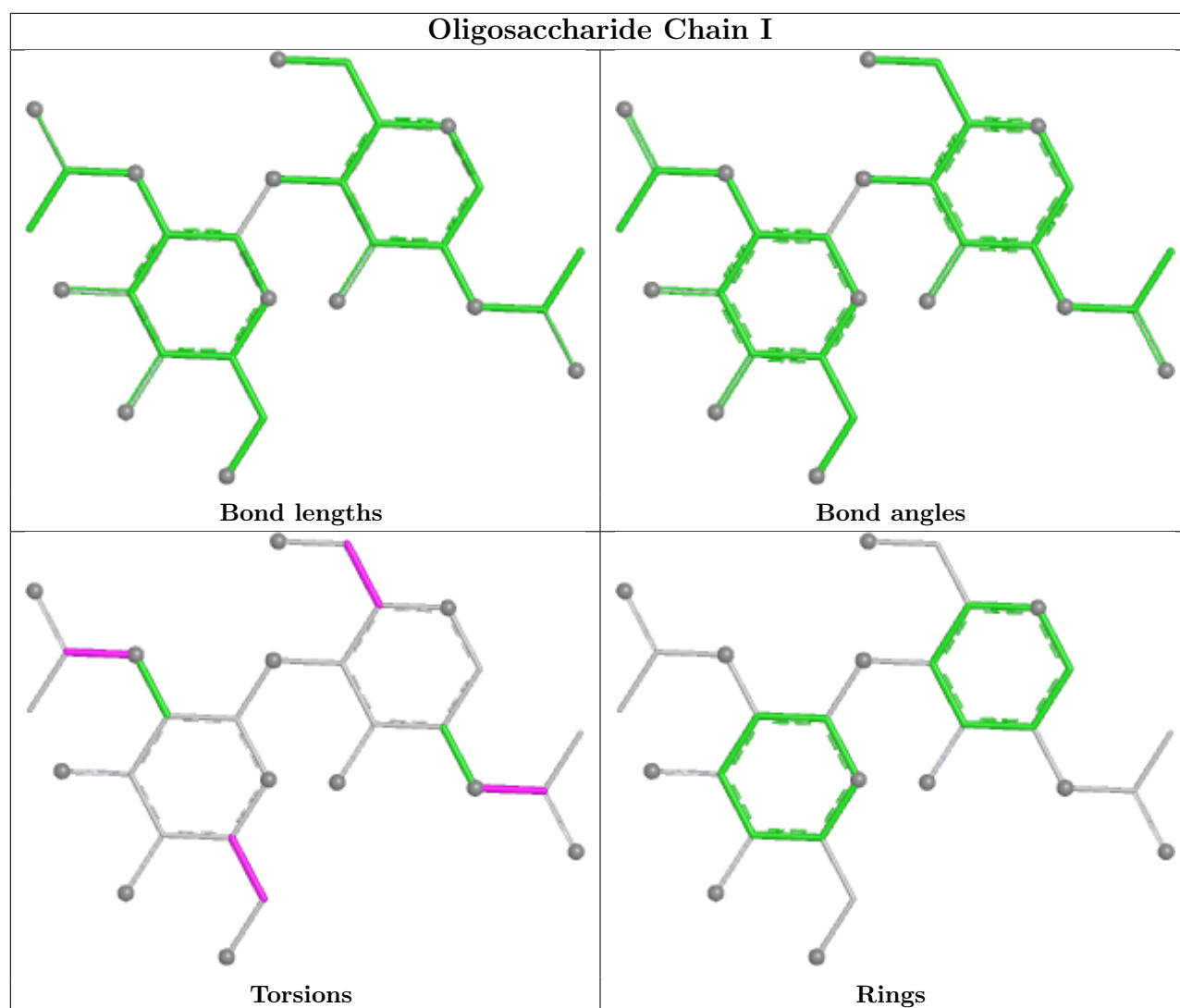
bond angles, torsion angles, and ring geometry for oligosaccharide.











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	$\# Z > 2$
4	NAG	C	1208	-	14,14,15	0.99	0	17,19,21	0.94	1 (5%)
4	NAG	B	1302	2	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	A	1205	2	14,14,15	0.25	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1202	-	14,14,15	2.70	7 (50%)	17,19,21	1.23	2 (11%)
4	NAG	C	1206	2	14,14,15	0.31	0	17,19,21	0.34	0
4	NAG	A	1208	2	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	A	1206	2	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	C	1205	2	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	B	1303	2	14,14,15	0.28	0	17,19,21	0.43	0
4	NAG	A	1203	2	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	B	1306	2	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	A	1201	2	14,14,15	0.50	0	17,19,21	0.76	1 (5%)
4	NAG	C	1207	2	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	C	1202	2	14,14,15	0.53	0	17,19,21	0.79	1 (5%)
4	NAG	C	1204	2	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	A	1209	2	14,14,15	0.43	0	17,19,21	0.35	0
4	NAG	C	1203	2	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	B	1304	2	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	C	1201	-	14,14,15	0.61	0	17,19,21	0.58	0
4	NAG	A	1204	2	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	B	1301	2	14,14,15	0.58	0	17,19,21	0.82	1 (5%)
4	NAG	B	1307	2	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	B	1305	-	14,14,15	1.65	2 (14%)	17,19,21	1.23	3 (17%)
4	NAG	A	1207	2	14,14,15	0.27	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	C	1208	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1302	2	-	4/6/23/26	0/1/1/1
4	NAG	A	1205	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1202	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1206	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1208	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1206	2	-	1/6/23/26	0/1/1/1
4	NAG	C	1205	2	-	1/6/23/26	0/1/1/1
4	NAG	B	1303	2	-	4/6/23/26	0/1/1/1
4	NAG	A	1203	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1306	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1201	2	-	4/6/23/26	0/1/1/1
4	NAG	C	1207	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1202	2	-	1/6/23/26	0/1/1/1
4	NAG	C	1204	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1209	2	-	3/6/23/26	0/1/1/1
4	NAG	C	1203	2	-	3/6/23/26	0/1/1/1
4	NAG	B	1304	2	-	4/6/23/26	0/1/1/1
4	NAG	C	1201	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1204	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1307	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1207	2	-	3/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1305	NAG	C1-C2	5.23	1.59	1.52
4	A	1202	NAG	O5-C5	4.45	1.52	1.43
4	A	1202	NAG	C3-C2	4.25	1.61	1.52
4	A	1202	NAG	C8-C7	-3.49	1.43	1.50
4	A	1202	NAG	C2-N2	-3.48	1.40	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1301	NAG	C1-O5-C5	3.04	116.27	112.19
4	A	1202	NAG	O7-C7-C8	-2.95	116.80	122.05
4	C	1202	NAG	C1-O5-C5	2.88	116.05	112.19
4	A	1201	NAG	C1-O5-C5	2.75	115.87	112.19
4	B	1305	NAG	O5-C5-C4	-2.72	104.20	110.83

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1204	NAG	C4-C5-C6-O6
4	A	1209	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1203	NAG	C4-C5-C6-O6
4	A	1205	NAG	O5-C5-C6-O6

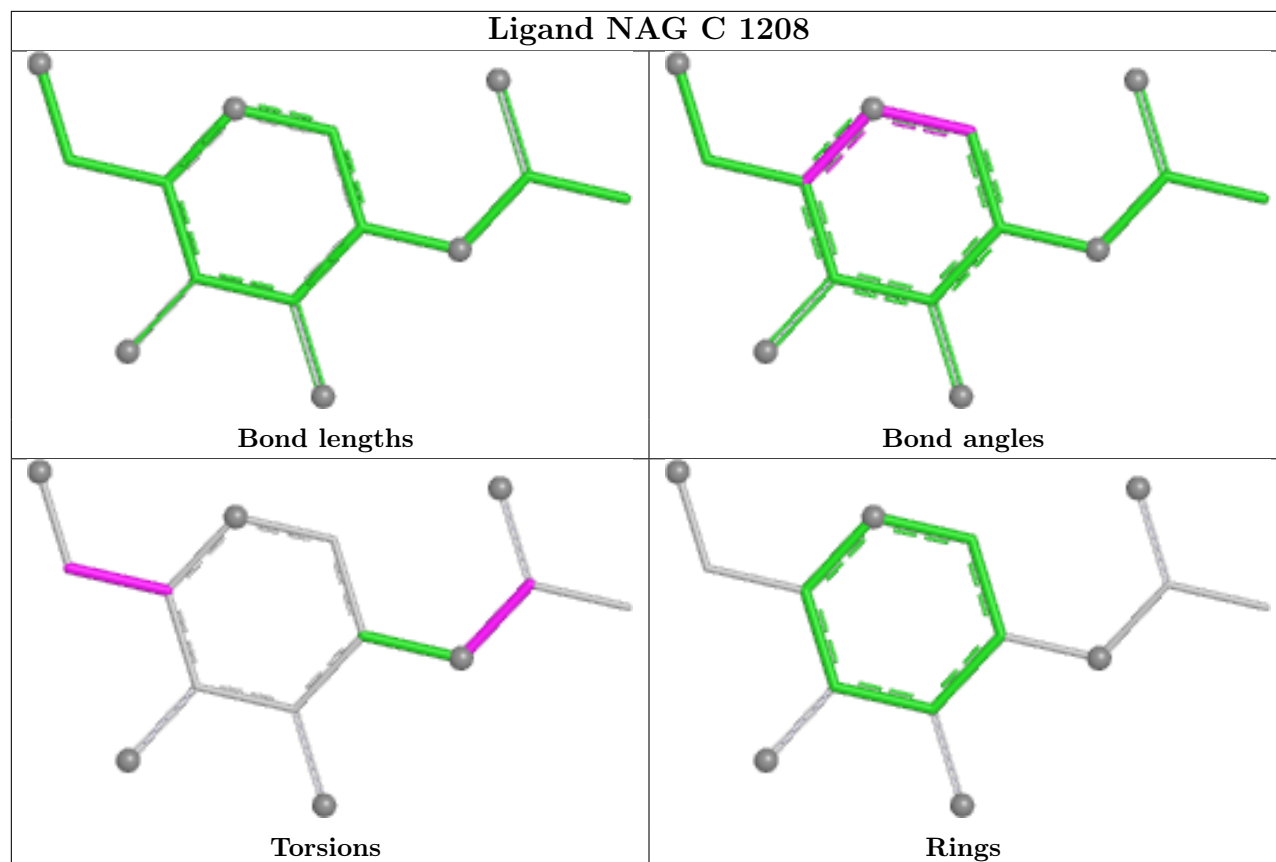
There are no ring outliers.

11 monomers are involved in 34 short contacts:

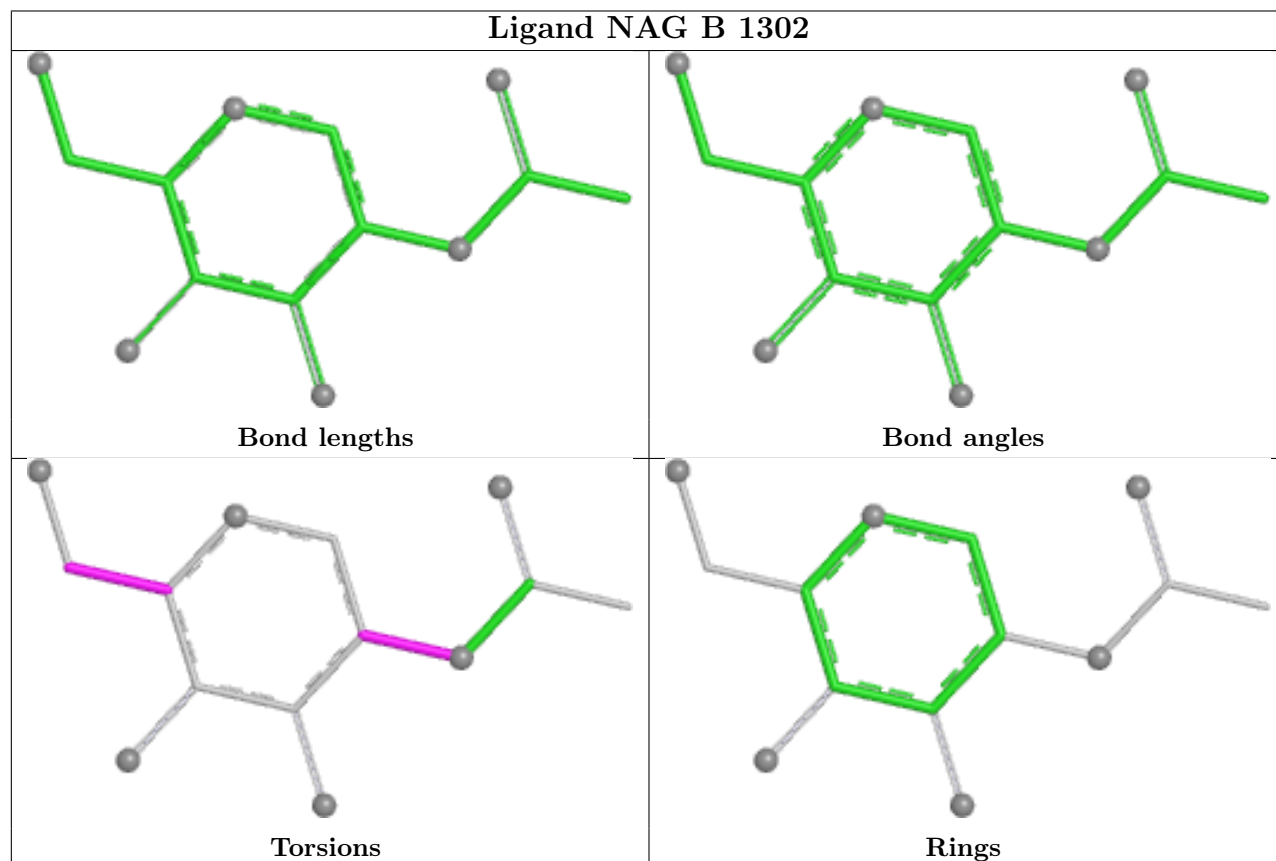
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1208	NAG	3	0
4	A	1202	NAG	5	0
4	C	1206	NAG	6	0
4	C	1205	NAG	1	0
4	B	1303	NAG	1	0
4	B	1304	NAG	1	0
4	C	1201	NAG	9	0
4	A	1204	NAG	3	0
4	B	1301	NAG	1	0
4	B	1307	NAG	3	0
4	A	1207	NAG	1	0

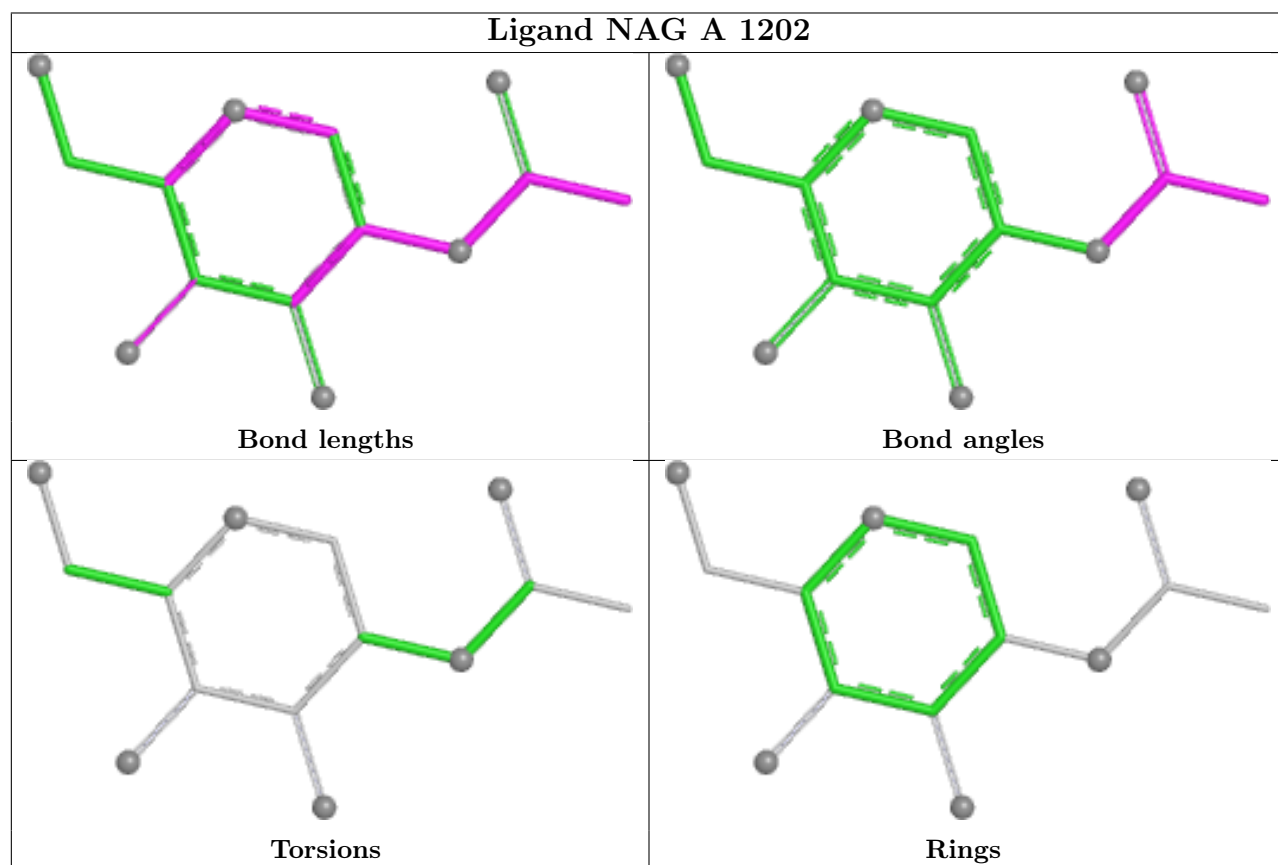
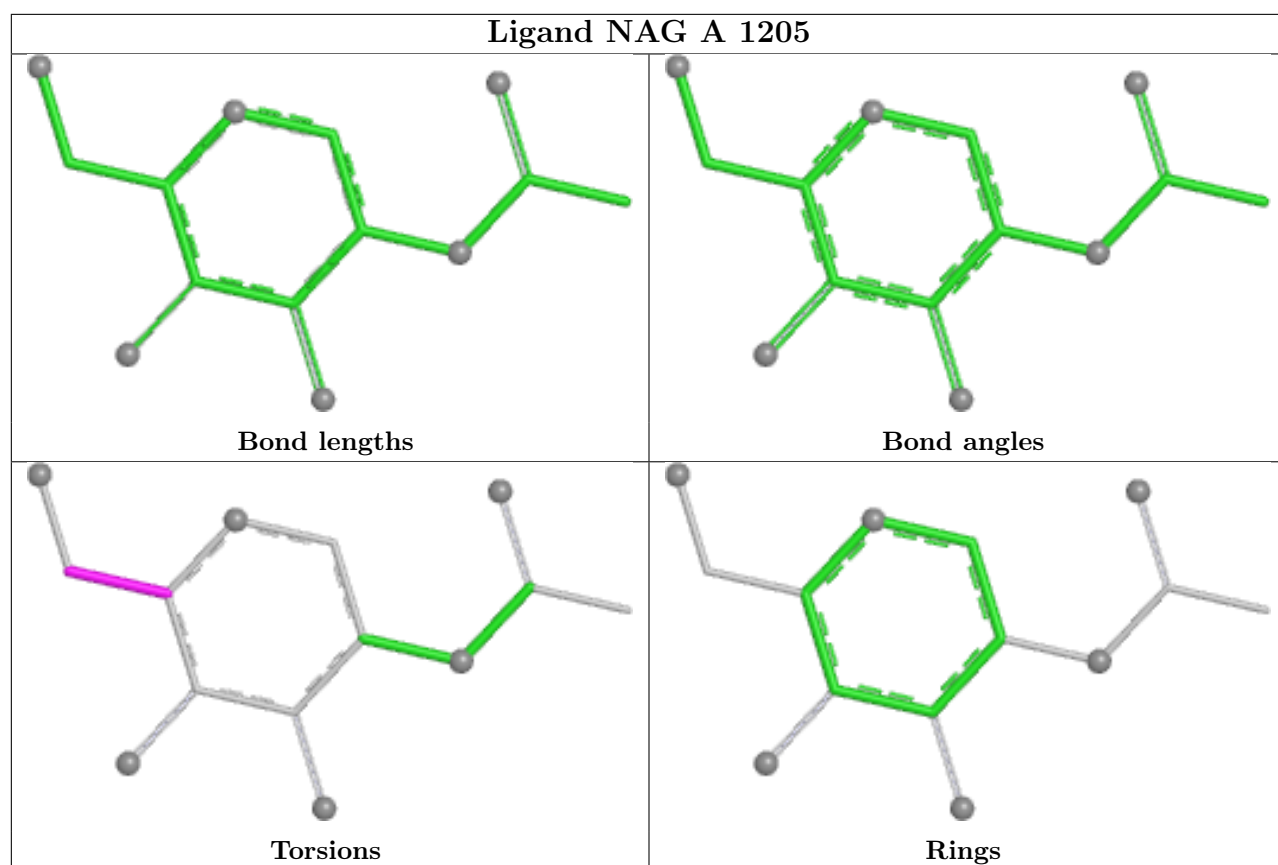
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 C 1208

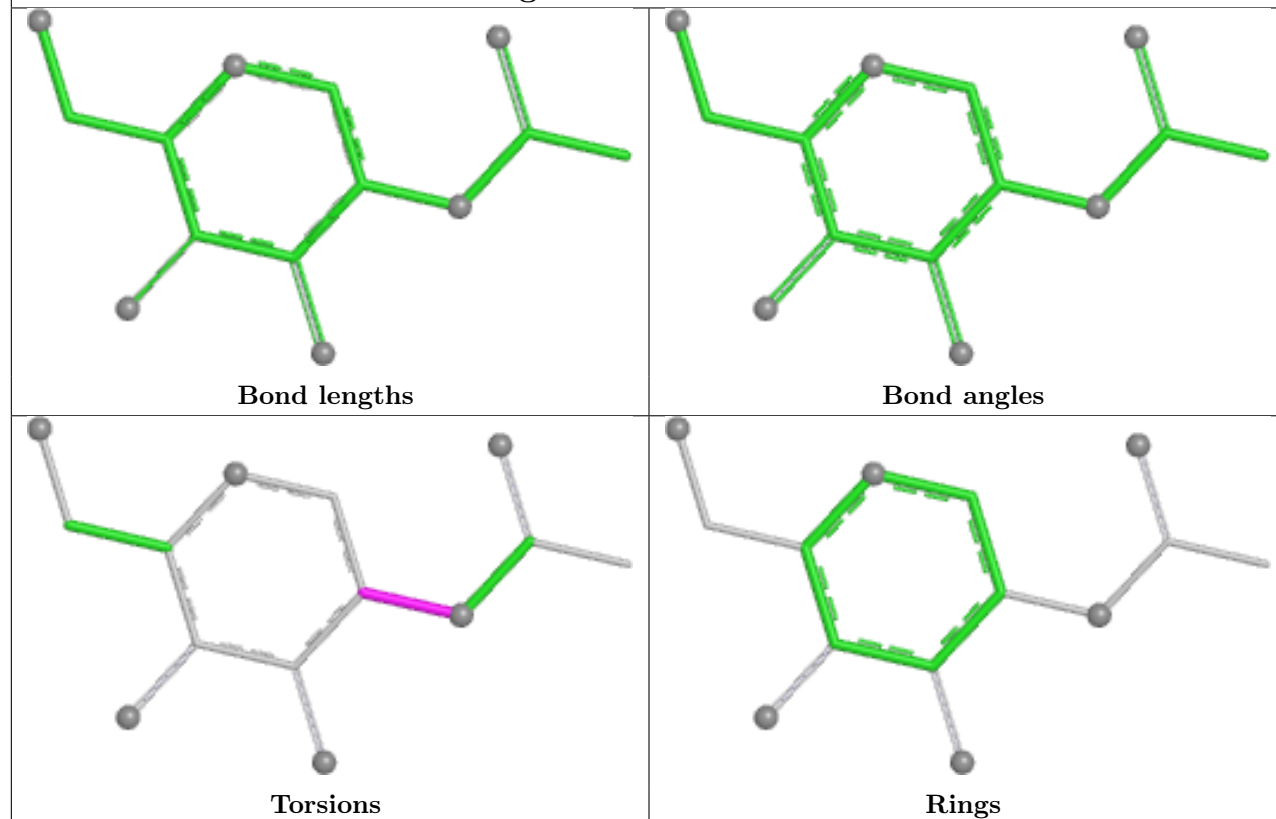


Ligand NAG B 1302

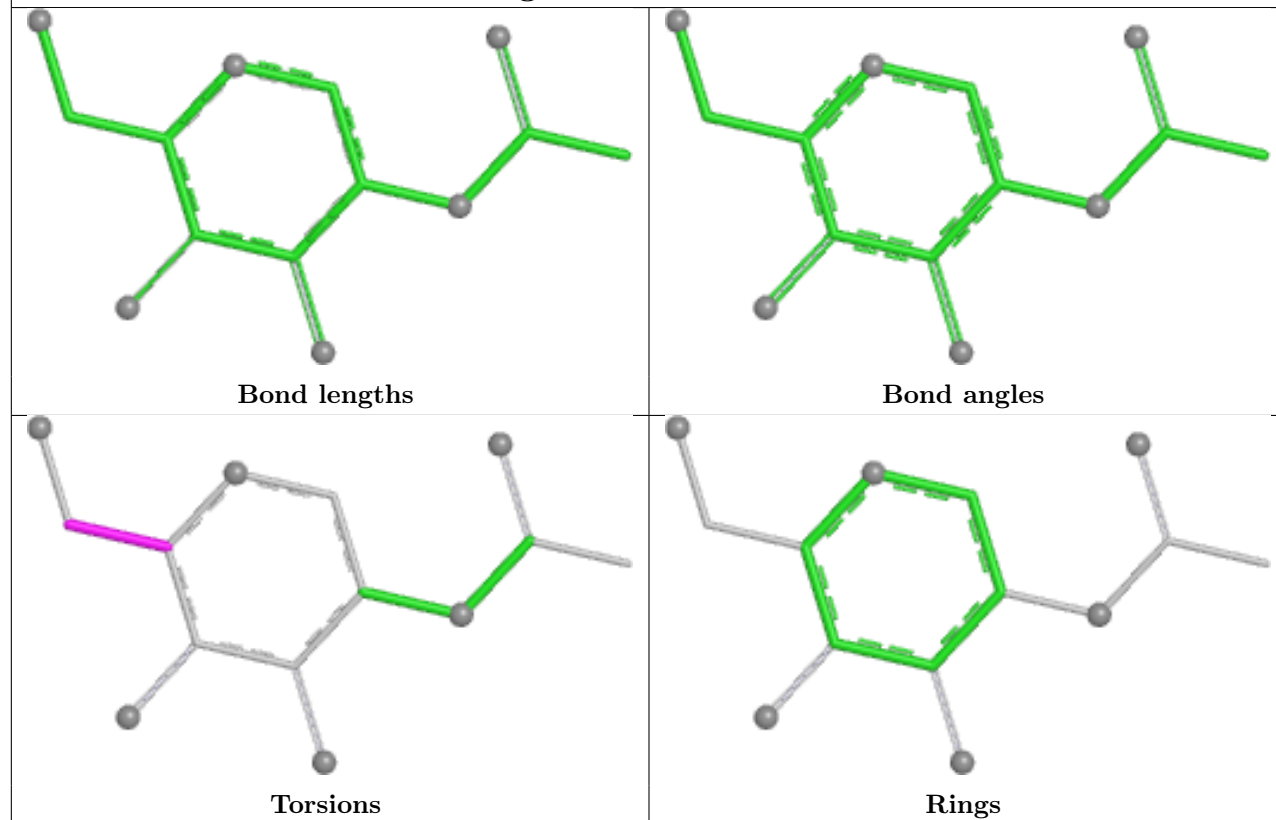


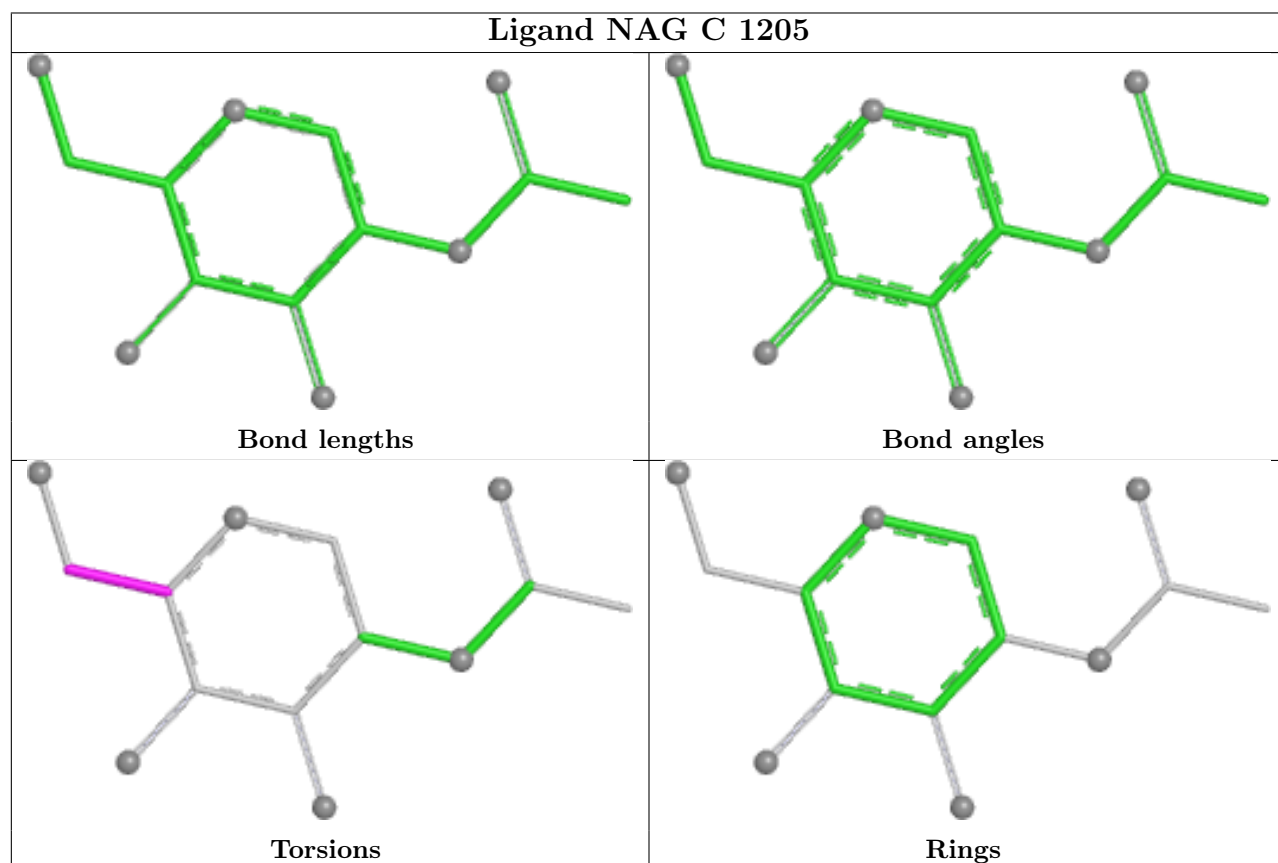
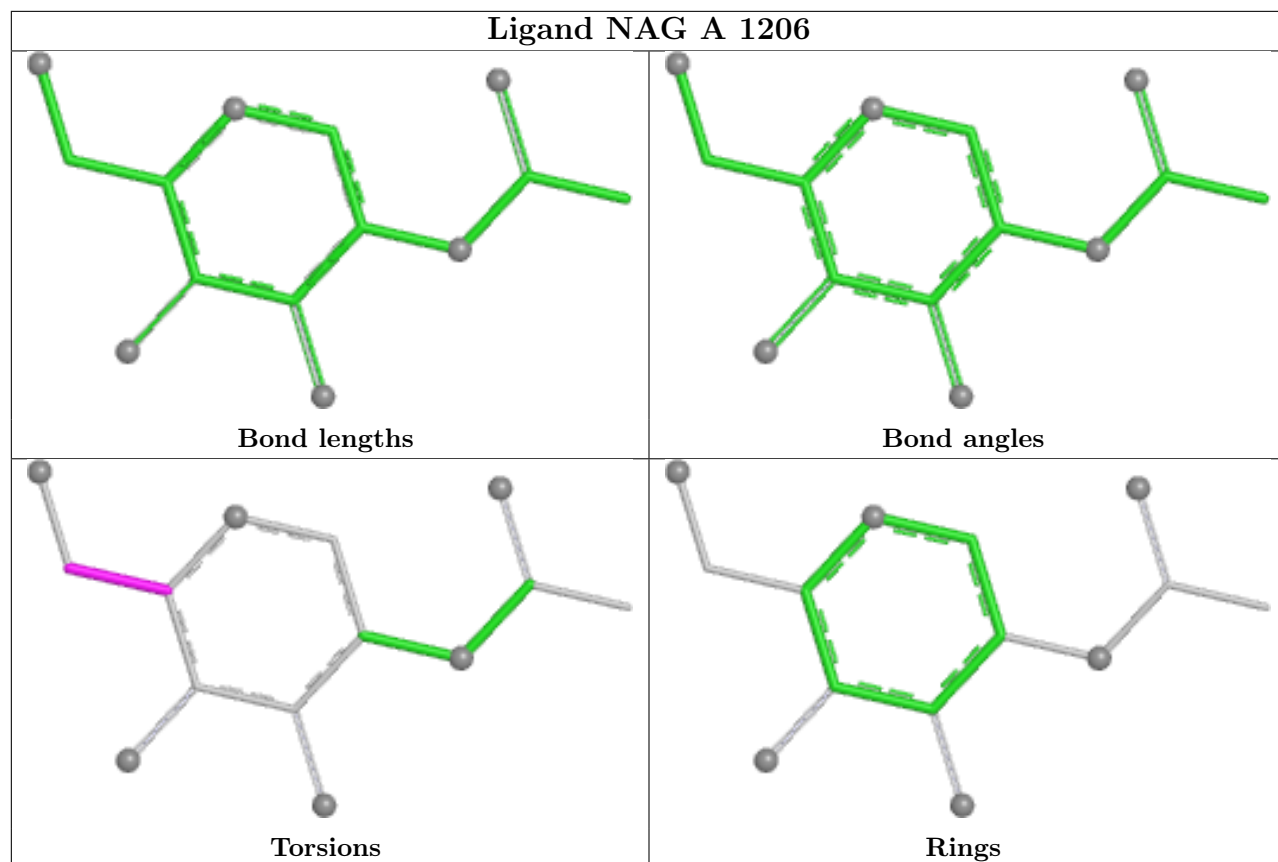


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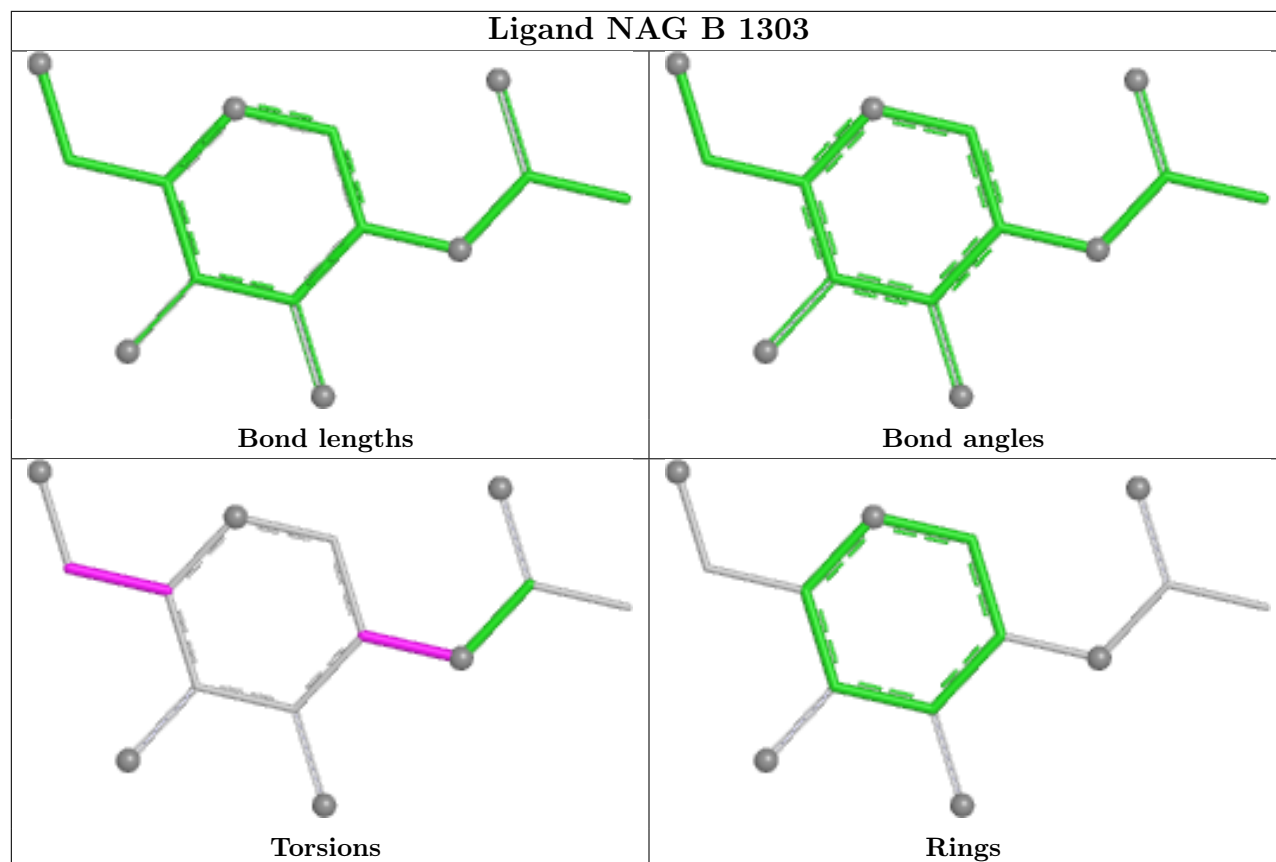


Ligand NAG A 1208

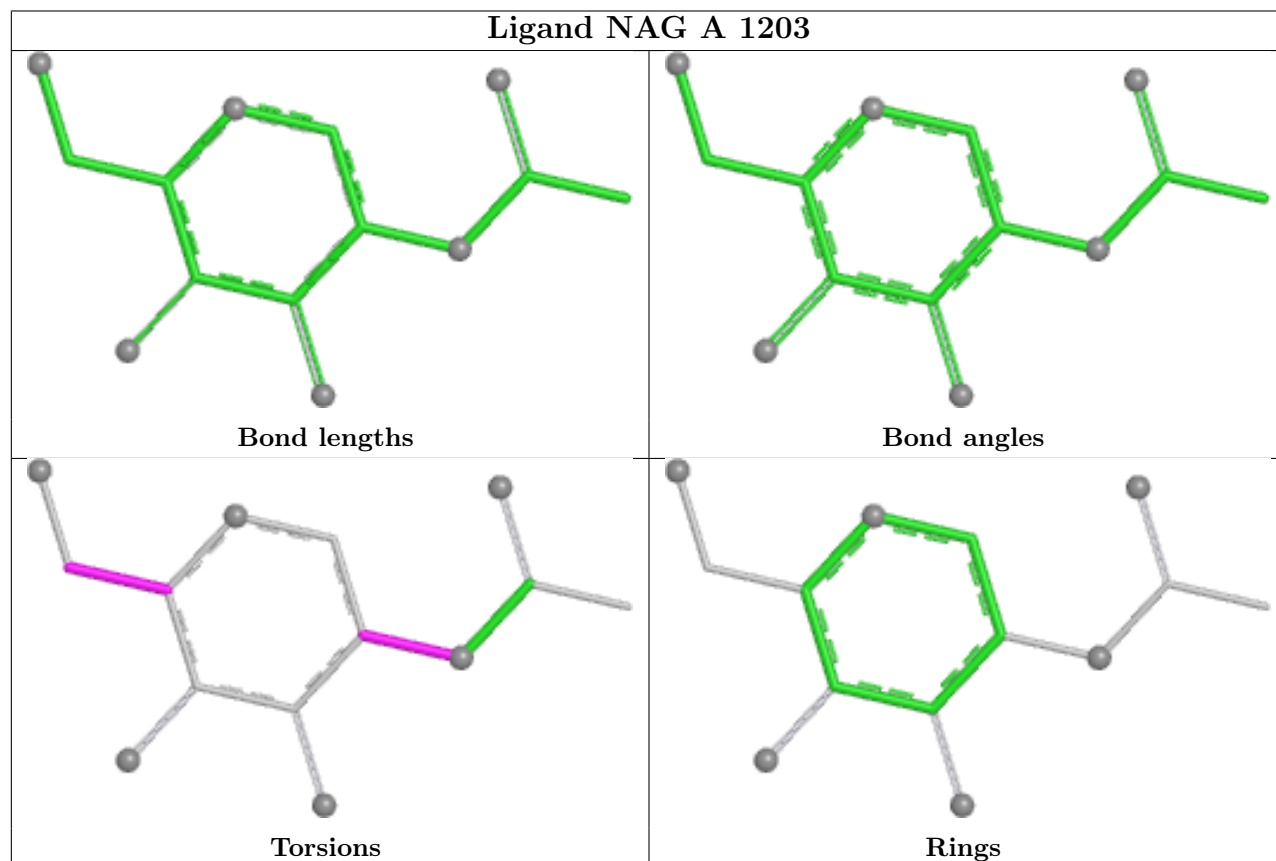


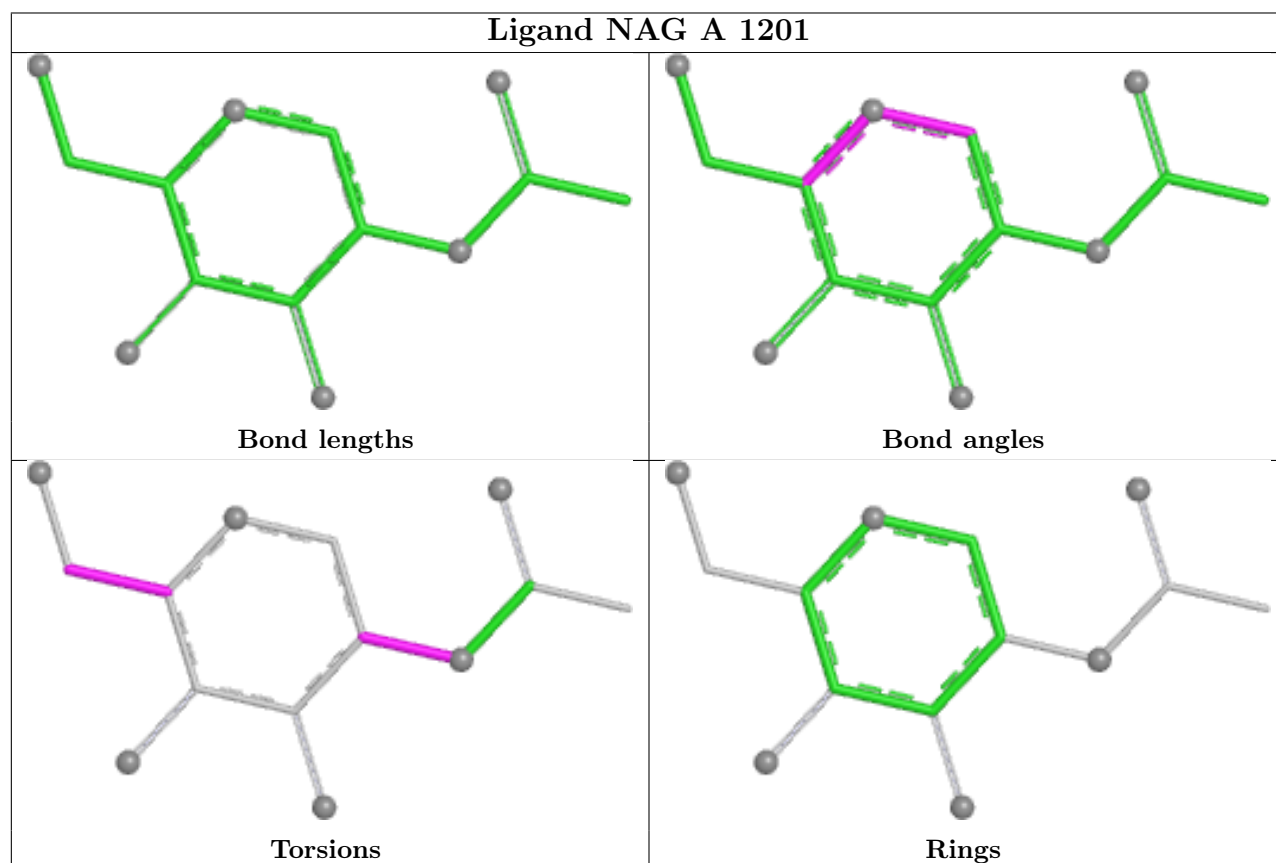
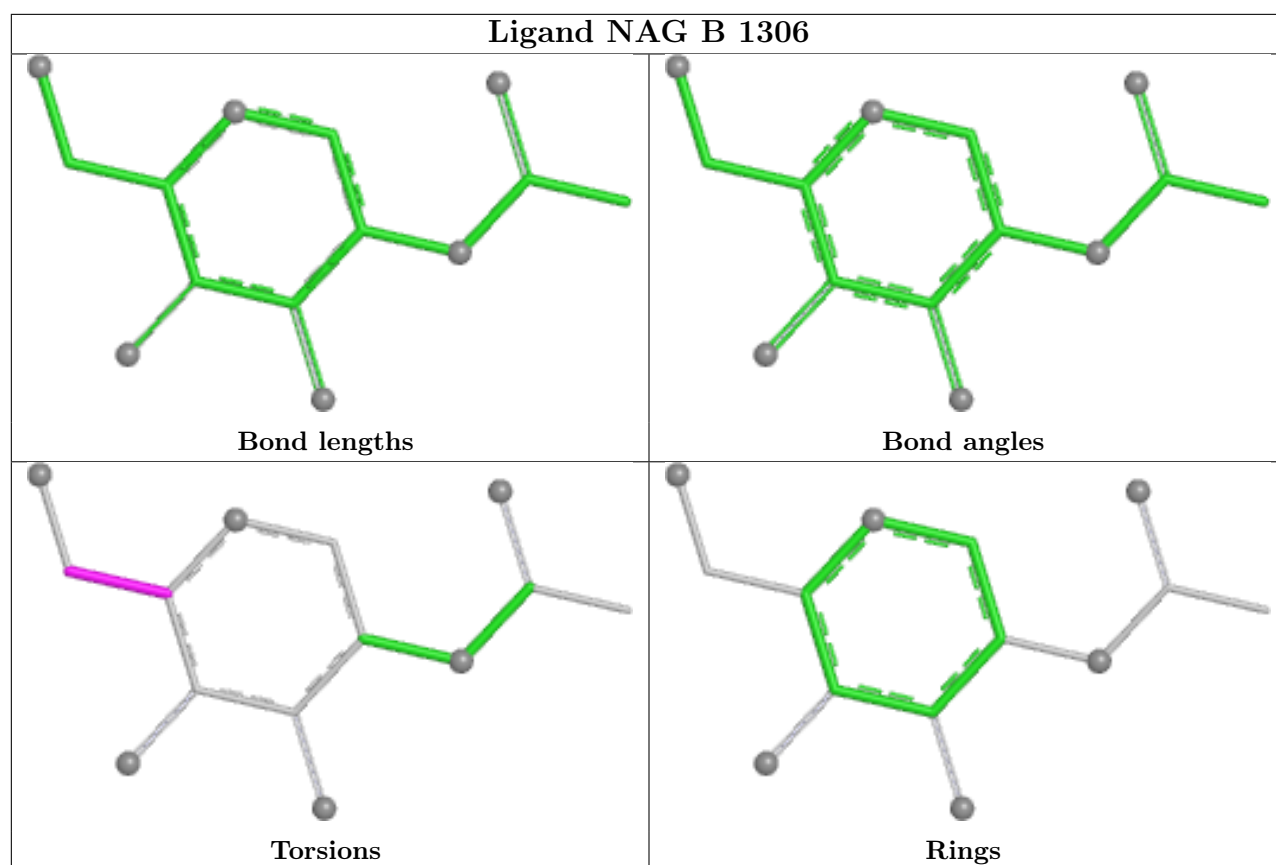


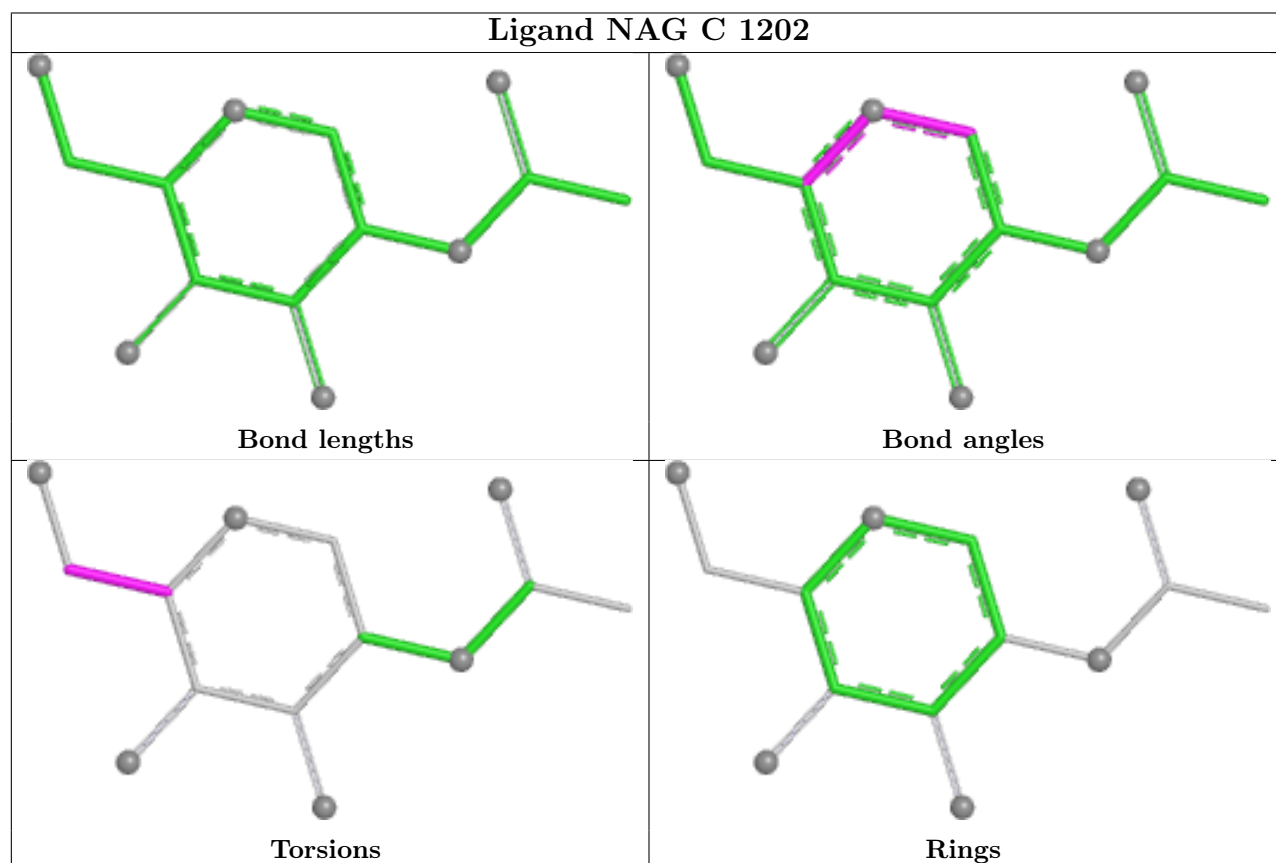
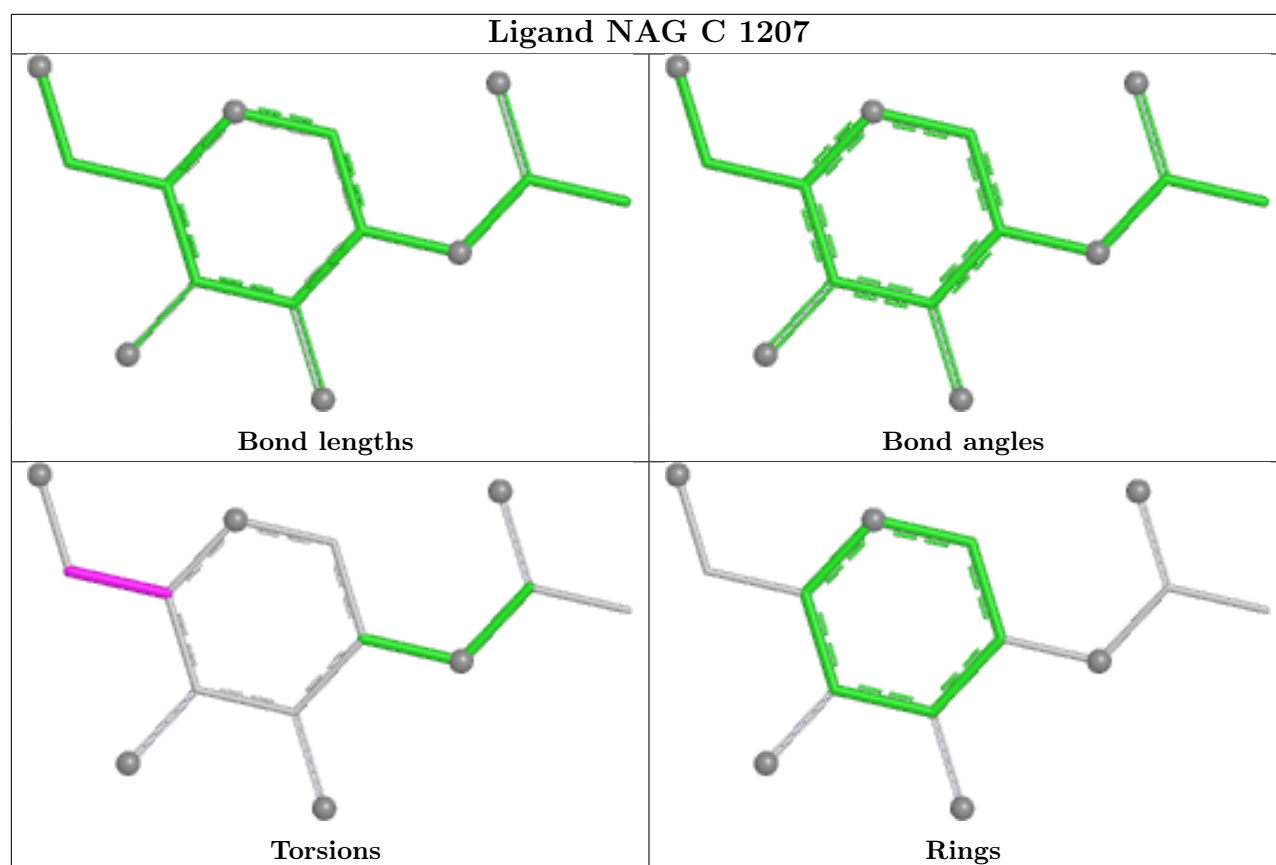
Ligand NAG B 1303

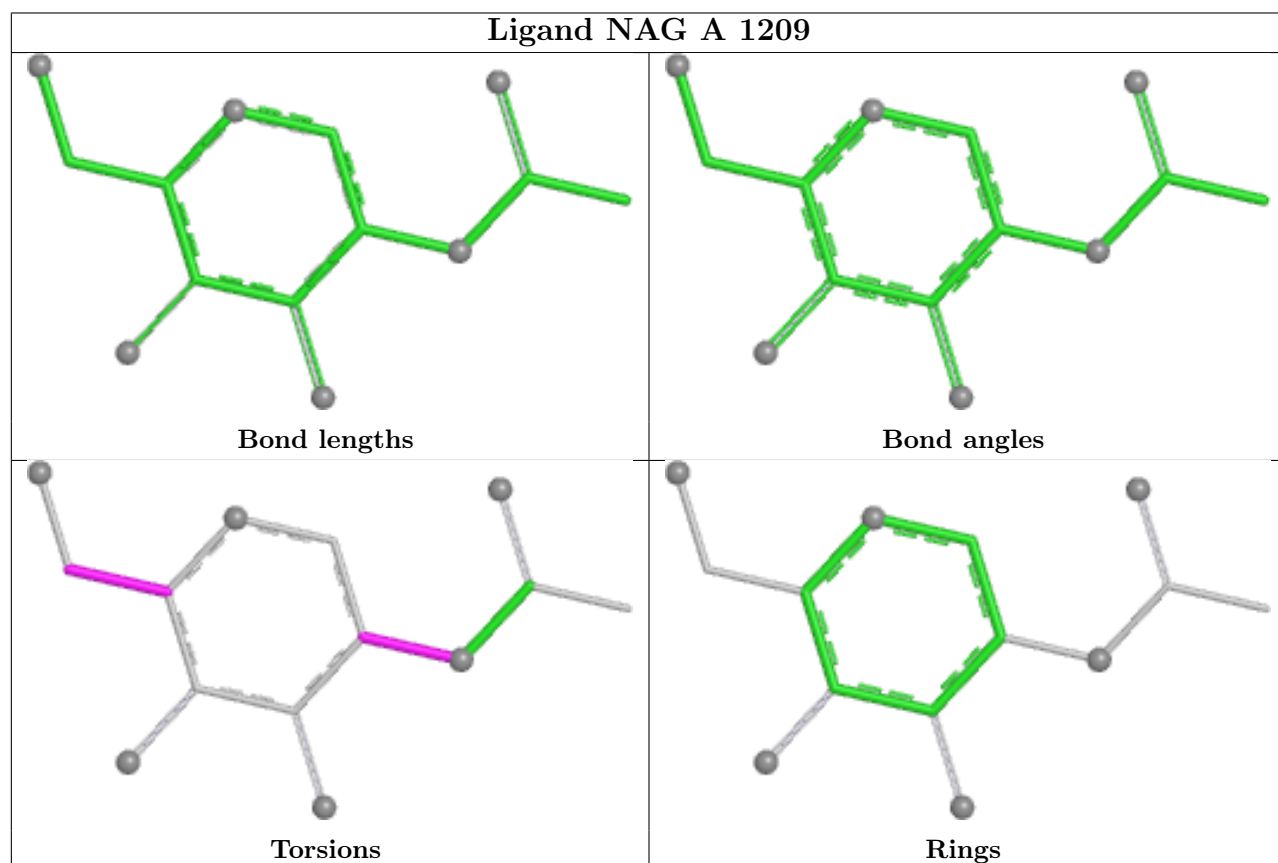
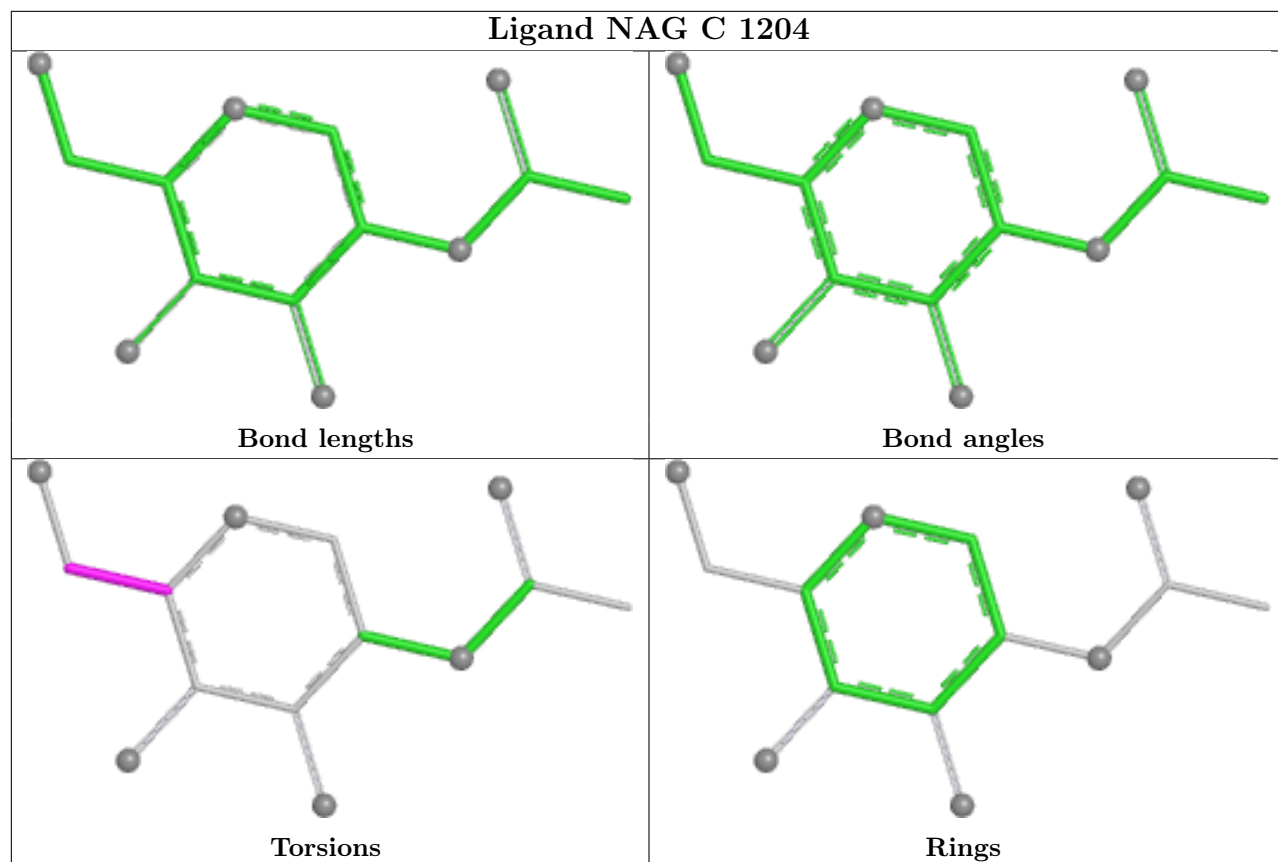


Ligand NAG A 1203

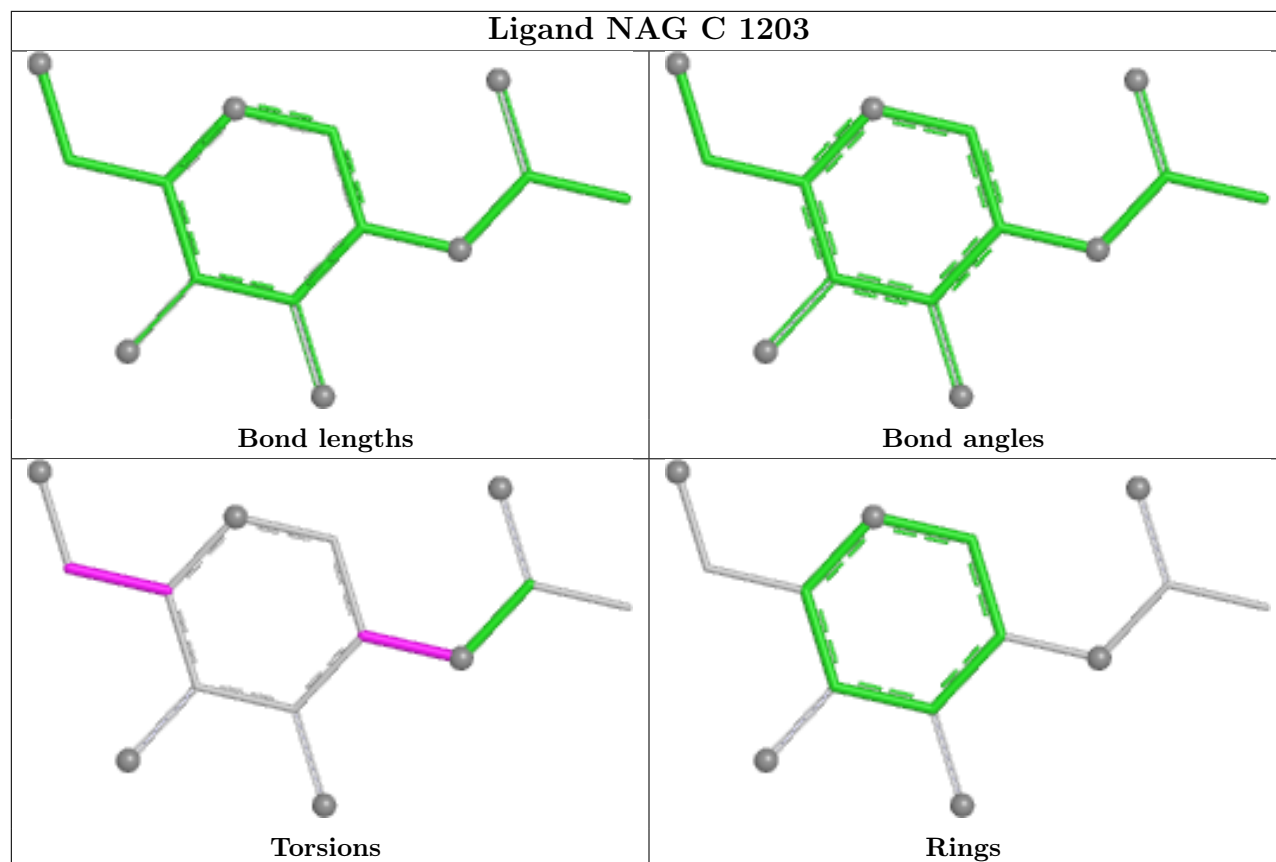




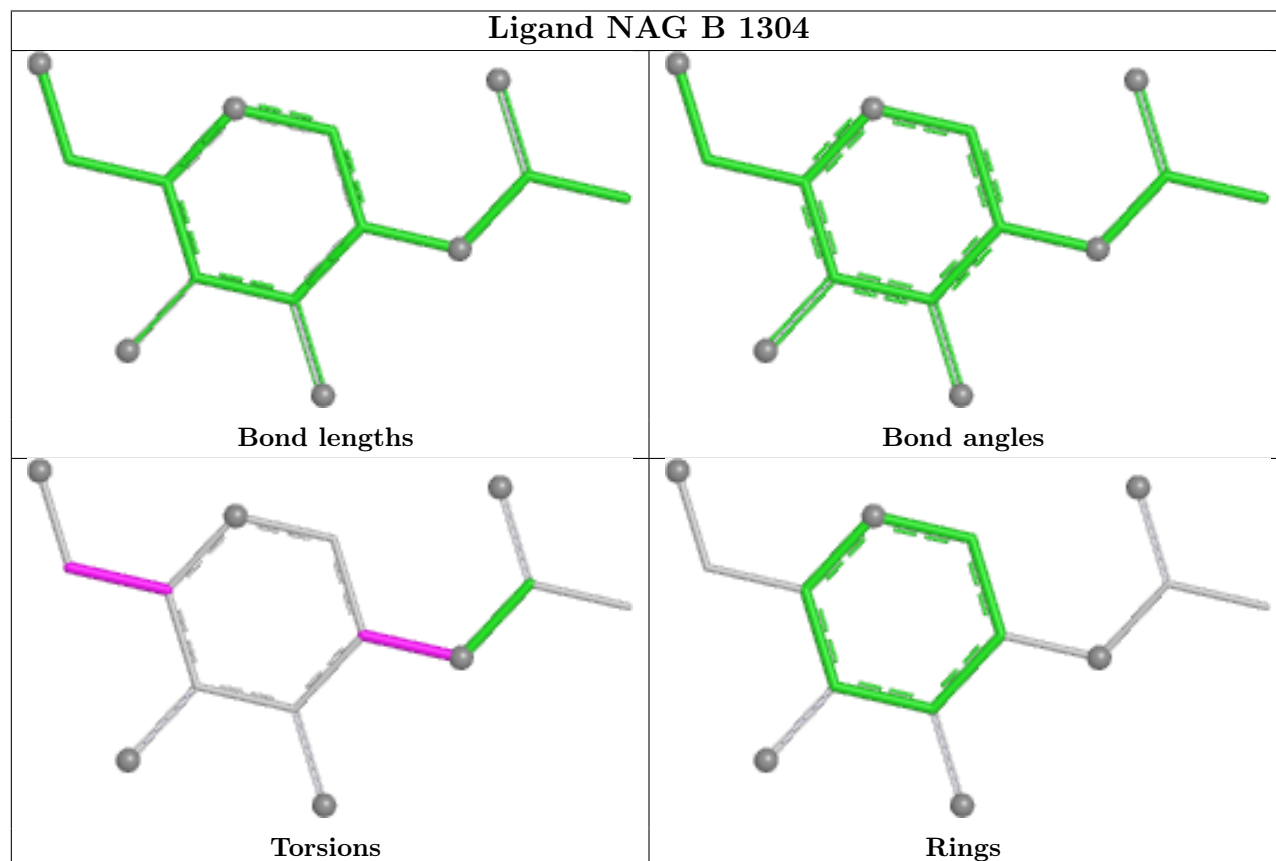


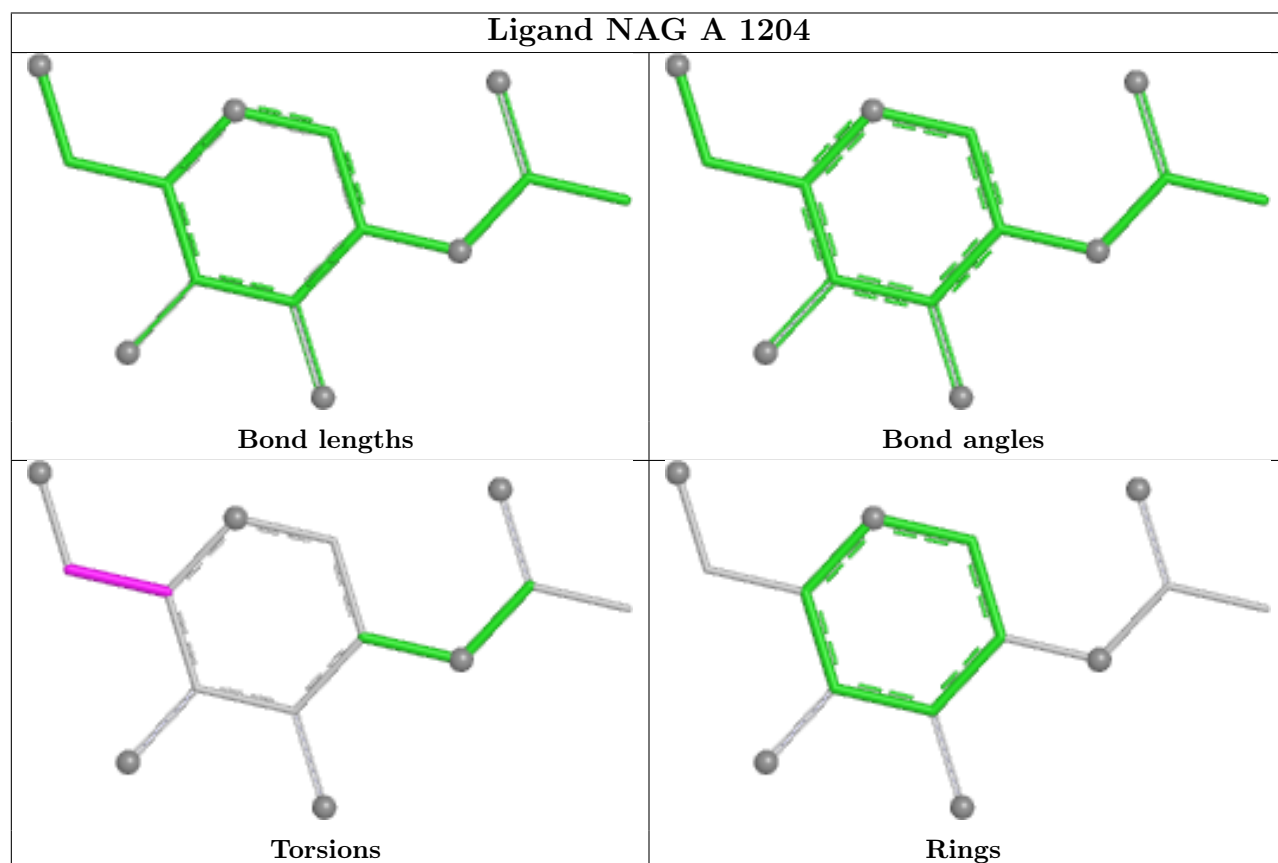
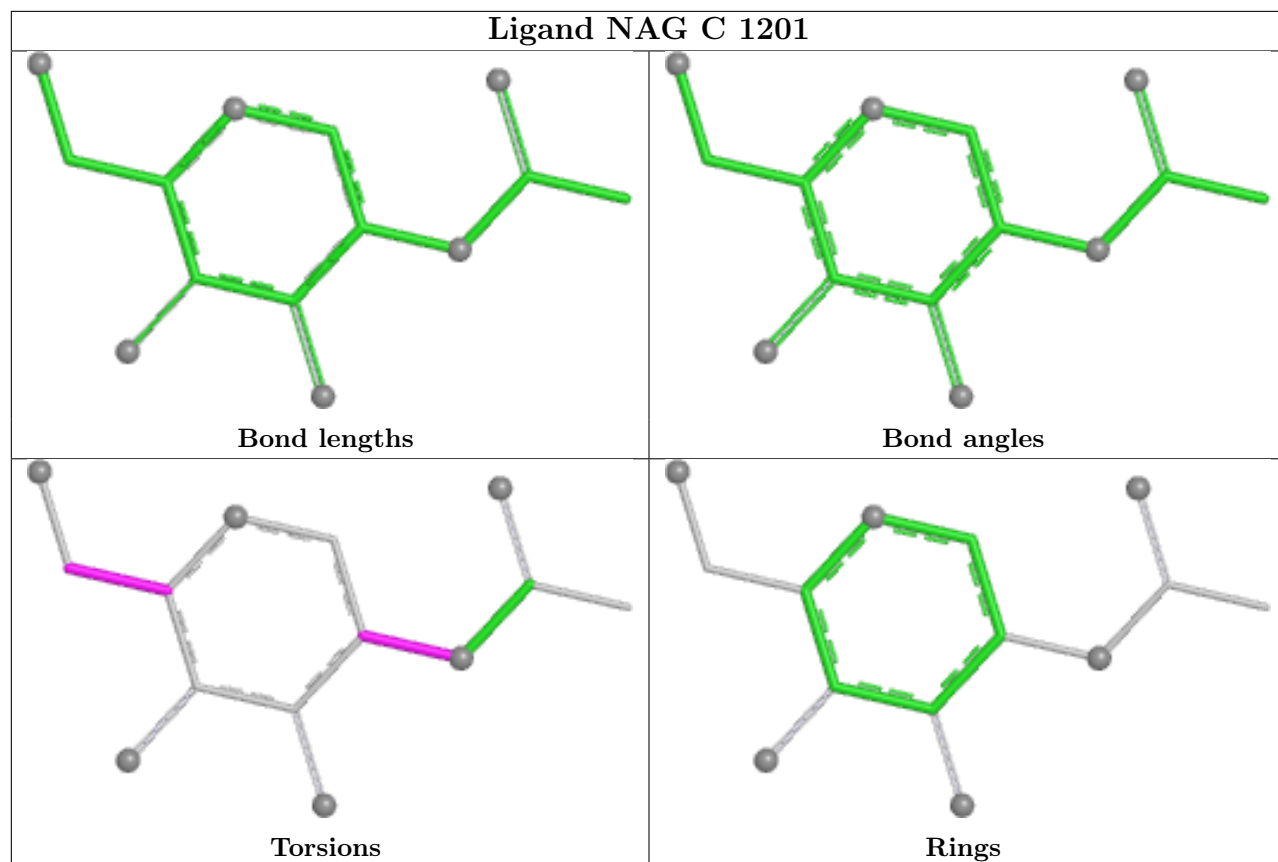


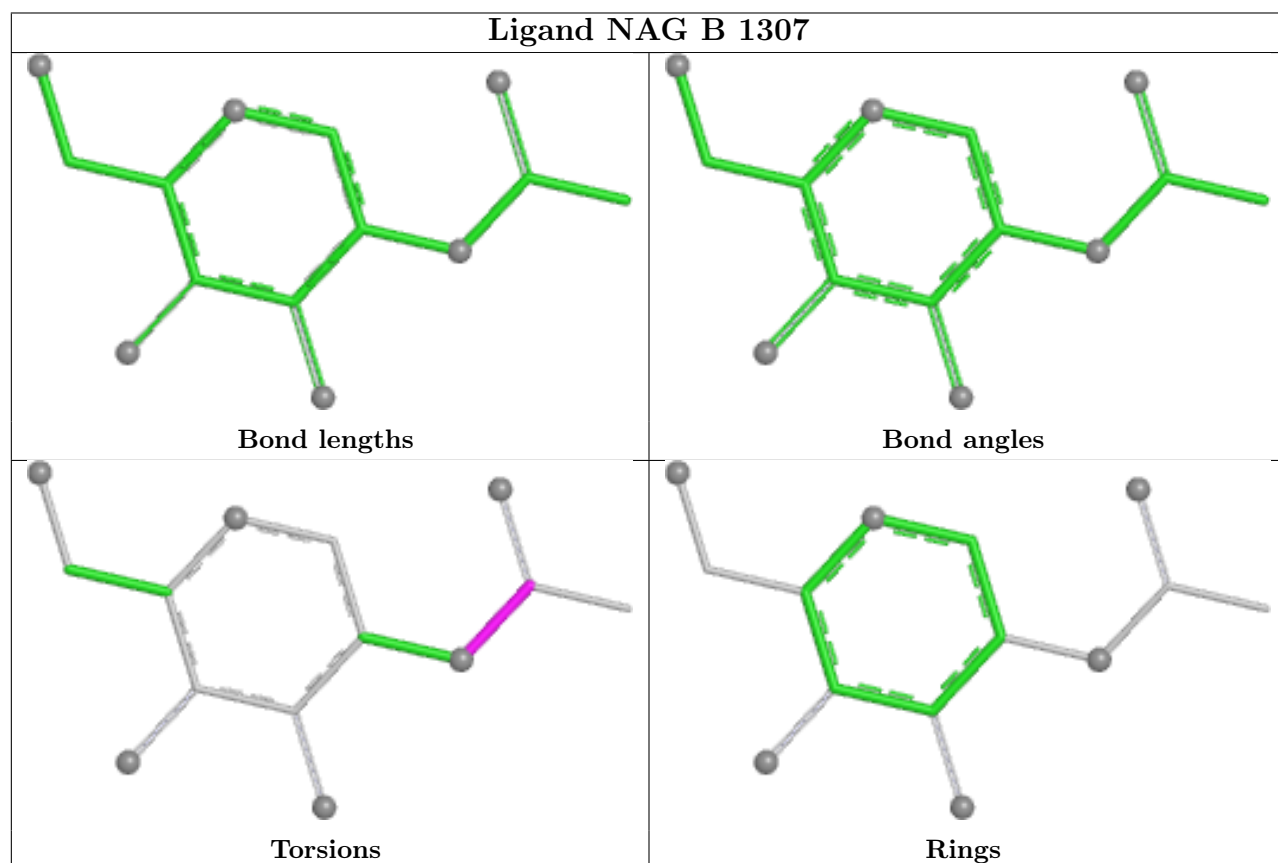
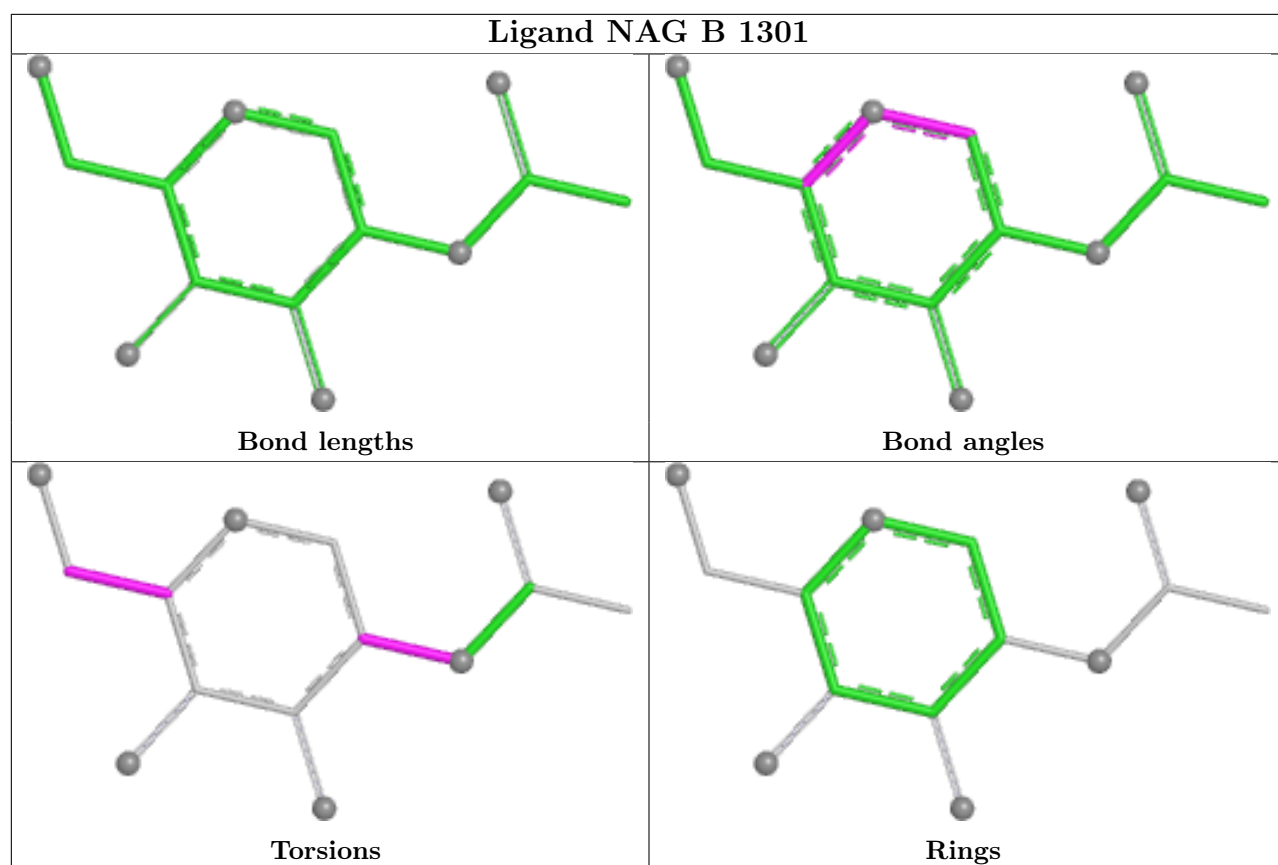
Ligand NAG C 1203



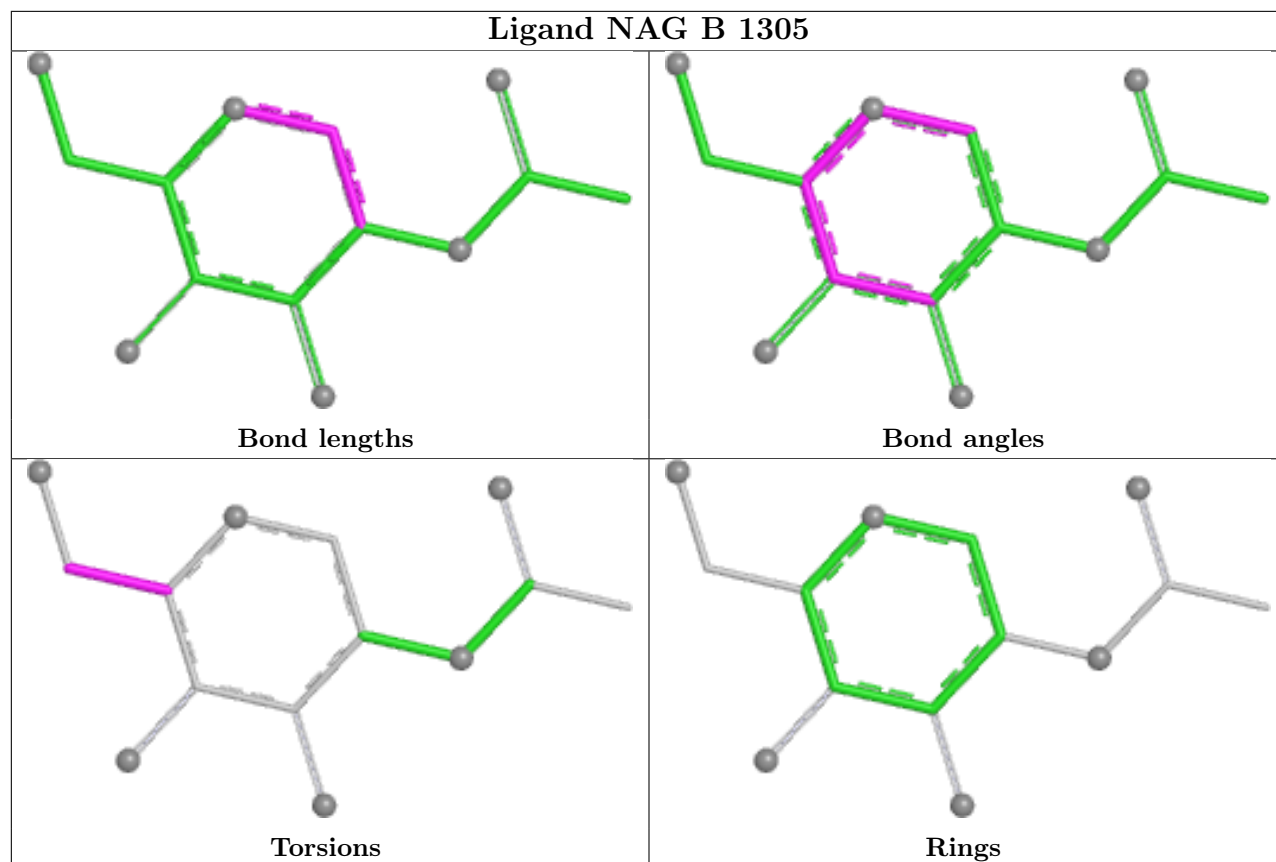
Ligand NAG B 1304



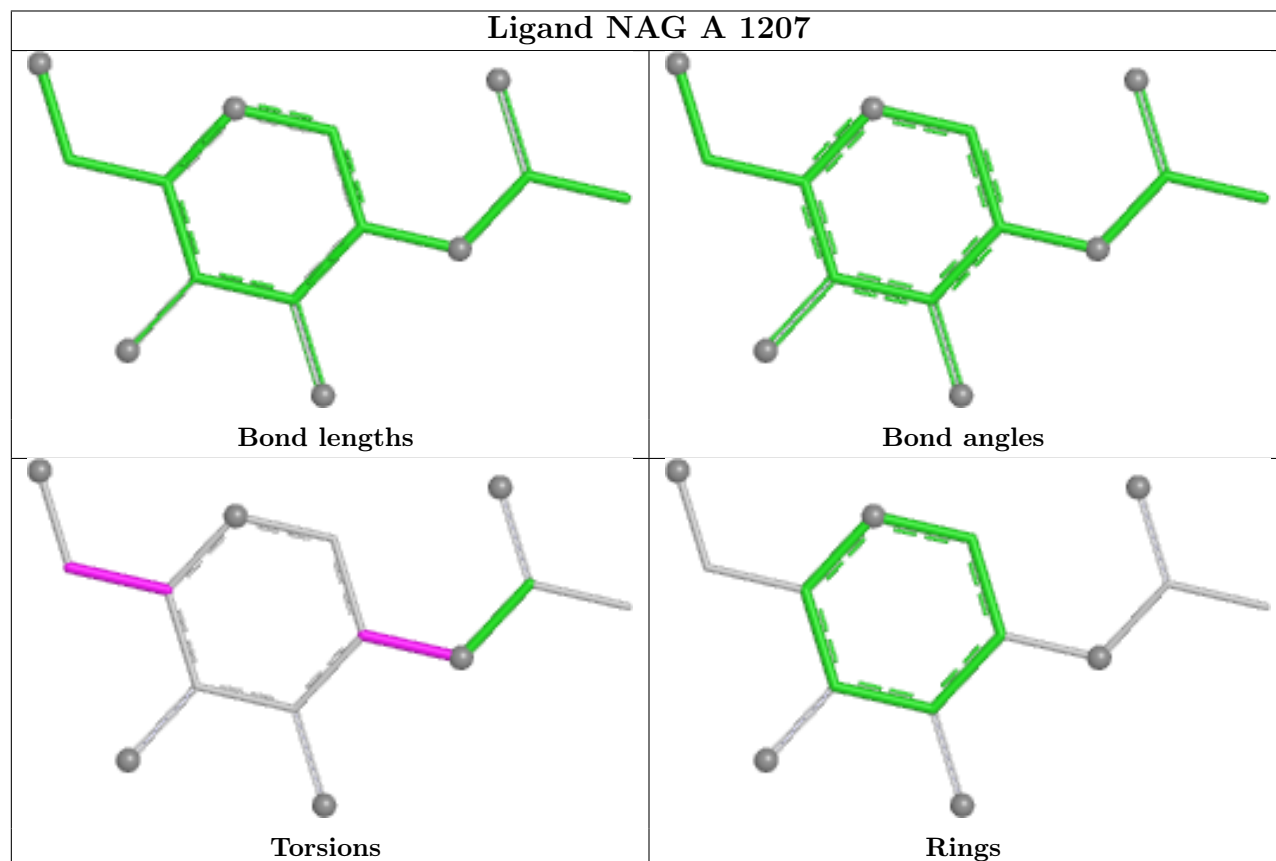




Ligand NAG B 1305



Ligand NAG A 1207



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.

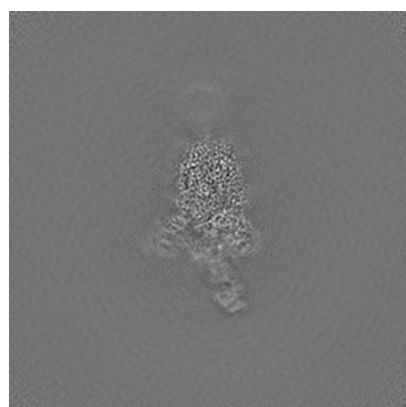
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28688. These allow visual inspection of the internal detail of the map and identification of artifacts.

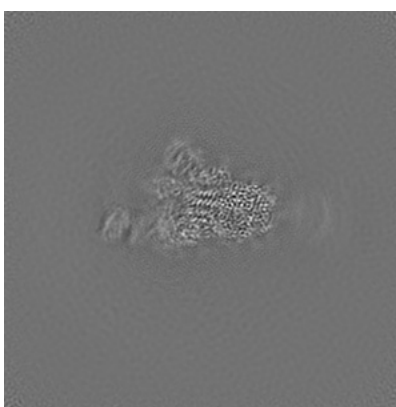
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

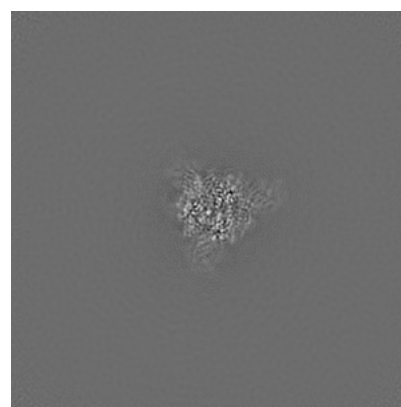
6.1.1 Primary map



X



Y

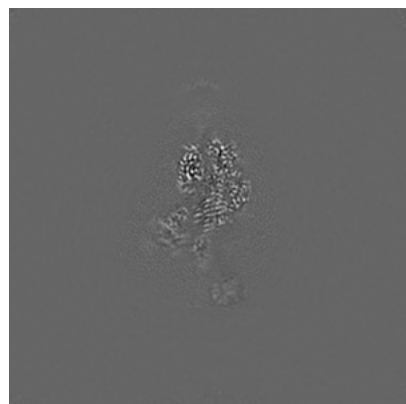


Z

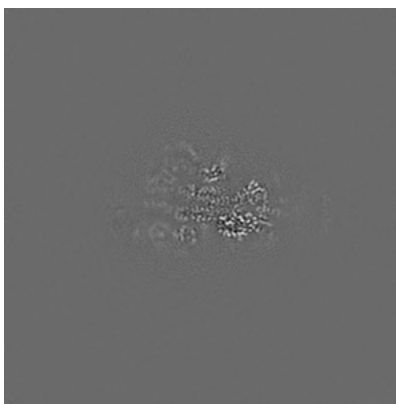
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

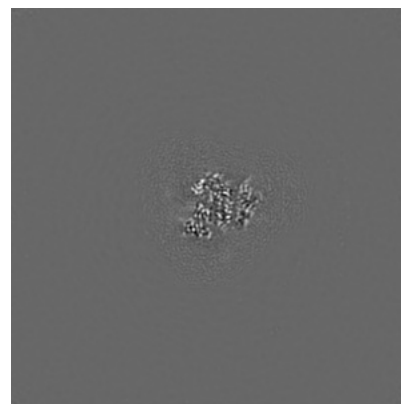
6.2.1 Primary map



X Index: 208



Y Index: 208



Z Index: 208

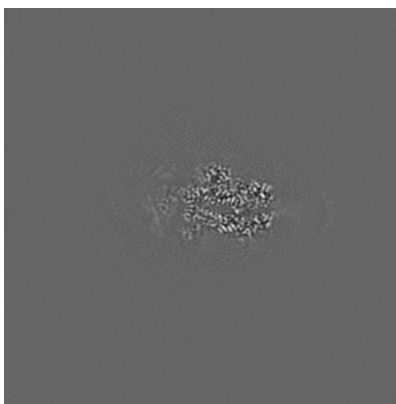
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

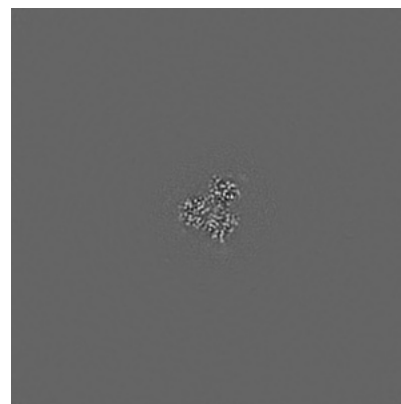
6.3.1 Primary map



X Index: 219



Y Index: 198

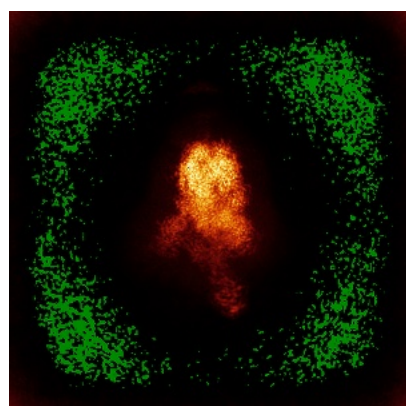


Z Index: 246

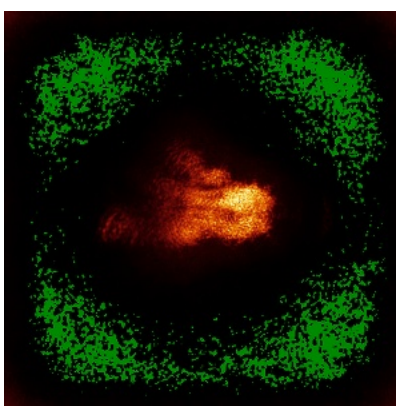
The images above show the largest variance slices of the map in three orthogonal directions.

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

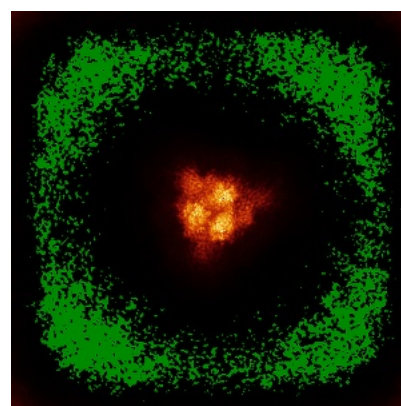
6.4.1 Primary map



X



Y



Z

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 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

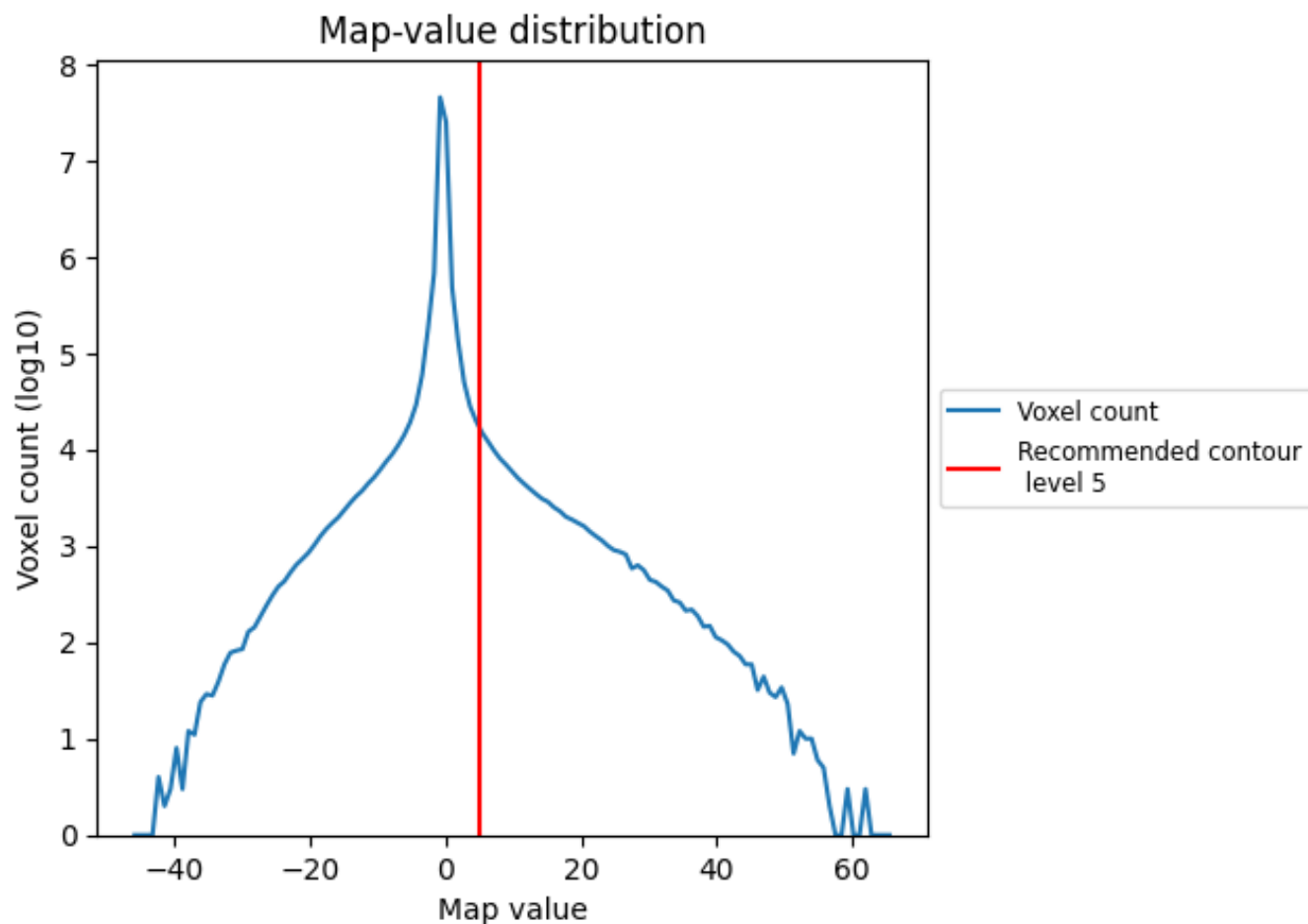
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

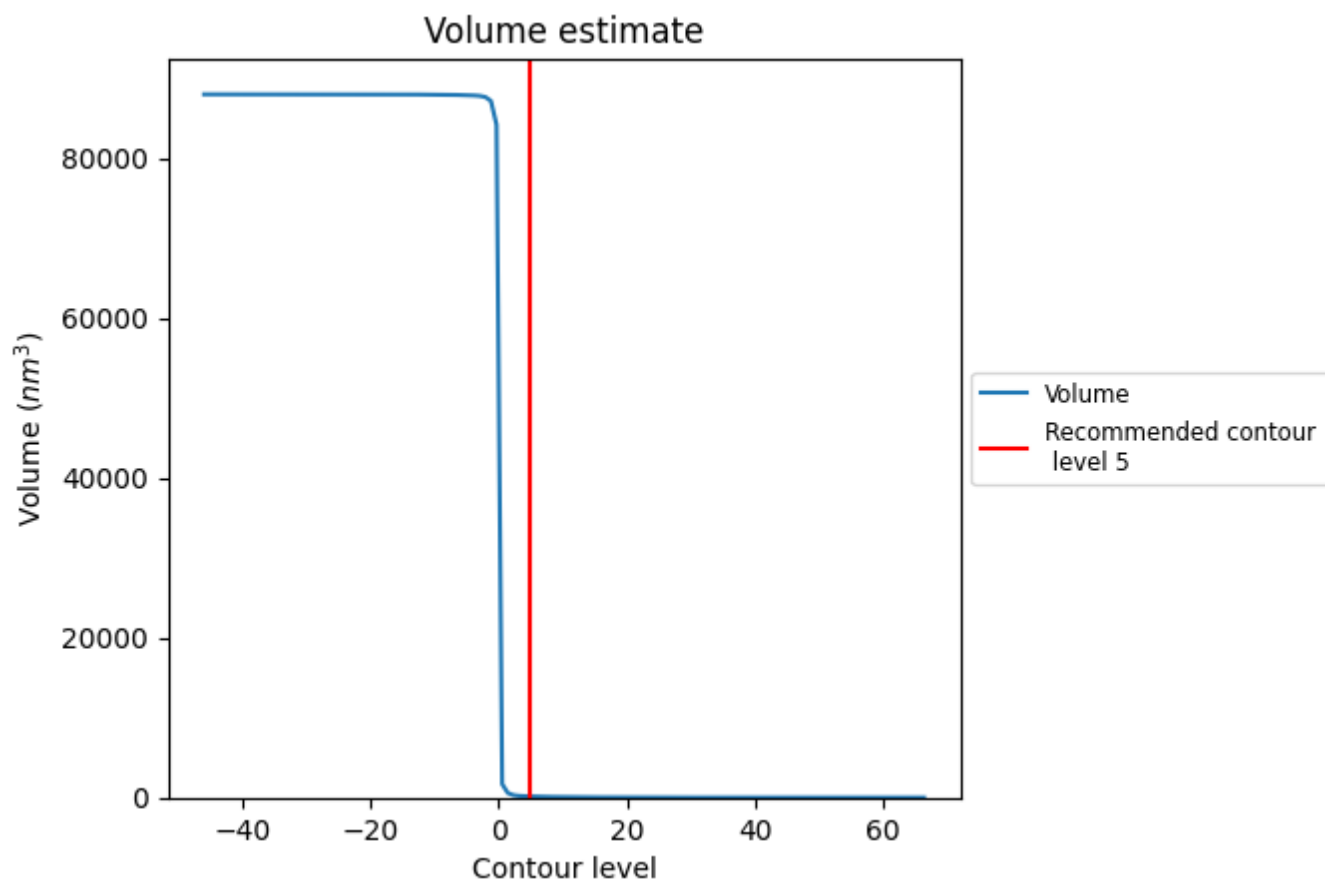
This section contains the results of statistical analysis of the map.

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.

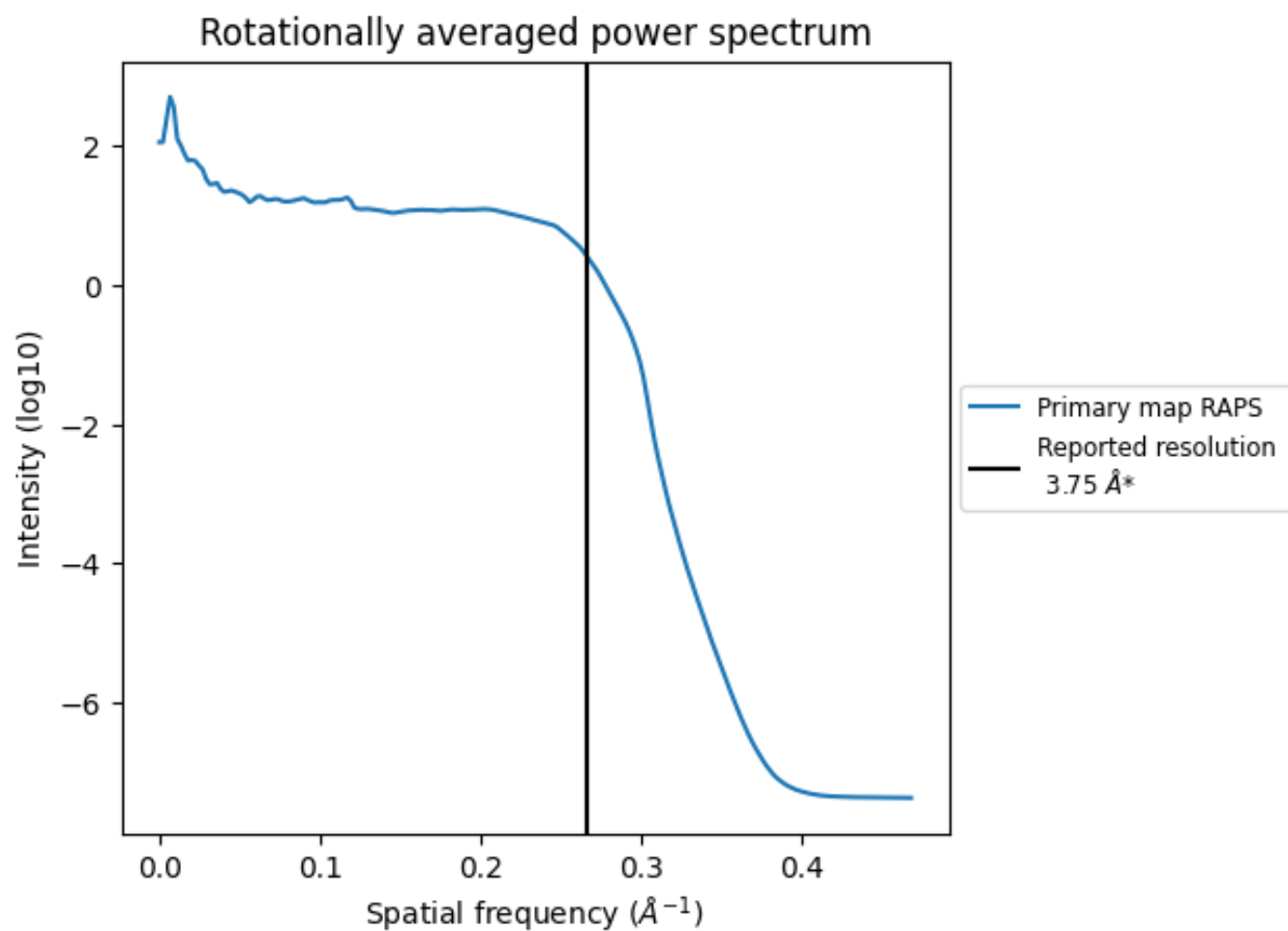
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm^3 ; this corresponds to an approximate mass of 125 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 ⓘ

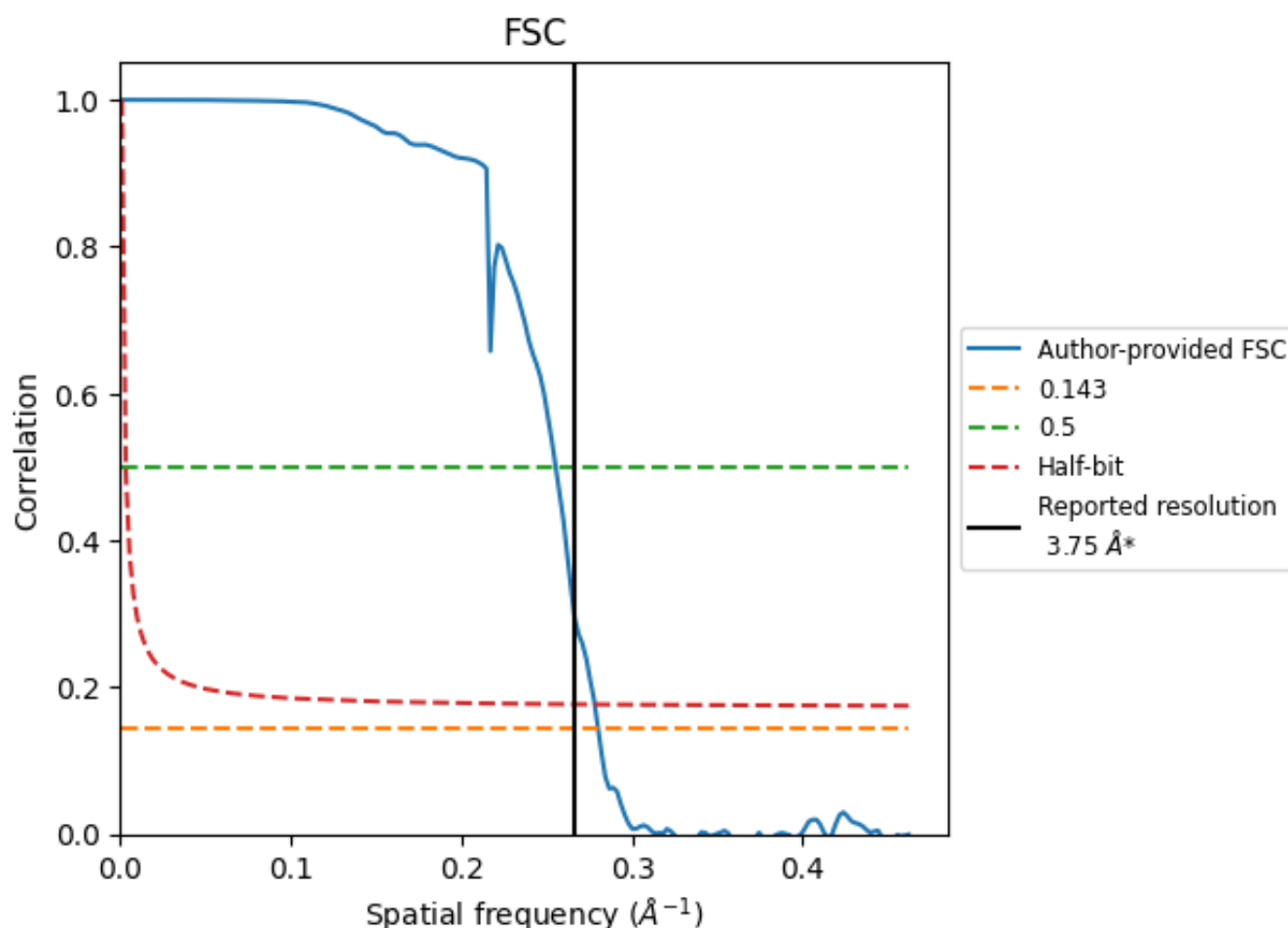


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

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 0.267 Å⁻¹

8.2 Resolution estimates [i](#)

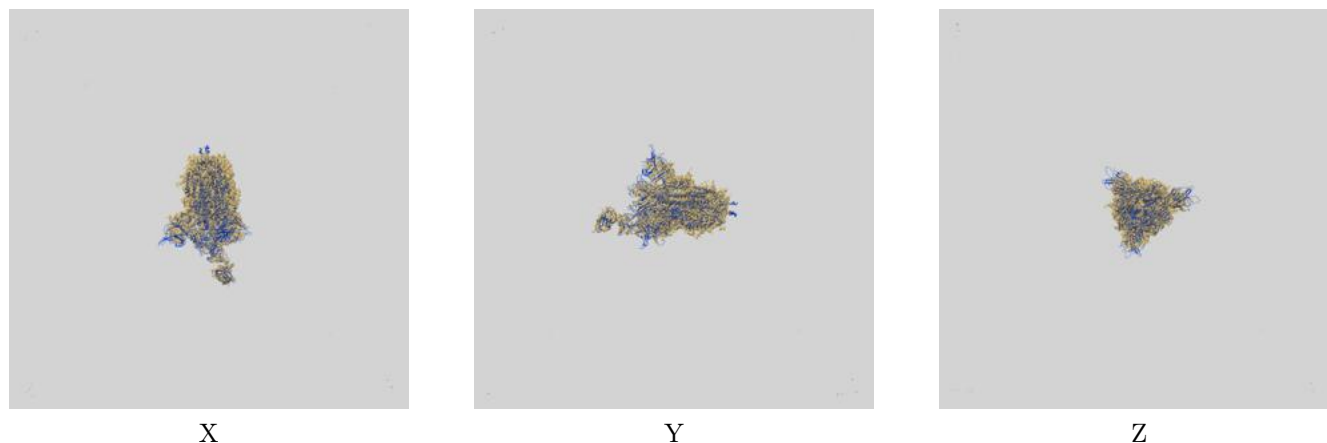
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.75	-
Author-provided FSC curve	3.57	3.92	3.60
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

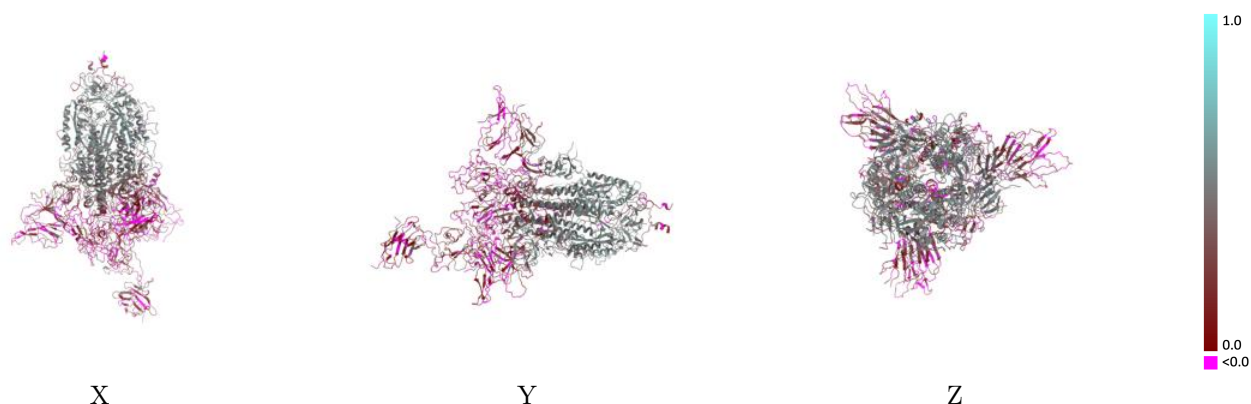
This section contains information regarding the fit between EMDB map EMD-28688 and PDB model 8EYH. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



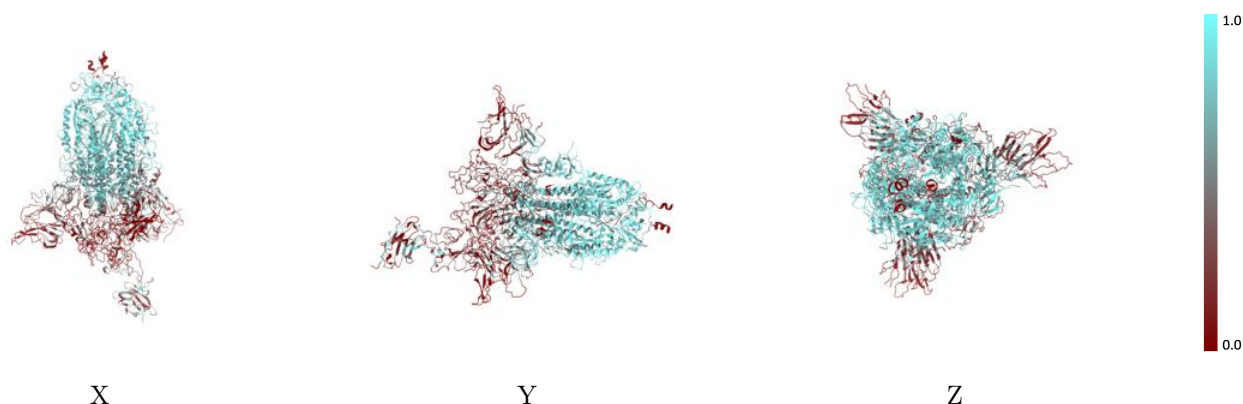
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



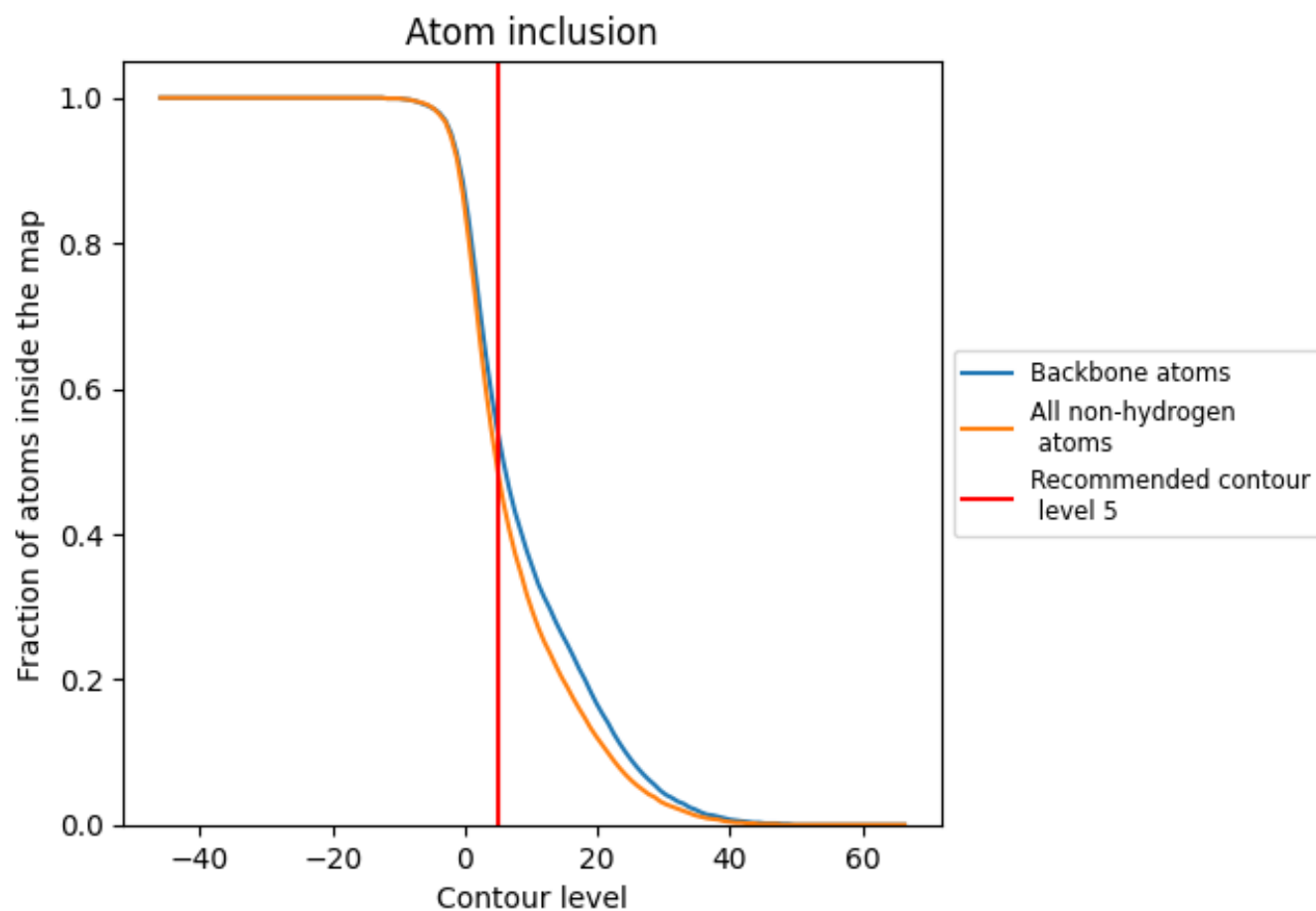
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 48% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4850	<div></div> 0.2870
A	<div></div> 0.4980	<div></div> 0.3080
B	<div></div> 0.5100	<div></div> 0.3000
C	<div></div> 0.4630	<div></div> 0.2720
D	<div></div> 0.3500	<div></div> 0.1460
E	<div></div> 0.3210	<div></div> 0.1470
F	<div></div> 0.1790	<div></div> 0.0860
G	<div></div> 0.3570	<div></div> 0.1290
H	<div></div> 0.2140	<div></div> 0.0730
I	<div></div> 0.0710	<div></div> -0.0470

1.0

0.0

<0.0