



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:36 PM UTC

PDB ID : 7UL7 / pdb_00007ul7
EMDB ID : EMD-26594
Title : Lineage I (Pinneo) Lassa virus glycoprotein bound to 18.5C-M30 Fab
Authors : Buck, T.K.; Enriquez, A.S.; Hastie, K.M.
Deposited on : 2022-04-04
Resolution : 3.59 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

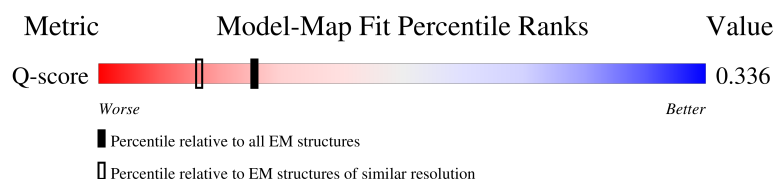
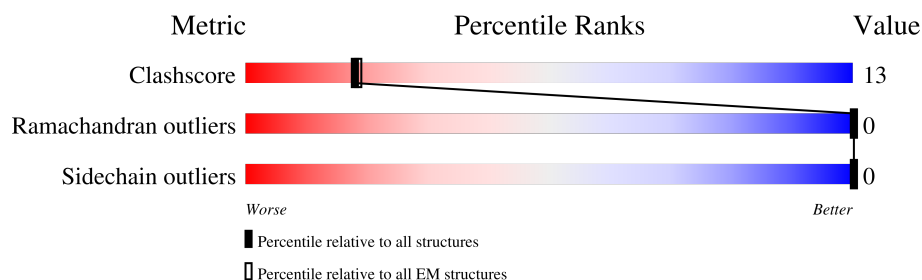
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.59 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12565 (3.09 - 4.09)

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	258	10% 39% 21% 40%
1	B	258	9% 44% 16% 40%
1	C	258	12% 38% 22% 40%
2	D	237	11% 64% 22% 14%

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Mol	Chain	Length	Quality of chain
2	F	237	
2	L	237	
3	E	249	
3	G	249	
3	H	249	
4	a	206	
4	b	206	
4	c	206	
5	I	2	
5	J	2	
5	K	2	
5	M	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17439 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 Glycoprotein G1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	155	Total	C	N	O	S	0	0
			1248	791	208	236	13		
1	A	155	Total	C	N	O	S	0	0
			1248	791	208	236	13		
1	B	155	Total	C	N	O	S	0	0
			1248	791	208	236	13		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	206	CYS	LYS	conflict	UNP Q9IMJ0
C	257	ARG	LEU	engineered mutation	UNP Q9IMJ0
C	258	ARG	LEU	engineered mutation	UNP Q9IMJ0
A	206	CYS	LYS	conflict	UNP Q9IMJ0
A	257	ARG	LEU	engineered mutation	UNP Q9IMJ0
A	258	ARG	LEU	engineered mutation	UNP Q9IMJ0
B	206	CYS	LYS	conflict	UNP Q9IMJ0
B	257	ARG	LEU	engineered mutation	UNP Q9IMJ0
B	258	ARG	LEU	engineered mutation	UNP Q9IMJ0

- Molecule 2 is a protein called 18.5C-M30 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	205	Total	C	N	O	S	0	0
			1579	999	263	313	4		
2	L	205	Total	C	N	O	S	0	0
			1579	999	263	313	4		
2	F	205	Total	C	N	O	S	0	0
			1579	999	263	313	4		

- Molecule 3 is a protein called 18.5C-M30 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	215	Total 1621	C 1021	N 286	O 307	S 7	0	0
3	H	215	Total 1621	C 1021	N 286	O 307	S 7	0	0
3	G	215	Total 1621	C 1021	N 286	O 307	S 7	0	0

- Molecule 4 is a protein called Glycoprotein G2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	151	Total 1225	C 771	N 207	O 234	S 13	0	0
4	b	151	Total 1225	C 771	N 207	O 234	S 13	0	0
4	a	151	Total 1225	C 771	N 207	O 234	S 13	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	328	PRO	GLU	conflict	UNP Q9IMJ0
c	359	CYS	GLY	conflict	UNP Q9IMJ0
c	419	LEU	-	expression tag	UNP Q9IMJ0
c	420	PRO	-	expression tag	UNP Q9IMJ0
c	421	GLU	-	expression tag	UNP Q9IMJ0
c	422	THR	-	expression tag	UNP Q9IMJ0
c	423	GLY	-	expression tag	UNP Q9IMJ0
c	424	LEU	-	expression tag	UNP Q9IMJ0
c	425	VAL	-	expression tag	UNP Q9IMJ0
c	426	ASP	-	expression tag	UNP Q9IMJ0
c	427	LEU	-	expression tag	UNP Q9IMJ0
c	428	GLU	-	expression tag	UNP Q9IMJ0
c	429	VAL	-	expression tag	UNP Q9IMJ0
c	430	ASP	-	expression tag	UNP Q9IMJ0
c	431	ASP	-	expression tag	UNP Q9IMJ0
c	432	ASP	-	expression tag	UNP Q9IMJ0
c	433	ASP	-	expression tag	UNP Q9IMJ0
c	434	LYS	-	expression tag	UNP Q9IMJ0
c	435	ALA	-	expression tag	UNP Q9IMJ0
c	436	GLY	-	expression tag	UNP Q9IMJ0
c	437	TRP	-	expression tag	UNP Q9IMJ0
c	438	SER	-	expression tag	UNP Q9IMJ0
c	439	HIS	-	expression tag	UNP Q9IMJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
c	440	PRO	-	expression tag	UNP Q9IMJ0
c	441	GLN	-	expression tag	UNP Q9IMJ0
c	442	PHE	-	expression tag	UNP Q9IMJ0
c	443	GLU	-	expression tag	UNP Q9IMJ0
c	444	LYS	-	expression tag	UNP Q9IMJ0
c	445	GLY	-	expression tag	UNP Q9IMJ0
c	446	GLY	-	expression tag	UNP Q9IMJ0
c	447	GLY	-	expression tag	UNP Q9IMJ0
c	448	SER	-	expression tag	UNP Q9IMJ0
c	449	GLY	-	expression tag	UNP Q9IMJ0
c	450	GLY	-	expression tag	UNP Q9IMJ0
c	451	GLY	-	expression tag	UNP Q9IMJ0
c	452	SER	-	expression tag	UNP Q9IMJ0
c	453	GLY	-	expression tag	UNP Q9IMJ0
c	454	GLY	-	expression tag	UNP Q9IMJ0
c	455	GLY	-	expression tag	UNP Q9IMJ0
c	456	SER	-	expression tag	UNP Q9IMJ0
c	457	TRP	-	expression tag	UNP Q9IMJ0
c	458	SER	-	expression tag	UNP Q9IMJ0
c	459	HIS	-	expression tag	UNP Q9IMJ0
c	460	PRO	-	expression tag	UNP Q9IMJ0
c	461	GLN	-	expression tag	UNP Q9IMJ0
c	462	PHE	-	expression tag	UNP Q9IMJ0
c	463	GLU	-	expression tag	UNP Q9IMJ0
c	464	LYS	-	expression tag	UNP Q9IMJ0
b	328	PRO	GLU	conflict	UNP Q9IMJ0
b	359	CYS	GLY	conflict	UNP Q9IMJ0
b	419	LEU	-	expression tag	UNP Q9IMJ0
b	420	PRO	-	expression tag	UNP Q9IMJ0
b	421	GLU	-	expression tag	UNP Q9IMJ0
b	422	THR	-	expression tag	UNP Q9IMJ0
b	423	GLY	-	expression tag	UNP Q9IMJ0
b	424	LEU	-	expression tag	UNP Q9IMJ0
b	425	VAL	-	expression tag	UNP Q9IMJ0
b	426	ASP	-	expression tag	UNP Q9IMJ0
b	427	LEU	-	expression tag	UNP Q9IMJ0
b	428	GLU	-	expression tag	UNP Q9IMJ0
b	429	VAL	-	expression tag	UNP Q9IMJ0
b	430	ASP	-	expression tag	UNP Q9IMJ0
b	431	ASP	-	expression tag	UNP Q9IMJ0
b	432	ASP	-	expression tag	UNP Q9IMJ0
b	433	ASP	-	expression tag	UNP Q9IMJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
b	434	LYS	-	expression tag	UNP Q9IMJ0
b	435	ALA	-	expression tag	UNP Q9IMJ0
b	436	GLY	-	expression tag	UNP Q9IMJ0
b	437	TRP	-	expression tag	UNP Q9IMJ0
b	438	SER	-	expression tag	UNP Q9IMJ0
b	439	HIS	-	expression tag	UNP Q9IMJ0
b	440	PRO	-	expression tag	UNP Q9IMJ0
b	441	GLN	-	expression tag	UNP Q9IMJ0
b	442	PHE	-	expression tag	UNP Q9IMJ0
b	443	GLU	-	expression tag	UNP Q9IMJ0
b	444	LYS	-	expression tag	UNP Q9IMJ0
b	445	GLY	-	expression tag	UNP Q9IMJ0
b	446	GLY	-	expression tag	UNP Q9IMJ0
b	447	GLY	-	expression tag	UNP Q9IMJ0
b	448	SER	-	expression tag	UNP Q9IMJ0
b	449	GLY	-	expression tag	UNP Q9IMJ0
b	450	GLY	-	expression tag	UNP Q9IMJ0
b	451	GLY	-	expression tag	UNP Q9IMJ0
b	452	SER	-	expression tag	UNP Q9IMJ0
b	453	GLY	-	expression tag	UNP Q9IMJ0
b	454	GLY	-	expression tag	UNP Q9IMJ0
b	455	GLY	-	expression tag	UNP Q9IMJ0
b	456	SER	-	expression tag	UNP Q9IMJ0
b	457	TRP	-	expression tag	UNP Q9IMJ0
b	458	SER	-	expression tag	UNP Q9IMJ0
b	459	HIS	-	expression tag	UNP Q9IMJ0
b	460	PRO	-	expression tag	UNP Q9IMJ0
b	461	GLN	-	expression tag	UNP Q9IMJ0
b	462	PHE	-	expression tag	UNP Q9IMJ0
b	463	GLU	-	expression tag	UNP Q9IMJ0
b	464	LYS	-	expression tag	UNP Q9IMJ0
a	328	PRO	GLU	conflict	UNP Q9IMJ0
a	359	CYS	GLY	conflict	UNP Q9IMJ0
a	419	LEU	-	expression tag	UNP Q9IMJ0
a	420	PRO	-	expression tag	UNP Q9IMJ0
a	421	GLU	-	expression tag	UNP Q9IMJ0
a	422	THR	-	expression tag	UNP Q9IMJ0
a	423	GLY	-	expression tag	UNP Q9IMJ0
a	424	LEU	-	expression tag	UNP Q9IMJ0
a	425	VAL	-	expression tag	UNP Q9IMJ0
a	426	ASP	-	expression tag	UNP Q9IMJ0
a	427	LEU	-	expression tag	UNP Q9IMJ0

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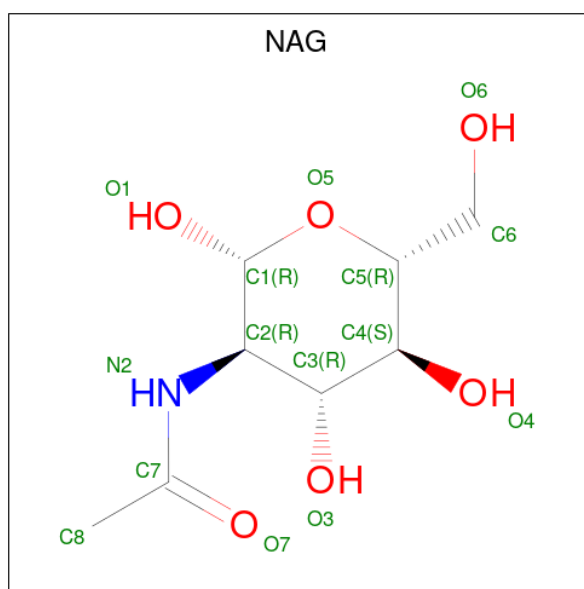
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a	428	GLU	-	expression tag	UNP Q9IMJ0
a	429	VAL	-	expression tag	UNP Q9IMJ0
a	430	ASP	-	expression tag	UNP Q9IMJ0
a	431	ASP	-	expression tag	UNP Q9IMJ0
a	432	ASP	-	expression tag	UNP Q9IMJ0
a	433	ASP	-	expression tag	UNP Q9IMJ0
a	434	LYS	-	expression tag	UNP Q9IMJ0
a	435	ALA	-	expression tag	UNP Q9IMJ0
a	436	GLY	-	expression tag	UNP Q9IMJ0
a	437	TRP	-	expression tag	UNP Q9IMJ0
a	438	SER	-	expression tag	UNP Q9IMJ0
a	439	HIS	-	expression tag	UNP Q9IMJ0
a	440	PRO	-	expression tag	UNP Q9IMJ0
a	441	GLN	-	expression tag	UNP Q9IMJ0
a	442	PHE	-	expression tag	UNP Q9IMJ0
a	443	GLU	-	expression tag	UNP Q9IMJ0
a	444	LYS	-	expression tag	UNP Q9IMJ0
a	445	GLY	-	expression tag	UNP Q9IMJ0
a	446	GLY	-	expression tag	UNP Q9IMJ0
a	447	GLY	-	expression tag	UNP Q9IMJ0
a	448	SER	-	expression tag	UNP Q9IMJ0
a	449	GLY	-	expression tag	UNP Q9IMJ0
a	450	GLY	-	expression tag	UNP Q9IMJ0
a	451	GLY	-	expression tag	UNP Q9IMJ0
a	452	SER	-	expression tag	UNP Q9IMJ0
a	453	GLY	-	expression tag	UNP Q9IMJ0
a	454	GLY	-	expression tag	UNP Q9IMJ0
a	455	GLY	-	expression tag	UNP Q9IMJ0
a	456	SER	-	expression tag	UNP Q9IMJ0
a	457	TRP	-	expression tag	UNP Q9IMJ0
a	458	SER	-	expression tag	UNP Q9IMJ0
a	459	HIS	-	expression tag	UNP Q9IMJ0
a	460	PRO	-	expression tag	UNP Q9IMJ0
a	461	GLN	-	expression tag	UNP Q9IMJ0
a	462	PHE	-	expression tag	UNP Q9IMJ0
a	463	GLU	-	expression tag	UNP Q9IMJ0
a	464	LYS	-	expression tag	UNP Q9IMJ0

- Molecule 5 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
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



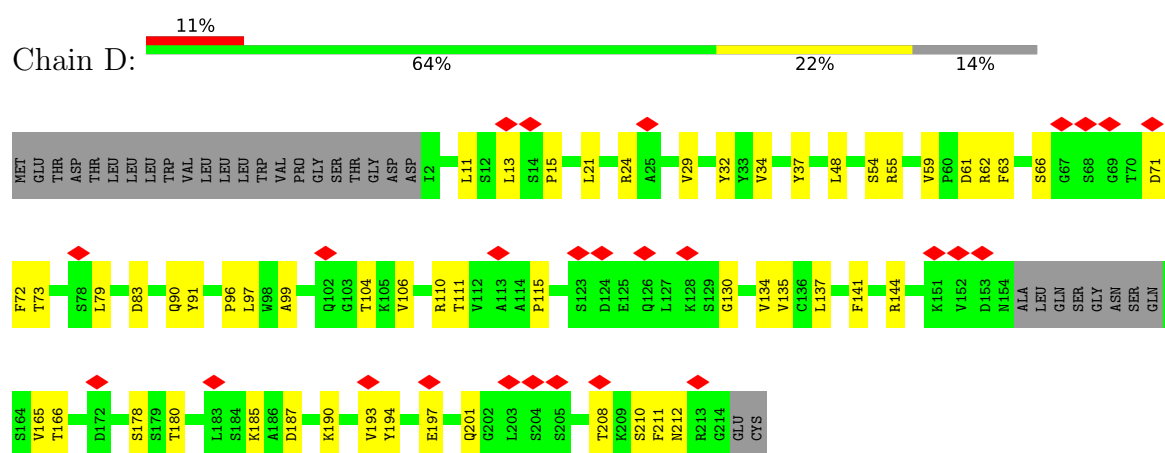
Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

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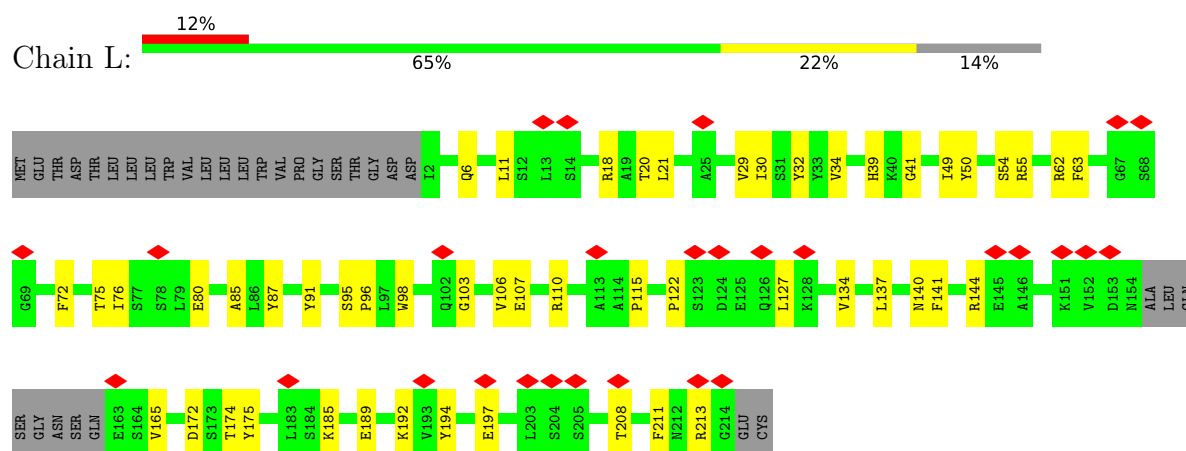
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Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C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

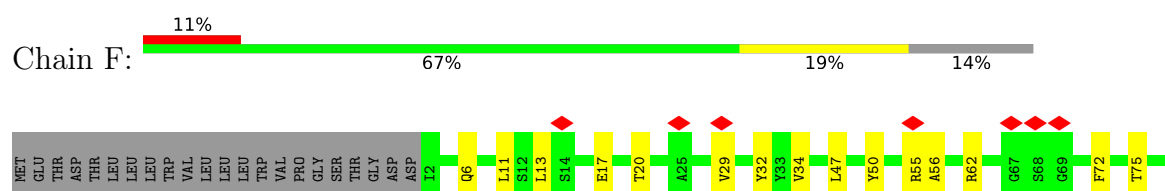
- Molecule 2: 18.5C-M30 Fab Light Chain

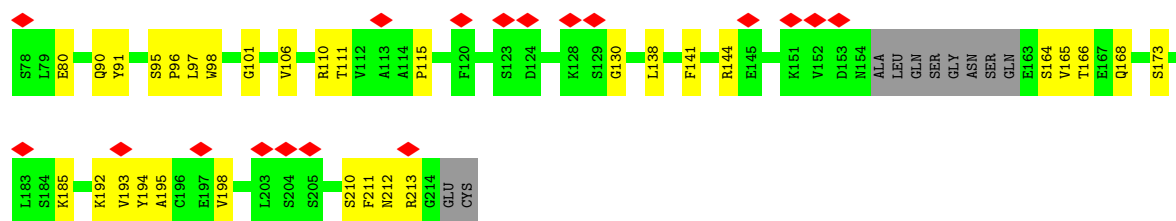


- Molecule 2: 18.5C-M30 Fab Light Chain

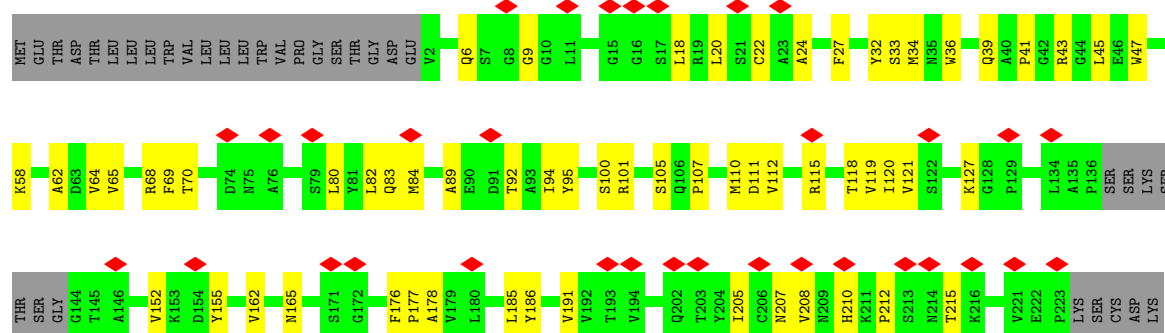


- Molecule 2: 18.5C-M30 Fab Light Chain

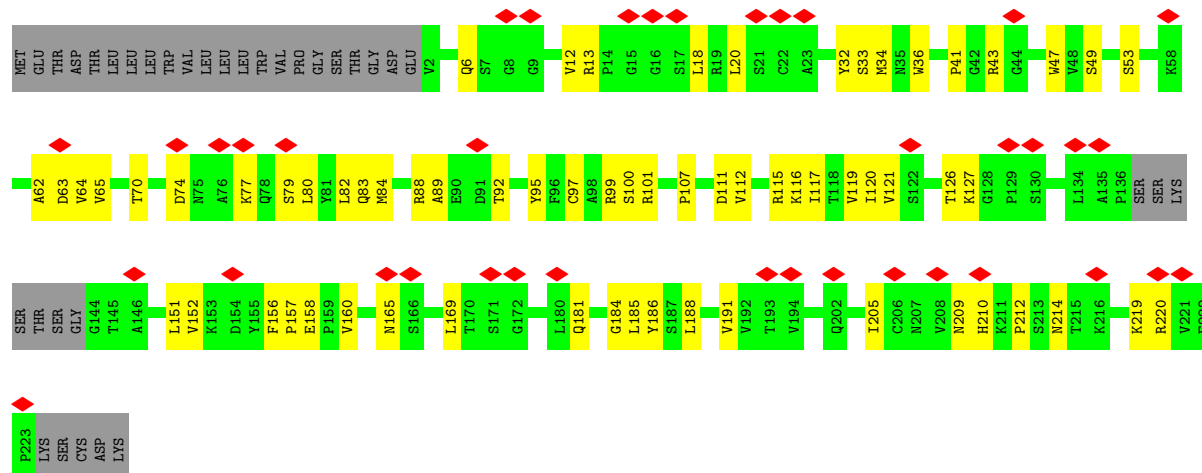




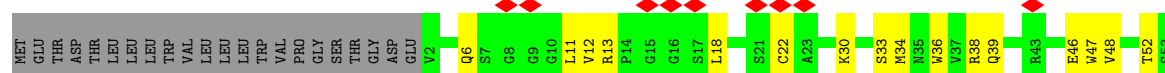
• Molecule 3: 18.5C-M30 Fab Heavy Chain

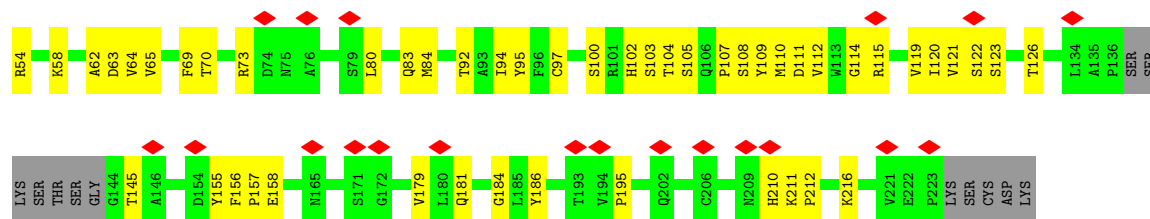


• Molecule 3: 18.5C-M30 Fab Heavy Chain

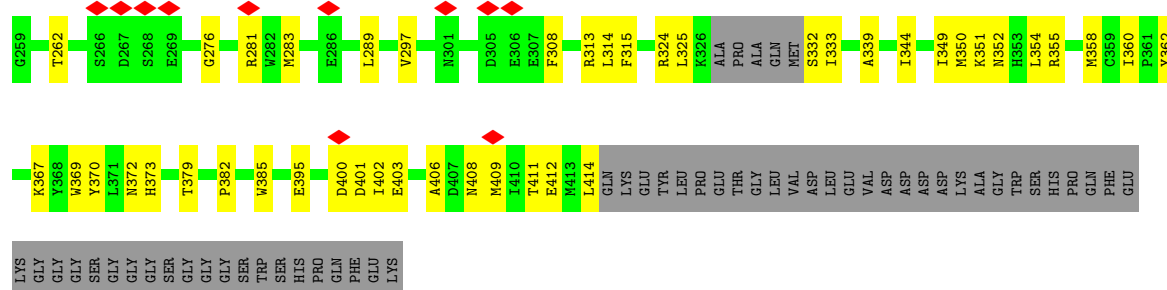


• Molecule 3: 18.5C-M30 Fab Heavy Chain

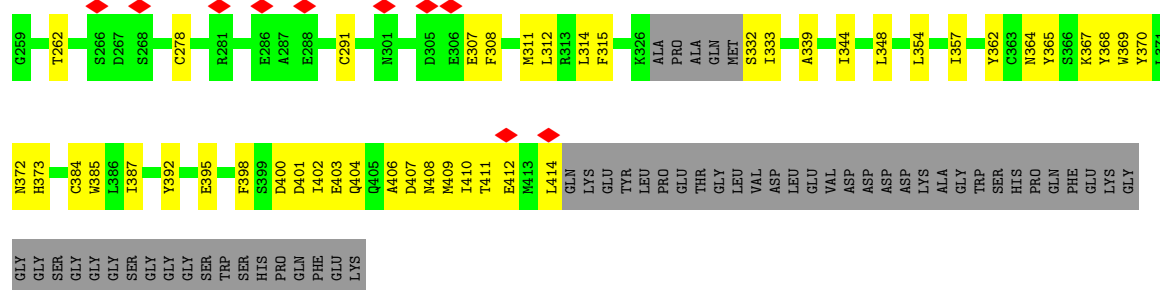




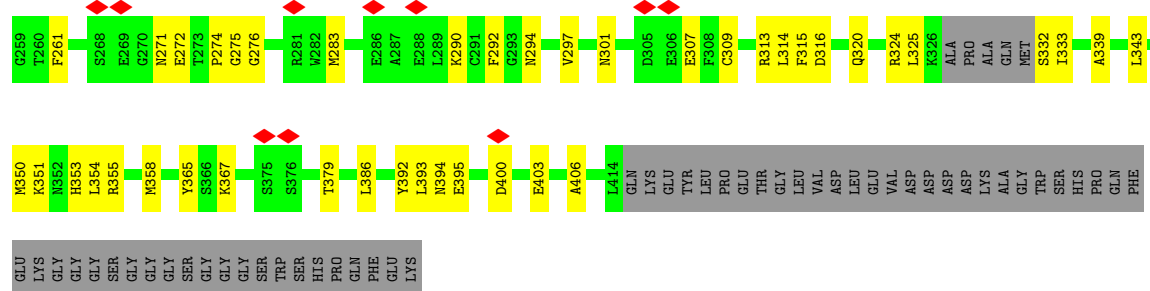
• Molecule 4: Glycoprotein G2



• Molecule 4: Glycoprotein G2



• Molecule 4: Glycoprotein G2



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	380210	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.245	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	539.136, 539.136, 539.136	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.296, 1.296, 1.296	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	0.15	0/1276	0.36	0/1729
1	B	0.16	0/1276	0.39	0/1729
1	C	0.18	0/1276	0.41	0/1729
2	D	0.18	0/1617	0.36	0/2197
2	F	0.17	0/1617	0.32	0/2197
2	L	0.15	0/1617	0.30	0/2197
3	E	0.17	0/1658	0.38	0/2253
3	G	0.18	0/1658	0.39	0/2253
3	H	0.16	0/1658	0.37	0/2253
4	a	0.19	0/1249	0.36	0/1685
4	b	0.19	0/1249	0.37	0/1685
4	c	0.19	0/1249	0.35	0/1685
All	All	0.17	0/17400	0.36	0/23592

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	1248	0	1191	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1248	0	1192	36	0
1	C	1248	0	1191	48	0
2	D	1579	0	1530	40	0
2	F	1579	0	1530	39	0
2	L	1579	0	1530	34	0
3	E	1621	0	1612	53	0
3	G	1621	0	1612	59	0
3	H	1621	0	1612	55	0
4	a	1225	0	1175	35	0
4	b	1225	0	1176	40	0
4	c	1225	0	1176	39	0
5	I	28	0	25	1	0
5	J	28	0	25	0	0
5	K	28	0	25	0	0
5	M	28	0	25	1	0
6	A	70	0	65	4	0
6	B	42	0	39	0	0
6	C	70	0	65	2	0
6	a	42	0	39	4	0
6	b	42	0	39	1	0
6	c	42	0	39	1	0
All	All	17439	0	16913	458	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 13.

All (458) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:210:HIS:O	3:H:214:ASN:HA	1.68	0.93
3:E:58:LYS:NZ	4:c:395:GLU:CD	2.31	0.89
2:F:90:GLN:HE22	3:G:110:MET:HE1	1.39	0.87
3:E:58:LYS:HZ3	4:c:395:GLU:CD	1.83	0.85
4:a:394:ASN:HB2	6:a:503:NAG:HN2	1.46	0.81
4:a:394:ASN:HB2	6:a:503:NAG:N2	1.98	0.79
2:F:144:ARG:HH12	2:F:165:VAL:HG11	1.48	0.78
1:C:227:GLU:CD	1:C:228:ASP:H	1.92	0.77
3:G:111:ASP:OD1	3:G:112:VAL:N	2.17	0.77
3:E:111:ASP:OD1	3:E:112:VAL:N	2.18	0.77
1:C:184:ASN:O	1:C:188:GLN:NE2	2.20	0.75
1:B:137:SER:HA	1:B:140:HIS:CE1	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:127:LEU:O	2:L:185:LYS:NZ	2.21	0.73
1:B:133:MET:HE1	1:B:161:ILE:HD12	1.71	0.73
3:E:6:GLN:NE2	3:E:115:ARG:O	2.22	0.72
3:E:6:GLN:HE22	3:E:115:ARG:H	1.37	0.71
1:C:121:ASP:HA	1:C:124:LYS:HB3	1.73	0.71
3:E:210:HIS:O	3:E:215:THR:HB	1.91	0.70
1:B:92:HIS:HB2	1:B:104:LEU:HB2	1.73	0.70
1:B:241:LEU:HD13	4:b:344:ILE:HD13	1.74	0.70
3:G:34:MET:HG2	3:G:80:LEU:HD11	1.71	0.70
2:D:115:PRO:HB3	2:D:141:PHE:HB3	1.72	0.70
2:L:144:ARG:HH12	2:L:165:VAL:HG21	1.57	0.68
1:C:114:HIS:NE2	1:C:154:CYS:O	2.26	0.68
3:H:210:HIS:O	3:H:214:ASN:CA	2.42	0.68
3:G:34:MET:HB3	3:G:80:LEU:HD21	1.76	0.68
3:G:13:ARG:NH1	3:G:123:SER:O	2.26	0.68
3:E:64:VAL:HG23	3:E:65:VAL:HG13	1.76	0.68
1:C:241:LEU:HD13	4:c:344:ILE:HD13	1.76	0.67
4:c:332:SER:OG	4:c:333:ILE:N	2.26	0.67
1:A:104:LEU:HD13	1:A:221:ILE:HG13	1.77	0.67
3:H:33:SER:HB3	3:H:100:SER:O	1.94	0.66
2:F:138:LEU:HD21	2:F:198:VAL:HG11	1.77	0.66
1:A:102:LEU:HD21	1:A:132:LEU:HD21	1.78	0.66
4:b:332:SER:OG	4:b:333:ILE:N	2.23	0.66
2:D:11:LEU:HB3	2:D:106:VAL:HG22	1.78	0.66
1:B:85:CYS:HB3	1:B:235:PRO:HB3	1.78	0.65
2:F:115:PRO:HB3	2:F:141:PHE:HB3	1.79	0.65
3:E:165:ASN:HA	3:E:205:ILE:HG22	1.78	0.65
1:B:223:ASN:OD1	1:B:224:THR:N	2.30	0.65
4:a:332:SER:OG	4:a:333:ILE:N	2.23	0.64
3:G:58:LYS:HZ3	4:b:395:GLU:CD	2.03	0.64
1:A:133:MET:HE1	1:A:136:ILE:HD11	1.78	0.64
1:C:107:THR:HG22	1:C:109:THR:H	1.61	0.64
3:H:64:VAL:HG23	3:H:65:VAL:HG13	1.79	0.64
1:A:126:ASN:OD1	1:A:130:HIS:NE2	2.31	0.63
3:E:9:GLY:HA3	3:E:118:THR:O	1.97	0.63
1:A:223:ASN:OD1	1:A:224:THR:N	2.32	0.63
2:F:47:LEU:HD11	3:G:109:TYR:HB2	1.80	0.63
3:H:32:TYR:HD2	3:H:99:ARG:HE	1.44	0.62
4:a:292:PHE:HD1	4:a:379:THR:HG21	1.64	0.62
1:B:152:MET:HA	1:B:165:TYR:HE1	1.64	0.62
4:b:408:ASN:O	4:b:412:GLU:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:88:ARG:HA	3:H:88:ARG:NH1	2.13	0.62
2:D:29:VAL:HG13	2:D:91:TYR:HE2	1.64	0.62
3:E:22:CYS:HB3	3:E:80:LEU:HD21	1.81	0.61
3:H:74:ASP:OD2	3:H:77:LYS:NZ	2.32	0.61
3:G:92:THR:HG22	3:G:120:ILE:HA	1.81	0.61
3:E:27:PHE:HA	4:a:272:GLU:HG3	1.81	0.61
1:A:218:TYR:HE1	6:A:303:NAG:HN2	1.47	0.60
2:D:37:TYR:OH	3:E:110:MET:SD	2.60	0.60
2:L:11:LEU:HB3	2:L:106:VAL:HG22	1.84	0.60
2:F:11:LEU:HB3	2:F:106:VAL:HG22	1.84	0.60
4:c:351:LYS:HE3	4:c:355:ARG:HH21	1.67	0.59
1:B:121:ASP:HA	1:B:124:LYS:HB3	1.84	0.59
3:G:54:ARG:HE	4:b:407:ASP:CG	2.10	0.59
1:C:87:LYS:HE3	1:C:87:LYS:HA	1.83	0.58
3:E:33:SER:HB3	3:E:100:SER:O	2.02	0.58
3:E:92:THR:HG22	3:E:121:VAL:H	1.67	0.58
2:F:32:TYR:HE1	4:c:324:ARG:HH12	1.51	0.58
2:L:34:VAL:HG21	2:L:72:PHE:CZ	2.38	0.58
1:B:153:SER:HB2	1:B:164:GLN:O	2.04	0.58
2:F:97:LEU:HB2	3:G:47:TRP:CH2	2.39	0.58
4:c:276:GLY:HA2	4:c:297:VAL:HG21	1.86	0.58
2:D:62:ARG:NH2	2:D:83:ASP:OD2	2.36	0.58
2:D:110:ARG:NH1	2:D:111:THR:OG1	2.37	0.58
4:b:406:ALA:O	4:b:409:MET:HB2	2.04	0.57
2:D:48:LEU:HD11	2:D:63:PHE:CD2	2.40	0.57
3:H:165:ASN:HD21	3:H:169:LEU:HB3	1.69	0.57
1:C:163:VAL:HB	1:C:221:ILE:HB	1.86	0.57
2:D:55:ARG:NH2	2:D:59:VAL:O	2.37	0.57
2:L:62:ARG:NH1	2:L:80:GLU:OE1	2.37	0.57
5:M:2:NAG:H3	5:M:2:NAG:H83	1.87	0.57
3:H:89:ALA:HA	3:H:121:VAL:HG11	1.87	0.57
1:C:192:ARG:NH2	4:c:350:MET:SD	2.70	0.56
1:C:223:ASN:OD1	1:C:224:THR:N	2.37	0.56
1:C:103:GLU:OE2	1:C:229:HIS:NE2	2.38	0.56
2:D:55:ARG:NH2	2:D:61:ASP:OD1	2.38	0.56
3:G:22:CYS:HB3	3:G:80:LEU:HB2	1.87	0.56
4:a:339:ALA:O	4:a:343:LEU:HG	2.05	0.56
1:C:81:MET:HE1	4:c:314:LEU:HD13	1.86	0.56
2:D:29:VAL:HG13	2:D:91:TYR:CE2	2.40	0.56
4:a:307:GLU:HG3	4:a:365:TYR:CZ	2.40	0.56
1:C:91:HIS:HA	1:C:104:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6:GLN:O	3:H:115:ARG:NH2	2.38	0.56
2:L:96:PRO:HB2	3:H:47:TRP:CZ3	2.41	0.56
4:c:324:ARG:O	4:c:325:LEU:HD22	2.05	0.55
2:D:96:PRO:HB2	3:E:47:TRP:CZ3	2.42	0.55
3:G:62:ALA:HB3	3:G:65:VAL:HG22	1.87	0.55
4:a:271:ASN:ND2	4:a:275:GLY:O	2.39	0.55
3:E:152:VAL:HG11	3:E:208:VAL:HG21	1.88	0.55
1:C:215:SER:HB3	6:C:302:NAG:H5	1.89	0.55
2:D:135:VAL:HG22	2:D:180:THR:HG22	1.88	0.55
3:E:62:ALA:HB3	3:E:65:VAL:HG22	1.88	0.55
1:C:160:LYS:HA	6:C:304:NAG:H5	1.89	0.55
3:H:70:THR:OG1	3:H:83:GLN:HB3	2.07	0.55
3:G:69:PHE:CD1	3:G:84:MET:HG2	2.42	0.55
1:C:70:LEU:HD23	4:c:370:TYR:HE2	1.72	0.55
2:D:201:GLN:N	2:D:201:GLN:OE1	2.40	0.54
3:E:89:ALA:HA	3:E:121:VAL:HG11	1.88	0.54
2:L:192:LYS:O	2:L:213:ARG:N	2.32	0.54
4:c:400:ASP:OD1	4:c:401:ASP:N	2.40	0.54
2:L:30:ILE:HG22	2:L:32:TYR:H	1.72	0.54
1:B:238:ILE:HD11	4:b:311:MET:HE3	1.88	0.54
2:F:20:THR:HG22	2:F:75:THR:HG22	1.89	0.54
2:F:192:LYS:HG2	2:F:213:ARG:HB3	1.89	0.54
2:L:107:GLU:OE1	2:L:175:TYR:OH	2.25	0.54
4:b:372:ASN:OD1	4:b:373:HIS:N	2.41	0.53
2:L:96:PRO:HB2	3:H:47:TRP:HZ3	1.73	0.53
4:b:401:ASP:OD1	4:b:404:GLN:NE2	2.41	0.53
3:H:111:ASP:OD1	3:H:112:VAL:N	2.39	0.53
3:E:18:LEU:HB3	3:E:84:MET:HG3	1.90	0.53
4:a:276:GLY:HA2	4:a:297:VAL:HG11	1.89	0.53
2:F:98:TRP:HD1	3:G:47:TRP:CE2	2.27	0.53
2:D:48:LEU:HD11	2:D:63:PHE:HD2	1.74	0.53
3:E:92:THR:HG22	3:E:120:ILE:HA	1.91	0.53
3:G:33:SER:HB3	3:G:100:SER:O	2.09	0.53
1:C:66:GLU:HG3	4:c:372:ASN:HB3	1.91	0.53
1:C:114:HIS:NE2	1:C:153:SER:OG	2.42	0.53
1:B:152:MET:HA	1:B:165:TYR:CE1	2.44	0.53
3:H:127:LYS:HD2	3:H:185:LEU:HD11	1.90	0.53
2:F:17:GLU:N	2:F:17:GLU:OE1	2.42	0.52
2:D:96:PRO:HB2	3:E:47:TRP:HZ3	1.75	0.52
1:A:114:HIS:ND1	1:A:116:PHE:O	2.42	0.52
3:H:32:TYR:CE1	3:H:101:ARG:HD3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:30:LYS:HB3	3:G:54:ARG:HB3	1.91	0.52
4:a:386:LEU:HB2	4:a:393:LEU:HD22	1.92	0.52
1:C:102:LEU:HD21	1:C:132:LEU:HD21	1.91	0.52
2:L:32:TYR:CZ	3:H:107:PRO:HG3	2.43	0.52
4:b:367:LYS:HD3	4:b:392:TYR:HE2	1.74	0.52
1:A:73:ASN:OD1	1:A:74:MET:N	2.41	0.52
3:G:36:TRP:CH2	3:G:97:CYS:HB3	2.44	0.52
6:b:503:NAG:H83	6:b:503:NAG:H3	1.90	0.52
4:a:403:GLU:O	4:a:406:ALA:HB3	2.09	0.52
3:G:12:VAL:HG21	3:G:18:LEU:HD22	1.91	0.52
4:b:400:ASP:OD1	4:b:401:ASP:N	2.43	0.52
1:C:104:LEU:CD2	1:C:221:ILE:HG12	2.40	0.52
3:E:6:GLN:HE22	3:E:115:ARG:N	2.07	0.52
3:G:38:ARG:HB3	3:G:95:TYR:CE1	2.45	0.52
1:C:190:PHE:HZ	1:C:219:LEU:HD13	1.75	0.51
3:E:9:GLY:HA2	3:E:119:VAL:HB	1.91	0.51
1:A:186:VAL:O	1:A:189:THR:OG1	2.26	0.51
2:F:144:ARG:NH1	2:F:165:VAL:HG11	2.24	0.51
3:H:13:ARG:HB2	3:H:13:ARG:NH1	2.25	0.51
3:H:160:VAL:HG11	3:H:210:HIS:ND1	2.25	0.51
4:c:370:TYR:HB3	4:c:382:PRO:HG3	1.91	0.51
4:c:403:GLU:O	4:c:406:ALA:HB3	2.10	0.51
3:E:70:THR:OG1	3:E:83:GLN:HB3	2.10	0.51
4:b:364:ASN:HB3	4:b:387:ILE:HD13	1.93	0.51
2:F:55:ARG:NH1	2:F:56:ALA:O	2.41	0.51
4:a:316:ASP:O	4:a:320:GLN:HG2	2.11	0.51
3:G:181:GLN:HE21	3:G:184:GLY:C	2.19	0.51
1:A:193:MET:HE3	1:A:243:LEU:HD22	1.93	0.51
3:H:83:GLN:NE2	3:H:84:MET:O	2.44	0.51
3:H:92:THR:HG22	3:H:120:ILE:HA	1.93	0.50
4:a:355:ARG:HG2	4:a:355:ARG:HH11	1.76	0.50
2:D:66:SER:OG	2:D:73:THR:OG1	2.29	0.50
3:G:58:LYS:NZ	4:b:395:GLU:OE2	2.38	0.50
3:H:88:ARG:HA	3:H:88:ARG:HH11	1.76	0.50
3:G:70:THR:OG1	3:G:83:GLN:HB3	2.11	0.50
3:E:34:MET:SD	3:E:80:LEU:HD22	2.51	0.50
3:H:18:LEU:H	3:H:84:MET:HB2	1.76	0.50
2:F:32:TYR:OH	3:G:105:SER:O	2.26	0.50
1:A:81:MET:SD	4:a:314:LEU:HD22	2.52	0.50
2:L:137:LEU:HD22	3:H:191:VAL:HG11	1.94	0.50
4:c:411:THR:HA	4:c:414:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LEU:HD23	1:C:221:ILE:HG12	1.93	0.50
3:E:94:ILE:HG22	3:E:118:THR:HG22	1.94	0.50
2:L:144:ARG:NH1	2:L:165:VAL:HG21	2.24	0.50
3:G:102:HIS:HE1	3:G:108:SER:HB3	1.76	0.50
1:B:227:GLU:HB2	1:B:229:HIS:HD2	1.76	0.50
2:F:62:ARG:NH2	2:F:80:GLU:OE1	2.45	0.50
3:G:63:ASP:OD1	3:G:64:VAL:N	2.44	0.50
1:A:94:ILE:HG13	1:A:102:LEU:HB2	1.93	0.49
1:A:121:ASP:HA	1:A:124:LYS:HB3	1.93	0.49
3:H:181:GLN:HE21	3:H:184:GLY:C	2.19	0.49
2:D:21:LEU:HD13	2:D:104:THR:HG21	1.94	0.49
3:G:210:HIS:CD2	3:G:212:PRO:HD2	2.47	0.49
3:E:92:THR:HA	3:E:119:VAL:O	2.12	0.49
1:B:146:PHE:CD2	1:B:148:GLN:HG3	2.47	0.49
3:G:69:PHE:CE1	3:G:84:MET:HG2	2.47	0.49
1:A:87:LYS:HD2	1:A:91:HIS:HD1	1.77	0.49
1:A:155:ASP:HB3	1:A:162:SER:OG	2.12	0.49
1:B:227:GLU:HB2	1:B:229:HIS:CD2	2.47	0.49
2:L:115:PRO:HB3	2:L:141:PHE:HB3	1.95	0.49
2:D:110:ARG:NH2	2:D:111:THR:O	2.45	0.49
3:E:41:PRO:O	3:E:43:ARG:NH1	2.45	0.49
2:F:194:TYR:HB2	2:F:211:PHE:CE1	2.48	0.49
3:G:48:VAL:HG21	3:G:95:TYR:HE1	1.77	0.49
1:C:96:VAL:HG23	1:C:100:THR:HB	1.94	0.48
2:F:32:TYR:CZ	3:G:107:PRO:HG3	2.47	0.48
3:G:157:PRO:HA	3:G:186:TYR:HD2	1.77	0.48
1:C:139:PHE:HB2	1:C:193:MET:HE1	1.94	0.48
1:B:156:PHE:HD1	1:B:161:ILE:HA	1.78	0.48
3:G:95:TYR:CE2	3:G:119:VAL:HG11	2.49	0.48
2:F:90:GLN:NE2	3:G:110:MET:HE1	2.19	0.48
2:L:189:GLU:OE1	2:L:213:ARG:NH2	2.46	0.48
3:H:41:PRO:O	3:H:43:ARG:NH1	2.47	0.48
3:H:157:PRO:HA	3:H:186:TYR:HD2	1.78	0.48
4:a:294:ASN:HA	4:a:297:VAL:HG12	1.96	0.48
3:E:155:TYR:CD2	3:E:186:TYR:HB3	2.49	0.48
4:a:400:ASP:O	4:a:403:GLU:HG3	2.13	0.48
3:E:20:LEU:HD12	3:E:82:LEU:HD23	1.95	0.48
2:L:18:ARG:HA	2:L:76:ILE:O	2.14	0.48
2:L:122:PRO:HD3	2:L:134:VAL:HG12	1.95	0.48
2:L:49:ILE:HD13	2:L:55:ARG:HA	1.96	0.48
4:b:278:CYS:HA	4:b:291:CYS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:96:PRO:HB2	3:G:47:TRP:CE3	2.49	0.47
1:B:146:PHE:HD2	1:B:148:GLN:HG3	1.79	0.47
3:G:92:THR:HA	3:G:119:VAL:O	2.14	0.47
3:E:65:VAL:HA	3:E:68:ARG:HH21	1.79	0.47
3:G:155:TYR:OH	3:G:158:GLU:O	2.23	0.47
3:G:211:LYS:CG	3:G:212:PRO:HD3	2.45	0.47
4:c:358:MET:HG2	4:a:325:LEU:HD11	1.96	0.47
1:B:228:ASP:OD1	1:B:228:ASP:N	2.44	0.47
2:F:29:VAL:HG13	2:F:91:TYR:CE2	2.49	0.47
1:A:81:MET:HE1	4:a:314:LEU:HD13	1.95	0.47
2:L:20:THR:HG22	2:L:75:THR:HG22	1.95	0.47
2:D:24:ARG:NH1	2:D:71:ASP:OD1	2.48	0.47
2:D:130:GLY:HA2	2:D:185:LYS:HE2	1.95	0.47
3:E:39:GLN:HB2	3:E:45:LEU:HD23	1.97	0.47
4:c:367:LYS:HZ3	4:c:385:TRP:CD1	2.33	0.47
4:b:307:GLU:CD	4:b:365:TYR:HE1	2.23	0.47
2:D:178:SER:HB3	3:E:176:PHE:HE2	1.79	0.47
1:A:192:ARG:HH22	4:a:350:MET:HE1	1.79	0.47
3:H:6:GLN:HE22	3:H:115:ARG:HB2	1.79	0.47
3:G:54:ARG:NE	4:b:407:ASP:OD2	2.44	0.47
4:b:398:PHE:HE1	4:b:402:ILE:HD11	1.79	0.47
2:F:6:GLN:HE22	2:F:101:GLY:HA3	1.80	0.47
3:G:103:SER:HB2	4:b:400:ASP:OD2	2.15	0.47
4:c:355:ARG:HD2	4:c:362:TYR:HB3	1.97	0.46
3:H:6:GLN:HE21	3:H:117:ILE:HD11	1.79	0.46
3:G:38:ARG:NE	3:G:46:GLU:OE1	2.42	0.46
3:G:39:GLN:HB3	3:G:94:ILE:HG13	1.95	0.46
4:c:379:THR:HG21	6:c:501:NAG:H82	1.96	0.46
4:c:409:MET:O	4:c:412:GLU:HB2	2.15	0.46
1:A:225:THR:HG23	1:A:227:GLU:HG3	1.97	0.46
1:B:77:LEU:HD21	4:b:315:PHE:HD1	1.80	0.46
3:H:152:VAL:HB	3:H:188:LEU:HD23	1.97	0.46
4:a:261:PHE:HD2	4:a:313:ARG:HH12	1.62	0.46
2:D:34:VAL:HG21	2:D:72:PHE:CZ	2.51	0.46
1:A:163:VAL:HB	1:A:221:ILE:HD13	1.96	0.46
2:F:34:VAL:HG21	2:F:72:PHE:CZ	2.51	0.46
3:G:155:TYR:O	3:G:186:TYR:N	2.48	0.46
4:c:372:ASN:OD1	4:c:373:HIS:N	2.49	0.46
3:E:32:TYR:HE1	4:a:274:PRO:HB3	1.79	0.46
1:A:92:HIS:HB2	1:A:104:LEU:HB2	1.98	0.46
1:B:70:LEU:HD23	4:b:370:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:90:GLN:HE21	2:F:98:TRP:HE3	1.64	0.46
4:c:308:PHE:CD2	4:c:382:PRO:HD2	2.51	0.46
1:C:70:LEU:HD23	4:c:370:TYR:CE2	2.51	0.46
1:A:123:HIS:HA	1:A:128:TYR:CE1	2.51	0.46
1:B:167:LEU:HD11	1:B:219:LEU:HD21	1.98	0.46
3:E:22:CYS:HB3	3:E:80:LEU:CD2	2.45	0.46
1:A:153:SER:OG	1:A:164:GLN:NE2	2.49	0.46
1:A:165:TYR:HB2	1:A:219:LEU:HD21	1.98	0.46
2:L:140:ASN:HA	2:L:174:THR:HG22	1.98	0.46
3:H:181:GLN:N	3:H:181:GLN:OE1	2.49	0.46
1:B:87:LYS:HE2	1:B:87:LYS:HA	1.97	0.46
1:A:195:TRP:HE1	4:a:353:HIS:HA	1.81	0.45
3:G:34:MET:HE1	3:G:73:ARG:CZ	2.46	0.45
1:C:184:ASN:CG	1:C:188:GLN:HE22	2.24	0.45
2:D:134:VAL:HG21	2:D:211:PHE:CE1	2.52	0.45
1:A:87:LYS:HA	1:A:232:PHE:H	1.81	0.45
1:C:183:ALA:O	1:C:187:LEU:HD23	2.16	0.45
2:L:98:TRP:HD1	3:H:47:TRP:CD2	2.34	0.45
2:F:13:LEU:HD23	2:F:13:LEU:HA	1.83	0.45
4:a:309:CYS:O	4:a:313:ARG:HG2	2.17	0.45
2:D:194:TYR:O	2:D:210:SER:OG	2.30	0.45
3:E:36:TRP:HZ3	3:E:95:TYR:HB3	1.81	0.45
2:D:32:TYR:CZ	3:E:107:PRO:HG3	2.52	0.45
3:E:24:ALA:HB1	3:E:27:PHE:CZ	2.52	0.45
1:C:114:HIS:CE1	1:C:153:SER:HG	2.34	0.45
2:D:13:LEU:HD23	2:D:13:LEU:HA	1.87	0.45
3:E:127:LYS:HE3	3:E:185:LEU:HD21	1.97	0.45
3:H:63:ASP:N	3:H:63:ASP:OD1	2.47	0.45
3:E:92:THR:HG23	3:E:121:VAL:HG12	1.98	0.45
2:L:197:GLU:HB2	2:L:208:THR:HG23	1.99	0.45
3:H:36:TRP:CZ3	3:H:95:TYR:HB3	2.52	0.45
3:G:216:LYS:HE3	3:G:216:LYS:HB2	1.87	0.45
1:A:134:SER:HA	1:A:137:SER:HB2	1.97	0.45
3:H:212:PRO:C	3:H:214:ASN:H	2.24	0.45
1:B:156:PHE:HE1	1:B:161:ILE:HG13	1.81	0.45
4:c:355:ARG:HG2	4:c:360:ILE:HB	1.98	0.45
2:L:41:GLY:O	3:H:116:LYS:NZ	2.50	0.44
4:c:262:THR:HG21	4:b:348:LEU:HD22	2.00	0.44
4:c:408:ASN:O	4:c:411:THR:OG1	2.32	0.44
3:H:165:ASN:OD1	3:H:169:LEU:N	2.41	0.44
2:F:144:ARG:HH22	2:F:165:VAL:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:165:VAL:HG12	2:F:166:THR:O	2.17	0.44
3:G:52:THR:O	3:G:73:ARG:NH1	2.48	0.44
3:G:111:ASP:OD1	3:G:112:VAL:HG23	2.18	0.44
1:B:147:ASN:OD1	1:B:149:TYR:N	2.43	0.44
2:F:130:GLY:H	2:F:185:LYS:NZ	2.16	0.44
2:F:168:GLN:HG2	2:F:173:SER:HA	2.00	0.44
4:b:262:THR:HB	4:a:351:LYS:HD2	2.00	0.44
4:b:368:TYR:HA	4:b:384:CYS:HA	1.98	0.44
2:F:195:ALA:HB2	2:F:210:SER:HB2	2.00	0.44
4:a:290:LYS:HB3	6:a:502:NAG:H81	1.99	0.44
4:b:278:CYS:HB3	4:b:291:CYS:HB2	1.83	0.44
4:a:394:ASN:OD1	4:a:395:GLU:N	2.50	0.44
2:D:166:THR:HG22	3:E:177:PRO:HD3	1.99	0.44
3:E:210:HIS:CG	3:E:212:PRO:HD2	2.52	0.44
1:A:133:MET:HE2	1:A:133:MET:HA	1.99	0.44
3:E:178:ALA:HB1	3:E:186:TYR:CD1	2.52	0.44
1:B:102:LEU:HD11	1:B:161:ILE:HD13	1.99	0.44
4:c:355:ARG:HA	4:c:358:MET:HE2	1.98	0.44
1:A:228:ASP:OD1	1:A:228:ASP:N	2.47	0.44
1:A:107:THR:O	1:A:218:TYR:HB2	2.18	0.43
3:H:34:MET:HG2	3:H:80:LEU:HD13	2.00	0.43
3:H:151:LEU:HD23	3:H:152:VAL:N	2.32	0.43
1:A:215:SER:HB3	6:A:302:NAG:H5	1.99	0.43
2:L:6:GLN:NE2	2:L:87:TYR:O	2.51	0.43
4:c:313:ARG:CZ	4:c:313:ARG:HB2	2.48	0.43
4:c:367:LYS:HB2	4:c:367:LYS:HE2	1.79	0.43
4:a:355:ARG:HG2	4:a:355:ARG:NH1	2.32	0.43
2:F:110:ARG:NH2	2:F:173:SER:OG	2.52	0.43
4:b:339:ALA:HB2	4:a:354:LEU:HD11	2.01	0.43
3:G:145:THR:HA	3:G:195:PRO:HA	2.00	0.43
3:E:162:VAL:HA	3:E:207:ASN:O	2.19	0.43
1:A:167:LEU:HB2	1:A:217:GLN:C	2.43	0.43
3:H:47:TRP:HE1	3:H:49:SER:C	2.26	0.43
4:b:400:ASP:HA	4:b:403:GLU:HG3	2.01	0.43
1:B:163:VAL:HB	1:B:221:ILE:HG13	2.01	0.43
2:D:144:ARG:HH12	2:D:165:VAL:HG21	1.83	0.43
2:L:21:LEU:HD12	2:L:87:TYR:HD2	1.84	0.43
1:B:91:HIS:O	1:B:92:HIS:ND1	2.52	0.43
1:B:134:SER:OG	4:b:333:ILE:HD11	2.18	0.43
4:a:324:ARG:C	4:a:325:LEU:HD12	2.44	0.43
1:C:105:THR:O	1:C:219:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:PHE:HD1	1:C:161:ILE:HA	1.84	0.43
3:E:32:TYR:CE1	3:E:101:ARG:HD3	2.53	0.43
1:B:107:THR:HG22	1:B:109:THR:H	1.84	0.43
2:F:193:VAL:HG22	2:F:212:ASN:OD1	2.18	0.43
1:C:72:LEU:HD23	1:C:72:LEU:HA	1.90	0.43
2:D:90:GLN:HA	2:D:99:ALA:O	2.19	0.43
2:L:194:TYR:HB2	2:L:211:PHE:CE1	2.53	0.43
4:b:308:PHE:CE2	4:b:312:LEU:HD11	2.54	0.43
1:C:195:TRP:HH2	4:c:352:ASN:HB3	1.84	0.43
3:G:92:THR:HG22	3:G:121:VAL:H	1.83	0.43
4:b:401:ASP:O	4:b:404:GLN:HG2	2.19	0.43
4:b:411:THR:HA	4:b:414:LEU:HD13	2.01	0.43
2:L:29:VAL:HG13	2:L:91:TYR:CE1	2.54	0.42
3:G:211:LYS:HG3	3:G:212:PRO:HD3	2.01	0.42
4:a:290:LYS:HD3	6:a:502:NAG:H81	2.00	0.42
1:C:190:PHE:HZ	1:C:219:LEU:CD1	2.33	0.42
2:L:141:PHE:CE1	2:L:175:TYR:HB2	2.54	0.42
3:H:20:LEU:HD12	3:H:82:LEU:HD23	2.00	0.42
1:C:186:VAL:O	1:C:189:THR:OG1	2.32	0.42
2:D:34:VAL:HG21	2:D:72:PHE:HZ	1.83	0.42
2:D:54:SER:OG	2:D:55:ARG:N	2.52	0.42
2:L:95:SER:HA	2:L:96:PRO:HA	1.87	0.42
3:H:62:ALA:HB3	3:H:65:VAL:HG22	2.01	0.42
4:b:410:ILE:H	4:b:410:ILE:HD12	1.83	0.42
1:C:124:LYS:HG3	1:B:149:TYR:HE2	1.84	0.42
3:H:77:LYS:HG3	3:H:79:SER:HB2	2.02	0.42
2:F:95:SER:HA	2:F:96:PRO:HA	1.89	0.42
3:E:9:GLY:CA	3:E:118:THR:O	2.64	0.42
1:A:134:SER:O	1:A:138:THR:HG22	2.20	0.42
3:H:219:LYS:HA	3:H:219:LYS:HD2	1.79	0.42
1:C:124:LYS:HG3	1:B:149:TYR:CE2	2.55	0.42
2:L:63:PHE:HD1	2:L:76:ILE:HG12	1.84	0.42
2:L:110:ARG:NH2	2:L:172:ASP:O	2.49	0.42
3:H:126:THR:HA	3:H:156:PHE:CD1	2.53	0.42
4:a:301:ASN:OD1	4:a:313:ARG:NH2	2.52	0.42
3:H:32:TYR:HD2	3:H:99:ARG:NE	2.15	0.42
2:D:15:PRO:HA	2:D:79:LEU:HB2	2.02	0.42
2:D:32:TYR:OH	3:E:105:SER:O	2.38	0.42
2:F:29:VAL:HG13	2:F:91:TYR:HE2	1.85	0.42
2:F:110:ARG:HG2	2:F:111:THR:N	2.35	0.42
1:A:187:LEU:HD11	1:A:214:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:210:HIS:NE2	3:G:212:PRO:HG2	2.35	0.42
4:b:401:ASP:HA	4:b:404:GLN:HG2	2.01	0.42
3:E:18:LEU:H	3:E:84:MET:HB2	1.85	0.42
3:G:95:TYR:HE2	3:G:119:VAL:HG11	1.85	0.42
4:b:367:LYS:HD3	4:b:392:TYR:CE2	2.54	0.42
1:C:78:ASN:HB2	5:I:1:NAG:O5	2.18	0.41
3:H:205:ILE:HD12	3:H:220:ARG:HG2	2.02	0.41
3:G:11:LEU:HD11	3:G:122:SER:HB3	2.01	0.41
4:c:369:TRP:CH2	4:c:402:ILE:HD13	2.55	0.41
4:b:369:TRP:CH2	4:b:402:ILE:HD13	2.55	0.41
1:C:123:HIS:HA	1:C:128:TYR:CE1	2.55	0.41
1:C:153:SER:HB3	1:C:164:GLN:HE21	1.84	0.41
3:E:34:MET:SD	3:E:80:LEU:HD13	2.61	0.41
2:L:39:HIS:O	2:L:85:ALA:HB1	2.20	0.41
3:H:156:PHE:HD2	3:H:158:GLU:HB2	1.85	0.41
1:B:137:SER:HA	1:B:140:HIS:HE1	1.78	0.41
1:B:210:ASP:OD1	1:B:210:ASP:N	2.53	0.41
4:b:314:LEU:HD23	4:b:314:LEU:HA	1.76	0.41
1:C:138:THR:HG21	1:C:240:TYR:HE1	1.85	0.41
3:H:36:TRP:CH2	3:H:97:CYS:HB3	2.56	0.41
4:c:283:MET:SD	4:c:283:MET:N	2.94	0.41
4:c:350:MET:HE2	4:c:350:MET:HB2	1.84	0.41
4:b:354:LEU:HA	4:b:357:ILE:HG22	2.03	0.41
1:A:91:HIS:NE2	1:A:103:GLU:HG3	2.35	0.41
1:C:86:THR:HG22	1:C:194:ALA:HB1	2.01	0.41
2:D:187:ASP:OD1	2:D:190:LYS:NZ	2.42	0.41
3:E:69:PHE:HE1	3:E:84:MET:SD	2.43	0.41
3:G:103:SER:OG	3:G:104:THR:N	2.54	0.41
1:C:135:ILE:O	1:C:138:THR:HG22	2.20	0.41
2:L:6:GLN:OE1	2:L:103:GLY:N	2.53	0.41
3:H:53:SER:OG	4:a:403:GLU:OE2	2.37	0.41
1:B:195:TRP:CH2	4:b:365:TYR:HE2	2.38	0.41
3:G:92:THR:HG23	3:G:121:VAL:HG12	2.02	0.41
4:a:283:MET:HE2	4:a:315:PHE:CG	2.56	0.41
1:C:156:PHE:CE1	1:C:161:ILE:HG13	2.55	0.41
1:A:85:CYS:HB3	1:A:235:PRO:HB3	2.03	0.41
1:A:121:ASP:OD2	6:A:305:NAG:N2	2.54	0.41
1:A:153:SER:HB3	1:A:164:GLN:HG2	2.02	0.41
3:G:34:MET:CB	3:G:80:LEU:HD21	2.49	0.41
1:C:90:SER:O	1:C:106:LEU:N	2.43	0.41
1:C:242:GLY:HA3	4:c:349:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:LEU:HD21	3:E:191:VAL:HG11	2.03	0.41
2:D:144:ARG:CZ	2:D:165:VAL:HG11	2.50	0.41
2:D:197:GLU:HB2	2:D:208:THR:HG23	2.02	0.41
3:E:36:TRP:CZ3	3:E:95:TYR:HB3	2.56	0.41
1:A:219:LEU:HD23	1:A:219:LEU:H	1.85	0.41
3:H:13:ARG:HB2	3:H:13:ARG:CZ	2.51	0.41
1:B:87:LYS:HZ1	1:B:232:PHE:N	2.18	0.41
1:B:147:ASN:OD1	1:B:148:GLN:N	2.54	0.41
1:B:164:GLN:HA	1:B:219:LEU:O	2.21	0.41
3:G:6:GLN:HE22	3:G:114:GLY:HA3	1.84	0.41
3:G:6:GLN:NE2	3:G:115:ARG:H	2.19	0.41
3:G:181:GLN:N	3:G:181:GLN:OE1	2.53	0.41
4:c:281:ARG:HB3	4:c:289:LEU:N	2.36	0.41
4:c:339:ALA:HB2	4:b:354:LEU:HD11	2.02	0.41
3:H:92:THR:HA	3:H:119:VAL:O	2.21	0.41
4:c:350:MET:HG3	4:c:354:LEU:HD23	2.02	0.41
4:a:354:LEU:O	4:a:358:MET:HG3	2.21	0.41
2:D:97:LEU:HB2	3:E:47:TRP:CH2	2.56	0.40
3:G:126:THR:HA	3:G:156:PHE:CD1	2.56	0.40
1:C:77:LEU:HD21	4:c:315:PHE:HD1	1.86	0.40
2:D:193:VAL:HG22	2:D:212:ASN:OD1	2.21	0.40
4:a:367:LYS:HG2	4:a:392:TYR:HE2	1.86	0.40
1:C:106:LEU:HD21	1:C:190:PHE:CE2	2.56	0.40
1:A:160:LYS:HG2	6:A:304:NAG:H3	2.03	0.40
3:H:160:VAL:HB	3:H:209:ASN:O	2.21	0.40
2:F:47:LEU:HD21	2:F:50:TYR:HB3	2.03	0.40
2:F:144:ARG:HH22	2:F:165:VAL:HG11	1.85	0.40
1:C:79:MET:SD	1:C:79:MET:N	2.94	0.40
3:H:12:VAL:HG22	3:H:120:ILE:O	2.22	0.40
2:F:164:SER:HA	3:G:179:VAL:HG11	2.04	0.40
4:b:362:TYR:CZ	4:b:387:ILE:HD11	2.56	0.40
4:b:385:TRP:HE1	4:b:392:TYR:HB3	1.87	0.40
2:D:194:TYR:HB2	2:D:211:PHE:CZ	2.56	0.40
2:L:50:TYR:O	2:L:54:SER:HB3	2.21	0.40
3:H:181:GLN:HG2	3:H:184:GLY:H	1.86	0.40
2:F:6:GLN:OE1	2:F:6:GLN:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	149/258 (58%)	139 (93%)	10 (7%)	0	100	100
1	B	149/258 (58%)	136 (91%)	13 (9%)	0	100	100
1	C	149/258 (58%)	137 (92%)	12 (8%)	0	100	100
2	D	201/237 (85%)	187 (93%)	14 (7%)	0	100	100
2	F	201/237 (85%)	188 (94%)	13 (6%)	0	100	100
2	L	201/237 (85%)	188 (94%)	13 (6%)	0	100	100
3	E	211/249 (85%)	203 (96%)	8 (4%)	0	100	100
3	G	211/249 (85%)	196 (93%)	15 (7%)	0	100	100
3	H	211/249 (85%)	200 (95%)	11 (5%)	0	100	100
4	a	147/206 (71%)	142 (97%)	5 (3%)	0	100	100
4	b	147/206 (71%)	143 (97%)	4 (3%)	0	100	100
4	c	147/206 (71%)	136 (92%)	11 (8%)	0	100	100
All	All	2124/2850 (74%)	1995 (94%)	129 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	143/225 (64%)	143 (100%)	0	100	100
1	B	143/225 (64%)	143 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	143/225 (64%)	143 (100%)	0	100	100
2	D	176/204 (86%)	176 (100%)	0	100	100
2	F	176/204 (86%)	176 (100%)	0	100	100
2	L	176/204 (86%)	176 (100%)	0	100	100
3	E	181/212 (85%)	181 (100%)	0	100	100
3	G	181/212 (85%)	181 (100%)	0	100	100
3	H	181/212 (85%)	181 (100%)	0	100	100
4	a	137/178 (77%)	137 (100%)	0	100	100
4	b	137/178 (77%)	137 (100%)	0	100	100
4	c	137/178 (77%)	137 (100%)	0	100	100
All	All	1911/2457 (78%)	1911 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	157	ASN
1	C	188	GLN
3	E	6	GLN
3	E	35	ASN
3	E	83	GLN
2	L	149	GLN
3	H	6	GLN
3	H	75	ASN
3	H	102	HIS
3	H	207	ASN
1	B	229	HIS
2	F	38	GLN
2	F	90	GLN
3	G	35	ASN
3	G	207	ASN
4	c	337	ASN
4	c	353	HIS
4	b	337	ASN
4	b	404	GLN
4	b	408	ASN
4	a	352	ASN

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Mol	Chain	Res	Type
4	a	373	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 ⓘ

8 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	$\# Z > 2$
5	NAG	I	1	1,5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	I	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	J	1	1,5	14,14,15	0.27	0	17,19,21	0.41	0
5	NAG	J	2	5	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	K	1	1,5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	K	2	5	14,14,15	0.18	0	17,19,21	0.42	0
5	NAG	M	1	1,5	14,14,15	0.37	0	17,19,21	0.41	0
5	NAG	M	2	5	14,14,15	0.50	0	17,19,21	1.36	2 (11%)

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	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	2	NAG	C2-N2-C7	4.52	128.96	122.90
5	M	2	NAG	C1-C2-N2	2.28	114.03	110.43

There are no chirality outliers.

All (18) torsion outliers are listed below:

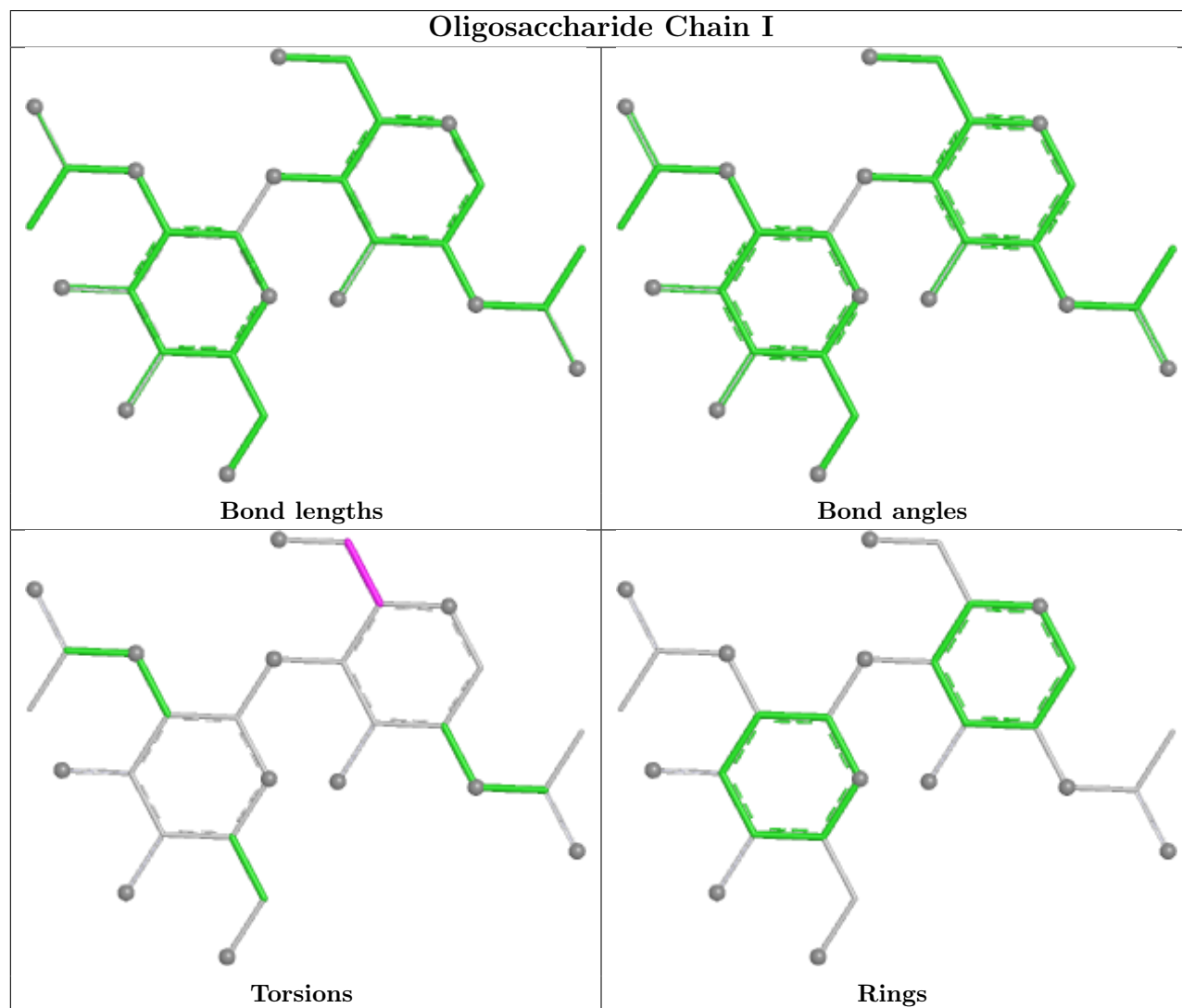
Mol	Chain	Res	Type	Atoms
5	J	2	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	J	1	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	M	2	NAG	C1-C2-N2-C7
5	M	2	NAG	C3-C2-N2-C7
5	I	1	NAG	O5-C5-C6-O6

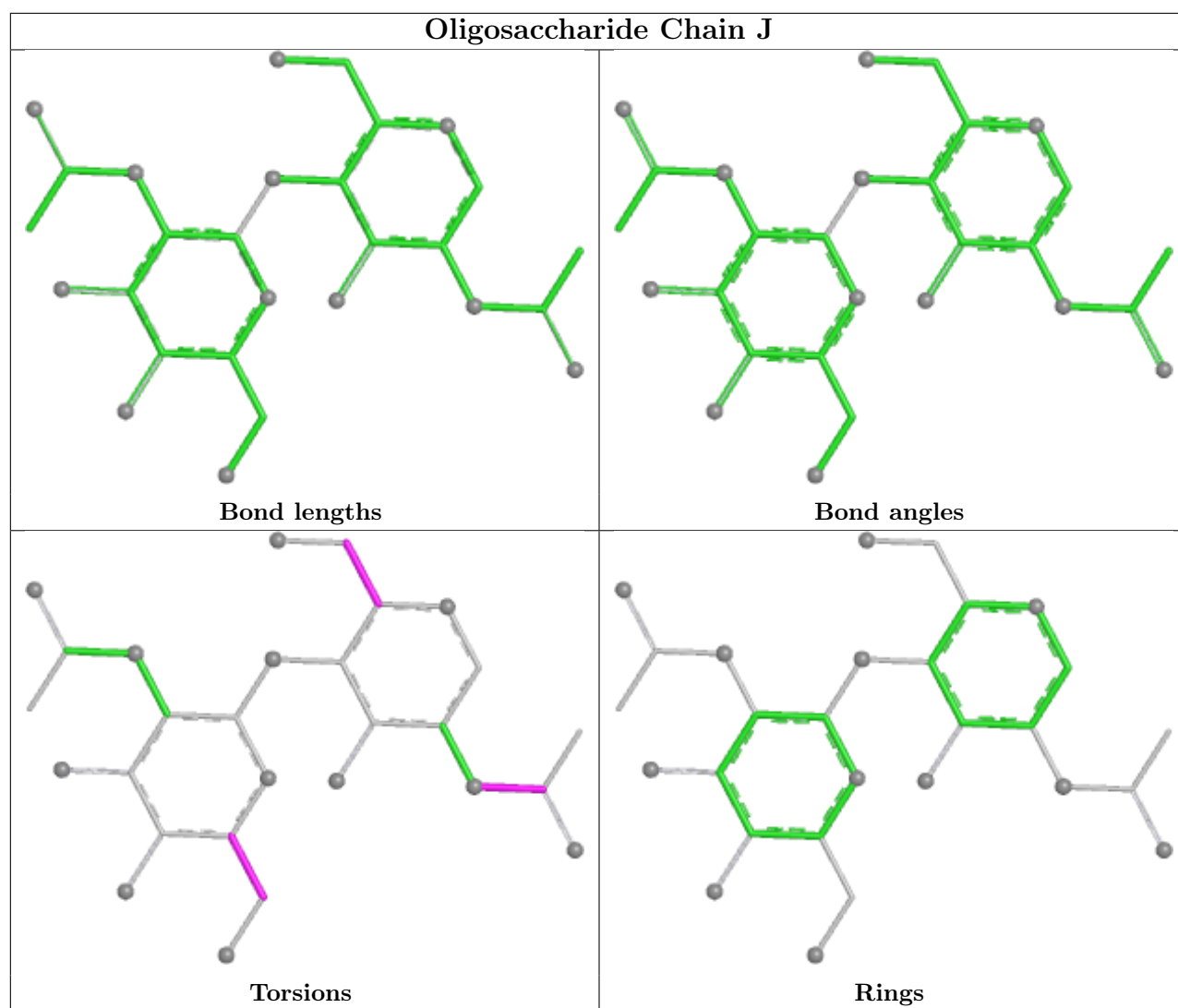
There are no ring outliers.

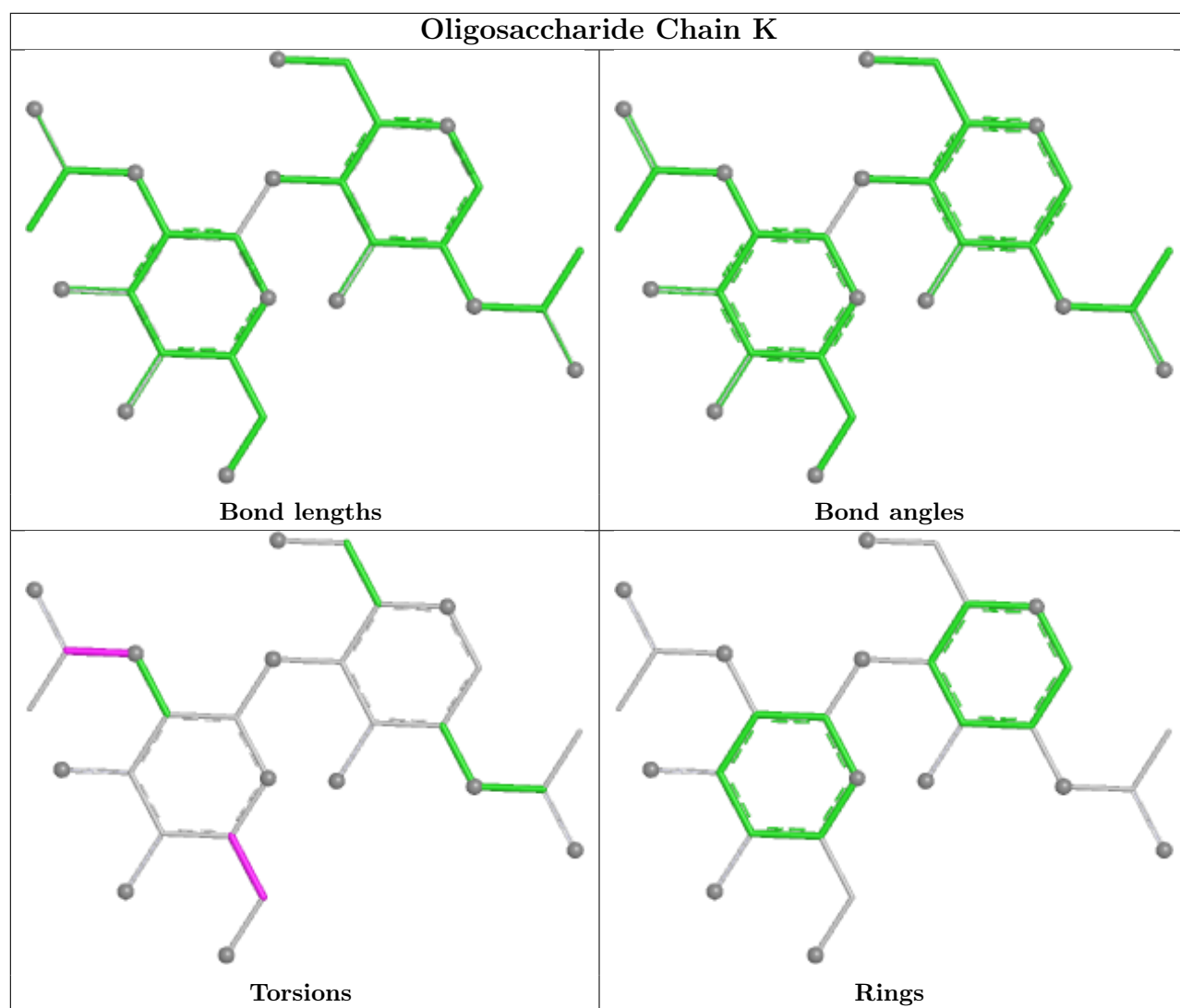
2 monomers are involved in 2 short contacts:

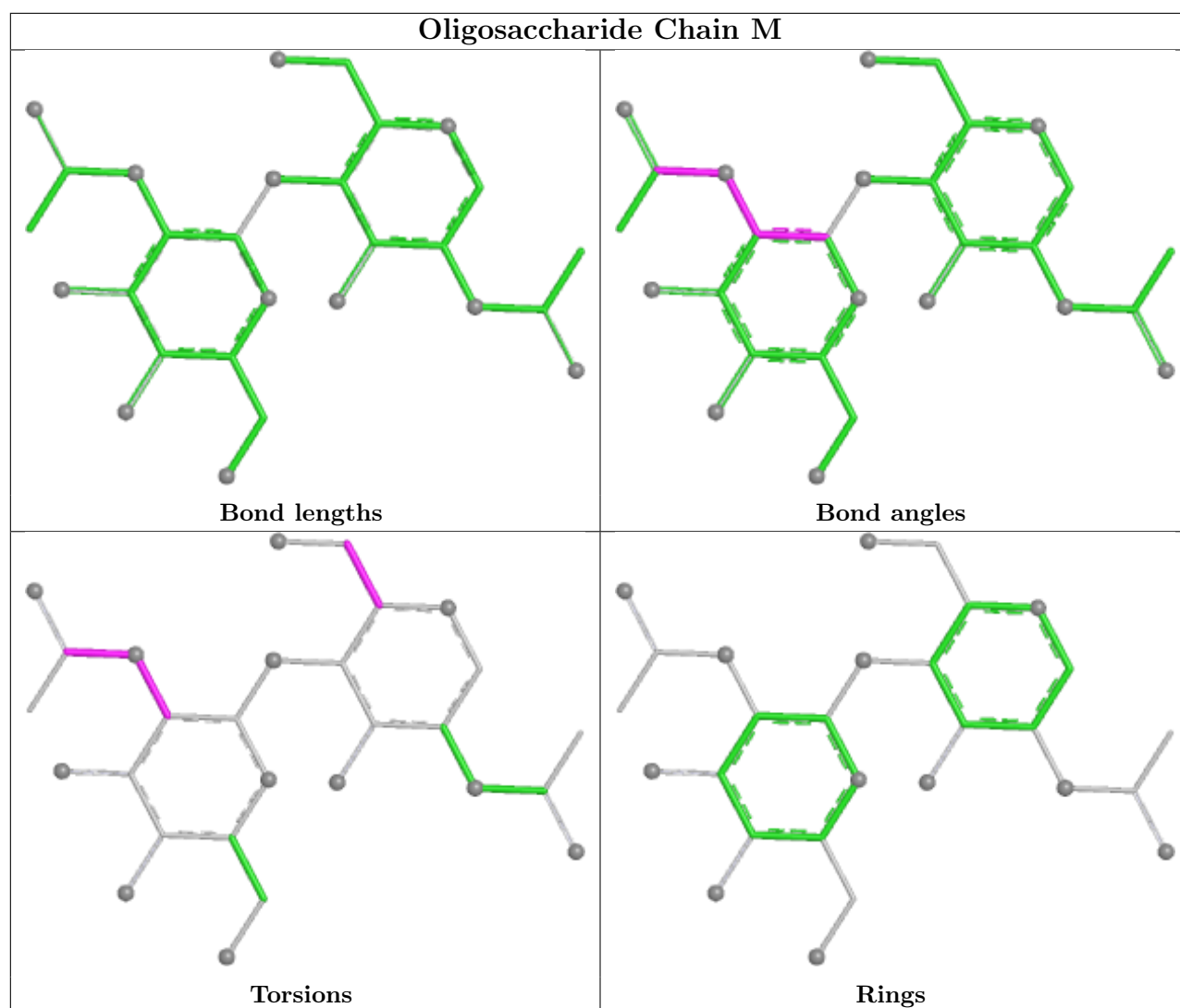
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	2	NAG	1	0
5	I	1	NAG	1	0

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](#)

22 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	$\# Z > 2$
6	NAG	A	304	1	14,14,15	0.30	0	17,19,21	0.58	0
6	NAG	a	501	4	14,14,15	0.31	0	17,19,21	0.60	0
6	NAG	C	304	1	14,14,15	0.25	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	b	502	4	14,14,15	0.24	0	17,19,21	0.58	0
6	NAG	A	305	1	14,14,15	0.39	0	17,19,21	0.59	0
6	NAG	C	302	1	14,14,15	0.19	0	17,19,21	0.45	0
6	NAG	b	503	4	14,14,15	0.32	0	17,19,21	1.36	2 (11%)
6	NAG	B	301	1	14,14,15	0.20	0	17,19,21	0.46	0
6	NAG	c	503	4	14,14,15	0.18	0	17,19,21	0.41	0
6	NAG	b	501	4	14,14,15	0.14	0	17,19,21	0.46	0
6	NAG	c	501	4	14,14,15	0.16	0	17,19,21	0.44	0
6	NAG	A	303	1	14,14,15	0.27	0	17,19,21	0.42	0
6	NAG	a	503	4	14,14,15	0.67	0	17,19,21	0.75	1 (5%)
6	NAG	C	303	1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	C	301	1	14,14,15	0.20	0	17,19,21	0.40	0
6	NAG	B	302	1	14,14,15	0.26	0	17,19,21	0.38	0
6	NAG	a	502	4	14,14,15	0.17	0	17,19,21	0.43	0
6	NAG	A	302	1	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	C	305	1	14,14,15	0.30	0	17,19,21	0.59	0
6	NAG	A	301	1	14,14,15	0.19	0	17,19,21	0.43	0
6	NAG	B	303	1	14,14,15	0.31	0	17,19,21	0.62	1 (5%)
6	NAG	c	502	4	14,14,15	0.23	0	17,19,21	0.53	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
6	NAG	A	304	1	-	0/6/23/26	0/1/1/1
6	NAG	a	501	4	-	3/6/23/26	0/1/1/1
6	NAG	C	304	1	-	4/6/23/26	0/1/1/1
6	NAG	b	502	4	-	4/6/23/26	0/1/1/1
6	NAG	A	305	1	-	4/6/23/26	0/1/1/1
6	NAG	C	302	1	-	2/6/23/26	0/1/1/1
6	NAG	b	503	4	-	6/6/23/26	0/1/1/1
6	NAG	B	301	1	-	2/6/23/26	0/1/1/1
6	NAG	c	503	4	-	0/6/23/26	0/1/1/1
6	NAG	b	501	4	-	2/6/23/26	0/1/1/1
6	NAG	c	501	4	-	2/6/23/26	0/1/1/1
6	NAG	A	303	1	-	2/6/23/26	0/1/1/1
6	NAG	a	503	4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	303	1	-	4/6/23/26	0/1/1/1
6	NAG	C	301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	302	1	-	0/6/23/26	0/1/1/1
6	NAG	a	502	4	-	2/6/23/26	0/1/1/1
6	NAG	A	302	1	-	2/6/23/26	0/1/1/1
6	NAG	C	305	1	-	4/6/23/26	0/1/1/1
6	NAG	A	301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	303	1	-	2/6/23/26	0/1/1/1
6	NAG	c	502	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	b	503	NAG	C2-N2-C7	4.64	129.12	122.90
6	a	503	NAG	C1-O5-C5	2.34	115.32	112.19
6	b	503	NAG	C1-C2-N2	2.27	114.01	110.43
6	B	303	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	302	NAG	O5-C5-C6-O6
6	a	503	NAG	O5-C5-C6-O6
6	A	302	NAG	O5-C5-C6-O6
6	a	502	NAG	O5-C5-C6-O6
6	C	303	NAG	O5-C5-C6-O6
6	A	305	NAG	O5-C5-C6-O6
6	C	304	NAG	C4-C5-C6-O6
6	C	305	NAG	C4-C5-C6-O6
6	C	302	NAG	C4-C5-C6-O6
6	b	503	NAG	O5-C5-C6-O6
6	b	503	NAG	C4-C5-C6-O6
6	a	503	NAG	C4-C5-C6-O6
6	A	302	NAG	C4-C5-C6-O6
6	A	305	NAG	C4-C5-C6-O6
6	C	304	NAG	O5-C5-C6-O6
6	a	502	NAG	C4-C5-C6-O6

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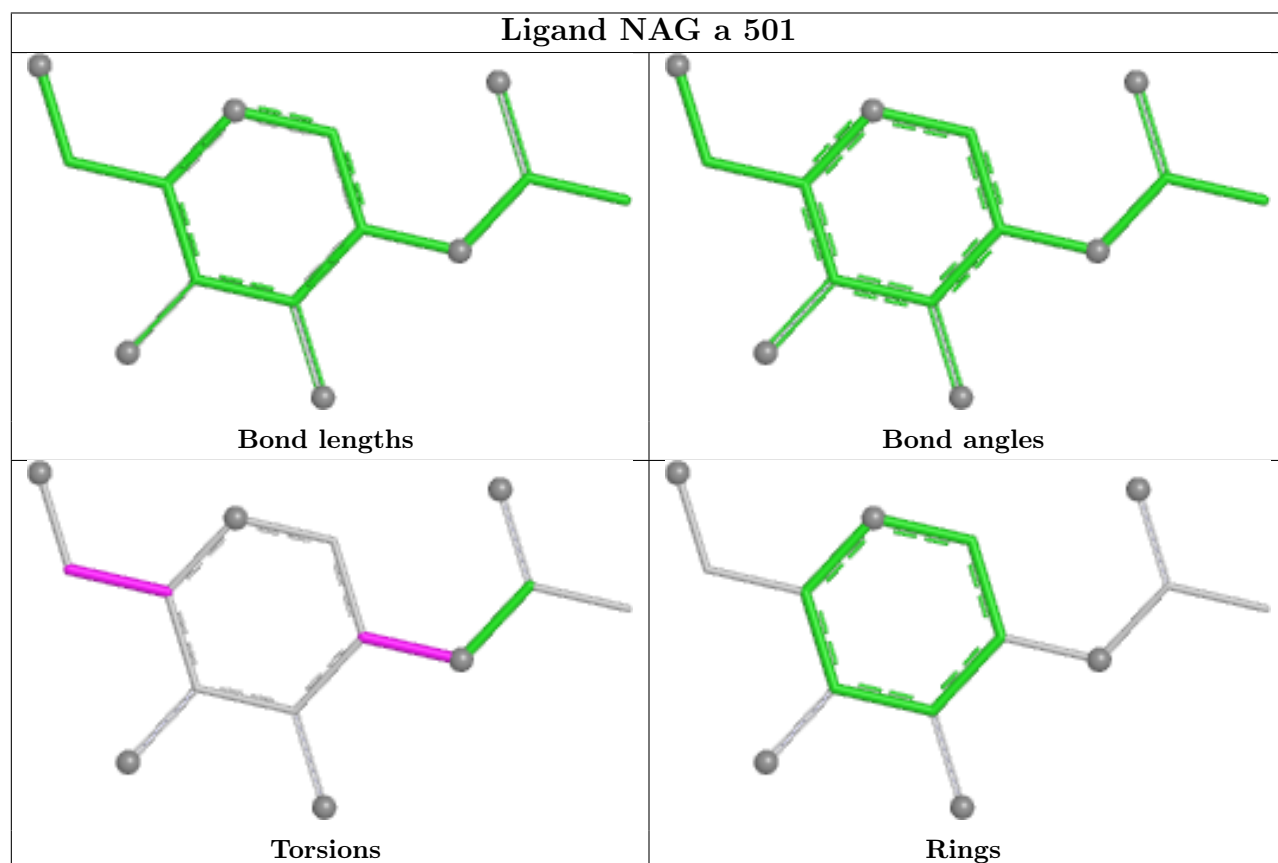
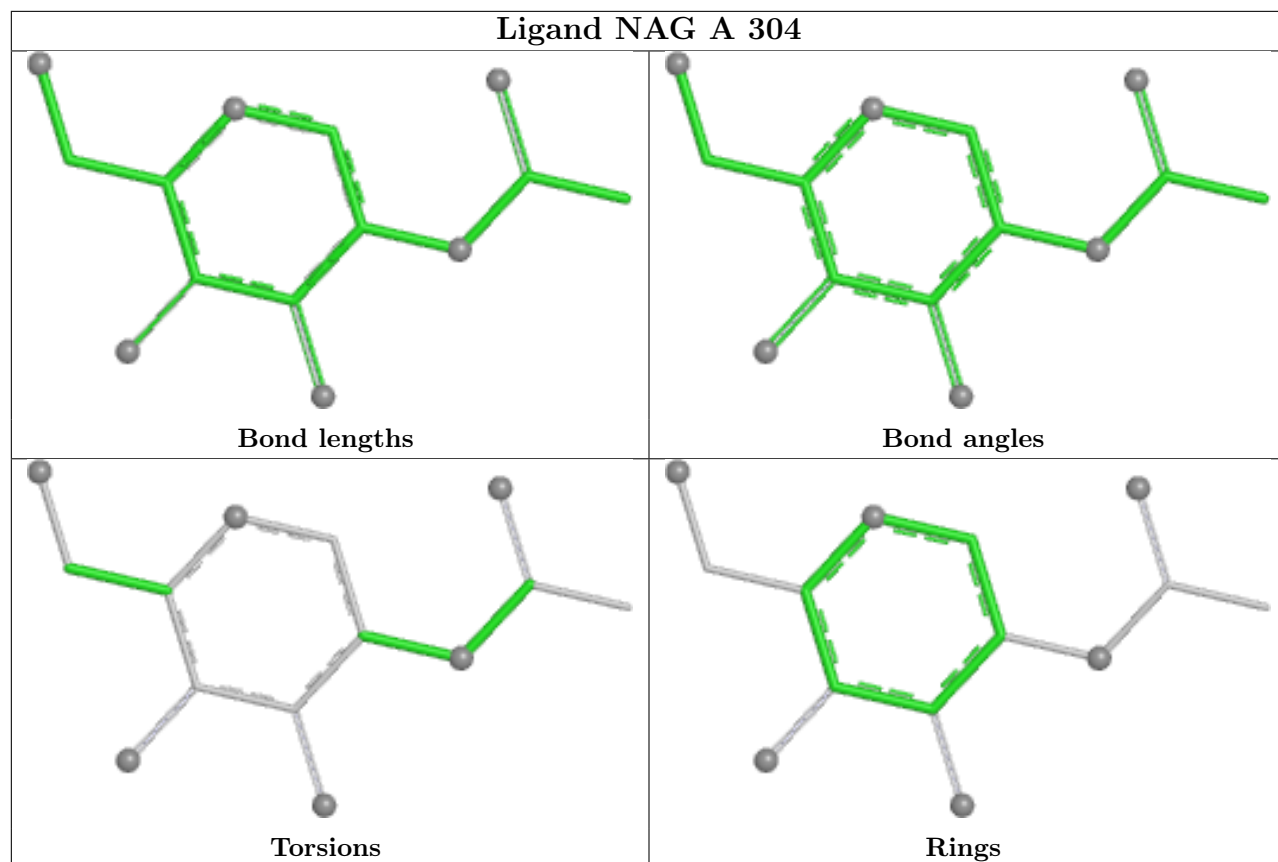
Mol	Chain	Res	Type	Atoms
6	C	305	NAG	O5-C5-C6-O6
6	c	502	NAG	C4-C5-C6-O6
6	C	303	NAG	C8-C7-N2-C2
6	C	303	NAG	O7-C7-N2-C2
6	C	304	NAG	C8-C7-N2-C2
6	C	304	NAG	O7-C7-N2-C2
6	A	303	NAG	C8-C7-N2-C2
6	A	303	NAG	O7-C7-N2-C2
6	B	301	NAG	C8-C7-N2-C2
6	B	301	NAG	O7-C7-N2-C2
6	b	503	NAG	C8-C7-N2-C2
6	b	503	NAG	O7-C7-N2-C2
6	A	301	NAG	O5-C5-C6-O6
6	C	301	NAG	O5-C5-C6-O6
6	C	303	NAG	C4-C5-C6-O6
6	A	301	NAG	C4-C5-C6-O6
6	B	303	NAG	C4-C5-C6-O6
6	c	502	NAG	O5-C5-C6-O6
6	c	501	NAG	O5-C5-C6-O6
6	B	303	NAG	O5-C5-C6-O6
6	b	502	NAG	C4-C5-C6-O6
6	a	501	NAG	O5-C5-C6-O6
6	C	305	NAG	C1-C2-N2-C7
6	c	502	NAG	C1-C2-N2-C7
6	b	502	NAG	O5-C5-C6-O6
6	b	501	NAG	C4-C5-C6-O6
6	C	305	NAG	C3-C2-N2-C7
6	A	305	NAG	C3-C2-N2-C7
6	c	502	NAG	C3-C2-N2-C7
6	b	502	NAG	C3-C2-N2-C7
6	a	501	NAG	C3-C2-N2-C7
6	C	301	NAG	C4-C5-C6-O6
6	b	501	NAG	O5-C5-C6-O6
6	c	501	NAG	C4-C5-C6-O6
6	A	305	NAG	C1-C2-N2-C7
6	b	502	NAG	C1-C2-N2-C7
6	b	503	NAG	C1-C2-N2-C7
6	a	501	NAG	C1-C2-N2-C7
6	b	503	NAG	C3-C2-N2-C7
6	a	503	NAG	C3-C2-N2-C7

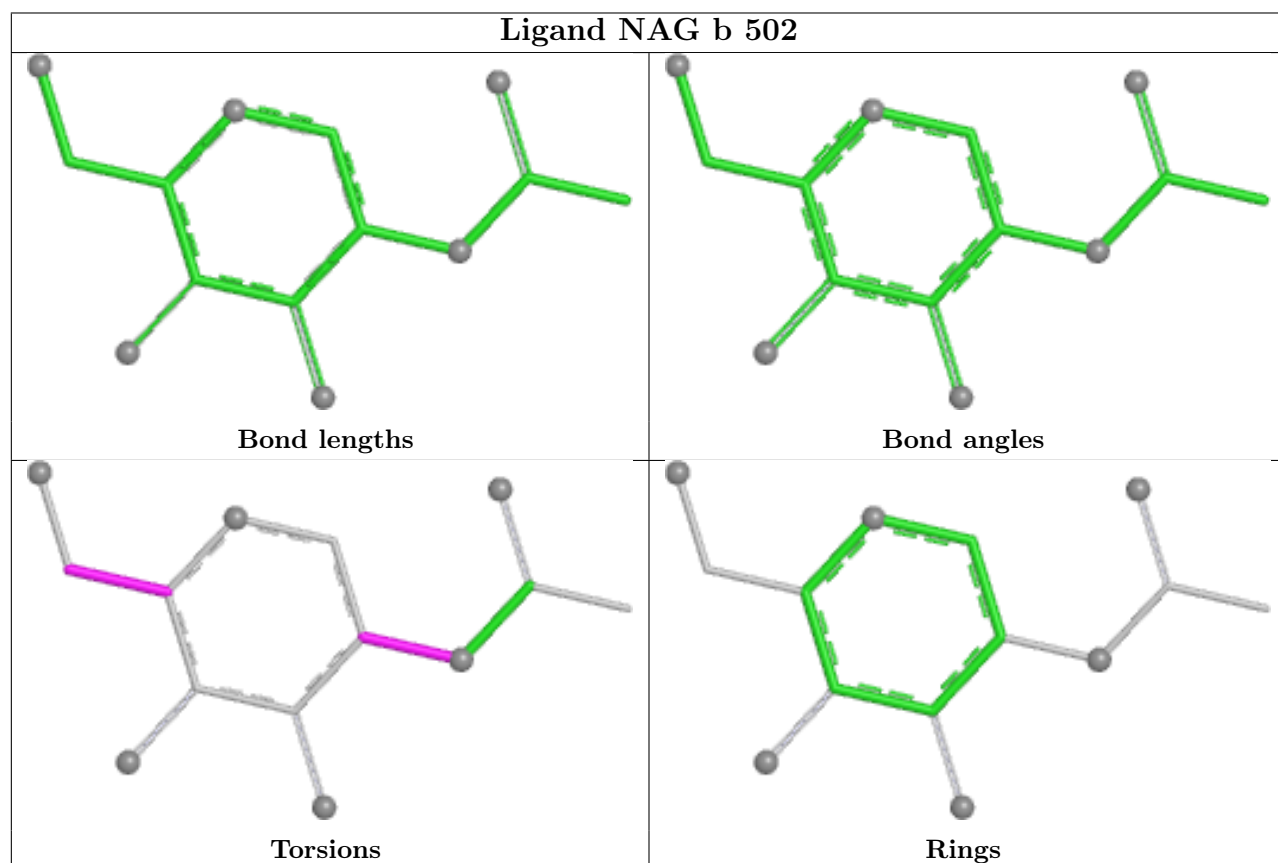
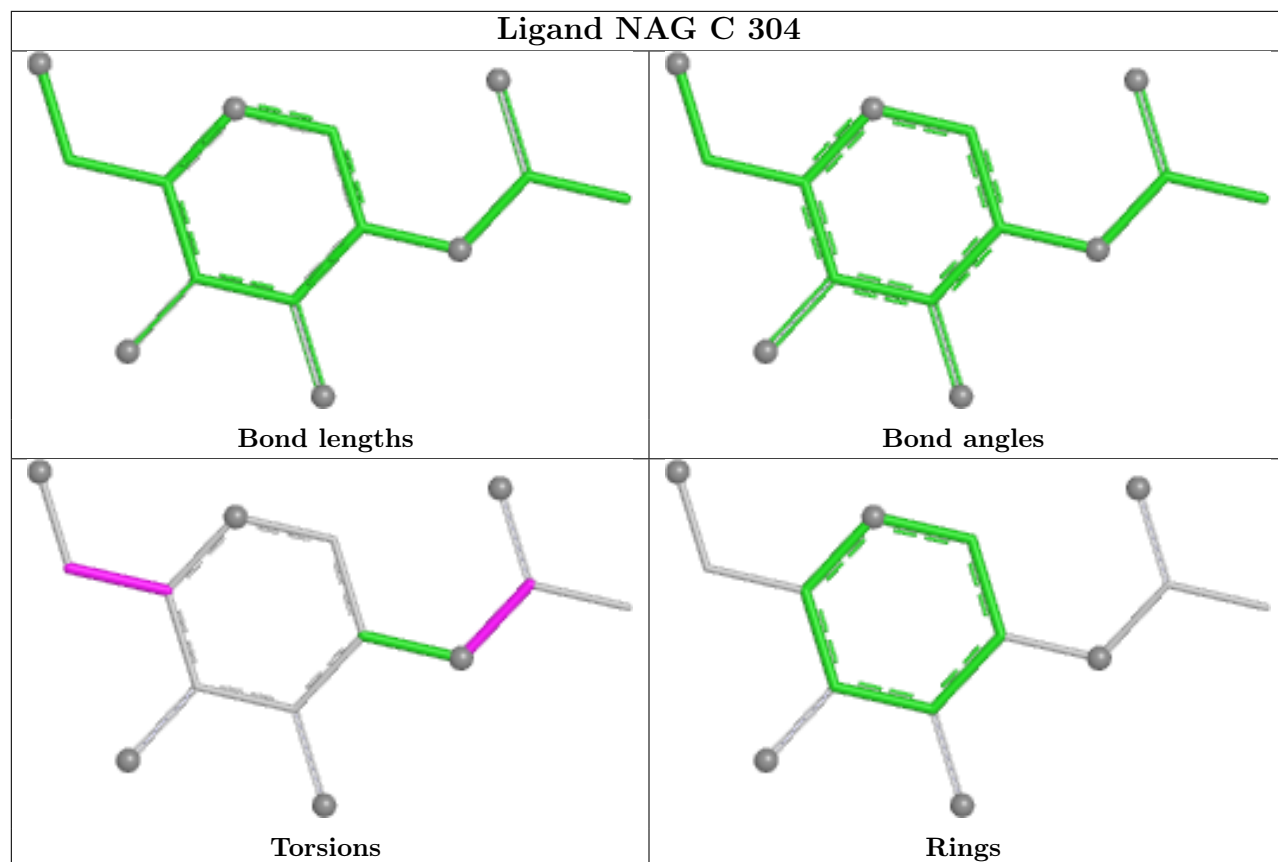
There are no ring outliers.

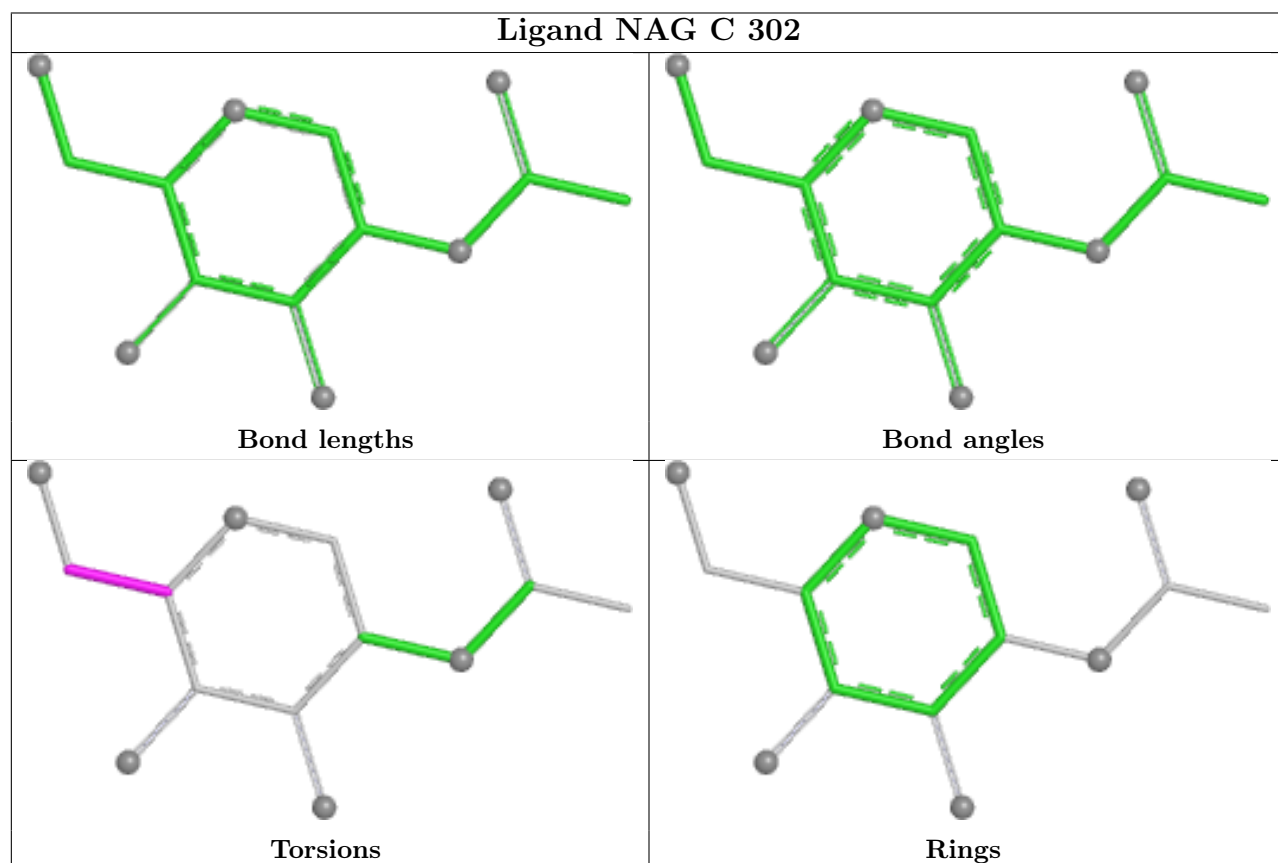
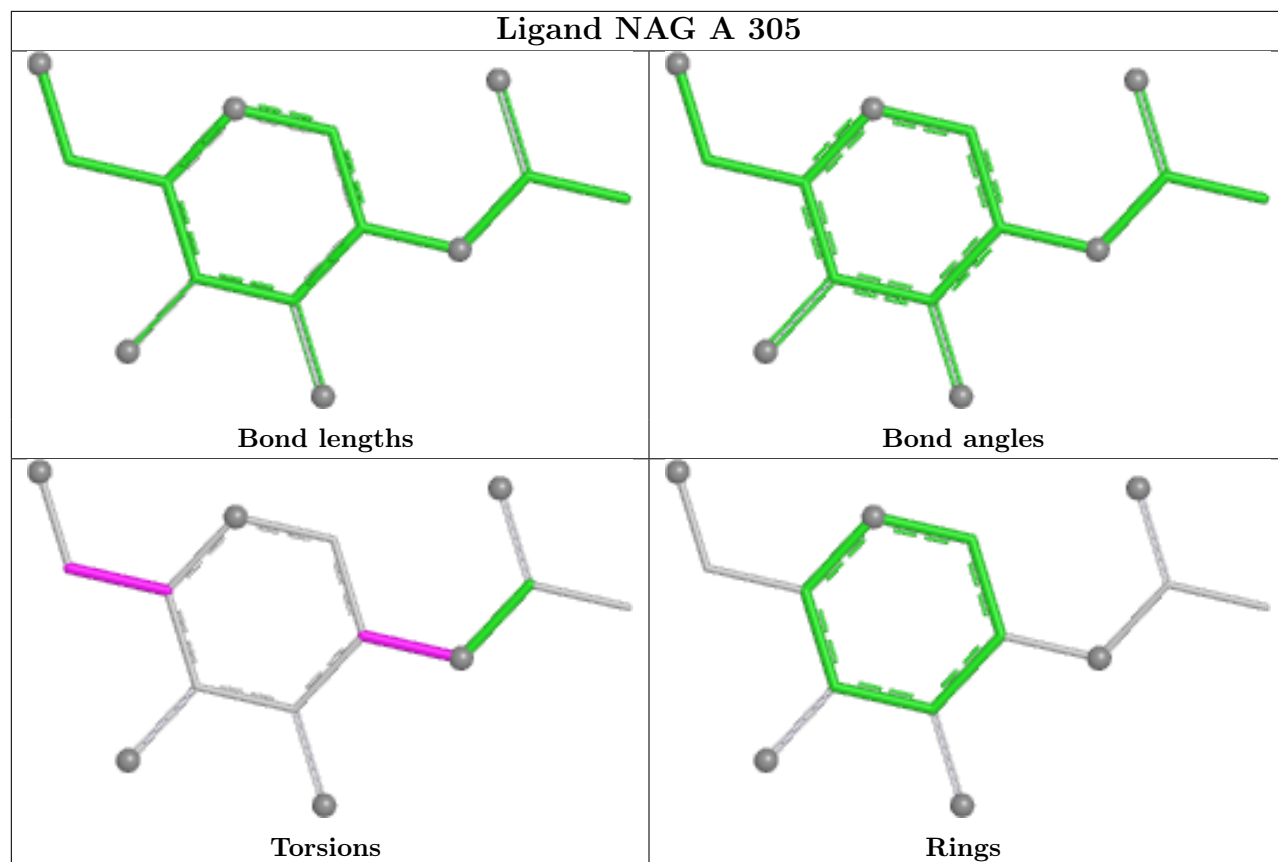
10 monomers are involved in 12 short contacts:

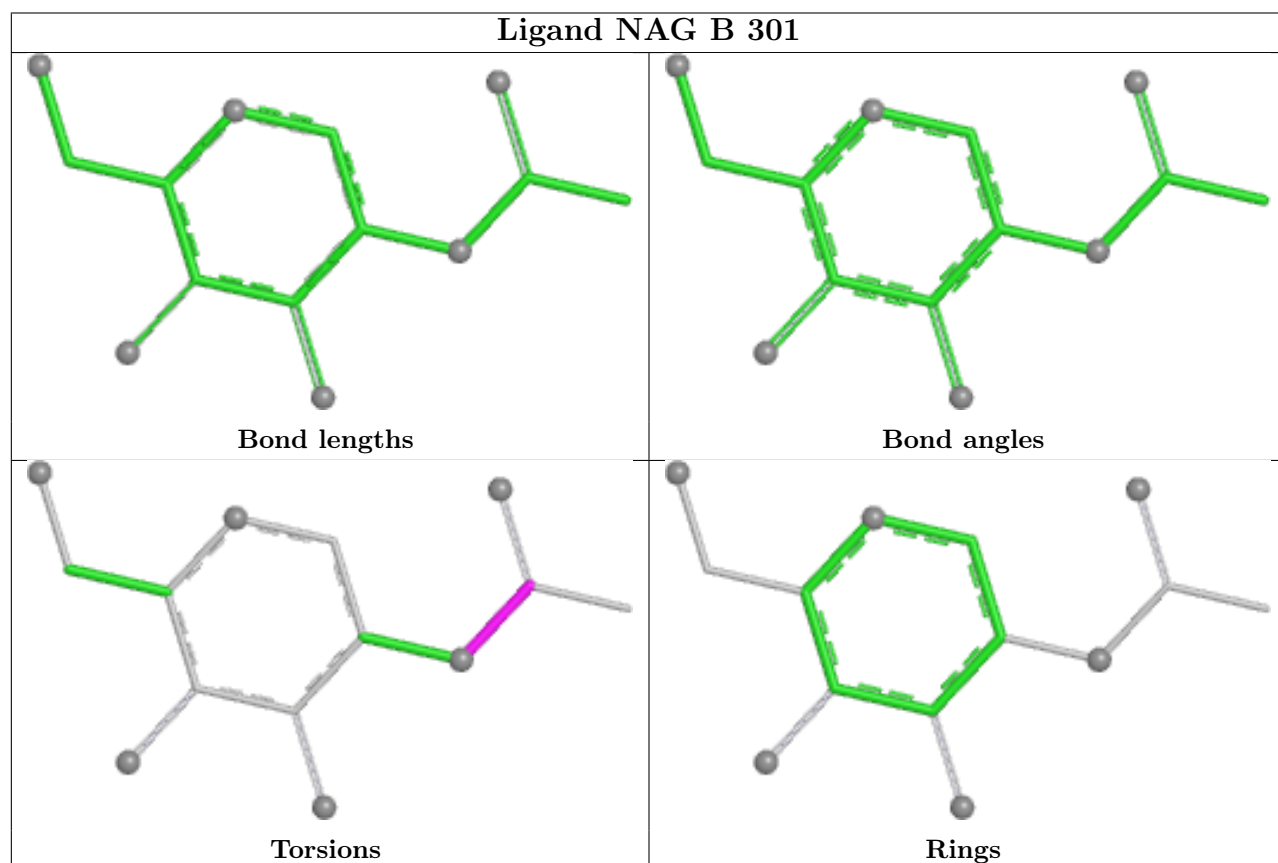
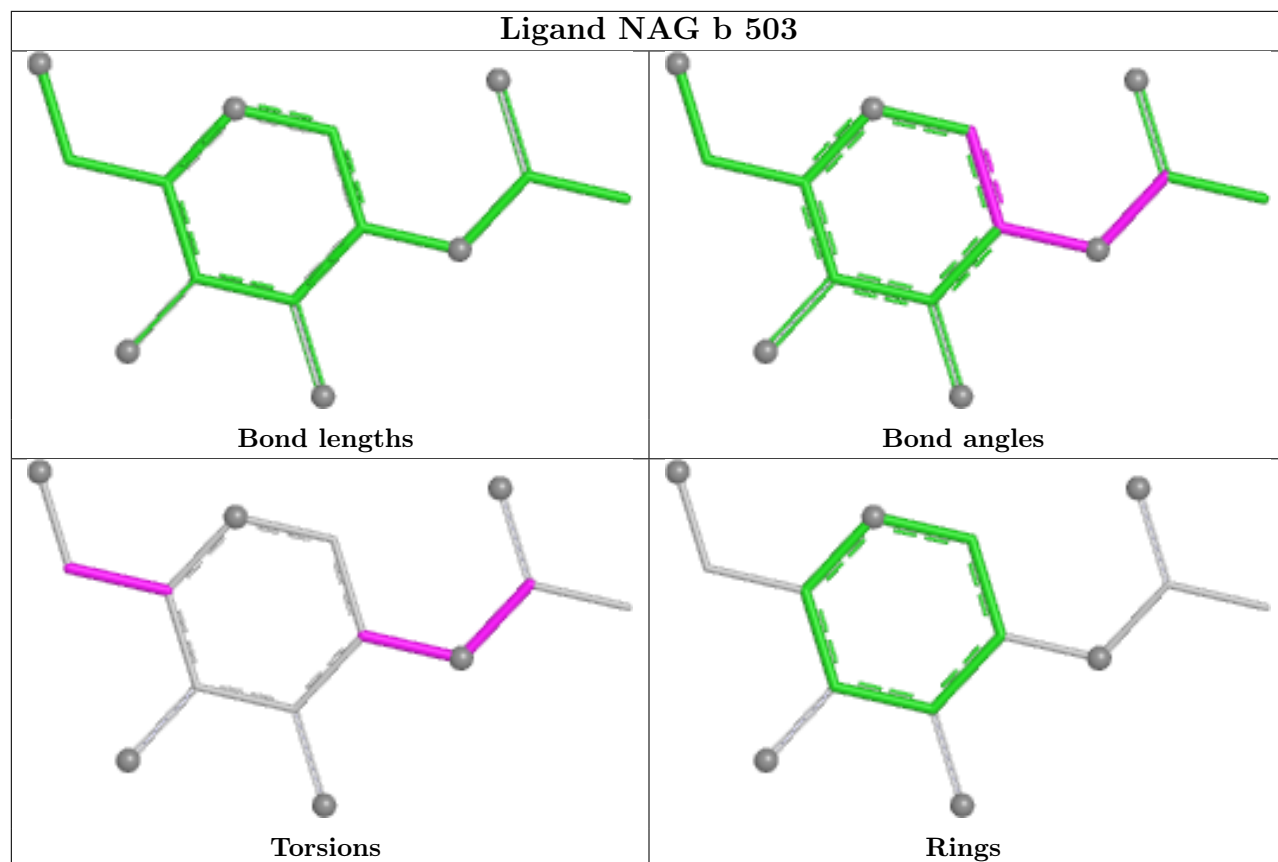
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	304	NAG	1	0
6	C	304	NAG	1	0
6	A	305	NAG	1	0
6	C	302	NAG	1	0
6	b	503	NAG	1	0
6	c	501	NAG	1	0
6	A	303	NAG	1	0
6	a	503	NAG	2	0
6	a	502	NAG	2	0
6	A	302	NAG	1	0

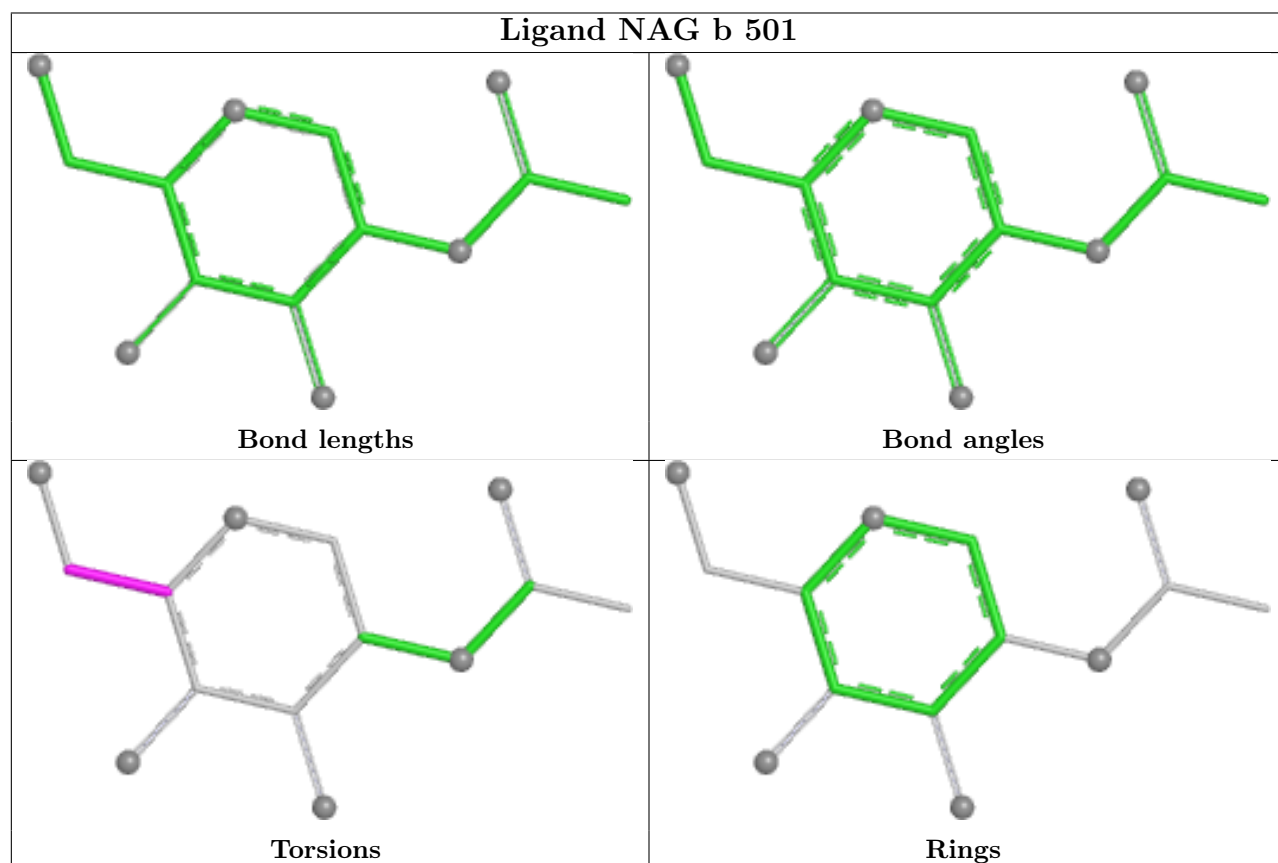
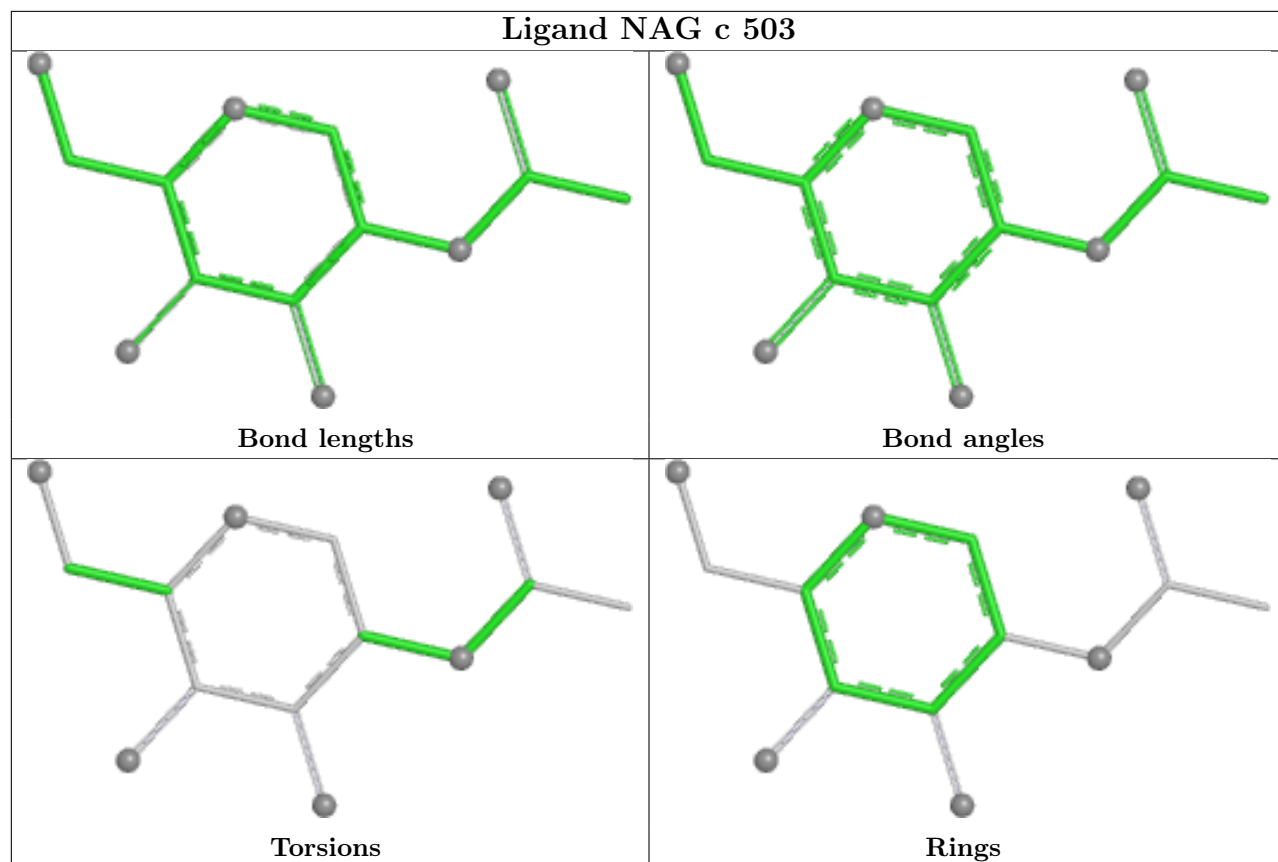
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

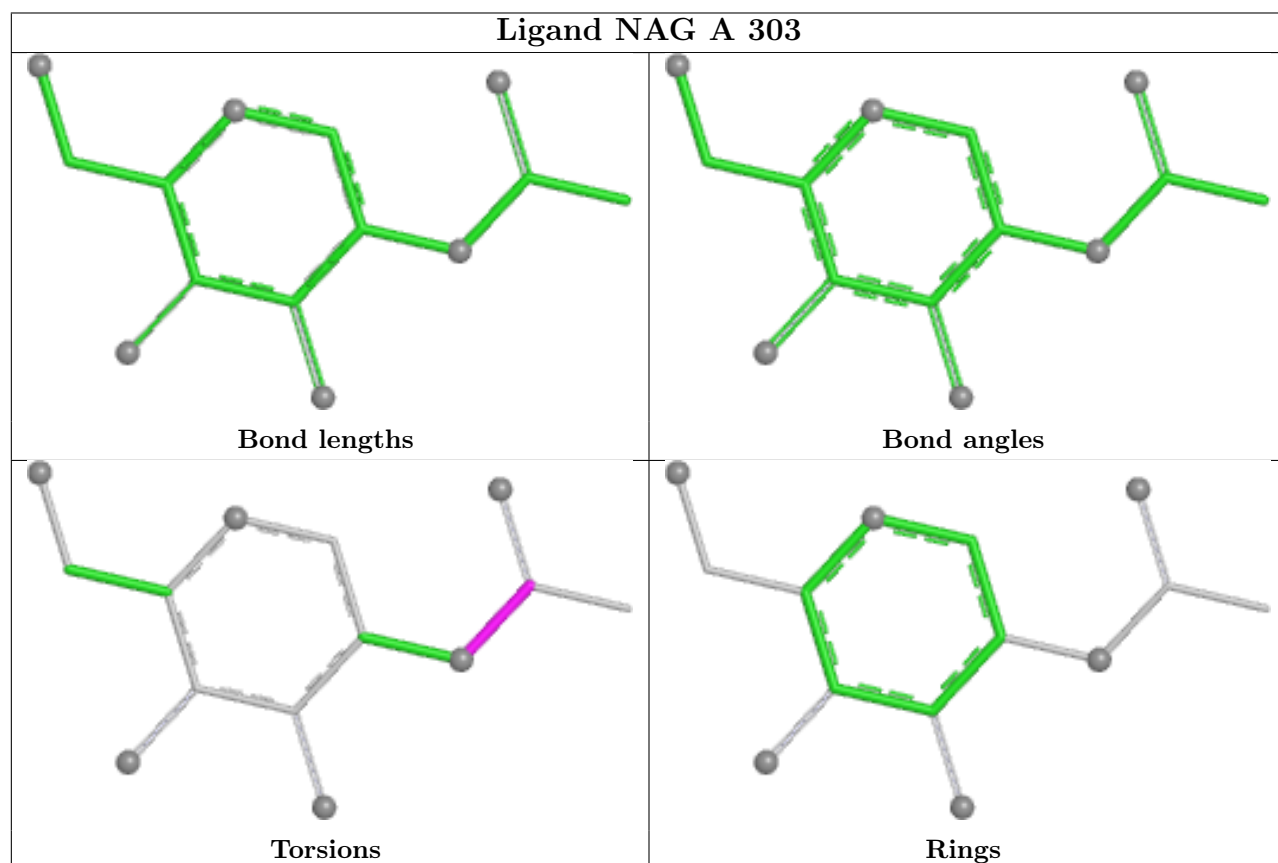
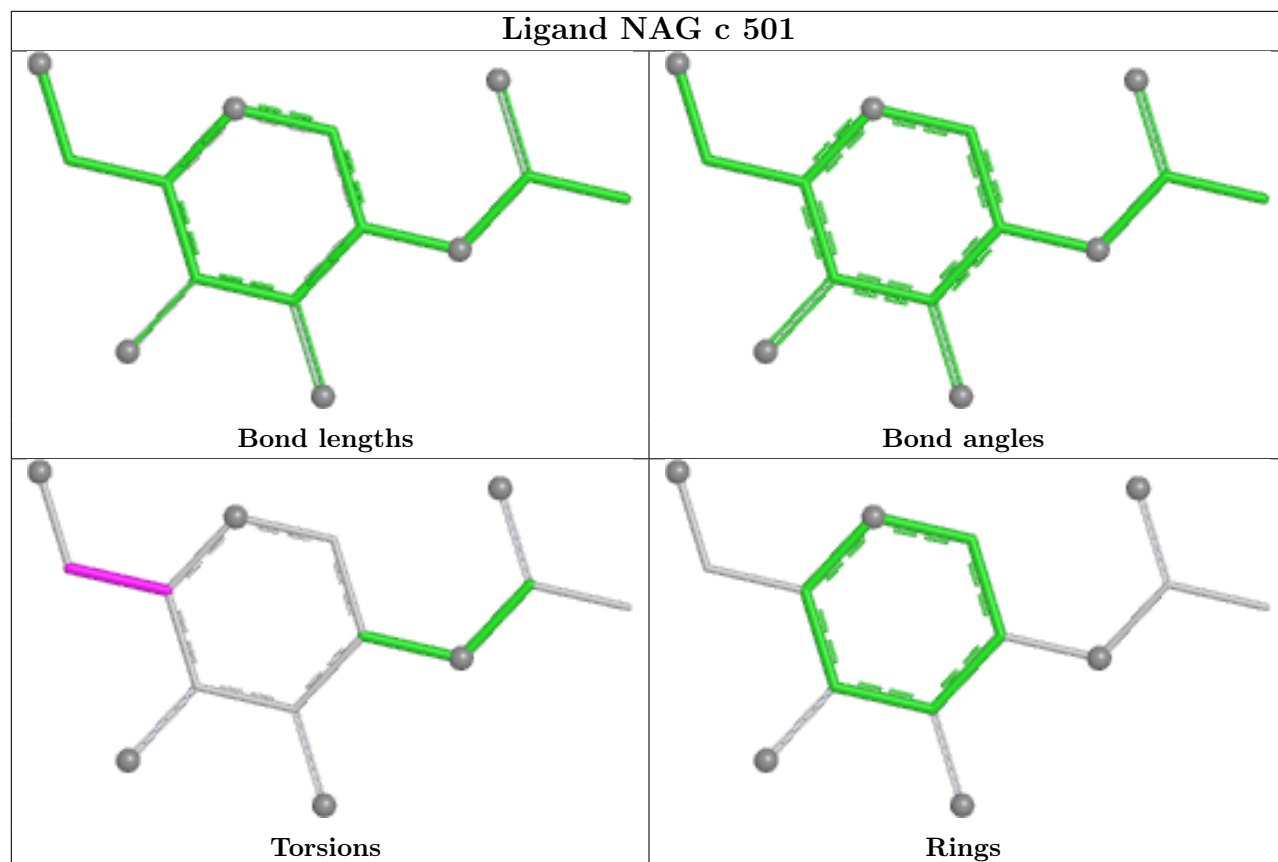


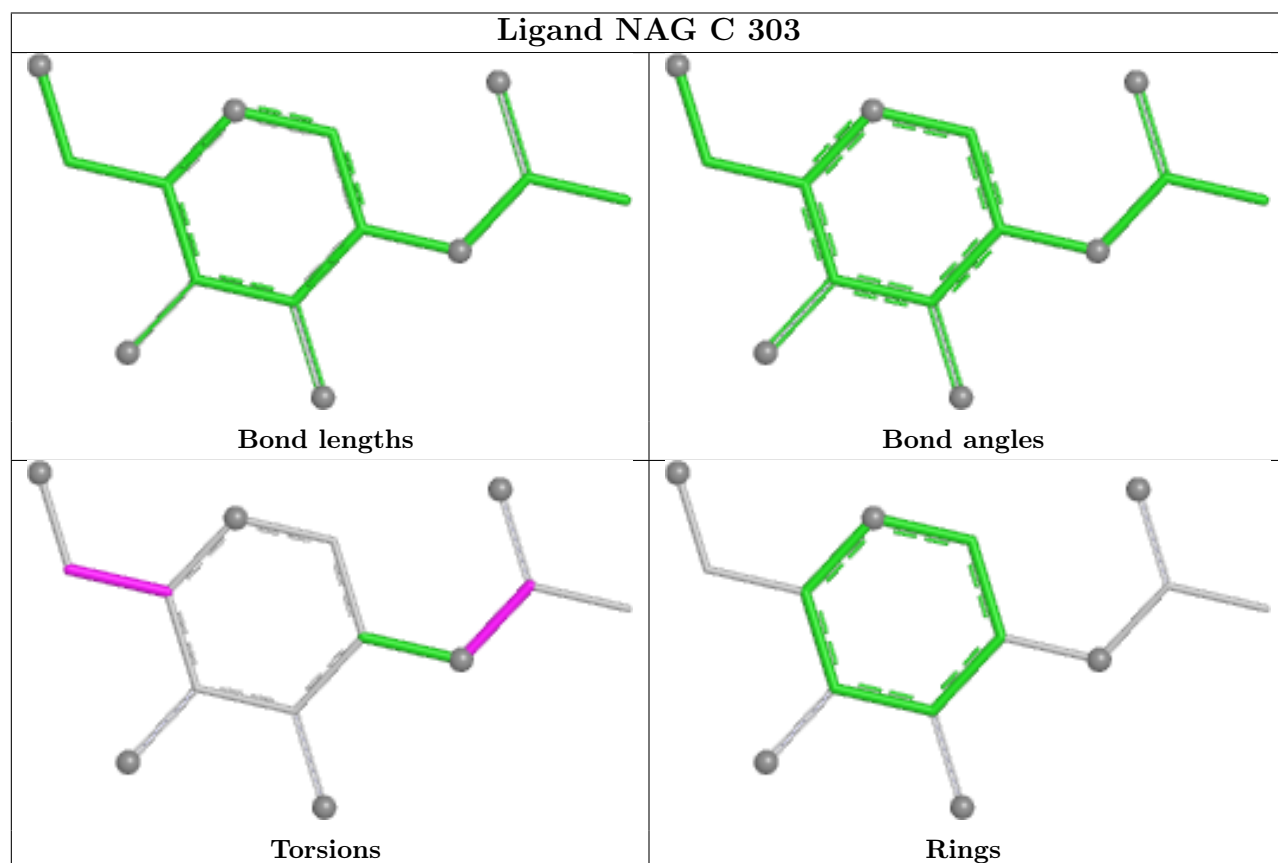
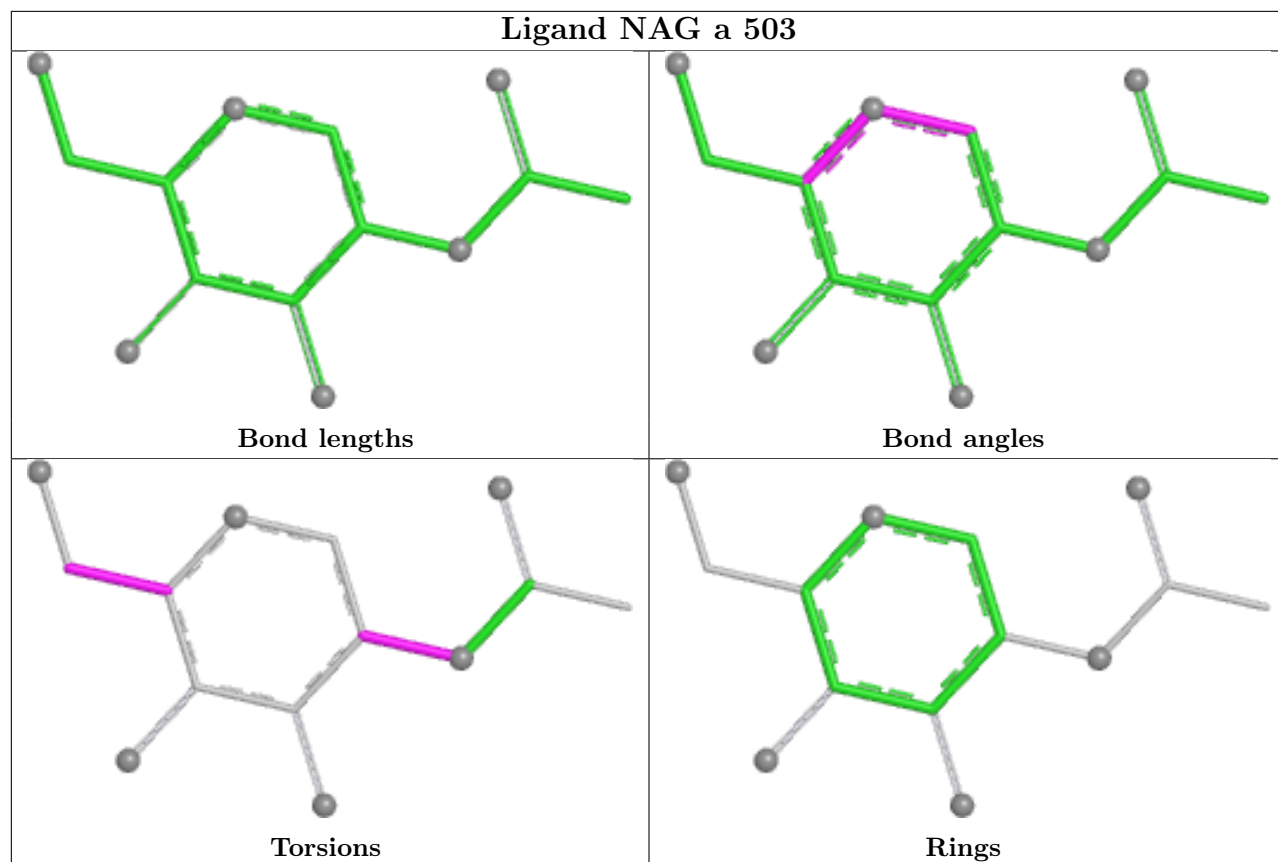


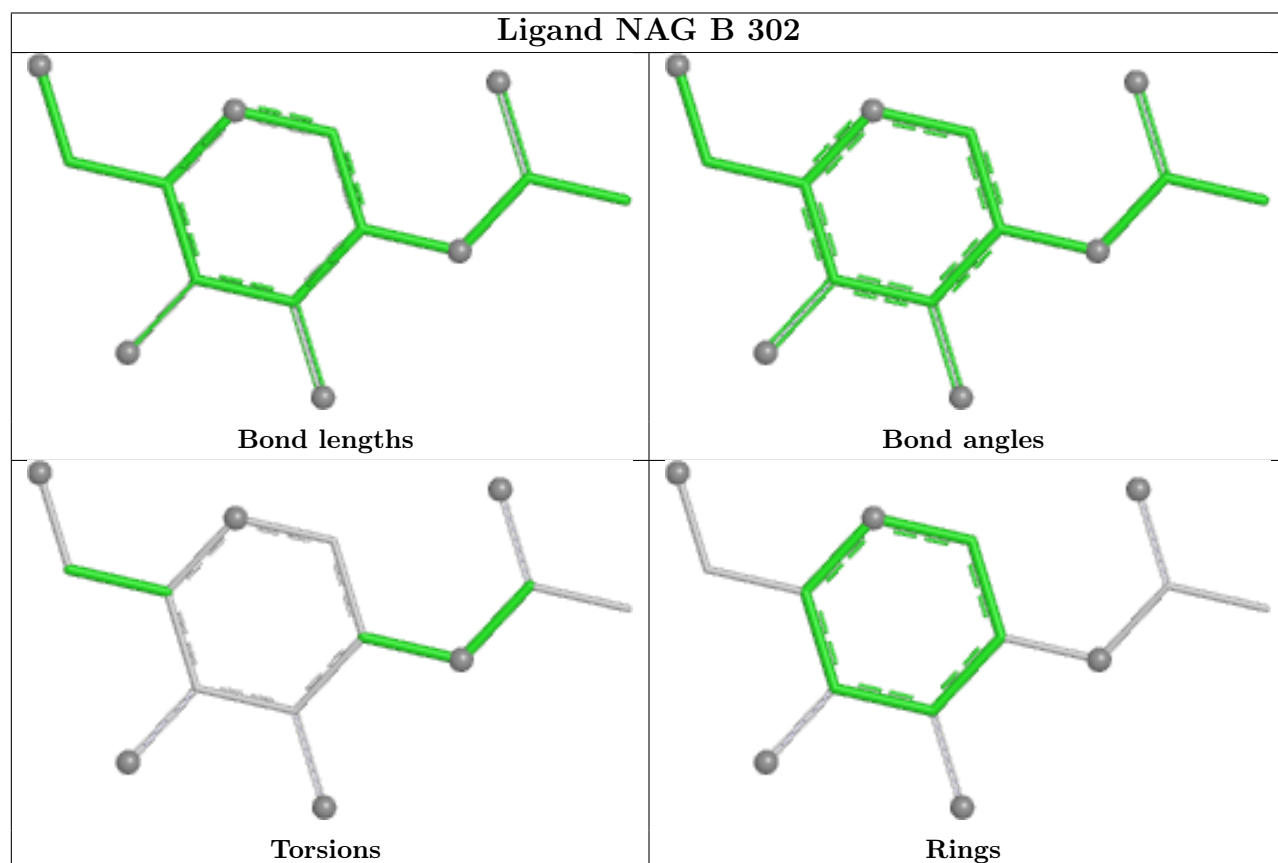
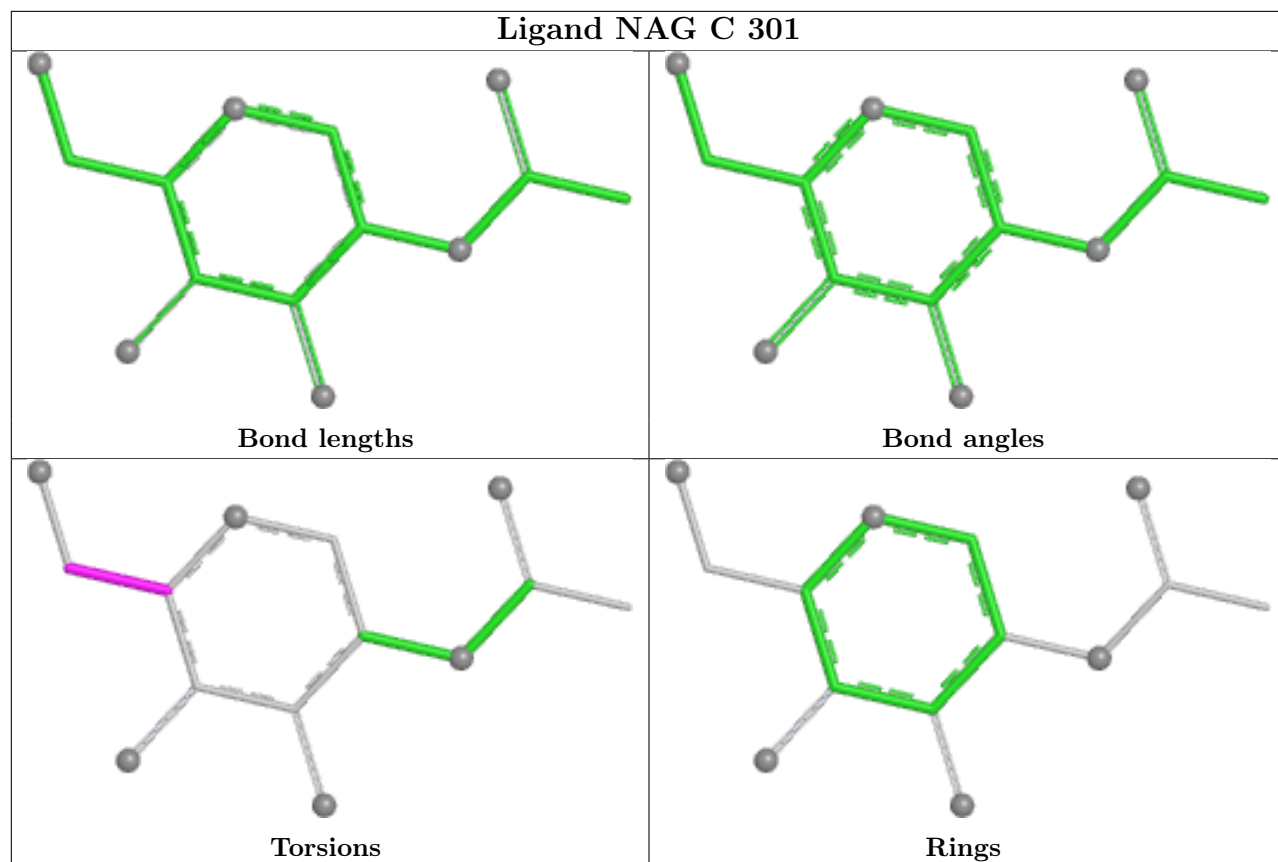


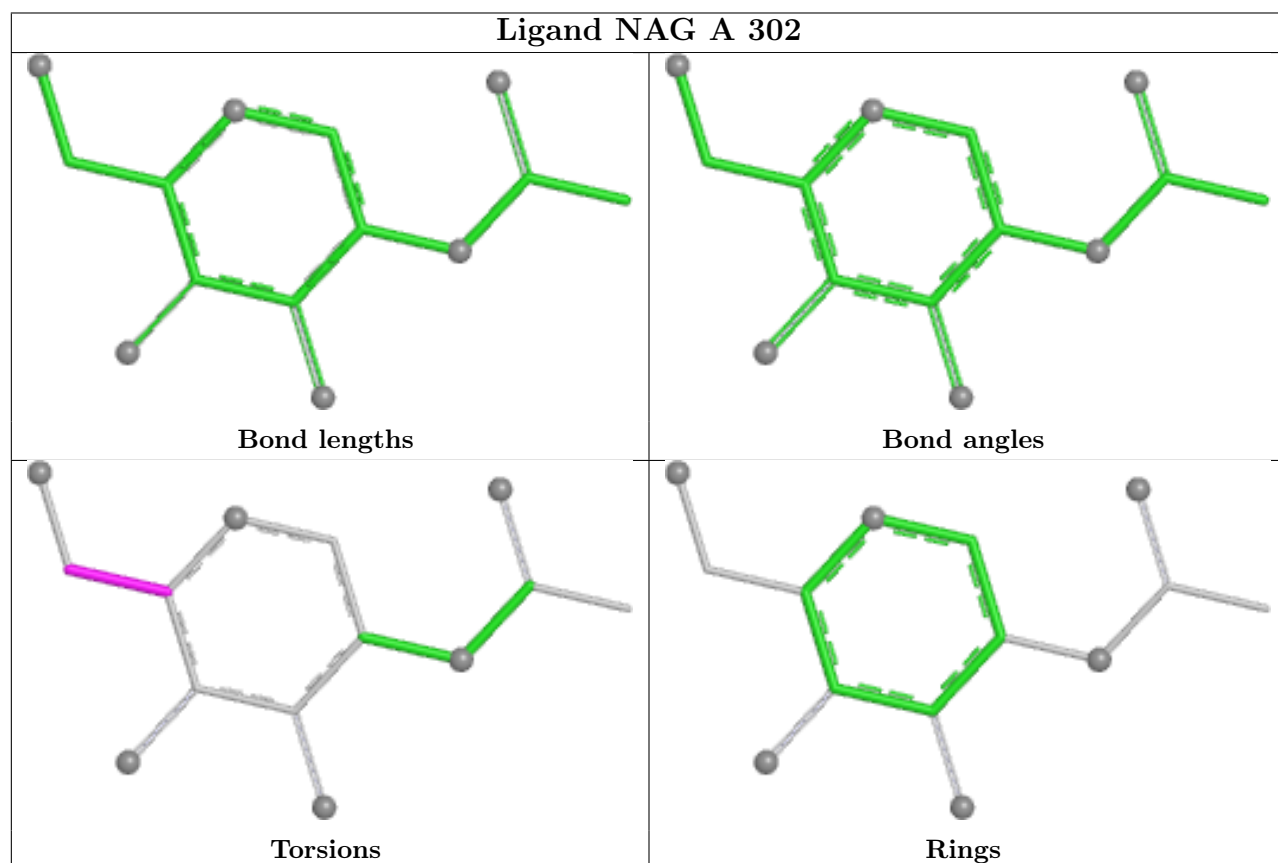
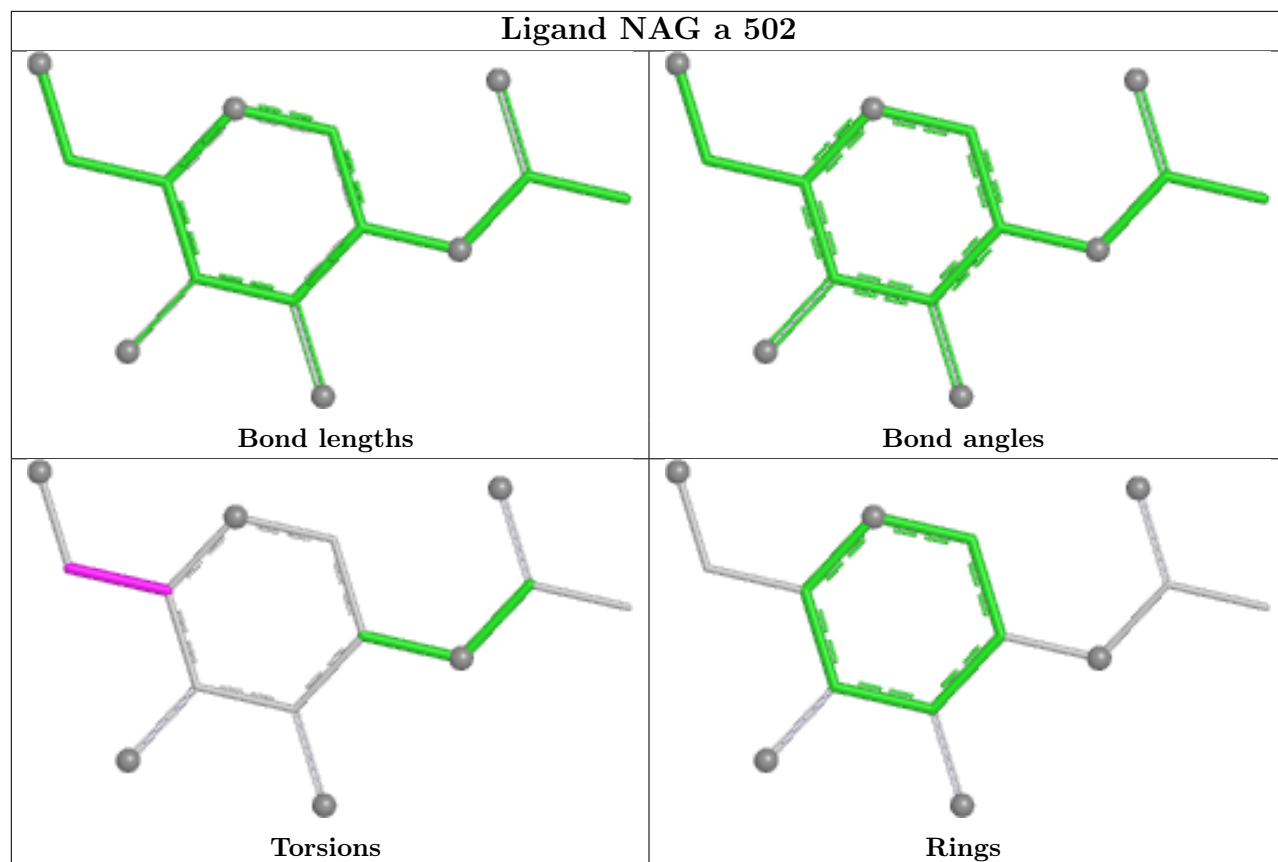


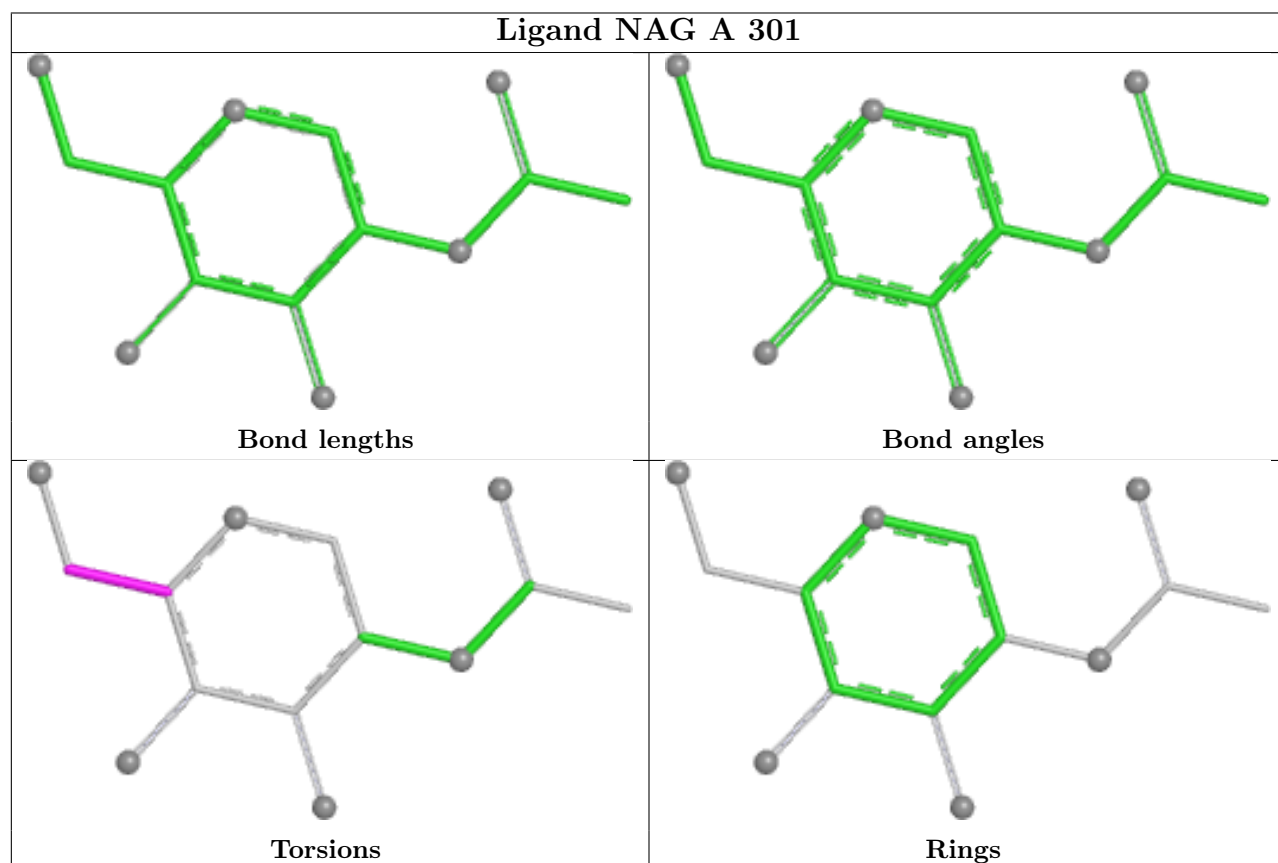
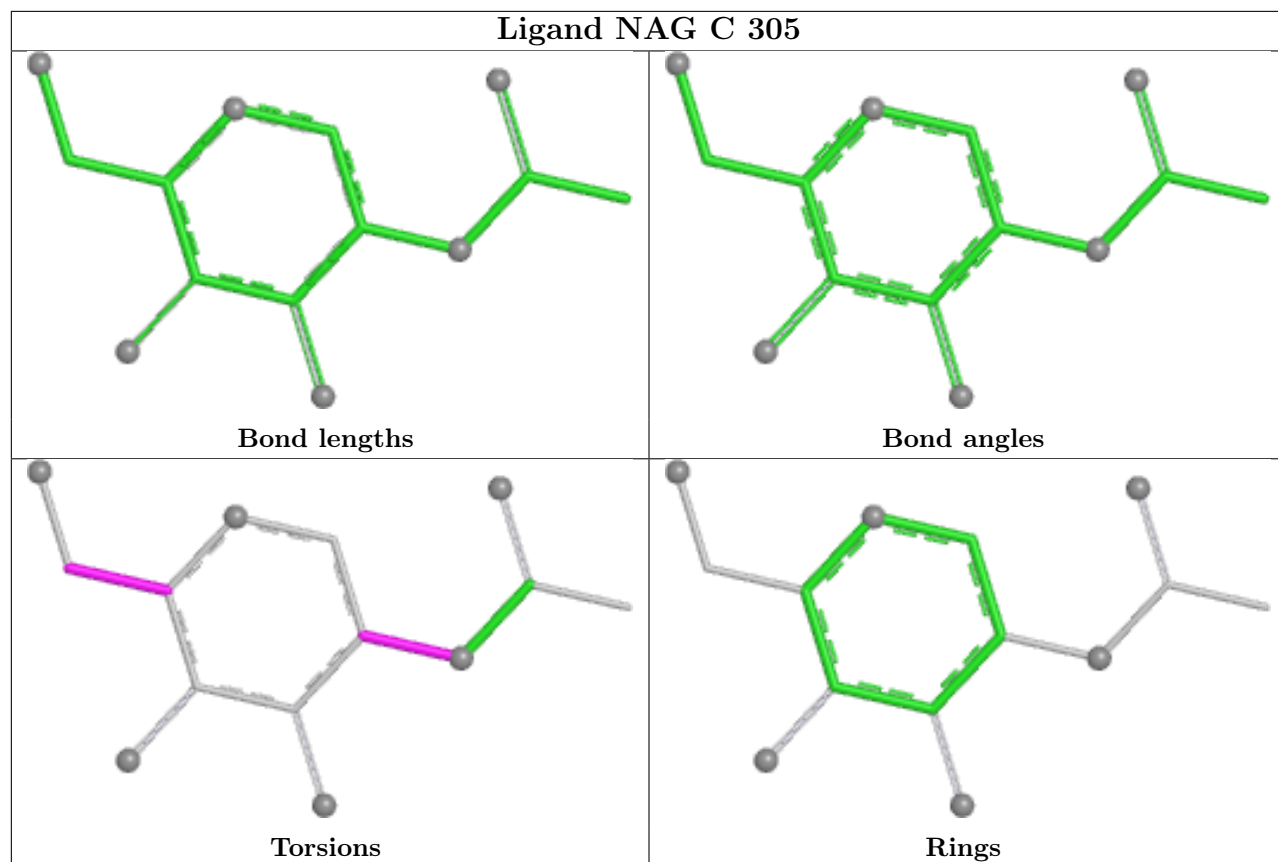


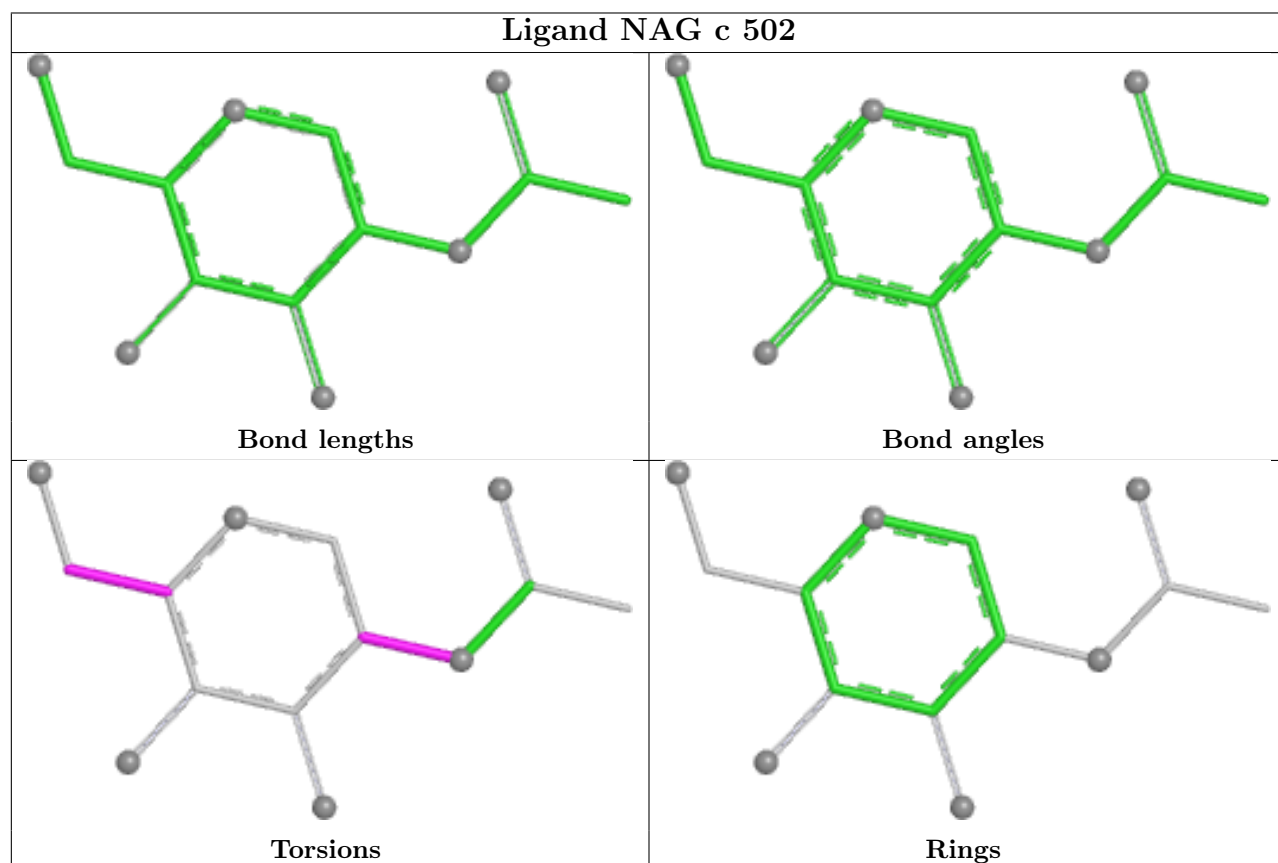
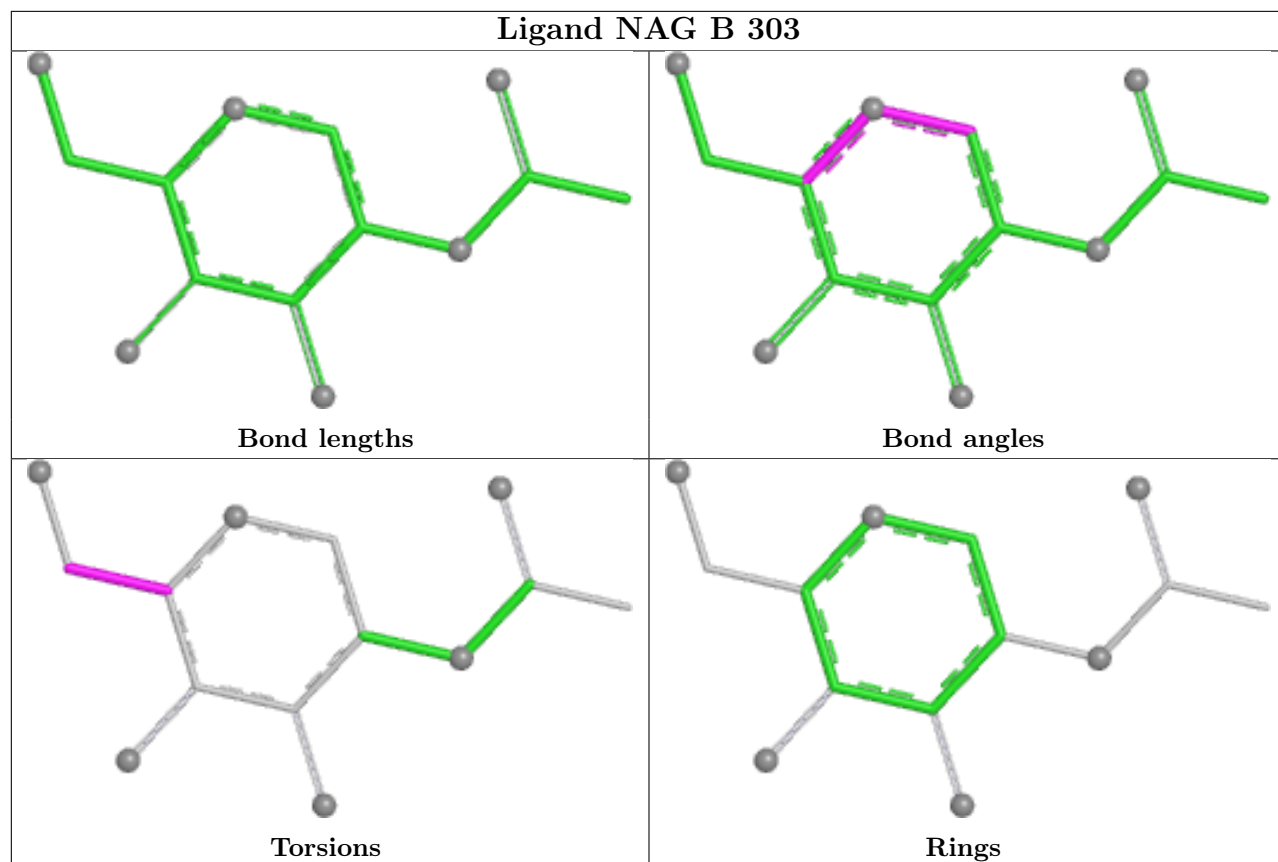












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

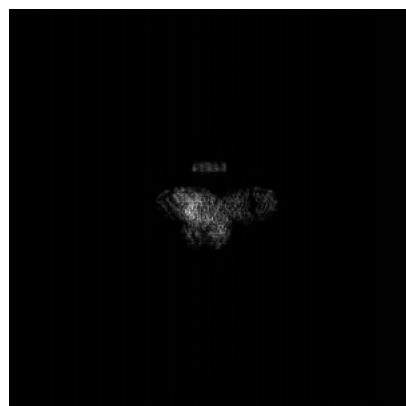
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26594. These allow visual inspection of the internal detail of the map and identification of artifacts.

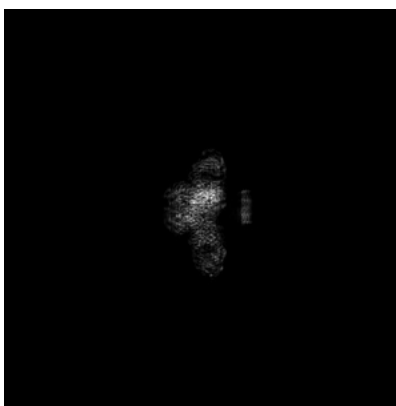
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

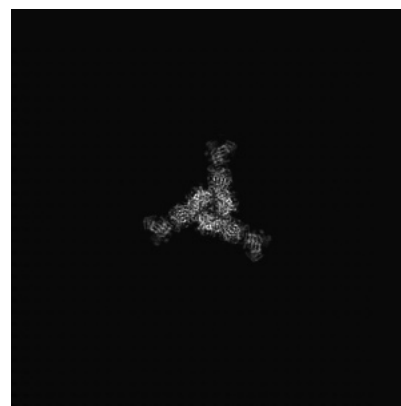
6.1.1 Primary map



X

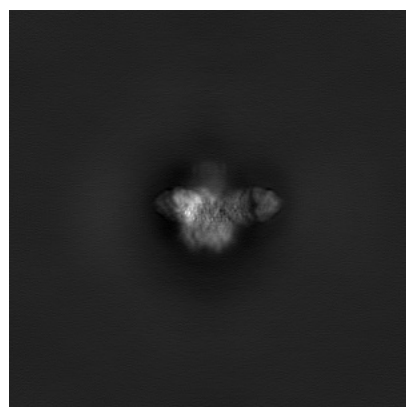


Y

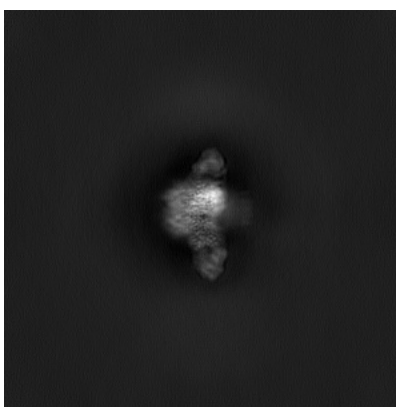


Z

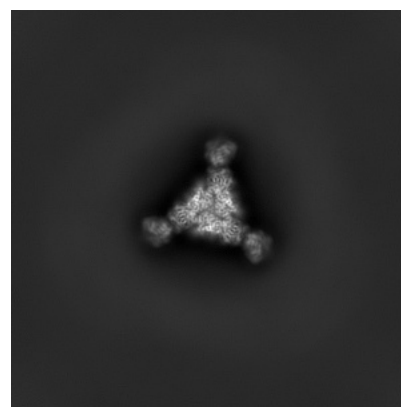
6.1.2 Raw map



X



Y



Z

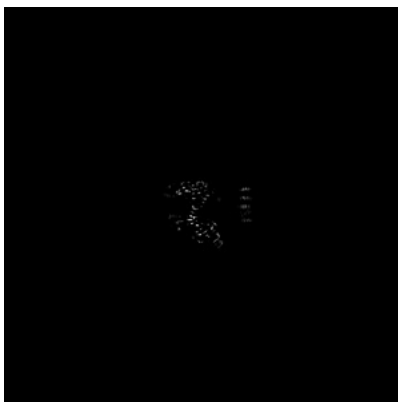
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 208

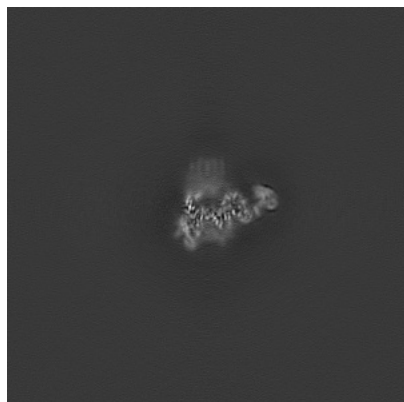


Y Index: 208

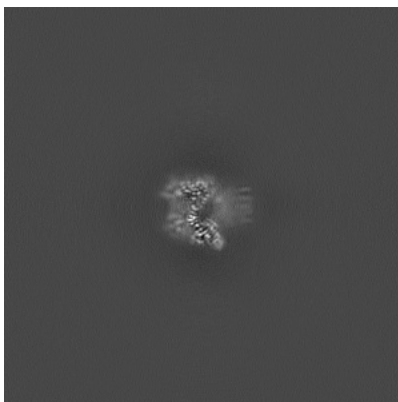


Z Index: 208

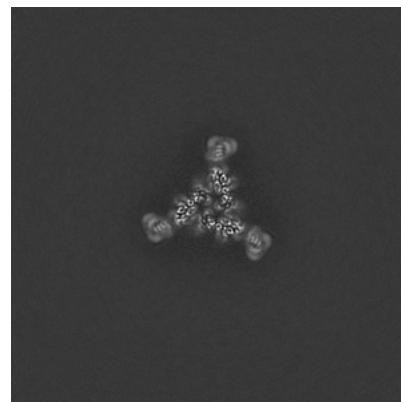
6.2.2 Raw map



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](#)

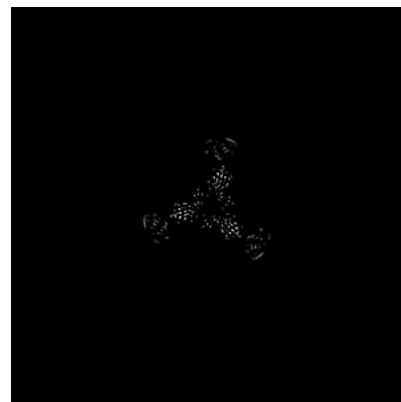
6.3.1 Primary map



X Index: 214

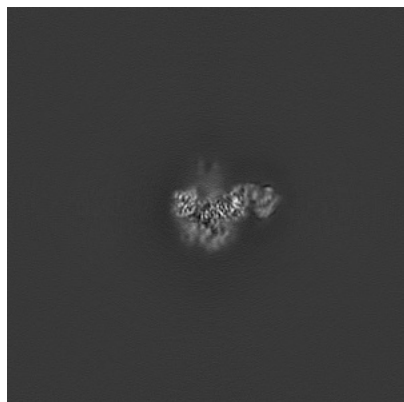


Y Index: 187

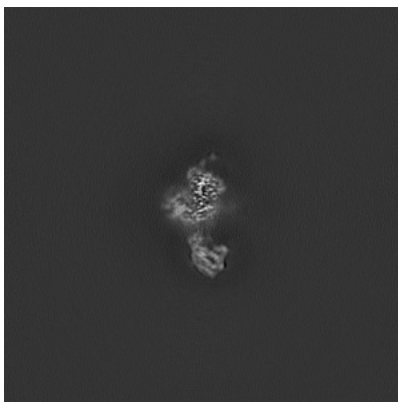


Z Index: 215

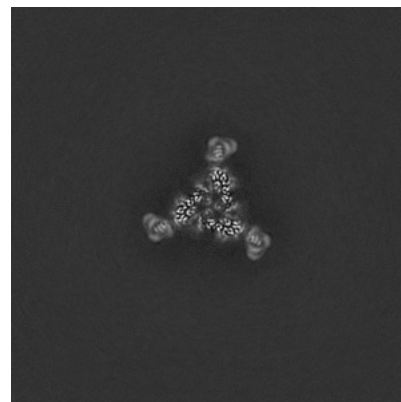
6.3.2 Raw map



X Index: 222



Y Index: 187

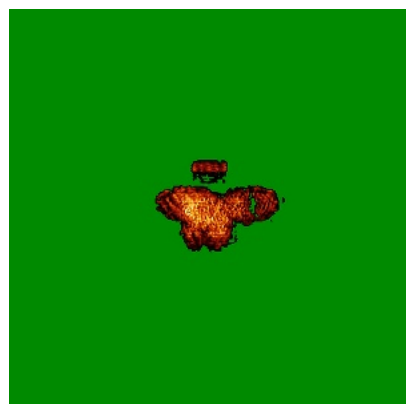


Z Index: 207

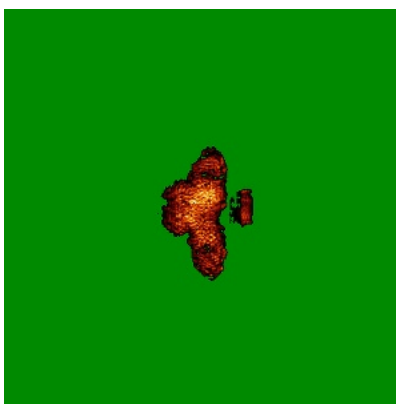
The images above show the largest variance slices of the map in three orthogonal directions.

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

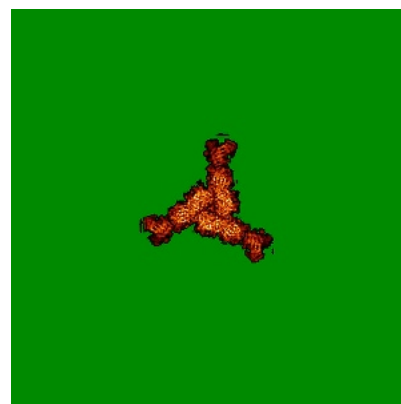
6.4.1 Primary map



X

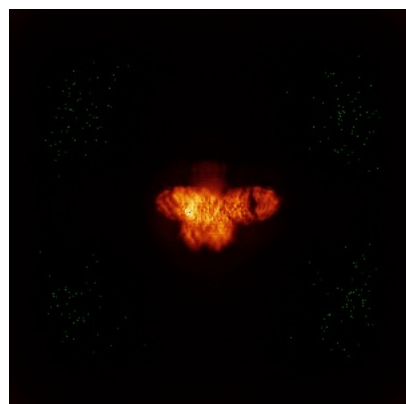


Y

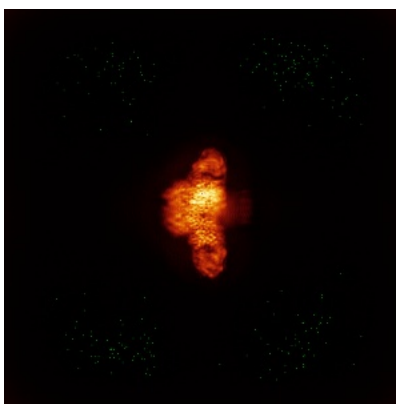


Z

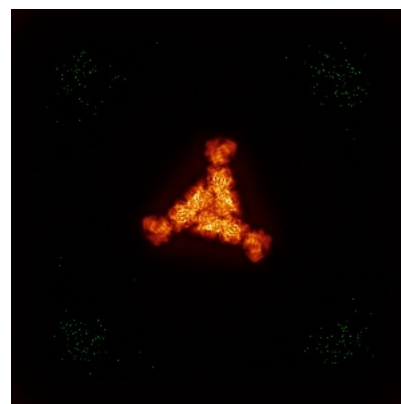
6.4.2 Raw map



X



Y

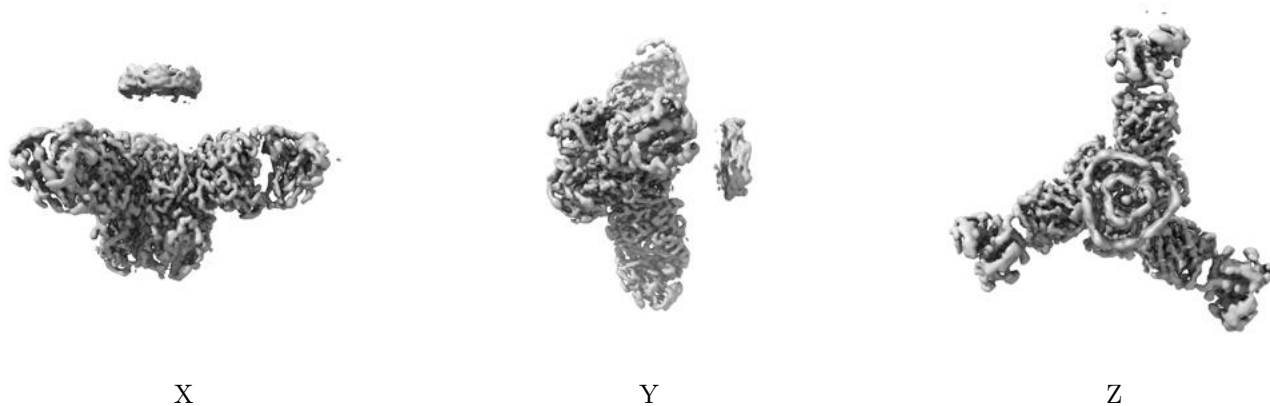


Z

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 0.1. 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.

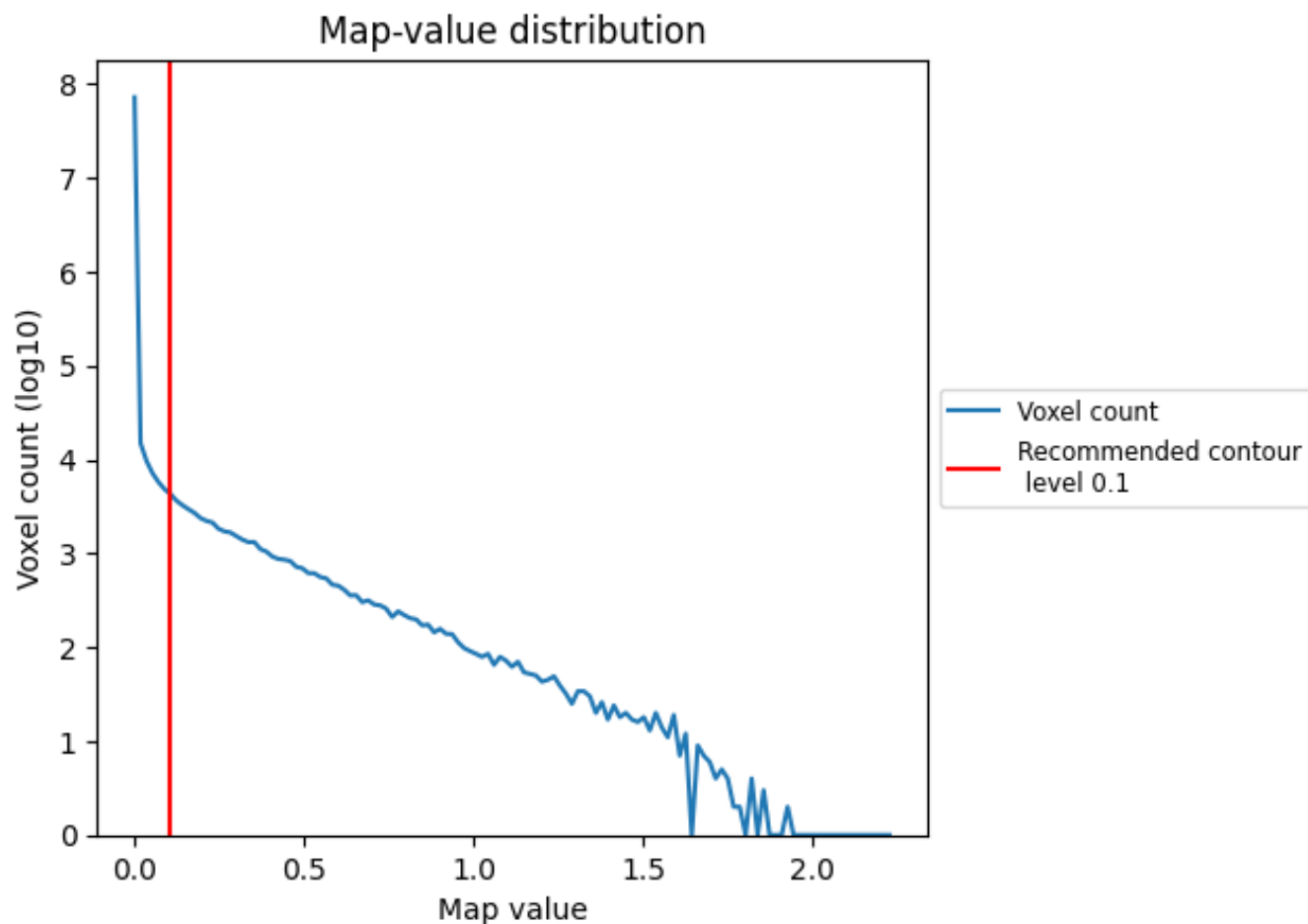
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

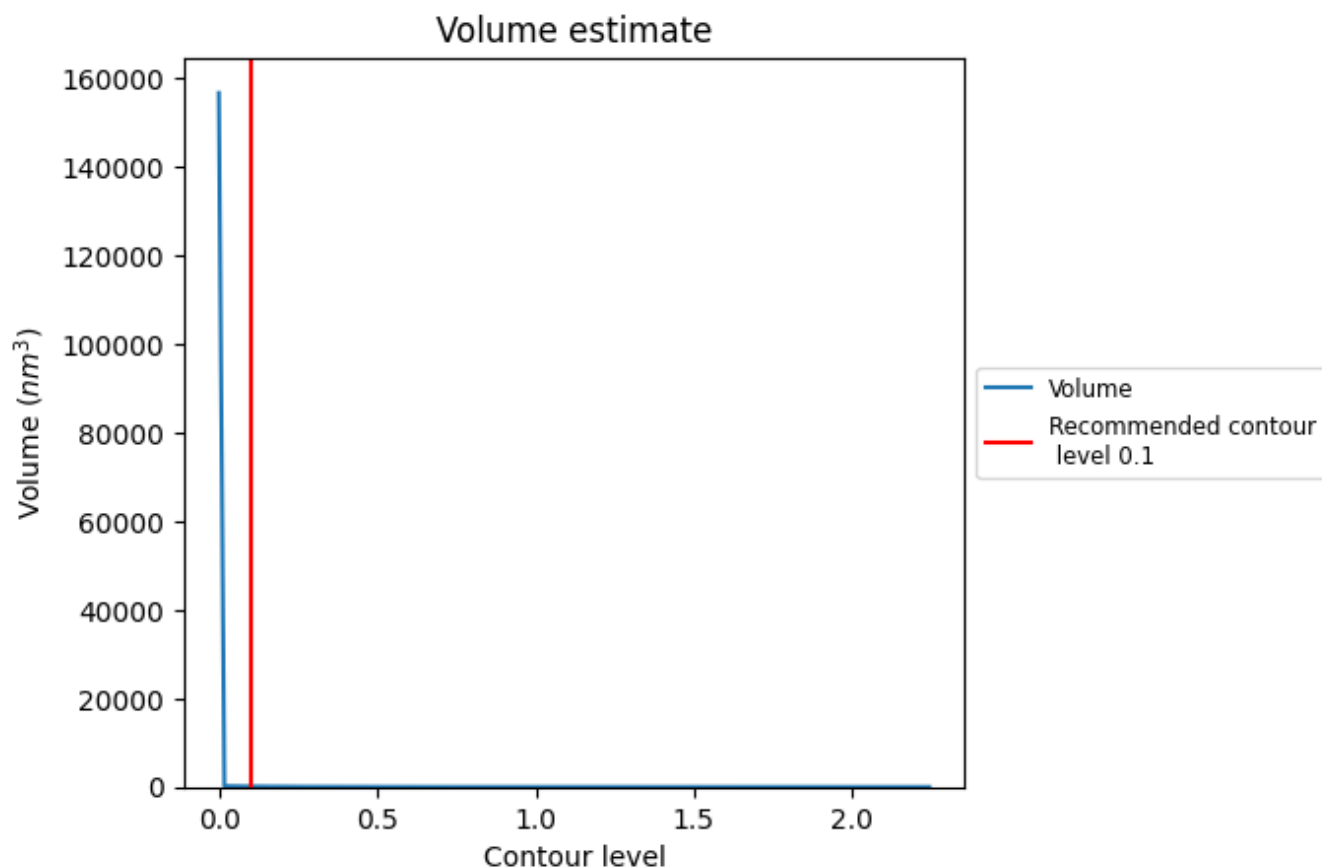
This section contains the results of statistical analysis of the map.

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.

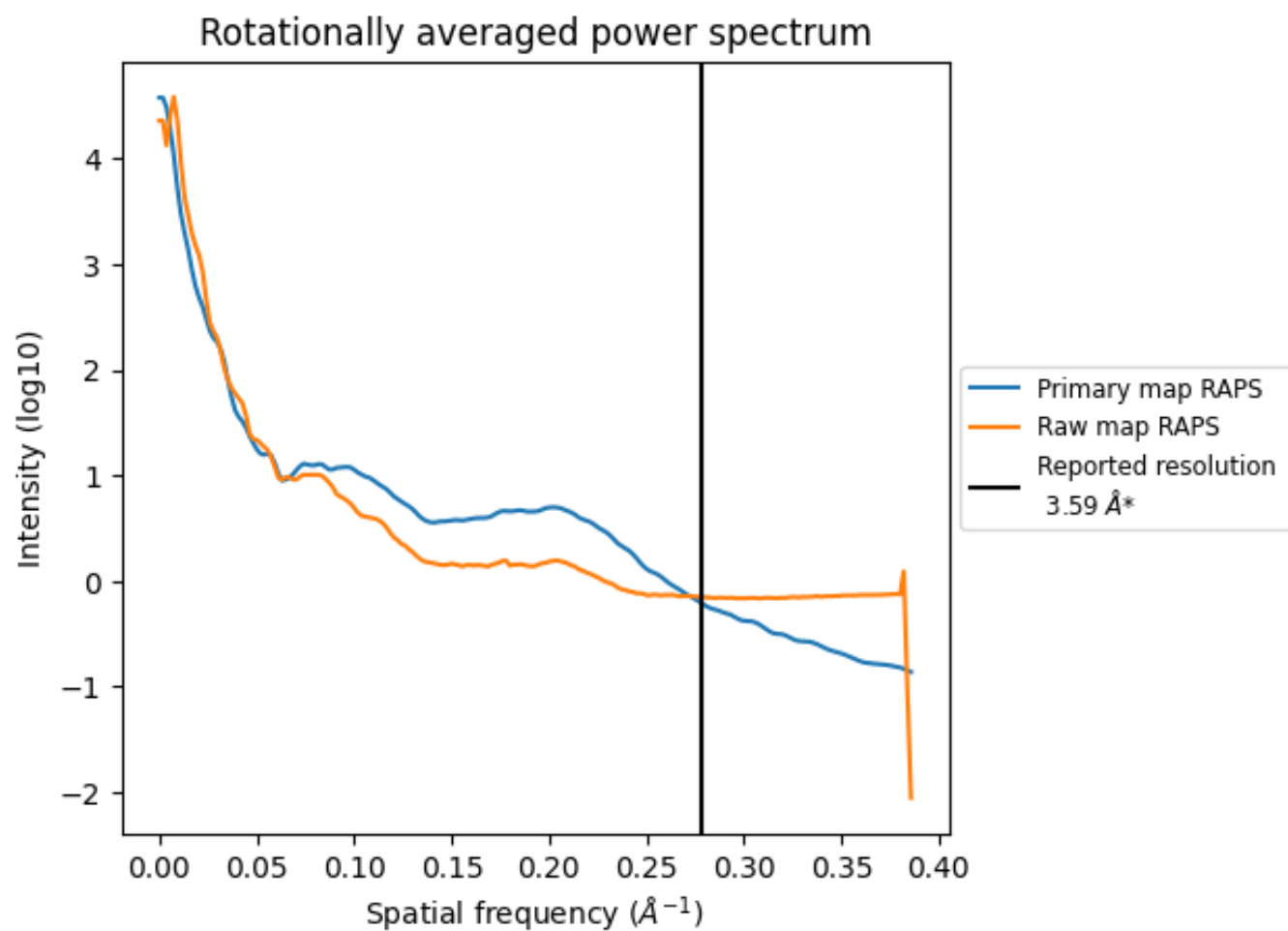
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm^3 ; this corresponds to an approximate mass of 102 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 ⓘ

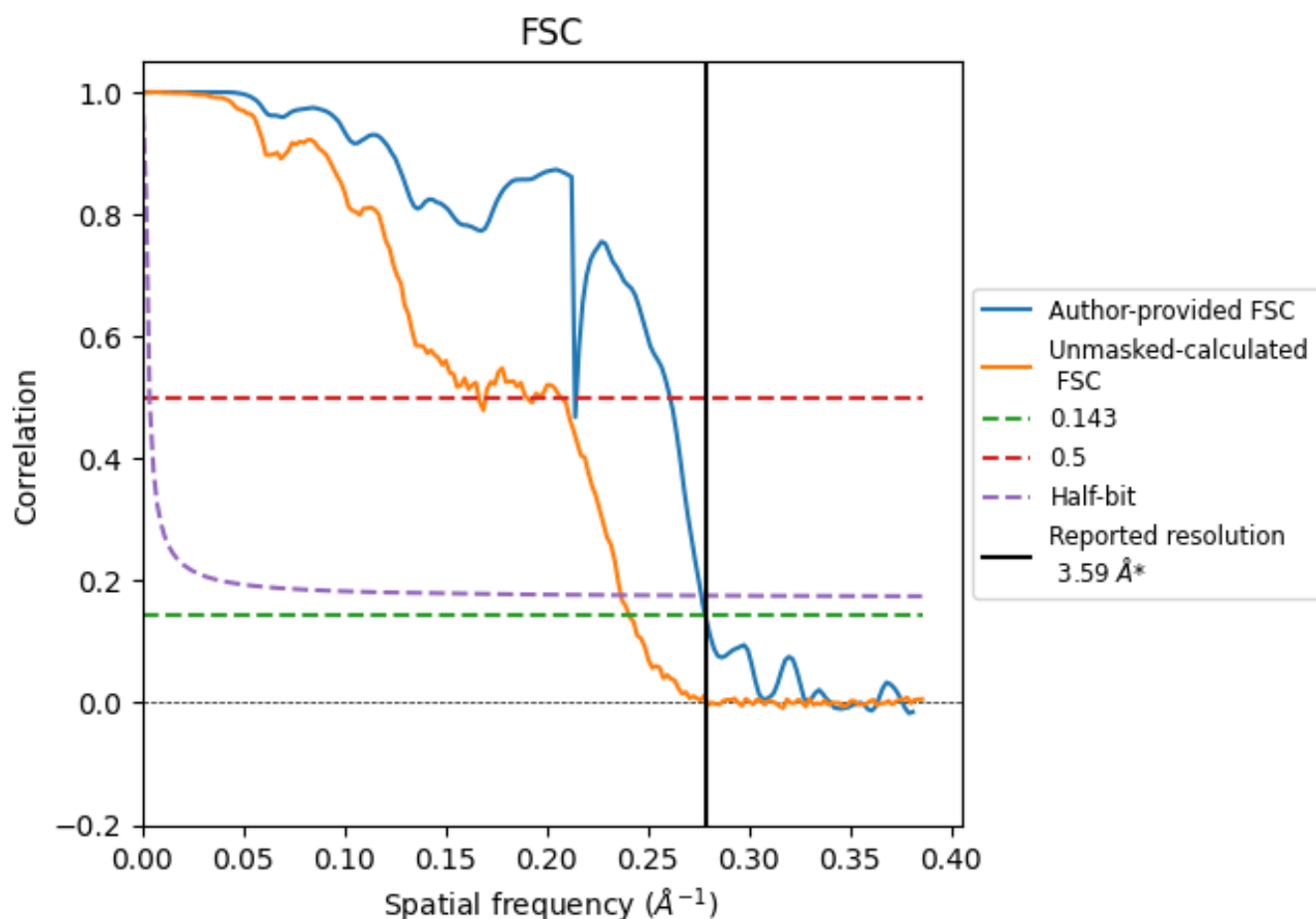


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

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 0.279 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

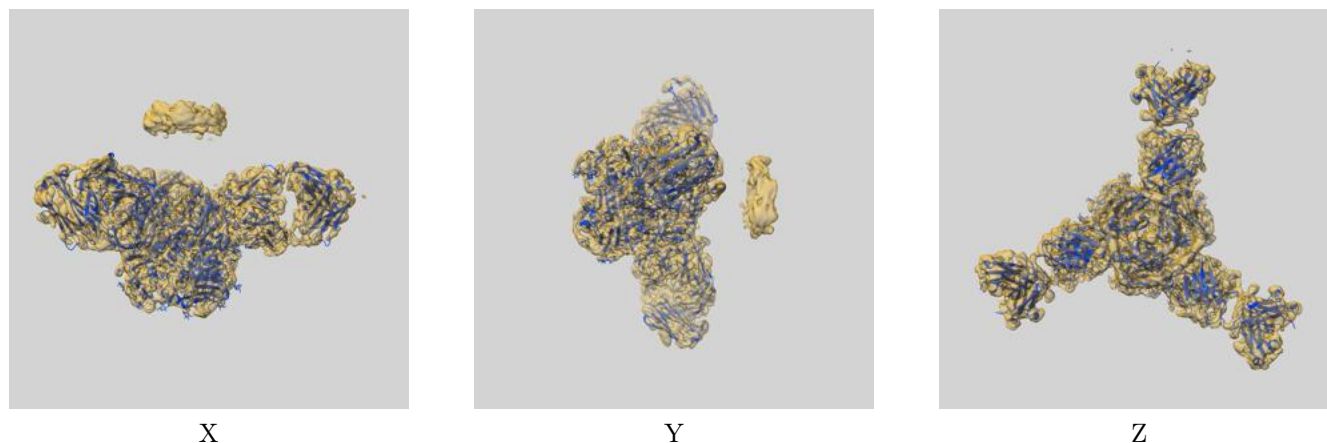
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.59	-	-
Author-provided FSC curve	3.59	4.67	3.62
Unmasked-calculated*	4.15	6.01	4.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.59 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26594 and PDB model 7UL7. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



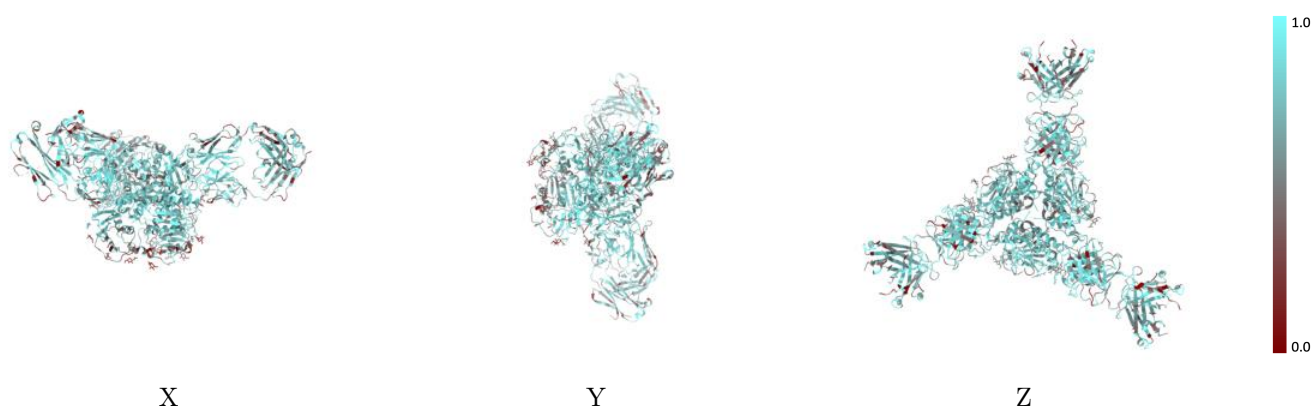
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



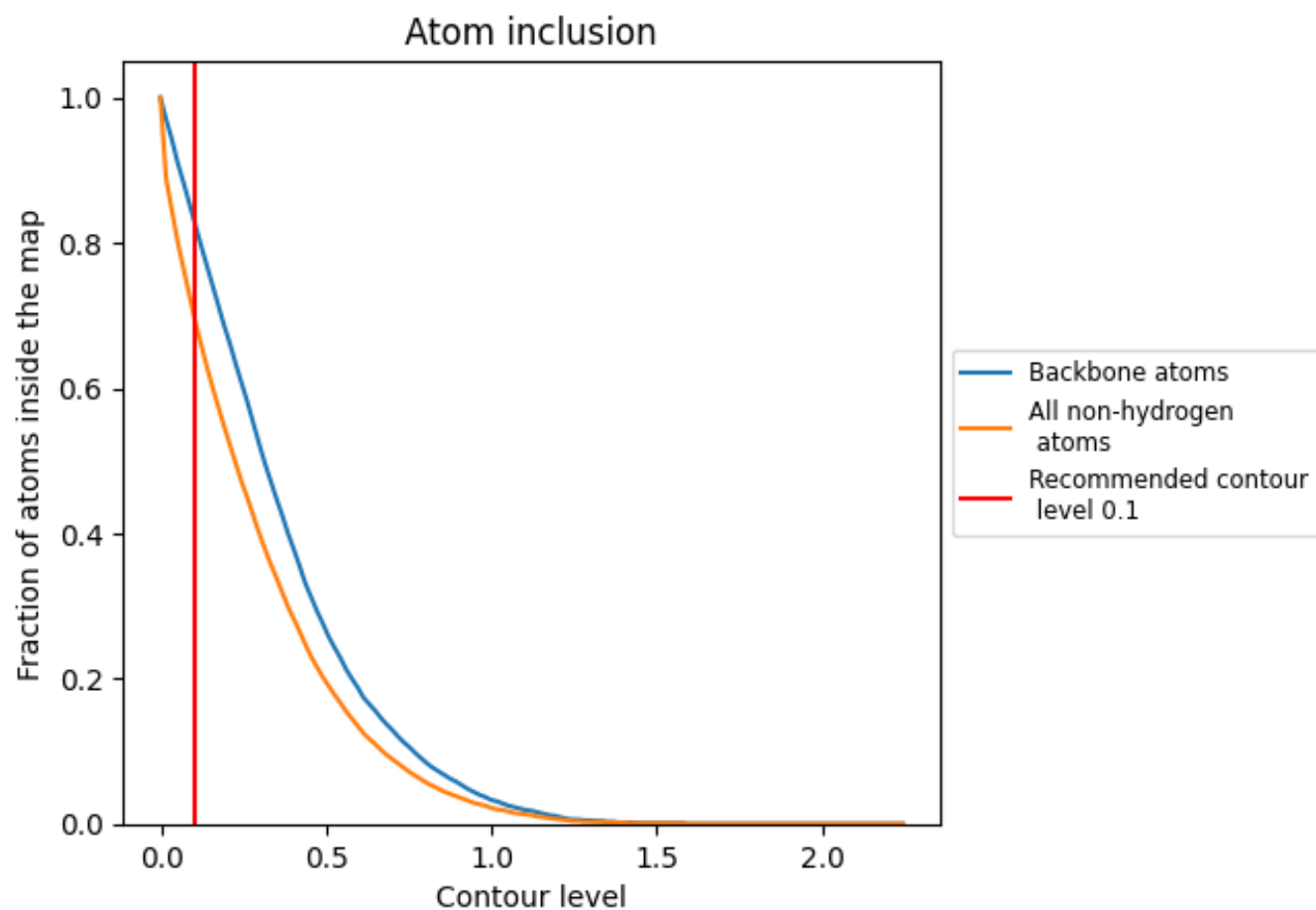
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 70% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6990	 0.3360
A	 0.6490	 0.2990
B	 0.6560	 0.2940
C	 0.6440	 0.2920
D	 0.7130	 0.3360
E	 0.6820	 0.3130
F	 0.7110	 0.3320
G	 0.6890	 0.3120
H	 0.6690	 0.3200
I	 0.6070	 0.3310
J	 0.5710	 0.3110
K	 0.5360	 0.3340
L	 0.6880	 0.3350
M	 0.5000	 0.2810
a	 0.7730	 0.4010
b	 0.7650	 0.4090
c	 0.7760	 0.4130

