



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 05:34 PM UTC

PDB ID : 8ONH / pdb_00008onh
Title : Variant Surface Glycoprotein VSG11wt-Oil
Authors : Zeelen, J.P.; Stebbins, C.E.; Foti, K.; Gkeka, A.; Vlachou, E.P.
Deposited on : 2023-04-03
Resolution : 2.59 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

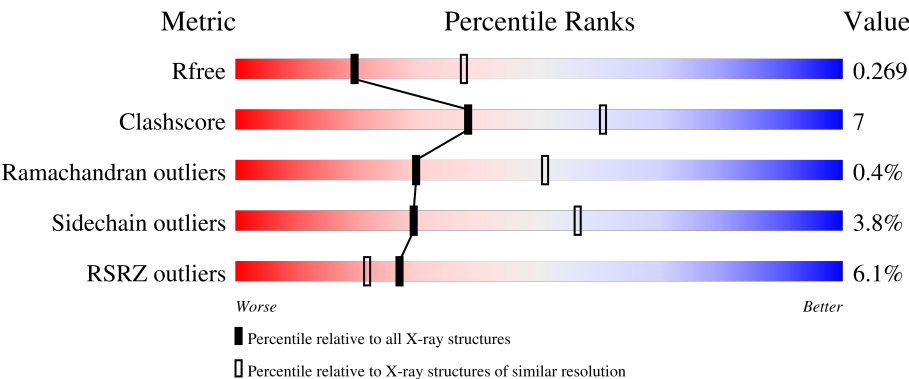
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	410	0% 77%11%11%
1	B	410	3% 78%10%11%
1	C	410	2% 74%15%11%
1	D	410	6% 64%13%22%
1	E	410	2% 55%15%30%

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Mol	Chain	Length	Quality of chain
1	F	410	
1	G	410	
1	H	410	
1	I	410	
1	J	410	
1	K	410	
1	L	410	
1	M	410	
1	N	410	
1	O	410	
1	P	410	
1	Q	410	
1	R	410	
2	S	6	
2	Z	6	
3	T	5	
4	U	3	
5	V	3	
5	X	3	
5	Y	3	
6	W	5	
6	c	5	
7	a	5	
7	b	5	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 43982 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Variant surface glycoprotein.

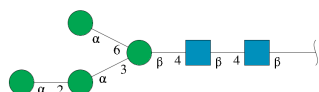
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2749	1699	490	547	13			
1	B	366	Total	C	N	O	S	0	0	0
			2704	1665	480	546	13			
1	C	366	Total	C	N	O	S	0	0	0
			2721	1679	485	544	13			
1	D	321	Total	C	N	O	S	0	0	0
			2332	1436	417	466	13			
1	E	285	Total	C	N	O	S	0	0	0
			2046	1250	363	421	12			
1	F	282	Total	C	N	O	S	0	0	0
			2044	1246	363	422	13			
1	G	365	Total	C	N	O	S	0	0	0
			2704	1672	475	544	13			
1	H	287	Total	C	N	O	S	0	0	0
			2057	1260	363	422	12			
1	I	343	Total	C	N	O	S	0	0	0
			2461	1517	433	500	11			
1	J	366	Total	C	N	O	S	0	0	0
			2741	1692	489	547	13			
1	K	365	Total	C	N	O	S	0	0	0
			2698	1668	478	539	13			
1	L	358	Total	C	N	O	S	0	0	0
			2660	1644	470	533	13			
1	M	287	Total	C	N	O	S	0	0	0
			2079	1270	372	425	12			
1	N	353	Total	C	N	O	S	0	0	0
			2618	1608	471	526	13			
1	O	301	Total	C	N	O	S	0	0	0
			2172	1332	382	445	13			
1	P	261	Total	C	N	O	S	0	0	0
			1882	1147	335	387	13			

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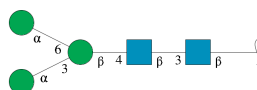
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	272	Total	C	N	O	S	0	0	0
			1967	1200	350	405	12			
1	R	310	Total	C	N	O	S	0	0	0
			2215	1363	390	449	13			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



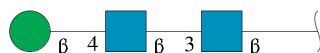
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	6	Total	C	N	O		0	0	0
			72	40	2	30				
2	Z	6	Total	C	N	O		0	0	0
			72	40	2	30				

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



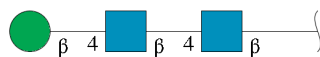
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	5	Total	C	N	O		0	0	0
			61	34	2	25				

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



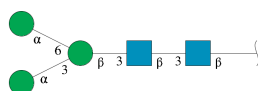
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	U	3	Total	C	N	O		0	0	0
			39	22	2	15				

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



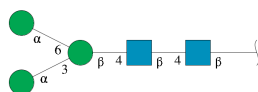
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	V	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	W	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	c	5	Total	C	N	O	0	0	0
			61	34	2	25			

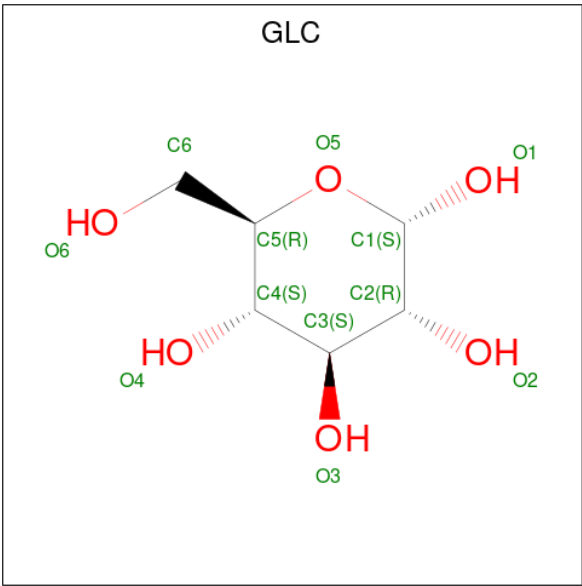
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	a	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	b	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆) (labeled as

"Ligand of Interest" by depositor).



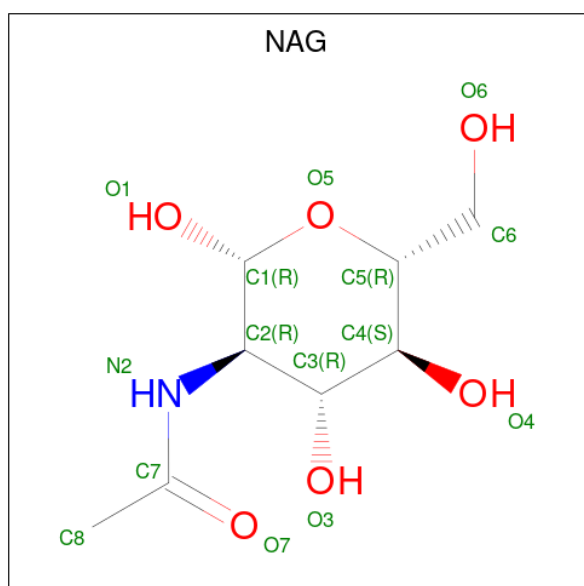
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		
8	B	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		
8	E	1	Total	C	O	0	0
			11	6	5		
8	F	1	Total	C	O	0	0
			11	6	5		
8	H	1	Total	C	O	0	0
			11	6	5		
8	I	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	K	1	Total	C	O	0	0
			11	6	5		
8	L	1	Total	C	O	0	0
			11	6	5		
8	M	1	Total	C	O	0	0
			11	6	5		
8	N	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	O	1	Total	C	O	0	0
			11	6	5		
8	P	1	Total	C	O	0	0
			11	6	5		
8	Q	1	Total	C	O	0	0
			11	6	5		
8	R	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	1	Total	C	N	O	0	0
			14	8	1	5		
9	O	1	Total	C	N	O	0	0
			14	8	1	5		
9	Q	1	Total	C	N	O	0	0
			14	8	1	5		
9	R	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	53	Total	O	0	0
			53	53		

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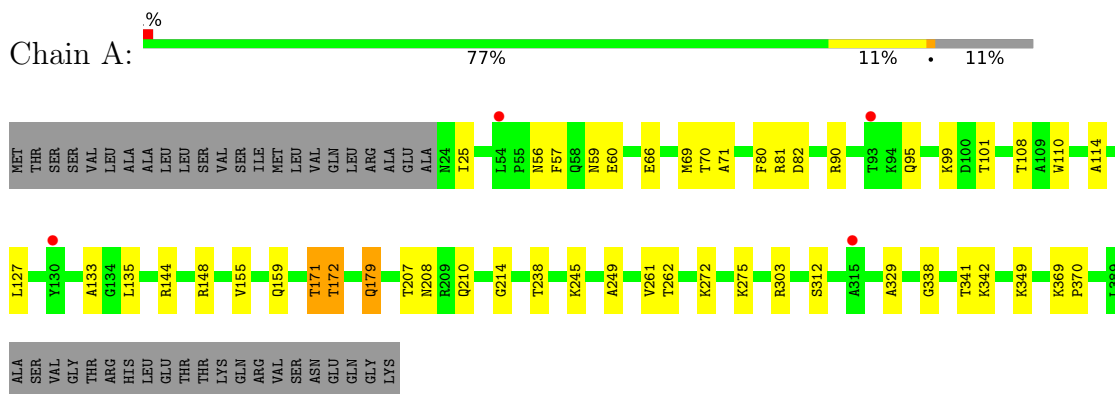
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	43	Total 43	O 43	0	0
10	C	28	Total 28	O 28	0	0
10	D	19	Total 19	O 19	0	0
10	E	4	Total 4	O 4	0	0
10	F	12	Total 12	O 12	0	0
10	J	51	Total 51	O 51	0	0
10	K	13	Total 13	O 13	0	0
10	L	15	Total 15	O 15	0	0
10	M	20	Total 20	O 20	0	0
10	N	19	Total 19	O 19	0	0
10	P	2	Total 2	O 2	0	0
10	R	5	Total 5	O 5	0	0

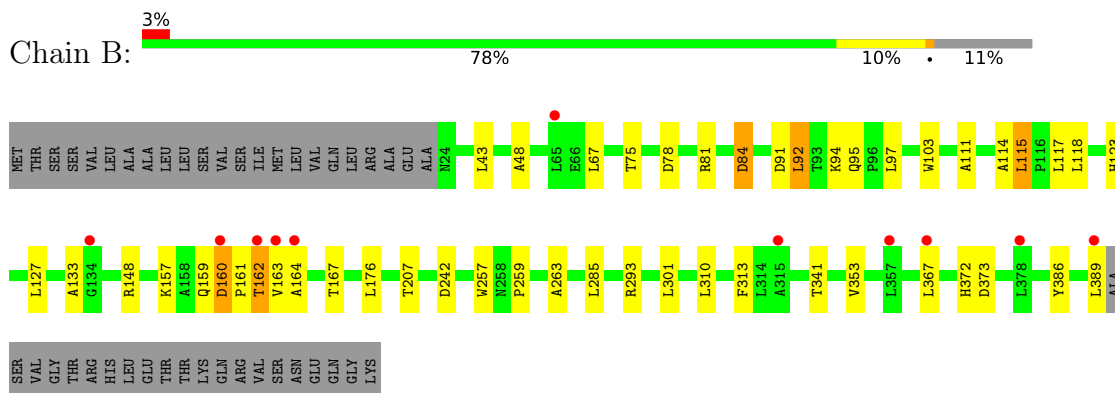
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

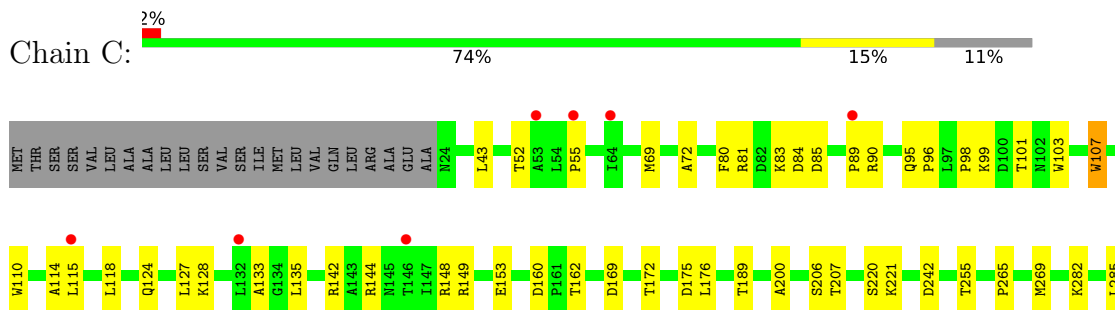
• Molecule 1: Variant surface glycoprotein

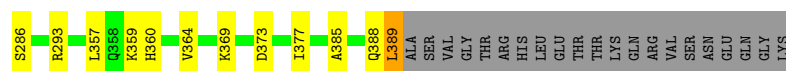


• Molecule 1: Variant surface glycoprotein

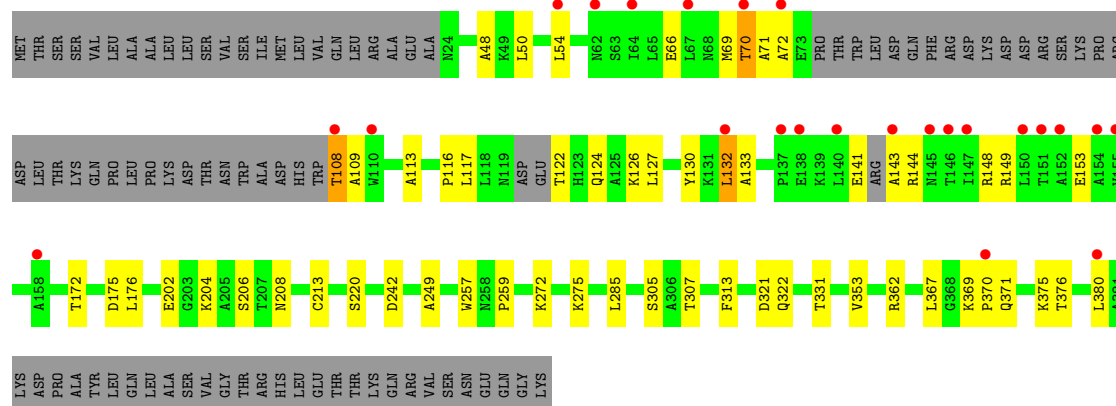


• Molecule 1: Variant surface glycoprotein

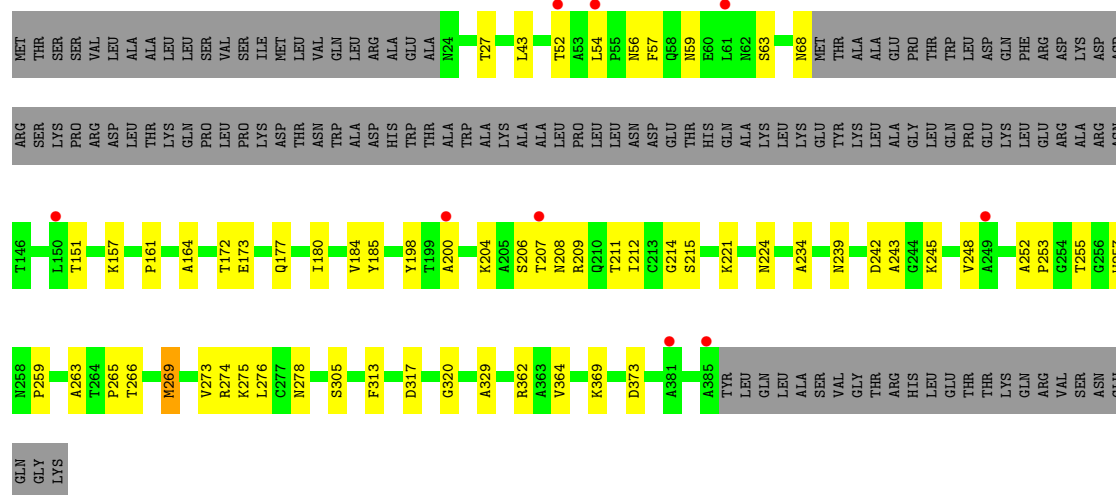




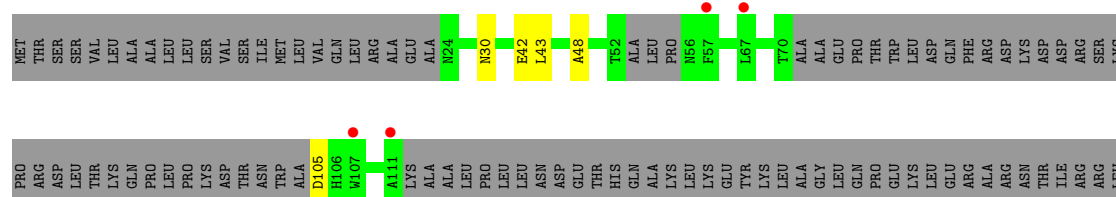
• Molecule 1: Variant surface glycoprotein

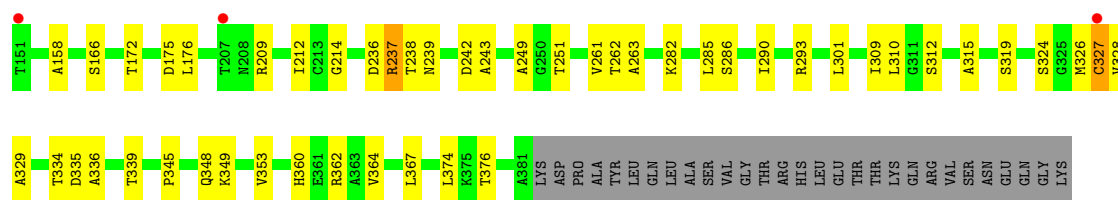


• Molecule 1: Variant surface glycoprotein

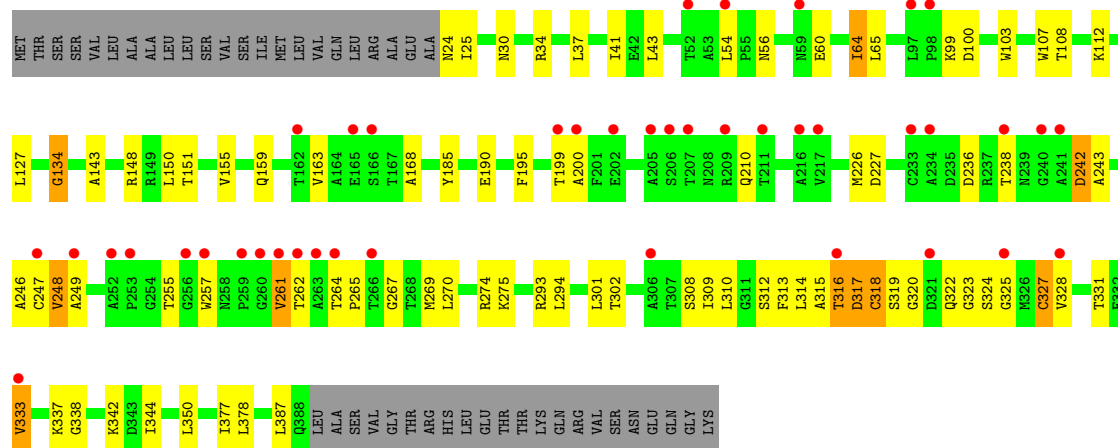


• Molecule 1: Variant surface glycoprotein

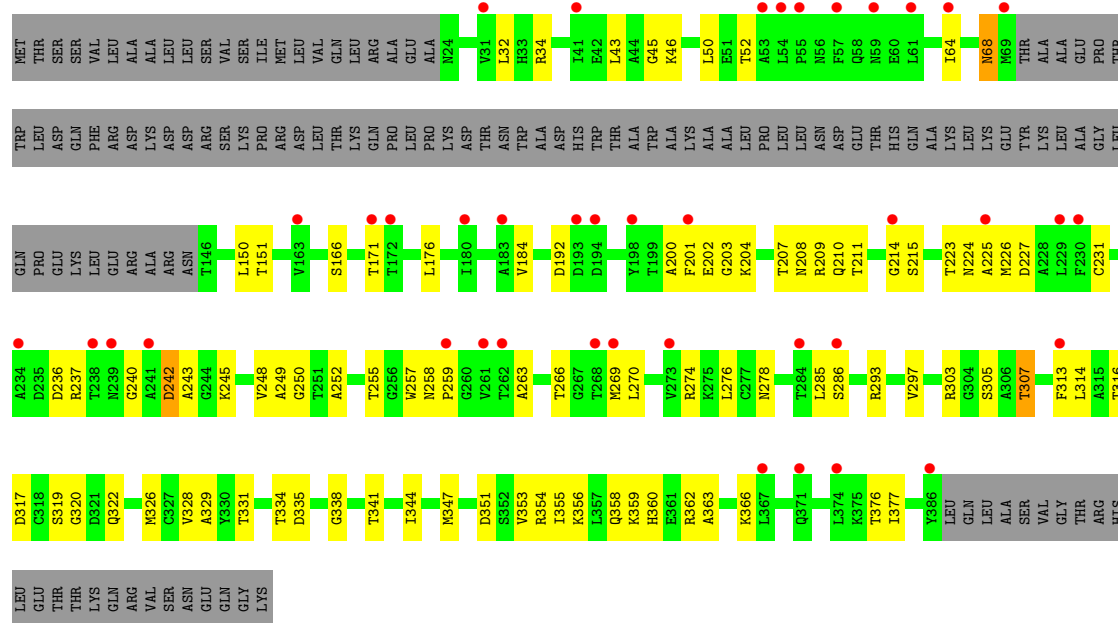




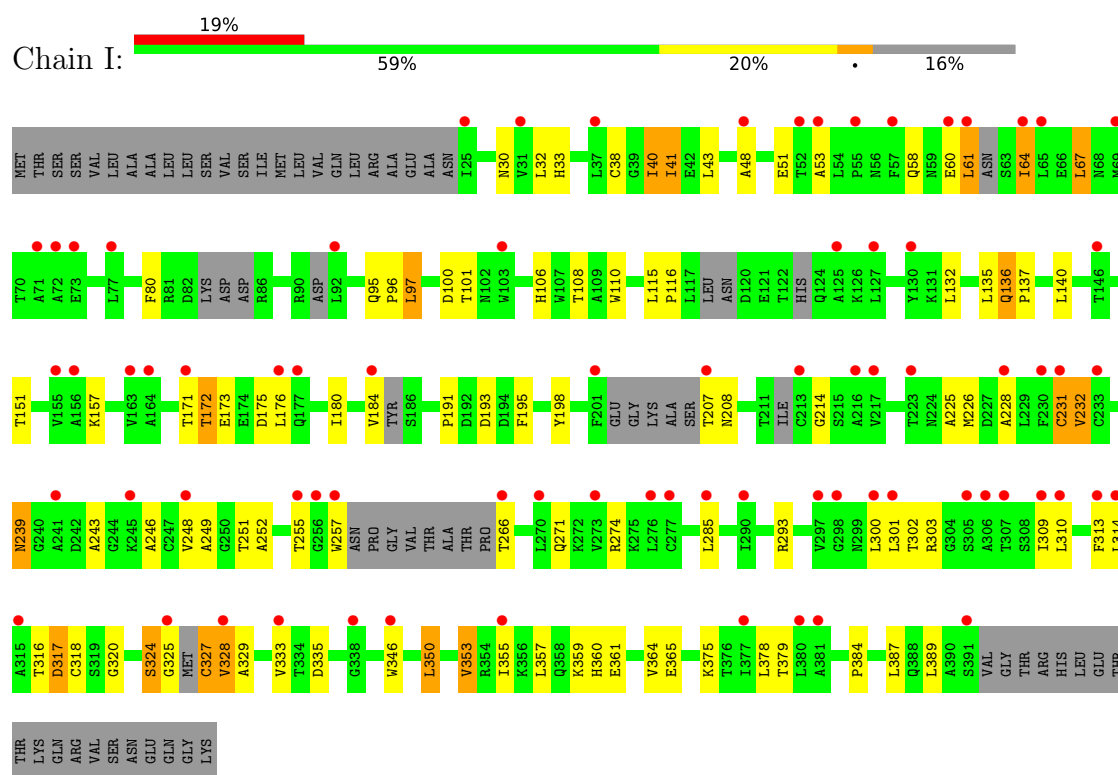
• Molecule 1: Variant surface glycoprotein



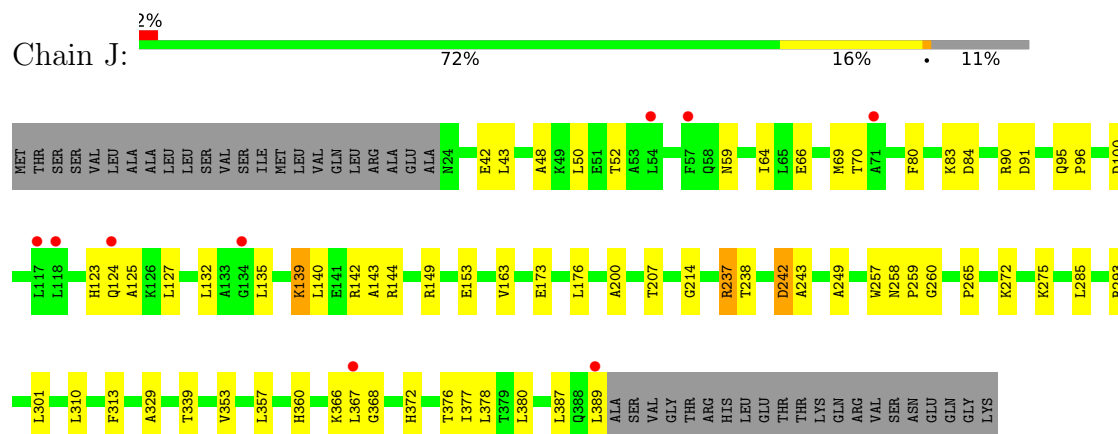
• Molecule 1: Variant surface glycoprotein



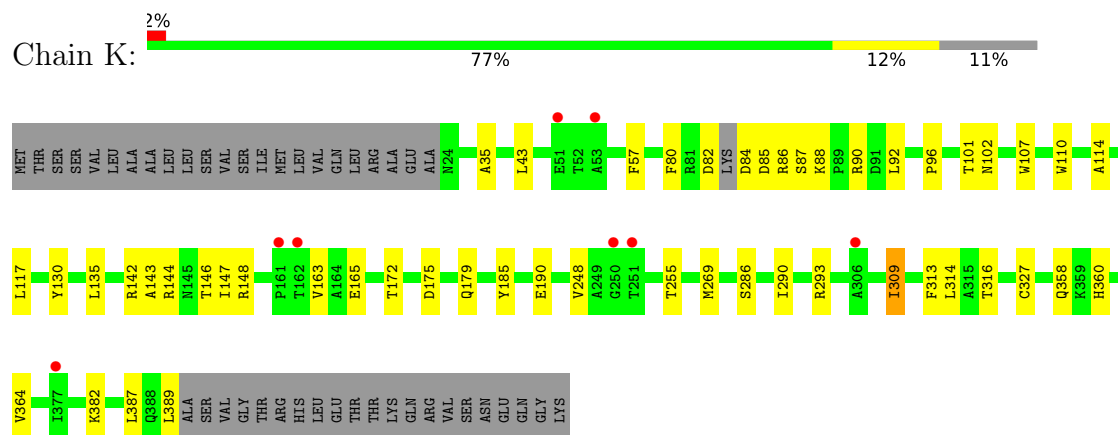
• Molecule 1: Variant surface glycoprotein



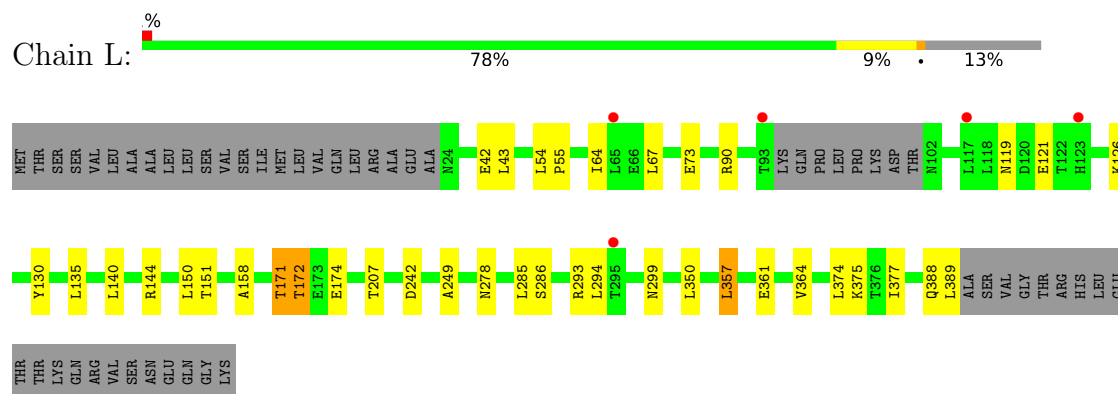
• Molecule 1: Variant surface glycoprotein



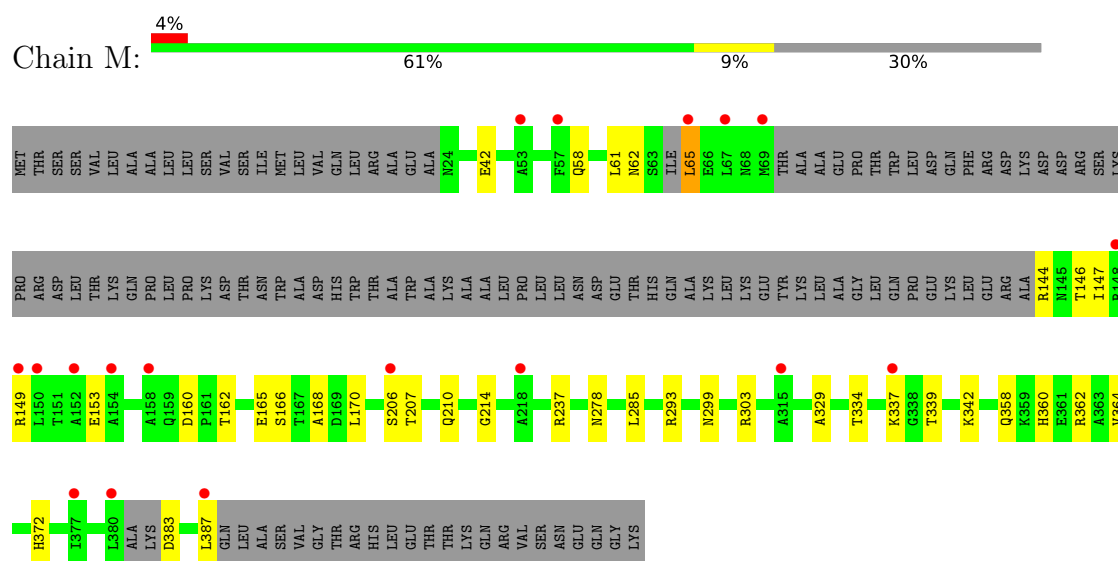
• Molecule 1: Variant surface glycoprotein



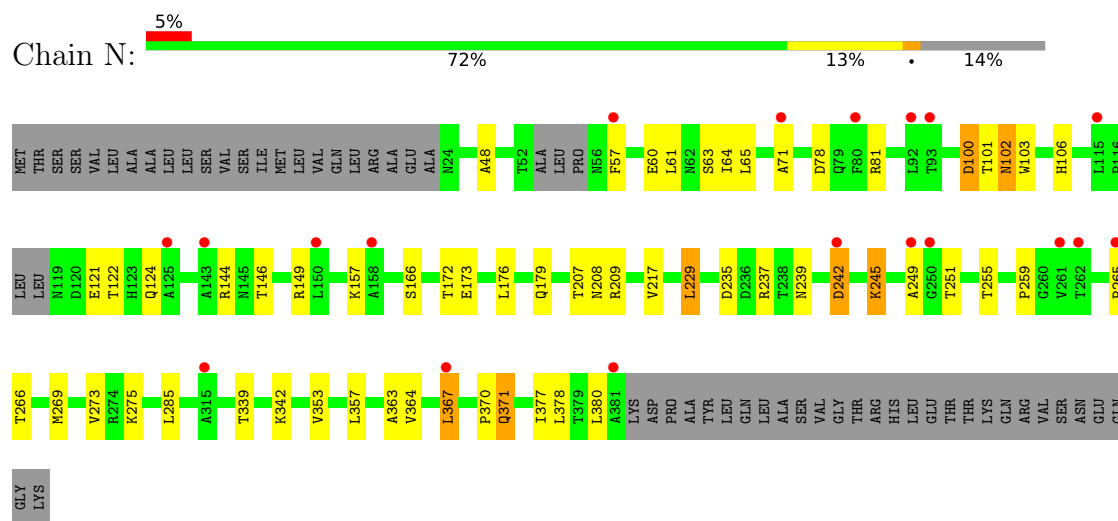
- Molecule 1: Variant surface glycoprotein



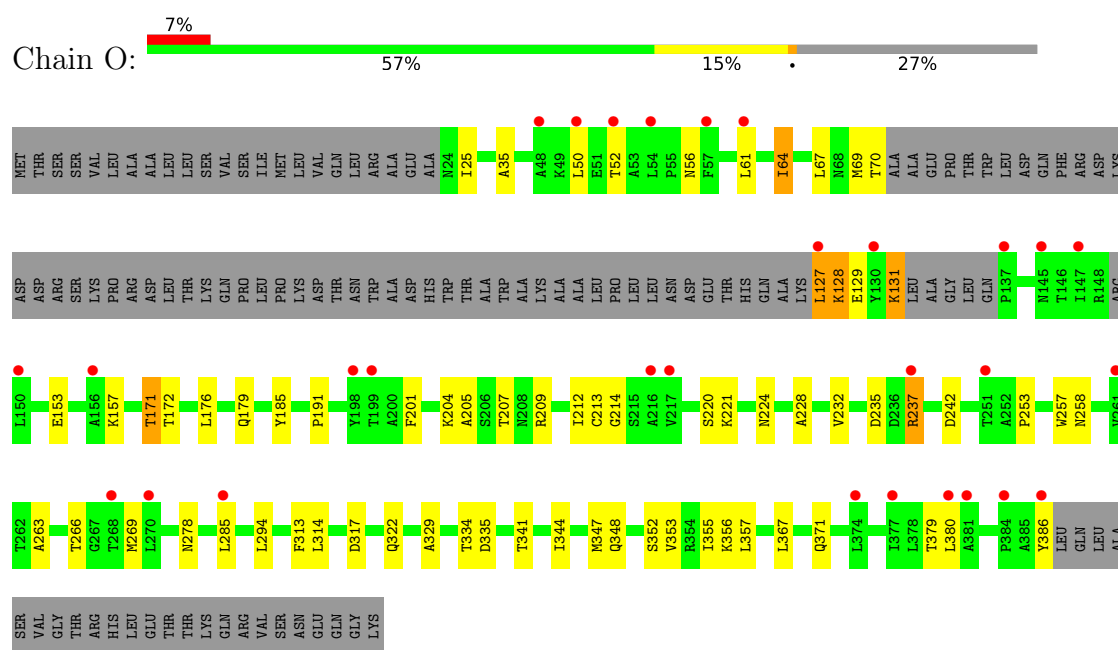
- Molecule 1: Variant surface glycoprotein



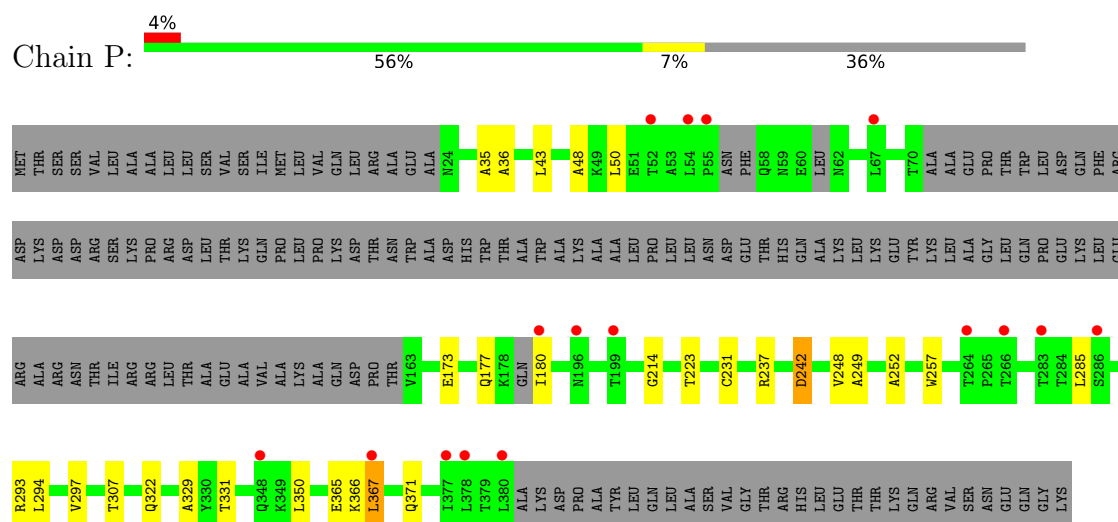
- Molecule 1: Variant surface glycoprotein



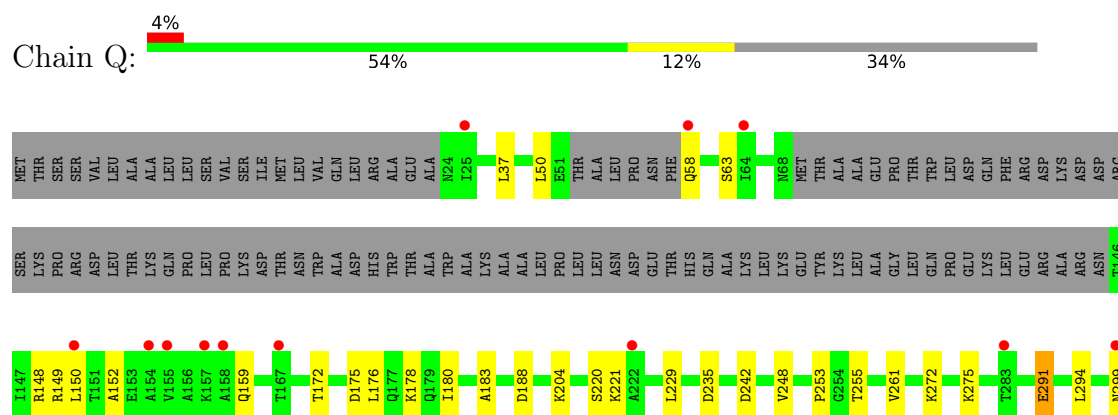
- Molecule 1: Variant surface glycoprotein

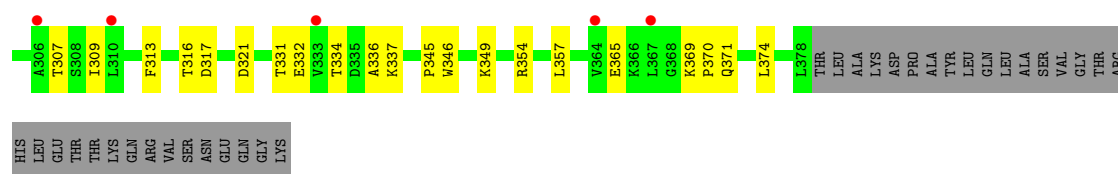


• Molecule 1: Variant surface glycoprotein

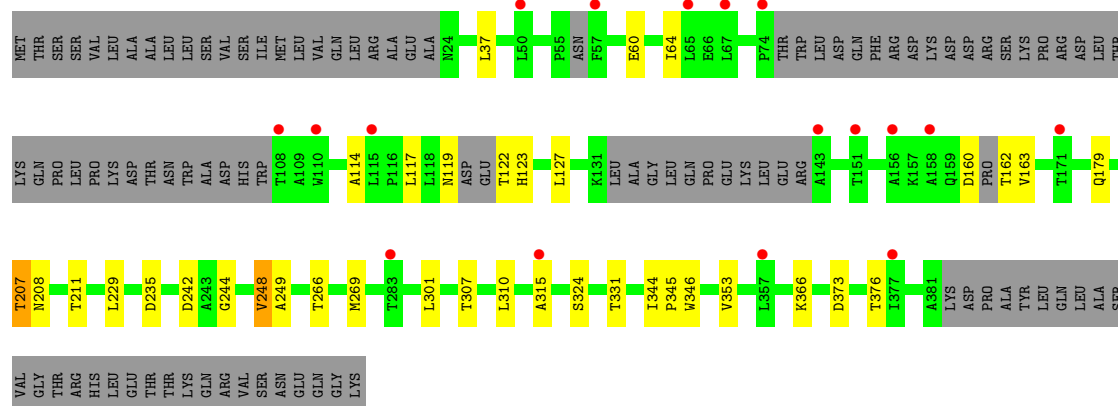


• Molecule 1: Variant surface glycoprotein

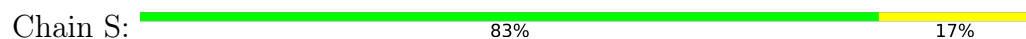




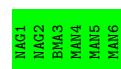
- Molecule 1: Variant surface glycoprotein



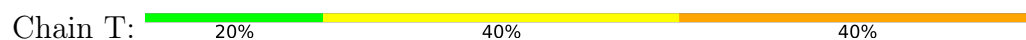
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain U:  33% 67%



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

Chain V:  100%



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

Chain X:  33% 67%



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

Chain Y:  33% 67%



- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  60% 20% 20%



- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  80% 20%



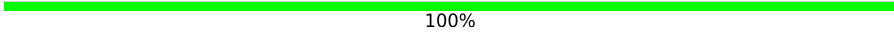
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

nose

Chain a:  40% 40% 20%

 MAG1
MAG2
BMA3
MAN4
MAN5

• Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain b:  100%

 MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.88Å 210.77Å 133.75Å 90.00° 104.54° 90.00°	Depositor
Resolution (Å)	48.81 – 2.59 48.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.81-2.59) 99.2 (48.81-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.229 , 0.270 0.229 , 0.269	Depositor DCC
R_{free} test set	10889 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	43982	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.16	0/2793	0.34	0/3795
1	B	0.17	0/2747	0.37	0/3744
1	C	0.15	0/2765	0.36	0/3761
1	D	0.16	0/2359	0.36	0/3196
1	E	0.15	0/2069	0.36	0/2810
1	F	0.14	0/2066	0.32	0/2801
1	G	0.14	0/2748	0.35	0/3742
1	H	0.14	0/2081	0.33	0/2830
1	I	0.15	0/2489	0.34	0/3386
1	J	0.19	0/2784	0.37	0/3782
1	K	0.15	0/2742	0.33	0/3736
1	L	0.14	0/2701	0.31	0/3672
1	M	0.15	0/2103	0.33	0/2855
1	N	0.15	0/2655	0.33	0/3602
1	O	0.14	0/2196	0.35	0/2980
1	P	0.14	0/1901	0.34	0/2575
1	Q	0.14	0/1987	0.35	1/2693 (0.0%)
1	R	0.14	0/2239	0.33	0/3042
All	All	0.15	0/43425	0.34	1/59002 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	261	VAL	N-CA-C	-6.25	106.71	112.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2749	0	2710	28	0
1	B	2704	0	2604	27	0
1	C	2721	0	2649	38	0
1	D	2332	0	2294	32	0
1	E	2046	0	1988	33	0
1	F	2044	0	1976	31	0
1	G	2704	0	2628	58	0
1	H	2057	0	1991	52	0
1	I	2461	0	2319	68	0
1	J	2741	0	2703	40	0
1	K	2698	0	2616	28	0
1	L	2660	0	2593	21	0
1	M	2079	0	2013	25	0
1	N	2618	0	2540	40	0
1	O	2172	0	2098	42	0
1	P	1882	0	1822	19	0
1	Q	1967	0	1916	31	0
1	R	2215	0	2143	18	0
2	S	72	0	61	1	0
2	Z	72	0	61	0	0
3	T	61	0	52	3	0
4	U	39	0	34	2	0
5	V	39	0	34	0	0
5	X	39	0	34	1	0
5	Y	39	0	34	2	0
6	W	61	0	52	2	0
6	c	61	0	52	0	0
7	a	61	0	52	3	0
7	b	61	0	52	0	0
8	A	11	0	10	0	0
8	B	11	0	10	0	0
8	C	11	0	10	0	0
8	D	11	0	10	0	0
8	E	11	0	10	0	0
8	F	11	0	10	0	0
8	H	11	0	10	0	0
8	I	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	11	0	10	0	0
8	K	11	0	10	0	0
8	L	11	0	10	0	0
8	M	11	0	10	0	0
8	N	11	0	10	0	0
8	O	11	0	10	0	0
8	P	11	0	10	0	0
8	Q	11	0	10	0	0
8	R	11	0	10	0	0
9	E	14	0	13	0	0
9	O	14	0	13	0	0
9	Q	14	0	13	0	0
9	R	14	0	13	0	0
10	A	53	0	0	3	0
10	B	43	0	0	0	0
10	C	28	0	0	0	0
10	D	19	0	0	0	0
10	E	4	0	0	0	0
10	F	12	0	0	0	0
10	J	51	0	0	0	0
10	K	13	0	0	0	0
10	L	15	0	0	0	0
10	M	20	0	0	0	0
10	N	19	0	0	0	0
10	P	2	0	0	0	0
10	R	5	0	0	0	0
All	All	43982	0	42343	596	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 7.

All (596) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:52:THR:HG21	1:J:360:HIS:HE2	1.38	0.87
1:C:127:LEU:HB3	1:C:133:ALA:HB2	1.63	0.80
1:B:92:LEU:HD21	1:B:97:LEU:HG	1.63	0.79
7:a:3:BMA:H62	7:a:5:MAN:H5	1.65	0.77
1:G:64:ILE:HG22	1:G:378:LEU:HD23	1.70	0.73
1:M:162:THR:HA	1:M:165:GLU:HG2	1.71	0.73
1:D:376:THR:HG21	1:E:157:LYS:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:119:ASN:HB3	1:R:122:THR:HB	1.72	0.72
1:K:147:ILE:HG13	1:K:387:LEU:HD11	1.72	0.72
1:A:69:MET:HE3	1:A:114:ALA:HB2	1.73	0.71
1:I:285:LEU:HG	1:I:357:LEU:HD11	1.73	0.71
1:J:272:LYS:HA	1:J:275:LYS:HE3	1.73	0.70
1:Q:334:THR:HG23	1:Q:336:ALA:H	1.58	0.69
1:N:285:LEU:HG	1:N:357:LEU:HD11	1.74	0.68
1:D:144:ARG:HG2	1:D:148:ARG:HD3	1.75	0.68
1:G:226:MET:HE1	1:G:274:ARG:HB2	1.76	0.67
1:C:90:ARG:NH2	1:C:96:PRO:O	2.27	0.67
1:G:317:ASP:CG	1:G:318:CYS:H	2.03	0.67
1:O:70:THR:HB	1:O:127:LEU:HD21	1.78	0.66
1:O:213:CYS:HA	1:O:220:SER:HB2	1.77	0.66
1:A:82:ASP:HA	1:A:95:GLN:HE22	1.60	0.66
1:E:245:LYS:HG2	1:E:252:ALA:HB2	1.78	0.66
1:H:303:ARG:NH2	1:H:338:GLY:O	2.29	0.66
1:I:300:LEU:HG	1:I:310:LEU:HD23	1.78	0.66
1:I:48:ALA:HB1	1:I:285:LEU:HD13	1.77	0.66
1:G:99:LYS:NZ	1:O:237:ARG:O	2.29	0.65
1:F:48:ALA:HB1	1:F:285:LEU:HG	1.76	0.65
1:Q:307:THR:HG22	1:Q:331:THR:HG22	1.79	0.65
1:A:101:THR:HG22	2:S:3:BMA:H4	1.78	0.65
1:C:52:THR:HG21	1:C:360:HIS:HE2	1.60	0.65
1:I:101:THR:HA	5:Y:3:BMA:H4	1.80	0.64
1:K:82:ASP:CG	1:K:84:ASP:H	2.04	0.64
1:D:127:LEU:HB3	1:D:133:ALA:HB2	1.78	0.64
1:D:202:GLU:HB2	1:D:204:LYS:HD3	1.78	0.64
1:F:212:ILE:HD11	1:F:263:ALA:HB1	1.80	0.64
1:G:37:LEU:HD21	1:G:310:LEU:HD21	1.79	0.64
1:G:34:ARG:HD3	1:G:247:CYS:HB3	1.80	0.64
1:O:209:ARG:HG3	1:O:212:ILE:HD11	1.80	0.64
1:O:201:PHE:HE2	1:O:212:ILE:HD13	1.63	0.63
1:C:98:PRO:HB2	1:C:101:THR:HB	1.80	0.63
1:P:36:ALA:HB1	1:P:297:VAL:HG12	1.81	0.63
1:N:249:ALA:HB1	1:O:313:PHE:HB3	1.80	0.63
1:D:116:PRO:O	1:D:122:THR:OG1	2.17	0.62
1:G:127:LEU:HD21	1:G:134:GLY:H	1.64	0.62
1:C:81:ARG:HG2	1:C:118:LEU:HD22	1.81	0.62
1:K:102:ASN:HB3	7:a:4:MAN:H62	1.81	0.62
1:R:179:GLN:HG2	1:R:353:VAL:HG23	1.80	0.62
1:M:146:THR:HG23	1:M:149:ARG:HH21	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:THR:HG21	1:H:356:LYS:HB3	1.82	0.62
1:H:255:THR:HB	1:H:269:MET:HB3	1.82	0.61
1:I:226:MET:HE1	1:I:274:ARG:HB3	1.81	0.61
1:I:228:ALA:HA	1:I:328:VAL:HG11	1.81	0.61
1:I:248:VAL:HG12	1:I:249:ALA:H	1.65	0.61
1:E:255:THR:HB	1:E:269:MET:HB3	1.82	0.61
1:J:64:ILE:HG13	1:J:378:LEU:HD23	1.81	0.61
1:F:172:THR:HG23	1:F:175:ASP:H	1.66	0.61
1:H:43:LEU:HD11	1:H:293:ARG:HD3	1.83	0.61
1:B:161:PRO:O	1:B:163:VAL:N	2.34	0.61
1:J:301:LEU:HD23	1:J:310:LEU:HB2	1.81	0.60
1:M:339:THR:HG23	1:O:278:ASN:HD21	1.67	0.60
1:N:176:LEU:HD22	1:N:353:VAL:HG13	1.82	0.60
1:O:237:ARG:NE	1:O:258:ASN:OD1	2.35	0.60
1:A:303:ARG:NH2	1:A:338:GLY:O	2.35	0.60
1:C:69:MET:HE3	1:C:114:ALA:HB2	1.84	0.60
1:P:307:THR:HG22	1:P:331:THR:HG22	1.84	0.60
1:F:334:THR:HG23	1:F:336:ALA:H	1.67	0.59
1:G:103:TRP:HZ2	6:W:3:BMA:H62	1.67	0.59
1:H:250:GLY:H	1:I:313:PHE:HE1	1.49	0.59
1:H:376:THR:HG21	1:I:157:LYS:HD3	1.84	0.59
1:M:299:ASN:HB3	1:O:35:ALA:HB1	1.82	0.59
1:B:81:ARG:NH2	1:B:118:LEU:O	2.34	0.59
1:L:285:LEU:HB3	1:L:357:LEU:HD11	1.83	0.59
1:D:69:MET:C	1:D:71:ALA:H	2.11	0.59
1:I:193:ASP:HA	1:I:271:GLN:HG3	1.84	0.59
1:I:384:PRO:HA	1:I:387:LEU:HD12	1.85	0.59
1:I:80:PHE:CE2	1:I:110:TRP:HB3	2.37	0.59
1:G:24:ASN:HA	1:G:314:LEU:HD11	1.84	0.58
1:D:172:THR:HG23	1:D:175:ASP:H	1.69	0.58
1:B:127:LEU:HB3	1:B:133:ALA:HB2	1.86	0.58
1:C:285:LEU:HD22	1:C:357:LEU:HD11	1.84	0.58
1:F:327:CYS:SG	1:F:328:VAL:N	2.76	0.58
1:I:318:CYS:HA	1:I:325:GLY:HA3	1.86	0.58
1:O:176:LEU:HG	1:O:353:VAL:HG13	1.85	0.58
1:N:64:ILE:HG12	1:N:378:LEU:HD23	1.86	0.58
1:K:43:LEU:HD11	1:K:293:ARG:HD3	1.86	0.58
1:B:78:ASP:HA	1:B:81:ARG:HD2	1.86	0.58
1:H:259:PRO:HA	1:H:263:ALA:HA	1.85	0.58
1:L:43:LEU:HD11	1:L:293:ARG:HD3	1.86	0.57
1:A:179:GLN:HE22	1:A:349:LYS:HG2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:THR:HG1	1:C:103:TRP:CG	2.21	0.57
1:C:148:ARG:HG2	4:U:1:NAG:H5	1.87	0.57
1:C:43:LEU:HD11	1:C:293:ARG:HD3	1.86	0.57
1:C:80:PHE:HA	1:C:107:TRP:HH2	1.70	0.57
1:N:60:GLU:CD	1:N:60:GLU:H	2.12	0.57
1:A:127:LEU:HB3	1:A:133:ALA:HB2	1.85	0.57
1:K:85:ASP:C	1:K:87:SER:H	2.12	0.57
1:D:72:ALA:HA	1:D:144:ARG:HE	1.69	0.56
1:I:232:VAL:HG23	1:I:327:CYS:HA	1.88	0.56
1:J:260:GLY:O	1:M:237:ARG:NH2	2.38	0.56
1:P:248:VAL:HG22	1:P:249:ALA:H	1.70	0.56
1:F:309:ILE:HG23	1:F:327:CYS:SG	2.46	0.56
1:I:361:GLU:O	1:I:365:GLU:HG2	2.06	0.56
1:J:48:ALA:HB1	1:J:285:LEU:HG	1.88	0.56
1:R:207:THR:OG1	1:R:211:THR:OG1	2.22	0.56
1:Q:365:GLU:O	1:Q:369:LYS:NZ	2.37	0.56
1:H:34:ARG:NH2	1:I:300:LEU:O	2.39	0.56
1:P:249:ALA:HB1	1:Q:313:PHE:HB3	1.88	0.56
1:D:272:LYS:HA	1:D:275:LYS:HD3	1.87	0.55
1:A:272:LYS:HA	1:A:275:LYS:HD2	1.87	0.55
1:E:275:LYS:HG2	1:F:335:ASP:HB2	1.87	0.55
1:R:207:THR:OG1	1:R:208:ASN:N	2.35	0.55
1:I:95:GLN:C	1:I:97:LEU:H	2.15	0.55
1:N:266:THR:H	1:N:269:MET:HE3	1.72	0.55
1:Q:58:GLN:HB2	1:Q:371:GLN:HB2	1.88	0.55
1:H:266:THR:H	1:H:269:MET:HE2	1.70	0.55
1:K:101:THR:HG22	7:a:3:BMA:H4	1.89	0.55
1:B:257:TRP:CE2	1:B:259:PRO:HG3	2.42	0.55
1:G:210:GLN:HG2	1:G:319:SER:HB2	1.88	0.55
1:H:200:ALA:HB2	1:H:270:LEU:HD11	1.87	0.55
1:C:83:LYS:H	1:C:95:GLN:NE2	2.05	0.55
1:I:136:GLN:HG2	1:I:137:PRO:HD2	1.88	0.55
1:J:90:ARG:HE	1:J:95:GLN:HB3	1.72	0.55
1:M:42:GLU:OE2	1:M:293:ARG:NH1	2.30	0.55
1:C:149:ARG:NH1	1:C:153:GLU:OE2	2.39	0.55
1:I:80:PHE:HE2	1:I:110:TRP:HB3	1.71	0.55
1:L:158:ALA:HB2	1:L:374:LEU:HD11	1.89	0.55
1:E:200:ALA:HB3	1:E:265:PRO:HD2	1.89	0.54
1:F:42:GLU:OE2	1:F:293:ARG:NH2	2.37	0.54
1:N:102:ASN:C	1:N:102:ASN:HD22	2.14	0.54
1:B:43:LEU:HD11	1:B:293:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:168:ALA:HB1	1:M:337:LYS:HD3	1.88	0.54
1:G:316:THR:OG1	1:G:324:SER:HA	2.08	0.54
1:E:209:ARG:HE	1:E:257:TRP:HZ3	1.56	0.54
1:Q:334:THR:HG22	1:Q:337:LYS:HG3	1.89	0.54
1:G:242:ASP:HB3	1:G:322:GLN:HG2	1.90	0.54
1:R:160:ASP:C	1:R:163:VAL:H	2.16	0.54
1:B:115:LEU:HA	1:B:118:LEU:HD13	1.90	0.54
1:K:143:ALA:HA	1:K:387:LEU:HD12	1.88	0.54
1:N:235:ASP:O	1:N:255:THR:OG1	2.23	0.54
1:O:242:ASP:OD2	1:O:322:GLN:NE2	2.39	0.54
1:G:342:LYS:C	1:G:344:ILE:H	2.16	0.54
1:C:89:PRO:HG3	1:C:115:LEU:HD11	1.91	0.53
1:L:172:THR:OG1	1:L:174:GLU:OE1	2.25	0.53
1:B:157:LYS:HD3	1:B:373:ASP:HB3	1.90	0.53
1:H:297:VAL:HG13	1:H:347:MET:HE2	1.91	0.53
1:H:34:ARG:HH12	1:I:302:THR:HA	1.73	0.53
1:P:50:LEU:HB3	1:P:173:GLU:HB2	1.90	0.53
1:A:369:LYS:HD2	1:C:369:LYS:HD3	1.90	0.53
1:K:172:THR:HG23	1:K:175:ASP:H	1.73	0.53
1:B:84:ASP:OD1	1:B:84:ASP:N	2.40	0.53
1:K:309:ILE:HG22	1:K:327:CYS:HB2	1.90	0.53
1:N:101:THR:HG23	1:N:103:TRP:H	1.73	0.53
1:N:377:ILE:HA	1:N:380:LEU:HD12	1.89	0.53
1:C:101:THR:HG23	1:C:103:TRP:H	1.73	0.53
1:H:150:LEU:HB3	1:H:377:ILE:HG23	1.90	0.53
1:G:200:ALA:HB2	1:G:270:LEU:HD11	1.91	0.53
1:G:248:VAL:HG12	1:G:249:ALA:H	1.74	0.53
1:J:257:TRP:CE2	1:J:259:PRO:HG3	2.43	0.52
1:N:78:ASP:OD1	1:N:81:ARG:NH2	2.42	0.52
1:J:83:LYS:H	1:J:95:GLN:HE22	1.57	0.52
1:D:307:THR:HG22	1:D:331:THR:HG22	1.92	0.52
1:M:372:HIS:NE2	1:N:370:PRO:HG3	2.25	0.52
1:G:314:LEU:HD12	1:G:323:GLY:HA2	1.91	0.52
1:H:257:TRP:CD1	1:H:258:ASN:H	2.28	0.52
1:E:206:SER:OG	1:E:207:THR:N	2.40	0.52
1:F:176:LEU:HD22	1:F:353:VAL:HG13	1.92	0.52
1:P:367:LEU:O	1:P:371:GLN:HG2	2.10	0.52
1:Q:172:THR:HG23	1:Q:175:ASP:H	1.74	0.52
1:I:316:THR:HB	1:I:324:SER:HB3	1.90	0.52
1:O:224:ASN:OD1	1:O:224:ASN:N	2.42	0.52
1:Q:346:TRP:HA	1:Q:349:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:GLY:HA3	1:F:329:ALA:HB3	1.92	0.52
1:I:251:THR:HG22	1:I:252:ALA:H	1.75	0.52
1:Q:309:ILE:HG21	1:Q:313:PHE:HB2	1.91	0.52
1:R:248:VAL:HG12	1:R:249:ALA:H	1.74	0.52
1:J:249:ALA:HB1	1:K:313:PHE:CD1	2.45	0.52
1:E:369:LYS:NZ	1:E:373:ASP:OD2	2.42	0.52
1:J:139:LYS:NZ	1:J:142:ARG:HE	2.08	0.52
1:N:57:PHE:HA	1:N:371:GLN:NE2	2.23	0.51
1:G:242:ASP:OD1	1:G:242:ASP:N	2.42	0.51
1:M:278:ASN:HD21	1:N:339:THR:HG23	1.74	0.51
1:R:315:ALA:HB3	1:R:324:SER:HA	1.92	0.51
1:K:130:TYR:HA	1:K:382:LYS:HE3	1.92	0.51
1:F:243:ALA:HB1	1:F:326:MET:HG3	1.92	0.51
1:H:192:ASP:OD1	1:H:192:ASP:N	2.44	0.51
1:N:101:THR:HG1	1:N:103:TRP:CD1	2.29	0.51
1:A:57:PHE:CE1	1:A:370:PRO:HB2	2.46	0.51
1:E:273:VAL:HA	1:E:276:LEU:HD12	1.93	0.51
1:F:315:ALA:HB3	1:F:324:SER:HA	1.93	0.51
1:K:144:ARG:O	1:K:148:ARG:HG3	2.10	0.51
1:J:123:HIS:C	1:J:125:ALA:H	2.19	0.51
1:K:57:PHE:HZ	1:K:163:VAL:HG11	1.76	0.51
1:E:242:ASP:OD1	1:E:243:ALA:N	2.42	0.50
1:J:66:GLU:O	1:J:70:THR:HG23	2.11	0.50
1:N:71:ALA:O	1:N:144:ARG:NH1	2.44	0.50
1:N:78:ASP:HA	1:N:81:ARG:HE	1.76	0.50
1:F:261:VAL:HG23	1:F:262:THR:HG23	1.94	0.50
1:I:375:LYS:O	1:I:379:THR:HG23	2.11	0.50
1:Q:316:THR:OG1	1:Q:317:ASP:OD1	2.29	0.50
1:L:64:ILE:HG22	1:L:151:THR:HG23	1.93	0.50
1:D:69:MET:C	1:D:71:ALA:N	2.70	0.50
1:D:122:THR:O	1:D:126:LYS:HG3	2.11	0.50
1:K:255:THR:HB	1:K:269:MET:HB3	1.94	0.50
1:G:148:ARG:HG2	6:W:1:NAG:H5	1.93	0.50
1:I:225:ALA:HB2	1:I:346:TRP:CE3	2.46	0.50
1:B:114:ALA:HA	1:B:117:LEU:HD12	1.92	0.50
1:D:371:GLN:HG2	1:D:375:LYS:HE3	1.94	0.50
1:G:301:LEU:HD23	1:G:310:LEU:HB2	1.93	0.50
1:R:373:ASP:HA	1:R:376:THR:HG22	1.94	0.50
1:D:369:LYS:HB2	1:D:370:PRO:HD3	1.94	0.50
1:B:91:ASP:HB2	1:B:94:LYS:HB2	1.93	0.50
1:B:148:ARG:HD3	3:T:1:NAG:O4	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:GLU:HA	1:D:113:ALA:HB1	1.93	0.50
1:O:242:ASP:OD1	1:O:242:ASP:N	2.44	0.50
1:Q:248:VAL:HG11	1:Q:253:PRO:HD3	1.94	0.50
1:E:185:TYR:OH	1:E:274:ARG:HD2	2.12	0.50
1:E:212:ILE:HD11	1:E:263:ALA:HB1	1.94	0.50
1:I:64:ILE:HG22	1:I:151:THR:HG22	1.94	0.49
1:I:303:ARG:HD3	1:I:335:ASP:HA	1.94	0.49
1:G:64:ILE:HG13	1:G:65:LEU:N	2.27	0.49
1:H:176:LEU:HD23	1:H:285:LEU:HD13	1.94	0.49
1:I:43:LEU:HD11	1:I:293:ARG:HD3	1.93	0.49
1:Q:220:SER:OG	1:Q:221:LYS:N	2.45	0.49
1:F:166:SER:HB2	1:F:367:LEU:HD13	1.93	0.49
1:Q:317:ASP:OD1	1:Q:317:ASP:N	2.46	0.49
1:A:208:ASN:OD1	1:A:210:GLN:HG2	2.12	0.49
1:G:261:VAL:HG12	1:G:262:THR:HG23	1.94	0.49
1:H:201:PHE:C	1:H:203:GLY:H	2.21	0.49
1:M:303:ARG:NH1	1:M:334:THR:O	2.44	0.49
1:O:294:LEU:HD22	1:O:347:MET:HE3	1.92	0.49
1:C:142:ARG:HD3	1:C:388:GLN:HA	1.94	0.49
1:G:25:ILE:HG13	1:G:325:GLY:HA2	1.94	0.49
1:G:30:ASN:HB2	1:G:246:ALA:HB1	1.93	0.49
1:D:141:GLU:O	1:D:143:ALA:N	2.46	0.49
1:E:239:ASN:HB2	1:E:243:ALA:HB3	1.94	0.49
1:R:235:ASP:HB3	1:R:244:GLY:HA3	1.94	0.49
1:A:82:ASP:HB3	1:A:90:ARG:HA	1.94	0.49
1:K:82:ASP:CG	1:K:84:ASP:N	2.71	0.49
1:R:301:LEU:HD23	1:R:310:LEU:HB2	1.95	0.49
1:P:294:LEU:HD21	1:P:350:LEU:HB3	1.94	0.49
1:B:164:ALA:H	1:B:167:THR:HG23	1.77	0.49
1:D:69:MET:O	1:D:71:ALA:N	2.46	0.48
1:A:56:ASN:OD1	1:A:59:ASN:ND2	2.46	0.48
1:G:317:ASP:OD1	1:G:319:SER:N	2.46	0.48
1:H:210:GLN:HB3	1:H:319:SER:HB3	1.95	0.48
1:I:64:ILE:HG12	1:I:378:LEU:HD23	1.95	0.48
1:L:171:THR:HG22	1:L:172:THR:H	1.78	0.48
1:J:285:LEU:HD22	1:J:357:LEU:HD11	1.96	0.48
1:J:366:LYS:C	1:J:368:GLY:H	2.22	0.48
1:N:121:GLU:O	1:N:124:GLN:NE2	2.46	0.48
1:O:56:ASN:O	1:O:371:GLN:NE2	2.44	0.48
1:G:257:TRP:CD1	1:G:269:MET:HE1	2.49	0.48
1:I:248:VAL:HG12	1:I:249:ALA:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:200:ALA:HB3	1:J:265:PRO:HD2	1.94	0.48
1:C:124:GLN:O	1:C:128:LYS:HD2	2.13	0.48
1:E:198:TYR:OH	1:E:224:ASN:ND2	2.43	0.48
1:J:237:ARG:HG3	1:J:258:ASN:HB2	1.94	0.48
1:Q:332:GLU:N	1:Q:332:GLU:OE1	2.46	0.48
1:Q:183:ALA:HB2	1:Q:349:LYS:HB2	1.96	0.48
1:A:57:PHE:HE1	1:A:370:PRO:HB2	1.78	0.48
1:B:372:HIS:NE2	1:C:162:THR:HG21	2.29	0.48
1:H:176:LEU:HG	1:H:353:VAL:HG13	1.96	0.48
1:N:146:THR:HG22	1:N:149:ARG:HH21	1.78	0.48
1:O:50:LEU:C	1:O:52:THR:H	2.21	0.48
1:R:307:THR:HG22	1:R:331:THR:HG22	1.95	0.48
1:C:55:PRO:HD3	1:C:364:VAL:HG22	1.95	0.48
1:D:70:THR:HB	1:D:117:LEU:HD11	1.96	0.48
1:I:38:CYS:HA	1:I:41:ILE:HG12	1.96	0.48
1:O:257:TRP:HD1	1:O:269:MET:HE1	1.78	0.48
1:O:317:ASP:OD1	1:O:317:ASP:N	2.47	0.48
1:Q:242:ASP:OD1	1:Q:242:ASP:N	2.45	0.48
1:H:209:ARG:NH1	1:H:326:MET:SD	2.87	0.47
1:I:214:GLY:HA3	1:I:329:ALA:HB3	1.95	0.47
1:I:309:ILE:HG13	1:I:328:VAL:O	2.14	0.47
1:G:317:ASP:O	1:G:318:CYS:HB2	2.13	0.47
1:O:25:ILE:HG13	1:O:314:LEU:HD12	1.96	0.47
1:D:70:THR:HG21	1:D:130:TYR:HD2	1.79	0.47
1:H:351:ASP:OD1	1:H:354:ARG:NH1	2.47	0.47
1:J:90:ARG:NH2	1:J:96:PRO:O	2.48	0.47
1:L:135:LEU:HD12	1:L:140:LEU:HD23	1.96	0.47
1:N:239:ASN:HB2	1:N:242:ASP:O	2.14	0.47
1:A:99:LYS:NZ	10:A:606:HOH:O	2.48	0.47
1:E:173:GLU:O	1:E:177:GLN:HG3	2.14	0.47
1:E:278:ASN:HD21	1:F:339:THR:HG23	1.79	0.47
1:N:229:LEU:HD13	1:N:273:VAL:HG12	1.96	0.47
1:P:365:GLU:HG3	1:P:366:LYS:HE2	1.97	0.47
1:C:80:PHE:HA	1:C:107:TRP:CH2	2.48	0.47
1:H:52:THR:HG21	1:H:360:HIS:CD2	2.49	0.47
1:H:184:VAL:HA	1:H:225:ALA:HB3	1.96	0.47
1:H:208:ASN:HA	1:H:259:PRO:HB2	1.96	0.47
1:I:173:GLU:C	1:I:175:ASP:H	2.23	0.47
1:J:90:ARG:NE	1:J:95:GLN:HB3	2.29	0.47
1:A:71:ALA:O	1:A:144:ARG:NE	2.47	0.47
1:G:319:SER:OG	1:G:320:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:344:ILE:HD11	1:H:347:MET:SD	2.55	0.47
1:K:360:HIS:O	1:K:364:VAL:HG13	2.15	0.47
1:Q:204:LYS:HE2	1:Q:221:LYS:HG2	1.96	0.47
1:Q:235:ASP:O	1:Q:255:THR:OG1	2.32	0.47
1:C:148:ARG:NH2	4:U:2:NAG:H83	2.30	0.47
1:B:111:ALA:O	1:B:115:LEU:N	2.43	0.47
1:F:105:ASP:OD1	1:F:105:ASP:N	2.45	0.47
1:H:214:GLY:HA3	1:H:329:ALA:HB3	1.97	0.47
1:J:339:THR:HG23	1:L:278:ASN:HD21	1.80	0.47
1:D:321:ASP:OD1	1:D:322:GLN:N	2.48	0.47
1:N:245:LYS:HE2	1:N:245:LYS:HB3	1.73	0.47
1:A:144:ARG:O	1:A:148:ARG:HG3	2.15	0.46
1:C:220:SER:OG	1:C:221:LYS:N	2.48	0.46
1:J:42:GLU:OE2	1:J:293:ARG:NH2	2.47	0.46
1:N:166:SER:HB3	1:N:363:ALA:HB1	1.97	0.46
1:Q:272:LYS:HA	1:Q:275:LYS:HE3	1.96	0.46
1:Q:345:PRO:O	1:Q:349:LYS:HG2	2.15	0.46
1:D:176:LEU:HG	1:D:353:VAL:HG13	1.96	0.46
1:H:202:GLU:OE1	1:H:204:LYS:HG2	2.16	0.46
1:I:195:PHE:CD1	1:I:271:GLN:HG2	2.50	0.46
1:N:100:ASP:OD1	1:N:100:ASP:N	2.49	0.46
1:G:265:PRO:HB3	1:G:269:MET:HE2	1.97	0.46
1:L:73:GLU:HG3	1:L:144:ARG:CZ	2.46	0.46
1:M:153:GLU:HA	1:O:380:LEU:HD11	1.98	0.46
1:M:206:SER:OG	1:M:207:THR:N	2.48	0.46
1:D:48:ALA:HB1	1:D:285:LEU:HG	1.97	0.46
1:K:35:ALA:HB1	1:L:299:ASN:HB3	1.98	0.46
1:O:352:SER:O	1:O:356:LYS:HG2	2.14	0.46
1:F:158:ALA:HB2	1:F:374:LEU:HD11	1.97	0.46
1:I:184:VAL:HG13	1:I:226:MET:HB2	1.98	0.46
1:O:128:LYS:HG2	1:O:131:LYS:HD3	1.98	0.46
1:A:80:PHE:CE2	1:A:110:TRP:HB3	2.50	0.46
1:B:103:TRP:HE1	3:T:2:NAG:H3	1.81	0.46
1:C:80:PHE:CE1	1:C:110:TRP:HB3	2.51	0.46
1:I:207:THR:OG1	1:I:208:ASN:N	2.49	0.46
1:J:242:ASP:HB2	1:J:243:ALA:H	1.55	0.46
1:K:92:LEU:HD11	1:K:107:TRP:CD1	2.50	0.46
1:N:237:ARG:HA	1:N:237:ARG:HD2	1.79	0.46
1:A:25:ILE:HD12	1:A:312:SER:HB3	1.97	0.46
1:H:215:SER:O	1:H:307:THR:HG21	2.16	0.46
1:J:132:LEU:HA	1:J:135:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:344:ILE:O	1:O:348:GLN:HG3	2.15	0.46
1:P:177:GLN:C	1:P:180:ILE:H	2.23	0.46
1:B:259:PRO:HA	1:B:263:ALA:HA	1.98	0.46
1:E:68:ASN:HA	1:E:151:THR:HG21	1.97	0.46
1:H:224:ASN:ND2	1:H:227:ASP:OD2	2.49	0.46
1:N:48:ALA:HB1	1:N:285:LEU:HD13	1.97	0.46
1:B:48:ALA:HB1	1:B:285:LEU:HG	1.97	0.46
1:F:301:LEU:HD23	1:F:310:LEU:HB2	1.98	0.46
1:H:208:ASN:ND2	1:H:210:GLN:OE1	2.41	0.46
1:I:191:PRO:HG2	1:I:195:PHE:CE2	2.51	0.46
1:L:119:ASN:OD1	1:L:121:GLU:N	2.49	0.46
1:I:239:ASN:ND2	1:I:320:GLY:O	2.44	0.46
1:J:100:ASP:OD1	1:J:100:ASP:N	2.46	0.46
1:A:342:LYS:NZ	10:A:608:HOH:O	2.49	0.45
1:J:313:PHE:CD1	1:L:249:ALA:HB1	2.51	0.45
1:P:366:LYS:HD3	1:P:366:LYS:HA	1.75	0.45
1:B:372:HIS:NE2	1:C:160:ASP:OD2	2.49	0.45
1:I:58:GLN:O	1:I:60:GLU:N	2.48	0.45
1:I:171:THR:OG1	1:I:172:THR:N	2.47	0.45
1:J:50:LEU:HB3	1:J:173:GLU:HB2	1.97	0.45
1:P:214:GLY:HA3	1:P:329:ALA:HB3	1.98	0.45
1:C:101:THR:C	1:C:103:TRP:H	2.24	0.45
1:J:43:LEU:HD11	1:J:293:ARG:HD3	1.99	0.45
1:N:208:ASN:OD1	1:N:208:ASN:N	2.50	0.45
1:F:209:ARG:HD3	1:F:319:SER:C	2.41	0.45
1:G:342:LYS:O	1:G:344:ILE:N	2.44	0.45
1:K:146:THR:OG1	1:K:387:LEU:HD13	2.16	0.45
1:C:172:THR:HG23	1:C:175:ASP:H	1.81	0.45
1:G:64:ILE:HD12	1:G:151:THR:HA	1.99	0.45
1:H:237:ARG:HD2	1:H:258:ASN:HB2	1.99	0.45
1:M:165:GLU:HG3	1:M:166:SER:N	2.31	0.45
1:N:342:LYS:HE2	1:N:342:LYS:HB2	1.78	0.45
1:Q:149:ARG:HA	1:Q:152:ALA:HB3	1.99	0.45
1:F:237:ARG:HD2	1:F:237:ARG:HA	1.70	0.45
1:H:45:GLY:C	1:H:46:LYS:HD2	2.41	0.45
1:R:60:GLU:CD	1:R:60:GLU:H	2.24	0.45
1:H:215:SER:HB2	1:H:317:ASP:HB3	1.98	0.45
1:J:124:GLN:HA	1:J:127:LEU:HD12	1.99	0.45
1:J:372:HIS:O	1:J:376:THR:HG23	2.17	0.45
1:P:248:VAL:HG11	1:P:252:ALA:HA	1.97	0.45
3:T:3:BMA:H61	3:T:5:MAN:H2	1.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:LYS:HA	1:E:221:LYS:HD3	1.76	0.45
1:H:334:THR:OG1	1:H:335:ASP:N	2.50	0.45
1:I:350:LEU:O	1:I:353:VAL:HG22	2.17	0.45
1:O:214:GLY:HA3	1:O:329:ALA:HB3	1.99	0.45
1:I:32:LEU:HD12	1:I:33:HIS:N	2.32	0.45
1:L:375:LYS:HB2	1:L:375:LYS:HE3	1.76	0.45
1:D:213:CYS:O	1:D:220:SER:HB2	2.17	0.45
1:E:248:VAL:HG21	1:E:253:PRO:HD3	1.99	0.45
1:G:150:LEU:HB3	1:G:377:ILE:HG23	1.99	0.45
1:L:357:LEU:O	1:L:361:GLU:HG3	2.16	0.45
1:G:60:GLU:O	1:G:64:ILE:HG23	2.17	0.44
1:I:132:LEU:HA	1:I:135:LEU:HD11	2.00	0.44
1:M:62:ASN:O	1:M:65:LEU:HG	2.16	0.44
1:Q:370:PRO:O	1:Q:374:LEU:HB2	2.16	0.44
1:C:84:ASP:OD1	1:C:85:ASP:N	2.50	0.44
1:G:100:ASP:OD1	1:G:100:ASP:N	2.49	0.44
1:G:275:LYS:HB2	1:H:335:ASP:HB2	1.99	0.44
1:H:243:ALA:HB2	1:H:322:GLN:HB3	1.99	0.44
1:H:249:ALA:HB1	1:I:313:PHE:CD1	2.51	0.44
1:M:58:GLN:O	1:M:61:LEU:N	2.49	0.44
1:M:372:HIS:CD2	1:N:157:LYS:HE3	2.52	0.44
1:H:358:GLN:OE1	1:H:362:ARG:NH2	2.51	0.44
1:O:334:THR:HG22	1:O:335:ASP:H	1.82	0.44
1:Q:178:LYS:HE2	1:Q:188:ASP:HB3	2.00	0.44
1:E:204:LYS:NZ	1:K:165:GLU:HG3	2.32	0.44
1:E:266:THR:HG22	1:E:269:MET:SD	2.57	0.44
1:F:345:PRO:O	1:F:348:GLN:HG3	2.16	0.44
1:L:150:LEU:HB3	1:L:377:ILE:HG23	2.00	0.44
1:Q:148:ARG:C	1:Q:150:LEU:H	2.25	0.44
1:D:257:TRP:CE2	1:D:259:PRO:HG3	2.52	0.44
1:G:43:LEU:HD11	1:G:293:ARG:HD3	1.99	0.44
1:K:142:ARG:NH2	1:K:389:LEU:O	2.51	0.44
1:N:172:THR:OG1	1:N:173:GLU:N	2.50	0.44
1:O:204:LYS:HB2	1:O:221:LYS:HG2	1.99	0.44
1:G:155:VAL:O	1:G:159:GLN:HB2	2.18	0.44
1:G:242:ASP:HB2	1:G:243:ALA:H	1.61	0.44
1:J:69:MET:HE1	1:J:80:PHE:CE1	2.52	0.44
1:B:386:TYR:CE1	1:C:149:ARG:HG3	2.53	0.44
1:I:61:LEU:HD12	1:I:61:LEU:HA	1.82	0.44
1:P:35:ALA:HB1	1:Q:299:ASN:HB3	1.99	0.44
1:P:48:ALA:HB1	1:P:285:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:ALA:HB1	1:H:313:PHE:CD1	2.53	0.44
1:H:278:ASN:HA	1:I:303:ARG:HH12	1.83	0.44
1:O:171:THR:HG22	1:O:172:THR:H	1.82	0.44
1:O:352:SER:HA	1:O:355:ILE:HG12	1.99	0.44
1:F:362:ARG:HE	1:F:362:ARG:HB2	1.46	0.44
1:J:50:LEU:HG	1:J:52:THR:HG22	2.00	0.44
1:J:149:ARG:O	1:J:153:GLU:HG3	2.17	0.44
1:N:275:LYS:HE2	1:O:335:ASP:HB2	2.00	0.44
1:C:373:ASP:O	1:C:377:ILE:HG12	2.18	0.43
1:E:161:PRO:O	1:E:164:ALA:N	2.50	0.43
1:E:214:GLY:HA3	1:E:329:ALA:HB3	1.99	0.43
1:O:185:TYR:CG	1:O:191:PRO:HD2	2.53	0.43
1:Q:369:LYS:N	1:Q:370:PRO:HD2	2.32	0.43
1:A:249:ALA:HB1	1:B:313:PHE:CD1	2.53	0.43
1:G:337:LYS:NZ	1:M:168:ALA:O	2.42	0.43
1:E:56:ASN:O	1:E:59:ASN:N	2.51	0.43
1:F:349:LYS:HB2	1:F:349:LYS:HE3	1.82	0.43
1:C:99:LYS:C	1:C:101:THR:H	2.27	0.43
1:I:251:THR:HG22	1:I:252:ALA:N	2.33	0.43
1:K:80:PHE:CZ	1:K:110:TRP:HB3	2.53	0.43
1:H:226:MET:HE1	1:H:274:ARG:HB2	2.00	0.43
1:E:215:SER:HA	1:E:317:ASP:HA	2.01	0.43
1:K:85:ASP:HB3	1:K:88:LYS:H	1.83	0.43
1:P:285:LEU:HD23	1:P:285:LEU:HA	1.75	0.43
1:E:362:ARG:HA	1:E:362:ARG:HD3	1.75	0.43
1:F:43:LEU:HD11	1:F:293:ARG:HD3	2.01	0.43
1:I:231:CYS:O	1:I:327:CYS:N	2.52	0.43
1:I:110:TRP:HE1	5:Y:1:NAG:H82	1.83	0.43
1:I:309:ILE:HD12	1:I:329:ALA:HB2	2.01	0.43
1:P:43:LEU:HD11	1:P:293:ARG:HD3	2.01	0.43
1:P:242:ASP:OD1	1:P:242:ASP:N	2.52	0.43
1:G:255:THR:HB	1:G:269:MET:HB3	2.01	0.43
1:G:308:SER:HB2	1:G:333:VAL:HG23	2.01	0.43
1:I:30:ASN:N	1:I:246:ALA:HB1	2.34	0.43
1:I:33:HIS:CD2	1:I:310:LEU:HG	2.54	0.43
1:M:144:ARG:HA	1:M:147:ILE:HD13	2.01	0.43
1:M:358:GLN:O	1:M:362:ARG:HG2	2.18	0.43
1:Q:294:LEU:HD23	1:Q:294:LEU:HA	1.78	0.43
1:G:318:CYS:SG	1:G:327:CYS:N	2.91	0.43
1:H:355:ILE:O	1:H:359:LYS:HG2	2.18	0.43
1:Q:176:LEU:O	1:Q:180:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:291:GLU:HG2	1:Q:354:ARG:HE	1.82	0.43
1:G:255:THR:O	1:G:269:MET:HG2	2.19	0.42
1:I:171:THR:HG22	1:I:360:HIS:HB2	2.01	0.42
1:K:114:ALA:HA	1:K:117:LEU:HD12	2.01	0.42
1:N:265:PRO:HA	1:N:269:MET:HE3	2.00	0.42
1:O:221:LYS:HD2	1:O:221:LYS:HA	1.80	0.42
1:O:357:LEU:HD23	1:O:357:LEU:HA	1.87	0.42
1:R:64:ILE:HD13	1:R:64:ILE:HA	1.86	0.42
1:A:171:THR:HG22	1:A:172:THR:H	1.83	0.42
1:D:124:GLN:HA	1:D:127:LEU:HD12	2.01	0.42
1:F:236:ASP:N	1:F:239:ASN:OD1	2.47	0.42
1:P:248:VAL:HG22	1:P:249:ALA:N	2.34	0.42
1:E:56:ASN:OD1	1:E:57:PHE:N	2.53	0.42
1:O:205:ALA:HB1	1:O:263:ALA:O	2.20	0.42
1:G:333:VAL:HG12	1:G:338:GLY:HA3	2.01	0.42
1:I:95:GLN:O	1:I:97:LEU:N	2.47	0.42
1:N:146:THR:HG22	1:N:149:ARG:NH2	2.35	0.42
1:R:37:LEU:HD13	1:R:229:LEU:HA	2.01	0.42
1:C:169:ASP:HB3	1:C:359:LYS:HB3	2.02	0.42
1:G:143:ALA:HB1	1:G:387:LEU:HD13	2.00	0.42
1:I:53:ALA:HB1	1:I:364:VAL:HG21	2.01	0.42
1:I:172:THR:OG1	1:I:173:GLU:N	2.53	0.42
1:J:380:LEU:HD23	1:J:380:LEU:HA	1.90	0.42
1:M:285:LEU:HD23	1:M:285:LEU:HA	1.91	0.42
1:O:380:LEU:HD22	1:O:386:TYR:CG	2.54	0.42
1:P:237:ARG:HG2	1:P:257:TRP:O	2.20	0.42
1:C:255:THR:O	1:C:269:MET:HG2	2.19	0.42
1:G:25:ILE:HD12	1:G:312:SER:HB3	2.01	0.42
1:G:185:TYR:CE2	1:G:190:GLU:HG3	2.55	0.42
1:H:166:SER:O	1:H:363:ALA:HB1	2.20	0.42
1:O:204:LYS:CB	1:O:221:LYS:HG2	2.49	0.42
1:Q:50:LEU:HD23	1:Q:50:LEU:HA	1.82	0.42
1:A:66:GLU:O	1:A:70:THR:HG23	2.19	0.42
1:C:385:ALA:O	1:C:389:LEU:HD13	2.20	0.42
1:F:360:HIS:O	1:F:364:VAL:HG23	2.20	0.42
1:I:180:ILE:HD11	1:I:353:VAL:HG11	2.01	0.42
1:M:214:GLY:HA3	1:M:329:ALA:HB3	2.02	0.42
1:N:61:LEU:HG	1:N:65:LEU:CD2	2.49	0.42
1:N:209:ARG:HB2	1:N:259:PRO:HG3	2.01	0.42
1:D:149:ARG:O	1:D:153:GLU:HG3	2.19	0.42
1:E:234:ALA:HB2	1:E:273:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:LEU:HD23	1:F:285:LEU:HA	1.84	0.42
1:I:30:ASN:H	1:I:246:ALA:HB1	1.84	0.42
1:L:42:GLU:OE2	1:L:293:ARG:NH2	2.51	0.42
1:O:153:GLU:O	1:O:157:LYS:HG3	2.19	0.42
1:A:135:LEU:HD12	1:A:135:LEU:HA	1.90	0.42
1:A:261:VAL:HG12	1:A:262:THR:HG23	2.00	0.42
1:D:108:THR:HG23	1:D:109:ALA:H	1.85	0.42
1:G:108:THR:O	1:G:112:LYS:HG2	2.20	0.42
1:H:248:VAL:HG12	1:H:276:LEU:HD21	2.02	0.42
1:L:294:LEU:HD11	1:L:350:LEU:HB3	2.02	0.42
1:O:61:LEU:HA	1:O:64:ILE:HD12	2.00	0.42
1:O:131:LYS:HA	1:O:131:LYS:HD2	1.63	0.42
1:A:245:LYS:NZ	10:A:604:HOH:O	2.45	0.41
1:E:54:LEU:HD23	1:E:364:VAL:HB	2.01	0.41
1:G:151:THR:O	1:G:155:VAL:HG13	2.20	0.41
1:H:366:LYS:HD3	1:H:366:LYS:HA	1.84	0.41
1:O:176:LEU:HD23	1:O:285:LEU:HD13	2.01	0.41
1:R:266:THR:HG23	1:R:269:MET:HE3	2.01	0.41
1:R:344:ILE:HG22	1:R:345:PRO:O	2.20	0.41
1:H:240:GLY:N	1:H:242:ASP:OD1	2.52	0.41
1:L:54:LEU:HA	1:L:54:LEU:HD23	1.81	0.41
1:C:200:ALA:HB3	1:C:265:PRO:HD2	2.02	0.41
1:F:282:LYS:HE3	1:F:282:LYS:HB2	1.92	0.41
1:R:114:ALA:O	1:R:117:LEU:N	2.54	0.41
1:R:123:HIS:O	1:R:127:LEU:HD22	2.20	0.41
5:X:2:NAG:H4	5:X:3:BMA:H2	1.92	0.41
1:C:206:SER:OG	1:C:207:THR:N	2.54	0.41
1:D:206:SER:O	1:D:208:ASN:N	2.53	0.41
1:I:355:ILE:O	1:I:359:LYS:HG3	2.21	0.41
1:J:366:LYS:O	1:J:367:LEU:HB2	2.20	0.41
1:B:163:VAL:HG12	1:B:164:ALA:N	2.35	0.41
1:B:176:LEU:HD22	1:B:353:VAL:HG13	2.02	0.41
1:E:180:ILE:O	1:E:184:VAL:HG23	2.20	0.41
1:F:30:ASN:OD1	1:F:312:SER:HB2	2.21	0.41
1:G:103:TRP:O	1:G:107:TRP:HB2	2.20	0.41
1:Q:37:LEU:HD13	1:Q:229:LEU:HA	2.03	0.41
1:D:362:ARG:HA	1:D:362:ARG:HD3	1.69	0.41
1:H:231:CYS:HB2	1:H:328:VAL:HG22	2.02	0.41
1:H:249:ALA:HB1	1:I:313:PHE:HD1	1.86	0.41
1:I:176:LEU:O	1:I:180:ILE:HD12	2.20	0.41
1:K:90:ARG:NH2	1:K:96:PRO:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:55:PRO:HD3	1:L:364:VAL:HG23	2.03	0.41
1:N:124:GLN:H	1:N:124:GLN:CD	2.28	0.41
1:O:228:ALA:O	1:O:232:VAL:HG23	2.20	0.41
1:A:56:ASN:O	1:A:60:GLU:HG2	2.20	0.41
1:E:259:PRO:HA	1:E:263:ALA:HA	2.02	0.41
1:G:294:LEU:HD21	1:G:350:LEU:HD23	2.03	0.41
1:G:302:THR:N	1:G:309:ILE:O	2.53	0.41
1:K:286:SER:O	1:K:290:ILE:HG12	2.20	0.41
1:A:155:VAL:O	1:A:159:GLN:HG3	2.20	0.41
1:B:159:GLN:O	1:B:160:ASP:C	2.64	0.41
1:C:72:ALA:HA	1:C:144:ARG:HD3	2.03	0.41
1:C:176:LEU:HD13	1:C:357:LEU:HD21	2.03	0.41
1:G:54:LEU:CD2	1:G:56:ASN:HB2	2.50	0.41
1:G:195:PHE:HB2	1:G:267:GLY:HA3	2.03	0.41
1:G:242:ASP:HB3	1:G:322:GLN:CG	2.49	0.41
1:H:320:GLY:HA2	1:H:326:MET:SD	2.61	0.41
1:I:115:LEU:HB3	1:I:116:PRO:HD3	2.02	0.41
1:I:257:TRP:HB2	1:I:266:THR:HB	2.02	0.41
1:J:91:ASP:OD1	1:J:91:ASP:C	2.64	0.41
1:J:285:LEU:HD23	1:J:285:LEU:HA	1.94	0.41
1:K:185:TYR:OH	1:K:190:GLU:OE2	2.35	0.41
1:L:389:LEU:HD12	1:L:389:LEU:HA	1.88	0.41
1:M:360:HIS:O	1:M:364:VAL:HG13	2.21	0.41
1:N:60:GLU:O	1:N:63:SER:OG	2.35	0.41
1:O:212:ILE:H	1:O:212:ILE:HG13	1.61	0.41
1:D:71:ALA:HB2	1:D:132:LEU:HD22	2.03	0.41
1:E:209:ARG:NH1	1:E:320:GLY:HA3	2.36	0.41
1:J:143:ALA:HA	1:J:387:LEU:HB3	2.03	0.41
1:M:160:ASP:OD1	1:M:162:THR:OG1	2.31	0.41
1:F:285:LEU:HD22	1:F:290:ILE:HD11	2.03	0.40
1:G:313:PHE:HE1	1:G:316:THR:C	2.30	0.40
1:H:64:ILE:HG22	1:H:151:THR:HG23	2.03	0.40
1:I:195:PHE:HD2	1:I:198:TYR:CD1	2.39	0.40
1:J:140:LEU:O	1:J:144:ARG:HB2	2.20	0.40
1:K:314:LEU:HD23	1:K:314:LEU:HA	1.93	0.40
1:M:342:LYS:HB3	1:M:342:LYS:HE2	1.93	0.40
1:N:364:VAL:HA	1:N:367:LEU:HD23	2.03	0.40
1:O:235:ASP:OD1	1:O:253:PRO:HG2	2.21	0.40
1:D:313:PHE:CD1	1:F:249:ALA:HB1	2.57	0.40
1:I:32:LEU:HD13	1:I:300:LEU:HD21	2.03	0.40
1:I:316:THR:HG22	1:I:317:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:176:LEU:HD22	1:J:353:VAL:HG13	2.04	0.40
1:A:214:GLY:HA3	1:A:329:ALA:HB3	2.03	0.40
1:H:245:LYS:HE2	1:H:249:ALA:O	2.21	0.40
1:L:67:LEU:HD13	1:L:130:TYR:CD1	2.57	0.40
1:M:210:GLN:H	1:M:210:GLN:HG2	1.52	0.40
1:N:285:LEU:HD12	1:N:285:LEU:HA	1.87	0.40
1:B:123:HIS:O	1:B:127:LEU:HB2	2.21	0.40
1:G:227:ASP:OD1	1:G:227:ASP:N	2.54	0.40
1:H:236:ASP:OD1	1:H:236:ASP:N	2.53	0.40
1:I:40:ILE:HG21	1:I:346:TRP:HZ3	1.86	0.40
1:I:67:LEU:HD23	1:I:67:LEU:HA	1.85	0.40
1:N:266:THR:H	1:N:269:MET:CE	2.33	0.40
1:B:301:LEU:HD23	1:B:310:LEU:HB2	2.03	0.40
1:D:249:ALA:HB1	1:E:313:PHE:CD1	2.56	0.40
1:J:214:GLY:HA3	1:J:329:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	364/410 (89%)	351 (96%)	12 (3%)	1 (0%)	36 58
1	B	364/410 (89%)	340 (93%)	21 (6%)	3 (1%)	16 34
1	C	364/410 (89%)	341 (94%)	23 (6%)	0	100 100
1	D	313/410 (76%)	297 (95%)	15 (5%)	1 (0%)	36 58
1	E	281/410 (68%)	254 (90%)	26 (9%)	1 (0%)	30 51
1	F	274/410 (67%)	253 (92%)	21 (8%)	0	100 100
1	G	363/410 (88%)	326 (90%)	33 (9%)	4 (1%)	11 25
1	H	283/410 (69%)	255 (90%)	23 (8%)	5 (2%)	6 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	323/410 (79%)	287 (89%)	32 (10%)	4 (1%)	10	23
1	J	364/410 (89%)	349 (96%)	14 (4%)	1 (0%)	36	58
1	K	363/410 (88%)	345 (95%)	17 (5%)	1 (0%)	36	58
1	L	354/410 (86%)	340 (96%)	13 (4%)	1 (0%)	36	58
1	M	281/410 (68%)	268 (95%)	13 (5%)	0	100	100
1	N	347/410 (85%)	329 (95%)	18 (5%)	0	100	100
1	O	293/410 (72%)	265 (90%)	28 (10%)	0	100	100
1	P	253/410 (62%)	237 (94%)	16 (6%)	0	100	100
1	Q	266/410 (65%)	246 (92%)	19 (7%)	1 (0%)	30	51
1	R	300/410 (73%)	282 (94%)	16 (5%)	2 (1%)	18	38
All	All	5750/7380 (78%)	5365 (93%)	360 (6%)	25 (0%)	30	51

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	THR
1	D	70	THR
1	E	208	ASN
1	G	134	GLY
1	G	318	CYS
1	Q	159	GLN
1	G	315	ALA
1	R	162	THR
1	H	68	ASN
1	I	301	LEU
1	K	135	LEU
1	L	207	THR
1	A	207	THR
1	H	207	THR
1	H	316	THR
1	B	207	THR
1	G	317	ASP
1	I	243	ALA
1	J	207	THR
1	B	160	ASP
1	H	242	ASP
1	I	97	LEU
1	R	207	THR

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Mol	Chain	Res	Type
1	H	252	ALA
1	I	96	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	288/330 (87%)	281 (98%)	7 (2%)	43	70
1	B	278/330 (84%)	267 (96%)	11 (4%)	28	55
1	C	281/330 (85%)	274 (98%)	7 (2%)	42	69
1	D	237/330 (72%)	229 (97%)	8 (3%)	32	60
1	E	211/330 (64%)	203 (96%)	8 (4%)	29	56
1	F	212/330 (64%)	205 (97%)	7 (3%)	33	61
1	G	280/330 (85%)	265 (95%)	15 (5%)	20	42
1	H	211/330 (64%)	200 (95%)	11 (5%)	21	44
1	I	243/330 (74%)	218 (90%)	25 (10%)	7	15
1	J	287/330 (87%)	278 (97%)	9 (3%)	35	63
1	K	277/330 (84%)	271 (98%)	6 (2%)	45	72
1	L	275/330 (83%)	267 (97%)	8 (3%)	37	65
1	M	215/330 (65%)	211 (98%)	4 (2%)	50	75
1	N	269/330 (82%)	256 (95%)	13 (5%)	23	47
1	O	222/330 (67%)	207 (93%)	15 (7%)	14	32
1	P	196/330 (59%)	191 (97%)	5 (3%)	40	68
1	Q	205/330 (62%)	201 (98%)	4 (2%)	48	74
1	R	223/330 (68%)	219 (98%)	4 (2%)	51	76
All	All	4410/5940 (74%)	4243 (96%)	167 (4%)	29	56

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	108	THR
1	A	171	THR
1	A	172	THR
1	A	179	GLN
1	A	238	THR
1	A	341	THR
1	B	67	LEU
1	B	75	THR
1	B	84	ASP
1	B	92	LEU
1	B	95	GLN
1	B	115	LEU
1	B	162	THR
1	B	242	ASP
1	B	341	THR
1	B	367	LEU
1	B	389	LEU
1	C	107	TRP
1	C	135	LEU
1	C	189	THR
1	C	242	ASP
1	C	282	LYS
1	C	286	SER
1	C	389	LEU
1	D	50	LEU
1	D	54	LEU
1	D	108	THR
1	D	132	LEU
1	D	242	ASP
1	D	305	SER
1	D	367	LEU
1	D	380	LEU
1	E	27	THR
1	E	43	LEU
1	E	52	THR
1	E	63	SER
1	E	172	THR
1	E	211	THR
1	E	269	MET
1	E	305	SER
1	F	237	ARG
1	F	238	THR

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Mol	Chain	Res	Type
1	F	242	ASP
1	F	251	THR
1	F	286	SER
1	F	327	CYS
1	F	376	THR
1	G	41	ILE
1	G	64	ILE
1	G	163	VAL
1	G	199	THR
1	G	236	ASP
1	G	238	THR
1	G	242	ASP
1	G	248	VAL
1	G	261	VAL
1	G	264	THR
1	G	316	THR
1	G	327	CYS
1	G	328	VAL
1	G	331	THR
1	G	333	VAL
1	H	32	LEU
1	H	50	LEU
1	H	68	ASN
1	H	211	THR
1	H	223	THR
1	H	286	SER
1	H	305	SER
1	H	307	THR
1	H	314	LEU
1	H	331	THR
1	H	341	THR
1	I	40	ILE
1	I	41	ILE
1	I	51	GLU
1	I	61	LEU
1	I	64	ILE
1	I	67	LEU
1	I	100	ASP
1	I	106	HIS
1	I	108	THR
1	I	136	GLN
1	I	140	LEU

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Mol	Chain	Res	Type
1	I	172	THR
1	I	231	CYS
1	I	232	VAL
1	I	239	ASN
1	I	255	THR
1	I	314	LEU
1	I	317	ASP
1	I	324	SER
1	I	327	CYS
1	I	328	VAL
1	I	333	VAL
1	I	350	LEU
1	I	353	VAL
1	I	389	LEU
1	J	59	ASN
1	J	84	ASP
1	J	139	LYS
1	J	163	VAL
1	J	237	ARG
1	J	238	THR
1	J	242	ASP
1	J	377	ILE
1	J	389	LEU
1	K	86	ARG
1	K	179	GLN
1	K	248	VAL
1	K	309	ILE
1	K	316	THR
1	K	358	GLN
1	L	90	ARG
1	L	126	LYS
1	L	171	THR
1	L	172	THR
1	L	242	ASP
1	L	286	SER
1	L	357	LEU
1	L	388	GLN
1	M	65	LEU
1	M	170	LEU
1	M	383	ASP
1	M	387	LEU
1	N	100	ASP

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Mol	Chain	Res	Type
1	N	102	ASN
1	N	106	HIS
1	N	122	THR
1	N	179	GLN
1	N	207	THR
1	N	217	VAL
1	N	229	LEU
1	N	242	ASP
1	N	245	LYS
1	N	251	THR
1	N	367	LEU
1	N	371	GLN
1	O	64	ILE
1	O	67	LEU
1	O	69	MET
1	O	127	LEU
1	O	128	LYS
1	O	129	GLU
1	O	131	LYS
1	O	171	THR
1	O	179	GLN
1	O	207	THR
1	O	237	ARG
1	O	266	THR
1	O	341	THR
1	O	367	LEU
1	O	379	THR
1	P	223	THR
1	P	231	CYS
1	P	242	ASP
1	P	322	GLN
1	P	367	LEU
1	Q	63	SER
1	Q	291	GLU
1	Q	321	ASP
1	Q	357	LEU
1	R	242	ASP
1	R	248	VAL
1	R	346	TRP
1	R	366	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	179	GLN
1	A	196	ASN
1	A	348	GLN
1	B	136	GLN
1	B	179	GLN
1	C	62	ASN
1	C	280	HIS
1	D	68	ASN
1	F	322	GLN
1	G	124	GLN
1	G	179	GLN
1	G	196	ASN
1	G	210	GLN
1	G	278	ASN
1	G	280	HIS
1	H	62	ASN
1	H	258	ASN
1	I	79	GLN
1	I	136	GLN
1	I	182	GLN
1	I	278	ASN
1	J	145	ASN
1	J	322	GLN
1	J	371	GLN
1	K	123	HIS
1	K	280	HIS
1	L	179	GLN
1	M	59	ASN
1	M	179	GLN
1	M	280	HIS
1	N	159	GLN
1	N	348	GLN
1	N	358	GLN
1	N	371	GLN
1	O	278	ASN
1	O	280	HIS
1	P	182	GLN
1	P	280	HIS
1	R	280	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 ⓘ

49 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	S	1	1,2	14,14,15	0.42	0	17,19,21	0.56	0
2	NAG	S	2	2	14,14,15	0.36	0	17,19,21	0.53	0
2	BMA	S	3	2	11,11,12	0.38	0	15,15,17	0.65	0
2	MAN	S	4	2	11,11,12	0.21	0	15,15,17	0.47	0
2	MAN	S	5	2	11,11,12	0.39	0	15,15,17	0.57	0
2	MAN	S	6	2	11,11,12	0.61	0	15,15,17	0.65	0
3	NAG	T	1	1,3	14,14,15	0.52	0	17,19,21	1.00	2 (11%)
3	NAG	T	2	3	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
3	BMA	T	3	3	11,11,12	0.24	0	15,15,17	0.77	0
3	MAN	T	4	3	11,11,12	0.41	0	15,15,17	0.54	0
3	MAN	T	5	3	11,11,12	0.37	0	15,15,17	0.49	0
4	NAG	U	1	4,1	14,14,15	0.51	0	17,19,21	0.79	1 (5%)
4	NAG	U	2	4	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
4	BMA	U	3	4	11,11,12	0.27	0	15,15,17	0.59	0
5	NAG	V	1	5,1	14,14,15	0.34	0	17,19,21	0.51	0
5	NAG	V	2	5	14,14,15	0.45	0	17,19,21	0.48	0
5	BMA	V	3	5	11,11,12	0.29	0	15,15,17	0.51	0
6	NAG	W	1	1,6	14,14,15	0.58	0	17,19,21	1.06	1 (5%)
6	NAG	W	2	6	14,14,15	0.41	0	17,19,21	0.72	0
6	BMA	W	3	6	11,11,12	0.34	0	15,15,17	0.57	0
6	MAN	W	4	6	11,11,12	0.32	0	15,15,17	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	W	5	6	11,11,12	0.38	0	15,15,17	0.56	0
5	NAG	X	1	5,1	14,14,15	0.38	0	17,19,21	0.52	0
5	NAG	X	2	5	14,14,15	0.37	0	17,19,21	0.61	0
5	BMA	X	3	5	11,11,12	0.29	0	15,15,17	0.49	0
5	NAG	Y	1	5,1	14,14,15	0.38	0	17,19,21	0.57	0
5	NAG	Y	2	5	14,14,15	0.35	0	17,19,21	0.62	0
5	BMA	Y	3	5	11,11,12	0.29	0	15,15,17	0.53	0
2	NAG	Z	1	1,2	14,14,15	0.36	0	17,19,21	0.61	0
2	NAG	Z	2	2	14,14,15	0.34	0	17,19,21	0.54	0
2	BMA	Z	3	2	11,11,12	0.36	0	15,15,17	0.56	0
2	MAN	Z	4	2	11,11,12	0.30	0	15,15,17	0.52	0
2	MAN	Z	5	2	11,11,12	0.32	0	15,15,17	0.49	0
2	MAN	Z	6	2	11,11,12	0.29	0	15,15,17	0.53	0
7	NAG	a	1	7,1	14,14,15	0.34	0	17,19,21	0.60	0
7	NAG	a	2	7	14,14,15	0.31	0	17,19,21	0.55	0
7	BMA	a	3	7	11,11,12	0.25	0	15,15,17	0.76	0
7	MAN	a	4	7	11,11,12	0.25	0	15,15,17	0.50	0
7	MAN	a	5	7	11,11,12	1.44	2 (18%)	15,15,17	0.78	0
7	NAG	b	1	7,1	14,14,15	0.33	0	17,19,21	0.56	0
7	NAG	b	2	7	14,14,15	0.31	0	17,19,21	0.55	0
7	BMA	b	3	7	11,11,12	0.23	0	15,15,17	0.53	0
7	MAN	b	4	7	11,11,12	0.38	0	15,15,17	0.55	0
7	MAN	b	5	7	11,11,12	0.22	0	15,15,17	0.52	0
6	NAG	c	1	1,6	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
6	NAG	c	2	6	14,14,15	0.55	0	17,19,21	0.65	0
6	BMA	c	3	6	11,11,12	0.46	0	15,15,17	0.67	0
6	MAN	c	4	6	11,11,12	0.38	0	15,15,17	0.55	0
6	MAN	c	5	6	11,11,12	0.27	0	15,15,17	0.51	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
2	NAG	S	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	BMA	S	3	2	-	0/2/19/22	0/1/1/1
2	MAN	S	4	2	-	0/2/19/22	0/1/1/1
2	MAN	S	5	2	-	0/2/19/22	0/1/1/1
2	MAN	S	6	2	-	0/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	MAN	T	4	3	-	1/2/19/22	0/1/1/1
3	MAN	T	5	3	-	2/2/19/22	0/1/1/1
4	NAG	U	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	BMA	U	3	4	-	0/2/19/22	0/1/1/1
5	NAG	V	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
5	BMA	V	3	5	-	1/2/19/22	0/1/1/1
6	NAG	W	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	W	2	6	-	3/6/23/26	0/1/1/1
6	BMA	W	3	6	-	2/2/19/22	0/1/1/1
6	MAN	W	4	6	-	0/2/19/22	0/1/1/1
6	MAN	W	5	6	-	0/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	3/6/23/26	0/1/1/1
5	BMA	X	3	5	-	0/2/19/22	0/1/1/1
5	NAG	Y	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
2	NAG	Z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/6/23/26	0/1/1/1
2	BMA	Z	3	2	-	0/2/19/22	0/1/1/1
2	MAN	Z	4	2	-	0/2/19/22	0/1/1/1
2	MAN	Z	5	2	-	1/2/19/22	0/1/1/1
2	MAN	Z	6	2	-	0/2/19/22	0/1/1/1
7	NAG	a	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	2/6/23/26	0/1/1/1
7	BMA	a	3	7	-	2/2/19/22	0/1/1/1
7	MAN	a	4	7	-	0/2/19/22	0/1/1/1
7	MAN	a	5	7	-	1/2/19/22	0/1/1/1
7	NAG	b	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	0/6/23/26	0/1/1/1
7	BMA	b	3	7	-	0/2/19/22	0/1/1/1
7	MAN	b	4	7	-	0/2/19/22	0/1/1/1
7	MAN	b	5	7	-	0/2/19/22	0/1/1/1
6	NAG	c	1	1,6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	c	2	6	-	4/6/23/26	0/1/1/1
6	BMA	c	3	6	-	2/2/19/22	0/1/1/1
6	MAN	c	4	6	-	0/2/19/22	0/1/1/1
6	MAN	c	5	6	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	5	MAN	O5-C1	3.87	1.50	1.43
7	a	5	MAN	C1-C2	2.59	1.58	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	1	NAG	O5-C1-C2	-2.48	107.45	111.29
3	T	2	NAG	O5-C1-C2	-2.47	107.47	111.29
4	U	2	NAG	O5-C1-C2	-2.38	107.61	111.29
3	T	1	NAG	C3-C4-C5	2.32	114.43	110.23
3	T	1	NAG	O5-C1-C2	-2.31	107.71	111.29
4	U	1	NAG	O5-C1-C2	-2.11	108.03	111.29
6	c	1	NAG	O5-C1-C2	-2.03	108.15	111.29

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Y	1	NAG	C8-C7-N2-C2
5	Y	1	NAG	O7-C7-N2-C2
6	W	1	NAG	C1-C2-N2-C7
6	W	1	NAG	C8-C7-N2-C2
6	W	1	NAG	O7-C7-N2-C2
6	W	2	NAG	C8-C7-N2-C2
6	W	2	NAG	O7-C7-N2-C2
6	W	3	BMA	C4-C5-C6-O6
6	c	5	MAN	C4-C5-C6-O6
6	c	5	MAN	O5-C5-C6-O6
7	b	1	NAG	C8-C7-N2-C2
7	b	1	NAG	O7-C7-N2-C2
6	W	3	BMA	O5-C5-C6-O6
3	T	5	MAN	C4-C5-C6-O6

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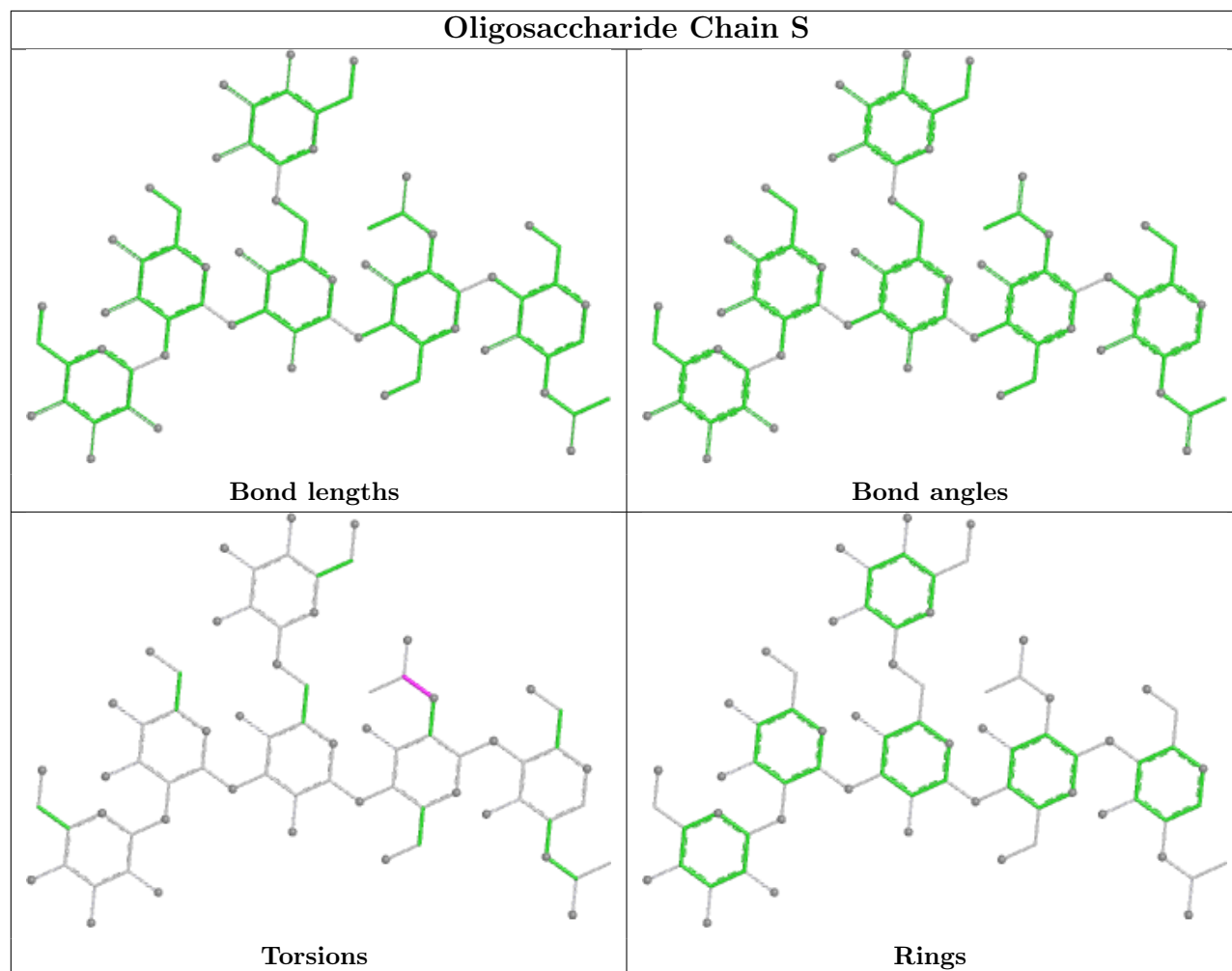
Mol	Chain	Res	Type	Atoms
3	T	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C8-C7-N2-C2
2	S	2	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
6	c	2	NAG	C8-C7-N2-C2
6	c	2	NAG	O5-C5-C6-O6
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
6	c	2	NAG	O7-C7-N2-C2
7	a	2	NAG	C8-C7-N2-C2
7	a	2	NAG	O7-C7-N2-C2
3	T	2	NAG	O5-C5-C6-O6
7	a	3	BMA	C4-C5-C6-O6
3	T	4	MAN	O5-C5-C6-O6
3	T	5	MAN	O5-C5-C6-O6
5	V	1	NAG	C8-C7-N2-C2
7	a	3	BMA	O5-C5-C6-O6
5	V	1	NAG	O7-C7-N2-C2
2	Z	1	NAG	C8-C7-N2-C2
2	Z	5	MAN	O5-C5-C6-O6
7	a	5	MAN	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	V	3	BMA	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
6	c	3	BMA	C4-C5-C6-O6
5	V	2	NAG	C1-C2-N2-C7
5	X	2	NAG	C1-C2-N2-C7
6	c	1	NAG	C8-C7-N2-C2
6	c	3	BMA	O5-C5-C6-O6
2	Z	1	NAG	O7-C7-N2-C2
5	V	2	NAG	C3-C2-N2-C7
5	X	2	NAG	C3-C2-N2-C7
6	c	1	NAG	O7-C7-N2-C2
6	W	1	NAG	C4-C5-C6-O6
6	c	2	NAG	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6

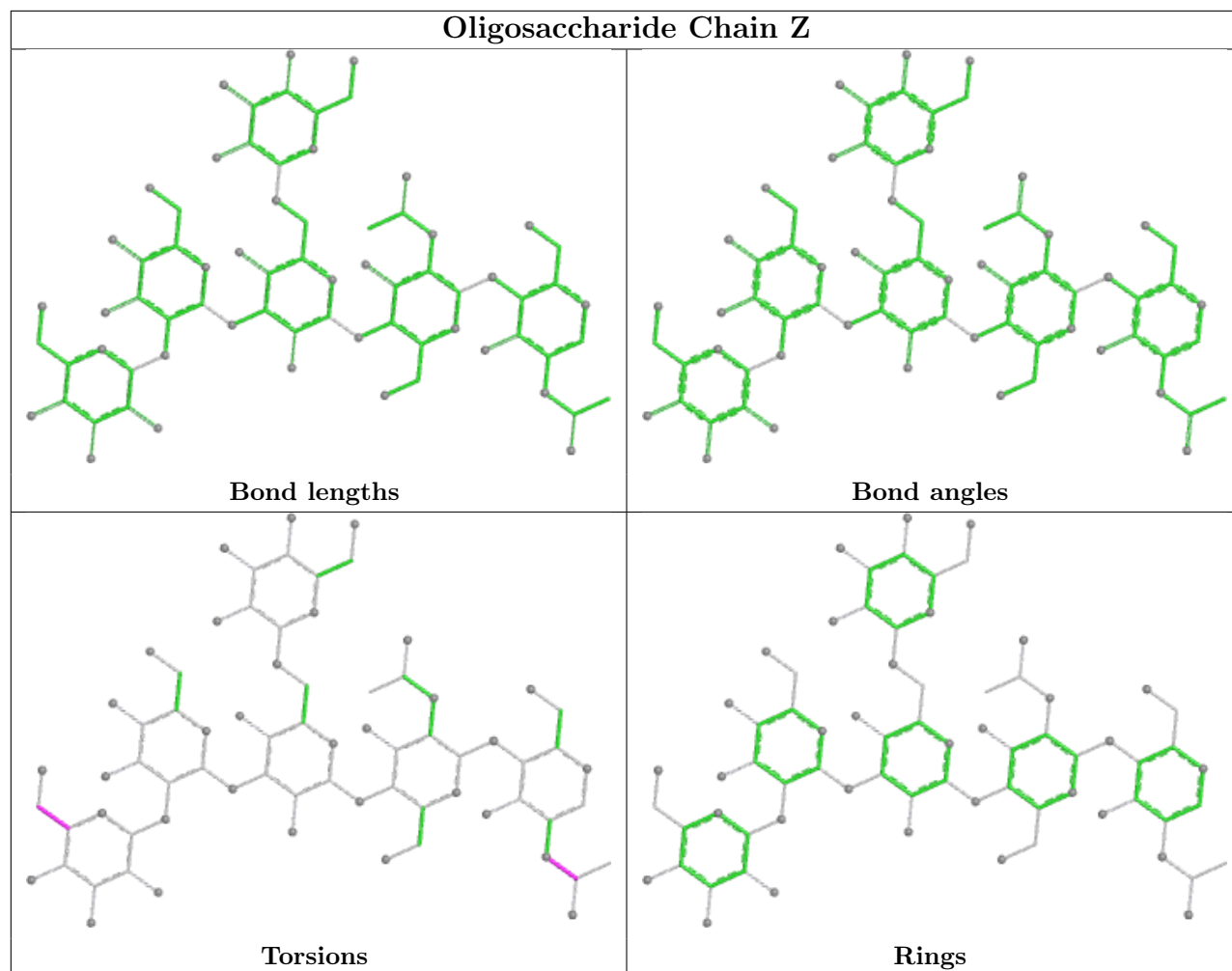
There are no ring outliers.

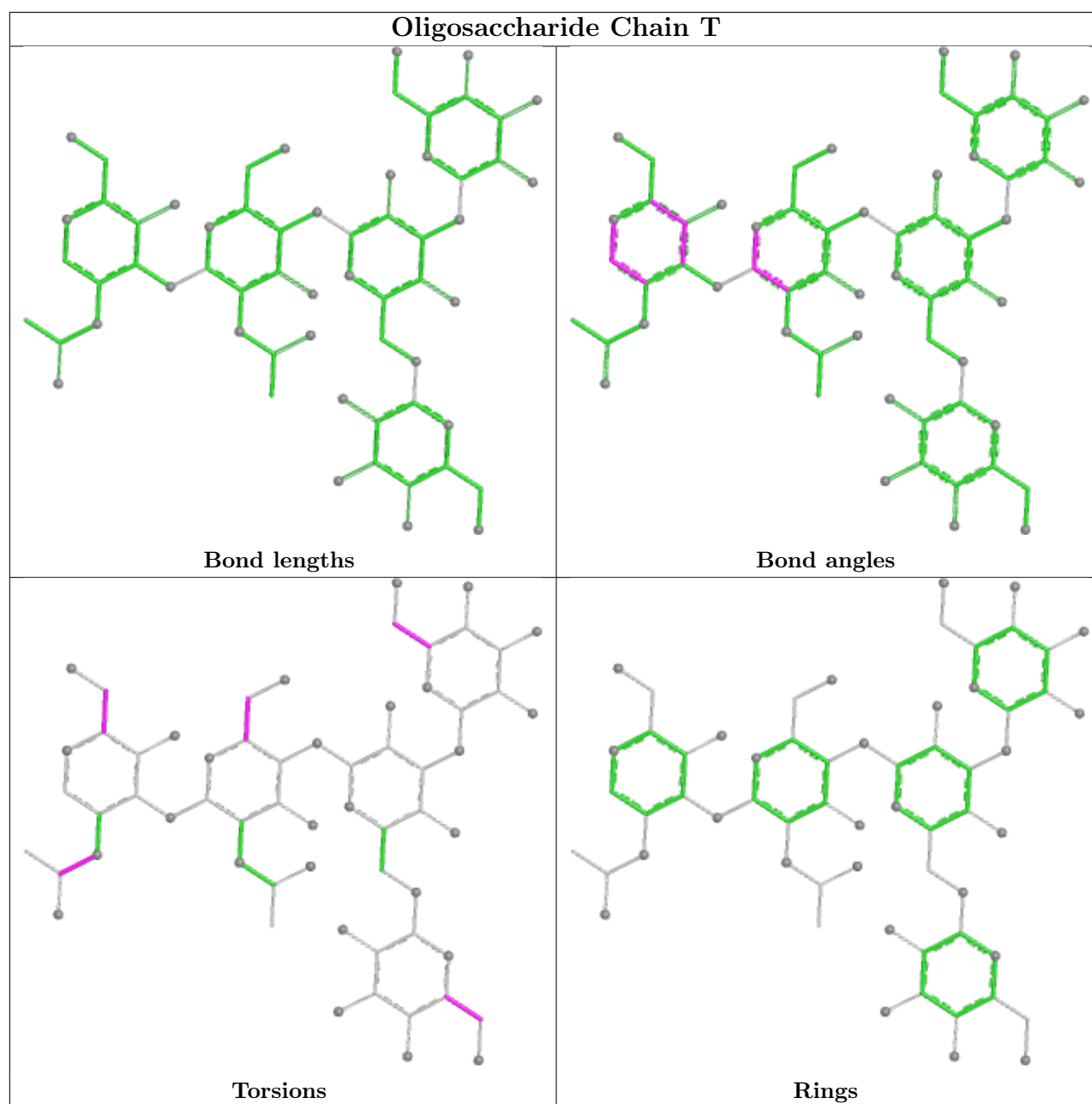
16 monomers are involved in 14 short contacts:

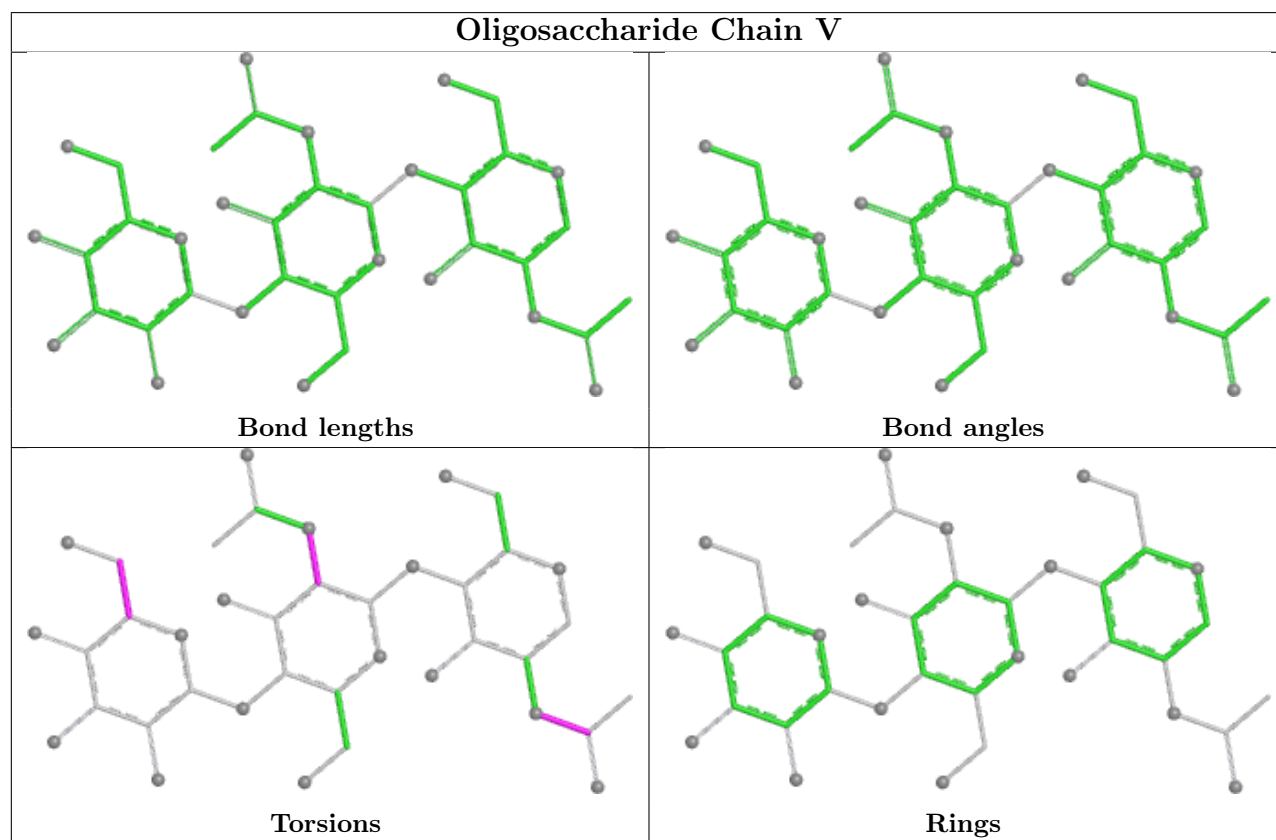
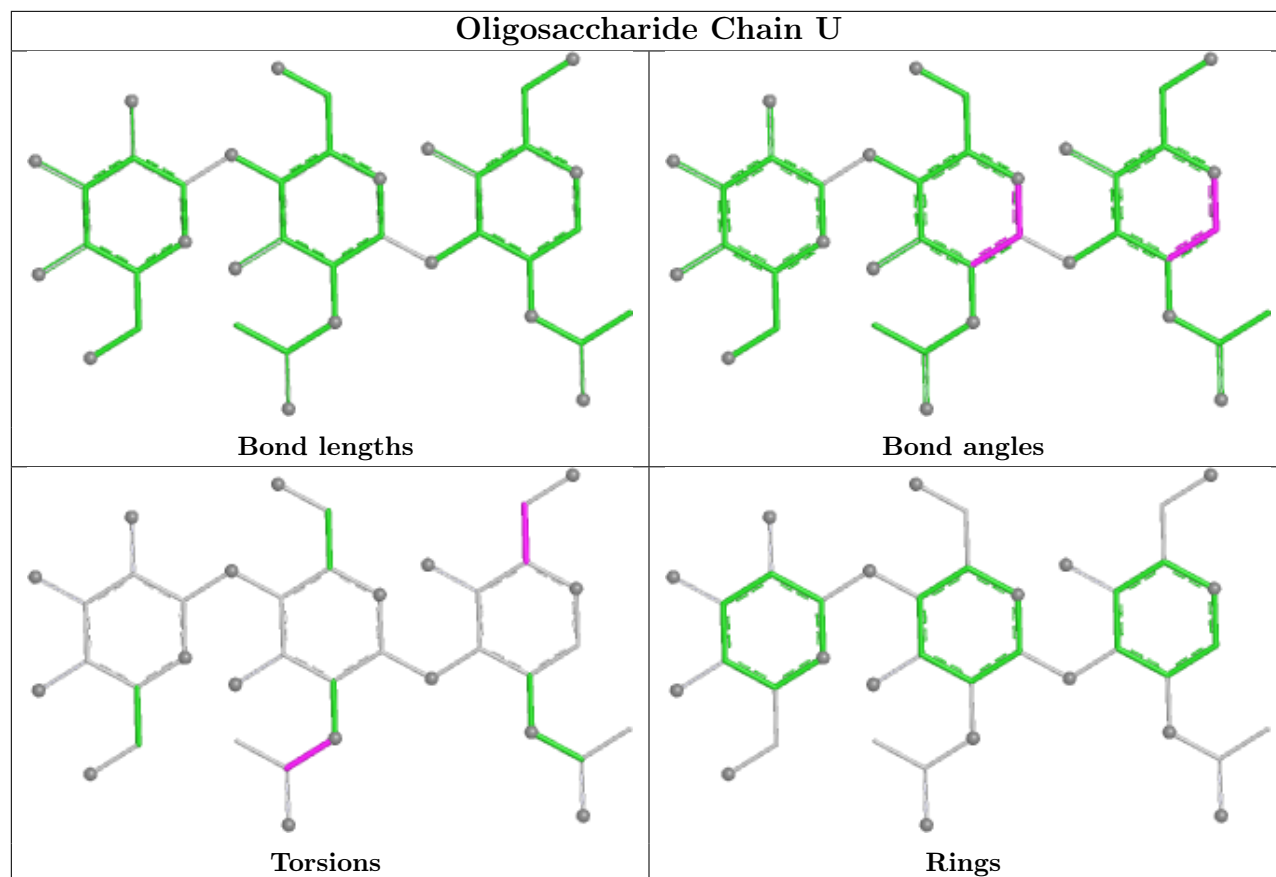
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	1	NAG	1	0
6	W	1	NAG	1	0
5	Y	3	BMA	1	0
7	a	4	MAN	1	0
3	T	5	MAN	1	0
7	a	5	MAN	1	0
6	W	3	BMA	1	0
4	U	2	NAG	1	0
3	T	3	BMA	1	0
2	S	3	BMA	1	0
5	Y	1	NAG	1	0
5	X	3	BMA	1	0
5	X	2	NAG	1	0
3	T	2	NAG	1	0
4	U	1	NAG	1	0
7	a	3	BMA	2	0

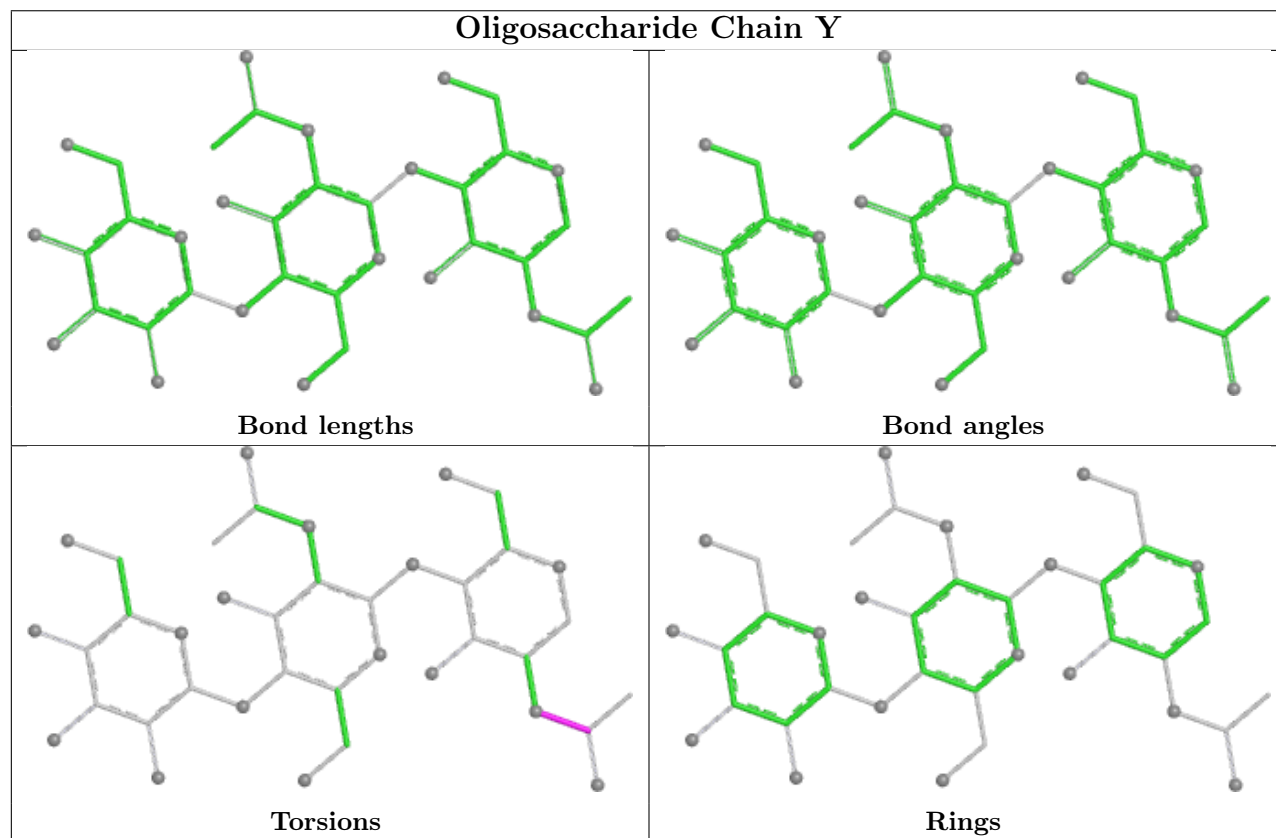
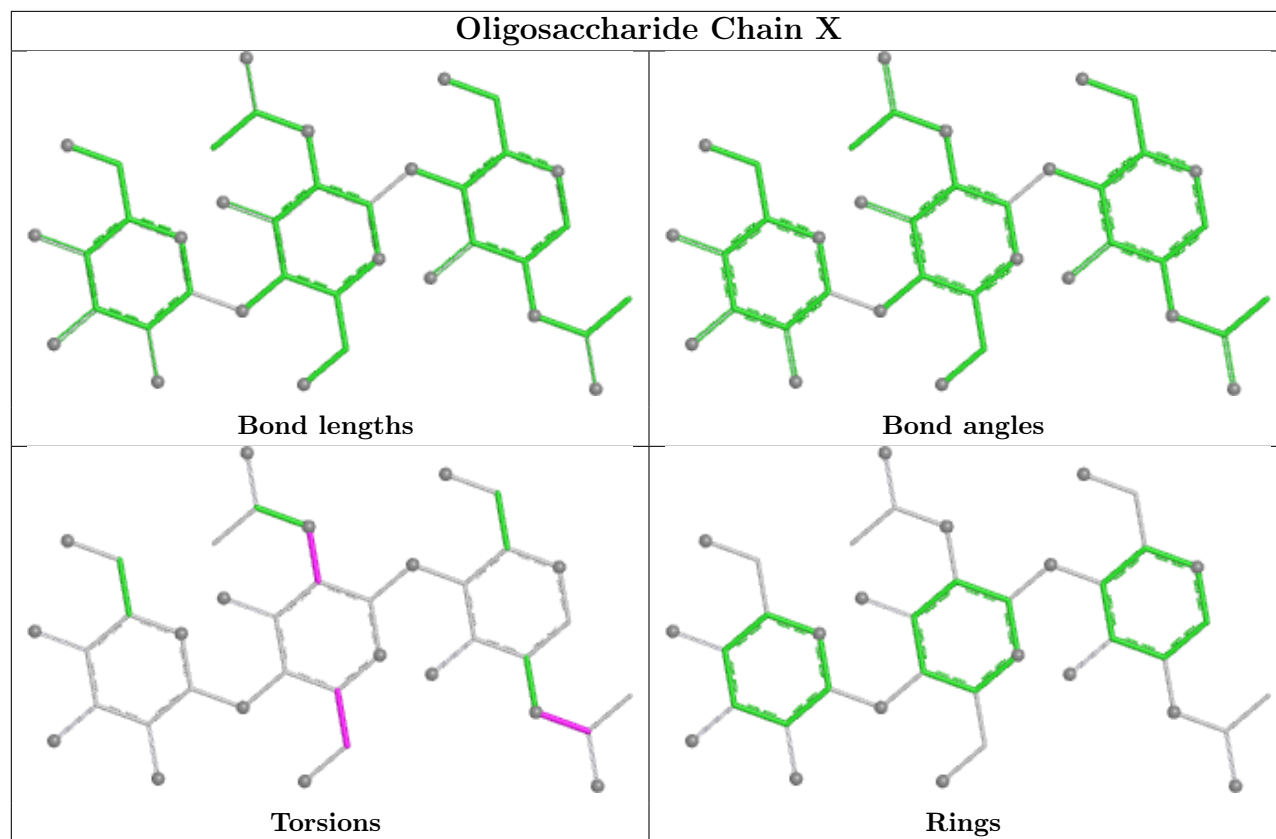
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

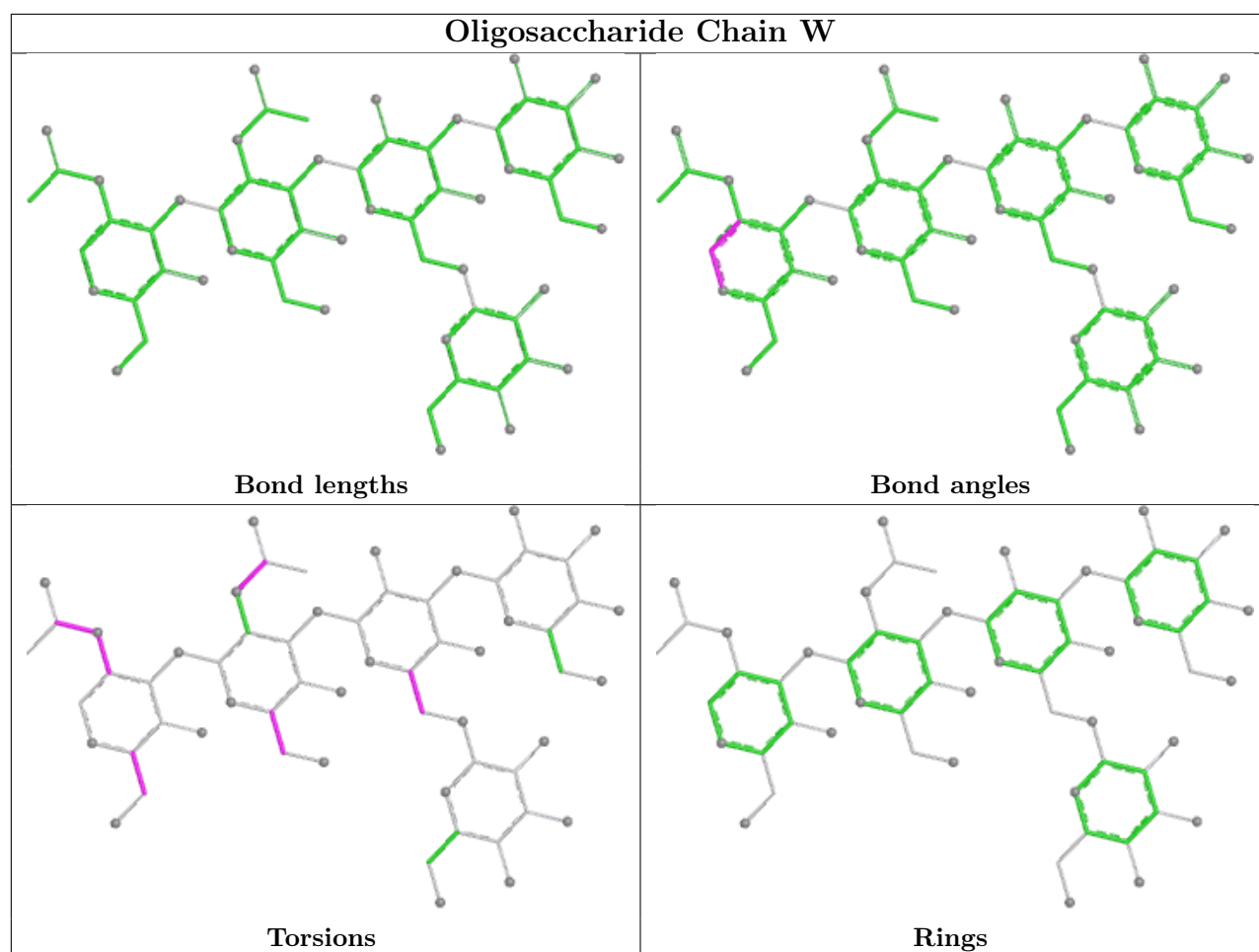


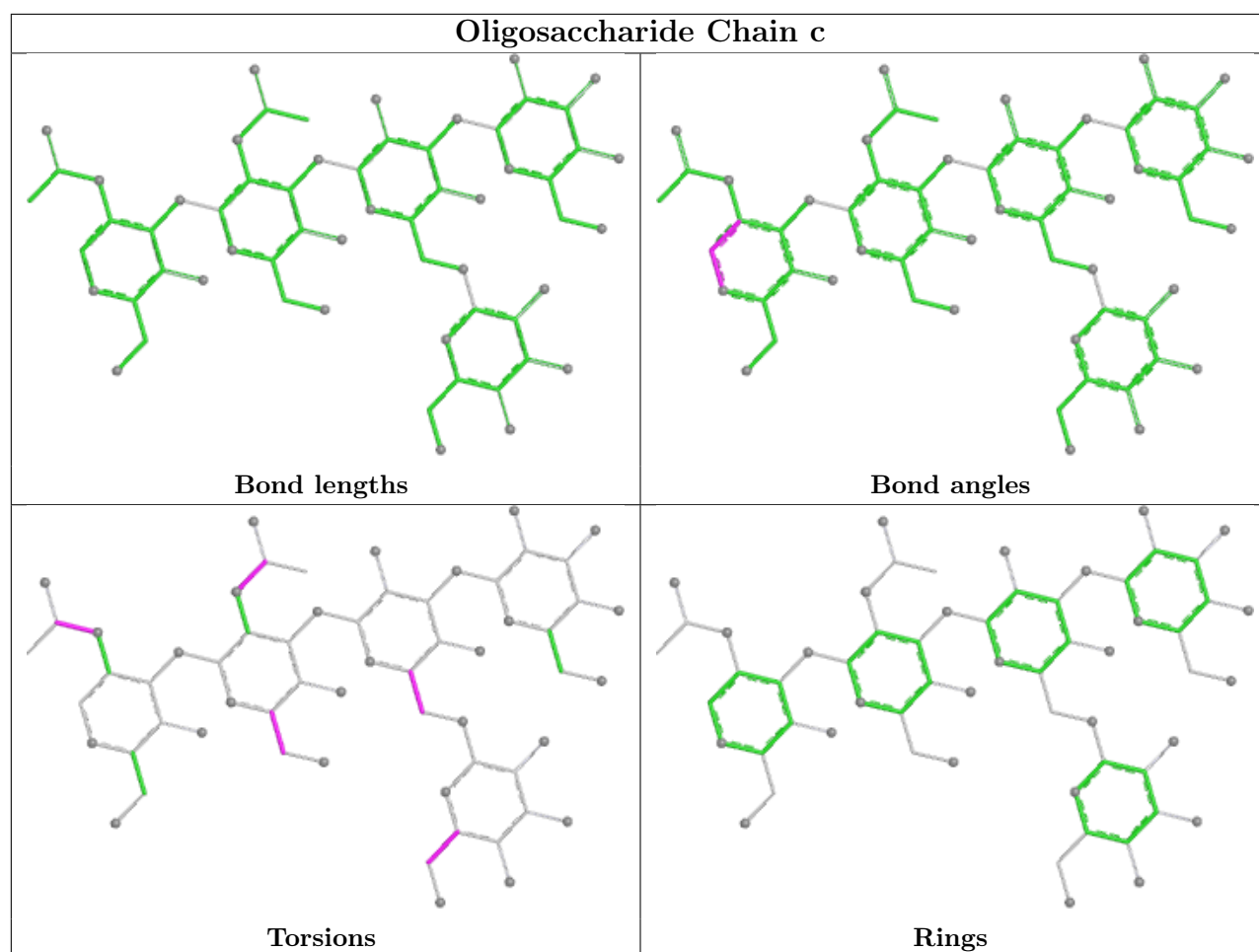


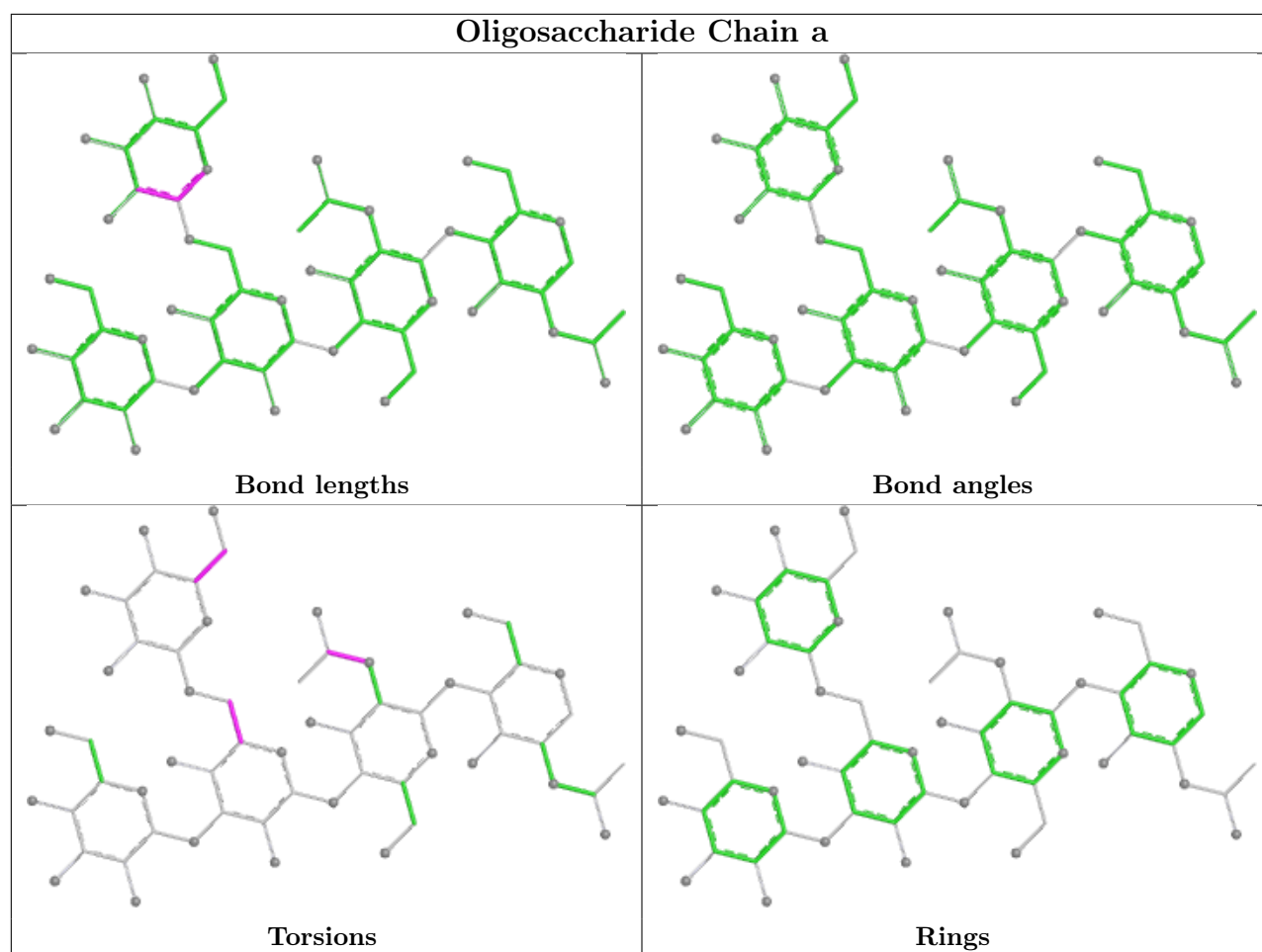


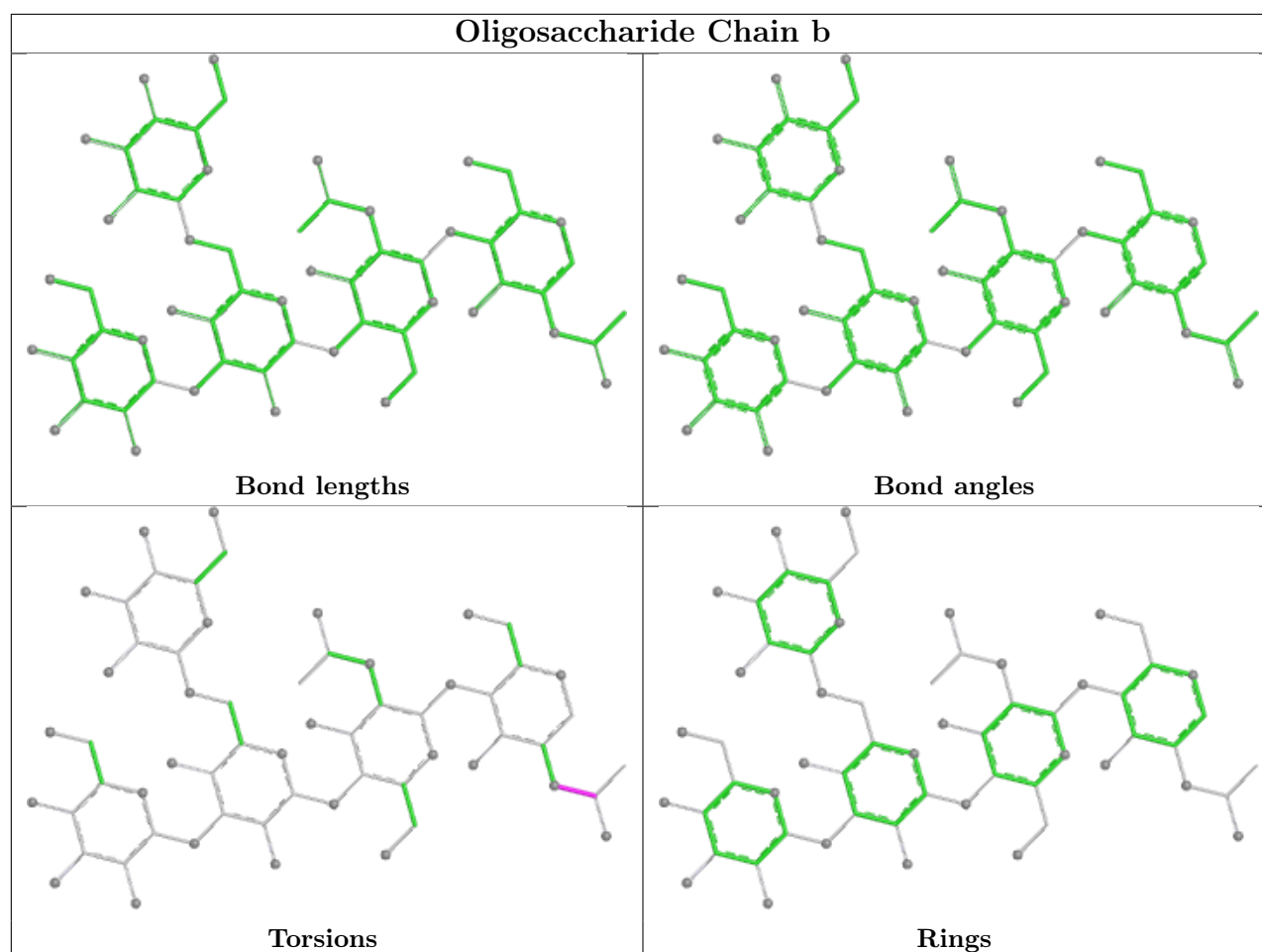












5.6 Ligand geometry [i](#)

21 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	$\# Z > 2$
8	GLC	I	501	1	11,11,12	0.81	0	15,15,17	0.51	0
8	GLC	K	501	1	11,11,12	0.81	0	15,15,17	0.50	0
8	GLC	D	501	1	11,11,12	0.78	0	15,15,17	0.50	0
8	GLC	P	501	1	11,11,12	0.81	0	15,15,17	0.52	0
8	GLC	J	501	1	11,11,12	0.81	0	15,15,17	0.50	0
9	NAG	O	502	1	14,14,15	0.28	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GLC	Q	502	1	11,11,12	0.80	0	15,15,17	0.49	0
9	NAG	Q	501	1	14,14,15	0.38	0	17,19,21	0.49	0
8	GLC	A	501	1	11,11,12	0.77	0	15,15,17	0.51	0
8	GLC	N	501	1	11,11,12	0.73	0	15,15,17	0.51	0
8	GLC	E	501	1	11,11,12	0.79	0	15,15,17	0.50	0
8	GLC	O	501	1	11,11,12	0.78	0	15,15,17	0.62	0
9	NAG	R	501	1	14,14,15	0.31	0	17,19,21	0.50	0
8	GLC	M	501	1	11,11,12	0.79	0	15,15,17	0.50	0
8	GLC	C	501	1	11,11,12	0.71	0	15,15,17	0.49	0
8	GLC	F	501	1	11,11,12	0.71	0	15,15,17	0.56	0
9	NAG	E	502	1	14,14,15	0.53	0	17,19,21	0.48	0
8	GLC	L	501	1	11,11,12	0.74	0	15,15,17	0.49	0
8	GLC	B	501	1	11,11,12	0.72	0	15,15,17	0.50	0
8	GLC	R	502	1	11,11,12	0.81	0	15,15,17	0.50	0
8	GLC	H	501	1	11,11,12	0.77	0	15,15,17	0.61	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
8	GLC	I	501	1	-	0/2/19/22	0/1/1/1
8	GLC	K	501	1	-	0/2/19/22	0/1/1/1
8	GLC	D	501	1	-	0/2/19/22	0/1/1/1
8	GLC	P	501	1	-	0/2/19/22	0/1/1/1
8	GLC	J	501	1	-	0/2/19/22	0/1/1/1
9	NAG	O	502	1	-	3/6/23/26	0/1/1/1
8	GLC	Q	502	1	-	0/2/19/22	0/1/1/1
9	NAG	Q	501	1	-	1/6/23/26	0/1/1/1
8	GLC	A	501	1	-	0/2/19/22	0/1/1/1
8	GLC	N	501	1	-	0/2/19/22	0/1/1/1
8	GLC	E	501	1	-	0/2/19/22	0/1/1/1
8	GLC	O	501	1	-	0/2/19/22	0/1/1/1
9	NAG	R	501	1	-	3/6/23/26	0/1/1/1
8	GLC	M	501	1	-	0/2/19/22	0/1/1/1
8	GLC	C	501	1	-	0/2/19/22	0/1/1/1
8	GLC	F	501	1	-	0/2/19/22	0/1/1/1
9	NAG	E	502	1	-	0/6/23/26	0/1/1/1
8	GLC	L	501	1	-	0/2/19/22	0/1/1/1
8	GLC	B	501	1	-	0/2/19/22	0/1/1/1
8	GLC	R	502	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GLC	H	501	1	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

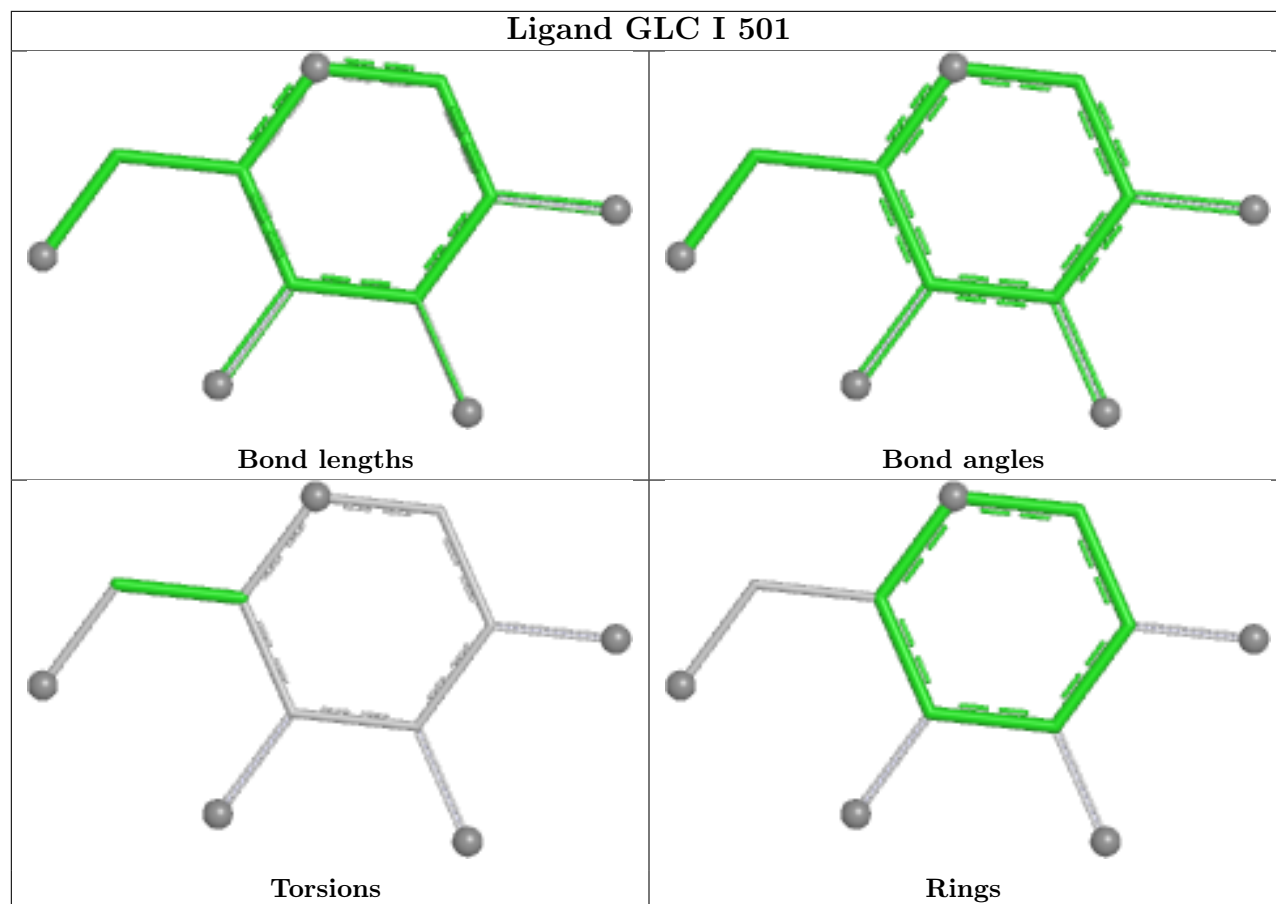
All (8) torsion outliers are listed below:

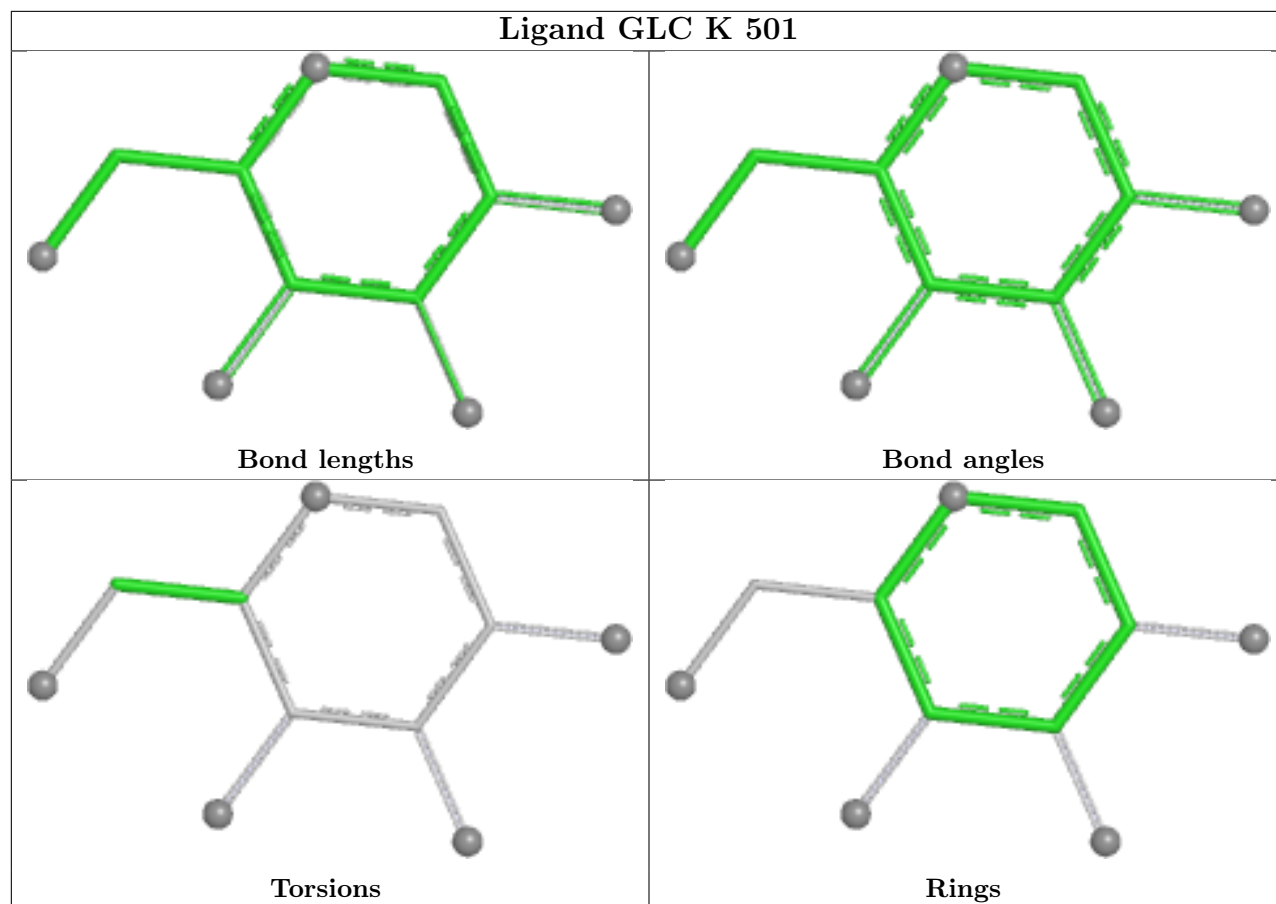
Mol	Chain	Res	Type	Atoms
9	O	502	NAG	C3-C2-N2-C7
9	O	502	NAG	C8-C7-N2-C2
9	O	502	NAG	O7-C7-N2-C2
9	R	501	NAG	C8-C7-N2-C2
9	R	501	NAG	O7-C7-N2-C2
9	R	501	NAG	O5-C5-C6-O6
8	H	501	GLC	O5-C5-C6-O6
9	Q	501	NAG	C3-C2-N2-C7

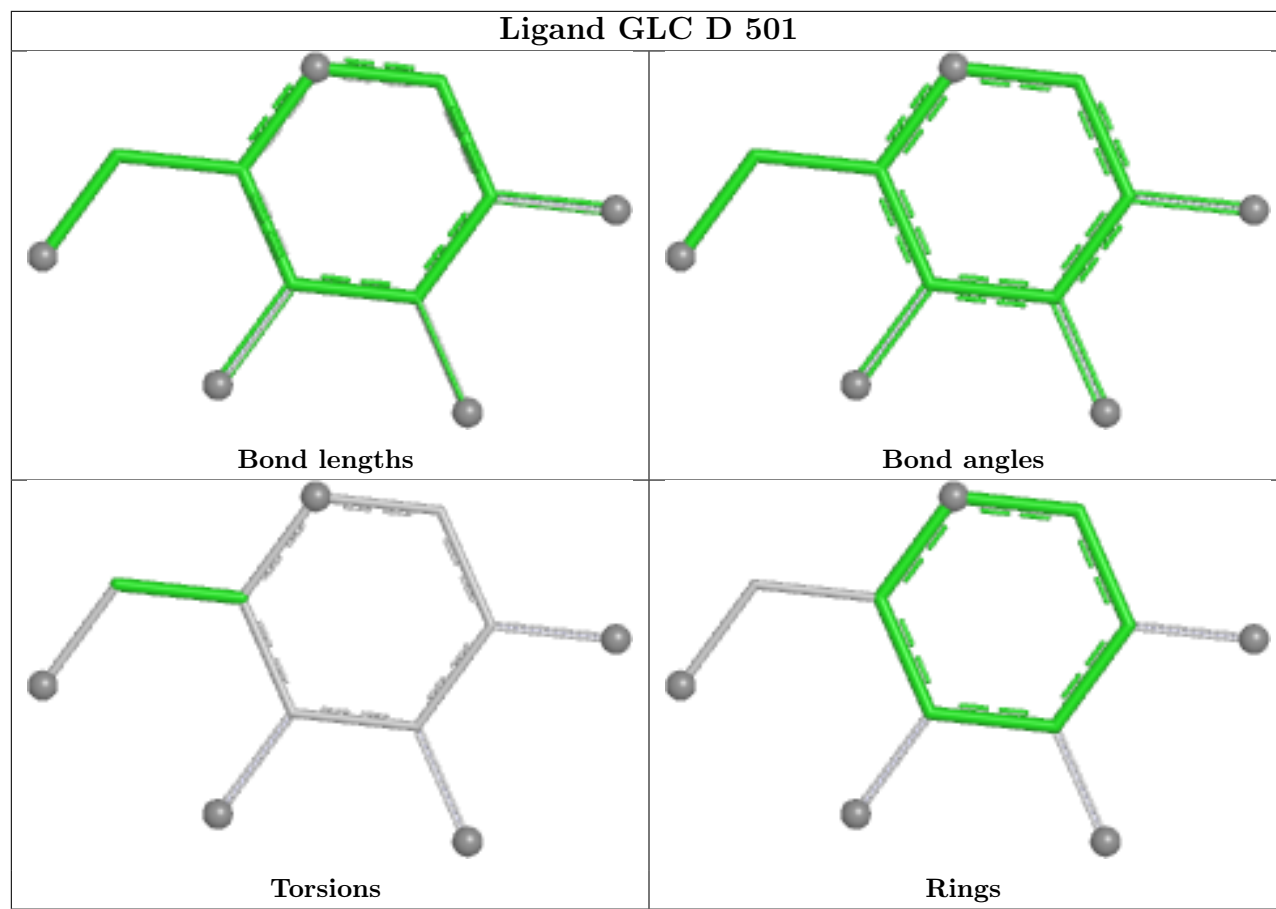
There are no ring outliers.

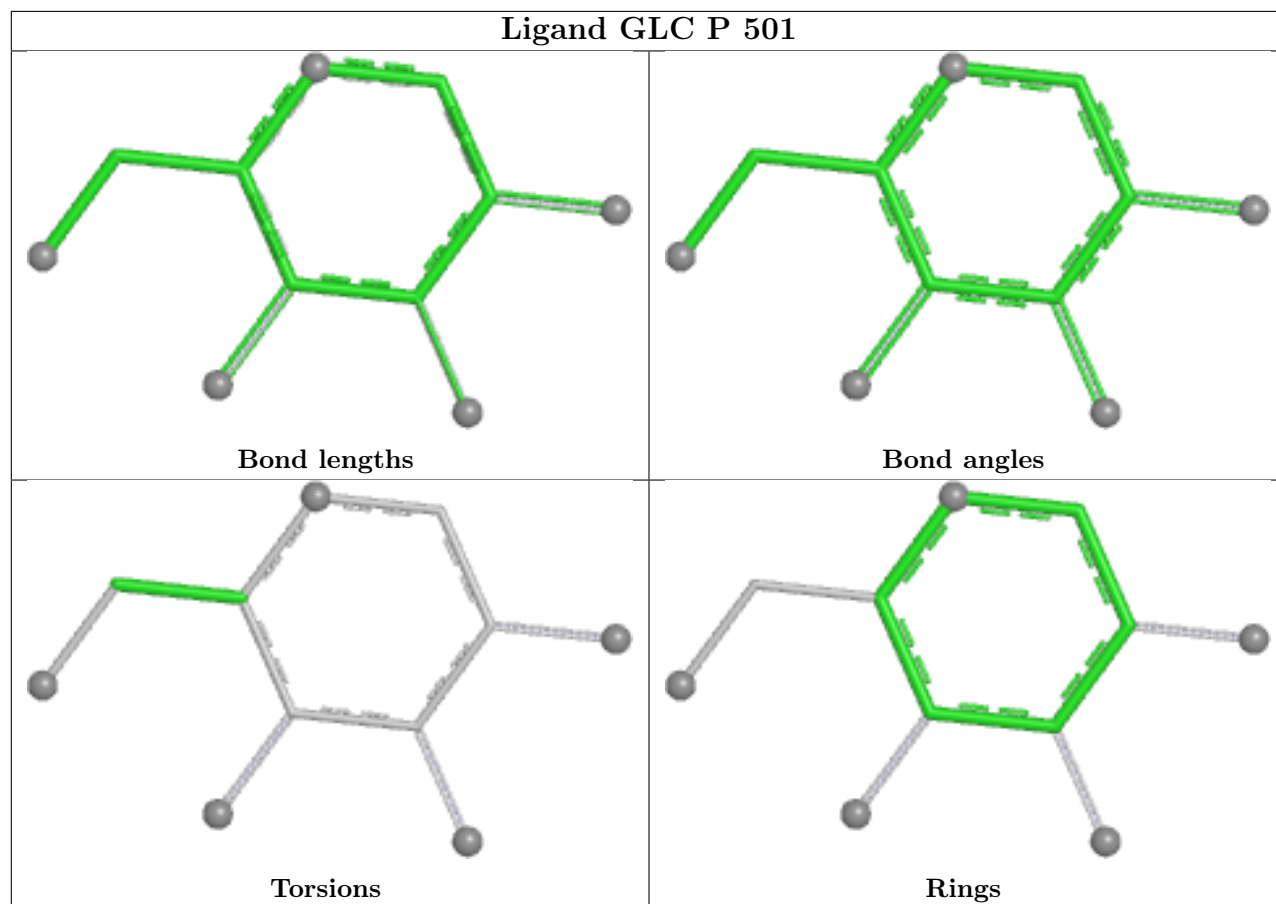
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

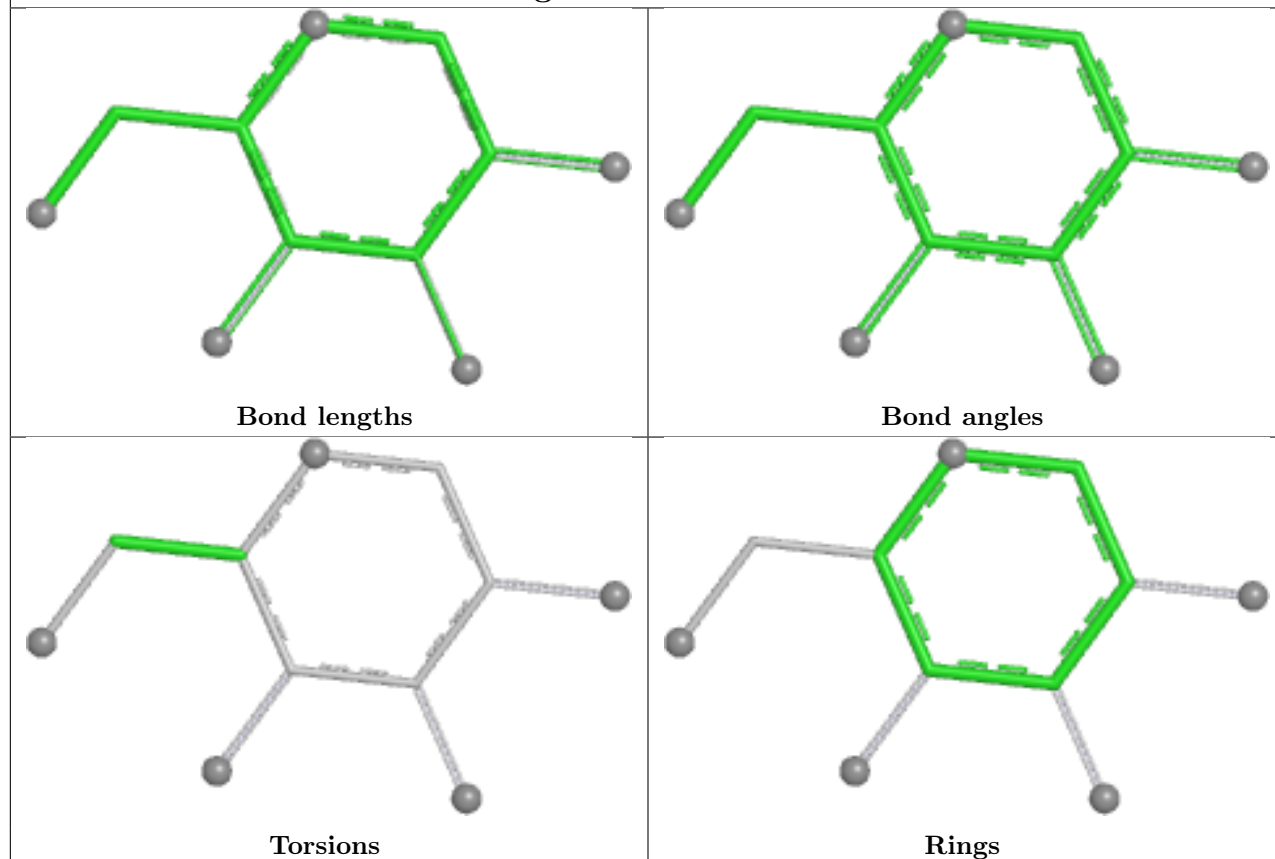




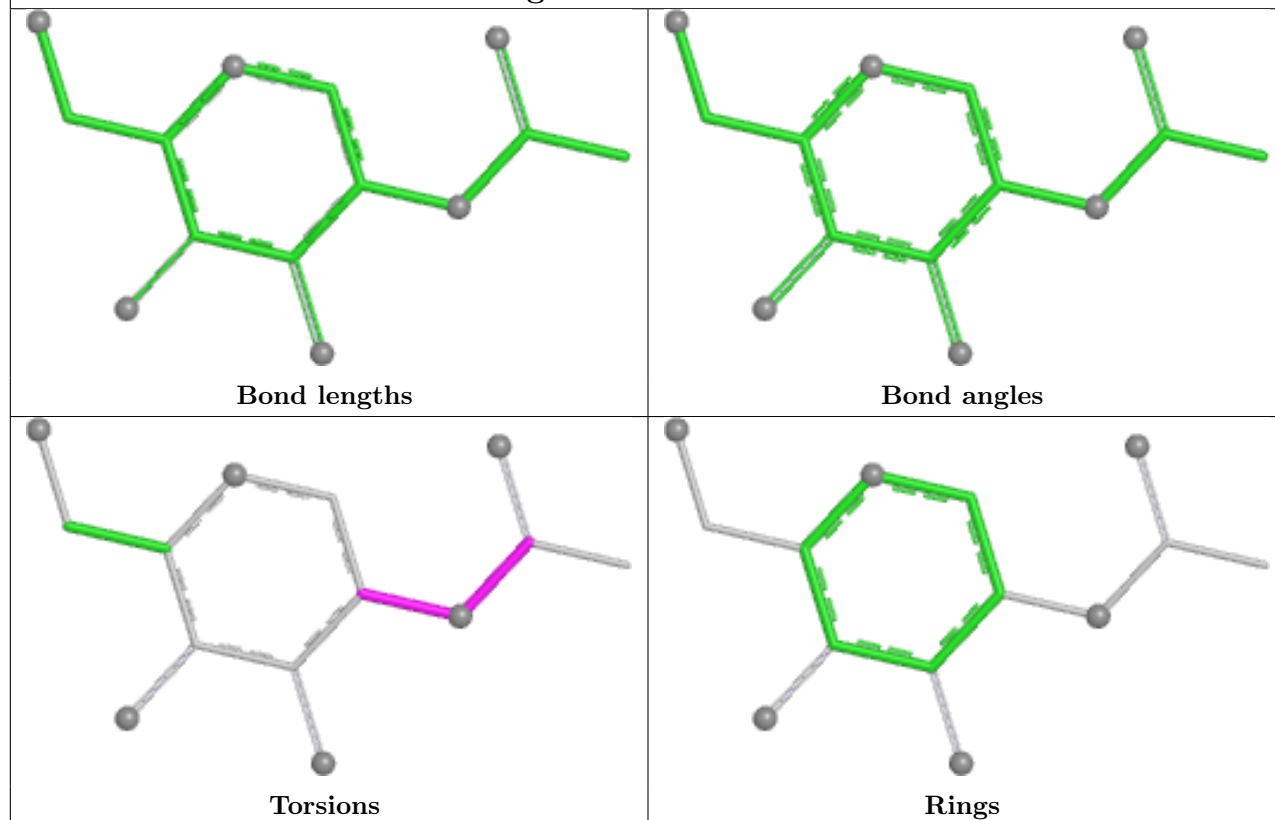




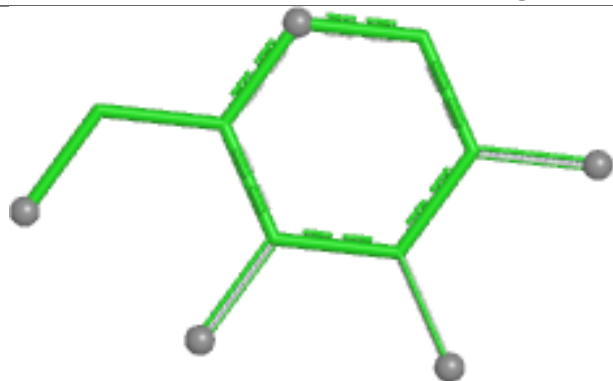
Ligand GLC J 501



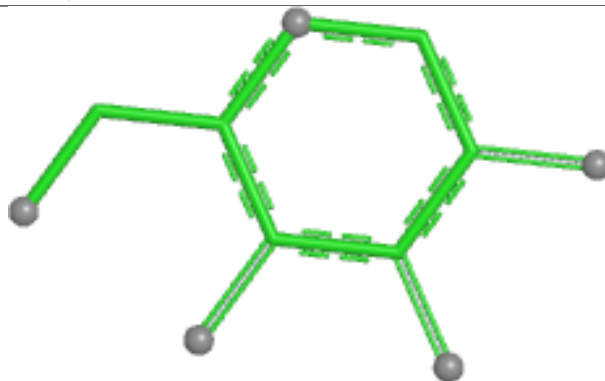
Ligand NAG O 502



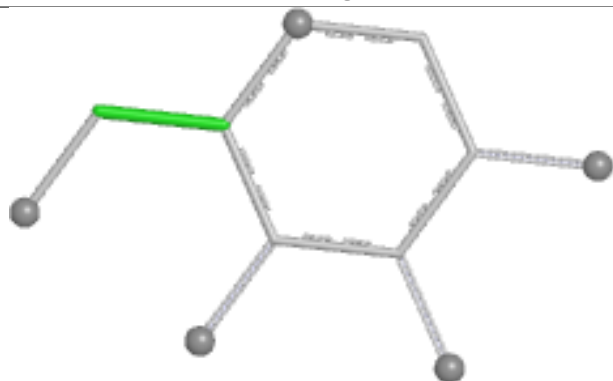
Ligand GLC Q 502



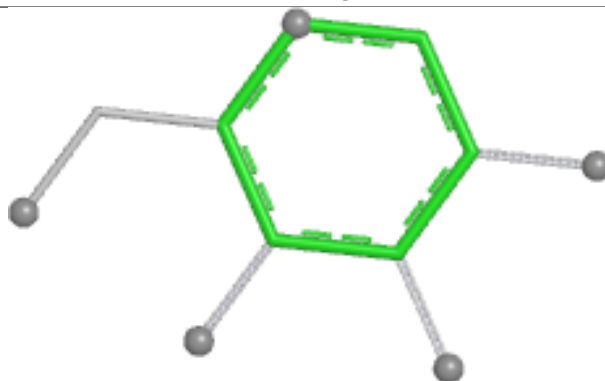
Bond lengths



Bond angles

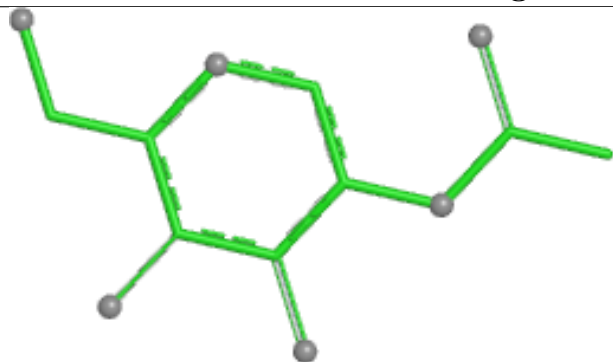


Torsions

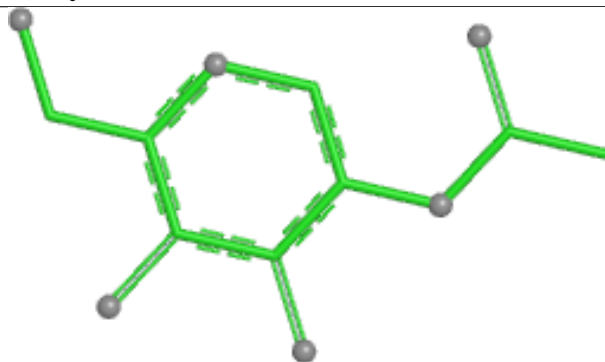


Rings

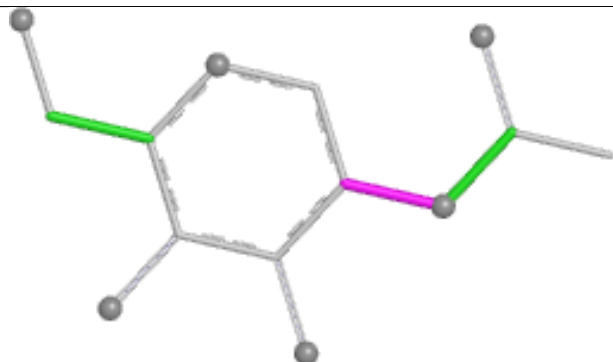
Ligand NAG Q 501



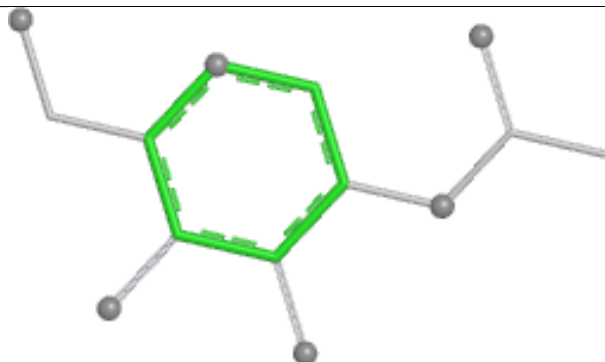
Bond lengths



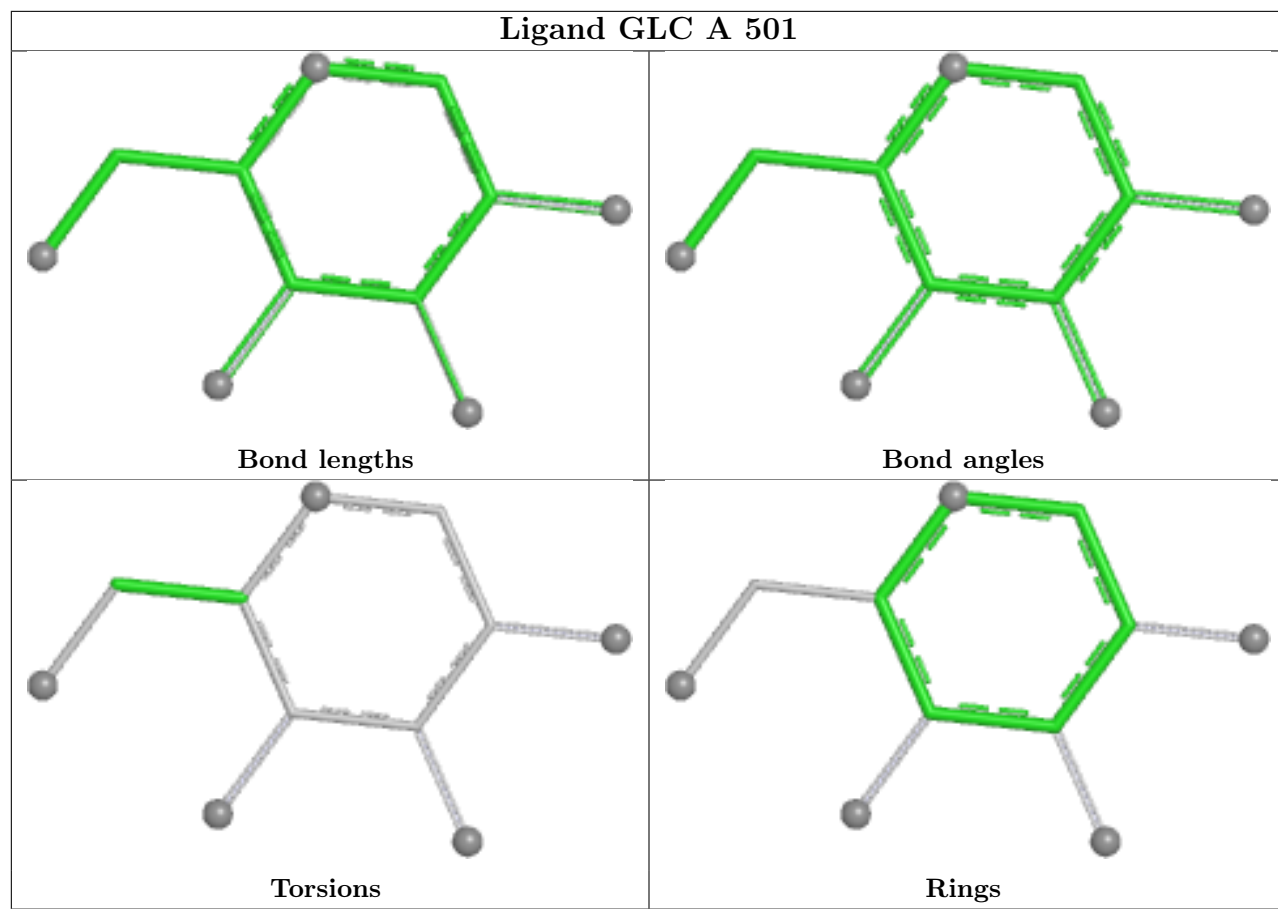
Bond angles

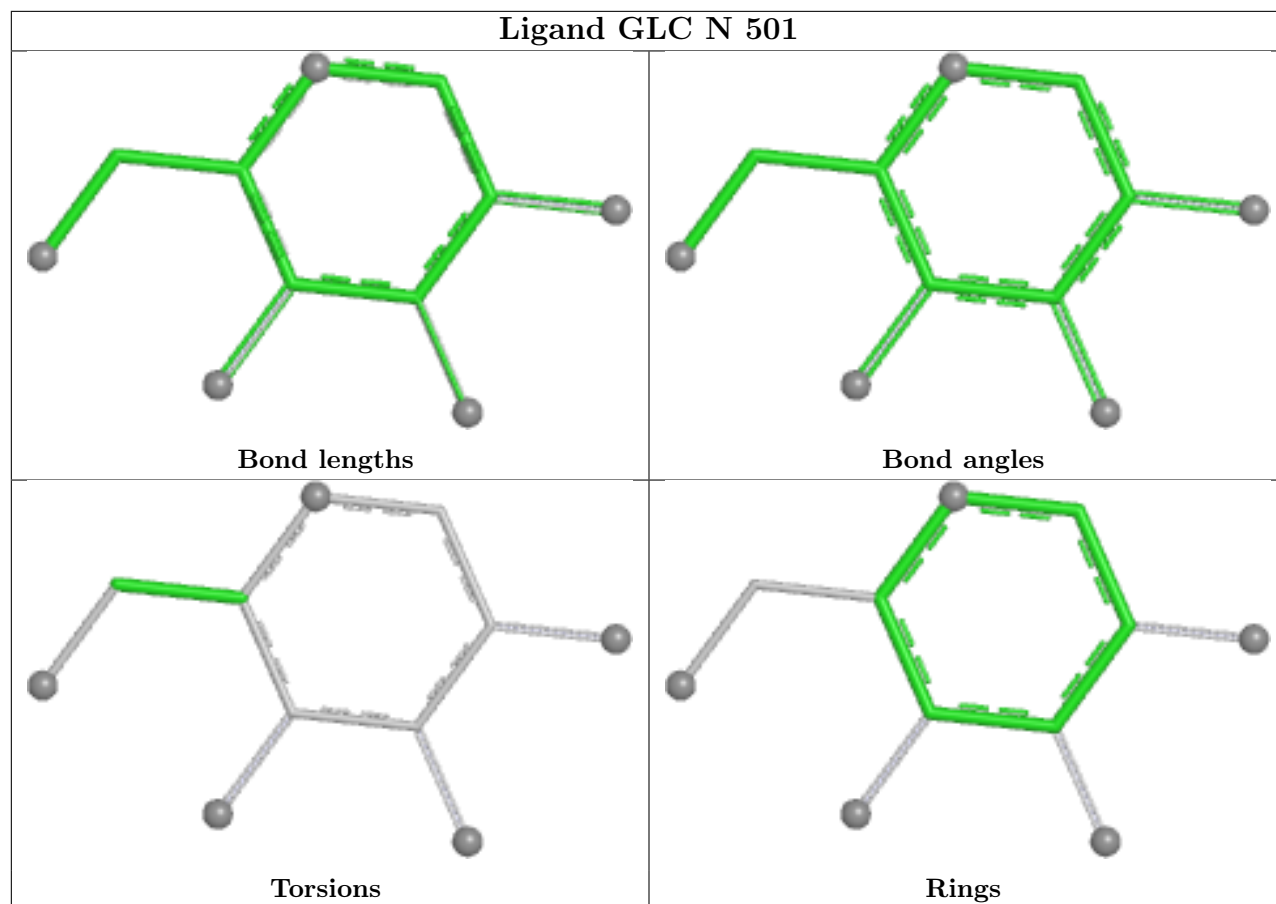


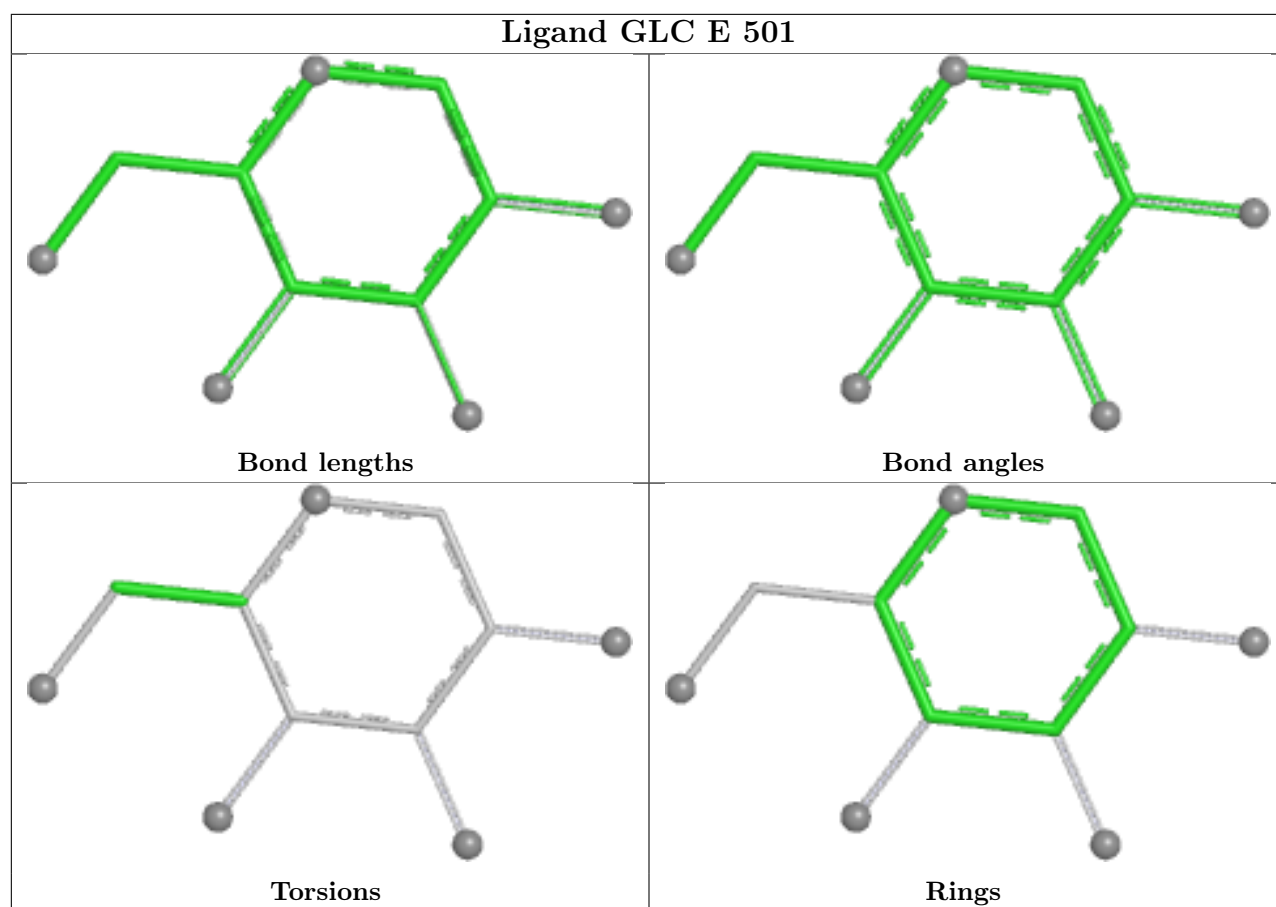
Torsions



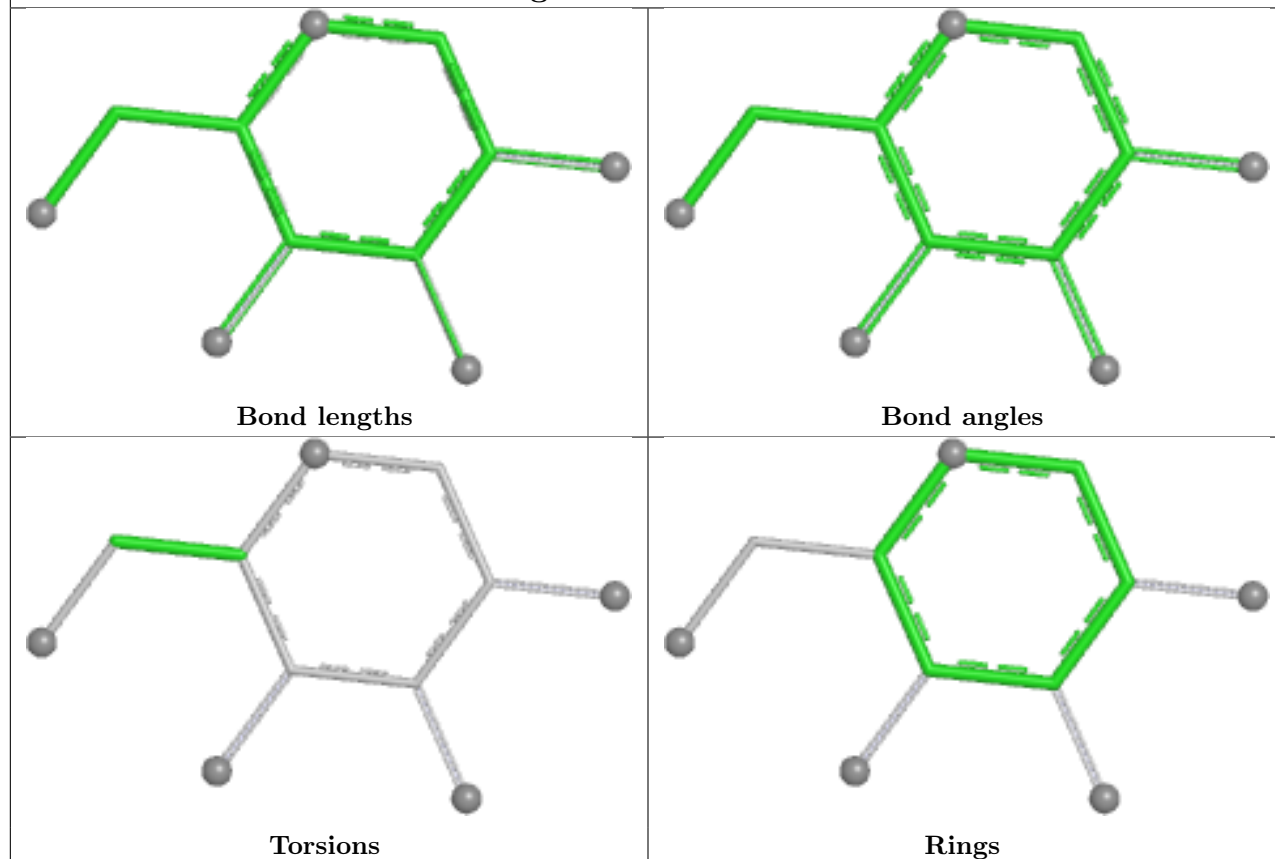
Rings



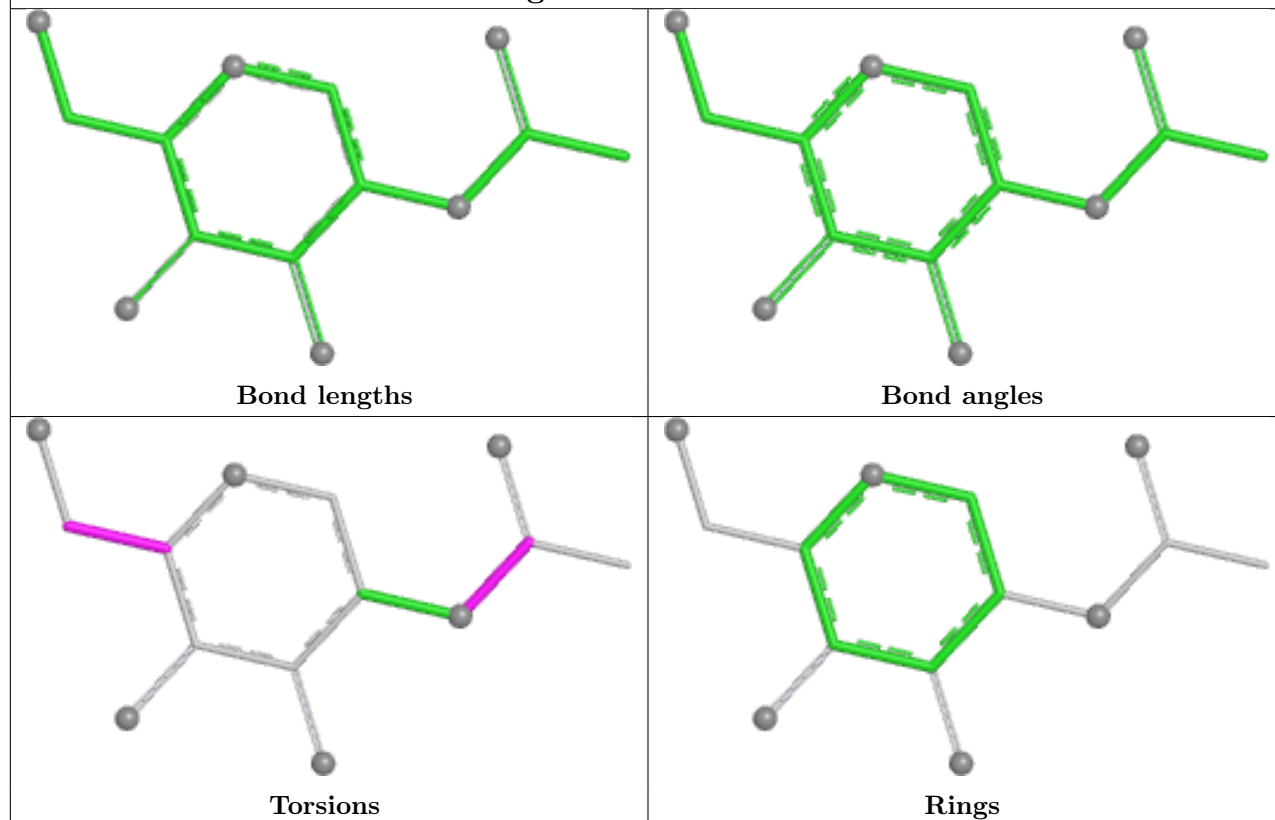


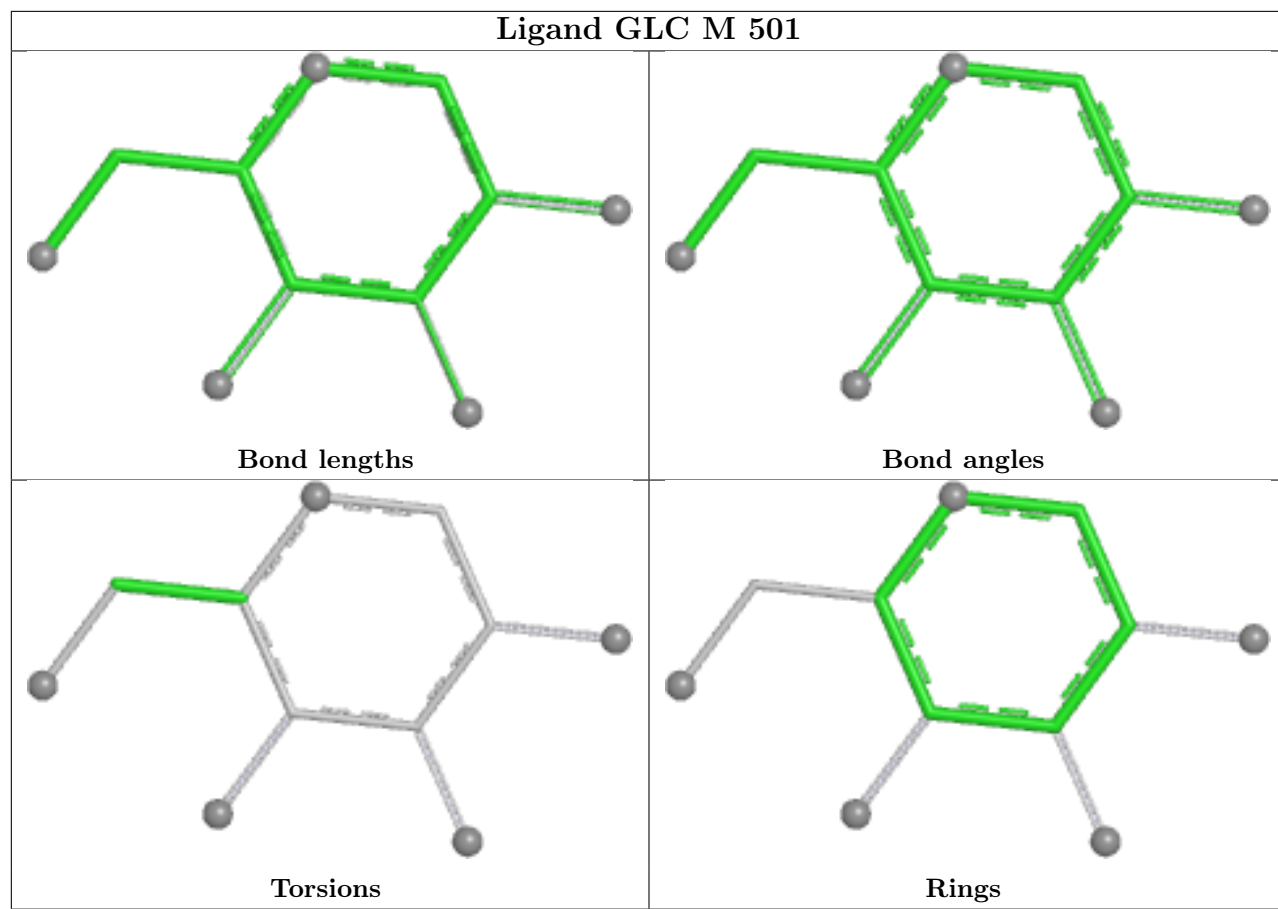


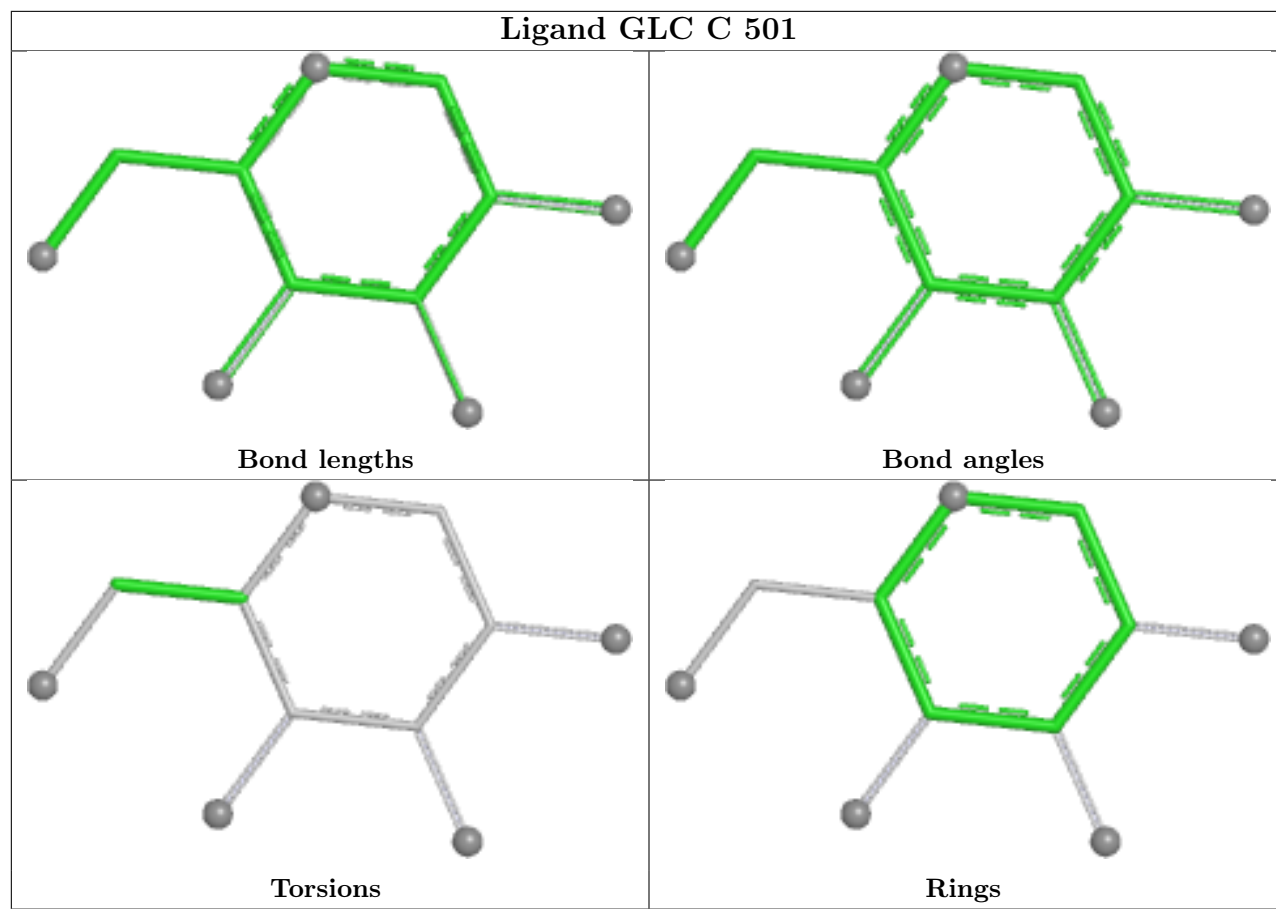
Ligand GLC O 501



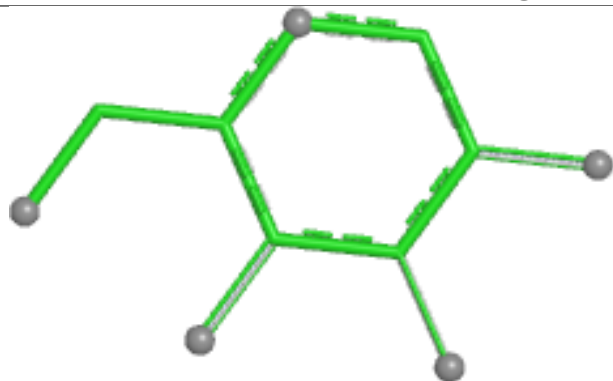
Ligand NAG R 501



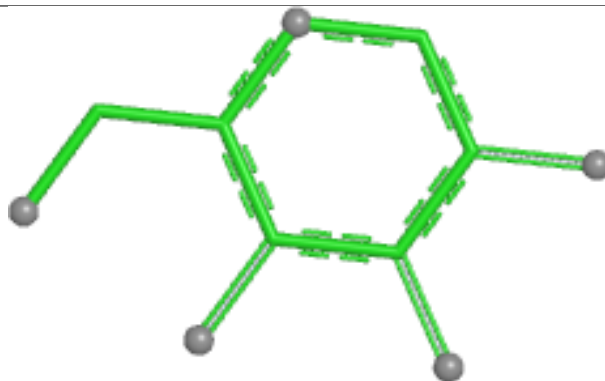




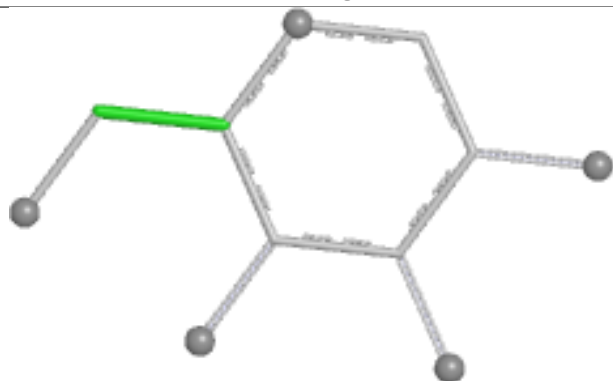
Ligand GLC F 501



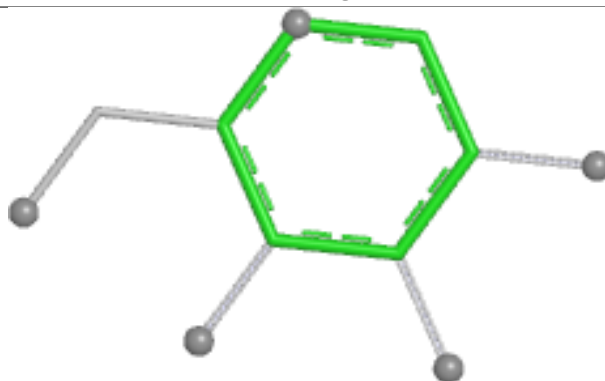
Bond lengths



Bond angles

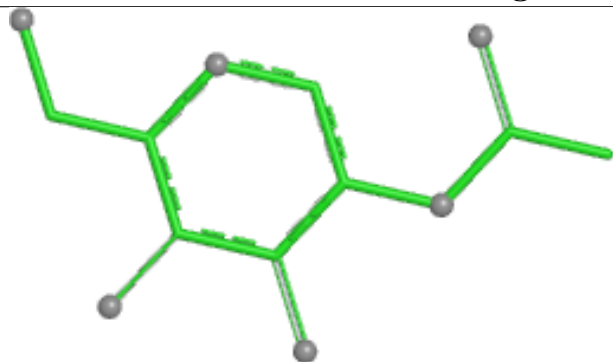


Torsions

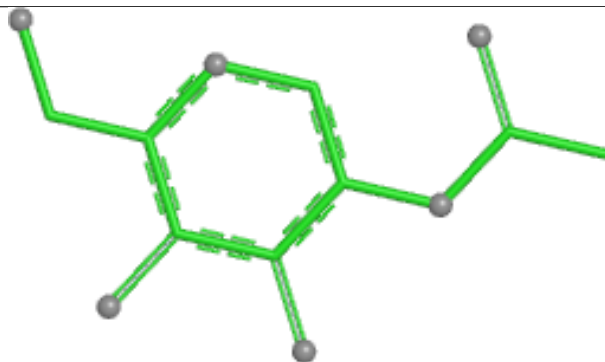


Rings

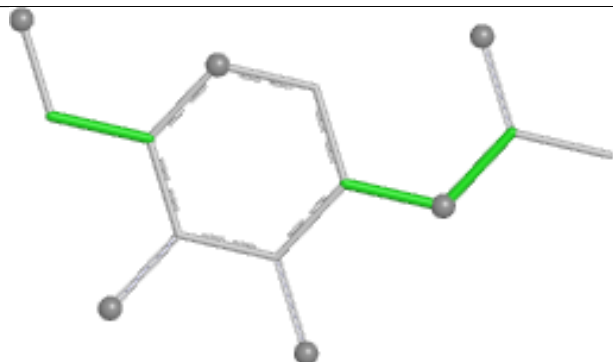
Ligand NAG E 502



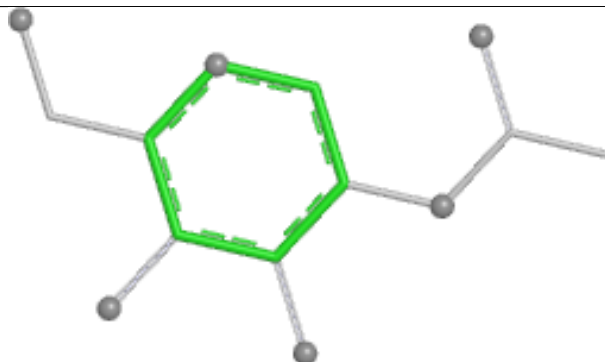
Bond lengths



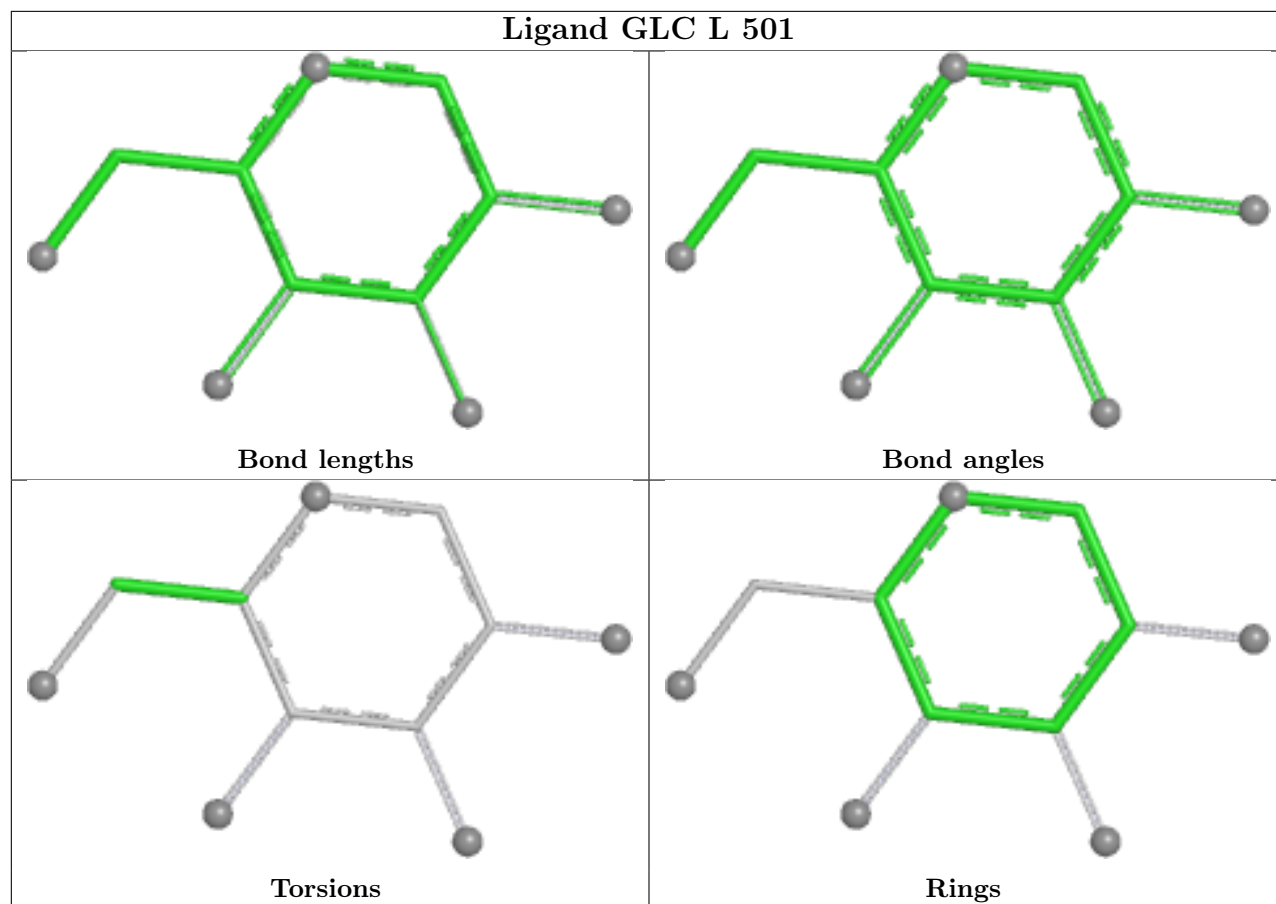
Bond angles

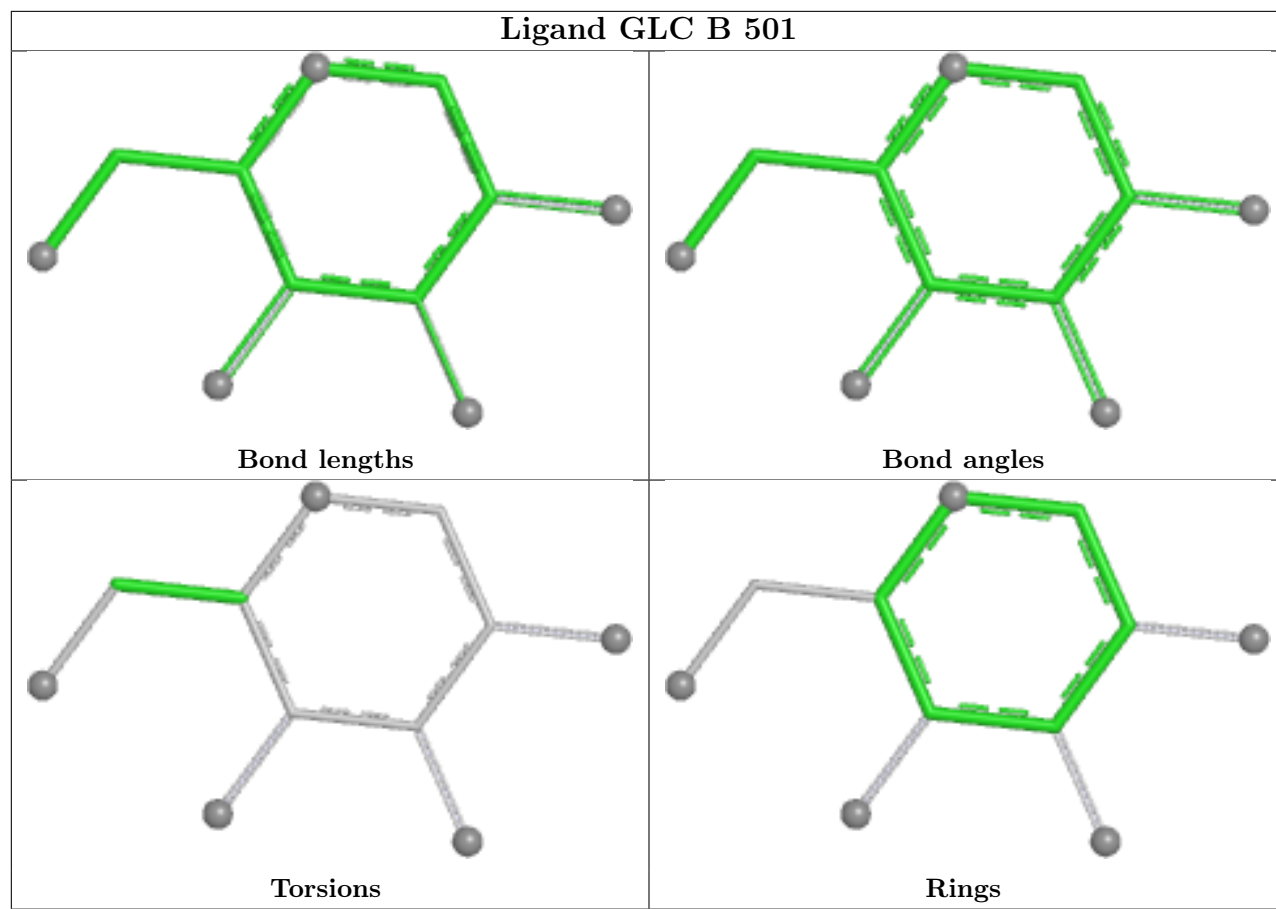


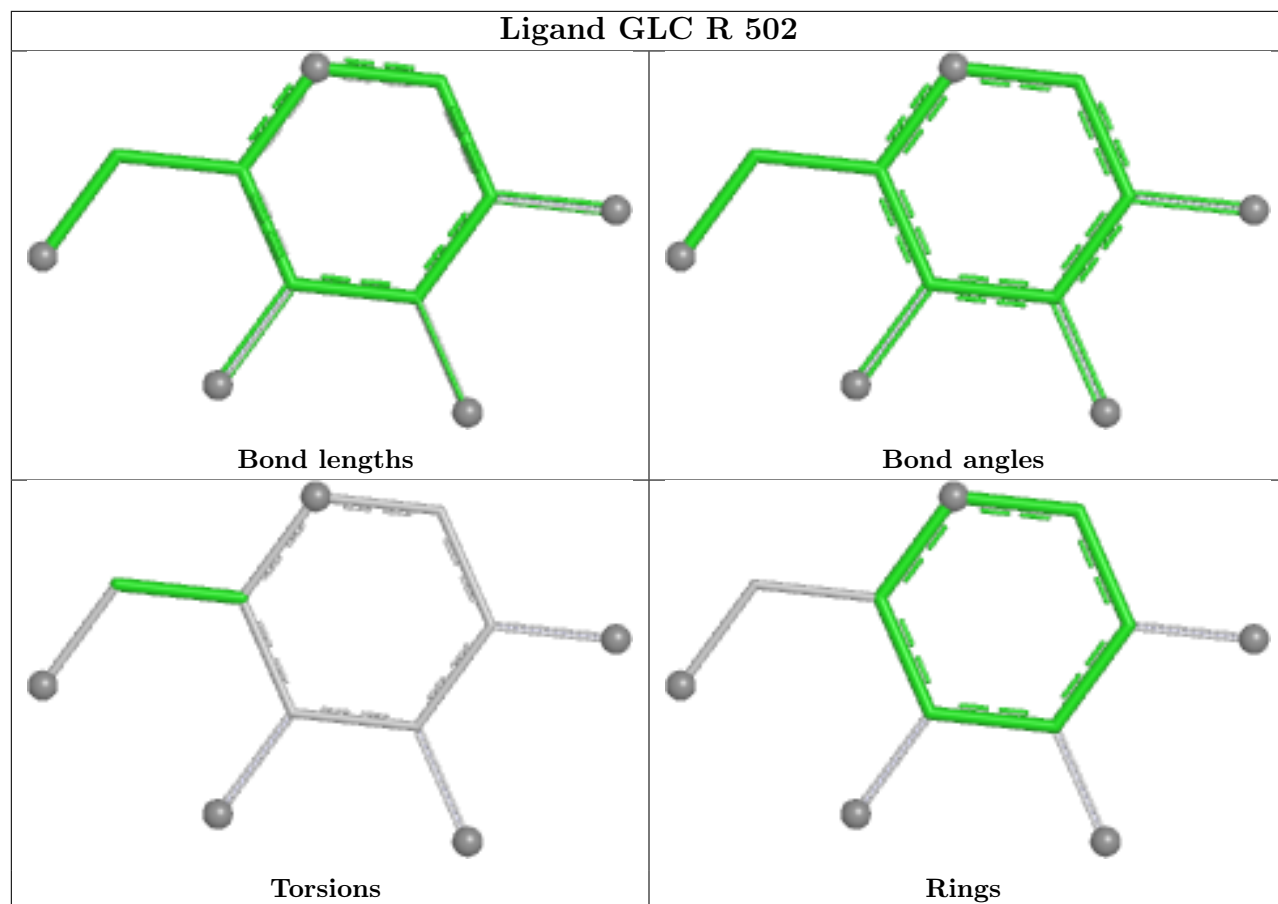
Torsions

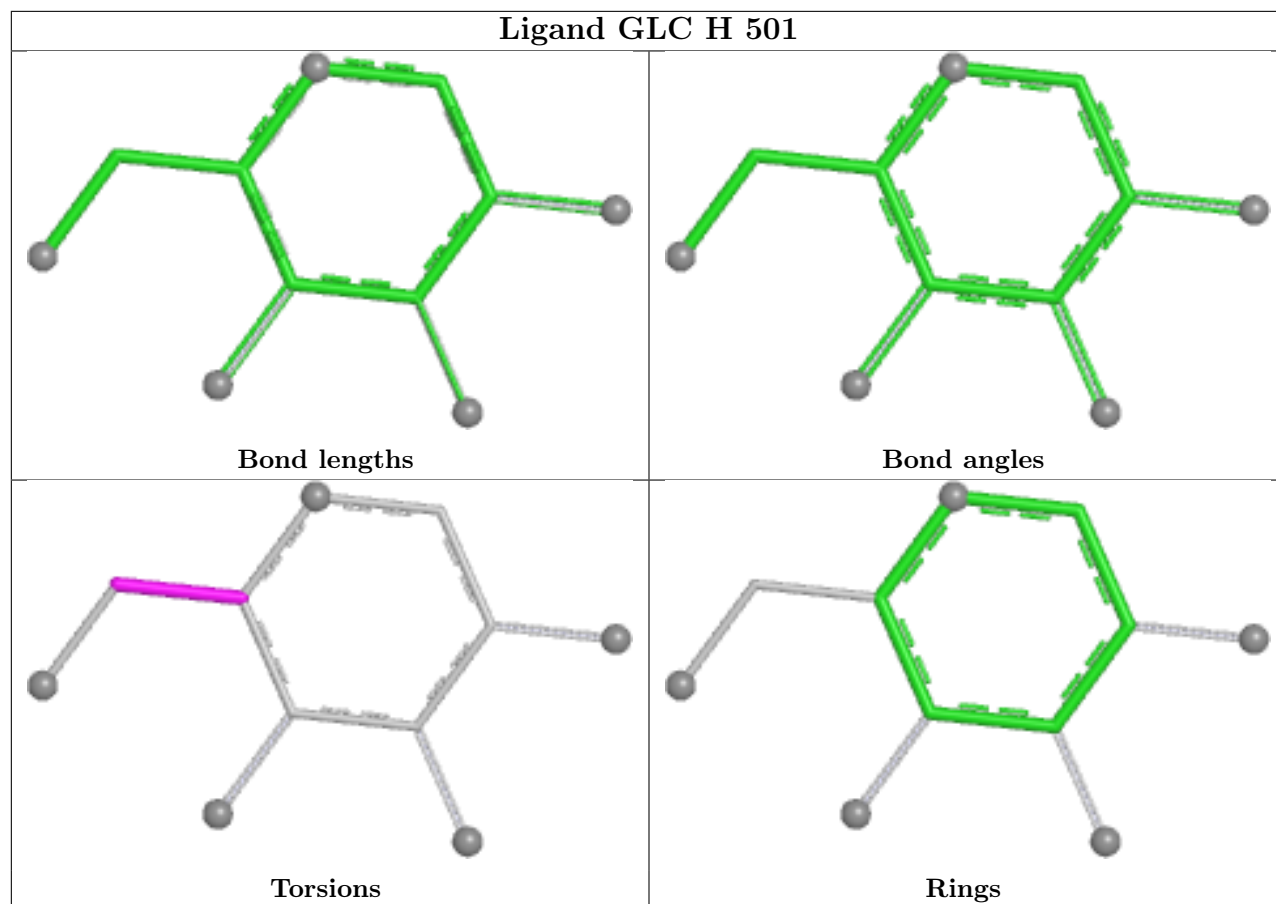


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	366/410 (89%)	0.06	4 (1%) 78 74	44, 61, 99, 114	0
1	B	366/410 (89%)	0.26	11 (3%) 52 47	45, 67, 132, 155	0
1	C	366/410 (89%)	0.26	7 (1%) 66 61	46, 72, 143, 173	0
1	D	321/410 (78%)	0.46	24 (7%) 20 16	51, 72, 141, 161	0
1	E	285/410 (69%)	0.54	9 (3%) 50 44	61, 98, 140, 148	0
1	F	282/410 (68%)	0.53	7 (2%) 58 52	58, 86, 152, 181	0
1	G	365/410 (89%)	1.01	42 (11%) 9 7	77, 106, 141, 153	0
1	H	287/410 (70%)	1.23	40 (13%) 6 5	96, 123, 148, 155	0
1	I	343/410 (83%)	1.43	76 (22%) 2 2	90, 136, 167, 185	0
1	J	366/410 (89%)	0.10	9 (2%) 58 52	44, 60, 118, 128	0
1	K	365/410 (89%)	0.38	8 (2%) 62 57	55, 83, 132, 143	0
1	L	358/410 (87%)	0.29	5 (1%) 73 69	52, 74, 138, 163	0
1	M	287/410 (70%)	0.42	18 (6%) 26 20	52, 71, 157, 166	0
1	N	353/410 (86%)	0.57	19 (5%) 31 26	55, 91, 154, 172	0
1	O	301/410 (73%)	0.98	29 (9%) 13 10	79, 125, 153, 178	0
1	P	261/410 (63%)	0.70	16 (6%) 27 22	67, 90, 144, 160	0
1	Q	272/410 (66%)	0.76	17 (6%) 26 20	73, 100, 162, 169	0
1	R	310/410 (75%)	0.55	17 (5%) 30 25	62, 82, 160, 171	0
All	All	5854/7380 (79%)	0.57	358 (6%) 27 22	44, 91, 151, 185	0

All (358) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	57	PHE	5.2
1	I	301	LEU	5.1
1	I	61	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	231	CYS	4.4
1	I	25	ILE	4.3
1	D	154	ALA	4.3
1	D	147	ILE	4.1
1	R	57	PHE	4.0
1	P	54	LEU	4.0
1	H	54	LEU	4.0
1	I	338	GLY	3.9
1	M	152	ALA	3.9
1	H	262	THR	3.8
1	H	238	THR	3.7
1	R	110	TRP	3.7
1	N	262	THR	3.7
1	I	184	VAL	3.7
1	I	266	THR	3.7
1	D	158	ALA	3.7
1	Q	299	ASN	3.7
1	N	242	ASP	3.6
1	I	217	VAL	3.6
1	P	199	THR	3.6
1	H	53	ALA	3.6
1	G	205	ALA	3.5
1	I	314	LEU	3.5
1	M	150	LEU	3.5
1	G	98	PRO	3.5
1	N	381	ALA	3.5
1	H	230	PHE	3.5
1	K	377	ILE	3.5
1	D	67	LEU	3.4
1	N	315	ALA	3.4
1	G	252	ALA	3.4
1	J	57	PHE	3.3
1	I	333	VAL	3.3
1	R	50	LEU	3.3
1	E	385	ALA	3.3
1	I	306	ALA	3.3
1	I	310	LEU	3.3
1	N	261	VAL	3.3
1	G	162	THR	3.3
1	H	386	TYR	3.3
1	O	57	PHE	3.2
1	M	65	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	O	127	LEU	3.2
1	I	315	ALA	3.2
1	M	315	ALA	3.2
1	B	65	LEU	3.2
1	I	276	LEU	3.2
1	M	67	LEU	3.2
1	N	57	PHE	3.2
1	D	137	PRO	3.2
1	D	108	THR	3.2
1	F	151	THR	3.2
1	R	158	ALA	3.1
1	G	325	GLY	3.1
1	O	147	ILE	3.1
1	F	327	CYS	3.1
1	G	233	CYS	3.1
1	I	380	LEU	3.1
1	H	171	THR	3.0
1	O	381	ALA	3.0
1	Q	154	ALA	3.0
1	I	77	LEU	3.0
1	M	57	PHE	3.0
1	Q	157	LYS	3.0
1	D	140	LEU	3.0
1	I	65	LEU	3.0
1	I	346	TRP	3.0
1	N	265	PRO	3.0
1	H	371	GLN	3.0
1	G	217	VAL	2.9
1	P	283	THR	2.9
1	M	377	ILE	2.9
1	G	266	THR	2.9
1	R	171	THR	2.9
1	D	152	ALA	2.9
1	O	237	ARG	2.9
1	L	65	LEU	2.9
1	N	150	LEU	2.9
1	G	260	GLY	2.9
1	I	31	VAL	2.8
1	F	57	PHE	2.8
1	H	273	VAL	2.8
1	I	328	VAL	2.8
1	G	207	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	154	ALA	2.8
1	N	143	ALA	2.8
1	I	163	VAL	2.8
1	G	216	ALA	2.8
1	I	241	ALA	2.8
1	J	71	ALA	2.8
1	G	261	VAL	2.8
1	D	72	ALA	2.8
1	G	211	THR	2.8
1	H	268	THR	2.8
1	I	307	THR	2.8
1	I	277	CYS	2.8
1	H	214	GLY	2.7
1	H	64	ILE	2.7
1	O	386	TYR	2.7
1	I	37	LEU	2.7
1	F	111	ALA	2.7
1	K	162	THR	2.7
1	O	268	THR	2.7
1	D	110	TRP	2.7
1	Q	367	LEU	2.7
1	E	52	THR	2.7
1	G	264	THR	2.7
1	G	256	GLY	2.7
1	I	377	ILE	2.7
1	D	54	LEU	2.7
1	N	367	LEU	2.7
1	R	143	ALA	2.7
1	H	194	ASP	2.7
1	I	201	PHE	2.7
1	G	253	PRO	2.7
1	H	163	VAL	2.7
1	I	130	TYR	2.7
1	B	315	ALA	2.7
1	D	151	THR	2.7
1	I	228	ALA	2.7
1	K	251	THR	2.7
1	Q	158	ALA	2.7
1	I	177	GLN	2.7
1	B	163	VAL	2.6
1	J	54	LEU	2.6
1	K	306	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	259	PRO	2.6
1	G	316	THR	2.6
1	M	53	ALA	2.6
1	M	158	ALA	2.6
1	M	218	ALA	2.6
1	I	64	ILE	2.6
1	H	313	PHE	2.6
1	F	67	LEU	2.6
1	I	176	LEU	2.6
1	I	213	CYS	2.6
1	P	380	LEU	2.6
1	I	155	VAL	2.6
1	O	198	TYR	2.6
1	I	256	GLY	2.6
1	H	261	VAL	2.6
1	C	53	ALA	2.6
1	G	166	SER	2.6
1	I	48	ALA	2.6
1	I	309	ILE	2.5
1	I	230	PHE	2.5
1	D	380	LEU	2.5
1	I	233	CYS	2.5
1	N	249	ALA	2.5
1	O	48	ALA	2.5
1	N	93	THR	2.5
1	O	377	ILE	2.5
1	H	239	ASN	2.5
1	Q	306	ALA	2.5
1	P	266	THR	2.5
1	M	69	MET	2.5
1	R	74	PRO	2.5
1	I	290	ILE	2.5
1	I	355	ILE	2.5
1	I	92	LEU	2.5
1	D	145	ASN	2.5
1	D	155	VAL	2.5
1	H	234	ALA	2.5
1	M	149	ARG	2.5
1	E	207	THR	2.5
1	G	52	THR	2.5
1	O	251	THR	2.5
1	G	247	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	384	PRO	2.5
1	J	117	LEU	2.5
1	N	92	LEU	2.5
1	O	374	LEU	2.5
1	P	367	LEU	2.5
1	I	248	VAL	2.5
1	E	381	ALA	2.5
1	N	158	ALA	2.5
1	I	391	SER	2.5
1	B	357	LEU	2.4
1	G	54	LEU	2.4
1	I	270	LEU	2.4
1	Q	310	LEU	2.4
1	R	115	LEU	2.4
1	I	313	PHE	2.4
1	O	145	ASN	2.4
1	N	71	ALA	2.4
1	C	115	LEU	2.4
1	R	357	LEU	2.4
1	I	125	ALA	2.4
1	B	389	LEU	2.4
1	J	124	GLN	2.4
1	G	209	ARG	2.4
1	M	148	ARG	2.4
1	I	156	ALA	2.4
1	M	206	SER	2.4
1	O	50	LEU	2.4
1	O	54	LEU	2.4
1	G	333	VAL	2.4
1	G	240	GLY	2.3
1	A	54	LEU	2.3
1	L	123	HIS	2.3
1	H	198	TYR	2.3
1	A	315	ALA	2.3
1	K	161	PRO	2.3
1	I	255	THR	2.3
1	B	378	LEU	2.3
1	M	380	LEU	2.3
1	O	285	LEU	2.3
1	I	60	GLU	2.3
1	G	59	ASN	2.3
1	H	59	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	222	ALA	2.3
1	I	146	THR	2.3
1	R	151	THR	2.3
1	K	250	GLY	2.3
1	C	132	LEU	2.3
1	O	150	LEU	2.3
1	H	183	ALA	2.3
1	O	156	ALA	2.3
1	C	146	THR	2.3
1	P	52	THR	2.3
1	R	108	THR	2.3
1	I	325	GLY	2.3
1	E	54	LEU	2.3
1	J	389	LEU	2.3
1	G	263	ALA	2.2
1	I	53	ALA	2.2
1	I	72	ALA	2.2
1	D	146	THR	2.2
1	H	284	THR	2.2
1	I	171	THR	2.2
1	L	93	THR	2.2
1	D	64	ILE	2.2
1	I	127	LEU	2.2
1	Q	150	LEU	2.2
1	I	273	VAL	2.2
1	O	261	VAL	2.2
1	D	143	ALA	2.2
1	G	306	ALA	2.2
1	G	199	THR	2.2
1	I	223	THR	2.2
1	P	264	THR	2.2
1	Q	167	THR	2.2
1	R	67	LEU	2.2
1	G	321	ASP	2.2
1	G	202	GLU	2.2
1	K	51	GLU	2.2
1	O	217	VAL	2.2
1	Q	364	VAL	2.2
1	D	62	ASN	2.2
1	K	53	ALA	2.2
1	N	125	ALA	2.2
1	B	162	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	58	GLN	2.2
1	D	150	LEU	2.2
1	H	61	LEU	2.2
1	N	250	GLY	2.2
1	O	61	LEU	2.2
1	H	41	ILE	2.2
1	H	286	SER	2.2
1	G	165	GLU	2.2
1	I	103	TRP	2.2
1	D	370	PRO	2.2
1	I	55	PRO	2.2
1	Q	333	VAL	2.2
1	G	200	ALA	2.2
1	I	71	ALA	2.2
1	I	164	ALA	2.2
1	H	269	MET	2.2
1	B	134	GLY	2.2
1	E	61	LEU	2.2
1	E	150	LEU	2.2
1	H	229	LEU	2.2
1	P	67	LEU	2.2
1	P	377	ILE	2.2
1	I	305	SER	2.2
1	B	160	ASP	2.2
1	D	138	GLU	2.2
1	C	89	PRO	2.2
1	F	107	TRP	2.2
1	E	249	ALA	2.1
1	F	207	THR	2.1
1	I	207	THR	2.1
1	J	118	LEU	2.1
1	N	115	LEU	2.1
1	O	52	THR	2.1
1	C	64	ILE	2.1
1	H	180	ILE	2.1
1	O	130	TYR	2.1
1	I	73	GLU	2.1
1	G	206	SER	2.1
1	C	55	PRO	2.1
1	P	55	PRO	2.1
1	H	201	PHE	2.1
1	H	69	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	69	MET	2.1
1	P	348	GLN	2.1
1	G	249	ALA	2.1
1	H	241	ALA	2.1
1	A	93	THR	2.1
1	D	132	LEU	2.1
1	G	238	THR	2.1
1	G	262	THR	2.1
1	L	117	LEU	2.1
1	R	65	LEU	2.1
1	R	283	THR	2.1
1	A	130	TYR	2.1
1	G	259	PRO	2.1
1	G	241	ALA	2.1
1	I	216	ALA	2.1
1	R	315	ALA	2.1
1	H	374	LEU	2.1
1	I	300	LEU	2.1
1	J	134	GLY	2.1
1	J	367	LEU	2.1
1	O	270	LEU	2.1
1	L	295	THR	2.1
1	Q	283	THR	2.1
1	Q	25	ILE	2.1
1	G	328	VAL	2.1
1	H	31	VAL	2.1
1	I	297	VAL	2.1
1	N	80	PHE	2.1
1	G	234	ALA	2.1
1	O	216	ALA	2.1
1	R	156	ALA	2.1
1	G	257	TRP	2.1
1	I	257	TRP	2.1
1	I	298	GLY	2.1
1	H	172	THR	2.1
1	P	180	ILE	2.1
1	M	337	LYS	2.1
1	P	286	SER	2.1
1	H	55	PRO	2.1
1	Q	155	VAL	2.0
1	E	200	ALA	2.0
1	H	225	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	367	LEU	2.0
1	O	380	LEU	2.0
1	D	70	THR	2.0
1	I	52	THR	2.0
1	Q	64	ILE	2.0
1	R	377	ILE	2.0
1	H	193	ASP	2.0
1	O	137	PRO	2.0
1	I	57	PHE	2.0
1	B	164	ALA	2.0
1	G	97	LEU	2.0
1	H	367	LEU	2.0
1	I	285	LEU	2.0
1	I	381	ALA	2.0
1	M	387	LEU	2.0
1	P	378	LEU	2.0
1	I	245	LYS	2.0
1	P	196	ASN	2.0
1	O	199	THR	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	X	2	14/15	0.33	0.12	151,160,163,163	0
5	NAG	X	1	14/15	0.38	0.14	149,154,160,161	0
5	BMA	X	3	11/12	0.41	0.13	158,166,170,173	0
5	NAG	V	2	14/15	0.42	0.12	144,157,161,162	0
4	BMA	U	3	11/12	0.54	0.16	112,134,140,145	0
3	MAN	T	5	11/12	0.55	0.19	122,128,133,134	0
5	BMA	Y	3	11/12	0.56	0.12	140,148,153,154	0
5	BMA	V	3	11/12	0.58	0.12	141,154,162,163	0
5	NAG	Y	1	14/15	0.62	0.15	113,124,130,130	0

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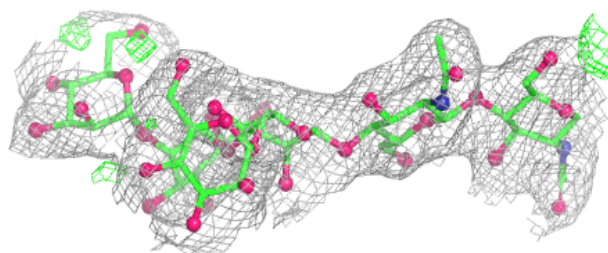
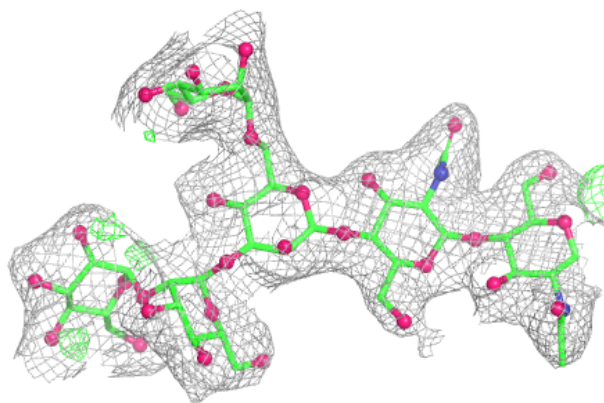
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	T	4	11/12	0.66	0.12	119,125,130,132	0
4	NAG	U	2	14/15	0.66	0.17	91,117,137,142	0
2	MAN	S	5	11/12	0.70	0.13	103,109,117,121	0
5	NAG	V	1	14/15	0.71	0.12	134,157,160,162	0
6	NAG	W	2	14/15	0.72	0.17	81,93,101,102	0
6	MAN	W	4	11/12	0.72	0.13	95,102,110,113	0
2	MAN	Z	5	11/12	0.74	0.12	102,102,102,102	0
4	NAG	U	1	14/15	0.74	0.16	78,104,117,119	0
6	NAG	W	1	14/15	0.77	0.16	77,84,97,97	0
5	NAG	Y	2	14/15	0.77	0.13	123,136,142,148	0
3	NAG	T	1	14/15	0.77	0.17	91,97,106,108	0
2	MAN	S	4	11/12	0.79	0.12	77,90,95,101	0
6	MAN	W	5	11/12	0.81	0.15	93,98,106,108	0
3	BMA	T	3	11/12	0.82	0.09	111,118,126,127	0
3	NAG	T	2	14/15	0.84	0.13	87,101,109,121	0
6	BMA	W	3	11/12	0.85	0.11	95,99,103,104	0
2	MAN	S	6	11/12	0.86	0.10	83,88,99,99	0
2	NAG	Z	1	14/15	0.89	0.12	75,84,87,91	0
2	MAN	Z	6	11/12	0.89	0.09	78,79,86,92	0
2	NAG	Z	2	14/15	0.89	0.10	67,83,89,90	0
2	BMA	S	3	11/12	0.90	0.09	73,87,92,93	0
2	MAN	Z	4	11/12	0.91	0.09	77,86,98,99	0
2	NAG	S	2	14/15	0.92	0.09	58,78,84,86	0
2	BMA	Z	3	11/12	0.93	0.07	74,83,86,93	0
2	NAG	S	1	14/15	0.93	0.09	69,75,82,85	0
6	NAG	c	1	14/15	-	-	132,137,141,144	0
6	NAG	c	2	14/15	-	-	129,138,151,157	0
6	BMA	c	3	11/12	-	-	137,141,145,147	0
6	MAN	c	4	11/12	-	-	142,146,150,151	0
6	MAN	c	5	11/12	-	-	139,144,149,149	0
7	NAG	a	1	14/15	-	-	92,104,110,113	0
7	NAG	a	2	14/15	-	-	104,113,123,129	0
7	BMA	a	3	11/12	-	-	122,127,134,137	0
7	MAN	a	4	11/12	-	-	124,134,137,138	0
7	MAN	a	5	11/12	-	-	126,131,132,133	0
7	NAG	b	1	14/15	-	-	101,113,122,123	0
7	NAG	b	2	14/15	-	-	113,124,135,144	0
7	BMA	b	3	11/12	-	-	135,139,140,141	0
7	MAN	b	4	11/12	-	-	132,141,146,148	0
7	MAN	b	5	11/12	-	-	132,134,139,143	0

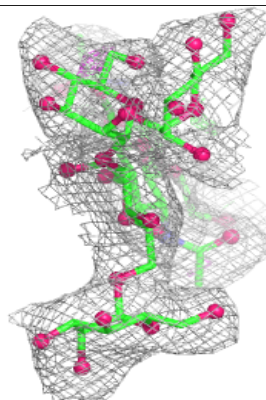
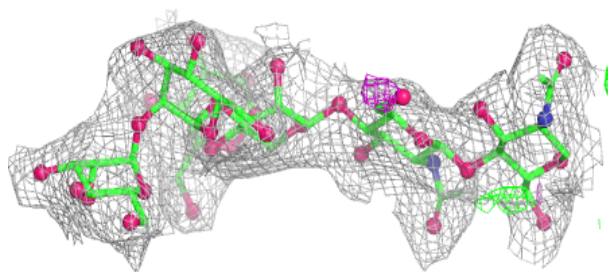
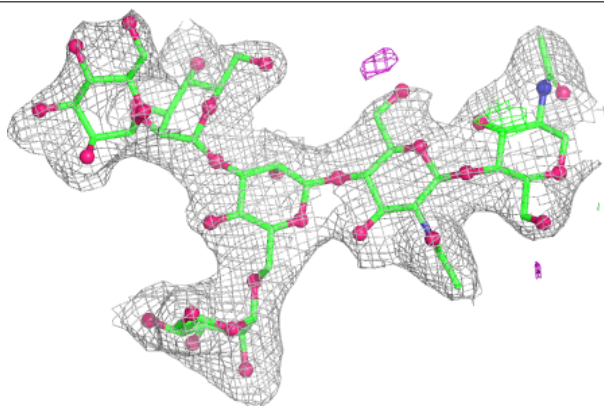
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain S:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

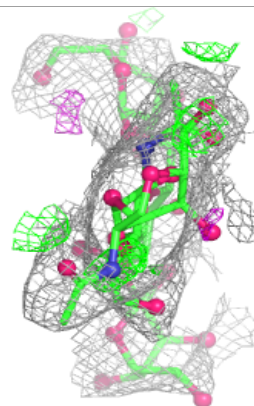
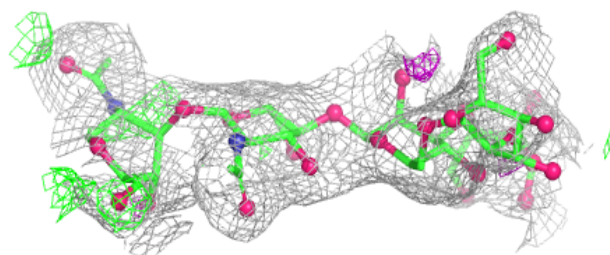
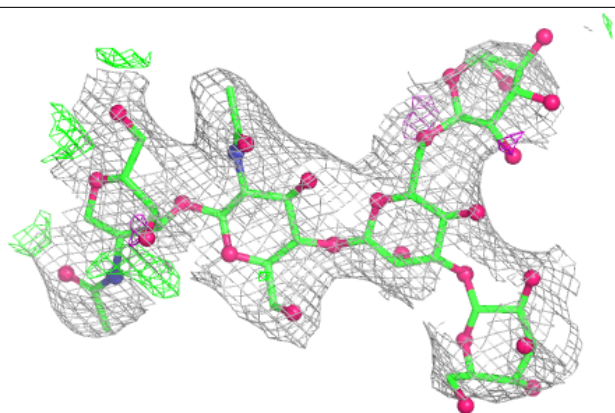
**Electron density around Chain Z:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

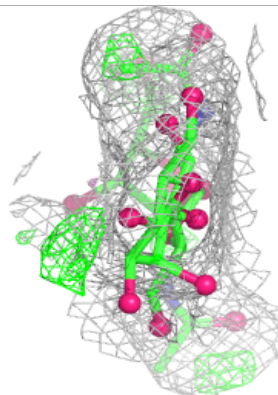
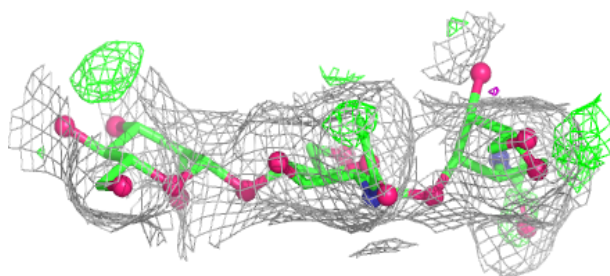
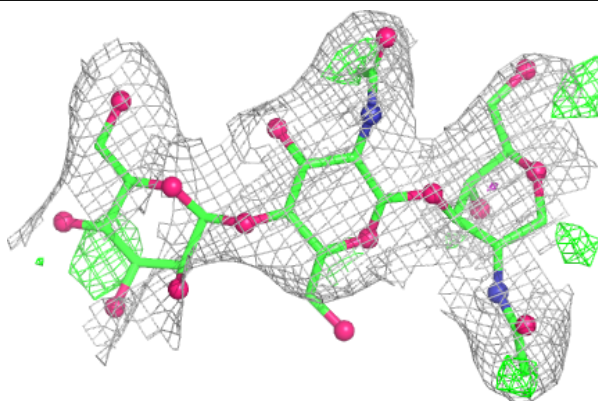


Electron density around Chain T:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

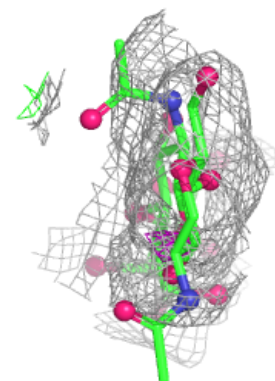
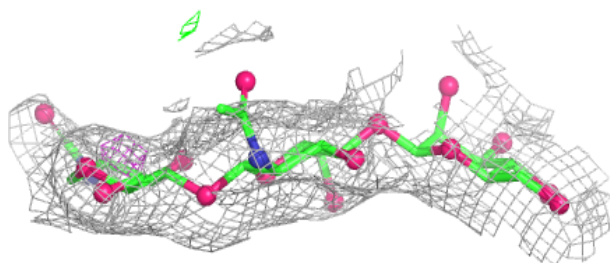
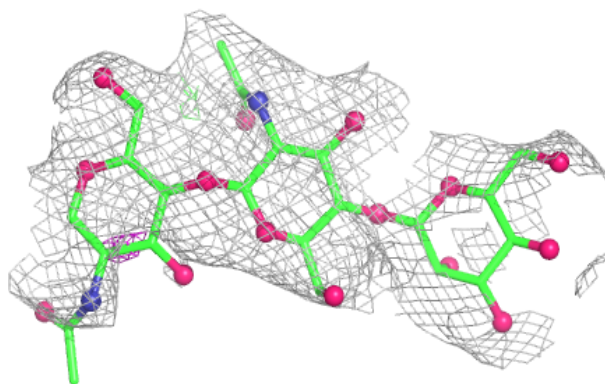
**Electron density around Chain U:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

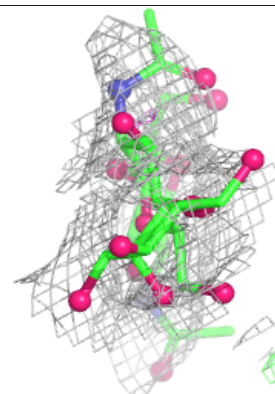
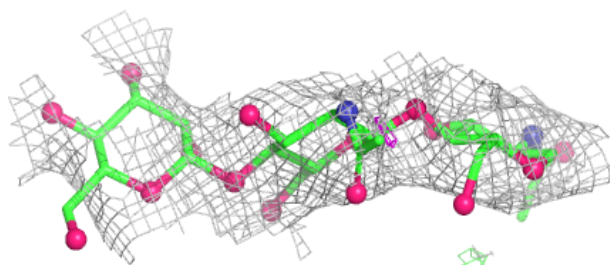
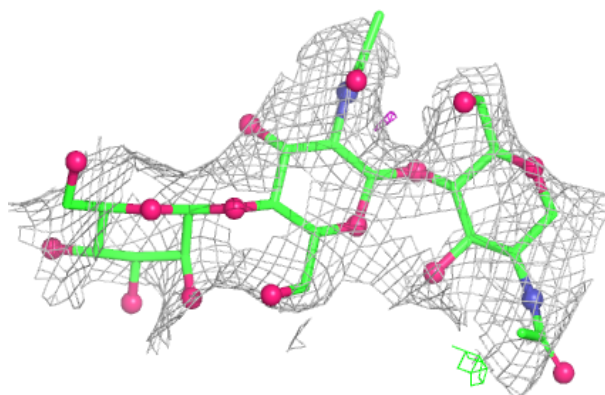


Electron density around Chain V:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

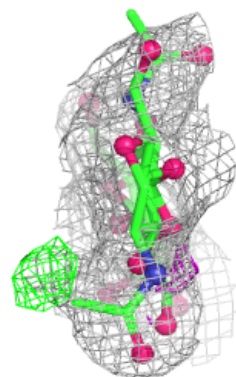
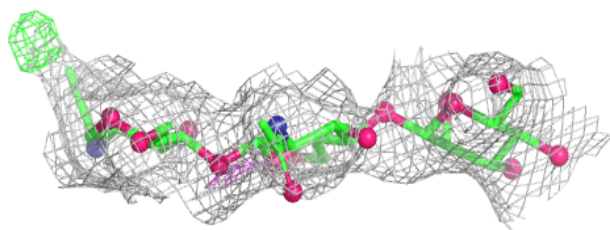
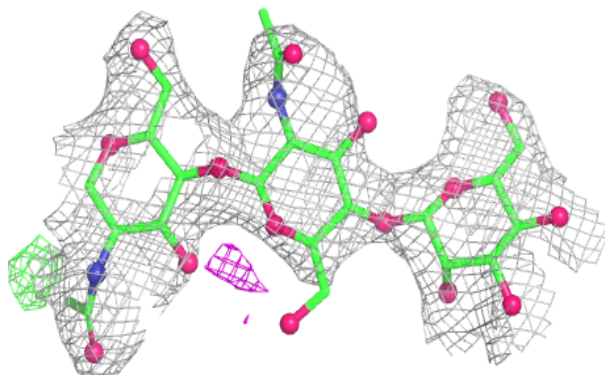
**Electron density around Chain X:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

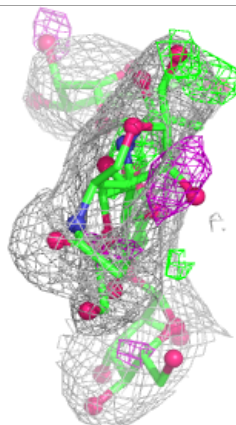
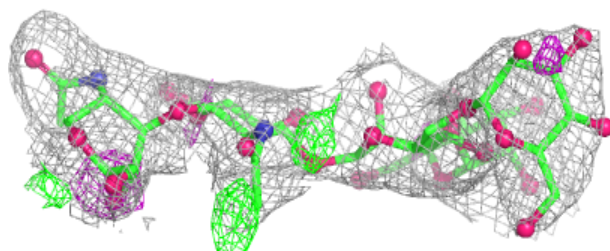
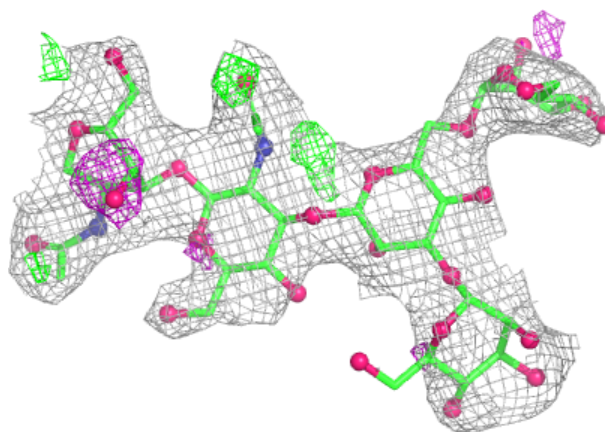


Electron density around Chain Y:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

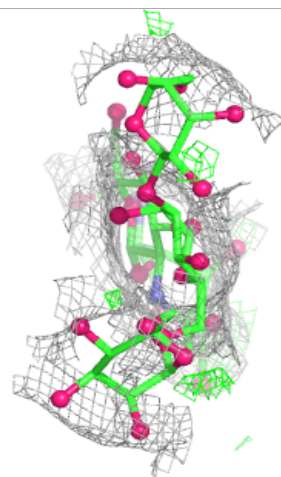
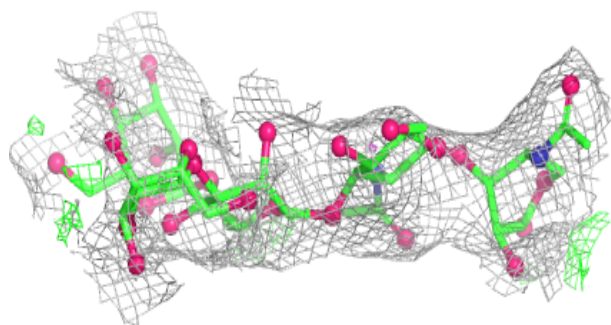
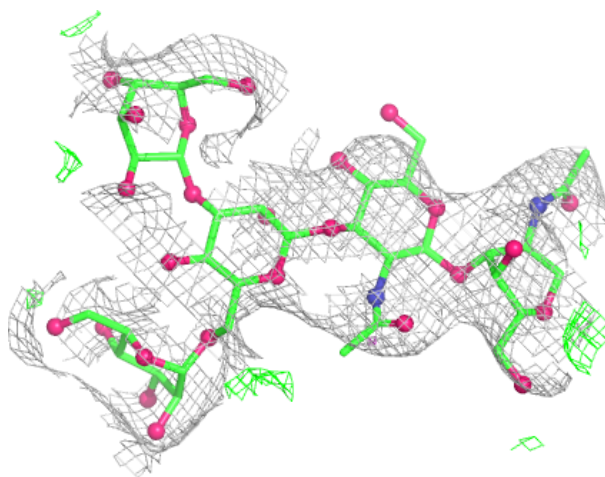
**Electron density around Chain W:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



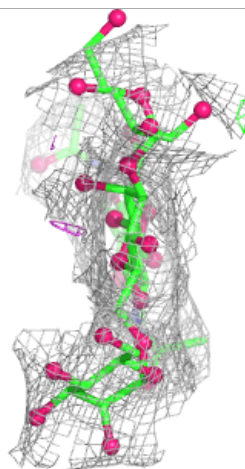
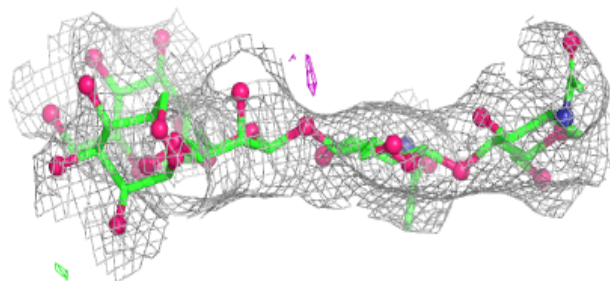
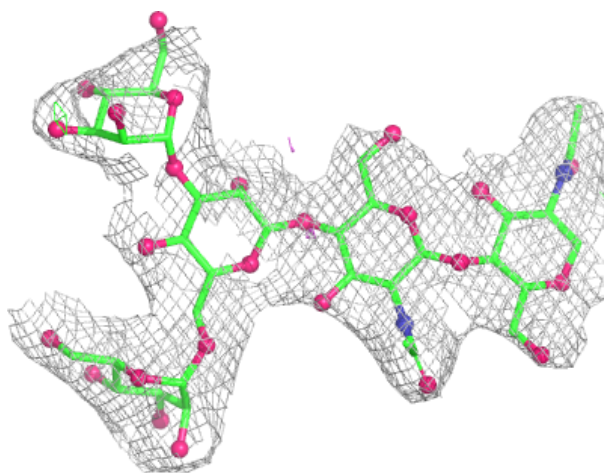
Electron density around Chain c:

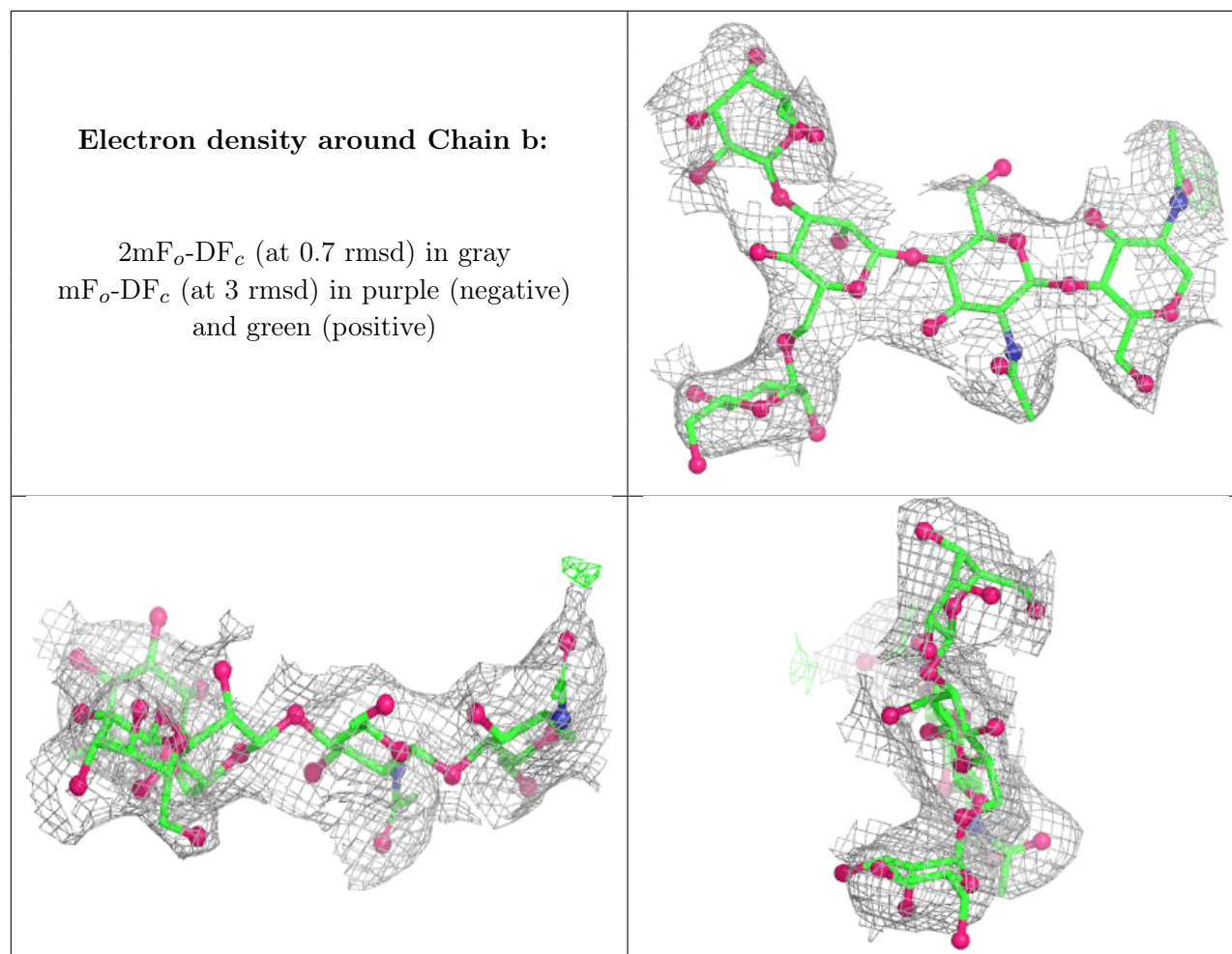
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain a:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

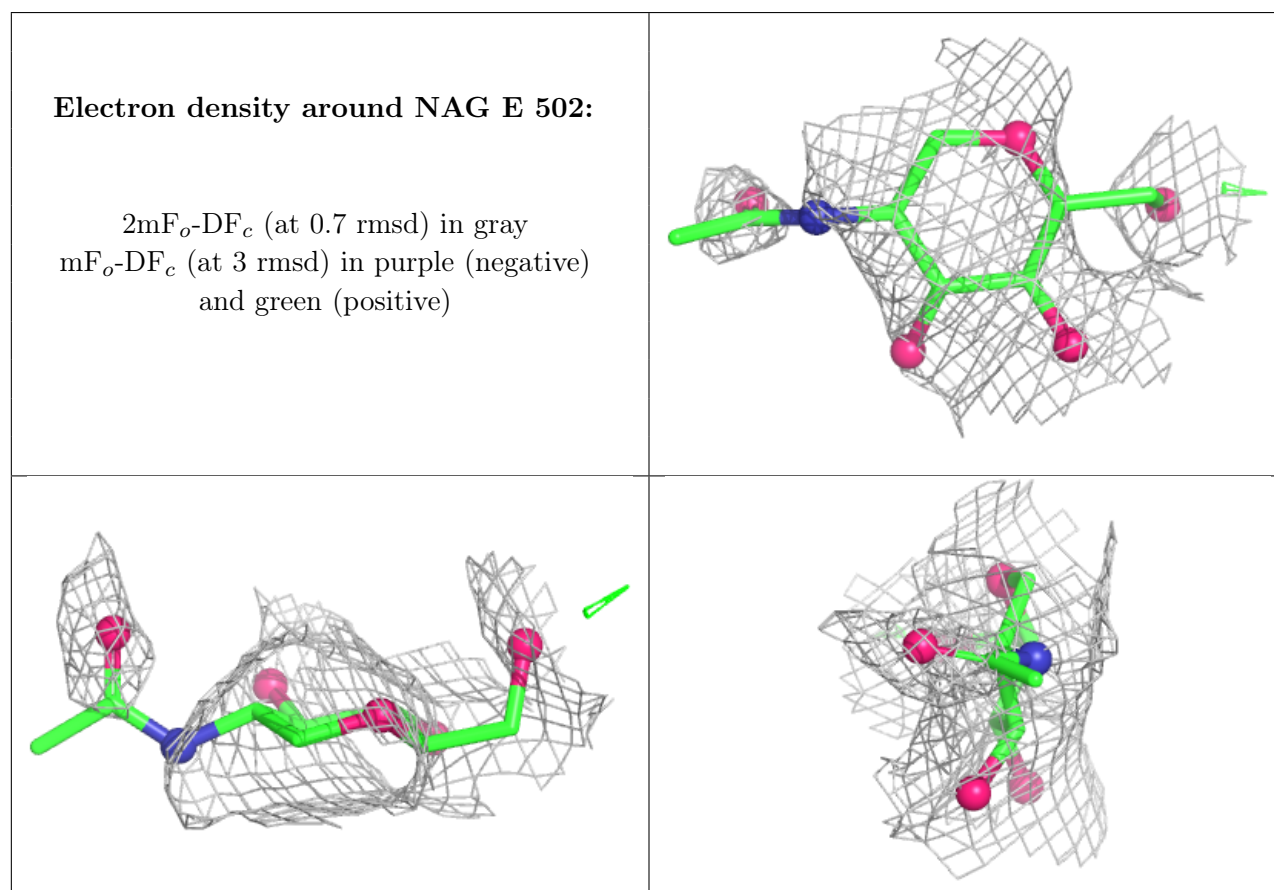
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	E	502	14/15	0.50	0.14	127,138,144,147	0
8	GLC	H	501	11/12	0.59	0.13	123,133,140,141	0
8	GLC	I	501	11/12	0.61	0.16	156,161,168,168	0
9	NAG	O	502	14/15	0.64	0.12	120,140,144,144	0
9	NAG	Q	501	14/15	0.65	0.12	152,161,166,168	0
9	NAG	R	501	14/15	0.66	0.13	160,164,169,172	0
8	GLC	N	501	11/12	0.82	0.09	84,86,92,93	0
8	GLC	O	501	11/12	0.83	0.10	103,115,118,122	0
8	GLC	Q	502	11/12	0.83	0.10	96,103,107,109	0
8	GLC	P	501	11/12	0.85	0.10	83,90,94,96	0

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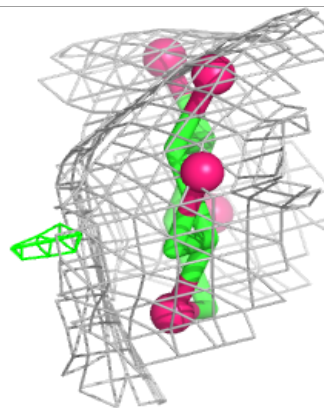
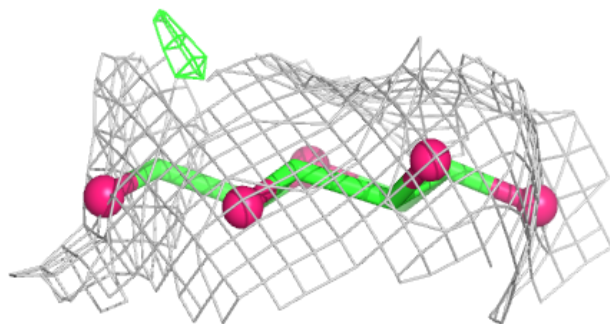
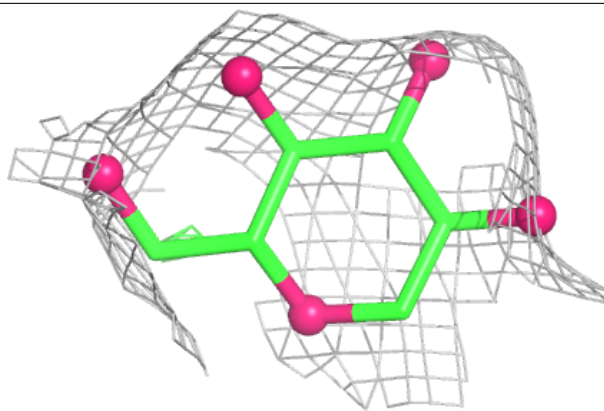
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GLC	L	501	11/12	0.86	0.10	67,72,78,83	0
8	GLC	R	502	11/12	0.87	0.10	81,91,98,103	0
8	GLC	F	501	11/12	0.88	0.09	90,100,105,105	0
8	GLC	K	501	11/12	0.88	0.08	65,74,78,78	0
8	GLC	E	501	11/12	0.88	0.09	90,93,98,104	0
8	GLC	A	501	11/12	0.90	0.08	49,59,71,71	0
8	GLC	M	501	11/12	0.92	0.09	74,80,86,94	0
8	GLC	D	501	11/12	0.92	0.06	73,79,83,84	0
8	GLC	B	501	11/12	0.93	0.07	54,59,66,71	0
8	GLC	J	501	11/12	0.94	0.06	56,60,66,68	0
8	GLC	C	501	11/12	0.96	0.07	58,61,65,68	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



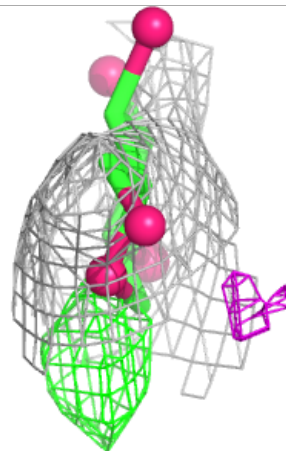
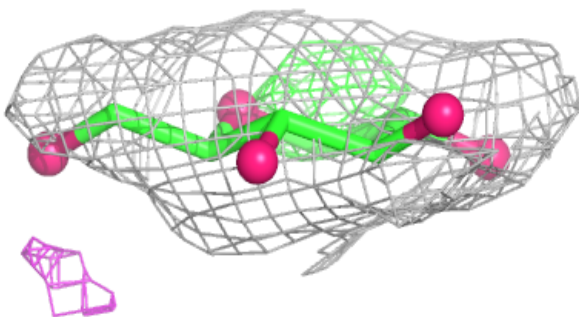
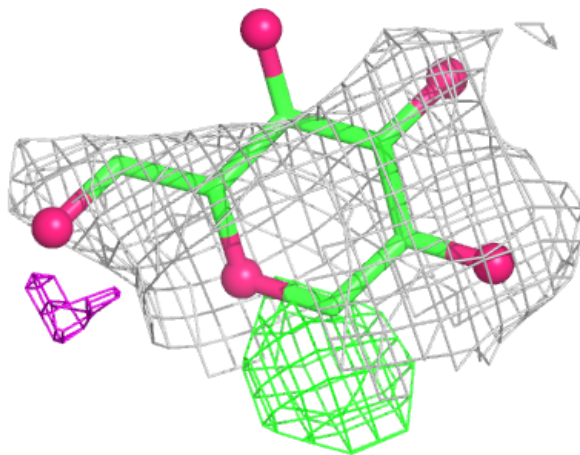
Electron density around GLC H 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



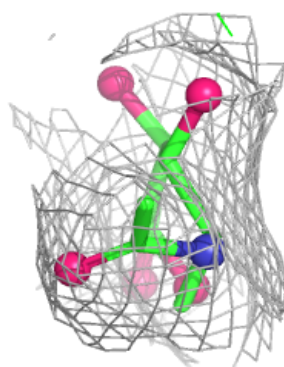
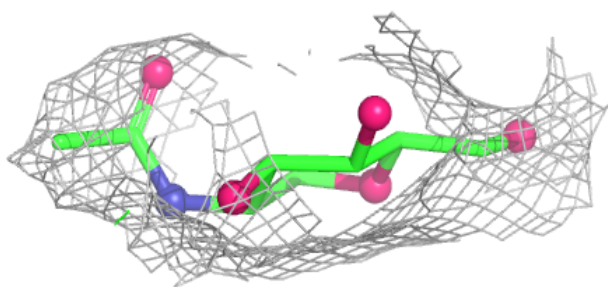
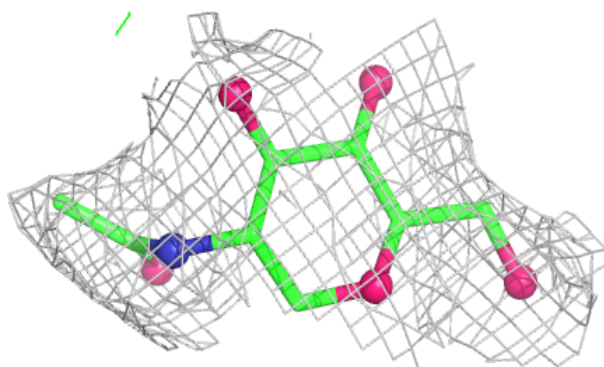
Electron density around GLC I 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

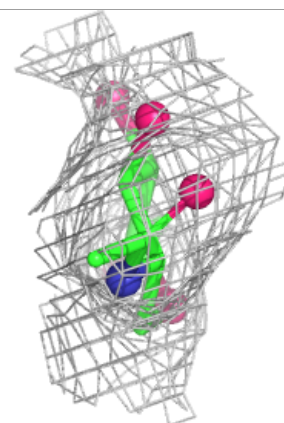
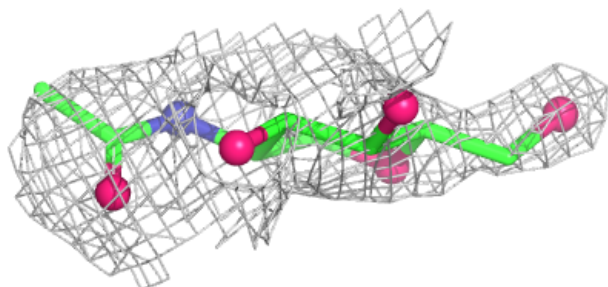
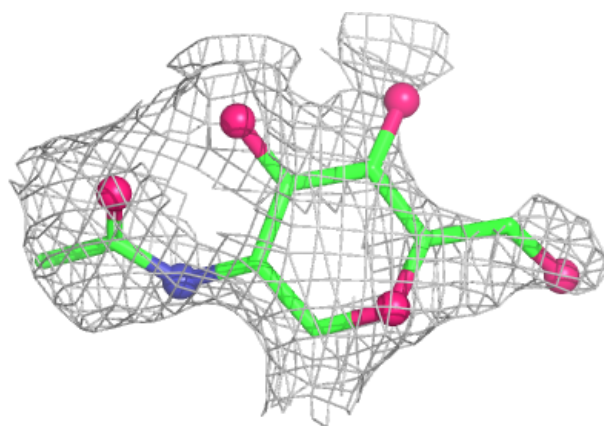


Electron density around NAG O 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

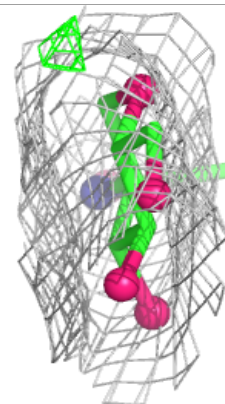
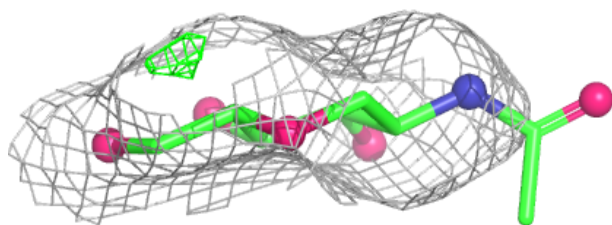
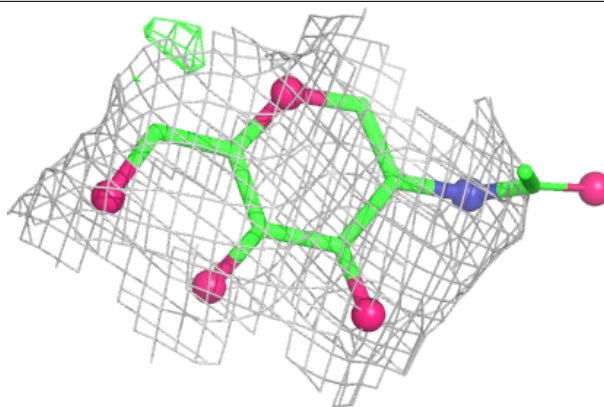
**Electron density around NAG Q 501:**

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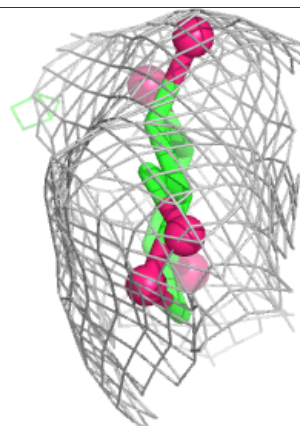
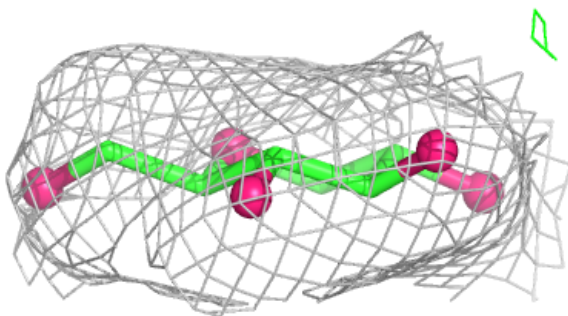
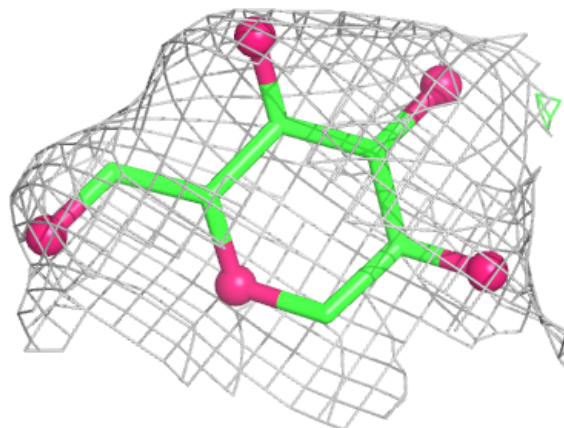


Electron density around NAG R 501:

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and green (positive)

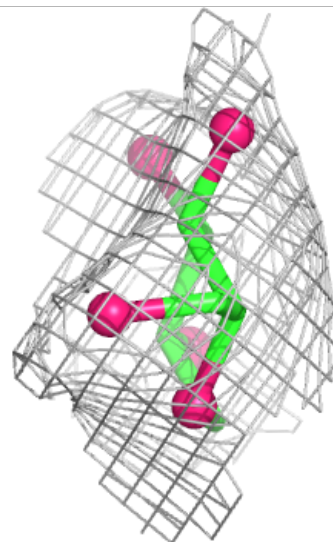
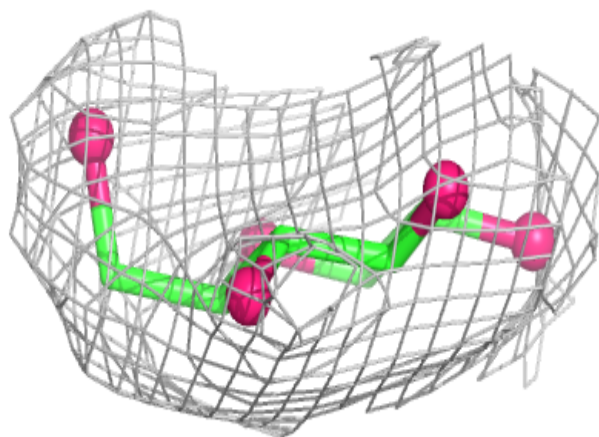
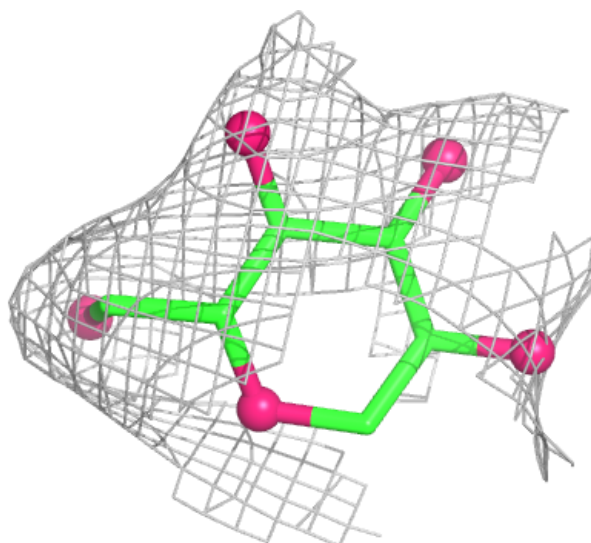
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



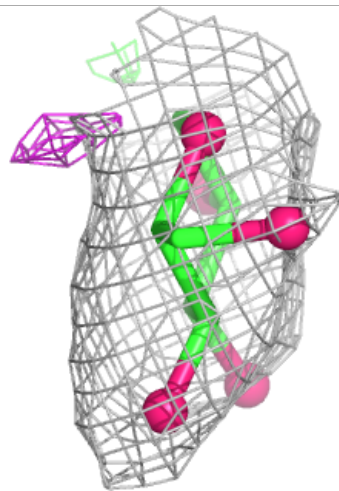
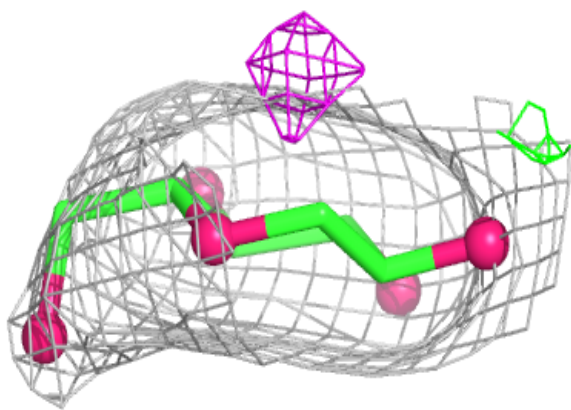
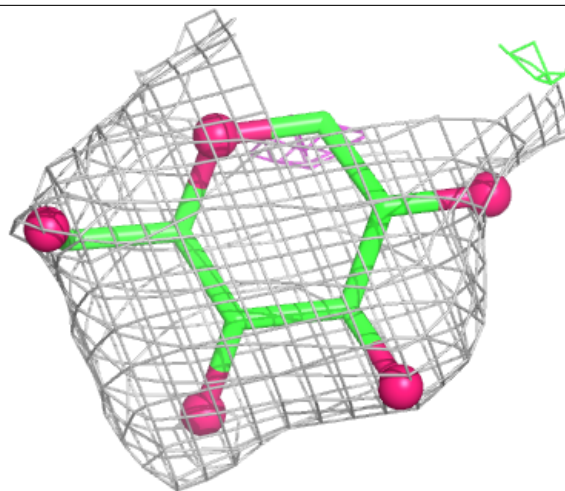
Electron density around GLC O 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



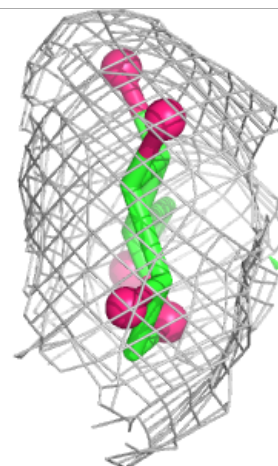
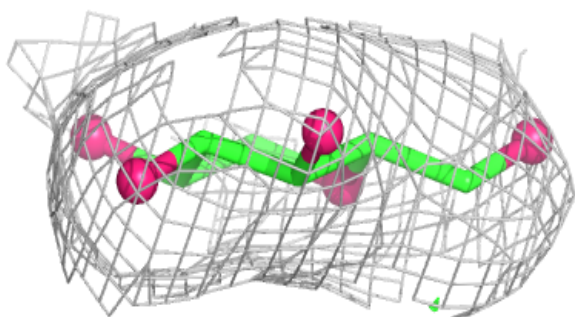
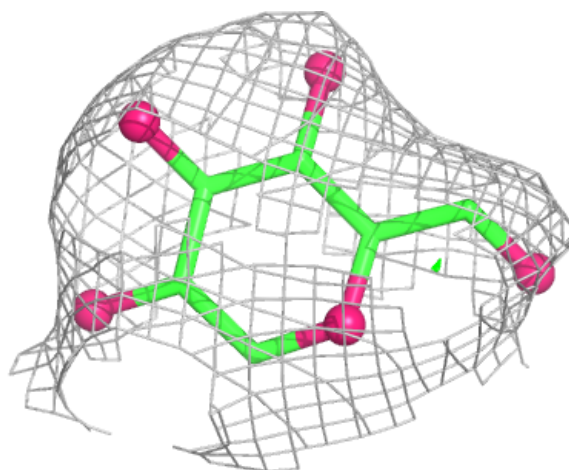
Electron density around GLC Q 502:

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and green (positive)



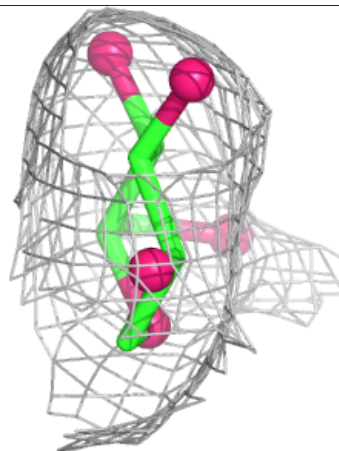
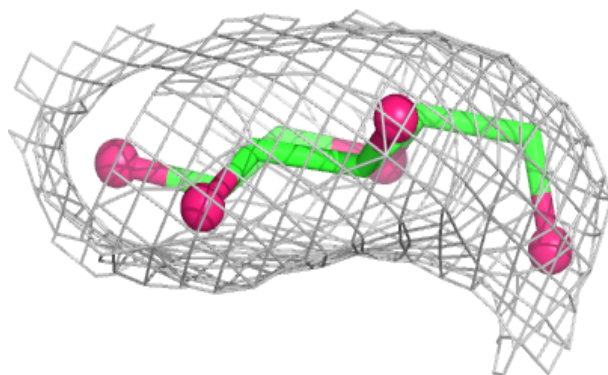
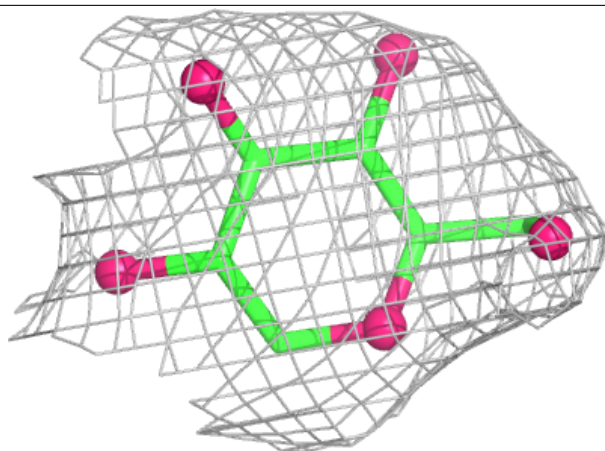
Electron density around GLC P 501:

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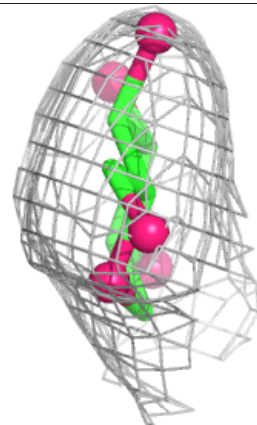
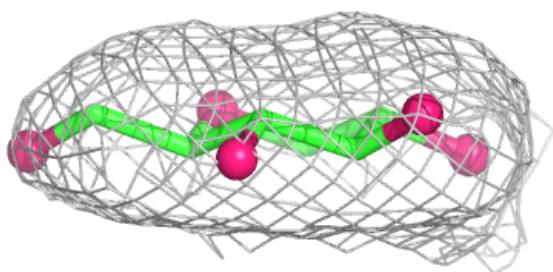
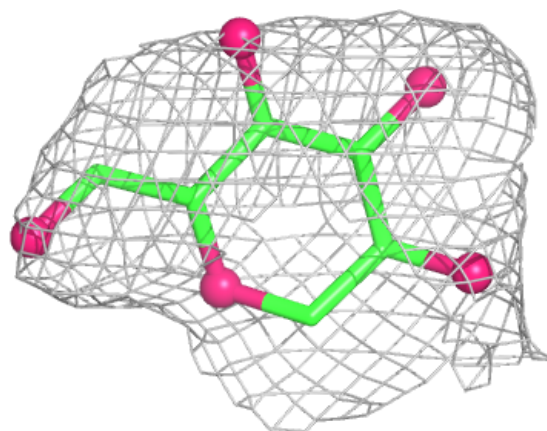
Electron density around GLC L 501:

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and green (positive)



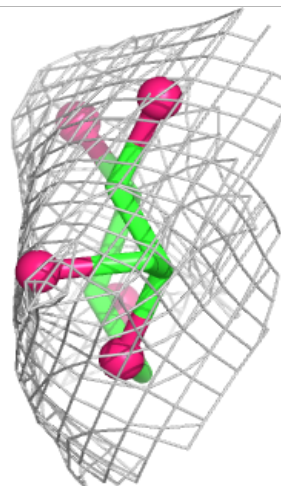
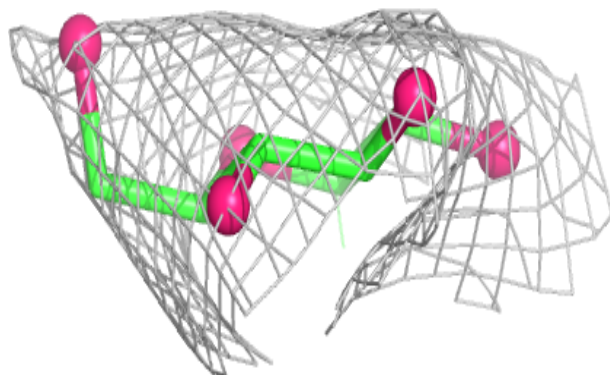
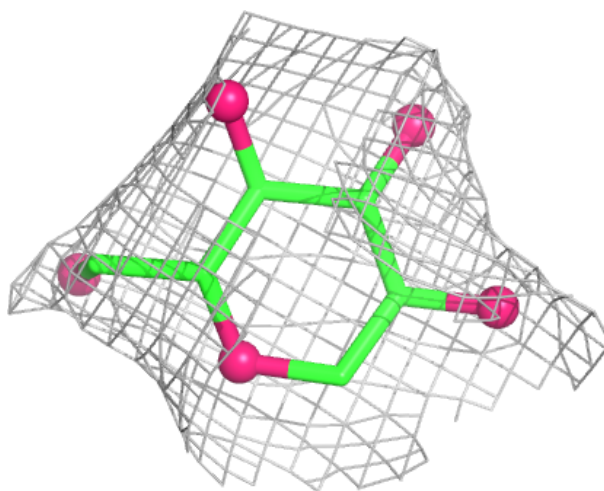
Electron density around GLC R 502:

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and green (positive)



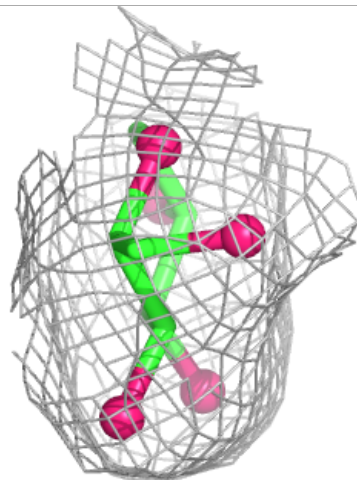
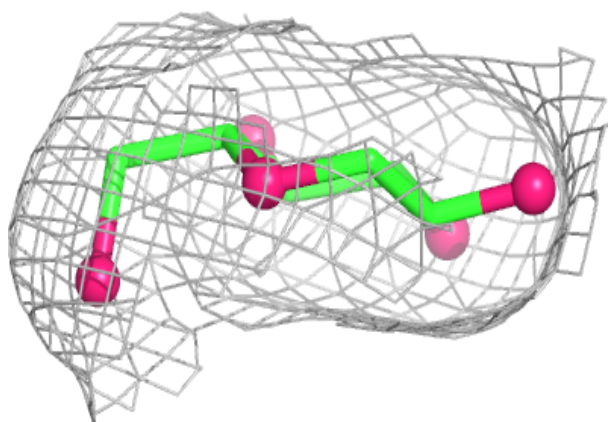
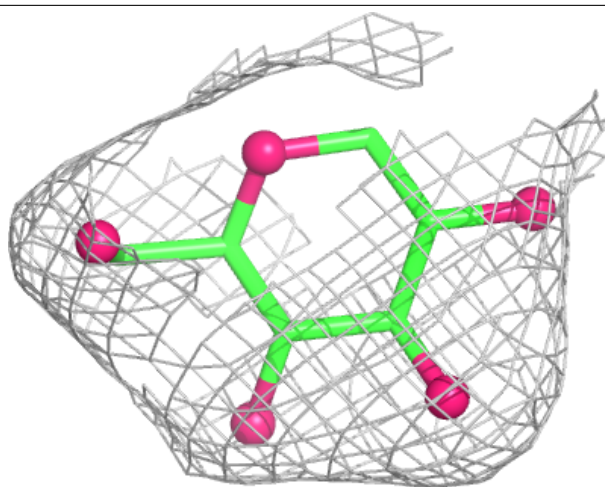
Electron density around GLC F 501:

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and green (positive)



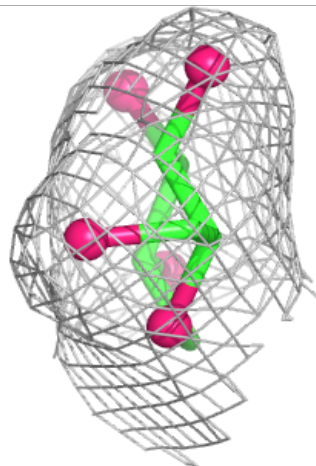
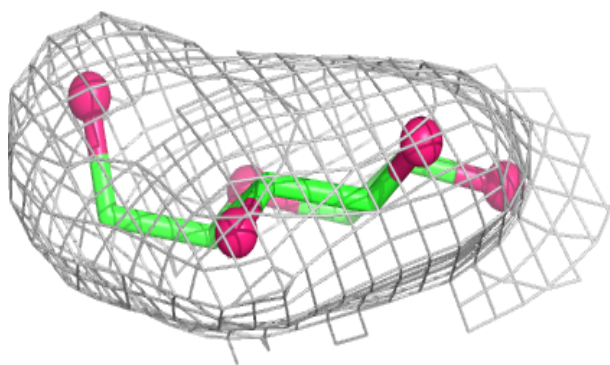
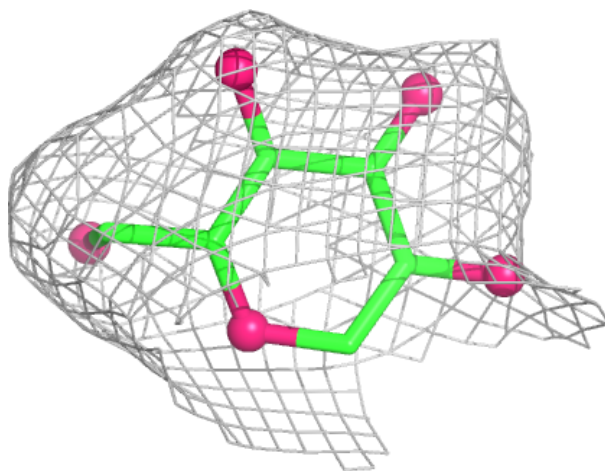
Electron density around GLC K 501:

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and green (positive)



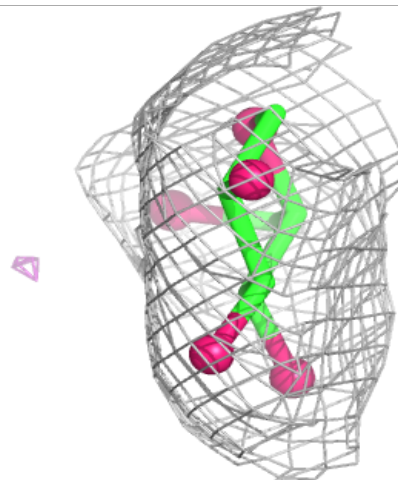
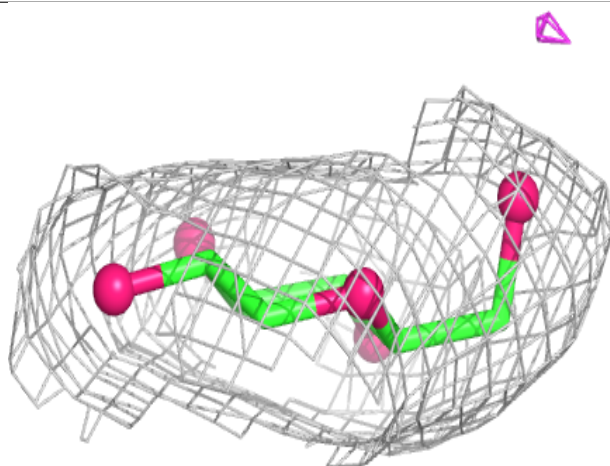
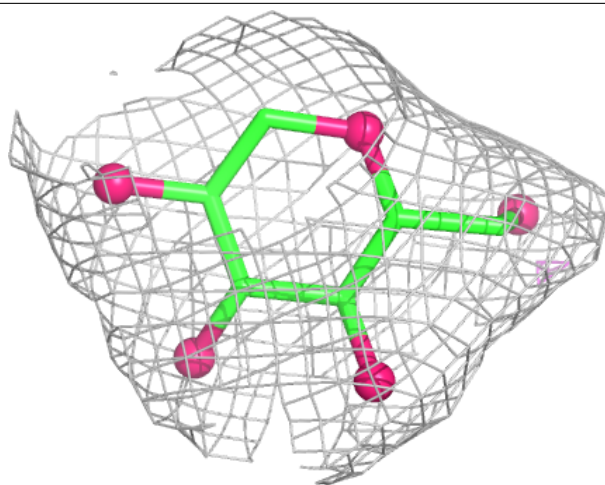
Electron density around GLC E 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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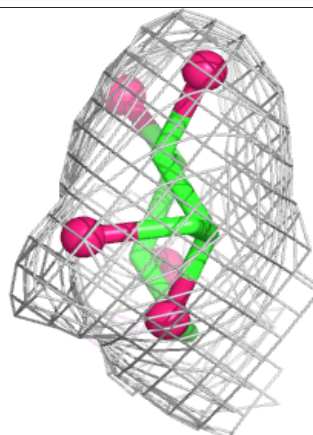
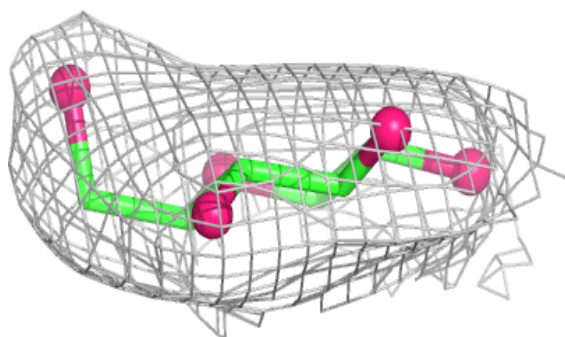
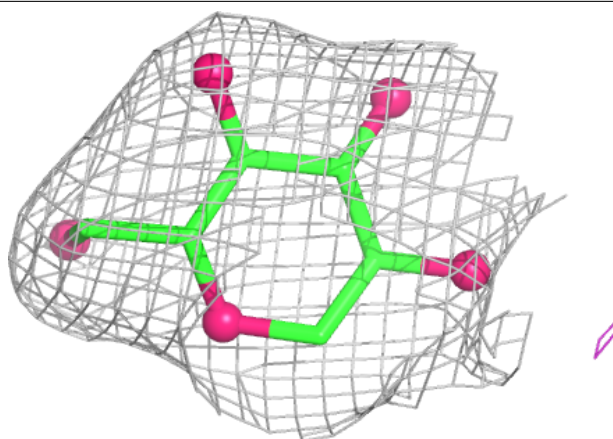
Electron density around GLC A 501:

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and green (positive)



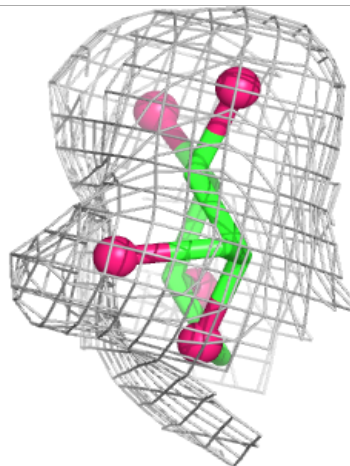
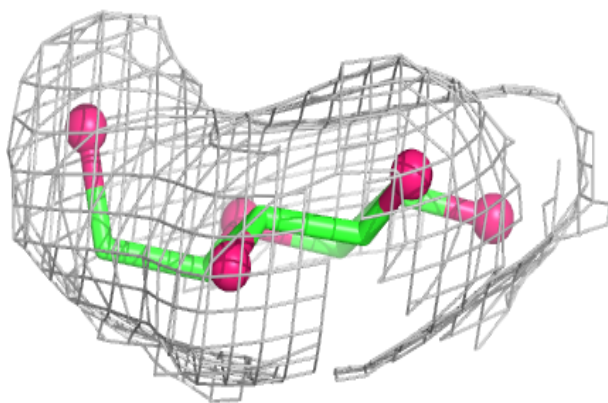
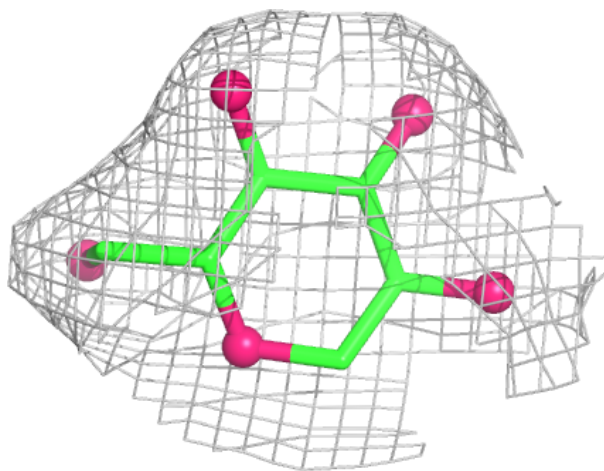
Electron density around GLC M 501:

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and green (positive)



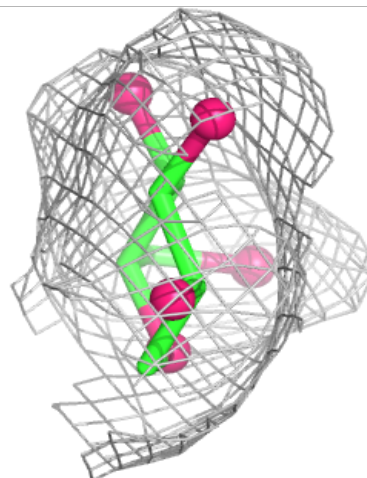
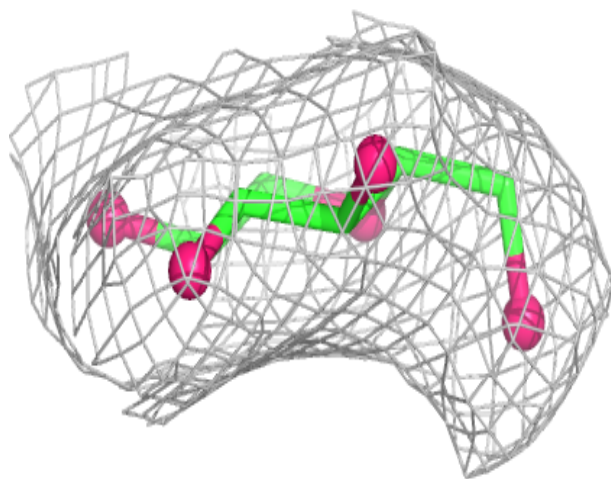
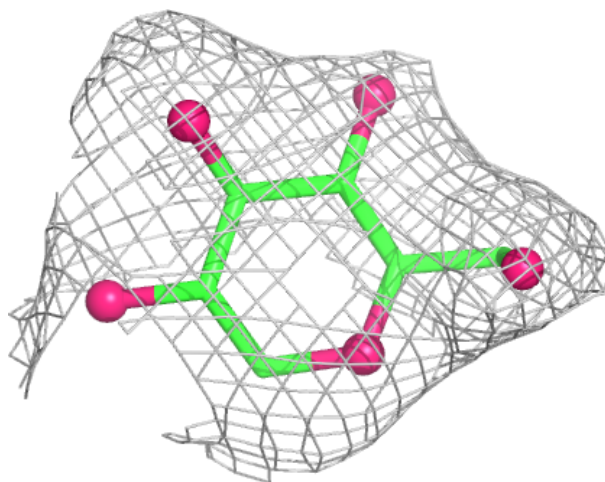
Electron density around GLC D 501:

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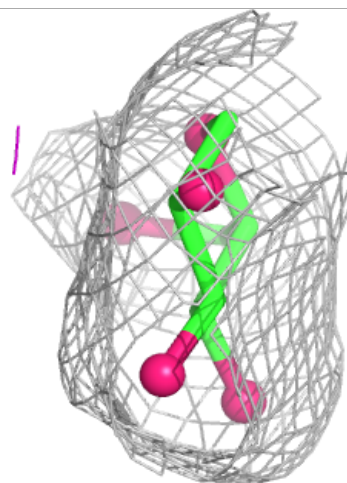
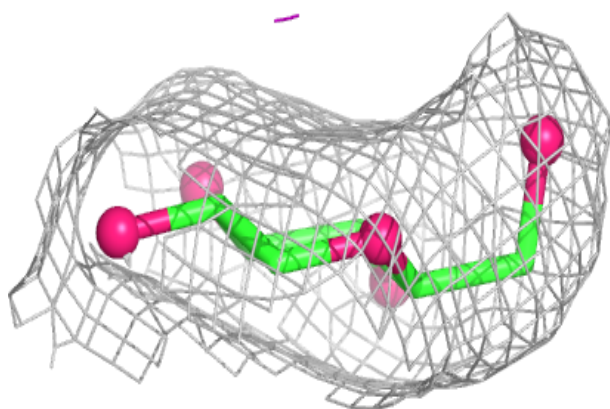
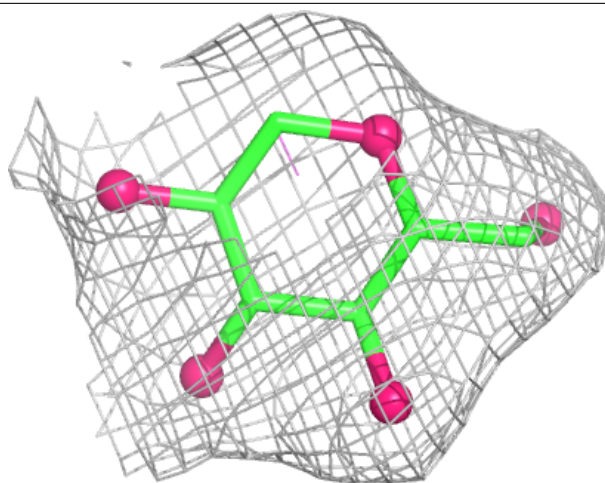
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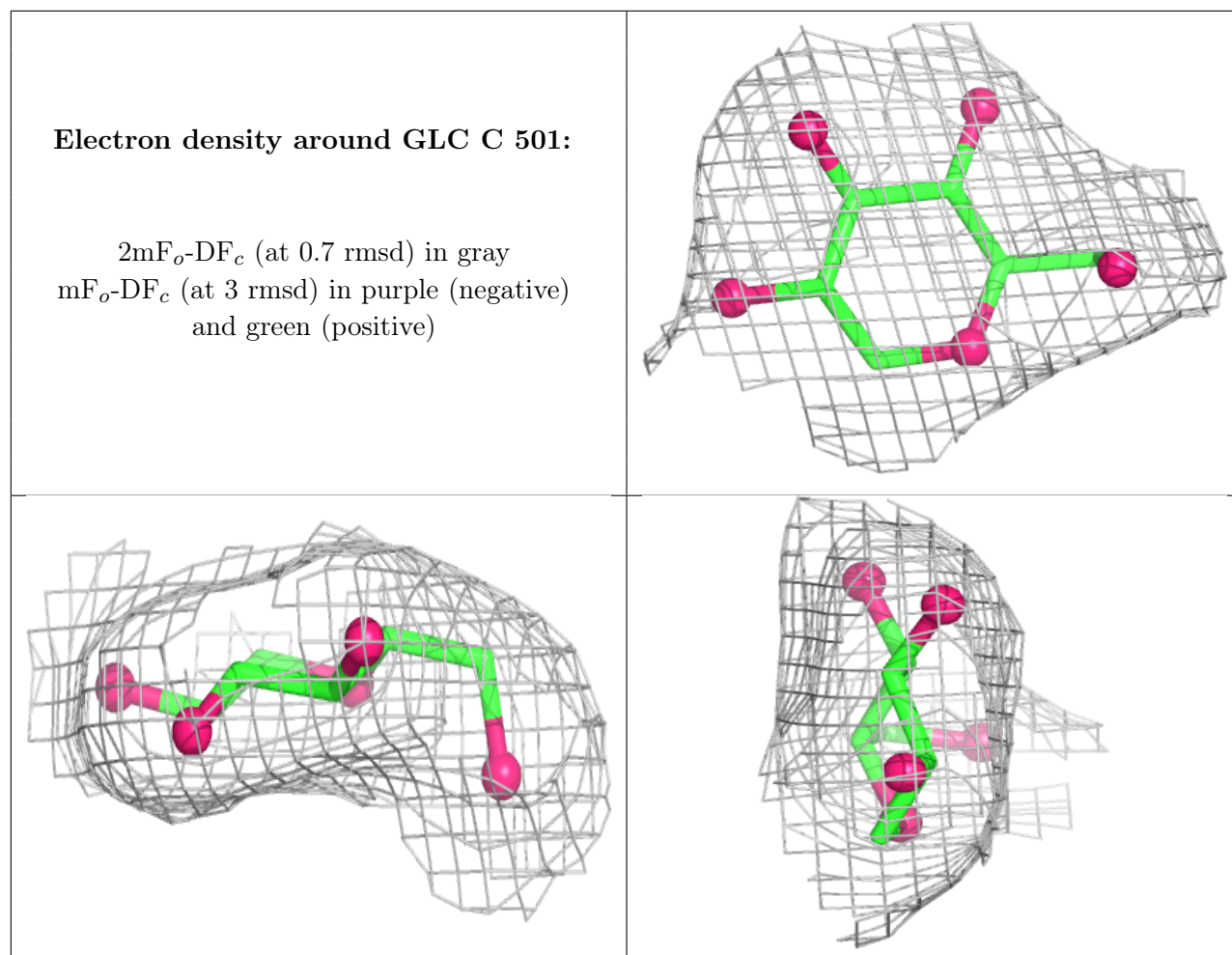
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



Electron density around GLC J 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.