



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 09:02 PM UTC

PDB ID : 9I9H / pdb\_00009i9h  
Title : Structure of FAB-fragment GB11 in complex with Sialyl Lewis A  
Authors : Freitag, A.; Khan-Kilji, S.; Nedielkov, R.; Murali Kumar, S.; Krummhaar, M.; Luehle, J.; Goerdeler, F.; Arndt, J.; Kamphues, C.; Mroginski, M.A.; Roth, C.; Seeberger, P.H.; Moeller, H.M.; Moscovitz, O.  
Deposited on : 2025-02-06  
Resolution : 2.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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>.

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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

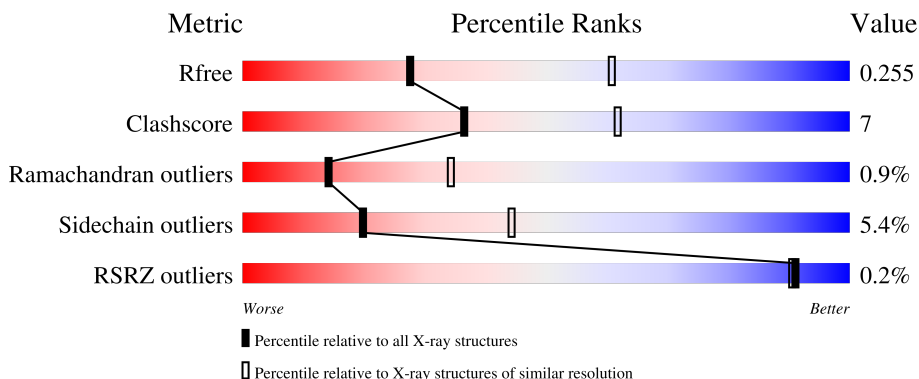
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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  $\geq 3$ , 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	217	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	C	217	<div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	E	217	<div> <div>65%</div> <div>31%</div> <div>..</div> </div>
1	H	217	<div> <div>80%</div> <div>19%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	212	 88% 11% .
2	D	212	 85% 13% .
2	F	212	 82% 16% .
2	L	212	 87% 11% .
3	T	3	 33% 67%
3	V	3	 67% 33%
4	U	4	 75% 25%
5	S	2	 50% 50%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 26531 atoms, of which 13027 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.

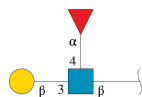
- Molecule 1 is a protein called IgG antibody FAB fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	217	Total	C	H	N	O	S	66	0	0
			3226	1037	1589	269	322	9			
1	H	217	Total	C	H	N	O	S	68	0	0
			3228	1037	1591	269	322	9			
1	C	217	Total	C	H	N	O	S	66	0	0
			3226	1037	1589	269	322	9			
1	E	217	Total	C	H	N	O	S	68	1	0
			3248	1046	1600	270	323	9			

- Molecule 2 is a protein called IgG antibody Fab fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	212	Total	C	H	N	O	S	64	0	0
			3263	1041	1596	281	337	8			
2	L	212	Total	C	H	N	O	S	64	0	0
			3263	1041	1596	281	337	8			
2	D	212	Total	C	H	N	O	S	68	0	0
			3267	1041	1600	281	337	8			
2	F	212	Total	C	H	N	O	S	68	0	0
			3267	1041	1600	281	337	8			

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



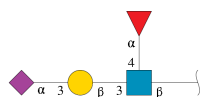
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	3	Total	C	H	N	O	10	0	0
			73	20	37	1	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	3	Total	C	H	N	O	10	0	0
			73	20	37	1	15			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



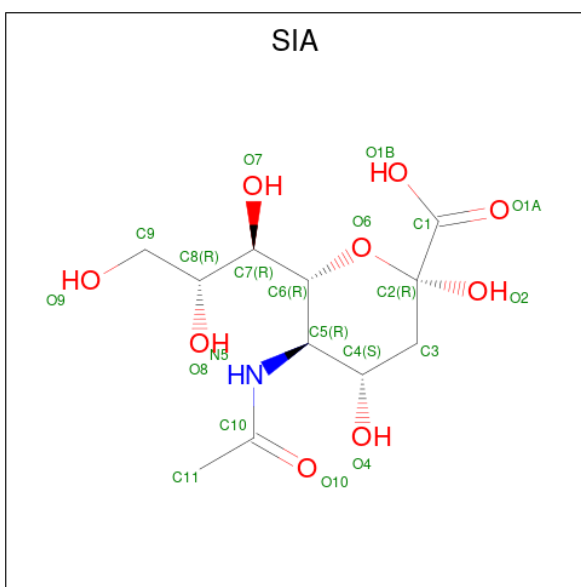
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	U	4	Total	C	H	N	O	14	0	0
			110	31	54	2	23			

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



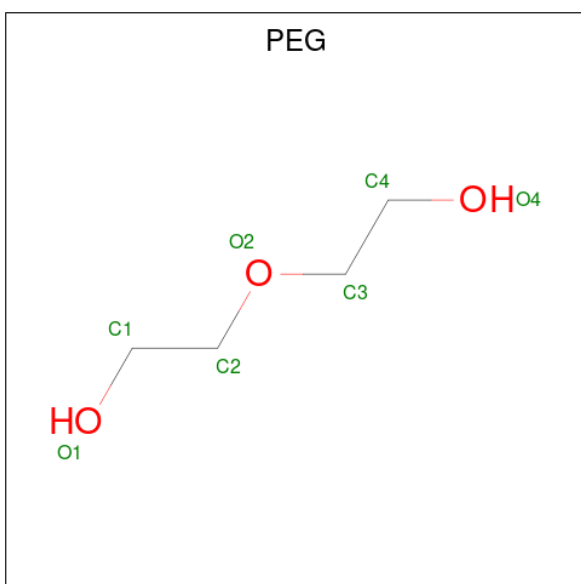
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S	2	Total	C	H	N	O	6	0	0
			51	14	26	1	10			

- Molecule 6 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>) (labeled as "Ligand of Interest" by depositor).



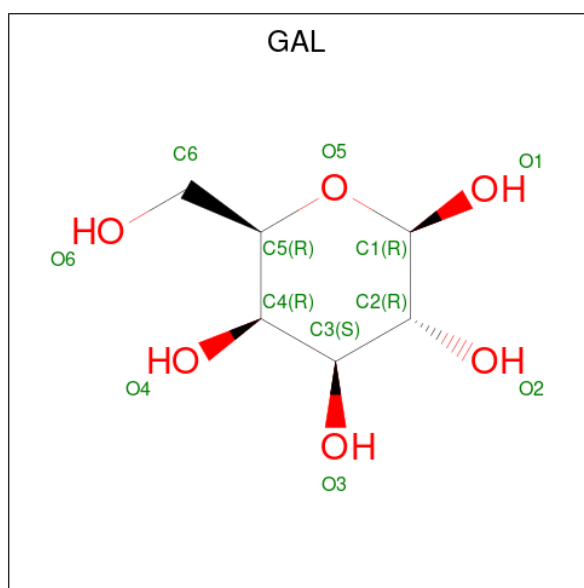
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	4	0
			37	11	17	1	8		
6	L	1	Total	C	H	N	O	4	0
			37	11	17	1	8		
6	F	1	Total	C	H	N	O	4	0
			37	11	17	1	8		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C H O 17 4 10 3	1	0
7	H	1	Total C H O 17 4 10 3	1	0
7	C	1	Total C H O 17 4 10 3	1	0
7	C	1	Total C H O 17 4 10 3	1	0
7	E	1	Total C H O 17 4 10 3	1	0

- Molecule 8 is beta-D-galactopyranose (CCD ID: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C H O 22 6 11 5	4	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total O 3 3	0	0
9	B	3	Total O 3 3	0	0
9	D	5	Total O 5 5	0	0

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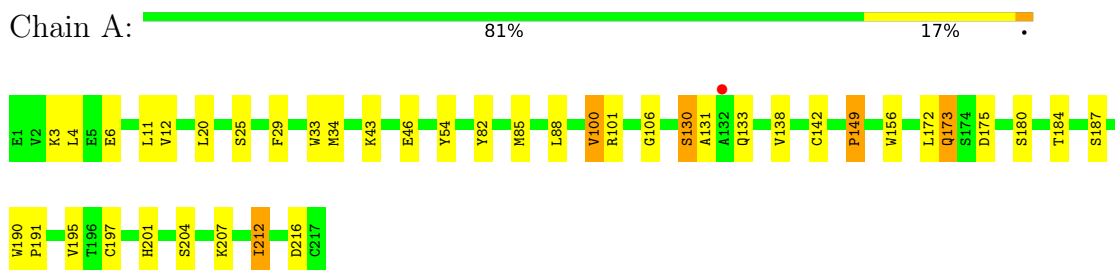
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	4	Total 4	O 4	0	0
9	C	3	Total 3	O 3	0	0



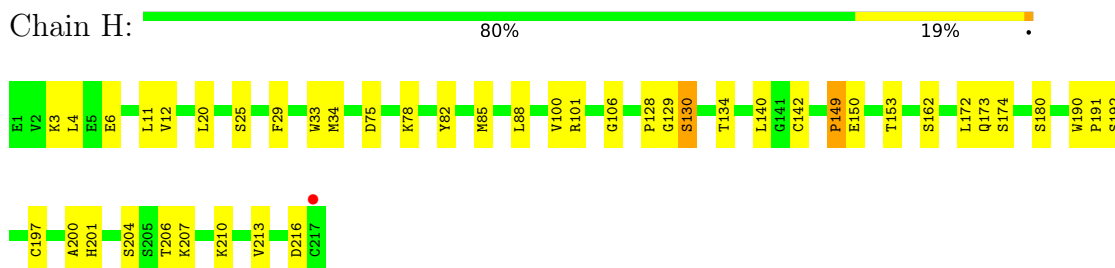
### 3 Residue-property plots [i](#)

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

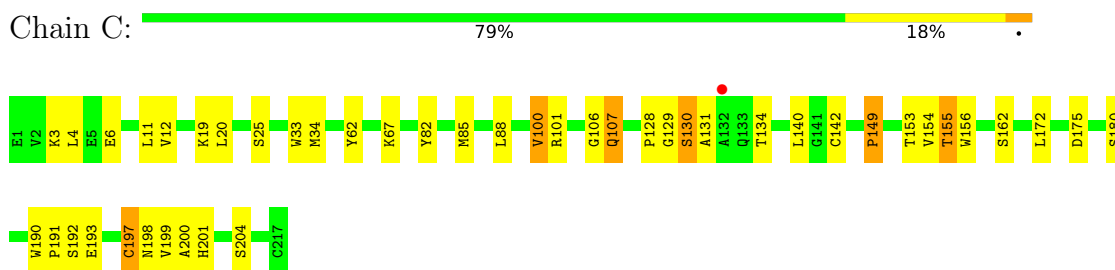
- Molecule 1: IgG antibody FAB fragment



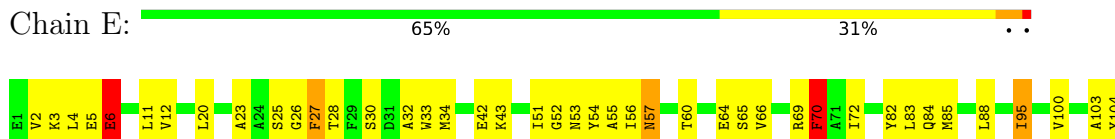
- Molecule 1: IgG antibody FAB fragment



- Molecule 1: IgG antibody FAB fragment



- Molecule 1: IgG antibody FAB fragment





- Molecule 2: IgG antibody Fab fragment

Chain B: 88% 11% .



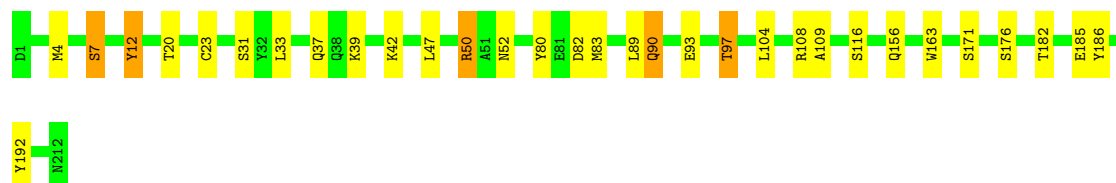
- Molecule 2: IgG antibody Fab fragment

Chain L: 87% 11% .



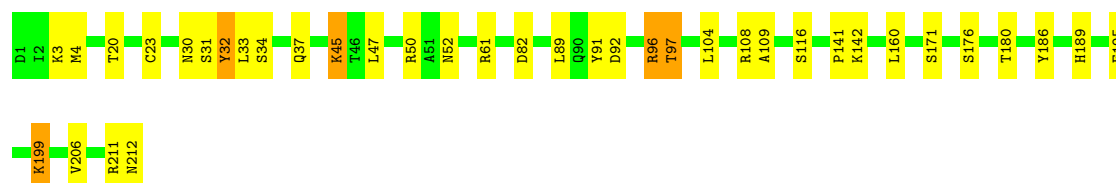
- Molecule 2: IgG antibody Fab fragment

Chain D: 85% 13% .



- Molecule 2: IgG antibody Fab fragment

Chain F: 82% 16% .



- Molecule 3: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 33% 67%



- Molecule 3: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 67% 33%



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 75% 25%



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

Chain S: 50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.84Å 108.70Å 108.92Å 89.60° 87.34° 89.25°	Depositor
Resolution (Å)	26.70 – 2.96 26.70 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.7 (26.70-2.96) 93.1 (26.70-2.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 2.94Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.210 , 0.248 0.217 , 0.255	Depositor DCC
$R_{free}$ test set	1994 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 66.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.076 for h,l,-k 0.076 for h,-l,k 0.084 for h,-k,-l 0.038 for -h,k,-l 0.027 for -h,-k,l 0.027 for -h,l,k 0.027 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	26531	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, SIA, FUC, NAG, GAL

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	0.55	0/1681	0.94	2/2297 (0.1%)
1	C	0.53	0/1681	0.93	1/2297 (0.0%)
1	E	0.56	0/1693	1.03	4/2313 (0.2%)
1	H	0.55	0/1681	0.92	0/2297
2	B	0.54	0/1705	0.91	0/2307
2	D	0.52	0/1705	0.92	0/2307
2	F	0.52	0/1705	0.92	0/2307
2	L	0.53	0/1705	0.92	0/2307
All	All	0.54	0/13556	0.94	7/18432 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
2	L	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLN	CB-CA-C	6.19	122.73	110.42
1	E	216	ASP	CB-CA-C	6.12	119.98	109.51
1	E	6	GLU	N-CA-CB	5.68	120.08	110.49
1	E	184	THR	CA-CB-OG1	-5.55	101.27	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	GLU	CB-CG-CD	-5.41	103.40	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	50	ARG	Sidechain
2	D	50	ARG	Sidechain
2	F	96	ARG	Sidechain
2	L	50	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1637	1589	1587	23	0
1	C	1637	1589	1587	20	2
1	E	1648	1600	1595	53	2
1	H	1637	1591	1587	19	2
2	B	1667	1596	1597	17	0
2	D	1667	1600	1597	20	0
2	F	1667	1600	1597	22	2
2	L	1667	1596	1597	18	0
3	T	36	37	32	0	0
3	V	36	37	32	4	0
4	U	56	54	49	1	0
5	S	25	26	23	1	0
6	B	20	17	17	0	0
6	F	20	17	17	2	0
6	L	20	17	17	1	0
7	C	14	20	20	0	0
7	E	7	10	10	0	0
7	H	7	10	10	0	0
7	L	7	10	10	0	0
8	H	11	11	9	1	0
9	A	3	0	0	0	0
9	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	3	0	0	0	0
9	D	5	0	0	2	0
9	H	4	0	0	1	0
All	All	13504	13027	12990	190	4

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.

The worst 5 of 190 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)
6:F:301:SIA:C2	3:V:2:GAL:O3	1.67	1.42
1:E:51:ILE:HG22	1:E:60:THR:HG22	1.57	0.86
2:L:83:MET:HE1	2:L:168:SER:HA	1.59	0.84
2:D:182:THR:HG23	2:D:185:GLU:H	1.46	0.80
1:E:83:LEU:HD23	1:E:85:MET:HE2	1.66	0.78

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:210:LYS:HZ2	1:E:206:THR:HG1[1_556]	1.13	0.47
2:F:92:ASP:OD2	1:C:19:LYS:NZ[1_565]	1.89	0.31
1:H:206:THR:HG1	1:E:210:LYS:HZ2[1_556]	1.34	0.26
2:F:92:ASP:OD2	1:C:19:LYS:HZ2[1_565]	1.43	0.17

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	215/217 (99%)	206 (96%)	7 (3%)	2 (1%)	14 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	215/217 (99%)	207 (96%)	7 (3%)	1 (0%)	24	49
1	E	216/217 (100%)	194 (90%)	12 (6%)	10 (5%)	2	4
1	H	215/217 (99%)	203 (94%)	9 (4%)	3 (1%)	9	24
2	B	210/212 (99%)	193 (92%)	17 (8%)	0	100	100
2	D	210/212 (99%)	195 (93%)	15 (7%)	0	100	100
2	F	210/212 (99%)	195 (93%)	15 (7%)	0	100	100
2	L	210/212 (99%)	195 (93%)	15 (7%)	0	100	100
All	All	1701/1716 (99%)	1588 (93%)	97 (6%)	16 (1%)	14	34

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ASP
1	E	6	GLU
1	E	27[A]	PHE
1	E	27[B]	PHE
1	E	28	THR

### 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	183/183 (100%)	172 (94%)	11 (6%)	17	40
1	C	183/183 (100%)	170 (93%)	13 (7%)	13	33
1	E	184/183 (100%)	170 (92%)	14 (8%)	12	31
1	H	183/183 (100%)	172 (94%)	11 (6%)	17	40
2	B	190/190 (100%)	185 (97%)	5 (3%)	40	65
2	D	190/190 (100%)	182 (96%)	8 (4%)	26	53
2	F	190/190 (100%)	178 (94%)	12 (6%)	16	38
2	L	190/190 (100%)	184 (97%)	6 (3%)	34	59
All	All	1493/1492 (100%)	1413 (95%)	80 (5%)	20	44



5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	142	CYS
1	E	149	PRO
1	C	155	THR
1	C	197	CYS
1	E	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	53	ASN
1	E	173	GLN
1	E	135	ASN
2	D	198	HIS
1	C	57	ASN

### 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 ⓘ

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	S	1	5	15,15,15	0.19	0	21,21,21	1.12	1 (4%)
5	FUC	S	2	5	10,10,11	0.62	0	14,14,16	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	T	1	3	15,15,15	0.26	0	21,21,21	0.66	1 (4%)
3	GAL	T	2	3	11,11,12	0.49	0	15,15,17	1.74	3 (20%)
3	FUC	T	3	3	10,10,11	0.61	0	14,14,16	0.75	0
4	NAG	U	1	4	15,15,15	0.24	0	21,21,21	1.44	2 (9%)
4	GAL	U	2	4	11,11,12	1.34	1 (9%)	15,15,17	1.45	1 (6%)
4	SIA	U	3	4	20,20,21	0.86	1 (5%)	21,28,31	0.92	1 (4%)
4	FUC	U	4	4	10,10,11	0.31	0	14,14,16	0.45	0
3	NAG	V	1	3	15,15,15	0.22	0	21,21,21	0.90	0
3	GAL	V	2	3	11,11,12	0.93	1 (9%)	15,15,17	1.51	2 (13%)
3	FUC	V	3	3	10,10,11	0.37	0	14,14,16	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	S	1	5	-	4/6/26/26	0/1/1/1
5	FUC	S	2	5	-	-	0/1/1/1
3	NAG	T	1	3	-	2/6/26/26	0/1/1/1
3	GAL	T	2	3	-	2/2/19/22	0/1/1/1
3	FUC	T	3	3	-	-	0/1/1/1
4	NAG	U	1	4	-	0/6/26/26	0/1/1/1
4	GAL	U	2	4	-	2/2/19/22	0/1/1/1
4	SIA	U	3	4	-	2/18/34/38	0/1/1/1
4	FUC	U	4	4	-	-	0/1/1/1
3	NAG	V	1	3	-	2/6/26/26	0/1/1/1
3	GAL	V	2	3	-	0/2/19/22	0/1/1/1
3	FUC	V	3	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	2	GAL	O3-C3	4.30	1.53	1.43
4	U	3	SIA	O1B-C1	-3.41	1.19	1.30
3	V	2	GAL	O3-C3	2.79	1.49	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	2	GAL	C1-O5-C5	5.36	119.37	112.19
4	U	1	NAG	C1-C2-N2	5.12	116.66	110.73
4	U	2	GAL	C3-C4-C5	-4.18	102.66	110.23
5	S	1	NAG	C1-C2-N2	3.82	115.16	110.73
3	V	2	GAL	C3-C4-C5	-3.70	103.53	110.23

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

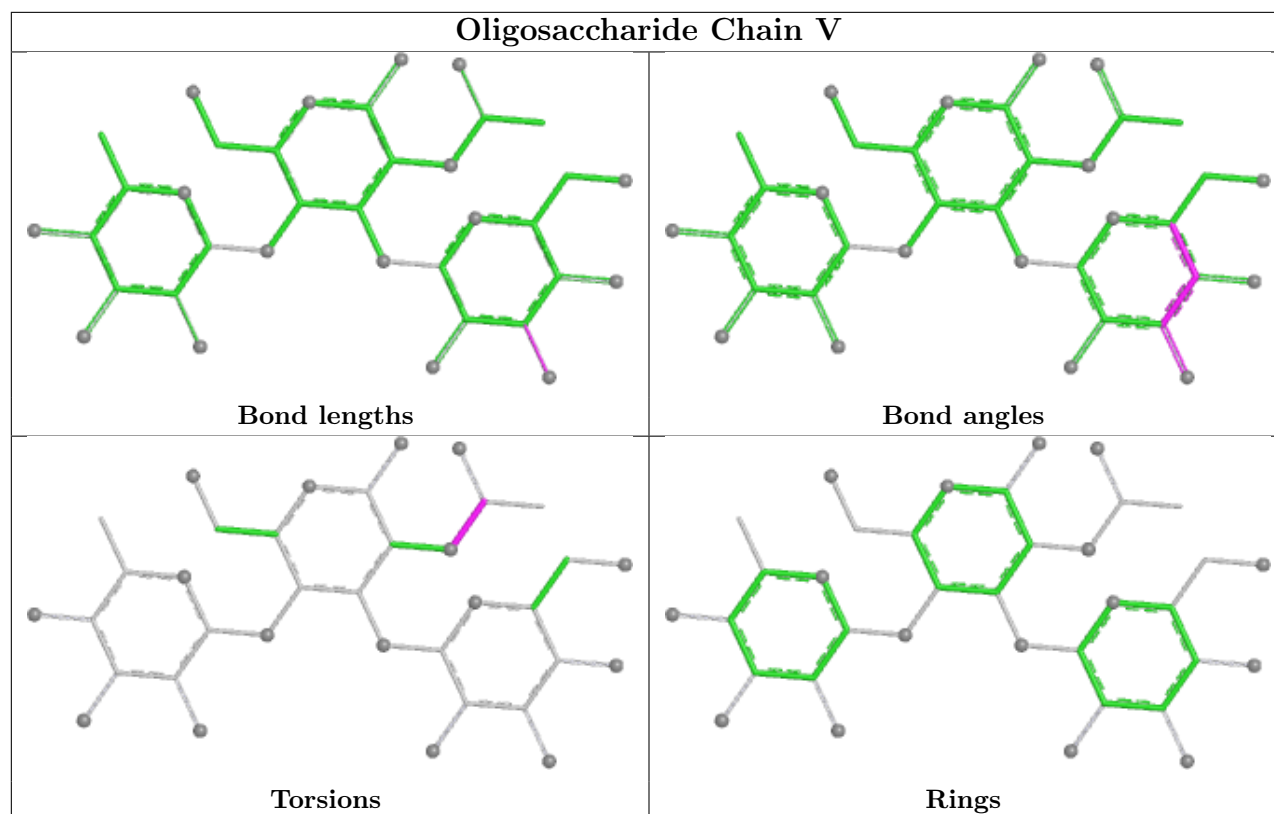
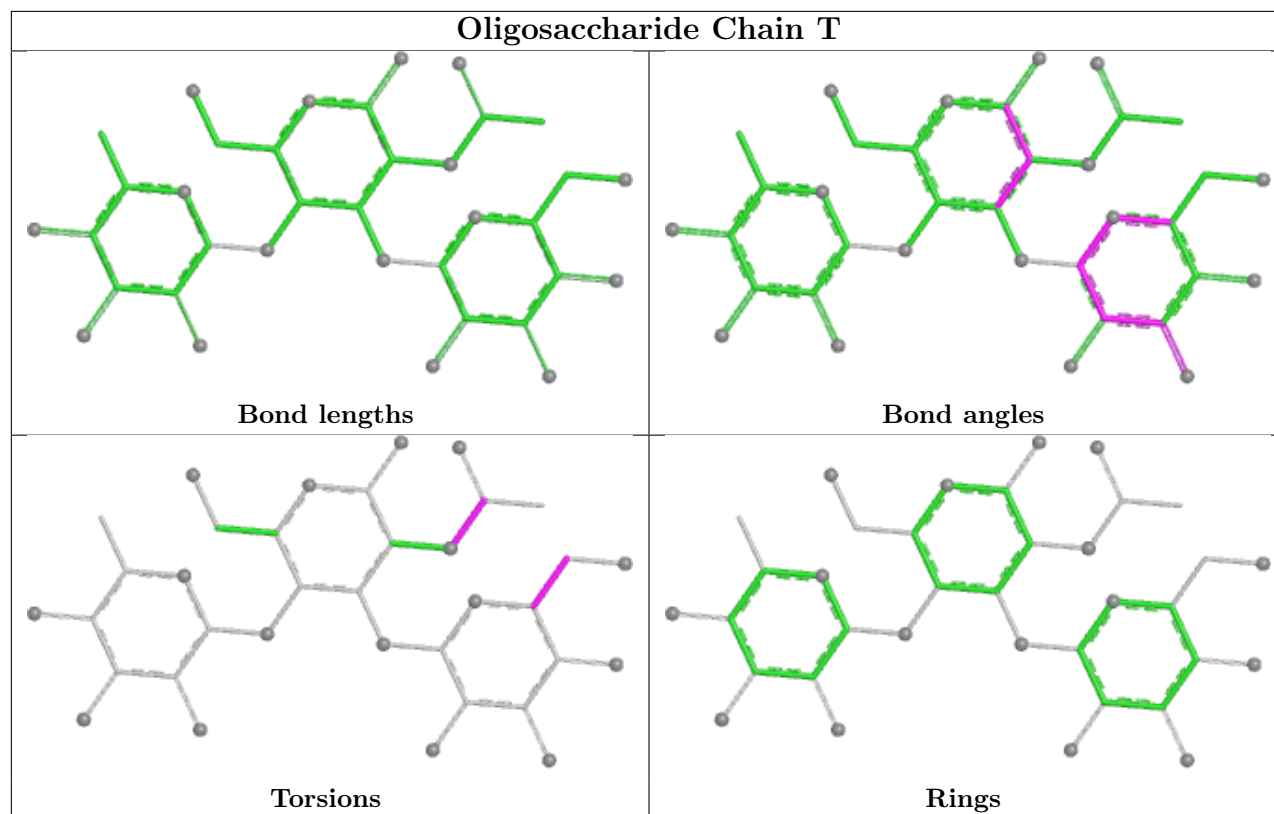
Mol	Chain	Res	Type	Atoms
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
4	U	3	SIA	O8-C8-C9-O9
4	U	2	GAL	O5-C5-C6-O6
4	U	3	SIA	C7-C8-C9-O9

There are no ring outliers.

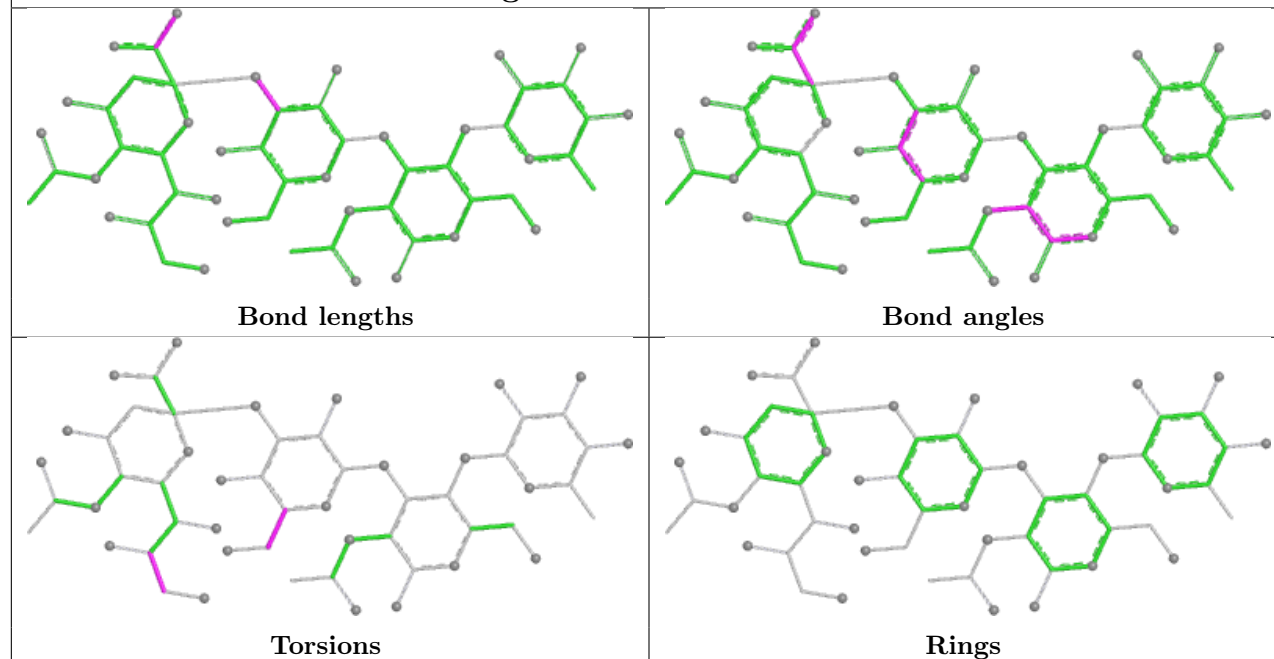
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	4	FUC	1	0
3	V	2	GAL	2	0
3	V	3	FUC	1	0
3	V	1	NAG	1	0
5	S	1	NAG	1	0
4	U	2	GAL	1	0

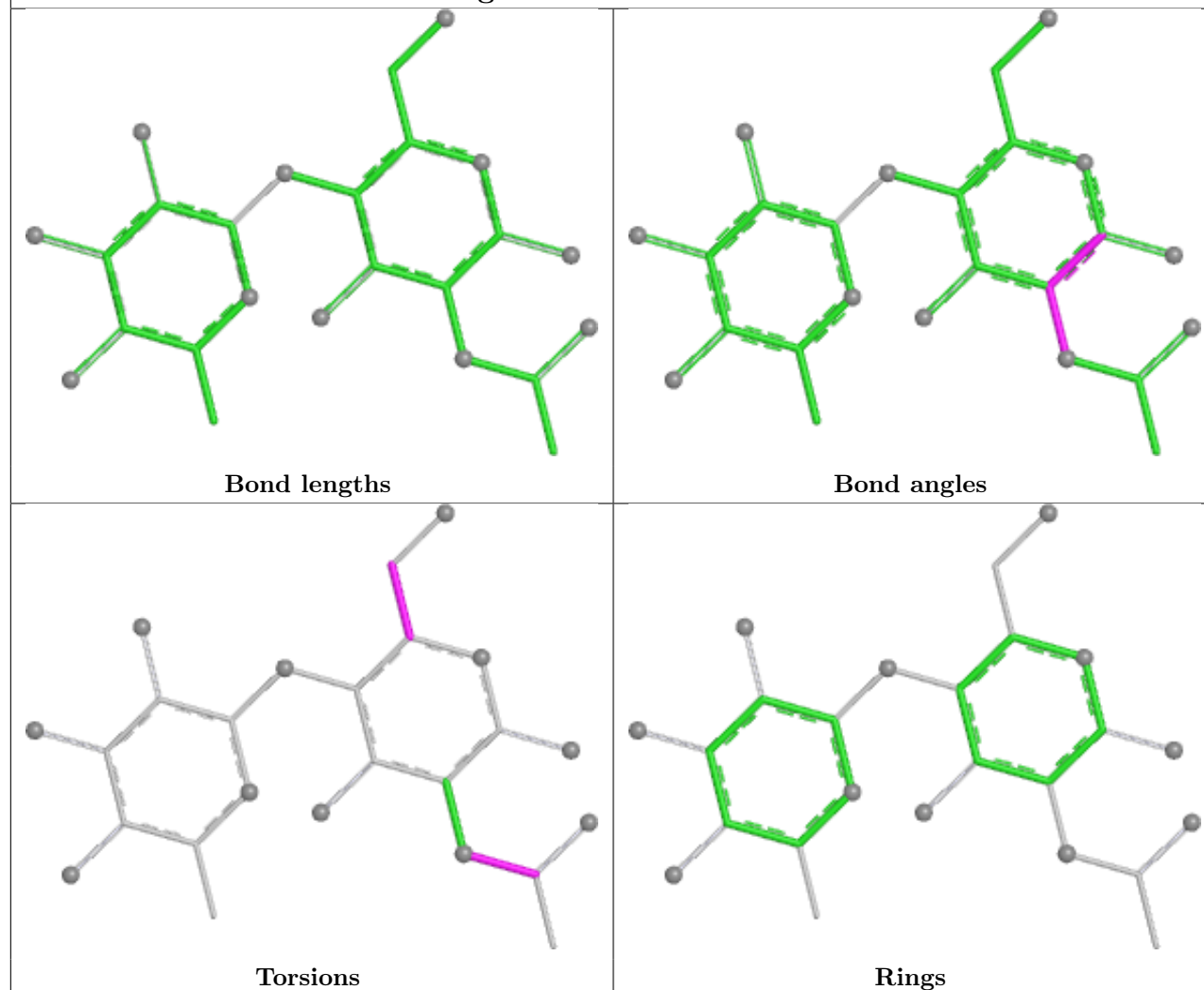
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## Oligosaccharide Chain U



## Oligosaccharide Chain S



## 5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SIA	B	301	-	20,20,21	0.78	1 (5%)	21,28,31	0.82	1 (4%)
7	PEG	C	301	-	6,6,6	0.27	0	5,5,5	0.15	0
7	PEG	E	301	-	6,6,6	0.37	0	5,5,5	0.24	0
6	SIA	L	301	-	20,20,21	0.98	2 (10%)	21,28,31	1.08	3 (14%)
8	GAL	H	301	-	11,11,12	0.66	0	15,15,17	1.43	1 (6%)
7	PEG	C	302	-	6,6,6	0.21	0	5,5,5	0.14	0
7	PEG	H	302	-	6,6,6	0.24	0	5,5,5	0.08	0
7	PEG	L	302	-	6,6,6	0.19	0	5,5,5	0.11	0
6	SIA	F	301	-	20,20,21	0.81	1 (5%)	21,28,31	0.82	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SIA	B	301	-	-	1/18/34/38	0/1/1/1
7	PEG	C	301	-	-	2/4/4/4	-
7	PEG	E	301	-	-	3/4/4/4	-
6	SIA	L	301	-	-	2/18/34/38	0/1/1/1
8	GAL	H	301	-	-	1/2/19/22	0/1/1/1
7	PEG	C	302	-	-	0/4/4/4	-
7	PEG	H	302	-	-	2/4/4/4	-
7	PEG	L	302	-	-	3/4/4/4	-
6	SIA	F	301	-	-	11/18/34/38	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	301	SIA	O1B-C1	-3.46	1.19	1.30
6	B	301	SIA	O1B-C1	-3.22	1.20	1.30
6	L	301	SIA	C2-C1	3.08	1.56	1.52
6	L	301	SIA	O1B-C1	-2.86	1.21	1.30

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	301	SIA	O1B-C1-C2	2.57	119.41	112.71
6	B	301	SIA	O1B-C1-C2	2.48	119.16	112.71
8	H	301	GAL	O5-C5-C6	2.47	112.47	107.66
6	F	301	SIA	O1B-C1-C2	2.47	119.13	112.71
6	L	301	SIA	O6-C2-C1	2.12	111.73	107.72

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	301	SIA	O8-C8-C9-O9
6	F	301	SIA	C5-C6-C7-C8
6	F	301	SIA	C5-C6-C7-O7
6	F	301	SIA	O6-C6-C7-C8
6	F	301	SIA	O6-C6-C7-O7

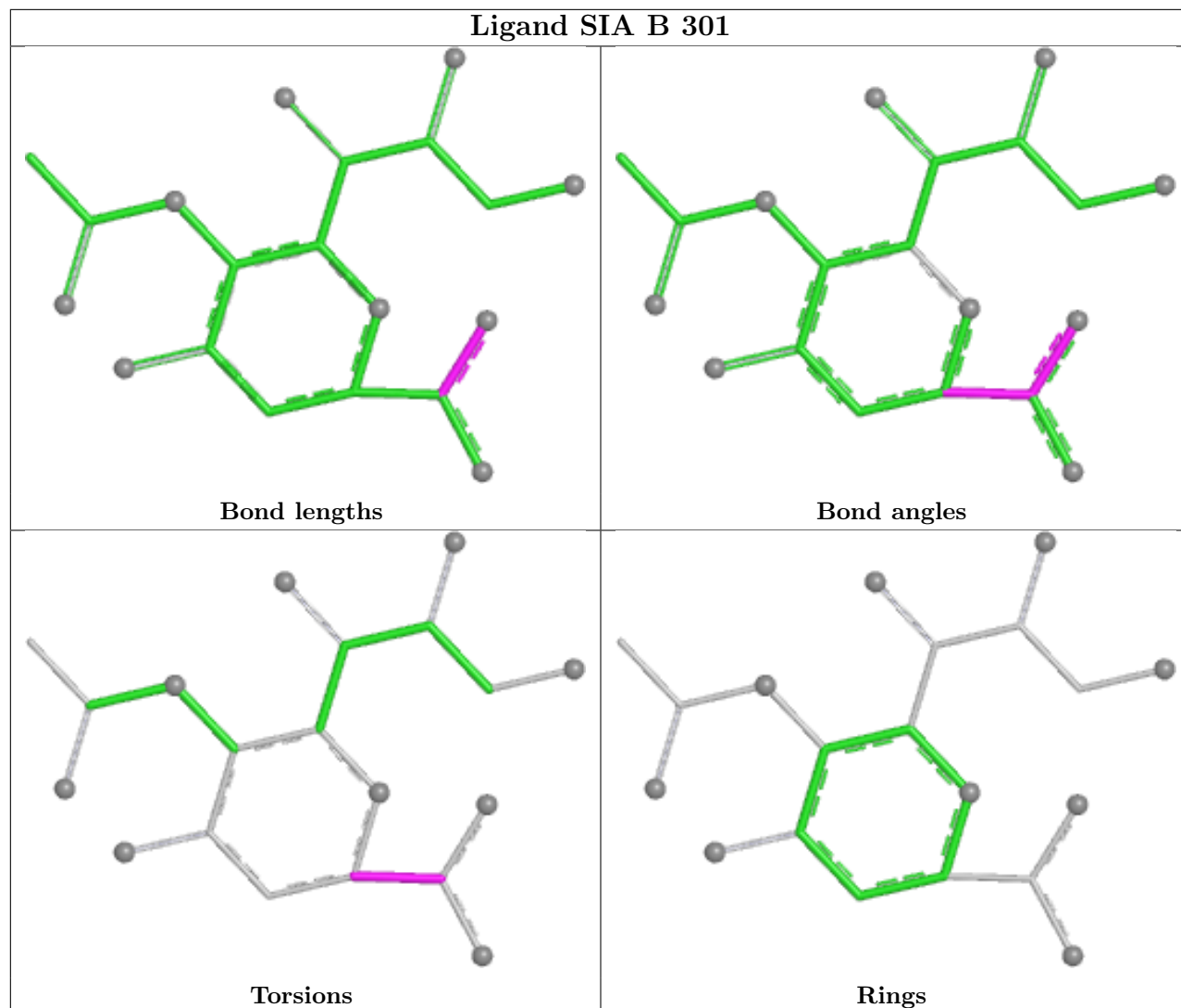
There are no ring outliers.

3 monomers are involved in 4 short contacts:

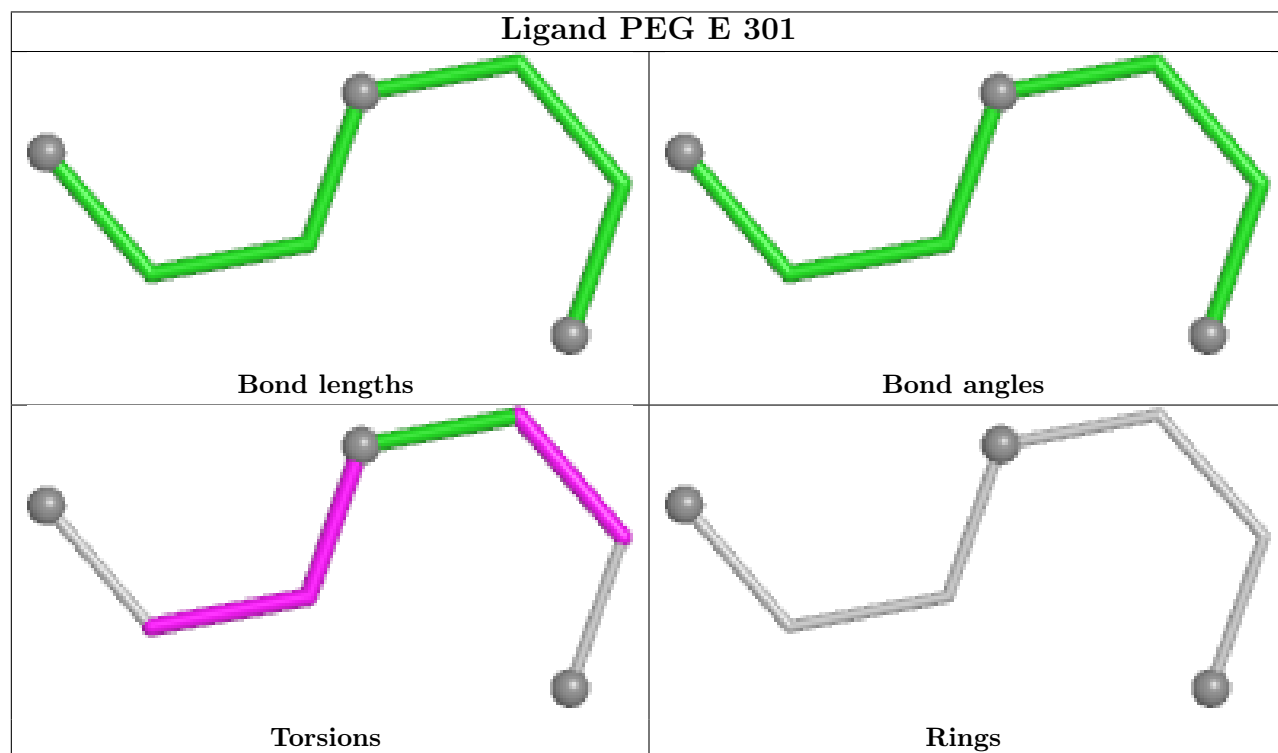
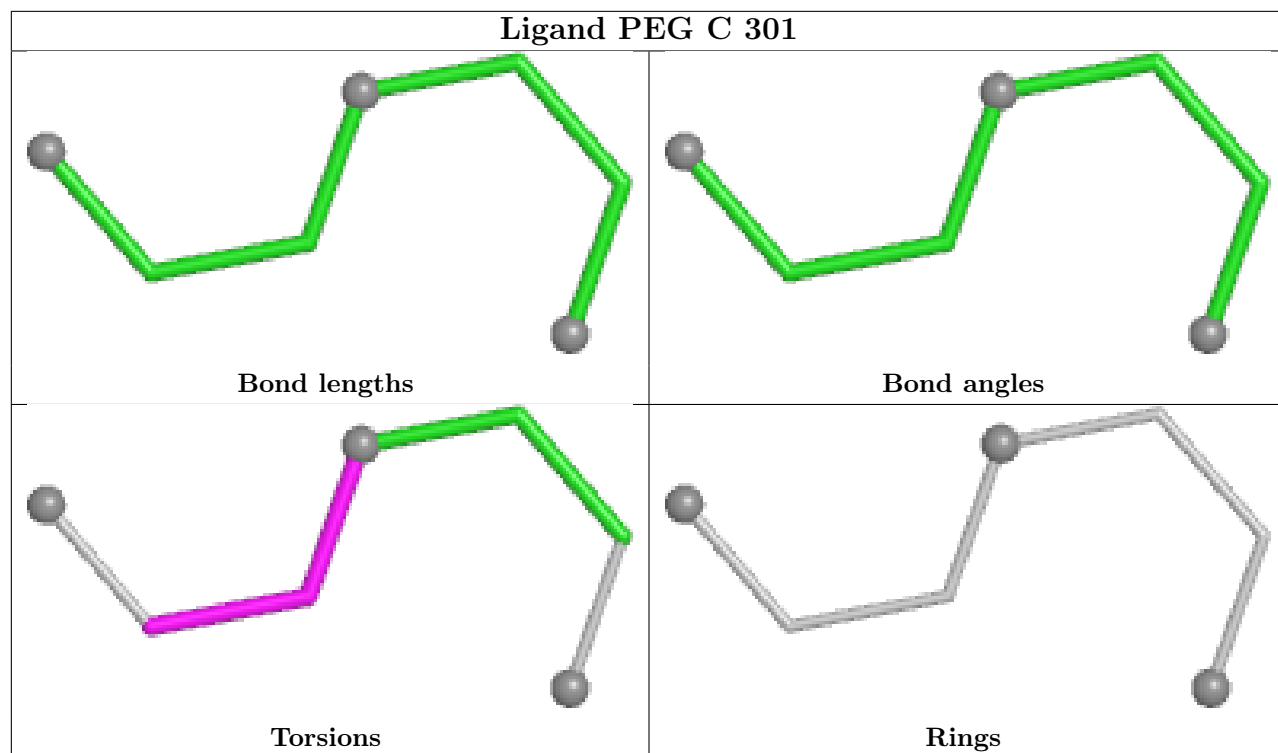
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	301	SIA	1	0
8	H	301	GAL	1	0
6	F	301	SIA	2	0

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

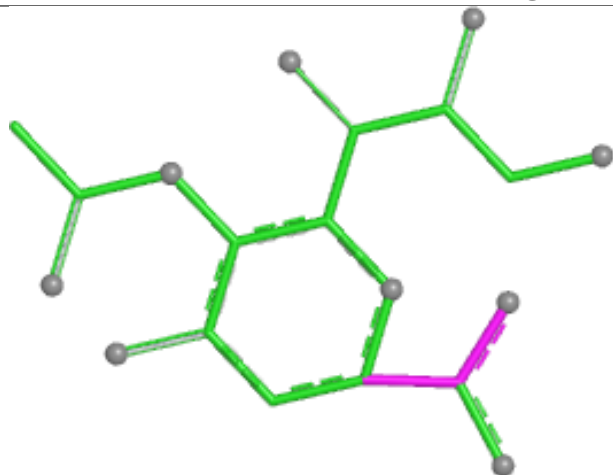
equivalents in the CSD to analyse the geometry.



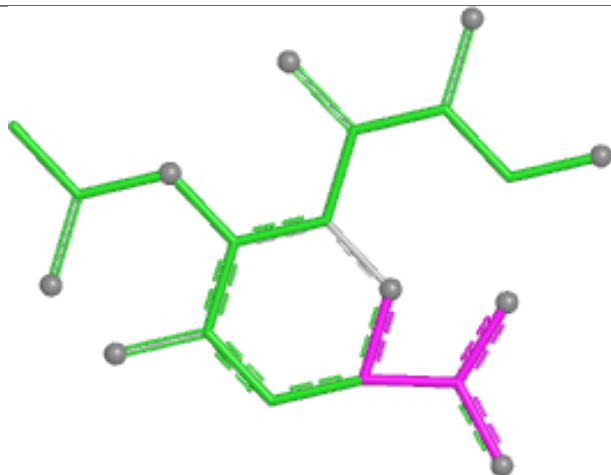




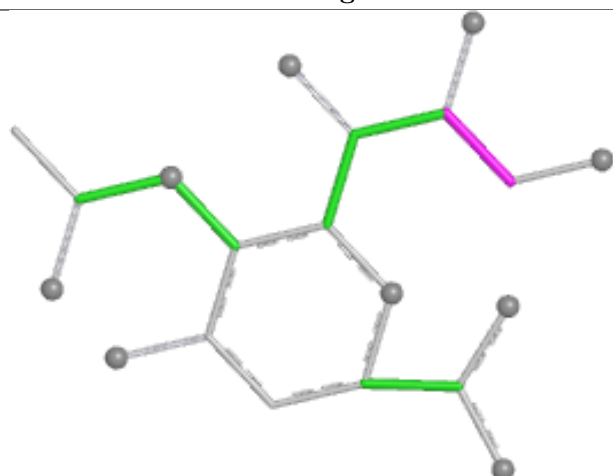
## Ligand SIA L 301



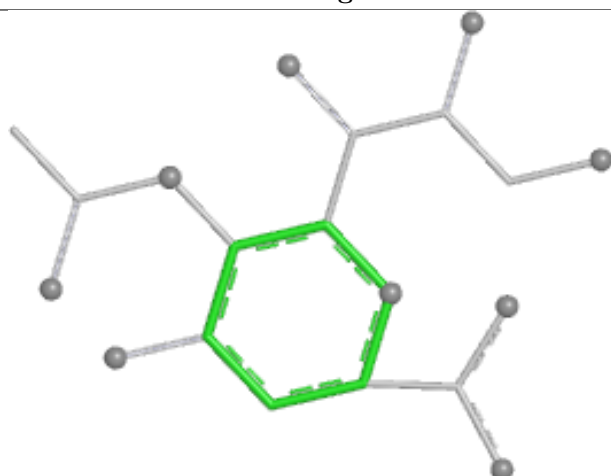
Bond lengths



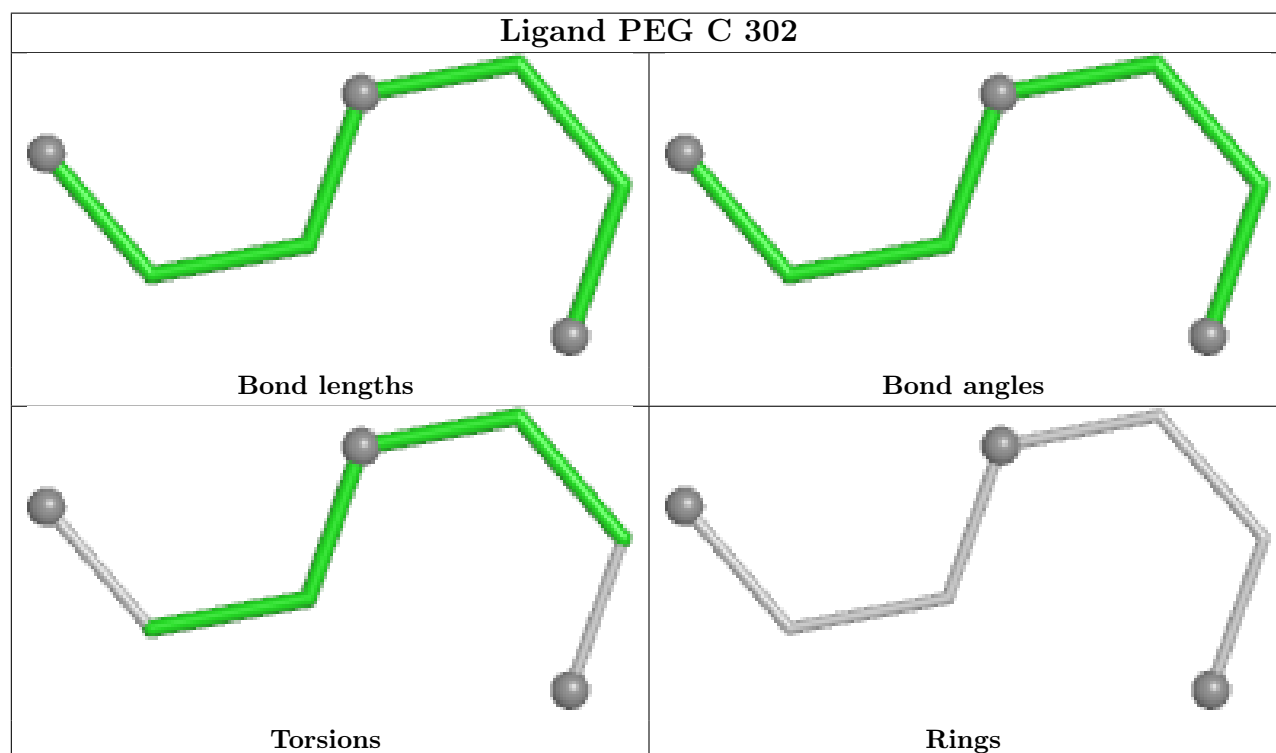
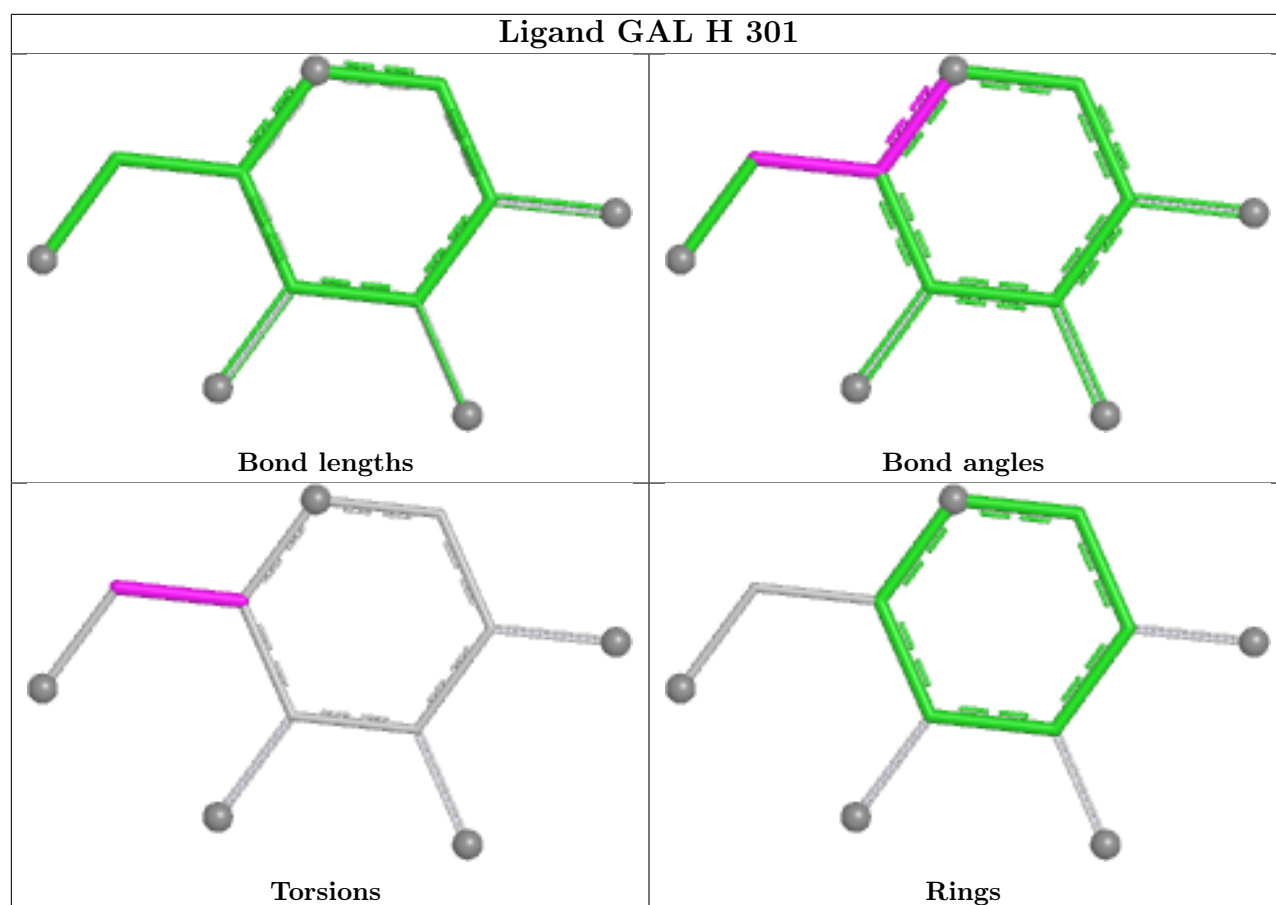
Bond angles

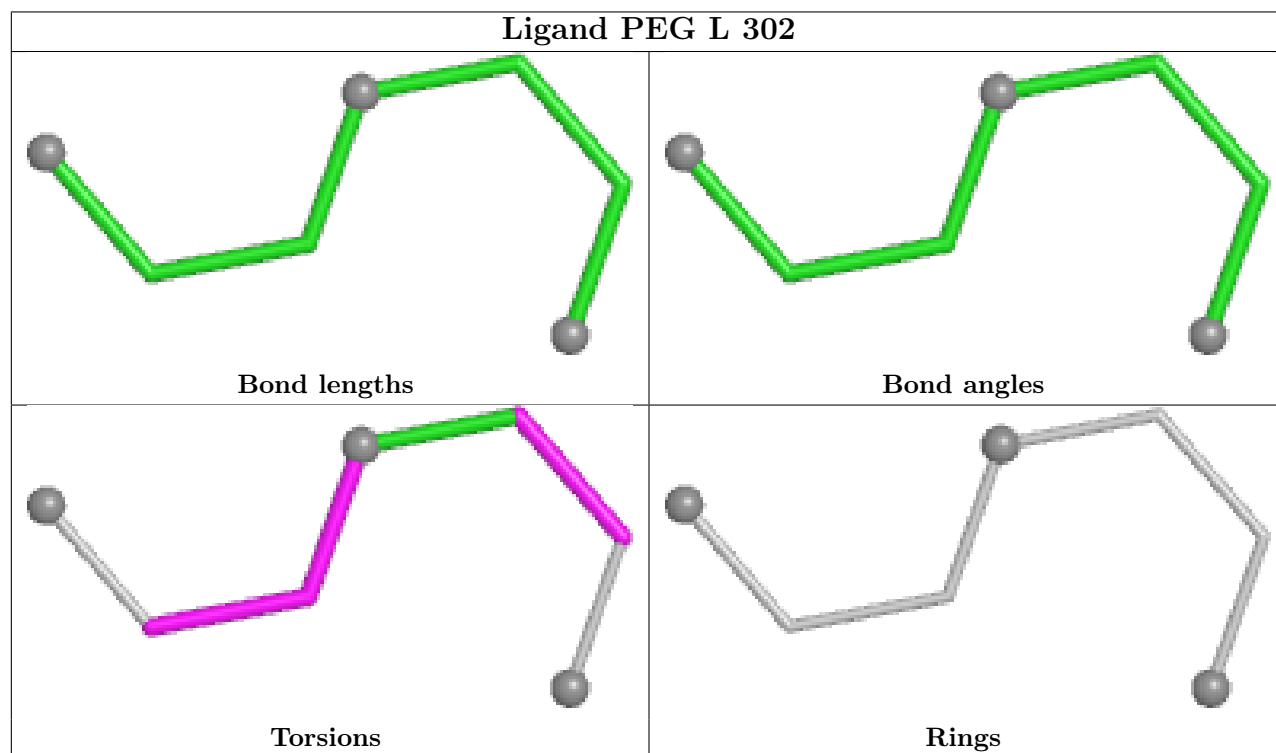
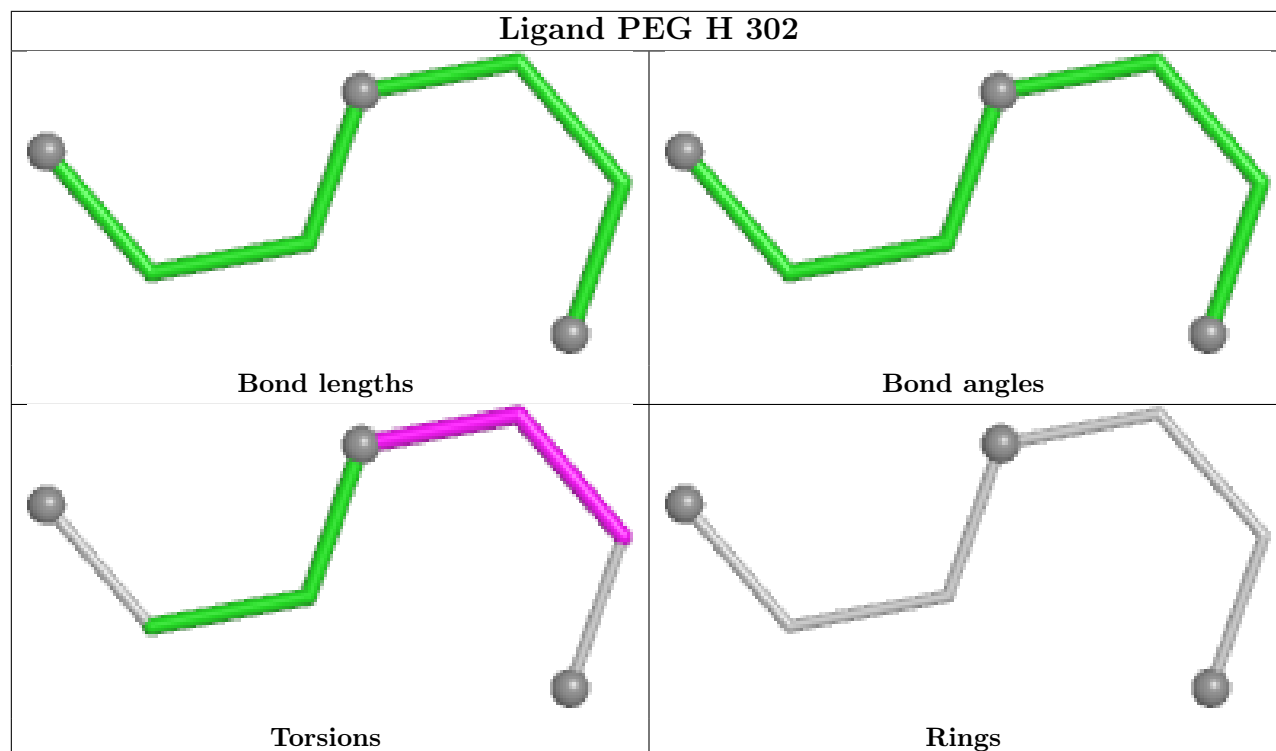


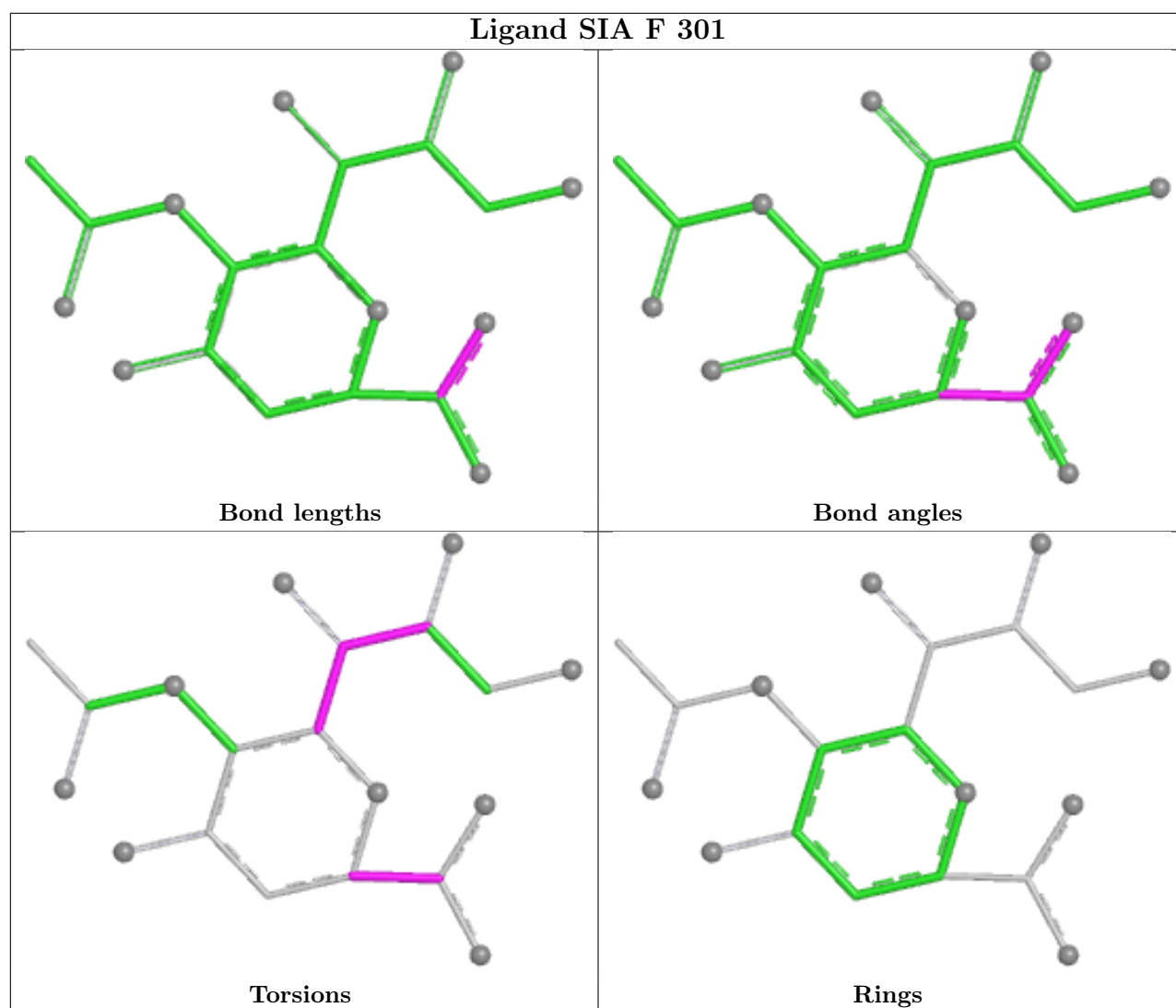
Torsions



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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	217/217 (100%)	-0.49	1 (0%) 87 83	34, 52, 97, 133	0
1	C	217/217 (100%)	-0.51	1 (0%) 87 83	35, 48, 83, 122	0
1	E	217/217 (100%)	-0.17	0 100 100	35, 66, 134, 154	1 (0%)
1	H	217/217 (100%)	-0.60	1 (0%) 87 83	32, 47, 78, 125	0
2	B	212/212 (100%)	-0.48	0 100 100	38, 60, 85, 108	0
2	D	212/212 (100%)	-0.38	0 100 100	31, 61, 88, 97	0
2	F	212/212 (100%)	-0.30	0 100 100	40, 70, 98, 123	0
2	L	212/212 (100%)	-0.55	0 100 100	32, 52, 81, 113	0
All	All	1716/1716 (100%)	-0.44	3 (0%) 91 90	31, 56, 100, 154	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	217	CYS	2.9
1	A	132	ALA	2.2
1	C	132	ALA	2.1

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

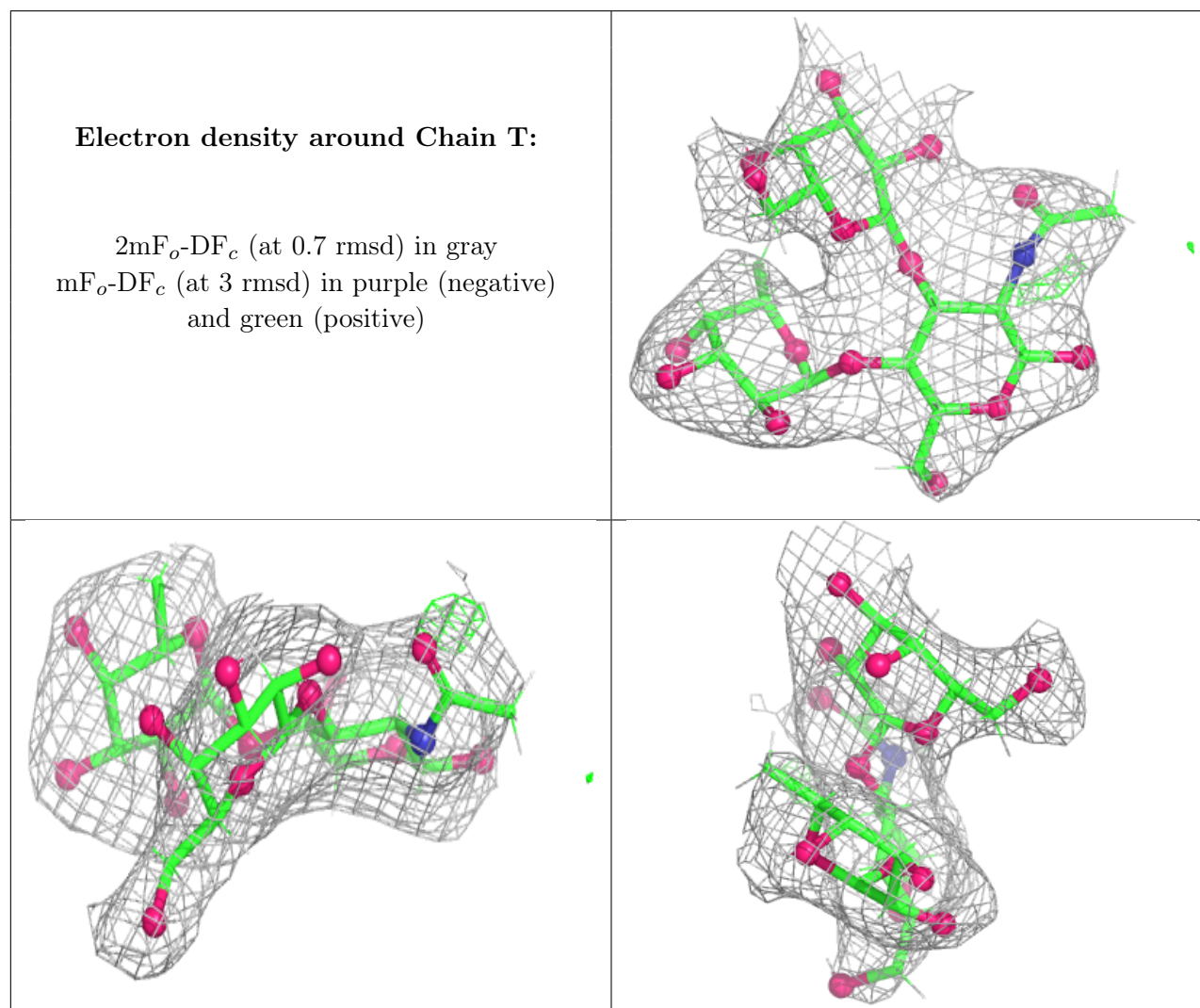
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> 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.

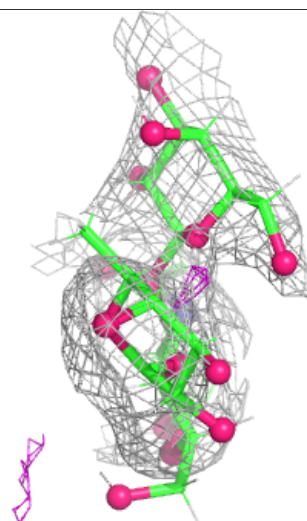
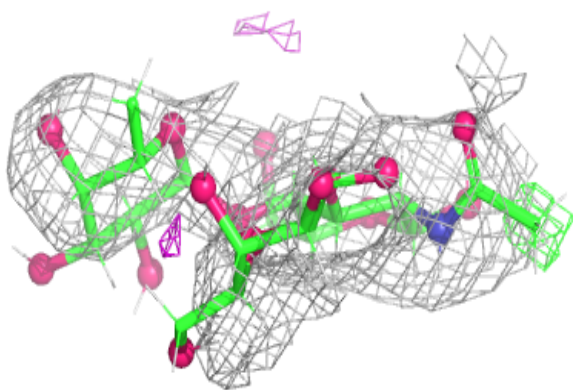
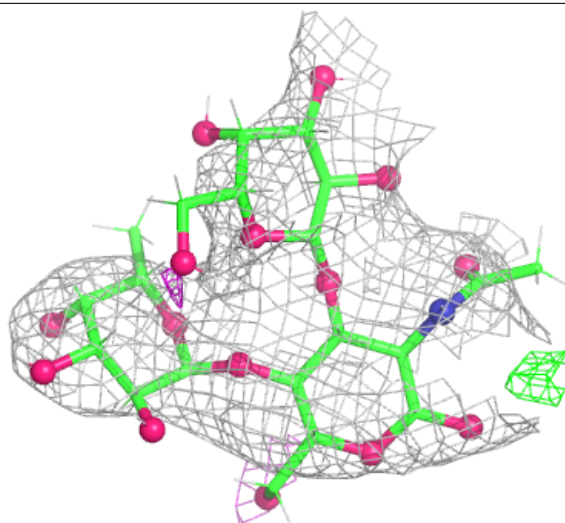
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	T	1	15/15	-	-	46,62,70,76	3
3	GAL	T	2	11/12	-	-	56,61,66,67	4
3	FUC	T	3	10/11	-	-	48,54,66,66	3
3	NAG	V	1	15/15	-	-	79,96,110,110	3
3	GAL	V	2	11/12	-	-	100,139,152,154	4
3	FUC	V	3	10/11	-	-	98,126,131,138	3
4	NAG	U	1	15/15	-	-	45,64,75,79	3
4	GAL	U	2	11/12	-	-	66,74,84,85	4
4	SIA	U	3	20/21	-	-	46,51,63,64	4
4	FUC	U	4	10/11	-	-	59,65,69,69	3
5	NAG	S	1	15/15	-	-	49,52,55,58	3
5	FUC	S	2	10/11	-	-	49,57,65,65	3

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 V:**

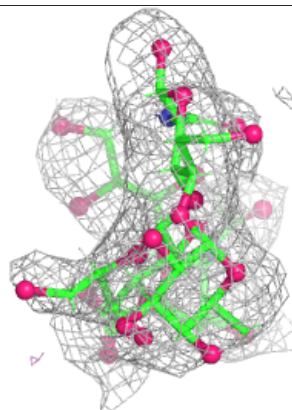
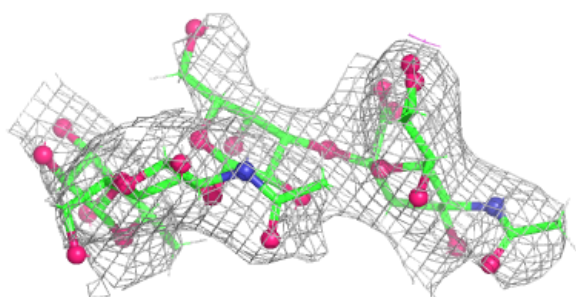
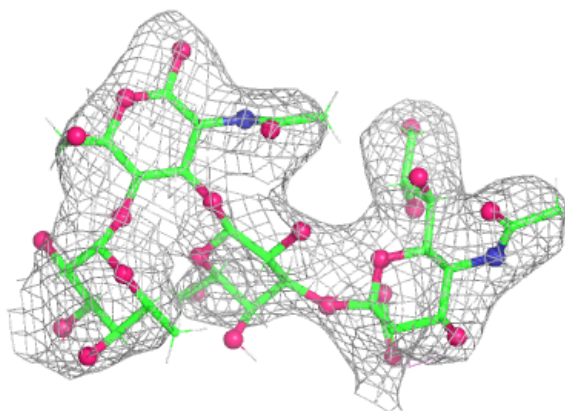
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



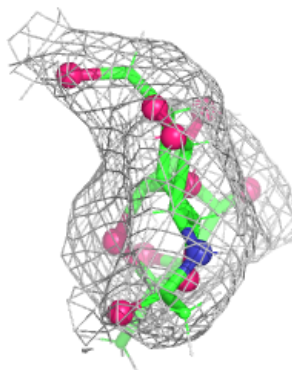
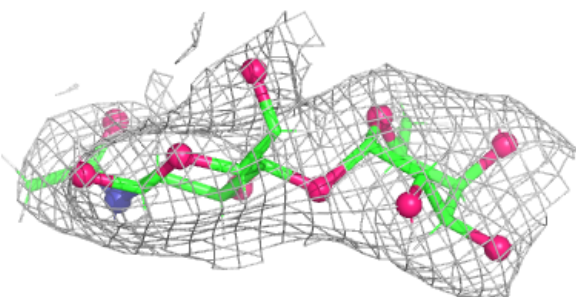
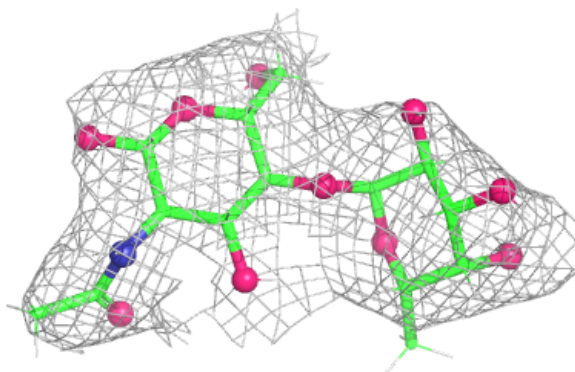


**Electron density around Chain U:**

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

**Electron density around Chain S:**

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



## 6.4 Ligands ⓘ

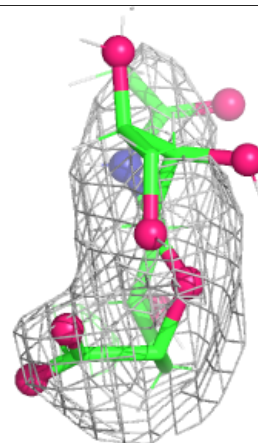
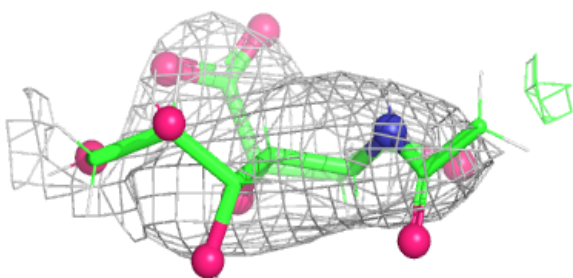
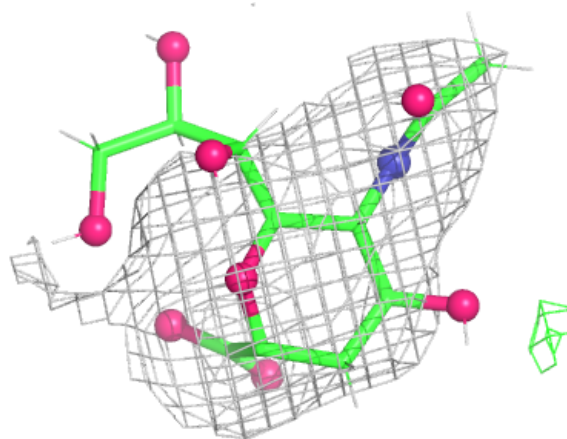
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SIA	F	301	20/21	0.75	0.14	86,104,142,142	4
7	PEG	H	302	7/7	0.83	0.14	54,69,86,86	1
7	PEG	E	301	7/7	0.88	0.10	57,63,67,67	1
7	PEG	C	302	7/7	0.89	0.10	42,53,60,60	1
7	PEG	L	302	7/7	0.89	0.09	53,59,62,62	1
7	PEG	C	301	7/7	0.92	0.09	32,44,62,62	1
6	SIA	B	301	20/21	0.93	0.07	42,50,67,68	4
6	SIA	L	301	20/21	0.93	0.07	49,55,58,60	4
8	GAL	H	301	11/12	0.94	0.06	42,50,52,53	4

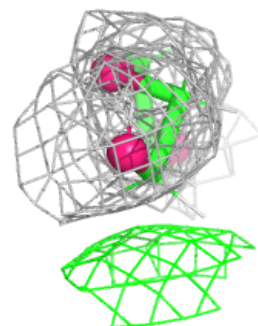
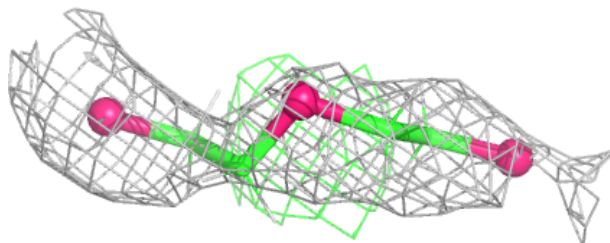
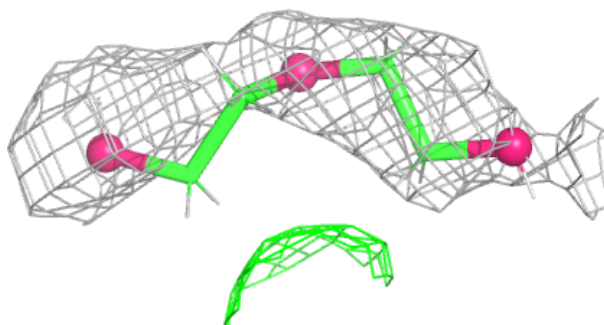
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SIA F 301:**

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

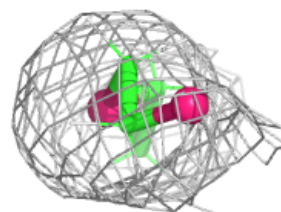
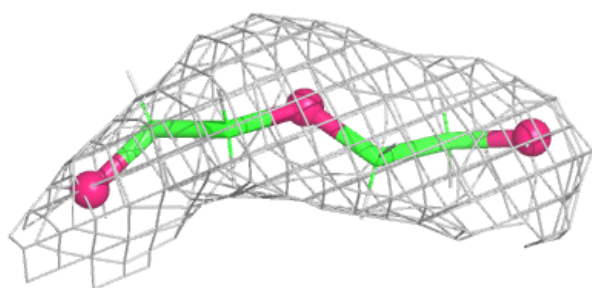
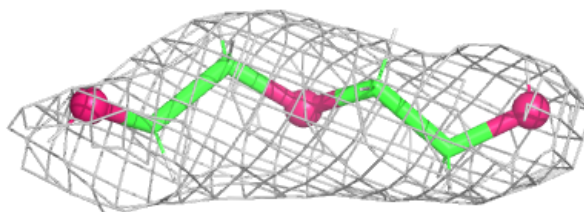
**Electron density around PEG H 302:**

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

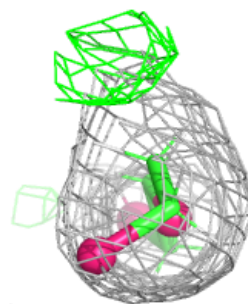
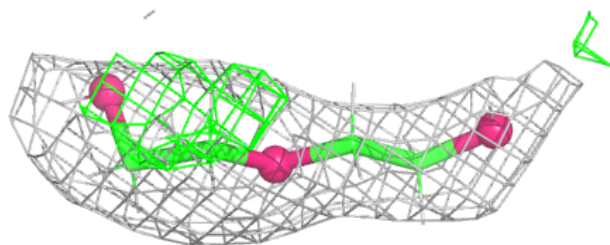
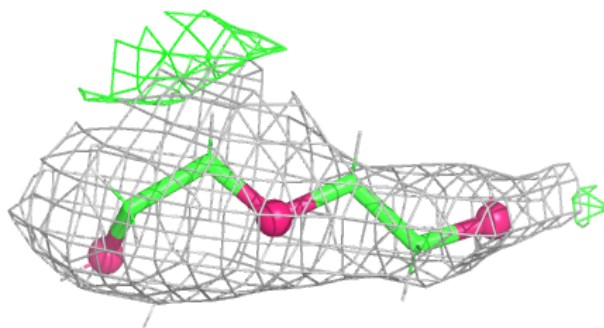


**Electron density around PEG E 301:**

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

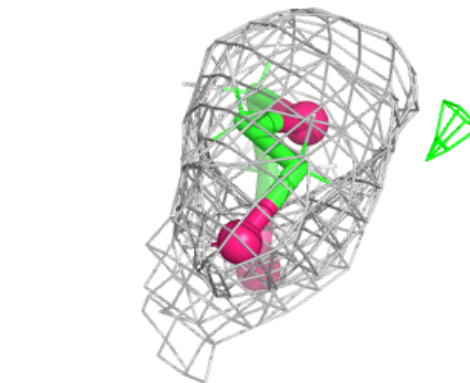
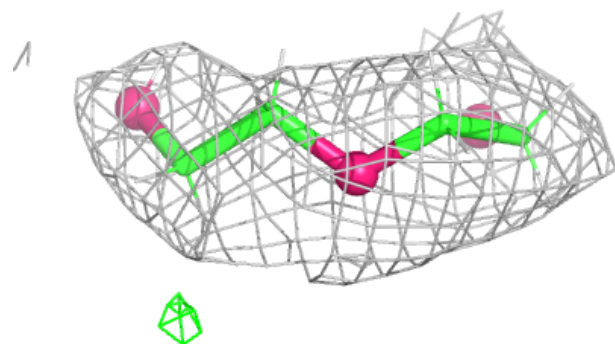
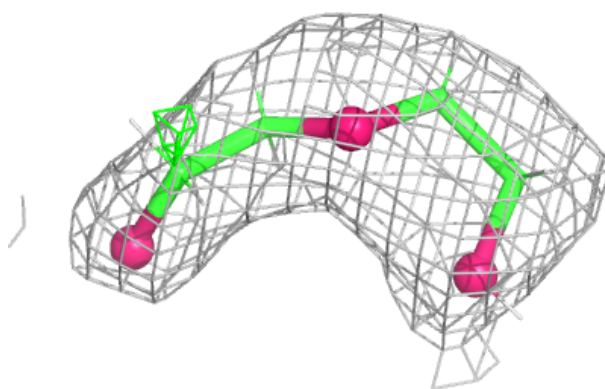
**Electron density around PEG C 302:**

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

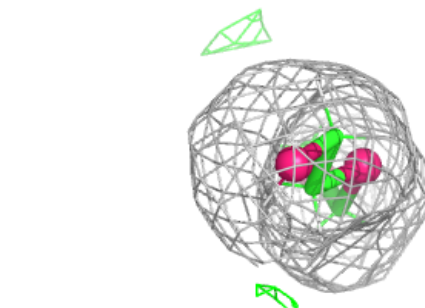
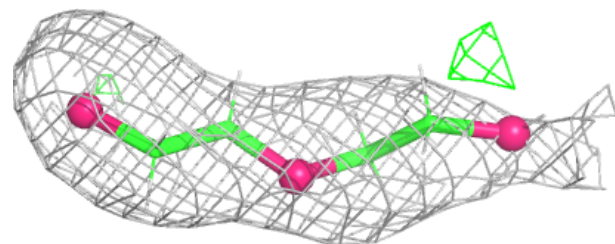
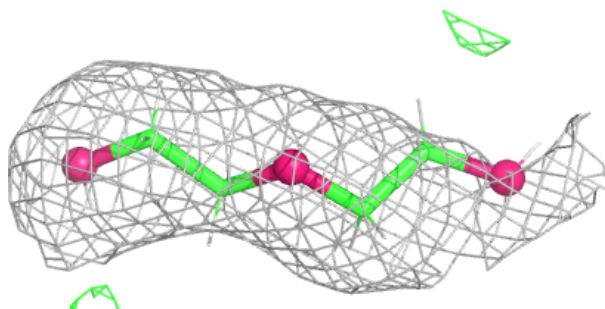


**Electron density around PEG L 302:**

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

**Electron density around PEG C 301:**

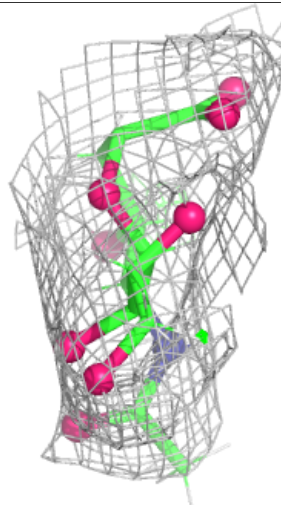
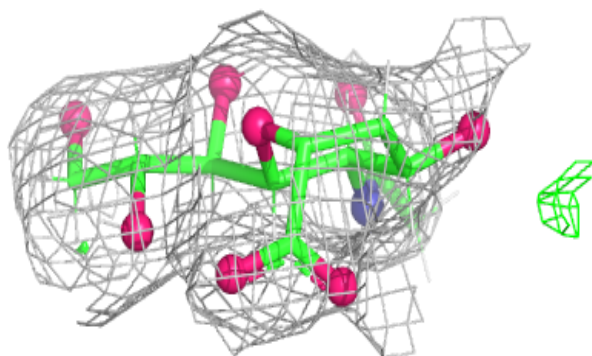
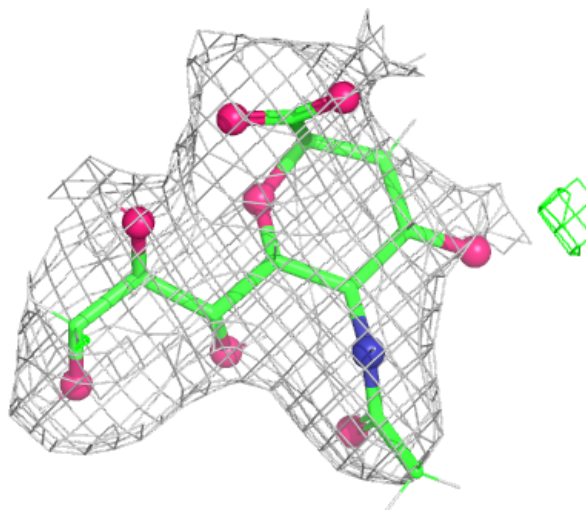
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





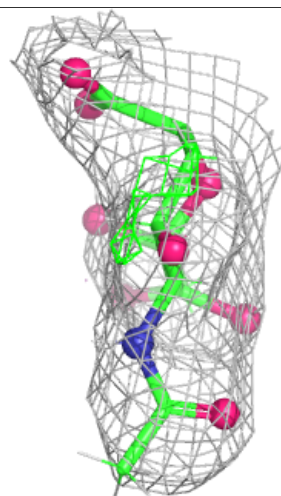
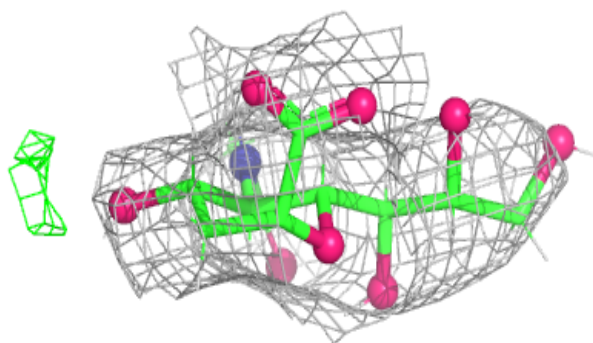
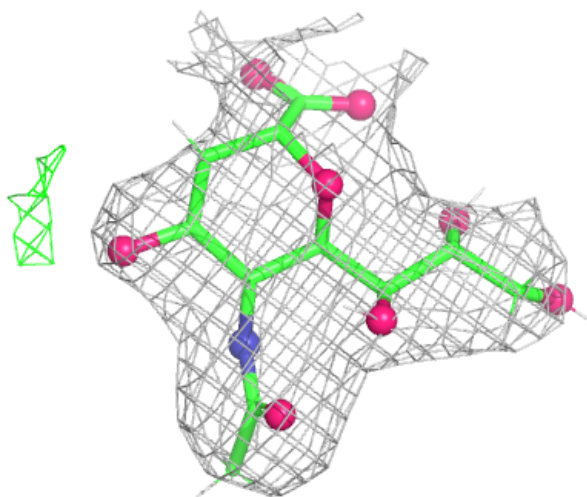
**Electron density around SIA B 301:**

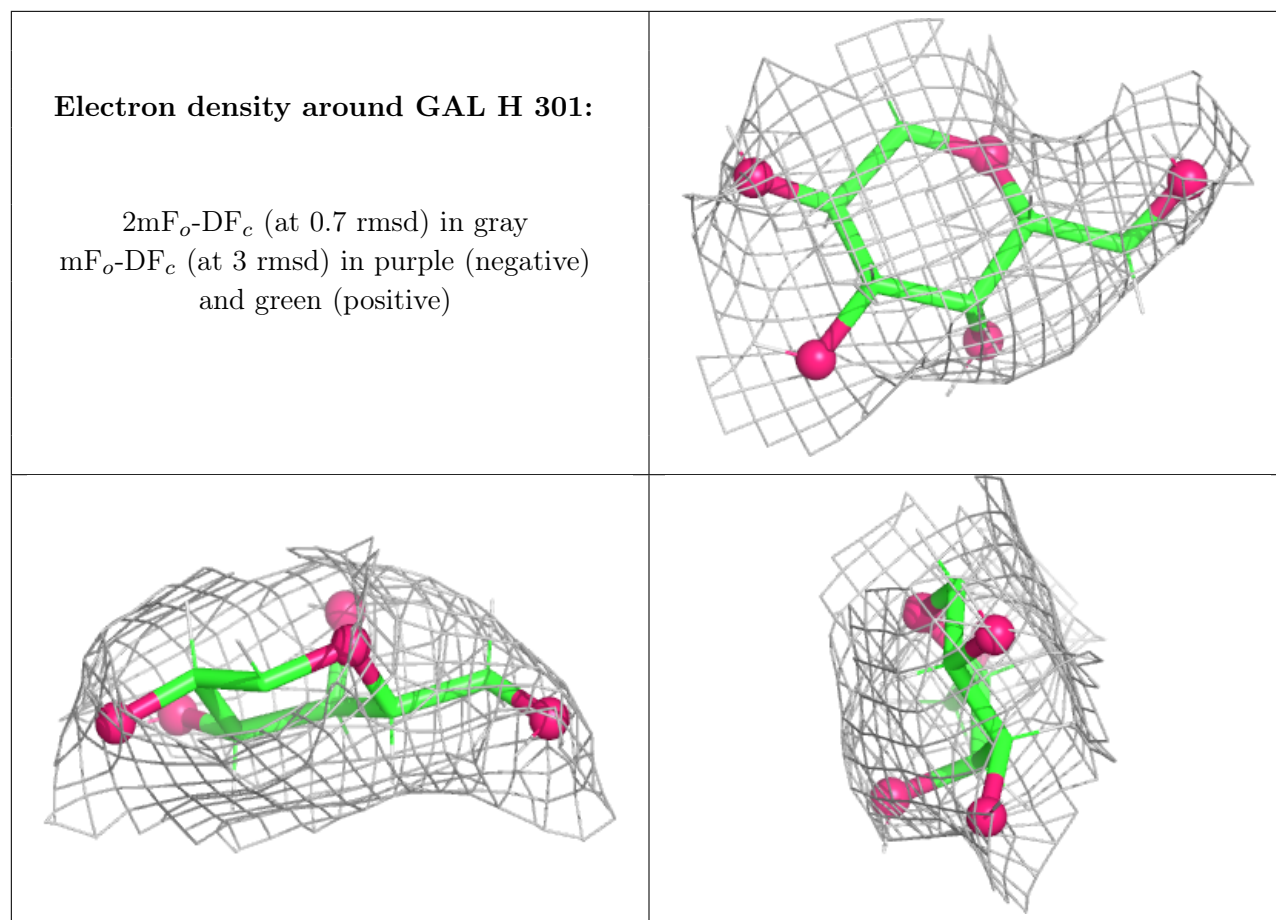
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SIA L 301:**

$2mF_o-DF_c$  (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.