



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:38 AM UTC

PDB ID : 8BJZ / pdb_00008bjz
Title : crystal structure of antibody Fab with SiaLac-amidine-Lys
Authors : Moynie, L.; Naismith, J.H.
Deposited on : 2022-11-08
Resolution : 1.89 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

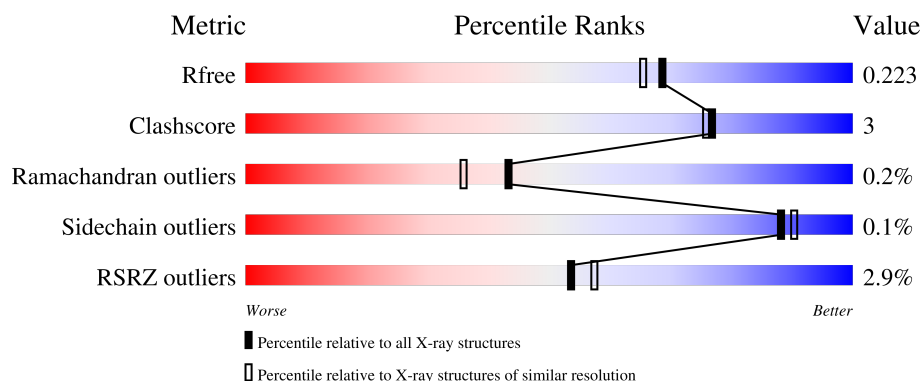
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	227	5% 89% 5% 5%
1	H	227	3% 90% 6% .
2	B	219	2% 89% 7% ..
2	L	219	% 86% 11% .
3	C	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	D	3	33% 67%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7047 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.

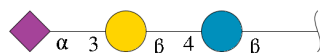
- Molecule 1 is a protein called BAR-1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	4	0
			1639	1039	270	321	9			
1	A	215	Total	C	N	O	S	0	4	0
			1620	1029	266	315	10			

- Molecule 2 is a protein called BAR-1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	2	0
			1663	1037	277	340	9			
2	B	211	Total	C	N	O	S	0	1	0
			1644	1027	274	335	8			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			42	23	1	18			
3	D	3	Total	C	N	O	0	0	0
			42	23	1	18			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

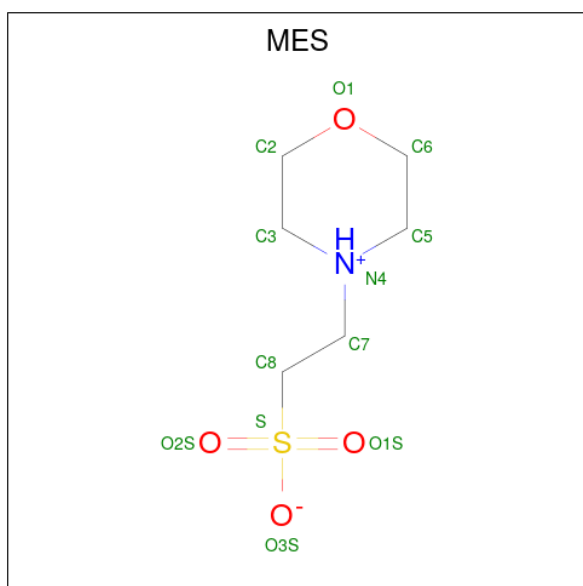
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	2	Total	Zn	0	0
			2	2		
4	A	1	Total	Zn	0	0
			1	1		
4	B	2	Total	Zn	0	0
			2	2		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



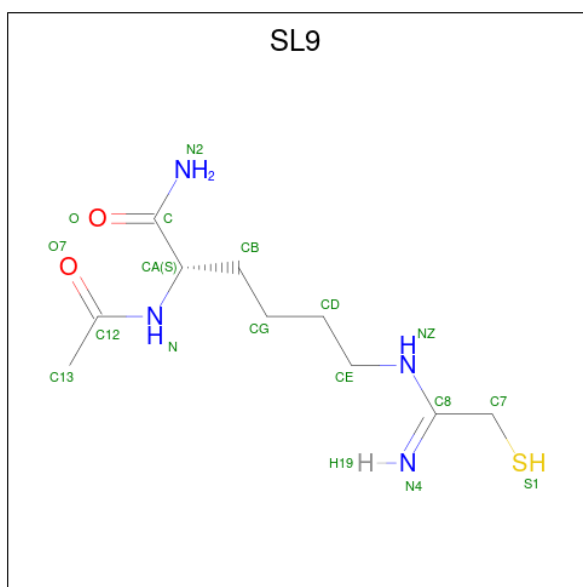
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is (2 {S})-2-acetamido-6-(2-sulfanylethanimidoylamino)hexanamide (CCD ID: SL9) (formula: C₁₀H₂₀N₄O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
7	B	1	Total	C	N	O	S	0	0
			17	10	4	2	1		

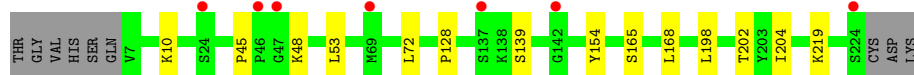
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	77	Total	O	0	0
			77	77		
8	L	87	Total	O	0	0
			87	87		
8	A	79	Total	O	0	0
			79	79		
8	B	60	Total	O	0	0
			60	60		

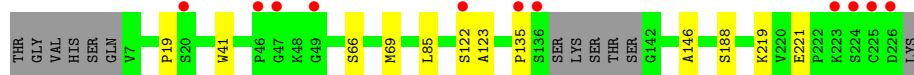
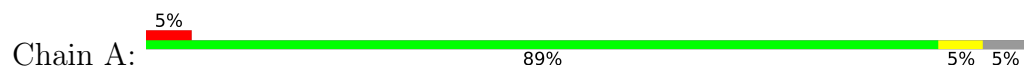
3 Residue-property plots [i](#)

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.

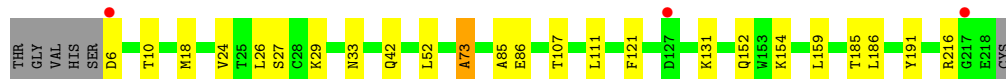
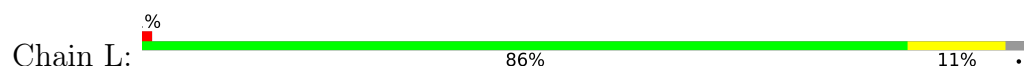
- Molecule 1: BAR-1 Fab heavy chain



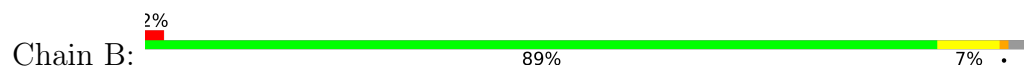
- Molecule 1: BAR-1 Fab heavy chain



- Molecule 2: BAR-1 Fab light chain



- Molecule 2: BAR-1 Fab light chain



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain D:  33% 67%

BCG1
GAL2
STAG

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.91Å 130.68Å 76.91Å 90.00° 123.66° 90.00°	Depositor
Resolution (Å)	48.24 – 1.89 48.24 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.24-1.89) 99.6 (48.24-1.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.186 , 0.223 0.187 , 0.223	Depositor DCC
R_{free} test set	4859 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SL9, GOL, ZN, MES, SIA, BGC, 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	0.36	0/1660	0.62	0/2264
1	H	0.37	0/1680	0.61	0/2291
2	B	0.36	0/1680	0.63	5/2280 (0.2%)
2	L	0.40	0/1699	0.67	3/2305 (0.1%)
All	All	0.37	0/6719	0.63	8/9140 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	131	LYS	CA-CB-CG	-7.63	98.85	114.10
2	L	86	GLU	CA-CB-CG	7.22	128.54	114.10
2	B	150	LYS	CB-CA-C	-7.12	96.68	109.71
2	B	194	HIS	CA-C-N	-6.75	110.48	122.42
2	B	194	HIS	C-N-CA	-6.75	110.48	122.42
2	L	131	LYS	CD-CE-NZ	-5.69	93.69	111.90
2	B	150	LYS	CA-CB-CG	5.33	124.76	114.10
2	B	195	LYS	CG-CD-CE	-5.21	99.31	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1620	0	1589	9	0
1	H	1639	0	1612	10	0
2	B	1644	0	1582	8	1
2	L	1663	0	1594	13	1
3	C	42	0	35	0	0
3	D	42	0	35	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	H	1	0	0	0	0
4	L	2	0	0	0	0
5	A	12	0	12	0	0
5	H	12	0	12	1	0
6	A	12	0	16	2	0
6	H	12	0	16	1	0
6	L	6	0	8	0	0
7	B	17	0	0	0	0
7	L	17	0	0	0	0
8	A	79	0	0	0	0
8	B	60	0	0	0	0
8	H	77	0	0	1	0
8	L	87	0	0	0	0
All	All	7047	0	6511	39	1

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 3.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:LYS:HB2	2:B:202:THR:HB	1.59	0.85
2:L:18:MET:HG3	2:L:24:VAL:HG22	1.71	0.73
1:A:19:PRO:HD2	1:A:122:SER:HB3	1.73	0.71
1:A:66:SER:HA	1:A:69:MET:HG2	1.74	0.68
1:H:168:LEU:HD12	6:H:304:GOL:H32	1.83	0.60
1:A:219:LYS:HD3	1:A:221:GLU:HG3	1.83	0.59
2:L:154:LYS:HG2	2:L:159:LEU:HD23	1.87	0.57
1:H:198:LEU:O	8:H:401:HOH:O	2.18	0.56
2:B:26:LEU:HD22	2:B:107:THR:HG21	1.88	0.56
1:H:165:SER:O	1:A:123:ALA:HA	2.09	0.53
1:H:45:PRO:HB2	1:H:48:LYS:HE3	1.91	0.52
2:B:18:MET:HG3	2:B:24:VAL:HG22	1.91	0.52
1:H:10:LYS:HA	1:H:10:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:VAL:HG22	2:B:180:LEU:HD12	1.94	0.50
1:H:202:THR:HG23	1:H:219:LYS:HE3	1.93	0.49
6:A:304:GOL:H12	2:B:183:THR:OG1	2.13	0.49
1:A:135:PRO:HB3	1:A:146:ALA:O	2.13	0.49
2:L:6:ASP:N	2:L:6:ASP:OD1	2.47	0.48
1:H:53:LEU:HB3	1:H:72:LEU:HD21	1.95	0.48
5:H:302:MES:H32	5:H:302:MES:H81	1.70	0.47
2:B:6:ASP:O	2:B:6:ASP:CG	2.58	0.46
1:H:139:SER:HA	2:L:121:PHE:CD1	2.51	0.45
2:L:42:GLN:HB2	2:L:52:LEU:HD11	1.99	0.45
2:L:85:ALA:HA	2:L:111:LEU:HD11	1.98	0.45
2:L:27:SER:OG	2:L:29:LYS:HE2	2.17	0.44
1:H:128:PRO:HB3	1:H:154:TYR:HB3	1.99	0.44
2:B:26:LEU:HD12	2:B:78:LEU:HD23	1.99	0.44
2:B:9:MET:HE3	2:B:28:CYS:SG	2.58	0.44
1:H:204:ILE:HD13	1:H:219:LYS:HA	2.00	0.43
1:A:219:LYS:CD	1:A:221:GLU:HG3	2.48	0.43
2:L:152:GLN:CD	2:L:159:LEU:HD22	2.44	0.43
1:A:188[A]:SER:OG	6:A:304:GOL:H32	2.19	0.43
2:L:26:LEU:HD22	2:L:107:THR:HG21	2.01	0.43
2:L:185:THR:O	2:L:186:LEU:HD23	2.18	0.42
2:L:10:THR:O	2:L:29:LYS:HE3	2.20	0.42
2:L:33:ASN:OD1	2:L:73:ALA:HA	2.21	0.41
2:L:191:TYR:CE2	2:L:216:ARG:HD2	2.56	0.41
1:A:41:TRP:CE2	1:A:85:LEU:HB2	2.56	0.41
1:A:19:PRO:CD	1:A:122:SER:HB3	2.46	0.40

All (1) 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)
2:L:6:ASP:N	2:B:86:GLU:OE1[1_556]	2.02	0.18

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	215/227 (95%)	211 (98%)	4 (2%)	0	100	100
1	H	220/227 (97%)	215 (98%)	5 (2%)	0	100	100
2	B	210/219 (96%)	205 (98%)	4 (2%)	1 (0%)	24	16
2	L	213/219 (97%)	208 (98%)	4 (2%)	1 (0%)	24	16
All	All	858/892 (96%)	839 (98%)	17 (2%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	73	ALA
2	B	73	ALA

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	186/193 (96%)	186 (100%)	0	100	100
1	H	189/193 (98%)	189 (100%)	0	100	100
2	B	189/194 (97%)	188 (100%)	1 (0%)	81	84
2	L	191/194 (98%)	191 (100%)	0	100	100
All	All	755/774 (98%)	754 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	195	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	105	ASN
2	L	152	GLN
1	A	105	ASN
2	B	8	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BGC	C	1	3,7	11,11,12	0.65	0	15,15,17	0.86	0
3	GAL	C	2	3	11,11,12	0.81	0	15,15,17	0.92	0
3	SIA	C	3	3	20,20,21	1.21	2 (10%)	21,28,31	1.39	3 (14%)
3	BGC	D	1	3,7	11,11,12	0.40	0	15,15,17	0.97	0
3	GAL	D	2	3	11,11,12	0.75	0	15,15,17	0.96	1 (6%)
3	SIA	D	3	3	20,20,21	1.12	1 (5%)	21,28,31	1.32	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	C	1	3,7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	C	2	3	-	0/2/19/22	0/1/1/1
3	SIA	C	3	3	-	0/18/34/38	0/1/1/1
3	BGC	D	1	3,7	-	0/2/19/22	0/1/1/1
3	GAL	D	2	3	-	1/2/19/22	0/1/1/1
3	SIA	D	3	3	-	0/18/34/38	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	SIA	C2-C1	2.83	1.55	1.52
3	D	3	SIA	C2-C1	2.80	1.55	1.52
3	C	3	SIA	C3-C2	2.20	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	SIA	C8-C7-C6	-3.42	106.62	113.05
3	C	3	SIA	C8-C7-C6	-3.35	106.76	113.05
3	C	3	SIA	O6-C2-C1	2.82	113.04	107.72
3	D	3	SIA	O6-C2-C1	2.57	112.56	107.72
3	D	2	GAL	O5-C5-C6	-2.37	103.05	107.66
3	C	3	SIA	C4-C5-N5	2.08	114.54	110.44

There are no chirality outliers.

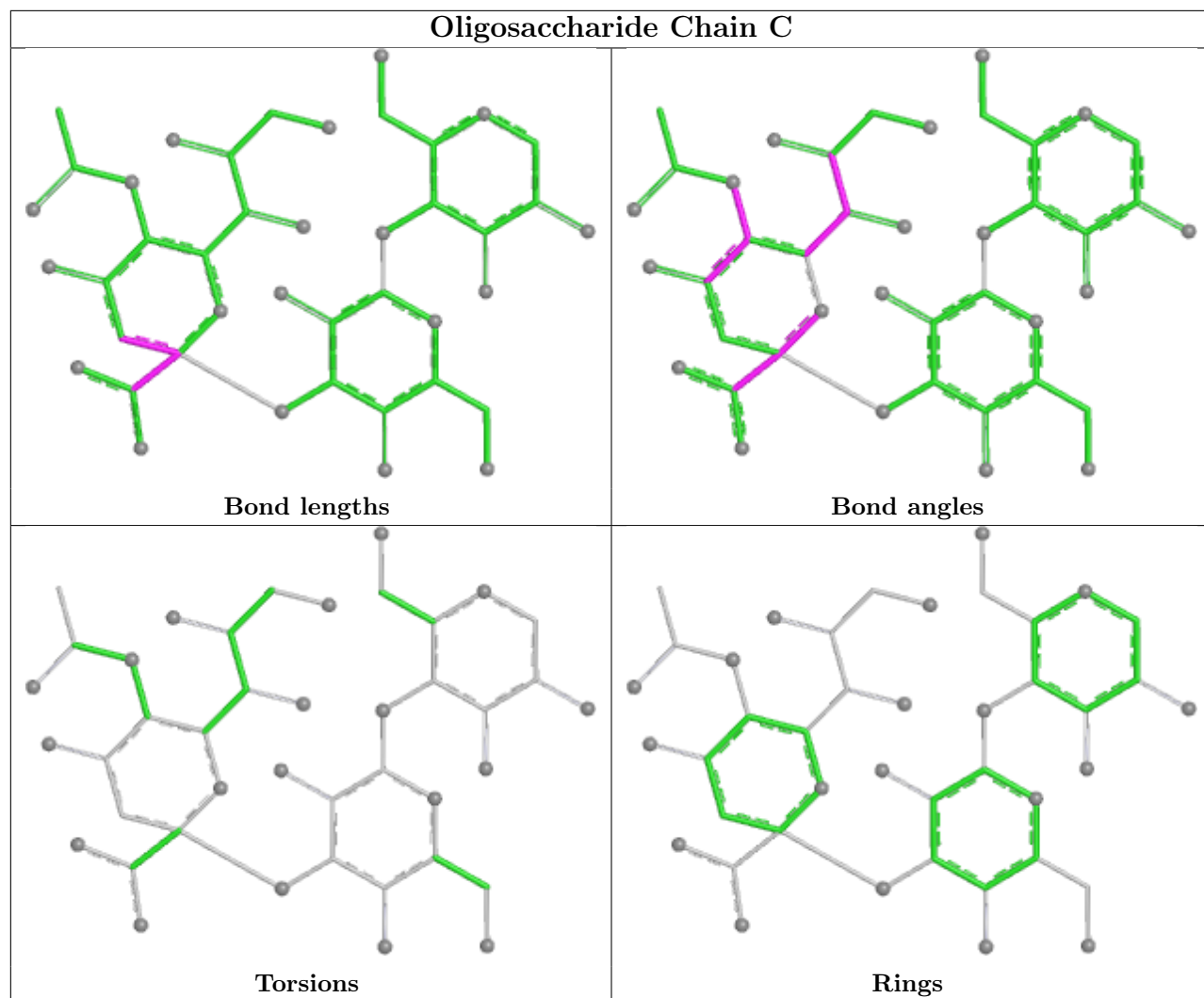
All (1) torsion outliers are listed below:

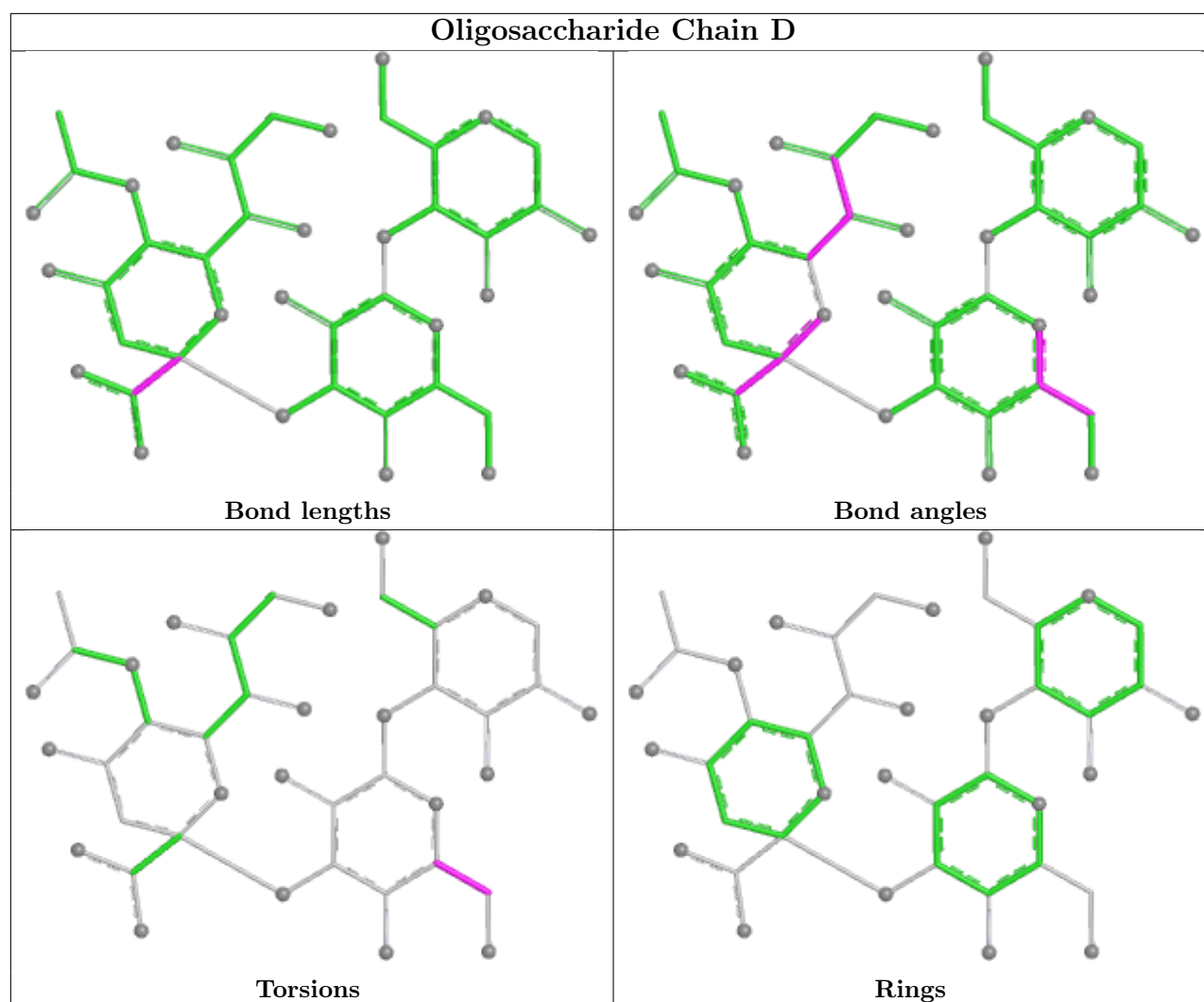
Mol	Chain	Res	Type	Atoms
3	D	2	GAL	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 for Mogul analysis.

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	GOL	H	303	-	5,5,5	0.86	0	5,5,5	0.99	0
5	MES	A	302	-	12,12,12	1.90	1 (8%)	15,16,16	1.54	2 (13%)
7	SL9	B	303	3	15,16,16	1.19	2 (13%)	17,19,19	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SL9	L	304	3	15,16,16	1.11	1 (6%)	17,19,19	0.83	0
6	GOL	L	301	-	5,5,5	0.97	0	5,5,5	0.93	0
6	GOL	H	304	-	5,5,5	1.00	0	5,5,5	1.05	0
5	MES	H	302	-	12,12,12	1.91	1 (8%)	15,16,16	2.23	6 (40%)
6	GOL	A	303	-	5,5,5	1.02	1 (20%)	5,5,5	1.20	0
6	GOL	A	304	-	5,5,5	0.75	0	5,5,5	1.23	1 (20%)

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	GOL	H	303	-	-	2/4/4/4	-
5	MES	A	302	-	-	1/6/14/14	0/1/1/1
7	SL9	B	303	3	-	7/16/18/18	-
7	SL9	L	304	3	-	4/16/18/18	-
6	GOL	L	301	-	-	4/4/4/4	-
6	GOL	H	304	-	-	1/4/4/4	-
5	MES	H	302	-	-	5/6/14/14	0/1/1/1
6	GOL	A	303	-	-	4/4/4/4	-
6	GOL	A	304	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	302	MES	C8-S	-6.18	1.68	1.77
5	A	302	MES	C8-S	-6.12	1.69	1.77
7	B	303	SL9	C8-N4	3.09	1.34	1.27
7	L	304	SL9	C8-N4	2.98	1.33	1.27
7	B	303	SL9	C7-S1	2.52	1.86	1.82
6	A	303	GOL	O2-C2	-2.02	1.37	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	302	MES	C2-C3-N4	-4.16	103.80	110.12
5	A	302	MES	C5-N4-C3	3.98	117.41	108.84
5	H	302	MES	O2S-S-C8	3.93	112.67	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	302	MES	C5-N4-C3	3.48	116.33	108.84
5	H	302	MES	C7-N4-C3	3.37	120.22	111.24
6	A	304	GOL	C3-C2-C1	-2.38	103.06	111.80
7	B	303	SL9	CB-CA-N	-2.37	106.21	110.91
5	A	302	MES	O3S-S-C8	2.37	110.65	106.00
5	H	302	MES	C7-N4-C5	2.20	117.11	111.24
5	H	302	MES	C6-C5-N4	-2.08	106.96	110.12

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	302	MES	C8-C7-N4-C3
5	H	302	MES	C7-C8-S-O1S
5	H	302	MES	C7-C8-S-O2S
6	H	303	GOL	C1-C2-C3-O3
6	A	303	GOL	O1-C1-C2-O2
6	A	303	GOL	O1-C1-C2-C3
6	A	303	GOL	C1-C2-C3-O3
7	B	303	SL9	N-CA-CB-CG
7	B	303	SL9	C-CA-CB-CG
7	L	304	SL9	O7-C12-N-CA
7	L	304	SL9	C13-C12-N-CA
7	B	303	SL9	O7-C12-N-CA
7	B	303	SL9	C13-C12-N-CA
6	L	301	GOL	O2-C2-C3-O3
6	L	301	GOL	O1-C1-C2-C3
6	L	301	GOL	C1-C2-C3-O3
6	A	304	GOL	O1-C1-C2-C3
6	A	303	GOL	O2-C2-C3-O3
6	A	304	GOL	O1-C1-C2-O2
5	H	302	MES	N4-C7-C8-S
7	B	303	SL9	CA-CB-CG-CD
6	H	303	GOL	O2-C2-C3-O3
6	L	301	GOL	O1-C1-C2-O2
7	L	304	SL9	CG-CD-CE-NZ
7	L	304	SL9	CE-CD-CG-CB
5	H	302	MES	C7-C8-S-O3S
6	H	304	GOL	O1-C1-C2-O2
7	B	303	SL9	CE-CD-CG-CB
5	A	302	MES	C8-C7-N4-C3
7	B	303	SL9	CG-CD-CE-NZ

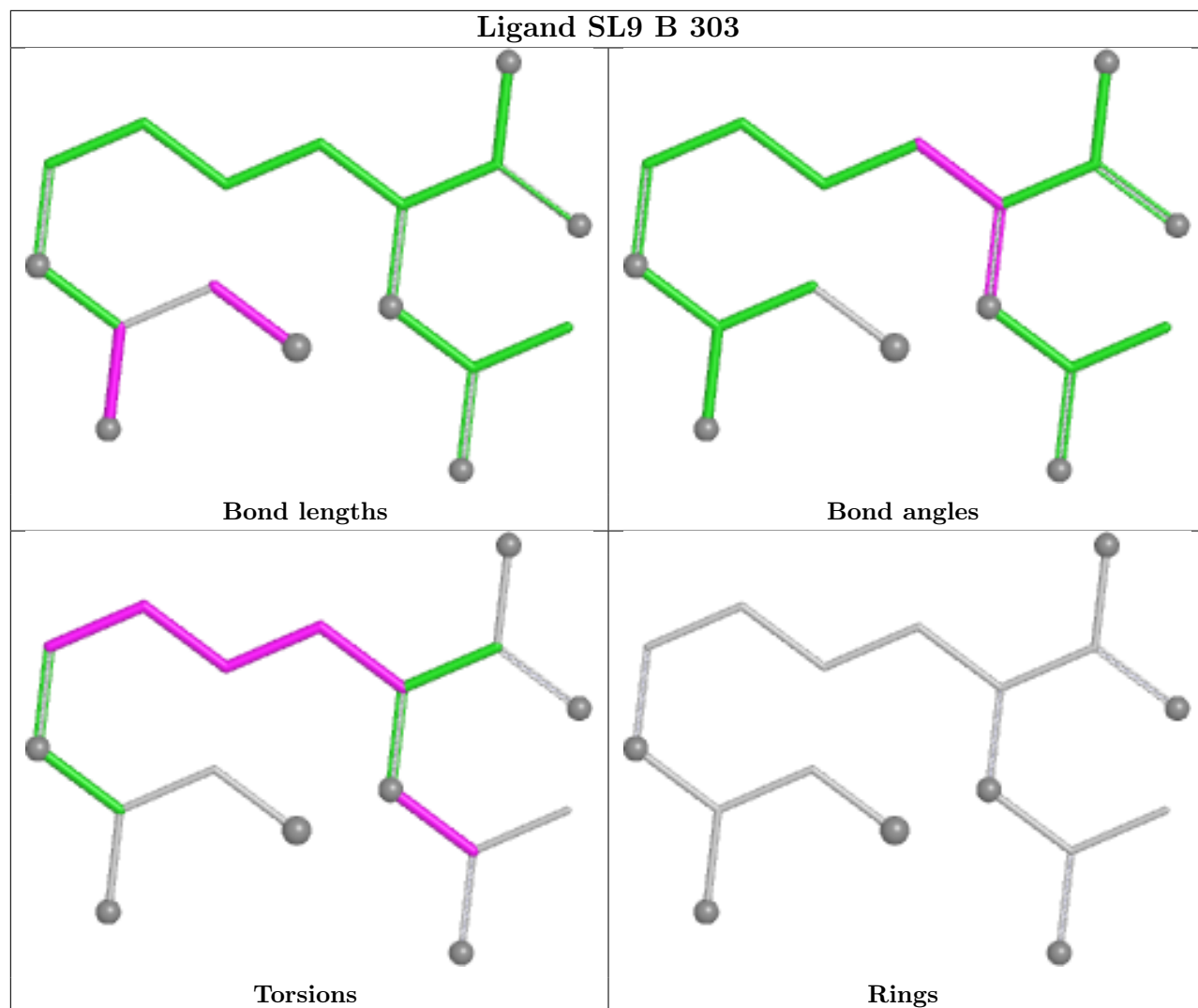
There are no ring outliers.

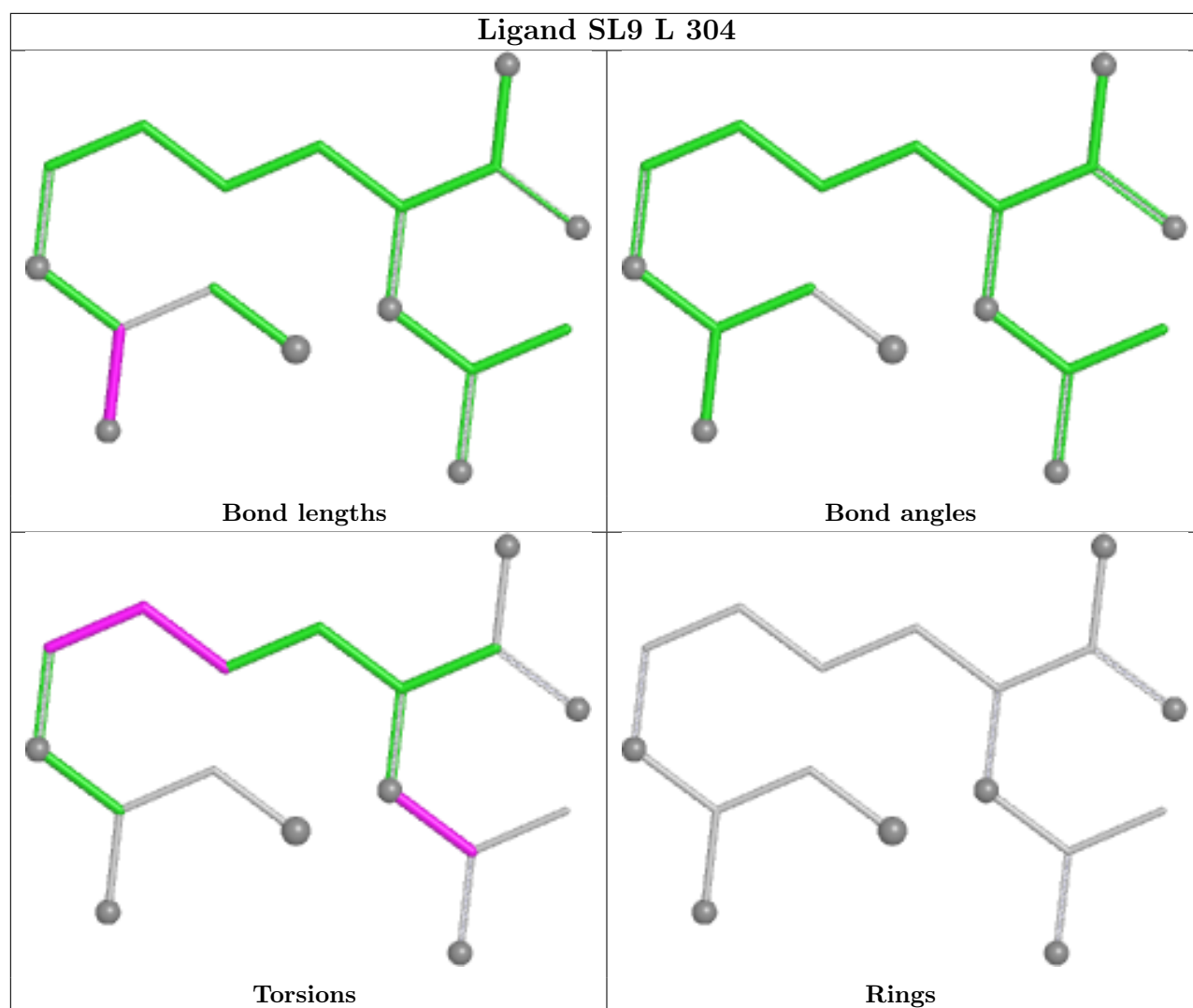
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	304	GOL	1	0
5	H	302	MES	1	0
6	A	304	GOL	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 SL9 B 303





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	215/227 (94%)	0.12	11 (5%) 33 36	12, 27, 47, 68	4 (1%)
1	H	218/227 (96%)	-0.05	7 (3%) 50 54	10, 26, 40, 70	4 (1%)
2	B	211/219 (96%)	0.18	4 (1%) 66 70	18, 31, 49, 59	1 (0%)
2	L	213/219 (97%)	-0.00	3 (1%) 73 76	11, 27, 40, 54	2 (0%)
All	All	857/892 (96%)	0.06	25 (2%) 53 57	10, 28, 46, 70	11 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLY	5.4
2	L	6	ASP	4.3
1	H	224	SER	3.9
2	B	159	LEU	3.2
1	A	20	SER	3.0
1	A	226	ASP	2.8
1	H	46	PRO	2.8
1	A	46	PRO	2.8
1	A	225	CYS	2.8
1	H	142	GLY	2.6
2	L	217	GLY	2.5
2	B	202	THR	2.4
1	A	223	LYS	2.4
2	B	6	ASP	2.4
1	H	137	SER	2.2
2	L	127	ASP	2.2
1	A	136	SER	2.2
1	H	24	SER	2.1
1	A	135	PRO	2.1
1	A	224	SER	2.1
1	H	69	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	122	SER	2.1
2	B	65	ASP	2.0
1	H	47	GLY	2.0
1	A	49	GLY	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](#)

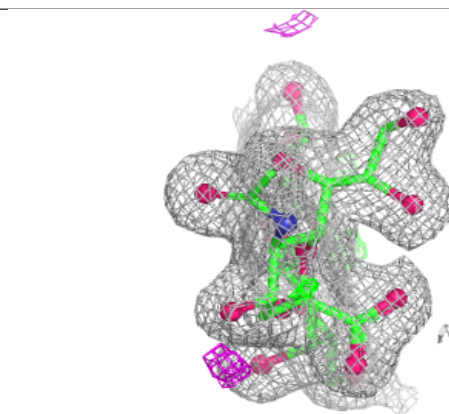
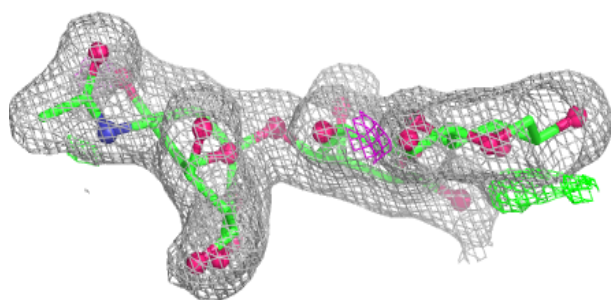
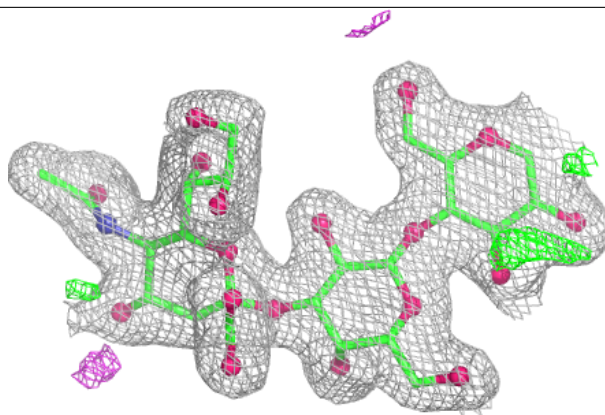
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	C	1	11/12	-	-	29,32,38,42	0
3	GAL	C	2	11/12	-	-	21,23,26,29	0
3	SIA	C	3	20/21	-	-	16,22,27,30	0
3	BGC	D	1	11/12	-	-	26,33,39,40	0
3	GAL	D	2	11/12	-	-	22,27,28,37	0
3	SIA	D	3	20/21	-	-	19,26,31,33	0

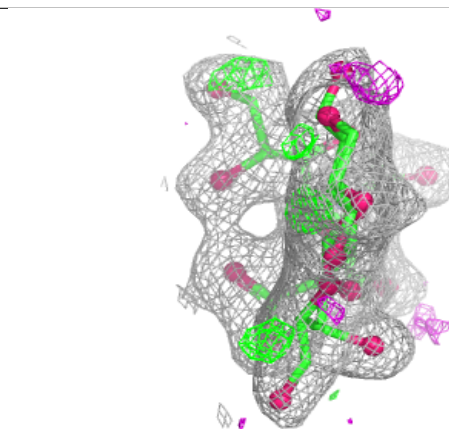
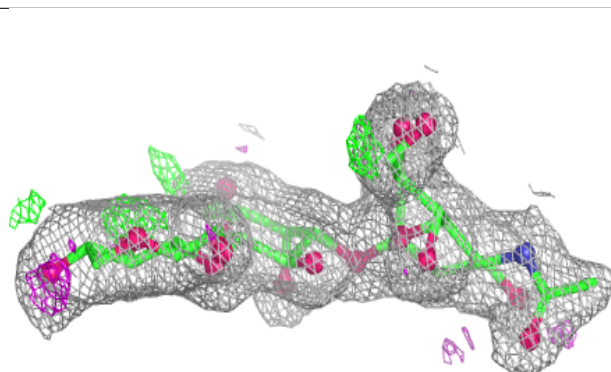
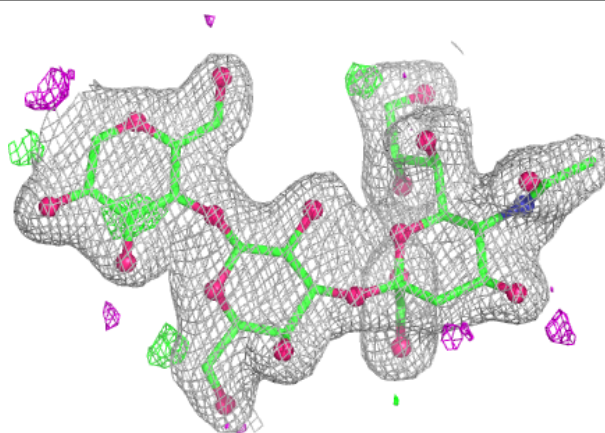
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain 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 D:**

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



6.4 Ligands

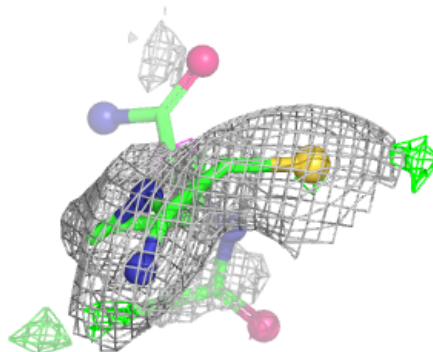
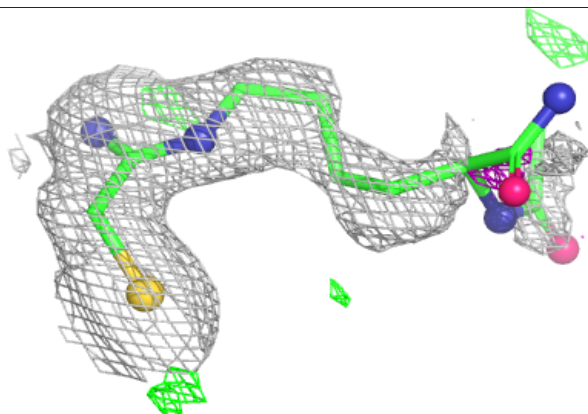
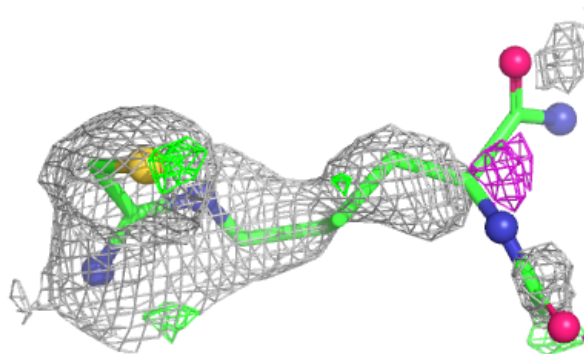
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SL9	L	304	17/17	0.81	0.18	34,55,80,82	0
7	SL9	B	303	17/17	0.85	0.16	33,48,75,78	0
6	GOL	A	304	6/6	0.88	0.11	29,37,40,42	0
6	GOL	H	303	6/6	0.89	0.10	36,40,41,41	0
5	MES	H	302	12/12	0.90	0.13	27,41,42,42	0
6	GOL	H	304	6/6	0.90	0.09	35,37,41,44	0
6	GOL	L	301	6/6	0.90	0.09	35,42,44,46	0
4	ZN	L	303	1/1	0.92	0.14	82,82,82,82	0
5	MES	A	302	12/12	0.93	0.11	24,36,45,45	0
4	ZN	B	302	1/1	0.93	0.09	82,82,82,82	0
6	GOL	A	303	6/6	0.93	0.10	30,33,40,40	0
4	ZN	H	301	1/1	0.94	0.07	57,57,57,57	0
4	ZN	A	301	1/1	0.98	0.09	56,56,56,56	0
4	ZN	B	301	1/1	0.98	0.04	37,37,37,37	0
4	ZN	L	302	1/1	0.99	0.03	42,42,42,42	0

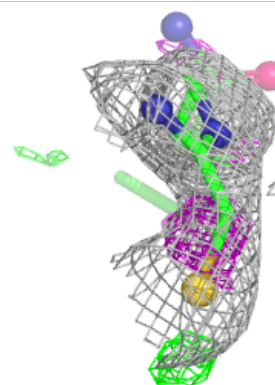
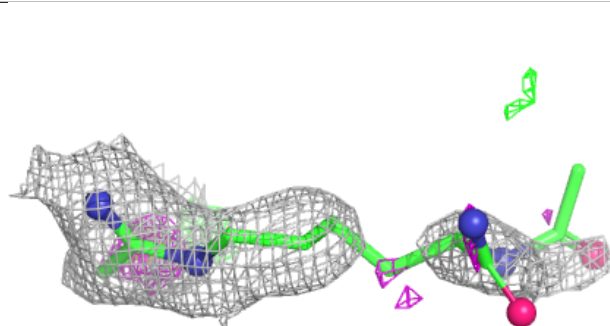
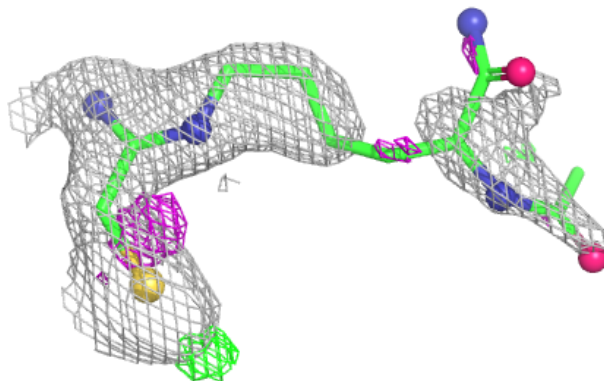
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SL9 L 304:

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

**Electron density around SL9 B 303:**

$2mF_o-DF_c$ (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.