Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 09:18 AM EDT

PDB ID	:	5WHU
Title	:	Crystal structure of 3'SL bound ArtB
Authors	:	Gao, X.; Galan, J.E.
Deposited on	:	2017-07-18
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

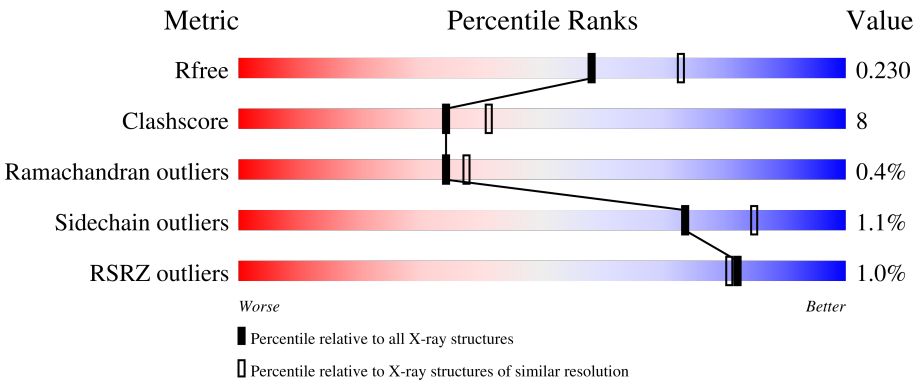
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	149	.% 66% 15% 19%
1	B	149	2% 66% 13% 20%
1	C	149	.% 70% 8% • 21%
1	D	149	74% 5% 21%
1	E	149	.% 70% 9% 20%

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Mol	Chain	Length	Quality of chain
1	F	149	62% 17% 21%
1	G	149	2% 66% 13% 21%
1	H	149	66% 16% 17%
1	I	149	70% 9% 21%
1	J	149	2% 68% 14% 17%
2	K	2	50% 50%
2	N	2	50% 50%
2	Q	2	50% 50%
3	L	3	33% 67%
3	M	3	33% 33% 33%
3	O	3	67% 33%
3	P	3	33% 67%
3	R	3	33% 67%
3	S	3	67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	B	202	-	-	X	-
5	PEG	F	203	-	-	X	-
5	PEG	H	208	-	-	X	-
5	PEG	H	209	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10677 atoms, of which 85 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 ArtB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	120	951	598	160	186	7	0	0	0
1	B	119	952	597	161	187	7	0	1	0
1	C	118	939	590	158	184	7	0	0	0
1	D	118	939	590	158	184	7	0	0	0
1	E	119	946	595	159	185	7	0	0	0
1	F	118	939	590	158	184	7	0	0	0
1	G	118	947	594	160	186	7	0	1	0
1	H	124	988	621	168	192	7	0	0	0
1	I	118	939	590	158	184	7	0	0	0
1	J	123	998	625	170	196	7	0	2	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	LEU	-	expression tag	UNP Q404H3
A	143	GLU	-	expression tag	UNP Q404H3
A	144	HIS	-	expression tag	UNP Q404H3
A	145	HIS	-	expression tag	UNP Q404H3
A	146	HIS	-	expression tag	UNP Q404H3
A	147	HIS	-	expression tag	UNP Q404H3
A	148	HIS	-	expression tag	UNP Q404H3
A	149	HIS	-	expression tag	UNP Q404H3
B	142	LEU	-	expression tag	UNP Q404H3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	143	GLU	-	expression tag	UNP Q404H3
B	144	HIS	-	expression tag	UNP Q404H3
B	145	HIS	-	expression tag	UNP Q404H3
B	146	HIS	-	expression tag	UNP Q404H3
B	147	HIS	-	expression tag	UNP Q404H3
B	148	HIS	-	expression tag	UNP Q404H3
B	149	HIS	-	expression tag	UNP Q404H3
C	142	LEU	-	expression tag	UNP Q404H3
C	143	GLU	-	expression tag	UNP Q404H3
C	144	HIS	-	expression tag	UNP Q404H3
C	145	HIS	-	expression tag	UNP Q404H3
C	146	HIS	-	expression tag	UNP Q404H3
C	147	HIS	-	expression tag	UNP Q404H3
C	148	HIS	-	expression tag	UNP Q404H3
C	149	HIS	-	expression tag	UNP Q404H3
D	142	LEU	-	expression tag	UNP Q404H3
D	143	GLU	-	expression tag	UNP Q404H3
D	144	HIS	-	expression tag	UNP Q404H3
D	145	HIS	-	expression tag	UNP Q404H3
D	146	HIS	-	expression tag	UNP Q404H3
D	147	HIS	-	expression tag	UNP Q404H3
D	148	HIS	-	expression tag	UNP Q404H3
D	149	HIS	-	expression tag	UNP Q404H3
E	142	LEU	-	expression tag	UNP Q404H3
E	143	GLU	-	expression tag	UNP Q404H3
E	144	HIS	-	expression tag	UNP Q404H3
E	145	HIS	-	expression tag	UNP Q404H3
E	146	HIS	-	expression tag	UNP Q404H3
E	147	HIS	-	expression tag	UNP Q404H3
E	148	HIS	-	expression tag	UNP Q404H3
E	149	HIS	-	expression tag	UNP Q404H3
F	142	LEU	-	expression tag	UNP Q404H3
F	143	GLU	-	expression tag	UNP Q404H3
F	144	HIS	-	expression tag	UNP Q404H3
F	145	HIS	-	expression tag	UNP Q404H3
F	146	HIS	-	expression tag	UNP Q404H3
F	147	HIS	-	expression tag	UNP Q404H3
F	148	HIS	-	expression tag	UNP Q404H3
F	149	HIS	-	expression tag	UNP Q404H3
G	142	LEU	-	expression tag	UNP Q404H3
G	143	GLU	-	expression tag	UNP Q404H3
G	144	HIS	-	expression tag	UNP Q404H3

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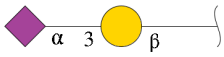
Chain	Residue	Modelled	Actual	Comment	Reference
G	145	HIS	-	expression tag	UNP Q404H3
G	146	HIS	-	expression tag	UNP Q404H3
G	147	HIS	-	expression tag	UNP Q404H3
G	148	HIS	-	expression tag	UNP Q404H3
G	149	HIS	-	expression tag	UNP Q404H3
H	142	LEU	-	expression tag	UNP Q404H3
H	143	GLU	-	expression tag	UNP Q404H3
H	144	HIS	-	expression tag	UNP Q404H3
H	145	HIS	-	expression tag	UNP Q404H3
H	146	HIS	-	expression tag	UNP Q404H3
H	147	HIS	-	expression tag	UNP Q404H3
H	148	HIS	-	expression tag	UNP Q404H3
H	149	HIS	-	expression tag	UNP Q404H3
I	142	LEU	-	expression tag	UNP Q404H3
I	143	GLU	-	expression tag	UNP Q404H3
I	144	HIS	-	expression tag	UNP Q404H3
I	145	HIS	-	expression tag	UNP Q404H3
I	146	HIS	-	expression tag	UNP Q404H3
I	147	HIS	-	expression tag	UNP Q404H3
I	148	HIS	-	expression tag	UNP Q404H3
I	149	HIS	-	expression tag	UNP Q404H3
J	142	LEU	-	expression tag	UNP Q404H3
J	143	GLU	-	expression tag	UNP Q404H3
J	144	HIS	-	expression tag	UNP Q404H3
J	145	HIS	-	expression tag	UNP Q404H3
J	146	HIS	-	expression tag	UNP Q404H3
J	147	HIS	-	expression tag	UNP Q404H3
J	148	HIS	-	expression tag	UNP Q404H3
J	149	HIS	-	expression tag	UNP Q404H3

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	K	2	32	17	1	14	0	0	0
			Total	C	N	O			
2	N	2	32	17	1	14	0	0	0

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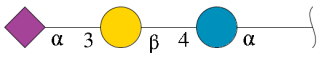
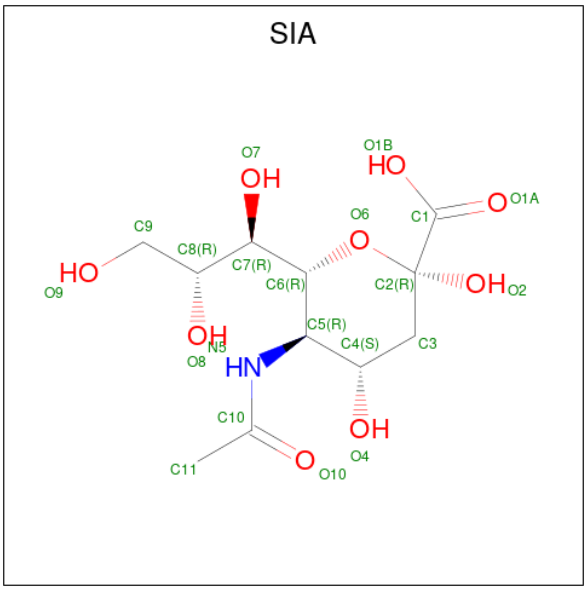
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Q	2	Total C N O 32 17 1 14	0	0	0

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



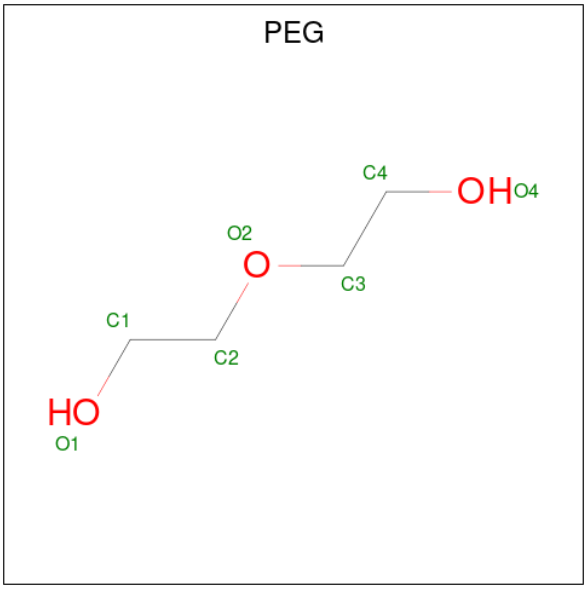
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	L	3	Total C H N O 55 23 12 1 19	0	0	0
3	M	3	Total C N O 43 23 1 19	0	0	0
3	O	3	Total C N O 43 23 1 19	0	0	0
3	P	3	Total C N O 43 23 1 19	0	0	0
3	R	3	Total C N O 43 23 1 19	0	0	0
3	S	3	Total C N O 43 23 1 19	0	0	0

- Molecule 4 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 21 11 1 9	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 17 4 10 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	E	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	F	1	Total C H O 17 4 10 3	0	0
5	G	1	Total C O 7 4 3	0	0
5	G	1	Total C H O 17 4 10 3	0	0
5	H	1	Total C H O 17 4 10 3	0	0
5	H	1	Total C O 7 4 3	0	0
5	H	1	Total C H O 17 4 10 3	0	0

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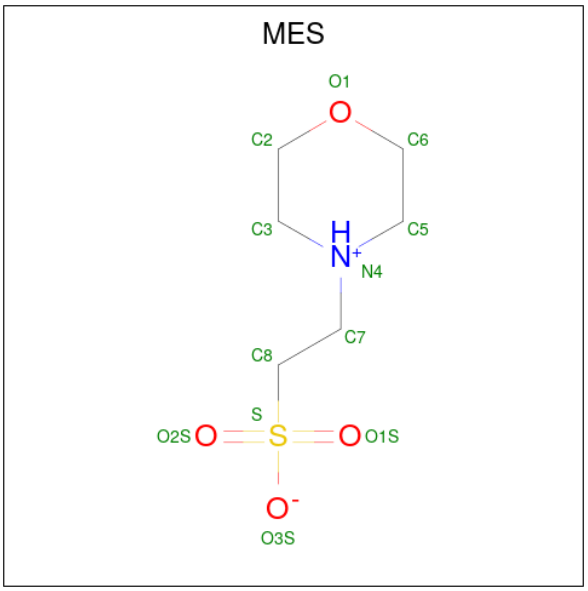
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	J	1	17	4	10	3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

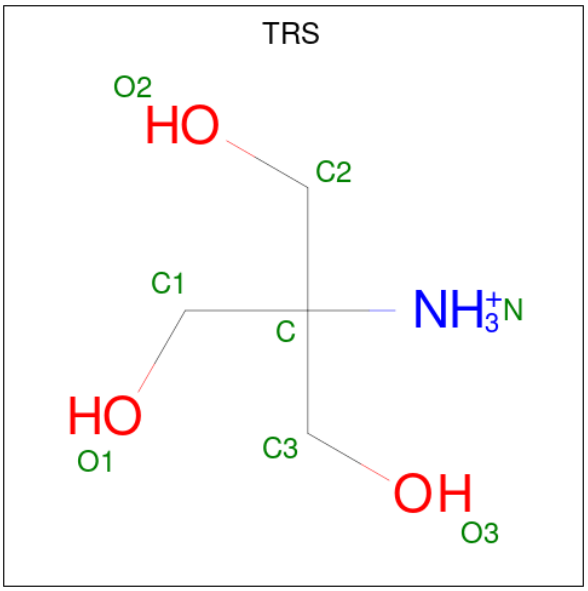
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	A	4	4	4	0	0
6	B	3	3	3	0	0
6	C	1	1	1	0	0
6	D	1	1	1	0	0
6	E	1	1	1	0	0
6	F	3	3	3	0	0
6	G	2	2	2	0	0
6	H	2	2	2	0	0
6	I	4	4	4	0	0
6	J	2	2	2	0	0

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C H N O S 25 6 13 1 4 1	0	0
7	C	1	Total C N O S 12 6 1 4 1	0	0
7	D	1	Total C N O S 12 6 1 4 1	0	0
7	G	1	Total C N O S 12 6 1 4 1	0	0
7	H	1	Total C N O S 12 6 1 4 1	0	0
7	J	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C N O 8 4 1 3	0	0
8	H	1	Total C N O 8 4 1 3	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total Ca 1 1	0	0
9	F	1	Total Ca 1 1	0	0
9	G	1	Total Ca 1 1	0	0
9	H	2	Total Ca 2 2	0	0
9	I	1	Total Ca 1 1	0	0
9	J	1	Total Ca 1 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	47	Total O 47 47	0	0

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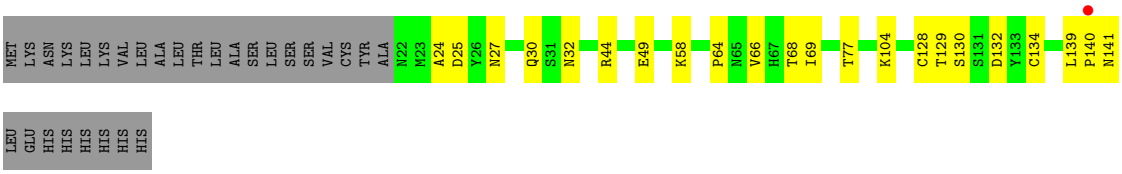
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	B	43	43	43	0	0
			Total	O		
10	C	46	46	46	0	0
			Total	O		
10	D	48	48	48	0	0
			Total	O		
10	E	43	43	43	0	0
			Total	O		
10	F	50	50	50	0	0
			Total	O		
10	G	46	46	46	0	0
			Total	O		
10	H	54	54	54	0	0
			Total	O		
10	I	49	49	49	0	0
			Total	O		
10	J	51	51	51	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.

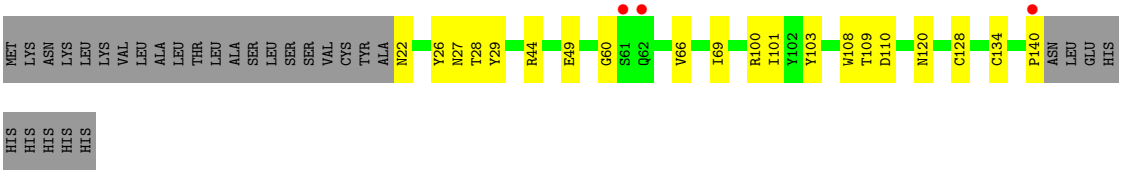
• Molecule 1: ArtB protein

Chain A:



• Molecule 1: ArtB protein

Chain B:

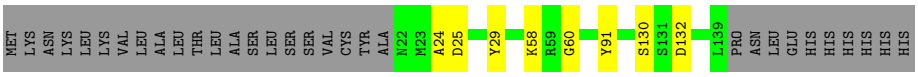


• Molecule 1: ArtB protein

Chain C:

• Molecule 1: ArtB protein

Chain D:



• Molecule 1: ArtB protein

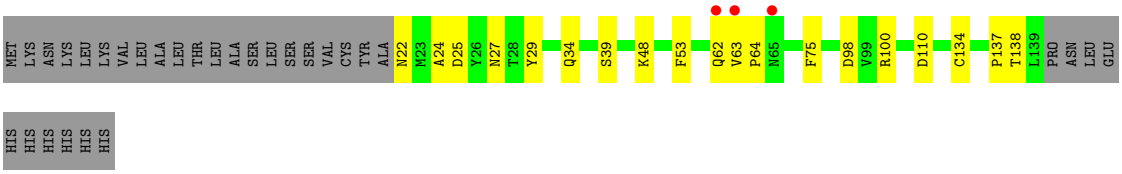
Chain E:

• Molecule 1: ArtB protein

Chain F:

• Molecule 1: ArtB protein

Chain G:



• Molecule 1: ArtB protein

Chain H:

• Molecule 1: ArtB protein

Chain I:

• Molecule 1: ArtB protein

Chain J:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain K:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain N:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

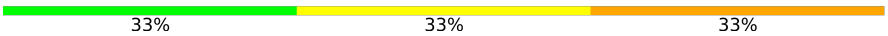
Chain Q:

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

Chain L:

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

Chain M:



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

Chain O:

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

Chain P:

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

Chain R:

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

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	137.91Å 94.21Å 123.96Å 90.00° 102.60° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 69.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.20) 97.7 (69.11-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.174 , 0.230 0.175 , 0.230	Depositor DCC
R_{free} test set	3851 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.981	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10677	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, TRS, GLC, GAL, CL, PEG, MES, SIA

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	0.40	0/973	0.57	0/1320
1	B	0.36	0/973	0.54	1/1319 (0.1%)
1	C	0.36	0/960	0.55	0/1301
1	D	0.38	0/960	0.56	0/1301
1	E	0.38	0/968	0.54	0/1313
1	F	0.37	0/960	0.53	0/1301
1	G	0.38	0/968	0.55	0/1312
1	H	0.37	0/1012	0.56	0/1373
1	I	0.40	0/960	0.56	0/1301
1	J	0.39	0/1021	0.60	0/1385
All	All	0.38	0/9755	0.56	1/13226 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	140	PRO	N-CA-CB	5.76	110.21	103.30

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	951	0	887	14	0
1	B	952	0	884	26	0
1	C	939	0	878	8	0
1	D	939	0	878	5	0
1	E	946	0	885	9	0
1	F	939	0	878	25	0
1	G	947	0	883	16	0
1	H	988	0	918	20	0
1	I	939	0	878	11	0
1	J	998	0	927	19	0
2	K	32	0	28	2	0
2	N	32	0	28	0	0
2	Q	32	0	28	3	0
3	L	43	12	37	0	0
3	M	43	0	37	1	0
3	O	43	0	37	0	0
3	P	43	0	37	2	0
3	R	43	0	37	0	0
3	S	43	0	37	0	0
4	A	21	0	18	0	0
5	A	7	10	10	0	0
5	B	7	0	10	9	0
5	E	7	0	10	2	0
5	F	21	10	30	13	0
5	G	14	10	20	2	0
5	H	21	20	30	11	0
5	J	7	10	10	1	0
6	A	4	0	0	1	0
6	B	3	0	0	1	0
6	C	1	0	0	1	0
6	D	1	0	0	0	0
6	E	1	0	0	1	0
6	F	3	0	0	0	0
6	G	2	0	0	1	0
6	H	2	0	0	0	0
6	I	4	0	0	0	0
6	J	2	0	0	0	0
7	B	12	13	12	1	0
7	C	12	0	12	0	0
7	D	12	0	12	2	0
7	G	12	0	12	2	0
7	H	12	0	12	0	0
7	J	12	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	8	0	12	2	0
8	H	8	0	12	1	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
9	H	2	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
10	A	47	0	0	1	0
10	B	43	0	0	2	0
10	C	46	0	0	1	0
10	D	48	0	0	2	0
10	E	43	0	0	2	0
10	F	50	0	0	1	0
10	G	46	0	0	0	0
10	H	54	0	0	1	0
10	I	49	0	0	2	0
10	J	51	0	0	0	0
All	All	10592	85	9436	165	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 8.

All (165) 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:F:82:PHE:H	5:F:203:PEG:H42	1.18	1.03
1:H:141:ASN:HA	5:H:208:PEG:H32	1.45	0.97
1:G:22:ASN:HA	5:H:209:PEG:H42	1.47	0.94
1:F:83:ASP:HB2	5:F:203:PEG:H21	1.50	0.92
1:G:24:ALA:O	1:G:25:ASP:HB2	1.83	0.79
1:B:27[B]:ASN:ND2	10:B:302:HOH:O	2.16	0.78
1:F:43:TYR:CE2	1:F:45:SER:HB2	2.18	0.77
1:F:82:PHE:N	5:F:203:PEG:H42	1.99	0.76
1:B:22:ASN:ND2	1:B:27[B]:ASN:HD21	1.84	0.75
6:C:205:CL:CL	10:C:328:HOH:O	2.41	0.75
1:A:24:ALA:O	1:A:25:ASP:HB2	1.87	0.75
1:F:83:ASP:CB	5:F:203:PEG:H21	2.17	0.74
1:B:109:THR:H	5:B:202:PEG:H32	1.53	0.74
1:G:22:ASN:HA	5:H:209:PEG:C4	2.18	0.74
1:H:141:ASN:HD22	5:H:208:PEG:H31	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASN:HB2	6:A:206:CL:CL	2.26	0.73
1:B:110:ASP:CB	5:B:202:PEG:H12	2.21	0.70
1:C:24:ALA:O	1:C:25:ASP:HB2	1.90	0.70
1:G:137:PRO:HA	5:H:209:PEG:H12	1.74	0.69
1:B:108:TRP:HA	5:B:202:PEG:H31	1.74	0.69
1:J:143:GLU:O	1:J:144:HIS:HB3	1.91	0.69
5:B:202:PEG:O1	10:B:301:HOH:O	2.09	0.68
1:F:63:VAL:HG21	5:F:202:PEG:H32	1.74	0.68
8:H:212:TRS:O1	10:H:301:HOH:O	2.10	0.67
1:A:30:GLN:NE2	1:A:66:VAL:O	2.27	0.67
1:H:141:ASN:HD22	5:H:208:PEG:C3	2.07	0.66
1:A:27:ASN:HB3	1:A:139:LEU:HD21	1.78	0.66
1:B:110:ASP:H	5:B:202:PEG:H12	1.61	0.66
1:B:128:CYS:O	6:B:204:CL:CL	2.50	0.66
1:J:66:VAL:HG13	1:J:120:ASN:ND2	2.11	0.66
1:I:30:GLN:NE2	1:I:66:VAL:HB	2.12	0.64
1:I:48:LYS:HE3	1:I:75:PHE:CE1	2.33	0.64
1:A:77:THR:HG21	1:A:104:LYS:HE2	1.80	0.64
1:F:116:ALA:HB1	1:H:137:PRO:HD3	1.82	0.61
1:H:34:GLN:OE1	1:H:58:LYS:NZ	2.27	0.61
2:Q:1:GAL:H4	2:Q:2:SIA:C1	2.30	0.61
1:G:29:TYR:O	7:G:201:MES:H31	2.01	0.61
1:J:66:VAL:HG21	1:J:103:TYR:CE2	2.36	0.60
1:I:30:GLN:HE22	1:I:66:VAL:HB	1.67	0.60
1:J:133:TYR:C	1:J:133:TYR:CD1	2.75	0.60
1:A:32:ASN:ND2	10:A:301:HOH:O	2.11	0.59
1:J:66:VAL:HG21	1:J:103:TYR:CZ	2.38	0.59
5:E:207:PEG:H32	10:E:331:HOH:O	2.02	0.59
1:G:138:THR:H	5:H:209:PEG:H12	1.68	0.59
2:K:2:SIA:O10	2:K:2:SIA:O7	2.20	0.59
1:A:77:THR:HG21	1:A:104:LYS:CE	2.33	0.58
1:E:24:ALA:O	1:E:25:ASP:HB2	2.03	0.58
1:D:29:TYR:O	7:D:201:MES:H52	2.02	0.58
1:B:69:ILE:HD13	1:B:103:TYR:HB3	1.85	0.58
1:F:24:ALA:O	1:F:25:ASP:HB2	2.05	0.57
1:B:110:ASP:HB2	5:B:202:PEG:H12	1.87	0.57
1:E:97:GLU:HA	5:E:207:PEG:H32	1.87	0.56
1:H:66:VAL:HG12	1:H:69:ILE:HD11	1.88	0.56
1:B:28:THR:HG22	1:B:103:TYR:CZ	2.41	0.56
1:A:130:SER:C	1:A:132:ASP:H	2.08	0.56
5:F:203:PEG:H32	10:F:316:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:ASN:HD22	1:G:27[A]:ASN:ND2	2.04	0.55
1:E:44:ARG:HD2	1:E:49:GLU:OE2	2.06	0.55
1:C:69:ILE:N	1:C:69:ILE:HD12	2.21	0.55
1:G:110:ASP:H	5:G:203:PEG:H12	1.72	0.55
1:I:22:ASN:N	1:J:112:ASN:OD1	2.41	0.54
1:B:29:TYR:H	7:B:201:MES:H22	1.73	0.54
7:D:201:MES:O3S	7:D:201:MES:H51	2.07	0.54
1:F:43:TYR:HE2	1:F:45:SER:HB2	1.69	0.54
1:B:22:ASN:HD22	1:B:27[B]:ASN:HD21	1.56	0.54
1:H:141:ASN:ND2	5:H:208:PEG:H31	2.23	0.54
1:I:30:GLN:OE1	1:I:64:PRO:HB2	2.08	0.53
1:H:128:CYS:HA	1:H:134:CYS:HA	1.91	0.53
1:E:77:THR:HG21	1:E:104:LYS:HE3	1.90	0.53
1:J:143:GLU:O	1:J:144:HIS:CB	2.57	0.53
1:A:58:LYS:HA	1:A:64:PRO:HD3	1.92	0.52
1:F:83:ASP:H	5:F:203:PEG:C2	2.22	0.52
1:I:25:ASP:OD1	1:I:25:ASP:N	2.38	0.52
1:A:128:CYS:HA	1:A:134:CYS:HA	1.92	0.52
1:H:116:ALA:HB2	5:H:209:PEG:H31	1.91	0.52
1:B:100:ARG:CZ	1:B:134:CYS:HB2	2.40	0.52
1:J:133:TYR:CD1	1:J:133:TYR:O	2.62	0.52
2:K:1:GAL:H4	2:K:2:SIA:C1	2.40	0.52
1:J:77:THR:HG21	1:J:104:LYS:HE2	1.92	0.52
1:B:22:ASN:ND2	1:B:27[B]:ASN:ND2	2.54	0.51
1:D:24:ALA:O	1:D:25:ASP:HB2	2.10	0.51
1:F:81:GLY:CA	5:F:203:PEG:H12	2.41	0.51
1:B:26:TYR:HH	1:C:52:PHE:HE2	1.58	0.51
1:G:22:ASN:HD22	1:G:27[A]:ASN:HD21	1.57	0.50
1:G:27[B]:ASN:ND2	1:G:27[B]:ASN:H	2.10	0.50
1:I:48:LYS:HE3	1:I:75:PHE:CZ	2.47	0.50
1:B:110:ASP:HB3	5:B:202:PEG:H12	1.93	0.49
1:E:48:LYS:HD3	1:E:75:PHE:CE1	2.47	0.49
1:C:39:SER:O	1:C:53:PHE:HA	2.12	0.49
1:F:82:PHE:H	5:F:203:PEG:C4	2.08	0.49
1:H:141:ASN:HA	5:H:208:PEG:C3	2.31	0.49
1:F:43:TYR:CD2	1:H:23:MET:CE	2.95	0.49
1:H:51:GLN:HG3	1:H:73:ASP:OD2	2.13	0.49
1:F:128:CYS:HA	1:F:134:CYS:HA	1.95	0.48
1:C:100:ARG:CZ	1:C:134:CYS:HB2	2.44	0.48
1:F:105:GLU:HG2	1:F:120:ASN:OD1	2.13	0.48
1:D:58:LYS:HD2	1:D:60:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:LYS:HD3	1:E:75:PHE:CZ	2.48	0.48
1:F:81:GLY:C	5:F:203:PEG:H12	2.33	0.48
1:F:83:ASP:H	5:F:203:PEG:H21	1.77	0.48
1:G:39:SER:O	1:G:53:PHE:HB2	2.13	0.48
1:J:144:HIS:ND1	5:J:206:PEG:H21	2.28	0.48
1:I:100:ARG:CZ	1:I:134:CYS:HB2	2.43	0.48
1:A:44:ARG:HD2	1:A:49:GLU:OE2	2.12	0.48
1:E:66:VAL:CG1	1:E:120:ASN:ND2	2.77	0.48
1:B:110:ASP:H	5:B:202:PEG:C1	2.26	0.48
1:J:69:ILE:HG22	1:J:122:LEU:HB2	1.96	0.47
1:B:22:ASN:HD22	1:B:27[B]:ASN:ND2	2.11	0.47
1:F:63:VAL:HG21	5:F:202:PEG:C3	2.44	0.47
1:I:48:LYS:CE	1:I:75:PHE:CE1	2.98	0.47
6:E:208:CL:CL	10:E:336:HOH:O	2.58	0.47
1:F:80:GLN:HA	5:F:203:PEG:H41	1.97	0.47
1:J:28:THR:HG22	1:J:103:TYR:CE2	2.50	0.47
1:B:66:VAL:HG13	1:B:120:ASN:ND2	2.29	0.46
1:F:77:THR:HG21	1:F:104:LYS:NZ	2.30	0.46
1:G:34:GLN:NE2	1:G:98:ASP:OD1	2.45	0.46
1:J:129:THR:OG1	1:J:133:TYR:CD1	2.68	0.46
8:D:206:TRS:O2	10:D:301:HOH:O	2.21	0.46
1:J:24:ALA:O	1:J:25:ASP:HB2	2.15	0.46
8:D:206:TRS:C2	10:D:301:HOH:O	2.63	0.46
1:C:34:GLN:NE2	1:C:98:ASP:OD1	2.49	0.46
1:H:39:SER:O	1:H:53:PHE:HA	2.16	0.46
1:J:69:ILE:HD12	1:J:69:ILE:N	2.31	0.46
1:G:48:LYS:HD2	1:G:75:PHE:CZ	2.51	0.45
1:G:100:ARG:CZ	1:G:134:CYS:HB2	2.47	0.45
1:H:43:TYR:CE2	1:H:45:SER:HB2	2.51	0.45
1:J:28:THR:HG22	1:J:103:TYR:CZ	2.51	0.45
1:J:30:GLN:HA	7:J:201:MES:O2S	2.17	0.44
1:B:69:ILE:HD12	1:B:101:ILE:HG21	1.99	0.44
1:B:100:ARG:NH2	1:B:134:CYS:HB2	2.33	0.44
1:A:130:SER:C	1:A:132:ASP:N	2.71	0.44
1:I:25:ASP:HB3	1:I:104:LYS:NZ	2.33	0.44
1:F:129:THR:HG23	1:I:37:ASN:HD21	1.83	0.44
5:G:203:PEG:H32	6:G:206:CL:CL	2.55	0.43
1:G:24:ALA:O	1:G:25:ASP:CB	2.60	0.43
1:E:100:ARG:NH1	1:E:138:THR:HG22	2.34	0.43
1:A:140:PRO:HA	1:A:141:ASN:HA	1.62	0.43
1:A:68:THR:C	1:A:69:ILE:HD13	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:VAL:HG21	1:B:103:TYR:CZ	2.53	0.43
7:J:201:MES:H82	7:J:201:MES:H51	1.28	0.43
1:J:68:THR:C	1:J:69:ILE:HD12	2.39	0.42
1:B:66:VAL:CG1	1:B:120:ASN:ND2	2.83	0.42
1:B:109:THR:H	5:B:202:PEG:C3	2.27	0.42
1:C:66:VAL:HG13	1:C:120:ASN:ND2	2.34	0.42
1:C:110:ASP:OD1	1:C:110:ASP:C	2.58	0.42
1:B:44:ARG:NE	1:B:49:GLU:OE2	2.51	0.42
10:I:302:HOH:O	2:Q:2:SIA:H113	2.19	0.42
1:E:96:GLY:HA3	1:F:59:ARG:CZ	2.50	0.41
1:F:68:THR:O	1:F:69:ILE:HD13	2.20	0.41
7:G:201:MES:H81	7:G:201:MES:H51	1.78	0.41
1:F:28:THR:HB	1:F:103:TYR:O	2.20	0.41
1:H:66:VAL:HG12	1:H:69:ILE:CD1	2.50	0.41
3:P:2:GAL:H3	3:P:3:SIA:O1A	2.20	0.41
1:H:141:ASN:CA	5:H:208:PEG:H32	2.32	0.41
1:H:27:ASN:HB2	1:H:139:LEU:HD13	2.01	0.41
1:D:130:SER:C	1:D:132:ASP:H	2.24	0.41
1:H:32:ASN:ND2	1:H:131:SER:HA	2.35	0.41
1:J:142:LEU:HD23	1:J:142:LEU:HA	1.82	0.41
10:I:302:HOH:O	2:Q:2:SIA:C10	2.69	0.41
1:G:62:GLN:HG2	1:G:63:VAL:N	2.37	0.40
1:B:69:ILE:HD13	1:B:103:TYR:CB	2.51	0.40
1:D:91:TYR:OH	1:F:62:GLN:OE1	2.32	0.40
1:H:72:ILE:HD12	3:P:3:SIA:H112	2.04	0.40
1:H:139:LEU:N	1:H:140:PRO:CD	2.85	0.40
3:M:2:GAL:H4	3:M:3:SIA:C1	2.51	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	118/149 (79%)	115 (98%)	3 (2%)	0	100	100
1	B	118/149 (79%)	113 (96%)	4 (3%)	1 (1%)	19	19
1	C	116/149 (78%)	112 (97%)	4 (3%)	0	100	100
1	D	116/149 (78%)	113 (97%)	3 (3%)	0	100	100
1	E	117/149 (78%)	114 (97%)	3 (3%)	0	100	100
1	F	116/149 (78%)	113 (97%)	2 (2%)	1 (1%)	17	16
1	G	117/149 (78%)	113 (97%)	3 (3%)	1 (1%)	17	16
1	H	122/149 (82%)	120 (98%)	2 (2%)	0	100	100
1	I	116/149 (78%)	114 (98%)	2 (2%)	0	100	100
1	J	123/149 (83%)	118 (96%)	3 (2%)	2 (2%)	9	7
All	All	1179/1490 (79%)	1145 (97%)	29 (2%)	5 (0%)	34	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	141	ASN
1	G	64	PRO
1	J	65	ASN
1	F	110	ASP
1	B	60	GLY

5.3.2 Protein sidechains (i)

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	103/130 (79%)	102 (99%)	1 (1%)	76	86
1	B	103/130 (79%)	103 (100%)	0	100	100
1	C	102/130 (78%)	101 (99%)	1 (1%)	76	86
1	D	102/130 (78%)	102 (100%)	0	100	100
1	E	103/130 (79%)	103 (100%)	0	100	100
1	F	102/130 (78%)	101 (99%)	1 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	103/130 (79%)	103 (100%)	0	100	100
1	H	107/130 (82%)	103 (96%)	4 (4%)	34	43
1	I	102/130 (78%)	99 (97%)	3 (3%)	42	54
1	J	109/130 (84%)	108 (99%)	1 (1%)	78	88
All	All	1036/1300 (80%)	1025 (99%)	11 (1%)	73	85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	C	98	ASP
1	F	131	SER
1	H	25	ASP
1	H	47	ASP
1	H	131	SER
1	H	145	HIS
1	I	47	ASP
1	I	98	ASP
1	I	129	THR
1	J	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	22	ASN
1	E	22	ASN
1	E	120	ASN
1	F	22	ASN
1	G	22	ASN
1	H	141	ASN
1	J	144	HIS

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)

24 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	GAL	K	1	2	12,12,12	0.56	0	17,17,17	0.66	0
2	SIA	K	2	2	20,20,21	2.18	6 (30%)	24,28,31	1.39	6 (25%)
3	GLC	L	1	3	12,12,12	0.58	0	17,17,17	0.68	0
3	GAL	L	2	3	11,11,12	0.32	0	15,15,17	0.99	1 (6%)
3	SIA	L	3	3	20,20,21	1.86	7 (35%)	24,28,31	1.31	4 (16%)
3	GLC	M	1	3	12,12,12	0.48	0	17,17,17	0.78	0
3	GAL	M	2	3	11,11,12	0.38	0	15,15,17	1.07	0
3	SIA	M	3	3	20,20,21	1.80	6 (30%)	24,28,31	1.41	4 (16%)
2	GAL	N	1	2	12,12,12	0.55	0	17,17,17	0.79	0
2	SIA	N	2	2	20,20,21	2.14	8 (40%)	24,28,31	1.08	1 (4%)
3	GLC	O	1	3	12,12,12	0.51	0	17,17,17	0.84	0
3	GAL	O	2	3	11,11,12	0.52	0	15,15,17	0.89	0
3	SIA	O	3	3	20,20,21	1.92	7 (35%)	24,28,31	1.19	2 (8%)
3	GLC	P	1	3	12,12,12	0.52	0	17,17,17	0.60	0
3	GAL	P	2	3	11,11,12	0.32	0	15,15,17	1.01	1 (6%)
3	SIA	P	3	3	20,20,21	1.80	7 (35%)	24,28,31	1.22	2 (8%)
2	GAL	Q	1	2	12,12,12	0.59	0	17,17,17	0.78	0
2	SIA	Q	2	2	20,20,21	2.16	8 (40%)	24,28,31	1.39	4 (16%)
3	GLC	R	1	3	12,12,12	0.56	0	17,17,17	1.17	1 (5%)
3	GAL	R	2	3	11,11,12	0.43	0	15,15,17	0.93	0
3	SIA	R	3	3	20,20,21	1.91	8 (40%)	24,28,31	1.36	4 (16%)
3	GLC	S	1	3	12,12,12	0.52	0	17,17,17	0.65	0
3	GAL	S	2	3	11,11,12	0.24	0	15,15,17	0.85	0
3	SIA	S	3	3	20,20,21	1.71	6 (30%)	24,28,31	1.17	3 (12%)

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	GAL	K	1	2	-	0/2/22/22	0/1/1/1
2	SIA	K	2	2	-	5/18/34/38	0/1/1/1
3	GLC	L	1	3	-	1/2/22/22	0/1/1/1
3	GAL	L	2	3	-	1/2/19/22	0/1/1/1
3	SIA	L	3	3	-	0/18/34/38	0/1/1/1
3	GLC	M	1	3	-	2/2/22/22	0/1/1/1
3	GAL	M	2	3	-	0/2/19/22	0/1/1/1
3	SIA	M	3	3	-	1/18/34/38	0/1/1/1
2	GAL	N	1	2	-	0/2/22/22	0/1/1/1
2	SIA	N	2	2	-	0/18/34/38	0/1/1/1
3	GLC	O	1	3	-	2/2/22/22	0/1/1/1
3	GAL	O	2	3	-	2/2/19/22	0/1/1/1
3	SIA	O	3	3	-	2/18/34/38	0/1/1/1
3	GLC	P	1	3	-	0/2/22/22	0/1/1/1
3	GAL	P	2	3	-	0/2/19/22	0/1/1/1
3	SIA	P	3	3	-	1/18/34/38	0/1/1/1
2	GAL	Q	1	2	-	0/2/22/22	0/1/1/1
2	SIA	Q	2	2	-	2/18/34/38	0/1/1/1
3	GLC	R	1	3	-	1/2/22/22	0/1/1/1
3	GAL	R	2	3	-	0/2/19/22	0/1/1/1
3	SIA	R	3	3	-	2/18/34/38	0/1/1/1
3	GLC	S	1	3	-	1/2/22/22	0/1/1/1
3	GAL	S	2	3	-	0/2/19/22	0/1/1/1
3	SIA	S	3	3	-	1/18/34/38	0/1/1/1

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	SIA	C4-C5	-6.25	1.47	1.53
2	Q	2	SIA	C4-C5	-6.20	1.47	1.53
2	N	2	SIA	C4-C5	-6.02	1.47	1.53
3	O	3	SIA	C4-C5	-4.43	1.49	1.53
3	R	3	SIA	C4-C5	-4.32	1.49	1.53
3	L	3	SIA	C4-C5	-4.02	1.49	1.53
3	M	3	SIA	C4-C5	-3.60	1.50	1.53
3	P	3	SIA	C4-C5	-3.50	1.50	1.53
3	S	3	SIA	C4-C5	-3.46	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	3	SIA	C10-N5	3.28	1.45	1.34
2	N	2	SIA	C10-N5	3.23	1.45	1.34
3	P	3	SIA	C10-N5	3.11	1.45	1.34
3	L	3	SIA	C10-N5	3.07	1.44	1.34
2	K	2	SIA	C10-N5	3.05	1.44	1.34
3	S	3	SIA	C10-N5	3.02	1.44	1.34
3	M	3	SIA	C10-N5	3.00	1.44	1.34
3	R	3	SIA	C10-N5	2.96	1.44	1.34
3	M	3	SIA	C6-C5	-2.89	1.48	1.53
2	Q	2	SIA	C10-N5	2.84	1.44	1.34
2	Q	2	SIA	O6-C2	-2.81	1.40	1.43
2	K	2	SIA	C6-C5	-2.74	1.48	1.53
2	K	2	SIA	O6-C2	-2.62	1.40	1.43
3	L	3	SIA	O8-C8	-2.61	1.37	1.43
3	R	3	SIA	O6-C6	-2.61	1.39	1.44
3	L	3	SIA	C6-C5	-2.54	1.48	1.53
3	S	3	SIA	O6-C6	-2.54	1.40	1.44
2	N	2	SIA	O8-C8	-2.52	1.38	1.43
2	N	2	SIA	C6-C5	-2.50	1.48	1.53
3	O	3	SIA	O8-C8	-2.49	1.38	1.43
3	M	3	SIA	O8-C8	-2.43	1.38	1.43
3	P	3	SIA	O6-C2	-2.43	1.40	1.43
3	O	3	SIA	C6-C5	-2.40	1.49	1.53
2	K	2	SIA	C8-C7	-2.39	1.49	1.53
2	Q	2	SIA	O6-C6	-2.39	1.40	1.44
2	K	2	SIA	O8-C8	-2.39	1.38	1.43
2	Q	2	SIA	C6-C5	-2.38	1.49	1.53
3	P	3	SIA	C6-C5	-2.35	1.49	1.53
3	M	3	SIA	O6-C6	-2.33	1.40	1.44
3	O	3	SIA	O6-C6	-2.33	1.40	1.44
3	P	3	SIA	O6-C6	-2.32	1.40	1.44
3	L	3	SIA	C8-C7	-2.30	1.49	1.53
2	N	2	SIA	O6-C2	-2.29	1.40	1.43
3	R	3	SIA	O8-C8	-2.26	1.38	1.43
3	O	3	SIA	C8-C7	-2.25	1.49	1.53
3	S	3	SIA	O6-C2	-2.25	1.40	1.43
2	N	2	SIA	O6-C6	-2.25	1.40	1.44
2	N	2	SIA	C8-C7	-2.25	1.49	1.53
2	Q	2	SIA	O8-C8	-2.25	1.38	1.43
3	R	3	SIA	C8-C7	-2.23	1.49	1.53
3	R	3	SIA	C6-C5	-2.21	1.49	1.53
2	Q	2	SIA	O4-C4	-2.18	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	2	SIA	O4-C4	-2.17	1.38	1.43
3	R	3	SIA	O6-C2	-2.13	1.40	1.43
3	L	3	SIA	O6-C6	-2.11	1.40	1.44
3	S	3	SIA	O8-C8	-2.10	1.38	1.43
3	M	3	SIA	C8-C7	-2.10	1.49	1.53
2	Q	2	SIA	C8-C7	-2.07	1.49	1.53
3	S	3	SIA	C6-C5	-2.06	1.49	1.53
3	O	3	SIA	O7-C7	-2.05	1.38	1.43
3	P	3	SIA	O8-C8	-2.05	1.39	1.43
3	P	3	SIA	C8-C7	-2.05	1.49	1.53
3	R	3	SIA	O4-C4	-2.02	1.39	1.43
3	L	3	SIA	O7-C7	-2.01	1.38	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	2	SIA	C4-C5-N5	-3.16	104.11	110.38
2	Q	2	SIA	C4-C5-N5	-3.15	104.13	110.38
3	R	1	GLC	C3-C4-C5	3.10	115.77	110.24
3	P	3	SIA	O1B-C1-C2	2.91	121.34	113.03
3	S	3	SIA	O6-C2-C3	2.90	114.45	110.46
3	M	3	SIA	O6-C2-C1	2.86	113.31	107.70
3	P	2	GAL	C1-C2-C3	2.86	113.18	109.67
2	Q	2	SIA	O1B-C1-C2	2.62	120.51	113.03
3	L	2	GAL	O5-C1-C2	-2.54	106.85	110.77
3	M	3	SIA	O6-C2-C3	2.48	113.88	110.46
2	Q	2	SIA	C8-C7-C6	-2.45	108.38	113.03
3	L	3	SIA	C6-O6-C2	2.43	116.54	111.34
3	R	3	SIA	O1B-C1-C2	2.43	119.96	113.03
3	L	3	SIA	O6-C2-C1	2.42	112.45	107.70
3	R	3	SIA	O6-C2-C3	2.41	113.78	110.46
3	P	3	SIA	C11-C10-N5	2.37	120.11	116.10
3	M	3	SIA	O1B-C1-C2	2.36	119.78	113.03
3	L	3	SIA	O1B-C1-C2	2.35	119.74	113.03
3	M	3	SIA	C6-O6-C2	2.32	116.30	111.34
2	K	2	SIA	O1B-C1-C2	2.32	119.64	113.03
3	R	3	SIA	C11-C10-N5	2.31	120.02	116.10
2	N	2	SIA	O1B-C1-C2	2.26	119.47	113.03
2	Q	2	SIA	C11-C10-N5	2.25	119.90	116.10
3	L	3	SIA	C4-C5-N5	-2.21	106.00	110.38
3	O	3	SIA	O1B-C1-C2	2.15	119.15	113.03
3	R	3	SIA	O6-C2-C1	2.11	111.84	107.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	3	SIA	O1B-C1-C2	2.10	119.02	113.03
2	K	2	SIA	C8-C7-C6	-2.07	109.10	113.03
2	K	2	SIA	C6-O6-C2	2.07	115.78	111.34
2	K	2	SIA	C6-C5-N5	2.04	114.31	110.91
3	O	3	SIA	C6-O6-C2	2.04	115.69	111.34
3	S	3	SIA	C11-C10-N5	2.03	119.53	116.10
2	K	2	SIA	C11-C10-N5	2.01	119.50	116.10

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	SIA	O6-C6-C7-C8
2	K	2	SIA	O6-C6-C7-O7
3	R	3	SIA	C7-C8-C9-O9
3	R	3	SIA	O8-C8-C9-O9
2	K	2	SIA	O8-C8-C9-O9
3	O	2	GAL	O5-C5-C6-O6
3	O	2	GAL	C4-C5-C6-O6
3	O	1	GLC	O5-C5-C6-O6
3	O	1	GLC	C4-C5-C6-O6
3	M	1	GLC	O5-C5-C6-O6
2	K	2	SIA	C7-C8-C9-O9
2	Q	2	SIA	O8-C8-C9-O9
3	O	3	SIA	O8-C8-C9-O9
3	R	1	GLC	O5-C5-C6-O6
3	S	1	GLC	O5-C5-C6-O6
3	L	1	GLC	O5-C5-C6-O6
3	L	2	GAL	C4-C5-C6-O6
2	Q	2	SIA	C7-C8-C9-O9
2	K	2	SIA	C5-C6-C7-O7
3	P	3	SIA	O1A-C1-C2-O6
3	M	1	GLC	C4-C5-C6-O6
3	S	3	SIA	O1A-C1-C2-O6
3	O	3	SIA	C7-C8-C9-O9
3	M	3	SIA	O1A-C1-C2-C3

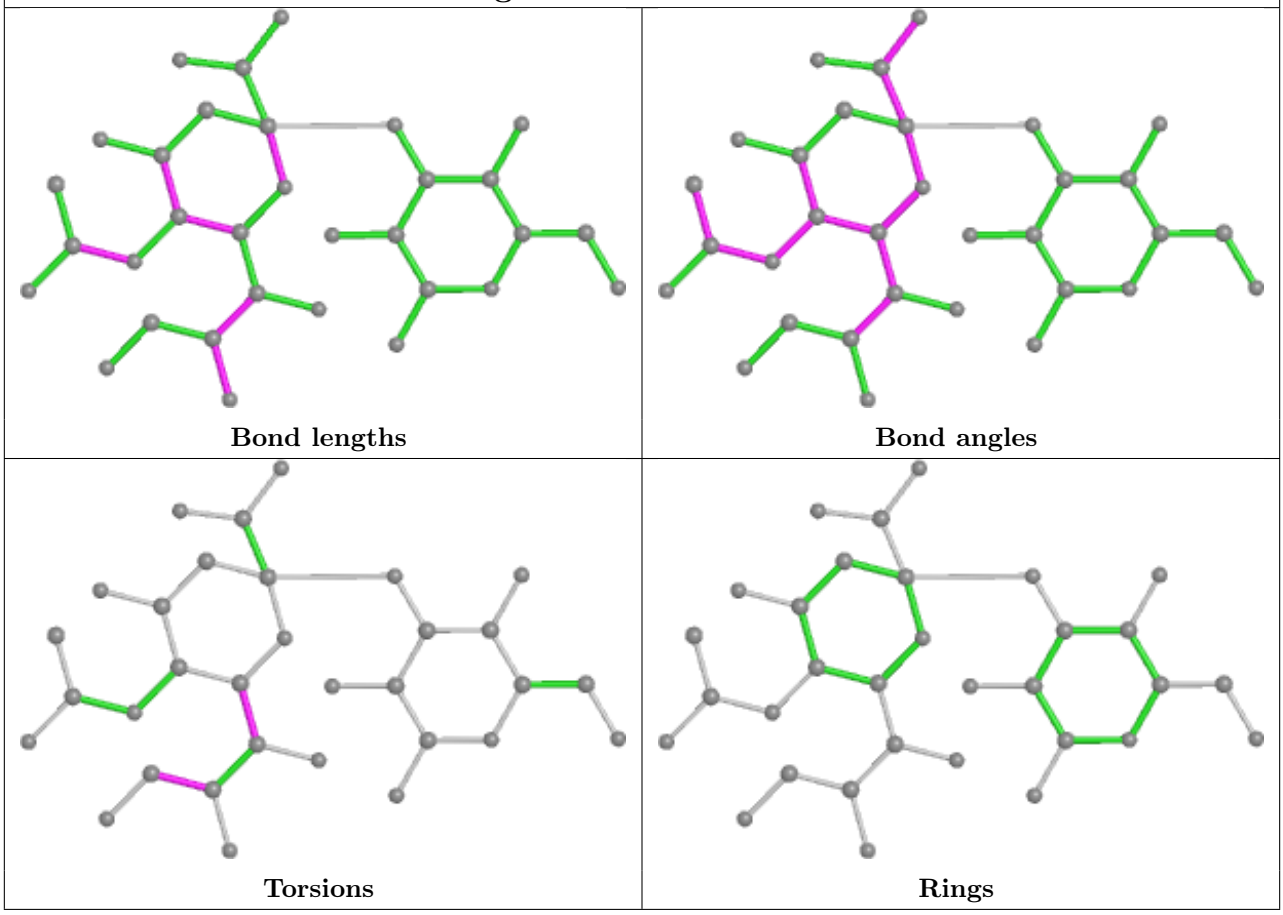
There are no ring outliers.

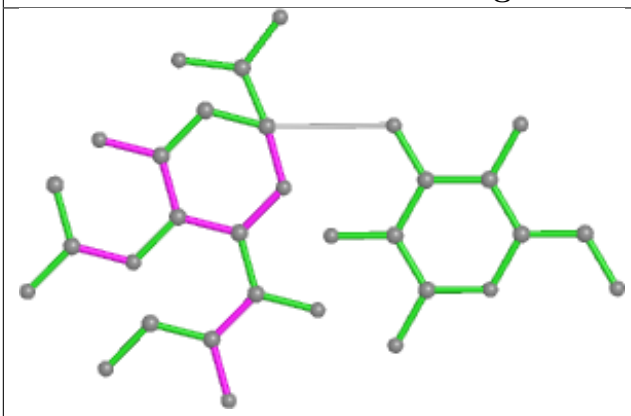
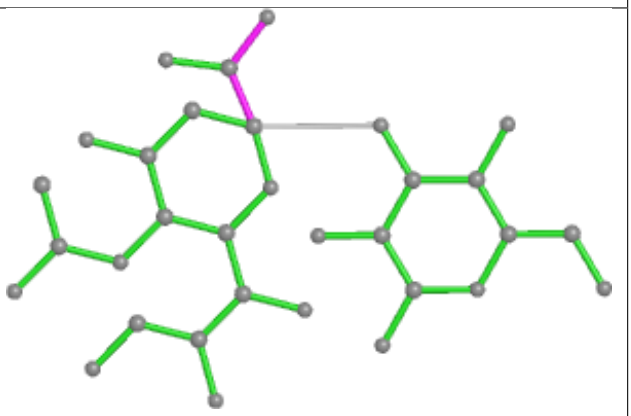
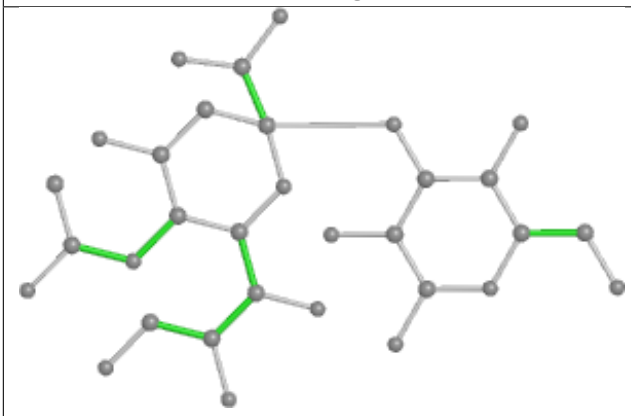
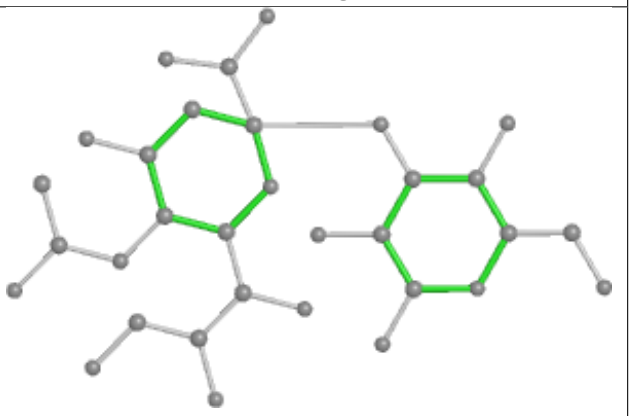
8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	SIA	2	0
2	Q	1	GAL	1	0
3	P	3	SIA	2	0
3	M	2	GAL	1	0
2	Q	2	SIA	3	0
2	K	1	GAL	1	0
3	M	3	SIA	1	0
3	P	2	GAL	1	0

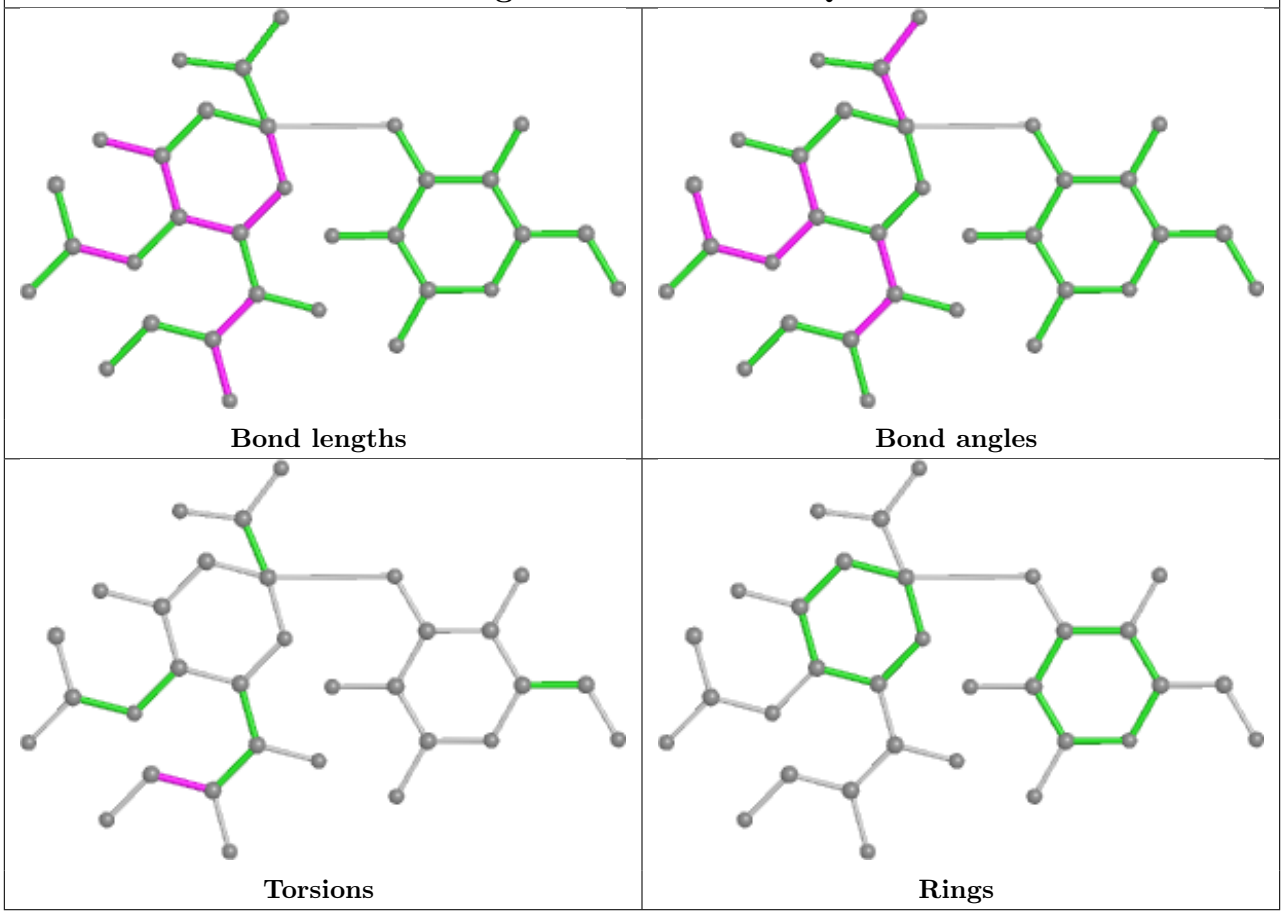
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain K

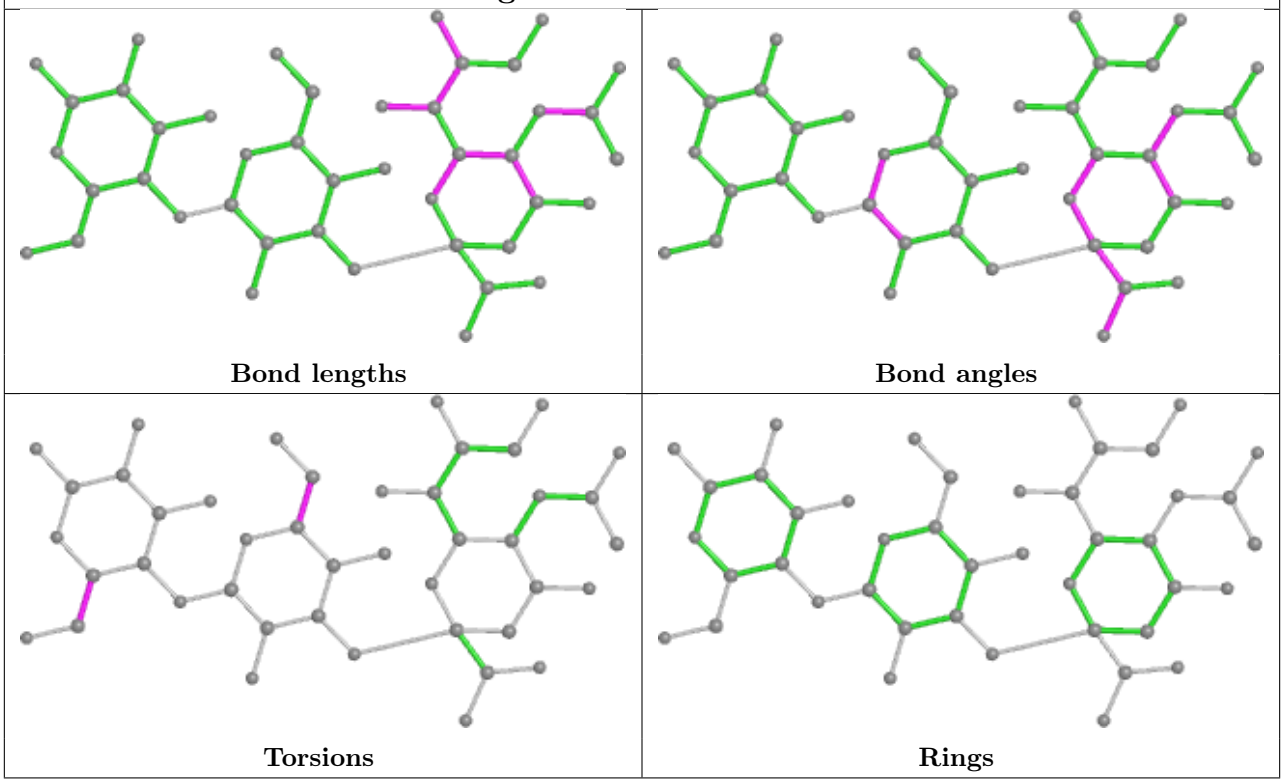


Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

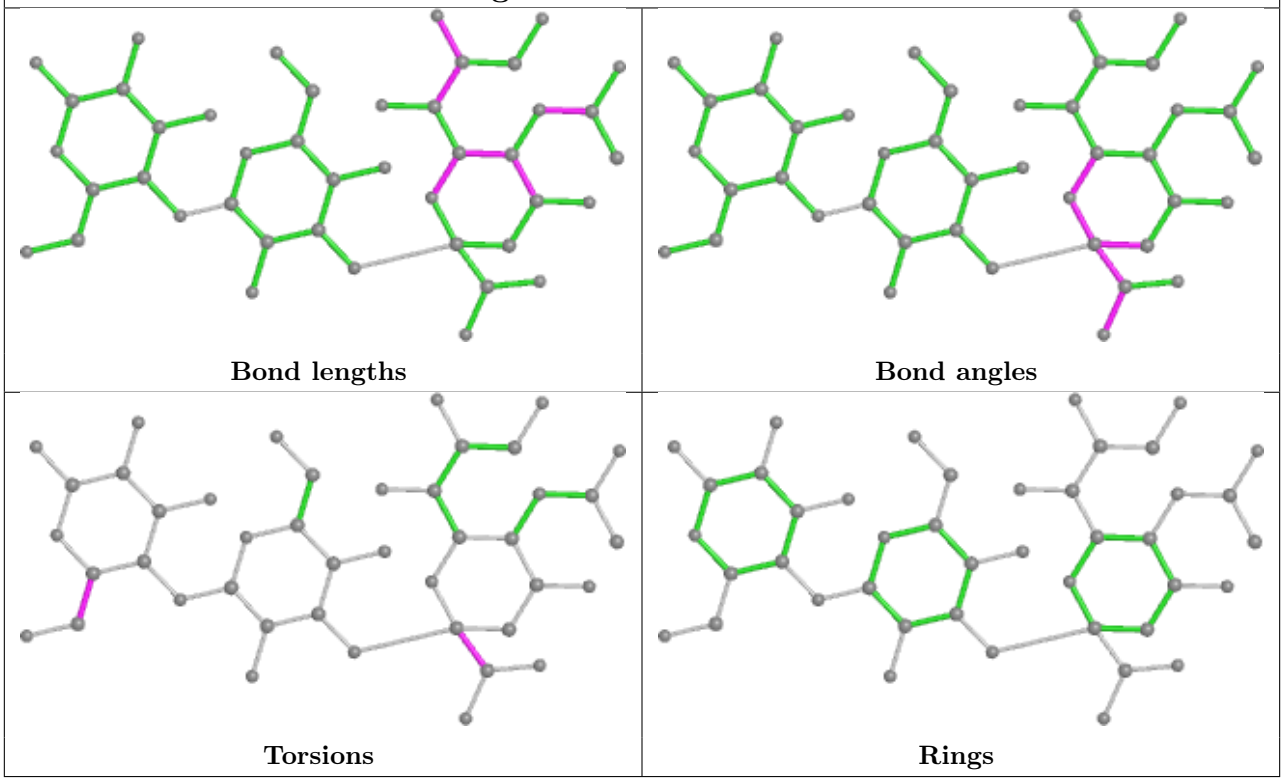
Oligosaccharide Chain Q



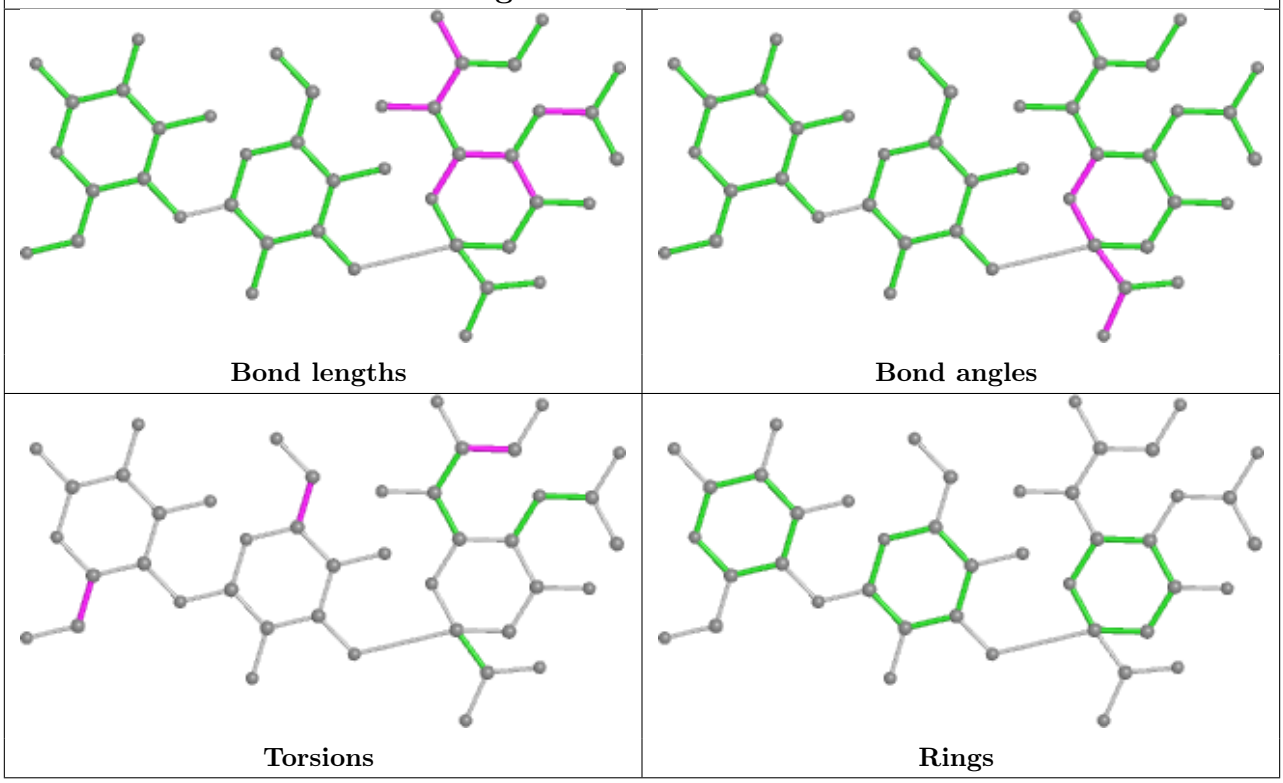
Oligosaccharide Chain L



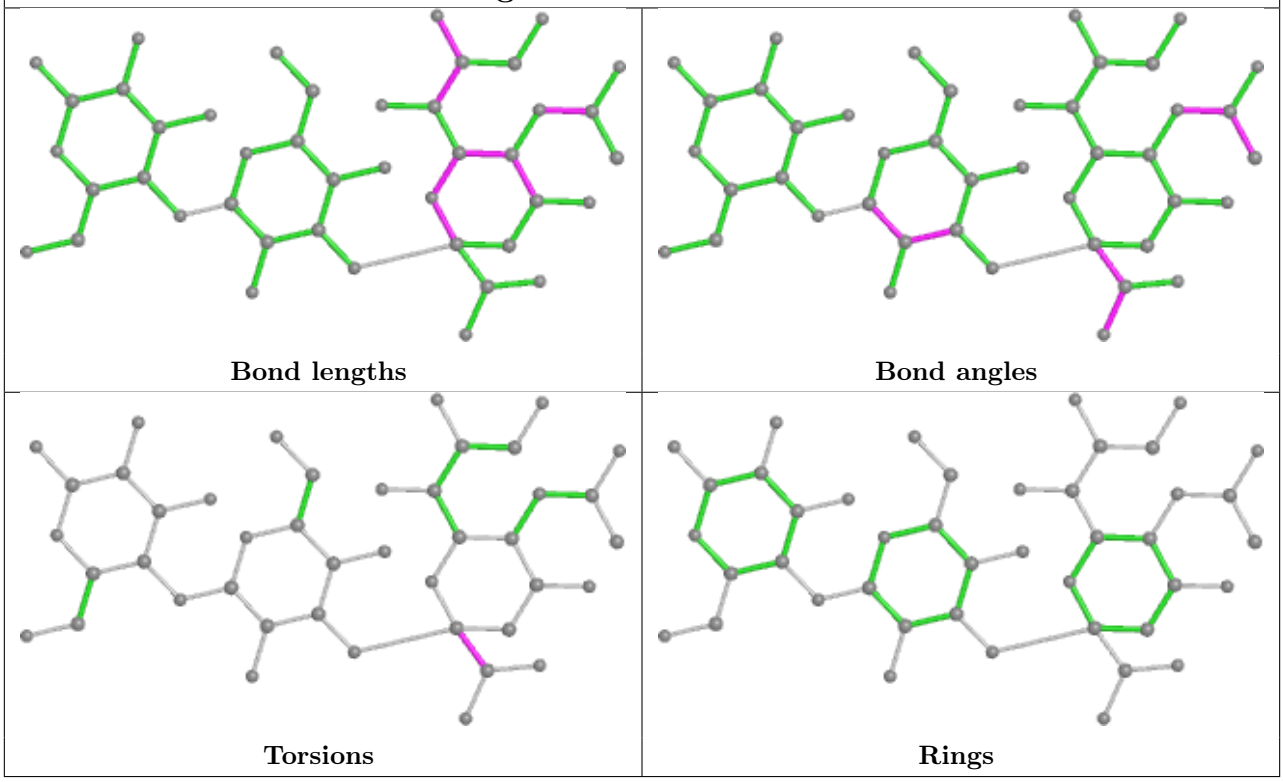
Oligosaccharide Chain M



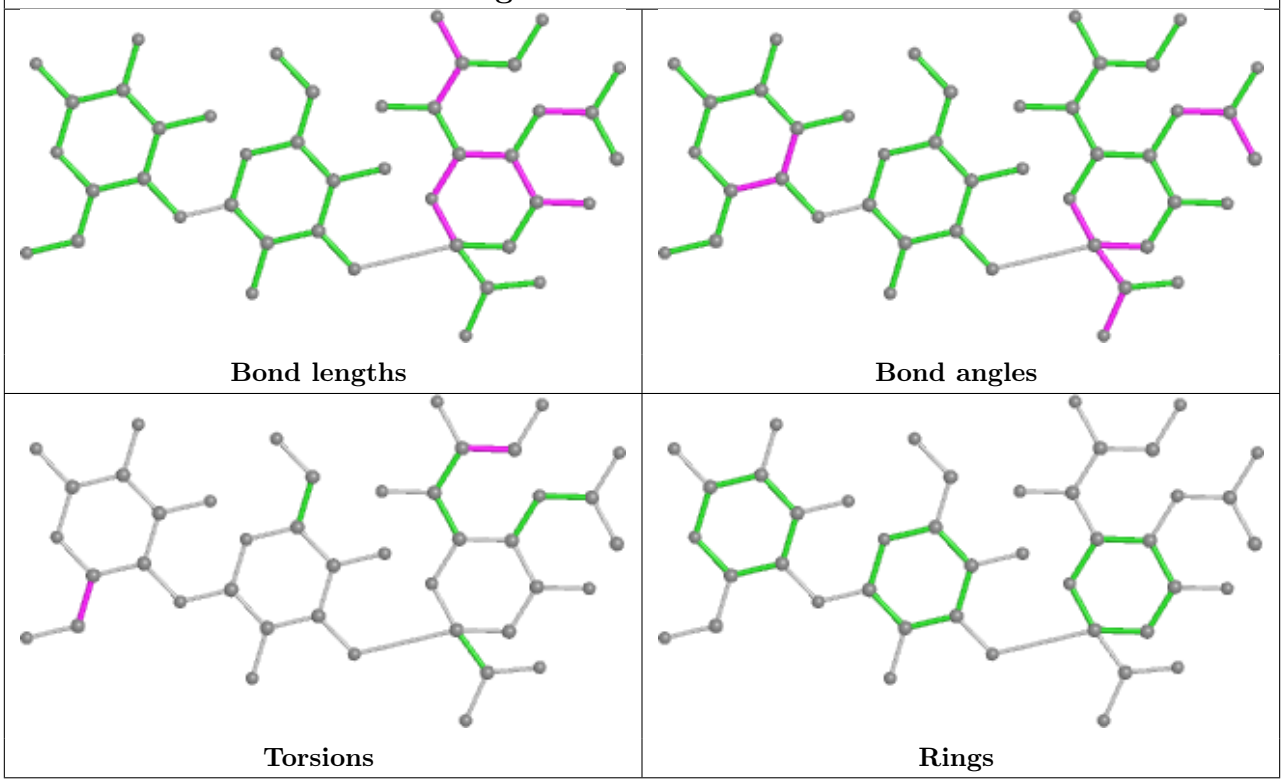
Oligosaccharide Chain O



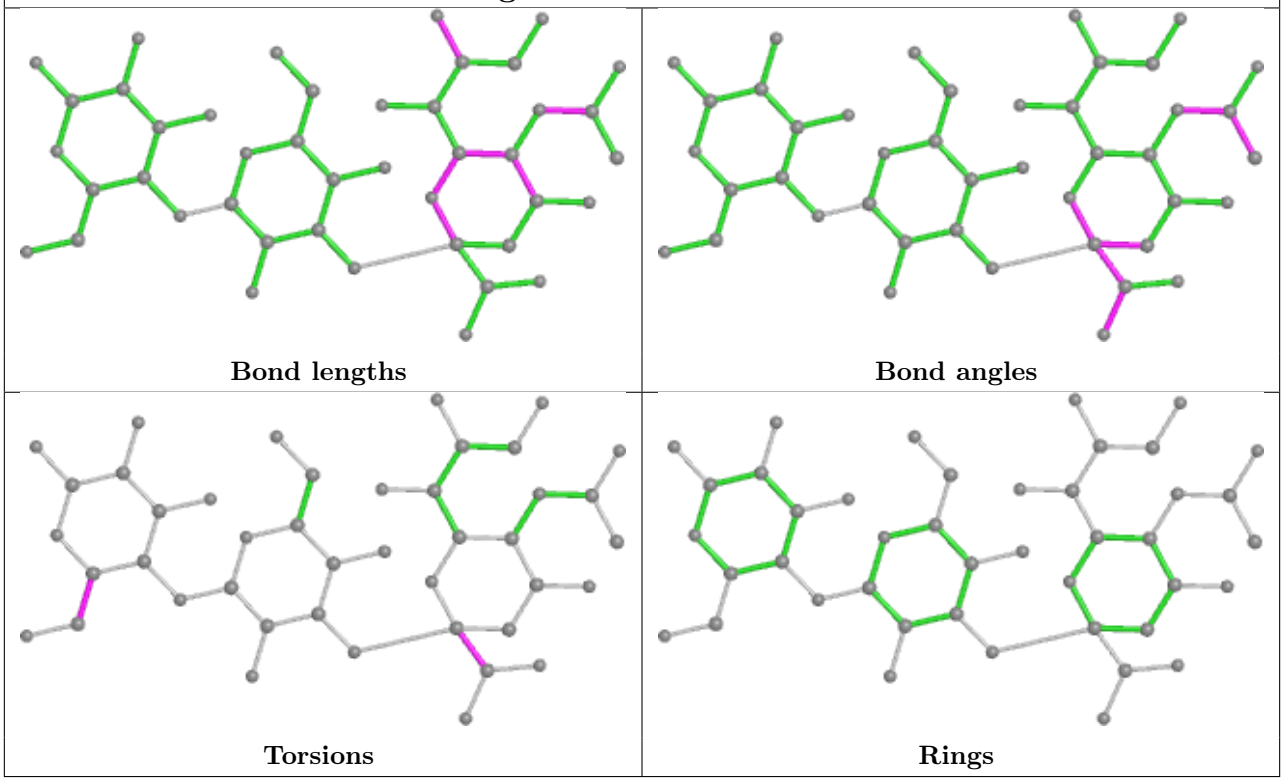
Oligosaccharide Chain P



Oligosaccharide Chain R



Oligosaccharide Chain S



5.6 Ligand geometry (i)

Of 51 ligands modelled in this entry, 30 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
7	MES	J	201	-	12,12,12	2.15	1 (8%)	14,16,16	2.04	7 (50%)
7	MES	G	201	-	12,12,12	2.26	1 (8%)	14,16,16	2.38	6 (42%)
5	PEG	H	207	-	6,6,6	0.48	0	5,5,5	0.20	0
5	PEG	G	203	-	6,6,6	0.50	0	5,5,5	0.32	0
5	PEG	F	202	-	6,6,6	0.50	0	5,5,5	0.27	0
7	MES	C	201	-	12,12,12	2.34	1 (8%)	14,16,16	2.04	4 (28%)
5	PEG	B	202	-	6,6,6	0.47	0	5,5,5	0.26	0
5	PEG	F	204	-	6,6,6	0.47	0	5,5,5	0.29	0
4	SIA	A	203	-	21,21,21	1.84	5 (23%)	25,31,31	1.33	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PEG	E	207	-	6,6,6	0.53	0	5,5,5	0.25	0
5	PEG	A	204	-	6,6,6	0.48	0	5,5,5	0.19	0
5	PEG	J	206	-	6,6,6	0.49	0	5,5,5	0.28	0
7	MES	H	201	-	12,12,12	2.35	1 (8%)	14,16,16	2.53	5 (35%)
7	MES	D	201	-	12,12,12	2.14	1 (8%)	14,16,16	2.09	6 (42%)
8	TRS	D	206	-	7,7,7	0.29	0	9,9,9	0.36	0
7	MES	B	201	-	12,12,12	2.43	1 (8%)	14,16,16	1.96	4 (28%)
5	PEG	G	204	-	6,6,6	0.47	0	5,5,5	0.16	0
5	PEG	F	203	-	6,6,6	0.56	0	5,5,5	0.24	0
5	PEG	H	209	-	6,6,6	0.46	0	5,5,5	0.42	0
5	PEG	H	208	-	6,6,6	0.48	0	5,5,5	0.30	0
8	TRS	H	212	-	7,7,7	0.28	0	9,9,9	0.29	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
7	MES	J	201	-	-	2/6/14/14	0/1/1/1
7	MES	G	201	-	-	1/6/14/14	0/1/1/1
5	PEG	H	207	-	-	1/4/4/4	-
5	PEG	G	203	-	-	1/4/4/4	-
5	PEG	F	202	-	-	2/4/4/4	-
7	MES	C	201	-	-	6/6/14/14	0/1/1/1
5	PEG	B	202	-	-	1/4/4/4	-
5	PEG	F	204	-	-	0/4/4/4	-
4	SIA	A	203	-	-	1/20/38/38	0/1/1/1
5	PEG	E	207	-	-	1/4/4/4	-
5	PEG	A	204	-	-	2/4/4/4	-
5	PEG	J	206	-	-	2/4/4/4	-
7	MES	H	201	-	-	4/6/14/14	0/1/1/1
7	MES	D	201	-	-	5/6/14/14	0/1/1/1
8	TRS	D	206	-	-	3/9/9/9	-
7	MES	B	201	-	-	3/6/14/14	0/1/1/1
5	PEG	G	204	-	-	2/4/4/4	-
5	PEG	F	203	-	-	4/4/4/4	-
5	PEG	H	209	-	-	2/4/4/4	-
5	PEG	H	208	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	TRS	H	212	-	-	5/9/9/9	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	201	MES	C8-S	-8.10	1.66	1.77
7	H	201	MES	C8-S	-7.87	1.66	1.77
7	C	201	MES	C8-S	-7.82	1.66	1.77
7	G	201	MES	C8-S	-7.51	1.66	1.77
7	J	201	MES	C8-S	-7.19	1.67	1.77
7	D	201	MES	C8-S	-7.08	1.67	1.77
4	A	203	SIA	C4-C5	-4.44	1.49	1.53
4	A	203	SIA	C10-N5	3.09	1.45	1.34
4	A	203	SIA	O8-C8	-2.35	1.38	1.43
4	A	203	SIA	C8-C7	-2.30	1.49	1.53
4	A	203	SIA	C6-C5	-2.20	1.49	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	201	MES	C5-N4-C3	5.42	121.02	108.83
7	C	201	MES	C5-N4-C3	5.32	120.80	108.83
7	G	201	MES	C5-N4-C3	5.25	120.65	108.83
7	D	201	MES	C5-N4-C3	4.22	118.34	108.83
7	J	201	MES	C5-N4-C3	4.22	118.33	108.83
7	G	201	MES	C6-C5-N4	-3.93	104.14	110.10
7	B	201	MES	C5-N4-C3	3.84	117.47	108.83
7	H	201	MES	C2-C3-N4	-3.65	104.56	110.10
7	H	201	MES	C7-N4-C5	3.27	119.60	111.23
7	H	201	MES	O1S-S-C8	3.25	110.83	106.92
4	A	203	SIA	C3-C2-C1	-3.18	107.08	113.00
7	H	201	MES	C7-N4-C3	3.17	119.35	111.23
7	B	201	MES	C6-C5-N4	-3.14	105.34	110.10
4	A	203	SIA	O1A-C1-C2	-2.98	119.08	123.59
7	D	201	MES	O1S-S-C8	2.92	110.44	106.92
7	G	201	MES	C7-N4-C5	2.87	118.57	111.23
7	J	201	MES	O1S-S-C8	2.86	110.36	106.92
7	D	201	MES	O3S-S-C8	2.83	110.34	105.77
7	D	201	MES	C7-N4-C5	2.78	118.35	111.23
7	G	201	MES	C7-N4-C3	2.72	118.19	111.23
7	G	201	MES	O1S-S-C8	2.72	110.19	106.92
7	J	201	MES	C6-C5-N4	-2.63	106.12	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	201	MES	C6-C5-N4	-2.56	106.21	110.10
7	B	201	MES	O1S-S-C8	2.54	109.98	106.92
7	C	201	MES	C7-N4-C5	2.51	117.64	111.23
4	A	203	SIA	O6-C6-C5	2.45	112.17	109.78
7	J	201	MES	C7-N4-C3	2.42	117.43	111.23
7	C	201	MES	O3S-S-C8	2.31	109.51	105.77
7	C	201	MES	C7-N4-C3	2.31	117.13	111.23
7	J	201	MES	O2S-S-C8	2.16	109.52	106.92
7	D	201	MES	C7-N4-C3	2.12	116.67	111.23
7	G	201	MES	O3S-S-C8	2.11	109.18	105.77
4	A	203	SIA	C8-C7-C6	-2.11	109.04	113.03
7	J	201	MES	O3S-S-C8	2.10	109.17	105.77
7	J	201	MES	C7-N4-C5	2.10	116.59	111.23
7	B	201	MES	C2-C3-N4	2.02	113.16	110.10

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	201	MES	N4-C7-C8-S
7	C	201	MES	C7-C8-S-O1S
7	C	201	MES	C7-C8-S-O3S
7	D	201	MES	N4-C7-C8-S
7	D	201	MES	C7-C8-S-O2S
7	D	201	MES	C7-C8-S-O3S
7	J	201	MES	C8-C7-N4-C5
7	J	201	MES	N4-C7-C8-S
8	H	212	TRS	N-C-C2-O2
8	H	212	TRS	C1-C-C3-O3
8	H	212	TRS	C2-C-C3-O3
5	H	208	PEG	O2-C3-C4-O4
7	H	201	MES	C7-C8-S-O3S
5	F	203	PEG	C1-C2-O2-C3
5	A	204	PEG	O2-C3-C4-O4
5	E	207	PEG	O1-C1-C2-O2
8	H	212	TRS	C3-C-C2-O2
5	F	202	PEG	O1-C1-C2-O2
5	F	203	PEG	O1-C1-C2-O2
5	H	209	PEG	O2-C3-C4-O4
5	J	206	PEG	O1-C1-C2-O2
7	C	201	MES	C8-C7-N4-C3
7	D	201	MES	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
7	G	201	MES	C8-C7-N4-C3
7	H	201	MES	C8-C7-N4-C3
7	B	201	MES	C7-C8-S-O3S
5	F	203	PEG	O2-C3-C4-O4
5	G	204	PEG	C1-C2-O2-C3
5	H	208	PEG	C4-C3-O2-C2
4	A	203	SIA	O1A-C1-C2-O6
5	F	202	PEG	C1-C2-O2-C3
5	A	204	PEG	C1-C2-O2-C3
5	F	203	PEG	C4-C3-O2-C2
8	D	206	TRS	C1-C-C3-O3
8	D	206	TRS	C2-C-C3-O3
8	H	212	TRS	N-C-C3-O3
5	J	206	PEG	C1-C2-O2-C3
5	B	202	PEG	C4-C3-O2-C2
7	B	201	MES	C7-C8-S-O1S
7	B	201	MES	C7-C8-S-O2S
7	C	201	MES	C7-C8-S-O2S
7	D	201	MES	C7-C8-S-O1S
7	H	201	MES	C7-C8-S-O1S
7	H	201	MES	C7-C8-S-O2S
5	G	203	PEG	O1-C1-C2-O2
5	G	204	PEG	O2-C3-C4-O4
7	C	201	MES	C8-C7-N4-C5
5	H	207	PEG	C1-C2-O2-C3
5	H	209	PEG	C1-C2-O2-C3
8	D	206	TRS	N-C-C3-O3

There are no ring outliers.

14 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	201	MES	2	0
7	G	201	MES	2	0
5	G	203	PEG	2	0
5	F	202	PEG	2	0
5	B	202	PEG	9	0
5	E	207	PEG	2	0
5	J	206	PEG	1	0
7	D	201	MES	2	0
8	D	206	TRS	2	0
7	B	201	MES	1	0

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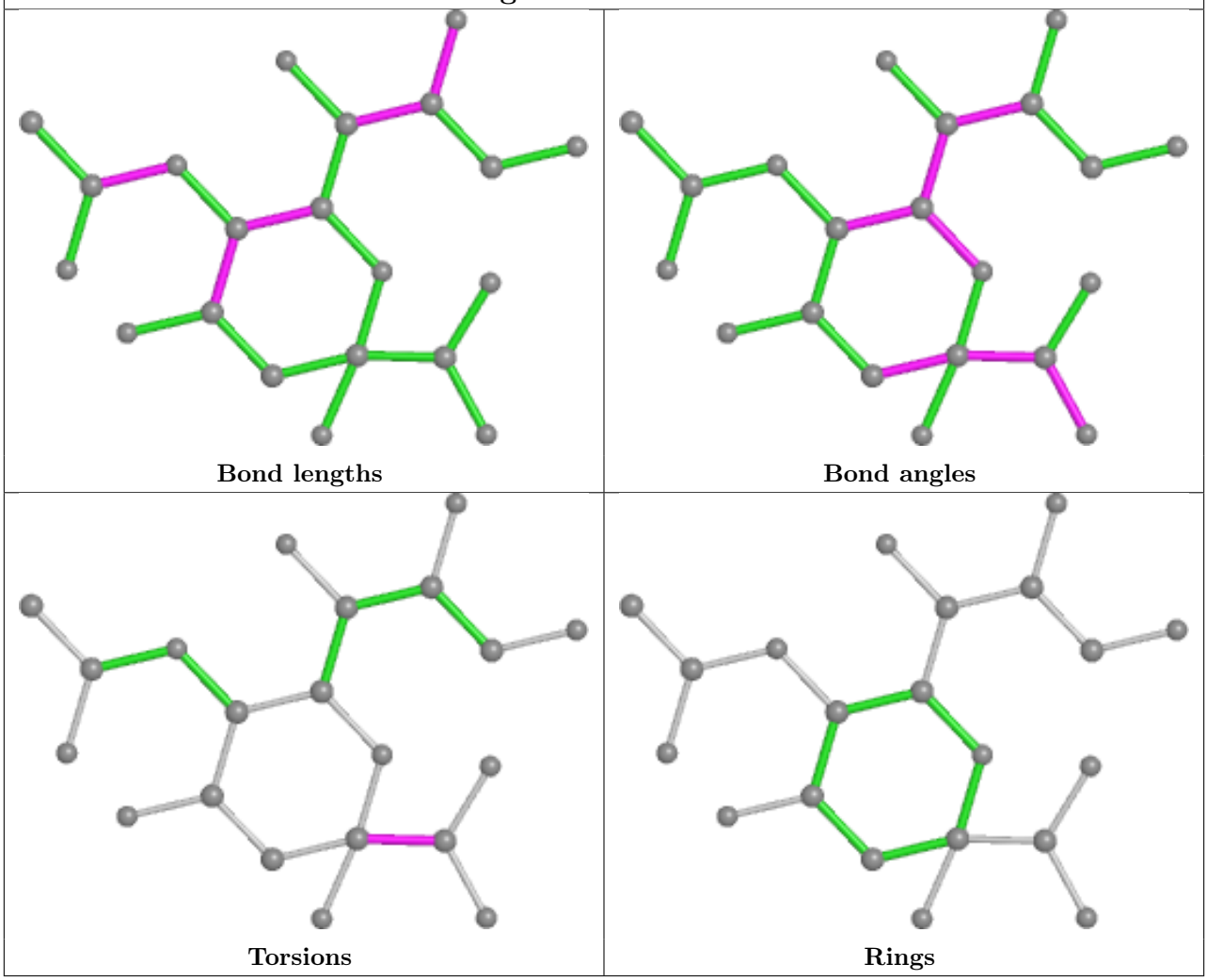
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	203	PEG	11	0
5	H	209	PEG	5	0
5	H	208	PEG	6	0
8	H	212	TRS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 A 203



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, 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	120/149 (80%)	-0.30	1 (0%)	86	85	12, 23, 41, 75	0
1	B	119/149 (79%)	-0.20	3 (2%)	57	55	13, 25, 55, 68	0
1	C	118/149 (79%)	-0.25	1 (0%)	86	85	12, 24, 51, 90	0
1	D	118/149 (79%)	-0.23	0	100	100	14, 24, 49, 68	0
1	E	119/149 (79%)	-0.21	1 (0%)	86	85	13, 25, 50, 83	0
1	F	118/149 (79%)	-0.29	0	100	100	12, 24, 49, 64	0
1	G	118/149 (79%)	-0.19	3 (2%)	57	55	12, 22, 52, 75	0
1	H	124/149 (83%)	-0.22	0	100	100	13, 22, 46, 63	0
1	I	118/149 (79%)	-0.31	0	100	100	13, 21, 42, 67	0
1	J	123/149 (82%)	-0.19	3 (2%)	59	56	13, 21, 56, 101	0
All	All	1195/1490 (80%)	-0.24	12 (1%)	82	81	12, 23, 51, 101	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	132	ASP	4.4
1	G	63	VAL	3.8
1	C	132	ASP	3.8
1	J	144	HIS	3.5
1	A	140	PRO	3.4
1	J	142	LEU	3.3
1	B	62	GLN	2.8
1	J	133	TYR	2.5
1	B	140	PRO	2.5
1	B	61	SER	2.5
1	G	62	GLN	2.3
1	G	65	ASN	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)

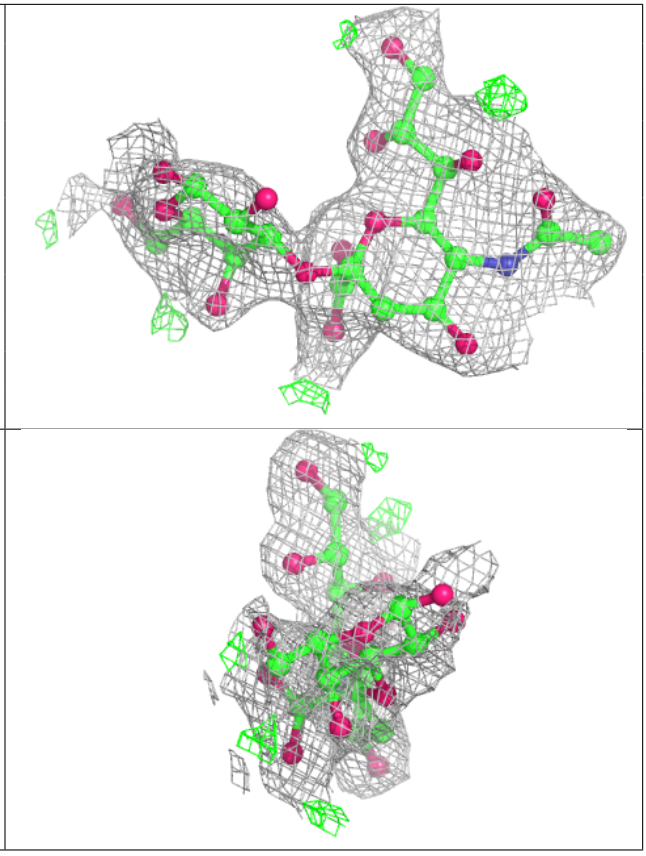
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

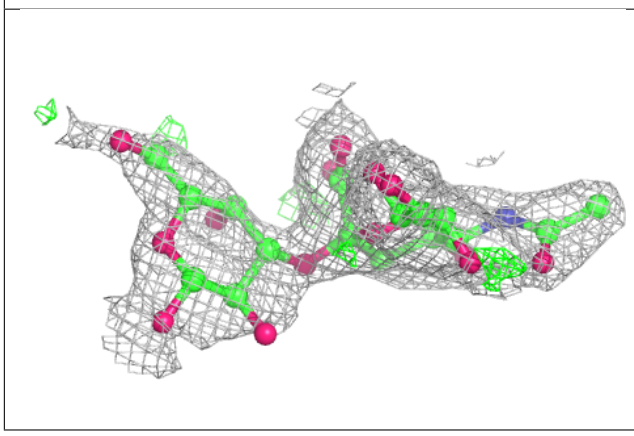
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	Q	1	12/12	0.66	0.24	61,70,72,74	0
2	GAL	N	1	12/12	0.73	0.30	65,73,75,77	0
3	GAL	O	2	11/12	0.76	0.23	45,54,61,63	0
2	GAL	K	1	12/12	0.77	0.31	55,67,70,71	0
3	GLC	O	1	12/12	0.81	0.23	47,61,68,77	0
3	GLC	P	1	12/12	0.82	0.25	36,51,60,64	0
3	GLC	L	1	12/12	0.86	0.28	55,72,83,88	0
3	GLC	R	1	12/12	0.86	0.20	32,54,58,60	0
2	SIA	Q	2	20/21	0.87	0.21	42,51,59,59	0
3	GLC	S	1	12/12	0.87	0.24	35,49,54,56	0
2	SIA	N	2	20/21	0.88	0.21	36,50,56,57	0
3	SIA	S	3	20/21	0.89	0.16	21,32,39,40	0
3	GLC	M	1	12/12	0.90	0.19	32,50,61,65	0
3	SIA	O	3	20/21	0.90	0.15	32,40,44,45	0
3	SIA	L	3	20/21	0.90	0.15	21,37,47,52	0
2	SIA	K	2	20/21	0.91	0.16	24,41,47,49	0
3	GAL	R	2	11/12	0.92	0.16	28,32,41,46	0
3	SIA	R	3	20/21	0.93	0.14	18,29,35,36	0
3	GAL	P	2	11/12	0.93	0.12	33,35,42,42	0
3	SIA	P	3	20/21	0.93	0.11	17,29,38,41	0
3	SIA	M	3	20/21	0.94	0.10	17,26,29,30	0
3	GAL	S	2	11/12	0.94	0.14	31,34,40,44	0
3	GAL	L	2	11/12	0.94	0.23	32,43,46,49	0
3	GAL	M	2	11/12	0.95	0.12	24,26,38,42	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 K:

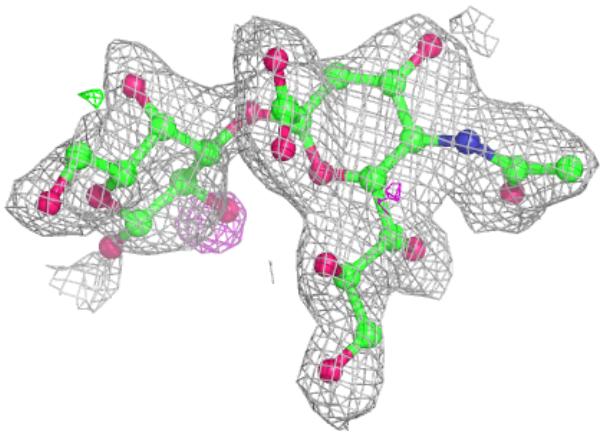
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

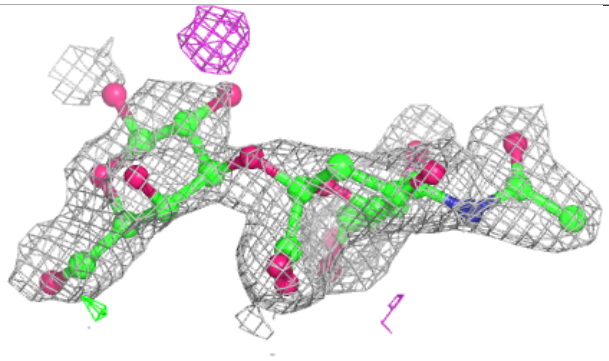




Electron density around Chain N:

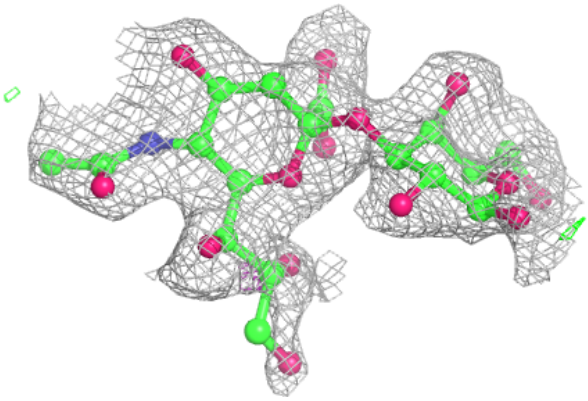
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

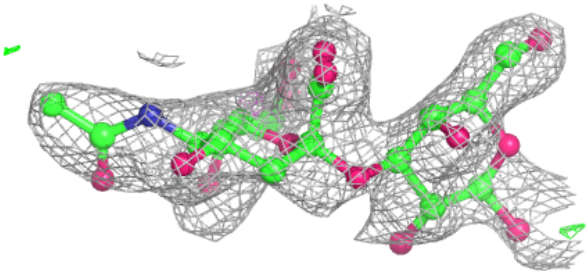


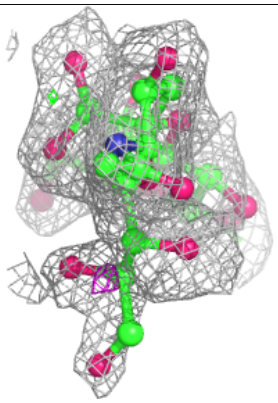


Electron density around Chain Q:

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

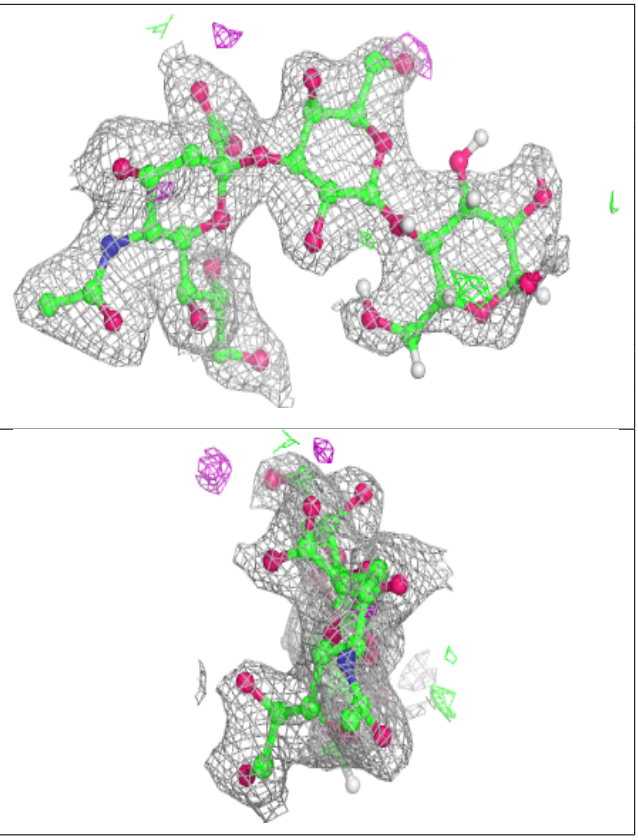


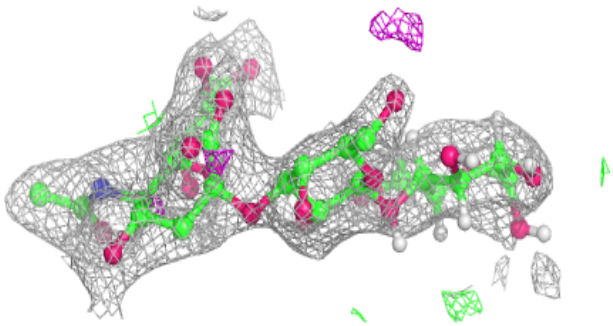




Electron density around Chain L:

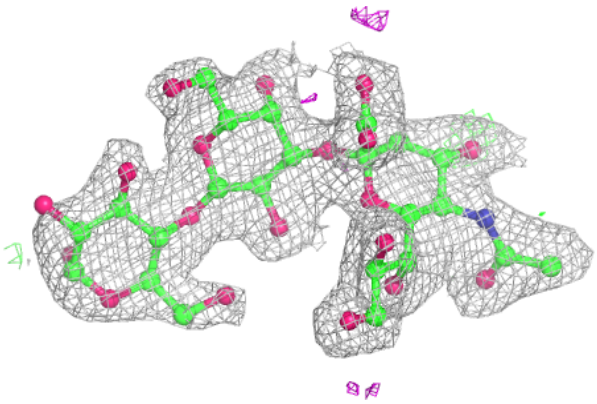
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

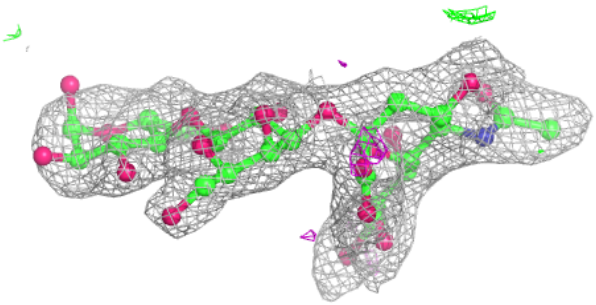


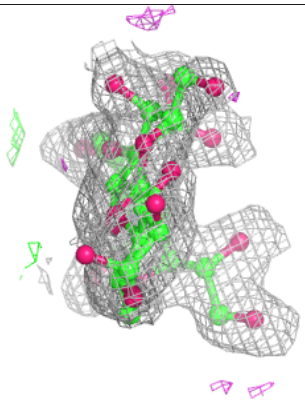


Electron density around Chain M:

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

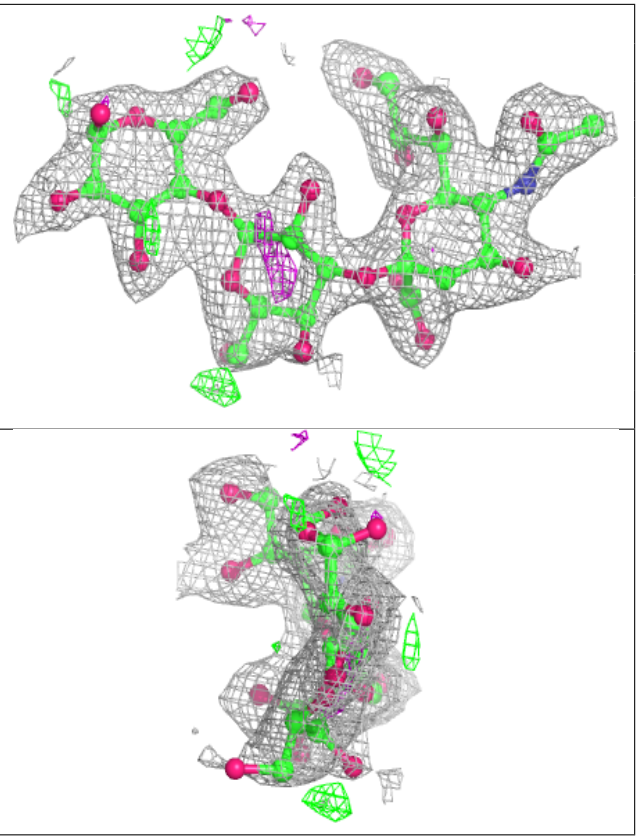


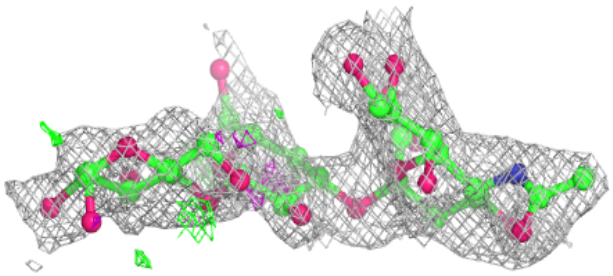




Electron density around Chain O:

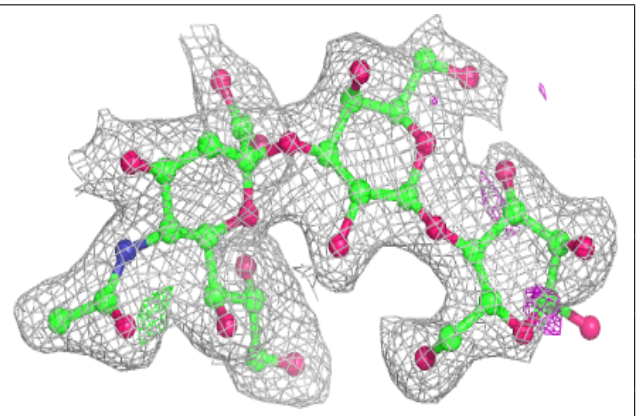
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

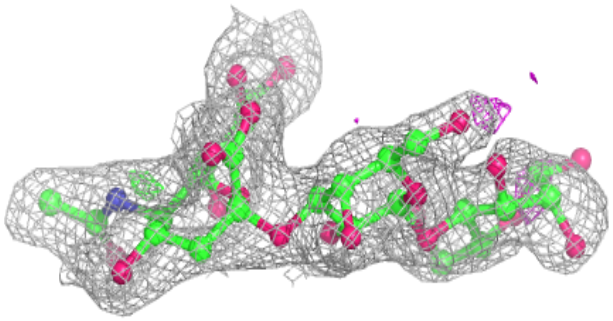


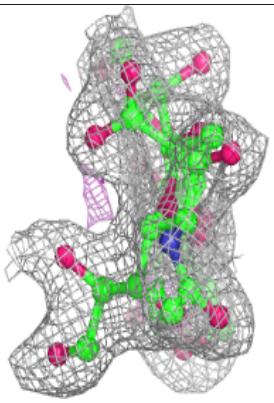


Electron density around Chain P:

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

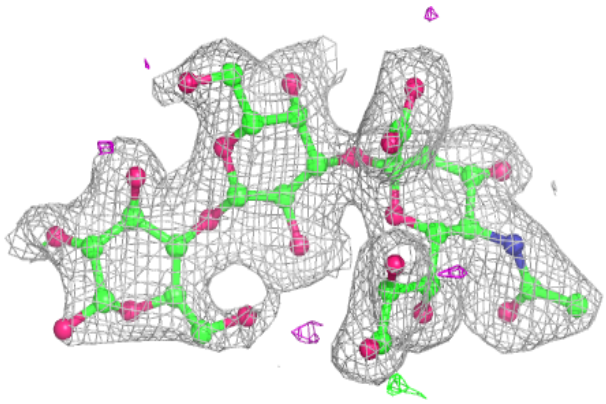


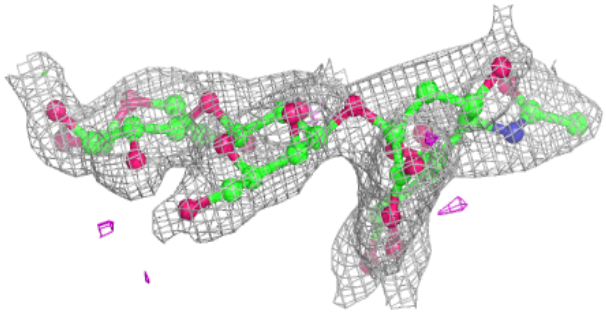


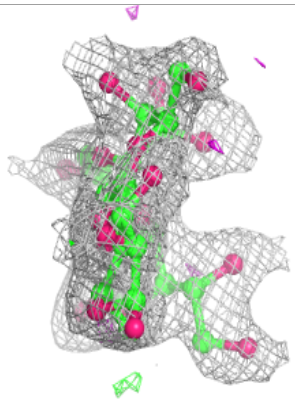


Electron density around Chain R:

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

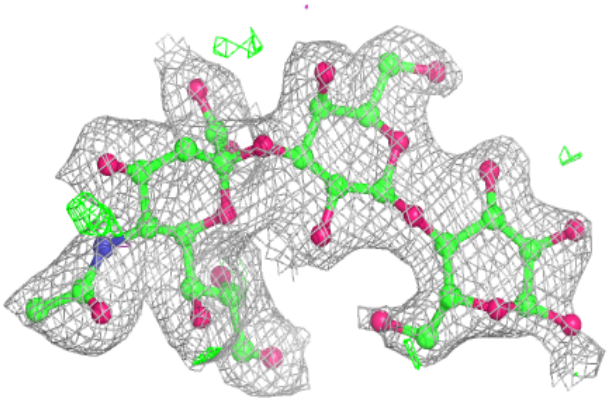


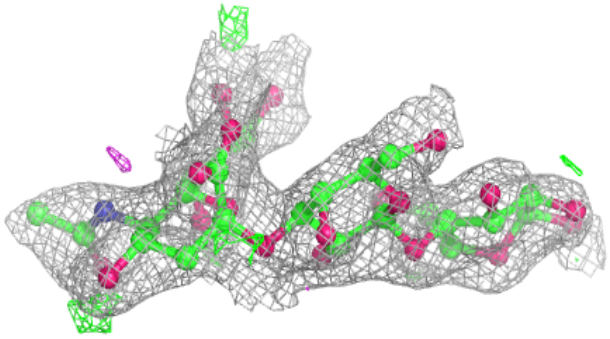


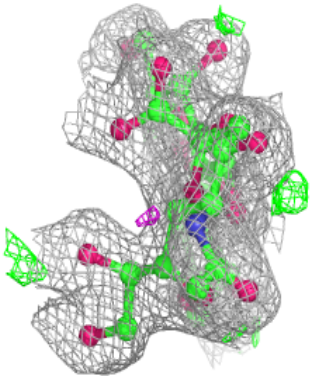


Electron density around Chain S:

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







6.4 Ligands (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
8	TRS	H	212	8/8	0.60	0.17	63,66,68,68	0
8	TRS	D	206	8/8	0.66	0.18	60,64,71,71	0
5	PEG	A	204	7/7	0.67	0.29	60,72,80,80	0
5	PEG	E	207	7/7	0.69	0.32	47,52,60,60	0
7	MES	D	201	12/12	0.72	0.24	60,64,93,95	0
7	MES	C	201	12/12	0.74	0.21	50,55,87,93	0
7	MES	G	201	12/12	0.75	0.23	53,59,82,82	0
5	PEG	G	204	7/7	0.78	0.28	51,62,74,74	0
5	PEG	F	204	7/7	0.79	0.23	49,58,66,66	0
5	PEG	J	206	7/7	0.80	0.17	47,57,63,63	0
6	CL	F	207	1/1	0.81	0.13	58,58,58,58	0
5	PEG	H	207	7/7	0.81	0.24	40,52,65,65	0
4	SIA	A	203	21/21	0.81	0.20	35,45,56,56	0
6	CL	G	206	1/1	0.82	0.12	68,68,68,68	0
5	PEG	B	202	7/7	0.82	0.13	34,37,43,47	0
6	CL	J	207	1/1	0.85	0.07	62,62,62,62	0
7	MES	J	201	12/12	0.86	0.25	42,53,105,106	0
7	MES	B	201	12/12	0.87	0.16	42,54,69,79	0
5	PEG	F	202	7/7	0.88	0.18	22,36,36,39	0
6	CL	A	208	1/1	0.88	0.17	53,53,53,53	0
5	PEG	G	203	7/7	0.88	0.17	33,39,41,44	0
5	PEG	H	208	7/7	0.89	0.17	42,45,49,50	0
6	CL	B	205	1/1	0.91	0.06	64,64,64,64	0
5	PEG	H	209	7/7	0.91	0.23	36,50,63,67	0
6	CL	B	204	1/1	0.91	0.11	49,49,49,49	0
6	CL	I	210	1/1	0.91	0.08	44,44,44,44	0
6	CL	B	203	1/1	0.92	0.08	43,43,43,43	0
5	PEG	F	203	7/7	0.92	0.23	28,35,38,41	0
6	CL	A	206	1/1	0.93	0.07	58,58,58,58	0
6	CL	G	205	1/1	0.93	0.11	44,44,44,44	0
7	MES	H	201	12/12	0.94	0.16	20,33,56,59	0
6	CL	A	205	1/1	0.94	0.09	57,57,57,57	0
9	CA	H	206	1/1	0.95	0.09	25,25,25,25	0
6	CL	F	206	1/1	0.96	0.09	55,55,55,55	0
6	CL	F	205	1/1	0.96	0.06	50,50,50,50	0
6	CL	J	208	1/1	0.96	0.07	47,47,47,47	0
6	CL	H	210	1/1	0.96	0.11	48,48,48,48	0

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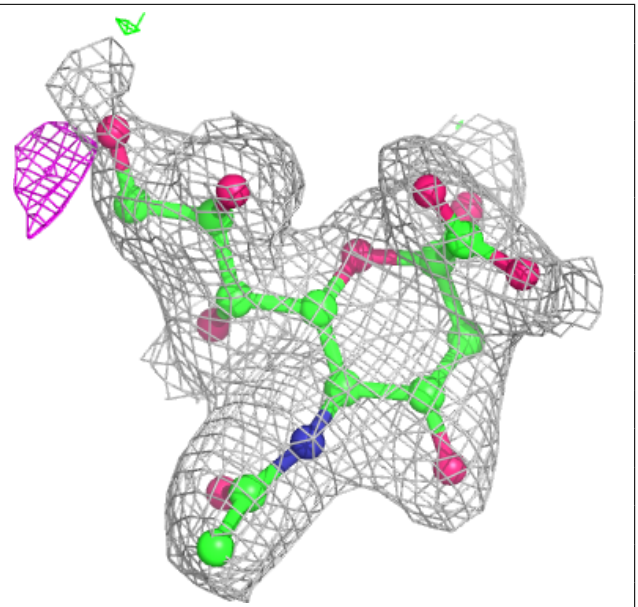
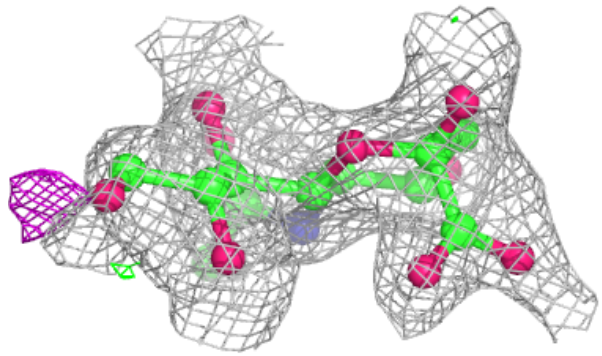
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	I	207	1/1	0.96	0.13	53,53,53,53	0
9	CA	F	201	1/1	0.96	0.06	32,32,32,32	0
6	CL	I	209	1/1	0.96	0.09	47,47,47,47	0
6	CL	C	205	1/1	0.97	0.07	40,40,40,40	0
6	CL	D	205	1/1	0.97	0.13	46,46,46,46	0
6	CL	H	211	1/1	0.97	0.07	60,60,60,60	0
9	CA	I	206	1/1	0.97	0.06	39,39,39,39	0
9	CA	G	202	1/1	0.98	0.04	32,32,32,32	0
9	CA	E	206	1/1	0.98	0.06	44,44,44,44	0
6	CL	E	208	1/1	0.98	0.12	34,34,34,34	0
9	CA	J	205	1/1	0.98	0.05	39,39,39,39	0
6	CL	I	208	1/1	0.99	0.08	37,37,37,37	0
6	CL	A	207	1/1	0.99	0.09	39,39,39,39	0
9	CA	H	205	1/1	0.99	0.09	18,18,18,18	0

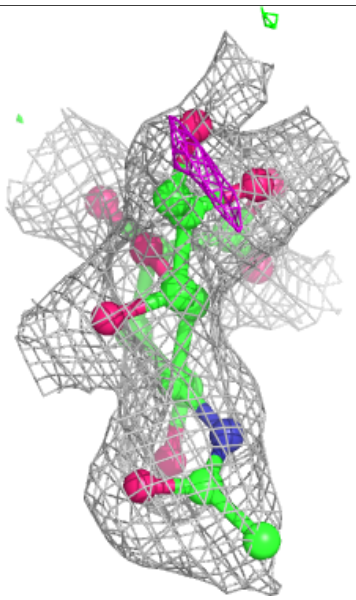
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SIA A 203:

$2mF_o$-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.