



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2024 – 10:32 AM EST

PDB ID : 8G82
Title : Vancomycin bound to D-Ala-D-Ser
Authors : Loll, P.J.; Park, J.H.
Deposited on : 2023-02-17
Resolution : 1.20 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 ⓘ 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

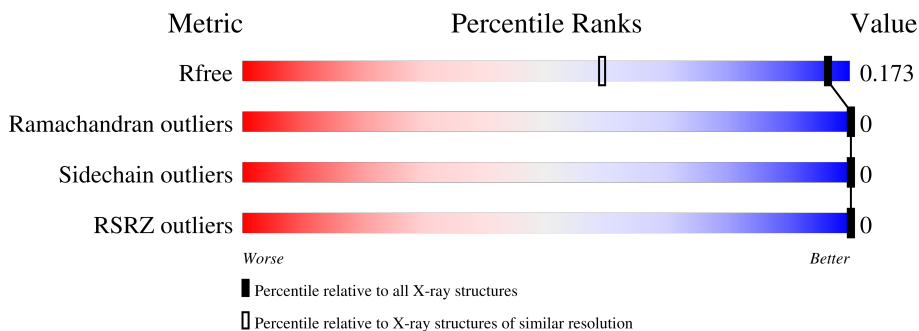
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

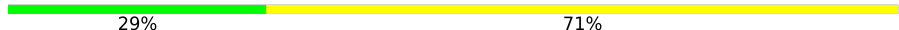
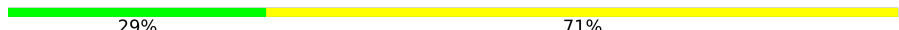
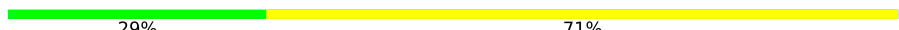

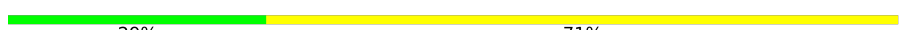

The reported resolution of this entry is 1.20 Å.

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	1223 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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	7	 29% 71%
1	B	7	 29% 71%
1	C	7	 29% 71%
1	D	7	 29% 71%
1	E	7	 29% 71%
1	F	7	 29% 71%

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Mol	Chain	Length	Quality of chain
1	G	7	29% 71%
1	H	7	14% 86%
1	I	7	14% 86%
1	J	7	43% 57%
2	K	3	100%
2	L	3	100%
2	M	3	100%
2	N	3	100%
2	O	3	100%
2	P	3	100%
2	Q	3	100%
2	R	3	100%
2	S	3	100%
2	T	3	100%
3	U	2	50% 50%
3	W	2	50% 50%
3	Y	2	50% 50%
3	a	2	100%
3	c	2	50% 50%
3	e	2	50% 50%
3	k	2	50% 50%
3	m	2	50% 50%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 1542 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 Vancomycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	Cl	N	O			
1	A	7	79	53	2	8	16	0	0	0
1	B	7	79	53	2	8	16	0	0	0
1	C	7	79	53	2	8	16	0	0	0
1	D	7	79	53	2	8	16	0	0	0
1	E	7	79	53	2	8	16	0	0	0
1	F	7	79	53	2	8	16	0	0	0
1	G	7	79	53	2	8	16	0	0	0
1	H	7	79	53	2	8	16	0	0	0
1	I	7	79	53	2	8	16	0	0	0
1	J	7	79	53	2	8	16	0	0	0

- Molecule 2 is a protein (with D amino acids) called D-Ala-D-Ser.

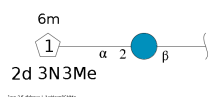
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	K	3	15	8	2	5	0	0	0
2	L	3	30	16	4	10	0	3	0
2	M	3	15	8	2	5	0	0	0
2	N	3	15	8	2	5	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	3	Total	C	N	O	0	0	0
			15	8	2	5			
2	P	3	Total	C	N	O	0	0	0
			15	8	2	5			
2	Q	3	Total	C	N	O	0	0	0
			15	8	2	5			
2	R	3	Total	C	N	O	0	0	0
			15	8	2	5			
2	S	3	Total	C	N	O	0	3	0
			30	16	4	10			
2	T	3	Total	C	N	O	0	0	0
			15	8	2	5			

- Molecule 3 is an oligosaccharide called vancosamine-(1-2)-beta-D-glucopyranose.



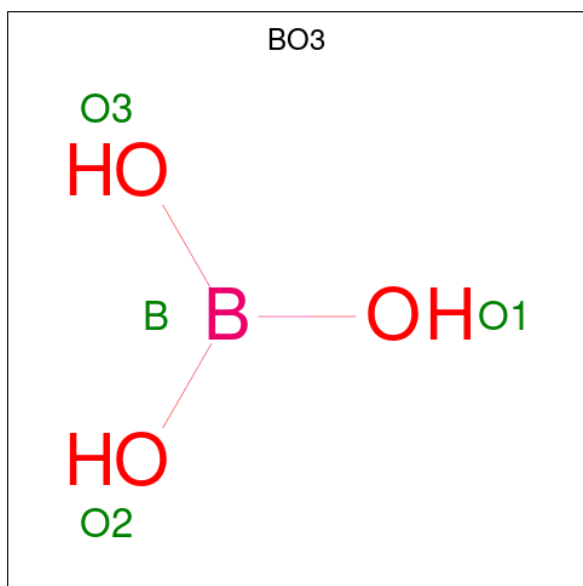
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	U	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	W	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	Y	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	a	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	c	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	e	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	k	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	m	2	Total	C	N	O	0	0	0
			22	13	1	8			

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



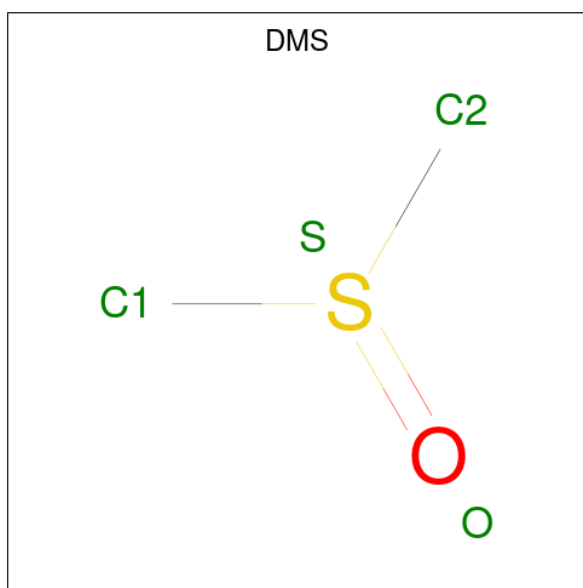
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is BORIC ACID (three-letter code: BO3) (formula: BH_3O_3).



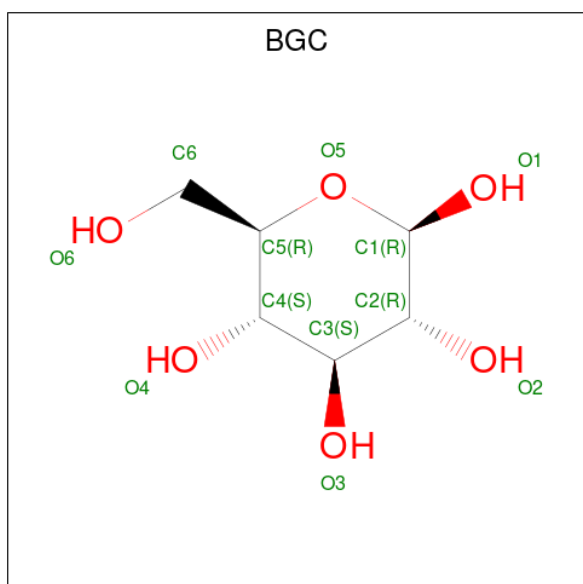
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	B	O	0	0
			4	1	3		
5	J	1	Total	B	O	0	0
			4	1	3		
5	O	1	Total	B	O	0	0
			4	1	3		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



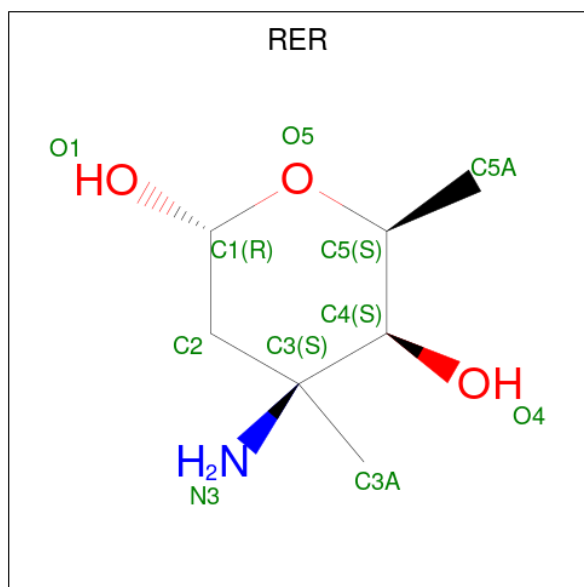
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			S
6	G	1	8	4	2	2	0	1
6	H	1	4	2	1	1	0	0
6	H	1	4	2	1	1	0	0
6	J	1	4	2	1	1	0	0

- Molecule 7 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total C O 24 12 12	0	1
7	H	1	Total C O 24 12 12	0	1

- Molecule 8 is vancosamine (three-letter code: RER) (formula: C₇H₁₅NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total C N O 20 14 2 4	0	1
8	H	1	Total C N O 20 14 2 4	0	1

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	19	Total O 19 19	0	2
9	B	16	Total O 17 17	0	1
9	C	26	Total O 26 26	0	5
9	D	22	Total O 22 22	0	3
9	E	25	Total O 26 26	0	1
9	F	19	Total O 20 20	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	22	Total O 23 23	0	1
9	H	18	Total O 19 19	0	5
9	I	13	Total O 14 14	0	1
9	J	17	Total O 17 17	0	0
9	K	7	Total O 7 7	0	0
9	L	6	Total O 6 6	0	1
9	M	11	Total O 12 12	0	2
9	N	5	Total O 5 5	0	0
9	O	8	Total O 8 8	0	0
9	P	5	Total O 6 6	0	1
9	Q	3	Total O 3 3	0	0
9	R	3	Total O 3 3	0	0
9	S	10	Total O 10 10	0	3
9	T	3	Total O 3 3	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

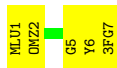
- Molecule 1: Vancomycin

Chain A:  29% 71%

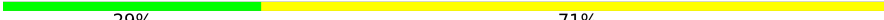


- Molecule 1: Vancomycin

Chain B:  29% 71%



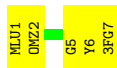
- Molecule 1: Vancomycin

Chain C:  29% 71%



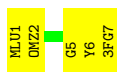
- Molecule 1: Vancomycin

Chain D:  29% 71%



- Molecule 1: Vancomycin

Chain E:  29% 71%



- Molecule 1: Vancomycin

Chain F:  29% 71%



- Molecule 1: Vancomycin



- Molecule 1: Vancomycin



- Molecule 1: Vancomycin



- Molecule 1: Vancomycin



- Molecule 2: D-Ala-D-Ser



There are no outlier residues recorded for this chain.

- Molecule 2: D-Ala-D-Ser



There are no outlier residues recorded for this chain.

- Molecule 2: D-Ala-D-Ser



There are no outlier residues recorded for this chain.

- Molecule 2: D-Ala-D-Ser



There are no outlier residues recorded for this chain.

- Molecule 2: D-Ala-D-Ser

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: D-Ala-D-Ser

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: D-Ala-D-Ser

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: D-Ala-D-Ser

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: D-Ala-D-Ser

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: D-Ala-D-Ser

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain U:  50% 50%

REC1
REC2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain W:  50% 50%


REC1
REC2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain Y:  50% 50%

BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain a:  100%BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain c:  50% 50%BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain e:  50% 50%BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain k:  50% 50%BGC1
RER2

- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain m:  50% 50%BGC1
RER2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	30.49Å 71.15Å 82.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.53 – 1.20 26.53 – 1.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (26.53-1.20) 93.0 (26.53-1.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.20Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.153 , 0.171 0.153 , 0.173	Depositor DCC
R_{free} test set	2000 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtrriage
Anisotropy	0.404	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1542	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.76% 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: MLU, PGE, GHP, DAL, BO3, BGC, 3FG, DSN, RER, OMZ, OMY, ACE, DMS

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	0.79	0/7	1.02	0/8
1	B	0.84	0/7	0.74	0/8
1	C	0.77	0/7	0.64	0/8
1	D	0.71	0/7	0.83	0/8
1	E	0.78	0/7	0.84	0/8
1	F	0.73	0/7	0.78	0/8
1	G	0.71	0/7	0.50	0/8
1	H	0.61	0/7	0.81	0/8
1	I	0.71	0/7	0.67	0/8
1	J	0.78	0/7	0.89	0/8
All	All	0.74	0/70	0.78	0/80

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	79	0	44	0	0
1	B	79	0	44	0	0
1	C	79	0	44	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	79	0	43	0	0
1	E	79	0	42	0	0
1	F	79	0	44	0	0
1	G	79	0	43	0	0
1	H	79	0	43	0	0
1	I	79	0	42	0	0
1	J	79	0	43	0	0
2	K	15	0	11	0	0
2	L	30	0	24	0	0
2	M	15	0	12	0	0
2	N	15	0	12	0	0
2	O	15	0	12	0	0
2	P	15	0	12	0	0
2	Q	15	0	12	0	0
2	R	15	0	12	0	0
2	S	30	0	24	0	0
2	T	15	0	12	0	0
3	U	22	0	23	0	0
3	W	22	0	23	0	0
3	Y	22	0	23	0	0
3	a	22	0	23	0	0
3	c	22	0	23	0	0
3	e	22	0	23	0	0
3	k	22	0	23	0	0
3	m	22	0	23	0	0
4	A	10	0	14	0	0
5	D	4	0	3	0	0
5	J	4	0	3	0	0
5	O	4	0	3	0	0
6	G	8	0	12	0	0
6	H	8	0	12	0	0
6	J	4	0	6	0	0
7	G	24	0	18	0	0
7	H	24	0	18	0	0
8	G	20	0	26	0	0
8	H	20	0	26	0	0
9	A	19	0	0	0	0
9	B	17	0	0	0	0
9	C	26	0	0	0	0
9	D	22	0	0	0	0
9	E	26	0	0	0	0
9	F	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	23	0	0	0	0
9	H	19	0	0	0	0
9	I	14	0	0	0	0
9	J	17	0	0	0	0
9	K	7	0	0	0	0
9	L	6	0	0	0	0
9	M	12	0	0	0	0
9	N	5	0	0	0	0
9	O	8	0	0	0	0
9	P	6	0	0	0	0
9	Q	3	0	0	0	0
9	R	3	0	0	0	0
9	S	10	0	0	0	0
9	T	3	0	0	0	0
All	All	1542	0	900	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1/7 (14%)	1 (100%)	0	0	100	100
1	B	1/7 (14%)	1 (100%)	0	0	100	100
1	C	1/7 (14%)	0	1 (100%)	0	100	100
1	D	1/7 (14%)	0	1 (100%)	0	100	100
1	E	1/7 (14%)	0	1 (100%)	0	100	100
1	F	1/7 (14%)	0	1 (100%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	1/7 (14%)	0	1 (100%)	0	100	100
1	H	1/7 (14%)	1 (100%)	0	0	100	100
1	I	1/7 (14%)	0	1 (100%)	0	100	100
1	J	1/7 (14%)	1 (100%)	0	0	100	100
All	All	10/70 (14%)	4 (40%)	6 (60%)	0	100	100

There are no Ramachandran outliers to report.

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	1/1 (100%)	1 (100%)	0	100	100
1	B	1/1 (100%)	1 (100%)	0	100	100
1	C	1/1 (100%)	1 (100%)	0	100	100
1	D	1/1 (100%)	1 (100%)	0	100	100
1	E	1/1 (100%)	1 (100%)	0	100	100
1	F	1/1 (100%)	1 (100%)	0	100	100
1	G	1/1 (100%)	1 (100%)	0	100	100
1	H	1/1 (100%)	1 (100%)	0	100	100
1	I	1/1 (100%)	1 (100%)	0	100	100
1	J	1/1 (100%)	1 (100%)	0	100	100
All	All	10/10 (100%)	10 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

84 non-standard protein/DNA/RNA residues 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
1	GHP	B	5	1	10,11,12	0.99	0	11,14,16	1.23	1 (9%)
1	MLU	G	1	1	7,8,9	0.66	0	6,9,11	1.16	1 (16%)
1	GHP	I	4	1	9,10,12	1.34	1 (11%)	9,12,16	0.78	0
1	GHP	H	5	1	10,11,12	1.48	1 (10%)	11,14,16	1.47	3 (27%)
1	OMY	E	6	1	12,14,15	2.47	3 (25%)	17,19,21	1.65	1 (5%)
1	3FG	G	7	1	12,13,13	1.02	1 (8%)	14,18,18	1.21	1 (7%)
1	OMZ	B	2	1	12,14,15	0.51	0	17,19,21	1.14	2 (11%)
1	OMZ	A	2	1	12,14,15	0.46	0	17,19,21	1.35	3 (17%)
1	OMZ	H	2	1	12,14,15	0.41	0	17,19,21	1.16	2 (11%)
1	GHP	C	4	1	9,10,12	1.14	0	9,12,16	1.03	0
1	GHP	J	4	1	9,10,12	1.02	0	9,12,16	0.61	0
1	GHP	F	4	1	9,10,12	0.84	0	9,12,16	0.41	0
1	OMY	A	6	1	12,14,15	2.17	1 (8%)	17,19,21	1.79	1 (5%)
1	GHP	A	4	1	9,10,12	0.96	0	9,12,16	0.62	0
1	3FG	C	7	1	12,13,13	1.00	1 (8%)	14,18,18	1.10	1 (7%)
1	OMY	D	6	1	12,14,15	2.15	1 (8%)	17,19,21	1.70	1 (5%)
1	OMY	J	6	1	12,14,15	2.71	2 (16%)	17,19,21	1.83	1 (5%)
1	MLU	A	1	1	7,8,9	0.59	0	6,9,11	1.12	1 (16%)
1	OMZ	F	2	1	12,14,15	0.48	0	17,19,21	1.10	2 (11%)
1	GHP	G	4	1	9,10,12	0.81	0	9,12,16	0.47	0
1	GHP	C	5	1	10,11,12	1.50	2 (20%)	11,14,16	1.47	1 (9%)
1	GHP	E	5	1	10,11,12	1.09	1 (10%)	11,14,16	1.32	2 (18%)
1	OMY	G	6	1	12,14,15	2.25	2 (16%)	17,19,21	1.50	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	3FG	A	7	1	12,13,13	0.94	0	14,18,18	0.79	1 (7%)
1	MLU	C	1	1	7,8,9	0.56	0	6,9,11	1.08	1 (16%)
1	OMY	F	6	1	12,14,15	2.09	1 (8%)	17,19,21	1.77	1 (5%)
1	OMZ	I	2	1	12,14,15	0.59	0	17,19,21	0.89	1 (5%)
1	GHP	H	4	1	9,10,12	0.97	1 (11%)	9,12,16	0.54	0
1	GHP	A	5	1	10,11,12	1.34	1 (10%)	11,14,16	1.29	1 (9%)
1	3FG	E	7	1	12,13,13	1.09	1 (8%)	14,18,18	0.91	1 (7%)
1	3FG	F	7	1	12,13,13	1.25	2 (16%)	14,18,18	1.08	1 (7%)
1	GHP	J	5	1	10,11,12	1.25	1 (10%)	11,14,16	1.14	1 (9%)
1	3FG	B	7	1	12,13,13	1.07	0	14,18,18	1.18	2 (14%)
1	3FG	H	7	1	12,13,13	1.10	1 (8%)	14,18,18	1.10	1 (7%)
1	MLU	B	1	1	7,8,9	0.57	0	6,9,11	1.06	1 (16%)
1	GHP	D	5	1	10,11,12	0.96	0	11,14,16	1.40	2 (18%)
1	GHP	F	5	1	10,11,12	1.09	0	11,14,16	1.27	2 (18%)
1	MLU	F	1	1	7,8,9	0.53	0	6,9,11	1.17	1 (16%)
1	GHP	E	4	1	9,10,12	0.96	0	9,12,16	0.65	0
1	OMY	I	6	1	12,14,15	2.40	1 (8%)	17,19,21	1.62	1 (5%)
1	OMY	C	6	1	12,14,15	2.28	2 (16%)	17,19,21	1.63	1 (5%)
1	OMZ	E	2	1	12,14,15	0.41	0	17,19,21	1.25	3 (17%)
1	OMY	H	6	1	12,14,15	2.04	2 (16%)	17,19,21	1.62	1 (5%)
1	OMZ	D	2	1	12,14,15	0.50	0	17,19,21	1.01	1 (5%)
1	OMZ	J	2	1	12,14,15	0.51	0	17,19,21	1.02	1 (5%)
1	3FG	I	7	1	12,13,13	1.32	2 (16%)	14,18,18	0.94	1 (7%)
1	GHP	D	4	1	9,10,12	0.82	0	9,12,16	0.51	0
1	GHP	I	5	1	10,11,12	0.97	0	11,14,16	1.19	1 (9%)
1	MLU	E	1	1	7,8,9	0.61	0	6,9,11	1.41	1 (16%)
1	OMY	B	6	1	12,14,15	1.78	1 (8%)	17,19,21	1.54	1 (5%)
1	MLU	D	1	1	7,8,9	0.43	0	6,9,11	1.21	1 (16%)
1	MLU	I	1	1	7,8,9	0.54	0	6,9,11	1.22	1 (16%)
1	OMZ	C	2	1	12,14,15	0.44	0	17,19,21	1.48	3 (17%)
1	3FG	J	7	1	12,13,13	0.91	0	14,18,18	0.80	0
1	OMZ	G	2	1	12,14,15	0.41	0	17,19,21	1.03	1 (5%)
1	3FG	D	7	1	12,13,13	0.99	0	14,18,18	1.06	1 (7%)
1	MLU	H	1	1	7,8,9	0.54	0	6,9,11	1.11	1 (16%)
1	GHP	B	4	1	9,10,12	0.97	0	9,12,16	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GHP	G	5	1	10,11,12	1.27	0	11,14,16	1.40	2 (18%)
1	MLU	J	1	1	7,8,9	0.58	0	6,9,11	1.11	1 (16%)

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
1	GHP	B	5	1	-	0/4/6/8	0/1/1/1
1	MLU	G	1	1	-	0/5/8/10	-
1	GHP	I	4	1	-	2/4/6/8	0/1/1/1
1	GHP	H	5	1	-	0/4/6/8	0/1/1/1
1	OMY	E	6	1	-	1/9/10/12	0/1/1/1
1	3FG	G	7	1	-	1/8/8/8	0/1/1/1
1	OMZ	B	2	1	-	0/9/10/12	0/1/1/1
1	OMZ	A	2	1	-	0/9/10/12	0/1/1/1
1	OMZ	H	2	1	-	1/9/10/12	0/1/1/1
1	GHP	C	4	1	-	1/4/6/8	0/1/1/1
1	GHP	J	4	1	-	2/4/6/8	0/1/1/1
1	GHP	F	4	1	-	3/4/6/8	0/1/1/1
1	OMY	A	6	1	-	1/9/10/12	0/1/1/1
1	GHP	A	4	1	-	2/4/6/8	0/1/1/1
1	3FG	C	7	1	-	5/8/8/8	0/1/1/1
1	OMY	D	6	1	-	1/9/10/12	0/1/1/1
1	OMY	J	6	1	-	1/9/10/12	0/1/1/1
1	MLU	A	1	1	-	0/5/8/10	-
1	OMZ	F	2	1	-	0/9/10/12	0/1/1/1
1	GHP	G	4	1	-	1/4/6/8	0/1/1/1
1	GHP	C	5	1	-	0/4/6/8	0/1/1/1
1	GHP	E	5	1	-	0/4/6/8	0/1/1/1
1	OMY	G	6	1	-	1/9/10/12	0/1/1/1
1	3FG	A	7	1	-	2/8/8/8	0/1/1/1
1	MLU	C	1	1	-	0/5/8/10	-
1	OMY	F	6	1	-	1/9/10/12	0/1/1/1
1	OMZ	I	2	1	-	0/9/10/12	0/1/1/1
1	GHP	H	4	1	-	2/4/6/8	0/1/1/1
1	GHP	A	5	1	-	0/4/6/8	0/1/1/1
1	3FG	E	7	1	-	4/8/8/8	0/1/1/1
1	3FG	F	7	1	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GHP	J	5	1	-	0/4/6/8	0/1/1/1
1	3FG	B	7	1	-	2/8/8/8	0/1/1/1
1	3FG	H	7	1	-	2/8/8/8	0/1/1/1
1	MLU	B	1	1	-	0/5/8/10	-
1	GHP	D	5	1	-	0/4/6/8	0/1/1/1
1	GHP	F	5	1	-	0/4/6/8	0/1/1/1
1	MLU	F	1	1	-	0/5/8/10	-
1	GHP	E	4	1	-	1/4/6/8	0/1/1/1
1	OMY	I	6	1	-	1/9/10/12	0/1/1/1
1	OMY	C	6	1	-	1/9/10/12	0/1/1/1
1	OMZ	E	2	1	-	0/9/10/12	0/1/1/1
1	OMY	H	6	1	-	1/9/10/12	0/1/1/1
1	OMZ	D	2	1	-	0/9/10/12	0/1/1/1
1	OMZ	J	2	1	-	0/9/10/12	0/1/1/1
1	3FG	I	7	1	-	2/8/8/8	0/1/1/1
1	GHP	D	4	1	-	2/4/6/8	0/1/1/1
1	GHP	I	5	1	-	0/4/6/8	0/1/1/1
1	MLU	E	1	1	-	0/5/8/10	-
1	OMY	B	6	1	-	1/9/10/12	0/1/1/1
1	MLU	D	1	1	-	0/5/8/10	-
1	MLU	I	1	1	-	0/5/8/10	-
1	OMZ	C	2	1	-	0/9/10/12	0/1/1/1
1	3FG	J	7	1	-	2/8/8/8	0/1/1/1
1	OMZ	G	2	1	-	1/9/10/12	0/1/1/1
1	3FG	D	7	1	-	3/8/8/8	0/1/1/1
1	MLU	H	1	1	-	0/5/8/10	-
1	GHP	B	4	1	-	2/4/6/8	0/1/1/1
1	GHP	G	5	1	-	0/4/6/8	0/1/1/1
1	MLU	J	1	1	-	0/5/8/10	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	6	OMY	CZ-CE1	8.82	1.47	1.39
1	I	6	OMY	CZ-CE1	7.69	1.46	1.39
1	E	6	OMY	CZ-CE1	7.58	1.46	1.39
1	C	6	OMY	CZ-CE1	6.95	1.46	1.39
1	A	6	OMY	CZ-CE1	6.87	1.46	1.39
1	G	6	OMY	CZ-CE1	6.78	1.46	1.39
1	D	6	OMY	CZ-CE1	6.68	1.45	1.39
1	F	6	OMY	CZ-CE1	6.26	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	6	OMY	CZ-CE1	6.02	1.45	1.39
1	B	6	OMY	CZ-CE1	5.24	1.44	1.39
1	H	5	GHP	C1-CA	-3.35	1.49	1.52
1	A	5	GHP	C1-CA	-3.34	1.49	1.52
1	J	5	GHP	C1-CA	-3.17	1.49	1.52
1	I	4	GHP	C1-CA	-3.04	1.49	1.52
1	C	5	GHP	C1-CA	-2.81	1.49	1.52
1	I	7	3FG	CG1-CD1	2.48	1.42	1.39
1	F	7	3FG	CG1-CD1	2.44	1.42	1.39
1	C	6	OMY	CD2-CG	2.42	1.43	1.39
1	H	6	OMY	CG-CB	-2.29	1.48	1.51
1	C	5	GHP	C2-C1	2.25	1.42	1.39
1	J	6	OMY	CG-CB	-2.23	1.48	1.51
1	H	7	3FG	CG1-CB	2.20	1.42	1.39
1	E	6	OMY	CG-CB	-2.17	1.48	1.51
1	G	6	OMY	CG-CB	-2.13	1.48	1.51
1	G	7	3FG	CG1-CB	2.11	1.42	1.39
1	F	7	3FG	CG1-CB	2.08	1.42	1.39
1	E	6	OMY	CD2-CG	2.08	1.42	1.39
1	I	7	3FG	CB-CA	2.07	1.55	1.52
1	C	7	3FG	CG1-CB	2.07	1.42	1.39
1	E	5	GHP	C1-CA	-2.04	1.50	1.52
1	H	4	GHP	C1-CA	-2.02	1.50	1.52
1	E	7	3FG	CG1-CB	2.01	1.42	1.39

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	OMY	CG-CB-CA	-6.70	102.52	111.49
1	J	6	OMY	CG-CB-CA	-6.62	102.63	111.49
1	F	6	OMY	CG-CB-CA	-6.50	102.79	111.49
1	D	6	OMY	CG-CB-CA	-6.11	103.31	111.49
1	H	6	OMY	CG-CB-CA	-6.02	103.43	111.49
1	E	6	OMY	CG-CB-CA	-5.94	103.53	111.49
1	C	6	OMY	CG-CB-CA	-5.85	103.66	111.49
1	I	6	OMY	CG-CB-CA	-5.80	103.72	111.49
1	B	6	OMY	CG-CB-CA	-5.66	103.91	111.49
1	G	6	OMY	CG-CB-CA	-5.45	104.19	111.49
1	G	7	3FG	CD1-CG1-CB	-3.68	116.96	120.11
1	B	7	3FG	CD1-CG1-CB	-3.37	117.22	120.11
1	C	7	3FG	CD1-CG1-CB	-3.35	117.24	120.11
1	F	2	OMZ	O-C-CA	-3.35	116.00	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	GHP	C1-CA-N	3.35	120.42	112.40
1	F	7	3FG	CD1-CG1-CB	-3.34	117.24	120.11
1	C	5	GHP	C1-CA-N	3.30	120.31	112.40
1	E	2	OMZ	O-C-CA	-3.25	116.26	124.78
1	B	5	GHP	C1-CA-N	3.24	120.17	112.40
1	H	7	3FG	CD1-CG1-CB	-3.23	117.34	120.11
1	I	5	GHP	C1-CA-N	3.20	120.06	112.40
1	D	7	3FG	CD1-CG1-CB	-3.18	117.38	120.11
1	C	2	OMZ	O-C-CA	-3.16	116.49	124.78
1	D	2	OMZ	O-C-CA	-3.13	116.57	124.78
1	G	5	GHP	C1-CA-N	3.09	119.80	112.40
1	H	5	GHP	C1-CA-N	3.06	119.73	112.40
1	B	2	OMZ	O-C-CA	-3.04	116.80	124.78
1	H	2	OMZ	O-C-CA	-3.03	116.83	124.78
1	E	5	GHP	C1-CA-N	3.03	119.65	112.40
1	J	5	GHP	C1-CA-N	2.98	119.53	112.40
1	A	2	OMZ	O-C-CA	-2.95	117.04	124.78
1	D	5	GHP	C1-CA-N	2.94	119.45	112.40
1	E	1	MLU	O-C-CA	-2.94	117.09	124.78
1	I	1	MLU	O-C-CA	-2.92	117.12	124.78
1	I	2	OMZ	O-C-CA	-2.90	117.17	124.78
1	C	2	OMZ	CD1-CE1-CZ	2.89	122.59	120.91
1	C	2	OMZ	OH-CZ-CE2	2.87	127.15	119.33
1	G	2	OMZ	O-C-CA	-2.82	117.38	124.78
1	G	1	MLU	O-C-CA	-2.82	117.39	124.78
1	F	1	MLU	O-C-CA	-2.78	117.48	124.78
1	F	5	GHP	C1-CA-N	2.78	119.06	112.40
1	D	1	MLU	O-C-CA	-2.76	117.53	124.78
1	B	2	OMZ	CD1-CE1-CZ	2.75	122.51	120.91
1	I	7	3FG	CD1-CG1-CB	-2.74	117.76	120.11
1	A	2	OMZ	CD1-CE1-CZ	2.72	122.49	120.91
1	E	7	3FG	CD1-CG1-CB	-2.72	117.78	120.11
1	H	1	MLU	O-C-CA	-2.71	117.67	124.78
1	J	1	MLU	O-C-CA	-2.67	117.78	124.78
1	J	2	OMZ	O-C-CA	-2.62	117.90	124.78
1	C	1	MLU	O-C-CA	-2.60	117.97	124.78
1	B	1	MLU	O-C-CA	-2.57	118.04	124.78
1	F	5	GHP	C2-C3-C4	-2.52	117.11	119.88
1	A	1	MLU	O-C-CA	-2.52	118.18	124.78
1	A	2	OMZ	OH-CZ-CE2	2.48	126.08	119.33
1	H	5	GHP	C5-C6-C1	-2.36	118.83	121.20
1	E	2	OMZ	CD1-CE1-CZ	2.36	122.28	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	2	OMZ	CD1-CE1-CZ	2.32	122.26	120.91
1	D	5	GHP	C2-C3-C4	-2.32	117.33	119.88
1	E	2	OMZ	OH-CZ-CE2	2.26	125.49	119.33
1	G	5	GHP	C2-C3-C4	-2.15	117.52	119.88
1	E	5	GHP	C2-C3-C4	-2.13	117.53	119.88
1	B	7	3FG	CG2-CB-CG1	2.12	121.10	118.08
1	F	2	OMZ	OH-CZ-CE2	2.11	125.07	119.33
1	A	7	3FG	CD1-CG1-CB	-2.05	118.36	120.11
1	H	5	GHP	C2-C3-C4	-2.04	117.64	119.88

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	6	OMY	O-C-CA-CB
1	B	6	OMY	O-C-CA-CB
1	C	6	OMY	O-C-CA-CB
1	D	6	OMY	O-C-CA-CB
1	E	6	OMY	O-C-CA-CB
1	F	6	OMY	O-C-CA-CB
1	H	6	OMY	O-C-CA-CB
1	I	6	OMY	O-C-CA-CB
1	J	6	OMY	O-C-CA-CB
1	C	7	3FG	C-CA-CB-CG2
1	C	7	3FG	O-C-CA-CB
1	C	7	3FG	OXT-C-CA-CB
1	D	7	3FG	O-C-CA-CB
1	D	7	3FG	OXT-C-CA-CB
1	E	7	3FG	O-C-CA-CB
1	E	7	3FG	OXT-C-CA-CB
1	C	7	3FG	C-CA-CB-CG1
1	A	7	3FG	C-CA-CB-CG2
1	B	7	3FG	C-CA-CB-CG1
1	B	7	3FG	C-CA-CB-CG2
1	I	7	3FG	C-CA-CB-CG2
1	J	7	3FG	C-CA-CB-CG2
1	A	7	3FG	C-CA-CB-CG1
1	E	7	3FG	C-CA-CB-CG2
1	G	7	3FG	C-CA-CB-CG2
1	H	7	3FG	C-CA-CB-CG1
1	H	7	3FG	C-CA-CB-CG2
1	I	7	3FG	C-CA-CB-CG1

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Mol	Chain	Res	Type	Atoms
1	J	7	3FG	C-CA-CB-CG1
1	C	7	3FG	OXT-C-CA-N
1	D	7	3FG	OXT-C-CA-N
1	E	7	3FG	OXT-C-CA-N
1	F	4	GHP	C2-C1-CA-N
1	G	2	OMZ	O-C-CA-CB
1	H	2	OMZ	O-C-CA-CB
1	G	6	OMY	O-C-CA-CB
1	A	4	GHP	C2-C1-CA-C
1	A	4	GHP	C6-C1-CA-C
1	B	4	GHP	C2-C1-CA-C
1	B	4	GHP	C6-C1-CA-C
1	F	4	GHP	C2-C1-CA-C
1	G	4	GHP	C6-C1-CA-C
1	H	4	GHP	C6-C1-CA-C
1	I	4	GHP	C2-C1-CA-C
1	I	4	GHP	C6-C1-CA-C
1	J	4	GHP	C6-C1-CA-C
1	C	4	GHP	C2-C1-CA-N
1	D	4	GHP	C2-C1-CA-N
1	D	4	GHP	C6-C1-CA-N
1	E	4	GHP	C2-C1-CA-N
1	F	4	GHP	C6-C1-CA-N
1	H	4	GHP	C2-C1-CA-N
1	J	4	GHP	C2-C1-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

16 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	U	1	3	12,12,12	0.48	0	17,17,17	0.68	0
3	RER	U	2	3	6,10,11	1.77	1 (16%)	6,15,17	1.43	2 (33%)
3	BGC	W	1	3	12,12,12	0.46	0	17,17,17	0.89	0
3	RER	W	2	3	6,10,11	1.71	1 (16%)	6,15,17	0.92	0
3	BGC	Y	1	3	12,12,12	0.52	0	17,17,17	0.72	0
3	RER	Y	2	3	6,10,11	1.80	2 (33%)	6,15,17	1.02	1 (16%)
3	BGC	a	1	3	12,12,12	0.39	0	17,17,17	0.98	1 (5%)
3	RER	a	2	3	6,10,11	1.40	1 (16%)	6,15,17	1.15	0
3	BGC	c	1	3	12,12,12	0.42	0	17,17,17	0.67	0
3	RER	c	2	3	6,10,11	1.71	1 (16%)	6,15,17	1.14	1 (16%)
3	BGC	e	1	3	12,12,12	0.45	0	17,17,17	0.94	0
3	RER	e	2	3	6,10,11	1.59	1 (16%)	6,15,17	1.02	1 (16%)
3	BGC	k	1	3	12,12,12	0.39	0	17,17,17	0.72	0
3	RER	k	2	3	6,10,11	1.70	2 (33%)	6,15,17	0.66	0
3	BGC	m	1	3	12,12,12	0.45	0	17,17,17	0.60	0
3	RER	m	2	3	6,10,11	1.67	1 (16%)	6,15,17	0.92	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	U	1	3	-	0/2/22/22	0/1/1/1
3	RER	U	2	3	-	-	0/1/1/1
3	BGC	W	1	3	-	0/2/22/22	0/1/1/1
3	RER	W	2	3	-	-	0/1/1/1
3	BGC	Y	1	3	-	0/2/22/22	0/1/1/1
3	RER	Y	2	3	-	-	0/1/1/1
3	BGC	a	1	3	-	0/2/22/22	0/1/1/1
3	RER	a	2	3	-	-	0/1/1/1
3	BGC	c	1	3	-	0/2/22/22	0/1/1/1
3	RER	c	2	3	-	-	0/1/1/1
3	BGC	e	1	3	-	0/2/22/22	0/1/1/1
3	RER	e	2	3	-	-	0/1/1/1
3	BGC	k	1	3	-	1/2/22/22	0/1/1/1
3	RER	k	2	3	-	-	0/1/1/1
3	BGC	m	1	3	-	0/2/22/22	0/1/1/1
3	RER	m	2	3	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	2	RER	O5-C5	3.42	1.50	1.43
3	m	2	RER	O5-C5	3.26	1.50	1.43
3	Y	2	RER	O5-C5	3.22	1.50	1.43
3	U	2	RER	O5-C5	3.20	1.50	1.43
3	k	2	RER	O5-C5	2.94	1.49	1.43
3	W	2	RER	O5-C5	2.86	1.49	1.43
3	e	2	RER	O5-C5	2.79	1.49	1.43
3	a	2	RER	O5-C5	2.60	1.49	1.43
3	Y	2	RER	C5A-C5	-2.20	1.46	1.51
3	k	2	RER	C5A-C5	-2.10	1.46	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	2	RER	O5-C1-C2	2.54	114.96	111.38
3	a	1	BGC	O5-C5-C6	2.52	112.70	106.44
3	e	2	RER	O5-C5-C4	-2.21	106.08	110.03
3	U	2	RER	C5A-C5-C4	2.20	116.32	112.57
3	Y	2	RER	O5-C1-C2	2.09	114.33	111.38
3	c	2	RER	O5-C1-C2	2.01	114.22	111.38

There are no chirality outliers.

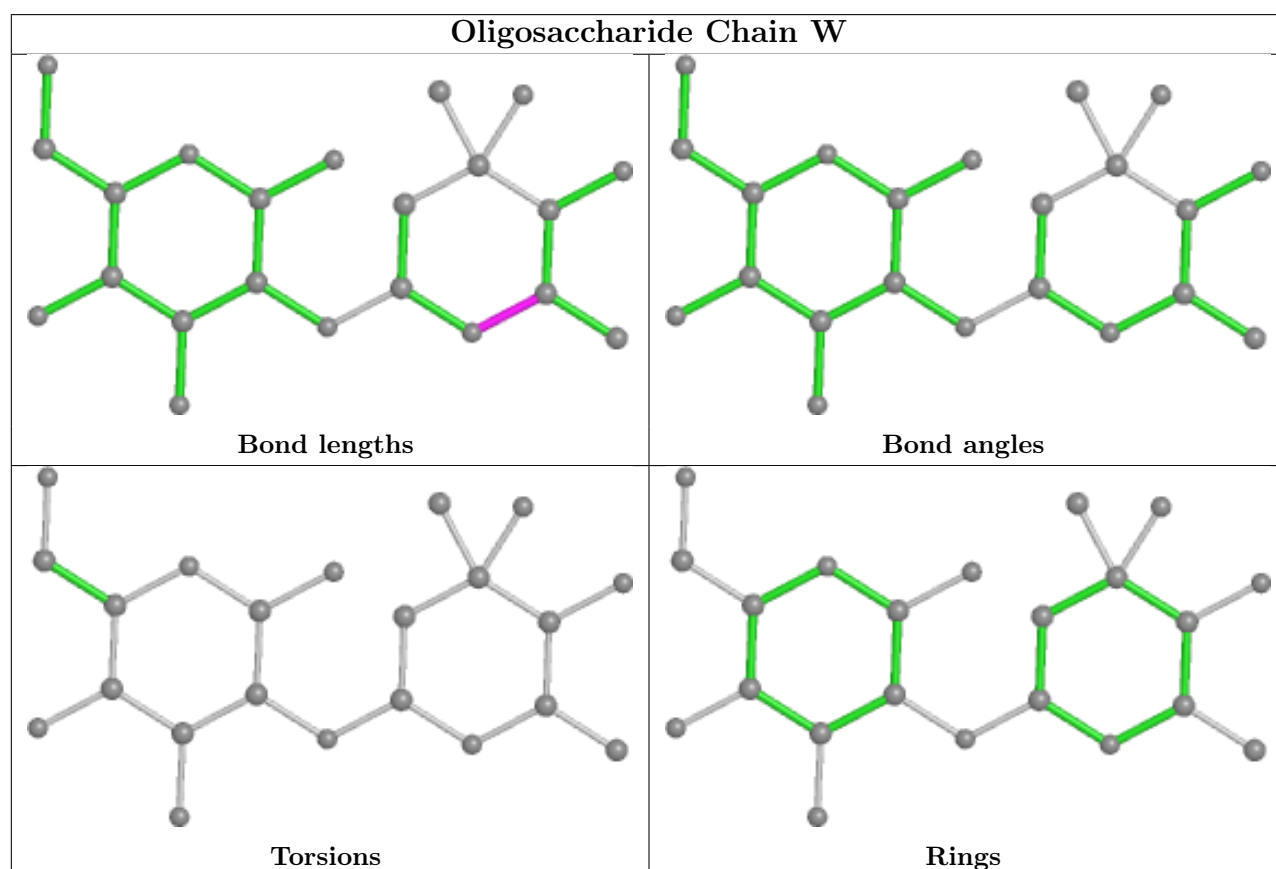
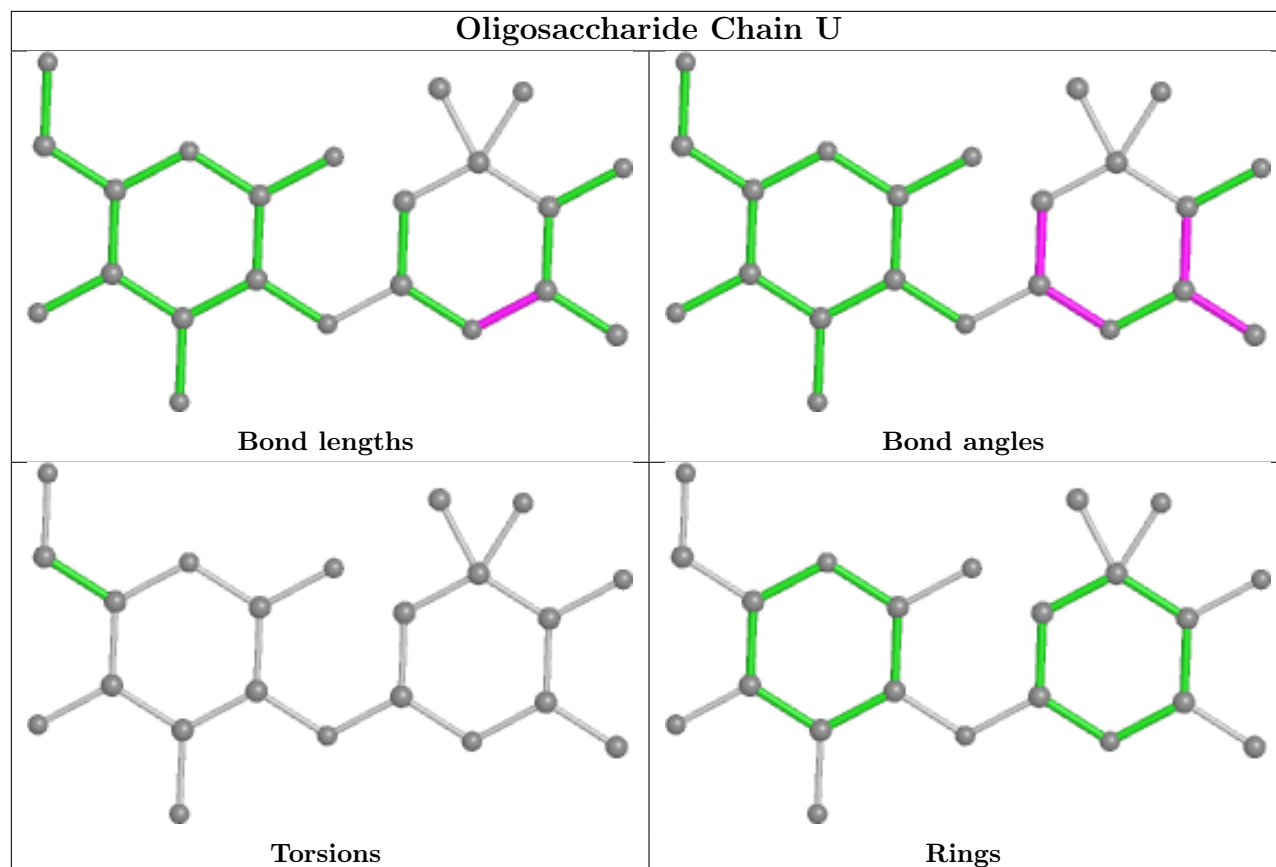
All (1) torsion outliers are listed below:

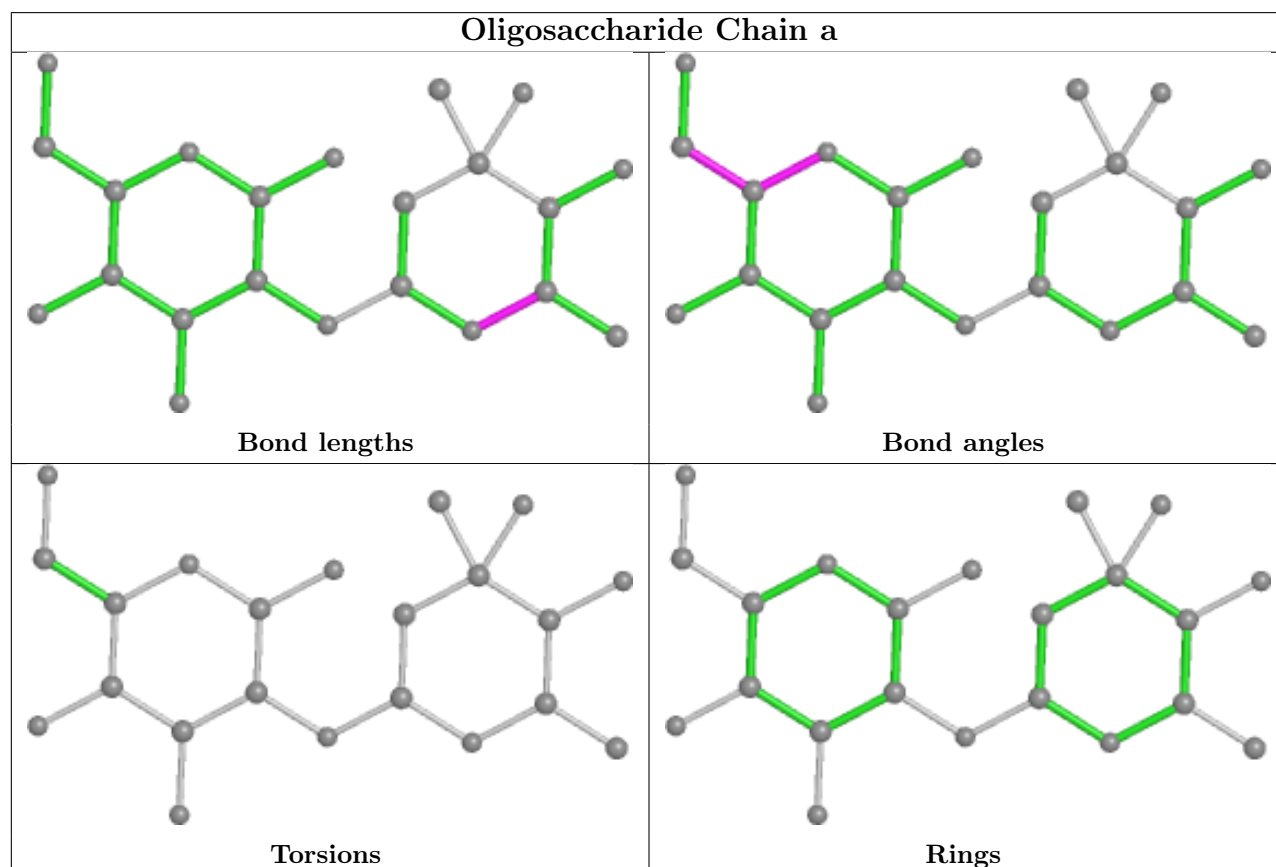
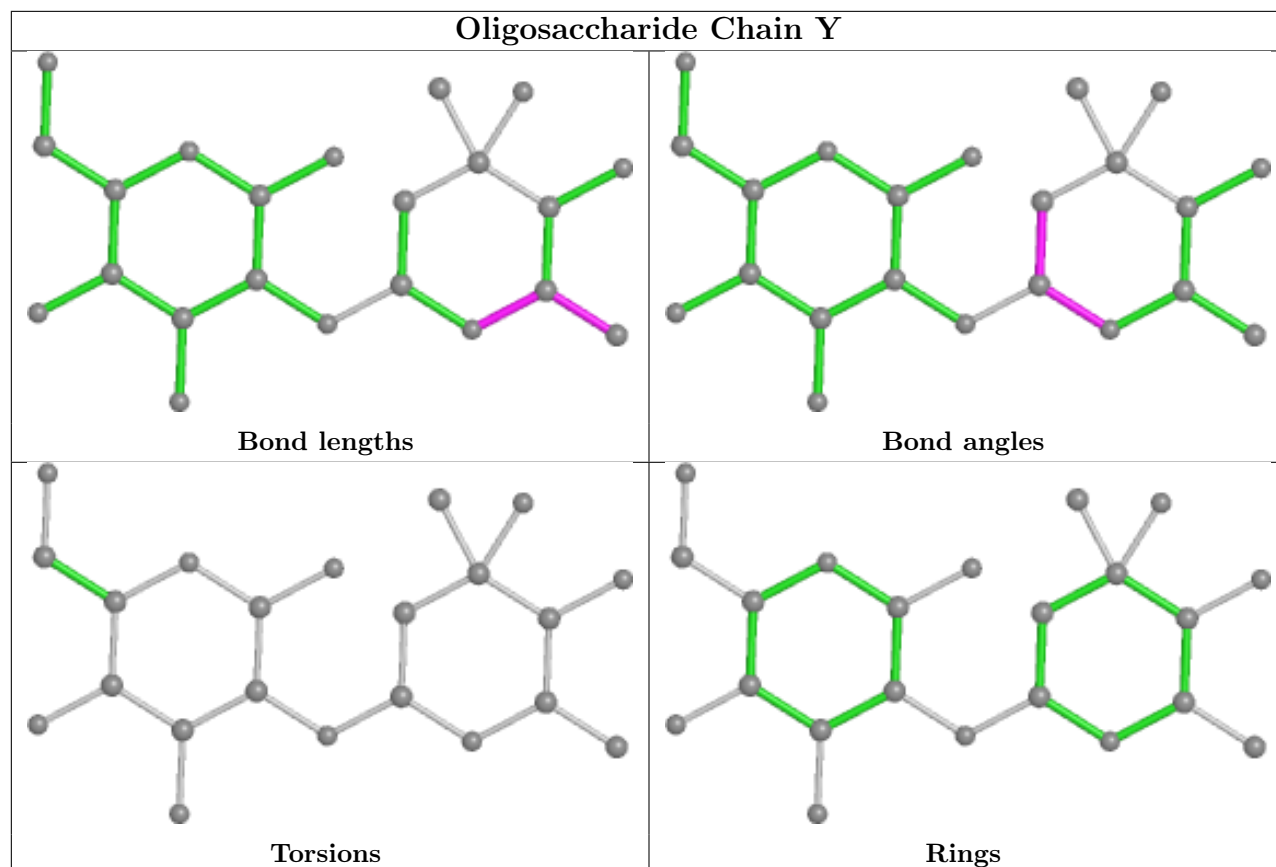
Mol	Chain	Res	Type	Atoms
3	k	1	BGC	O5-C5-C6-O6

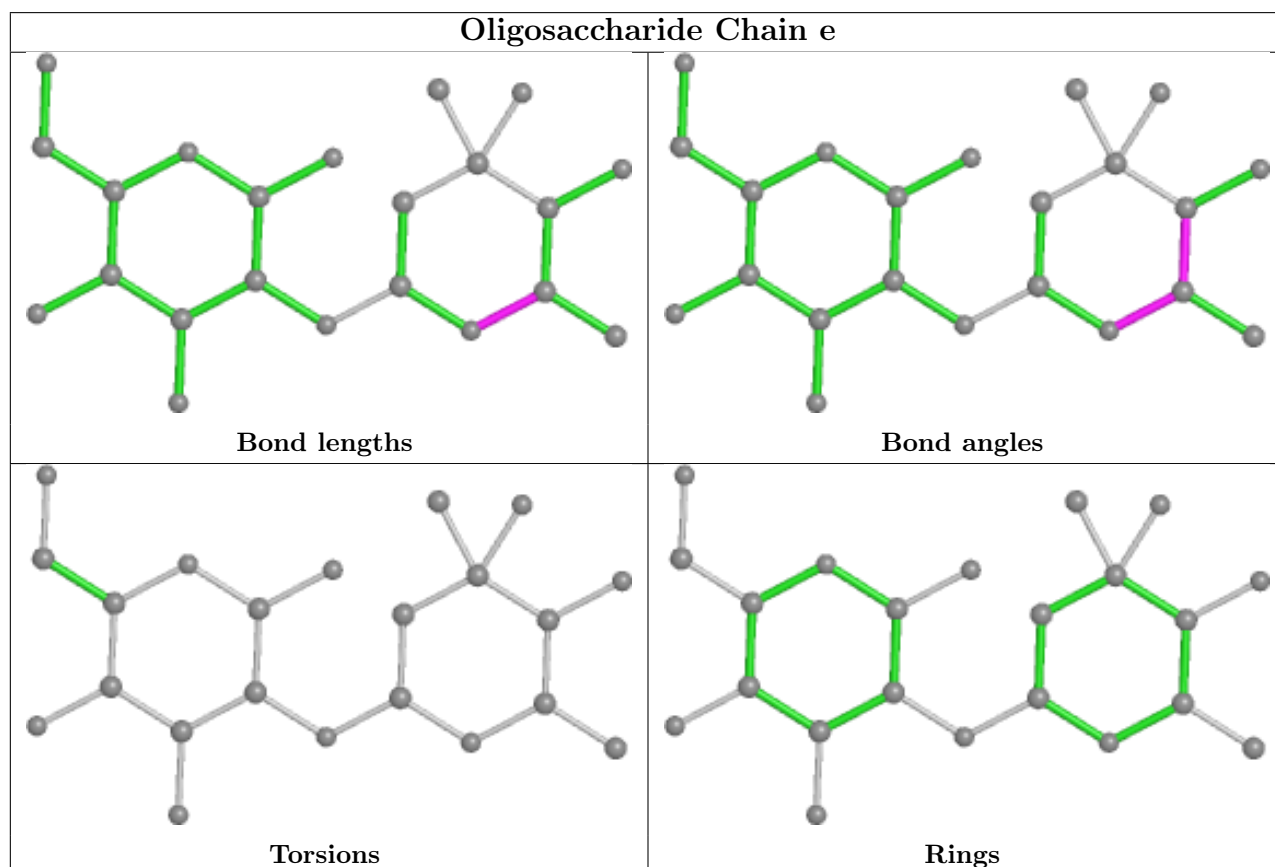
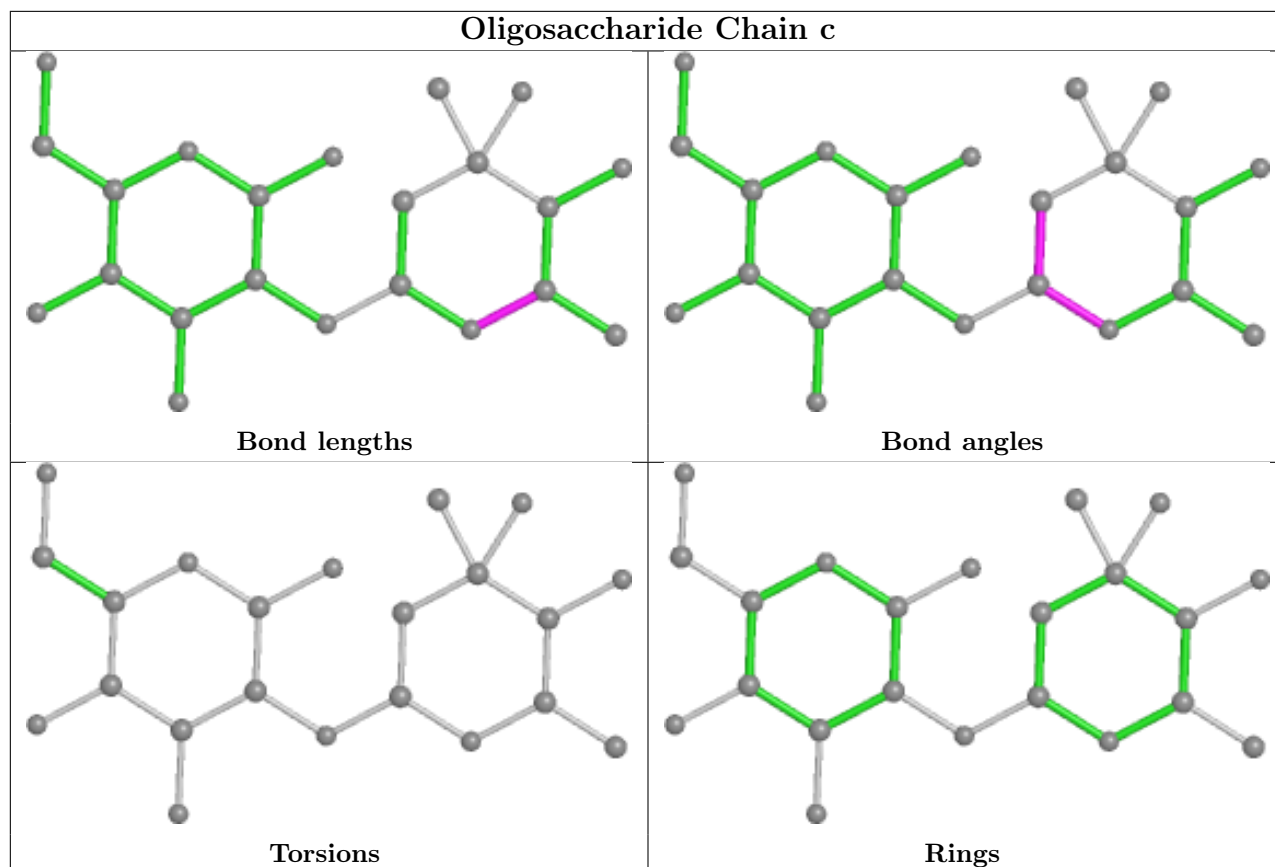
There are no ring outliers.

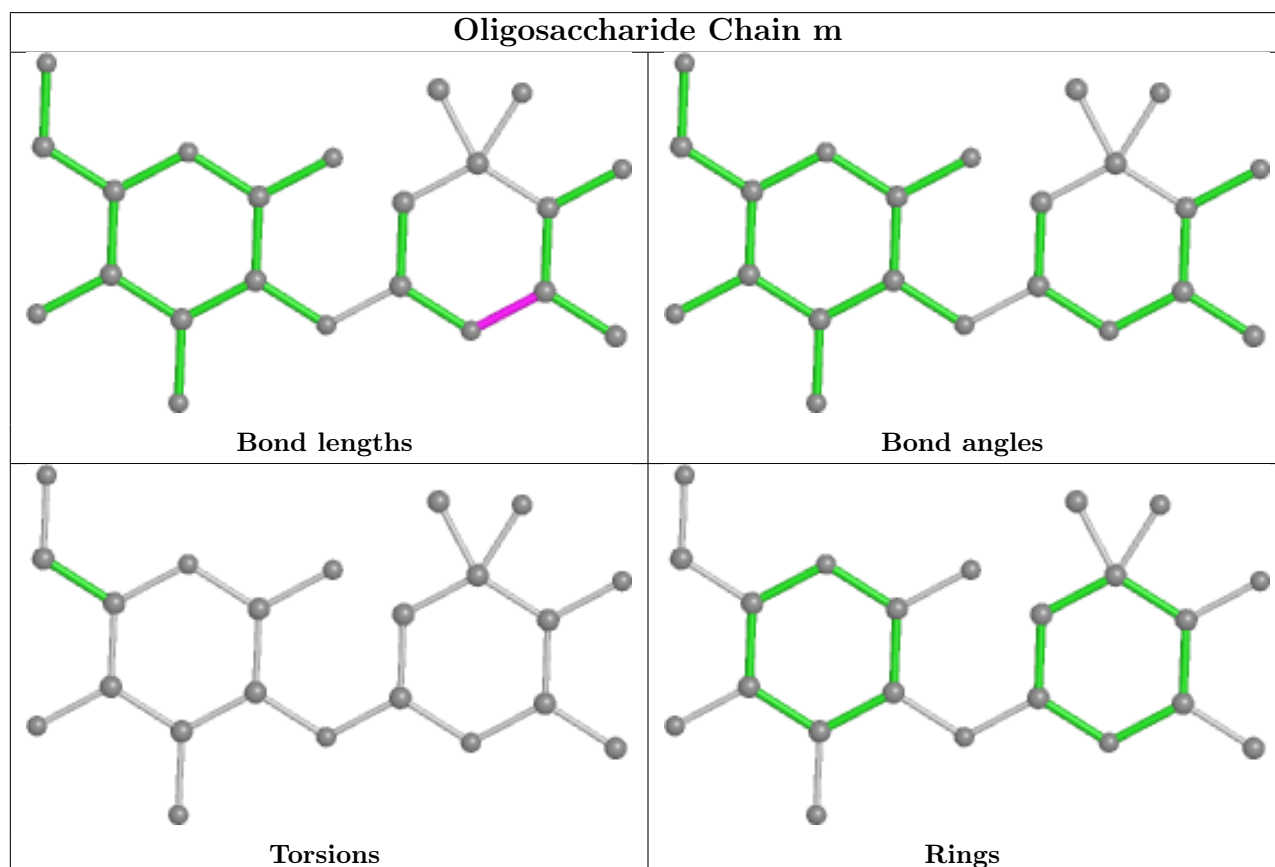
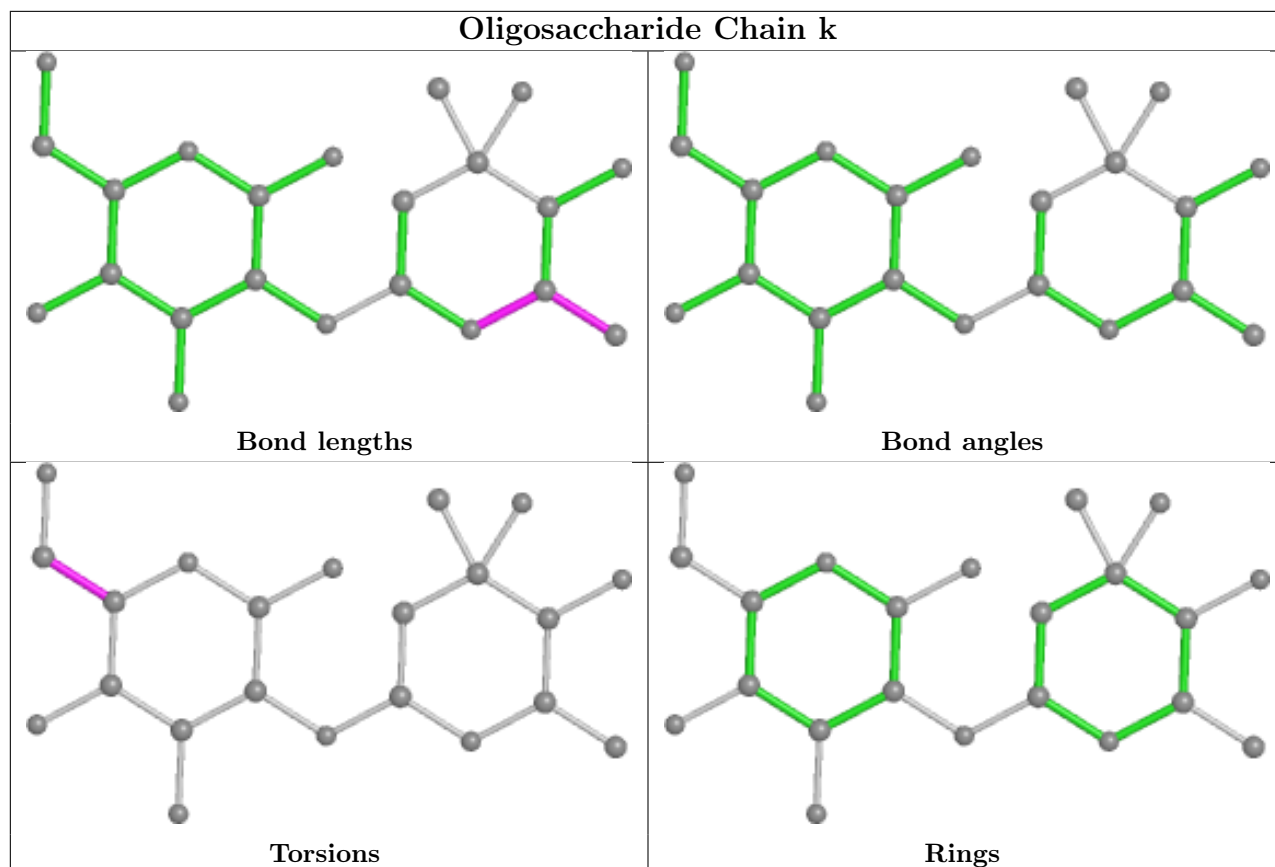
No monomer is involved in short contacts.

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](#)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PGE	A	101	-	9,9,9	0.52	0	8,8,8	0.36	0
7	BGC	H	103[A]	8	12,12,12	0.56	0	17,17,17	0.52	0
8	RER	G	103[B]	7	6,10,11	1.99	2 (33%)	6,15,17	1.52	1 (16%)
5	BO3	J	101	-	3,3,3	0.50	0	3,3,3	0.06	0
6	DMS	G	101[A]	-	3,3,3	0.56	0	3,3,3	0.23	0
6	DMS	H	102	-	3,3,3	0.46	0	3,3,3	0.51	0
7	BGC	G	102[B]	8	12,12,12	0.56	0	17,17,17	0.88	0
6	DMS	H	101	-	3,3,3	0.68	0	3,3,3	0.49	0
8	RER	H	104[B]	7	6,10,11	1.94	2 (33%)	6,15,17	1.71	1 (16%)
6	DMS	J	102	-	3,3,3	0.67	0	3,3,3	0.47	0
8	RER	G	103[A]	7	6,10,11	1.70	2 (33%)	6,15,17	1.14	1 (16%)
8	RER	H	104[A]	7	6,10,11	1.92	2 (33%)	6,15,17	0.91	0
7	BGC	G	102[A]	8	12,12,12	0.64	0	17,17,17	0.79	0
5	BO3	D	101	-	3,3,3	0.45	0	3,3,3	0.07	0
5	BO3	O	101	-	3,3,3	0.44	0	3,3,3	0.06	0
6	DMS	G	101[B]	-	3,3,3	0.61	0	3,3,3	0.50	0
7	BGC	H	103[B]	8	12,12,12	0.50	0	17,17,17	0.68	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. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	A	101	-	-	2/7/7/7	-
7	BGC	H	103[A]	8	-	0/2/22/22	0/1/1/1
8	RER	G	103[B]	7	-	-	0/1/1/1
7	BGC	G	102[B]	8	-	0/2/22/22	0/1/1/1
8	RER	H	104[B]	7	-	-	0/1/1/1
8	RER	G	103[A]	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	RER	H	104[A]	7	-	-	0/1/1/1
7	BGC	G	102[A]	8	-	0/2/22/22	0/1/1/1
7	BGC	H	103[B]	8	-	0/2/22/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	104[A]	RER	O5-C5	3.58	1.51	1.43
8	G	103[B]	RER	O5-C5	3.57	1.51	1.43
8	H	104[B]	RER	O5-C5	3.49	1.51	1.43
8	G	103[A]	RER	O5-C5	2.92	1.49	1.43
8	H	104[B]	RER	C5A-C5	-2.35	1.45	1.51
8	G	103[B]	RER	C5A-C5	-2.30	1.46	1.51
8	G	103[A]	RER	C5A-C5	-2.11	1.46	1.51
8	H	104[A]	RER	C5A-C5	-2.00	1.46	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	104[B]	RER	O5-C5-C4	3.18	115.72	110.03
8	G	103[B]	RER	O5-C1-C2	2.62	115.08	111.38
8	G	103[A]	RER	O5-C1-C2	2.35	114.69	111.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101	PGE	C1-C2-O2-C3
4	A	101	PGE	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1/7 (14%)	0.25	0 100 100	18, 18, 18, 18	0
1	B	1/7 (14%)	-0.19	0 100 100	13, 13, 13, 13	0
1	C	1/7 (14%)	-0.50	0 100 100	15, 15, 15, 15	0
1	D	1/7 (14%)	-0.62	0 100 100	12, 12, 12, 12	0
1	E	1/7 (14%)	-0.32	0 100 100	14, 14, 14, 14	0
1	F	1/7 (14%)	-0.68	0 100 100	13, 13, 13, 13	0
1	G	1/7 (14%)	-0.42	0 100 100	13, 13, 13, 13	0
1	H	1/7 (14%)	-0.68	0 100 100	13, 13, 13, 13	0
1	I	1/7 (14%)	-0.25	0 100 100	14, 14, 14, 14	0
1	J	1/7 (14%)	0.15	0 100 100	21, 21, 21, 21	0
2	K	0/3	-	-	-	-
2	L	0/3	-	-	-	-
2	M	0/3	-	-	-	-
2	N	0/3	-	-	-	-
2	O	0/3	-	-	-	-
2	P	0/3	-	-	-	-
2	Q	0/3	-	-	-	-
2	R	0/3	-	-	-	-
2	S	0/3	-	-	-	-
2	T	0/3	-	-	-	-
All	All	10/100 (10%)	-0.33	0 100 100	12, 13, 18, 21	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MLU	A	1	9/10	0.88	0.22	20,25,30,31	0
1	MLU	C	1	9/10	0.93	0.11	15,17,20,22	0
1	MLU	J	1	9/10	0.94	0.18	24,28,33,35	0
1	3FG	A	7	13/13	0.94	0.12	16,17,22,23	0
1	GHP	A	5	11/12	0.95	0.08	12,13,15,17	0
1	MLU	B	1	9/10	0.95	0.09	12,13,15,16	0
2	DSN	O	3	7/7	0.95	0.09	16,17,19,22	0
1	OMZ	E	2	14/15	0.96	0.07	14,16,17,18	1
1	MLU	E	1	9/10	0.96	0.10	16,19,21,22	0
1	GHP	J	5	11/12	0.96	0.06	14,15,19,21	0
1	OMZ	A	2	14/15	0.96	0.07	12,13,15,16	1
1	3FG	J	7	13/13	0.96	0.14	19,22,24,25	0
2	DAL	K	2	5/6	0.96	0.07	18,18,19,20	0
2	DAL	M	2	5/6	0.96	0.09	18,18,18,19	0
1	OMZ	C	2	14/15	0.96	0.10	13,14,15,16	1
2	DSN	T	3	7/7	0.96	0.09	19,19,20,20	0
1	3FG	E	7	13/13	0.97	0.07	13,14,16,17	0
1	3FG	G	7	13/13	0.97	0.07	11,13,17,19	0
1	3FG	I	7	13/13	0.97	0.07	12,13,18,18	0
1	GHP	E	4	10/12	0.97	0.07	12,13,14,14	0
1	GHP	J	4	10/12	0.97	0.06	13,14,15,15	0
1	MLU	H	1	9/10	0.97	0.08	13,14,16,16	0
2	DAL	N	2	5/6	0.97	0.07	13,13,14,16	0
2	DAL	O	2	5/6	0.97	0.05	18,18,19,19	0
2	DAL	S	2[A]	5/6	0.97	0.07	11,12,12,13	5
2	DAL	S	2[B]	5/6	0.97	0.07	13,13,13,14	5
2	DAL	T	2	5/6	0.97	0.08	21,22,22,23	0
2	DSN	M	3	7/7	0.97	0.07	16,16,17,18	0
1	MLU	I	1	9/10	0.97	0.12	12,14,16,17	0
1	OMZ	J	2	14/15	0.97	0.07	15,17,19,21	1
1	GHP	H	5	11/12	0.98	0.07	11,12,12,13	0
1	GHP	I	5	11/12	0.98	0.06	12,12,13,14	0
1	OMZ	F	2	14/15	0.98	0.06	12,13,13,13	1
1	OMY	B	6	14/15	0.98	0.07	12,12,14,14	1
1	OMY	C	6	14/15	0.98	0.08	11,12,13,13	1
1	OMY	F	6	14/15	0.98	0.07	12,13,14,14	1
1	OMY	J	6	14/15	0.98	0.07	14,15,18,18	1
1	OMZ	H	2	14/15	0.98	0.05	11,13,14,14	1
1	3FG	B	7	13/13	0.98	0.05	10,11,16,16	0
1	3FG	C	7	13/13	0.98	0.05	11,13,15,16	0
1	3FG	D	7	13/13	0.98	0.05	11,12,14,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OMZ	I	2	14/15	0.98	0.07	12,13,14,14	1
1	3FG	F	7	13/13	0.98	0.06	11,12,14,16	0
1	MLU	D	1	9/10	0.98	0.05	14,16,19,21	0
1	3FG	H	7	13/13	0.98	0.06	12,13,17,18	0
1	GHP	B	4	10/12	0.98	0.08	11,11,12,12	0
1	GHP	C	4	10/12	0.98	0.06	11,12,13,14	0
1	GHP	D	4	10/12	0.98	0.06	10,11,12,12	0
1	OMZ	B	2	14/15	0.98	0.06	11,12,13,13	1
1	GHP	F	4	10/12	0.98	0.06	11,12,13,13	0
1	GHP	G	4	10/12	0.98	0.06	10,11,12,12	0
2	DAL	P	2	5/6	0.98	0.06	14,14,14,15	0
2	DAL	Q	2	5/6	0.98	0.09	11,11,13,13	0
1	GHP	H	4	10/12	0.98	0.06	11,12,13,13	0
1	GHP	I	4	10/12	0.98	0.07	11,12,13,13	0
1	MLU	F	1	9/10	0.98	0.05	15,17,19,21	0
2	DSN	K	3	7/7	0.98	0.08	16,17,17,19	0
1	MLU	G	1	9/10	0.98	0.08	12,12,14,14	0
2	DSN	N	3	7/7	0.98	0.06	13,13,14,16	0
1	GHP	E	5	11/12	0.98	0.08	11,12,13,13	0
2	DSN	P	3	7/7	0.98	0.07	14,14,15,16	0
2	DSN	Q	3	7/7	0.98	0.05	11,11,13,16	0
2	DSN	R	3	7/7	0.98	0.07	13,13,14,18	0
2	DSN	S	3[A]	7/7	0.98	0.07	9,10,12,15	7
2	DSN	S	3[B]	7/7	0.98	0.07	15,16,17,17	7
1	GHP	F	5	11/12	0.98	0.08	11,12,12,12	0
1	GHP	B	5	11/12	0.99	0.06	11,11,12,12	0
1	GHP	C	5	11/12	0.99	0.07	11,11,12,12	0
2	DAL	R	2	5/6	0.99	0.05	12,13,14,15	0
1	OMY	A	6	14/15	0.99	0.06	13,14,16,16	1
1	GHP	D	5	11/12	0.99	0.07	10,11,12,12	0
1	OMZ	D	2	14/15	0.99	0.05	11,12,12,13	1
1	OMY	D	6	14/15	0.99	0.05	11,13,13,13	1
2	DSN	L	3[A]	7/7	0.99	0.07	10,10,12,14	7
2	DSN	L	3[B]	7/7	0.99	0.07	14,15,15,16	7
1	OMY	E	6	14/15	0.99	0.07	12,13,14,15	1
1	GHP	A	4	10/12	0.99	0.05	11,12,13,13	0
1	OMY	G	6	14/15	0.99	0.05	12,13,14,14	1
1	OMY	H	6	14/15	0.99	0.04	12,13,15,16	1
2	DAL	L	2[A]	5/6	0.99	0.09	10,10,10,11	5
2	DAL	L	2[B]	5/6	0.99	0.09	16,17,17,18	5
1	OMY	I	6	14/15	0.99	0.04	13,14,15,15	1
1	GHP	G	5	11/12	0.99	0.07	11,11,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OMZ	G	2	14/15	0.99	0.05	11,12,13,14	1

6.3 Carbohydrates [i](#)

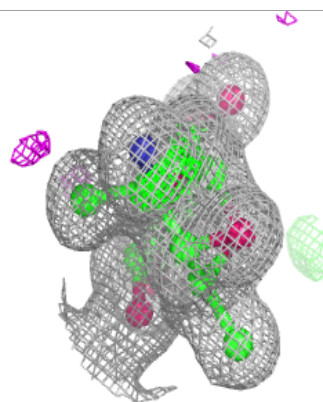
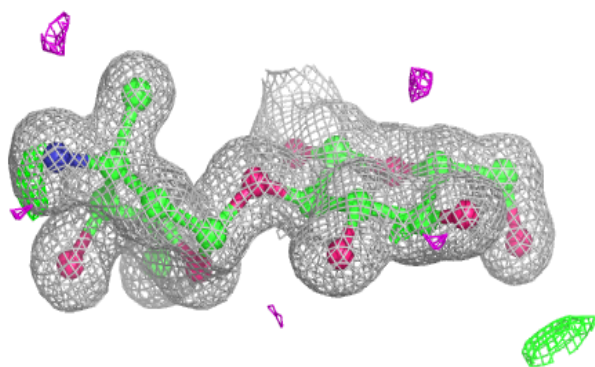
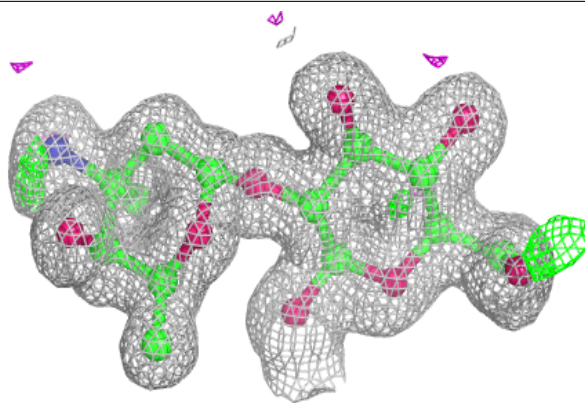
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	RER	U	2	10/11	0.94	0.07	15,16,18,19	0
3	RER	Y	2	10/11	0.95	0.07	17,19,21,22	0
3	RER	a	2	10/11	0.96	0.07	12,13,14,15	0
3	RER	k	2	10/11	0.96	0.06	18,19,21,22	0
3	RER	m	2	10/11	0.96	0.07	15,16,19,19	0
3	RER	c	2	10/11	0.97	0.06	17,18,20,21	0
3	BGC	e	1	12/12	0.97	0.07	13,17,22,23	0
3	RER	e	2	10/11	0.97	0.06	12,13,15,15	0
3	BGC	k	1	12/12	0.97	0.06	13,16,17,18	0
3	BGC	W	1	12/12	0.97	0.06	13,19,22,24	0
3	BGC	m	1	12/12	0.97	0.06	14,16,19,20	0
3	RER	W	2	10/11	0.97	0.07	14,15,16,17	0
3	BGC	c	1	12/12	0.98	0.05	14,16,20,23	0
3	BGC	U	1	12/12	0.98	0.07	13,16,19,23	0
3	BGC	a	1	12/12	0.98	0.05	12,15,20,21	0
3	BGC	Y	1	12/12	0.98	0.06	13,15,17,18	0

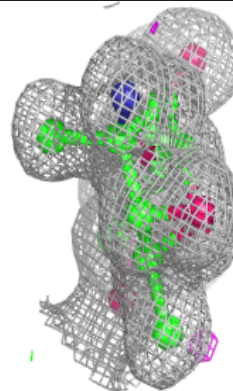
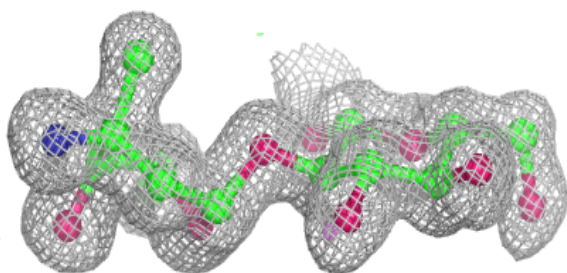
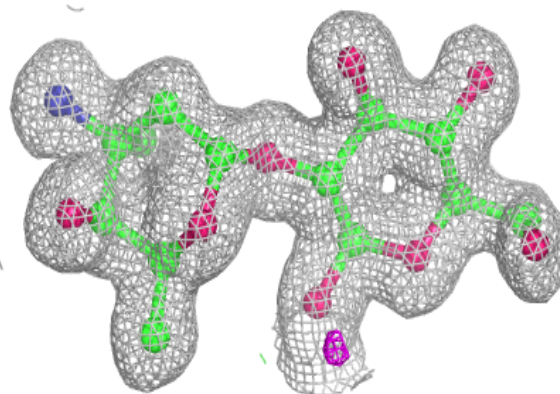
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain U:

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

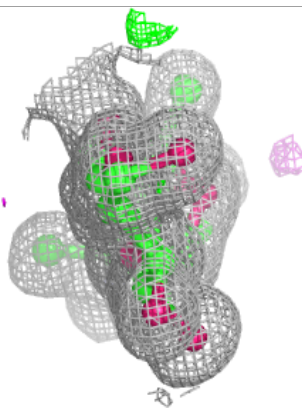
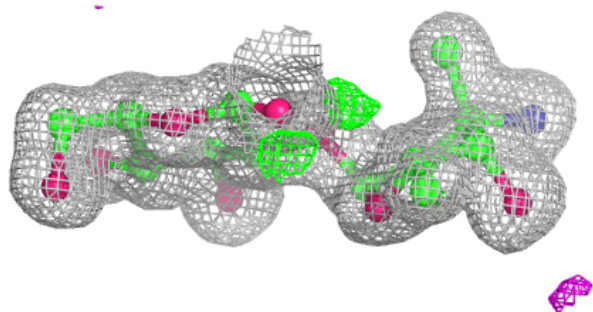
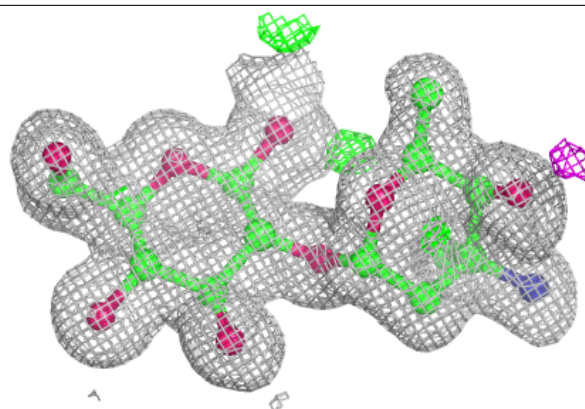
**Electron density around Chain W:**

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

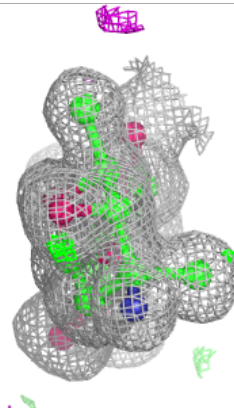
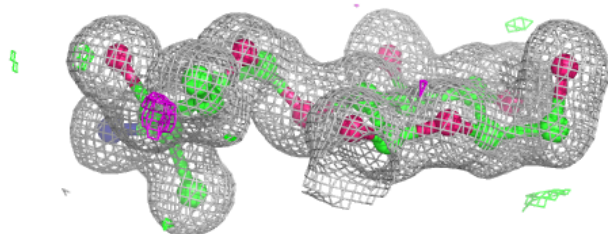
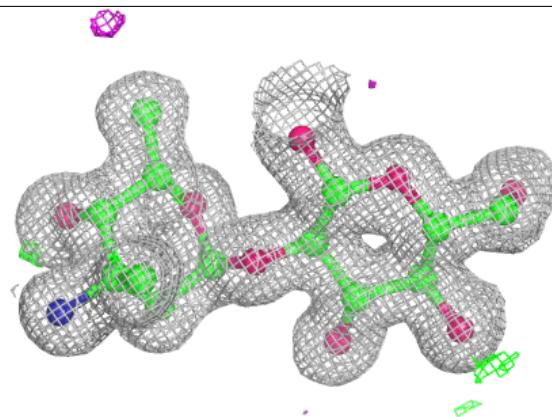


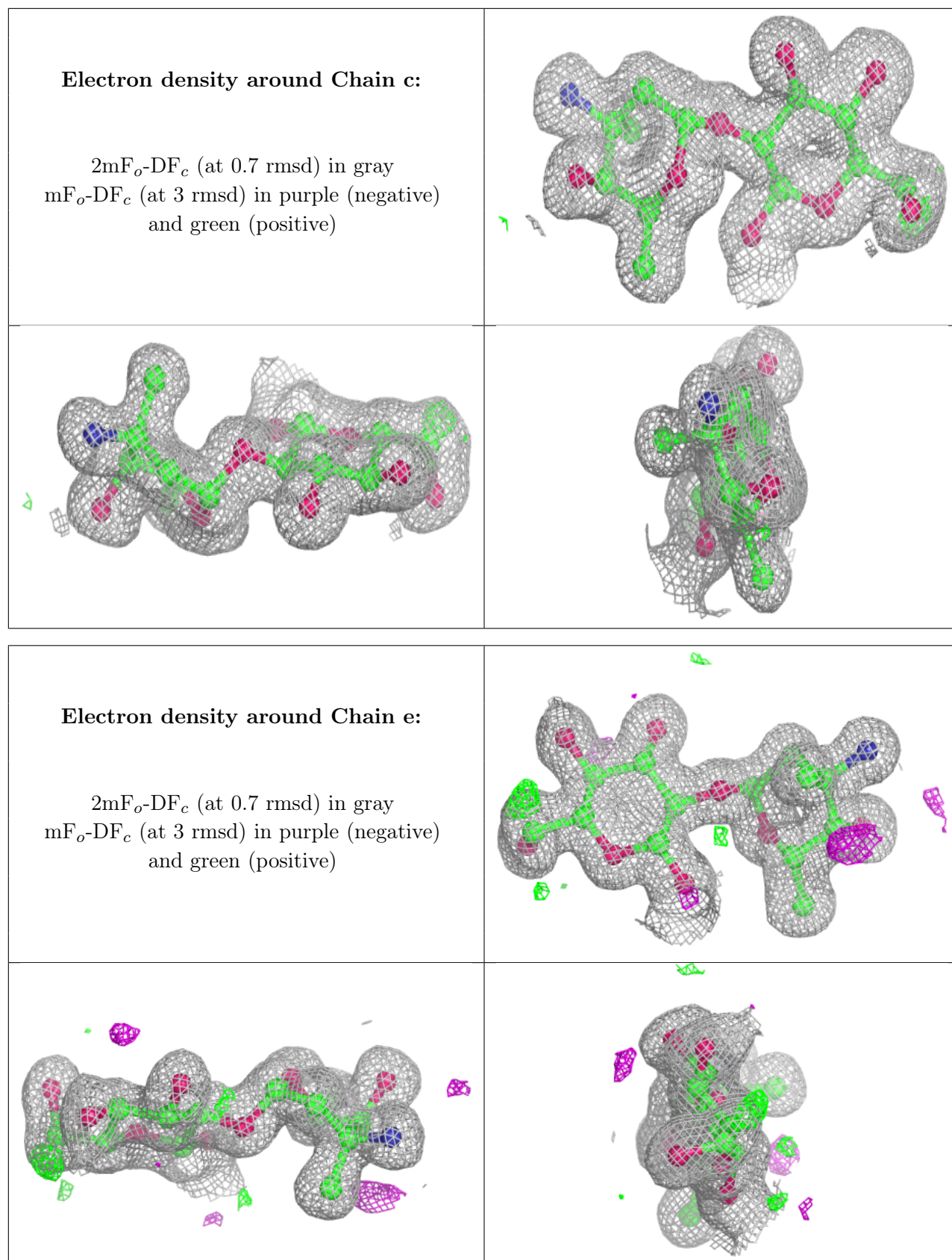
Electron density around Chain Y:

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

**Electron density around Chain a:**

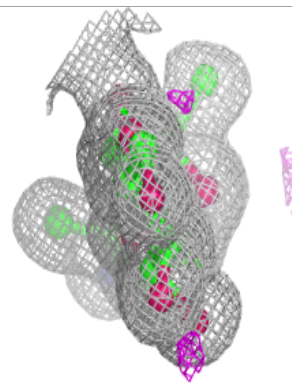
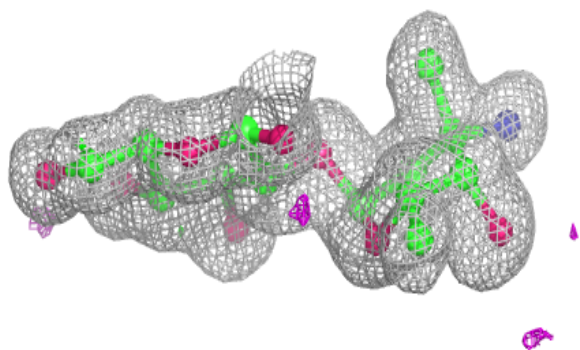
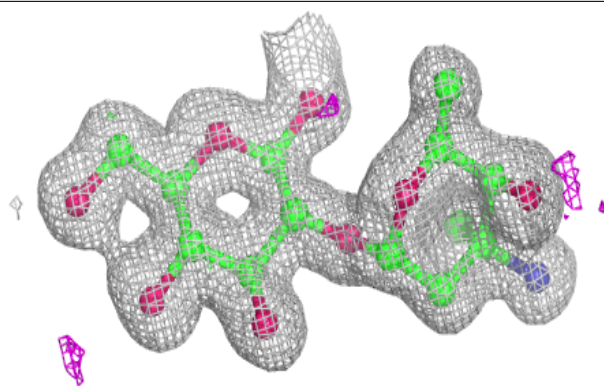
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



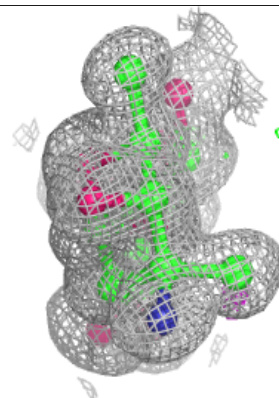
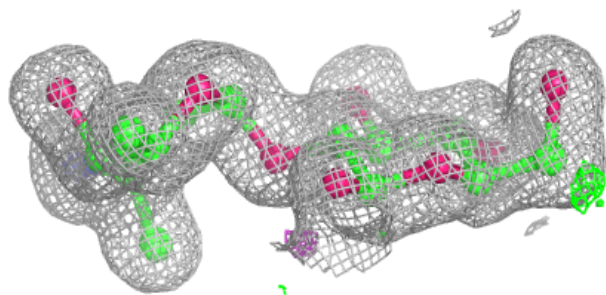
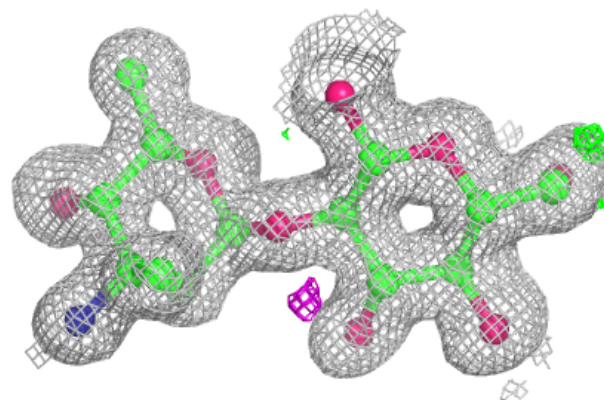


Electron density around Chain k:

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

**Electron density around Chain m:**

$2mF_o-DF_c$ (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
4	PGE	A	101	10/10	0.86	0.08	26,35,45,60	0
5	BO3	D	101	4/4	0.88	0.15	14,38,42,55	0
8	RER	H	104[A]	10/11	0.89	0.17	16,19,21,21	10
8	RER	H	104[B]	10/11	0.89	0.17	21,23,24,26	10
6	DMS	H	101	4/4	0.90	0.16	49,67,68,78	0
8	RER	G	103[B]	10/11	0.92	0.13	20,23,24,24	10
5	BO3	J	101	4/4	0.92	0.23	13,32,49,52	0
8	RER	G	103[A]	10/11	0.92	0.13	13,14,15,16	10
5	BO3	O	101	4/4	0.93	0.13	13,25,38,54	0
7	BGC	H	103[A]	12/12	0.96	0.11	12,13,15,15	12
7	BGC	H	103[B]	12/12	0.96	0.11	15,21,24,24	12
6	DMS	H	102	4/4	0.97	0.08	19,19,20,20	0
7	BGC	G	102[A]	12/12	0.97	0.11	12,13,18,19	12
7	BGC	G	102[B]	12/12	0.97	0.11	14,18,20,21	12
6	DMS	J	102	4/4	0.98	0.11	20,24,25,26	0
6	DMS	G	101[A]	4/4	0.98	0.07	16,16,18,27	4
6	DMS	G	101[B]	4/4	0.98	0.07	10,14,22,26	4

6.5 Other polymers [i](#)

There are no such residues in this entry.