



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:24 AM UTC

PDB ID : 8G82 / pdb_00008g82
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

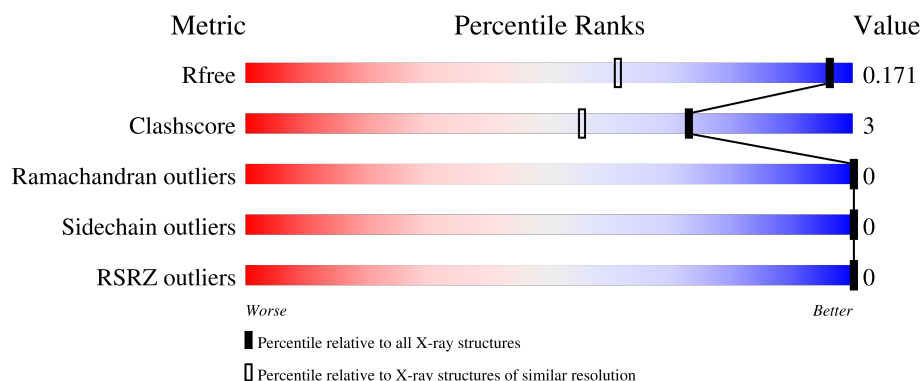
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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.



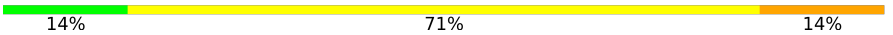
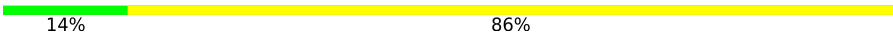
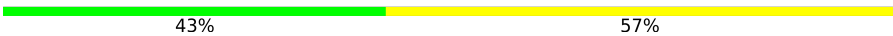
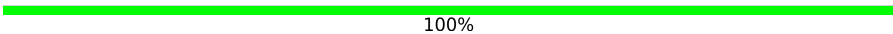
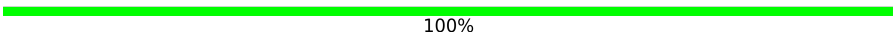
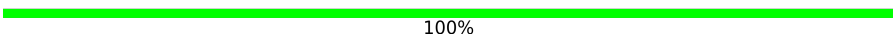
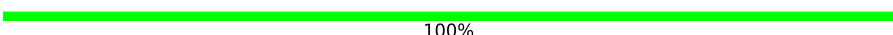
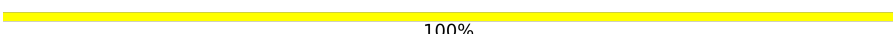
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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 $\leq 5\%$. 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	14% 86%
1	D	7	29% 71%
1	E	7	29% 71%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	7	
1	G	7	
1	H	7	
1	I	7	
1	J	7	
2	K	3	
2	L	3	
2	M	3	
2	N	3	
2	O	3	
2	P	3	
2	Q	3	
2	R	3	
2	S	3	
2	T	3	
3	U	2	
3	W	2	
3	Y	2	
3	a	2	
3	c	2	
3	e	2	
3	k	2	
3	m	2	

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
1	A	7	Total	C	Cl	N	O	0	0	0
			79	53	2	8	16			
1	B	7	Total	C	Cl	N	O	0	0	0
			79	53	2	8	16			
1	C	7	Total	C	Cl	N	O	0	0	0
			79	53	2	8	16			
1	D	7	Total	C	Cl	N	O	0	0	0
			79	53	2	8	16			
1	E	7	Total	C	Cl	N	O	0	0	0
			79	53	2	8	16			
1	F	7	Total	C	Cl	N	O	0	0	0
			79	53	2	8	16			
1	G	7	Total	C	Cl	N	O	0	0	0
			79	53	2	8	16			
1	H	7	Total	C	Cl	N	O	0	0	0
			79	53	2	8	16			
1	I	7	Total	C	Cl	N	O	0	0	0
			79	53	2	8	16			
1	J	7	Total	C	Cl	N	O	0	0	0
			79	53	2	8	16			

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

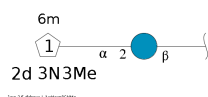
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	3	Total	C	N	O	0	0	0
			15	8	2	5			
2	L	3	Total	C	N	O	0	3	0
			30	16	4	10			
2	M	3	Total	C	N	O	0	0	0
			15	8	2	5			
2	N	3	Total	C	N	O	0	0	0
			15	8	2	5			

Continued on next page...

Continued from previous page...

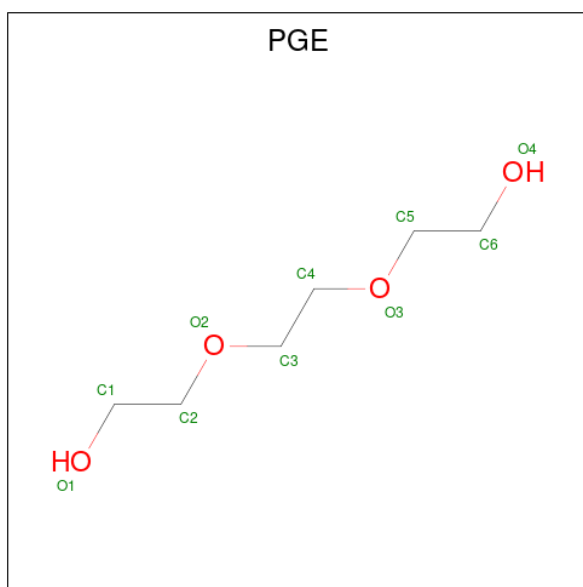
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	3	Total	C	N	O	0	0	0
			15	8	2	5			
2	P	3	Total	C	N	O	0	0	0
			15	8	2	5			
2	Q	3	Total	C	N	O	0	0	0
			15	8	2	5			
2	R	3	Total	C	N	O	0	0	0
			15	8	2	5			
2	S	3	Total	C	N	O	0	3	0
			30	16	4	10			
2	T	3	Total	C	N	O	0	0	0
			15	8	2	5			

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



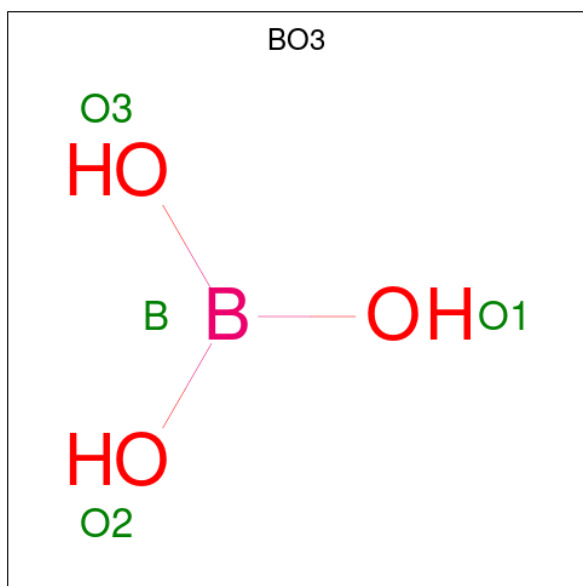
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	U	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	W	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	Y	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	a	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	c	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	e	2	Total	C	N	O	0	0	0
			22	13	1	8			
3	k	2	Total	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 (CCD ID: PGE) (formula: C₆H₁₄O₄).



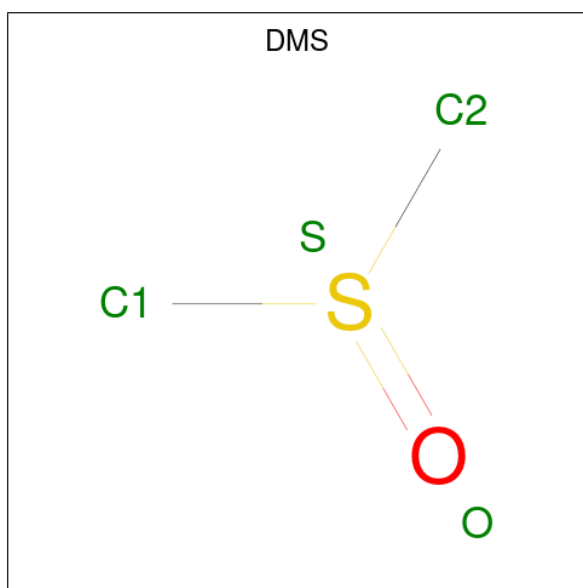
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is BORIC ACID (CCD ID: BO3) (formula: BH_3O_3).



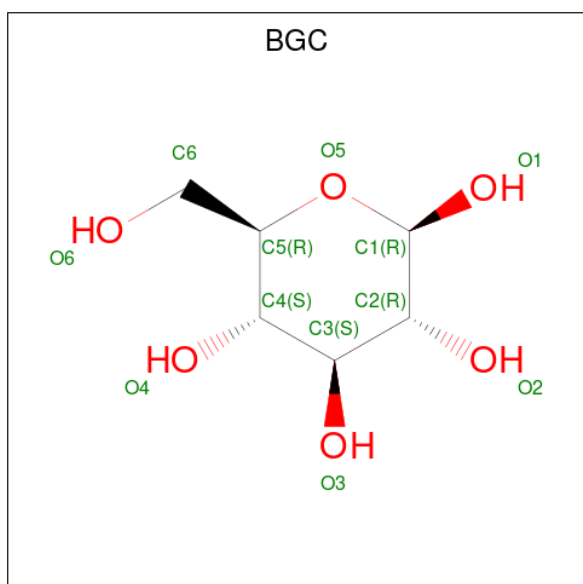
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	B	O	0	0
			4	1	3		
5	J	1	Total	B	O	0	0
			4	1	3		
5	O	1	Total	B	O	0	0
			4	1	3		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



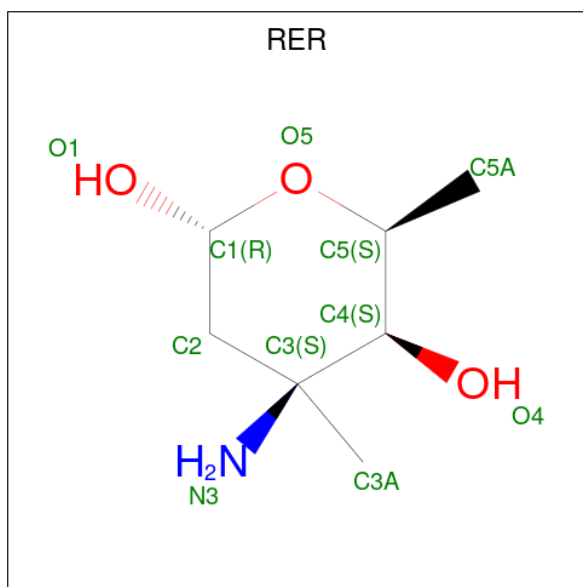
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	O	S	0	1
			8	4	2	2		
6	H	1	Total	C	O	S	0	0
			4	2	1	1		
6	H	1	Total	C	O	S	0	0
			4	2	1	1		
6	J	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



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

- Molecule 8 is vancosamine (CCD ID: RER) (formula: $C_7H_{15}NO_3$).



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

- Molecule 9 is water.

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

Continued on next page...

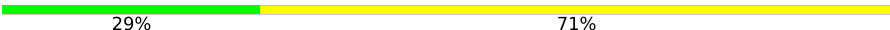
Continued from previous page...

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

3 Residue-property plots [i](#)

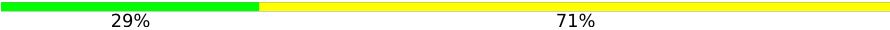
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

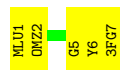
● Molecule 1: Vancomycin

Chain A:  29% 71%

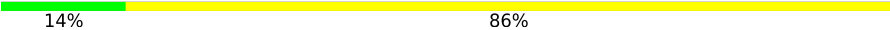


● Molecule 1: Vancomycin

Chain B:  29% 71%



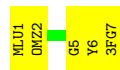
● Molecule 1: Vancomycin

Chain C:  14% 86%



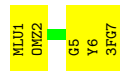
● Molecule 1: Vancomycin

Chain D:  29% 71%

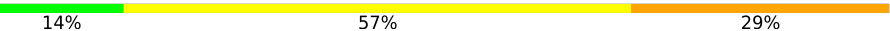


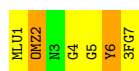
● Molecule 1: Vancomycin

Chain E:  29% 71%



● Molecule 1: Vancomycin

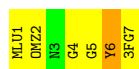
Chain F:  14% 57% 29%



- 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



- 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:  33% 67%



- 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%



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

Chain W:  50% 50%

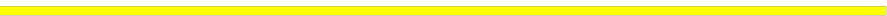


- Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose

Chain Y:  50% 50%

BCG1
RER2

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

Chain a:  100%

BCG1
RER2

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

Chain c:  50% 50%

BCG1
RER2

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

Chain e:  50% 50%

BCG1
RER2

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

Chain k:  50% 50%

BCG1
RER2

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

Chain m:  50% 50%

BCG1
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)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.153 , 0.171 0.153 , 0.171	Depositor DCC
R_{free} test set	2000 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1542	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage'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: RER, OMY, MLU, PGE, ACE, 3FG, BO3, DMS, OMZ, DAL, BGC, GHP, DSN

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	0.81	0/7	1.31	0/8
1	B	0.80	0/7	0.97	0/8
1	C	0.76	0/7	0.78	0/8
1	D	0.75	0/7	1.09	0/8
1	E	0.81	0/7	1.04	0/8
1	F	0.72	0/7	1.01	0/8
1	G	0.69	0/7	0.83	0/8
1	H	0.62	0/7	0.96	0/8
1	I	0.71	0/7	1.11	0/8
1	J	0.80	0/7	0.99	0/8
All	All	0.75	0/70	1.02	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	1	0
1	C	79	0	44	0	0

Continued on next page...

Continued from previous page...

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	2	0
1	G	79	0	43	1	0
1	H	79	0	43	1	0
1	I	79	0	42	1	0
1	J	79	0	43	0	0
2	K	15	0	11	0	0
2	L	30	0	24	1	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	2	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	1	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	1	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	1	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

Continued on next page...

Continued from previous page...

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	7	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 3.

All (7) 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:G:7:3FG:HA	6:G:101[B]:DMS:H11	1.95	0.47
2:S:3[B]:DSN:OG	3:k:2:RER:H5A2	2.16	0.45
1:I:5:GHP:HC2	2:S:1[A]:ACE:O	2.16	0.45
1:F:4:GHP:C3	1:F:6:OMY:CL	3.02	0.44
1:H:6:OMY:CL	7:H:103[B]:BGC:H6C2	2.55	0.44
1:B:5:GHP:HC2	2:L:1[A]:ACE:O	2.18	0.43
1:F:2:OMZ:CE1	1:F:4:GHP:H6	2.48	0.42

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
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 ⓘ

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	3FG	I	7	1	12,13,13	1.35	2 (16%)	14,18,18	0.93	1 (7%)
1	MLU	G	1	1	7,8,9	0.67	0	7,9,11	1.16	1 (14%)
1	GHP	J	4	1	9,10,12	1.10	0	9,12,16	0.88	0
1	GHP	F	5	1	10,11,12	1.18	1 (10%)	11,14,16	1.11	1 (9%)
1	GHP	H	4	1	9,10,12	1.03	1 (11%)	9,12,16	0.77	0
1	GHP	I	5	1	10,11,12	1.05	0	11,14,16	0.82	0
1	OMY	A	6	1	12,14,15	2.13	1 (8%)	17,19,21	1.84	1 (5%)
1	MLU	H	1	1	7,8,9	0.58	0	7,9,11	1.12	1 (14%)
1	GHP	C	5	1	10,11,12	1.60	3 (30%)	11,14,16	1.25	0
1	MLU	A	1	1	7,8,9	0.60	0	7,9,11	1.18	1 (14%)
1	OMZ	G	2	1	12,14,15	0.42	0	17,19,21	1.05	1 (5%)
1	OMY	G	6	1	12,14,15	2.22	2 (16%)	17,19,21	1.53	1 (5%)
1	MLU	D	1	1	7,8,9	0.42	0	7,9,11	1.47	2 (28%)

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	0.98	0	14,18,18	0.78	1 (7%)
1	3FG	E	7	1	12,13,13	1.13	1 (8%)	14,18,18	0.90	1 (7%)
1	GHP	C	4	1	9,10,12	1.25	0	9,12,16	1.29	1 (11%)
1	OMY	C	6	1	12,14,15	2.25	2 (16%)	17,19,21	1.67	1 (5%)
1	3FG	F	7	1	12,13,13	1.28	2 (16%)	14,18,18	1.08	1 (7%)
1	GHP	B	4	1	9,10,12	1.03	0	9,12,16	0.98	0
1	GHP	A	5	1	10,11,12	1.42	1 (10%)	11,14,16	1.08	1 (9%)
1	OMZ	I	2	1	12,14,15	0.60	0	17,19,21	0.90	1 (5%)
1	GHP	D	4	1	9,10,12	0.87	0	9,12,16	0.65	0
1	GHP	E	5	1	10,11,12	1.16	1 (10%)	11,14,16	1.07	1 (9%)
1	GHP	I	4	1	9,10,12	1.44	1 (11%)	9,12,16	0.95	0
1	3FG	D	7	1	12,13,13	1.03	0	14,18,18	1.06	1 (7%)
1	GHP	G	5	1	10,11,12	1.33	1 (10%)	11,14,16	1.13	1 (9%)
1	GHP	H	5	1	10,11,12	1.56	1 (10%)	11,14,16	1.24	2 (18%)
1	OMY	F	6	1	12,14,15	2.06	1 (8%)	17,19,21	1.82	1 (5%)
1	OMZ	J	2	1	12,14,15	0.52	0	17,19,21	1.04	1 (5%)
1	OMZ	H	2	1	12,14,15	0.43	0	17,19,21	1.17	2 (11%)
1	GHP	B	5	1	10,11,12	1.04	0	11,14,16	0.90	0
1	OMY	I	6	1	12,14,15	2.36	1 (8%)	17,19,21	1.65	1 (5%)
1	OMY	J	6	1	12,14,15	2.66	2 (16%)	17,19,21	1.88	1 (5%)
1	OMZ	C	2	1	12,14,15	0.45	0	17,19,21	1.50	3 (17%)
1	MLU	E	1	1	7,8,9	0.62	0	7,9,11	1.83	2 (28%)
1	OMZ	A	2	1	12,14,15	0.47	0	17,19,21	1.37	3 (17%)
1	GHP	A	4	1	9,10,12	1.00	0	9,12,16	0.82	0
1	OMZ	E	2	1	12,14,15	0.43	0	17,19,21	1.27	3 (17%)
1	OMZ	F	2	1	12,14,15	0.48	0	17,19,21	1.12	2 (11%)
1	MLU	C	1	1	7,8,9	0.64	0	7,9,11	1.28	2 (28%)
1	OMY	E	6	1	12,14,15	2.43	3 (25%)	17,19,21	1.69	1 (5%)
1	MLU	F	1	1	7,8,9	0.53	0	7,9,11	1.42	2 (28%)
1	GHP	E	4	1	9,10,12	1.05	0	9,12,16	0.82	0
1	OMZ	B	2	1	12,14,15	0.52	0	17,19,21	1.15	2 (11%)
1	GHP	D	5	1	10,11,12	1.03	0	11,14,16	1.23	1 (9%)
1	OMY	H	6	1	12,14,15	2.01	2 (16%)	17,19,21	1.66	1 (5%)
1	3FG	J	7	1	12,13,13	0.93	0	14,18,18	0.80	0
1	MLU	B	1	1	7,8,9	0.63	0	7,9,11	1.07	1 (14%)
1	OMZ	D	2	1	12,14,15	0.50	0	17,19,21	1.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GHP	F	4	1	9,10,12	0.91	0	9,12,16	0.64	0
1	GHP	G	4	1	9,10,12	0.85	0	9,12,16	0.63	0
1	GHP	J	5	1	10,11,12	1.34	1 (10%)	11,14,16	0.86	0
1	MLU	I	1	1	7,8,9	0.55	0	7,9,11	1.25	1 (14%)
1	3FG	G	7	1	12,13,13	1.06	1 (8%)	14,18,18	1.21	1 (7%)
1	3FG	H	7	1	12,13,13	1.14	1 (8%)	14,18,18	1.09	1 (7%)
1	OMY	D	6	1	12,14,15	2.11	1 (8%)	17,19,21	1.75	1 (5%)
1	3FG	C	7	1	12,13,13	1.04	1 (8%)	14,18,18	1.10	2 (14%)
1	3FG	B	7	1	12,13,13	1.10	1 (8%)	14,18,18	1.18	2 (14%)
1	OMY	B	6	1	12,14,15	1.75	1 (8%)	17,19,21	1.58	1 (5%)
1	MLU	J	1	1	7,8,9	0.59	0	7,9,11	1.21	1 (14%)

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

Continued on next page...

Continued from previous page...

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

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	6	OMY	CZ-CE1	8.61	1.47	1.39
1	I	6	OMY	CZ-CE1	7.50	1.46	1.39
1	E	6	OMY	CZ-CE1	7.38	1.46	1.39
1	C	6	OMY	CZ-CE1	6.77	1.46	1.39
1	A	6	OMY	CZ-CE1	6.69	1.46	1.39
1	G	6	OMY	CZ-CE1	6.60	1.46	1.39
1	D	6	OMY	CZ-CE1	6.50	1.45	1.39
1	F	6	OMY	CZ-CE1	6.08	1.45	1.39
1	H	6	OMY	CZ-CE1	5.86	1.45	1.39
1	B	6	OMY	CZ-CE1	5.08	1.44	1.39
1	H	5	GHP	C1-CA	-3.56	1.49	1.52
1	A	5	GHP	C1-CA	-3.56	1.49	1.52
1	J	5	GHP	C1-CA	-3.37	1.49	1.52
1	I	4	GHP	C1-CA	-3.24	1.49	1.52
1	C	5	GHP	C1-CA	-3.00	1.49	1.52
1	I	7	3FG	CG1-CD1	2.46	1.42	1.39
1	F	7	3FG	CG1-CD1	2.43	1.42	1.39
1	C	6	OMY	CD2-CG	2.43	1.43	1.39
1	H	7	3FG	CG1-CB	2.32	1.42	1.39
1	H	6	OMY	CG-CB	-2.31	1.48	1.51
1	C	5	GHP	C2-C1	2.25	1.42	1.39
1	J	6	OMY	CG-CB	-2.25	1.48	1.51
1	G	7	3FG	CG1-CB	2.22	1.42	1.39
1	E	5	GHP	C1-CA	-2.19	1.50	1.52
1	E	6	OMY	CG-CB	-2.18	1.48	1.51
1	F	7	3FG	CG1-CB	2.18	1.42	1.39
1	I	7	3FG	CB-CA	2.18	1.55	1.52
1	C	5	GHP	CA-C	2.18	1.54	1.51
1	C	7	3FG	CG1-CB	2.17	1.42	1.39
1	H	4	GHP	C1-CA	-2.16	1.50	1.52
1	G	5	GHP	C1-CA	-2.14	1.50	1.52
1	G	6	OMY	CG-CB	-2.14	1.48	1.51
1	E	7	3FG	CG1-CB	2.11	1.42	1.39
1	E	6	OMY	CD2-CG	2.07	1.42	1.39
1	F	5	GHP	C3-C2	2.05	1.42	1.38
1	B	7	3FG	CG1-CB	2.03	1.42	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	OMY	CG-CB-CA	-6.90	102.52	111.58
1	J	6	OMY	CG-CB-CA	-6.82	102.63	111.58
1	F	6	OMY	CG-CB-CA	-6.70	102.79	111.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	6	OMY	CG-CB-CA	-6.30	103.31	111.58
1	H	6	OMY	CG-CB-CA	-6.21	103.43	111.58
1	E	6	OMY	CG-CB-CA	-6.13	103.53	111.58
1	C	6	OMY	CG-CB-CA	-6.03	103.66	111.58
1	I	6	OMY	CG-CB-CA	-5.98	103.72	111.58
1	B	6	OMY	CG-CB-CA	-5.84	103.91	111.58
1	G	6	OMY	CG-CB-CA	-5.63	104.19	111.58
1	E	1	MLU	CB-CA-C	-3.70	105.30	110.99
1	G	7	3FG	CD1-CG1-CB	-3.63	116.96	120.09
1	F	2	OMZ	O-C-CA	-3.41	116.00	124.77
1	B	7	3FG	CD1-CG1-CB	-3.32	117.22	120.09
1	E	2	OMZ	O-C-CA	-3.31	116.26	124.77
1	C	7	3FG	CD1-CG1-CB	-3.30	117.24	120.09
1	F	7	3FG	CD1-CG1-CB	-3.30	117.24	120.09
1	C	2	OMZ	O-C-CA	-3.22	116.49	124.77
1	D	2	OMZ	O-C-CA	-3.19	116.57	124.77
1	H	7	3FG	CD1-CG1-CB	-3.18	117.34	120.09
1	D	7	3FG	CD1-CG1-CB	-3.14	117.38	120.09
1	B	2	OMZ	O-C-CA	-3.10	116.80	124.77
1	H	2	OMZ	O-C-CA	-3.09	116.83	124.77
1	A	2	OMZ	O-C-CA	-3.01	117.04	124.77
1	E	1	MLU	O-C-CA	-2.99	117.09	124.77
1	I	1	MLU	O-C-CA	-2.98	117.12	124.77
1	I	2	OMZ	O-C-CA	-2.95	117.17	124.77
1	C	2	OMZ	OH-CZ-CE2	2.90	127.15	119.36
1	G	2	OMZ	O-C-CA	-2.87	117.38	124.77
1	G	1	MLU	O-C-CA	-2.87	117.39	124.77
1	C	2	OMZ	CD1-CE1-CZ	2.85	122.59	120.92
1	F	1	MLU	O-C-CA	-2.83	117.48	124.77
1	D	1	MLU	O-C-CA	-2.81	117.53	124.77
1	H	1	MLU	O-C-CA	-2.76	117.67	124.77
1	B	2	OMZ	CD1-CE1-CZ	2.72	122.51	120.92
1	J	1	MLU	O-C-CA	-2.72	117.78	124.77
1	I	7	3FG	CD1-CG1-CB	-2.69	117.76	120.09
1	A	2	OMZ	CD1-CE1-CZ	2.69	122.49	120.92
1	E	7	3FG	CD1-CG1-CB	-2.67	117.78	120.09
1	J	2	OMZ	O-C-CA	-2.67	117.90	124.77
1	C	1	MLU	O-C-CA	-2.64	117.97	124.77
1	B	1	MLU	O-C-CA	-2.62	118.04	124.77
1	F	5	GHP	C2-C3-C4	-2.62	117.11	119.88
1	A	1	MLU	O-C-CA	-2.56	118.18	124.77
1	A	2	OMZ	OH-CZ-CE2	2.51	126.08	119.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	MLU	CB-CA-C	-2.48	107.18	110.99
1	D	5	GHP	C2-C3-C4	-2.41	117.33	119.88
1	H	5	GHP	C5-C6-C1	-2.36	118.83	121.18
1	A	5	GHP	C1-CA-C	-2.35	105.49	112.09
1	E	2	OMZ	CD1-CE1-CZ	2.32	122.28	120.92
1	F	1	MLU	CB-CA-C	-2.31	107.44	110.99
1	H	2	OMZ	CD1-CE1-CZ	2.29	122.26	120.92
1	E	2	OMZ	OH-CZ-CE2	2.28	125.49	119.36
1	G	5	GHP	C2-C3-C4	-2.23	117.52	119.88
1	E	5	GHP	C2-C3-C4	-2.22	117.53	119.88
1	B	7	3FG	CG2-CB-CG1	2.20	121.10	118.09
1	C	4	GHP	C4-C5-C6	-2.14	117.60	120.24
1	F	2	OMZ	OH-CZ-CE2	2.13	125.07	119.36
1	H	5	GHP	C2-C3-C4	-2.12	117.64	119.88
1	C	7	3FG	CG2-CB-CG1	2.03	120.86	118.09
1	C	1	MLU	CB-CA-C	-2.03	107.87	110.99
1	A	7	3FG	CD1-CG1-CB	-2.01	118.36	120.09

There are no chirality outliers.

All (43) 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	E	7	3FG	O-C-CA-CB
1	E	7	3FG	OXT-C-CA-CB
1	C	7	3FG	C-CA-CB-CG2
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	C	7	3FG	O-C-CA-CB
1	C	7	3FG	OXT-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	D	7	3FG	O-C-CA-CB
1	D	7	3FG	OXT-C-CA-CB
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
1	J	7	3FG	C-CA-CB-CG1
1	C	4	GHP	C6-C1-CA-C
1	D	4	GHP	C6-C1-CA-C
1	E	4	GHP	C6-C1-CA-C
1	F	4	GHP	C2-C1-CA-C
1	F	4	GHP	C6-C1-CA-C
1	J	4	GHP	C6-C1-CA-C
1	D	7	3FG	C-CA-CB-CG1
1	E	7	3FG	C-CA-CB-CG1
1	F	7	3FG	C-CA-CB-CG1
1	G	7	3FG	C-CA-CB-CG1
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

There are no ring outliers.

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	5	GHP	1	0
1	F	6	OMY	1	0
1	B	5	GHP	1	0
1	F	2	OMZ	1	0
1	H	6	OMY	1	0
1	F	4	GHP	2	0
1	G	7	3FG	1	0

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	0.47	0	17,17,17	0.68	0
3	RER	U	2	3	7,10,11	2.20	2 (28%)	6,15,17	1.47	2 (33%)
3	BGC	W	1	3	12,12,12	0.45	0	17,17,17	0.88	0
3	RER	W	2	3	7,10,11	2.04	2 (28%)	6,15,17	0.94	0
3	BGC	Y	1	3	12,12,12	0.51	0	17,17,17	0.72	0
3	RER	Y	2	3	7,10,11	2.16	3 (42%)	6,15,17	1.04	1 (16%)
3	BGC	a	1	3	12,12,12	0.39	0	17,17,17	0.97	1 (5%)
3	RER	a	2	3	7,10,11	1.79	2 (28%)	6,15,17	1.16	0
3	BGC	c	1	3	12,12,12	0.42	0	17,17,17	0.66	0
3	RER	c	2	3	7,10,11	2.29	2 (28%)	6,15,17	1.16	1 (16%)
3	BGC	e	1	3	12,12,12	0.45	0	17,17,17	0.94	0
3	RER	e	2	3	7,10,11	1.96	2 (28%)	6,15,17	1.04	1 (16%)
3	BGC	k	1	3	12,12,12	0.39	0	17,17,17	0.72	0
3	RER	k	2	3	7,10,11	2.24	3 (42%)	6,15,17	0.67	0
3	BGC	m	1	3	12,12,12	0.44	0	17,17,17	0.60	0
3	RER	m	2	3	7,10,11	2.10	2 (28%)	6,15,17	0.94	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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	2	RER	C2-C3	-4.16	1.48	1.54
3	k	2	RER	C2-C3	-4.02	1.48	1.54
3	c	2	RER	O5-C5	3.69	1.50	1.43
3	U	2	RER	C2-C3	-3.62	1.49	1.54
3	m	2	RER	O5-C5	3.51	1.50	1.43
3	m	2	RER	C2-C3	-3.50	1.49	1.54
3	Y	2	RER	O5-C5	3.47	1.50	1.43
3	U	2	RER	O5-C5	3.45	1.50	1.43
3	Y	2	RER	C2-C3	-3.34	1.49	1.54
3	e	2	RER	C2-C3	-3.21	1.50	1.54
3	k	2	RER	O5-C5	3.17	1.49	1.43
3	W	2	RER	C2-C3	-3.14	1.50	1.54
3	a	2	RER	C2-C3	-3.08	1.50	1.54
3	W	2	RER	O5-C5	3.08	1.49	1.43
3	e	2	RER	O5-C5	3.01	1.49	1.43
3	a	2	RER	O5-C5	2.80	1.49	1.43
3	Y	2	RER	C5A-C5	-2.19	1.46	1.51
3	k	2	RER	C5A-C5	-2.09	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	2.64	114.96	111.38
3	a	1	BGC	O5-C5-C6	2.53	112.70	106.44
3	e	2	RER	O5-C5-C4	-2.30	106.08	110.04
3	U	2	RER	C5A-C5-C4	2.25	116.32	112.58
3	Y	2	RER	O5-C1-C2	2.17	114.33	111.38
3	c	2	RER	O5-C1-C2	2.09	114.22	111.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

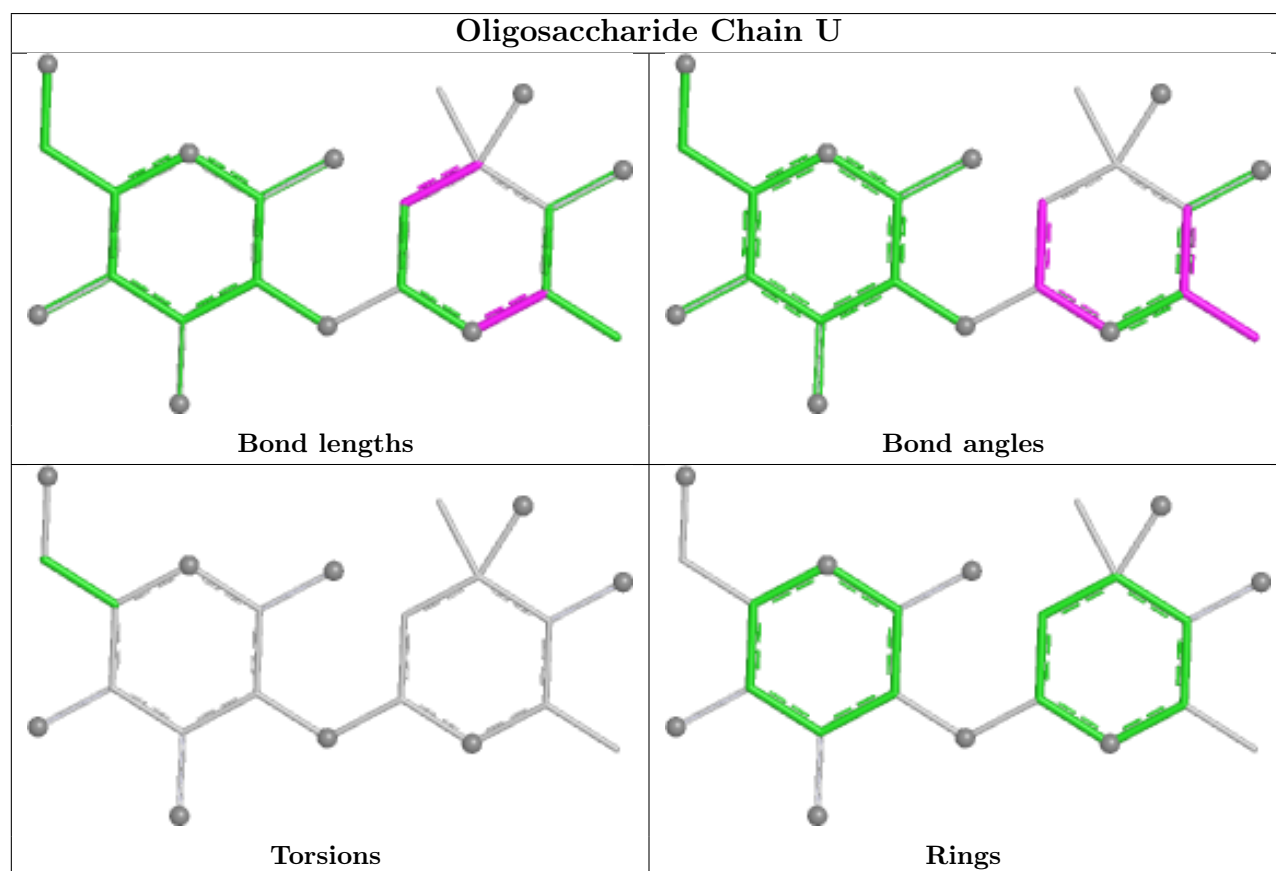
Mol	Chain	Res	Type	Atoms
3	k	1	BGC	O5-C5-C6-O6

There are no ring outliers.

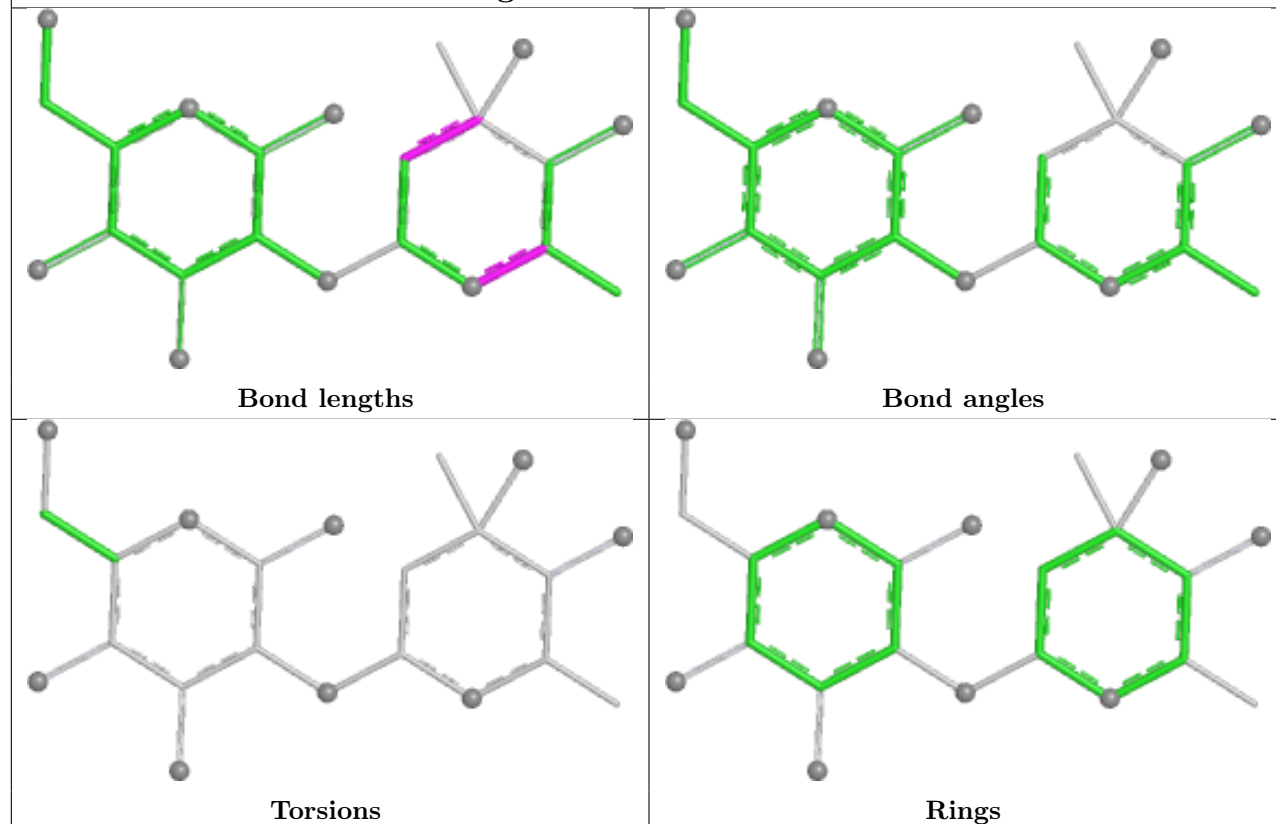
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	k	2	RER	1	0

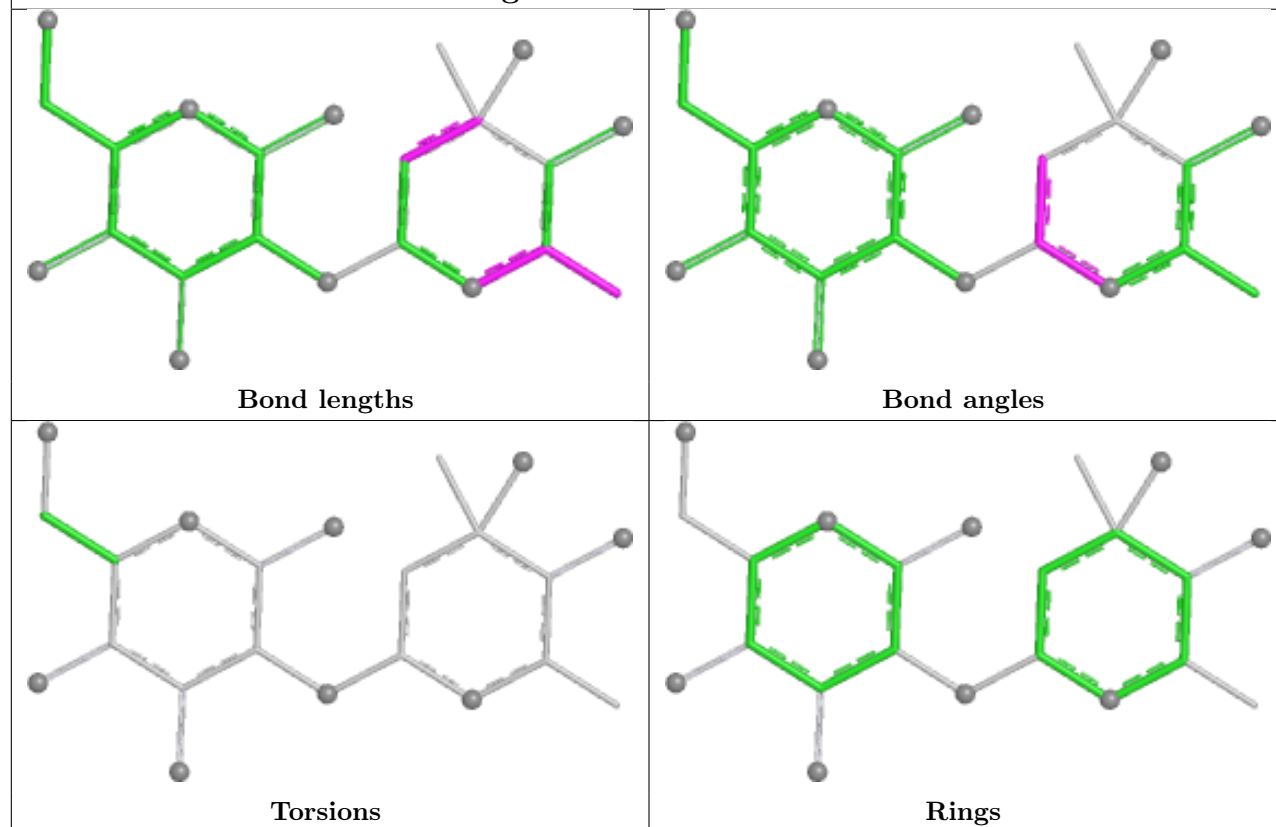
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

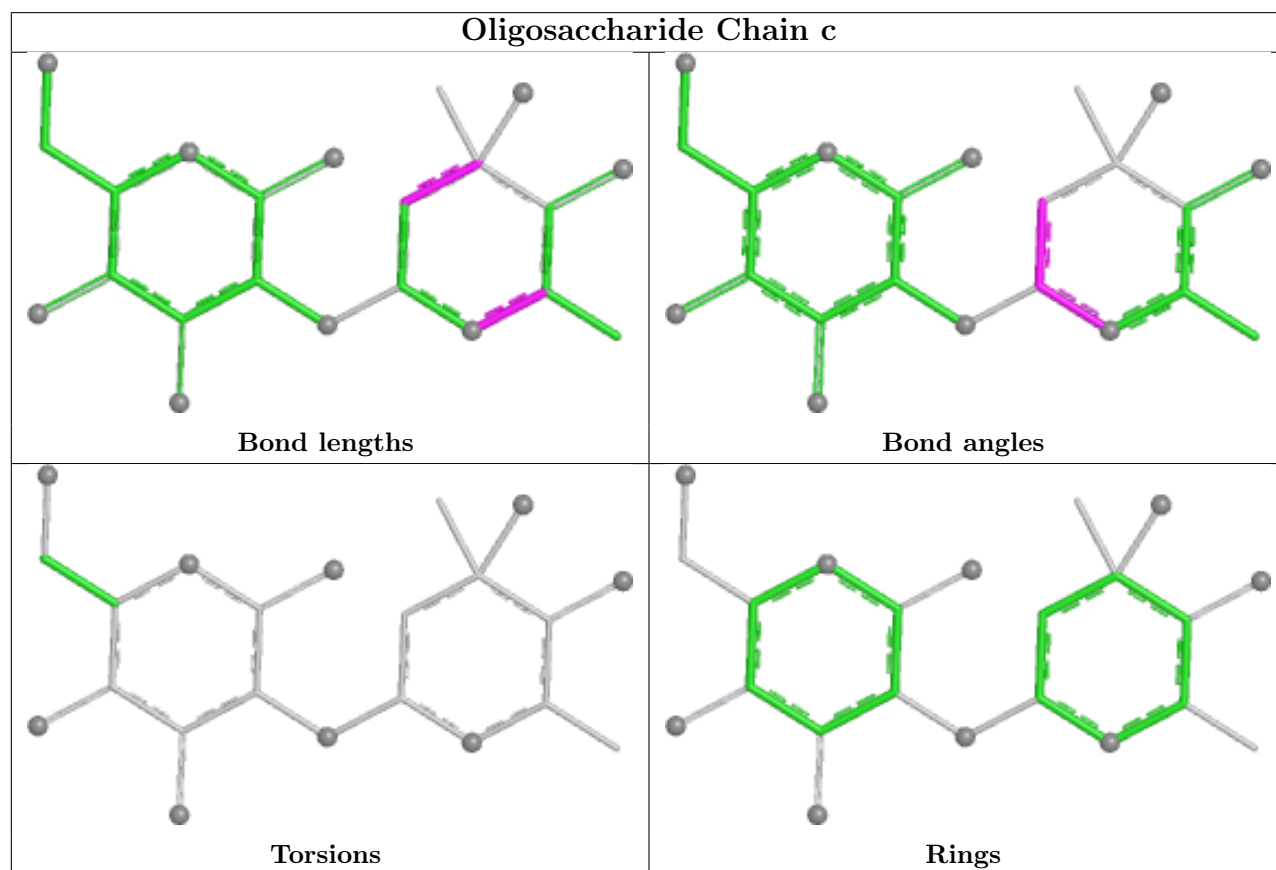
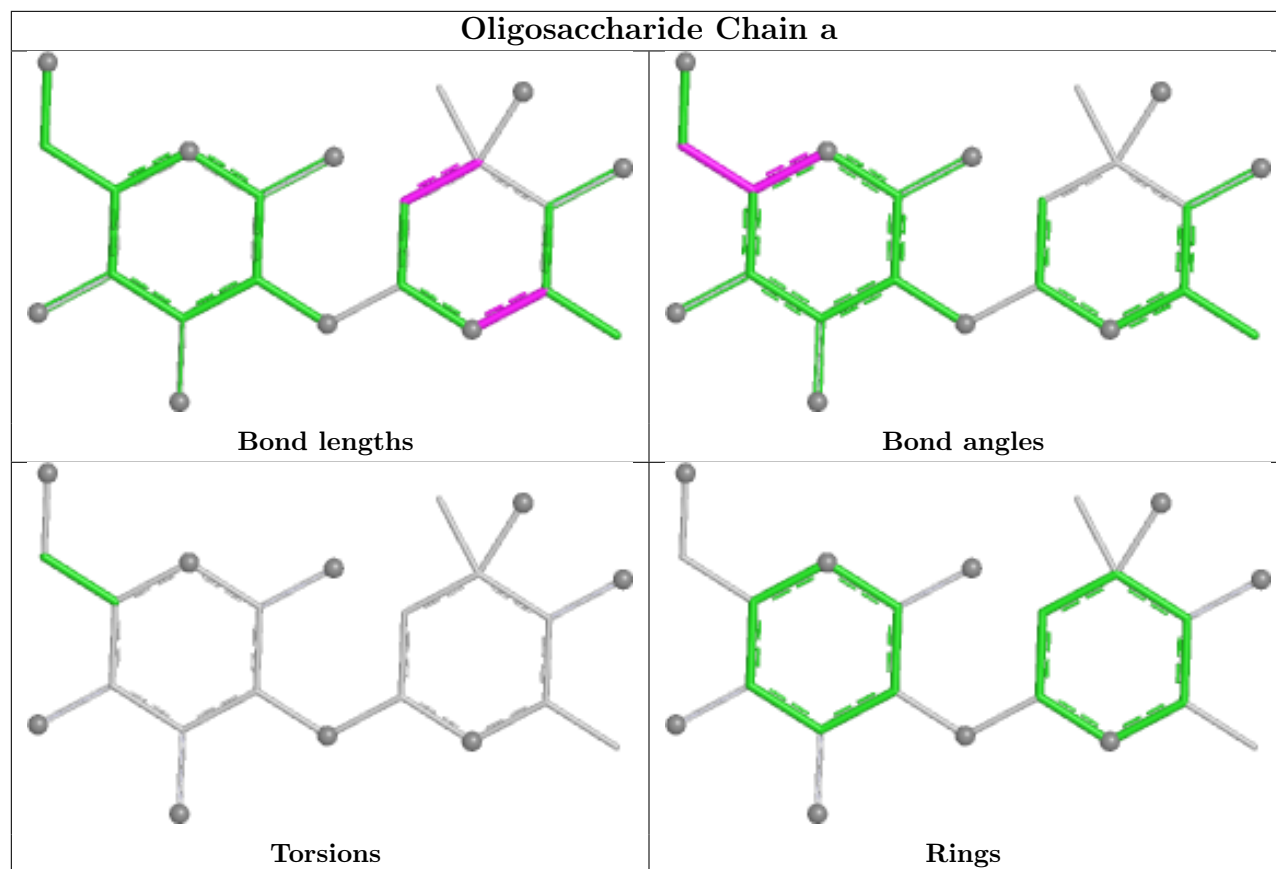


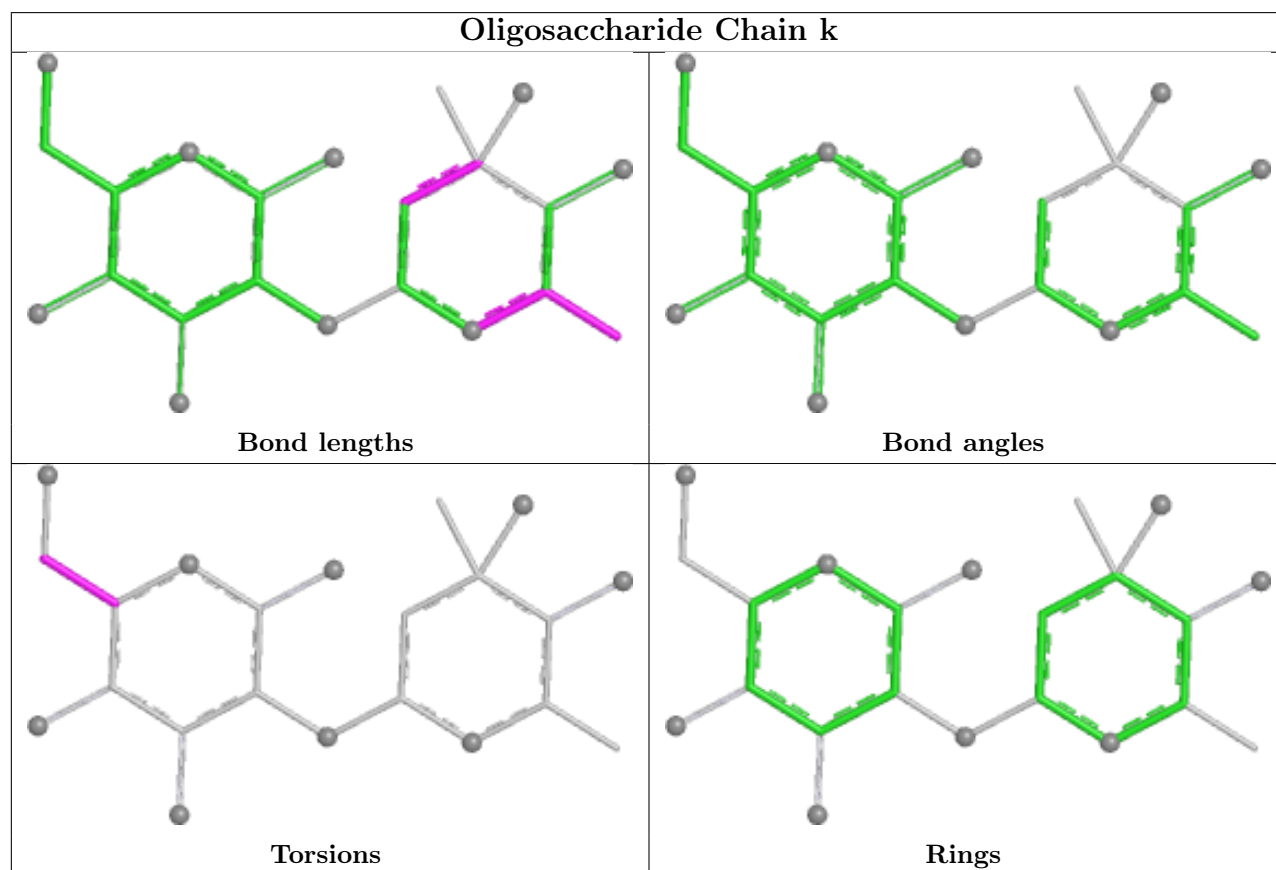
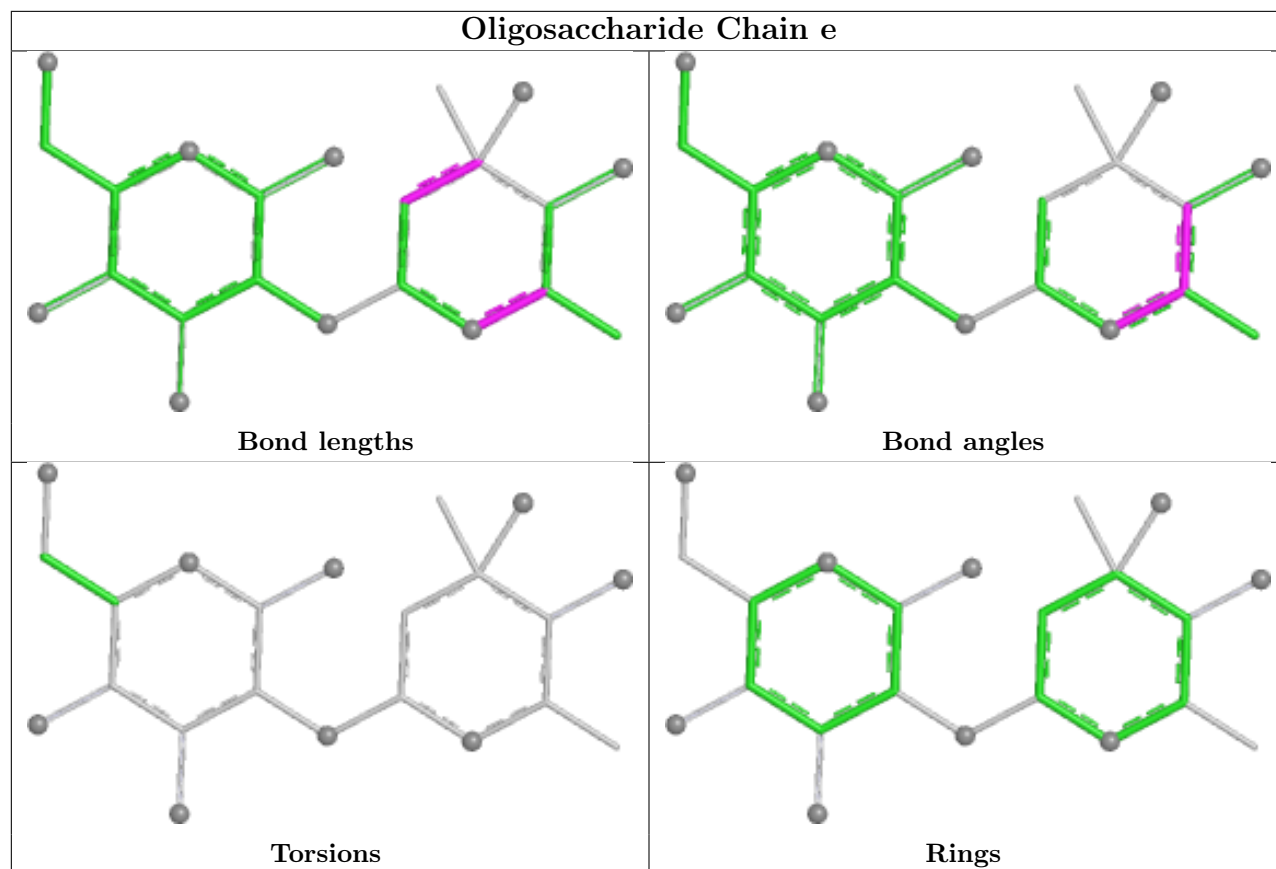
Oligosaccharide Chain W

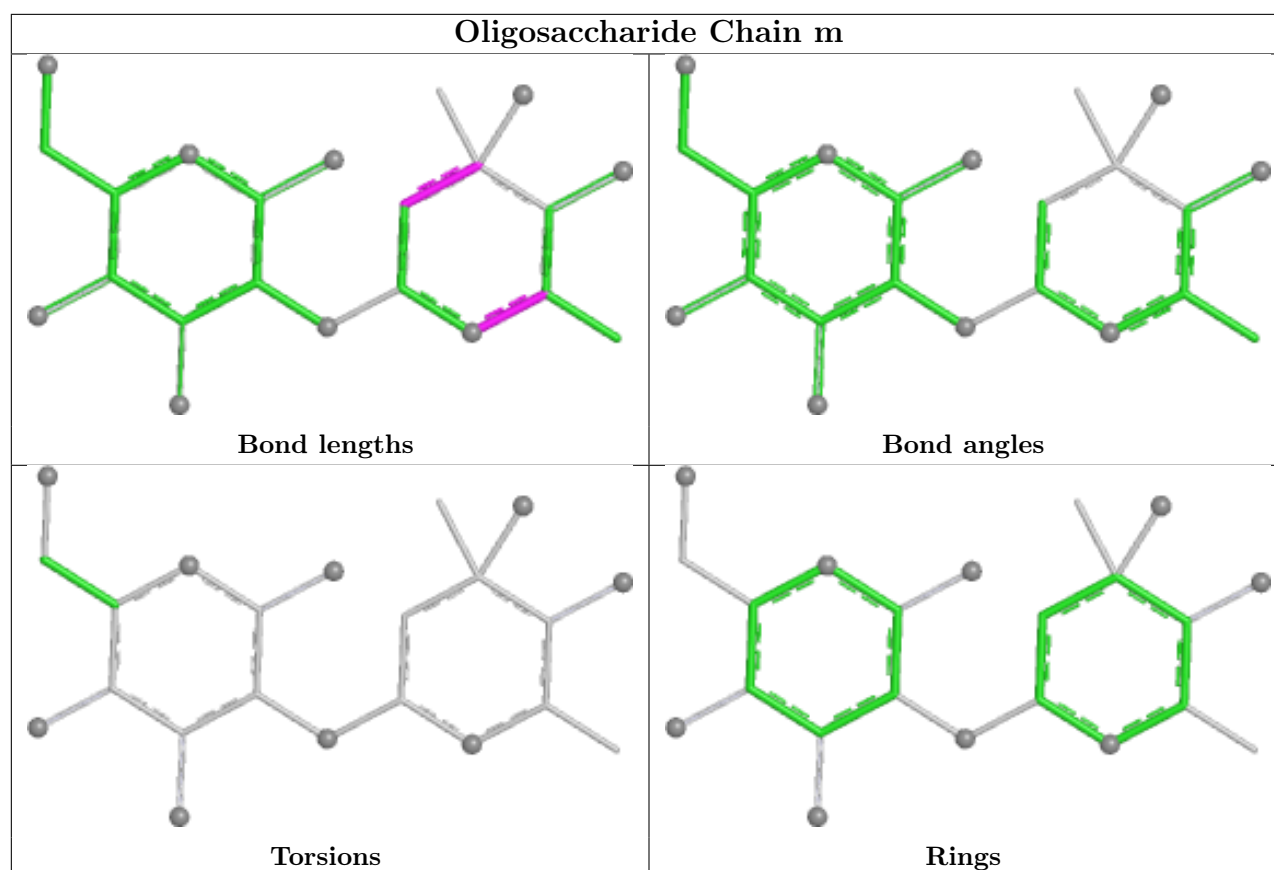


Oligosaccharide Chain Y









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	$\# Z > 2$
6	DMS	H	102	-	3,3,3	0.47	0	3,3,3	0.53	0
8	RER	H	104[B]	7	7,10,11	2.58	3 (42%)	6,15,17	1.75	1 (16%)
4	PGE	A	101	-	9,9,9	0.53	0	8,8,8	0.36	0
5	BO3	D	101	-	3,3,3	0.52	0	3,3,3	0.06	0
8	RER	G	103[B]	7	7,10,11	2.64	4 (57%)	6,15,17	1.56	1 (16%)
7	BGC	H	103[B]	8	12,12,12	0.49	0	17,17,17	0.67	0
5	BO3	J	101	-	3,3,3	0.58	0	3,3,3	0.05	0
6	DMS	G	101[B]	-	3,3,3	0.62	0	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	RER	G	103[A]	7	7,10,11	2.24	3 (42%)	6,15,17	1.18	1 (16%)
6	DMS	H	101	-	3,3,3	0.69	0	3,3,3	0.51	0
6	DMS	J	102	-	3,3,3	0.68	0	3,3,3	0.49	0
7	BGC	G	102[A]	8	12,12,12	0.64	0	17,17,17	0.79	0
6	DMS	G	101[A]	-	3,3,3	0.56	0	3,3,3	0.24	0
7	BGC	G	102[B]	8	12,12,12	0.55	0	17,17,17	0.88	0
7	BGC	H	103[A]	8	12,12,12	0.55	0	17,17,17	0.52	0
8	RER	H	104[A]	7	7,10,11	2.63	2 (28%)	6,15,17	0.91	0
5	BO3	O	101	-	3,3,3	0.50	0	3,3,3	0.05	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
4	PGE	A	101	-	-	2/7/7/7	-
8	RER	G	103[B]	7	-	-	0/1/1/1
7	BGC	H	103[B]	8	-	0/2/22/22	0/1/1/1
8	RER	G	103[A]	7	-	-	0/1/1/1
7	BGC	G	102[A]	8	-	0/2/22/22	0/1/1/1
7	BGC	G	102[B]	8	-	0/2/22/22	0/1/1/1
7	BGC	H	103[A]	8	-	0/2/22/22	0/1/1/1
8	RER	H	104[A]	7	-	-	0/1/1/1
8	RER	H	104[B]	7	-	-	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	104[A]	RER	C2-C3	-4.87	1.47	1.54
8	G	103[B]	RER	C2-C3	-4.77	1.47	1.54
8	H	104[B]	RER	C2-C3	-4.63	1.48	1.54
8	G	103[A]	RER	C2-C3	-4.01	1.48	1.54
8	H	104[A]	RER	O5-C5	3.87	1.51	1.43
8	G	103[B]	RER	O5-C5	3.86	1.51	1.43
8	H	104[B]	RER	O5-C5	3.76	1.51	1.43
8	G	103[A]	RER	O5-C5	3.14	1.49	1.43
8	H	104[B]	RER	C5A-C5	-2.34	1.45	1.51
8	G	103[B]	RER	C5A-C5	-2.29	1.46	1.51
8	G	103[A]	RER	C5A-C5	-2.10	1.46	1.51
8	G	103[B]	RER	C5-C4	-2.04	1.48	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	104[B]	RER	O5-C5-C4	3.30	115.72	110.04
8	G	103[B]	RER	O5-C1-C2	2.72	115.08	111.38
8	G	103[A]	RER	O5-C1-C2	2.44	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	103[B]	BGC	1	0
6	G	101[B]	DMS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1/7 (14%)	0.02	0 100 100	18, 18, 18, 18	0
1	B	1/7 (14%)	-0.62	0 100 100	13, 13, 13, 13	0
1	C	1/7 (14%)	-0.48	0 100 100	15, 15, 15, 15	0
1	D	1/7 (14%)	-0.76	0 100 100	12, 12, 12, 12	0
1	E	1/7 (14%)	-0.65	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%)	-0.90	0 100 100	13, 13, 13, 13	0
1	H	1/7 (14%)	-0.54	0 100 100	13, 13, 13, 13	0
1	I	1/7 (14%)	-0.85	0 100 100	14, 14, 14, 14	0
1	J	1/7 (14%)	0.61	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%)	-0.49	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 ⓘ

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	0.90	0.12	20,25,30,31	0
1	MLU	C	1	9/10	0.93	0.10	15,17,20,22	0
1	MLU	J	1	9/10	0.93	0.10	24,28,33,35	0
1	MLU	E	1	9/10	0.94	0.10	16,19,21,22	0
1	3FG	A	7	13/13	0.95	0.07	16,17,22,23	0
2	DAL	K	2	5/6	0.95	0.07	18,18,19,20	0
2	DAL	S	2[A]	5/6	0.95	0.07	11,12,12,13	5
2	DAL	S	2[B]	5/6	0.95	0.07	13,13,13,14	5
2	DAL	T	2	5/6	0.95	0.07	21,22,22,23	0
1	OMZ	C	2	14/15	0.96	0.08	13,14,15,16	1
2	DAL	M	2	5/6	0.96	0.07	18,18,18,19	0
1	GHP	A	5	11/12	0.96	0.07	12,13,15,17	0
1	MLU	I	1	9/10	0.96	0.08	12,14,16,17	0
1	3FG	J	7	13/13	0.96	0.06	19,22,24,25	0
2	DSN	O	3	7/7	0.96	0.07	16,17,19,22	0
2	DSN	T	3	7/7	0.96	0.07	19,19,20,20	0
1	MLU	B	1	9/10	0.97	0.06	12,13,15,16	0
1	OMZ	E	2	14/15	0.97	0.06	14,16,17,18	1
1	OMZ	F	2	14/15	0.97	0.06	12,13,13,13	1
2	DAL	N	2	5/6	0.97	0.06	13,13,14,16	0
2	DAL	O	2	5/6	0.97	0.07	18,18,19,19	0
1	GHP	E	4	10/12	0.97	0.05	12,13,14,14	0
1	MLU	H	1	9/10	0.97	0.06	13,14,16,16	0
1	OMZ	A	2	14/15	0.97	0.05	12,13,15,16	1
2	DSN	M	3	7/7	0.97	0.06	16,16,17,18	0
1	3FG	E	7	13/13	0.97	0.06	13,14,16,17	0
2	DSN	S	3[A]	7/7	0.97	0.06	9,10,12,15	7
2	DSN	S	3[B]	7/7	0.97	0.06	15,16,17,17	7
1	3FG	I	7	13/13	0.97	0.05	12,13,18,18	0
1	GHP	D	5	11/12	0.98	0.04	10,11,12,12	0
1	GHP	F	5	11/12	0.98	0.04	11,12,12,12	0
1	GHP	H	5	11/12	0.98	0.05	11,12,12,13	0
1	GHP	I	5	11/12	0.98	0.05	12,12,13,14	0
1	GHP	J	5	11/12	0.98	0.05	14,15,19,21	0
1	OMY	A	6	14/15	0.98	0.05	13,14,16,16	1
1	OMY	C	6	14/15	0.98	0.05	11,12,13,13	1
1	OMY	F	6	14/15	0.98	0.05	12,13,14,14	1
1	OMY	J	6	14/15	0.98	0.05	14,15,18,18	1
1	MLU	D	1	9/10	0.98	0.05	14,16,19,21	0
1	3FG	C	7	13/13	0.98	0.04	11,13,15,16	0
1	3FG	D	7	13/13	0.98	0.04	11,12,14,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMZ	H	2	14/15	0.98	0.04	11,13,14,14	1
1	3FG	F	7	13/13	0.98	0.05	11,12,14,16	0
1	3FG	G	7	13/13	0.98	0.05	11,13,17,19	0
1	3FG	H	7	13/13	0.98	0.04	12,13,17,18	0
1	OMZ	I	2	14/15	0.98	0.05	12,13,14,14	1
1	OMZ	J	2	14/15	0.98	0.05	15,17,19,21	1
1	GHP	B	4	10/12	0.98	0.04	11,11,12,12	0
1	GHP	C	4	10/12	0.98	0.04	11,12,13,14	0
1	GHP	D	4	10/12	0.98	0.04	10,11,12,12	0
1	MLU	F	1	9/10	0.98	0.05	15,17,19,21	0
2	DAL	P	2	5/6	0.98	0.05	14,14,14,15	0
2	DAL	Q	2	5/6	0.98	0.05	11,11,13,13	0
1	GHP	F	4	10/12	0.98	0.04	11,12,13,13	0
1	GHP	G	4	10/12	0.98	0.04	10,11,12,12	0
1	GHP	H	4	10/12	0.98	0.05	11,12,13,13	0
2	DSN	K	3	7/7	0.98	0.04	16,17,17,19	0
1	GHP	I	4	10/12	0.98	0.04	11,12,13,13	0
2	DSN	N	3	7/7	0.98	0.06	13,13,14,16	0
1	GHP	J	4	10/12	0.98	0.06	13,14,15,15	0
2	DSN	P	3	7/7	0.98	0.06	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	0.05	13,13,14,18	0
1	MLU	G	1	9/10	0.98	0.05	12,12,14,14	0
1	GHP	B	5	11/12	0.98	0.04	11,11,12,12	0
1	GHP	C	5	11/12	0.98	0.04	11,11,12,12	0
1	3FG	B	7	13/13	0.99	0.04	10,11,16,16	0
1	OMZ	B	2	14/15	0.99	0.04	11,12,13,13	1
2	DAL	R	2	5/6	0.99	0.04	12,13,14,15	0
1	GHP	E	5	11/12	0.99	0.04	11,12,13,13	0
1	OMY	B	6	14/15	0.99	0.04	12,12,14,14	1
1	OMZ	D	2	14/15	0.99	0.04	11,12,12,13	1
1	OMY	D	6	14/15	0.99	0.04	11,13,13,13	1
2	DSN	L	3[A]	7/7	0.99	0.04	10,10,12,14	7
2	DSN	L	3[B]	7/7	0.99	0.04	14,15,15,16	7
1	OMY	E	6	14/15	0.99	0.04	12,13,14,15	1
1	GHP	G	5	11/12	0.99	0.04	11,11,12,12	0
1	OMY	G	6	14/15	0.99	0.04	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	0.03	10,10,10,11	5
2	DAL	L	2[B]	5/6	0.99	0.03	16,17,17,18	5
1	OMY	I	6	14/15	0.99	0.04	13,14,15,15	1
1	OMZ	G	2	14/15	0.99	0.04	11,12,13,14	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	GHP	A	4	10/12	0.99	0.04	11,12,13,13	0

6.3 Carbohydrates

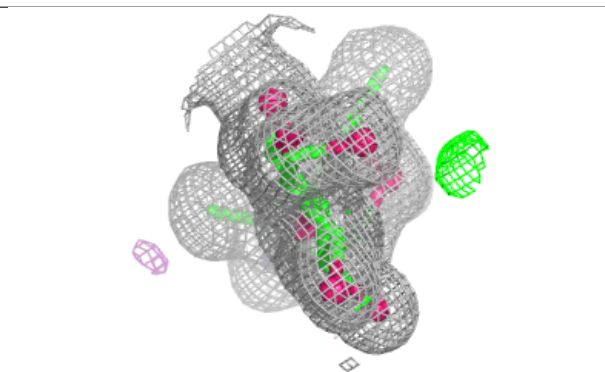
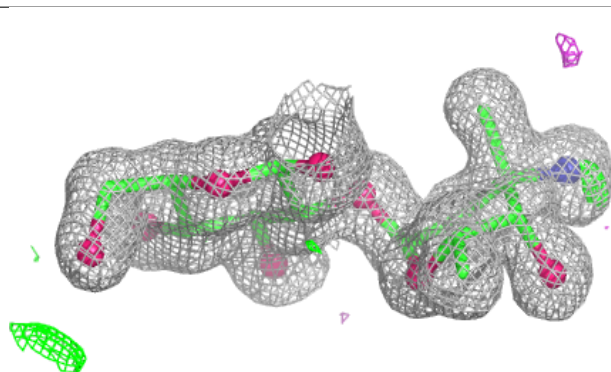
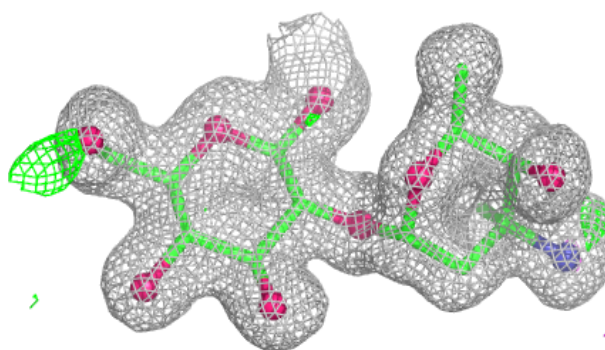
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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

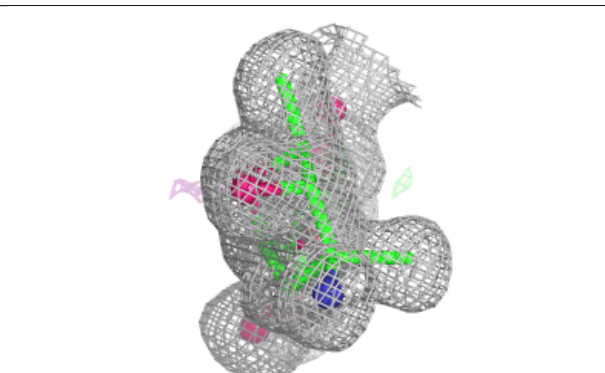
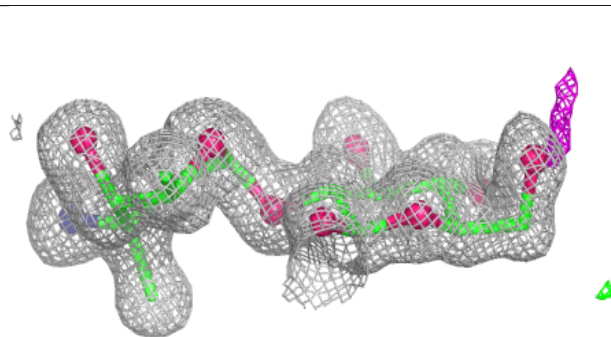
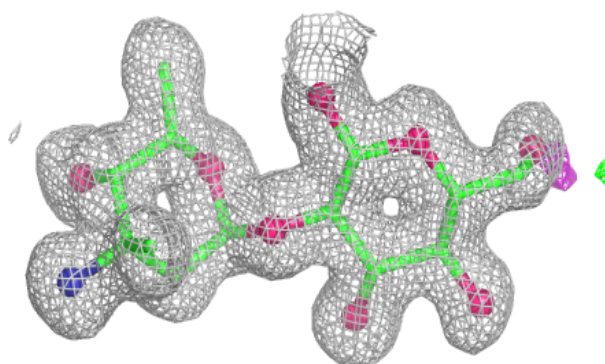
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

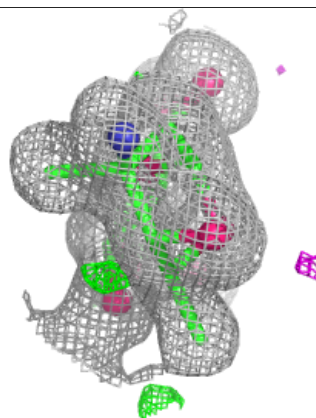
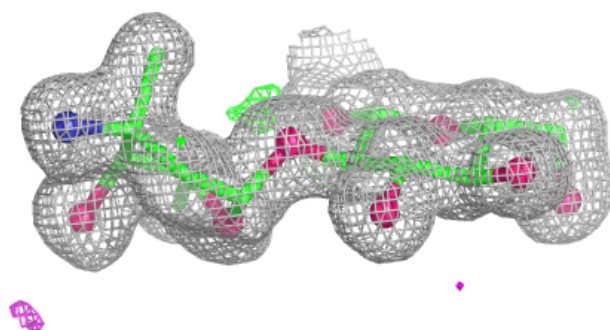
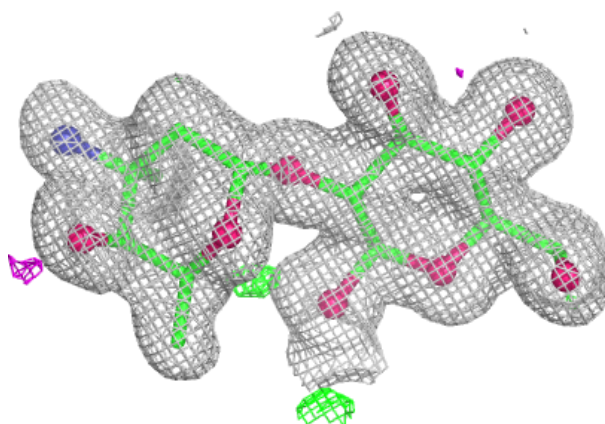
**Electron density around Chain W:**

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



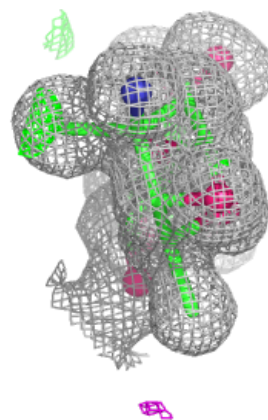
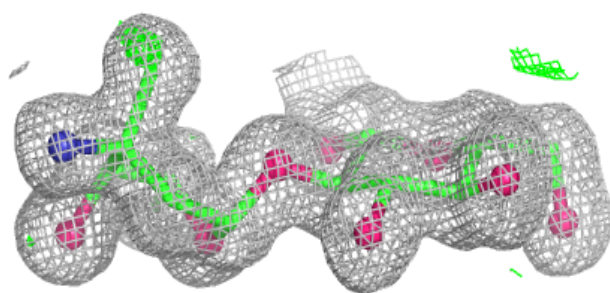
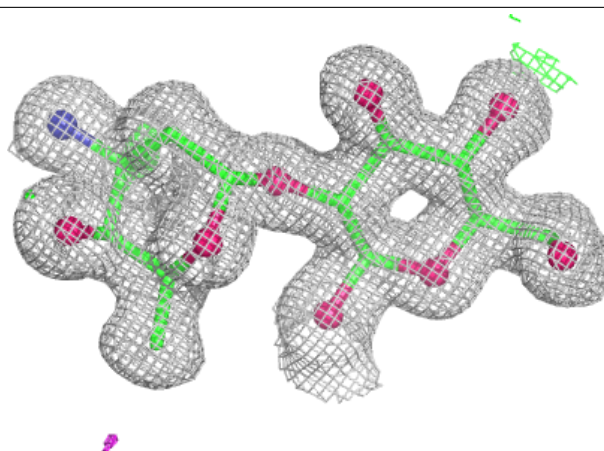
Electron density around Chain Y:

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

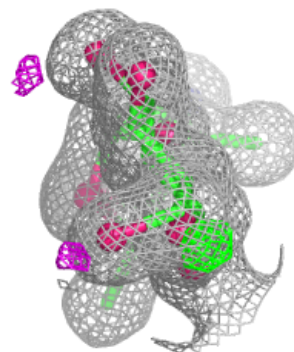
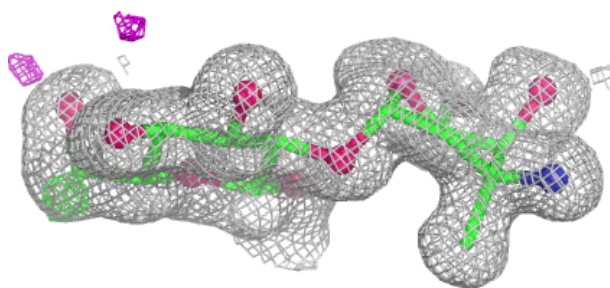
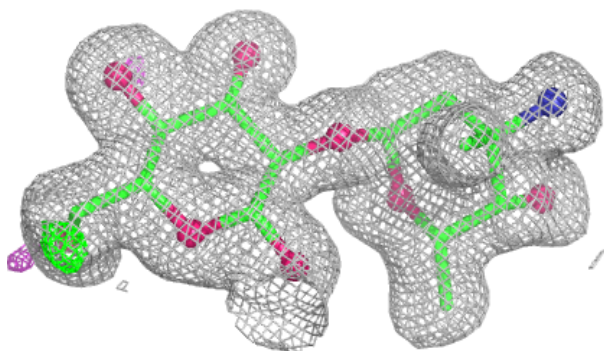


Electron density around Chain a:

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

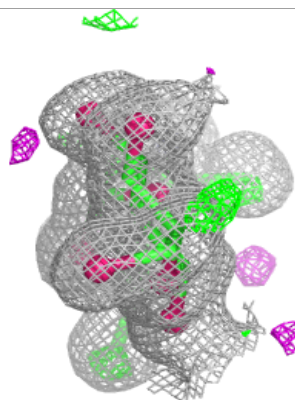
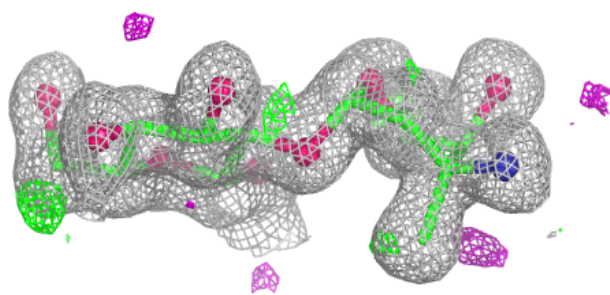
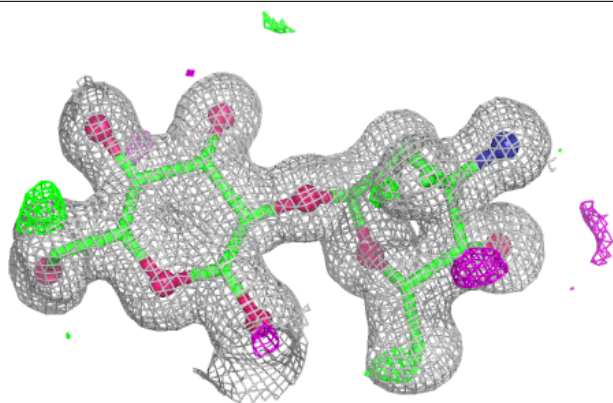
**Electron density around Chain c:**

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

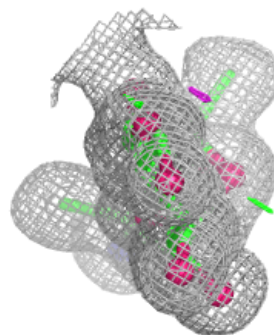
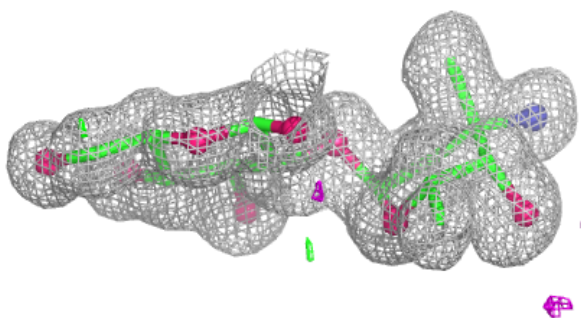
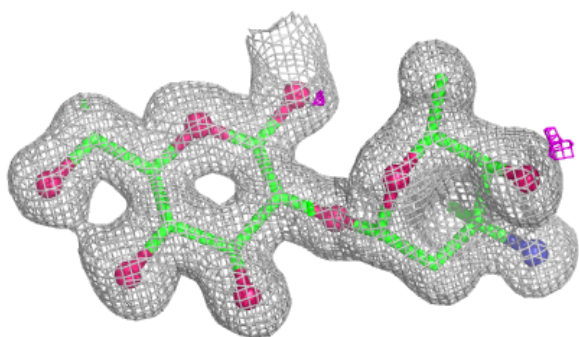


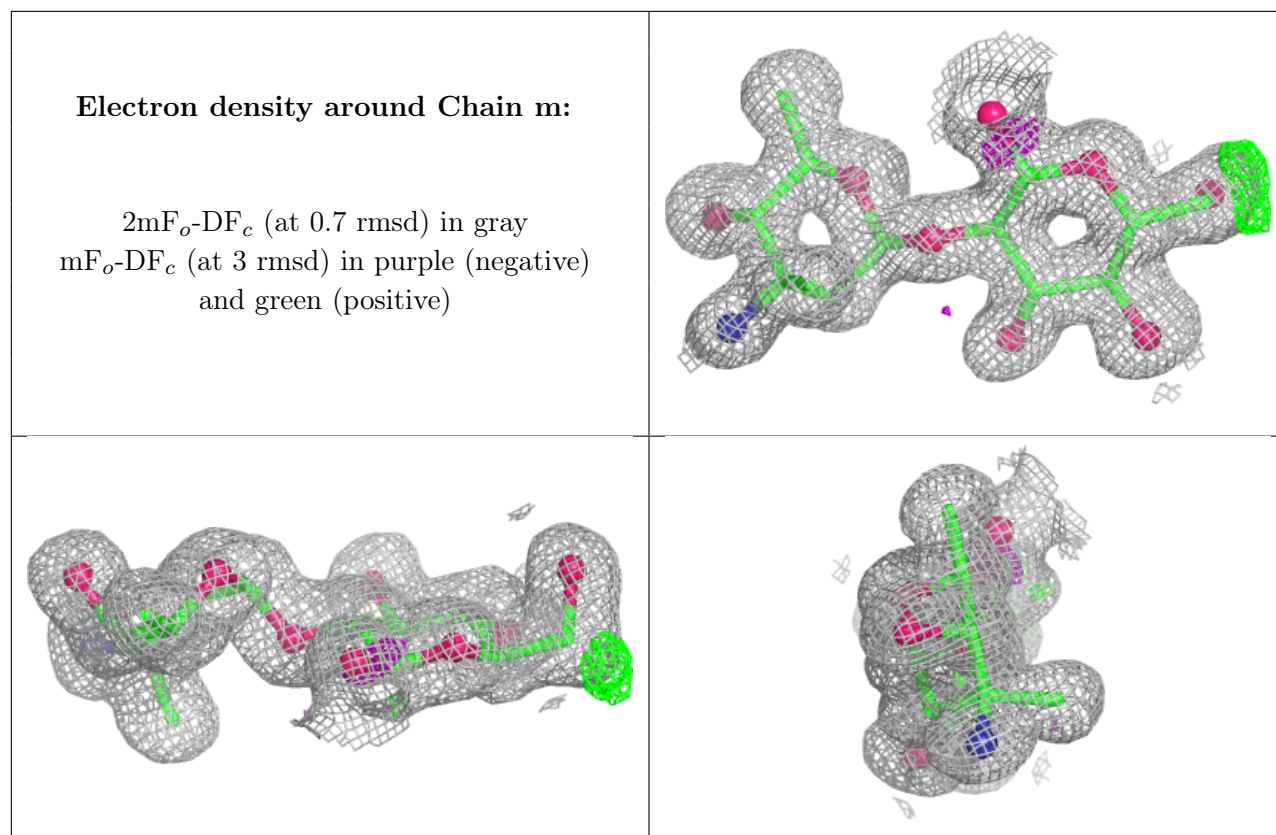
Electron density around Chain e:

$2mF_o-DF_c$ (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)





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
6	DMS	H	101	4/4	0.81	0.21	49,67,68,78	0
8	RER	G	103[A]	10/11	0.84	0.12	13,14,15,16	10
8	RER	G	103[B]	10/11	0.84	0.12	20,23,24,24	10
5	BO3	D	101	4/4	0.87	0.16	14,38,42,55	0
4	PGE	A	101	10/10	0.88	0.13	26,35,45,60	0
5	BO3	J	101	4/4	0.89	0.26	13,32,49,52	0
5	BO3	O	101	4/4	0.92	0.15	13,25,38,54	0
8	RER	H	104[A]	10/11	0.93	0.09	16,19,21,21	10
8	RER	H	104[B]	10/11	0.93	0.09	21,23,24,26	10
7	BGC	G	102[A]	12/12	0.96	0.07	12,13,18,19	12
7	BGC	G	102[B]	12/12	0.96	0.07	14,18,20,21	12
6	DMS	H	102	4/4	0.97	0.10	19,19,20,20	0
6	DMS	J	102	4/4	0.97	0.11	20,24,25,26	0
7	BGC	H	103[A]	12/12	0.97	0.06	12,13,15,15	12

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	BGC	H	103[B]	12/12	0.97	0.06	15,21,24,24	12
6	DMS	G	101[B]	4/4	0.98	0.07	10,14,22,26	4
6	DMS	G	101[A]	4/4	0.98	0.07	16,16,18,27	4

6.5 Other polymers [i](#)

There are no such residues in this entry.