



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 08:54 AM UTC

PDB ID : 4TZ3 / pdb_00004tz3
Title : Ensemble refinement of the E502A variant of sacteLam55A from Streptomyces sp. SirexAA-E in complex with laminaritetraose
Authors : Bianchetti, C.M.; Takasuka, T.E.; Yik, E.J.; Bergeman, L.F.; Fox, B.G.
Deposited on : 2014-07-09
Resolution : 1.90 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	:	FAILED
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

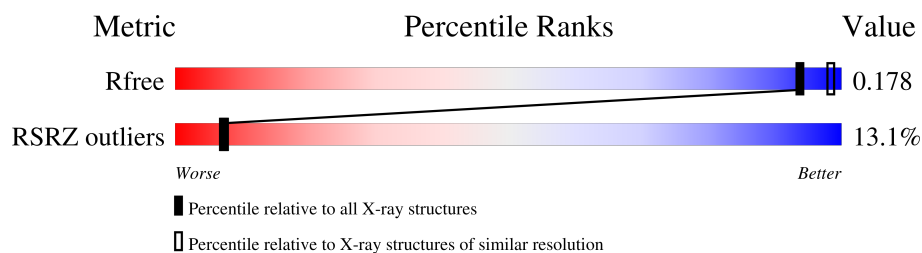
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 210296 atoms, of which 98125 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 Putative secreted protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	2-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	3-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	4-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	5-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	6-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	7-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	8-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	9-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	10-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	11-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	12-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	13-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	14-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	15-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	16-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	18-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	19-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	20-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	21-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	22-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	23-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	24-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	25-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	ALA	GLU	engineered mutation	UNP G2NFJ9

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	1-B	4	Total	C	O	0	0	0
			45	24	21			
2	2-B	4	Total	C	O	0	0	0
			45	24	21			
2	3-B	4	Total	C	O	0	0	0
			45	24	21			
2	4-B	4	Total	C	O	0	0	0
			45	24	21			
2	5-B	4	Total	C	O	0	0	0
			45	24	21			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	6-B	4	Total	C	O	0	0	0
			45	24	21			
2	7-B	4	Total	C	O	0	0	0
			45	24	21			
2	8-B	4	Total	C	O	0	0	0
			45	24	21			
2	9-B	4	Total	C	O	0	0	0
			45	24	21			
2	10-B	4	Total	C	O	0	0	0
			45	24	21			
2	11-B	4	Total	C	O	0	0	0
			45	24	21			
2	12-B	4	Total	C	O	0	0	0
			45	24	21			
2	13-B	4	Total	C	O	0	0	0
			45	24	21			
2	14-B	4	Total	C	O	0	0	0
			45	24	21			
2	15-B	4	Total	C	O	0	0	0
			45	24	21			
2	16-B	4	Total	C	O	0	0	0
			45	24	21			
2	17-B	4	Total	C	O	0	0	0
			45	24	21			
2	18-B	4	Total	C	O	0	0	0
			45	24	21			
2	19-B	4	Total	C	O	0	0	0
			45	24	21			
2	20-B	4	Total	C	O	0	0	0
			45	24	21			
2	21-B	4	Total	C	O	0	0	0
			45	24	21			
2	22-B	4	Total	C	O	0	0	0
			45	24	21			
2	23-B	4	Total	C	O	0	0	0
			45	24	21			
2	24-B	4	Total	C	O	0	0	0
			45	24	21			
2	25-B	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



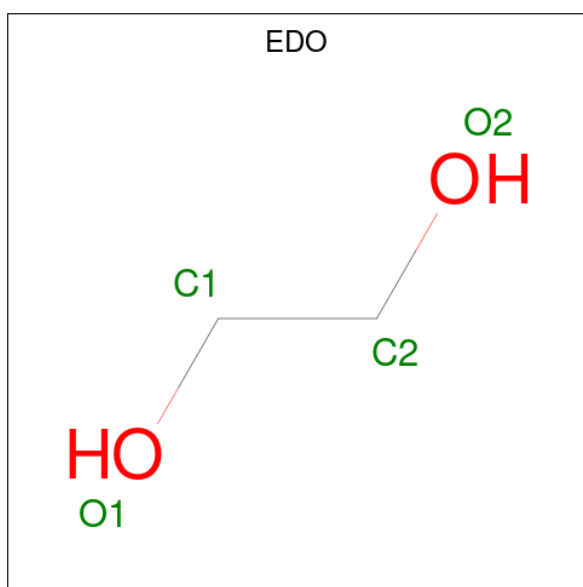
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total	C	O	0	0
			11	6	5		
3	2-A	1	Total	C	O	0	0
			11	6	5		
3	3-A	1	Total	C	O	0	0
			11	6	5		
3	4-A	1	Total	C	O	0	0
			11	6	5		
3	5-A	1	Total	C	O	0	0
			11	6	5		
3	6-A	1	Total	C	O	0	0
			11	6	5		
3	7-A	1	Total	C	O	0	0
			11	6	5		
3	8-A	1	Total	C	O	0	0
			11	6	5		
3	9-A	1	Total	C	O	0	0
			11	6	5		
3	10-A	1	Total	C	O	0	0
			11	6	5		
3	11-A	1	Total	C	O	0	0
			11	6	5		
3	12-A	1	Total	C	O	0	0
			11	6	5		
3	13-A	1	Total	C	O	0	0
			11	6	5		
3	14-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	15-A	1	Total	C	O	0	0
			11	6	5		
3	16-A	1	Total	C	O	0	0
			11	6	5		
3	17-A	1	Total	C	O	0	0
			11	6	5		
3	18-A	1	Total	C	O	0	0
			11	6	5		
3	19-A	1	Total	C	O	0	0
			11	6	5		
3	20-A	1	Total	C	O	0	0
			11	6	5		
3	21-A	1	Total	C	O	0	0
			11	6	5		
3	22-A	1	Total	C	O	0	0
			11	6	5		
3	23-A	1	Total	C	O	0	0
			11	6	5		
3	24-A	1	Total	C	O	0	0
			11	6	5		
3	25-A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	1-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	2-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	3-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	4-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	5-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	6-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	7-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	8-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	9-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	10-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	11-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	12-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	13-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	14-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	15-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	16-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	17-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	18-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	19-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	20-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	21-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	22-A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	23-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	24-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	25-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	1-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	2-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	3-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	4-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	5-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	6-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	7-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	8-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	9-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	10-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	11-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	12-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	13-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	14-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	15-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	16-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	17-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	18-A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	19-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	20-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	21-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	22-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	23-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	24-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	25-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	1-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	2-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	3-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	4-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	5-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	6-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	7-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	8-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	9-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	10-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	11-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	12-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	13-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	14-A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	15-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	16-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	17-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	18-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	19-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	20-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	21-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	22-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	23-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	24-A	1	Total	C	H	O	0	0
			10	2	6	2		
4	25-A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	253	Total	O	0	0
			253	253		
5	2-A	248	Total	O	0	0
			248	248		
5	3-A	259	Total	O	0	0
			259	259		
5	4-A	249	Total	O	0	0
			249	249		
5	5-A	246	Total	O	0	0
			246	246		
5	6-A	245	Total	O	0	0
			245	245		
5	7-A	258	Total	O	0	0
			258	258		
5	8-A	264	Total	O	0	0
			264	264		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	9-A	251	Total 251	O 251	0	0
5	10-A	248	Total 248	O 248	0	0
5	11-A	264	Total 264	O 264	0	0
5	12-A	246	Total 246	O 246	0	0
5	13-A	247	Total 247	O 247	0	0
5	14-A	242	Total 242	O 242	0	0
5	15-A	262	Total 262	O 262	0	0
5	16-A	252	Total 252	O 252	0	0
5	17-A	243	Total 243	O 243	0	0
5	18-A	255	Total 255	O 255	0	0
5	19-A	274	Total 274	O 274	0	0
5	20-A	242	Total 242	O 242	0	0
5	21-A	240	Total 240	O 240	0	0
5	22-A	250	Total 250	O 250	0	0
5	23-A	259	Total 259	O 259	0	0
5	24-A	250	Total 250	O 250	0	0
5	25-A	249	Total 249	O 249	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.28Å 100.21Å 54.22Å 90.00° 99.46° 90.00°	Depositor
Resolution (Å)	28.33 – 1.90 28.33 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.2 (28.33-1.90) 90.3 (28.33-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.9_1692)	Depositor
R, R_{free}	0.113 , 0.151 0.143 , 0.178	Depositor DCC
R_{free} test set	1989 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 23.3	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	0.91	EDS
Total number of atoms	210296	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 6.90% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

100 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	1-B	1	2	12,12,12	2.45	4 (33%)	17,17,17	3.24	7 (41%)
2	BGC	1-B	2	2	11,11,12	2.72	4 (36%)	15,15,17	1.58	2 (13%)
2	BGC	1-B	3	2	11,11,12	3.02	5 (45%)	15,15,17	1.84	5 (33%)
2	BGC	1-B	4	2	11,11,12	2.84	5 (45%)	15,15,17	2.91	4 (26%)
2	BGC	10-B	1	2	12,12,12	2.24	5 (41%)	17,17,17	1.31	2 (11%)
2	BGC	10-B	2	2	11,11,12	2.93	5 (45%)	15,15,17	1.91	5 (33%)
2	BGC	10-B	3	2	11,11,12	3.19	6 (54%)	15,15,17	1.78	4 (26%)
2	BGC	10-B	4	2	11,11,12	2.64	5 (45%)	15,15,17	2.26	5 (33%)
2	BGC	11-B	1	2	12,12,12	2.30	5 (41%)	17,17,17	1.21	1 (5%)
2	BGC	11-B	2	2	11,11,12	2.85	5 (45%)	15,15,17	1.85	2 (13%)
2	BGC	11-B	3	2	11,11,12	2.88	5 (45%)	15,15,17	1.82	4 (26%)
2	BGC	11-B	4	2	11,11,12	2.67	5 (45%)	15,15,17	2.23	4 (26%)
2	BGC	12-B	1	2	12,12,12	2.42	5 (41%)	17,17,17	0.80	0
2	BGC	12-B	2	2	11,11,12	2.83	4 (36%)	15,15,17	1.41	1 (6%)
2	BGC	12-B	3	2	11,11,12	2.99	5 (45%)	15,15,17	1.81	4 (26%)
2	BGC	12-B	4	2	11,11,12	2.71	4 (36%)	15,15,17	1.72	4 (26%)
2	BGC	13-B	1	2	12,12,12	2.33	5 (41%)	17,17,17	1.22	2 (11%)
2	BGC	13-B	2	2	11,11,12	2.84	4 (36%)	15,15,17	1.41	2 (13%)
2	BGC	13-B	3	2	11,11,12	3.01	6 (54%)	15,15,17	1.80	4 (26%)
2	BGC	13-B	4	2	11,11,12	2.65	5 (45%)	15,15,17	2.09	4 (26%)
2	BGC	14-B	1	2	12,12,12	2.30	5 (41%)	17,17,17	0.96	0
2	BGC	14-B	2	2	11,11,12	2.89	5 (45%)	15,15,17	1.69	4 (26%)
2	BGC	14-B	3	2	11,11,12	3.06	5 (45%)	15,15,17	1.87	3 (20%)
2	BGC	14-B	4	2	11,11,12	2.68	5 (45%)	15,15,17	2.17	6 (40%)
2	BGC	15-B	1	2	12,12,12	2.23	5 (41%)	17,17,17	1.63	5 (29%)
2	BGC	15-B	2	2	11,11,12	2.94	5 (45%)	15,15,17	2.15	5 (33%)
2	BGC	15-B	3	2	11,11,12	2.85	6 (54%)	15,15,17	1.75	3 (20%)
2	BGC	15-B	4	2	11,11,12	2.60	4 (36%)	15,15,17	2.23	5 (33%)
2	BGC	16-B	1	2	12,12,12	2.19	5 (41%)	17,17,17	1.70	2 (11%)
2	BGC	16-B	2	2	11,11,12	2.91	6 (54%)	15,15,17	1.75	4 (26%)
2	BGC	16-B	3	2	11,11,12	3.11	6 (54%)	15,15,17	1.88	4 (26%)
2	BGC	16-B	4	2	11,11,12	2.78	5 (45%)	15,15,17	2.25	5 (33%)
2	BGC	17-B	1	2	12,12,12	2.46	5 (41%)	17,17,17	1.35	3 (17%)
2	BGC	17-B	2	2	11,11,12	3.05	5 (45%)	15,15,17	1.47	3 (20%)
2	BGC	17-B	3	2	11,11,12	2.92	6 (54%)	15,15,17	1.50	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	17-B	4	2	11,11,12	2.62	5 (45%)	15,15,17	2.09	5 (33%)
2	BGC	18-B	1	2	12,12,12	2.33	5 (41%)	17,17,17	1.13	1 (5%)
2	BGC	18-B	2	2	11,11,12	2.92	5 (45%)	15,15,17	1.60	1 (6%)
2	BGC	18-B	3	2	11,11,12	2.84	5 (45%)	15,15,17	1.91	3 (20%)
2	BGC	18-B	4	2	11,11,12	2.67	5 (45%)	15,15,17	2.38	7 (46%)
2	BGC	19-B	1	2	12,12,12	2.24	5 (41%)	17,17,17	1.77	3 (17%)
2	BGC	19-B	2	2	11,11,12	2.91	4 (36%)	15,15,17	1.77	4 (26%)
2	BGC	19-B	3	2	11,11,12	3.05	6 (54%)	15,15,17	1.95	5 (33%)
2	BGC	19-B	4	2	11,11,12	2.73	5 (45%)	15,15,17	2.60	4 (26%)
2	BGC	2-B	1	2	12,12,12	2.35	5 (41%)	17,17,17	1.08	2 (11%)
2	BGC	2-B	2	2	11,11,12	3.02	6 (54%)	15,15,17	1.69	2 (13%)
2	BGC	2-B	3	2	11,11,12	3.08	5 (45%)	15,15,17	1.55	3 (20%)
2	BGC	2-B	4	2	11,11,12	2.75	5 (45%)	15,15,17	2.23	5 (33%)
2	BGC	20-B	1	2	12,12,12	2.42	5 (41%)	17,17,17	1.09	0
2	BGC	20-B	2	2	11,11,12	2.97	5 (45%)	15,15,17	1.89	4 (26%)
2	BGC	20-B	3	2	11,11,12	2.94	6 (54%)	15,15,17	1.51	2 (13%)
2	BGC	20-B	4	2	11,11,12	2.80	5 (45%)	15,15,17	2.83	5 (33%)
2	BGC	21-B	1	2	12,12,12	2.31	5 (41%)	17,17,17	1.12	1 (5%)
2	BGC	21-B	2	2	11,11,12	3.01	5 (45%)	15,15,17	2.19	6 (40%)
2	BGC	21-B	3	2	11,11,12	2.99	6 (54%)	15,15,17	1.61	2 (13%)
2	BGC	21-B	4	2	11,11,12	2.76	5 (45%)	15,15,17	2.26	4 (26%)
2	BGC	22-B	1	2	12,12,12	2.32	5 (41%)	17,17,17	1.10	0
2	BGC	22-B	2	2	11,11,12	2.81	5 (45%)	15,15,17	2.05	3 (20%)
2	BGC	22-B	3	2	11,11,12	3.12	5 (45%)	15,15,17	1.22	1 (6%)
2	BGC	22-B	4	2	11,11,12	2.73	5 (45%)	15,15,17	2.31	4 (26%)
2	BGC	23-B	1	2	12,12,12	2.39	6 (50%)	17,17,17	1.87	6 (35%)
2	BGC	23-B	2	2	11,11,12	3.02	6 (54%)	15,15,17	1.92	5 (33%)
2	BGC	23-B	3	2	11,11,12	3.01	5 (45%)	15,15,17	2.13	5 (33%)
2	BGC	23-B	4	2	11,11,12	2.62	5 (45%)	15,15,17	2.33	6 (40%)
2	BGC	24-B	1	2	12,12,12	2.23	5 (41%)	17,17,17	1.50	2 (11%)
2	BGC	24-B	2	2	11,11,12	3.01	6 (54%)	15,15,17	1.55	2 (13%)
2	BGC	24-B	3	2	11,11,12	3.12	6 (54%)	15,15,17	1.37	1 (6%)
2	BGC	24-B	4	2	11,11,12	2.66	4 (36%)	15,15,17	2.26	5 (33%)
2	BGC	25-B	1	2	12,12,12	2.34	5 (41%)	17,17,17	1.37	3 (17%)
2	BGC	25-B	2	2	11,11,12	3.00	5 (45%)	15,15,17	1.86	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	25-B	3	2	11,11,12	3.02	5 (45%)	15,15,17	1.73	3 (20%)
2	BGC	25-B	4	2	11,11,12	2.62	5 (45%)	15,15,17	1.93	4 (26%)
2	BGC	3-B	1	2	12,12,12	2.38	6 (50%)	17,17,17	1.11	1 (5%)
2	BGC	3-B	2	2	11,11,12	2.90	5 (45%)	15,15,17	1.50	3 (20%)
2	BGC	3-B	3	2	11,11,12	2.92	6 (54%)	15,15,17	1.61	2 (13%)
2	BGC	3-B	4	2	11,11,12	2.68	4 (36%)	15,15,17	2.03	6 (40%)
2	BGC	4-B	1	2	12,12,12	2.23	5 (41%)	17,17,17	1.56	4 (23%)
2	BGC	4-B	2	2	11,11,12	2.90	4 (36%)	15,15,17	1.79	3 (20%)
2	BGC	4-B	3	2	11,11,12	2.90	6 (54%)	15,15,17	1.65	2 (13%)
2	BGC	4-B	4	2	11,11,12	2.63	5 (45%)	15,15,17	1.95	4 (26%)
2	BGC	5-B	1	2	12,12,12	2.32	5 (41%)	17,17,17	1.40	3 (17%)
2	BGC	5-B	2	2	11,11,12	3.02	5 (45%)	15,15,17	2.39	7 (46%)
2	BGC	5-B	3	2	11,11,12	3.17	5 (45%)	15,15,17	1.49	2 (13%)
2	BGC	5-B	4	2	11,11,12	2.73	6 (54%)	15,15,17	2.12	5 (33%)
2	BGC	6-B	1	2	12,12,12	2.30	5 (41%)	17,17,17	1.17	0
2	BGC	6-B	2	2	11,11,12	2.85	5 (45%)	15,15,17	1.38	2 (13%)
2	BGC	6-B	3	2	11,11,12	2.95	5 (45%)	15,15,17	1.52	3 (20%)
2	BGC	6-B	4	2	11,11,12	2.78	4 (36%)	15,15,17	2.70	5 (33%)
2	BGC	7-B	1	2	12,12,12	2.47	5 (41%)	17,17,17	1.27	3 (17%)
2	BGC	7-B	2	2	11,11,12	2.84	4 (36%)	15,15,17	1.51	2 (13%)
2	BGC	7-B	3	2	11,11,12	3.07	6 (54%)	15,15,17	2.16	6 (40%)
2	BGC	7-B	4	2	11,11,12	2.78	5 (45%)	15,15,17	2.09	5 (33%)
2	BGC	8-B	1	2	12,12,12	2.31	5 (41%)	17,17,17	1.40	3 (17%)
2	BGC	8-B	2	2	11,11,12	2.94	6 (54%)	15,15,17	1.83	2 (13%)
2	BGC	8-B	3	2	11,11,12	2.95	6 (54%)	15,15,17	1.45	2 (13%)
2	BGC	8-B	4	2	11,11,12	2.62	5 (45%)	15,15,17	2.73	4 (26%)
2	BGC	9-B	1	2	12,12,12	2.48	5 (41%)	17,17,17	1.22	1 (5%)
2	BGC	9-B	2	2	11,11,12	3.07	5 (45%)	15,15,17	1.82	3 (20%)
2	BGC	9-B	3	2	11,11,12	3.11	5 (45%)	15,15,17	1.46	1 (6%)
2	BGC	9-B	4	2	11,11,12	2.89	5 (45%)	15,15,17	2.28	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	1-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	1-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	1-B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	1-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	10-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	10-B	2	2	-	1/2/19/22	0/1/1/1
2	BGC	10-B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	10-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	11-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	11-B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	11-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	11-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	12-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	12-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	12-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	12-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	13-B	1	2	-	2/2/22/22	0/1/1/1
2	BGC	13-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	13-B	3	2	-	1/2/19/22	0/1/1/1
2	BGC	13-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	14-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	14-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	14-B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	14-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	15-B	1	2	-	2/2/22/22	0/1/1/1
2	BGC	15-B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	15-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	15-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	16-B	1	2	-	2/2/22/22	0/1/1/1
2	BGC	16-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	16-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	16-B	4	2	-	1/2/19/22	0/1/1/1
2	BGC	17-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	17-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	17-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	17-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	18-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	18-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	18-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	18-B	4	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	19-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	19-B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	19-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	19-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	2-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	2-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	2-B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	2-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	20-B	1	2	-	1/2/22/22	0/1/1/1
2	BGC	20-B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	20-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	20-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	21-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	21-B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	21-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	21-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	22-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	22-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	22-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	22-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	23-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	23-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	23-B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	23-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	24-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	24-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	24-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	24-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	25-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	25-B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	25-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	25-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	3-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	3-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	3-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	3-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	4-B	1	2	-	2/2/22/22	0/1/1/1
2	BGC	4-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	4-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	4-B	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	5-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	5-B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	5-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	5-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	6-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	6-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	6-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	6-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	7-B	1	2	-	2/2/22/22	0/1/1/1
2	BGC	7-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	7-B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	7-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	8-B	1	2	-	2/2/22/22	0/1/1/1
2	BGC	8-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	8-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	8-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	9-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	9-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	9-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	9-B	4	2	-	0/2/19/22	0/1/1/1

All (509) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-B	3	BGC	C2-C3	-6.95	1.41	1.52
2	23-B	2	BGC	C2-C3	-6.80	1.42	1.52
2	22-B	3	BGC	C2-C3	-6.74	1.42	1.52
2	9-B	2	BGC	C2-C3	-6.68	1.42	1.52
2	2-B	2	BGC	C2-C3	-6.66	1.42	1.52
2	9-B	3	BGC	C2-C3	-6.65	1.42	1.52
2	24-B	2	BGC	C2-C3	-6.53	1.42	1.52
2	5-B	3	BGC	C2-C3	-6.53	1.42	1.52
2	24-B	3	BGC	C2-C3	-6.46	1.42	1.52
2	25-B	2	BGC	C2-C3	-6.39	1.42	1.52
2	5-B	2	BGC	C2-C3	-6.36	1.42	1.52
2	17-B	2	BGC	C2-C3	-6.33	1.42	1.52
2	2-B	3	BGC	C2-C3	-6.33	1.42	1.52
2	13-B	3	BGC	C2-C3	-6.31	1.42	1.52
2	16-B	3	BGC	C2-C3	-6.31	1.42	1.52
2	7-B	3	BGC	C2-C3	-6.26	1.42	1.52
2	12-B	3	BGC	C2-C3	-6.23	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	19-B	2	BGC	C2-C3	-6.20	1.43	1.52
2	6-B	3	BGC	C2-C3	-6.19	1.43	1.52
2	14-B	3	BGC	C2-C3	-6.17	1.43	1.52
2	20-B	2	BGC	C2-C3	-6.16	1.43	1.52
2	8-B	3	BGC	C2-C3	-6.15	1.43	1.52
2	11-B	3	BGC	C2-C3	-6.15	1.43	1.52
2	21-B	2	BGC	C2-C3	-6.12	1.43	1.52
2	18-B	2	BGC	C2-C3	-6.12	1.43	1.52
2	16-B	2	BGC	C2-C3	-6.11	1.43	1.52
2	13-B	2	BGC	C2-C3	-6.09	1.43	1.52
2	7-B	2	BGC	C2-C3	-6.06	1.43	1.52
2	8-B	2	BGC	C2-C3	-6.05	1.43	1.52
2	10-B	2	BGC	C2-C3	-6.05	1.43	1.52
2	4-B	3	BGC	C2-C3	-6.04	1.43	1.52
2	21-B	3	BGC	C2-C3	-6.04	1.43	1.52
2	3-B	3	BGC	C2-C3	-6.02	1.43	1.52
2	3-B	2	BGC	C2-C3	-5.98	1.43	1.52
2	1-B	3	BGC	C2-C3	-5.95	1.43	1.52
2	14-B	2	BGC	C2-C3	-5.94	1.43	1.52
2	25-B	3	BGC	C2-C3	-5.93	1.43	1.52
2	19-B	3	BGC	C2-C3	-5.92	1.43	1.52
2	15-B	3	BGC	C2-C3	-5.90	1.43	1.52
2	15-B	2	BGC	C2-C3	-5.89	1.43	1.52
2	12-B	2	BGC	C2-C3	-5.88	1.43	1.52
2	6-B	2	BGC	C2-C3	-5.86	1.43	1.52
2	23-B	3	BGC	C2-C3	-5.86	1.43	1.52
2	4-B	2	BGC	C2-C3	-5.83	1.43	1.52
2	11-B	2	BGC	C2-C3	-5.74	1.43	1.52
2	18-B	3	BGC	C2-C3	-5.74	1.43	1.52
2	17-B	3	BGC	C2-C3	-5.68	1.43	1.52
2	1-B	2	BGC	C2-C3	-5.59	1.43	1.52
2	22-B	2	BGC	C2-C3	-5.57	1.44	1.52
2	20-B	3	BGC	C2-C3	-5.55	1.44	1.52
2	21-B	1	BGC	C6-C5	-5.34	1.33	1.51
2	9-B	1	BGC	C6-C5	-5.29	1.34	1.51
2	5-B	1	BGC	C6-C5	-5.25	1.34	1.51
2	9-B	4	BGC	C6-C5	-5.24	1.34	1.51
2	7-B	4	BGC	C2-C3	-5.24	1.44	1.52
2	18-B	1	BGC	C6-C5	-5.23	1.34	1.51
2	11-B	1	BGC	C6-C5	-5.21	1.34	1.51
2	2-B	1	BGC	C6-C5	-5.20	1.34	1.51
2	16-B	4	BGC	C2-C3	-5.19	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	19-B	4	BGC	C2-C3	-5.19	1.44	1.52
2	6-B	1	BGC	C6-C5	-5.18	1.34	1.51
2	6-B	4	BGC	O5-C5	5.18	1.53	1.43
2	2-B	4	BGC	C2-C3	-5.15	1.44	1.52
2	1-B	4	BGC	O5-C5	5.13	1.53	1.43
2	22-B	1	BGC	C6-C5	-5.09	1.34	1.51
2	20-B	1	BGC	C6-C5	-5.08	1.34	1.51
2	14-B	1	BGC	C6-C5	-5.08	1.34	1.51
2	1-B	4	BGC	C2-C3	-5.07	1.44	1.52
2	22-B	4	BGC	O5-C5	5.07	1.53	1.43
2	19-B	1	BGC	C6-C5	-5.06	1.34	1.51
2	14-B	3	BGC	C6-C5	-5.04	1.34	1.51
2	25-B	1	BGC	C6-C5	-5.03	1.34	1.51
2	25-B	3	BGC	C6-C5	-5.00	1.35	1.51
2	24-B	1	BGC	C6-C5	-5.00	1.35	1.51
2	12-B	1	BGC	C6-C5	-5.00	1.35	1.51
2	10-B	1	BGC	C6-C5	-5.00	1.35	1.51
2	23-B	1	BGC	C6-C5	-4.99	1.35	1.51
2	16-B	1	BGC	C6-C5	-4.99	1.35	1.51
2	20-B	4	BGC	O5-C5	4.95	1.53	1.43
2	7-B	3	BGC	C6-C5	-4.94	1.35	1.51
2	1-B	1	BGC	C6-C5	-4.94	1.35	1.51
2	7-B	1	BGC	C6-C5	-4.94	1.35	1.51
2	3-B	1	BGC	C6-C5	-4.93	1.35	1.51
2	12-B	4	BGC	C6-C5	-4.93	1.35	1.51
2	17-B	1	BGC	C6-C5	-4.92	1.35	1.51
2	21-B	4	BGC	O5-C5	4.91	1.53	1.43
2	13-B	3	BGC	C6-C5	-4.89	1.35	1.51
2	20-B	4	BGC	C2-C3	-4.88	1.45	1.52
2	24-B	4	BGC	C2-C3	-4.88	1.45	1.52
2	12-B	4	BGC	C2-C3	-4.87	1.45	1.52
2	10-B	3	BGC	C6-C5	-4.87	1.35	1.51
2	9-B	4	BGC	O5-C5	4.86	1.52	1.43
2	2-B	3	BGC	C6-C5	-4.86	1.35	1.51
2	5-B	3	BGC	C6-C5	-4.85	1.35	1.51
2	18-B	3	BGC	C6-C5	-4.85	1.35	1.51
2	16-B	3	BGC	C6-C5	-4.85	1.35	1.51
2	19-B	3	BGC	C6-C5	-4.85	1.35	1.51
2	11-B	4	BGC	O5-C5	4.84	1.52	1.43
2	16-B	4	BGC	O5-C5	4.83	1.52	1.43
2	20-B	4	BGC	C6-C5	-4.83	1.35	1.51
2	22-B	3	BGC	C6-C5	-4.80	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-B	1	BGC	C6-C5	-4.80	1.35	1.51
2	4-B	1	BGC	C6-C5	-4.80	1.35	1.51
2	14-B	4	BGC	C2-C3	-4.79	1.45	1.52
2	1-B	3	BGC	C6-C5	-4.79	1.35	1.51
2	18-B	4	BGC	C2-C3	-4.78	1.45	1.52
2	15-B	1	BGC	C6-C5	-4.78	1.35	1.51
2	4-B	2	BGC	C6-C5	-4.78	1.35	1.51
2	6-B	3	BGC	C6-C5	-4.77	1.35	1.51
2	3-B	4	BGC	C6-C5	-4.76	1.35	1.51
2	6-B	4	BGC	C2-C3	-4.76	1.45	1.52
2	9-B	4	BGC	C2-C3	-4.76	1.45	1.52
2	8-B	1	BGC	C6-C5	-4.76	1.35	1.51
2	24-B	3	BGC	C6-C5	-4.73	1.36	1.51
2	13-B	4	BGC	O5-C5	4.72	1.52	1.43
2	8-B	4	BGC	C2-C3	-4.72	1.45	1.52
2	25-B	4	BGC	O5-C5	4.71	1.52	1.43
2	17-B	4	BGC	O5-C5	4.69	1.52	1.43
2	9-B	2	BGC	C6-C5	-4.69	1.36	1.51
2	3-B	3	BGC	C6-C5	-4.68	1.36	1.51
2	25-B	2	BGC	C6-C5	-4.68	1.36	1.51
2	21-B	2	BGC	C6-C5	-4.67	1.36	1.51
2	5-B	4	BGC	O5-C5	4.66	1.52	1.43
2	18-B	4	BGC	O5-C5	4.66	1.52	1.43
2	8-B	3	BGC	C6-C5	-4.66	1.36	1.51
2	2-B	4	BGC	O5-C5	4.65	1.52	1.43
2	7-B	4	BGC	O5-C5	4.65	1.52	1.43
2	15-B	2	BGC	C6-C5	-4.64	1.36	1.51
2	16-B	2	BGC	C6-C5	-4.64	1.36	1.51
2	5-B	4	BGC	C2-C3	-4.64	1.45	1.52
2	22-B	4	BGC	C2-C3	-4.64	1.45	1.52
2	21-B	3	BGC	C6-C5	-4.64	1.36	1.51
2	20-B	2	BGC	C6-C5	-4.63	1.36	1.51
2	3-B	2	BGC	C6-C5	-4.62	1.36	1.51
2	5-B	2	BGC	C6-C5	-4.62	1.36	1.51
2	12-B	3	BGC	C6-C5	-4.62	1.36	1.51
2	15-B	4	BGC	C2-C3	-4.61	1.45	1.52
2	21-B	2	BGC	O5-C5	4.61	1.52	1.43
2	20-B	3	BGC	C6-C5	-4.60	1.36	1.51
2	21-B	4	BGC	C6-C5	-4.58	1.36	1.51
2	3-B	4	BGC	O5-C5	4.58	1.52	1.43
2	14-B	4	BGC	O5-C5	4.57	1.52	1.43
2	9-B	3	BGC	C6-C5	-4.57	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-B	2	BGC	C6-C5	-4.57	1.36	1.51
2	24-B	2	BGC	C6-C5	-4.57	1.36	1.51
2	8-B	2	BGC	C6-C5	-4.57	1.36	1.51
2	15-B	2	BGC	O5-C5	4.56	1.52	1.43
2	17-B	3	BGC	C6-C5	-4.56	1.36	1.51
2	23-B	4	BGC	C2-C3	-4.56	1.45	1.52
2	23-B	2	BGC	C6-C5	-4.55	1.36	1.51
2	11-B	4	BGC	C2-C3	-4.55	1.45	1.52
2	16-B	4	BGC	C6-C5	-4.55	1.36	1.51
2	1-B	3	BGC	O5-C5	4.55	1.52	1.43
2	23-B	3	BGC	C6-C5	-4.55	1.36	1.51
2	4-B	4	BGC	C2-C3	-4.54	1.45	1.52
2	4-B	4	BGC	O5-C5	4.54	1.52	1.43
2	19-B	4	BGC	O5-C5	4.53	1.52	1.43
2	15-B	3	BGC	C6-C5	-4.52	1.36	1.51
2	11-B	2	BGC	C6-C5	-4.52	1.36	1.51
2	15-B	4	BGC	C6-C5	-4.51	1.36	1.51
2	13-B	4	BGC	C2-C3	-4.50	1.45	1.52
2	21-B	4	BGC	C2-C3	-4.50	1.45	1.52
2	17-B	2	BGC	C6-C5	-4.50	1.36	1.51
2	10-B	4	BGC	O5-C5	4.49	1.52	1.43
2	17-B	2	BGC	O5-C5	4.49	1.52	1.43
2	1-B	4	BGC	C6-C5	-4.48	1.36	1.51
2	4-B	3	BGC	C6-C5	-4.48	1.36	1.51
2	7-B	2	BGC	C6-C5	-4.47	1.36	1.51
2	1-B	2	BGC	C6-C5	-4.45	1.36	1.51
2	6-B	2	BGC	C6-C5	-4.45	1.36	1.51
2	11-B	3	BGC	C6-C5	-4.45	1.36	1.51
2	23-B	4	BGC	O5-C5	4.44	1.52	1.43
2	24-B	4	BGC	C6-C5	-4.44	1.36	1.51
2	22-B	2	BGC	C6-C5	-4.44	1.36	1.51
2	13-B	2	BGC	C6-C5	-4.43	1.37	1.51
2	12-B	2	BGC	C6-C5	-4.42	1.37	1.51
2	2-B	2	BGC	C6-C5	-4.42	1.37	1.51
2	6-B	4	BGC	C6-C5	-4.41	1.37	1.51
2	19-B	2	BGC	C6-C5	-4.40	1.37	1.51
2	18-B	2	BGC	C6-C5	-4.40	1.37	1.51
2	7-B	4	BGC	C6-C5	-4.40	1.37	1.51
2	17-B	4	BGC	C6-C5	-4.39	1.37	1.51
2	14-B	4	BGC	C6-C5	-4.39	1.37	1.51
2	4-B	2	BGC	O5-C5	4.39	1.52	1.43
2	11-B	4	BGC	C6-C5	-4.38	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-B	2	BGC	C6-C5	-4.37	1.37	1.51
2	12-B	4	BGC	O5-C5	4.36	1.51	1.43
2	13-B	4	BGC	C6-C5	-4.35	1.37	1.51
2	25-B	4	BGC	C6-C5	-4.34	1.37	1.51
2	9-B	2	BGC	O5-C5	4.33	1.51	1.43
2	8-B	2	BGC	O5-C5	4.33	1.51	1.43
2	3-B	4	BGC	C2-C3	-4.33	1.45	1.52
2	25-B	4	BGC	C2-C3	-4.31	1.45	1.52
2	19-B	3	BGC	O5-C5	4.30	1.51	1.43
2	2-B	4	BGC	C6-C5	-4.30	1.37	1.51
2	19-B	2	BGC	O5-C5	4.29	1.51	1.43
2	22-B	2	BGC	O5-C5	4.28	1.51	1.43
2	20-B	3	BGC	O5-C5	4.27	1.51	1.43
2	17-B	4	BGC	C2-C3	-4.26	1.46	1.52
2	24-B	2	BGC	O5-C5	4.25	1.51	1.43
2	18-B	2	BGC	O5-C5	4.25	1.51	1.43
2	5-B	2	BGC	O5-C5	4.25	1.51	1.43
2	25-B	2	BGC	O5-C5	4.24	1.51	1.43
2	20-B	2	BGC	O5-C5	4.23	1.51	1.43
2	10-B	4	BGC	C2-C3	-4.22	1.46	1.52
2	22-B	4	BGC	C6-C5	-4.20	1.37	1.51
2	3-B	2	BGC	O5-C5	4.20	1.51	1.43
2	10-B	4	BGC	C6-C5	-4.19	1.37	1.51
2	4-B	4	BGC	C6-C5	-4.19	1.37	1.51
2	19-B	4	BGC	C6-C5	-4.18	1.37	1.51
2	8-B	4	BGC	O5-C5	4.18	1.51	1.43
2	6-B	2	BGC	O5-C5	4.17	1.51	1.43
2	1-B	1	BGC	O3-C3	4.17	1.53	1.43
2	24-B	3	BGC	O5-C5	4.15	1.51	1.43
2	24-B	4	BGC	O5-C5	4.15	1.51	1.43
2	11-B	2	BGC	O5-C5	4.15	1.51	1.43
2	5-B	3	BGC	O5-C5	4.13	1.51	1.43
2	5-B	4	BGC	C6-C5	-4.13	1.38	1.51
2	23-B	4	BGC	C6-C5	-4.12	1.38	1.51
2	14-B	3	BGC	O5-C5	4.11	1.51	1.43
2	12-B	2	BGC	O5-C5	4.09	1.51	1.43
2	15-B	4	BGC	O5-C5	4.06	1.51	1.43
2	10-B	2	BGC	O5-C5	4.05	1.51	1.43
2	23-B	2	BGC	O5-C5	4.05	1.51	1.43
2	21-B	3	BGC	O5-C5	4.04	1.51	1.43
2	2-B	2	BGC	O5-C5	4.02	1.51	1.43
2	9-B	3	BGC	O5-C5	3.99	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-B	3	BGC	O5-C5	3.98	1.51	1.43
2	2-B	3	BGC	O5-C5	3.98	1.51	1.43
2	25-B	3	BGC	O5-C5	3.97	1.51	1.43
2	16-B	3	BGC	O3-C3	3.96	1.52	1.43
2	12-B	3	BGC	O5-C5	3.94	1.51	1.43
2	14-B	2	BGC	O5-C5	3.94	1.51	1.43
2	16-B	2	BGC	O5-C5	3.94	1.51	1.43
2	15-B	3	BGC	O5-C5	3.92	1.51	1.43
2	7-B	3	BGC	O5-C5	3.91	1.51	1.43
2	3-B	3	BGC	O5-C5	3.91	1.51	1.43
2	7-B	2	BGC	O5-C5	3.88	1.51	1.43
2	8-B	4	BGC	C6-C5	-3.88	1.38	1.51
2	16-B	3	BGC	O5-C5	3.84	1.50	1.43
2	22-B	3	BGC	O5-C5	3.83	1.50	1.43
2	17-B	3	BGC	O5-C5	3.79	1.50	1.43
2	13-B	3	BGC	O5-C5	3.77	1.50	1.43
2	18-B	3	BGC	O5-C5	3.74	1.50	1.43
2	4-B	3	BGC	O5-C5	3.74	1.50	1.43
2	1-B	2	BGC	O5-C5	3.73	1.50	1.43
2	8-B	3	BGC	O5-C5	3.73	1.50	1.43
2	18-B	4	BGC	C6-C5	-3.71	1.39	1.51
2	6-B	3	BGC	O5-C5	3.71	1.50	1.43
2	13-B	2	BGC	O5-C5	3.70	1.50	1.43
2	23-B	3	BGC	O5-C5	3.54	1.50	1.43
2	23-B	3	BGC	O3-C3	3.54	1.51	1.43
2	1-B	1	BGC	C3-C2	-3.48	1.43	1.52
2	7-B	3	BGC	O3-C3	3.47	1.51	1.43
2	11-B	3	BGC	O5-C5	3.45	1.50	1.43
2	7-B	1	BGC	C3-C2	-3.41	1.43	1.52
2	17-B	1	BGC	O5-C5	3.36	1.52	1.44
2	20-B	1	BGC	O5-C5	3.35	1.52	1.44
2	20-B	3	BGC	O3-C3	3.35	1.51	1.43
2	23-B	3	BGC	C4-C5	3.33	1.60	1.53
2	13-B	3	BGC	O3-C3	3.31	1.51	1.43
2	9-B	1	BGC	O5-C5	3.31	1.52	1.44
2	17-B	1	BGC	C3-C2	-3.30	1.43	1.52
2	19-B	3	BGC	O3-C3	3.30	1.51	1.43
2	12-B	3	BGC	O3-C3	3.29	1.51	1.43
2	12-B	1	BGC	O5-C5	3.29	1.52	1.44
2	17-B	3	BGC	O3-C3	3.27	1.51	1.43
2	9-B	3	BGC	O3-C3	3.26	1.51	1.43
2	25-B	1	BGC	O5-C5	3.26	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	19-B	1	BGC	O3-C3	3.25	1.51	1.43
2	2-B	3	BGC	O3-C3	3.25	1.51	1.43
2	5-B	3	BGC	O3-C3	3.22	1.50	1.43
2	13-B	1	BGC	C3-C2	-3.21	1.44	1.52
2	8-B	1	BGC	O5-C5	3.19	1.52	1.44
2	14-B	3	BGC	O3-C3	3.19	1.50	1.43
2	11-B	3	BGC	O3-C3	3.19	1.50	1.43
2	6-B	1	BGC	O3-C3	3.19	1.50	1.43
2	1-B	3	BGC	O3-C3	3.15	1.50	1.43
2	18-B	1	BGC	O3-C3	3.14	1.50	1.43
2	23-B	1	BGC	O3-C3	3.14	1.50	1.43
2	7-B	1	BGC	O5-C5	3.14	1.52	1.44
2	10-B	3	BGC	O3-C3	3.13	1.50	1.43
2	3-B	1	BGC	C3-C2	-3.12	1.44	1.52
2	15-B	1	BGC	O3-C3	3.11	1.50	1.43
2	21-B	1	BGC	C3-C2	-3.08	1.44	1.52
2	20-B	1	BGC	C3-C2	-3.07	1.44	1.52
2	9-B	1	BGC	C3-C2	-3.06	1.44	1.52
2	17-B	1	BGC	C1-C2	-3.06	1.45	1.52
2	21-B	3	BGC	O3-C3	3.05	1.50	1.43
2	3-B	1	BGC	O3-C3	3.05	1.50	1.43
2	22-B	1	BGC	C3-C2	-3.05	1.44	1.52
2	8-B	1	BGC	C3-C2	-3.04	1.44	1.52
2	12-B	1	BGC	C3-C2	-3.00	1.44	1.52
2	13-B	1	BGC	O5-C5	2.99	1.51	1.44
2	4-B	3	BGC	O3-C3	2.99	1.50	1.43
2	9-B	1	BGC	O3-C3	2.98	1.50	1.43
2	11-B	1	BGC	O3-C3	2.96	1.50	1.43
2	5-B	1	BGC	O5-C5	2.96	1.51	1.44
2	18-B	4	BGC	O3-C3	2.95	1.50	1.43
2	25-B	3	BGC	O3-C3	2.94	1.50	1.43
2	22-B	3	BGC	O3-C3	2.94	1.50	1.43
2	23-B	1	BGC	O5-C5	2.93	1.51	1.44
2	7-B	1	BGC	C1-C2	-2.93	1.45	1.52
2	2-B	1	BGC	C3-C2	-2.90	1.44	1.52
2	22-B	1	BGC	O3-C3	2.89	1.50	1.43
2	7-B	4	BGC	O2-C2	2.89	1.49	1.43
2	4-B	1	BGC	O5-C5	2.88	1.51	1.44
2	12-B	1	BGC	O3-C3	2.88	1.50	1.43
2	4-B	1	BGC	C3-C2	-2.87	1.44	1.52
2	14-B	1	BGC	C3-C2	-2.86	1.44	1.52
2	18-B	2	BGC	O3-C3	2.85	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-B	4	BGC	O3-C3	2.84	1.50	1.43
2	24-B	4	BGC	O3-C3	2.84	1.50	1.43
2	8-B	4	BGC	O3-C3	2.84	1.50	1.43
2	5-B	4	BGC	O3-C3	2.84	1.50	1.43
2	10-B	1	BGC	O3-C3	2.82	1.49	1.43
2	25-B	1	BGC	C3-C2	-2.82	1.45	1.52
2	21-B	4	BGC	O3-C3	2.82	1.49	1.43
2	14-B	1	BGC	O3-C3	2.81	1.49	1.43
2	4-B	1	BGC	O3-C3	2.81	1.49	1.43
2	8-B	1	BGC	O3-C3	2.80	1.49	1.43
2	3-B	1	BGC	O5-C5	2.79	1.51	1.44
2	6-B	1	BGC	C3-C2	-2.79	1.45	1.52
2	8-B	3	BGC	O3-C3	2.79	1.49	1.43
2	25-B	3	BGC	C4-C3	-2.79	1.45	1.52
2	5-B	1	BGC	O3-C3	2.78	1.49	1.43
2	24-B	3	BGC	O3-C3	2.78	1.49	1.43
2	20-B	3	BGC	C4-C5	2.78	1.59	1.53
2	24-B	1	BGC	C3-C2	-2.77	1.45	1.52
2	2-B	1	BGC	C1-C2	-2.77	1.45	1.52
2	1-B	2	BGC	O3-C3	2.76	1.49	1.43
2	17-B	2	BGC	O3-C3	2.76	1.49	1.43
2	13-B	1	BGC	C1-C2	-2.76	1.45	1.52
2	17-B	3	BGC	C4-C5	2.75	1.58	1.53
2	19-B	3	BGC	C4-C5	2.74	1.58	1.53
2	20-B	2	BGC	O3-C3	2.74	1.49	1.43
2	10-B	4	BGC	O3-C3	2.74	1.49	1.43
2	18-B	1	BGC	O5-C5	2.74	1.51	1.44
2	10-B	1	BGC	C3-C2	-2.73	1.45	1.52
2	16-B	1	BGC	C3-C2	-2.73	1.45	1.52
2	14-B	2	BGC	O3-C3	2.72	1.49	1.43
2	18-B	3	BGC	O3-C3	2.70	1.49	1.43
2	2-B	1	BGC	O5-C5	2.70	1.51	1.44
2	11-B	1	BGC	O5-C5	2.70	1.51	1.44
2	3-B	3	BGC	O3-C3	2.70	1.49	1.43
2	24-B	1	BGC	O3-C3	2.70	1.49	1.43
2	11-B	2	BGC	O3-C3	2.70	1.49	1.43
2	16-B	1	BGC	O5-C5	2.69	1.51	1.44
2	15-B	4	BGC	O3-C3	2.68	1.49	1.43
2	5-B	2	BGC	O3-C3	2.68	1.49	1.43
2	7-B	1	BGC	O3-C3	2.68	1.49	1.43
2	3-B	4	BGC	O3-C3	2.68	1.49	1.43
2	15-B	1	BGC	C3-C2	-2.67	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	22-B	4	BGC	O3-C3	2.67	1.49	1.43
2	4-B	4	BGC	O3-C3	2.67	1.49	1.43
2	22-B	1	BGC	O5-C5	2.67	1.50	1.44
2	20-B	1	BGC	C1-C2	-2.66	1.46	1.52
2	19-B	4	BGC	O3-C3	2.65	1.49	1.43
2	6-B	3	BGC	O3-C3	2.65	1.49	1.43
2	15-B	3	BGC	O3-C3	2.65	1.49	1.43
2	21-B	4	BGC	O2-C2	2.63	1.48	1.43
2	24-B	3	BGC	C4-C3	-2.61	1.45	1.52
2	21-B	3	BGC	C4-C5	2.61	1.58	1.53
2	11-B	4	BGC	O3-C3	2.61	1.49	1.43
2	25-B	1	BGC	O3-C3	2.60	1.49	1.43
2	2-B	1	BGC	O3-C3	2.60	1.49	1.43
2	5-B	3	BGC	C4-C3	-2.60	1.45	1.52
2	16-B	1	BGC	O3-C3	2.59	1.49	1.43
2	13-B	4	BGC	O3-C3	2.59	1.49	1.43
2	23-B	1	BGC	C4-C5	2.59	1.58	1.53
2	23-B	4	BGC	O3-C3	2.59	1.49	1.43
2	11-B	1	BGC	C3-C2	-2.59	1.45	1.52
2	12-B	2	BGC	O3-C3	2.59	1.49	1.43
2	16-B	3	BGC	C4-C5	2.58	1.58	1.53
2	15-B	1	BGC	O5-C5	2.57	1.50	1.44
2	14-B	3	BGC	C4-C3	-2.57	1.45	1.52
2	9-B	4	BGC	O3-C3	2.57	1.49	1.43
2	21-B	1	BGC	C1-C2	-2.56	1.46	1.52
2	5-B	1	BGC	C3-C2	-2.56	1.45	1.52
2	8-B	3	BGC	C4-C5	2.56	1.58	1.53
2	7-B	2	BGC	O3-C3	2.55	1.49	1.43
2	6-B	3	BGC	C4-C3	-2.55	1.45	1.52
2	14-B	1	BGC	C1-C2	-2.55	1.46	1.52
2	10-B	2	BGC	O3-C3	2.54	1.49	1.43
2	23-B	1	BGC	C1-C2	-2.54	1.46	1.52
2	17-B	1	BGC	O3-C3	2.54	1.49	1.43
2	2-B	3	BGC	C4-C3	-2.54	1.45	1.52
2	6-B	1	BGC	O5-C5	2.53	1.50	1.44
2	14-B	1	BGC	O5-C5	2.52	1.50	1.44
2	13-B	1	BGC	O3-C3	2.51	1.49	1.43
2	25-B	1	BGC	C1-C2	-2.50	1.46	1.52
2	1-B	3	BGC	C4-C3	-2.50	1.45	1.52
2	9-B	1	BGC	C1-C2	-2.50	1.46	1.52
2	25-B	2	BGC	O2-C2	2.49	1.48	1.43
2	24-B	1	BGC	O5-C5	2.49	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-B	4	BGC	O3-C3	2.48	1.49	1.43
2	17-B	2	BGC	O2-C2	2.48	1.48	1.43
2	23-B	1	BGC	C3-C2	-2.48	1.45	1.52
2	1-B	1	BGC	O5-C5	2.48	1.50	1.44
2	10-B	3	BGC	C4-C3	-2.47	1.45	1.52
2	19-B	1	BGC	O5-C5	2.46	1.50	1.44
2	17-B	4	BGC	O3-C3	2.46	1.49	1.43
2	9-B	3	BGC	C4-C3	-2.46	1.46	1.52
2	9-B	2	BGC	O3-C3	2.46	1.49	1.43
2	18-B	1	BGC	C3-C2	-2.46	1.46	1.52
2	25-B	4	BGC	O2-C2	2.46	1.48	1.43
2	5-B	4	BGC	O2-C2	2.45	1.48	1.43
2	22-B	3	BGC	C4-C3	-2.45	1.46	1.52
2	13-B	2	BGC	O3-C3	2.43	1.49	1.43
2	10-B	1	BGC	C1-C2	-2.43	1.46	1.52
2	2-B	2	BGC	O3-C3	2.42	1.49	1.43
2	10-B	2	BGC	O2-C2	2.42	1.48	1.43
2	12-B	1	BGC	C1-C2	-2.42	1.46	1.52
2	12-B	4	BGC	O2-C2	2.42	1.48	1.43
2	5-B	1	BGC	C1-C2	-2.41	1.46	1.52
2	21-B	1	BGC	O3-C3	2.40	1.48	1.43
2	19-B	2	BGC	O3-C3	2.40	1.48	1.43
2	4-B	4	BGC	O2-C2	2.40	1.48	1.43
2	12-B	3	BGC	C4-C5	2.40	1.58	1.53
2	11-B	3	BGC	C4-C5	2.39	1.58	1.53
2	19-B	1	BGC	C3-C2	-2.38	1.46	1.52
2	21-B	2	BGC	O2-C2	2.38	1.48	1.43
2	22-B	2	BGC	O3-C3	2.38	1.48	1.43
2	10-B	1	BGC	O5-C5	2.37	1.50	1.44
2	3-B	2	BGC	O3-C3	2.37	1.48	1.43
2	6-B	2	BGC	O3-C3	2.37	1.48	1.43
2	4-B	3	BGC	C4-C5	2.37	1.58	1.53
2	8-B	4	BGC	C4-C5	2.37	1.58	1.53
2	3-B	1	BGC	C1-C2	-2.36	1.46	1.52
2	4-B	2	BGC	O3-C3	2.36	1.48	1.43
2	2-B	4	BGC	O3-C3	2.35	1.48	1.43
2	15-B	3	BGC	C4-C3	-2.35	1.46	1.52
2	10-B	4	BGC	C4-C5	2.35	1.58	1.53
2	2-B	2	BGC	O2-C2	2.34	1.48	1.43
2	15-B	2	BGC	O3-C3	2.34	1.48	1.43
2	20-B	4	BGC	O3-C3	2.33	1.48	1.43
2	5-B	4	BGC	C4-C5	2.33	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	25-B	2	BGC	O3-C3	2.33	1.48	1.43
2	8-B	2	BGC	O3-C3	2.33	1.48	1.43
2	20-B	1	BGC	O3-C3	2.32	1.48	1.43
2	25-B	4	BGC	O3-C3	2.30	1.48	1.43
2	24-B	2	BGC	O3-C3	2.30	1.48	1.43
2	21-B	2	BGC	O3-C3	2.29	1.48	1.43
2	3-B	3	BGC	C4-C3	-2.29	1.46	1.52
2	13-B	3	BGC	C4-C5	2.28	1.57	1.53
2	8-B	1	BGC	C1-C2	-2.28	1.47	1.52
2	16-B	2	BGC	O3-C3	2.27	1.48	1.43
2	19-B	3	BGC	C4-C3	-2.27	1.46	1.52
2	20-B	4	BGC	O2-C2	2.26	1.48	1.43
2	7-B	3	BGC	C4-C3	-2.26	1.46	1.52
2	16-B	4	BGC	O3-C3	2.25	1.48	1.43
2	21-B	1	BGC	O5-C5	2.24	1.49	1.44
2	1-B	4	BGC	O3-C3	2.24	1.48	1.43
2	19-B	1	BGC	C1-C2	-2.24	1.47	1.52
2	22-B	1	BGC	C1-C2	-2.23	1.47	1.52
2	23-B	2	BGC	C1-C2	-2.23	1.46	1.52
2	11-B	1	BGC	C1-C2	-2.23	1.47	1.52
2	16-B	4	BGC	O2-C2	2.23	1.48	1.43
2	11-B	4	BGC	O2-C2	2.22	1.48	1.43
2	7-B	3	BGC	C4-C5	2.21	1.57	1.53
2	17-B	4	BGC	O2-C2	2.20	1.48	1.43
2	18-B	3	BGC	C4-C3	-2.20	1.46	1.52
2	6-B	1	BGC	C1-C2	-2.20	1.47	1.52
2	3-B	3	BGC	C4-C5	2.20	1.57	1.53
2	20-B	2	BGC	O2-C2	2.19	1.47	1.43
2	13-B	4	BGC	O2-C2	2.19	1.47	1.43
2	10-B	3	BGC	C4-C5	2.18	1.57	1.53
2	2-B	4	BGC	O2-C2	2.18	1.47	1.43
2	21-B	3	BGC	C4-C3	-2.17	1.46	1.52
2	16-B	2	BGC	O2-C2	2.17	1.47	1.43
2	24-B	3	BGC	C4-C5	2.16	1.57	1.53
2	15-B	3	BGC	C4-C5	2.16	1.57	1.53
2	15-B	1	BGC	C1-C2	-2.16	1.47	1.52
2	5-B	2	BGC	O2-C2	2.15	1.47	1.43
2	6-B	2	BGC	O2-C2	2.15	1.47	1.43
2	18-B	1	BGC	C1-C2	-2.15	1.47	1.52
2	14-B	4	BGC	O2-C2	2.15	1.47	1.43
2	23-B	4	BGC	O2-C2	2.15	1.47	1.43
2	22-B	4	BGC	O2-C2	2.13	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	24-B	1	BGC	C1-C2	-2.13	1.47	1.52
2	17-B	3	BGC	C4-C3	-2.13	1.46	1.52
2	4-B	1	BGC	C1-C2	-2.12	1.47	1.52
2	18-B	4	BGC	C4-C5	2.11	1.57	1.53
2	23-B	2	BGC	O2-C2	2.10	1.47	1.43
2	15-B	2	BGC	O2-C2	2.08	1.47	1.43
2	16-B	3	BGC	C4-C3	-2.08	1.46	1.52
2	1-B	4	BGC	O2-C2	2.08	1.47	1.43
2	8-B	2	BGC	C1-C2	-2.08	1.47	1.52
2	8-B	3	BGC	C4-C3	-2.08	1.47	1.52
2	8-B	2	BGC	O2-C2	2.07	1.47	1.43
2	16-B	1	BGC	C1-C2	-2.06	1.47	1.52
2	24-B	2	BGC	C1-C2	-2.05	1.47	1.52
2	7-B	4	BGC	O3-C3	2.05	1.48	1.43
2	13-B	3	BGC	C4-C3	-2.05	1.47	1.52
2	23-B	2	BGC	O3-C3	2.04	1.48	1.43
2	2-B	2	BGC	C1-C2	-2.04	1.47	1.52
2	4-B	3	BGC	C4-C3	-2.03	1.47	1.52
2	24-B	2	BGC	O2-C2	2.03	1.47	1.43
2	20-B	3	BGC	C4-C3	-2.03	1.47	1.52
2	19-B	4	BGC	O2-C2	2.02	1.47	1.43
2	16-B	2	BGC	C1-C2	-2.02	1.47	1.52
2	3-B	2	BGC	O2-C2	2.02	1.47	1.43
2	22-B	2	BGC	O2-C2	2.02	1.47	1.43
2	11-B	2	BGC	O2-C2	2.02	1.47	1.43
2	9-B	4	BGC	O6-C6	-2.02	1.33	1.42
2	14-B	2	BGC	C4-C5	2.02	1.57	1.53
2	18-B	2	BGC	O2-C2	2.01	1.47	1.43
2	3-B	1	BGC	O2-C2	2.01	1.47	1.43
2	9-B	2	BGC	O2-C2	2.01	1.47	1.43

All (333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-B	4	BGC	C1-O5-C5	8.61	123.72	112.19
2	1-B	1	BGC	C3-C4-C5	7.93	124.61	110.23
2	1-B	1	BGC	O4-C4-C5	-7.83	90.05	109.32
2	19-B	4	BGC	C1-O5-C5	7.36	122.05	112.19
2	20-B	4	BGC	C1-O5-C5	7.20	121.83	112.19
2	20-B	4	BGC	C1-C2-C3	6.50	119.11	109.64
2	6-B	4	BGC	C1-O5-C5	6.40	120.76	112.19
2	8-B	4	BGC	C1-O5-C5	5.85	120.03	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	15-B	4	BGC	C1-O5-C5	5.83	120.00	112.19
2	6-B	4	BGC	C1-C2-C3	5.70	117.95	109.64
2	7-B	3	BGC	C1-C2-C3	5.38	117.47	109.64
2	14-B	4	BGC	C1-O5-C5	5.36	119.37	112.19
2	24-B	4	BGC	C1-C2-C3	5.35	117.44	109.64
2	22-B	4	BGC	C1-O5-C5	5.33	119.34	112.19
2	18-B	2	BGC	C1-C2-C3	5.33	117.41	109.64
2	2-B	4	BGC	C1-C2-C3	5.29	117.35	109.64
2	22-B	4	BGC	C1-C2-C3	5.28	117.33	109.64
2	4-B	2	BGC	C1-C2-C3	5.20	117.22	109.64
2	22-B	2	BGC	C1-C2-C3	5.19	117.21	109.64
2	16-B	3	BGC	C1-C2-C3	5.18	117.19	109.64
2	9-B	2	BGC	C1-C2-C3	5.17	117.17	109.64
2	21-B	4	BGC	C1-O5-C5	5.14	119.08	112.19
2	5-B	2	BGC	C1-C2-C3	5.11	117.08	109.64
2	8-B	2	BGC	C1-C2-C3	5.09	117.06	109.64
2	10-B	2	BGC	C1-C2-C3	5.08	117.04	109.64
2	3-B	4	BGC	C1-C2-C3	5.03	116.96	109.64
2	21-B	4	BGC	C1-C2-C3	5.02	116.95	109.64
2	13-B	4	BGC	C1-C2-C3	4.98	116.90	109.64
2	11-B	4	BGC	C1-O5-C5	4.97	118.85	112.19
2	23-B	4	BGC	C1-C2-C3	4.92	116.81	109.64
2	9-B	4	BGC	C1-C2-C3	4.81	116.66	109.64
2	1-B	2	BGC	C1-C2-C3	4.74	116.54	109.64
2	11-B	4	BGC	C1-C2-C3	4.73	116.53	109.64
2	10-B	4	BGC	O5-C5-C4	-4.73	99.33	110.83
2	8-B	4	BGC	C1-C2-C3	4.71	116.50	109.64
2	19-B	1	BGC	O5-C5-C4	-4.71	101.22	109.70
2	5-B	4	BGC	C1-C2-C3	4.62	116.37	109.64
2	3-B	2	BGC	C1-C2-C3	4.61	116.35	109.64
2	21-B	2	BGC	O5-C5-C4	-4.60	99.63	110.83
2	18-B	4	BGC	C6-C5-C4	4.60	124.31	113.02
2	19-B	4	BGC	C1-C2-C3	4.59	116.33	109.64
2	25-B	4	BGC	C1-C2-C3	4.57	116.30	109.64
2	11-B	2	BGC	O5-C5-C4	-4.57	99.71	110.83
2	4-B	4	BGC	C1-C2-C3	4.57	116.30	109.64
2	12-B	3	BGC	C1-C2-C3	4.56	116.29	109.64
2	14-B	3	BGC	C1-C2-C3	4.55	116.27	109.64
2	23-B	4	BGC	O5-C5-C4	-4.55	99.76	110.83
2	8-B	4	BGC	C6-C5-C4	4.54	124.16	113.02
2	15-B	2	BGC	O5-C5-C4	-4.53	99.80	110.83
2	16-B	2	BGC	O5-C5-C4	-4.52	99.83	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	23-B	3	BGC	C1-C2-C3	4.52	116.22	109.64
2	12-B	2	BGC	C1-C2-C3	4.51	116.22	109.64
2	17-B	3	BGC	C1-C2-C3	4.47	116.16	109.64
2	20-B	3	BGC	C1-C2-C3	4.46	116.14	109.64
2	1-B	3	BGC	C1-C2-C3	4.46	116.13	109.64
2	2-B	2	BGC	C1-C2-C3	4.45	116.12	109.64
2	16-B	1	BGC	O5-C5-C4	-4.43	101.71	109.70
2	1-B	4	BGC	C1-C2-C3	4.42	116.07	109.64
2	23-B	2	BGC	O3-C3-C2	-4.36	101.16	110.05
2	17-B	4	BGC	C1-C2-C3	4.35	115.98	109.64
2	17-B	4	BGC	C1-O5-C5	4.34	118.00	112.19
2	16-B	4	BGC	C1-C2-C3	4.34	115.96	109.64
2	15-B	4	BGC	C1-C2-C3	4.31	115.92	109.64
2	5-B	2	BGC	O5-C5-C4	-4.31	100.35	110.83
2	2-B	4	BGC	C1-O5-C5	4.30	117.95	112.19
2	24-B	4	BGC	C1-O5-C5	4.28	117.92	112.19
2	19-B	3	BGC	C1-C2-C3	4.27	115.86	109.64
2	15-B	3	BGC	C1-C2-C3	4.24	115.81	109.64
2	18-B	3	BGC	C1-C2-C3	4.20	115.76	109.64
2	24-B	1	BGC	O5-C5-C4	-4.20	102.13	109.70
2	12-B	4	BGC	C1-C2-C3	4.19	115.75	109.64
2	14-B	2	BGC	C1-C2-C3	4.14	115.67	109.64
2	11-B	2	BGC	C1-C2-C3	4.14	115.67	109.64
2	10-B	4	BGC	C6-C5-C4	4.14	123.18	113.02
2	11-B	3	BGC	C1-C2-C3	4.13	115.66	109.64
2	5-B	4	BGC	C6-C5-C4	4.12	123.14	113.02
2	9-B	3	BGC	C1-C2-C3	4.12	115.64	109.64
2	14-B	4	BGC	C1-C2-C3	4.11	115.63	109.64
2	10-B	3	BGC	C1-C2-C3	4.10	115.61	109.64
2	17-B	2	BGC	C1-C2-C3	4.08	115.58	109.64
2	7-B	4	BGC	C1-O5-C5	4.07	117.65	112.19
2	25-B	3	BGC	C1-C2-C3	4.06	115.55	109.64
2	13-B	3	BGC	O5-C5-C4	-4.04	101.00	110.83
2	8-B	4	BGC	O5-C5-C4	-4.02	101.04	110.83
2	2-B	3	BGC	C1-C2-C3	4.01	115.49	109.64
2	6-B	2	BGC	C1-C2-C3	4.01	115.48	109.64
2	15-B	2	BGC	C1-C2-C3	4.00	115.46	109.64
2	20-B	2	BGC	C1-C2-C3	3.99	115.46	109.64
2	21-B	3	BGC	O5-C5-C4	-3.98	101.15	110.83
2	19-B	2	BGC	O5-C5-C4	-3.98	101.15	110.83
2	3-B	3	BGC	C1-C2-C3	3.97	115.43	109.64
2	18-B	4	BGC	O6-C6-C5	3.97	124.85	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-B	3	BGC	O5-C5-C4	-3.97	101.18	110.83
2	7-B	3	BGC	C1-O5-C5	3.95	117.48	112.19
2	20-B	2	BGC	O5-C5-C4	-3.94	101.25	110.83
2	10-B	4	BGC	C1-C2-C3	3.92	115.35	109.64
2	13-B	3	BGC	C1-C2-C3	3.92	115.35	109.64
2	1-B	1	BGC	O3-C3-C4	3.89	119.54	110.38
2	5-B	3	BGC	C1-C2-C3	3.87	115.28	109.64
2	7-B	4	BGC	O5-C5-C4	-3.86	101.43	110.83
2	4-B	4	BGC	C1-O5-C5	3.86	117.36	112.19
2	11-B	3	BGC	O5-C5-C4	-3.84	101.48	110.83
2	2-B	2	BGC	O3-C3-C2	-3.84	102.21	110.05
2	23-B	2	BGC	C1-C2-C3	3.84	115.24	109.64
2	7-B	2	BGC	C1-C2-C3	3.82	115.20	109.64
2	19-B	3	BGC	O5-C5-C4	-3.82	101.54	110.83
2	24-B	2	BGC	C1-C2-C3	3.80	115.18	109.64
2	14-B	3	BGC	O5-C5-C4	-3.79	101.60	110.83
2	22-B	2	BGC	O3-C3-C2	-3.78	102.34	110.05
2	25-B	3	BGC	O5-C5-C4	-3.77	101.66	110.83
2	16-B	4	BGC	O4-C4-C3	3.77	119.26	110.38
2	19-B	2	BGC	C1-C2-C3	3.73	115.08	109.64
2	23-B	1	BGC	O2-C2-C1	-3.73	100.64	109.25
2	23-B	3	BGC	C1-O5-C5	-3.71	107.22	112.19
2	16-B	4	BGC	O5-C5-C4	-3.67	101.89	110.83
2	21-B	2	BGC	C1-C2-C3	3.67	114.98	109.64
2	13-B	2	BGC	C1-C2-C3	3.64	114.95	109.64
2	24-B	3	BGC	C1-C2-C3	3.58	114.86	109.64
2	11-B	4	BGC	O4-C4-C3	3.55	118.75	110.38
2	21-B	3	BGC	C1-C2-C3	3.55	114.81	109.64
2	25-B	2	BGC	O5-C5-C4	-3.54	102.21	110.83
2	18-B	4	BGC	C1-O5-C5	3.50	116.88	112.19
2	8-B	2	BGC	O3-C3-C2	-3.49	102.93	110.05
2	25-B	2	BGC	C1-C2-C3	3.45	114.67	109.64
2	1-B	1	BGC	O2-C2-C3	-3.44	102.26	110.38
2	19-B	4	BGC	C3-C4-C5	3.40	116.39	110.23
2	23-B	3	BGC	C6-C5-C4	3.37	121.29	113.02
2	4-B	1	BGC	C3-C4-C5	3.36	116.32	110.23
2	7-B	4	BGC	C1-C2-C3	3.34	114.51	109.64
2	9-B	2	BGC	O3-C3-C2	-3.31	103.31	110.05
2	4-B	3	BGC	C1-C2-C3	3.28	114.42	109.64
2	6-B	3	BGC	O3-C3-C4	-3.27	102.66	110.38
2	13-B	4	BGC	O5-C5-C4	-3.26	102.90	110.83
2	18-B	3	BGC	O3-C3-C4	-3.26	102.70	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	16-B	4	BGC	C1-O5-C5	3.25	116.55	112.19
2	9-B	4	BGC	O5-C5-C6	3.24	113.97	107.66
2	22-B	2	BGC	O5-C5-C4	-3.23	102.96	110.83
2	8-B	3	BGC	C1-C2-C3	3.22	114.34	109.64
2	6-B	3	BGC	C1-C2-C3	3.22	114.34	109.64
2	7-B	2	BGC	O5-C5-C4	-3.21	103.01	110.83
2	16-B	3	BGC	O5-C5-C4	-3.21	103.01	110.83
2	23-B	4	BGC	C1-O5-C5	3.19	116.47	112.19
2	13-B	4	BGC	C1-O5-C5	3.17	116.44	112.19
2	23-B	4	BGC	C6-C5-C4	3.17	120.81	113.02
2	9-B	4	BGC	C6-C5-C4	-3.16	105.25	113.02
2	14-B	2	BGC	O5-C5-C4	-3.14	103.19	110.83
2	9-B	4	BGC	O3-C3-C4	-3.13	103.00	110.38
2	15-B	1	BGC	O5-C5-C4	-3.13	104.06	109.70
2	23-B	3	BGC	O5-C5-C4	-3.12	103.23	110.83
2	5-B	1	BGC	C1-O5-C5	-3.12	107.61	113.65
2	15-B	3	BGC	O5-C5-C4	-3.11	103.25	110.83
2	24-B	2	BGC	O3-C3-C2	-3.11	103.71	110.05
2	12-B	3	BGC	O5-C5-C4	-3.09	103.31	110.83
2	24-B	4	BGC	O5-C5-C4	-3.04	103.43	110.83
2	23-B	1	BGC	C4-C3-C2	3.03	116.15	110.83
2	21-B	2	BGC	C1-O5-C5	-3.02	108.14	112.19
2	16-B	2	BGC	C1-C2-C3	2.97	113.97	109.64
2	13-B	4	BGC	O4-C4-C3	2.97	117.38	110.38
2	3-B	3	BGC	O5-C5-C4	-2.96	103.62	110.83
2	6-B	3	BGC	O5-C5-C4	-2.96	103.63	110.83
2	3-B	4	BGC	O5-C5-C4	-2.94	103.67	110.83
2	20-B	4	BGC	O4-C4-C3	2.93	117.28	110.38
2	25-B	1	BGC	C3-C4-C5	2.93	115.54	110.23
2	8-B	3	BGC	O5-C5-C4	-2.91	103.75	110.83
2	18-B	4	BGC	C1-C2-C3	2.91	113.87	109.64
2	25-B	4	BGC	C1-O5-C5	2.90	116.07	112.19
2	25-B	4	BGC	O5-C5-C4	-2.89	103.79	110.83
2	5-B	2	BGC	O6-C6-C5	2.89	121.17	111.33
2	5-B	4	BGC	O5-C5-C4	-2.88	103.81	110.83
2	21-B	4	BGC	O4-C4-C3	2.88	117.16	110.38
2	1-B	3	BGC	O5-C5-C4	-2.88	103.83	110.83
2	5-B	2	BGC	O3-C3-C2	-2.87	104.19	110.05
2	15-B	2	BGC	O5-C5-C6	2.85	113.22	107.66
2	20-B	4	BGC	O3-C3-C4	-2.85	103.66	110.38
2	21-B	4	BGC	O5-C5-C4	-2.85	103.90	110.83
2	6-B	4	BGC	O4-C4-C3	2.84	117.07	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-B	4	BGC	C3-C4-C5	2.83	115.37	110.23
2	8-B	1	BGC	C3-C4-C5	2.82	115.35	110.23
2	16-B	1	BGC	C1-O5-C5	-2.82	108.20	113.65
2	23-B	1	BGC	C1-C2-C3	2.82	116.10	110.36
2	17-B	4	BGC	O5-C5-C4	-2.81	104.00	110.83
2	8-B	1	BGC	C6-C5-C4	-2.80	106.14	113.02
2	11-B	4	BGC	O5-C5-C4	-2.78	104.06	110.83
2	18-B	4	BGC	C2-C3-C4	2.77	115.74	110.86
2	2-B	4	BGC	O5-C5-C4	-2.75	104.13	110.83
2	18-B	3	BGC	O5-C5-C4	-2.75	104.14	110.83
2	19-B	3	BGC	C1-O5-C5	-2.74	108.51	112.19
2	9-B	1	BGC	C4-C3-C2	2.72	115.61	110.83
2	12-B	3	BGC	O3-C3-C2	-2.72	104.50	110.05
2	5-B	2	BGC	O5-C5-C6	2.72	112.95	107.66
2	10-B	2	BGC	C6-C5-C4	2.72	119.69	113.02
2	21-B	2	BGC	O5-C5-C6	2.72	112.95	107.66
2	24-B	4	BGC	O4-C4-C3	2.71	116.77	110.38
2	10-B	2	BGC	C1-O5-C5	2.70	115.81	112.19
2	17-B	1	BGC	O5-C1-C2	-2.69	105.57	110.30
2	6-B	4	BGC	O6-C6-C5	2.68	120.47	111.33
2	7-B	4	BGC	O4-C4-C3	2.67	116.67	110.38
2	10-B	3	BGC	O5-C5-C4	-2.67	104.34	110.83
2	14-B	3	BGC	O4-C4-C3	2.66	116.64	110.38
2	18-B	4	BGC	O2-C2-C1	-2.65	103.16	109.22
2	15-B	1	BGC	C1-O5-C5	-2.63	108.56	113.65
2	13-B	3	BGC	O4-C4-C3	2.63	116.56	110.38
2	15-B	2	BGC	O6-C6-C5	2.62	120.25	111.33
2	10-B	3	BGC	O3-C3-C2	-2.62	104.72	110.05
2	9-B	2	BGC	O5-C5-C4	-2.61	104.48	110.83
2	17-B	4	BGC	O4-C4-C3	2.60	116.51	110.38
2	25-B	2	BGC	C1-O5-C5	-2.59	108.71	112.19
2	1-B	1	BGC	O5-C5-C6	2.59	112.85	106.44
2	1-B	4	BGC	O3-C3-C4	-2.57	104.31	110.38
2	4-B	2	BGC	O3-C3-C2	-2.57	104.80	110.05
2	4-B	2	BGC	O5-C5-C4	-2.57	104.57	110.83
2	7-B	4	BGC	O3-C3-C4	-2.56	104.34	110.38
2	19-B	1	BGC	C1-O5-C5	-2.55	108.72	113.65
2	12-B	4	BGC	O4-C4-C3	2.54	116.37	110.38
2	15-B	1	BGC	C3-C4-C5	2.53	114.83	110.23
2	25-B	4	BGC	O4-C4-C3	2.53	116.35	110.38
2	5-B	1	BGC	O2-C2-C1	-2.53	103.40	109.25
2	7-B	3	BGC	O5-C5-C4	-2.53	104.68	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	14-B	4	BGC	O4-C4-C3	2.53	116.33	110.38
2	22-B	3	BGC	C1-C2-C3	2.50	113.29	109.64
2	15-B	2	BGC	C1-O5-C5	-2.50	108.83	112.19
2	7-B	3	BGC	O4-C4-C3	2.50	116.27	110.38
2	15-B	1	BGC	O6-C6-C5	2.50	119.83	111.33
2	7-B	1	BGC	C3-C4-C5	2.49	114.75	110.23
2	16-B	4	BGC	O6-C6-C5	2.49	119.81	111.33
2	3-B	4	BGC	O4-C4-C3	2.48	116.23	110.38
2	23-B	1	BGC	O4-C4-C5	2.48	115.42	109.32
2	12-B	4	BGC	O3-C3-C4	-2.46	104.57	110.38
2	11-B	3	BGC	O4-C4-C3	2.45	116.14	110.38
2	10-B	2	BGC	O3-C3-C2	-2.44	105.06	110.05
2	17-B	3	BGC	O5-C5-C4	-2.44	104.89	110.83
2	21-B	2	BGC	O6-C6-C5	2.43	119.62	111.33
2	6-B	4	BGC	O5-C5-C4	-2.42	104.93	110.83
2	10-B	4	BGC	O2-C2-C3	2.42	115.17	110.15
2	23-B	2	BGC	C1-O5-C5	2.41	115.41	112.19
2	1-B	2	BGC	O5-C5-C4	-2.41	104.97	110.83
2	10-B	1	BGC	O2-C2-C1	-2.40	103.71	109.25
2	23-B	4	BGC	O4-C4-C3	2.39	116.01	110.38
2	1-B	3	BGC	O3-C3-C4	-2.39	104.75	110.38
2	12-B	4	BGC	C1-O5-C5	2.38	115.38	112.19
2	10-B	4	BGC	O4-C4-C5	2.38	115.19	109.32
2	16-B	3	BGC	O4-C4-C3	2.37	115.96	110.38
2	18-B	1	BGC	C1-O5-C5	-2.37	109.08	113.65
2	4-B	1	BGC	C6-C5-C4	-2.36	107.22	113.02
2	25-B	1	BGC	O5-C1-C2	-2.36	106.15	110.30
2	25-B	3	BGC	O3-C3-C4	-2.35	104.83	110.38
2	14-B	4	BGC	O5-C5-C4	-2.35	105.11	110.83
2	2-B	4	BGC	O4-C4-C3	2.35	115.91	110.38
2	9-B	4	BGC	O4-C4-C3	2.35	115.90	110.38
2	20-B	2	BGC	O3-C3-C2	-2.34	105.29	110.05
2	13-B	1	BGC	C3-C4-C5	2.33	114.46	110.23
2	4-B	4	BGC	O5-C5-C4	-2.33	105.15	110.83
2	3-B	4	BGC	O3-C3-C4	-2.33	104.89	110.38
2	5-B	2	BGC	C1-O5-C5	-2.32	109.08	112.19
2	17-B	1	BGC	C1-O5-C5	-2.31	109.18	113.65
2	5-B	4	BGC	O2-C2-C3	2.31	114.93	110.15
2	12-B	3	BGC	O4-C4-C3	2.30	115.80	110.38
2	20-B	2	BGC	O6-C6-C5	2.30	119.16	111.33
2	19-B	1	BGC	O1-C1-C2	2.30	115.65	108.98
2	23-B	2	BGC	O5-C5-C4	-2.30	105.24	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-B	1	BGC	O2-C2-C1	-2.29	103.96	109.25
2	19-B	3	BGC	O4-C4-C3	2.29	115.77	110.38
2	15-B	4	BGC	C2-C3-C4	2.28	114.88	110.86
2	5-B	4	BGC	O4-C4-C3	2.27	115.73	110.38
2	4-B	1	BGC	O6-C6-C5	2.27	119.05	111.33
2	19-B	3	BGC	O2-C2-C1	-2.26	104.06	109.22
2	5-B	1	BGC	O1-C1-C2	2.25	115.51	108.98
2	15-B	4	BGC	O5-C5-C4	-2.25	105.36	110.83
2	18-B	4	BGC	O5-C5-C4	-2.25	105.36	110.83
2	1-B	1	BGC	O4-C4-C3	-2.25	105.08	110.38
2	10-B	1	BGC	O4-C4-C3	2.25	115.67	110.38
2	25-B	2	BGC	O6-C6-C5	2.24	118.97	111.33
2	11-B	1	BGC	O1-C1-C2	2.24	115.48	108.98
2	5-B	3	BGC	O5-C5-C6	2.24	112.02	107.66
2	17-B	2	BGC	O3-C3-C2	-2.23	105.49	110.05
2	13-B	2	BGC	O3-C3-C2	-2.23	105.50	110.05
2	16-B	2	BGC	O2-C2-C3	2.22	114.76	110.15
2	19-B	4	BGC	O4-C4-C3	2.22	115.61	110.38
2	4-B	4	BGC	O4-C4-C3	2.22	115.60	110.38
2	17-B	4	BGC	C6-C5-C4	2.22	118.46	113.02
2	10-B	2	BGC	C2-C3-C4	2.21	114.76	110.86
2	7-B	1	BGC	O2-C2-C1	-2.21	104.14	109.25
2	21-B	1	BGC	O5-C5-C4	-2.21	105.71	109.70
2	13-B	1	BGC	C6-C5-C4	-2.21	107.59	113.02
2	7-B	1	BGC	C6-C5-C4	-2.21	107.59	113.02
2	22-B	4	BGC	O4-C4-C3	2.21	115.58	110.38
2	1-B	3	BGC	C6-C5-C4	-2.21	107.60	113.02
2	2-B	3	BGC	O2-C2-C3	-2.20	105.59	110.15
2	6-B	2	BGC	O3-C3-C2	-2.20	105.57	110.05
2	22-B	4	BGC	O5-C5-C4	-2.18	105.53	110.83
2	2-B	1	BGC	C4-C3-C2	2.17	114.64	110.83
2	3-B	1	BGC	C3-C4-C5	2.17	114.17	110.23
2	20-B	3	BGC	O5-C5-C4	-2.16	105.56	110.83
2	7-B	3	BGC	O3-C3-C2	-2.16	105.64	110.05
2	2-B	4	BGC	O3-C3-C4	-2.16	105.29	110.38
2	4-B	1	BGC	O4-C4-C3	2.14	115.43	110.38
2	20-B	4	BGC	O2-C2-C3	2.14	114.59	110.15
2	2-B	3	BGC	O5-C5-C6	2.14	111.82	107.66
2	3-B	4	BGC	O5-C5-C6	2.13	111.81	107.66
2	10-B	3	BGC	O4-C4-C3	2.13	115.39	110.38
2	7-B	3	BGC	O6-C6-C5	2.13	118.58	111.33
2	13-B	3	BGC	O6-C6-C5	2.12	118.56	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	15-B	4	BGC	C6-C5-C4	2.12	118.23	113.02
2	3-B	2	BGC	O3-C3-C2	-2.12	105.73	110.05
2	19-B	2	BGC	O3-C3-C2	-2.12	105.73	110.05
2	17-B	1	BGC	C3-C4-C5	2.11	114.06	110.23
2	3-B	4	BGC	O2-C2-C3	2.10	114.51	110.15
2	23-B	3	BGC	O5-C5-C6	-2.10	103.57	107.66
2	11-B	3	BGC	O3-C3-C2	-2.10	105.77	110.05
2	16-B	3	BGC	O3-C3-C2	-2.09	105.78	110.05
2	19-B	2	BGC	O6-C6-C5	2.09	118.45	111.33
2	14-B	4	BGC	C6-C5-C4	2.09	118.14	113.02
2	23-B	1	BGC	O6-C6-C5	2.08	118.43	111.33
2	21-B	2	BGC	C3-C4-C5	-2.06	106.50	110.23
2	1-B	3	BGC	O4-C4-C3	2.05	115.22	110.38
2	17-B	2	BGC	O5-C5-C4	-2.05	105.83	110.83
2	15-B	3	BGC	O3-C3-C2	-2.05	105.87	110.05
2	8-B	1	BGC	O6-C6-C5	2.05	118.30	111.33
2	5-B	2	BGC	O3-C3-C4	2.04	115.19	110.38
2	25-B	2	BGC	O5-C5-C6	2.04	111.64	107.66
2	25-B	1	BGC	C6-C5-C4	-2.04	108.02	113.02
2	23-B	4	BGC	O4-C4-C5	2.03	114.33	109.32
2	24-B	1	BGC	C4-C3-C2	2.03	114.39	110.83
2	15-B	1	BGC	O1-C1-C2	2.03	114.86	108.98
2	16-B	2	BGC	O6-C6-C5	2.02	118.22	111.33
2	23-B	2	BGC	C2-C3-C4	2.02	114.42	110.86
2	1-B	1	BGC	O1-C1-C2	2.02	114.84	108.98
2	14-B	2	BGC	C6-C5-C4	2.02	117.97	113.02
2	23-B	1	BGC	O1-C1-C2	2.01	114.82	108.98
2	3-B	2	BGC	O5-C5-C4	-2.01	105.94	110.83
2	14-B	2	BGC	O3-C3-C2	-2.01	105.96	110.05
2	14-B	4	BGC	O2-C2-C3	2.00	114.30	110.15
2	24-B	4	BGC	O6-C6-C5	2.00	118.14	111.33

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	23-B	3	BGC	C4-C5-C6-O6
2	1-B	4	BGC	O5-C5-C6-O6
2	8-B	4	BGC	C4-C5-C6-O6
2	23-B	3	BGC	O5-C5-C6-O6
2	4-B	1	BGC	O5-C5-C6-O6
2	15-B	1	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	21-B	2	BGC	O5-C5-C6-O6
2	8-B	4	BGC	O5-C5-C6-O6
2	21-B	2	BGC	C4-C5-C6-O6
2	18-B	4	BGC	C4-C5-C6-O6
2	23-B	4	BGC	C4-C5-C6-O6
2	14-B	3	BGC	O5-C5-C6-O6
2	15-B	4	BGC	O5-C5-C6-O6
2	14-B	3	BGC	C4-C5-C6-O6
2	12-B	4	BGC	C4-C5-C6-O6
2	15-B	2	BGC	O5-C5-C6-O6
2	4-B	1	BGC	C4-C5-C6-O6
2	1-B	4	BGC	C4-C5-C6-O6
2	23-B	4	BGC	O5-C5-C6-O6
2	15-B	2	BGC	C4-C5-C6-O6
2	10-B	4	BGC	C4-C5-C6-O6
2	12-B	4	BGC	O5-C5-C6-O6
2	5-B	2	BGC	O5-C5-C6-O6
2	18-B	4	BGC	O5-C5-C6-O6
2	5-B	2	BGC	C4-C5-C6-O6
2	2-B	3	BGC	C4-C5-C6-O6
2	5-B	4	BGC	C4-C5-C6-O6
2	15-B	1	BGC	C4-C5-C6-O6
2	2-B	3	BGC	O5-C5-C6-O6
2	20-B	2	BGC	O5-C5-C6-O6
2	20-B	2	BGC	C4-C5-C6-O6
2	15-B	4	BGC	C4-C5-C6-O6
2	5-B	4	BGC	O5-C5-C6-O6
2	25-B	2	BGC	O5-C5-C6-O6
2	25-B	2	BGC	C4-C5-C6-O6
2	7-B	3	BGC	O5-C5-C6-O6
2	8-B	1	BGC	O5-C5-C6-O6
2	1-B	3	BGC	O5-C5-C6-O6
2	16-B	1	BGC	C4-C5-C6-O6
2	1-B	3	BGC	C4-C5-C6-O6
2	7-B	3	BGC	C4-C5-C6-O6
2	16-B	1	BGC	O5-C5-C6-O6
2	10-B	4	BGC	O5-C5-C6-O6
2	16-B	4	BGC	O5-C5-C6-O6
2	3-B	4	BGC	O5-C5-C6-O6
2	7-B	1	BGC	O5-C5-C6-O6
2	11-B	2	BGC	C4-C5-C6-O6
2	13-B	1	BGC	O5-C5-C6-O6

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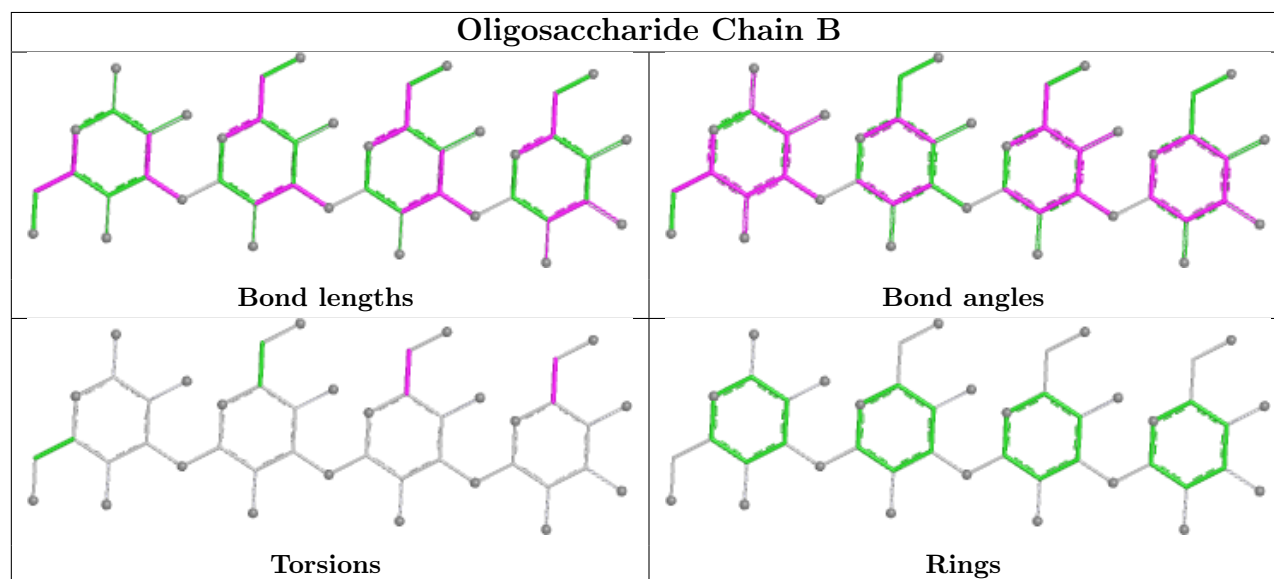
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Mol	Chain	Res	Type	Atoms
2	19-B	2	BGC	C4-C5-C6-O6
2	19-B	2	BGC	O5-C5-C6-O6
2	10-B	3	BGC	O5-C5-C6-O6
2	10-B	3	BGC	C4-C5-C6-O6
2	10-B	2	BGC	C4-C5-C6-O6
2	8-B	1	BGC	C4-C5-C6-O6
2	20-B	1	BGC	O5-C5-C6-O6
2	7-B	1	BGC	C4-C5-C6-O6
2	11-B	2	BGC	O5-C5-C6-O6
2	3-B	4	BGC	C4-C5-C6-O6
2	13-B	1	BGC	C4-C5-C6-O6
2	13-B	3	BGC	C4-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.



4.6 Ligand geometry [i](#)

100 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	EDO	5-A	704	-	3,3,3	0.60	0	2,2,2	0.17	0
4	EDO	2-A	704	-	3,3,3	0.62	0	2,2,2	0.16	0
4	EDO	18-A	703	-	3,3,3	0.44	0	2,2,2	0.12	0
4	EDO	11-A	704	-	3,3,3	0.50	0	2,2,2	0.51	0
3	BGC	22-A	701	-	11,11,12	1.05	0	15,15,17	3.47	9 (60%)
4	EDO	2-A	703	-	3,3,3	0.46	0	2,2,2	0.14	0
4	EDO	22-A	704	-	3,3,3	0.59	0	2,2,2	0.28	0
3	BGC	17-A	701	-	11,11,12	0.78	0	15,15,17	2.19	4 (26%)
4	EDO	5-A	703	-	3,3,3	0.45	0	2,2,2	0.14	0
4	EDO	11-A	703	-	3,3,3	0.51	0	2,2,2	0.08	0
3	BGC	14-A	701	-	11,11,12	0.86	0	15,15,17	2.82	7 (46%)
4	EDO	4-A	703	-	3,3,3	0.47	0	2,2,2	0.11	0
4	EDO	6-A	702	-	3,3,3	0.40	0	2,2,2	0.40	0
4	EDO	11-A	702	-	3,3,3	0.46	0	2,2,2	0.43	0
4	EDO	9-A	703	-	3,3,3	0.50	0	2,2,2	0.21	0
4	EDO	20-A	702	-	3,3,3	0.38	0	2,2,2	0.27	0
4	EDO	21-A	702	-	3,3,3	0.42	0	2,2,2	0.70	0
3	BGC	19-A	701	-	11,11,12	0.75	0	15,15,17	1.77	4 (26%)
3	BGC	12-A	701	-	11,11,12	0.84	0	15,15,17	2.02	5 (33%)
4	EDO	24-A	703	-	3,3,3	0.48	0	2,2,2	0.09	0
4	EDO	16-A	704	-	3,3,3	0.57	0	2,2,2	0.15	0
4	EDO	16-A	703	-	3,3,3	0.48	0	2,2,2	0.15	0
4	EDO	1-A	702	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EDO	17-A	704	-	3,3,3	0.60	0	2,2,2	0.28	0
3	BGC	8-A	701	-	11,11,12	1.02	0	15,15,17	1.80	5 (33%)
4	EDO	18-A	702	-	3,3,3	0.45	0	2,2,2	0.32	0
4	EDO	15-A	703	-	3,3,3	0.47	0	2,2,2	0.15	0
4	EDO	20-A	703	-	3,3,3	0.38	0	2,2,2	0.25	0
4	EDO	15-A	704	-	3,3,3	0.52	0	2,2,2	0.13	0
4	EDO	7-A	704	-	3,3,3	0.50	0	2,2,2	0.08	0
4	EDO	14-A	704	-	3,3,3	0.51	0	2,2,2	0.54	0
4	EDO	14-A	703	-	3,3,3	0.48	0	2,2,2	0.09	0
4	EDO	23-A	704	-	3,3,3	0.38	0	2,2,2	0.35	0
3	BGC	20-A	701	-	11,11,12	0.78	0	15,15,17	2.00	6 (40%)
4	EDO	19-A	704	-	3,3,3	0.60	0	2,2,2	0.26	0
4	EDO	10-A	704	-	3,3,3	0.56	0	2,2,2	0.15	0
4	EDO	19-A	702	-	3,3,3	0.37	0	2,2,2	0.27	0
4	EDO	21-A	704	-	3,3,3	0.53	0	2,2,2	0.22	0
4	EDO	3-A	702	-	3,3,3	0.38	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	9-A	704	-	3,3,3	0.57	0	2,2,2	0.27	0
4	EDO	12-A	704	-	3,3,3	0.55	0	2,2,2	0.51	0
4	EDO	25-A	702	-	3,3,3	0.42	0	2,2,2	0.23	0
3	BGC	1-A	701	-	11,11,12	0.71	0	15,15,17	1.16	1 (6%)
4	EDO	5-A	702	-	3,3,3	0.48	0	2,2,2	0.18	0
4	EDO	7-A	702	-	3,3,3	0.57	0	2,2,2	0.19	0
3	BGC	2-A	701	-	11,11,12	0.88	0	15,15,17	3.12	8 (53%)
4	EDO	8-A	704	-	3,3,3	0.58	0	2,2,2	0.35	0
4	EDO	3-A	703	-	3,3,3	0.45	0	2,2,2	0.15	0
4	EDO	18-A	704	-	3,3,3	0.59	0	2,2,2	0.19	0
3	BGC	25-A	701	-	11,11,12	0.58	0	15,15,17	2.06	4 (26%)
4	EDO	25-A	703	-	3,3,3	0.40	0	2,2,2	0.36	0
4	EDO	24-A	704	-	3,3,3	0.59	0	2,2,2	0.14	0
4	EDO	23-A	703	-	3,3,3	0.44	0	2,2,2	0.28	0
4	EDO	22-A	702	-	3,3,3	0.35	0	2,2,2	0.35	0
4	EDO	1-A	703	-	3,3,3	0.35	0	2,2,2	0.27	0
4	EDO	4-A	702	-	3,3,3	0.40	0	2,2,2	0.19	0
4	EDO	21-A	703	-	3,3,3	0.51	0	2,2,2	0.16	0
3	BGC	7-A	701	-	11,11,12	0.81	0	15,15,17	1.59	3 (20%)
3	BGC	6-A	701	-	11,11,12	0.77	0	15,15,17	1.23	2 (13%)
4	EDO	13-A	704	-	3,3,3	0.58	0	2,2,2	0.38	0
3	BGC	23-A	701	-	11,11,12	0.74	0	15,15,17	1.56	3 (20%)
4	EDO	19-A	703	-	3,3,3	0.33	0	2,2,2	0.43	0
4	EDO	10-A	703	-	3,3,3	0.45	0	2,2,2	0.10	0
4	EDO	1-A	704	-	3,3,3	0.38	0	2,2,2	0.13	0
4	EDO	25-A	704	-	3,3,3	0.29	0	2,2,2	0.34	0
4	EDO	10-A	702	-	3,3,3	0.37	0	2,2,2	0.23	0
4	EDO	17-A	703	-	3,3,3	0.61	0	2,2,2	0.09	0
4	EDO	15-A	702	-	3,3,3	0.40	0	2,2,2	0.46	0
3	BGC	11-A	701	-	11,11,12	1.07	1 (9%)	15,15,17	2.11	6 (40%)
4	EDO	12-A	702	-	3,3,3	0.40	0	2,2,2	0.36	0
4	EDO	16-A	702	-	3,3,3	0.38	0	2,2,2	0.45	0
3	BGC	4-A	701	-	11,11,12	0.67	0	15,15,17	0.85	0
3	BGC	9-A	701	-	11,11,12	0.67	0	15,15,17	1.71	3 (20%)
3	BGC	18-A	701	-	11,11,12	0.68	0	15,15,17	1.39	2 (13%)
3	BGC	15-A	701	-	11,11,12	1.03	1 (9%)	15,15,17	2.54	4 (26%)
4	EDO	6-A	704	-	3,3,3	0.64	0	2,2,2	0.14	0
4	EDO	4-A	704	-	3,3,3	0.61	0	2,2,2	0.16	0
4	EDO	20-A	704	-	3,3,3	0.32	0	2,2,2	0.56	0
4	EDO	23-A	702	-	3,3,3	0.46	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	10-A	701	-	11,11,12	1.18	1 (9%)	15,15,17	2.07	6 (40%)
4	EDO	22-A	703	-	3,3,3	0.47	0	2,2,2	0.13	0
4	EDO	13-A	703	-	3,3,3	0.57	0	2,2,2	0.05	0
4	EDO	3-A	704	-	3,3,3	0.56	0	2,2,2	0.17	0
4	EDO	9-A	702	-	3,3,3	0.57	0	2,2,2	0.15	0
4	EDO	24-A	702	-	3,3,3	0.39	0	2,2,2	0.10	0
3	BGC	5-A	701	-	11,11,12	0.78	0	15,15,17	1.63	2 (13%)
4	EDO	7-A	703	-	3,3,3	0.34	0	2,2,2	0.30	0
4	EDO	2-A	702	-	3,3,3	0.36	0	2,2,2	0.42	0
4	EDO	12-A	703	-	3,3,3	0.51	0	2,2,2	0.05	0
3	BGC	13-A	701	-	11,11,12	0.76	0	15,15,17	1.78	4 (26%)
4	EDO	8-A	703	-	3,3,3	0.46	0	2,2,2	0.39	0
3	BGC	16-A	701	-	11,11,12	0.90	0	15,15,17	2.54	7 (46%)
4	EDO	8-A	702	-	3,3,3	0.42	0	2,2,2	0.14	0
3	BGC	3-A	701	-	11,11,12	1.16	1 (9%)	15,15,17	2.67	5 (33%)
3	BGC	21-A	701	-	11,11,12	0.84	0	15,15,17	2.24	4 (26%)
4	EDO	14-A	702	-	3,3,3	0.41	0	2,2,2	0.33	0
3	BGC	24-A	701	-	11,11,12	1.17	1 (9%)	15,15,17	1.68	3 (20%)
4	EDO	13-A	702	-	3,3,3	0.39	0	2,2,2	0.56	0
4	EDO	6-A	703	-	3,3,3	0.51	0	2,2,2	0.02	0
4	EDO	17-A	702	-	3,3,3	0.47	0	2,2,2	0.41	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	EDO	5-A	704	-	-	0/1/1/1	-
4	EDO	2-A	704	-	-	0/1/1/1	-
4	EDO	18-A	703	-	-	0/1/1/1	-
4	EDO	11-A	704	-	-	1/1/1/1	-
3	BGC	22-A	701	-	-	1/2/19/22	0/1/1/1
4	EDO	2-A	703	-	-	1/1/1/1	-
4	EDO	22-A	704	-	-	0/1/1/1	-
3	BGC	17-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	5-A	703	-	-	0/1/1/1	-
4	EDO	11-A	703	-	-	0/1/1/1	-
3	BGC	14-A	701	-	-	1/2/19/22	0/1/1/1
4	EDO	4-A	703	-	-	0/1/1/1	-
4	EDO	6-A	702	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	11-A	702	-	-	0/1/1/1	-
4	EDO	9-A	703	-	-	0/1/1/1	-
4	EDO	20-A	702	-	-	0/1/1/1	-
4	EDO	21-A	702	-	-	0/1/1/1	-
3	BGC	19-A	701	-	-	1/2/19/22	0/1/1/1
3	BGC	12-A	701	-	-	1/2/19/22	0/1/1/1
4	EDO	24-A	703	-	-	0/1/1/1	-
4	EDO	16-A	704	-	-	0/1/1/1	-
4	EDO	16-A	703	-	-	0/1/1/1	-
4	EDO	1-A	702	-	-	0/1/1/1	-
4	EDO	17-A	704	-	-	0/1/1/1	-
3	BGC	8-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	18-A	702	-	-	0/1/1/1	-
4	EDO	15-A	703	-	-	0/1/1/1	-
4	EDO	20-A	703	-	-	0/1/1/1	-
4	EDO	15-A	704	-	-	0/1/1/1	-
4	EDO	7-A	704	-	-	0/1/1/1	-
4	EDO	14-A	704	-	-	0/1/1/1	-
4	EDO	14-A	703	-	-	0/1/1/1	-
4	EDO	23-A	704	-	-	1/1/1/1	-
3	BGC	20-A	701	-	-	1/2/19/22	0/1/1/1
4	EDO	19-A	704	-	-	0/1/1/1	-
4	EDO	10-A	704	-	-	1/1/1/1	-
4	EDO	19-A	702	-	-	0/1/1/1	-
4	EDO	21-A	704	-	-	0/1/1/1	-
4	EDO	3-A	702	-	-	0/1/1/1	-
4	EDO	9-A	704	-	-	0/1/1/1	-
4	EDO	12-A	704	-	-	0/1/1/1	-
4	EDO	25-A	702	-	-	1/1/1/1	-
3	BGC	1-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	5-A	702	-	-	1/1/1/1	-
4	EDO	7-A	702	-	-	1/1/1/1	-
3	BGC	2-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	8-A	704	-	-	0/1/1/1	-
4	EDO	3-A	703	-	-	0/1/1/1	-
4	EDO	18-A	704	-	-	0/1/1/1	-
3	BGC	25-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	25-A	703	-	-	0/1/1/1	-
4	EDO	24-A	704	-	-	0/1/1/1	-
4	EDO	23-A	703	-	-	0/1/1/1	-
4	EDO	22-A	702	-	-	0/1/1/1	-
4	EDO	1-A	703	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	4-A	702	-	-	0/1/1/1	-
4	EDO	21-A	703	-	-	0/1/1/1	-
3	BGC	7-A	701	-	-	0/2/19/22	0/1/1/1
3	BGC	6-A	701	-	-	1/2/19/22	0/1/1/1
4	EDO	13-A	704	-	-	1/1/1/1	-
3	BGC	23-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	19-A	703	-	-	0/1/1/1	-
4	EDO	10-A	703	-	-	0/1/1/1	-
4	EDO	1-A	704	-	-	0/1/1/1	-
4	EDO	25-A	704	-	-	0/1/1/1	-
4	EDO	10-A	702	-	-	0/1/1/1	-
4	EDO	17-A	703	-	-	1/1/1/1	-
4	EDO	15-A	702	-	-	0/1/1/1	-
3	BGC	11-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	12-A	702	-	-	0/1/1/1	-
4	EDO	16-A	702	-	-	0/1/1/1	-
3	BGC	4-A	701	-	-	0/2/19/22	0/1/1/1
3	BGC	9-A	701	-	-	2/2/19/22	0/1/1/1
3	BGC	18-A	701	-	-	0/2/19/22	0/1/1/1
3	BGC	15-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	6-A	704	-	-	0/1/1/1	-
4	EDO	4-A	704	-	-	0/1/1/1	-
4	EDO	20-A	704	-	-	1/1/1/1	-
4	EDO	23-A	702	-	-	1/1/1/1	-
3	BGC	10-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	22-A	703	-	-	1/1/1/1	-
4	EDO	13-A	703	-	-	0/1/1/1	-
4	EDO	3-A	704	-	-	0/1/1/1	-
4	EDO	9-A	702	-	-	1/1/1/1	-
4	EDO	24-A	702	-	-	1/1/1/1	-
3	BGC	5-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	7-A	703	-	-	0/1/1/1	-
4	EDO	2-A	702	-	-	0/1/1/1	-
4	EDO	12-A	703	-	-	0/1/1/1	-
3	BGC	13-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	8-A	703	-	-	0/1/1/1	-
3	BGC	16-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	8-A	702	-	-	1/1/1/1	-
3	BGC	3-A	701	-	-	1/2/19/22	0/1/1/1
3	BGC	21-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	14-A	702	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	24-A	701	-	-	1/2/19/22	0/1/1/1
4	EDO	13-A	702	-	-	0/1/1/1	-
4	EDO	6-A	703	-	-	1/1/1/1	-
4	EDO	17-A	702	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	10-A	701	BGC	O5-C1	-3.46	1.37	1.43
3	3-A	701	BGC	O5-C1	-2.62	1.39	1.43
3	24-A	701	BGC	O2-C2	-2.29	1.38	1.43
3	15-A	701	BGC	C2-C3	2.20	1.55	1.52
3	11-A	701	BGC	O5-C1	-2.09	1.40	1.43

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	22-A	701	BGC	C1-O5-C5	9.11	124.39	112.19
3	14-A	701	BGC	C1-O5-C5	8.15	123.11	112.19
3	2-A	701	BGC	C1-C2-C3	6.78	119.52	109.64
3	3-A	701	BGC	C3-C4-C5	-6.02	99.32	110.23
3	15-A	701	BGC	C1-O5-C5	6.01	120.24	112.19
3	16-A	701	BGC	C1-O5-C5	5.85	120.02	112.19
3	22-A	701	BGC	C1-C2-C3	5.57	117.76	109.64
3	2-A	701	BGC	C1-O5-C5	-5.46	104.86	112.19
3	3-A	701	BGC	O5-C5-C6	5.08	117.55	107.66
3	21-A	701	BGC	O5-C5-C6	4.92	117.24	107.66
3	17-A	701	BGC	C1-O5-C5	4.88	118.73	112.19
3	15-A	701	BGC	C6-C5-C4	-4.84	101.15	113.02
3	25-A	701	BGC	C1-O5-C5	4.80	118.61	112.19
3	20-A	701	BGC	C1-C2-C3	4.67	116.44	109.64
3	3-A	701	BGC	C1-C2-C3	4.66	116.43	109.64
3	13-A	701	BGC	C1-O5-C5	4.47	118.18	112.19
3	24-A	701	BGC	O2-C2-C3	-4.44	100.96	110.15
3	11-A	701	BGC	O2-C2-C3	4.41	119.28	110.15
3	17-A	701	BGC	C2-C3-C4	4.32	118.46	110.86
3	9-A	701	BGC	C1-O5-C5	4.26	117.90	112.19
3	2-A	701	BGC	O3-C3-C4	4.09	120.01	110.38
3	10-A	701	BGC	C1-O5-C5	4.01	117.55	112.19
3	21-A	701	BGC	C1-C2-C3	3.90	115.32	109.64
3	12-A	701	BGC	C1-C2-C3	3.85	115.25	109.64
3	2-A	701	BGC	C6-C5-C4	3.82	122.41	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-A	701	BGC	C1-O5-C5	-3.77	107.14	112.19
3	14-A	701	BGC	C1-C2-C3	3.71	115.04	109.64
3	25-A	701	BGC	C3-C4-C5	3.70	116.94	110.23
3	16-A	701	BGC	O5-C1-C2	3.66	119.53	110.79
3	9-A	701	BGC	C1-C2-C3	3.58	114.86	109.64
3	19-A	701	BGC	C2-C3-C4	3.55	117.11	110.86
3	8-A	701	BGC	O3-C3-C4	-3.48	102.17	110.38
3	7-A	701	BGC	O5-C5-C6	3.46	114.39	107.66
3	10-A	701	BGC	C1-C2-C3	3.46	114.68	109.64
3	21-A	701	BGC	C1-O5-C5	3.45	116.81	112.19
3	8-A	701	BGC	C2-C3-C4	3.42	116.88	110.86
3	23-A	701	BGC	O5-C5-C6	3.33	114.14	107.66
3	19-A	701	BGC	C1-C2-C3	3.32	114.48	109.64
3	15-A	701	BGC	C1-C2-C3	3.31	114.46	109.64
3	12-A	701	BGC	O5-C5-C6	3.28	114.05	107.66
3	2-A	701	BGC	C3-C4-C5	-3.23	104.37	110.23
3	11-A	701	BGC	C1-O5-C5	-3.22	107.87	112.19
3	13-A	701	BGC	C3-C4-C5	3.17	115.98	110.23
3	14-A	701	BGC	C3-C4-C5	-3.15	104.51	110.23
3	16-A	701	BGC	O2-C2-C3	3.13	116.63	110.15
3	16-A	701	BGC	O5-C5-C6	3.05	113.59	107.66
3	15-A	701	BGC	O5-C5-C6	3.04	113.58	107.66
3	2-A	701	BGC	O4-C4-C3	-3.04	103.20	110.38
3	22-A	701	BGC	O4-C4-C5	3.03	116.78	109.32
3	17-A	701	BGC	C6-C5-C4	-3.02	105.60	113.02
3	16-A	701	BGC	C3-C4-C5	3.00	115.67	110.23
3	17-A	701	BGC	C1-C2-C3	2.99	114.00	109.64
3	22-A	701	BGC	O4-C4-C3	-2.98	103.35	110.38
3	11-A	701	BGC	C1-C2-C3	-2.93	105.38	109.64
3	16-A	701	BGC	O3-C3-C2	-2.92	104.10	110.05
3	10-A	701	BGC	O5-C5-C6	2.91	113.32	107.66
3	22-A	701	BGC	O3-C3-C2	2.88	115.93	110.05
3	21-A	701	BGC	C2-C3-C4	2.85	115.87	110.86
3	22-A	701	BGC	O5-C5-C6	2.82	113.16	107.66
3	23-A	701	BGC	C2-C3-C4	2.75	115.70	110.86
3	25-A	701	BGC	C1-C2-C3	-2.75	105.64	109.64
3	18-A	701	BGC	C1-O5-C5	2.74	115.85	112.19
3	19-A	701	BGC	C1-O5-C5	2.72	115.84	112.19
3	12-A	701	BGC	O2-C2-C3	-2.71	104.54	110.15
3	2-A	701	BGC	O3-C3-C2	2.69	115.55	110.05
3	11-A	701	BGC	O2-C2-C1	-2.65	103.15	109.22
3	14-A	701	BGC	O3-C3-C2	2.64	115.45	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	20-A	701	BGC	O6-C6-C5	-2.62	102.41	111.33
3	23-A	701	BGC	C6-C5-C4	-2.59	106.66	113.02
3	20-A	701	BGC	O5-C1-C2	-2.59	104.61	110.79
3	20-A	701	BGC	C6-C5-C4	-2.57	106.71	113.02
3	16-A	701	BGC	O2-C2-C1	2.56	115.09	109.22
3	5-A	701	BGC	O5-C5-C6	2.56	112.64	107.66
3	14-A	701	BGC	O2-C2-C3	2.55	115.43	110.15
3	14-A	701	BGC	O5-C1-C2	2.54	116.86	110.79
3	7-A	701	BGC	C1-C2-C3	2.53	113.32	109.64
3	12-A	701	BGC	C2-C3-C4	2.49	115.25	110.86
3	20-A	701	BGC	C2-C3-C4	2.49	115.24	110.86
3	22-A	701	BGC	C6-C5-C4	-2.48	106.92	113.02
3	11-A	701	BGC	O5-C1-C2	-2.46	104.92	110.79
3	2-A	701	BGC	O2-C2-C3	-2.45	105.08	110.15
3	25-A	701	BGC	O4-C4-C5	-2.45	103.30	109.32
3	12-A	701	BGC	C3-C4-C5	-2.44	105.80	110.23
3	13-A	701	BGC	C6-C5-C4	-2.42	107.08	113.02
3	7-A	701	BGC	C1-O5-C5	2.39	115.39	112.19
3	10-A	701	BGC	O4-C4-C3	2.39	116.01	110.38
3	10-A	701	BGC	C6-C5-C4	-2.38	107.17	113.02
3	9-A	701	BGC	C6-C5-C4	-2.38	107.17	113.02
3	22-A	701	BGC	O2-C2-C3	-2.37	105.25	110.15
3	11-A	701	BGC	O4-C4-C3	2.32	115.85	110.38
3	10-A	701	BGC	O3-C3-C2	-2.32	105.32	110.05
3	22-A	701	BGC	C2-C3-C4	2.31	114.92	110.86
3	3-A	701	BGC	O2-C2-C3	-2.27	105.44	110.15
3	1-A	701	BGC	C6-C5-C4	-2.24	107.53	113.02
3	6-A	701	BGC	O5-C5-C6	-2.22	103.34	107.66
3	3-A	701	BGC	O4-C4-C5	2.22	114.78	109.32
3	20-A	701	BGC	O5-C5-C6	2.21	111.97	107.66
3	6-A	701	BGC	C1-C2-C3	2.20	112.85	109.64
3	8-A	701	BGC	O5-C1-C2	-2.20	105.55	110.79
3	24-A	701	BGC	C3-C4-C5	2.16	114.16	110.23
3	8-A	701	BGC	C6-C5-C4	-2.15	107.74	113.02
3	8-A	701	BGC	C1-C2-C3	2.14	112.75	109.64
3	13-A	701	BGC	C2-C3-C4	2.13	114.60	110.86
3	19-A	701	BGC	O5-C5-C6	2.11	111.77	107.66
3	18-A	701	BGC	C3-C4-C5	2.11	114.06	110.23
3	24-A	701	BGC	C1-O5-C5	-2.09	109.39	112.19
3	14-A	701	BGC	O4-C4-C3	2.00	115.10	110.38

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	21-A	701	BGC	O5-C5-C6-O6
3	15-A	701	BGC	O5-C5-C6-O6
3	23-A	701	BGC	O5-C5-C6-O6
3	1-A	701	BGC	O5-C5-C6-O6
3	9-A	701	BGC	O5-C5-C6-O6
3	21-A	701	BGC	C4-C5-C6-O6
3	9-A	701	BGC	C4-C5-C6-O6
3	15-A	701	BGC	C4-C5-C6-O6
3	1-A	701	BGC	C4-C5-C6-O6
3	23-A	701	BGC	C4-C5-C6-O6
3	10-A	701	BGC	O5-C5-C6-O6
3	11-A	701	BGC	O5-C5-C6-O6
3	3-A	701	BGC	O5-C5-C6-O6
3	11-A	701	BGC	C4-C5-C6-O6
3	24-A	701	BGC	O5-C5-C6-O6
3	20-A	701	BGC	O5-C5-C6-O6
3	6-A	701	BGC	O5-C5-C6-O6
3	12-A	701	BGC	O5-C5-C6-O6
3	10-A	701	BGC	C4-C5-C6-O6
3	14-A	701	BGC	O5-C5-C6-O6
3	19-A	701	BGC	C4-C5-C6-O6
4	7-A	702	EDO	O1-C1-C2-O2
4	9-A	702	EDO	O1-C1-C2-O2
4	23-A	702	EDO	O1-C1-C2-O2
4	24-A	702	EDO	O1-C1-C2-O2
4	25-A	702	EDO	O1-C1-C2-O2
4	2-A	703	EDO	O1-C1-C2-O2
4	22-A	703	EDO	O1-C1-C2-O2
4	13-A	704	EDO	O1-C1-C2-O2
4	20-A	704	EDO	O1-C1-C2-O2
4	17-A	703	EDO	O1-C1-C2-O2
4	10-A	704	EDO	O1-C1-C2-O2
4	11-A	704	EDO	O1-C1-C2-O2
4	23-A	704	EDO	O1-C1-C2-O2
3	22-A	701	BGC	C4-C5-C6-O6
4	5-A	702	EDO	O1-C1-C2-O2
4	8-A	702	EDO	O1-C1-C2-O2
4	6-A	703	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	1-A	549/549 (100%)	0.96	72 (13%) 7 7	1, 1, 1, 1	549 (100%)
1	2-A	0/549	-	-	-	-
1	3-A	0/549	-	-	-	-
1	4-A	0/549	-	-	-	-
1	5-A	0/549	-	-	-	-
1	6-A	0/549	-	-	-	-
1	7-A	0/549	-	-	-	-
1	8-A	0/549	-	-	-	-
1	9-A	0/549	-	-	-	-
1	10-A	0/549	-	-	-	-
1	11-A	0/549	-	-	-	-
1	12-A	0/549	-	-	-	-
1	13-A	0/549	-	-	-	-
1	14-A	0/549	-	-	-	-
1	15-A	0/549	-	-	-	-
1	16-A	0/549	-	-	-	-
1	17-A	0/549	-	-	-	-
1	18-A	0/549	-	-	-	-
1	19-A	0/549	-	-	-	-
1	20-A	0/549	-	-	-	-
1	21-A	0/549	-	-	-	-
1	22-A	0/549	-	-	-	-
1	23-A	0/549	-	-	-	-
1	24-A	0/549	-	-	-	-
1	25-A	0/549	-	-	-	-
All	All	549/13725 (4%)	0.96	72 (13%) 7 7	1, 1, 1, 1	549 (100%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	296	THR	6.8
1	1-A	58	VAL	6.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	293	GLY	6.5
1	1-A	295	GLY	5.9
1	1-A	298	GLU	5.7
1	1-A	294	ASN	5.5
1	1-A	276	TYR	4.9
1	1-A	273	GLY	4.8
1	1-A	66	PRO	4.8
1	1-A	87	ARG	4.4
1	1-A	88	LYS	4.4
1	1-A	236	MET	4.3
1	1-A	545	ASN	3.9
1	1-A	297	PRO	3.9
1	1-A	312	PRO	3.9
1	1-A	57	GLU	3.9
1	1-A	455	GLY	3.7
1	1-A	505	TYR	3.7
1	1-A	274	ASP	3.6
1	1-A	306	GLN	3.5
1	1-A	80	GLY	3.5
1	1-A	63	ASP	3.4
1	1-A	194	TYR	3.4
1	1-A	126	LEU	3.4
1	1-A	302	LEU	3.3
1	1-A	324	ASP	3.3
1	1-A	214	TYR	3.3
1	1-A	586	ASP	3.3
1	1-A	471	ASN	3.2
1	1-A	277	LYS	3.2
1	1-A	326	GLY	3.2
1	1-A	144	PHE	3.2
1	1-A	272	ASP	3.1
1	1-A	517	ASP	3.1
1	1-A	127	ASN	3.1
1	1-A	76	PRO	3.1
1	1-A	75	THR	3.0
1	1-A	536	TRP	2.9
1	1-A	251	GLU	2.8
1	1-A	292	TRP	2.8
1	1-A	195	GLY	2.8
1	1-A	77	ASP	2.7
1	1-A	528	ASP	2.7
1	1-A	399	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	1-A	340	GLN	2.7
1	1-A	160	ALA	2.7
1	1-A	300	GLU	2.5
1	1-A	71	PHE	2.5
1	1-A	114	GLN	2.5
1	1-A	587	ILE	2.4
1	1-A	532	THR	2.4
1	1-A	145	ASP	2.4
1	1-A	146	GLY	2.4
1	1-A	529	SER	2.4
1	1-A	120	SER	2.4
1	1-A	313	GLY	2.3
1	1-A	102	MET	2.3
1	1-A	258	GLU	2.3
1	1-A	323	VAL	2.3
1	1-A	246	ALA	2.2
1	1-A	402	SER	2.2
1	1-A	305	ASP	2.2
1	1-A	107	THR	2.2
1	1-A	304	LEU	2.2
1	1-A	250	PRO	2.2
1	1-A	560	VAL	2.1
1	1-A	601	VAL	2.1
1	1-A	424	PRO	2.1
1	1-A	270	TYR	2.1
1	1-A	514	GLN	2.0
1	1-A	69	LEU	2.0
1	1-A	91	SER	2.0

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

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

5.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	1-B	1	12/12	0.69	0.18	18,21,31,34	12
2	BGC	2-B	1	12/12	-	-	18,21,31,34	12
2	BGC	3-B	1	12/12	-	-	18,21,31,34	12
2	BGC	4-B	1	12/12	-	-	18,21,31,34	12
2	BGC	5-B	1	12/12	-	-	18,21,31,34	12
2	BGC	6-B	1	12/12	-	-	18,21,31,34	12
2	BGC	7-B	1	12/12	-	-	18,21,31,34	12
2	BGC	8-B	1	12/12	-	-	18,21,31,34	12
2	BGC	9-B	1	12/12	-	-	18,21,31,34	12
2	BGC	10-B	1	12/12	-	-	18,21,31,34	12
2	BGC	11-B	1	12/12	-	-	18,21,31,34	12
2	BGC	12-B	1	12/12	-	-	18,21,31,34	12
2	BGC	13-B	1	12/12	-	-	18,21,31,34	12
2	BGC	14-B	1	12/12	-	-	18,21,31,34	12
2	BGC	15-B	1	12/12	-	-	18,21,31,34	12
2	BGC	16-B	1	12/12	-	-	18,21,31,34	12
2	BGC	17-B	1	12/12	-	-	18,21,31,34	12
2	BGC	18-B	1	12/12	-	-	18,21,31,34	12
2	BGC	19-B	1	12/12	-	-	18,21,31,34	12
2	BGC	20-B	1	12/12	-	-	18,21,31,34	12
2	BGC	21-B	1	12/12	-	-	18,21,31,34	12
2	BGC	22-B	1	12/12	-	-	18,21,31,34	12
2	BGC	23-B	1	12/12	-	-	18,21,31,34	12
2	BGC	24-B	1	12/12	-	-	18,21,31,34	12
2	BGC	25-B	1	12/12	-	-	18,21,31,34	12
2	BGC	1-B	2	11/12	0.84	0.12	16,20,21,23	11
2	BGC	2-B	2	11/12	-	-	16,20,21,23	11
2	BGC	3-B	2	11/12	-	-	16,20,21,23	11
2	BGC	4-B	2	11/12	-	-	16,20,21,23	11
2	BGC	5-B	2	11/12	-	-	16,20,21,23	11
2	BGC	6-B	2	11/12	-	-	16,20,21,23	11
2	BGC	7-B	2	11/12	-	-	16,20,21,23	11
2	BGC	8-B	2	11/12	-	-	16,20,21,23	11
2	BGC	9-B	2	11/12	-	-	16,20,21,23	11
2	BGC	10-B	2	11/12	-	-	16,20,21,23	11
2	BGC	11-B	2	11/12	-	-	16,20,21,23	11
2	BGC	12-B	2	11/12	-	-	16,20,21,23	11
2	BGC	13-B	2	11/12	-	-	16,20,21,23	11
2	BGC	14-B	2	11/12	-	-	16,20,21,23	11
2	BGC	15-B	2	11/12	-	-	16,20,21,23	11
2	BGC	16-B	2	11/12	-	-	16,20,21,23	11
2	BGC	17-B	2	11/12	-	-	16,20,21,23	11
2	BGC	18-B	2	11/12	-	-	16,20,21,23	11

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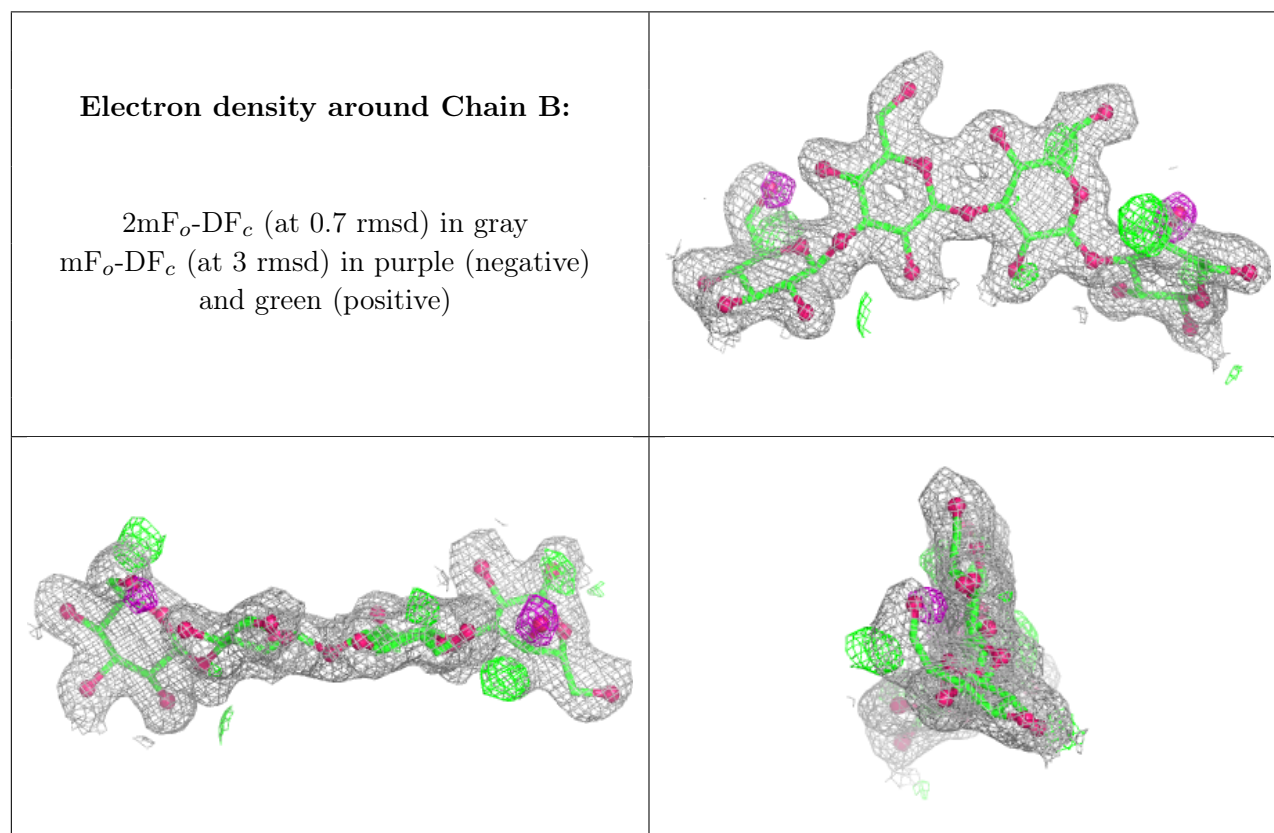
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	19-B	2	11/12	-	-	16,20,21,23	11
2	BGC	20-B	2	11/12	-	-	16,20,21,23	11
2	BGC	21-B	2	11/12	-	-	16,20,21,23	11
2	BGC	22-B	2	11/12	-	-	16,20,21,23	11
2	BGC	23-B	2	11/12	-	-	16,20,21,23	11
2	BGC	24-B	2	11/12	-	-	16,20,21,23	11
2	BGC	25-B	2	11/12	-	-	16,20,21,23	11
2	BGC	1-B	4	11/12	0.84	0.11	14,17,18,18	11
2	BGC	2-B	3	11/12	-	-	15,17,22,23	11
2	BGC	3-B	3	11/12	-	-	15,17,22,23	11
2	BGC	4-B	3	11/12	-	-	15,17,22,23	11
2	BGC	5-B	3	11/12	-	-	15,17,22,23	11
2	BGC	6-B	3	11/12	-	-	15,17,22,23	11
2	BGC	7-B	3	11/12	-	-	15,17,22,23	11
2	BGC	8-B	3	11/12	-	-	15,17,22,23	11
2	BGC	9-B	3	11/12	-	-	15,17,22,23	11
2	BGC	10-B	3	11/12	-	-	15,17,22,23	11
2	BGC	11-B	3	11/12	-	-	15,17,22,23	11
2	BGC	12-B	3	11/12	-	-	15,17,22,23	11
2	BGC	13-B	3	11/12	-	-	15,17,22,23	11
2	BGC	14-B	3	11/12	-	-	15,17,22,23	11
2	BGC	15-B	3	11/12	-	-	15,17,22,23	11
2	BGC	16-B	3	11/12	-	-	15,17,22,23	11
2	BGC	17-B	3	11/12	-	-	15,17,22,23	11
2	BGC	18-B	3	11/12	-	-	15,17,22,23	11
2	BGC	19-B	3	11/12	-	-	15,17,22,23	11
2	BGC	20-B	3	11/12	-	-	15,17,22,23	11
2	BGC	21-B	3	11/12	-	-	15,17,22,23	11
2	BGC	22-B	3	11/12	-	-	15,17,22,23	11
2	BGC	23-B	3	11/12	-	-	15,17,22,23	11
2	BGC	24-B	3	11/12	-	-	15,17,22,23	11
2	BGC	25-B	3	11/12	-	-	15,17,22,23	11
2	BGC	1-B	3	11/12	0.89	0.11	15,17,22,23	11
2	BGC	2-B	4	11/12	-	-	14,17,18,18	11
2	BGC	3-B	4	11/12	-	-	14,17,18,18	11
2	BGC	4-B	4	11/12	-	-	14,17,18,18	11
2	BGC	5-B	4	11/12	-	-	14,17,18,18	11
2	BGC	6-B	4	11/12	-	-	14,17,18,18	11
2	BGC	7-B	4	11/12	-	-	14,17,18,18	11
2	BGC	8-B	4	11/12	-	-	14,17,18,18	11
2	BGC	9-B	4	11/12	-	-	14,17,18,18	11
2	BGC	10-B	4	11/12	-	-	14,17,18,18	11

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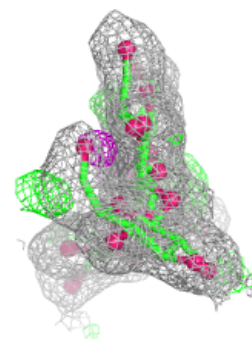
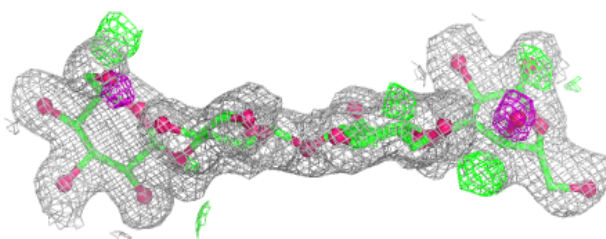
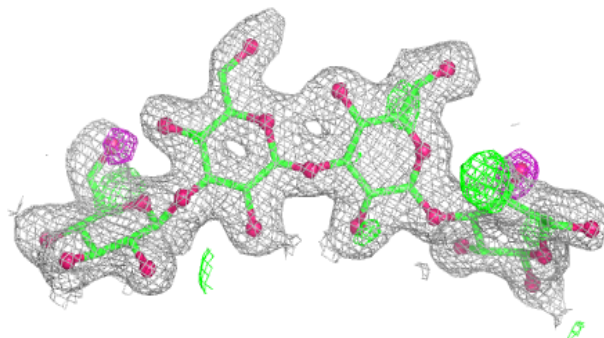
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	11-B	4	11/12	-	-	14,17,18,18	11
2	BGC	12-B	4	11/12	-	-	14,17,18,18	11
2	BGC	13-B	4	11/12	-	-	14,17,18,18	11
2	BGC	14-B	4	11/12	-	-	14,17,18,18	11
2	BGC	15-B	4	11/12	-	-	14,17,18,18	11
2	BGC	16-B	4	11/12	-	-	14,17,18,18	11
2	BGC	17-B	4	11/12	-	-	14,17,18,18	11
2	BGC	18-B	4	11/12	-	-	14,17,18,18	11
2	BGC	19-B	4	11/12	-	-	14,17,18,18	11
2	BGC	20-B	4	11/12	-	-	14,17,18,18	11
2	BGC	21-B	4	11/12	-	-	14,17,18,18	11
2	BGC	22-B	4	11/12	-	-	14,17,18,18	11
2	BGC	23-B	4	11/12	-	-	14,17,18,18	11
2	BGC	24-B	4	11/12	-	-	14,17,18,18	11
2	BGC	25-B	4	11/12	-	-	14,17,18,18	11

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.

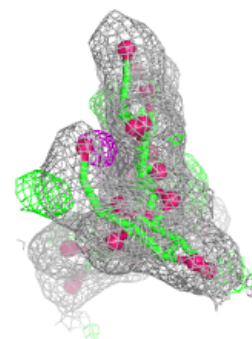
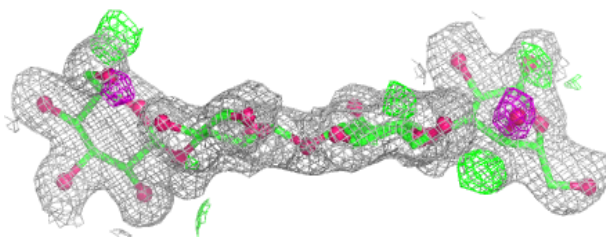
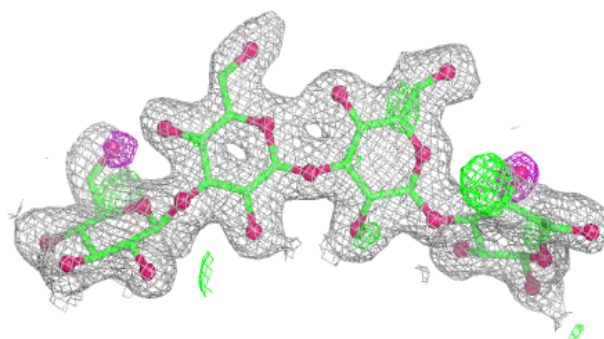


Electron density around Chain B:

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

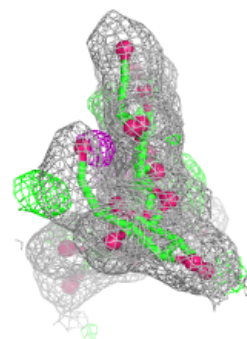
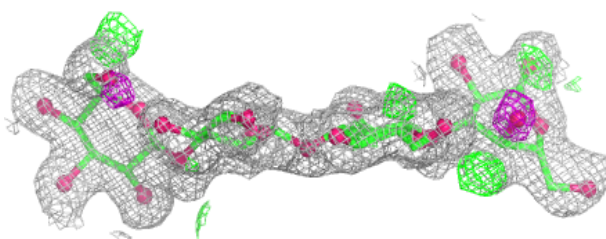
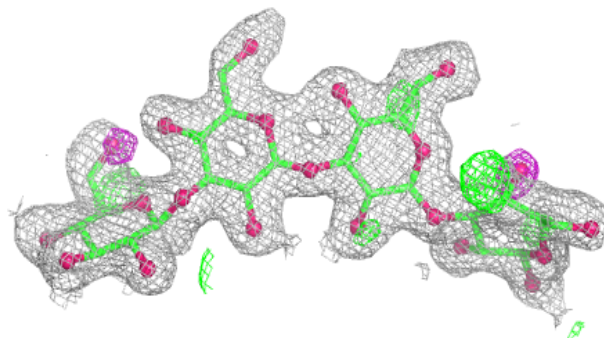
**Electron density around Chain B:**

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

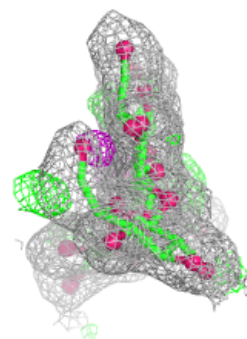
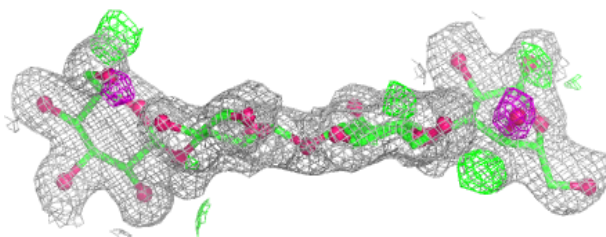
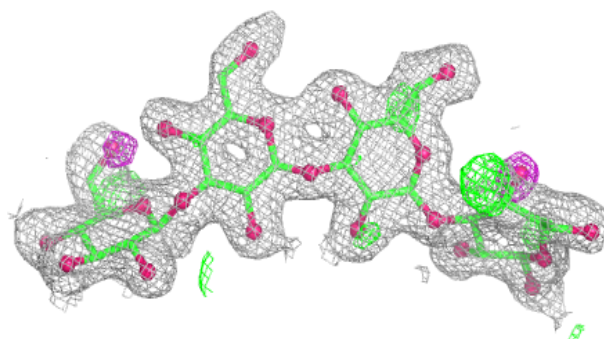


Electron density around Chain B:

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

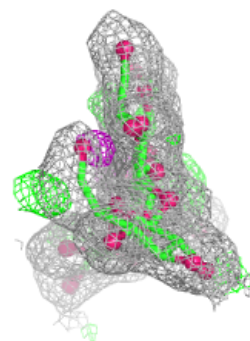
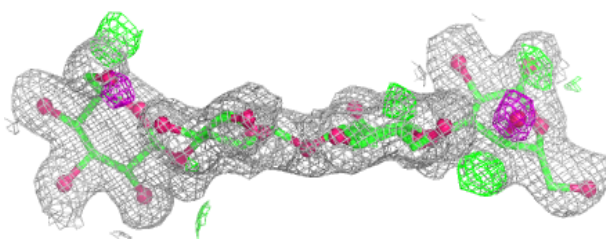
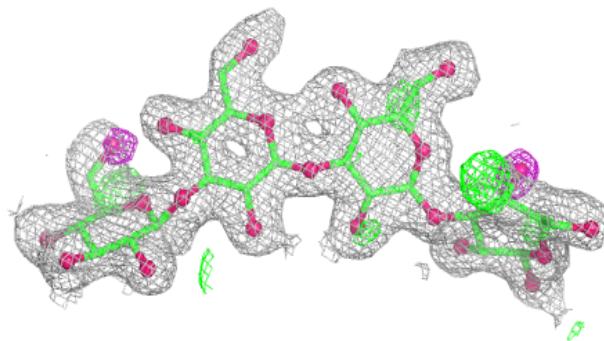
**Electron density around Chain B:**

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

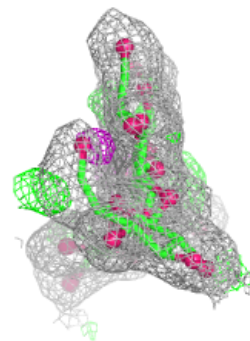
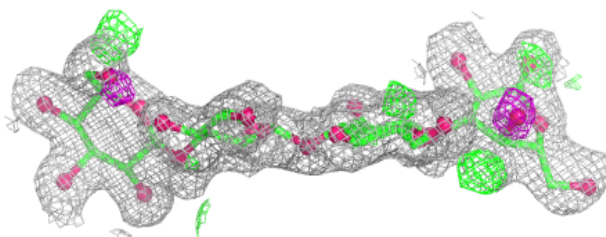
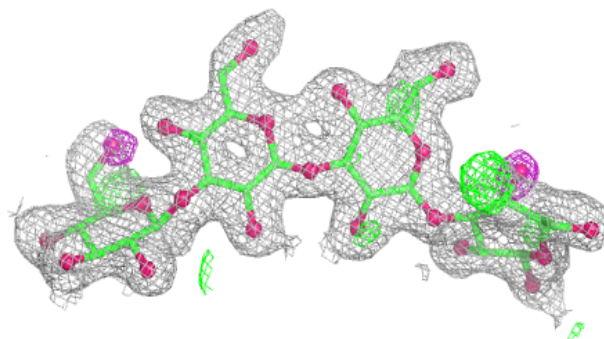


Electron density around Chain B:

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

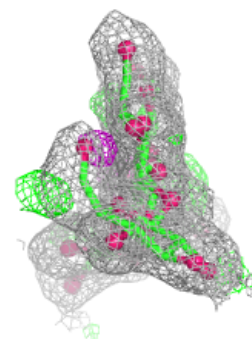
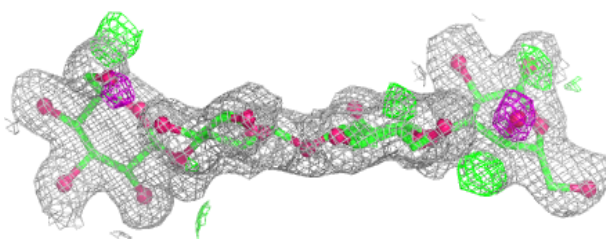
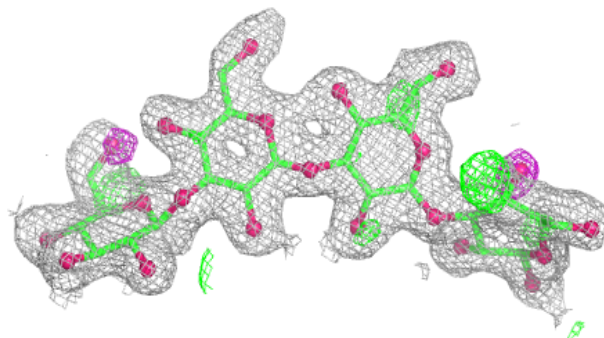
**Electron density around Chain B:**

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

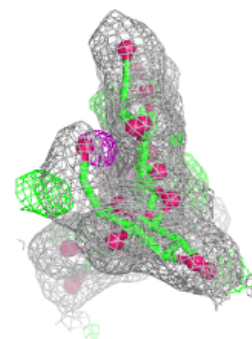
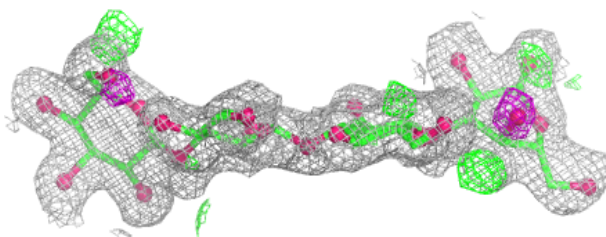
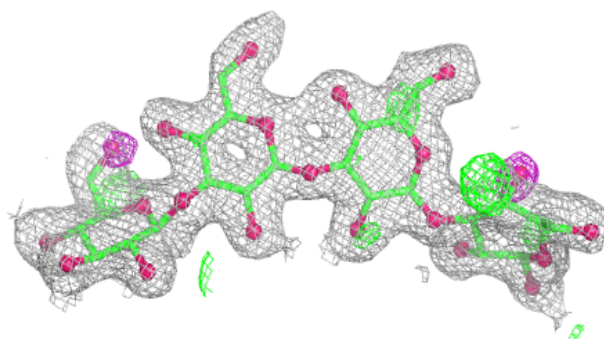


Electron density around Chain B:

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

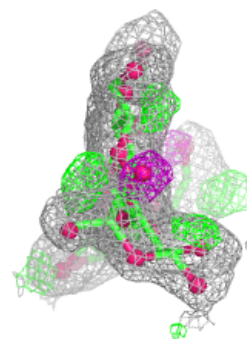
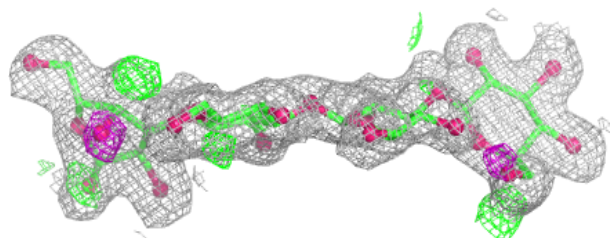
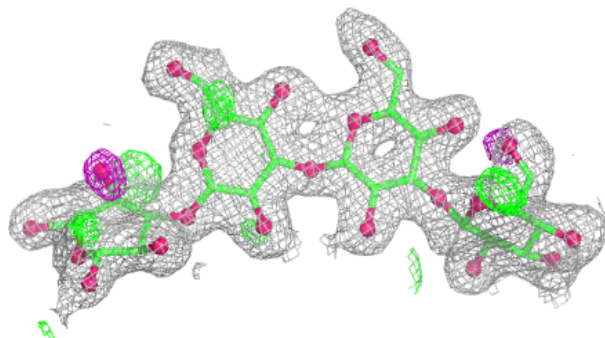
**Electron density around Chain B:**

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

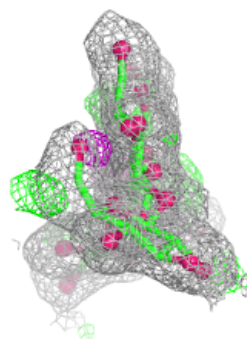
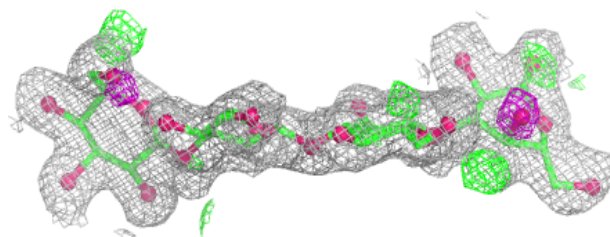
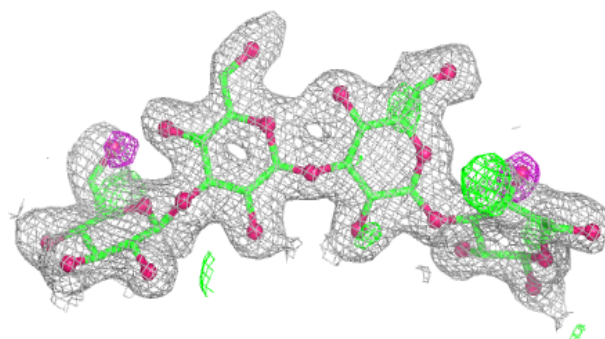


Electron density around Chain B:

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

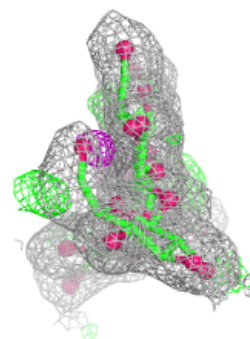
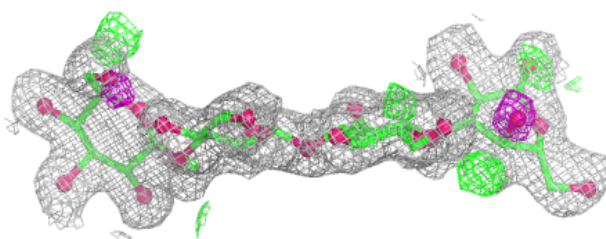
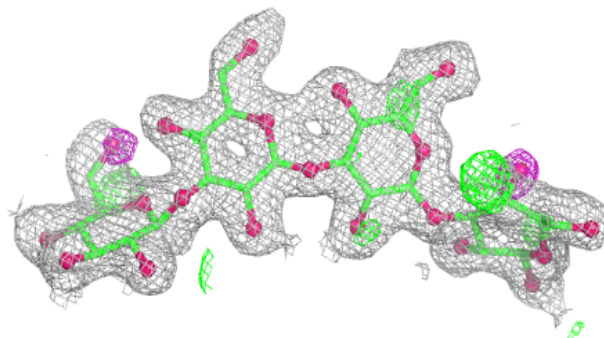
**Electron density around Chain B:**

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

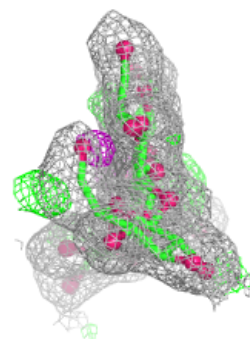
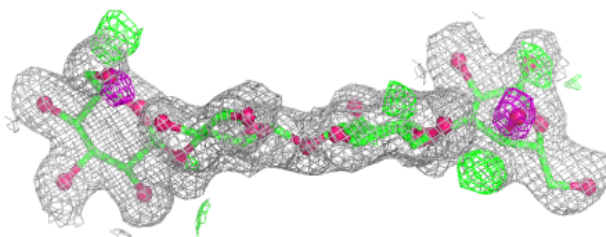
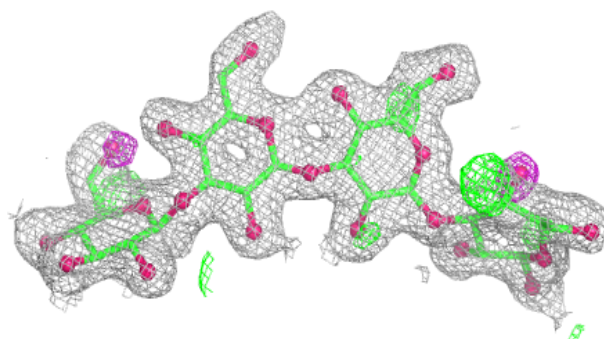


Electron density around Chain B:

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

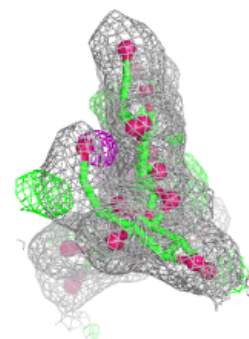
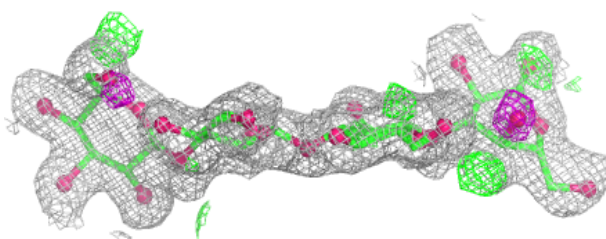
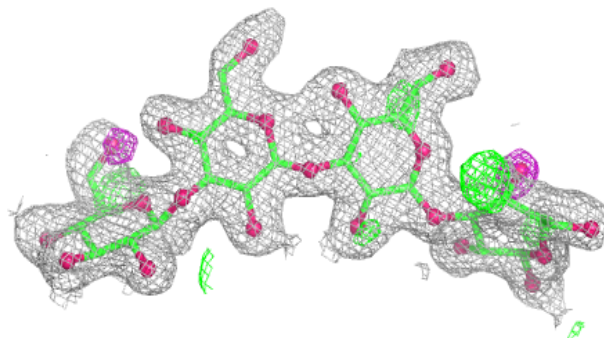
**Electron density around Chain B:**

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

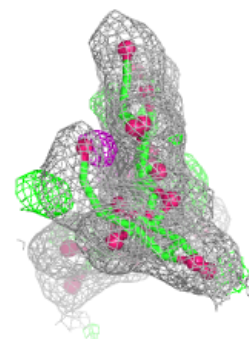
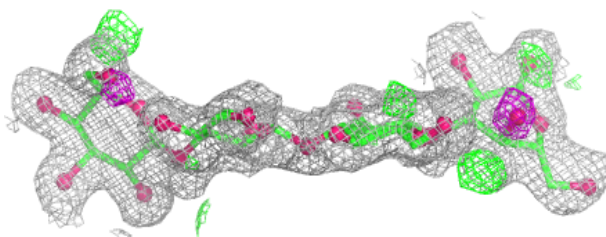
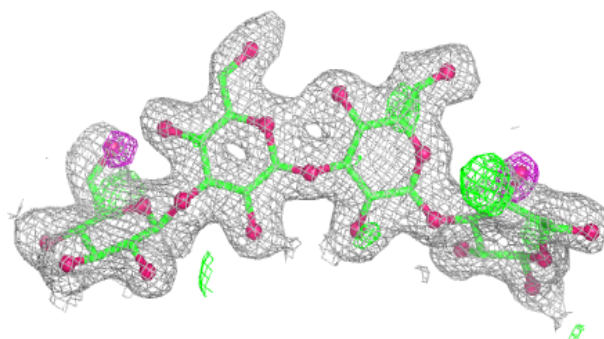


Electron density around Chain B:

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

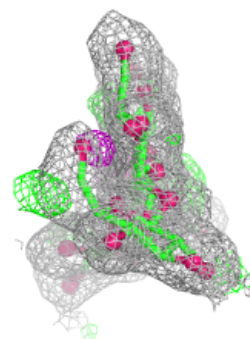
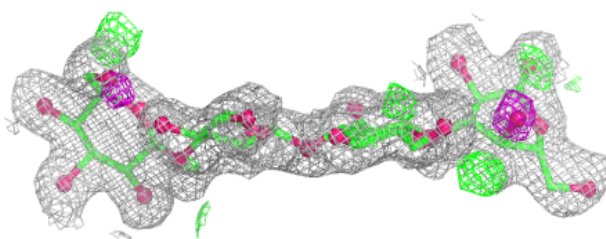
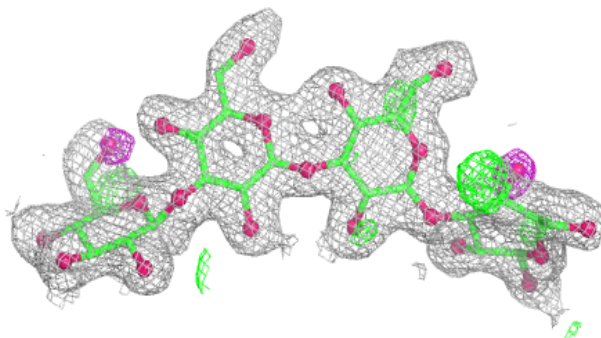
**Electron density around Chain B:**

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

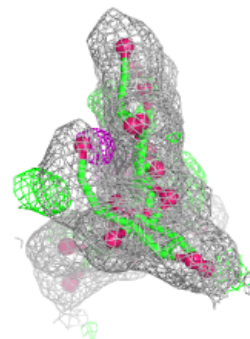
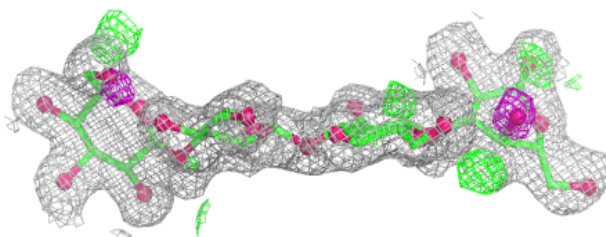
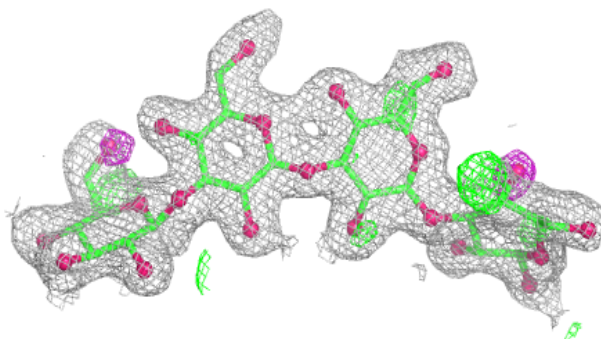


Electron density around Chain B:

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

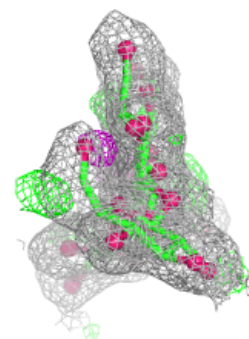
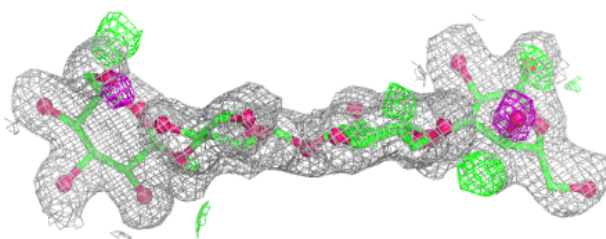
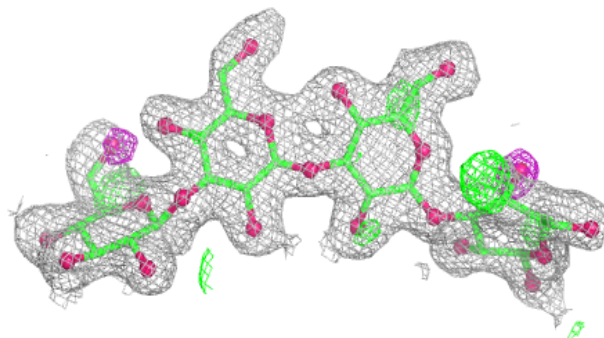
**Electron density around Chain B:**

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

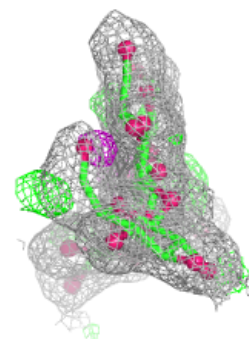
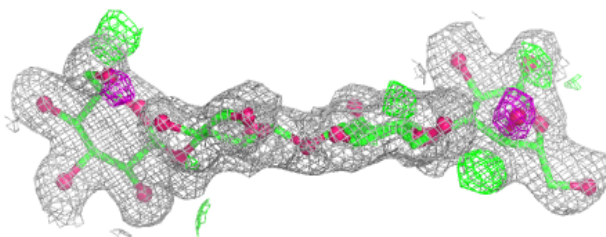
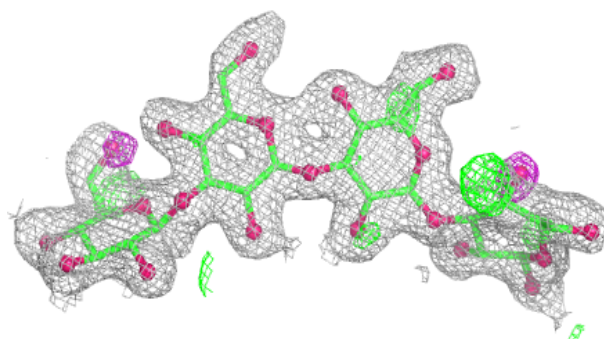


Electron density around Chain B:

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

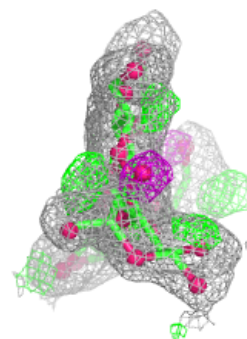
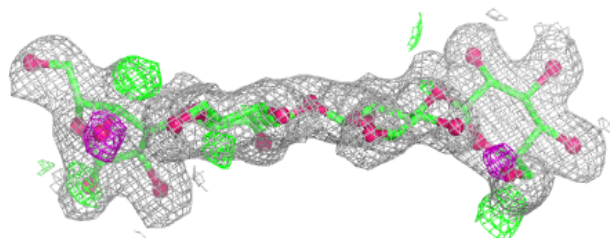
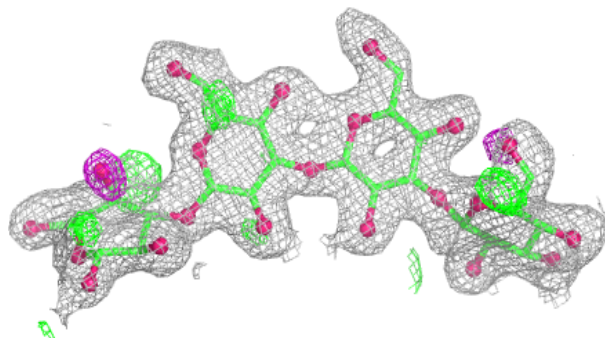
**Electron density around Chain B:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

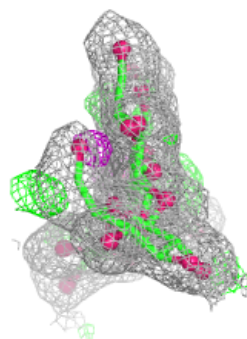
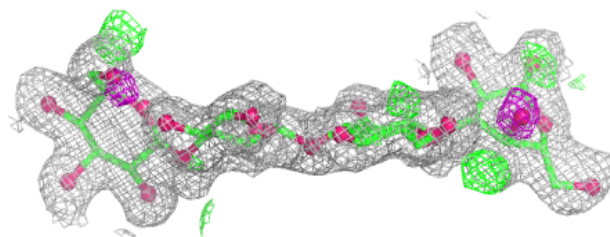
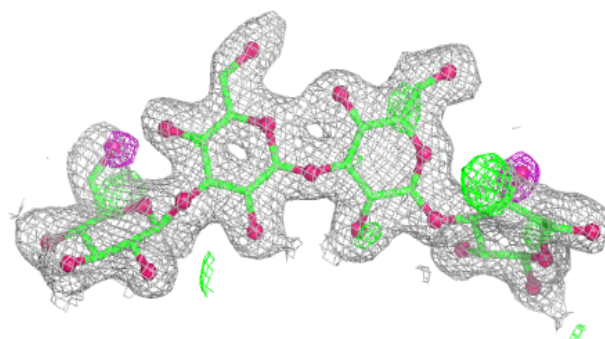


Electron density around Chain B:

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

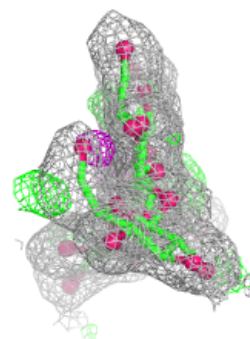
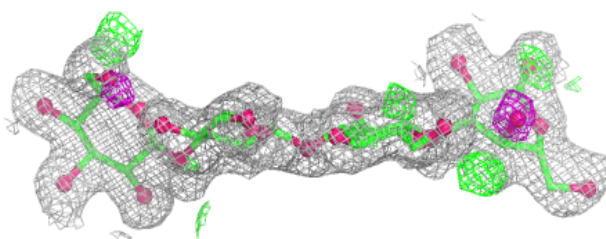
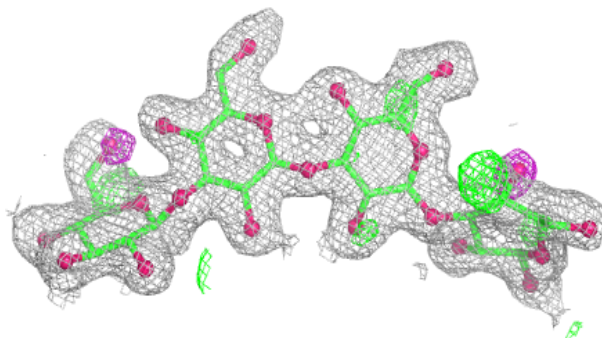
**Electron density around Chain B:**

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

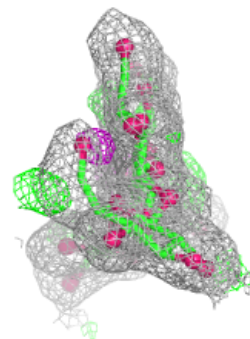
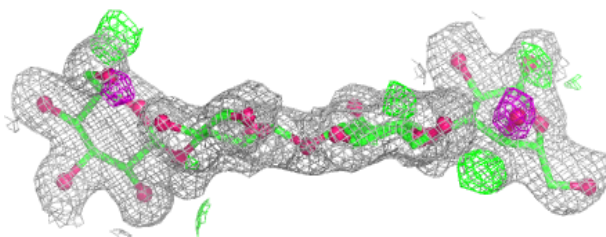
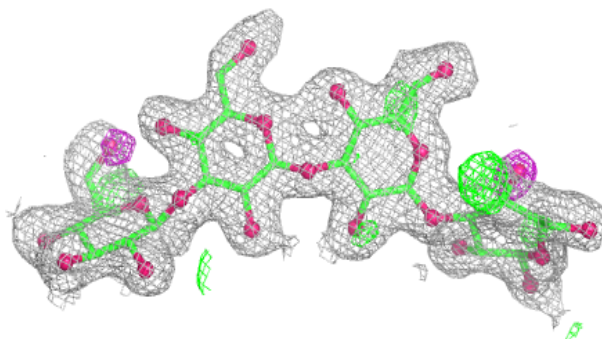


Electron density around Chain B:

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

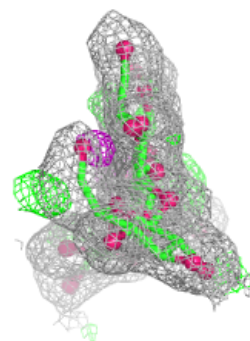
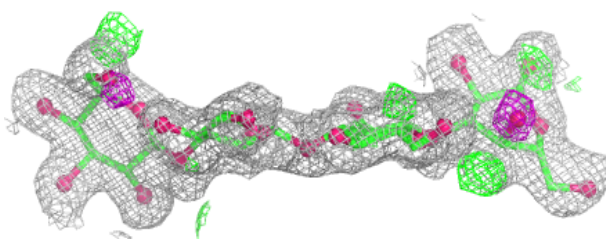
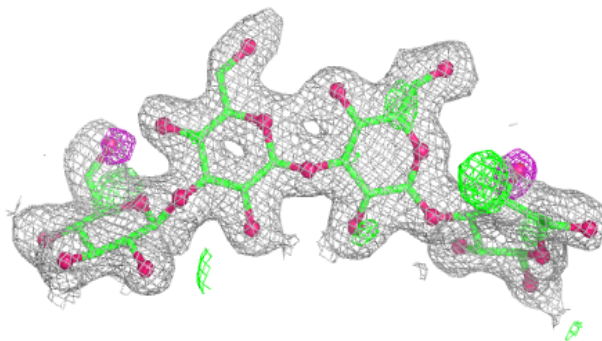
**Electron density around Chain B:**

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

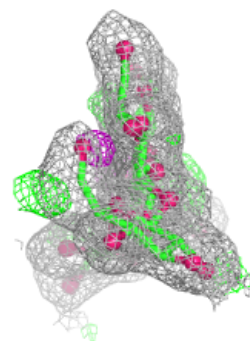
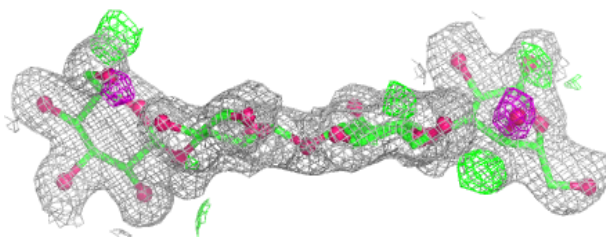
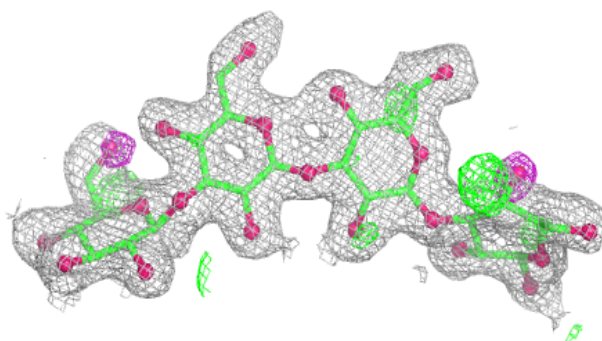


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**Electron density around Chain B:**

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



5.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	1-A	701	11/12	0.43	0.24	21,26,31,34	11
3	BGC	2-A	701	11/12	-	-	21,26,31,34	11
3	BGC	3-A	701	11/12	-	-	21,26,31,34	11
3	BGC	4-A	701	11/12	-	-	21,26,31,34	11
3	BGC	5-A	701	11/12	-	-	21,26,31,34	11
3	BGC	6-A	701	11/12	-	-	21,26,31,34	11
3	BGC	7-A	701	11/12	-	-	21,26,31,34	11
3	BGC	8-A	701	11/12	-	-	21,26,31,34	11
3	BGC	9-A	701	11/12	-	-	21,26,31,34	11
3	BGC	10-A	701	11/12	-	-	21,26,31,34	11
3	BGC	11-A	701	11/12	-	-	21,26,31,34	11
3	BGC	12-A	701	11/12	-	-	21,26,31,34	11
3	BGC	13-A	701	11/12	-	-	21,26,31,34	11
3	BGC	14-A	701	11/12	-	-	21,26,31,34	11
3	BGC	15-A	701	11/12	-	-	21,26,31,34	11
3	BGC	16-A	701	11/12	-	-	21,26,31,34	11
3	BGC	17-A	701	11/12	-	-	21,26,31,34	11
3	BGC	18-A	701	11/12	-	-	21,26,31,34	11
3	BGC	19-A	701	11/12	-	-	21,26,31,34	11
3	BGC	20-A	701	11/12	-	-	21,26,31,34	11
3	BGC	21-A	701	11/12	-	-	21,26,31,34	11
3	BGC	22-A	701	11/12	-	-	21,26,31,34	11
3	BGC	23-A	701	11/12	-	-	21,26,31,34	11
3	BGC	24-A	701	11/12	-	-	21,26,31,34	11
3	BGC	25-A	701	11/12	-	-	21,26,31,34	11
4	EDO	1-A	704	4/4	0.58	0.22	30,32,35,35	10
4	EDO	2-A	702	4/4	-	-	15,17,21,21	10
4	EDO	3-A	702	4/4	-	-	15,17,21,21	10
4	EDO	4-A	702	4/4	-	-	15,17,21,21	10
4	EDO	5-A	702	4/4	-	-	15,17,21,21	10
4	EDO	6-A	702	4/4	-	-	15,17,21,21	10
4	EDO	7-A	702	4/4	-	-	15,17,21,21	10
4	EDO	8-A	702	4/4	-	-	15,17,21,21	10
4	EDO	9-A	702	4/4	-	-	15,17,21,21	10
4	EDO	10-A	702	4/4	-	-	15,17,21,21	10
4	EDO	11-A	702	4/4	-	-	15,17,21,21	10
4	EDO	12-A	702	4/4	-	-	15,17,21,21	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	13-A	702	4/4	-	-	15,17,21,21	10
4	EDO	14-A	702	4/4	-	-	15,17,21,21	10
4	EDO	15-A	702	4/4	-	-	15,17,21,21	10
4	EDO	16-A	702	4/4	-	-	15,17,21,21	10
4	EDO	17-A	702	4/4	-	-	15,17,21,21	10
4	EDO	18-A	702	4/4	-	-	15,17,21,21	10
4	EDO	19-A	702	4/4	-	-	15,17,21,21	10
4	EDO	20-A	702	4/4	-	-	15,17,21,21	10
4	EDO	21-A	702	4/4	-	-	15,17,21,21	10
4	EDO	22-A	702	4/4	-	-	15,17,21,21	10
4	EDO	23-A	702	4/4	-	-	15,17,21,21	10
4	EDO	24-A	702	4/4	-	-	15,17,21,21	10
4	EDO	25-A	702	4/4	-	-	15,17,21,21	10
4	EDO	1-A	703	4/4	0.86	0.11	17,17,22,22	10
4	EDO	2-A	703	4/4	-	-	17,17,22,22	10
4	EDO	3-A	703	4/4	-	-	17,17,22,22	10
4	EDO	4-A	703	4/4	-	-	17,17,22,22	10
4	EDO	5-A	703	4/4	-	-	17,17,22,22	10
4	EDO	6-A	703	4/4	-	-	17,17,22,22	10
4	EDO	7-A	703	4/4	-	-	17,17,22,22	10
4	EDO	8-A	703	4/4	-	-	17,17,22,22	10
4	EDO	9-A	703	4/4	-	-	17,17,22,22	10
4	EDO	10-A	703	4/4	-	-	17,17,22,22	10
4	EDO	11-A	703	4/4	-	-	17,17,22,22	10
4	EDO	12-A	703	4/4	-	-	17,17,22,22	10
4	EDO	13-A	703	4/4	-	-	17,17,22,22	10
4	EDO	14-A	703	4/4	-	-	17,17,22,22	10
4	EDO	15-A	703	4/4	-	-	17,17,22,22	10
4	EDO	16-A	703	4/4	-	-	17,17,22,22	10
4	EDO	17-A	703	4/4	-	-	17,17,22,22	10
4	EDO	18-A	703	4/4	-	-	17,17,22,22	10
4	EDO	19-A	703	4/4	-	-	17,17,22,22	10
4	EDO	20-A	703	4/4	-	-	17,17,22,22	10
4	EDO	21-A	703	4/4	-	-	17,17,22,22	10
4	EDO	22-A	703	4/4	-	-	17,17,22,22	10
4	EDO	23-A	703	4/4	-	-	17,17,22,22	10
4	EDO	24-A	703	4/4	-	-	17,17,22,22	10
4	EDO	25-A	703	4/4	-	-	17,17,22,22	10
4	EDO	1-A	702	4/4	0.89	0.10	15,17,21,21	10
4	EDO	2-A	704	4/4	-	-	30,32,35,35	10
4	EDO	3-A	704	4/4	-	-	30,32,35,35	10
4	EDO	4-A	704	4/4	-	-	30,32,35,35	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	5-A	704	4/4	-	-	30,32,35,35	10
4	EDO	6-A	704	4/4	-	-	30,32,35,35	10
4	EDO	7-A	704	4/4	-	-	30,32,35,35	10
4	EDO	8-A	704	4/4	-	-	30,32,35,35	10
4	EDO	9-A	704	4/4	-	-	30,32,35,35	10
4	EDO	10-A	704	4/4	-	-	30,32,35,35	10
4	EDO	11-A	704	4/4	-	-	30,32,35,35	10
4	EDO	12-A	704	4/4	-	-	30,32,35,35	10
4	EDO	13-A	704	4/4	-	-	30,32,35,35	10
4	EDO	14-A	704	4/4	-	-	30,32,35,35	10
4	EDO	15-A	704	4/4	-	-	30,32,35,35	10
4	EDO	16-A	704	4/4	-	-	30,32,35,35	10
4	EDO	17-A	704	4/4	-	-	30,32,35,35	10
4	EDO	18-A	704	4/4	-	-	30,32,35,35	10
4	EDO	19-A	704	4/4	-	-	30,32,35,35	10
4	EDO	20-A	704	4/4	-	-	30,32,35,35	10
4	EDO	21-A	704	4/4	-	-	30,32,35,35	10
4	EDO	22-A	704	4/4	-	-	30,32,35,35	10
4	EDO	23-A	704	4/4	-	-	30,32,35,35	10
4	EDO	24-A	704	4/4	-	-	30,32,35,35	10
4	EDO	25-A	704	4/4	-	-	30,32,35,35	10

5.5 Other polymers

There are no such residues in this entry.