



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 01:20 PM UTC

PDB ID : 4TZ5 / pdb_00004tz5
Title : Ensemble refinement of the E502A variant of sacteLam55A from Streptomyces sp. SirexAA-E in complex with laminarihexaose
Authors : Bianchetti, C.M.; Takasuka, T.E.; Yik, E.J.; Bergeman, L.F.; Fox, B.G.
Deposited on : 2014-07-09
Resolution : 1.75 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

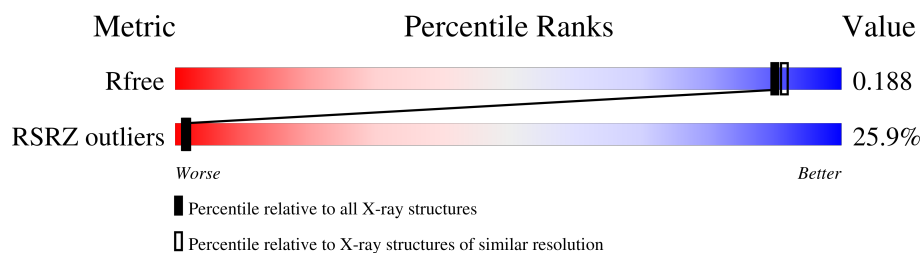
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 427968 atoms, of which 195500 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 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	18-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	19-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	20-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	21-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	22-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	23-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	24-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	25-A	549	Total 8074	C 2629	H 3907	N 708	O 825	S 5	0	0	0
1	1-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	2-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	3-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	4-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	5-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	6-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	7-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	8-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	9-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	10-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	11-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	12-B	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	13-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	14-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	15-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	16-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	17-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	18-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	19-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	20-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	21-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	22-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	23-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	24-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	25-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	ALA	GLU	engineered mutation	UNP G2NFJ9
B	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-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	1-C	6	Total 67	C 36	O 31	0	0	0
2	2-C	6	Total 67	C 36	O 31	0	0	0
2	3-C	6	Total 67	C 36	O 31	0	0	0
2	4-C	6	Total 67	C 36	O 31	0	0	0
2	5-C	6	Total 67	C 36	O 31	0	0	0
2	6-C	6	Total 67	C 36	O 31	0	0	0
2	7-C	6	Total 67	C 36	O 31	0	0	0
2	8-C	6	Total 67	C 36	O 31	0	0	0
2	9-C	6	Total 67	C 36	O 31	0	0	0
2	10-C	6	Total 67	C 36	O 31	0	0	0
2	11-C	6	Total 67	C 36	O 31	0	0	0
2	12-C	6	Total 67	C 36	O 31	0	0	0
2	13-C	6	Total 67	C 36	O 31	0	0	0
2	14-C	6	Total 67	C 36	O 31	0	0	0
2	15-C	6	Total 67	C 36	O 31	0	0	0
2	16-C	6	Total 67	C 36	O 31	0	0	0
2	17-C	6	Total 67	C 36	O 31	0	0	0
2	18-C	6	Total 67	C 36	O 31	0	0	0
2	19-C	6	Total 67	C 36	O 31	0	0	0
2	20-C	6	Total 67	C 36	O 31	0	0	0
2	21-C	6	Total 67	C 36	O 31	0	0	0
2	22-C	6	Total 67	C 36	O 31	0	0	0

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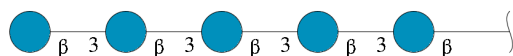
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	23-C	6	Total	C	O	0	0	0
			67	36	31			
2	24-C	6	Total	C	O	0	0	0
			67	36	31			
2	25-C	6	Total	C	O	0	0	0
			67	36	31			
2	1-E	6	Total	C	O	0	0	0
			67	36	31			
2	2-E	6	Total	C	O	0	0	0
			67	36	31			
2	3-E	6	Total	C	O	0	0	0
			67	36	31			
2	4-E	6	Total	C	O	0	0	0
			67	36	31			
2	5-E	6	Total	C	O	0	0	0
			67	36	31			
2	6-E	6	Total	C	O	0	0	0
			67	36	31			
2	7-E	6	Total	C	O	0	0	0
			67	36	31			
2	8-E	6	Total	C	O	0	0	0
			67	36	31			
2	9-E	6	Total	C	O	0	0	0
			67	36	31			
2	10-E	6	Total	C	O	0	0	0
			67	36	31			
2	11-E	6	Total	C	O	0	0	0
			67	36	31			
2	12-E	6	Total	C	O	0	0	0
			67	36	31			
2	13-E	6	Total	C	O	0	0	0
			67	36	31			
2	14-E	6	Total	C	O	0	0	0
			67	36	31			
2	15-E	6	Total	C	O	0	0	0
			67	36	31			
2	16-E	6	Total	C	O	0	0	0
			67	36	31			
2	17-E	6	Total	C	O	0	0	0
			67	36	31			
2	18-E	6	Total	C	O	0	0	0
			67	36	31			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	19-E	6	Total	C	O	0	0	0
			67	36	31			
2	20-E	6	Total	C	O	0	0	0
			67	36	31			
2	21-E	6	Total	C	O	0	0	0
			67	36	31			
2	22-E	6	Total	C	O	0	0	0
			67	36	31			
2	23-E	6	Total	C	O	0	0	0
			67	36	31			
2	24-E	6	Total	C	O	0	0	0
			67	36	31			
2	25-E	6	Total	C	O	0	0	0
			67	36	31			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-3)-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
3	1-D	5	Total	C	O	0	0	0
			56	30	26			
3	2-D	5	Total	C	O	0	0	0
			56	30	26			
3	3-D	5	Total	C	O	0	0	0
			56	30	26			
3	4-D	5	Total	C	O	0	0	0
			56	30	26			
3	5-D	5	Total	C	O	0	0	0
			56	30	26			
3	6-D	5	Total	C	O	0	0	0
			56	30	26			
3	7-D	5	Total	C	O	0	0	0
			56	30	26			
3	8-D	5	Total	C	O	0	0	0
			56	30	26			
3	9-D	5	Total	C	O	0	0	0
			56	30	26			
3	10-D	5	Total	C	O	0	0	0
			56	30	26			

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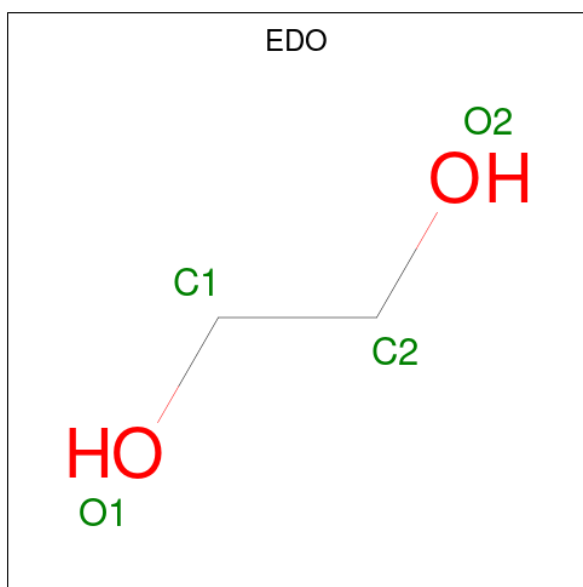
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	11-D	5	Total	C	O	0	0	0
			56	30	26			
3	12-D	5	Total	C	O	0	0	0
			56	30	26			
3	13-D	5	Total	C	O	0	0	0
			56	30	26			
3	14-D	5	Total	C	O	0	0	0
			56	30	26			
3	15-D	5	Total	C	O	0	0	0
			56	30	26			
3	16-D	5	Total	C	O	0	0	0
			56	30	26			
3	17-D	5	Total	C	O	0	0	0
			56	30	26			
3	18-D	5	Total	C	O	0	0	0
			56	30	26			
3	19-D	5	Total	C	O	0	0	0
			56	30	26			
3	20-D	5	Total	C	O	0	0	0
			56	30	26			
3	21-D	5	Total	C	O	0	0	0
			56	30	26			
3	22-D	5	Total	C	O	0	0	0
			56	30	26			
3	23-D	5	Total	C	O	0	0	0
			56	30	26			
3	24-D	5	Total	C	O	0	0	0
			56	30	26			
3	25-D	5	Total	C	O	0	0	0
			56	30	26			
3	1-F	5	Total	C	O	0	0	0
			56	30	26			
3	2-F	5	Total	C	O	0	0	0
			56	30	26			
3	3-F	5	Total	C	O	0	0	0
			56	30	26			
3	4-F	5	Total	C	O	0	0	0
			56	30	26			
3	5-F	5	Total	C	O	0	0	0
			56	30	26			
3	6-F	5	Total	C	O	0	0	0
			56	30	26			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	7-F	5	Total	C	O	0	0	0
			56	30	26			
3	8-F	5	Total	C	O	0	0	0
			56	30	26			
3	9-F	5	Total	C	O	0	0	0
			56	30	26			
3	10-F	5	Total	C	O	0	0	0
			56	30	26			
3	11-F	5	Total	C	O	0	0	0
			56	30	26			
3	12-F	5	Total	C	O	0	0	0
			56	30	26			
3	13-F	5	Total	C	O	0	0	0
			56	30	26			
3	14-F	5	Total	C	O	0	0	0
			56	30	26			
3	15-F	5	Total	C	O	0	0	0
			56	30	26			
3	16-F	5	Total	C	O	0	0	0
			56	30	26			
3	17-F	5	Total	C	O	0	0	0
			56	30	26			
3	18-F	5	Total	C	O	0	0	0
			56	30	26			
3	19-F	5	Total	C	O	0	0	0
			56	30	26			
3	20-F	5	Total	C	O	0	0	0
			56	30	26			
3	21-F	5	Total	C	O	0	0	0
			56	30	26			
3	22-F	5	Total	C	O	0	0	0
			56	30	26			
3	23-F	5	Total	C	O	0	0	0
			56	30	26			
3	24-F	5	Total	C	O	0	0	0
			56	30	26			
3	25-F	5	Total	C	O	0	0	0
			56	30	26			

- 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		

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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		
4	1-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	2-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	3-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	4-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	5-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	6-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	7-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	8-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	9-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	10-B	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	11-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	12-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	13-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	14-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	15-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	16-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	17-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	18-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	19-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	20-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	21-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	22-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	23-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	24-B	1	Total	C	H	O	0	0
			10	2	6	2		
4	25-B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	355	Total	O	0	0
			355	355		
5	2-A	362	Total	O	0	0
			362	362		
5	3-A	360	Total	O	0	0
			360	360		
5	4-A	370	Total	O	0	0
			370	370		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	5-A	364	Total 364	O 364	0	0
5	6-A	356	Total 356	O 356	0	0
5	7-A	325	Total 325	O 325	0	0
5	8-A	356	Total 356	O 356	0	0
5	9-A	327	Total 327	O 327	0	0
5	10-A	365	Total 365	O 365	0	0
5	11-A	361	Total 361	O 361	0	0
5	12-A	360	Total 360	O 360	0	0
5	13-A	335	Total 335	O 335	0	0
5	14-A	359	Total 359	O 359	0	0
5	15-A	348	Total 348	O 348	0	0
5	16-A	369	Total 369	O 369	0	0
5	17-A	351	Total 351	O 351	0	0
5	18-A	349	Total 349	O 349	0	0
5	19-A	346	Total 346	O 346	0	0
5	20-A	324	Total 324	O 324	0	0
5	21-A	347	Total 347	O 347	0	0
5	22-A	338	Total 338	O 338	0	0
5	23-A	366	Total 366	O 366	0	0
5	24-A	364	Total 364	O 364	0	0
5	25-A	359	Total 359	O 359	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-B	381	Total 381	O 381	0	0
5	2-B	369	Total 369	O 369	0	0
5	3-B	348	Total 348	O 348	0	0
5	4-B	377	Total 377	O 377	0	0
5	5-B	350	Total 350	O 350	0	0
5	6-B	364	Total 364	O 364	0	0
5	7-B	377	Total 377	O 377	0	0
5	8-B	372	Total 372	O 372	0	0
5	9-B	353	Total 353	O 353	0	0
5	10-B	367	Total 367	O 367	0	0
5	11-B	357	Total 357	O 357	0	0
5	12-B	379	Total 379	O 379	0	0
5	13-B	360	Total 360	O 360	0	0
5	14-B	392	Total 392	O 392	0	0
5	15-B	373	Total 373	O 373	0	0
5	16-B	361	Total 361	O 361	0	0
5	17-B	377	Total 377	O 377	0	0
5	18-B	373	Total 373	O 373	0	0
5	19-B	355	Total 355	O 355	0	0
5	20-B	372	Total 372	O 372	0	0
5	21-B	370	Total 370	O 370	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	22-B	386	Total 386	O 386	0	0
5	23-B	332	Total 332	O 332	0	0
5	24-B	360	Total 360	O 360	0	0
5	25-B	372	Total 372	O 372	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.10Å 100.96Å 104.18Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	30.30 – 1.75 30.30 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.30-1.75) 93.6 (30.30-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.9_1692)	Depositor
R, R_{free}	0.122 , 0.163 0.148 , 0.188	Depositor DCC
R_{free} test set	5640 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	427968	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0959e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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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](#)

550 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-C	1	2	12,12,12	1.56	3 (25%)	17,17,17	1.35	2 (11%)
2	BGC	1-C	2	2	11,11,12	1.36	3 (27%)	15,15,17	1.31	2 (13%)
2	BGC	1-C	3	2	11,11,12	1.46	3 (27%)	15,15,17	1.13	0
2	BGC	1-C	4	2	11,11,12	0.95	1 (9%)	15,15,17	1.49	2 (13%)
2	BGC	1-C	5	2	11,11,12	1.11	1 (9%)	15,15,17	1.31	2 (13%)
2	BGC	1-C	6	2	11,11,12	1.31	1 (9%)	15,15,17	1.31	3 (20%)
3	BGC	1-D	1	3	12,12,12	1.28	1 (8%)	17,17,17	1.07	0
3	BGC	1-D	2	3	11,11,12	1.43	1 (9%)	15,15,17	1.35	1 (6%)
3	BGC	1-D	3	3	11,11,12	1.24	1 (9%)	15,15,17	1.44	2 (13%)
3	BGC	1-D	4	3	11,11,12	1.29	1 (9%)	15,15,17	1.16	1 (6%)
3	BGC	1-D	5	3	11,11,12	1.50	1 (9%)	15,15,17	1.02	1 (6%)
2	BGC	1-E	1	2	12,12,12	1.54	3 (25%)	17,17,17	1.07	0
2	BGC	1-E	2	2	11,11,12	1.44	3 (27%)	15,15,17	1.16	1 (6%)
2	BGC	1-E	3	2	11,11,12	1.33	1 (9%)	15,15,17	1.13	2 (13%)
2	BGC	1-E	4	2	11,11,12	0.81	1 (9%)	15,15,17	1.28	2 (13%)
2	BGC	1-E	5	2	11,11,12	1.24	2 (18%)	15,15,17	1.82	2 (13%)
2	BGC	1-E	6	2	11,11,12	1.38	2 (18%)	15,15,17	1.01	1 (6%)
3	BGC	1-F	1	3	12,12,12	1.30	2 (16%)	17,17,17	0.99	1 (5%)
3	BGC	1-F	2	3	11,11,12	1.52	1 (9%)	15,15,17	1.48	2 (13%)
3	BGC	1-F	3	3	11,11,12	1.30	1 (9%)	15,15,17	2.84	3 (20%)
3	BGC	1-F	4	3	11,11,12	1.17	2 (18%)	15,15,17	0.89	0
3	BGC	1-F	5	3	11,11,12	1.69	1 (9%)	15,15,17	0.77	0
2	BGC	10-C	1	2	12,12,12	1.62	3 (25%)	17,17,17	1.07	1 (5%)
2	BGC	10-C	2	2	11,11,12	1.33	3 (27%)	15,15,17	1.35	2 (13%)
2	BGC	10-C	3	2	11,11,12	1.32	3 (27%)	15,15,17	1.14	1 (6%)
2	BGC	10-C	4	2	11,11,12	0.85	0	15,15,17	1.04	1 (6%)
2	BGC	10-C	5	2	11,11,12	1.20	1 (9%)	15,15,17	1.41	2 (13%)
2	BGC	10-C	6	2	11,11,12	1.32	2 (18%)	15,15,17	1.00	0
3	BGC	10-D	1	3	12,12,12	1.29	1 (8%)	17,17,17	1.20	0
3	BGC	10-D	2	3	11,11,12	1.41	1 (9%)	15,15,17	1.47	2 (13%)
3	BGC	10-D	3	3	11,11,12	1.26	1 (9%)	15,15,17	1.43	2 (13%)
3	BGC	10-D	4	3	11,11,12	1.18	2 (18%)	15,15,17	1.11	0
3	BGC	10-D	5	3	11,11,12	1.55	1 (9%)	15,15,17	1.29	2 (13%)
2	BGC	10-E	1	2	12,12,12	1.65	3 (25%)	17,17,17	1.01	1 (5%)
2	BGC	10-E	2	2	11,11,12	1.52	3 (27%)	15,15,17	1.06	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	10-E	3	2	11,11,12	1.34	2 (18%)	15,15,17	1.01	0
2	BGC	10-E	4	2	11,11,12	0.79	1 (9%)	15,15,17	1.28	2 (13%)
2	BGC	10-E	5	2	11,11,12	1.32	3 (27%)	15,15,17	1.26	2 (13%)
2	BGC	10-E	6	2	11,11,12	1.42	2 (18%)	15,15,17	2.02	4 (26%)
3	BGC	10-F	1	3	12,12,12	1.32	1 (8%)	17,17,17	1.01	0
3	BGC	10-F	2	3	11,11,12	1.54	2 (18%)	15,15,17	1.28	2 (13%)
3	BGC	10-F	3	3	11,11,12	1.06	1 (9%)	15,15,17	1.43	3 (20%)
3	BGC	10-F	4	3	11,11,12	1.38	2 (18%)	15,15,17	1.03	1 (6%)
3	BGC	10-F	5	3	11,11,12	1.58	1 (9%)	15,15,17	0.82	0
2	BGC	11-C	1	2	12,12,12	1.64	3 (25%)	17,17,17	1.03	1 (5%)
2	BGC	11-C	2	2	11,11,12	1.44	3 (27%)	15,15,17	1.62	2 (13%)
2	BGC	11-C	3	2	11,11,12	1.29	3 (27%)	15,15,17	1.07	2 (13%)
2	BGC	11-C	4	2	11,11,12	0.97	0	15,15,17	1.17	1 (6%)
2	BGC	11-C	5	2	11,11,12	1.23	1 (9%)	15,15,17	1.40	1 (6%)
2	BGC	11-C	6	2	11,11,12	1.33	2 (18%)	15,15,17	1.44	4 (26%)
3	BGC	11-D	1	3	12,12,12	1.28	1 (8%)	17,17,17	1.38	2 (11%)
3	BGC	11-D	2	3	11,11,12	1.29	1 (9%)	15,15,17	1.42	3 (20%)
3	BGC	11-D	3	3	11,11,12	1.31	1 (9%)	15,15,17	1.60	4 (26%)
3	BGC	11-D	4	3	11,11,12	1.51	2 (18%)	15,15,17	2.28	6 (40%)
3	BGC	11-D	5	3	11,11,12	1.64	1 (9%)	15,15,17	1.62	2 (13%)
2	BGC	11-E	1	2	12,12,12	1.66	3 (25%)	17,17,17	1.44	4 (23%)
2	BGC	11-E	2	2	11,11,12	1.47	3 (27%)	15,15,17	0.97	0
2	BGC	11-E	3	2	11,11,12	1.27	1 (9%)	15,15,17	1.26	2 (13%)
2	BGC	11-E	4	2	11,11,12	0.91	1 (9%)	15,15,17	1.13	2 (13%)
2	BGC	11-E	5	2	11,11,12	1.16	1 (9%)	15,15,17	1.41	2 (13%)
2	BGC	11-E	6	2	11,11,12	1.38	2 (18%)	15,15,17	1.26	1 (6%)
3	BGC	11-F	1	3	12,12,12	1.33	2 (16%)	17,17,17	1.27	3 (17%)
3	BGC	11-F	2	3	11,11,12	1.60	2 (18%)	15,15,17	1.37	2 (13%)
3	BGC	11-F	3	3	11,11,12	1.35	2 (18%)	15,15,17	1.96	2 (13%)
3	BGC	11-F	4	3	11,11,12	1.08	1 (9%)	15,15,17	0.91	0
3	BGC	11-F	5	3	11,11,12	1.54	1 (9%)	15,15,17	0.88	1 (6%)
2	BGC	12-C	1	2	12,12,12	1.72	3 (25%)	17,17,17	1.62	5 (29%)
2	BGC	12-C	2	2	11,11,12	1.37	3 (27%)	15,15,17	1.33	3 (20%)
2	BGC	12-C	3	2	11,11,12	1.38	3 (27%)	15,15,17	1.32	4 (26%)
2	BGC	12-C	4	2	11,11,12	0.84	0	15,15,17	1.15	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	12-C	5	2	11,11,12	1.29	1 (9%)	15,15,17	1.13	1 (6%)
2	BGC	12-C	6	2	11,11,12	1.41	2 (18%)	15,15,17	1.58	4 (26%)
3	BGC	12-D	1	3	12,12,12	1.31	2 (16%)	17,17,17	1.36	3 (17%)
3	BGC	12-D	2	3	11,11,12	1.52	2 (18%)	15,15,17	1.82	2 (13%)
3	BGC	12-D	3	3	11,11,12	1.42	1 (9%)	15,15,17	1.47	3 (20%)
3	BGC	12-D	4	3	11,11,12	1.23	1 (9%)	15,15,17	1.23	2 (13%)
3	BGC	12-D	5	3	11,11,12	1.57	1 (9%)	15,15,17	1.16	1 (6%)
2	BGC	12-E	1	2	12,12,12	1.67	3 (25%)	17,17,17	1.31	3 (17%)
2	BGC	12-E	2	2	11,11,12	1.36	3 (27%)	15,15,17	1.21	1 (6%)
2	BGC	12-E	3	2	11,11,12	1.21	1 (9%)	15,15,17	1.15	1 (6%)
2	BGC	12-E	4	2	11,11,12	0.65	0	15,15,17	1.31	1 (6%)
2	BGC	12-E	5	2	11,11,12	1.44	3 (27%)	15,15,17	1.79	3 (20%)
2	BGC	12-E	6	2	11,11,12	1.42	2 (18%)	15,15,17	1.16	2 (13%)
3	BGC	12-F	1	3	12,12,12	1.27	2 (16%)	17,17,17	0.98	1 (5%)
3	BGC	12-F	2	3	11,11,12	1.53	2 (18%)	15,15,17	1.37	2 (13%)
3	BGC	12-F	3	3	11,11,12	1.19	1 (9%)	15,15,17	1.16	1 (6%)
3	BGC	12-F	4	3	11,11,12	1.31	2 (18%)	15,15,17	0.99	0
3	BGC	12-F	5	3	11,11,12	1.67	1 (9%)	15,15,17	0.66	0
2	BGC	13-C	1	2	12,12,12	1.73	3 (25%)	17,17,17	1.63	2 (11%)
2	BGC	13-C	2	2	11,11,12	1.38	3 (27%)	15,15,17	1.34	2 (13%)
2	BGC	13-C	3	2	11,11,12	1.58	3 (27%)	15,15,17	1.20	2 (13%)
2	BGC	13-C	4	2	11,11,12	0.96	1 (9%)	15,15,17	1.75	3 (20%)
2	BGC	13-C	5	2	11,11,12	1.28	1 (9%)	15,15,17	1.14	2 (13%)
2	BGC	13-C	6	2	11,11,12	1.35	1 (9%)	15,15,17	2.23	5 (33%)
3	BGC	13-D	1	3	12,12,12	1.28	1 (8%)	17,17,17	1.21	1 (5%)
3	BGC	13-D	2	3	11,11,12	1.34	1 (9%)	15,15,17	1.72	2 (13%)
3	BGC	13-D	3	3	11,11,12	1.40	1 (9%)	15,15,17	1.50	3 (20%)
3	BGC	13-D	4	3	11,11,12	1.39	2 (18%)	15,15,17	2.24	2 (13%)
3	BGC	13-D	5	3	11,11,12	1.38	1 (9%)	15,15,17	1.90	4 (26%)
2	BGC	13-E	1	2	12,12,12	1.63	3 (25%)	17,17,17	1.15	2 (11%)
2	BGC	13-E	2	2	11,11,12	1.26	2 (18%)	15,15,17	1.10	1 (6%)
2	BGC	13-E	3	2	11,11,12	1.36	1 (9%)	15,15,17	1.20	2 (13%)
2	BGC	13-E	4	2	11,11,12	0.69	0	15,15,17	1.35	2 (13%)
2	BGC	13-E	5	2	11,11,12	1.13	1 (9%)	15,15,17	2.19	3 (20%)
2	BGC	13-E	6	2	11,11,12	1.39	2 (18%)	15,15,17	1.20	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	13-F	1	3	12,12,12	1.31	1 (8%)	17,17,17	1.20	1 (5%)
3	BGC	13-F	2	3	11,11,12	1.48	1 (9%)	15,15,17	1.39	2 (13%)
3	BGC	13-F	3	3	11,11,12	1.28	2 (18%)	15,15,17	1.14	1 (6%)
3	BGC	13-F	4	3	11,11,12	1.43	2 (18%)	15,15,17	1.09	1 (6%)
3	BGC	13-F	5	3	11,11,12	1.45	1 (9%)	15,15,17	0.89	1 (6%)
2	BGC	14-C	1	2	12,12,12	1.68	3 (25%)	17,17,17	1.06	1 (5%)
2	BGC	14-C	2	2	11,11,12	1.33	3 (27%)	15,15,17	1.40	2 (13%)
2	BGC	14-C	3	2	11,11,12	1.33	3 (27%)	15,15,17	1.12	1 (6%)
2	BGC	14-C	4	2	11,11,12	0.88	1 (9%)	15,15,17	1.21	2 (13%)
2	BGC	14-C	5	2	11,11,12	1.24	1 (9%)	15,15,17	1.40	2 (13%)
2	BGC	14-C	6	2	11,11,12	1.30	1 (9%)	15,15,17	1.23	2 (13%)
3	BGC	14-D	1	3	12,12,12	1.30	1 (8%)	17,17,17	1.40	3 (17%)
3	BGC	14-D	2	3	11,11,12	1.53	1 (9%)	15,15,17	1.30	2 (13%)
3	BGC	14-D	3	3	11,11,12	1.28	1 (9%)	15,15,17	1.60	2 (13%)
3	BGC	14-D	4	3	11,11,12	1.34	1 (9%)	15,15,17	1.50	2 (13%)
3	BGC	14-D	5	3	11,11,12	1.52	1 (9%)	15,15,17	0.90	1 (6%)
2	BGC	14-E	1	2	12,12,12	1.75	3 (25%)	17,17,17	1.68	2 (11%)
2	BGC	14-E	2	2	11,11,12	1.63	3 (27%)	15,15,17	1.26	2 (13%)
2	BGC	14-E	3	2	11,11,12	1.37	2 (18%)	15,15,17	1.41	2 (13%)
2	BGC	14-E	4	2	11,11,12	0.59	0	15,15,17	1.15	1 (6%)
2	BGC	14-E	5	2	11,11,12	1.29	3 (27%)	15,15,17	1.28	2 (13%)
2	BGC	14-E	6	2	11,11,12	1.45	2 (18%)	15,15,17	1.26	2 (13%)
3	BGC	14-F	1	3	12,12,12	1.31	1 (8%)	17,17,17	1.15	1 (5%)
3	BGC	14-F	2	3	11,11,12	1.60	2 (18%)	15,15,17	1.35	1 (6%)
3	BGC	14-F	3	3	11,11,12	1.28	2 (18%)	15,15,17	1.38	1 (6%)
3	BGC	14-F	4	3	11,11,12	1.20	1 (9%)	15,15,17	0.55	0
3	BGC	14-F	5	3	11,11,12	1.55	1 (9%)	15,15,17	0.69	0
2	BGC	15-C	1	2	12,12,12	1.66	3 (25%)	17,17,17	1.24	2 (11%)
2	BGC	15-C	2	2	11,11,12	1.51	3 (27%)	15,15,17	1.70	2 (13%)
2	BGC	15-C	3	2	11,11,12	1.28	2 (18%)	15,15,17	1.09	2 (13%)
2	BGC	15-C	4	2	11,11,12	0.93	1 (9%)	15,15,17	1.22	2 (13%)
2	BGC	15-C	5	2	11,11,12	1.23	1 (9%)	15,15,17	1.23	1 (6%)
2	BGC	15-C	6	2	11,11,12	1.37	1 (9%)	15,15,17	1.10	1 (6%)
3	BGC	15-D	1	3	12,12,12	1.42	2 (16%)	17,17,17	1.54	4 (23%)
3	BGC	15-D	2	3	11,11,12	1.26	1 (9%)	15,15,17	2.25	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	15-D	3	3	11,11,12	1.45	2 (18%)	15,15,17	1.49	1 (6%)
3	BGC	15-D	4	3	11,11,12	1.31	2 (18%)	15,15,17	1.21	2 (13%)
3	BGC	15-D	5	3	11,11,12	1.51	1 (9%)	15,15,17	1.47	1 (6%)
2	BGC	15-E	1	2	12,12,12	1.57	3 (25%)	17,17,17	1.70	4 (23%)
2	BGC	15-E	2	2	11,11,12	1.44	3 (27%)	15,15,17	1.30	2 (13%)
2	BGC	15-E	3	2	11,11,12	1.20	2 (18%)	15,15,17	1.30	3 (20%)
2	BGC	15-E	4	2	11,11,12	0.85	1 (9%)	15,15,17	1.25	2 (13%)
2	BGC	15-E	5	2	11,11,12	1.29	2 (18%)	15,15,17	1.57	4 (26%)
2	BGC	15-E	6	2	11,11,12	1.48	2 (18%)	15,15,17	1.23	1 (6%)
3	BGC	15-F	1	3	12,12,12	1.41	2 (16%)	17,17,17	1.05	0
3	BGC	15-F	2	3	11,11,12	1.54	1 (9%)	15,15,17	1.42	2 (13%)
3	BGC	15-F	3	3	11,11,12	1.31	1 (9%)	15,15,17	1.03	0
3	BGC	15-F	4	3	11,11,12	1.25	2 (18%)	15,15,17	0.97	0
3	BGC	15-F	5	3	11,11,12	1.59	1 (9%)	15,15,17	0.84	1 (6%)
2	BGC	16-C	1	2	12,12,12	1.63	3 (25%)	17,17,17	1.12	0
2	BGC	16-C	2	2	11,11,12	1.32	3 (27%)	15,15,17	1.18	2 (13%)
2	BGC	16-C	3	2	11,11,12	1.38	3 (27%)	15,15,17	1.05	1 (6%)
2	BGC	16-C	4	2	11,11,12	0.87	0	15,15,17	1.18	2 (13%)
2	BGC	16-C	5	2	11,11,12	1.27	1 (9%)	15,15,17	1.43	2 (13%)
2	BGC	16-C	6	2	11,11,12	1.52	2 (18%)	15,15,17	1.23	2 (13%)
3	BGC	16-D	1	3	12,12,12	1.32	1 (8%)	17,17,17	1.02	1 (5%)
3	BGC	16-D	2	3	11,11,12	1.39	1 (9%)	15,15,17	1.71	2 (13%)
3	BGC	16-D	3	3	11,11,12	1.28	2 (18%)	15,15,17	1.68	3 (20%)
3	BGC	16-D	4	3	11,11,12	1.13	1 (9%)	15,15,17	1.37	3 (20%)
3	BGC	16-D	5	3	11,11,12	1.56	1 (9%)	15,15,17	0.71	0
2	BGC	16-E	1	2	12,12,12	1.51	3 (25%)	17,17,17	1.17	2 (11%)
2	BGC	16-E	2	2	11,11,12	1.43	2 (18%)	15,15,17	1.13	1 (6%)
2	BGC	16-E	3	2	11,11,12	1.36	1 (9%)	15,15,17	1.33	1 (6%)
2	BGC	16-E	4	2	11,11,12	0.71	0	15,15,17	1.17	2 (13%)
2	BGC	16-E	5	2	11,11,12	1.40	2 (18%)	15,15,17	1.59	3 (20%)
2	BGC	16-E	6	2	11,11,12	1.47	2 (18%)	15,15,17	2.76	4 (26%)
3	BGC	16-F	1	3	12,12,12	1.25	2 (16%)	17,17,17	1.00	1 (5%)
3	BGC	16-F	2	3	11,11,12	1.53	2 (18%)	15,15,17	1.52	3 (20%)
3	BGC	16-F	3	3	11,11,12	1.28	2 (18%)	15,15,17	1.23	2 (13%)
3	BGC	16-F	4	3	11,11,12	1.16	1 (9%)	15,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	16-F	5	3	11,11,12	1.62	1 (9%)	15,15,17	0.70	1 (6%)
2	BGC	17-C	1	2	12,12,12	1.66	4 (33%)	17,17,17	1.39	2 (11%)
2	BGC	17-C	2	2	11,11,12	1.32	3 (27%)	15,15,17	1.39	2 (13%)
2	BGC	17-C	3	2	11,11,12	1.41	3 (27%)	15,15,17	1.05	1 (6%)
2	BGC	17-C	4	2	11,11,12	0.82	0	15,15,17	1.21	1 (6%)
2	BGC	17-C	5	2	11,11,12	1.25	1 (9%)	15,15,17	1.32	2 (13%)
2	BGC	17-C	6	2	11,11,12	1.38	1 (9%)	15,15,17	1.33	4 (26%)
3	BGC	17-D	1	3	12,12,12	1.28	1 (8%)	17,17,17	1.53	4 (23%)
3	BGC	17-D	2	3	11,11,12	1.34	1 (9%)	15,15,17	1.86	2 (13%)
3	BGC	17-D	3	3	11,11,12	1.27	1 (9%)	15,15,17	1.15	1 (6%)
3	BGC	17-D	4	3	11,11,12	1.32	2 (18%)	15,15,17	1.14	1 (6%)
3	BGC	17-D	5	3	11,11,12	1.48	1 (9%)	15,15,17	0.94	0
2	BGC	17-E	1	2	12,12,12	1.58	3 (25%)	17,17,17	1.33	3 (17%)
2	BGC	17-E	2	2	11,11,12	1.37	3 (27%)	15,15,17	1.23	1 (6%)
2	BGC	17-E	3	2	11,11,12	1.35	1 (9%)	15,15,17	1.19	1 (6%)
2	BGC	17-E	4	2	11,11,12	0.70	0	15,15,17	1.02	2 (13%)
2	BGC	17-E	5	2	11,11,12	1.25	2 (18%)	15,15,17	1.27	1 (6%)
2	BGC	17-E	6	2	11,11,12	1.82	3 (27%)	15,15,17	2.58	4 (26%)
3	BGC	17-F	1	3	12,12,12	1.44	3 (25%)	17,17,17	1.87	4 (23%)
3	BGC	17-F	2	3	11,11,12	1.64	1 (9%)	15,15,17	1.44	3 (20%)
3	BGC	17-F	3	3	11,11,12	1.19	1 (9%)	15,15,17	1.17	2 (13%)
3	BGC	17-F	4	3	11,11,12	1.19	2 (18%)	15,15,17	1.23	1 (6%)
3	BGC	17-F	5	3	11,11,12	1.58	1 (9%)	15,15,17	0.78	0
2	BGC	18-C	1	2	12,12,12	1.65	3 (25%)	17,17,17	1.05	1 (5%)
2	BGC	18-C	2	2	11,11,12	1.31	3 (27%)	15,15,17	1.37	2 (13%)
2	BGC	18-C	3	2	11,11,12	1.45	2 (18%)	15,15,17	1.38	2 (13%)
2	BGC	18-C	4	2	11,11,12	0.83	0	15,15,17	1.09	2 (13%)
2	BGC	18-C	5	2	11,11,12	1.37	1 (9%)	15,15,17	1.34	1 (6%)
2	BGC	18-C	6	2	11,11,12	1.35	2 (18%)	15,15,17	1.66	5 (33%)
3	BGC	18-D	1	3	12,12,12	1.39	2 (16%)	17,17,17	1.50	5 (29%)
3	BGC	18-D	2	3	11,11,12	1.23	0	15,15,17	1.91	4 (26%)
3	BGC	18-D	3	3	11,11,12	1.29	1 (9%)	15,15,17	1.59	1 (6%)
3	BGC	18-D	4	3	11,11,12	1.12	1 (9%)	15,15,17	1.18	0
3	BGC	18-D	5	3	11,11,12	1.43	1 (9%)	15,15,17	1.60	4 (26%)
2	BGC	18-E	1	2	12,12,12	1.49	3 (25%)	17,17,17	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	18-E	2	2	11,11,12	1.43	2 (18%)	15,15,17	1.38	3 (20%)
2	BGC	18-E	3	2	11,11,12	1.30	2 (18%)	15,15,17	1.74	3 (20%)
2	BGC	18-E	4	2	11,11,12	0.73	0	15,15,17	1.26	2 (13%)
2	BGC	18-E	5	2	11,11,12	1.21	2 (18%)	15,15,17	1.33	3 (20%)
2	BGC	18-E	6	2	11,11,12	1.33	2 (18%)	15,15,17	1.41	4 (26%)
3	BGC	18-F	1	3	12,12,12	1.34	2 (16%)	17,17,17	1.13	1 (5%)
3	BGC	18-F	2	3	11,11,12	1.65	1 (9%)	15,15,17	1.53	2 (13%)
3	BGC	18-F	3	3	11,11,12	1.18	2 (18%)	15,15,17	1.15	1 (6%)
3	BGC	18-F	4	3	11,11,12	1.31	2 (18%)	15,15,17	0.90	0
3	BGC	18-F	5	3	11,11,12	1.62	1 (9%)	15,15,17	0.89	1 (6%)
2	BGC	19-C	1	2	12,12,12	1.72	3 (25%)	17,17,17	1.79	6 (35%)
2	BGC	19-C	2	2	11,11,12	1.37	2 (18%)	15,15,17	1.75	3 (20%)
2	BGC	19-C	3	2	11,11,12	1.26	2 (18%)	15,15,17	1.08	1 (6%)
2	BGC	19-C	4	2	11,11,12	1.12	1 (9%)	15,15,17	1.58	3 (20%)
2	BGC	19-C	5	2	11,11,12	1.26	2 (18%)	15,15,17	1.35	1 (6%)
2	BGC	19-C	6	2	11,11,12	1.36	2 (18%)	15,15,17	1.17	1 (6%)
3	BGC	19-D	1	3	12,12,12	1.23	1 (8%)	17,17,17	1.16	2 (11%)
3	BGC	19-D	2	3	11,11,12	1.33	1 (9%)	15,15,17	2.19	5 (33%)
3	BGC	19-D	3	3	11,11,12	1.27	2 (18%)	15,15,17	2.03	5 (33%)
3	BGC	19-D	4	3	11,11,12	1.31	2 (18%)	15,15,17	1.13	1 (6%)
3	BGC	19-D	5	3	11,11,12	1.45	1 (9%)	15,15,17	1.17	2 (13%)
2	BGC	19-E	1	2	12,12,12	1.55	3 (25%)	17,17,17	1.04	2 (11%)
2	BGC	19-E	2	2	11,11,12	1.40	3 (27%)	15,15,17	1.28	1 (6%)
2	BGC	19-E	3	2	11,11,12	1.28	1 (9%)	15,15,17	1.16	0
2	BGC	19-E	4	2	11,11,12	0.63	0	15,15,17	1.03	1 (6%)
2	BGC	19-E	5	2	11,11,12	1.31	3 (27%)	15,15,17	1.22	1 (6%)
2	BGC	19-E	6	2	11,11,12	1.39	2 (18%)	15,15,17	2.03	4 (26%)
3	BGC	19-F	1	3	12,12,12	1.31	1 (8%)	17,17,17	1.14	2 (11%)
3	BGC	19-F	2	3	11,11,12	1.42	1 (9%)	15,15,17	1.55	2 (13%)
3	BGC	19-F	3	3	11,11,12	1.24	1 (9%)	15,15,17	1.26	2 (13%)
3	BGC	19-F	4	3	11,11,12	1.27	2 (18%)	15,15,17	0.82	0
3	BGC	19-F	5	3	11,11,12	1.54	1 (9%)	15,15,17	0.86	1 (6%)
2	BGC	2-C	1	2	12,12,12	1.57	3 (25%)	17,17,17	0.87	0
2	BGC	2-C	2	2	11,11,12	1.26	2 (18%)	15,15,17	1.51	3 (20%)
2	BGC	2-C	3	2	11,11,12	1.30	2 (18%)	15,15,17	1.02	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	2-C	4	2	11,11,12	0.77	0	15,15,17	1.40	1 (6%)
2	BGC	2-C	5	2	11,11,12	1.29	1 (9%)	15,15,17	1.37	2 (13%)
2	BGC	2-C	6	2	11,11,12	1.52	2 (18%)	15,15,17	1.50	4 (26%)
3	BGC	2-D	1	3	12,12,12	1.32	2 (16%)	17,17,17	1.38	2 (11%)
3	BGC	2-D	2	3	11,11,12	1.23	0	15,15,17	1.45	1 (6%)
3	BGC	2-D	3	3	11,11,12	1.29	2 (18%)	15,15,17	1.48	4 (26%)
3	BGC	2-D	4	3	11,11,12	1.27	2 (18%)	15,15,17	1.05	1 (6%)
3	BGC	2-D	5	3	11,11,12	1.60	1 (9%)	15,15,17	1.16	2 (13%)
2	BGC	2-E	1	2	12,12,12	1.61	3 (25%)	17,17,17	0.95	0
2	BGC	2-E	2	2	11,11,12	1.33	3 (27%)	15,15,17	1.38	2 (13%)
2	BGC	2-E	3	2	11,11,12	1.20	1 (9%)	15,15,17	1.14	0
2	BGC	2-E	4	2	11,11,12	0.52	0	15,15,17	1.06	1 (6%)
2	BGC	2-E	5	2	11,11,12	1.31	2 (18%)	15,15,17	1.31	2 (13%)
2	BGC	2-E	6	2	11,11,12	1.44	2 (18%)	15,15,17	1.32	3 (20%)
3	BGC	2-F	1	3	12,12,12	1.36	2 (16%)	17,17,17	1.17	1 (5%)
3	BGC	2-F	2	3	11,11,12	1.62	1 (9%)	15,15,17	1.72	3 (20%)
3	BGC	2-F	3	3	11,11,12	1.25	1 (9%)	15,15,17	1.06	2 (13%)
3	BGC	2-F	4	3	11,11,12	1.18	2 (18%)	15,15,17	0.95	0
3	BGC	2-F	5	3	11,11,12	1.54	1 (9%)	15,15,17	0.81	1 (6%)
2	BGC	20-C	1	2	12,12,12	1.67	3 (25%)	17,17,17	1.04	1 (5%)
2	BGC	20-C	2	2	11,11,12	1.39	3 (27%)	15,15,17	1.63	3 (20%)
2	BGC	20-C	3	2	11,11,12	1.28	3 (27%)	15,15,17	1.20	1 (6%)
2	BGC	20-C	4	2	11,11,12	0.97	1 (9%)	15,15,17	1.28	2 (13%)
2	BGC	20-C	5	2	11,11,12	1.37	1 (9%)	15,15,17	1.41	2 (13%)
2	BGC	20-C	6	2	11,11,12	1.26	2 (18%)	15,15,17	1.34	2 (13%)
3	BGC	20-D	1	3	12,12,12	1.28	1 (8%)	17,17,17	1.20	2 (11%)
3	BGC	20-D	2	3	11,11,12	1.50	1 (9%)	15,15,17	1.52	2 (13%)
3	BGC	20-D	3	3	11,11,12	1.38	1 (9%)	15,15,17	1.42	2 (13%)
3	BGC	20-D	4	3	11,11,12	1.26	1 (9%)	15,15,17	0.87	0
3	BGC	20-D	5	3	11,11,12	1.51	1 (9%)	15,15,17	1.09	1 (6%)
2	BGC	20-E	1	2	12,12,12	1.62	3 (25%)	17,17,17	0.95	1 (5%)
2	BGC	20-E	2	2	11,11,12	1.42	3 (27%)	15,15,17	1.19	1 (6%)
2	BGC	20-E	3	2	11,11,12	1.27	1 (9%)	15,15,17	1.44	1 (6%)
2	BGC	20-E	4	2	11,11,12	0.58	0	15,15,17	1.21	2 (13%)
2	BGC	20-E	5	2	11,11,12	1.33	2 (18%)	15,15,17	1.34	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	20-E	6	2	11,11,12	1.34	2 (18%)	15,15,17	1.01	1 (6%)
3	BGC	20-F	1	3	12,12,12	1.27	2 (16%)	17,17,17	1.13	1 (5%)
3	BGC	20-F	2	3	11,11,12	1.63	3 (27%)	15,15,17	1.57	2 (13%)
3	BGC	20-F	3	3	11,11,12	1.27	2 (18%)	15,15,17	1.13	2 (13%)
3	BGC	20-F	4	3	11,11,12	1.34	2 (18%)	15,15,17	0.81	0
3	BGC	20-F	5	3	11,11,12	1.62	1 (9%)	15,15,17	0.71	0
2	BGC	21-C	1	2	12,12,12	1.69	3 (25%)	17,17,17	1.23	1 (5%)
2	BGC	21-C	2	2	11,11,12	1.65	3 (27%)	15,15,17	1.86	5 (33%)
2	BGC	21-C	3	2	11,11,12	1.38	3 (27%)	15,15,17	1.20	2 (13%)
2	BGC	21-C	4	2	11,11,12	0.90	1 (9%)	15,15,17	1.07	1 (6%)
2	BGC	21-C	5	2	11,11,12	1.33	1 (9%)	15,15,17	1.49	3 (20%)
2	BGC	21-C	6	2	11,11,12	1.41	2 (18%)	15,15,17	1.12	0
3	BGC	21-D	1	3	12,12,12	1.34	2 (16%)	17,17,17	1.30	2 (11%)
3	BGC	21-D	2	3	11,11,12	1.33	2 (18%)	15,15,17	1.89	2 (13%)
3	BGC	21-D	3	3	11,11,12	1.25	0	15,15,17	1.26	3 (20%)
3	BGC	21-D	4	3	11,11,12	1.29	2 (18%)	15,15,17	1.16	1 (6%)
3	BGC	21-D	5	3	11,11,12	1.59	1 (9%)	15,15,17	1.09	1 (6%)
2	BGC	21-E	1	2	12,12,12	1.84	4 (33%)	17,17,17	1.49	3 (17%)
2	BGC	21-E	2	2	11,11,12	1.49	3 (27%)	15,15,17	1.40	2 (13%)
2	BGC	21-E	3	2	11,11,12	1.32	1 (9%)	15,15,17	1.06	1 (6%)
2	BGC	21-E	4	2	11,11,12	0.86	1 (9%)	15,15,17	1.55	3 (20%)
2	BGC	21-E	5	2	11,11,12	1.40	3 (27%)	15,15,17	1.84	5 (33%)
2	BGC	21-E	6	2	11,11,12	1.32	3 (27%)	15,15,17	1.37	2 (13%)
3	BGC	21-F	1	3	12,12,12	1.25	1 (8%)	17,17,17	0.93	0
3	BGC	21-F	2	3	11,11,12	1.62	2 (18%)	15,15,17	1.48	1 (6%)
3	BGC	21-F	3	3	11,11,12	1.30	2 (18%)	15,15,17	1.36	2 (13%)
3	BGC	21-F	4	3	11,11,12	1.18	1 (9%)	15,15,17	0.93	0
3	BGC	21-F	5	3	11,11,12	1.67	1 (9%)	15,15,17	0.77	0
2	BGC	22-C	1	2	12,12,12	1.57	3 (25%)	17,17,17	1.04	0
2	BGC	22-C	2	2	11,11,12	1.40	3 (27%)	15,15,17	1.52	3 (20%)
2	BGC	22-C	3	2	11,11,12	1.22	2 (18%)	15,15,17	1.23	2 (13%)
2	BGC	22-C	4	2	11,11,12	1.04	1 (9%)	15,15,17	1.10	1 (6%)
2	BGC	22-C	5	2	11,11,12	1.45	1 (9%)	15,15,17	1.38	1 (6%)
2	BGC	22-C	6	2	11,11,12	1.39	1 (9%)	15,15,17	2.01	5 (33%)
3	BGC	22-D	1	3	12,12,12	1.28	1 (8%)	17,17,17	1.89	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	22-D	2	3	11,11,12	1.33	1 (9%)	15,15,17	1.68	3 (20%)
3	BGC	22-D	3	3	11,11,12	1.27	1 (9%)	15,15,17	1.57	2 (13%)
3	BGC	22-D	4	3	11,11,12	1.20	2 (18%)	15,15,17	1.02	0
3	BGC	22-D	5	3	11,11,12	1.34	1 (9%)	15,15,17	1.38	2 (13%)
2	BGC	22-E	1	2	12,12,12	1.53	3 (25%)	17,17,17	1.27	2 (11%)
2	BGC	22-E	2	2	11,11,12	1.43	3 (27%)	15,15,17	1.24	2 (13%)
2	BGC	22-E	3	2	11,11,12	1.20	1 (9%)	15,15,17	1.13	0
2	BGC	22-E	4	2	11,11,12	0.76	0	15,15,17	1.41	2 (13%)
2	BGC	22-E	5	2	11,11,12	1.44	2 (18%)	15,15,17	1.20	1 (6%)
2	BGC	22-E	6	2	11,11,12	1.49	2 (18%)	15,15,17	1.01	1 (6%)
3	BGC	22-F	1	3	12,12,12	1.30	1 (8%)	17,17,17	1.27	2 (11%)
3	BGC	22-F	2	3	11,11,12	1.39	2 (18%)	15,15,17	1.27	1 (6%)
3	BGC	22-F	3	3	11,11,12	1.24	1 (9%)	15,15,17	1.18	2 (13%)
3	BGC	22-F	4	3	11,11,12	1.38	2 (18%)	15,15,17	1.01	0
3	BGC	22-F	5	3	11,11,12	1.52	1 (9%)	15,15,17	0.72	0
2	BGC	23-C	1	2	12,12,12	1.60	3 (25%)	17,17,17	1.55	3 (17%)
2	BGC	23-C	2	2	11,11,12	1.41	3 (27%)	15,15,17	1.52	2 (13%)
2	BGC	23-C	3	2	11,11,12	1.29	3 (27%)	15,15,17	1.15	1 (6%)
2	BGC	23-C	4	2	11,11,12	0.80	0	15,15,17	1.80	4 (26%)
2	BGC	23-C	5	2	11,11,12	1.18	1 (9%)	15,15,17	1.33	2 (13%)
2	BGC	23-C	6	2	11,11,12	1.48	2 (18%)	15,15,17	1.60	4 (26%)
3	BGC	23-D	1	3	12,12,12	1.32	2 (16%)	17,17,17	1.62	5 (29%)
3	BGC	23-D	2	3	11,11,12	1.40	1 (9%)	15,15,17	1.33	1 (6%)
3	BGC	23-D	3	3	11,11,12	1.30	1 (9%)	15,15,17	1.50	2 (13%)
3	BGC	23-D	4	3	11,11,12	1.27	2 (18%)	15,15,17	1.22	2 (13%)
3	BGC	23-D	5	3	11,11,12	1.49	1 (9%)	15,15,17	1.17	2 (13%)
2	BGC	23-E	1	2	12,12,12	1.53	3 (25%)	17,17,17	1.10	2 (11%)
2	BGC	23-E	2	2	11,11,12	1.37	2 (18%)	15,15,17	1.12	2 (13%)
2	BGC	23-E	3	2	11,11,12	1.35	1 (9%)	15,15,17	1.47	1 (6%)
2	BGC	23-E	4	2	11,11,12	0.85	1 (9%)	15,15,17	1.68	2 (13%)
2	BGC	23-E	5	2	11,11,12	1.23	1 (9%)	15,15,17	1.23	2 (13%)
2	BGC	23-E	6	2	11,11,12	1.39	2 (18%)	15,15,17	1.82	3 (20%)
3	BGC	23-F	1	3	12,12,12	1.43	2 (16%)	17,17,17	1.76	6 (35%)
3	BGC	23-F	2	3	11,11,12	1.42	2 (18%)	15,15,17	1.33	3 (20%)
3	BGC	23-F	3	3	11,11,12	1.10	1 (9%)	15,15,17	1.37	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	23-F	4	3	11,11,12	1.33	2 (18%)	15,15,17	1.04	0
3	BGC	23-F	5	3	11,11,12	1.56	1 (9%)	15,15,17	1.82	2 (13%)
2	BGC	24-C	1	2	12,12,12	1.51	3 (25%)	17,17,17	1.42	3 (17%)
2	BGC	24-C	2	2	11,11,12	1.46	3 (27%)	15,15,17	1.41	2 (13%)
2	BGC	24-C	3	2	11,11,12	1.41	2 (18%)	15,15,17	1.17	1 (6%)
2	BGC	24-C	4	2	11,11,12	0.90	0	15,15,17	1.24	2 (13%)
2	BGC	24-C	5	2	11,11,12	1.20	1 (9%)	15,15,17	1.38	2 (13%)
2	BGC	24-C	6	2	11,11,12	1.36	2 (18%)	15,15,17	2.14	3 (20%)
3	BGC	24-D	1	3	12,12,12	1.30	1 (8%)	17,17,17	1.34	2 (11%)
3	BGC	24-D	2	3	11,11,12	1.20	0	15,15,17	1.47	1 (6%)
3	BGC	24-D	3	3	11,11,12	1.33	2 (18%)	15,15,17	1.28	3 (20%)
3	BGC	24-D	4	3	11,11,12	1.29	2 (18%)	15,15,17	1.23	1 (6%)
3	BGC	24-D	5	3	11,11,12	1.58	1 (9%)	15,15,17	1.11	1 (6%)
2	BGC	24-E	1	2	12,12,12	1.56	3 (25%)	17,17,17	1.36	2 (11%)
2	BGC	24-E	2	2	11,11,12	1.55	2 (18%)	15,15,17	0.88	0
2	BGC	24-E	3	2	11,11,12	1.23	1 (9%)	15,15,17	1.00	1 (6%)
2	BGC	24-E	4	2	11,11,12	0.82	1 (9%)	15,15,17	1.30	2 (13%)
2	BGC	24-E	5	2	11,11,12	1.33	2 (18%)	15,15,17	1.34	2 (13%)
2	BGC	24-E	6	2	11,11,12	1.46	2 (18%)	15,15,17	1.54	5 (33%)
3	BGC	24-F	1	3	12,12,12	1.33	2 (16%)	17,17,17	1.10	1 (5%)
3	BGC	24-F	2	3	11,11,12	1.54	1 (9%)	15,15,17	1.54	3 (20%)
3	BGC	24-F	3	3	11,11,12	1.20	1 (9%)	15,15,17	1.43	2 (13%)
3	BGC	24-F	4	3	11,11,12	1.28	2 (18%)	15,15,17	1.00	0
3	BGC	24-F	5	3	11,11,12	1.62	1 (9%)	15,15,17	0.76	0
2	BGC	25-C	1	2	12,12,12	1.59	3 (25%)	17,17,17	1.02	0
2	BGC	25-C	2	2	11,11,12	1.35	3 (27%)	15,15,17	1.33	2 (13%)
2	BGC	25-C	3	2	11,11,12	1.25	3 (27%)	15,15,17	1.15	3 (20%)
2	BGC	25-C	4	2	11,11,12	0.80	0	15,15,17	1.34	4 (26%)
2	BGC	25-C	5	2	11,11,12	1.32	1 (9%)	15,15,17	1.37	2 (13%)
2	BGC	25-C	6	2	11,11,12	1.22	1 (9%)	15,15,17	1.70	3 (20%)
3	BGC	25-D	1	3	12,12,12	1.33	2 (16%)	17,17,17	1.39	2 (11%)
3	BGC	25-D	2	3	11,11,12	1.34	1 (9%)	15,15,17	1.90	4 (26%)
3	BGC	25-D	3	3	11,11,12	1.31	1 (9%)	15,15,17	1.46	2 (13%)
3	BGC	25-D	4	3	11,11,12	1.33	1 (9%)	15,15,17	1.21	2 (13%)
3	BGC	25-D	5	3	11,11,12	1.53	1 (9%)	15,15,17	1.08	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	25-E	1	2	12,12,12	1.61	3 (25%)	17,17,17	1.57	5 (29%)
2	BGC	25-E	2	2	11,11,12	1.35	3 (27%)	15,15,17	1.28	1 (6%)
2	BGC	25-E	3	2	11,11,12	1.26	1 (9%)	15,15,17	1.27	2 (13%)
2	BGC	25-E	4	2	11,11,12	0.68	0	15,15,17	1.49	4 (26%)
2	BGC	25-E	5	2	11,11,12	1.26	3 (27%)	15,15,17	1.25	2 (13%)
2	BGC	25-E	6	2	11,11,12	1.29	2 (18%)	15,15,17	0.96	0
3	BGC	25-F	1	3	12,12,12	1.33	2 (16%)	17,17,17	1.08	0
3	BGC	25-F	2	3	11,11,12	1.54	3 (27%)	15,15,17	1.79	1 (6%)
3	BGC	25-F	3	3	11,11,12	1.42	2 (18%)	15,15,17	1.84	4 (26%)
3	BGC	25-F	4	3	11,11,12	1.24	2 (18%)	15,15,17	1.64	2 (13%)
3	BGC	25-F	5	3	11,11,12	1.47	1 (9%)	15,15,17	0.94	1 (6%)
2	BGC	3-C	1	2	12,12,12	1.63	3 (25%)	17,17,17	1.04	1 (5%)
2	BGC	3-C	2	2	11,11,12	1.36	3 (27%)	15,15,17	1.48	2 (13%)
2	BGC	3-C	3	2	11,11,12	1.34	2 (18%)	15,15,17	0.95	0
2	BGC	3-C	4	2	11,11,12	0.91	1 (9%)	15,15,17	1.19	1 (6%)
2	BGC	3-C	5	2	11,11,12	1.30	1 (9%)	15,15,17	1.92	5 (33%)
2	BGC	3-C	6	2	11,11,12	1.33	2 (18%)	15,15,17	1.25	1 (6%)
3	BGC	3-D	1	3	12,12,12	1.33	1 (8%)	17,17,17	1.45	4 (23%)
3	BGC	3-D	2	3	11,11,12	1.38	1 (9%)	15,15,17	1.49	2 (13%)
3	BGC	3-D	3	3	11,11,12	1.31	1 (9%)	15,15,17	1.48	2 (13%)
3	BGC	3-D	4	3	11,11,12	1.14	1 (9%)	15,15,17	1.44	1 (6%)
3	BGC	3-D	5	3	11,11,12	1.66	1 (9%)	15,15,17	1.10	1 (6%)
2	BGC	3-E	1	2	12,12,12	1.65	4 (33%)	17,17,17	0.98	1 (5%)
2	BGC	3-E	2	2	11,11,12	1.44	2 (18%)	15,15,17	1.36	2 (13%)
2	BGC	3-E	3	2	11,11,12	1.52	2 (18%)	15,15,17	1.15	1 (6%)
2	BGC	3-E	4	2	11,11,12	0.97	1 (9%)	15,15,17	3.26	7 (46%)
2	BGC	3-E	5	2	11,11,12	1.18	2 (18%)	15,15,17	1.17	2 (13%)
2	BGC	3-E	6	2	11,11,12	1.41	2 (18%)	15,15,17	1.53	3 (20%)
3	BGC	3-F	1	3	12,12,12	1.30	2 (16%)	17,17,17	0.99	0
3	BGC	3-F	2	3	11,11,12	1.45	1 (9%)	15,15,17	1.58	2 (13%)
3	BGC	3-F	3	3	11,11,12	1.37	2 (18%)	15,15,17	1.18	2 (13%)
3	BGC	3-F	4	3	11,11,12	1.25	2 (18%)	15,15,17	0.99	0
3	BGC	3-F	5	3	11,11,12	1.59	1 (9%)	15,15,17	0.79	0
2	BGC	4-C	1	2	12,12,12	1.69	3 (25%)	17,17,17	1.21	2 (11%)
2	BGC	4-C	2	2	11,11,12	1.42	3 (27%)	15,15,17	1.42	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	4-C	3	2	11,11,12	1.47	3 (27%)	15,15,17	1.15	3 (20%)
2	BGC	4-C	4	2	11,11,12	0.86	0	15,15,17	0.99	1 (6%)
2	BGC	4-C	5	2	11,11,12	1.41	1 (9%)	15,15,17	1.26	1 (6%)
2	BGC	4-C	6	2	11,11,12	1.57	2 (18%)	15,15,17	1.62	4 (26%)
3	BGC	4-D	1	3	12,12,12	1.27	1 (8%)	17,17,17	1.23	3 (17%)
3	BGC	4-D	2	3	11,11,12	1.39	1 (9%)	15,15,17	1.70	4 (26%)
3	BGC	4-D	3	3	11,11,12	1.43	2 (18%)	15,15,17	1.84	3 (20%)
3	BGC	4-D	4	3	11,11,12	1.65	2 (18%)	15,15,17	1.46	3 (20%)
3	BGC	4-D	5	3	11,11,12	1.58	1 (9%)	15,15,17	1.19	2 (13%)
2	BGC	4-E	1	2	12,12,12	1.61	3 (25%)	17,17,17	1.21	3 (17%)
2	BGC	4-E	2	2	11,11,12	1.44	2 (18%)	15,15,17	1.23	2 (13%)
2	BGC	4-E	3	2	11,11,12	1.33	1 (9%)	15,15,17	1.08	0
2	BGC	4-E	4	2	11,11,12	0.77	0	15,15,17	1.25	3 (20%)
2	BGC	4-E	5	2	11,11,12	1.21	2 (18%)	15,15,17	1.05	2 (13%)
2	BGC	4-E	6	2	11,11,12	1.42	3 (27%)	15,15,17	1.42	2 (13%)
3	BGC	4-F	1	3	12,12,12	1.32	1 (8%)	17,17,17	0.90	0
3	BGC	4-F	2	3	11,11,12	1.41	1 (9%)	15,15,17	1.50	2 (13%)
3	BGC	4-F	3	3	11,11,12	1.38	1 (9%)	15,15,17	1.21	1 (6%)
3	BGC	4-F	4	3	11,11,12	1.25	2 (18%)	15,15,17	1.00	0
3	BGC	4-F	5	3	11,11,12	1.53	1 (9%)	15,15,17	1.20	2 (13%)
2	BGC	5-C	1	2	12,12,12	1.67	3 (25%)	17,17,17	1.68	5 (29%)
2	BGC	5-C	2	2	11,11,12	1.46	3 (27%)	15,15,17	1.63	3 (20%)
2	BGC	5-C	3	2	11,11,12	1.40	3 (27%)	15,15,17	1.30	1 (6%)
2	BGC	5-C	4	2	11,11,12	0.86	0	15,15,17	1.23	2 (13%)
2	BGC	5-C	5	2	11,11,12	1.39	1 (9%)	15,15,17	1.21	1 (6%)
2	BGC	5-C	6	2	11,11,12	1.56	2 (18%)	15,15,17	1.23	2 (13%)
3	BGC	5-D	1	3	12,12,12	1.33	1 (8%)	17,17,17	1.41	1 (5%)
3	BGC	5-D	2	3	11,11,12	1.30	1 (9%)	15,15,17	1.69	4 (26%)
3	BGC	5-D	3	3	11,11,12	1.41	2 (18%)	15,15,17	1.72	4 (26%)
3	BGC	5-D	4	3	11,11,12	1.20	1 (9%)	15,15,17	1.26	2 (13%)
3	BGC	5-D	5	3	11,11,12	1.51	1 (9%)	15,15,17	0.87	0
2	BGC	5-E	1	2	12,12,12	1.54	3 (25%)	17,17,17	1.05	1 (5%)
2	BGC	5-E	2	2	11,11,12	1.62	3 (27%)	15,15,17	0.85	0
2	BGC	5-E	3	2	11,11,12	1.38	1 (9%)	15,15,17	1.16	0
2	BGC	5-E	4	2	11,11,12	0.87	1 (9%)	15,15,17	1.49	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	5-E	5	2	11,11,12	1.32	2 (18%)	15,15,17	1.19	2 (13%)
2	BGC	5-E	6	2	11,11,12	1.38	2 (18%)	15,15,17	1.42	4 (26%)
3	BGC	5-F	1	3	12,12,12	1.42	3 (25%)	17,17,17	1.80	4 (23%)
3	BGC	5-F	2	3	11,11,12	1.70	2 (18%)	15,15,17	1.57	2 (13%)
3	BGC	5-F	3	3	11,11,12	1.30	1 (9%)	15,15,17	1.01	0
3	BGC	5-F	4	3	11,11,12	1.36	2 (18%)	15,15,17	1.23	1 (6%)
3	BGC	5-F	5	3	11,11,12	1.61	1 (9%)	15,15,17	1.06	2 (13%)
2	BGC	6-C	1	2	12,12,12	1.57	3 (25%)	17,17,17	1.19	3 (17%)
2	BGC	6-C	2	2	11,11,12	1.39	3 (27%)	15,15,17	1.54	3 (20%)
2	BGC	6-C	3	2	11,11,12	1.33	3 (27%)	15,15,17	1.38	2 (13%)
2	BGC	6-C	4	2	11,11,12	0.77	0	15,15,17	1.05	2 (13%)
2	BGC	6-C	5	2	11,11,12	1.36	2 (18%)	15,15,17	1.27	2 (13%)
2	BGC	6-C	6	2	11,11,12	1.35	1 (9%)	15,15,17	1.44	2 (13%)
3	BGC	6-D	1	3	12,12,12	1.33	1 (8%)	17,17,17	1.99	5 (29%)
3	BGC	6-D	2	3	11,11,12	1.75	3 (27%)	15,15,17	2.49	6 (40%)
3	BGC	6-D	3	3	11,11,12	1.23	1 (9%)	15,15,17	1.54	4 (26%)
3	BGC	6-D	4	3	11,11,12	1.20	1 (9%)	15,15,17	1.12	2 (13%)
3	BGC	6-D	5	3	11,11,12	1.39	1 (9%)	15,15,17	1.44	3 (20%)
2	BGC	6-E	1	2	12,12,12	1.63	3 (25%)	17,17,17	1.40	1 (5%)
2	BGC	6-E	2	2	11,11,12	1.48	3 (27%)	15,15,17	1.15	2 (13%)
2	BGC	6-E	3	2	11,11,12	1.16	0	15,15,17	1.37	1 (6%)
2	BGC	6-E	4	2	11,11,12	0.82	1 (9%)	15,15,17	1.22	1 (6%)
2	BGC	6-E	5	2	11,11,12	1.19	2 (18%)	15,15,17	1.22	2 (13%)
2	BGC	6-E	6	2	11,11,12	1.29	2 (18%)	15,15,17	1.09	1 (6%)
3	BGC	6-F	1	3	12,12,12	1.27	1 (8%)	17,17,17	0.88	0
3	BGC	6-F	2	3	11,11,12	1.55	1 (9%)	15,15,17	1.82	4 (26%)
3	BGC	6-F	3	3	11,11,12	1.38	3 (27%)	15,15,17	1.39	2 (13%)
3	BGC	6-F	4	3	11,11,12	1.25	2 (18%)	15,15,17	0.68	0
3	BGC	6-F	5	3	11,11,12	1.71	1 (9%)	15,15,17	0.81	0
2	BGC	7-C	1	2	12,12,12	1.64	3 (25%)	17,17,17	1.67	5 (29%)
2	BGC	7-C	2	2	11,11,12	1.58	3 (27%)	15,15,17	3.78	5 (33%)
2	BGC	7-C	3	2	11,11,12	1.41	2 (18%)	15,15,17	1.11	0
2	BGC	7-C	4	2	11,11,12	0.98	1 (9%)	15,15,17	1.22	2 (13%)
2	BGC	7-C	5	2	11,11,12	1.45	2 (18%)	15,15,17	1.31	2 (13%)
2	BGC	7-C	6	2	11,11,12	1.37	1 (9%)	15,15,17	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	7-D	1	3	12,12,12	1.24	1 (8%)	17,17,17	1.24	2 (11%)
3	BGC	7-D	2	3	11,11,12	1.42	1 (9%)	15,15,17	1.53	1 (6%)
3	BGC	7-D	3	3	11,11,12	1.28	2 (18%)	15,15,17	1.53	5 (33%)
3	BGC	7-D	4	3	11,11,12	1.36	2 (18%)	15,15,17	1.08	1 (6%)
3	BGC	7-D	5	3	11,11,12	1.42	1 (9%)	15,15,17	1.32	2 (13%)
2	BGC	7-E	1	2	12,12,12	1.54	3 (25%)	17,17,17	1.06	2 (11%)
2	BGC	7-E	2	2	11,11,12	1.34	2 (18%)	15,15,17	1.17	1 (6%)
2	BGC	7-E	3	2	11,11,12	1.25	1 (9%)	15,15,17	1.20	2 (13%)
2	BGC	7-E	4	2	11,11,12	0.73	0	15,15,17	1.22	1 (6%)
2	BGC	7-E	5	2	11,11,12	1.26	2 (18%)	15,15,17	1.28	2 (13%)
2	BGC	7-E	6	2	11,11,12	1.39	2 (18%)	15,15,17	1.21	2 (13%)
3	BGC	7-F	1	3	12,12,12	1.21	1 (8%)	17,17,17	1.16	1 (5%)
3	BGC	7-F	2	3	11,11,12	1.47	3 (27%)	15,15,17	1.67	2 (13%)
3	BGC	7-F	3	3	11,11,12	1.22	2 (18%)	15,15,17	1.30	2 (13%)
3	BGC	7-F	4	3	11,11,12	1.44	2 (18%)	15,15,17	0.95	0
3	BGC	7-F	5	3	11,11,12	1.58	1 (9%)	15,15,17	0.72	0
2	BGC	8-C	1	2	12,12,12	1.67	3 (25%)	17,17,17	1.36	2 (11%)
2	BGC	8-C	2	2	11,11,12	1.41	3 (27%)	15,15,17	1.39	2 (13%)
2	BGC	8-C	3	2	11,11,12	1.39	2 (18%)	15,15,17	1.11	1 (6%)
2	BGC	8-C	4	2	11,11,12	1.04	1 (9%)	15,15,17	1.33	2 (13%)
2	BGC	8-C	5	2	11,11,12	1.18	1 (9%)	15,15,17	0.94	0
2	BGC	8-C	6	2	11,11,12	1.37	2 (18%)	15,15,17	1.70	3 (20%)
3	BGC	8-D	1	3	12,12,12	1.25	1 (8%)	17,17,17	1.28	1 (5%)
3	BGC	8-D	2	3	11,11,12	1.43	1 (9%)	15,15,17	1.46	2 (13%)
3	BGC	8-D	3	3	11,11,12	1.26	1 (9%)	15,15,17	1.36	1 (6%)
3	BGC	8-D	4	3	11,11,12	1.18	1 (9%)	15,15,17	1.15	1 (6%)
3	BGC	8-D	5	3	11,11,12	1.63	1 (9%)	15,15,17	1.57	2 (13%)
2	BGC	8-E	1	2	12,12,12	1.63	3 (25%)	17,17,17	1.37	3 (17%)
2	BGC	8-E	2	2	11,11,12	1.54	2 (18%)	15,15,17	1.92	5 (33%)
2	BGC	8-E	3	2	11,11,12	1.34	1 (9%)	15,15,17	1.50	2 (13%)
2	BGC	8-E	4	2	11,11,12	0.74	0	15,15,17	1.31	2 (13%)
2	BGC	8-E	5	2	11,11,12	1.43	2 (18%)	15,15,17	1.30	2 (13%)
2	BGC	8-E	6	2	11,11,12	1.27	2 (18%)	15,15,17	1.02	0
3	BGC	8-F	1	3	12,12,12	1.31	1 (8%)	17,17,17	0.96	1 (5%)
3	BGC	8-F	2	3	11,11,12	1.50	2 (18%)	15,15,17	1.78	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	8-F	3	3	11,11,12	1.27	1 (9%)	15,15,17	1.32	1 (6%)
3	BGC	8-F	4	3	11,11,12	1.30	2 (18%)	15,15,17	1.08	0
3	BGC	8-F	5	3	11,11,12	1.65	2 (18%)	15,15,17	0.74	0
2	BGC	9-C	1	2	12,12,12	1.71	3 (25%)	17,17,17	1.59	4 (23%)
2	BGC	9-C	2	2	11,11,12	1.37	2 (18%)	15,15,17	1.69	3 (20%)
2	BGC	9-C	3	2	11,11,12	1.31	2 (18%)	15,15,17	0.98	0
2	BGC	9-C	4	2	11,11,12	0.86	0	15,15,17	1.02	1 (6%)
2	BGC	9-C	5	2	11,11,12	1.36	1 (9%)	15,15,17	1.24	1 (6%)
2	BGC	9-C	6	2	11,11,12	1.29	2 (18%)	15,15,17	1.60	3 (20%)
3	BGC	9-D	1	3	12,12,12	1.33	1 (8%)	17,17,17	1.33	4 (23%)
3	BGC	9-D	2	3	11,11,12	1.26	1 (9%)	15,15,17	1.67	2 (13%)
3	BGC	9-D	3	3	11,11,12	1.15	1 (9%)	15,15,17	1.71	3 (20%)
3	BGC	9-D	4	3	11,11,12	1.15	1 (9%)	15,15,17	1.19	1 (6%)
3	BGC	9-D	5	3	11,11,12	1.60	1 (9%)	15,15,17	0.95	1 (6%)
2	BGC	9-E	1	2	12,12,12	1.72	3 (25%)	17,17,17	1.38	2 (11%)
2	BGC	9-E	2	2	11,11,12	1.39	2 (18%)	15,15,17	1.91	4 (26%)
2	BGC	9-E	3	2	11,11,12	1.33	1 (9%)	15,15,17	1.04	0
2	BGC	9-E	4	2	11,11,12	0.73	0	15,15,17	1.05	1 (6%)
2	BGC	9-E	5	2	11,11,12	1.23	2 (18%)	15,15,17	1.60	4 (26%)
2	BGC	9-E	6	2	11,11,12	1.44	2 (18%)	15,15,17	1.35	2 (13%)
3	BGC	9-F	1	3	12,12,12	1.29	2 (16%)	17,17,17	0.98	0
3	BGC	9-F	2	3	11,11,12	1.50	2 (18%)	15,15,17	1.33	2 (13%)
3	BGC	9-F	3	3	11,11,12	1.17	1 (9%)	15,15,17	1.46	3 (20%)
3	BGC	9-F	4	3	11,11,12	1.17	2 (18%)	15,15,17	1.06	0
3	BGC	9-F	5	3	11,11,12	1.91	1 (9%)	15,15,17	1.03	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
2	BGC	1-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	1-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	1-C	3	2	-	2/2/19/22	0/1/1/1
2	BGC	1-C	4	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	1-C	5	2	-	2/2/19/22	0/1/1/1
2	BGC	1-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	1-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	1-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	1-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	1-D	4	3	-	2/2/19/22	0/1/1/1
3	BGC	1-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	1-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	1-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	1-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	1-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	1-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	1-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	1-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	1-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	1-F	3	3	-	1/2/19/22	0/1/1/1
3	BGC	1-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	1-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	10-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	10-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	10-C	3	2	-	2/2/19/22	0/1/1/1
2	BGC	10-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	10-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	10-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	10-D	1	3	-	1/2/22/22	0/1/1/1
3	BGC	10-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	10-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	10-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	10-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	10-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	10-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	10-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	10-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	10-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	10-E	6	2	-	1/2/19/22	0/1/1/1
3	BGC	10-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	10-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	10-F	3	3	-	2/2/19/22	0/1/1/1
3	BGC	10-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	10-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	11-C	1	2	-	1/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	11-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	11-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	11-C	4	2	-	1/2/19/22	0/1/1/1
2	BGC	11-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	11-C	6	2	-	1/2/19/22	0/1/1/1
3	BGC	11-D	1	3	-	0/2/22/22	0/1/1/1
3	BGC	11-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	11-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	11-D	4	3	-	2/2/19/22	0/1/1/1
3	BGC	11-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	11-E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	11-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	11-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	11-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	11-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	11-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	11-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	11-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	11-F	3	3	-	2/2/19/22	0/1/1/1
3	BGC	11-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	11-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	12-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	12-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	12-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	12-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	12-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	12-C	6	2	-	1/2/19/22	0/1/1/1
3	BGC	12-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	12-D	2	3	-	1/2/19/22	0/1/1/1
3	BGC	12-D	3	3	-	1/2/19/22	0/1/1/1
3	BGC	12-D	4	3	-	2/2/19/22	0/1/1/1
3	BGC	12-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	12-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	12-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	12-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	12-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	12-E	5	2	-	2/2/19/22	0/1/1/1
2	BGC	12-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	12-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	12-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	12-F	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	12-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	12-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	13-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	13-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	13-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	13-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	13-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	13-C	6	2	-	1/2/19/22	0/1/1/1
3	BGC	13-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	13-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	13-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	13-D	4	3	-	2/2/19/22	0/1/1/1
3	BGC	13-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	13-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	13-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	13-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	13-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	13-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	13-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	13-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	13-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	13-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	13-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	13-F	5	3	-	1/2/19/22	0/1/1/1
2	BGC	14-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	14-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	14-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	14-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	14-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	14-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	14-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	14-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	14-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	14-D	4	3	-	1/2/19/22	0/1/1/1
3	BGC	14-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	14-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	14-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	14-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	14-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	14-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	14-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	14-F	1	3	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	14-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	14-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	14-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	14-F	5	3	-	2/2/19/22	0/1/1/1
2	BGC	15-C	1	2	-	1/2/22/22	0/1/1/1
2	BGC	15-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	15-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	15-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	15-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	15-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	15-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	15-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	15-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	15-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	15-D	5	3	-	1/2/19/22	0/1/1/1
2	BGC	15-E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	15-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	15-E	3	2	-	1/2/19/22	0/1/1/1
2	BGC	15-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	15-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	15-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	15-F	1	3	-	2/2/22/22	0/1/1/1
3	BGC	15-F	2	3	-	1/2/19/22	0/1/1/1
3	BGC	15-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	15-F	4	3	-	2/2/19/22	0/1/1/1
3	BGC	15-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	16-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	16-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	16-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	16-C	4	2	-	2/2/19/22	0/1/1/1
2	BGC	16-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	16-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	16-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	16-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	16-D	3	3	-	1/2/19/22	0/1/1/1
3	BGC	16-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	16-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	16-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	16-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	16-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	16-E	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	16-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	16-E	6	2	-	1/2/19/22	0/1/1/1
3	BGC	16-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	16-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	16-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	16-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	16-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	17-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	17-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	17-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	17-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	17-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	17-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	17-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	17-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	17-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	17-D	4	3	-	2/2/19/22	0/1/1/1
3	BGC	17-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	17-E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	17-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	17-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	17-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	17-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	17-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	17-F	1	3	-	2/2/22/22	0/1/1/1
3	BGC	17-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	17-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	17-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	17-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	18-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	18-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	18-C	3	2	-	2/2/19/22	0/1/1/1
2	BGC	18-C	4	2	-	1/2/19/22	0/1/1/1
2	BGC	18-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	18-C	6	2	-	2/2/19/22	0/1/1/1
3	BGC	18-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	18-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	18-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	18-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	18-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	18-E	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	18-E	2	2	-	1/2/19/22	0/1/1/1
2	BGC	18-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	18-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	18-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	18-E	6	2	-	2/2/19/22	0/1/1/1
3	BGC	18-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	18-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	18-F	3	3	-	2/2/19/22	0/1/1/1
3	BGC	18-F	4	3	-	1/2/19/22	0/1/1/1
3	BGC	18-F	5	3	-	2/2/19/22	0/1/1/1
2	BGC	19-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	19-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	19-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	19-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	19-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	19-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	19-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	19-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	19-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	19-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	19-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	19-E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	19-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	19-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	19-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	19-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	19-E	6	2	-	2/2/19/22	0/1/1/1
3	BGC	19-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	19-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	19-F	3	3	-	1/2/19/22	0/1/1/1
3	BGC	19-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	19-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	2-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	2-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	2-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	2-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	2-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	2-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	2-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	2-D	2	3	-	1/2/19/22	0/1/1/1
3	BGC	2-D	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	2-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	2-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	2-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	2-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	2-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	2-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	2-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	2-E	6	2	-	1/2/19/22	0/1/1/1
3	BGC	2-F	1	3	-	2/2/22/22	0/1/1/1
3	BGC	2-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	2-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	2-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	2-F	5	3	-	1/2/19/22	0/1/1/1
2	BGC	20-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	20-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	20-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	20-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	20-C	5	2	-	2/2/19/22	0/1/1/1
2	BGC	20-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	20-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	20-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	20-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	20-D	4	3	-	2/2/19/22	0/1/1/1
3	BGC	20-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	20-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	20-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	20-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	20-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	20-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	20-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	20-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	20-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	20-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	20-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	20-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	21-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	21-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	21-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	21-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	21-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	21-C	6	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	21-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	21-D	2	3	-	1/2/19/22	0/1/1/1
3	BGC	21-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	21-D	4	3	-	2/2/19/22	0/1/1/1
3	BGC	21-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	21-E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	21-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	21-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	21-E	4	2	-	2/2/19/22	0/1/1/1
2	BGC	21-E	5	2	-	2/2/19/22	0/1/1/1
2	BGC	21-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	21-F	1	3	-	1/2/22/22	0/1/1/1
3	BGC	21-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	21-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	21-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	21-F	5	3	-	2/2/19/22	0/1/1/1
2	BGC	22-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	22-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	22-C	3	2	-	1/2/19/22	0/1/1/1
2	BGC	22-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	22-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	22-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	22-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	22-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	22-D	3	3	-	1/2/19/22	0/1/1/1
3	BGC	22-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	22-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	22-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	22-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	22-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	22-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	22-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	22-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	22-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	22-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	22-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	22-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	22-F	5	3	-	2/2/19/22	0/1/1/1
2	BGC	23-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	23-C	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	23-C	3	2	-	2/2/19/22	0/1/1/1
2	BGC	23-C	4	2	-	2/2/19/22	0/1/1/1
2	BGC	23-C	5	2	-	2/2/19/22	0/1/1/1
2	BGC	23-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	23-D	1	3	-	1/2/22/22	0/1/1/1
3	BGC	23-D	2	3	-	2/2/19/22	0/1/1/1
3	BGC	23-D	3	3	-	2/2/19/22	0/1/1/1
3	BGC	23-D	4	3	-	2/2/19/22	0/1/1/1
3	BGC	23-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	23-E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	23-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	23-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	23-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	23-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	23-E	6	2	-	2/2/19/22	0/1/1/1
3	BGC	23-F	1	3	-	2/2/22/22	0/1/1/1
3	BGC	23-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	23-F	3	3	-	2/2/19/22	0/1/1/1
3	BGC	23-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	23-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	24-C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	24-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	24-C	3	2	-	1/2/19/22	0/1/1/1
2	BGC	24-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	24-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	24-C	6	2	-	2/2/19/22	0/1/1/1
3	BGC	24-D	1	3	-	1/2/22/22	0/1/1/1
3	BGC	24-D	2	3	-	1/2/19/22	0/1/1/1
3	BGC	24-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	24-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	24-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	24-E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	24-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	24-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	24-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	24-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	24-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	24-F	1	3	-	2/2/22/22	0/1/1/1
3	BGC	24-F	2	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	24-F	3	3	-	2/2/19/22	0/1/1/1
3	BGC	24-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	24-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	25-C	1	2	-	1/2/22/22	0/1/1/1
2	BGC	25-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	25-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	25-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	25-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	25-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	25-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	25-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	25-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	25-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	25-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	25-E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	25-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	25-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	25-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	25-E	5	2	-	2/2/19/22	0/1/1/1
2	BGC	25-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	25-F	1	3	-	2/2/22/22	0/1/1/1
3	BGC	25-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	25-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	25-F	4	3	-	2/2/19/22	0/1/1/1
3	BGC	25-F	5	3	-	1/2/19/22	0/1/1/1
2	BGC	3-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	3-C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	3-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	3-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	3-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	3-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	3-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	3-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	3-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	3-D	4	3	-	1/2/19/22	0/1/1/1
3	BGC	3-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	3-E	1	2	-	1/2/22/22	0/1/1/1
2	BGC	3-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	3-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	3-E	4	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	3-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	3-E	6	2	-	2/2/19/22	0/1/1/1
3	BGC	3-F	1	3	-	1/2/22/22	0/1/1/1
3	BGC	3-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	3-F	3	3	-	2/2/19/22	0/1/1/1
3	BGC	3-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	3-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	4-C	1	2	-	1/2/22/22	0/1/1/1
2	BGC	4-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	4-C	3	2	-	2/2/19/22	0/1/1/1
2	BGC	4-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	4-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	4-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	4-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	4-D	2	3	-	1/2/19/22	0/1/1/1
3	BGC	4-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	4-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	4-D	5	3	-	2/2/19/22	0/1/1/1
2	BGC	4-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	4-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	4-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	4-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	4-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	4-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	4-F	1	3	-	2/2/22/22	0/1/1/1
3	BGC	4-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	4-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	4-F	4	3	-	2/2/19/22	0/1/1/1
3	BGC	4-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	5-C	1	2	-	1/2/22/22	0/1/1/1
2	BGC	5-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	5-C	3	2	-	2/2/19/22	0/1/1/1
2	BGC	5-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	5-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	5-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	5-D	1	3	-	1/2/22/22	0/1/1/1
3	BGC	5-D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	5-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	5-D	4	3	-	0/2/19/22	0/1/1/1
3	BGC	5-D	5	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	5-E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	5-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	5-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	5-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	5-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	5-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	5-F	1	3	-	2/2/22/22	0/1/1/1
3	BGC	5-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	5-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	5-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	5-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	6-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	6-C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	6-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	6-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	6-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	6-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	6-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	6-D	2	3	-	1/2/19/22	0/1/1/1
3	BGC	6-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	6-D	4	3	-	2/2/19/22	0/1/1/1
3	BGC	6-D	5	3	-	0/2/19/22	0/1/1/1
2	BGC	6-E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	6-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	6-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	6-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	6-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	6-E	6	2	-	0/2/19/22	0/1/1/1
3	BGC	6-F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	6-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	6-F	3	3	-	2/2/19/22	0/1/1/1
3	BGC	6-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	6-F	5	3	-	0/2/19/22	0/1/1/1
2	BGC	7-C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	7-C	2	2	-	1/2/19/22	0/1/1/1
2	BGC	7-C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	7-C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	7-C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	7-C	6	2	-	0/2/19/22	0/1/1/1
3	BGC	7-D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	7-D	2	3	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	9-C	6	2	-	2/2/19/22	0/1/1/1
3	BGC	9-D	1	3	-	0/2/22/22	0/1/1/1
3	BGC	9-D	2	3	-	1/2/19/22	0/1/1/1
3	BGC	9-D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	9-D	4	3	-	2/2/19/22	0/1/1/1
3	BGC	9-D	5	3	-	1/2/19/22	0/1/1/1
2	BGC	9-E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	9-E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	9-E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	9-E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	9-E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	9-E	6	2	-	1/2/19/22	0/1/1/1
3	BGC	9-F	1	3	-	1/2/22/22	0/1/1/1
3	BGC	9-F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	9-F	3	3	-	0/2/19/22	0/1/1/1
3	BGC	9-F	4	3	-	0/2/19/22	0/1/1/1
3	BGC	9-F	5	3	-	2/2/19/22	0/1/1/1

All (926) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-F	5	BGC	C2-C3	-5.62	1.43	1.52
3	3-D	5	BGC	C2-C3	-4.90	1.45	1.52
3	6-F	5	BGC	C2-C3	-4.83	1.45	1.52
3	9-D	5	BGC	C2-C3	-4.78	1.45	1.52
3	8-D	5	BGC	C2-C3	-4.70	1.45	1.52
3	4-D	5	BGC	C2-C3	-4.69	1.45	1.52
3	21-F	5	BGC	C2-C3	-4.68	1.45	1.52
3	12-F	5	BGC	C2-C3	-4.66	1.45	1.52
3	12-D	5	BGC	C2-C3	-4.66	1.45	1.52
3	21-D	5	BGC	C2-C3	-4.64	1.45	1.52
3	18-F	5	BGC	C2-C3	-4.61	1.45	1.52
3	2-D	5	BGC	C2-C3	-4.60	1.45	1.52
3	24-D	5	BGC	C2-C3	-4.60	1.45	1.52
3	16-F	5	BGC	C2-C3	-4.59	1.45	1.52
3	16-D	5	BGC	C2-C3	-4.57	1.45	1.52
3	11-D	5	BGC	C2-C3	-4.49	1.45	1.52
3	1-F	5	BGC	C2-C3	-4.48	1.45	1.52
3	10-D	5	BGC	C2-C3	-4.46	1.45	1.52
3	17-F	5	BGC	C2-C3	-4.43	1.45	1.52
3	20-D	5	BGC	C2-C3	-4.41	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	20-F	5	BGC	C2-C3	-4.39	1.45	1.52
3	15-D	5	BGC	C2-C3	-4.37	1.45	1.52
3	25-D	5	BGC	C2-C3	-4.35	1.45	1.52
3	14-D	5	BGC	C2-C3	-4.35	1.45	1.52
3	3-F	5	BGC	C2-C3	-4.35	1.45	1.52
3	19-F	5	BGC	C2-C3	-4.31	1.45	1.52
3	23-D	5	BGC	C2-C3	-4.30	1.45	1.52
3	5-D	5	BGC	C2-C3	-4.29	1.45	1.52
3	24-F	5	BGC	C2-C3	-4.29	1.45	1.52
3	5-F	5	BGC	C2-C3	-4.27	1.45	1.52
3	8-F	5	BGC	C2-C3	-4.27	1.45	1.52
3	4-F	5	BGC	C2-C3	-4.25	1.46	1.52
3	17-D	5	BGC	C2-C3	-4.24	1.46	1.52
3	23-F	5	BGC	C2-C3	-4.23	1.46	1.52
3	1-D	5	BGC	C2-C3	-4.21	1.46	1.52
3	15-F	5	BGC	C2-C3	-4.19	1.46	1.52
3	7-F	5	BGC	C2-C3	-4.16	1.46	1.52
3	18-D	5	BGC	C2-C3	-4.13	1.46	1.52
3	19-D	5	BGC	C2-C3	-4.13	1.46	1.52
3	4-D	4	BGC	C2-C3	-4.11	1.46	1.52
3	10-F	5	BGC	C2-C3	-4.11	1.46	1.52
3	7-D	5	BGC	C2-C3	-4.07	1.46	1.52
3	2-F	5	BGC	C2-C3	-4.06	1.46	1.52
3	14-F	5	BGC	C2-C3	-4.03	1.46	1.52
3	11-F	5	BGC	C2-C3	-4.02	1.46	1.52
3	22-F	5	BGC	C2-C3	-4.00	1.46	1.52
3	25-F	5	BGC	C2-C3	-3.86	1.46	1.52
3	5-F	2	BGC	O5-C1	3.83	1.50	1.43
3	17-F	2	BGC	O5-C1	3.82	1.50	1.43
3	18-F	2	BGC	O5-C1	3.81	1.50	1.43
3	13-D	5	BGC	C2-C3	-3.79	1.46	1.52
3	22-D	5	BGC	C2-C3	-3.76	1.46	1.52
3	11-D	4	BGC	C2-C3	-3.76	1.46	1.52
2	14-E	1	BGC	C3-C2	-3.69	1.42	1.52
3	11-F	2	BGC	O5-C1	3.66	1.49	1.43
3	20-F	2	BGC	O5-C1	3.62	1.49	1.43
3	21-F	2	BGC	O5-C1	3.60	1.49	1.43
2	13-C	3	BGC	C2-C3	-3.60	1.47	1.52
2	9-E	1	BGC	C3-C2	-3.57	1.43	1.52
3	14-F	2	BGC	O5-C1	3.55	1.49	1.43
2	12-E	1	BGC	C3-C2	-3.54	1.43	1.52
2	25-E	1	BGC	O3-C3	3.52	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	13-F	5	BGC	C2-C3	-3.52	1.47	1.52
2	14-E	2	BGC	C2-C3	-3.52	1.47	1.52
3	6-D	5	BGC	C2-C3	-3.51	1.47	1.52
2	9-C	1	BGC	C3-C2	-3.50	1.43	1.52
3	2-F	2	BGC	O5-C1	3.47	1.49	1.43
3	6-D	2	BGC	C2-C3	-3.43	1.47	1.52
2	21-E	1	BGC	C3-C2	-3.43	1.43	1.52
2	21-C	2	BGC	C2-C3	-3.42	1.47	1.52
2	20-C	1	BGC	O3-C3	3.42	1.51	1.43
2	15-C	2	BGC	C2-C3	-3.38	1.47	1.52
2	11-E	1	BGC	C3-C2	-3.38	1.43	1.52
3	17-D	4	BGC	C2-C3	-3.37	1.47	1.52
3	24-F	2	BGC	O5-C1	3.36	1.49	1.43
3	23-F	1	BGC	C3-C2	-3.35	1.43	1.52
3	13-D	4	BGC	C2-C3	-3.35	1.47	1.52
3	16-F	2	BGC	O5-C1	3.35	1.49	1.43
2	5-E	2	BGC	C2-C3	-3.34	1.47	1.52
3	12-F	2	BGC	O5-C1	3.34	1.49	1.43
2	24-E	2	BGC	C2-C3	-3.34	1.47	1.52
2	3-E	1	BGC	O3-C3	3.34	1.51	1.43
3	1-F	2	BGC	O5-C1	3.31	1.49	1.43
2	19-C	1	BGC	C3-C2	-3.30	1.43	1.52
2	8-C	1	BGC	O3-C3	3.30	1.51	1.43
2	10-E	2	BGC	C2-C3	-3.30	1.47	1.52
2	21-C	1	BGC	C3-C2	-3.30	1.43	1.52
3	6-F	2	BGC	O5-C1	3.30	1.49	1.43
2	24-C	3	BGC	C2-C3	-3.30	1.47	1.52
2	7-C	3	BGC	C2-C3	-3.29	1.47	1.52
2	3-E	3	BGC	C2-C3	-3.29	1.47	1.52
2	10-E	6	BGC	C2-C3	-3.29	1.47	1.52
2	13-C	1	BGC	C3-C2	-3.28	1.43	1.52
2	21-E	2	BGC	C2-C3	-3.28	1.47	1.52
2	3-C	1	BGC	O3-C3	3.28	1.51	1.43
3	15-F	2	BGC	O5-C1	3.27	1.49	1.43
3	15-D	1	BGC	C3-C2	-3.26	1.43	1.52
2	21-C	1	BGC	O3-C3	3.26	1.51	1.43
2	4-C	1	BGC	C3-C2	-3.25	1.43	1.52
3	3-F	2	BGC	O5-C1	3.25	1.49	1.43
3	1-D	4	BGC	C2-C3	-3.25	1.47	1.52
2	12-C	1	BGC	C3-C2	-3.25	1.43	1.52
2	11-C	1	BGC	O3-C3	3.24	1.51	1.43
2	17-E	6	BGC	C4-C3	-3.24	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-E	1	BGC	C3-C2	-3.24	1.43	1.52
3	25-D	4	BGC	C2-C3	-3.24	1.47	1.52
3	14-D	4	BGC	C2-C3	-3.23	1.47	1.52
3	9-F	2	BGC	O5-C1	3.22	1.49	1.43
2	5-C	6	BGC	C4-C3	-3.22	1.44	1.52
2	16-E	3	BGC	C2-C3	-3.22	1.47	1.52
2	6-E	2	BGC	C2-C3	-3.22	1.47	1.52
2	10-E	1	BGC	C3-C2	-3.22	1.44	1.52
2	4-C	3	BGC	C2-C3	-3.21	1.47	1.52
2	14-C	1	BGC	O3-C3	3.20	1.50	1.43
3	10-F	2	BGC	O5-C1	3.20	1.49	1.43
2	18-C	1	BGC	O3-C3	3.20	1.50	1.43
3	20-D	4	BGC	C2-C3	-3.19	1.47	1.52
3	13-F	4	BGC	C2-C3	-3.19	1.47	1.52
2	5-E	1	BGC	C3-C2	-3.19	1.44	1.52
2	2-C	1	BGC	O3-C3	3.19	1.50	1.43
2	7-C	2	BGC	C4-C3	-3.19	1.44	1.52
2	16-C	1	BGC	O3-C3	3.18	1.50	1.43
2	8-E	1	BGC	C3-C2	-3.18	1.44	1.52
2	13-C	1	BGC	O1-C1	-3.17	1.29	1.39
2	17-C	1	BGC	O3-C3	3.17	1.50	1.43
2	23-C	6	BGC	C4-C3	-3.17	1.44	1.52
2	17-E	6	BGC	C2-C3	-3.17	1.47	1.52
2	22-E	2	BGC	C2-C3	-3.16	1.47	1.52
2	4-C	1	BGC	O3-C3	3.16	1.50	1.43
2	12-C	1	BGC	O3-C3	3.16	1.50	1.43
2	14-C	1	BGC	C3-C2	-3.14	1.44	1.52
2	7-C	1	BGC	C3-C2	-3.13	1.44	1.52
2	20-E	1	BGC	C3-C2	-3.13	1.44	1.52
2	4-E	2	BGC	C2-C3	-3.13	1.47	1.52
2	8-E	2	BGC	C4-C3	-3.13	1.44	1.52
3	7-F	2	BGC	O5-C1	3.12	1.48	1.43
2	4-E	1	BGC	C3-C2	-3.12	1.44	1.52
2	17-C	3	BGC	C2-C3	-3.11	1.47	1.52
2	24-E	1	BGC	C3-C2	-3.11	1.44	1.52
2	16-C	1	BGC	C3-C2	-3.11	1.44	1.52
3	20-D	3	BGC	C2-C3	-3.11	1.47	1.52
2	15-C	1	BGC	C3-C2	-3.09	1.44	1.52
2	11-E	2	BGC	C2-C3	-3.09	1.47	1.52
2	2-C	5	BGC	O3-C3	3.09	1.50	1.43
2	1-C	1	BGC	O3-C3	3.08	1.50	1.43
2	25-C	1	BGC	O3-C3	3.08	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	15-E	6	BGC	C2-C3	-3.08	1.47	1.52
2	24-E	6	BGC	C4-C3	-3.07	1.44	1.52
2	6-E	1	BGC	C3-C2	-3.07	1.44	1.52
2	16-C	6	BGC	C4-C3	-3.07	1.44	1.52
2	19-C	1	BGC	O1-C1	-3.07	1.30	1.39
2	12-C	3	BGC	C2-C3	-3.07	1.47	1.52
3	15-F	1	BGC	C3-C2	-3.06	1.44	1.52
3	13-F	2	BGC	O5-C1	3.05	1.48	1.43
2	11-C	1	BGC	C3-C2	-3.05	1.44	1.52
3	17-F	1	BGC	C3-C2	-3.05	1.44	1.52
3	9-D	1	BGC	C3-C2	-3.04	1.44	1.52
2	10-C	1	BGC	O3-C3	3.04	1.50	1.43
2	5-C	1	BGC	O1-C1	-3.04	1.30	1.39
2	1-E	1	BGC	C3-C2	-3.04	1.44	1.52
2	9-C	1	BGC	O3-C3	3.03	1.50	1.43
3	18-D	1	BGC	C3-C2	-3.03	1.44	1.52
2	24-C	2	BGC	C2-C3	-3.03	1.47	1.52
2	8-C	3	BGC	C2-C3	-3.02	1.47	1.52
2	16-C	3	BGC	C2-C3	-3.02	1.47	1.52
3	19-F	2	BGC	O5-C1	3.02	1.48	1.43
2	20-E	2	BGC	C2-C3	-3.02	1.47	1.52
3	12-D	4	BGC	C2-C3	-3.02	1.47	1.52
2	3-C	3	BGC	C2-C3	-3.01	1.47	1.52
3	11-D	3	BGC	C2-C3	-3.01	1.47	1.52
2	23-C	1	BGC	O3-C3	3.01	1.50	1.43
2	15-E	2	BGC	C2-C3	-3.01	1.47	1.52
3	6-D	2	BGC	O5-C1	3.01	1.48	1.43
2	23-E	1	BGC	C3-C2	-3.01	1.44	1.52
2	5-E	2	BGC	C4-C3	-3.01	1.44	1.52
3	21-D	4	BGC	C2-C3	-3.01	1.47	1.52
2	16-E	1	BGC	C3-C2	-3.00	1.44	1.52
3	3-D	1	BGC	C3-C2	-3.00	1.44	1.52
2	16-E	5	BGC	C2-C3	-3.00	1.47	1.52
3	23-D	1	BGC	C3-C2	-2.99	1.44	1.52
2	2-E	1	BGC	O3-C3	2.99	1.50	1.43
2	7-E	1	BGC	C3-C2	-2.99	1.44	1.52
3	24-D	4	BGC	C2-C3	-2.99	1.47	1.52
2	4-C	5	BGC	O3-C3	2.99	1.50	1.43
3	23-D	4	BGC	C2-C3	-2.99	1.47	1.52
3	22-F	4	BGC	O5-C1	2.98	1.48	1.43
2	22-C	1	BGC	O3-C3	2.98	1.50	1.43
3	5-D	1	BGC	C3-C2	-2.98	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-C	1	BGC	O1-C1	-2.98	1.30	1.39
2	5-C	1	BGC	O3-C3	2.98	1.50	1.43
3	7-F	4	BGC	C2-C3	-2.98	1.47	1.52
2	18-C	5	BGC	O3-C3	2.97	1.50	1.43
2	22-E	5	BGC	C2-C3	-2.97	1.47	1.52
2	18-C	1	BGC	C3-C2	-2.97	1.44	1.52
2	3-C	5	BGC	O3-C3	2.97	1.50	1.43
2	22-C	5	BGC	O3-C3	2.97	1.50	1.43
3	15-D	4	BGC	C2-C3	-2.97	1.47	1.52
2	23-E	3	BGC	C2-C3	-2.97	1.47	1.52
2	13-E	3	BGC	C2-C3	-2.96	1.47	1.52
2	2-C	6	BGC	C4-C3	-2.96	1.44	1.52
2	12-C	1	BGC	O1-C1	-2.96	1.30	1.39
2	4-C	6	BGC	C4-C3	-2.95	1.44	1.52
2	9-E	6	BGC	C2-C3	-2.95	1.48	1.52
3	2-D	1	BGC	C3-C2	-2.95	1.44	1.52
2	23-C	1	BGC	O1-C1	-2.95	1.30	1.39
2	19-C	1	BGC	O3-C3	2.94	1.50	1.43
2	20-C	1	BGC	C3-C2	-2.94	1.44	1.52
2	22-C	1	BGC	C3-C2	-2.94	1.44	1.52
3	16-D	1	BGC	C3-C2	-2.94	1.44	1.52
2	9-C	1	BGC	O1-C1	-2.94	1.30	1.39
2	3-E	2	BGC	C2-C3	-2.94	1.48	1.52
2	17-E	6	BGC	O6-C6	-2.94	1.30	1.42
2	23-C	1	BGC	C3-C2	-2.93	1.44	1.52
2	24-E	2	BGC	C4-C3	-2.93	1.44	1.52
2	12-E	2	BGC	C2-C3	-2.93	1.48	1.52
3	7-D	4	BGC	C2-C3	-2.93	1.48	1.52
2	5-C	1	BGC	C3-C2	-2.93	1.44	1.52
2	12-E	6	BGC	C4-C3	-2.93	1.44	1.52
2	15-C	1	BGC	O3-C3	2.93	1.50	1.43
2	3-C	1	BGC	C3-C2	-2.93	1.44	1.52
2	22-E	6	BGC	C2-C3	-2.93	1.48	1.52
3	5-F	1	BGC	C3-C2	-2.93	1.44	1.52
2	14-E	6	BGC	C2-C3	-2.92	1.48	1.52
3	6-D	4	BGC	C2-C3	-2.92	1.48	1.52
3	13-F	1	BGC	C3-C2	-2.92	1.44	1.52
2	10-E	1	BGC	O3-C3	2.92	1.50	1.43
2	21-C	3	BGC	C2-C3	-2.92	1.48	1.52
2	6-C	6	BGC	C4-C3	-2.92	1.44	1.52
3	8-F	2	BGC	O5-C1	2.92	1.48	1.43
3	19-D	4	BGC	C2-C3	-2.91	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	22-D	1	BGC	C3-C2	-2.91	1.44	1.52
2	2-E	1	BGC	C3-C2	-2.91	1.44	1.52
2	22-E	1	BGC	C3-C2	-2.91	1.44	1.52
2	23-E	6	BGC	C2-C3	-2.91	1.48	1.52
2	20-E	1	BGC	O3-C3	2.90	1.50	1.43
2	8-C	2	BGC	C2-C3	-2.90	1.48	1.52
3	10-F	4	BGC	O5-C1	2.90	1.48	1.43
3	4-F	1	BGC	C3-C2	-2.90	1.44	1.52
2	4-E	6	BGC	C2-C3	-2.90	1.48	1.52
2	8-C	1	BGC	C3-C2	-2.90	1.44	1.52
2	8-E	2	BGC	C2-C3	-2.89	1.48	1.52
2	14-E	2	BGC	C4-C3	-2.89	1.44	1.52
2	15-C	1	BGC	O1-C1	-2.89	1.30	1.39
3	19-F	1	BGC	C3-C2	-2.89	1.44	1.52
3	6-D	1	BGC	C3-C2	-2.89	1.44	1.52
2	13-C	1	BGC	O3-C3	2.89	1.50	1.43
2	6-C	1	BGC	O3-C3	2.88	1.50	1.43
2	25-E	3	BGC	C2-C3	-2.88	1.48	1.52
2	3-E	6	BGC	C2-C3	-2.88	1.48	1.52
2	22-E	1	BGC	O3-C3	2.88	1.50	1.43
3	17-D	1	BGC	C3-C2	-2.88	1.44	1.52
3	22-F	1	BGC	C3-C2	-2.88	1.44	1.52
3	14-D	2	BGC	O5-C1	2.88	1.48	1.43
2	21-C	2	BGC	C4-C3	-2.87	1.44	1.52
3	4-F	2	BGC	O5-C1	2.87	1.48	1.43
2	13-C	3	BGC	O3-C3	2.87	1.50	1.43
2	16-E	2	BGC	C2-C3	-2.87	1.48	1.52
3	25-F	2	BGC	O5-C1	2.87	1.48	1.43
3	25-F	3	BGC	C2-C3	-2.87	1.48	1.52
2	14-E	1	BGC	O1-C1	-2.87	1.30	1.39
2	2-C	1	BGC	C3-C2	-2.87	1.44	1.52
3	12-D	1	BGC	C3-C2	-2.87	1.44	1.52
3	10-F	4	BGC	C2-C3	-2.86	1.48	1.52
2	17-C	1	BGC	C3-C2	-2.86	1.44	1.52
3	23-F	2	BGC	O5-C1	2.86	1.48	1.43
2	1-E	2	BGC	C2-C3	-2.86	1.48	1.52
2	19-E	1	BGC	C3-C2	-2.86	1.44	1.52
2	19-C	4	BGC	O5-C1	2.86	1.48	1.43
3	21-D	1	BGC	C3-C2	-2.85	1.44	1.52
2	20-C	5	BGC	O3-C3	2.85	1.50	1.43
3	14-D	1	BGC	C3-C2	-2.85	1.44	1.52
2	12-E	6	BGC	C2-C3	-2.85	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-D	4	BGC	C2-C3	-2.85	1.48	1.52
2	1-C	3	BGC	C2-C3	-2.85	1.48	1.52
2	18-E	1	BGC	C3-C2	-2.85	1.45	1.52
3	23-F	4	BGC	C2-C3	-2.85	1.48	1.52
3	8-D	4	BGC	C2-C3	-2.84	1.48	1.52
2	6-C	1	BGC	C3-C2	-2.84	1.45	1.52
2	23-C	2	BGC	C2-C3	-2.84	1.48	1.52
2	13-C	2	BGC	C2-C3	-2.84	1.48	1.52
3	14-F	1	BGC	C3-C2	-2.84	1.45	1.52
3	24-D	1	BGC	C3-C2	-2.83	1.45	1.52
3	5-D	4	BGC	C2-C3	-2.83	1.48	1.52
3	7-F	4	BGC	O5-C1	2.83	1.48	1.43
2	17-E	1	BGC	C3-C2	-2.83	1.45	1.52
3	2-F	1	BGC	C3-C2	-2.83	1.45	1.52
3	13-D	1	BGC	C3-C2	-2.83	1.45	1.52
2	21-E	1	BGC	O1-C1	-2.83	1.30	1.39
3	10-F	1	BGC	C3-C2	-2.83	1.45	1.52
2	5-C	2	BGC	C2-C3	-2.82	1.48	1.52
3	13-F	4	BGC	O5-C1	2.82	1.48	1.43
2	10-E	3	BGC	C2-C3	-2.82	1.48	1.52
2	24-C	1	BGC	O3-C3	2.82	1.49	1.43
2	24-E	6	BGC	C2-C3	-2.82	1.48	1.52
2	1-C	1	BGC	C3-C2	-2.81	1.45	1.52
2	25-C	1	BGC	C3-C2	-2.81	1.45	1.52
2	19-C	6	BGC	C4-C3	-2.81	1.45	1.52
2	7-C	1	BGC	O3-C3	2.81	1.49	1.43
2	10-C	1	BGC	C3-C2	-2.81	1.45	1.52
3	4-F	3	BGC	C2-C3	-2.81	1.48	1.52
3	18-F	1	BGC	C3-C2	-2.81	1.45	1.52
3	4-D	1	BGC	C3-C2	-2.81	1.45	1.52
2	9-E	1	BGC	O1-C1	-2.80	1.30	1.39
3	10-D	1	BGC	C3-C2	-2.80	1.45	1.52
2	1-C	6	BGC	C4-C3	-2.80	1.45	1.52
3	19-D	1	BGC	C3-C2	-2.80	1.45	1.52
2	8-E	3	BGC	C2-C3	-2.79	1.48	1.52
2	13-E	6	BGC	C2-C3	-2.79	1.48	1.52
2	8-E	5	BGC	C2-C3	-2.79	1.48	1.52
3	25-D	1	BGC	C3-C2	-2.79	1.45	1.52
2	14-C	6	BGC	C4-C3	-2.78	1.45	1.52
2	16-E	6	BGC	C2-C3	-2.78	1.48	1.52
3	11-F	1	BGC	C3-C2	-2.78	1.45	1.52
2	18-C	3	BGC	C2-C3	-2.78	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	19-E	2	BGC	C2-C3	-2.78	1.48	1.52
2	15-E	1	BGC	C3-C2	-2.78	1.45	1.52
2	21-E	3	BGC	C2-C3	-2.78	1.48	1.52
3	20-D	2	BGC	O5-C1	2.78	1.48	1.43
2	25-C	5	BGC	O3-C3	2.77	1.49	1.43
2	16-C	6	BGC	C2-C3	-2.77	1.48	1.52
2	5-C	3	BGC	C2-C3	-2.77	1.48	1.52
2	1-E	3	BGC	C2-C3	-2.77	1.48	1.52
2	8-C	4	BGC	O5-C1	2.77	1.48	1.43
2	25-E	2	BGC	C4-C3	-2.77	1.45	1.52
2	9-E	2	BGC	C2-C3	-2.76	1.48	1.52
2	11-E	6	BGC	C4-C3	-2.76	1.45	1.52
2	3-E	6	BGC	C4-C3	-2.76	1.45	1.52
3	12-D	2	BGC	O5-C1	2.76	1.48	1.43
2	17-E	2	BGC	C2-C3	-2.75	1.48	1.52
2	24-E	5	BGC	C2-C3	-2.75	1.48	1.52
2	15-E	1	BGC	O3-C3	2.75	1.49	1.43
2	21-E	1	BGC	O3-C3	2.75	1.49	1.43
2	4-C	1	BGC	O1-C1	-2.75	1.31	1.39
3	13-D	3	BGC	C2-C3	-2.75	1.48	1.52
3	5-F	4	BGC	C2-C3	-2.75	1.48	1.52
2	22-C	2	BGC	C2-C3	-2.74	1.48	1.52
3	12-D	3	BGC	C2-C3	-2.74	1.48	1.52
3	13-F	3	BGC	C2-C3	-2.74	1.48	1.52
3	24-F	1	BGC	C3-C2	-2.74	1.45	1.52
2	5-E	6	BGC	C4-C3	-2.74	1.45	1.52
2	4-E	1	BGC	O3-C3	2.74	1.49	1.43
2	10-C	1	BGC	O1-C1	-2.74	1.31	1.39
2	24-C	1	BGC	O1-C1	-2.74	1.31	1.39
2	2-E	6	BGC	C2-C3	-2.74	1.48	1.52
3	12-F	4	BGC	C2-C3	-2.73	1.48	1.52
2	25-E	6	BGC	C4-C3	-2.73	1.45	1.52
2	17-E	5	BGC	C2-C3	-2.73	1.48	1.52
3	1-D	2	BGC	O5-C1	2.73	1.48	1.43
2	9-C	3	BGC	C2-C3	-2.73	1.48	1.52
2	23-E	2	BGC	C2-C3	-2.73	1.48	1.52
2	19-E	1	BGC	O3-C3	2.72	1.49	1.43
2	11-C	3	BGC	C2-C3	-2.72	1.48	1.52
2	17-C	6	BGC	C4-C3	-2.72	1.45	1.52
2	9-E	6	BGC	C4-C3	-2.72	1.45	1.52
2	9-C	5	BGC	O3-C3	2.72	1.49	1.43
2	17-C	1	BGC	O1-C1	-2.72	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-C	6	BGC	C4-C3	-2.72	1.45	1.52
2	8-C	1	BGC	O1-C1	-2.72	1.31	1.39
2	20-E	6	BGC	C4-C3	-2.72	1.45	1.52
2	2-E	6	BGC	C4-C3	-2.71	1.45	1.52
2	14-E	6	BGC	C4-C3	-2.71	1.45	1.52
3	18-D	4	BGC	C2-C3	-2.71	1.48	1.52
2	4-C	2	BGC	C2-C3	-2.71	1.48	1.52
2	7-C	6	BGC	C4-C3	-2.71	1.45	1.52
2	9-E	3	BGC	C2-C3	-2.71	1.48	1.52
2	13-E	6	BGC	C4-C3	-2.71	1.45	1.52
2	12-E	1	BGC	O1-C1	-2.70	1.31	1.39
2	6-C	1	BGC	O1-C1	-2.70	1.31	1.39
2	18-E	2	BGC	C2-C3	-2.70	1.48	1.52
3	1-D	1	BGC	C3-C2	-2.70	1.45	1.52
2	5-E	6	BGC	C2-C3	-2.70	1.48	1.52
2	18-C	1	BGC	O1-C1	-2.70	1.31	1.39
3	8-F	4	BGC	C2-C3	-2.70	1.48	1.52
3	3-D	3	BGC	C2-C3	-2.69	1.48	1.52
3	3-D	4	BGC	C2-C3	-2.69	1.48	1.52
2	23-C	5	BGC	O3-C3	2.69	1.49	1.43
3	22-F	2	BGC	O5-C1	2.69	1.48	1.43
2	7-E	6	BGC	C4-C3	-2.69	1.45	1.52
2	16-C	1	BGC	O1-C1	-2.69	1.31	1.39
2	9-C	6	BGC	C4-C3	-2.68	1.45	1.52
2	3-E	2	BGC	C4-C3	-2.68	1.45	1.52
2	4-E	6	BGC	C4-C3	-2.68	1.45	1.52
3	21-F	1	BGC	C3-C2	-2.68	1.45	1.52
2	25-C	3	BGC	C2-C3	-2.68	1.48	1.52
2	21-C	1	BGC	O1-C1	-2.68	1.31	1.39
2	16-E	2	BGC	C4-C3	-2.68	1.45	1.52
2	20-C	1	BGC	O1-C1	-2.68	1.31	1.39
3	8-D	2	BGC	O5-C1	2.67	1.48	1.43
3	8-F	1	BGC	C3-C2	-2.67	1.45	1.52
3	16-D	2	BGC	O5-C1	2.67	1.48	1.43
2	8-E	1	BGC	O1-C1	-2.67	1.31	1.39
2	23-C	2	BGC	O3-C3	2.66	1.49	1.43
2	20-C	2	BGC	C2-C3	-2.66	1.48	1.52
3	15-F	3	BGC	C2-C3	-2.66	1.48	1.52
2	23-E	6	BGC	C4-C3	-2.66	1.45	1.52
2	10-E	2	BGC	C4-C3	-2.66	1.45	1.52
2	10-C	3	BGC	C2-C3	-2.66	1.48	1.52
2	1-E	2	BGC	C4-C3	-2.66	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-C	3	BGC	C2-C3	-2.66	1.48	1.52
2	20-E	5	BGC	C2-C3	-2.66	1.48	1.52
3	4-D	2	BGC	O5-C1	2.66	1.48	1.43
2	3-C	1	BGC	O1-C1	-2.66	1.31	1.39
3	5-F	4	BGC	O5-C1	2.66	1.48	1.43
3	7-D	1	BGC	C3-C2	-2.66	1.45	1.52
2	3-E	1	BGC	C3-C2	-2.66	1.45	1.52
2	12-C	5	BGC	O3-C3	2.65	1.49	1.43
2	1-C	2	BGC	C2-C3	-2.65	1.48	1.52
2	1-C	5	BGC	O3-C3	2.65	1.49	1.43
3	8-F	3	BGC	C2-C3	-2.65	1.48	1.52
3	6-F	1	BGC	C3-C2	-2.65	1.45	1.52
2	12-C	6	BGC	C4-C3	-2.65	1.45	1.52
3	7-D	2	BGC	O5-C1	2.65	1.48	1.43
2	15-C	6	BGC	C4-C3	-2.64	1.45	1.52
3	11-F	3	BGC	C2-C3	-2.64	1.48	1.52
3	11-D	1	BGC	C3-C2	-2.64	1.45	1.52
2	11-E	6	BGC	C2-C3	-2.64	1.48	1.52
3	22-D	4	BGC	C2-C3	-2.64	1.48	1.52
3	15-F	4	BGC	C2-C3	-2.64	1.48	1.52
2	14-C	1	BGC	O1-C1	-2.64	1.31	1.39
2	3-C	2	BGC	C2-C3	-2.64	1.48	1.52
2	9-C	2	BGC	C2-C3	-2.64	1.48	1.52
2	6-E	6	BGC	C4-C3	-2.63	1.45	1.52
2	6-C	5	BGC	O3-C3	2.63	1.49	1.43
2	24-C	1	BGC	C3-C2	-2.63	1.45	1.52
2	15-E	5	BGC	O3-C3	2.63	1.49	1.43
2	15-E	1	BGC	O1-C1	-2.63	1.31	1.39
2	17-E	1	BGC	O3-C3	2.63	1.49	1.43
2	22-E	6	BGC	C4-C3	-2.63	1.45	1.52
3	10-D	4	BGC	C2-C3	-2.63	1.48	1.52
2	19-C	2	BGC	C2-C3	-2.63	1.48	1.52
2	4-E	3	BGC	C2-C3	-2.63	1.48	1.52
3	9-F	1	BGC	C3-C2	-2.63	1.45	1.52
3	14-F	3	BGC	C2-C3	-2.63	1.48	1.52
2	15-C	5	BGC	O3-C3	2.62	1.49	1.43
2	16-E	6	BGC	C4-C3	-2.62	1.45	1.52
3	9-D	4	BGC	C2-C3	-2.62	1.48	1.52
2	21-E	2	BGC	C4-C3	-2.62	1.45	1.52
2	4-C	6	BGC	O3-C3	2.62	1.49	1.43
2	11-E	1	BGC	O3-C3	2.61	1.49	1.43
3	20-F	4	BGC	O5-C1	2.61	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	11-E	1	BGC	O1-C1	-2.61	1.31	1.39
2	19-E	5	BGC	O3-C3	2.60	1.49	1.43
2	7-E	1	BGC	O3-C3	2.60	1.49	1.43
2	1-E	6	BGC	C4-C3	-2.60	1.45	1.52
2	22-C	1	BGC	O1-C1	-2.60	1.31	1.39
2	6-E	1	BGC	O1-C1	-2.60	1.31	1.39
3	17-D	2	BGC	O5-C1	2.60	1.48	1.43
3	8-D	1	BGC	C3-C2	-2.60	1.45	1.52
2	18-E	1	BGC	O3-C3	2.60	1.49	1.43
2	7-E	2	BGC	C2-C3	-2.60	1.48	1.52
2	11-E	3	BGC	C2-C3	-2.60	1.48	1.52
3	20-F	4	BGC	C2-C3	-2.60	1.48	1.52
2	15-C	3	BGC	C2-C3	-2.60	1.48	1.52
3	3-F	1	BGC	C3-C2	-2.60	1.45	1.52
2	11-C	1	BGC	O1-C1	-2.60	1.31	1.39
3	16-D	4	BGC	C2-C3	-2.60	1.48	1.52
2	15-E	6	BGC	C4-C3	-2.60	1.45	1.52
2	13-E	1	BGC	O3-C3	2.59	1.49	1.43
2	23-E	1	BGC	O3-C3	2.59	1.49	1.43
2	5-C	5	BGC	O3-C3	2.59	1.49	1.43
3	19-D	3	BGC	O3-C3	2.59	1.49	1.43
3	24-F	4	BGC	C2-C3	-2.59	1.48	1.52
2	12-C	2	BGC	C2-C3	-2.59	1.48	1.52
2	2-C	3	BGC	C2-C3	-2.58	1.48	1.52
3	19-F	4	BGC	O5-C1	2.58	1.48	1.43
2	11-C	2	BGC	C2-C3	-2.58	1.48	1.52
2	11-E	2	BGC	C4-C3	-2.58	1.45	1.52
2	16-C	2	BGC	C2-C3	-2.57	1.48	1.52
3	20-F	1	BGC	O3-C3	2.57	1.49	1.43
2	5-E	3	BGC	C2-C3	-2.57	1.48	1.52
2	18-C	6	BGC	C4-C3	-2.57	1.45	1.52
2	7-E	6	BGC	C2-C3	-2.57	1.48	1.52
2	25-C	2	BGC	O3-C3	2.57	1.49	1.43
2	8-C	3	BGC	O3-C3	2.57	1.49	1.43
3	20-D	1	BGC	C3-C2	-2.57	1.45	1.52
3	15-D	3	BGC	C2-C3	-2.56	1.48	1.52
2	11-C	2	BGC	O3-C3	2.56	1.49	1.43
2	6-C	3	BGC	C2-C3	-2.56	1.48	1.52
2	20-E	2	BGC	C4-C3	-2.56	1.45	1.52
2	13-C	5	BGC	O3-C3	2.55	1.49	1.43
3	6-F	4	BGC	C2-C3	-2.55	1.48	1.52
2	14-E	3	BGC	C2-C3	-2.55	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	25-C	2	BGC	C2-C3	-2.55	1.48	1.52
2	24-C	6	BGC	C2-C3	-2.55	1.48	1.52
2	11-C	5	BGC	O3-C3	2.54	1.49	1.43
2	12-E	5	BGC	O3-C3	2.54	1.49	1.43
2	25-C	1	BGC	O1-C1	-2.54	1.31	1.39
2	24-E	3	BGC	C2-C3	-2.54	1.48	1.52
2	8-E	6	BGC	C4-C3	-2.54	1.45	1.52
2	10-C	2	BGC	C2-C3	-2.54	1.48	1.52
2	13-E	2	BGC	C2-C3	-2.54	1.48	1.52
3	25-F	1	BGC	C3-C2	-2.53	1.45	1.52
2	13-E	1	BGC	O1-C1	-2.53	1.31	1.39
3	22-F	4	BGC	C2-C3	-2.53	1.48	1.52
2	14-C	5	BGC	O3-C3	2.53	1.49	1.43
2	19-C	3	BGC	O3-C3	2.53	1.49	1.43
2	1-E	1	BGC	O3-C3	2.53	1.49	1.43
3	5-D	2	BGC	O5-C1	2.53	1.47	1.43
3	14-D	3	BGC	C2-C3	-2.53	1.48	1.52
2	18-E	3	BGC	C2-C3	-2.53	1.48	1.52
3	16-F	1	BGC	C3-C2	-2.53	1.45	1.52
2	20-C	6	BGC	C4-C3	-2.52	1.45	1.52
2	2-C	3	BGC	O3-C3	2.52	1.49	1.43
3	8-D	3	BGC	C2-C3	-2.52	1.48	1.52
3	12-F	1	BGC	C3-C2	-2.52	1.45	1.52
2	18-E	2	BGC	C4-C3	-2.52	1.45	1.52
2	7-E	1	BGC	O1-C1	-2.52	1.31	1.39
3	4-F	4	BGC	O5-C1	2.52	1.47	1.43
2	10-E	1	BGC	O1-C1	-2.52	1.31	1.39
2	19-E	2	BGC	C4-C3	-2.52	1.45	1.52
2	18-E	6	BGC	C4-C3	-2.52	1.45	1.52
3	14-F	4	BGC	C2-C3	-2.51	1.48	1.52
2	21-C	5	BGC	O3-C3	2.51	1.49	1.43
2	15-E	5	BGC	C2-C3	-2.51	1.48	1.52
3	1-F	1	BGC	C3-C2	-2.51	1.45	1.52
3	1-D	3	BGC	C2-C3	-2.51	1.48	1.52
2	6-E	2	BGC	C4-C3	-2.51	1.45	1.52
3	5-F	3	BGC	C2-C3	-2.51	1.48	1.52
2	16-E	1	BGC	O3-C3	2.51	1.49	1.43
2	20-E	3	BGC	C2-C3	-2.51	1.48	1.52
2	5-E	1	BGC	O1-C1	-2.51	1.31	1.39
3	4-D	3	BGC	C2-C3	-2.51	1.48	1.52
2	2-E	1	BGC	O1-C1	-2.50	1.31	1.39
2	21-E	5	BGC	C2-C3	-2.50	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	24-D	3	BGC	C2-C3	-2.50	1.48	1.52
3	23-F	4	BGC	O5-C1	2.50	1.47	1.43
2	1-E	6	BGC	C2-C3	-2.50	1.48	1.52
2	3-E	4	BGC	C2-C3	-2.49	1.48	1.52
2	12-E	1	BGC	O3-C3	2.49	1.49	1.43
2	12-C	6	BGC	O3-C3	2.49	1.49	1.43
2	7-E	2	BGC	C4-C3	-2.49	1.45	1.52
2	20-C	3	BGC	C2-C3	-2.49	1.48	1.52
2	1-E	1	BGC	O1-C1	-2.48	1.31	1.39
2	21-E	6	BGC	C4-C3	-2.48	1.45	1.52
3	22-F	3	BGC	C2-C3	-2.48	1.48	1.52
2	9-C	2	BGC	O3-C3	2.48	1.49	1.43
2	24-C	6	BGC	C4-C3	-2.48	1.45	1.52
2	12-E	3	BGC	C2-C3	-2.48	1.48	1.52
2	14-E	1	BGC	O3-C3	2.48	1.49	1.43
2	23-E	1	BGC	O1-C1	-2.47	1.31	1.39
2	14-C	2	BGC	C2-C3	-2.47	1.48	1.52
3	3-F	4	BGC	O5-C1	2.47	1.47	1.43
2	18-C	2	BGC	C4-C3	-2.47	1.45	1.52
2	4-E	1	BGC	O1-C1	-2.47	1.31	1.39
3	25-F	4	BGC	C2-C3	-2.47	1.48	1.52
2	10-E	6	BGC	C4-C3	-2.47	1.45	1.52
2	10-C	6	BGC	C4-C3	-2.47	1.45	1.52
2	5-C	2	BGC	C4-C3	-2.46	1.45	1.52
3	15-D	1	BGC	O3-C3	2.46	1.49	1.43
2	25-E	6	BGC	C2-C3	-2.46	1.48	1.52
2	18-C	6	BGC	C2-C3	-2.46	1.48	1.52
3	16-D	3	BGC	O3-C3	2.46	1.49	1.43
2	11-C	6	BGC	C4-C3	-2.46	1.46	1.52
2	19-E	6	BGC	C2-C3	-2.46	1.48	1.52
2	22-C	3	BGC	C2-C3	-2.46	1.48	1.52
2	12-E	5	BGC	C2-C3	-2.46	1.48	1.52
2	1-E	5	BGC	O3-C3	2.45	1.49	1.43
2	24-E	1	BGC	O1-C1	-2.45	1.31	1.39
3	22-D	2	BGC	O5-C1	2.45	1.47	1.43
3	21-F	3	BGC	C2-C3	-2.45	1.48	1.52
2	16-C	5	BGC	O3-C3	2.45	1.49	1.43
2	24-E	1	BGC	O3-C3	2.45	1.49	1.43
2	1-C	1	BGC	O1-C1	-2.45	1.31	1.39
3	18-F	4	BGC	O5-C1	2.45	1.47	1.43
3	20-F	1	BGC	C3-C2	-2.45	1.46	1.52
2	6-E	6	BGC	C2-C3	-2.45	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	17-F	4	BGC	C2-C3	-2.45	1.48	1.52
3	21-F	4	BGC	O5-C1	2.44	1.47	1.43
2	21-C	6	BGC	C4-C3	-2.44	1.46	1.52
3	23-D	2	BGC	O5-C1	2.44	1.47	1.43
2	22-E	1	BGC	O1-C1	-2.44	1.31	1.39
2	2-C	1	BGC	O1-C1	-2.44	1.31	1.39
3	24-F	3	BGC	C2-C3	-2.44	1.48	1.52
2	20-E	1	BGC	O1-C1	-2.44	1.31	1.39
2	6-E	5	BGC	C2-C3	-2.44	1.48	1.52
3	8-F	4	BGC	O5-C1	2.44	1.47	1.43
3	18-D	3	BGC	C2-C3	-2.44	1.48	1.52
2	7-C	5	BGC	O3-C3	2.44	1.49	1.43
2	1-E	5	BGC	C2-C3	-2.43	1.48	1.52
3	19-D	2	BGC	O5-C1	2.43	1.47	1.43
2	2-E	5	BGC	C2-C3	-2.43	1.48	1.52
2	6-E	1	BGC	O3-C3	2.43	1.49	1.43
2	5-E	1	BGC	O3-C3	2.43	1.49	1.43
2	2-E	5	BGC	O3-C3	2.43	1.49	1.43
3	18-F	4	BGC	C2-C3	-2.43	1.48	1.52
2	14-C	3	BGC	O3-C3	2.42	1.49	1.43
2	5-E	5	BGC	C2-C3	-2.42	1.48	1.52
2	21-C	3	BGC	O3-C3	2.42	1.48	1.43
2	25-C	6	BGC	C4-C3	-2.42	1.46	1.52
2	4-E	2	BGC	C4-C3	-2.42	1.46	1.52
3	7-F	1	BGC	C3-C2	-2.42	1.46	1.52
2	19-C	3	BGC	C2-C3	-2.41	1.48	1.52
2	12-E	5	BGC	O5-C1	2.41	1.47	1.43
2	14-C	2	BGC	O3-C3	2.41	1.48	1.43
2	4-C	2	BGC	C4-C3	-2.41	1.46	1.52
2	17-C	2	BGC	C2-C3	-2.41	1.48	1.52
2	8-C	6	BGC	C2-C3	-2.41	1.48	1.52
3	25-D	3	BGC	C2-C3	-2.41	1.48	1.52
2	17-C	5	BGC	O3-C3	2.41	1.48	1.43
3	10-D	2	BGC	O5-C1	2.41	1.47	1.43
3	9-D	3	BGC	O3-C3	2.41	1.48	1.43
3	18-F	1	BGC	O3-C3	2.40	1.48	1.43
2	20-E	6	BGC	C2-C3	-2.40	1.48	1.52
3	25-F	1	BGC	O3-C3	2.40	1.48	1.43
2	15-C	2	BGC	O3-C3	2.40	1.48	1.43
2	19-C	2	BGC	O3-C3	2.40	1.48	1.43
2	23-C	3	BGC	C2-C3	-2.40	1.48	1.52
2	22-E	2	BGC	C4-C3	-2.40	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	23-E	2	BGC	C4-C3	-2.39	1.46	1.52
3	19-D	4	BGC	O5-C1	2.39	1.47	1.43
3	2-D	3	BGC	O3-C3	2.39	1.48	1.43
2	17-E	2	BGC	C4-C3	-2.39	1.46	1.52
2	8-E	1	BGC	O3-C3	2.39	1.48	1.43
2	8-E	5	BGC	O3-C3	2.39	1.48	1.43
2	25-E	5	BGC	C2-C3	-2.39	1.48	1.52
2	23-C	6	BGC	C2-C3	-2.39	1.48	1.52
3	19-F	4	BGC	C2-C3	-2.39	1.48	1.52
2	3-E	1	BGC	O1-C1	-2.39	1.32	1.39
3	12-F	4	BGC	O5-C1	2.39	1.47	1.43
2	16-E	1	BGC	O1-C1	-2.39	1.32	1.39
2	6-C	2	BGC	C4-C3	-2.38	1.46	1.52
2	15-C	3	BGC	O3-C3	2.38	1.48	1.43
2	19-C	5	BGC	O3-C3	2.38	1.48	1.43
2	17-C	2	BGC	O3-C3	2.38	1.48	1.43
2	10-E	5	BGC	C2-C3	-2.38	1.48	1.52
2	7-E	3	BGC	C2-C3	-2.37	1.48	1.52
2	7-E	5	BGC	O3-C3	2.37	1.48	1.43
3	21-D	1	BGC	O3-C3	2.37	1.48	1.43
2	24-E	5	BGC	O3-C3	2.37	1.48	1.43
2	9-E	5	BGC	O3-C3	2.37	1.48	1.43
2	18-E	1	BGC	O1-C1	-2.37	1.32	1.39
2	3-C	2	BGC	O3-C3	2.37	1.48	1.43
3	7-F	3	BGC	C2-C3	-2.37	1.48	1.52
3	10-D	3	BGC	C2-C3	-2.37	1.48	1.52
2	24-C	5	BGC	O3-C3	2.36	1.48	1.43
2	24-C	2	BGC	O3-C3	2.36	1.48	1.43
2	6-C	2	BGC	C2-C3	-2.36	1.48	1.52
2	18-C	3	BGC	C4-C3	-2.36	1.46	1.52
2	18-E	6	BGC	C2-C3	-2.36	1.48	1.52
3	5-D	3	BGC	C2-C3	-2.36	1.48	1.52
2	12-C	2	BGC	O3-C3	2.35	1.48	1.43
2	2-E	2	BGC	C2-C3	-2.35	1.48	1.52
2	3-E	5	BGC	O3-C3	2.35	1.48	1.43
2	15-E	2	BGC	C4-C3	-2.35	1.46	1.52
2	18-E	5	BGC	C2-C3	-2.35	1.48	1.52
3	3-F	3	BGC	C2-C3	-2.35	1.48	1.52
3	18-D	1	BGC	O3-C3	2.35	1.48	1.43
2	1-C	3	BGC	C4-C3	-2.35	1.46	1.52
2	14-C	2	BGC	C4-C3	-2.34	1.46	1.52
3	5-D	3	BGC	O5-C1	2.34	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	17-D	3	BGC	C2-C3	-2.34	1.48	1.52
2	8-E	6	BGC	C2-C3	-2.34	1.48	1.52
2	21-C	2	BGC	O3-C3	2.34	1.48	1.43
3	13-D	2	BGC	O5-C1	2.34	1.47	1.43
3	7-D	3	BGC	O3-C3	2.34	1.48	1.43
3	24-F	4	BGC	O5-C1	2.33	1.47	1.43
2	8-C	6	BGC	C4-C3	-2.33	1.46	1.52
2	9-E	1	BGC	O3-C3	2.33	1.48	1.43
3	16-F	4	BGC	C2-C3	-2.33	1.48	1.52
2	1-C	3	BGC	O3-C3	2.33	1.48	1.43
2	16-C	3	BGC	O3-C3	2.33	1.48	1.43
2	14-E	2	BGC	O3-C3	2.33	1.48	1.43
3	3-F	3	BGC	C4-C3	-2.33	1.46	1.52
2	23-E	5	BGC	C2-C3	-2.33	1.48	1.52
2	22-C	6	BGC	O3-C3	2.33	1.48	1.43
2	25-E	5	BGC	O3-C3	2.33	1.48	1.43
3	16-D	3	BGC	C2-C3	-2.32	1.48	1.52
2	13-E	5	BGC	O3-C3	2.32	1.48	1.43
3	7-D	4	BGC	O5-C1	2.32	1.47	1.43
2	21-C	6	BGC	C2-C3	-2.32	1.48	1.52
2	19-C	6	BGC	C2-C3	-2.31	1.48	1.52
2	6-C	5	BGC	C2-C3	-2.31	1.48	1.52
3	16-F	3	BGC	C2-C3	-2.31	1.48	1.52
3	9-F	4	BGC	O5-C1	2.31	1.47	1.43
2	11-E	4	BGC	C2-C3	-2.31	1.48	1.52
3	17-F	3	BGC	C2-C3	-2.31	1.48	1.52
2	21-E	4	BGC	C2-C3	-2.31	1.48	1.52
2	2-C	2	BGC	O3-C3	2.31	1.48	1.43
2	16-E	5	BGC	O3-C3	2.31	1.48	1.43
3	6-D	3	BGC	C2-C3	-2.31	1.49	1.52
2	5-C	3	BGC	O3-C3	2.31	1.48	1.43
2	10-E	5	BGC	O5-C1	2.30	1.47	1.43
2	13-C	2	BGC	O3-C3	2.30	1.48	1.43
2	2-E	2	BGC	C4-C3	-2.30	1.46	1.52
3	2-F	4	BGC	C2-C3	-2.30	1.49	1.52
2	5-E	5	BGC	O3-C3	2.30	1.48	1.43
3	25-D	2	BGC	O5-C1	2.30	1.47	1.43
2	10-C	3	BGC	O3-C3	2.30	1.48	1.43
2	21-E	5	BGC	O5-C1	2.29	1.47	1.43
2	7-E	5	BGC	C2-C3	-2.29	1.49	1.52
2	11-E	5	BGC	O3-C3	2.29	1.48	1.43
2	17-E	1	BGC	O1-C1	-2.29	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-C	5	BGC	O3-C3	2.28	1.48	1.43
2	7-C	2	BGC	C2-C3	-2.28	1.49	1.52
2	6-C	3	BGC	O3-C3	2.28	1.48	1.43
3	23-D	3	BGC	C2-C3	-2.27	1.49	1.52
2	17-C	3	BGC	C4-C3	-2.27	1.46	1.52
2	19-E	1	BGC	O1-C1	-2.27	1.32	1.39
2	1-E	4	BGC	C2-C3	-2.27	1.49	1.52
3	20-F	3	BGC	C2-C3	-2.27	1.49	1.52
2	2-E	2	BGC	O3-C3	2.27	1.48	1.43
2	2-E	3	BGC	C2-C3	-2.27	1.49	1.52
2	9-C	3	BGC	O3-C3	2.26	1.48	1.43
3	3-F	4	BGC	C2-C3	-2.26	1.49	1.52
2	4-E	5	BGC	O3-C3	2.26	1.48	1.43
3	1-F	1	BGC	O3-C3	2.26	1.48	1.43
3	21-D	2	BGC	C1-C2	2.26	1.57	1.52
2	20-E	5	BGC	O3-C3	2.25	1.48	1.43
2	1-C	2	BGC	O3-C3	2.25	1.48	1.43
2	19-E	3	BGC	C2-C3	-2.25	1.49	1.52
3	15-F	4	BGC	O5-C1	2.25	1.47	1.43
3	24-D	3	BGC	O3-C3	2.25	1.48	1.43
2	20-C	2	BGC	C4-C3	-2.25	1.46	1.52
3	17-F	1	BGC	O3-C3	2.24	1.48	1.43
2	12-C	2	BGC	C4-C3	-2.24	1.46	1.52
2	20-C	3	BGC	O3-C3	2.24	1.48	1.43
3	1-F	3	BGC	C2-C3	-2.24	1.49	1.52
3	15-D	4	BGC	O5-C1	2.24	1.47	1.43
3	17-F	4	BGC	O5-C1	2.24	1.47	1.43
2	10-C	3	BGC	C4-C3	-2.23	1.46	1.52
3	6-F	4	BGC	O5-C1	2.23	1.47	1.43
3	6-F	3	BGC	C4-C3	-2.23	1.46	1.52
2	21-E	5	BGC	O3-C3	2.23	1.48	1.43
2	4-C	2	BGC	O3-C3	2.23	1.48	1.43
3	15-F	1	BGC	O3-C3	2.23	1.48	1.43
2	4-C	3	BGC	C4-C3	-2.23	1.46	1.52
2	22-C	2	BGC	C4-C3	-2.22	1.46	1.52
2	13-C	4	BGC	O5-C1	2.22	1.47	1.43
3	4-D	4	BGC	O5-C1	2.22	1.47	1.43
2	5-E	4	BGC	C2-C3	-2.22	1.49	1.52
2	24-C	2	BGC	C4-C3	-2.22	1.46	1.52
3	7-D	3	BGC	C2-C3	-2.22	1.49	1.52
3	5-F	1	BGC	O5-C1	2.22	1.48	1.42
2	6-E	5	BGC	O3-C3	2.21	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	18-C	2	BGC	O3-C3	2.21	1.48	1.43
2	19-E	5	BGC	C2-C3	-2.21	1.49	1.52
2	12-E	2	BGC	C4-C3	-2.21	1.46	1.52
2	2-C	6	BGC	C2-C3	-2.21	1.49	1.52
3	20-F	2	BGC	O5-C5	2.21	1.47	1.43
2	13-E	2	BGC	C4-C3	-2.21	1.46	1.52
3	12-D	2	BGC	C1-C2	2.21	1.57	1.52
2	6-C	2	BGC	O3-C3	2.21	1.48	1.43
2	15-E	2	BGC	O3-C3	2.21	1.48	1.43
2	12-C	3	BGC	O3-C3	2.20	1.48	1.43
3	2-D	3	BGC	C2-C3	-2.20	1.49	1.52
2	10-E	5	BGC	O3-C3	2.20	1.48	1.43
2	1-C	2	BGC	C4-C3	-2.20	1.46	1.52
3	16-F	3	BGC	C4-C3	-2.20	1.46	1.52
3	9-F	4	BGC	C2-C3	-2.20	1.49	1.52
2	15-C	2	BGC	C4-C3	-2.20	1.46	1.52
2	7-C	2	BGC	C4-C5	-2.20	1.48	1.53
2	22-C	2	BGC	O3-C3	2.20	1.48	1.43
2	25-E	2	BGC	C2-C3	-2.20	1.49	1.52
2	9-E	2	BGC	O3-C3	2.20	1.48	1.43
2	16-C	2	BGC	C4-C3	-2.20	1.46	1.52
2	8-C	5	BGC	O3-C3	2.19	1.48	1.43
2	2-C	2	BGC	C4-C3	-2.19	1.46	1.52
3	4-F	4	BGC	C2-C3	-2.19	1.49	1.52
3	12-F	1	BGC	O3-C3	2.19	1.48	1.43
2	3-C	3	BGC	O3-C3	2.19	1.48	1.43
3	9-F	3	BGC	C2-C3	-2.19	1.49	1.52
3	12-F	3	BGC	C4-C3	-2.19	1.46	1.52
3	22-F	2	BGC	C6-C5	-2.18	1.44	1.51
2	22-C	3	BGC	O3-C3	2.18	1.48	1.43
2	6-E	4	BGC	C2-C3	-2.18	1.49	1.52
2	23-E	4	BGC	C2-C3	-2.18	1.49	1.52
3	11-F	1	BGC	O3-C3	2.18	1.48	1.43
2	21-C	3	BGC	C4-C3	-2.18	1.46	1.52
2	14-E	3	BGC	C4-C3	-2.17	1.46	1.52
2	16-C	2	BGC	O3-C3	2.17	1.48	1.43
3	4-D	3	BGC	O5-C1	2.17	1.47	1.43
3	6-F	3	BGC	O5-C1	2.17	1.47	1.43
2	10-C	2	BGC	O3-C3	2.17	1.48	1.43
2	17-E	3	BGC	C2-C3	-2.17	1.49	1.52
3	2-D	4	BGC	O5-C1	2.17	1.47	1.43
2	9-C	6	BGC	C2-C3	-2.17	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	21-C	4	BGC	O5-C1	2.17	1.47	1.43
2	1-E	2	BGC	O3-C3	2.16	1.48	1.43
2	19-C	5	BGC	C2-C3	-2.16	1.49	1.52
2	11-C	2	BGC	C4-C3	-2.16	1.46	1.52
2	20-C	3	BGC	C4-C3	-2.16	1.46	1.52
2	7-C	5	BGC	C2-C3	-2.16	1.49	1.52
2	10-E	4	BGC	C2-C3	-2.16	1.49	1.52
3	6-F	3	BGC	C2-C3	-2.16	1.49	1.52
2	3-C	6	BGC	C2-C3	-2.16	1.49	1.52
3	7-F	2	BGC	O5-C5	2.15	1.47	1.43
3	21-D	2	BGC	O5-C1	2.15	1.47	1.43
3	12-D	1	BGC	O3-C3	2.15	1.48	1.43
2	13-C	6	BGC	O3-C3	2.15	1.48	1.43
2	15-E	4	BGC	C2-C3	-2.15	1.49	1.52
2	25-E	1	BGC	C3-C2	-2.15	1.46	1.52
3	10-F	2	BGC	C6-C5	-2.14	1.44	1.51
2	14-E	5	BGC	C2-C3	-2.14	1.49	1.52
3	18-F	3	BGC	C4-C3	-2.14	1.46	1.52
2	25-E	1	BGC	O1-C1	-2.14	1.32	1.39
2	14-E	5	BGC	O5-C1	2.13	1.47	1.43
2	3-E	1	BGC	O4-C4	-2.13	1.37	1.43
3	19-F	3	BGC	C2-C3	-2.13	1.49	1.52
3	3-D	2	BGC	O5-C1	2.13	1.47	1.43
3	15-D	3	BGC	O3-C3	2.13	1.48	1.43
2	3-E	3	BGC	C4-C3	-2.13	1.46	1.52
3	8-F	2	BGC	C6-C5	-2.13	1.44	1.51
3	24-D	4	BGC	O5-C1	2.13	1.47	1.43
2	13-C	2	BGC	C4-C3	-2.13	1.46	1.52
3	3-F	1	BGC	O3-C3	2.13	1.48	1.43
2	4-E	5	BGC	C2-C3	-2.13	1.49	1.52
3	23-D	1	BGC	O3-C3	2.13	1.48	1.43
2	22-C	4	BGC	O5-C1	2.13	1.47	1.43
3	23-F	3	BGC	C2-C3	-2.12	1.49	1.52
2	8-C	2	BGC	O3-C3	2.12	1.48	1.43
2	14-C	3	BGC	C4-C3	-2.12	1.46	1.52
2	3-C	2	BGC	C4-C3	-2.12	1.46	1.52
3	14-F	2	BGC	C6-C5	-2.12	1.44	1.51
2	25-C	2	BGC	C4-C3	-2.12	1.46	1.52
3	11-F	4	BGC	C2-C3	-2.11	1.49	1.52
2	8-C	2	BGC	C4-C3	-2.11	1.46	1.52
2	10-C	2	BGC	C4-C3	-2.11	1.46	1.52
3	11-F	3	BGC	C4-C3	-2.11	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	24-E	4	BGC	C2-C3	-2.11	1.49	1.52
2	22-E	5	BGC	O3-C3	2.11	1.48	1.43
3	11-D	4	BGC	O5-C1	2.11	1.47	1.43
2	6-C	3	BGC	C4-C3	-2.11	1.46	1.52
2	3-E	5	BGC	C2-C3	-2.11	1.49	1.52
2	19-E	2	BGC	O3-C3	2.10	1.48	1.43
3	14-F	3	BGC	C4-C3	-2.10	1.46	1.52
2	18-C	2	BGC	C2-C3	-2.10	1.49	1.52
3	19-D	3	BGC	C2-C3	-2.10	1.49	1.52
3	1-F	4	BGC	C2-C3	-2.10	1.49	1.52
2	5-C	2	BGC	O3-C3	2.10	1.48	1.43
3	7-F	2	BGC	C6-C5	-2.10	1.44	1.51
3	23-F	1	BGC	O3-C3	2.10	1.48	1.43
2	1-C	4	BGC	O5-C1	2.10	1.47	1.43
2	15-E	3	BGC	O3-C3	2.10	1.48	1.43
3	9-D	2	BGC	O5-C1	2.10	1.47	1.43
2	17-C	2	BGC	C4-C3	-2.09	1.46	1.52
2	18-E	5	BGC	O3-C3	2.09	1.48	1.43
2	20-C	2	BGC	O3-C3	2.09	1.48	1.43
2	5-C	6	BGC	C2-C3	-2.09	1.49	1.52
2	22-E	2	BGC	O3-C3	2.09	1.48	1.43
2	10-E	2	BGC	O3-C3	2.09	1.48	1.43
2	5-C	3	BGC	C4-C3	-2.09	1.46	1.52
2	11-C	3	BGC	O3-C3	2.09	1.48	1.43
2	12-C	3	BGC	C4-C3	-2.09	1.46	1.52
2	24-C	3	BGC	C4-C3	-2.09	1.46	1.52
2	17-E	2	BGC	O3-C3	2.09	1.48	1.43
2	7-C	4	BGC	O5-C1	2.09	1.47	1.43
3	13-D	4	BGC	O5-C1	2.09	1.47	1.43
3	1-F	4	BGC	O5-C1	2.09	1.47	1.43
2	18-E	3	BGC	C4-C3	-2.08	1.46	1.52
2	5-E	2	BGC	O3-C3	2.08	1.48	1.43
2	17-C	1	BGC	O5-C1	2.08	1.48	1.42
3	17-F	1	BGC	O5-C1	2.08	1.48	1.42
3	22-D	3	BGC	C2-C3	-2.08	1.49	1.52
3	2-F	4	BGC	O5-C1	2.08	1.47	1.43
2	25-C	3	BGC	O3-C3	2.08	1.48	1.43
3	22-D	4	BGC	O5-C1	2.08	1.47	1.43
3	21-F	2	BGC	C6-C5	-2.07	1.44	1.51
2	25-C	3	BGC	C4-C3	-2.07	1.47	1.52
3	25-F	2	BGC	C1-C2	2.07	1.57	1.52
2	20-C	4	BGC	O5-C1	2.07	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	22-E	3	BGC	O3-C3	2.07	1.48	1.43
3	15-D	2	BGC	O5-C1	2.07	1.47	1.43
3	7-F	3	BGC	C4-C3	-2.07	1.47	1.52
2	16-C	3	BGC	C4-C3	-2.06	1.47	1.52
2	21-E	6	BGC	O3-C3	2.06	1.48	1.43
3	11-D	2	BGC	O5-C1	2.06	1.47	1.43
2	21-E	6	BGC	C2-C3	-2.06	1.49	1.52
2	20-E	2	BGC	O3-C3	2.06	1.48	1.43
2	11-C	3	BGC	C4-C3	-2.06	1.47	1.52
2	15-E	3	BGC	C2-C3	-2.06	1.49	1.52
3	17-D	4	BGC	O5-C1	2.06	1.47	1.43
3	9-F	2	BGC	C6-C5	-2.06	1.44	1.51
2	14-E	5	BGC	O3-C3	2.06	1.48	1.43
2	25-E	2	BGC	O3-C3	2.05	1.48	1.43
2	9-E	5	BGC	O5-C1	2.05	1.47	1.43
3	11-F	2	BGC	C6-C5	-2.05	1.44	1.51
3	16-F	2	BGC	C6-C5	-2.05	1.44	1.51
3	25-F	3	BGC	C4-C3	-2.05	1.47	1.52
2	11-E	2	BGC	O3-C3	2.05	1.48	1.43
2	15-C	4	BGC	O5-C1	2.05	1.47	1.43
2	11-C	6	BGC	O3-C3	2.05	1.48	1.43
3	21-F	3	BGC	C4-C3	-2.05	1.47	1.52
3	16-F	1	BGC	O3-C3	2.05	1.48	1.43
2	23-C	3	BGC	C4-C3	-2.05	1.47	1.52
3	12-F	2	BGC	C6-C5	-2.05	1.45	1.51
2	17-E	5	BGC	O3-C3	2.04	1.48	1.43
2	6-E	2	BGC	O3-C3	2.04	1.48	1.43
2	17-C	3	BGC	O3-C3	2.04	1.48	1.43
3	8-F	5	BGC	C4-C5	-2.04	1.48	1.53
2	19-E	5	BGC	O5-C1	2.04	1.47	1.43
2	13-C	3	BGC	C4-C3	-2.04	1.47	1.52
3	10-F	3	BGC	C2-C3	-2.04	1.49	1.52
2	3-C	4	BGC	O5-C1	2.04	1.47	1.43
3	10-D	4	BGC	O5-C1	2.04	1.47	1.43
3	20-F	3	BGC	C4-C3	-2.04	1.47	1.52
3	2-F	3	BGC	C2-C3	-2.03	1.49	1.52
2	14-C	4	BGC	O5-C1	2.03	1.47	1.43
3	25-F	2	BGC	C6-C5	-2.03	1.45	1.51
3	5-F	1	BGC	O3-C3	2.03	1.48	1.43
3	24-F	1	BGC	O3-C3	2.03	1.48	1.43
3	23-F	2	BGC	C6-C5	-2.03	1.45	1.51
3	9-F	1	BGC	O3-C3	2.03	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	18-F	3	BGC	C2-C3	-2.03	1.49	1.52
2	21-E	2	BGC	O3-C3	2.02	1.48	1.43
3	21-D	4	BGC	O5-C1	2.02	1.47	1.43
2	25-E	5	BGC	O5-C1	2.02	1.47	1.43
2	4-C	3	BGC	O3-C3	2.02	1.47	1.43
3	25-F	4	BGC	O5-C1	2.02	1.47	1.43
3	25-D	1	BGC	O3-C3	2.02	1.47	1.43
2	10-C	6	BGC	O3-C3	2.02	1.47	1.43
2	4-E	6	BGC	O3-C3	2.01	1.47	1.43
3	13-F	3	BGC	C4-C3	-2.01	1.47	1.52
3	2-F	1	BGC	O3-C3	2.01	1.47	1.43
3	6-D	2	BGC	O5-C5	2.01	1.47	1.43
2	10-E	3	BGC	C4-C3	-2.01	1.47	1.52
2	20-C	6	BGC	O3-C3	2.01	1.47	1.43
2	19-E	6	BGC	C4-C3	-2.01	1.47	1.52
3	5-F	2	BGC	O5-C5	2.01	1.47	1.43
2	21-E	1	BGC	O5-C1	2.01	1.47	1.42
3	20-F	2	BGC	C6-C5	-2.01	1.45	1.51
3	2-D	1	BGC	O3-C3	2.01	1.47	1.43
2	7-C	3	BGC	O3-C3	2.00	1.47	1.43
2	23-C	3	BGC	O3-C3	2.00	1.47	1.43
3	23-D	4	BGC	O5-C1	2.00	1.47	1.43
2	12-E	2	BGC	O3-C3	2.00	1.47	1.43
2	23-C	2	BGC	C4-C3	-2.00	1.47	1.52

All (1022) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-E	4	BGC	O5-C5-C6	-9.51	89.16	107.66
3	1-F	3	BGC	C1-O5-C5	9.47	124.88	112.19
2	7-C	2	BGC	C1-O5-C5	-8.38	100.96	112.19
2	7-C	2	BGC	O5-C5-C6	7.90	123.05	107.66
2	17-E	6	BGC	C6-C5-C4	-7.81	93.84	113.02
2	16-E	6	BGC	C3-C4-C5	-7.17	97.23	110.23
2	7-C	2	BGC	C3-C4-C5	-7.00	97.54	110.23
3	6-D	2	BGC	C1-O5-C5	6.83	121.34	112.19
3	13-D	4	BGC	C1-O5-C5	6.83	121.34	112.19
3	11-F	3	BGC	C1-O5-C5	6.04	120.28	112.19
3	8-F	2	BGC	C1-C2-C3	5.73	117.99	109.64
2	13-E	5	BGC	O5-C5-C6	-5.69	96.59	107.66
3	21-D	2	BGC	C1-C2-C3	5.65	117.88	109.64
2	16-E	6	BGC	C1-O5-C5	-5.63	104.64	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-E	5	BGC	O5-C5-C6	-5.62	96.73	107.66
3	25-F	2	BGC	C1-C2-C3	5.47	117.61	109.64
3	12-D	2	BGC	C1-C2-C3	5.33	117.40	109.64
3	7-D	2	BGC	C1-C2-C3	5.03	116.97	109.64
3	19-D	2	BGC	C1-C2-C3	5.00	116.93	109.64
2	9-E	2	BGC	C6-C5-C4	4.98	125.24	113.02
3	2-F	2	BGC	C1-C2-C3	4.97	116.87	109.64
2	15-C	2	BGC	O3-C3-C2	-4.96	99.92	110.05
2	24-C	6	BGC	C1-O5-C5	4.93	118.80	112.19
3	16-D	2	BGC	C1-C2-C3	4.92	116.80	109.64
3	9-D	2	BGC	C1-C2-C3	4.89	116.77	109.64
3	15-D	2	BGC	C3-C4-C5	4.89	119.10	110.23
3	4-D	3	BGC	C1-O5-C5	4.89	118.74	112.19
3	5-F	1	BGC	C1-O5-C5	4.87	123.06	113.65
2	13-C	6	BGC	C6-C5-C4	4.85	124.94	113.02
3	11-D	5	BGC	C1-O5-C5	4.85	118.69	112.19
3	17-D	2	BGC	C1-O5-C5	-4.84	105.70	112.19
2	18-E	3	BGC	C1-O5-C5	-4.83	105.72	112.19
3	17-F	1	BGC	C1-O5-C5	4.75	122.84	113.65
3	6-F	2	BGC	C1-C2-C3	4.72	116.51	109.64
2	14-E	1	BGC	O5-C1-C2	-4.69	102.06	110.30
3	25-F	3	BGC	C1-O5-C5	4.67	118.45	112.19
3	3-D	2	BGC	C1-C2-C3	4.65	116.42	109.64
3	8-D	2	BGC	C1-C2-C3	4.62	116.37	109.64
3	15-D	3	BGC	C1-O5-C5	4.61	118.36	112.19
2	13-C	1	BGC	C4-C3-C2	4.60	118.91	110.83
2	22-C	6	BGC	C6-C5-C4	4.60	124.31	113.02
3	25-F	4	BGC	C1-O5-C5	-4.57	106.06	112.19
3	8-D	5	BGC	C1-O5-C5	4.55	118.29	112.19
3	23-D	2	BGC	C1-C2-C3	4.54	116.25	109.64
2	22-C	5	BGC	C1-C2-C3	4.52	116.22	109.64
3	18-D	3	BGC	C1-O5-C5	4.48	118.19	112.19
3	5-D	3	BGC	C1-O5-C5	4.45	118.14	112.19
3	3-F	2	BGC	C1-C2-C3	4.44	116.10	109.64
3	2-D	2	BGC	C1-C2-C3	4.41	116.07	109.64
2	10-E	6	BGC	O6-C6-C5	4.41	126.34	111.33
3	25-D	2	BGC	C1-C2-C3	4.41	116.06	109.64
3	10-D	2	BGC	C1-C2-C3	4.39	116.04	109.64
2	23-E	6	BGC	O6-C6-C5	4.37	126.21	111.33
2	23-E	3	BGC	C1-O5-C5	-4.35	106.35	112.19
3	9-D	3	BGC	C2-C3-C4	4.34	118.49	110.86
3	23-D	3	BGC	C1-O5-C5	4.31	117.96	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	19-E	6	BGC	O5-C5-C4	-4.31	100.34	110.83
3	1-D	2	BGC	C1-C2-C3	4.29	115.89	109.64
2	19-C	2	BGC	O3-C3-C2	-4.29	101.31	110.05
2	13-C	4	BGC	C1-C2-C3	4.28	115.87	109.64
3	20-D	2	BGC	C1-C2-C3	4.25	115.83	109.64
2	17-C	1	BGC	O2-C2-C3	4.24	120.38	110.38
3	19-D	2	BGC	C1-O5-C5	-4.22	106.53	112.19
3	4-F	2	BGC	C1-C2-C3	4.22	115.78	109.64
3	20-F	2	BGC	C1-C2-C3	4.21	115.78	109.64
3	18-D	2	BGC	C1-C2-C3	4.21	115.78	109.64
2	16-E	5	BGC	O5-C5-C6	-4.19	99.50	107.66
3	14-D	3	BGC	C1-O5-C5	4.17	117.78	112.19
2	24-C	6	BGC	O5-C5-C6	-4.17	99.55	107.66
3	23-F	5	BGC	C1-O5-C5	-4.16	106.61	112.19
3	15-D	2	BGC	C1-O5-C5	4.16	117.76	112.19
2	6-E	1	BGC	C1-O5-C5	-4.15	105.62	113.65
2	9-C	2	BGC	O3-C3-C2	-4.15	101.59	110.05
2	2-C	4	BGC	C1-C2-C3	4.14	115.68	109.64
3	11-D	4	BGC	O6-C6-C5	4.12	125.37	111.33
3	22-D	1	BGC	O5-C5-C4	4.12	117.12	109.70
3	14-D	4	BGC	C1-O5-C5	4.12	117.71	112.19
2	21-C	2	BGC	C2-C3-C4	-4.12	103.62	110.86
2	23-E	4	BGC	C1-C2-C3	4.08	115.58	109.64
3	24-D	2	BGC	C1-C2-C3	4.08	115.58	109.64
3	13-D	2	BGC	C1-O5-C5	-4.07	106.72	112.19
2	12-E	5	BGC	C6-C5-C4	-4.06	103.06	113.02
2	23-E	4	BGC	O3-C3-C2	-4.04	101.80	110.05
2	14-C	5	BGC	C1-C2-C3	4.04	115.53	109.64
2	20-E	3	BGC	C1-O5-C5	-4.03	106.79	112.19
2	19-C	4	BGC	C1-O5-C5	4.02	117.57	112.19
2	11-C	5	BGC	C1-C2-C3	4.02	115.49	109.64
3	25-D	3	BGC	C1-O5-C5	4.01	117.56	112.19
3	1-F	2	BGC	C1-C2-C3	3.99	115.46	109.64
2	21-E	4	BGC	C6-C5-C4	-3.98	103.24	113.02
2	3-C	5	BGC	C1-C2-C3	3.95	115.40	109.64
3	4-D	2	BGC	C1-C2-C3	3.94	115.39	109.64
2	8-E	2	BGC	O5-C5-C6	3.94	115.34	107.66
3	18-F	2	BGC	C1-C2-C3	3.93	115.37	109.64
3	13-D	2	BGC	C1-C2-C3	3.93	115.36	109.64
2	3-E	4	BGC	C6-C5-C4	3.93	122.66	113.02
3	16-F	2	BGC	C1-C2-C3	3.92	115.35	109.64
3	12-F	2	BGC	C1-C2-C3	3.91	115.33	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-D	2	BGC	C2-C3-C4	-3.91	103.99	110.86
2	8-C	6	BGC	O4-C4-C3	3.91	119.58	110.38
2	18-C	5	BGC	C1-C2-C3	3.90	115.32	109.64
3	19-D	3	BGC	C3-C4-C5	3.89	117.29	110.23
3	22-D	3	BGC	C1-O5-C5	3.89	117.40	112.19
2	20-C	2	BGC	O3-C3-C2	-3.88	102.14	110.05
3	21-F	2	BGC	C1-C2-C3	3.87	115.28	109.64
2	23-C	4	BGC	C1-C2-C3	3.87	115.27	109.64
3	22-D	2	BGC	C1-C2-C3	3.86	115.26	109.64
3	6-D	1	BGC	O5-C5-C4	3.85	116.64	109.70
3	5-D	2	BGC	C1-C2-C3	3.83	115.22	109.64
2	19-E	6	BGC	C6-C5-C4	3.82	122.41	113.02
2	21-E	5	BGC	C1-O5-C5	-3.82	107.07	112.19
3	8-D	3	BGC	C1-O5-C5	3.82	117.30	112.19
2	16-E	3	BGC	C1-O5-C5	-3.80	107.09	112.19
3	17-D	2	BGC	C1-C2-C3	3.80	115.18	109.64
2	21-E	1	BGC	C1-O5-C5	-3.80	106.30	113.65
3	6-D	1	BGC	C3-C4-C5	3.80	117.12	110.23
2	10-C	5	BGC	C1-C2-C3	3.80	115.17	109.64
3	24-F	3	BGC	C1-O5-C5	3.80	117.27	112.19
3	19-D	3	BGC	C2-C3-C4	3.79	117.53	110.86
2	25-E	2	BGC	C1-C2-C3	3.79	115.16	109.64
3	13-D	5	BGC	C1-O5-C5	-3.79	107.11	112.19
3	25-D	2	BGC	C3-C4-C5	3.78	117.08	110.23
2	24-C	6	BGC	O6-C6-C5	3.77	124.16	111.33
2	10-E	6	BGC	C1-O5-C5	3.76	117.22	112.19
3	3-D	3	BGC	C1-O5-C5	3.75	117.22	112.19
2	3-E	4	BGC	C1-C2-C3	3.75	115.10	109.64
2	19-E	2	BGC	C1-C2-C3	3.74	115.10	109.64
2	19-E	6	BGC	O5-C5-C6	-3.74	100.38	107.66
3	23-F	5	BGC	O5-C5-C4	-3.74	101.74	110.83
2	11-E	5	BGC	O5-C5-C6	-3.73	100.40	107.66
2	23-C	2	BGC	O3-C3-C2	-3.72	102.46	110.05
3	19-D	3	BGC	C1-O5-C5	3.71	117.16	112.19
3	5-F	2	BGC	C1-C2-C3	3.71	115.05	109.64
3	7-F	2	BGC	C1-C2-C3	3.71	115.05	109.64
3	10-D	3	BGC	C1-O5-C5	3.71	117.16	112.19
3	15-D	2	BGC	C1-C2-C3	3.71	115.04	109.64
3	11-F	2	BGC	C1-C2-C3	3.71	115.04	109.64
2	23-E	6	BGC	C1-O5-C5	3.70	117.15	112.19
3	11-D	4	BGC	C1-O5-C5	3.70	117.15	112.19
2	13-E	5	BGC	C1-C2-C3	3.68	115.00	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	13-D	4	BGC	O5-C5-C4	3.68	119.78	110.83
2	24-E	5	BGC	O5-C5-C6	-3.68	100.51	107.66
3	9-F	3	BGC	C1-O5-C5	3.67	117.11	112.19
3	15-F	2	BGC	C1-C2-C3	3.67	114.99	109.64
2	24-C	5	BGC	C1-C2-C3	3.66	114.98	109.64
2	17-C	2	BGC	O3-C3-C2	-3.66	102.59	110.05
3	14-D	2	BGC	C1-C2-C3	3.65	114.96	109.64
2	25-C	6	BGC	O5-C5-C6	-3.64	100.57	107.66
2	21-C	5	BGC	C1-C2-C3	3.64	114.95	109.64
3	8-F	3	BGC	C1-O5-C5	3.64	117.06	112.19
3	19-F	2	BGC	C1-C2-C3	3.63	114.93	109.64
2	3-E	4	BGC	O3-C3-C2	-3.63	102.65	110.05
2	24-C	1	BGC	O4-C4-C3	3.60	118.87	110.38
2	5-E	4	BGC	O3-C3-C2	-3.60	102.71	110.05
2	15-E	1	BGC	O5-C5-C4	3.59	116.17	109.70
2	8-C	6	BGC	O5-C5-C4	-3.59	102.09	110.83
2	7-C	2	BGC	C1-C2-C3	3.59	114.87	109.64
2	16-C	5	BGC	C1-C2-C3	3.59	114.87	109.64
3	18-D	2	BGC	C3-C4-C5	3.58	116.73	110.23
3	24-F	2	BGC	C1-C2-C3	3.58	114.86	109.64
2	11-C	2	BGC	O3-C3-C2	-3.58	102.75	110.05
3	22-D	1	BGC	C3-C4-C5	3.58	116.72	110.23
3	15-D	5	BGC	C1-O5-C5	3.56	116.96	112.19
2	3-C	2	BGC	O3-C3-C2	-3.56	102.79	110.05
2	3-C	5	BGC	C6-C5-C4	-3.55	104.31	113.02
3	7-F	2	BGC	O2-C2-C3	3.54	117.49	110.15
3	23-F	1	BGC	C3-C4-C5	3.54	116.64	110.23
3	4-D	3	BGC	C1-C2-C3	3.53	114.79	109.64
2	7-C	1	BGC	C1-O5-C5	-3.53	106.82	113.65
3	23-D	1	BGC	O5-C5-C4	3.53	116.06	109.70
2	8-C	4	BGC	C1-C2-C3	3.53	114.78	109.64
2	24-E	1	BGC	C4-C3-C2	3.52	117.02	110.83
2	9-E	1	BGC	O2-C2-C3	3.52	118.68	110.38
3	5-D	2	BGC	C3-C4-C5	3.50	116.58	110.23
3	15-D	1	BGC	O3-C3-C4	3.50	118.62	110.38
3	6-F	3	BGC	O5-C5-C6	3.49	114.47	107.66
2	22-E	4	BGC	O3-C3-C2	-3.49	102.92	110.05
2	1-C	4	BGC	C1-C2-C3	3.49	114.72	109.64
2	8-E	3	BGC	C1-O5-C5	-3.48	107.52	112.19
2	3-E	2	BGC	C1-C2-C3	3.47	114.69	109.64
2	15-C	5	BGC	C1-C2-C3	3.47	114.69	109.64
3	9-F	2	BGC	C1-C2-C3	3.45	114.67	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-C	5	BGC	C1-C2-C3	3.45	114.67	109.64
2	6-C	5	BGC	C1-C2-C3	3.45	114.67	109.64
2	6-E	5	BGC	O5-C5-C6	-3.44	100.97	107.66
3	12-D	3	BGC	C1-C2-C3	3.43	114.64	109.64
3	16-D	3	BGC	C3-C4-C5	3.43	116.45	110.23
2	12-C	1	BGC	C1-O5-C5	-3.43	107.02	113.65
2	5-C	1	BGC	O2-C2-C3	3.43	118.45	110.38
2	25-E	4	BGC	C1-O5-C5	-3.43	107.59	112.19
2	24-C	2	BGC	C1-O5-C5	-3.42	107.61	112.19
3	14-F	3	BGC	C1-O5-C5	3.42	116.77	112.19
2	13-C	1	BGC	C1-O5-C5	-3.42	107.04	113.65
2	7-C	5	BGC	C1-C2-C3	3.42	114.62	109.64
2	15-E	5	BGC	O5-C5-C6	-3.42	101.01	107.66
2	4-E	6	BGC	O5-C5-C6	-3.41	101.03	107.66
3	3-F	3	BGC	C1-O5-C5	3.40	116.75	112.19
2	24-C	3	BGC	O3-C3-C2	-3.40	103.11	110.05
2	22-C	2	BGC	O3-C3-C2	-3.40	103.11	110.05
2	14-C	2	BGC	C1-C2-C3	3.40	114.60	109.64
2	2-E	5	BGC	O5-C5-C6	-3.40	101.05	107.66
3	18-D	5	BGC	C1-O5-C5	3.39	116.73	112.19
2	21-E	2	BGC	C1-C2-C3	3.38	114.57	109.64
2	20-C	5	BGC	C1-O5-C5	-3.37	107.67	112.19
2	13-C	6	BGC	O4-C4-C5	3.36	117.61	109.32
2	20-E	2	BGC	C1-C2-C3	3.35	114.53	109.64
3	11-D	2	BGC	C1-C2-C3	3.35	114.52	109.64
3	23-F	2	BGC	C1-C2-C3	3.35	114.52	109.64
2	1-E	4	BGC	O3-C3-C2	-3.35	103.22	110.05
2	2-C	2	BGC	O3-C3-C2	-3.35	103.23	110.05
2	17-C	5	BGC	C1-C2-C3	3.34	114.51	109.64
2	25-C	2	BGC	O3-C3-C2	-3.33	103.25	110.05
3	11-D	3	BGC	C1-O5-C5	3.33	116.66	112.19
3	9-D	3	BGC	C3-C4-C5	3.33	116.28	110.23
3	17-F	2	BGC	C1-C2-C3	3.32	114.48	109.64
3	16-D	3	BGC	C2-C3-C4	3.31	116.69	110.86
2	11-C	2	BGC	C1-C2-C3	3.31	114.47	109.64
3	23-F	1	BGC	O5-C5-C4	3.31	115.66	109.70
2	12-E	5	BGC	C1-C2-C3	3.31	114.46	109.64
2	4-C	5	BGC	C1-C2-C3	3.30	114.45	109.64
2	3-C	4	BGC	C1-C2-C3	3.30	114.45	109.64
3	21-F	3	BGC	C1-O5-C5	3.30	116.61	112.19
2	8-C	2	BGC	O3-C3-C2	-3.30	103.32	110.05
3	22-D	2	BGC	C1-O5-C5	-3.29	107.77	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	15-E	1	BGC	C1-O5-C5	3.29	120.02	113.65
2	19-C	5	BGC	C1-C2-C3	3.28	114.42	109.64
3	13-D	5	BGC	C3-C4-C5	-3.28	104.29	110.23
2	19-E	5	BGC	C1-C2-C3	3.28	114.41	109.64
2	3-C	5	BGC	O5-C5-C6	-3.27	101.30	107.66
3	6-D	3	BGC	C1-O5-C5	3.27	116.56	112.19
3	19-F	2	BGC	C3-C4-C5	3.26	116.14	110.23
2	9-E	2	BGC	O5-C5-C6	-3.25	101.34	107.66
2	4-C	6	BGC	C6-C5-C4	-3.25	105.05	113.02
2	19-C	1	BGC	O2-C2-C3	3.24	118.02	110.38
3	17-F	1	BGC	O5-C5-C4	3.24	115.53	109.70
3	12-D	3	BGC	C1-O5-C5	3.24	116.53	112.19
3	13-F	2	BGC	C1-C2-C3	3.23	114.35	109.64
2	20-E	5	BGC	O5-C5-C6	-3.23	101.37	107.66
2	1-C	2	BGC	O3-C3-C2	-3.23	103.46	110.05
2	5-E	5	BGC	O5-C5-C6	-3.23	101.38	107.66
2	5-C	2	BGC	C1-O5-C5	-3.22	107.86	112.19
2	14-E	5	BGC	C1-C2-C3	3.22	114.34	109.64
2	15-E	4	BGC	C1-C2-C3	3.22	114.33	109.64
3	11-D	4	BGC	C2-C3-C4	-3.22	105.20	110.86
2	7-E	4	BGC	O3-C3-C2	-3.21	103.50	110.05
2	8-E	4	BGC	C1-C2-C3	3.21	114.32	109.64
2	22-C	6	BGC	O5-C5-C4	-3.21	103.02	110.83
2	24-E	4	BGC	O3-C3-C2	-3.21	103.51	110.05
2	16-E	6	BGC	O5-C5-C6	3.20	113.89	107.66
2	5-C	2	BGC	O3-C3-C2	-3.20	103.52	110.05
2	7-C	2	BGC	O4-C4-C3	3.19	117.91	110.38
2	18-C	6	BGC	O6-C6-C5	3.19	122.20	111.33
2	15-E	2	BGC	C1-C2-C3	3.19	114.29	109.64
2	10-C	2	BGC	O3-C3-C2	-3.18	103.56	110.05
2	5-E	4	BGC	C1-C2-C3	3.18	114.27	109.64
2	9-C	1	BGC	O3-C3-C4	3.18	117.86	110.38
2	17-E	5	BGC	O5-C5-C6	-3.17	101.49	107.66
3	14-F	2	BGC	C1-C2-C3	3.17	114.26	109.64
2	18-E	4	BGC	C1-C2-C3	3.16	114.25	109.64
3	1-F	3	BGC	C3-C4-C5	3.16	115.96	110.23
3	3-D	1	BGC	O5-C5-C4	3.15	115.37	109.70
2	19-C	1	BGC	C1-O5-C5	-3.15	107.56	113.65
2	9-E	1	BGC	O5-C1-C2	-3.14	104.77	110.30
2	9-C	6	BGC	C1-C2-C3	3.14	114.22	109.64
2	12-C	5	BGC	C1-C2-C3	3.13	114.20	109.64
2	9-C	1	BGC	O5-C1-C2	-3.13	104.79	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-E	5	BGC	O5-C5-C6	-3.13	101.57	107.66
2	22-C	4	BGC	C1-C2-C3	3.13	114.19	109.64
2	22-C	6	BGC	C1-O5-C5	3.12	116.37	112.19
2	9-C	5	BGC	C1-C2-C3	3.12	114.19	109.64
2	13-C	6	BGC	O5-C5-C4	-3.12	103.25	110.83
2	19-C	4	BGC	O3-C3-C2	-3.11	103.71	110.05
3	19-D	2	BGC	O4-C4-C5	-3.11	101.67	109.32
3	3-D	1	BGC	C1-O5-C5	3.11	119.66	113.65
3	22-F	2	BGC	C1-C2-C3	3.10	114.16	109.64
2	20-C	4	BGC	C1-C2-C3	3.10	114.16	109.64
2	2-C	2	BGC	C1-C2-C3	3.10	114.15	109.64
2	3-E	6	BGC	C1-C2-C3	3.09	114.15	109.64
2	9-E	5	BGC	C1-C2-C3	3.09	114.14	109.64
2	8-E	5	BGC	C1-C2-C3	3.08	114.13	109.64
2	1-C	6	BGC	C1-O5-C5	3.08	116.31	112.19
3	13-D	3	BGC	C1-O5-C5	3.08	116.31	112.19
3	11-D	4	BGC	O3-C3-C2	3.07	116.33	110.05
2	8-E	2	BGC	C1-O5-C5	-3.07	108.07	112.19
2	24-C	4	BGC	C1-C2-C3	3.07	114.11	109.64
2	12-E	1	BGC	O5-C1-C2	-3.06	104.91	110.30
2	7-E	2	BGC	C1-C2-C3	3.06	114.10	109.64
2	2-E	2	BGC	C1-C2-C3	3.06	114.09	109.64
2	13-C	6	BGC	O5-C5-C6	-3.05	101.72	107.66
3	24-D	4	BGC	C1-O5-C5	3.05	116.28	112.19
2	20-C	4	BGC	O3-C3-C2	-3.05	103.83	110.05
2	21-E	5	BGC	O5-C5-C4	-3.05	103.41	110.83
3	10-F	2	BGC	C1-C2-C3	3.05	114.08	109.64
2	5-C	5	BGC	C1-C2-C3	3.05	114.08	109.64
3	6-D	1	BGC	C1-O5-C5	3.04	119.54	113.65
2	24-E	6	BGC	C3-C4-C5	-3.04	104.71	110.23
2	15-C	4	BGC	C1-C2-C3	3.04	114.07	109.64
2	18-C	2	BGC	C1-C2-C3	3.04	114.07	109.64
2	12-C	1	BGC	O5-C1-C2	-3.04	104.96	110.30
2	1-C	1	BGC	C4-C3-C2	3.03	116.16	110.83
2	14-E	1	BGC	O2-C2-C3	3.03	117.52	110.38
2	23-C	1	BGC	O5-C1-C2	-3.03	104.98	110.30
3	11-D	3	BGC	C2-C3-C4	3.02	116.18	110.86
2	6-C	6	BGC	O3-C3-C4	-3.02	103.25	110.38
2	8-C	2	BGC	C1-O5-C5	-3.02	108.14	112.19
2	21-C	2	BGC	O5-C5-C4	-3.02	103.49	110.83
2	17-E	6	BGC	O3-C3-C4	-3.02	103.27	110.38
2	18-E	2	BGC	C1-C2-C3	3.01	114.03	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-C	6	BGC	O3-C3-C2	3.01	116.21	110.05
3	5-F	1	BGC	O5-C5-C4	3.01	115.12	109.70
2	25-C	6	BGC	C1-O5-C5	3.01	116.22	112.19
2	21-E	3	BGC	O3-C3-C2	-3.00	103.92	110.05
2	16-E	5	BGC	C1-C2-C3	3.00	114.02	109.64
2	25-C	5	BGC	C1-C2-C3	2.99	114.00	109.64
2	22-E	4	BGC	C1-C2-C3	2.99	114.00	109.64
3	8-F	2	BGC	C1-O5-C5	-2.99	108.18	112.19
2	1-E	4	BGC	C1-C2-C3	2.99	114.00	109.64
3	7-F	1	BGC	C4-C3-C2	2.99	116.08	110.83
2	6-C	2	BGC	O3-C3-C2	-2.99	103.96	110.05
2	13-C	2	BGC	O3-C3-C2	-2.98	103.97	110.05
3	18-D	5	BGC	C2-C3-C4	2.98	116.10	110.86
2	21-C	5	BGC	O3-C3-C4	-2.98	103.36	110.38
2	22-E	5	BGC	O5-C5-C6	-2.97	101.87	107.66
2	4-C	2	BGC	O3-C3-C2	-2.97	103.99	110.05
3	5-F	1	BGC	O5-C1-C2	2.97	115.51	110.30
2	7-C	1	BGC	O2-C2-C3	2.96	117.36	110.38
2	14-C	4	BGC	C1-C2-C3	2.96	113.95	109.64
3	10-D	5	BGC	C1-O5-C5	2.96	116.15	112.19
2	23-C	2	BGC	C1-C2-C3	2.96	113.95	109.64
2	5-C	1	BGC	O5-C1-C2	-2.95	105.11	110.30
2	7-C	4	BGC	O3-C3-C2	-2.95	104.03	110.05
3	6-D	3	BGC	C2-C3-C4	2.95	116.05	110.86
3	10-F	3	BGC	C1-O5-C5	2.94	116.13	112.19
2	8-C	3	BGC	O3-C3-C2	-2.94	104.05	110.05
2	19-C	2	BGC	C1-C2-C3	2.94	113.92	109.64
2	5-E	6	BGC	C1-C2-C3	2.93	113.91	109.64
2	12-C	2	BGC	O3-C3-C2	-2.93	104.07	110.05
2	4-E	4	BGC	O3-C3-C2	-2.93	104.08	110.05
3	6-F	2	BGC	O3-C3-C2	2.92	116.02	110.05
3	25-D	2	BGC	O4-C4-C5	-2.92	102.13	109.32
2	7-C	4	BGC	C1-C2-C3	2.92	113.89	109.64
3	25-F	3	BGC	C1-C2-C3	2.92	113.89	109.64
2	8-E	1	BGC	O5-C1-C2	-2.91	105.17	110.30
2	18-E	4	BGC	O3-C3-C2	-2.91	104.12	110.05
2	12-C	6	BGC	C6-C5-C4	-2.91	105.89	113.02
2	18-C	1	BGC	C1-O5-C5	-2.90	108.05	113.65
2	23-C	4	BGC	O3-C3-C2	-2.89	104.15	110.05
2	10-E	4	BGC	C1-C2-C3	2.89	113.86	109.64
2	18-E	5	BGC	O5-C5-C6	-2.89	102.04	107.66
3	7-D	5	BGC	C2-C3-C4	2.88	115.93	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6-C	3	BGC	O5-C1-C2	-2.88	103.91	110.79
2	3-E	5	BGC	O5-C5-C6	-2.88	102.05	107.66
2	6-E	4	BGC	O3-C3-C2	-2.88	104.17	110.05
3	23-D	1	BGC	C3-C4-C5	2.88	115.46	110.23
2	15-E	5	BGC	C1-C2-C3	2.88	113.84	109.64
3	4-F	3	BGC	C1-O5-C5	2.87	116.04	112.19
3	4-D	5	BGC	O6-C6-C5	2.87	121.11	111.33
2	14-E	3	BGC	C2-C3-C4	2.87	115.91	110.86
2	11-E	5	BGC	C1-C2-C3	2.86	113.81	109.64
2	21-C	2	BGC	C1-C2-C3	2.86	113.80	109.64
2	22-E	1	BGC	C1-O5-C5	-2.85	108.13	113.65
2	8-E	1	BGC	O2-C2-C3	2.85	117.10	110.38
2	23-C	1	BGC	O2-C2-C3	2.85	117.10	110.38
3	1-D	3	BGC	C1-O5-C5	2.85	116.00	112.19
2	16-E	6	BGC	C1-C2-C3	2.84	113.78	109.64
2	8-E	1	BGC	C1-O5-C5	-2.83	108.17	113.65
2	16-E	4	BGC	C1-C2-C3	2.83	113.77	109.64
2	2-C	6	BGC	C3-C4-C5	-2.83	105.09	110.23
2	21-C	4	BGC	C1-C2-C3	2.83	113.77	109.64
2	20-C	2	BGC	C1-C2-C3	2.83	113.77	109.64
2	9-E	6	BGC	O5-C5-C4	-2.82	103.96	110.83
2	9-C	2	BGC	C1-C2-C3	2.82	113.76	109.64
2	19-C	6	BGC	O3-C3-C4	-2.82	103.73	110.38
3	5-F	2	BGC	O5-C5-C6	2.82	113.15	107.66
2	23-C	5	BGC	C1-O5-C5	-2.82	108.41	112.19
2	9-C	4	BGC	C1-C2-C3	2.81	113.74	109.64
2	23-C	6	BGC	O5-C5-C4	-2.81	103.99	110.83
2	1-C	6	BGC	O3-C3-C4	-2.81	103.75	110.38
2	17-E	2	BGC	C1-C2-C3	2.81	113.73	109.64
3	16-F	3	BGC	C1-O5-C5	2.81	115.95	112.19
2	1-C	5	BGC	C1-C2-C3	2.81	113.73	109.64
2	3-C	2	BGC	C1-C2-C3	2.81	113.73	109.64
2	3-E	3	BGC	C1-O5-C5	-2.81	108.43	112.19
2	20-C	5	BGC	C1-C2-C3	2.81	113.73	109.64
3	2-D	3	BGC	C3-C4-C5	2.81	115.32	110.23
2	19-C	1	BGC	C1-C2-C3	-2.80	104.65	110.36
3	16-D	4	BGC	O6-C6-C5	2.80	120.86	111.33
2	3-E	4	BGC	O5-C1-C2	-2.79	104.12	110.79
2	23-C	1	BGC	O5-C5-C6	-2.79	99.52	106.44
2	21-E	6	BGC	C1-C2-C3	2.79	113.71	109.64
3	7-D	3	BGC	C3-C4-C5	2.79	115.28	110.23
2	13-C	6	BGC	C1-O5-C5	2.78	115.91	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-F	3	BGC	O6-C6-C5	2.78	120.80	111.33
2	24-E	6	BGC	O5-C5-C4	-2.77	104.08	110.83
2	17-E	6	BGC	O6-C6-C5	2.77	120.76	111.33
2	24-C	2	BGC	O3-C3-C2	-2.77	104.41	110.05
2	10-E	5	BGC	C1-O5-C5	2.76	115.89	112.19
2	14-C	2	BGC	O3-C3-C2	-2.76	104.42	110.05
3	22-D	5	BGC	O2-C2-C1	-2.76	102.90	109.22
2	4-E	1	BGC	C1-O5-C5	-2.76	108.31	113.65
3	19-D	3	BGC	C1-C2-C3	2.76	113.66	109.64
2	5-C	3	BGC	O5-C5-C4	-2.75	104.14	110.83
2	23-E	5	BGC	C1-C2-C3	2.75	113.65	109.64
2	23-C	6	BGC	C1-C2-C3	2.75	113.64	109.64
3	1-D	3	BGC	C2-C3-C4	2.74	115.69	110.86
2	23-C	3	BGC	O3-C3-C2	-2.74	104.46	110.05
3	21-D	3	BGC	C1-O5-C5	2.74	115.86	112.19
2	2-E	5	BGC	C1-C2-C3	2.74	113.63	109.64
3	13-D	5	BGC	C1-C2-C3	2.74	113.63	109.64
2	20-E	5	BGC	C1-C2-C3	2.73	113.62	109.64
2	12-E	4	BGC	O2-C2-C3	2.73	115.81	110.15
2	25-E	1	BGC	C1-C2-C3	2.73	115.93	110.36
2	1-C	4	BGC	O3-C3-C2	-2.73	104.49	110.05
2	8-E	2	BGC	C6-C5-C4	-2.72	106.33	113.02
3	22-F	1	BGC	C4-C3-C2	2.72	115.61	110.83
2	17-E	6	BGC	C1-O5-C5	2.72	115.84	112.19
2	22-E	2	BGC	C1-C2-C3	2.72	113.61	109.64
2	13-C	4	BGC	O3-C3-C2	-2.72	104.50	110.05
3	10-D	5	BGC	C2-C3-C4	2.72	115.64	110.86
2	12-C	6	BGC	O4-C4-C3	2.72	116.78	110.38
2	3-E	6	BGC	O5-C5-C4	-2.72	104.22	110.83
2	8-C	1	BGC	C4-C3-C2	2.72	115.60	110.83
3	23-D	5	BGC	C2-C3-C4	2.72	115.64	110.86
3	17-F	1	BGC	O5-C1-C2	2.71	115.07	110.30
3	19-D	1	BGC	C4-C3-C2	2.71	115.59	110.83
3	6-D	2	BGC	O2-C2-C3	2.71	115.77	110.15
3	4-D	2	BGC	C1-O5-C5	-2.71	108.55	112.19
2	12-C	1	BGC	O5-C5-C4	2.71	114.59	109.70
3	17-D	1	BGC	O5-C5-C4	2.71	114.59	109.70
3	2-F	2	BGC	C3-C4-C5	2.71	115.14	110.23
2	22-C	2	BGC	C1-C2-C3	2.71	113.59	109.64
2	12-C	4	BGC	C1-C2-C3	2.71	113.58	109.64
2	15-C	2	BGC	C1-C2-C3	2.70	113.58	109.64
2	14-C	6	BGC	C1-C2-C3	2.70	113.58	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	17-E	4	BGC	O3-C3-C2	-2.70	104.55	110.05
2	25-E	1	BGC	O2-C2-C3	2.70	116.73	110.38
2	17-C	4	BGC	C1-C2-C3	2.69	113.57	109.64
3	15-D	2	BGC	O5-C5-C4	2.69	117.37	110.83
2	25-E	5	BGC	C1-C2-C3	2.69	113.56	109.64
2	4-E	4	BGC	C1-C2-C3	2.69	113.56	109.64
2	3-C	6	BGC	O5-C5-C6	-2.68	102.44	107.66
3	13-F	2	BGC	C3-C4-C5	2.68	115.09	110.23
2	4-C	6	BGC	O3-C3-C4	-2.68	104.06	110.38
2	13-E	4	BGC	O3-C3-C2	-2.68	104.58	110.05
3	13-D	3	BGC	C2-C3-C4	2.68	115.57	110.86
2	8-E	2	BGC	C1-C2-C3	2.68	113.54	109.64
3	25-D	5	BGC	C1-O5-C5	2.68	115.78	112.19
2	13-E	5	BGC	C1-O5-C5	-2.66	108.62	112.19
2	2-E	4	BGC	O2-C2-C3	2.66	115.66	110.15
2	7-E	6	BGC	O5-C5-C4	-2.66	104.36	110.83
2	1-E	2	BGC	C1-C2-C3	2.66	113.51	109.64
2	14-E	4	BGC	O3-C3-C2	-2.66	104.63	110.05
2	14-E	2	BGC	C1-C2-C3	2.66	113.51	109.64
2	23-C	4	BGC	C1-O5-C5	-2.65	108.63	112.19
2	23-C	4	BGC	C3-C4-C5	-2.65	105.42	110.23
2	12-E	2	BGC	O3-C3-C2	-2.65	104.64	110.05
2	19-E	6	BGC	O6-C6-C5	-2.65	102.31	111.33
3	6-D	2	BGC	O5-C5-C4	2.65	117.27	110.83
2	14-E	3	BGC	O3-C3-C4	-2.65	104.13	110.38
2	11-E	1	BGC	O5-C1-C2	-2.65	105.64	110.30
3	11-D	2	BGC	O2-C2-C3	2.64	115.63	110.15
3	4-D	4	BGC	C2-C3-C4	-2.64	106.21	110.86
2	8-E	4	BGC	O3-C3-C2	-2.64	104.66	110.05
2	10-C	1	BGC	C4-C3-C2	2.64	115.47	110.83
2	9-E	2	BGC	C2-C3-C4	2.64	115.50	110.86
3	7-D	5	BGC	C1-C2-C3	2.64	113.49	109.64
3	1-F	2	BGC	C3-C4-C5	2.64	115.01	110.23
2	16-E	4	BGC	O3-C3-C2	-2.63	104.68	110.05
2	21-E	5	BGC	O4-C4-C5	2.63	115.80	109.32
2	16-C	4	BGC	C1-C2-C3	2.63	113.47	109.64
3	5-F	4	BGC	O3-C3-C2	-2.63	104.69	110.05
3	4-F	2	BGC	C3-C4-C5	2.63	115.00	110.23
3	7-D	3	BGC	C2-C3-C4	2.63	115.48	110.86
2	6-C	2	BGC	C1-C2-C3	2.63	113.47	109.64
2	15-E	4	BGC	O3-C3-C2	-2.63	104.69	110.05
2	21-E	6	BGC	O5-C5-C4	-2.62	104.44	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-C	4	BGC	C1-C2-C3	2.62	113.46	109.64
2	11-E	4	BGC	O3-C3-C2	-2.62	104.70	110.05
3	23-F	1	BGC	O3-C3-C2	-2.62	104.19	110.38
2	14-C	3	BGC	O5-C1-C2	-2.62	104.54	110.79
3	6-D	5	BGC	C1-C2-C3	2.62	113.46	109.64
2	21-E	1	BGC	C6-C5-C4	-2.62	106.59	113.02
2	9-C	6	BGC	O6-C6-C5	2.61	120.24	111.33
3	5-D	4	BGC	C1-O5-C5	2.61	115.68	112.19
2	25-E	3	BGC	C1-O5-C5	-2.61	108.69	112.19
2	22-E	6	BGC	C1-O5-C5	2.60	115.68	112.19
2	16-C	5	BGC	O3-C3-C4	-2.60	104.25	110.38
2	25-C	6	BGC	O3-C3-C4	-2.60	104.25	110.38
2	10-E	4	BGC	O3-C3-C2	-2.60	104.75	110.05
2	11-C	4	BGC	C1-C2-C3	2.59	113.42	109.64
2	4-E	1	BGC	O5-C1-C2	-2.59	105.74	110.30
3	16-D	4	BGC	C1-C2-C3	2.59	113.42	109.64
2	15-C	3	BGC	O3-C3-C2	-2.59	104.77	110.05
3	6-D	1	BGC	C6-C5-C4	-2.59	106.66	113.02
2	6-E	3	BGC	C1-O5-C5	2.59	115.66	112.19
2	5-C	4	BGC	C1-C2-C3	2.59	113.41	109.64
2	25-C	4	BGC	C1-C2-C3	2.58	113.40	109.64
3	12-D	1	BGC	O5-C5-C4	2.58	114.35	109.70
2	3-E	5	BGC	C1-C2-C3	2.58	113.40	109.64
3	21-D	5	BGC	C1-O5-C5	2.58	115.64	112.19
2	10-E	6	BGC	C1-C2-C3	2.58	113.40	109.64
2	8-E	5	BGC	O5-C5-C6	-2.58	102.65	107.66
3	2-D	3	BGC	C2-C3-C4	2.57	115.39	110.86
3	16-F	2	BGC	C1-O5-C5	-2.57	108.74	112.19
2	15-E	6	BGC	C1-C2-C3	2.57	113.39	109.64
3	9-D	1	BGC	O3-C3-C2	-2.57	104.31	110.38
3	17-D	1	BGC	C4-C3-C2	2.57	115.34	110.83
3	22-D	1	BGC	C1-O5-C5	2.57	118.62	113.65
3	11-D	4	BGC	O2-C2-C3	2.57	115.47	110.15
2	18-C	4	BGC	C1-C2-C3	2.57	113.38	109.64
2	14-C	6	BGC	C1-O5-C5	2.57	115.62	112.19
3	17-D	1	BGC	O3-C3-C2	-2.56	104.34	110.38
3	21-D	4	BGC	C1-O5-C5	2.56	115.61	112.19
3	17-F	1	BGC	O6-C6-C5	2.55	120.03	111.33
2	6-C	6	BGC	C1-O5-C5	-2.55	108.77	112.19
2	10-E	6	BGC	O3-C3-C4	-2.55	104.36	110.38
2	15-E	3	BGC	C1-O5-C5	-2.55	108.77	112.19
2	11-C	3	BGC	O3-C3-C2	-2.55	104.85	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	18-D	2	BGC	C1-O5-C5	2.55	115.60	112.19
2	18-E	5	BGC	C1-C2-C3	2.55	113.35	109.64
2	18-C	2	BGC	O3-C3-C2	-2.55	104.86	110.05
2	19-C	4	BGC	C1-C2-C3	2.54	113.35	109.64
3	6-D	2	BGC	C1-C2-C3	2.54	113.34	109.64
3	25-F	4	BGC	O5-C5-C6	2.54	112.61	107.66
3	2-D	3	BGC	C1-O5-C5	2.54	115.59	112.19
3	25-D	3	BGC	C1-C2-C3	2.54	113.34	109.64
2	16-C	2	BGC	O3-C3-C2	-2.53	104.88	110.05
2	15-E	5	BGC	O5-C1-C2	-2.53	104.74	110.79
2	9-E	5	BGC	O5-C5-C6	-2.53	102.73	107.66
3	24-F	2	BGC	O2-C2-C3	2.53	115.40	110.15
2	16-E	1	BGC	C1-O5-C5	-2.53	108.75	113.65
2	5-C	4	BGC	O3-C3-C2	-2.53	104.90	110.05
3	20-D	2	BGC	C1-O5-C5	2.52	115.56	112.19
3	11-D	2	BGC	C2-C3-C4	2.52	115.30	110.86
3	3-D	5	BGC	C1-C2-C3	2.52	113.31	109.64
3	15-D	4	BGC	C1-C2-C3	2.51	113.31	109.64
3	18-D	1	BGC	O5-C5-C4	2.51	114.22	109.70
3	22-D	5	BGC	C1-C2-C3	2.51	113.30	109.64
2	12-C	3	BGC	O3-C3-C4	-2.51	104.47	110.38
2	20-C	2	BGC	O5-C1-C2	-2.51	104.81	110.79
2	21-E	4	BGC	O3-C3-C2	-2.50	104.95	110.05
3	21-D	1	BGC	O5-C5-C4	2.50	114.21	109.70
2	23-E	6	BGC	O3-C3-C4	-2.50	104.49	110.38
2	1-C	1	BGC	C1-C2-C3	2.50	115.45	110.36
3	14-D	1	BGC	O5-C5-C4	2.50	114.20	109.70
3	11-D	4	BGC	C6-C5-C4	2.50	119.15	113.02
3	11-D	5	BGC	C1-C2-C3	2.49	113.28	109.64
2	5-E	5	BGC	C1-C2-C3	2.49	113.28	109.64
3	24-D	1	BGC	O5-C5-C4	2.49	114.19	109.70
2	5-C	6	BGC	C1-C2-C3	2.49	113.27	109.64
3	11-D	1	BGC	O5-C5-C4	2.49	114.18	109.70
2	24-E	1	BGC	C1-O5-C5	-2.48	108.85	113.65
2	15-E	1	BGC	O5-C5-C6	2.48	112.59	106.44
2	17-E	1	BGC	C1-O5-C5	-2.48	108.85	113.65
2	19-E	1	BGC	C1-O5-C5	-2.48	108.86	113.65
2	25-C	2	BGC	C1-C2-C3	2.48	113.25	109.64
3	1-D	5	BGC	C1-C2-C3	2.48	113.25	109.64
2	13-C	4	BGC	O5-C5-C4	-2.47	104.81	110.83
3	16-F	2	BGC	O2-C2-C3	2.47	115.27	110.15
2	18-E	3	BGC	O5-C1-C2	-2.47	104.89	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	23-D	5	BGC	C1-C2-C3	2.47	113.24	109.64
2	8-C	4	BGC	O3-C3-C2	-2.47	105.02	110.05
2	16-C	3	BGC	C1-O5-C5	-2.47	108.88	112.19
3	9-D	2	BGC	C3-C4-C5	2.47	114.70	110.23
3	23-F	3	BGC	O6-C6-C5	2.46	119.72	111.33
3	4-F	5	BGC	C2-C3-C4	2.46	115.19	110.86
3	20-D	3	BGC	C1-O5-C5	2.46	115.48	112.19
2	23-C	6	BGC	O3-C3-C4	-2.46	104.57	110.38
3	3-F	2	BGC	O2-C2-C3	2.46	115.24	110.15
2	16-E	2	BGC	C1-O5-C5	-2.46	108.89	112.19
2	24-E	4	BGC	C1-C2-C3	2.46	113.22	109.64
2	13-C	3	BGC	O5-C1-C2	-2.46	104.93	110.79
2	16-C	4	BGC	O3-C3-C2	-2.45	105.05	110.05
2	4-C	6	BGC	C1-O5-C5	2.45	115.47	112.19
2	1-E	3	BGC	O3-C3-C2	-2.45	105.05	110.05
3	15-F	5	BGC	C2-C3-C4	2.45	115.17	110.86
2	21-E	4	BGC	O6-C6-C5	2.45	119.67	111.33
2	17-C	6	BGC	C1-C2-C3	2.45	113.21	109.64
3	6-F	3	BGC	C1-C2-C3	2.45	113.21	109.64
2	12-E	1	BGC	O2-C2-C3	2.45	116.14	110.38
2	7-E	5	BGC	C1-C2-C3	2.44	113.20	109.64
3	3-D	4	BGC	O6-C6-C5	2.44	119.65	111.33
2	13-E	6	BGC	C1-O5-C5	2.44	115.45	112.19
3	2-D	5	BGC	C2-C3-C4	2.44	115.15	110.86
2	20-E	4	BGC	C1-C2-C3	2.44	113.19	109.64
2	22-C	6	BGC	O6-C6-C5	2.43	119.62	111.33
3	9-F	2	BGC	C3-C4-C5	2.43	114.64	110.23
3	23-F	3	BGC	O2-C2-C3	2.43	115.18	110.15
2	11-C	6	BGC	O6-C6-C5	2.43	119.60	111.33
2	9-C	2	BGC	C1-O5-C5	-2.43	108.93	112.19
2	12-E	6	BGC	C1-O5-C5	2.43	115.44	112.19
3	15-D	1	BGC	O5-C5-C4	2.43	114.07	109.70
3	21-D	1	BGC	O3-C3-C4	2.42	116.09	110.38
2	19-C	1	BGC	O5-C5-C4	2.42	114.07	109.70
3	25-D	4	BGC	O6-C6-C5	2.42	119.59	111.33
3	16-D	4	BGC	C1-O5-C5	2.42	115.43	112.19
3	5-F	1	BGC	O6-C6-C5	2.42	119.58	111.33
2	25-E	5	BGC	O5-C5-C6	-2.42	102.95	107.66
3	11-D	1	BGC	C4-C3-C2	2.41	115.07	110.83
2	14-C	4	BGC	O3-C3-C2	-2.41	105.13	110.05
2	1-E	5	BGC	C1-C2-C3	2.41	113.16	109.64
3	18-D	1	BGC	C3-C4-C5	2.41	114.60	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-C	6	BGC	C1-O5-C5	2.41	115.42	112.19
3	23-F	1	BGC	O6-C6-C5	2.41	119.54	111.33
2	6-C	4	BGC	O3-C3-C2	-2.41	105.14	110.05
3	10-F	3	BGC	O2-C2-C3	2.41	115.13	110.15
2	12-E	3	BGC	O3-C3-C2	-2.40	105.15	110.05
2	11-E	6	BGC	O3-C3-C4	-2.40	104.71	110.38
3	20-D	5	BGC	C1-O5-C5	2.40	115.40	112.19
2	13-C	3	BGC	O3-C3-C2	-2.40	105.15	110.05
3	22-D	1	BGC	C6-C5-C4	-2.40	107.13	113.02
3	6-F	2	BGC	O2-C2-C3	2.40	115.12	110.15
3	23-D	4	BGC	C3-C4-C5	-2.40	105.89	110.23
2	3-E	6	BGC	O3-C3-C4	-2.40	104.73	110.38
3	15-D	4	BGC	O6-C6-C5	2.39	119.48	111.33
3	23-D	1	BGC	O6-C6-C5	2.39	119.47	111.33
2	2-E	2	BGC	O3-C3-C2	-2.39	105.18	110.05
2	21-C	5	BGC	C6-C5-C4	-2.39	107.16	113.02
3	19-D	4	BGC	O6-C6-C5	2.39	119.46	111.33
3	15-F	2	BGC	C3-C4-C5	2.38	114.56	110.23
2	8-C	1	BGC	C1-C2-C3	2.38	115.22	110.36
3	16-D	2	BGC	C1-O5-C5	-2.38	108.99	112.19
3	18-D	2	BGC	O5-C5-C4	2.38	116.61	110.83
2	25-E	4	BGC	O3-C3-C2	-2.38	105.20	110.05
2	7-C	1	BGC	C1-C2-C3	-2.38	105.50	110.36
2	17-C	6	BGC	O5-C5-C4	-2.37	105.05	110.83
2	16-C	2	BGC	C1-C2-C3	2.37	113.10	109.64
2	12-C	6	BGC	O5-C5-C4	-2.37	105.05	110.83
2	17-C	2	BGC	C1-C2-C3	2.37	113.10	109.64
3	7-D	3	BGC	C1-O5-C5	2.37	115.36	112.19
2	20-C	3	BGC	O5-C1-C2	-2.37	105.15	110.79
3	17-F	2	BGC	O5-C5-C6	2.36	112.26	107.66
2	15-C	4	BGC	O3-C3-C2	-2.36	105.23	110.05
2	10-E	5	BGC	O5-C5-C6	-2.36	103.06	107.66
2	17-C	1	BGC	O5-C5-C4	2.36	113.95	109.70
2	2-C	6	BGC	C1-C2-C3	2.36	113.08	109.64
2	13-E	4	BGC	C1-C2-C3	2.36	113.08	109.64
2	2-C	6	BGC	O6-C6-C5	2.35	119.32	111.33
3	9-D	3	BGC	C1-C2-C3	2.35	113.06	109.64
2	4-E	2	BGC	C1-O5-C5	-2.35	109.04	112.19
2	10-C	4	BGC	C1-C2-C3	2.34	113.06	109.64
2	2-E	6	BGC	O5-C5-C4	-2.34	105.13	110.83
2	15-E	2	BGC	O3-C3-C2	-2.34	105.28	110.05
2	5-E	1	BGC	O3-C3-C2	-2.34	104.86	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	12-C	6	BGC	O3-C3-C2	2.34	114.83	110.05
2	16-E	5	BGC	O5-C1-C2	-2.34	105.21	110.79
3	14-F	1	BGC	C4-C3-C2	2.34	114.93	110.83
2	24-E	6	BGC	O6-C6-C5	2.34	119.29	111.33
2	18-E	6	BGC	O6-C6-C5	2.34	119.28	111.33
3	9-D	5	BGC	C1-O5-C5	2.33	115.31	112.19
2	9-E	2	BGC	O3-C3-C2	-2.33	105.29	110.05
2	22-E	1	BGC	O2-C2-C3	2.33	115.88	110.38
3	6-D	1	BGC	C4-C3-C2	2.33	114.93	110.83
3	5-D	1	BGC	O5-C5-C4	2.33	113.90	109.70
3	1-F	1	BGC	O6-C6-C5	2.33	119.27	111.33
2	18-C	6	BGC	C1-C2-C3	2.33	113.04	109.64
2	12-C	4	BGC	O3-C3-C2	-2.33	105.30	110.05
2	4-E	1	BGC	O2-C2-C3	2.33	115.86	110.38
3	18-F	3	BGC	C1-O5-C5	2.33	115.30	112.19
2	20-C	6	BGC	C1-C2-C3	2.32	113.03	109.64
3	7-D	4	BGC	O5-C5-C6	2.32	112.18	107.66
2	23-C	5	BGC	C1-C2-C3	2.32	113.02	109.64
3	14-D	1	BGC	C3-C4-C5	2.32	114.44	110.23
2	16-C	6	BGC	O3-C3-C4	-2.32	104.91	110.38
2	4-E	5	BGC	C1-O5-C5	-2.32	109.08	112.19
3	12-D	4	BGC	O6-C6-C5	2.32	119.23	111.33
3	4-D	2	BGC	O3-C3-C2	2.32	114.78	110.05
2	24-E	6	BGC	C6-C5-C4	2.31	118.69	113.02
2	8-E	3	BGC	O3-C3-C2	-2.31	105.34	110.05
3	24-D	5	BGC	C1-C2-C3	2.31	113.01	109.64
2	6-E	5	BGC	C1-C2-C3	2.31	113.00	109.64
3	14-D	5	BGC	C1-C2-C3	2.30	113.00	109.64
3	17-D	3	BGC	C1-O5-C5	2.30	115.27	112.19
3	3-D	2	BGC	C2-C3-C4	2.30	114.91	110.86
3	14-D	1	BGC	O3-C3-C2	-2.30	104.95	110.38
2	21-C	1	BGC	O3-C3-C4	2.30	115.80	110.38
2	18-C	6	BGC	O5-C5-C6	-2.30	103.18	107.66
2	11-C	6	BGC	O5-C5-C4	-2.30	105.23	110.83
2	12-E	1	BGC	C1-O5-C5	-2.30	109.20	113.65
3	24-F	1	BGC	C4-C3-C2	2.30	114.87	110.83
3	24-D	3	BGC	C1-O5-C5	2.30	115.27	112.19
3	5-D	3	BGC	O5-C5-C6	2.30	112.14	107.66
3	25-F	3	BGC	O3-C3-C2	-2.30	105.36	110.05
2	25-E	1	BGC	O5-C1-C2	-2.30	106.26	110.30
2	24-E	5	BGC	C1-C2-C3	2.29	112.98	109.64
2	25-C	5	BGC	C6-C5-C4	-2.29	107.39	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-E	2	BGC	O4-C4-C5	-2.29	103.67	109.32
3	18-D	1	BGC	O3-C3-C4	2.29	115.78	110.38
3	21-D	3	BGC	C1-C2-C3	2.29	112.98	109.64
3	10-F	3	BGC	O3-C3-C2	-2.29	105.38	110.05
2	25-E	4	BGC	C3-C4-C5	-2.29	106.08	110.23
2	18-C	6	BGC	C6-C5-C4	2.29	118.64	113.02
3	20-F	2	BGC	O5-C5-C6	2.28	112.11	107.66
2	22-E	2	BGC	O3-C3-C2	-2.28	105.39	110.05
2	15-C	1	BGC	O2-C2-C3	2.28	115.76	110.38
2	25-E	1	BGC	C4-C3-C2	-2.28	106.82	110.83
2	10-C	5	BGC	C6-C5-C4	-2.28	107.42	113.02
3	2-F	5	BGC	C2-C3-C4	2.28	114.87	110.86
3	25-D	1	BGC	O4-C4-C3	2.28	115.75	110.38
2	25-C	3	BGC	O5-C1-C2	-2.28	105.35	110.79
3	7-F	3	BGC	C1-O5-C5	2.28	115.24	112.19
2	11-E	1	BGC	O2-C2-C3	2.28	115.74	110.38
2	23-E	2	BGC	C1-C2-C3	2.28	112.96	109.64
2	12-E	6	BGC	O3-C3-C4	-2.28	105.01	110.38
2	18-E	6	BGC	O5-C5-C4	-2.28	105.29	110.83
2	17-C	6	BGC	C3-C4-C5	-2.27	106.11	110.23
3	23-D	3	BGC	C1-C2-C3	2.27	112.95	109.64
2	12-C	3	BGC	C1-C2-C3	2.27	112.95	109.64
2	4-E	2	BGC	O3-C3-C2	-2.26	105.44	110.05
3	22-F	1	BGC	O3-C3-C2	-2.26	105.04	110.38
3	11-D	3	BGC	O3-C3-C2	-2.26	105.44	110.05
3	8-D	1	BGC	O5-C5-C4	2.26	113.77	109.70
2	13-E	1	BGC	O2-C2-C3	2.26	115.70	110.38
3	4-D	4	BGC	O6-C6-C5	2.26	119.02	111.33
2	11-C	6	BGC	C6-C5-C4	2.26	118.56	113.02
2	22-C	3	BGC	O5-C1-C2	-2.25	105.41	110.79
2	14-C	1	BGC	C1-O5-C5	-2.25	109.29	113.65
2	13-C	2	BGC	C1-O5-C5	-2.25	109.17	112.19
2	19-C	1	BGC	O3-C3-C4	2.25	115.68	110.38
3	18-F	5	BGC	C2-C3-C4	2.25	114.82	110.86
2	5-E	6	BGC	O3-C3-C4	-2.25	105.07	110.38
2	12-C	1	BGC	O2-C2-C3	2.25	115.68	110.38
2	5-C	1	BGC	O6-C6-C5	2.25	119.00	111.33
3	7-D	1	BGC	O5-C5-C4	2.25	113.75	109.70
2	9-E	4	BGC	O2-C2-C3	2.25	114.80	110.15
2	10-C	3	BGC	C1-O5-C5	-2.24	109.18	112.19
3	23-F	1	BGC	C4-C3-C2	2.24	114.77	110.83
3	19-D	5	BGC	C1-C2-C3	2.24	112.91	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	13-D	1	BGC	O3-C3-C2	-2.24	105.09	110.38
3	7-D	3	BGC	C1-C2-C3	2.24	112.91	109.64
2	5-C	1	BGC	O5-C5-C4	2.24	113.74	109.70
2	23-C	6	BGC	C3-C4-C5	-2.24	106.17	110.23
2	11-E	1	BGC	C1-O5-C5	-2.24	109.32	113.65
3	8-D	4	BGC	C1-C2-C3	2.24	112.90	109.64
2	25-E	4	BGC	C1-C2-C3	2.24	112.90	109.64
3	7-D	1	BGC	C4-C3-C2	2.24	114.75	110.83
3	13-F	3	BGC	O2-C2-C3	2.23	114.78	110.15
2	6-C	4	BGC	C1-C2-C3	2.23	112.90	109.64
2	1-C	2	BGC	C1-C2-C3	2.23	112.89	109.64
3	9-D	4	BGC	O6-C6-C5	2.23	118.93	111.33
3	3-F	3	BGC	C1-C2-C3	2.23	112.89	109.64
3	24-D	1	BGC	O3-C3-C2	-2.23	105.12	110.38
3	16-D	3	BGC	O6-C6-C5	2.23	118.92	111.33
2	9-E	5	BGC	C2-C3-C4	2.23	114.78	110.86
2	3-C	5	BGC	C3-C4-C5	2.23	114.27	110.23
3	22-D	1	BGC	O3-C3-C2	-2.23	105.12	110.38
2	25-C	4	BGC	O3-C3-C2	-2.23	105.51	110.05
3	4-F	5	BGC	O5-C5-C4	-2.22	105.42	110.83
3	22-F	3	BGC	C1-O5-C5	2.22	115.17	112.19
3	2-D	1	BGC	O5-C5-C4	2.22	113.70	109.70
2	6-E	2	BGC	C1-C2-C3	2.22	112.88	109.64
3	13-F	1	BGC	C4-C3-C2	2.22	114.73	110.83
2	24-C	4	BGC	O3-C3-C2	-2.22	105.53	110.05
3	21-D	2	BGC	C3-C4-C5	2.22	114.25	110.23
3	12-D	5	BGC	C2-C3-C4	2.22	114.76	110.86
2	19-C	1	BGC	O5-C1-C2	-2.22	106.40	110.30
2	20-C	6	BGC	O3-C3-C4	-2.22	105.15	110.38
2	15-E	5	BGC	O3-C3-C2	-2.22	105.53	110.05
3	17-D	4	BGC	O6-C6-C5	2.21	118.87	111.33
2	10-E	2	BGC	C1-C2-C3	2.21	112.86	109.64
2	2-C	3	BGC	O5-C1-C2	-2.21	105.51	110.79
3	19-F	3	BGC	O6-C6-C5	2.21	118.86	111.33
2	7-E	1	BGC	O2-C2-C3	2.21	115.58	110.38
2	19-C	3	BGC	O3-C3-C2	-2.21	105.55	110.05
2	18-E	2	BGC	O6-C6-C5	2.21	118.85	111.33
2	4-C	1	BGC	O5-C5-C4	2.21	113.67	109.70
2	23-E	2	BGC	C2-C3-C4	2.20	114.74	110.86
3	5-D	3	BGC	O6-C6-C5	2.20	118.84	111.33
3	23-D	1	BGC	O3-C3-C2	-2.20	105.19	110.38
2	9-E	5	BGC	C6-C5-C4	-2.20	107.62	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-E	1	BGC	C1-O5-C5	-2.20	109.40	113.65
3	17-F	4	BGC	O3-C3-C2	-2.20	105.57	110.05
3	8-F	1	BGC	C4-C3-C2	2.20	114.69	110.83
2	3-E	4	BGC	O4-C4-C5	2.20	114.73	109.32
3	9-D	1	BGC	O3-C3-C4	2.20	115.55	110.38
2	18-C	4	BGC	O3-C3-C2	-2.19	105.58	110.05
2	24-C	1	BGC	O3-C3-C2	-2.19	105.20	110.38
3	23-F	2	BGC	O2-C2-C3	2.19	114.69	110.15
3	4-D	3	BGC	C2-C3-C4	2.19	114.72	110.86
3	5-D	2	BGC	O3-C3-C4	2.19	115.55	110.38
3	19-D	5	BGC	C1-O5-C5	2.19	115.12	112.19
3	5-F	5	BGC	C2-C3-C4	2.19	114.71	110.86
3	23-F	2	BGC	C3-C4-C5	2.19	114.20	110.23
3	24-D	3	BGC	C1-C2-C3	2.19	112.83	109.64
2	13-E	1	BGC	C1-O5-C5	-2.19	109.42	113.65
2	17-E	1	BGC	O5-C5-C6	2.19	111.86	106.44
3	18-F	2	BGC	O5-C5-C6	2.19	111.92	107.66
3	15-D	1	BGC	O3-C3-C2	-2.19	105.22	110.38
2	23-E	1	BGC	O3-C3-C2	-2.18	105.23	110.38
2	12-C	3	BGC	O5-C1-C2	-2.18	105.58	110.79
3	11-F	3	BGC	C3-C4-C5	2.18	114.19	110.23
3	6-D	3	BGC	C1-C2-C3	2.18	112.82	109.64
3	18-D	5	BGC	O2-C2-C1	-2.18	104.23	109.22
2	10-E	1	BGC	C1-O5-C5	-2.18	109.44	113.65
3	10-D	2	BGC	C1-O5-C5	-2.18	109.27	112.19
3	5-D	2	BGC	O4-C4-C5	-2.18	103.96	109.32
2	21-E	2	BGC	O2-C2-C3	-2.18	105.64	110.15
3	1-D	4	BGC	O6-C6-C5	2.18	118.75	111.33
2	17-C	6	BGC	O4-C4-C3	2.18	115.51	110.38
3	6-F	2	BGC	C1-O5-C5	-2.18	109.27	112.19
2	21-E	5	BGC	O6-C6-C5	2.18	118.74	111.33
3	16-D	1	BGC	O5-C5-C4	2.18	113.62	109.70
2	12-C	3	BGC	O3-C3-C2	-2.18	105.61	110.05
3	4-D	5	BGC	C1-C2-C3	2.17	112.81	109.64
3	17-F	3	BGC	O6-C6-C5	2.17	118.73	111.33
3	12-F	2	BGC	C3-C4-C5	2.17	114.17	110.23
3	14-D	2	BGC	C1-O5-C5	-2.17	109.28	112.19
2	16-E	1	BGC	O2-C2-C3	2.17	115.49	110.38
3	12-F	1	BGC	C4-C3-C2	2.17	114.64	110.83
2	6-E	6	BGC	C3-C4-C5	-2.17	106.30	110.23
3	22-D	3	BGC	O6-C6-C5	2.17	118.72	111.33
2	7-C	1	BGC	O5-C5-C4	2.17	113.61	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	25-D	2	BGC	O5-C5-C4	2.17	116.10	110.83
3	13-F	4	BGC	O3-C3-C2	-2.17	105.63	110.05
2	18-E	3	BGC	C1-C2-C3	2.17	112.80	109.64
2	14-E	6	BGC	O5-C5-C4	-2.17	105.56	110.83
2	7-C	1	BGC	O5-C1-C2	-2.17	106.49	110.30
2	2-E	6	BGC	C1-O5-C5	2.17	115.09	112.19
2	7-C	5	BGC	C2-C3-C4	-2.16	107.06	110.86
2	18-E	2	BGC	C2-C3-C4	2.16	114.67	110.86
2	21-E	1	BGC	O5-C1-C2	2.16	114.10	110.30
3	12-F	3	BGC	C1-O5-C5	2.16	115.08	112.19
2	9-C	1	BGC	O2-C2-C3	2.16	115.47	110.38
2	15-C	1	BGC	O5-C5-C4	2.16	113.59	109.70
2	15-E	3	BGC	O5-C1-C2	-2.16	105.64	110.79
2	15-E	1	BGC	O2-C2-C1	-2.16	104.26	109.25
3	19-F	3	BGC	O5-C5-C6	2.16	111.86	107.66
3	11-D	3	BGC	C3-C4-C5	2.16	114.15	110.23
2	14-E	5	BGC	C1-O5-C5	-2.16	109.29	112.19
3	23-D	1	BGC	C1-O5-C5	2.16	117.83	113.65
2	14-C	5	BGC	O3-C3-C4	-2.16	105.29	110.38
3	20-D	1	BGC	O6-C6-C5	2.15	118.67	111.33
3	6-D	2	BGC	O3-C3-C4	2.15	115.45	110.38
2	3-C	5	BGC	O3-C3-C2	-2.15	105.66	110.05
2	23-E	5	BGC	O5-C5-C6	-2.15	103.48	107.66
2	4-C	2	BGC	C1-C2-C3	2.15	112.77	109.64
2	7-E	3	BGC	C2-C3-C4	2.15	114.64	110.86
3	5-D	3	BGC	C2-C3-C4	2.15	114.64	110.86
3	2-D	1	BGC	O3-C3-C2	-2.14	105.32	110.38
2	4-C	2	BGC	C6-C5-C4	-2.14	107.76	113.02
2	18-E	6	BGC	O2-C2-C3	2.14	114.59	110.15
2	1-E	3	BGC	O5-C1-C2	-2.14	105.68	110.79
3	9-F	3	BGC	O6-C6-C5	2.14	118.62	111.33
3	10-F	2	BGC	O2-C2-C1	2.14	114.12	109.22
3	2-D	4	BGC	C1-C2-C3	2.14	112.76	109.64
2	20-E	1	BGC	C1-O5-C5	-2.14	109.52	113.65
3	17-D	1	BGC	C3-C4-C5	2.14	114.11	110.23
2	15-C	3	BGC	O5-C1-C2	-2.14	105.69	110.79
2	17-E	1	BGC	C1-C2-C3	2.13	114.71	110.36
2	21-C	3	BGC	O3-C3-C4	-2.13	105.34	110.38
3	19-F	1	BGC	C4-C3-C2	2.13	114.57	110.83
3	20-F	3	BGC	C1-C2-C3	2.13	112.75	109.64
3	11-F	2	BGC	O2-C2-C1	2.13	114.10	109.22
3	2-D	3	BGC	C1-C2-C3	2.13	112.75	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	18-D	1	BGC	O3-C3-C2	-2.13	105.36	110.38
3	18-F	1	BGC	O6-C6-C5	2.13	118.58	111.33
2	11-E	4	BGC	C1-C2-C3	2.13	112.74	109.64
3	20-D	3	BGC	C2-C3-C4	2.13	114.60	110.86
2	10-E	2	BGC	O3-C3-C2	-2.13	105.72	110.05
2	11-C	3	BGC	O5-C1-C2	-2.12	105.72	110.79
2	1-C	5	BGC	C1-O5-C5	-2.12	109.34	112.19
3	16-F	5	BGC	C2-C3-C4	2.12	114.59	110.86
3	8-D	5	BGC	O5-C5-C4	2.12	115.99	110.83
3	11-F	5	BGC	C2-C3-C4	2.12	114.59	110.86
3	20-F	1	BGC	O6-C6-C5	2.12	118.55	111.33
2	25-C	3	BGC	C1-C2-C3	2.12	112.73	109.64
2	24-C	1	BGC	C1-O5-C5	-2.12	109.55	113.65
2	25-C	3	BGC	O3-C3-C2	-2.12	105.73	110.05
3	13-D	5	BGC	C2-C3-C4	2.12	114.58	110.86
3	6-D	5	BGC	C6-C5-C4	-2.12	107.82	113.02
2	9-C	1	BGC	O5-C5-C4	2.11	113.51	109.70
3	23-D	4	BGC	O6-C6-C5	2.11	118.53	111.33
2	21-C	2	BGC	C3-C4-C5	-2.11	106.40	110.23
2	5-C	1	BGC	O3-C3-C4	2.11	115.36	110.38
2	6-C	2	BGC	O6-C6-C5	2.11	118.52	111.33
3	22-D	2	BGC	O2-C2-C3	2.11	114.52	110.15
3	19-D	2	BGC	O2-C2-C3	2.11	114.52	110.15
3	10-D	3	BGC	C1-C2-C3	2.11	112.72	109.64
2	17-C	3	BGC	O5-C1-C2	-2.11	105.76	110.79
2	11-E	1	BGC	O4-C4-C5	-2.11	104.13	109.32
3	6-D	4	BGC	C1-O5-C5	2.11	115.01	112.19
3	25-D	1	BGC	O5-C5-C4	2.11	113.50	109.70
3	15-D	1	BGC	O6-C6-C5	2.11	118.51	111.33
2	20-C	1	BGC	C1-O5-C5	-2.11	109.58	113.65
2	5-E	6	BGC	O5-C5-C6	-2.10	103.57	107.66
2	4-C	3	BGC	O5-C1-C2	-2.10	105.77	110.79
3	12-D	1	BGC	O3-C3-C2	-2.10	105.42	110.38
3	5-F	5	BGC	C1-O5-C5	-2.10	109.37	112.19
3	4-D	1	BGC	C4-C3-C2	2.10	114.52	110.83
2	2-C	2	BGC	O5-C1-C2	-2.10	105.78	110.79
3	19-F	5	BGC	C2-C3-C4	2.10	114.55	110.86
3	17-F	3	BGC	C1-O5-C5	2.10	115.00	112.19
3	5-D	4	BGC	O6-C6-C5	2.10	118.48	111.33
2	1-E	6	BGC	O3-C3-C4	-2.10	105.43	110.38
2	11-C	1	BGC	O5-C5-C4	2.10	113.48	109.70
3	19-D	3	BGC	O6-C6-C5	2.10	118.47	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	19-C	2	BGC	C1-O5-C5	-2.10	109.38	112.19
3	13-D	3	BGC	C1-C2-C3	2.10	112.69	109.64
3	10-F	4	BGC	O3-C3-C2	-2.09	105.78	110.05
2	11-E	3	BGC	O5-C1-C2	-2.09	105.79	110.79
2	3-E	2	BGC	O2-C2-C3	-2.09	105.81	110.15
3	16-F	1	BGC	C4-C3-C2	2.09	114.51	110.83
3	9-D	1	BGC	O4-C4-C3	2.09	115.31	110.38
2	20-E	6	BGC	O3-C3-C4	-2.09	105.44	110.38
2	12-C	2	BGC	C1-O5-C5	-2.09	109.38	112.19
3	12-D	2	BGC	C3-C4-C5	2.09	114.02	110.23
2	25-C	4	BGC	O5-C5-C4	-2.09	105.74	110.83
2	19-E	4	BGC	O3-C3-C2	-2.09	105.79	110.05
3	21-F	3	BGC	C1-C2-C3	2.09	112.69	109.64
3	4-D	4	BGC	O5-C5-C4	-2.09	105.74	110.83
2	5-C	2	BGC	C1-C2-C3	2.09	112.69	109.64
2	24-E	6	BGC	C1-O5-C5	-2.09	109.39	112.19
2	22-C	6	BGC	C1-C2-C3	2.09	112.68	109.64
3	11-F	1	BGC	O3-C3-C2	-2.08	105.47	110.38
2	20-E	4	BGC	O3-C3-C2	-2.08	105.81	110.05
2	2-C	5	BGC	O3-C3-C4	-2.08	105.47	110.38
2	6-C	1	BGC	O5-C5-C4	2.08	113.44	109.70
2	12-C	1	BGC	O3-C3-C4	2.08	115.27	110.38
2	6-C	5	BGC	O3-C3-C4	-2.08	105.48	110.38
2	15-E	3	BGC	O3-C3-C2	-2.07	105.83	110.05
2	13-C	5	BGC	O3-C3-C4	-2.07	105.50	110.38
2	14-E	6	BGC	O3-C3-C4	-2.07	105.50	110.38
3	9-F	3	BGC	C2-C3-C4	2.07	114.50	110.86
3	25-F	3	BGC	O5-C5-C4	2.07	115.86	110.83
2	13-E	3	BGC	C2-C3-C4	2.07	114.50	110.86
2	2-E	6	BGC	O3-C3-C4	-2.07	105.50	110.38
2	14-E	2	BGC	O2-C2-C3	-2.07	105.87	110.15
2	5-C	6	BGC	O3-C3-C4	-2.07	105.51	110.38
2	13-E	3	BGC	O3-C3-C2	-2.06	105.84	110.05
2	4-C	3	BGC	O3-C3-C4	-2.06	105.51	110.38
2	18-C	3	BGC	C6-C5-C4	-2.06	107.95	113.02
3	12-D	3	BGC	O2-C2-C3	-2.06	105.88	110.15
3	25-D	4	BGC	C3-C4-C5	-2.06	106.50	110.23
3	3-D	1	BGC	O3-C3-C2	-2.06	105.52	110.38
2	25-C	4	BGC	O6-C6-C5	2.06	118.34	111.33
2	12-C	2	BGC	C1-C2-C3	2.06	112.64	109.64
2	6-E	2	BGC	O3-C3-C2	-2.06	105.86	110.05
3	12-D	4	BGC	C3-C4-C5	-2.06	106.50	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	11-F	1	BGC	C4-C3-C2	2.06	114.44	110.83
2	21-C	2	BGC	O6-C6-C5	2.05	118.33	111.33
2	6-C	1	BGC	O2-C2-C3	2.05	115.22	110.38
2	25-E	3	BGC	O3-C3-C2	-2.05	105.87	110.05
2	21-C	3	BGC	O5-C1-C2	-2.05	105.90	110.79
3	21-D	3	BGC	C2-C3-C4	2.05	114.47	110.86
3	6-D	4	BGC	O6-C6-C5	2.05	118.31	111.33
2	6-C	3	BGC	O4-C4-C3	2.05	115.20	110.38
3	14-D	4	BGC	C6-C5-C4	-2.05	107.99	113.02
3	2-D	5	BGC	C1-C2-C3	2.05	112.62	109.64
2	5-E	6	BGC	O5-C5-C4	-2.05	105.85	110.83
2	2-C	6	BGC	O3-C3-C4	-2.05	105.56	110.38
3	11-F	1	BGC	C1-C2-C3	2.04	114.52	110.36
3	6-D	3	BGC	C3-C4-C5	2.04	113.94	110.23
2	17-E	4	BGC	C1-C2-C3	2.04	112.62	109.64
3	6-D	5	BGC	O5-C1-C2	-2.04	105.92	110.79
3	8-D	2	BGC	O2-C2-C1	2.04	113.90	109.22
2	22-C	2	BGC	C1-O5-C5	-2.04	109.45	112.19
3	23-F	1	BGC	C1-O5-C5	2.04	117.60	113.65
2	4-E	5	BGC	O5-C5-C4	-2.04	105.86	110.83
2	3-C	1	BGC	C1-O5-C5	-2.04	109.71	113.65
2	22-C	3	BGC	O3-C3-C2	-2.04	105.90	110.05
2	4-C	1	BGC	O3-C3-C4	2.04	115.18	110.38
3	19-D	1	BGC	O5-C5-C4	2.04	113.37	109.70
3	20-F	3	BGC	C1-O5-C5	2.04	114.91	112.19
3	18-D	1	BGC	O6-C6-C5	2.04	118.26	111.33
3	3-D	1	BGC	O6-C6-C5	2.03	118.26	111.33
2	24-C	5	BGC	O3-C3-C4	-2.03	105.58	110.38
2	18-C	6	BGC	O3-C3-C2	-2.03	105.90	110.05
2	15-C	6	BGC	O5-C5-C4	-2.03	105.88	110.83
3	2-F	2	BGC	O3-C3-C2	2.03	114.20	110.05
2	18-E	6	BGC	O3-C3-C4	-2.03	105.58	110.38
3	2-F	1	BGC	O6-C6-C5	2.03	118.25	111.33
3	24-F	2	BGC	C3-C4-C5	2.03	113.92	110.23
2	10-C	2	BGC	C1-O5-C5	-2.03	109.47	112.19
3	4-D	1	BGC	O5-C5-C4	2.03	113.36	109.70
3	13-F	5	BGC	C2-C3-C4	2.03	114.43	110.86
3	14-D	3	BGC	O6-C6-C5	2.03	118.24	111.33
2	12-E	5	BGC	C3-C4-C5	2.03	113.91	110.23
3	19-D	2	BGC	C3-C4-C5	2.03	113.91	110.23
2	23-E	1	BGC	O2-C2-C3	2.03	115.16	110.38
3	20-D	1	BGC	O5-C5-C6	2.03	111.46	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-E	4	BGC	C1-O5-C5	2.03	114.90	112.19
2	9-E	6	BGC	C1-C2-C3	2.03	112.59	109.64
2	1-C	6	BGC	O5-C5-C6	-2.03	103.72	107.66
3	12-D	1	BGC	O6-C6-C5	2.03	118.23	111.33
3	25-F	5	BGC	C1-C2-C3	2.03	112.59	109.64
3	9-D	1	BGC	O5-C5-C4	2.03	113.35	109.70
2	3-E	1	BGC	O2-C2-C3	2.02	115.15	110.38
3	4-D	2	BGC	O5-C5-C6	2.02	111.60	107.66
2	19-E	1	BGC	O2-C2-C3	2.02	115.15	110.38
2	18-E	5	BGC	O4-C4-C5	2.02	114.31	109.32
2	4-E	6	BGC	C1-C2-C3	2.02	112.59	109.64
3	4-D	1	BGC	O3-C3-C2	-2.02	105.61	110.38
3	16-F	3	BGC	C1-C2-C3	2.02	112.59	109.64
2	24-E	3	BGC	O5-C1-C2	-2.02	105.97	110.79
2	25-E	1	BGC	C1-O5-C5	-2.02	109.74	113.65
3	19-F	1	BGC	O6-C6-C5	2.02	118.21	111.33
2	11-E	3	BGC	C1-O5-C5	-2.02	109.48	112.19
2	11-C	6	BGC	O5-C5-C6	-2.02	103.73	107.66
3	24-D	3	BGC	O6-C6-C5	2.02	118.20	111.33
2	16-C	6	BGC	C1-C2-C3	2.02	112.58	109.64
2	17-E	3	BGC	C2-C3-C4	2.02	114.41	110.86
3	24-F	3	BGC	O3-C3-C2	-2.02	105.94	110.05
2	13-C	5	BGC	C1-C2-C3	2.02	112.58	109.64
2	17-C	5	BGC	O5-C5-C6	-2.02	103.74	107.66
2	4-E	4	BGC	O2-C2-C3	2.01	114.32	110.15
2	7-E	6	BGC	C1-C2-C3	2.01	112.58	109.64
2	4-C	3	BGC	O3-C3-C2	-2.01	105.95	110.05
3	18-D	5	BGC	C1-C2-C3	2.01	112.57	109.64
3	2-F	3	BGC	C1-O5-C5	2.01	114.88	112.19
2	6-C	1	BGC	O5-C1-C2	-2.01	106.76	110.30
2	7-E	3	BGC	O5-C1-C2	-2.01	106.00	110.79
3	17-F	2	BGC	C1-O5-C5	-2.01	109.49	112.19
3	7-D	3	BGC	O6-C6-C5	2.01	118.17	111.33
3	3-D	3	BGC	O6-C6-C5	2.01	118.17	111.33
2	21-E	5	BGC	C1-C2-C3	2.01	112.57	109.64
2	13-E	2	BGC	C2-C3-C4	2.01	114.39	110.86
3	2-F	3	BGC	C1-C2-C3	2.01	112.56	109.64
3	22-F	3	BGC	O6-C6-C5	2.00	118.16	111.33
2	9-C	6	BGC	O5-C5-C4	-2.00	105.95	110.83
3	7-F	3	BGC	O6-C6-C5	2.00	118.15	111.33
2	18-C	3	BGC	O5-C1-C2	-2.00	106.01	110.79
2	4-C	2	BGC	O6-C6-C5	2.00	118.15	111.33

There are no chirality outliers.

All (251) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	18-D	1	BGC	C4-C5-C6-O6
2	6-C	2	BGC	C4-C5-C6-O6
2	9-C	6	BGC	C4-C5-C6-O6
3	9-D	4	BGC	C4-C5-C6-O6
2	21-E	1	BGC	O5-C5-C6-O6
3	17-D	4	BGC	C4-C5-C6-O6
2	18-C	6	BGC	C4-C5-C6-O6
3	6-D	1	BGC	C4-C5-C6-O6
3	6-D	4	BGC	C4-C5-C6-O6
2	5-C	3	BGC	O5-C5-C6-O6
2	18-C	3	BGC	O5-C5-C6-O6
3	9-D	4	BGC	O5-C5-C6-O6
3	6-F	3	BGC	O5-C5-C6-O6
3	15-F	4	BGC	C4-C5-C6-O6
2	6-C	2	BGC	O5-C5-C6-O6
3	17-D	4	BGC	O5-C5-C6-O6
3	15-F	1	BGC	O5-C5-C6-O6
2	21-C	6	BGC	C4-C5-C6-O6
3	4-F	4	BGC	C4-C5-C6-O6
3	8-F	4	BGC	C4-C5-C6-O6
2	9-C	6	BGC	O5-C5-C6-O6
3	13-D	1	BGC	O5-C5-C6-O6
3	17-F	1	BGC	C4-C5-C6-O6
3	1-D	1	BGC	O5-C5-C6-O6
3	20-D	1	BGC	O5-C5-C6-O6
3	8-F	1	BGC	O5-C5-C6-O6
2	15-E	1	BGC	C4-C5-C6-O6
2	3-E	6	BGC	C4-C5-C6-O6
3	3-D	1	BGC	C4-C5-C6-O6
3	12-D	4	BGC	C4-C5-C6-O6
2	4-C	3	BGC	O5-C5-C6-O6
3	1-D	4	BGC	O5-C5-C6-O6
3	13-D	4	BGC	O5-C5-C6-O6
3	4-F	1	BGC	C4-C5-C6-O6
3	23-F	1	BGC	C4-C5-C6-O6
3	25-F	4	BGC	C4-C5-C6-O6
2	24-C	6	BGC	O5-C5-C6-O6
2	12-E	5	BGC	O5-C5-C6-O6
2	23-E	6	BGC	O5-C5-C6-O6
3	22-D	1	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	17-F	1	BGC	O5-C5-C6-O6
3	23-F	1	BGC	O5-C5-C6-O6
3	25-F	4	BGC	O5-C5-C6-O6
2	18-C	3	BGC	C4-C5-C6-O6
3	2-F	1	BGC	C4-C5-C6-O6
3	8-F	1	BGC	C4-C5-C6-O6
2	6-E	1	BGC	O5-C5-C6-O6
3	12-D	1	BGC	O5-C5-C6-O6
3	22-D	1	BGC	C4-C5-C6-O6
3	2-D	1	BGC	O5-C5-C6-O6
3	17-D	1	BGC	O5-C5-C6-O6
3	18-D	1	BGC	O5-C5-C6-O6
3	15-F	1	BGC	C4-C5-C6-O6
2	18-C	6	BGC	O5-C5-C6-O6
2	3-E	4	BGC	O5-C5-C6-O6
3	11-D	4	BGC	O5-C5-C6-O6
2	21-E	1	BGC	C4-C5-C6-O6
3	1-D	1	BGC	C4-C5-C6-O6
2	23-C	3	BGC	O5-C5-C6-O6
3	6-D	4	BGC	O5-C5-C6-O6
2	12-E	5	BGC	C4-C5-C6-O6
2	19-E	6	BGC	C4-C5-C6-O6
3	6-F	3	BGC	C4-C5-C6-O6
2	24-C	1	BGC	O5-C5-C6-O6
3	3-D	1	BGC	O5-C5-C6-O6
3	4-F	4	BGC	O5-C5-C6-O6
3	15-F	4	BGC	O5-C5-C6-O6
3	6-D	1	BGC	O5-C5-C6-O6
3	16-D	1	BGC	O5-C5-C6-O6
3	8-F	4	BGC	O5-C5-C6-O6
2	8-E	2	BGC	O5-C5-C6-O6
3	3-F	3	BGC	O5-C5-C6-O6
2	4-C	2	BGC	C4-C5-C6-O6
2	4-C	3	BGC	C4-C5-C6-O6
2	6-E	1	BGC	C4-C5-C6-O6
3	16-D	1	BGC	C4-C5-C6-O6
3	20-D	1	BGC	C4-C5-C6-O6
2	9-C	1	BGC	O5-C5-C6-O6
2	5-C	3	BGC	C4-C5-C6-O6
3	24-F	1	BGC	C4-C5-C6-O6
3	23-D	2	BGC	O5-C5-C6-O6
2	23-C	5	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	15-D	1	BGC	C4-C5-C6-O6
3	17-D	1	BGC	C4-C5-C6-O6
2	16-C	4	BGC	O5-C5-C6-O6
2	23-C	1	BGC	O5-C5-C6-O6
2	21-C	6	BGC	O5-C5-C6-O6
3	12-D	4	BGC	O5-C5-C6-O6
3	4-F	1	BGC	O5-C5-C6-O6
2	1-C	5	BGC	C4-C5-C6-O6
3	21-D	1	BGC	C4-C5-C6-O6
2	23-C	5	BGC	O5-C5-C6-O6
2	15-E	1	BGC	O5-C5-C6-O6
2	17-E	1	BGC	O5-C5-C6-O6
3	2-F	1	BGC	O5-C5-C6-O6
2	3-E	4	BGC	C4-C5-C6-O6
3	12-D	1	BGC	C4-C5-C6-O6
3	1-D	4	BGC	C4-C5-C6-O6
3	13-D	1	BGC	C4-C5-C6-O6
3	11-F	3	BGC	C4-C5-C6-O6
2	10-C	3	BGC	O5-C5-C6-O6
3	8-D	1	BGC	C4-C5-C6-O6
2	1-C	5	BGC	O5-C5-C6-O6
2	1-C	3	BGC	O5-C5-C6-O6
3	8-D	1	BGC	O5-C5-C6-O6
3	15-D	1	BGC	O5-C5-C6-O6
3	11-F	3	BGC	O5-C5-C6-O6
2	17-E	1	BGC	C4-C5-C6-O6
2	21-E	5	BGC	C4-C5-C6-O6
3	25-F	1	BGC	C4-C5-C6-O6
3	14-F	5	BGC	C4-C5-C6-O6
2	24-C	1	BGC	C4-C5-C6-O6
2	23-C	3	BGC	C4-C5-C6-O6
2	10-E	6	BGC	O5-C5-C6-O6
2	15-C	1	BGC	O5-C5-C6-O6
2	18-E	6	BGC	O5-C5-C6-O6
3	7-D	4	BGC	O5-C5-C6-O6
3	24-F	1	BGC	O5-C5-C6-O6
2	4-C	2	BGC	O5-C5-C6-O6
3	14-D	1	BGC	C4-C5-C6-O6
3	19-D	1	BGC	C4-C5-C6-O6
3	18-F	3	BGC	C4-C5-C6-O6
3	2-D	1	BGC	C4-C5-C6-O6
3	21-D	4	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	6-D	2	BGC	O5-C5-C6-O6
3	23-D	1	BGC	O5-C5-C6-O6
3	10-F	3	BGC	O5-C5-C6-O6
2	21-E	5	BGC	O5-C5-C6-O6
3	21-D	2	BGC	O5-C5-C6-O6
2	25-E	1	BGC	C4-C5-C6-O6
3	21-F	5	BGC	C4-C5-C6-O6
2	5-C	2	BGC	O5-C5-C6-O6
3	21-D	4	BGC	O5-C5-C6-O6
3	9-F	5	BGC	O5-C5-C6-O6
3	25-D	1	BGC	C4-C5-C6-O6
3	5-F	1	BGC	O5-C5-C6-O6
3	18-F	3	BGC	O5-C5-C6-O6
2	10-C	3	BGC	C4-C5-C6-O6
2	16-C	4	BGC	C4-C5-C6-O6
3	9-F	5	BGC	C4-C5-C6-O6
3	23-F	3	BGC	O5-C5-C6-O6
3	21-F	5	BGC	O5-C5-C6-O6
2	21-E	4	BGC	O5-C5-C6-O6
2	5-C	2	BGC	C4-C5-C6-O6
3	4-D	1	BGC	C4-C5-C6-O6
2	7-C	2	BGC	C4-C5-C6-O6
2	11-E	1	BGC	O5-C5-C6-O6
3	9-D	2	BGC	O5-C5-C6-O6
3	18-F	5	BGC	O5-C5-C6-O6
3	14-D	1	BGC	O5-C5-C6-O6
3	23-F	3	BGC	C4-C5-C6-O6
2	23-C	1	BGC	C4-C5-C6-O6
2	1-C	4	BGC	O5-C5-C6-O6
3	7-D	1	BGC	C4-C5-C6-O6
2	23-E	1	BGC	O5-C5-C6-O6
3	2-D	2	BGC	O5-C5-C6-O6
2	21-E	4	BGC	C4-C5-C6-O6
3	13-D	4	BGC	C4-C5-C6-O6
2	3-E	6	BGC	O5-C5-C6-O6
3	14-F	5	BGC	O5-C5-C6-O6
2	9-E	1	BGC	O5-C5-C6-O6
3	19-D	1	BGC	O5-C5-C6-O6
2	5-C	1	BGC	O5-C5-C6-O6
3	24-D	2	BGC	O5-C5-C6-O6
3	10-D	1	BGC	O5-C5-C6-O6
3	9-F	1	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	9-C	1	BGC	C4-C5-C6-O6
2	20-C	5	BGC	O5-C5-C6-O6
3	4-D	2	BGC	C4-C5-C6-O6
3	25-F	1	BGC	O5-C5-C6-O6
3	24-F	3	BGC	O5-C5-C6-O6
3	4-D	5	BGC	C4-C5-C6-O6
3	4-D	5	BGC	O5-C5-C6-O6
2	20-C	5	BGC	C4-C5-C6-O6
2	23-E	6	BGC	C4-C5-C6-O6
3	3-F	3	BGC	C4-C5-C6-O6
2	19-E	1	BGC	C4-C5-C6-O6
3	1-F	3	BGC	O5-C5-C6-O6
2	18-E	6	BGC	C4-C5-C6-O6
2	11-C	6	BGC	O5-C5-C6-O6
3	12-D	2	BGC	C4-C5-C6-O6
3	8-F	3	BGC	O5-C5-C6-O6
2	24-E	1	BGC	C4-C5-C6-O6
2	1-C	3	BGC	C4-C5-C6-O6
3	4-D	1	BGC	O5-C5-C6-O6
2	15-E	3	BGC	C4-C5-C6-O6
3	22-F	5	BGC	C4-C5-C6-O6
2	25-E	1	BGC	O5-C5-C6-O6
3	23-D	2	BGC	C4-C5-C6-O6
3	24-F	3	BGC	C4-C5-C6-O6
3	21-F	1	BGC	O5-C5-C6-O6
2	24-C	6	BGC	C4-C5-C6-O6
3	20-D	4	BGC	C4-C5-C6-O6
3	21-D	1	BGC	O5-C5-C6-O6
3	23-D	3	BGC	O5-C5-C6-O6
2	11-C	1	BGC	O5-C5-C6-O6
2	25-E	5	BGC	O5-C5-C6-O6
3	5-F	1	BGC	C4-C5-C6-O6
3	11-D	4	BGC	C4-C5-C6-O6
3	13-F	5	BGC	C4-C5-C6-O6
3	3-F	1	BGC	C4-C5-C6-O6
3	23-D	4	BGC	O5-C5-C6-O6
2	25-E	5	BGC	C4-C5-C6-O6
3	23-D	4	BGC	C4-C5-C6-O6
3	15-D	5	BGC	C4-C5-C6-O6
2	9-E	6	BGC	O5-C5-C6-O6
3	25-D	1	BGC	O5-C5-C6-O6
2	3-E	1	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	7-F	5	BGC	C4-C5-C6-O6
3	23-D	3	BGC	C4-C5-C6-O6
2	24-E	1	BGC	O5-C5-C6-O6
2	12-C	6	BGC	O5-C5-C6-O6
2	7-E	3	BGC	O5-C5-C6-O6
2	1-C	4	BGC	C4-C5-C6-O6
3	24-D	1	BGC	C4-C5-C6-O6
3	19-F	3	BGC	O5-C5-C6-O6
3	16-D	3	BGC	C4-C5-C6-O6
3	10-F	3	BGC	C4-C5-C6-O6
2	23-C	4	BGC	O5-C5-C6-O6
2	23-E	1	BGC	C4-C5-C6-O6
3	7-D	1	BGC	O5-C5-C6-O6
2	19-E	6	BGC	O5-C5-C6-O6
2	8-E	2	BGC	C4-C5-C6-O6
3	18-F	5	BGC	C4-C5-C6-O6
2	11-E	1	BGC	C4-C5-C6-O6
2	22-C	3	BGC	C4-C5-C6-O6
3	5-D	1	BGC	C4-C5-C6-O6
3	20-D	4	BGC	O5-C5-C6-O6
3	22-D	3	BGC	O5-C5-C6-O6
3	3-D	4	BGC	C4-C5-C6-O6
3	22-F	5	BGC	O5-C5-C6-O6
3	18-F	4	BGC	C4-C5-C6-O6
3	9-D	5	BGC	C4-C5-C6-O6
3	12-D	3	BGC	O5-C5-C6-O6
2	13-C	6	BGC	O5-C5-C6-O6
2	4-C	1	BGC	C4-C5-C6-O6
2	11-C	4	BGC	C4-C5-C6-O6
3	14-D	4	BGC	C4-C5-C6-O6
2	25-C	1	BGC	O5-C5-C6-O6
3	15-F	2	BGC	C4-C5-C6-O6
3	7-D	5	BGC	C4-C5-C6-O6
2	19-E	1	BGC	O5-C5-C6-O6
2	24-C	3	BGC	O5-C5-C6-O6
2	18-C	4	BGC	C4-C5-C6-O6
3	2-F	5	BGC	C4-C5-C6-O6
2	18-E	2	BGC	O5-C5-C6-O6
2	16-E	6	BGC	C4-C5-C6-O6
3	25-F	5	BGC	C4-C5-C6-O6
2	9-E	1	BGC	C4-C5-C6-O6
2	23-C	4	BGC	C4-C5-C6-O6

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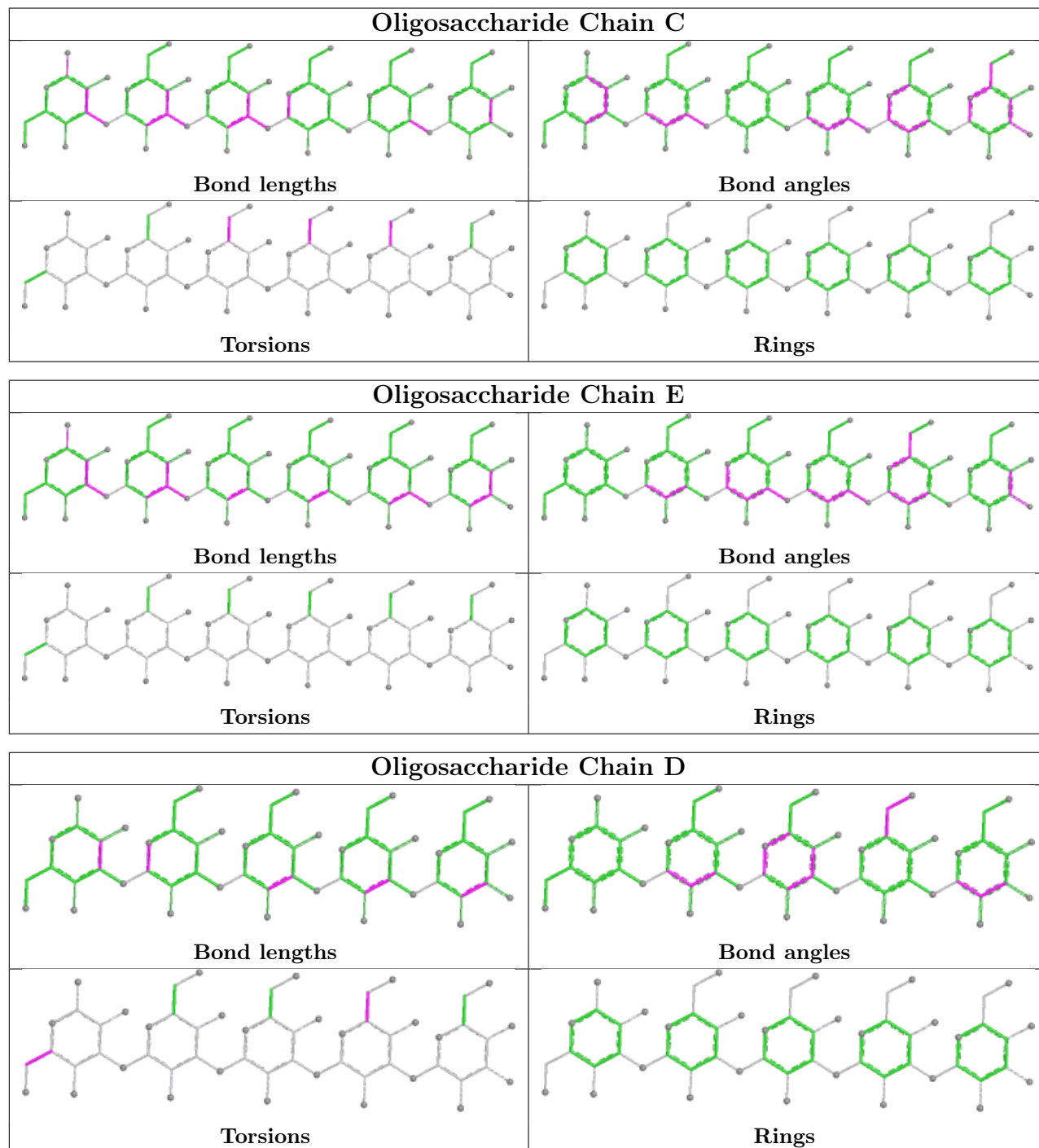
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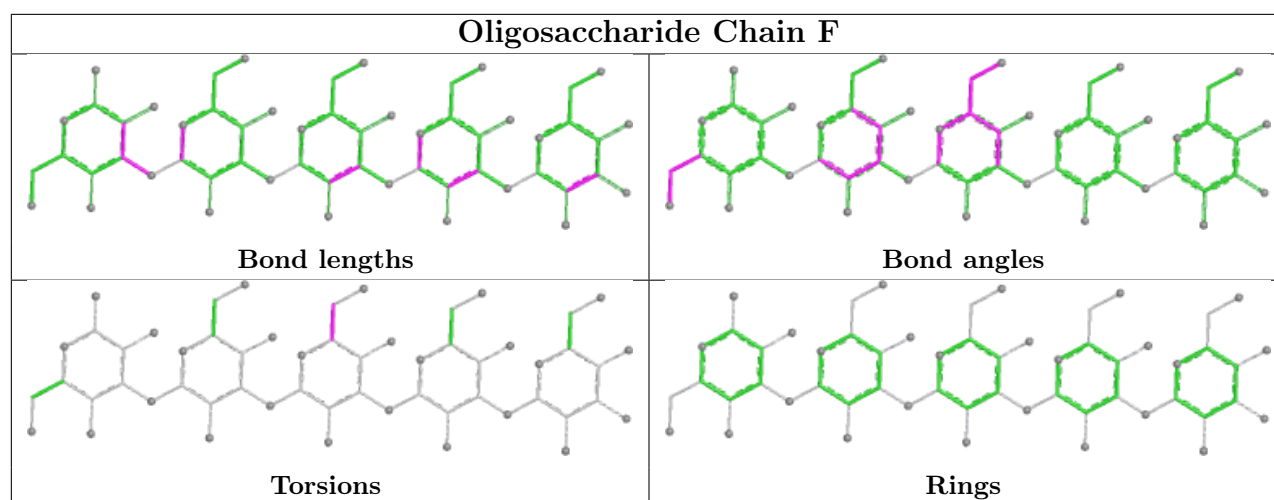
Mol	Chain	Res	Type	Atoms
2	2-E	6	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





4.6 Ligand geometry [i](#)

50 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	6-A	701	-	3,3,3	0.40	0	2,2,2	0.59	0
4	EDO	23-A	701	-	3,3,3	0.38	0	2,2,2	0.49	0
4	EDO	11-A	701	-	3,3,3	0.40	0	2,2,2	0.31	0
4	EDO	13-A	701	-	3,3,3	0.50	0	2,2,2	0.09	0
4	EDO	3-B	701	-	3,3,3	0.35	0	2,2,2	0.52	0
4	EDO	8-B	701	-	3,3,3	0.31	0	2,2,2	0.76	0
4	EDO	9-B	701	-	3,3,3	0.46	0	2,2,2	0.11	0
4	EDO	11-B	701	-	3,3,3	0.34	0	2,2,2	0.21	0
4	EDO	10-B	701	-	3,3,3	0.75	0	2,2,2	0.74	0
4	EDO	21-A	701	-	3,3,3	0.46	0	2,2,2	0.49	0
4	EDO	17-A	701	-	3,3,3	0.44	0	2,2,2	0.76	0
4	EDO	4-A	701	-	3,3,3	0.44	0	2,2,2	0.21	0
4	EDO	9-A	701	-	3,3,3	0.37	0	2,2,2	0.33	0
4	EDO	16-A	701	-	3,3,3	0.53	0	2,2,2	0.35	0
4	EDO	24-A	701	-	3,3,3	0.41	0	2,2,2	0.54	0
4	EDO	1-A	701	-	3,3,3	0.49	0	2,2,2	0.16	0
4	EDO	5-B	701	-	3,3,3	0.48	0	2,2,2	0.69	0
4	EDO	15-B	701	-	3,3,3	0.49	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	19-B	701	-	3,3,3	0.59	0	2,2,2	0.34	0
4	EDO	25-A	701	-	3,3,3	0.46	0	2,2,2	0.25	0
4	EDO	13-B	701	-	3,3,3	0.51	0	2,2,2	0.28	0
4	EDO	14-B	701	-	3,3,3	0.37	0	2,2,2	0.56	0
4	EDO	23-B	701	-	3,3,3	0.79	0	2,2,2	0.41	0
4	EDO	2-A	701	-	3,3,3	0.44	0	2,2,2	0.37	0
4	EDO	22-B	701	-	3,3,3	0.36	0	2,2,2	0.34	0
4	EDO	12-A	701	-	3,3,3	0.55	0	2,2,2	0.23	0
4	EDO	21-B	701	-	3,3,3	0.38	0	2,2,2	0.34	0
4	EDO	2-B	701	-	3,3,3	0.60	0	2,2,2	0.39	0
4	EDO	25-B	701	-	3,3,3	0.44	0	2,2,2	0.50	0
4	EDO	1-B	701	-	3,3,3	0.59	0	2,2,2	0.63	0
4	EDO	4-B	701	-	3,3,3	0.63	0	2,2,2	0.42	0
4	EDO	7-A	701	-	3,3,3	0.55	0	2,2,2	0.36	0
4	EDO	15-A	701	-	3,3,3	0.42	0	2,2,2	0.34	0
4	EDO	20-A	701	-	3,3,3	0.38	0	2,2,2	0.47	0
4	EDO	7-B	701	-	3,3,3	0.40	0	2,2,2	0.23	0
4	EDO	12-B	701	-	3,3,3	0.53	0	2,2,2	0.26	0
4	EDO	16-B	701	-	3,3,3	0.73	0	2,2,2	0.34	0
4	EDO	24-B	701	-	3,3,3	0.68	0	2,2,2	1.27	0
4	EDO	3-A	701	-	3,3,3	0.23	0	2,2,2	0.95	0
4	EDO	8-A	701	-	3,3,3	0.47	0	2,2,2	0.78	0
4	EDO	10-A	701	-	3,3,3	0.40	0	2,2,2	0.44	0
4	EDO	18-A	701	-	3,3,3	0.43	0	2,2,2	0.17	0
4	EDO	17-B	701	-	3,3,3	0.39	0	2,2,2	1.11	0
4	EDO	20-B	701	-	3,3,3	0.64	0	2,2,2	0.43	0
4	EDO	5-A	701	-	3,3,3	0.73	0	2,2,2	0.19	0
4	EDO	18-B	701	-	3,3,3	0.37	0	2,2,2	0.35	0
4	EDO	19-A	701	-	3,3,3	0.40	0	2,2,2	0.20	0
4	EDO	6-B	701	-	3,3,3	0.51	0	2,2,2	1.66	1 (50%)
4	EDO	14-A	701	-	3,3,3	0.48	0	2,2,2	0.13	0
4	EDO	22-A	701	-	3,3,3	0.54	0	2,2,2	0.33	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	6-A	701	-	-	0/1/1/1	-
4	EDO	23-A	701	-	-	0/1/1/1	-
4	EDO	11-A	701	-	-	0/1/1/1	-

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	18-B	701	-	-	0/1/1/1	-
4	EDO	19-A	701	-	-	1/1/1/1	-
4	EDO	6-B	701	-	-	1/1/1/1	-
4	EDO	14-A	701	-	-	0/1/1/1	-
4	EDO	22-A	701	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	6-B	701	EDO	O2-C2-C1	-2.26	95.20	112.39

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	5-A	701	EDO	O1-C1-C2-O2
4	12-A	701	EDO	O1-C1-C2-O2
4	10-B	701	EDO	O1-C1-C2-O2
4	19-B	701	EDO	O1-C1-C2-O2
4	8-A	701	EDO	O1-C1-C2-O2
4	14-B	701	EDO	O1-C1-C2-O2
4	17-B	701	EDO	O1-C1-C2-O2
4	16-B	701	EDO	O1-C1-C2-O2
4	8-B	701	EDO	O1-C1-C2-O2
4	3-A	701	EDO	O1-C1-C2-O2
4	4-B	701	EDO	O1-C1-C2-O2
4	22-B	701	EDO	O1-C1-C2-O2
4	16-A	701	EDO	O1-C1-C2-O2
4	5-B	701	EDO	O1-C1-C2-O2
4	11-B	701	EDO	O1-C1-C2-O2
4	7-A	701	EDO	O1-C1-C2-O2
4	13-A	701	EDO	O1-C1-C2-O2
4	19-A	701	EDO	O1-C1-C2-O2
4	2-B	701	EDO	O1-C1-C2-O2
4	6-B	701	EDO	O1-C1-C2-O2
4	1-B	701	EDO	O1-C1-C2-O2
4	9-B	701	EDO	O1-C1-C2-O2
4	20-B	701	EDO	O1-C1-C2-O2
4	10-A	701	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%)	1.68	146 (26%) 1 1	1, 1, 1, 1	549 (100%)
1	1-B	548/549 (99%)	1.68	138 (25%) 1 2	1, 1, 1, 1	548 (100%)
1	2-A	0/549	-	-	-	-
1	2-B	0/549	-	-	-	-
1	3-A	0/549	-	-	-	-
1	3-B	0/549	-	-	-	-
1	4-A	0/549	-	-	-	-
1	4-B	0/549	-	-	-	-
1	5-A	0/549	-	-	-	-
1	5-B	0/549	-	-	-	-
1	6-A	0/549	-	-	-	-
1	6-B	0/549	-	-	-	-
1	7-A	0/549	-	-	-	-
1	7-B	0/549	-	-	-	-
1	8-A	0/549	-	-	-	-
1	8-B	0/549	-	-	-	-
1	9-A	0/549	-	-	-	-
1	9-B	0/549	-	-	-	-
1	10-A	0/549	-	-	-	-
1	10-B	0/549	-	-	-	-
1	11-A	0/549	-	-	-	-
1	11-B	0/549	-	-	-	-
1	12-A	0/549	-	-	-	-
1	12-B	0/549	-	-	-	-
1	13-A	0/549	-	-	-	-
1	13-B	0/549	-	-	-	-
1	14-A	0/549	-	-	-	-
1	14-B	0/549	-	-	-	-
1	15-A	0/549	-	-	-	-
1	15-B	0/549	-	-	-	-
1	16-A	0/549	-	-	-	-
1	16-B	0/549	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	17-A	0/549	-	-	-	-
1	17-B	0/549	-	-	-	-
1	18-A	0/549	-	-	-	-
1	18-B	0/549	-	-	-	-
1	19-A	0/549	-	-	-	-
1	19-B	0/549	-	-	-	-
1	20-A	0/549	-	-	-	-
1	20-B	0/549	-	-	-	-
1	21-A	0/549	-	-	-	-
1	21-B	0/549	-	-	-	-
1	22-A	0/549	-	-	-	-
1	22-B	0/549	-	-	-	-
1	23-A	0/549	-	-	-	-
1	23-B	0/549	-	-	-	-
1	24-A	0/549	-	-	-	-
1	24-B	0/549	-	-	-	-
1	25-A	0/549	-	-	-	-
1	25-B	0/549	-	-	-	-
All	All	1097/27450 (3%)	1.68	284 (25%) 1 2	1, 1, 1, 1	1097 (100%)

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	298	GLU	15.0
1	1-B	294	ASN	13.3
1	1-B	293	GLY	13.2
1	1-A	58	VAL	12.6
1	1-B	296	THR	11.5
1	1-B	299	GLY	11.2
1	1-B	400	GLY	10.4
1	1-A	294	ASN	9.8
1	1-B	194	TYR	9.5
1	1-B	126	LEU	8.8
1	1-A	57	GLU	8.8
1	1-A	295	GLY	8.6
1	1-A	312	PRO	8.4
1	1-A	293	GLY	8.3
1	1-A	399	ASP	8.2
1	1-A	560	VAL	8.0
1	1-B	402	SER	8.0
1	1-A	62	GLY	7.9
1	1-B	273	GLY	7.8

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Mol	Chain	Res	Type	RSRZ
1	1-B	317	GLU	7.3
1	1-B	398	SER	7.2
1	1-A	60	GLY	7.1
1	1-A	596	THR	7.0
1	1-B	302	LEU	7.0
1	1-A	274	ASP	6.7
1	1-A	273	GLY	6.6
1	1-A	272	ASP	6.5
1	1-B	58	VAL	6.5
1	1-B	336	TYR	6.5
1	1-A	323	VAL	6.5
1	1-A	605	PRO	6.4
1	1-B	399	ASP	6.4
1	1-B	232	GLY	6.2
1	1-A	402	SER	6.1
1	1-A	84	GLU	6.1
1	1-A	296	THR	6.1
1	1-B	274	ASP	6.0
1	1-A	604	PHE	6.0
1	1-B	528	ASP	6.0
1	1-A	74	SER	5.9
1	1-A	63	ASP	5.9
1	1-A	517	ASP	5.9
1	1-B	312	PRO	5.8
1	1-A	88	LYS	5.8
1	1-A	320	ASN	5.8
1	1-A	145	ASP	5.5
1	1-B	300	GLU	5.5
1	1-A	304	LEU	5.5
1	1-B	310	VAL	5.5
1	1-A	401	ALA	5.4
1	1-A	298	GLU	5.4
1	1-B	295	GLY	5.4
1	1-B	279	PHE	5.4
1	1-B	109	ASN	5.4
1	1-B	127	ASN	5.4
1	1-A	457	GLU	5.4
1	1-B	272	ASP	5.3
1	1-B	297	PRO	5.3
1	1-B	102	MET	5.3
1	1-A	400	GLY	5.2
1	1-B	313	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	1-B	59	VAL	5.2
1	1-A	324	ASP	5.2
1	1-A	126	LEU	5.2
1	1-A	460	ARG	5.0
1	1-B	145	ASP	5.0
1	1-B	324	ASP	5.0
1	1-B	589	ASP	5.0
1	1-B	600	GLN	4.9
1	1-B	107	THR	4.9
1	1-B	271	LEU	4.9
1	1-A	144	PHE	4.8
1	1-B	110	ASP	4.8
1	1-A	603	SER	4.8
1	1-B	515	ASN	4.7
1	1-A	251	GLU	4.7
1	1-B	285	THR	4.7
1	1-A	286	ASN	4.6
1	1-A	297	PRO	4.5
1	1-B	77	ASP	4.5
1	1-B	460	ARG	4.5
1	1-B	517	ASP	4.5
1	1-A	308	TYR	4.4
1	1-A	346	ARG	4.4
1	1-A	111	ILE	4.4
1	1-A	433	VAL	4.3
1	1-A	454	VAL	4.3
1	1-A	104	LYS	4.3
1	1-B	597	ILE	4.3
1	1-A	225	SER	4.2
1	1-A	143	TRP	4.2
1	1-A	313	GLY	4.2
1	1-B	345	ASP	4.1
1	1-B	276	TYR	4.1
1	1-A	78	ILE	4.1
1	1-B	401	ALA	4.1
1	1-A	306	GLN	4.1
1	1-A	300	GLU	4.1
1	1-A	59	VAL	4.0
1	1-B	343	GLU	4.0
1	1-B	440	ILE	3.9
1	1-A	194	TYR	3.9
1	1-B	275	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	1-B	144	PHE	3.9
1	1-A	317	GLU	3.9
1	1-A	545	ASN	3.9
1	1-A	61	GLY	3.9
1	1-B	67	ASN	3.8
1	1-B	132	THR	3.8
1	1-A	391	GLU	3.8
1	1-B	143	TRP	3.8
1	1-A	277	LYS	3.7
1	1-A	516	GLY	3.7
1	1-A	518	ILE	3.7
1	1-B	404	ASP	3.7
1	1-B	63	ASP	3.7
1	1-A	597	ILE	3.6
1	1-B	559	PRO	3.6
1	1-B	340	GLN	3.6
1	1-A	99	TYR	3.6
1	1-A	452	GLU	3.6
1	1-A	280	VAL	3.6
1	1-B	518	ILE	3.5
1	1-A	232	GLY	3.5
1	1-B	452	GLU	3.5
1	1-A	227	GLY	3.5
1	1-A	340	GLN	3.5
1	1-A	73	PRO	3.5
1	1-A	188	ASN	3.4
1	1-B	325	GLN	3.4
1	1-A	485	TYR	3.3
1	1-A	505	TYR	3.3
1	1-B	466	HIS	3.3
1	1-A	587	ILE	3.3
1	1-B	60	GLY	3.3
1	1-B	251	GLU	3.3
1	1-A	87	ARG	3.3
1	1-B	301	SER	3.2
1	1-B	490	SER	3.2
1	1-A	72	ASP	3.2
1	1-A	310	VAL	3.2
1	1-B	230	GLY	3.2
1	1-A	463	TYR	3.2
1	1-B	368	LEU	3.2
1	1-A	112	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	1-B	112	ASN	3.2
1	1-B	262	VAL	3.2
1	1-B	596	THR	3.2
1	1-A	381	LEU	3.1
1	1-B	193	GLY	3.1
1	1-A	282	ALA	3.1
1	1-A	284	ARG	3.1
1	1-A	559	PRO	3.1
1	1-B	519	LYS	3.1
1	1-B	309	VAL	3.1
1	1-B	603	SER	3.1
1	1-A	146	GLY	3.1
1	1-A	96	THR	3.1
1	1-A	595	THR	3.1
1	1-B	527	ASP	3.1
1	1-B	514	GLN	3.0
1	1-B	373	VAL	3.0
1	1-B	516	GLY	3.0
1	1-A	285	THR	3.0
1	1-A	302	LEU	3.0
1	1-A	257	LEU	3.0
1	1-B	78	ILE	3.0
1	1-B	381	LEU	3.0
1	1-A	263	SER	2.9
1	1-B	75	THR	2.9
1	1-A	558	ALA	2.9
1	1-B	82	VAL	2.9
1	1-B	605	PRO	2.9
1	1-B	604	PHE	2.8
1	1-B	560	VAL	2.8
1	1-B	403	GLY	2.8
1	1-B	69	LEU	2.8
1	1-A	419	ILE	2.8
1	1-A	157	GLU	2.8
1	1-B	74	SER	2.8
1	1-A	301	SER	2.8
1	1-A	127	ASN	2.8
1	1-A	525	LYS	2.8
1	1-A	83	ASP	2.8
1	1-B	305	ASP	2.8
1	1-A	245	PRO	2.7
1	1-B	283	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	1-A	529	SER	2.7
1	1-B	457	GLU	2.7
1	1-A	564	VAL	2.7
1	1-A	214	TYR	2.7
1	1-A	276	TYR	2.7
1	1-B	86	PHE	2.7
1	1-A	266	LYS	2.7
1	1-A	97	ASP	2.7
1	1-A	528	ASP	2.7
1	1-A	321	ALA	2.7
1	1-B	248	SER	2.6
1	1-A	299	GLY	2.6
1	1-A	336	TYR	2.6
1	1-B	587	ILE	2.6
1	1-A	129	ASP	2.6
1	1-A	76	PRO	2.6
1	1-A	326	GLY	2.6
1	1-B	87	ARG	2.6
1	1-B	72	ASP	2.6
1	1-B	97	ASP	2.6
1	1-B	330	LEU	2.6
1	1-B	382	LEU	2.6
1	1-A	262	VAL	2.6
1	1-B	211	VAL	2.6
1	1-A	303	PRO	2.6
1	1-B	468	LYS	2.6
1	1-B	147	ASN	2.6
1	1-A	69	LEU	2.6
1	1-A	322	ALA	2.6
1	1-B	180	ARG	2.6
1	1-B	130	ASP	2.5
1	1-A	184	LYS	2.5
1	1-B	505	TYR	2.5
1	1-B	292	TRP	2.5
1	1-A	130	ASP	2.5
1	1-B	380	GLY	2.5
1	1-B	488	GLN	2.5
1	1-A	178	PHE	2.5
1	1-B	356	LEU	2.5
1	1-A	314	ALA	2.5
1	1-A	82	VAL	2.5
1	1-B	111	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-B	454	VAL	2.5
1	1-A	77	ASP	2.4
1	1-B	352	LEU	2.4
1	1-B	508	PRO	2.4
1	1-B	99	TYR	2.4
1	1-A	253	PRO	2.4
1	1-A	271	LEU	2.4
1	1-A	570	LEU	2.4
1	1-B	123	GLY	2.4
1	1-A	206	LYS	2.4
1	1-B	565	LYS	2.4
1	1-B	207	ILE	2.4
1	1-B	370	VAL	2.4
1	1-A	387	PRO	2.3
1	1-A	75	THR	2.3
1	1-A	406	ALA	2.3
1	1-A	311	LYS	2.3
1	1-B	306	GLN	2.3
1	1-A	584	ILE	2.3
1	1-A	309	VAL	2.3
1	1-B	233	VAL	2.3
1	1-A	218	GLN	2.3
1	1-A	283	LYS	2.3
1	1-A	565	LYS	2.3
1	1-B	188	ASN	2.2
1	1-B	412	LEU	2.2
1	1-A	586	ASP	2.2
1	1-A	575	GLY	2.2
1	1-A	567	HIS	2.2
1	1-B	266	LYS	2.2
1	1-B	545	ASN	2.2
1	1-A	488	GLN	2.1
1	1-B	64	LEU	2.1
1	1-A	562	PRO	2.1
1	1-B	210	GLU	2.1
1	1-B	244	ALA	2.1
1	1-B	432	VAL	2.1
1	1-B	408	ASN	2.1
1	1-A	229	TRP	2.1
1	1-B	424	PRO	2.1
1	1-B	88	LYS	2.1
1	1-A	530	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	339	ASP	2.1
1	1-B	214	TYR	2.1
1	1-A	368	LEU	2.0
1	1-B	281	PRO	2.0
1	1-A	515	ASN	2.0
1	1-A	79	GLN	2.0
1	1-A	195	GLY	2.0
1	1-B	451	GLY	2.0
1	1-B	513	ILE	2.0
1	1-B	372	ASP	2.0
1	1-A	490	SER	2.0
1	1-A	278	VAL	2.0
1	1-A	467	VAL	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(Å ²)	Q<0.9
3	BGC	1-D	1	12/12	0.63	0.20	35,43,47,53	12
2	BGC	2-C	1	12/12	-	-	20,24,32,37	12
2	BGC	3-C	1	12/12	-	-	20,24,32,37	12
2	BGC	4-C	1	12/12	-	-	20,24,32,37	12
2	BGC	5-C	1	12/12	-	-	20,24,32,37	12
2	BGC	6-C	1	12/12	-	-	20,24,32,37	12
2	BGC	7-C	1	12/12	-	-	20,24,32,37	12
2	BGC	8-C	1	12/12	-	-	20,24,32,37	12
2	BGC	9-C	1	12/12	-	-	20,24,32,37	12
2	BGC	10-C	1	12/12	-	-	20,24,32,37	12
2	BGC	11-C	1	12/12	-	-	20,24,32,37	12
2	BGC	12-C	1	12/12	-	-	20,24,32,37	12
2	BGC	13-C	1	12/12	-	-	20,24,32,37	12
2	BGC	14-C	1	12/12	-	-	20,24,32,37	12
2	BGC	15-C	1	12/12	-	-	20,24,32,37	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	16-C	1	12/12	-	-	20,24,32,37	12
2	BGC	17-C	1	12/12	-	-	20,24,32,37	12
2	BGC	18-C	1	12/12	-	-	20,24,32,37	12
2	BGC	19-C	1	12/12	-	-	20,24,32,37	12
2	BGC	20-C	1	12/12	-	-	20,24,32,37	12
2	BGC	21-C	1	12/12	-	-	20,24,32,37	12
2	BGC	22-C	1	12/12	-	-	20,24,32,37	12
2	BGC	23-C	1	12/12	-	-	20,24,32,37	12
2	BGC	24-C	1	12/12	-	-	20,24,32,37	12
2	BGC	25-C	1	12/12	-	-	20,24,32,37	12
3	BGC	1-F	1	12/12	0.67	0.20	27,35,46,66	12
2	BGC	2-C	2	11/12	-	-	13,17,24,24	11
2	BGC	3-C	2	11/12	-	-	13,17,24,24	11
2	BGC	4-C	2	11/12	-	-	13,17,24,24	11
2	BGC	5-C	2	11/12	-	-	13,17,24,24	11
2	BGC	6-C	2	11/12	-	-	13,17,24,24	11
2	BGC	7-C	2	11/12	-	-	13,17,24,24	11
2	BGC	8-C	2	11/12	-	-	13,17,24,24	11
2	BGC	9-C	2	11/12	-	-	13,17,24,24	11
2	BGC	10-C	2	11/12	-	-	13,17,24,24	11
2	BGC	11-C	2	11/12	-	-	13,17,24,24	11
2	BGC	12-C	2	11/12	-	-	13,17,24,24	11
2	BGC	13-C	2	11/12	-	-	13,17,24,24	11
2	BGC	14-C	2	11/12	-	-	13,17,24,24	11
2	BGC	15-C	2	11/12	-	-	13,17,24,24	11
2	BGC	16-C	2	11/12	-	-	13,17,24,24	11
2	BGC	17-C	2	11/12	-	-	13,17,24,24	11
2	BGC	18-C	2	11/12	-	-	13,17,24,24	11
2	BGC	19-C	2	11/12	-	-	13,17,24,24	11
2	BGC	20-C	2	11/12	-	-	13,17,24,24	11
2	BGC	21-C	2	11/12	-	-	13,17,24,24	11
2	BGC	22-C	2	11/12	-	-	13,17,24,24	11
2	BGC	23-C	2	11/12	-	-	13,17,24,24	11
2	BGC	24-C	2	11/12	-	-	13,17,24,24	11
2	BGC	25-C	2	11/12	-	-	13,17,24,24	11
2	BGC	1-C	1	12/12	0.76	0.16	20,24,32,37	12
2	BGC	2-C	3	11/12	-	-	12,13,18,26	11
2	BGC	3-C	3	11/12	-	-	12,13,18,26	11
2	BGC	4-C	3	11/12	-	-	12,13,18,26	11
2	BGC	5-C	3	11/12	-	-	12,13,18,26	11
2	BGC	6-C	3	11/12	-	-	12,13,18,26	11
2	BGC	7-C	3	11/12	-	-	12,13,18,26	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	8-C	3	11/12	-	-	12,13,18,26	11
2	BGC	9-C	3	11/12	-	-	12,13,18,26	11
2	BGC	10-C	3	11/12	-	-	12,13,18,26	11
2	BGC	11-C	3	11/12	-	-	12,13,18,26	11
2	BGC	12-C	3	11/12	-	-	12,13,18,26	11
2	BGC	13-C	3	11/12	-	-	12,13,18,26	11
2	BGC	14-C	3	11/12	-	-	12,13,18,26	11
2	BGC	15-C	3	11/12	-	-	12,13,18,26	11
2	BGC	16-C	3	11/12	-	-	12,13,18,26	11
2	BGC	17-C	3	11/12	-	-	12,13,18,26	11
2	BGC	18-C	3	11/12	-	-	12,13,18,26	11
2	BGC	19-C	3	11/12	-	-	12,13,18,26	11
2	BGC	20-C	3	11/12	-	-	12,13,18,26	11
2	BGC	21-C	3	11/12	-	-	12,13,18,26	11
2	BGC	22-C	3	11/12	-	-	12,13,18,26	11
2	BGC	23-C	3	11/12	-	-	12,13,18,26	11
2	BGC	24-C	3	11/12	-	-	12,13,18,26	11
2	BGC	25-C	3	11/12	-	-	12,13,18,26	11
3	BGC	1-F	3	11/12	0.79	0.17	19,23,30,35	11
2	BGC	2-C	4	11/12	-	-	11,12,16,17	11
2	BGC	3-C	4	11/12	-	-	11,12,16,17	11
2	BGC	4-C	4	11/12	-	-	11,12,16,17	11
2	BGC	5-C	4	11/12	-	-	11,12,16,17	11
2	BGC	6-C	4	11/12	-	-	11,12,16,17	11
2	BGC	7-C	4	11/12	-	-	11,12,16,17	11
2	BGC	8-C	4	11/12	-	-	11,12,16,17	11
2	BGC	9-C	4	11/12	-	-	11,12,16,17	11
2	BGC	10-C	4	11/12	-	-	11,12,16,17	11
2	BGC	11-C	4	11/12	-	-	11,12,16,17	11
2	BGC	12-C	4	11/12	-	-	11,12,16,17	11
2	BGC	13-C	4	11/12	-	-	11,12,16,17	11
2	BGC	14-C	4	11/12	-	-	11,12,16,17	11
2	BGC	15-C	4	11/12	-	-	11,12,16,17	11
2	BGC	16-C	4	11/12	-	-	11,12,16,17	11
2	BGC	17-C	4	11/12	-	-	11,12,16,17	11
2	BGC	18-C	4	11/12	-	-	11,12,16,17	11
2	BGC	19-C	4	11/12	-	-	11,12,16,17	11
2	BGC	20-C	4	11/12	-	-	11,12,16,17	11
2	BGC	21-C	4	11/12	-	-	11,12,16,17	11
2	BGC	22-C	4	11/12	-	-	11,12,16,17	11
2	BGC	23-C	4	11/12	-	-	11,12,16,17	11
2	BGC	24-C	4	11/12	-	-	11,12,16,17	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	25-C	4	11/12	-	-	11,12,16,17	11
3	BGC	1-F	2	11/12	0.81	0.15	24,27,30,33	11
2	BGC	2-C	5	11/12	-	-	10,12,18,22	11
2	BGC	3-C	5	11/12	-	-	10,12,18,22	11
2	BGC	4-C	5	11/12	-	-	10,12,18,22	11
2	BGC	5-C	5	11/12	-	-	10,12,18,22	11
2	BGC	6-C	5	11/12	-	-	10,12,18,22	11
2	BGC	7-C	5	11/12	-	-	10,12,18,22	11
2	BGC	8-C	5	11/12	-	-	10,12,18,22	11
2	BGC	9-C	5	11/12	-	-	10,12,18,22	11
2	BGC	10-C	5	11/12	-	-	10,12,18,22	11
2	BGC	11-C	5	11/12	-	-	10,12,18,22	11
2	BGC	12-C	5	11/12	-	-	10,12,18,22	11
2	BGC	13-C	5	11/12	-	-	10,12,18,22	11
2	BGC	14-C	5	11/12	-	-	10,12,18,22	11
2	BGC	15-C	5	11/12	-	-	10,12,18,22	11
2	BGC	16-C	5	11/12	-	-	10,12,18,22	11
2	BGC	17-C	5	11/12	-	-	10,12,18,22	11
2	BGC	18-C	5	11/12	-	-	10,12,18,22	11
2	BGC	19-C	5	11/12	-	-	10,12,18,22	11
2	BGC	20-C	5	11/12	-	-	10,12,18,22	11
2	BGC	21-C	5	11/12	-	-	10,12,18,22	11
2	BGC	22-C	5	11/12	-	-	10,12,18,22	11
2	BGC	23-C	5	11/12	-	-	10,12,18,22	11
2	BGC	24-C	5	11/12	-	-	10,12,18,22	11
2	BGC	25-C	5	11/12	-	-	10,12,18,22	11
3	BGC	1-D	5	11/12	0.81	0.17	16,19,23,27	11
2	BGC	2-C	6	11/12	-	-	9,12,14,14	11
2	BGC	3-C	6	11/12	-	-	9,12,14,14	11
2	BGC	4-C	6	11/12	-	-	9,12,14,14	11
2	BGC	5-C	6	11/12	-	-	9,12,14,14	11
2	BGC	6-C	6	11/12	-	-	9,12,14,14	11
2	BGC	7-C	6	11/12	-	-	9,12,14,14	11
2	BGC	8-C	6	11/12	-	-	9,12,14,14	11
2	BGC	9-C	6	11/12	-	-	9,12,14,14	11
2	BGC	10-C	6	11/12	-	-	9,12,14,14	11
2	BGC	11-C	6	11/12	-	-	9,12,14,14	11
2	BGC	12-C	6	11/12	-	-	9,12,14,14	11
2	BGC	13-C	6	11/12	-	-	9,12,14,14	11
2	BGC	14-C	6	11/12	-	-	9,12,14,14	11
2	BGC	15-C	6	11/12	-	-	9,12,14,14	11
2	BGC	16-C	6	11/12	-	-	9,12,14,14	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	17-C	6	11/12	-	-	9,12,14,14	11
2	BGC	18-C	6	11/12	-	-	9,12,14,14	11
2	BGC	19-C	6	11/12	-	-	9,12,14,14	11
2	BGC	20-C	6	11/12	-	-	9,12,14,14	11
2	BGC	21-C	6	11/12	-	-	9,12,14,14	11
2	BGC	22-C	6	11/12	-	-	9,12,14,14	11
2	BGC	23-C	6	11/12	-	-	9,12,14,14	11
2	BGC	24-C	6	11/12	-	-	9,12,14,14	11
2	BGC	25-C	6	11/12	-	-	9,12,14,14	11
2	BGC	1-E	3	11/12	0.82	0.14	11,14,19,23	11
2	BGC	2-E	1	12/12	-	-	17,20,30,39	12
2	BGC	3-E	1	12/12	-	-	17,20,30,39	12
2	BGC	4-E	1	12/12	-	-	17,20,30,39	12
2	BGC	5-E	1	12/12	-	-	17,20,30,39	12
2	BGC	6-E	1	12/12	-	-	17,20,30,39	12
2	BGC	7-E	1	12/12	-	-	17,20,30,39	12
2	BGC	8-E	1	12/12	-	-	17,20,30,39	12
2	BGC	9-E	1	12/12	-	-	17,20,30,39	12
2	BGC	10-E	1	12/12	-	-	17,20,30,39	12
2	BGC	11-E	1	12/12	-	-	17,20,30,39	12
2	BGC	12-E	1	12/12	-	-	17,20,30,39	12
2	BGC	13-E	1	12/12	-	-	17,20,30,39	12
2	BGC	14-E	1	12/12	-	-	17,20,30,39	12
2	BGC	15-E	1	12/12	-	-	17,20,30,39	12
2	BGC	16-E	1	12/12	-	-	17,20,30,39	12
2	BGC	17-E	1	12/12	-	-	17,20,30,39	12
2	BGC	18-E	1	12/12	-	-	17,20,30,39	12
2	BGC	19-E	1	12/12	-	-	17,20,30,39	12
2	BGC	20-E	1	12/12	-	-	17,20,30,39	12
2	BGC	21-E	1	12/12	-	-	17,20,30,39	12
2	BGC	22-E	1	12/12	-	-	17,20,30,39	12
2	BGC	23-E	1	12/12	-	-	17,20,30,39	12
2	BGC	24-E	1	12/12	-	-	17,20,30,39	12
2	BGC	25-E	1	12/12	-	-	17,20,30,39	12
2	BGC	1-E	1	12/12	0.82	0.14	17,20,30,39	12
2	BGC	2-E	2	11/12	-	-	15,17,23,23	11
2	BGC	3-E	2	11/12	-	-	15,17,23,23	11
2	BGC	4-E	2	11/12	-	-	15,17,23,23	11
2	BGC	5-E	2	11/12	-	-	15,17,23,23	11
2	BGC	6-E	2	11/12	-	-	15,17,23,23	11
2	BGC	7-E	2	11/12	-	-	15,17,23,23	11
2	BGC	8-E	2	11/12	-	-	15,17,23,23	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	9-E	2	11/12	-	-	15,17,23,23	11
2	BGC	10-E	2	11/12	-	-	15,17,23,23	11
2	BGC	11-E	2	11/12	-	-	15,17,23,23	11
2	BGC	12-E	2	11/12	-	-	15,17,23,23	11
2	BGC	13-E	2	11/12	-	-	15,17,23,23	11
2	BGC	14-E	2	11/12	-	-	15,17,23,23	11
2	BGC	15-E	2	11/12	-	-	15,17,23,23	11
2	BGC	16-E	2	11/12	-	-	15,17,23,23	11
2	BGC	17-E	2	11/12	-	-	15,17,23,23	11
2	BGC	18-E	2	11/12	-	-	15,17,23,23	11
2	BGC	19-E	2	11/12	-	-	15,17,23,23	11
2	BGC	20-E	2	11/12	-	-	15,17,23,23	11
2	BGC	21-E	2	11/12	-	-	15,17,23,23	11
2	BGC	22-E	2	11/12	-	-	15,17,23,23	11
2	BGC	23-E	2	11/12	-	-	15,17,23,23	11
2	BGC	24-E	2	11/12	-	-	15,17,23,23	11
2	BGC	25-E	2	11/12	-	-	15,17,23,23	11
3	BGC	1-D	2	11/12	0.83	0.12	21,28,33,36	11
2	BGC	2-E	3	11/12	-	-	11,14,19,23	11
2	BGC	3-E	3	11/12	-	-	11,14,19,23	11
2	BGC	4-E	3	11/12	-	-	11,14,19,23	11
2	BGC	5-E	3	11/12	-	-	11,14,19,23	11
2	BGC	6-E	3	11/12	-	-	11,14,19,23	11
2	BGC	7-E	3	11/12	-	-	11,14,19,23	11
2	BGC	8-E	3	11/12	-	-	11,14,19,23	11
2	BGC	9-E	3	11/12	-	-	11,14,19,23	11
2	BGC	10-E	3	11/12	-	-	11,14,19,23	11
2	BGC	11-E	3	11/12	-	-	11,14,19,23	11
2	BGC	12-E	3	11/12	-	-	11,14,19,23	11
2	BGC	13-E	3	11/12	-	-	11,14,19,23	11
2	BGC	14-E	3	11/12	-	-	11,14,19,23	11
2	BGC	15-E	3	11/12	-	-	11,14,19,23	11
2	BGC	16-E	3	11/12	-	-	11,14,19,23	11
2	BGC	17-E	3	11/12	-	-	11,14,19,23	11
2	BGC	18-E	3	11/12	-	-	11,14,19,23	11
2	BGC	19-E	3	11/12	-	-	11,14,19,23	11
2	BGC	20-E	3	11/12	-	-	11,14,19,23	11
2	BGC	21-E	3	11/12	-	-	11,14,19,23	11
2	BGC	22-E	3	11/12	-	-	11,14,19,23	11
2	BGC	23-E	3	11/12	-	-	11,14,19,23	11
2	BGC	24-E	3	11/12	-	-	11,14,19,23	11
2	BGC	25-E	3	11/12	-	-	11,14,19,23	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	1-D	4	11/12	0.83	0.13	18,20,25,28	11
2	BGC	2-E	4	11/12	-	-	11,12,17,18	11
2	BGC	3-E	4	11/12	-	-	11,12,17,18	11
2	BGC	4-E	4	11/12	-	-	11,12,17,18	11
2	BGC	5-E	4	11/12	-	-	11,12,17,18	11
2	BGC	6-E	4	11/12	-	-	11,12,17,18	11
2	BGC	7-E	4	11/12	-	-	11,12,17,18	11
2	BGC	8-E	4	11/12	-	-	11,12,17,18	11
2	BGC	9-E	4	11/12	-	-	11,12,17,18	11
2	BGC	10-E	4	11/12	-	-	11,12,17,18	11
2	BGC	11-E	4	11/12	-	-	11,12,17,18	11
2	BGC	12-E	4	11/12	-	-	11,12,17,18	11
2	BGC	13-E	4	11/12	-	-	11,12,17,18	11
2	BGC	14-E	4	11/12	-	-	11,12,17,18	11
2	BGC	15-E	4	11/12	-	-	11,12,17,18	11
2	BGC	16-E	4	11/12	-	-	11,12,17,18	11
2	BGC	17-E	4	11/12	-	-	11,12,17,18	11
2	BGC	18-E	4	11/12	-	-	11,12,17,18	11
2	BGC	19-E	4	11/12	-	-	11,12,17,18	11
2	BGC	20-E	4	11/12	-	-	11,12,17,18	11
2	BGC	21-E	4	11/12	-	-	11,12,17,18	11
2	BGC	22-E	4	11/12	-	-	11,12,17,18	11
2	BGC	23-E	4	11/12	-	-	11,12,17,18	11
2	BGC	24-E	4	11/12	-	-	11,12,17,18	11
2	BGC	25-E	4	11/12	-	-	11,12,17,18	11
2	BGC	1-E	5	11/12	0.85	0.12	11,13,18,20	11
2	BGC	2-E	5	11/12	-	-	11,13,18,20	11
2	BGC	3-E	5	11/12	-	-	11,13,18,20	11
2	BGC	4-E	5	11/12	-	-	11,13,18,20	11
2	BGC	5-E	5	11/12	-	-	11,13,18,20	11
2	BGC	6-E	5	11/12	-	-	11,13,18,20	11
2	BGC	7-E	5	11/12	-	-	11,13,18,20	11
2	BGC	8-E	5	11/12	-	-	11,13,18,20	11
2	BGC	9-E	5	11/12	-	-	11,13,18,20	11
2	BGC	10-E	5	11/12	-	-	11,13,18,20	11
2	BGC	11-E	5	11/12	-	-	11,13,18,20	11
2	BGC	12-E	5	11/12	-	-	11,13,18,20	11
2	BGC	13-E	5	11/12	-	-	11,13,18,20	11
2	BGC	14-E	5	11/12	-	-	11,13,18,20	11
2	BGC	15-E	5	11/12	-	-	11,13,18,20	11
2	BGC	16-E	5	11/12	-	-	11,13,18,20	11
2	BGC	17-E	5	11/12	-	-	11,13,18,20	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	18-E	5	11/12	-	-	11,13,18,20	11
2	BGC	19-E	5	11/12	-	-	11,13,18,20	11
2	BGC	20-E	5	11/12	-	-	11,13,18,20	11
2	BGC	21-E	5	11/12	-	-	11,13,18,20	11
2	BGC	22-E	5	11/12	-	-	11,13,18,20	11
2	BGC	23-E	5	11/12	-	-	11,13,18,20	11
2	BGC	24-E	5	11/12	-	-	11,13,18,20	11
2	BGC	25-E	5	11/12	-	-	11,13,18,20	11
3	BGC	1-F	4	11/12	0.85	0.13	15,19,22,29	11
2	BGC	2-E	6	11/12	-	-	10,12,13,14	11
2	BGC	3-E	6	11/12	-	-	10,12,13,14	11
2	BGC	4-E	6	11/12	-	-	10,12,13,14	11
2	BGC	5-E	6	11/12	-	-	10,12,13,14	11
2	BGC	6-E	6	11/12	-	-	10,12,13,14	11
2	BGC	7-E	6	11/12	-	-	10,12,13,14	11
2	BGC	8-E	6	11/12	-	-	10,12,13,14	11
2	BGC	9-E	6	11/12	-	-	10,12,13,14	11
2	BGC	10-E	6	11/12	-	-	10,12,13,14	11
2	BGC	11-E	6	11/12	-	-	10,12,13,14	11
2	BGC	12-E	6	11/12	-	-	10,12,13,14	11
2	BGC	13-E	6	11/12	-	-	10,12,13,14	11
2	BGC	14-E	6	11/12	-	-	10,12,13,14	11
2	BGC	15-E	6	11/12	-	-	10,12,13,14	11
2	BGC	16-E	6	11/12	-	-	10,12,13,14	11
2	BGC	17-E	6	11/12	-	-	10,12,13,14	11
2	BGC	18-E	6	11/12	-	-	10,12,13,14	11
2	BGC	19-E	6	11/12	-	-	10,12,13,14	11
2	BGC	20-E	6	11/12	-	-	10,12,13,14	11
2	BGC	21-E	6	11/12	-	-	10,12,13,14	11
2	BGC	22-E	6	11/12	-	-	10,12,13,14	11
2	BGC	23-E	6	11/12	-	-	10,12,13,14	11
2	BGC	24-E	6	11/12	-	-	10,12,13,14	11
2	BGC	25-E	6	11/12	-	-	10,12,13,14	11
3	BGC	1-F	5	11/12	0.85	0.14	15,17,22,25	11
3	BGC	2-D	1	12/12	-	-	35,43,47,53	12
3	BGC	3-D	1	12/12	-	-	35,43,47,53	12
3	BGC	4-D	1	12/12	-	-	35,43,47,53	12
3	BGC	5-D	1	12/12	-	-	35,43,47,53	12
3	BGC	6-D	1	12/12	-	-	35,43,47,53	12
3	BGC	7-D	1	12/12	-	-	35,43,47,53	12
3	BGC	8-D	1	12/12	-	-	35,43,47,53	12
3	BGC	9-D	1	12/12	-	-	35,43,47,53	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	10-D	1	12/12	-	-	35,43,47,53	12
3	BGC	11-D	1	12/12	-	-	35,43,47,53	12
3	BGC	12-D	1	12/12	-	-	35,43,47,53	12
3	BGC	13-D	1	12/12	-	-	35,43,47,53	12
3	BGC	14-D	1	12/12	-	-	35,43,47,53	12
3	BGC	15-D	1	12/12	-	-	35,43,47,53	12
3	BGC	16-D	1	12/12	-	-	35,43,47,53	12
3	BGC	17-D	1	12/12	-	-	35,43,47,53	12
3	BGC	18-D	1	12/12	-	-	35,43,47,53	12
3	BGC	19-D	1	12/12	-	-	35,43,47,53	12
3	BGC	20-D	1	12/12	-	-	35,43,47,53	12
3	BGC	21-D	1	12/12	-	-	35,43,47,53	12
3	BGC	22-D	1	12/12	-	-	35,43,47,53	12
3	BGC	23-D	1	12/12	-	-	35,43,47,53	12
3	BGC	24-D	1	12/12	-	-	35,43,47,53	12
3	BGC	25-D	1	12/12	-	-	35,43,47,53	12
3	BGC	1-D	3	11/12	0.86	0.13	21,25,31,42	11
3	BGC	2-D	2	11/12	-	-	21,28,33,36	11
3	BGC	3-D	2	11/12	-	-	21,28,33,36	11
3	BGC	4-D	2	11/12	-	-	21,28,33,36	11
3	BGC	5-D	2	11/12	-	-	21,28,33,36	11
3	BGC	6-D	2	11/12	-	-	21,28,33,36	11
3	BGC	7-D	2	11/12	-	-	21,28,33,36	11
3	BGC	8-D	2	11/12	-	-	21,28,33,36	11
3	BGC	9-D	2	11/12	-	-	21,28,33,36	11
3	BGC	10-D	2	11/12	-	-	21,28,33,36	11
3	BGC	11-D	2	11/12	-	-	21,28,33,36	11
3	BGC	12-D	2	11/12	-	-	21,28,33,36	11
3	BGC	13-D	2	11/12	-	-	21,28,33,36	11
3	BGC	14-D	2	11/12	-	-	21,28,33,36	11
3	BGC	15-D	2	11/12	-	-	21,28,33,36	11
3	BGC	16-D	2	11/12	-	-	21,28,33,36	11
3	BGC	17-D	2	11/12	-	-	21,28,33,36	11
3	BGC	18-D	2	11/12	-	-	21,28,33,36	11
3	BGC	19-D	2	11/12	-	-	21,28,33,36	11
3	BGC	20-D	2	11/12	-	-	21,28,33,36	11
3	BGC	21-D	2	11/12	-	-	21,28,33,36	11
3	BGC	22-D	2	11/12	-	-	21,28,33,36	11
3	BGC	23-D	2	11/12	-	-	21,28,33,36	11
3	BGC	24-D	2	11/12	-	-	21,28,33,36	11
3	BGC	25-D	2	11/12	-	-	21,28,33,36	11
2	BGC	1-C	6	11/12	0.86	0.11	9,12,14,14	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	2-D	3	11/12	-	-	21,25,31,42	11
3	BGC	3-D	3	11/12	-	-	21,25,31,42	11
3	BGC	4-D	3	11/12	-	-	21,25,31,42	11
3	BGC	5-D	3	11/12	-	-	21,25,31,42	11
3	BGC	6-D	3	11/12	-	-	21,25,31,42	11
3	BGC	7-D	3	11/12	-	-	21,25,31,42	11
3	BGC	8-D	3	11/12	-	-	21,25,31,42	11
3	BGC	9-D	3	11/12	-	-	21,25,31,42	11
3	BGC	10-D	3	11/12	-	-	21,25,31,42	11
3	BGC	11-D	3	11/12	-	-	21,25,31,42	11
3	BGC	12-D	3	11/12	-	-	21,25,31,42	11
3	BGC	13-D	3	11/12	-	-	21,25,31,42	11
3	BGC	14-D	3	11/12	-	-	21,25,31,42	11
3	BGC	15-D	3	11/12	-	-	21,25,31,42	11
3	BGC	16-D	3	11/12	-	-	21,25,31,42	11
3	BGC	17-D	3	11/12	-	-	21,25,31,42	11
3	BGC	18-D	3	11/12	-	-	21,25,31,42	11
3	BGC	19-D	3	11/12	-	-	21,25,31,42	11
3	BGC	20-D	3	11/12	-	-	21,25,31,42	11
3	BGC	21-D	3	11/12	-	-	21,25,31,42	11
3	BGC	22-D	3	11/12	-	-	21,25,31,42	11
3	BGC	23-D	3	11/12	-	-	21,25,31,42	11
3	BGC	24-D	3	11/12	-	-	21,25,31,42	11
3	BGC	25-D	3	11/12	-	-	21,25,31,42	11
2	BGC	1-E	4	11/12	0.88	0.11	11,12,17,18	11
3	BGC	2-D	4	11/12	-	-	18,20,25,28	11
3	BGC	3-D	4	11/12	-	-	18,20,25,28	11
3	BGC	4-D	4	11/12	-	-	18,20,25,28	11
3	BGC	5-D	4	11/12	-	-	18,20,25,28	11
3	BGC	6-D	4	11/12	-	-	18,20,25,28	11
3	BGC	7-D	4	11/12	-	-	18,20,25,28	11
3	BGC	8-D	4	11/12	-	-	18,20,25,28	11
3	BGC	9-D	4	11/12	-	-	18,20,25,28	11
3	BGC	10-D	4	11/12	-	-	18,20,25,28	11
3	BGC	11-D	4	11/12	-	-	18,20,25,28	11
3	BGC	12-D	4	11/12	-	-	18,20,25,28	11
3	BGC	13-D	4	11/12	-	-	18,20,25,28	11
3	BGC	14-D	4	11/12	-	-	18,20,25,28	11
3	BGC	15-D	4	11/12	-	-	18,20,25,28	11
3	BGC	16-D	4	11/12	-	-	18,20,25,28	11
3	BGC	17-D	4	11/12	-	-	18,20,25,28	11
3	BGC	18-D	4	11/12	-	-	18,20,25,28	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	19-D	4	11/12	-	-	18,20,25,28	11
3	BGC	20-D	4	11/12	-	-	18,20,25,28	11
3	BGC	21-D	4	11/12	-	-	18,20,25,28	11
3	BGC	22-D	4	11/12	-	-	18,20,25,28	11
3	BGC	23-D	4	11/12	-	-	18,20,25,28	11
3	BGC	24-D	4	11/12	-	-	18,20,25,28	11
3	BGC	25-D	4	11/12	-	-	18,20,25,28	11
2	BGC	1-C	4	11/12	0.89	0.10	11,12,16,17	11
3	BGC	2-D	5	11/12	-	-	16,19,23,27	11
3	BGC	3-D	5	11/12	-	-	16,19,23,27	11
3	BGC	4-D	5	11/12	-	-	16,19,23,27	11
3	BGC	5-D	5	11/12	-	-	16,19,23,27	11
3	BGC	6-D	5	11/12	-	-	16,19,23,27	11
3	BGC	7-D	5	11/12	-	-	16,19,23,27	11
3	BGC	8-D	5	11/12	-	-	16,19,23,27	11
3	BGC	9-D	5	11/12	-	-	16,19,23,27	11
3	BGC	10-D	5	11/12	-	-	16,19,23,27	11
3	BGC	11-D	5	11/12	-	-	16,19,23,27	11
3	BGC	12-D	5	11/12	-	-	16,19,23,27	11
3	BGC	13-D	5	11/12	-	-	16,19,23,27	11
3	BGC	14-D	5	11/12	-	-	16,19,23,27	11
3	BGC	15-D	5	11/12	-	-	16,19,23,27	11
3	BGC	16-D	5	11/12	-	-	16,19,23,27	11
3	BGC	17-D	5	11/12	-	-	16,19,23,27	11
3	BGC	18-D	5	11/12	-	-	16,19,23,27	11
3	BGC	19-D	5	11/12	-	-	16,19,23,27	11
3	BGC	20-D	5	11/12	-	-	16,19,23,27	11
3	BGC	21-D	5	11/12	-	-	16,19,23,27	11
3	BGC	22-D	5	11/12	-	-	16,19,23,27	11
3	BGC	23-D	5	11/12	-	-	16,19,23,27	11
3	BGC	24-D	5	11/12	-	-	16,19,23,27	11
3	BGC	25-D	5	11/12	-	-	16,19,23,27	11
2	BGC	1-E	6	11/12	0.89	0.10	10,12,13,14	11
3	BGC	2-F	1	12/12	-	-	27,35,46,66	12
3	BGC	3-F	1	12/12	-	-	27,35,46,66	12
3	BGC	4-F	1	12/12	-	-	27,35,46,66	12
3	BGC	5-F	1	12/12	-	-	27,35,46,66	12
3	BGC	6-F	1	12/12	-	-	27,35,46,66	12
3	BGC	7-F	1	12/12	-	-	27,35,46,66	12
3	BGC	8-F	1	12/12	-	-	27,35,46,66	12
3	BGC	9-F	1	12/12	-	-	27,35,46,66	12
3	BGC	10-F	1	12/12	-	-	27,35,46,66	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	11-F	1	12/12	-	-	27,35,46,66	12
3	BGC	12-F	1	12/12	-	-	27,35,46,66	12
3	BGC	13-F	1	12/12	-	-	27,35,46,66	12
3	BGC	14-F	1	12/12	-	-	27,35,46,66	12
3	BGC	15-F	1	12/12	-	-	27,35,46,66	12
3	BGC	16-F	1	12/12	-	-	27,35,46,66	12
3	BGC	17-F	1	12/12	-	-	27,35,46,66	12
3	BGC	18-F	1	12/12	-	-	27,35,46,66	12
3	BGC	19-F	1	12/12	-	-	27,35,46,66	12
3	BGC	20-F	1	12/12	-	-	27,35,46,66	12
3	BGC	21-F	1	12/12	-	-	27,35,46,66	12
3	BGC	22-F	1	12/12	-	-	27,35,46,66	12
3	BGC	23-F	1	12/12	-	-	27,35,46,66	12
3	BGC	24-F	1	12/12	-	-	27,35,46,66	12
3	BGC	25-F	1	12/12	-	-	27,35,46,66	12
2	BGC	1-C	5	11/12	0.89	0.11	10,12,18,22	11
3	BGC	2-F	2	11/12	-	-	24,27,30,33	11
3	BGC	3-F	2	11/12	-	-	24,27,30,33	11
3	BGC	4-F	2	11/12	-	-	24,27,30,33	11
3	BGC	5-F	2	11/12	-	-	24,27,30,33	11
3	BGC	6-F	2	11/12	-	-	24,27,30,33	11
3	BGC	7-F	2	11/12	-	-	24,27,30,33	11
3	BGC	8-F	2	11/12	-	-	24,27,30,33	11
3	BGC	9-F	2	11/12	-	-	24,27,30,33	11
3	BGC	10-F	2	11/12	-	-	24,27,30,33	11
3	BGC	11-F	2	11/12	-	-	24,27,30,33	11
3	BGC	12-F	2	11/12	-	-	24,27,30,33	11
3	BGC	13-F	2	11/12	-	-	24,27,30,33	11
3	BGC	14-F	2	11/12	-	-	24,27,30,33	11
3	BGC	15-F	2	11/12	-	-	24,27,30,33	11
3	BGC	16-F	2	11/12	-	-	24,27,30,33	11
3	BGC	17-F	2	11/12	-	-	24,27,30,33	11
3	BGC	18-F	2	11/12	-	-	24,27,30,33	11
3	BGC	19-F	2	11/12	-	-	24,27,30,33	11
3	BGC	20-F	2	11/12	-	-	24,27,30,33	11
3	BGC	21-F	2	11/12	-	-	24,27,30,33	11
3	BGC	22-F	2	11/12	-	-	24,27,30,33	11
3	BGC	23-F	2	11/12	-	-	24,27,30,33	11
3	BGC	24-F	2	11/12	-	-	24,27,30,33	11
3	BGC	25-F	2	11/12	-	-	24,27,30,33	11
2	BGC	1-C	2	11/12	0.91	0.10	13,17,24,24	11
3	BGC	2-F	3	11/12	-	-	19,23,30,35	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	3-F	3	11/12	-	-	19,23,30,35	11
3	BGC	4-F	3	11/12	-	-	19,23,30,35	11
3	BGC	5-F	3	11/12	-	-	19,23,30,35	11
3	BGC	6-F	3	11/12	-	-	19,23,30,35	11
3	BGC	7-F	3	11/12	-	-	19,23,30,35	11
3	BGC	8-F	3	11/12	-	-	19,23,30,35	11
3	BGC	9-F	3	11/12	-	-	19,23,30,35	11
3	BGC	10-F	3	11/12	-	-	19,23,30,35	11
3	BGC	11-F	3	11/12	-	-	19,23,30,35	11
3	BGC	12-F	3	11/12	-	-	19,23,30,35	11
3	BGC	13-F	3	11/12	-	-	19,23,30,35	11
3	BGC	14-F	3	11/12	-	-	19,23,30,35	11
3	BGC	15-F	3	11/12	-	-	19,23,30,35	11
3	BGC	16-F	3	11/12	-	-	19,23,30,35	11
3	BGC	17-F	3	11/12	-	-	19,23,30,35	11
3	BGC	18-F	3	11/12	-	-	19,23,30,35	11
3	BGC	19-F	3	11/12	-	-	19,23,30,35	11
3	BGC	20-F	3	11/12	-	-	19,23,30,35	11
3	BGC	21-F	3	11/12	-	-	19,23,30,35	11
3	BGC	22-F	3	11/12	-	-	19,23,30,35	11
3	BGC	23-F	3	11/12	-	-	19,23,30,35	11
3	BGC	24-F	3	11/12	-	-	19,23,30,35	11
3	BGC	25-F	3	11/12	-	-	19,23,30,35	11
2	BGC	1-C	3	11/12	0.91	0.09	12,13,18,26	11
3	BGC	2-F	4	11/12	-	-	15,19,22,29	11
3	BGC	3-F	4	11/12	-	-	15,19,22,29	11
3	BGC	4-F	4	11/12	-	-	15,19,22,29	11
3	BGC	5-F	4	11/12	-	-	15,19,22,29	11
3	BGC	6-F	4	11/12	-	-	15,19,22,29	11
3	BGC	7-F	4	11/12	-	-	15,19,22,29	11
3	BGC	8-F	4	11/12	-	-	15,19,22,29	11
3	BGC	9-F	4	11/12	-	-	15,19,22,29	11
3	BGC	10-F	4	11/12	-	-	15,19,22,29	11
3	BGC	11-F	4	11/12	-	-	15,19,22,29	11
3	BGC	12-F	4	11/12	-	-	15,19,22,29	11
3	BGC	13-F	4	11/12	-	-	15,19,22,29	11
3	BGC	14-F	4	11/12	-	-	15,19,22,29	11
3	BGC	15-F	4	11/12	-	-	15,19,22,29	11
3	BGC	16-F	4	11/12	-	-	15,19,22,29	11
3	BGC	17-F	4	11/12	-	-	15,19,22,29	11
3	BGC	18-F	4	11/12	-	-	15,19,22,29	11
3	BGC	19-F	4	11/12	-	-	15,19,22,29	11

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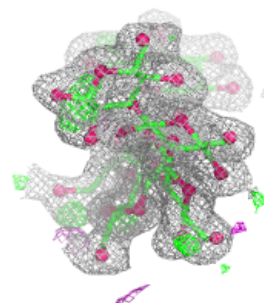
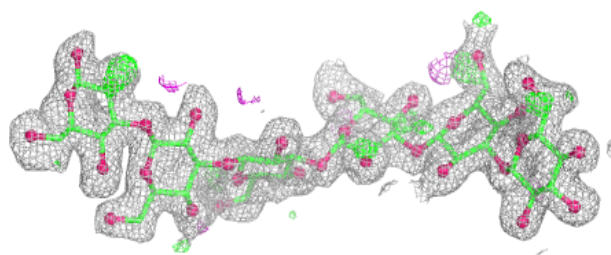
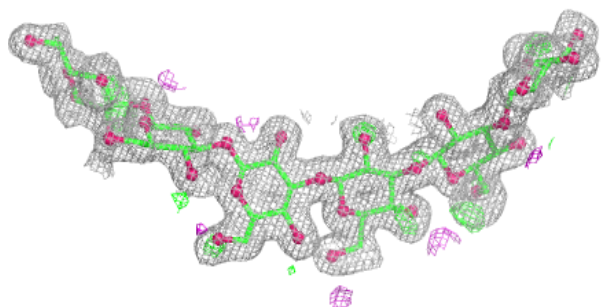
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	20-F	4	11/12	-	-	15,19,22,29	11
3	BGC	21-F	4	11/12	-	-	15,19,22,29	11
3	BGC	22-F	4	11/12	-	-	15,19,22,29	11
3	BGC	23-F	4	11/12	-	-	15,19,22,29	11
3	BGC	24-F	4	11/12	-	-	15,19,22,29	11
3	BGC	25-F	4	11/12	-	-	15,19,22,29	11
2	BGC	1-E	2	11/12	0.93	0.10	15,17,23,23	11
3	BGC	2-F	5	11/12	-	-	15,17,22,25	11
3	BGC	3-F	5	11/12	-	-	15,17,22,25	11
3	BGC	4-F	5	11/12	-	-	15,17,22,25	11
3	BGC	5-F	5	11/12	-	-	15,17,22,25	11
3	BGC	6-F	5	11/12	-	-	15,17,22,25	11
3	BGC	7-F	5	11/12	-	-	15,17,22,25	11
3	BGC	8-F	5	11/12	-	-	15,17,22,25	11
3	BGC	9-F	5	11/12	-	-	15,17,22,25	11
3	BGC	10-F	5	11/12	-	-	15,17,22,25	11
3	BGC	11-F	5	11/12	-	-	15,17,22,25	11
3	BGC	12-F	5	11/12	-	-	15,17,22,25	11
3	BGC	13-F	5	11/12	-	-	15,17,22,25	11
3	BGC	14-F	5	11/12	-	-	15,17,22,25	11
3	BGC	15-F	5	11/12	-	-	15,17,22,25	11
3	BGC	16-F	5	11/12	-	-	15,17,22,25	11
3	BGC	17-F	5	11/12	-	-	15,17,22,25	11
3	BGC	18-F	5	11/12	-	-	15,17,22,25	11
3	BGC	19-F	5	11/12	-	-	15,17,22,25	11
3	BGC	20-F	5	11/12	-	-	15,17,22,25	11
3	BGC	21-F	5	11/12	-	-	15,17,22,25	11
3	BGC	22-F	5	11/12	-	-	15,17,22,25	11
3	BGC	23-F	5	11/12	-	-	15,17,22,25	11
3	BGC	24-F	5	11/12	-	-	15,17,22,25	11
3	BGC	25-F	5	11/12	-	-	15,17,22,25	11

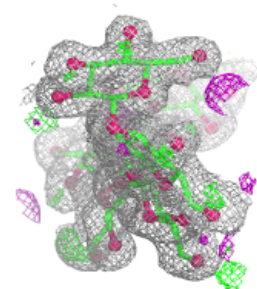
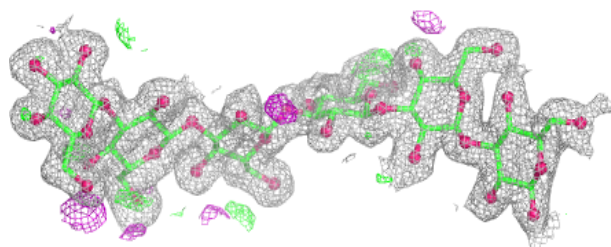
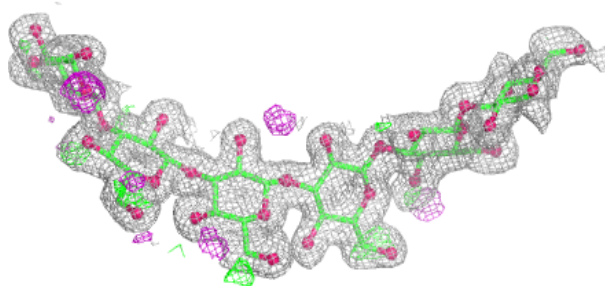
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

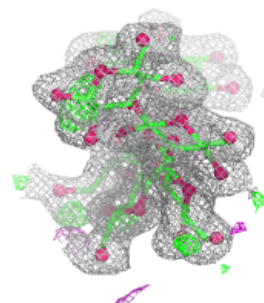
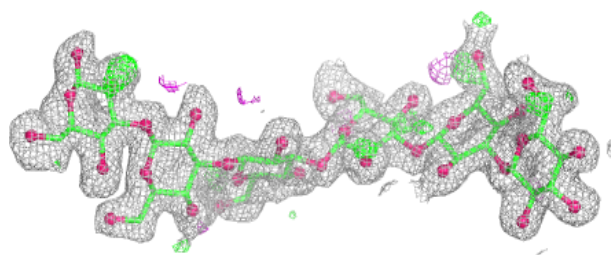
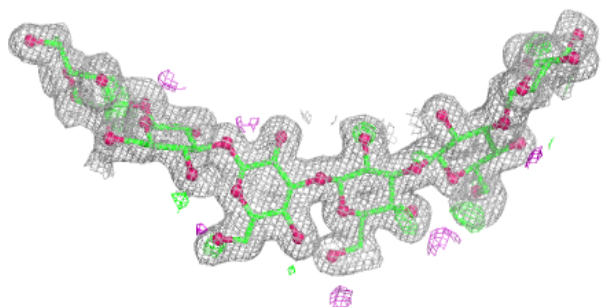
**Electron density around Chain E:**

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

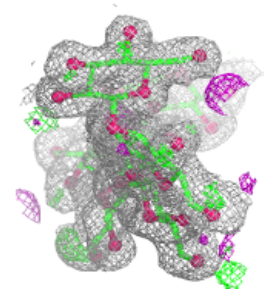
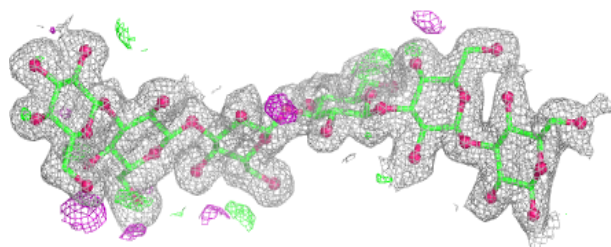
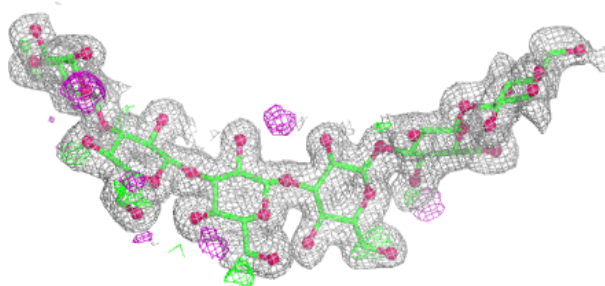


Electron density around Chain C:

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

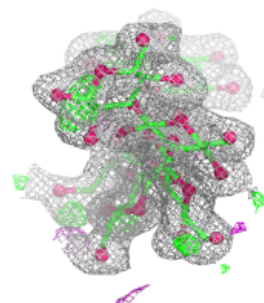
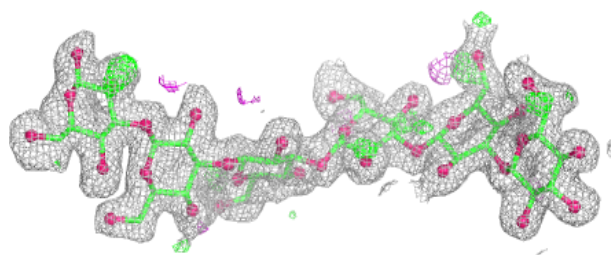
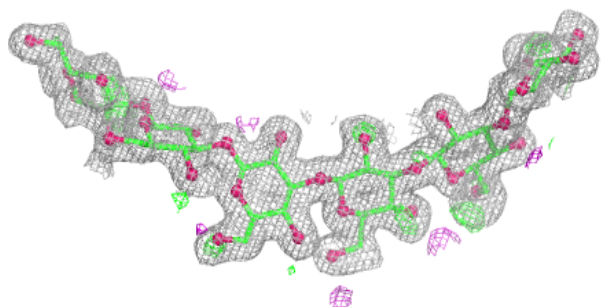
**Electron density around Chain E:**

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

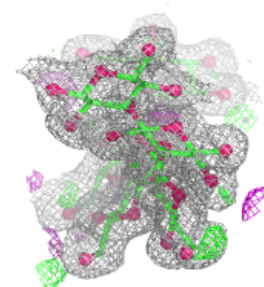
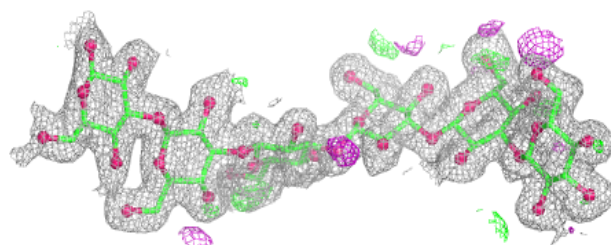
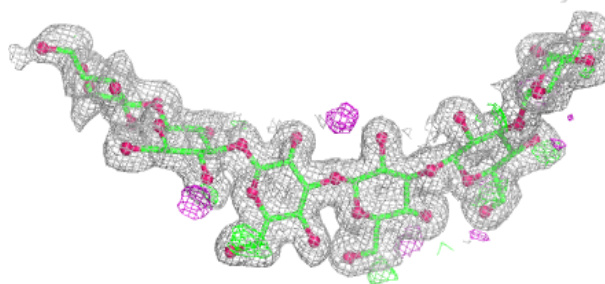


Electron density around Chain C:

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

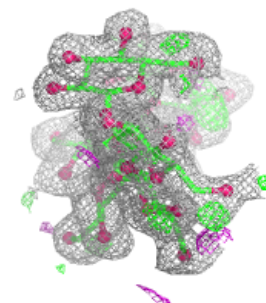
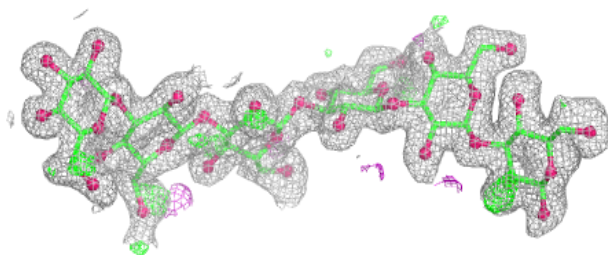
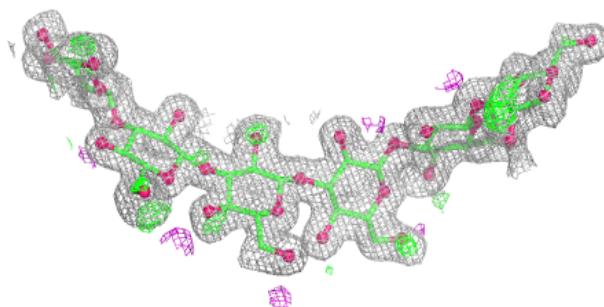
**Electron density around Chain E:**

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

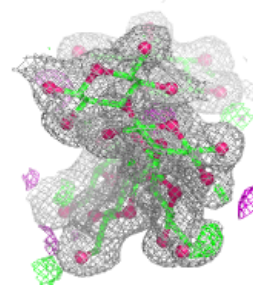
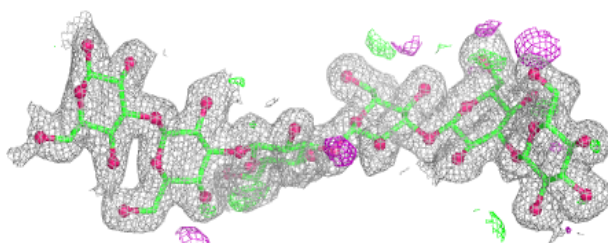
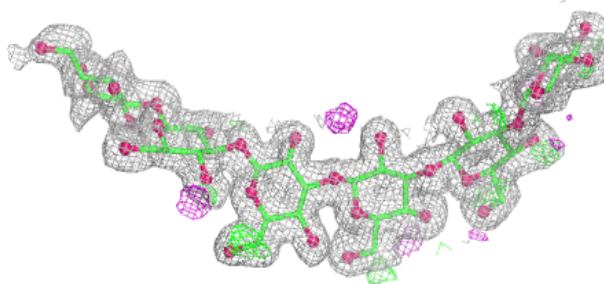


Electron density around Chain C:

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

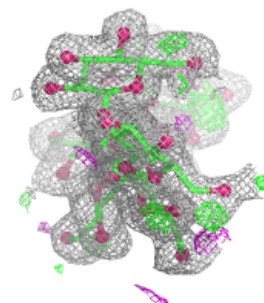
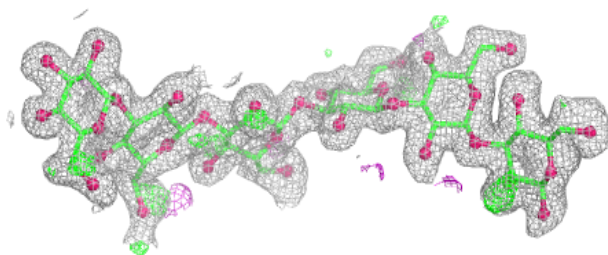
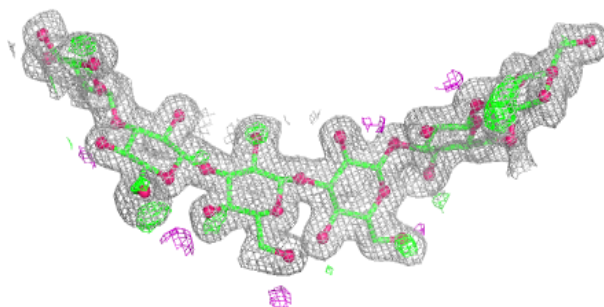
**Electron density around Chain E:**

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

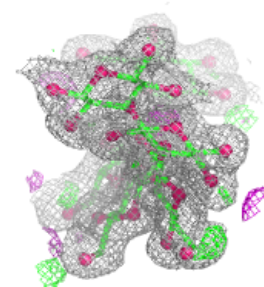
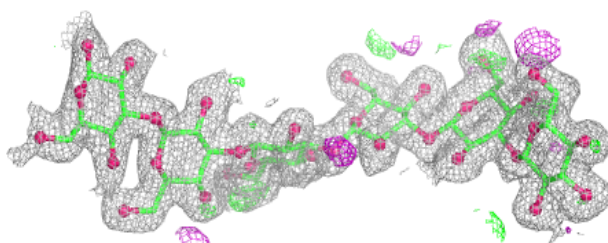
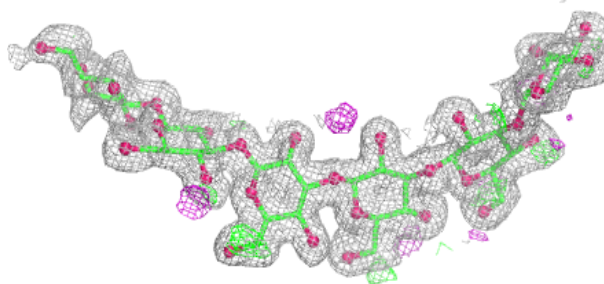


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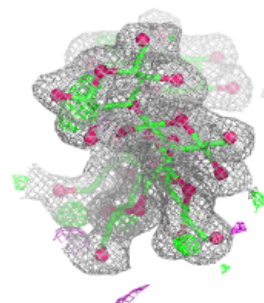
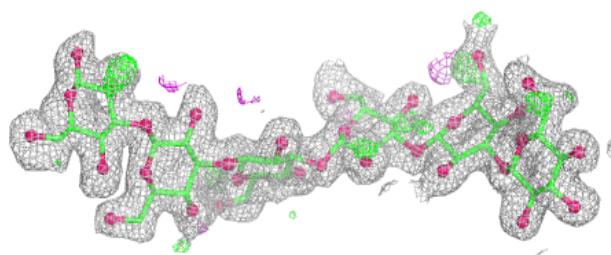
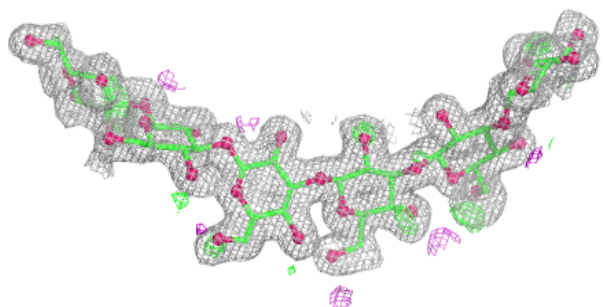
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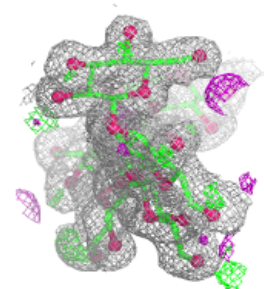
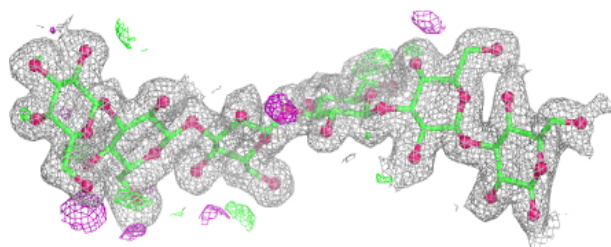
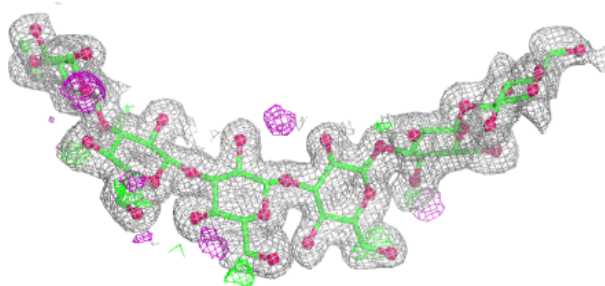


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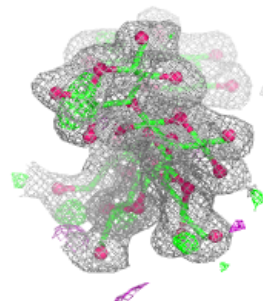
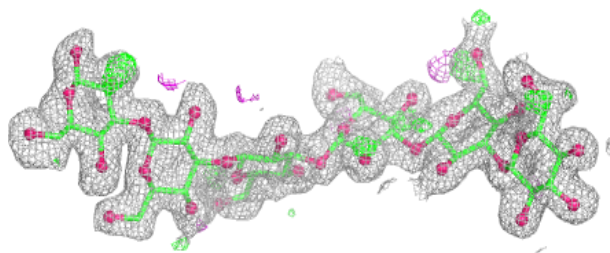
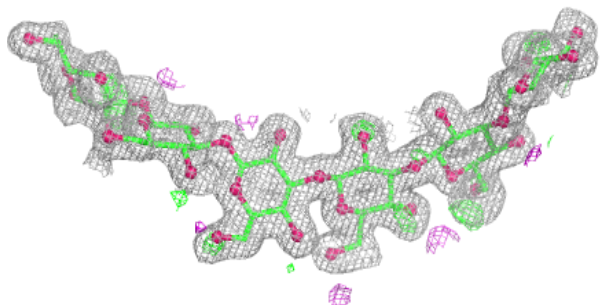
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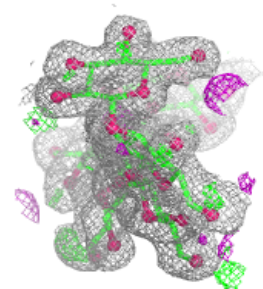
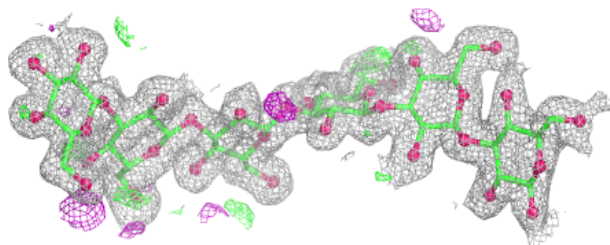
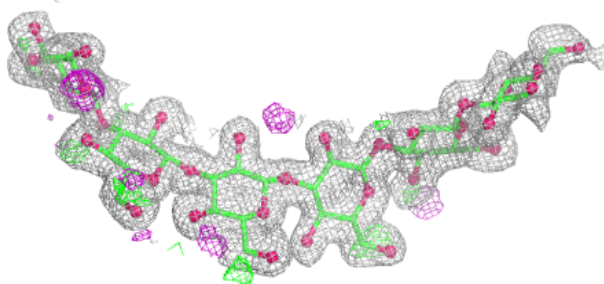


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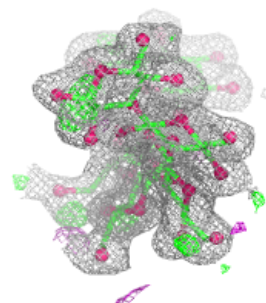
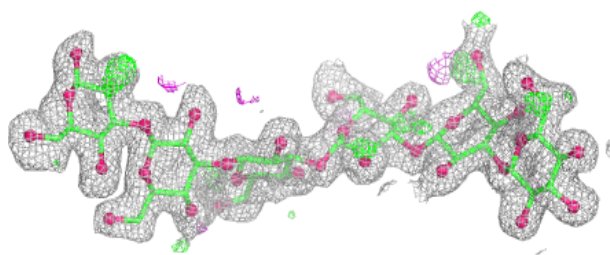
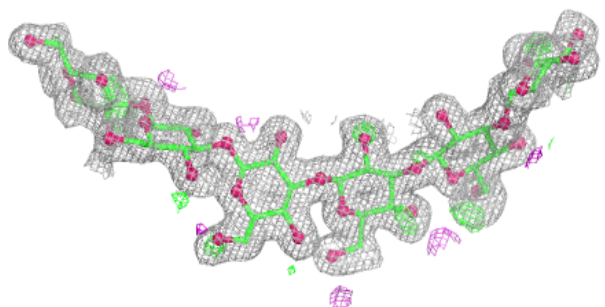
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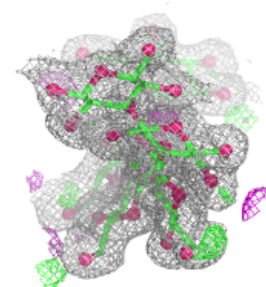
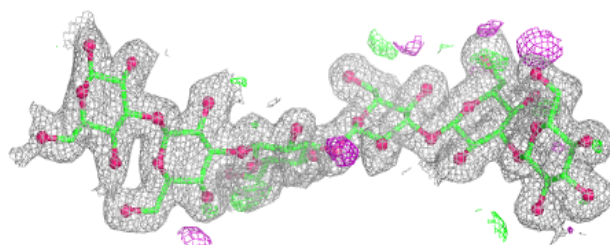
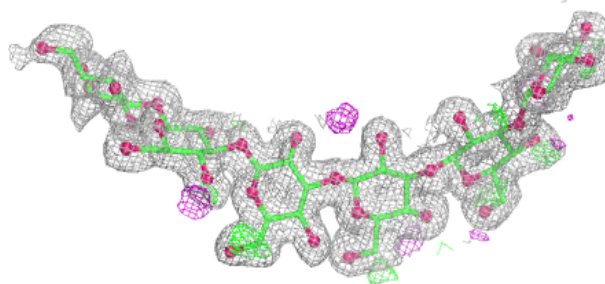


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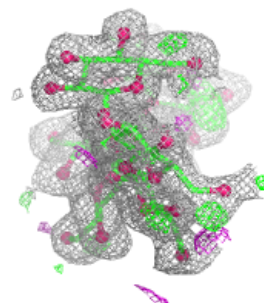
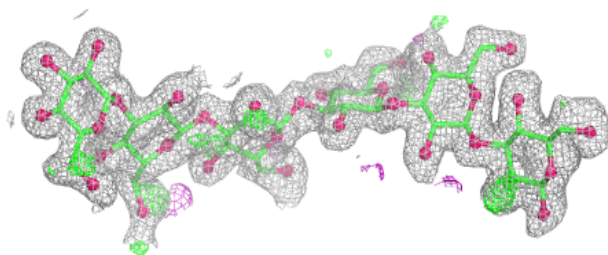
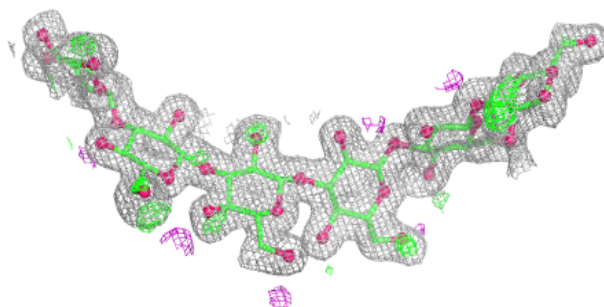
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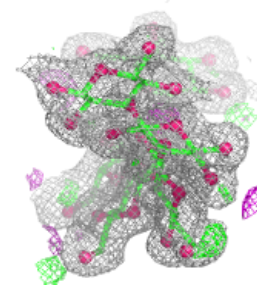
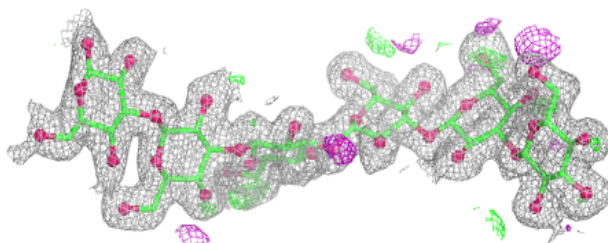
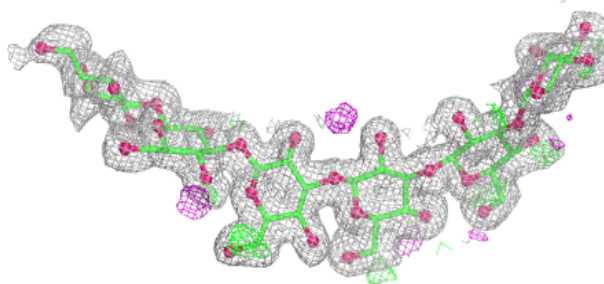


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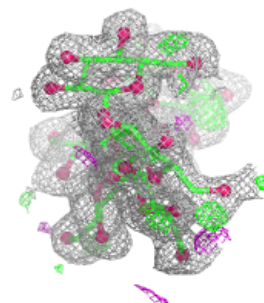
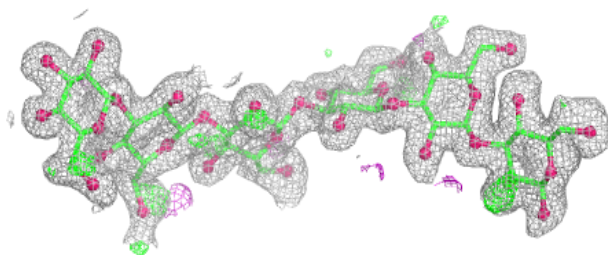
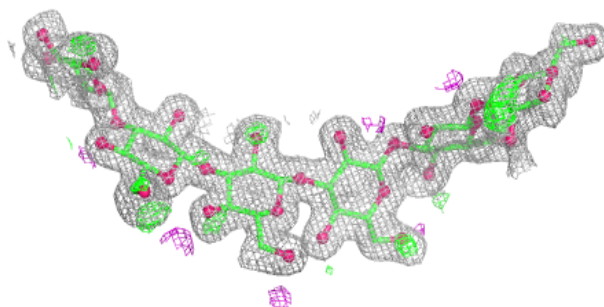
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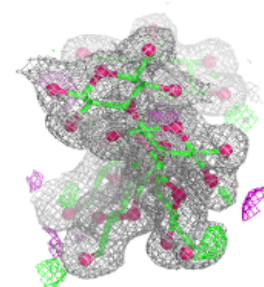
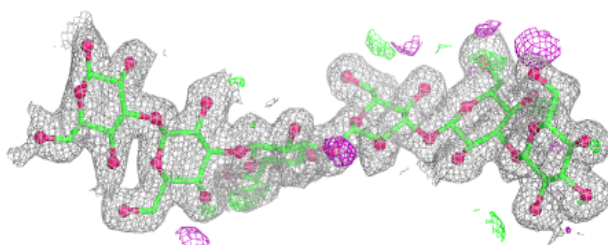
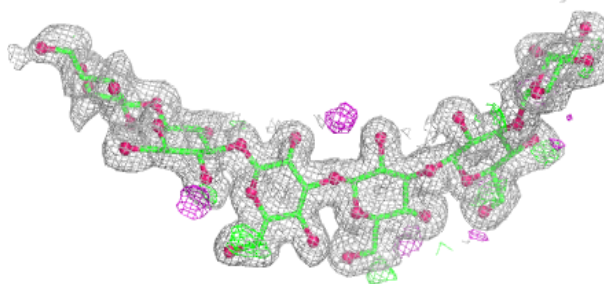


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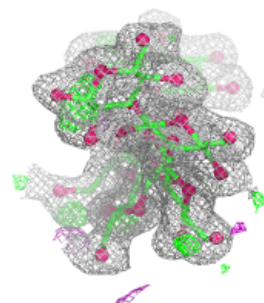
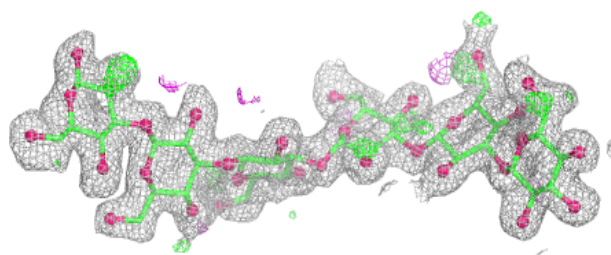
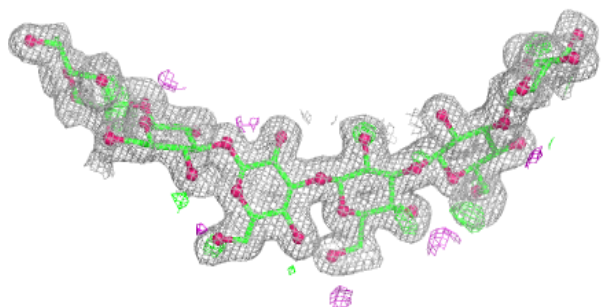
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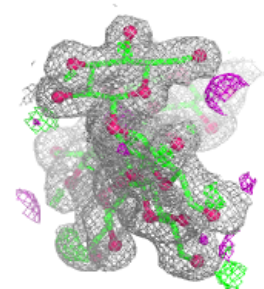
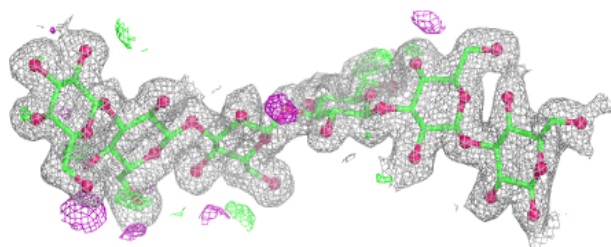
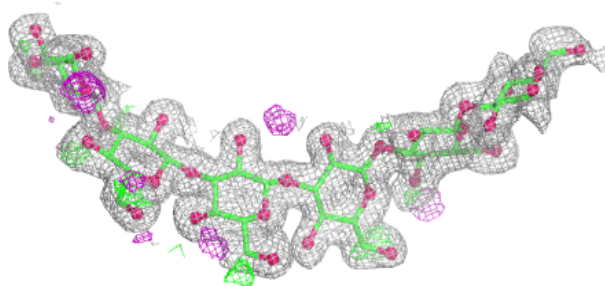


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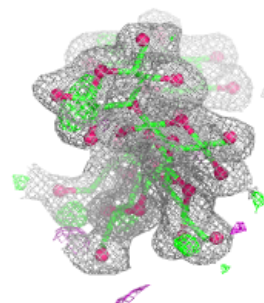
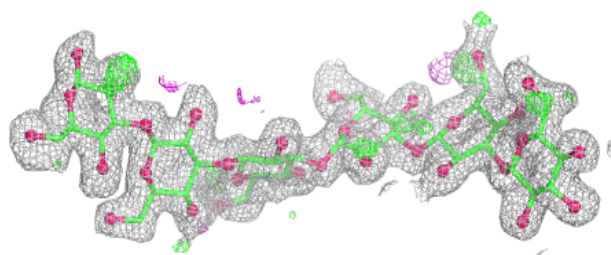
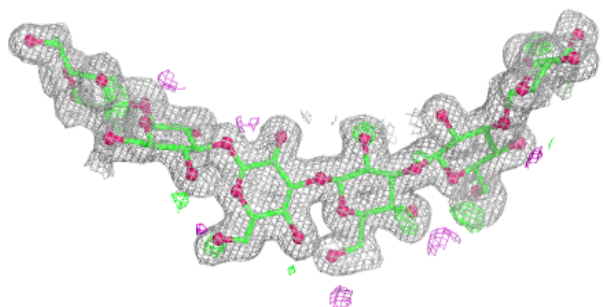
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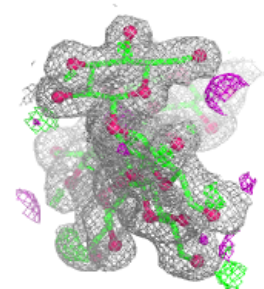
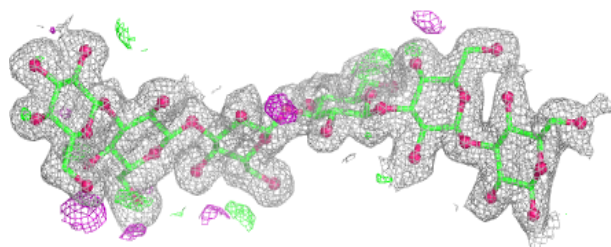
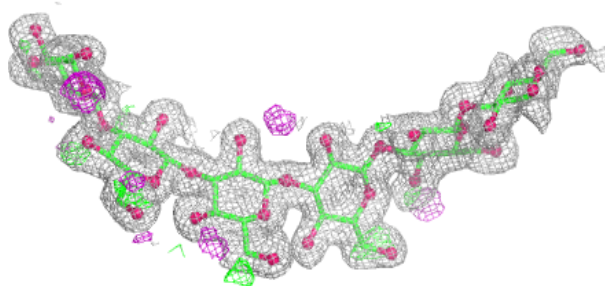


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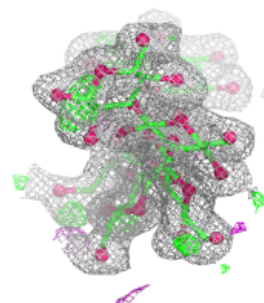
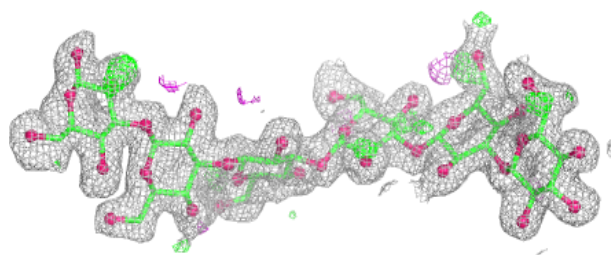
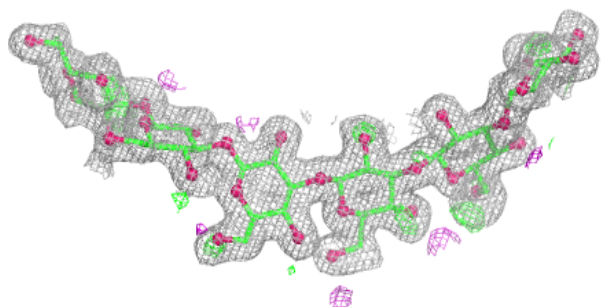
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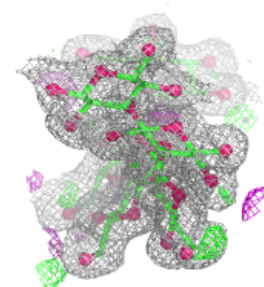
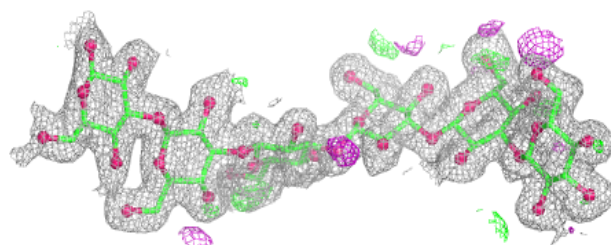
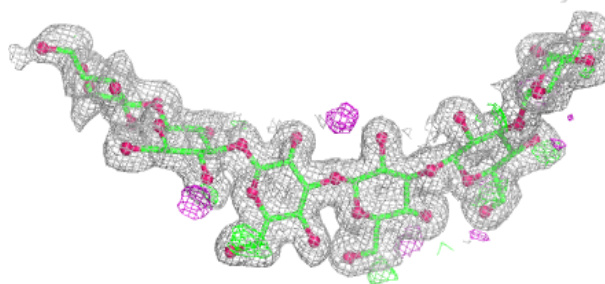


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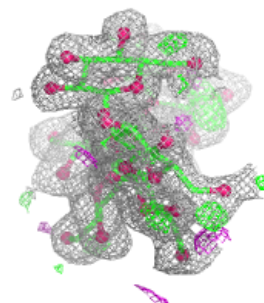
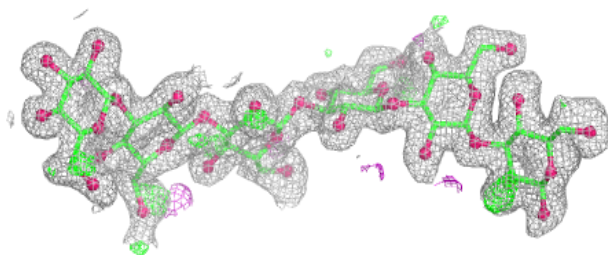
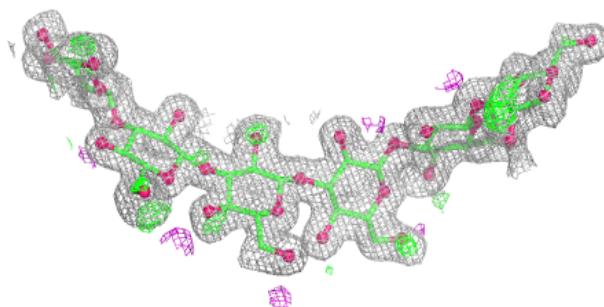
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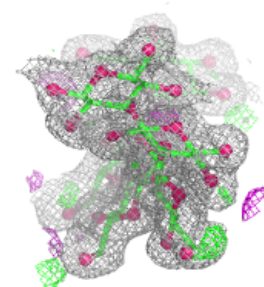
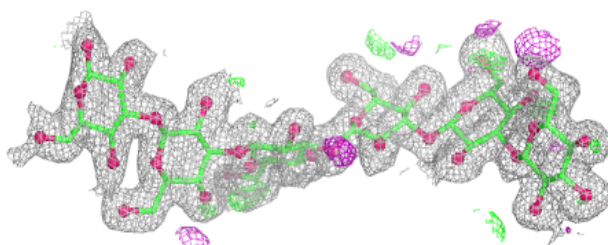
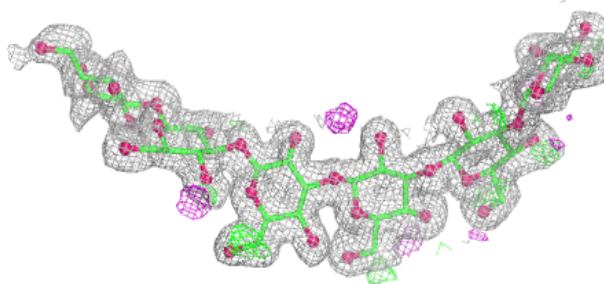


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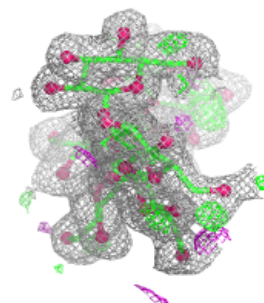
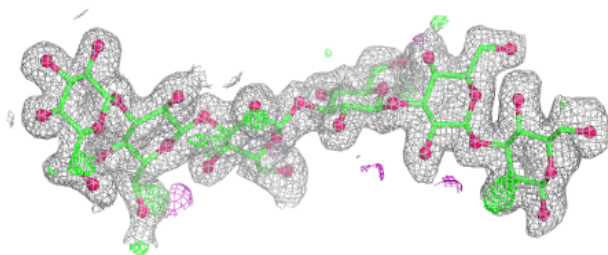
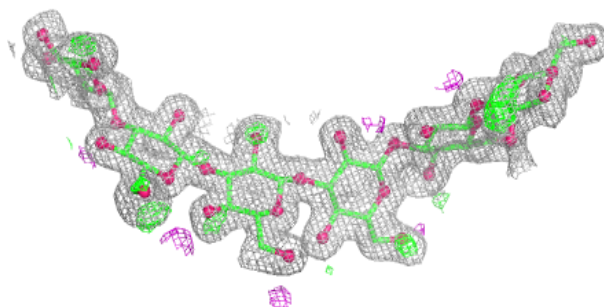
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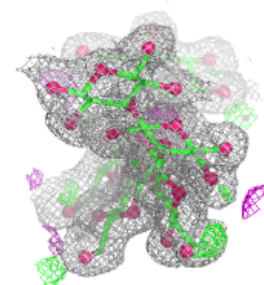
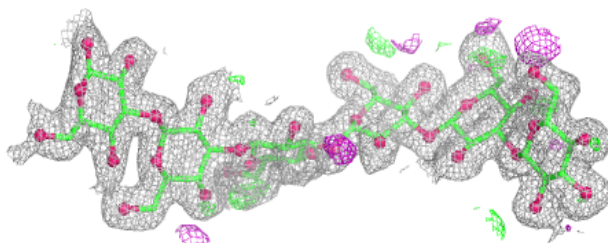
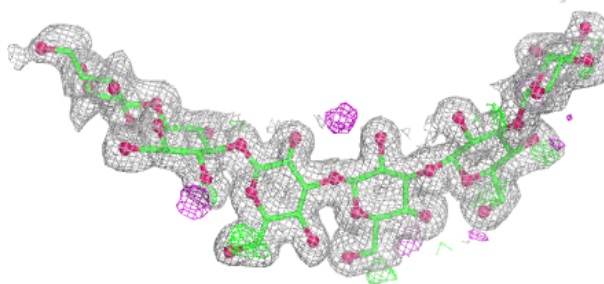


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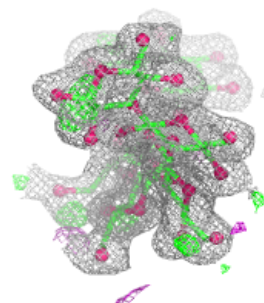
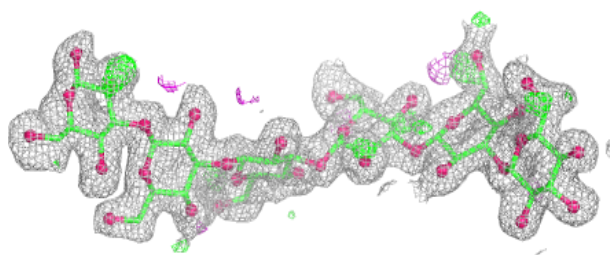
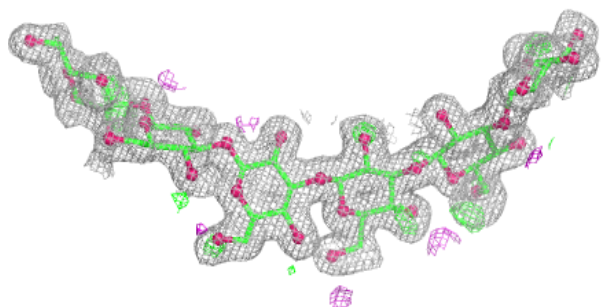
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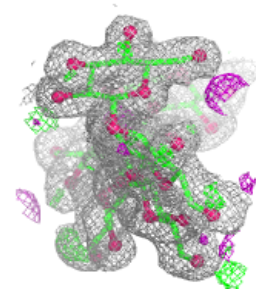
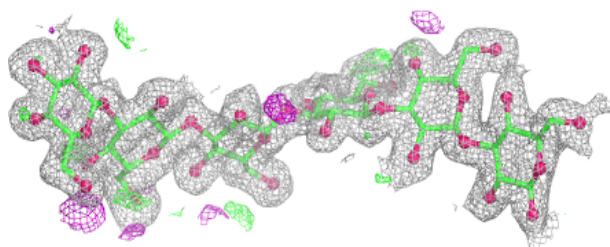
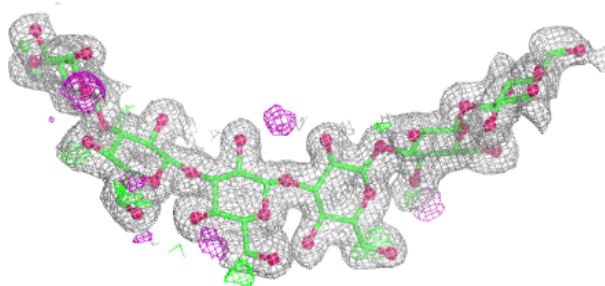


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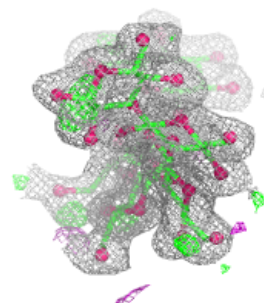
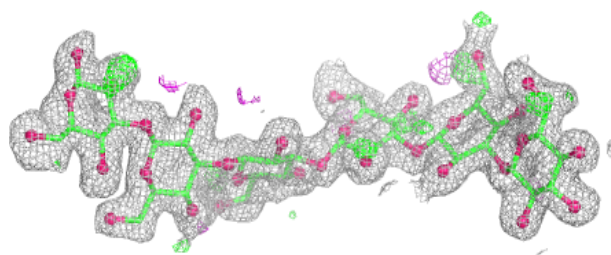
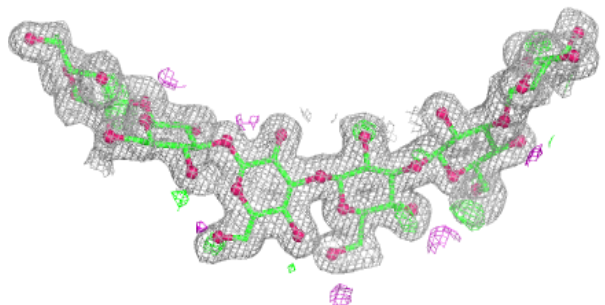
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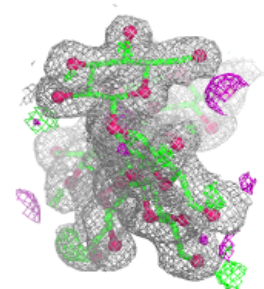
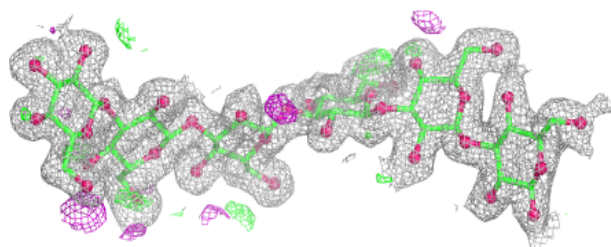
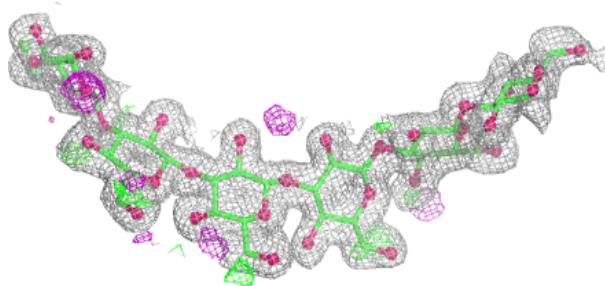


Electron density around Chain C:

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

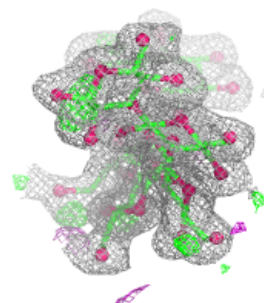
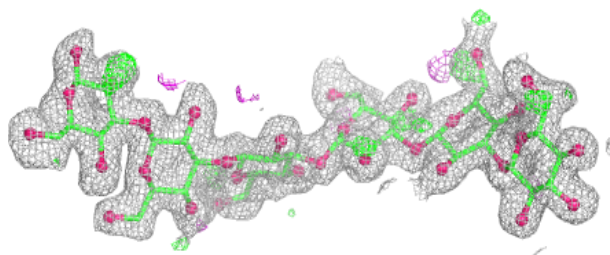
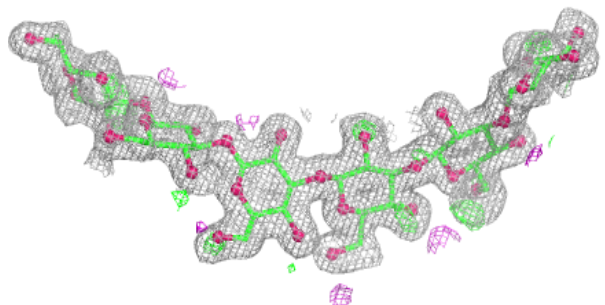
**Electron density around Chain E:**

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

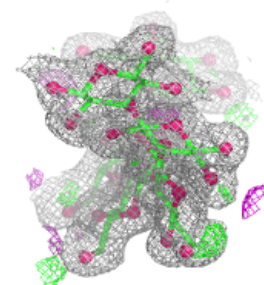
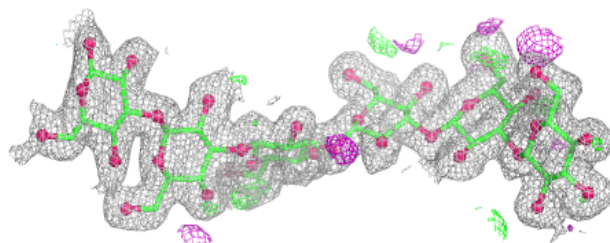
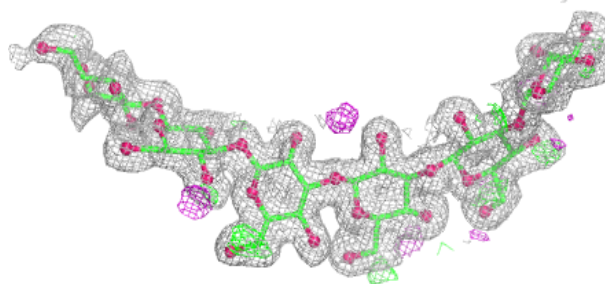


Electron density around Chain C:

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

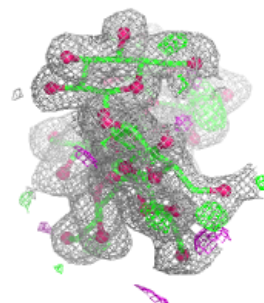
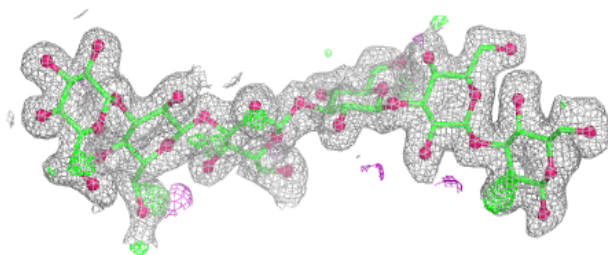
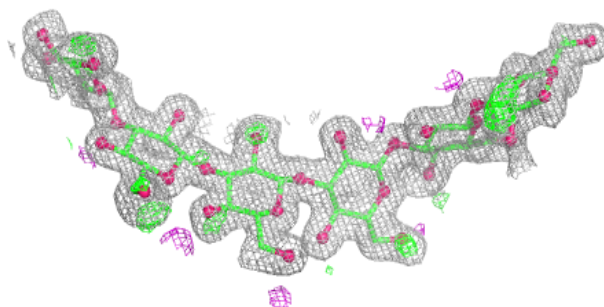
**Electron density around Chain E:**

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

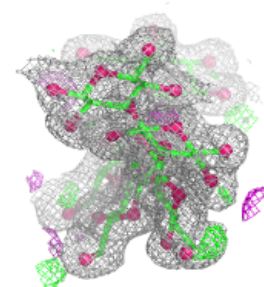
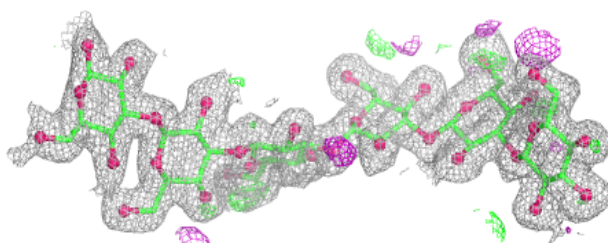
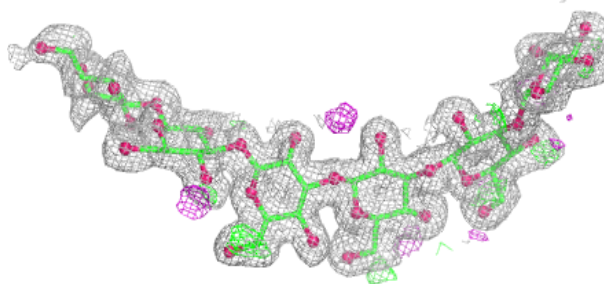


Electron density around Chain C:

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

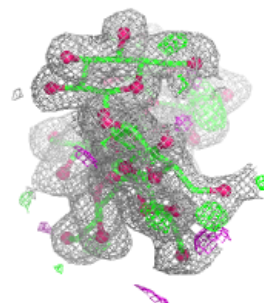
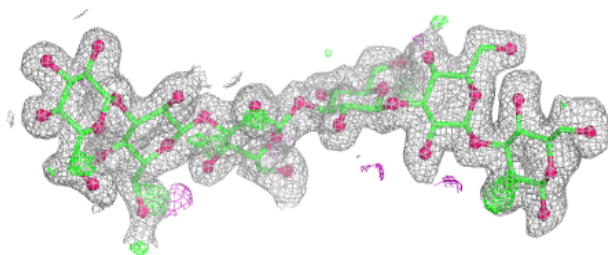
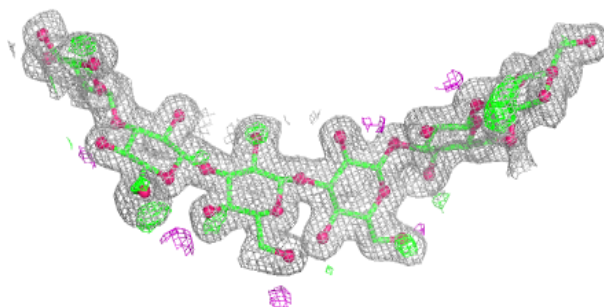
**Electron density around Chain E:**

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

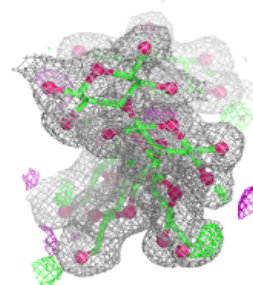
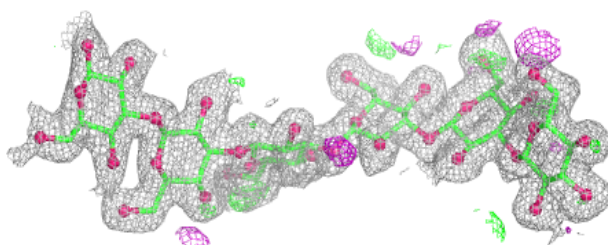
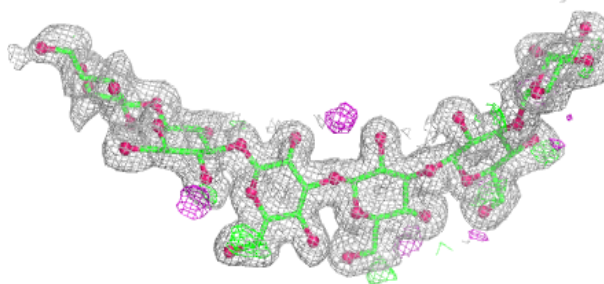


Electron density around Chain C:

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

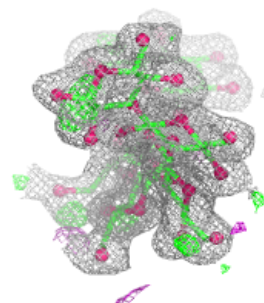
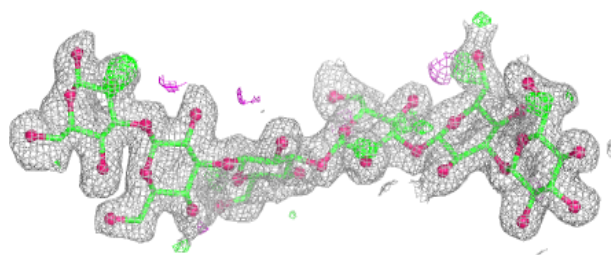
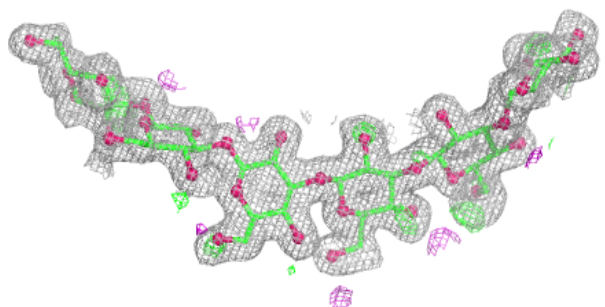
**Electron density around Chain E:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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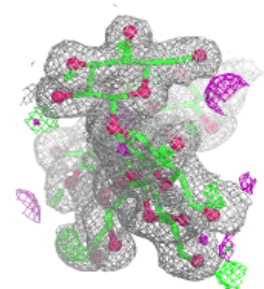
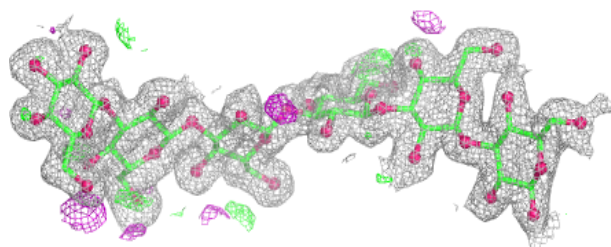
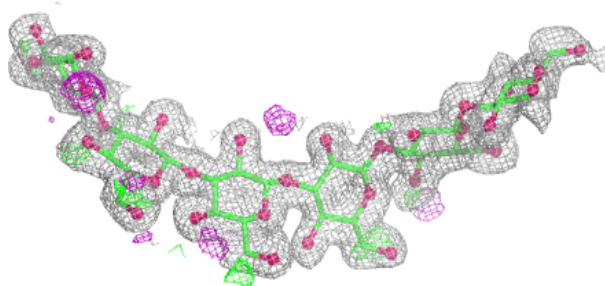


Electron density around Chain C:

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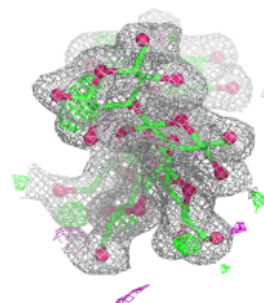
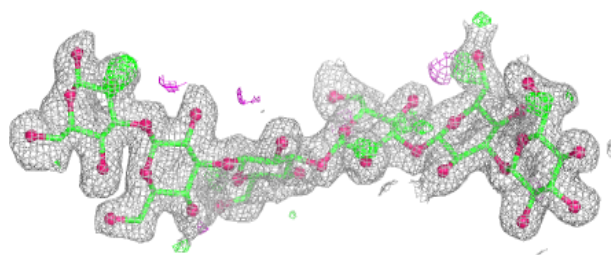
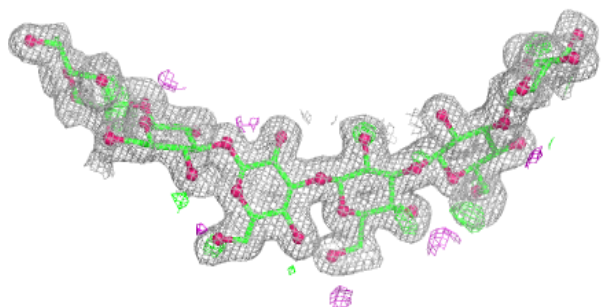
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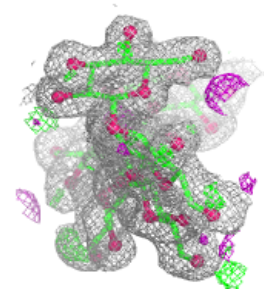
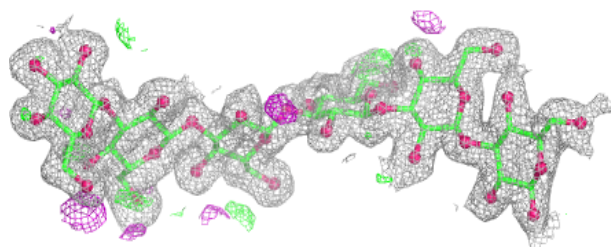
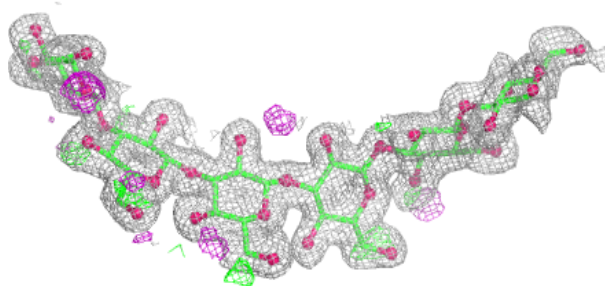


Electron density around Chain C:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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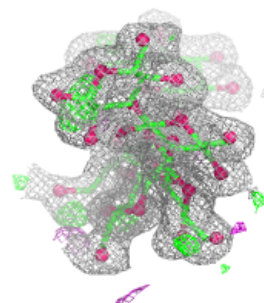
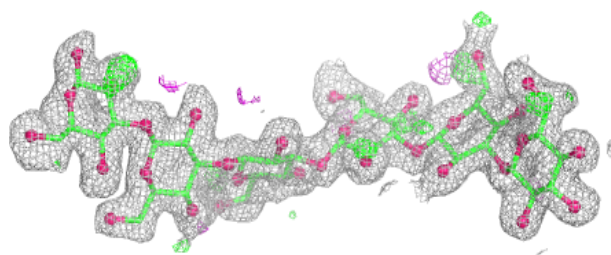
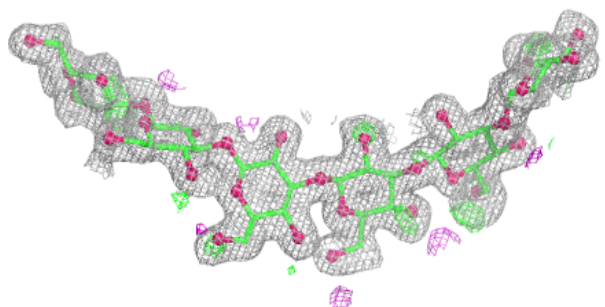
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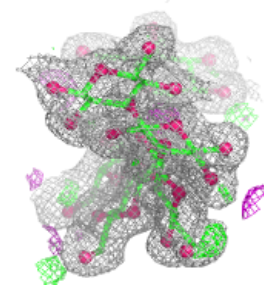
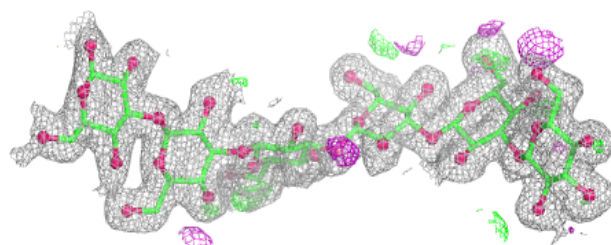
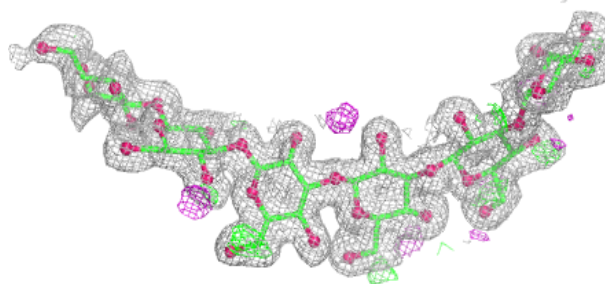


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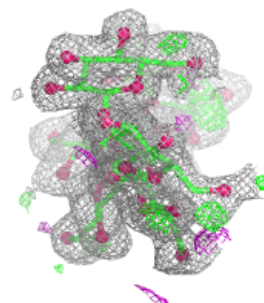
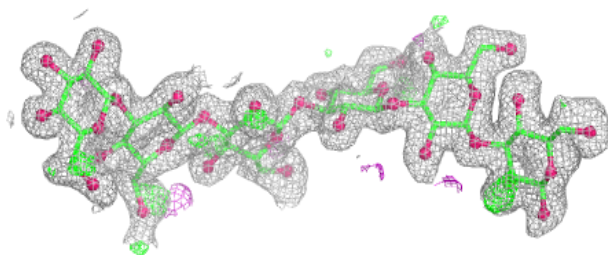
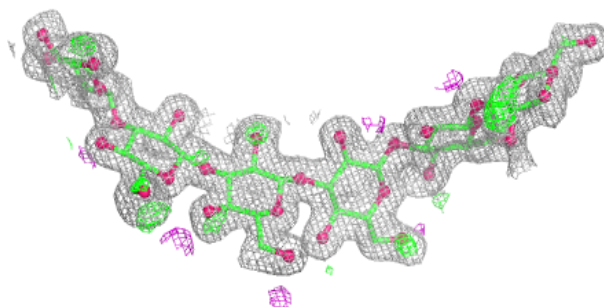
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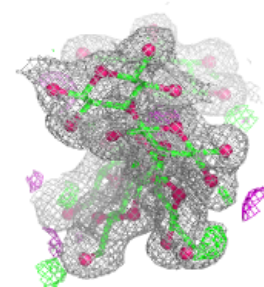
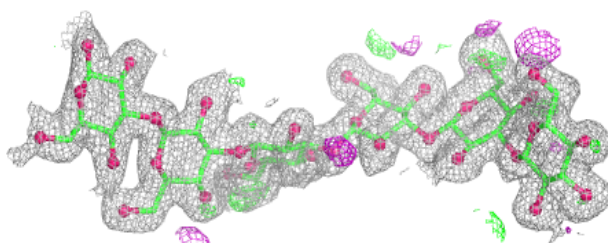
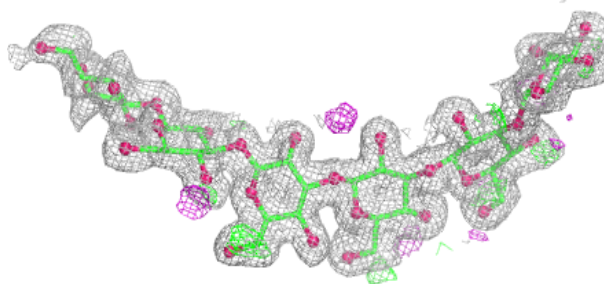


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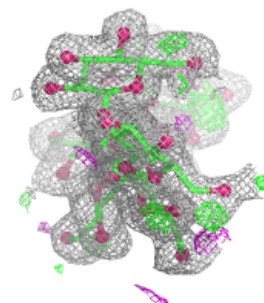
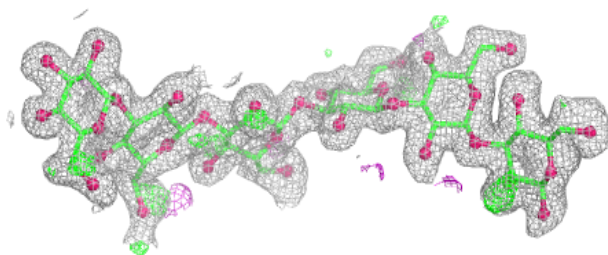
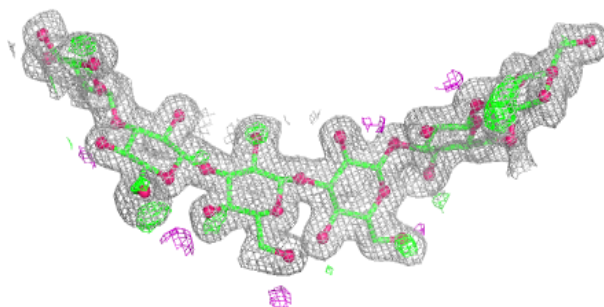
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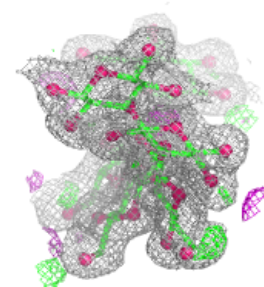
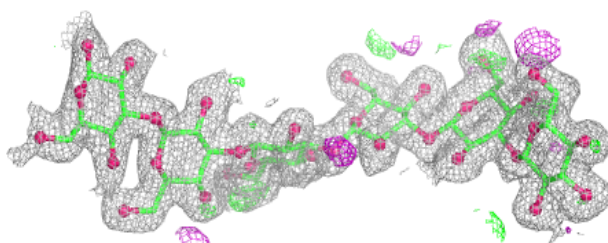
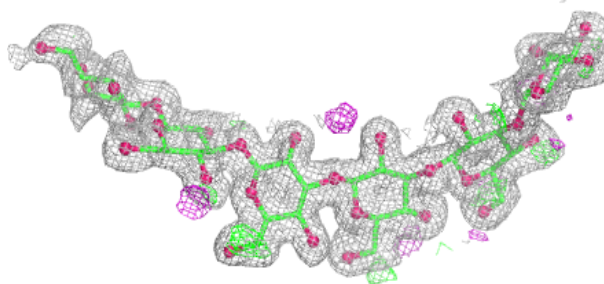


Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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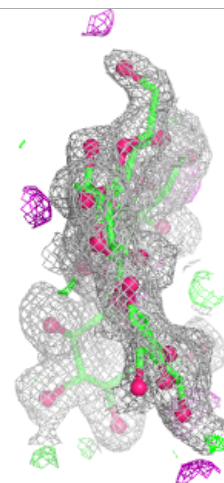
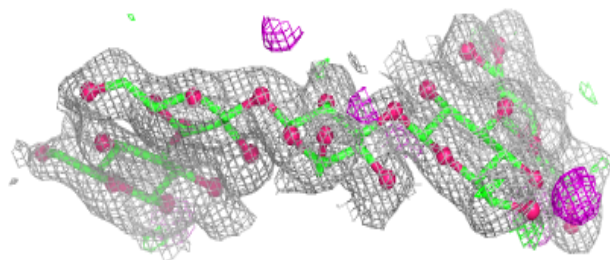
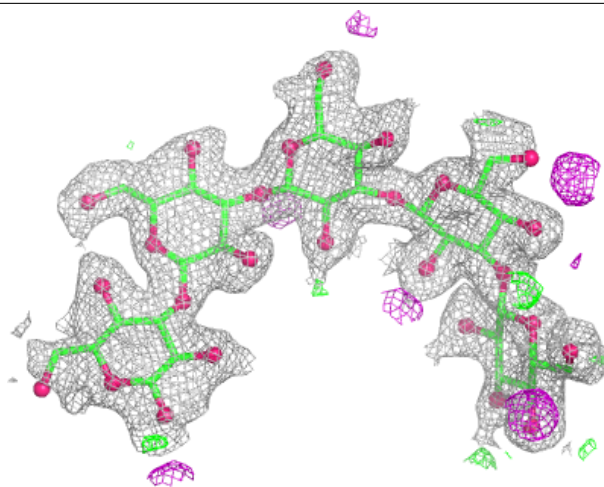
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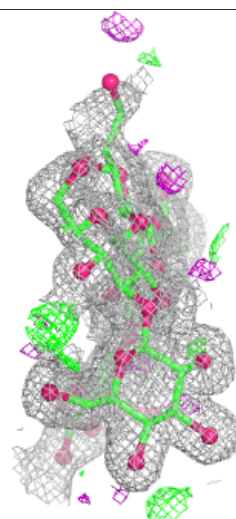
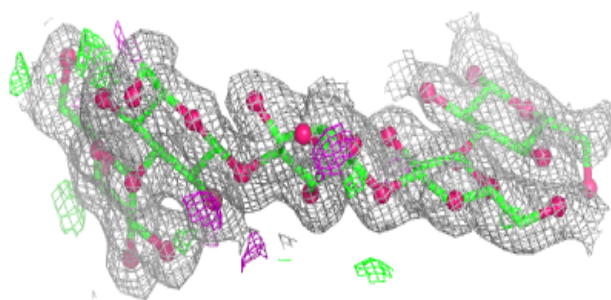
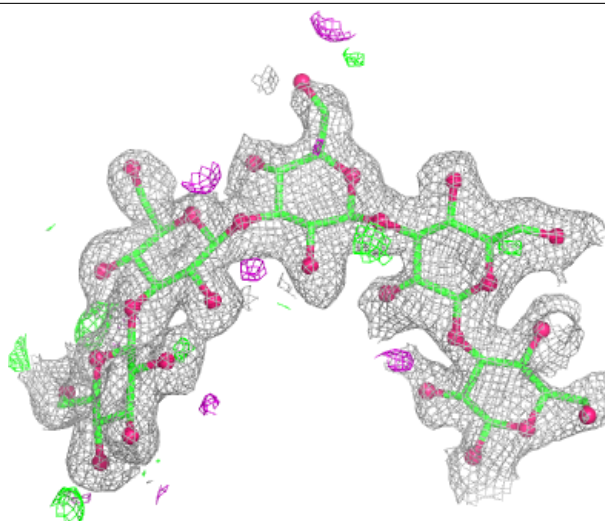
Electron density around Chain D:

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



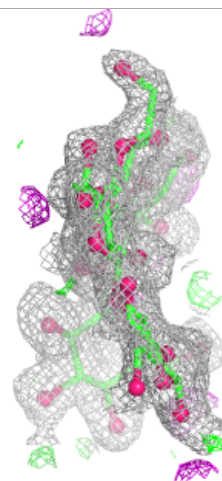
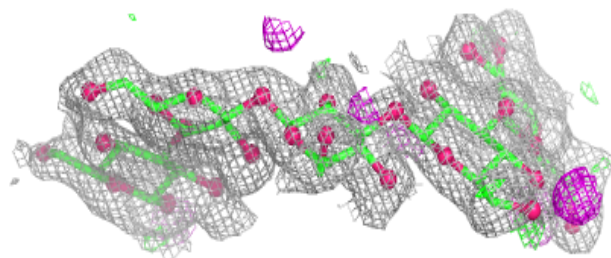
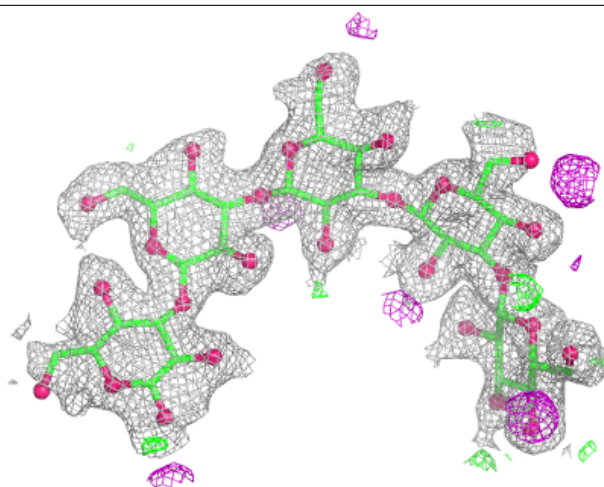
Electron density around Chain F:

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



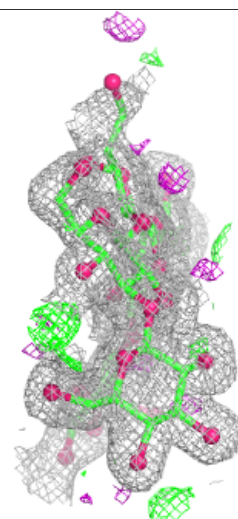
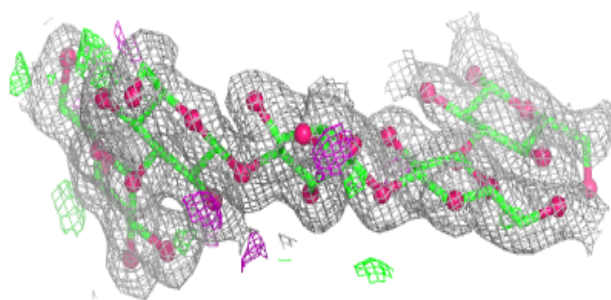
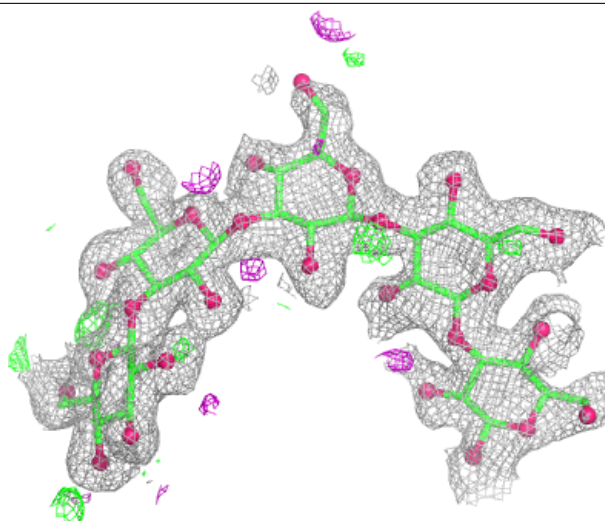
Electron density around Chain D:

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



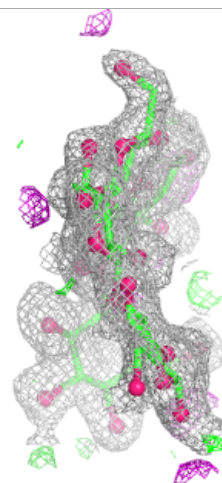
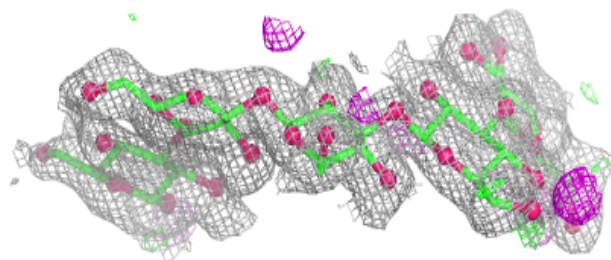
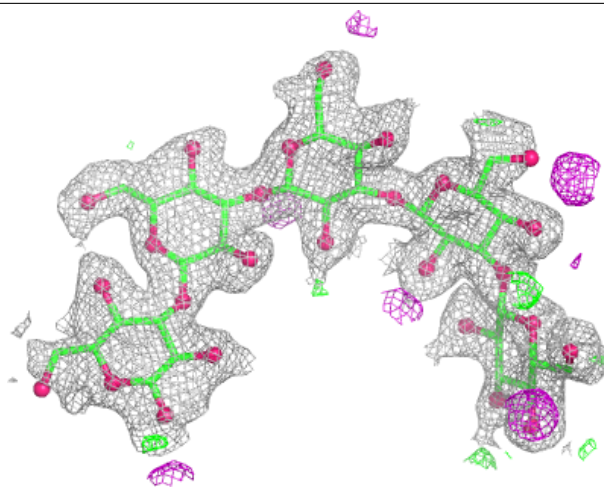
Electron density around Chain F:

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



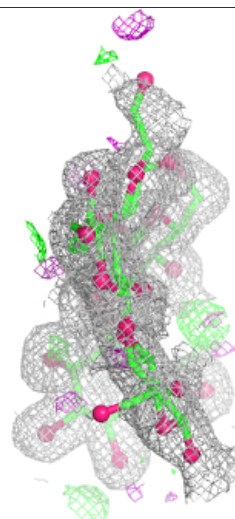
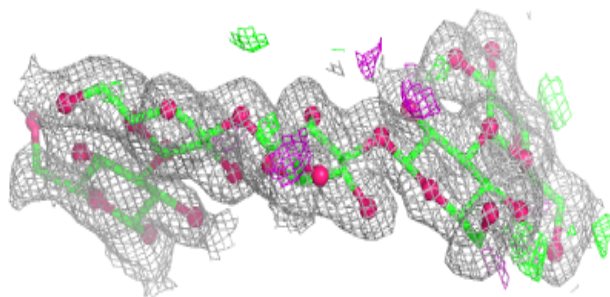
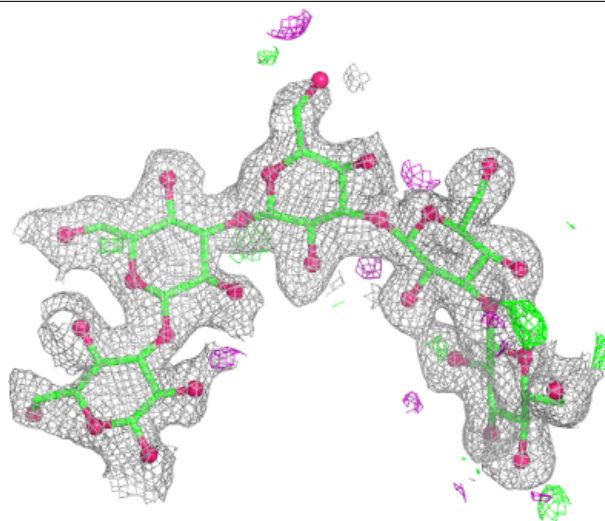
Electron density around Chain D:

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



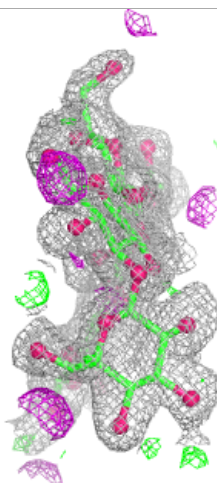
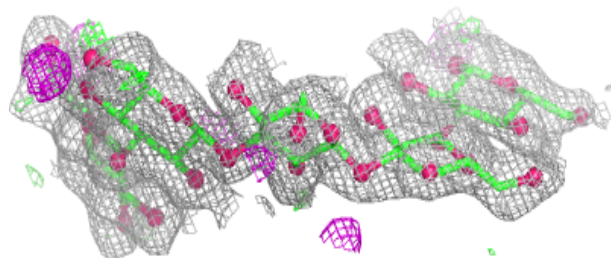
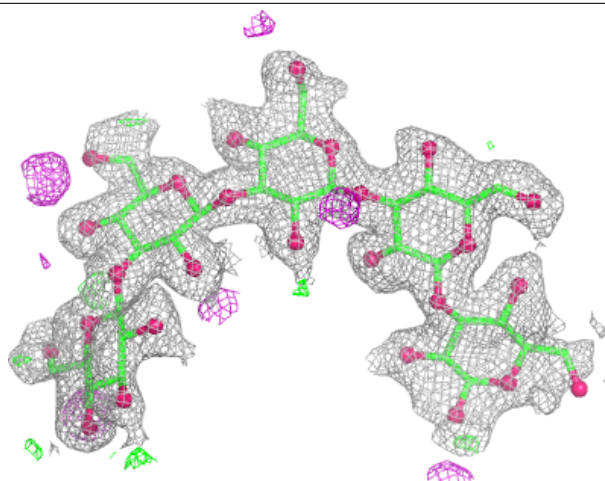
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



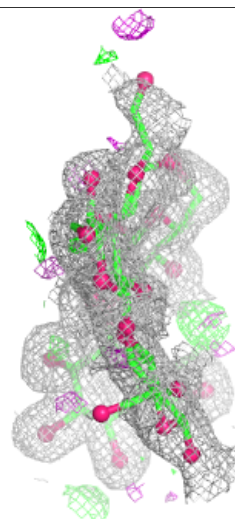
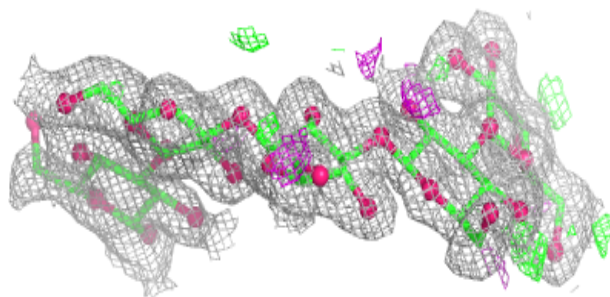
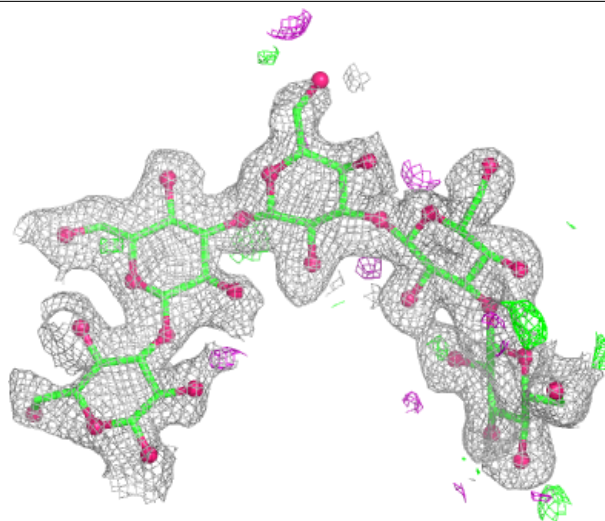
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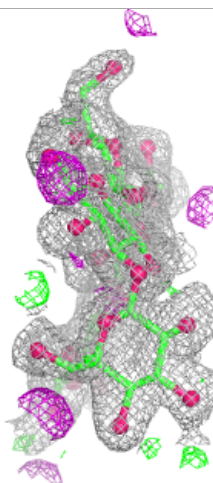
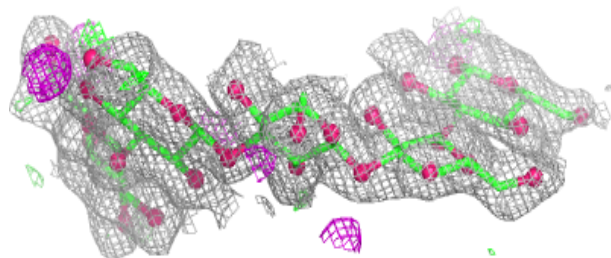
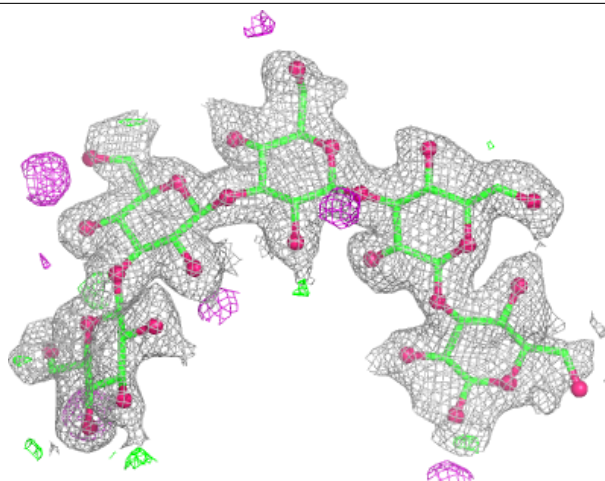
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and green (positive)



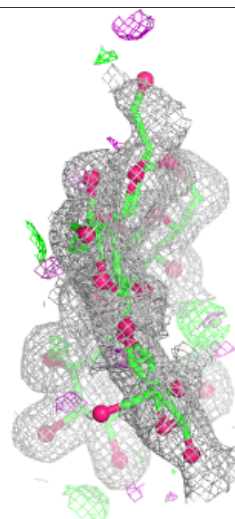
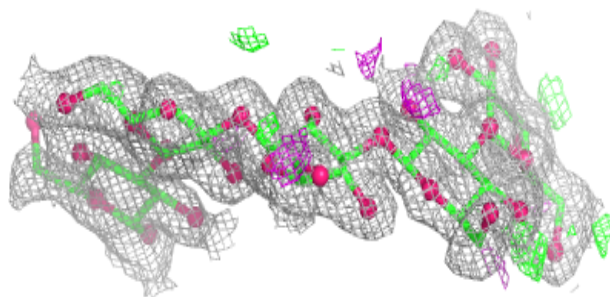
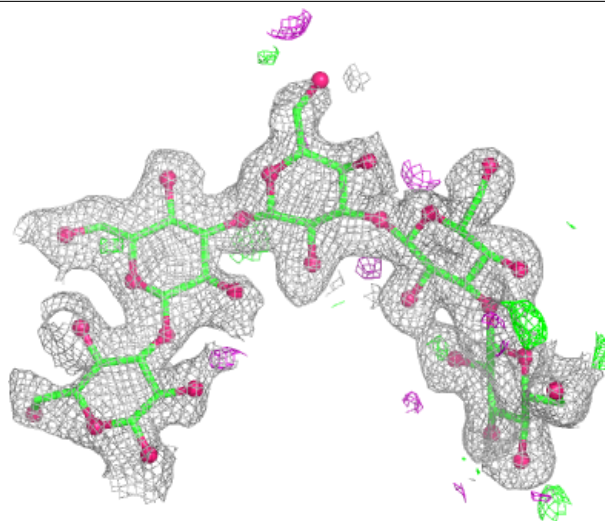
Electron density around Chain D:

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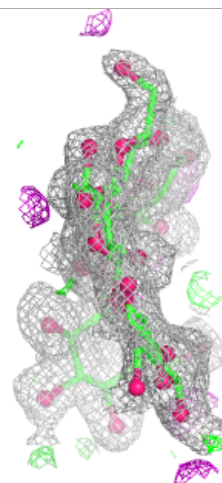
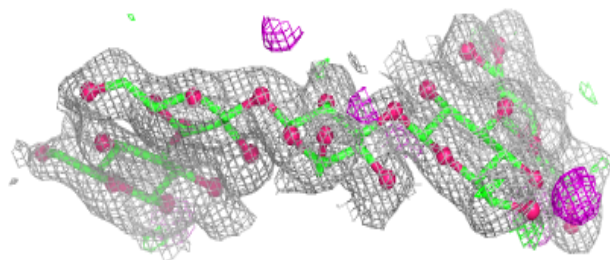
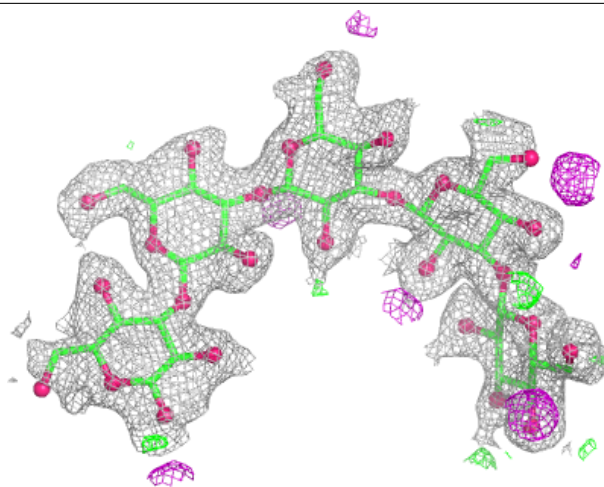
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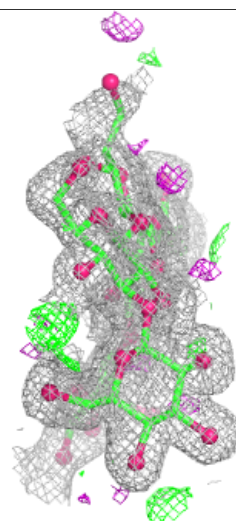
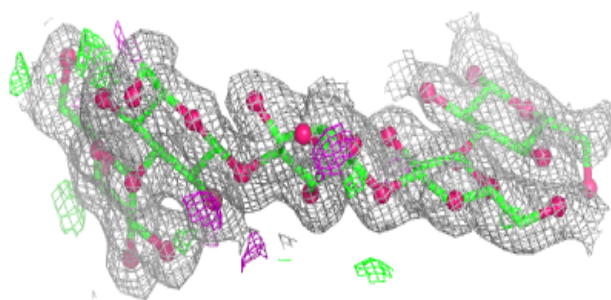
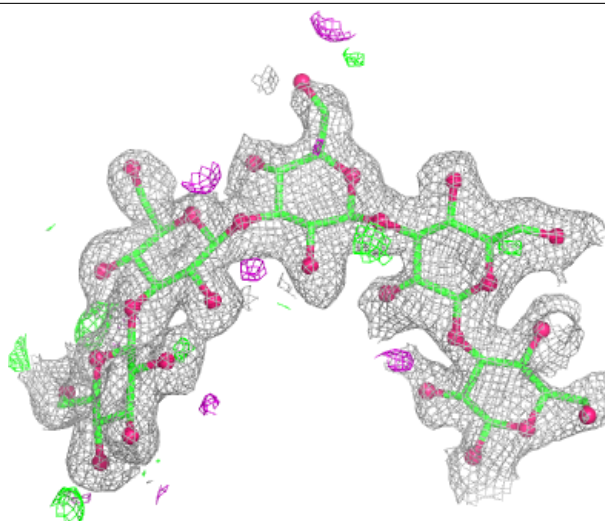
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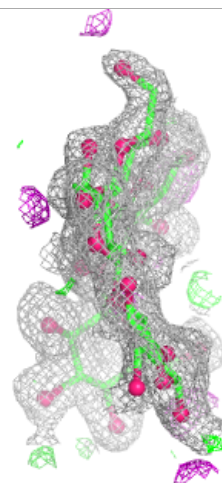
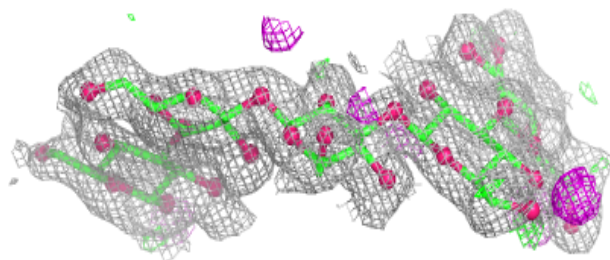
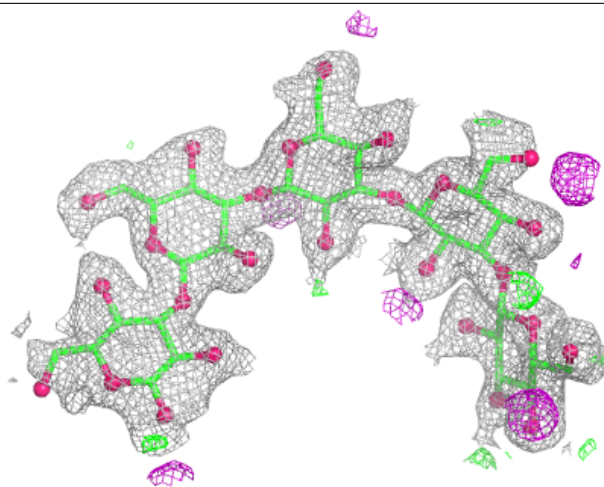
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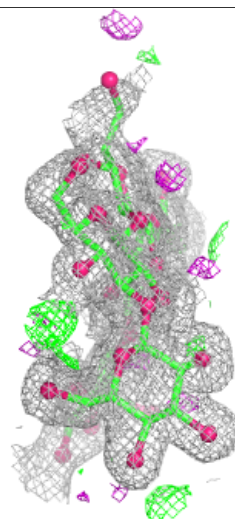
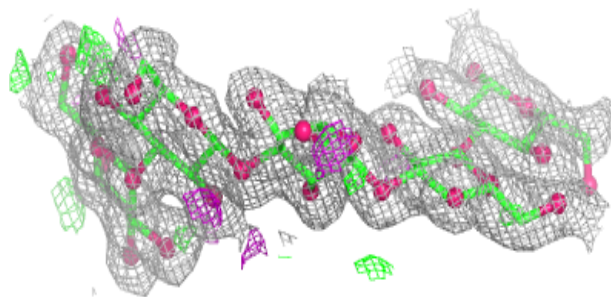
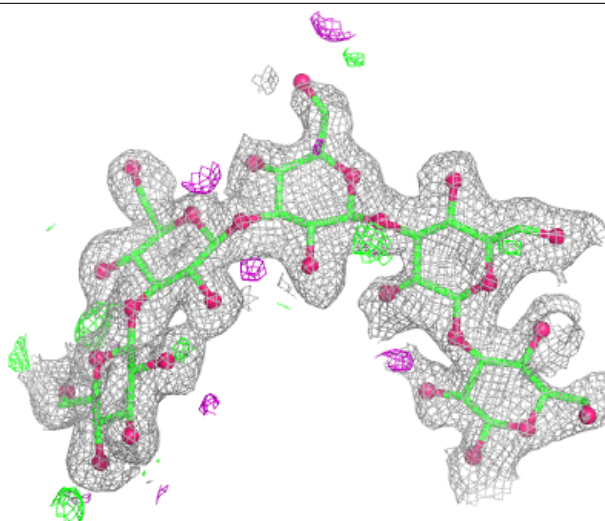
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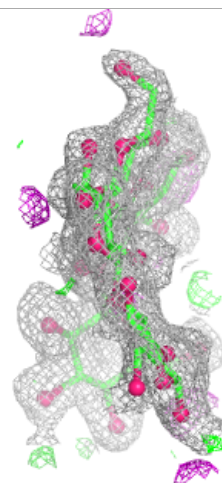
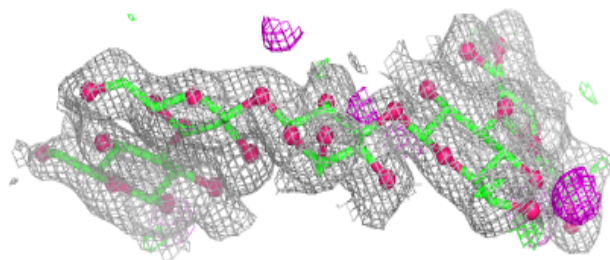
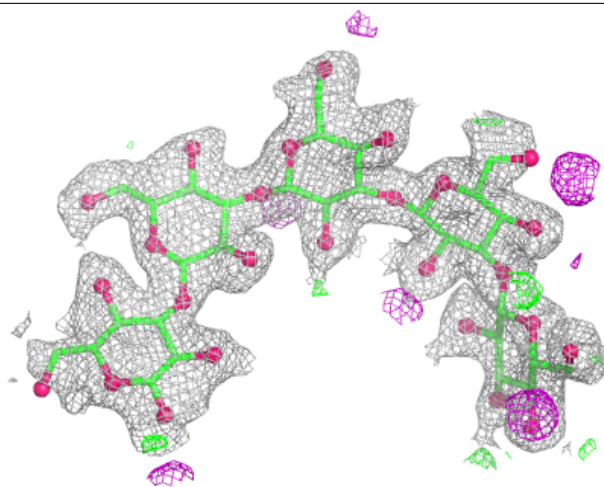
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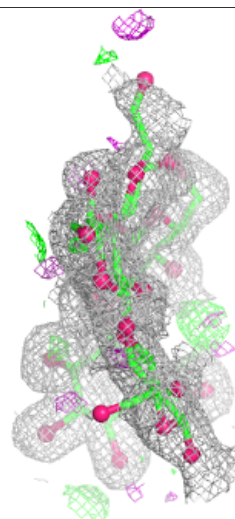
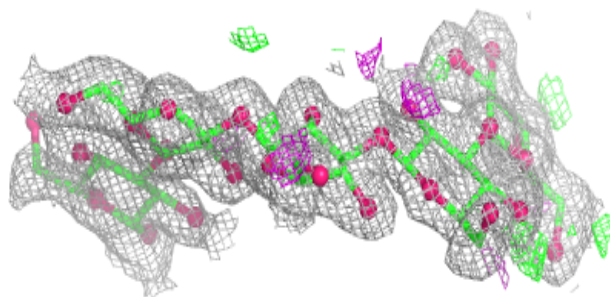
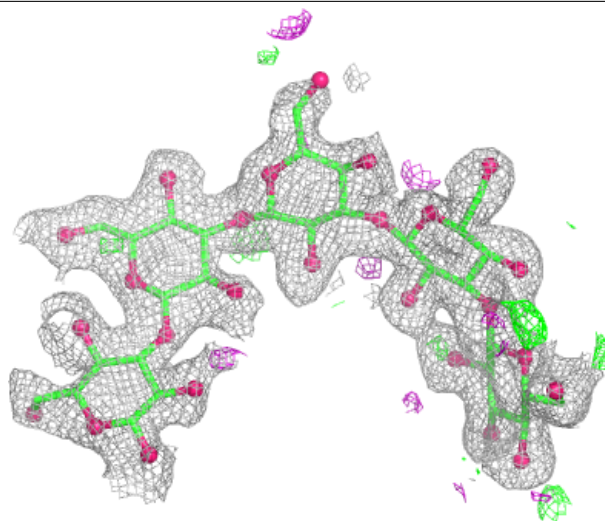
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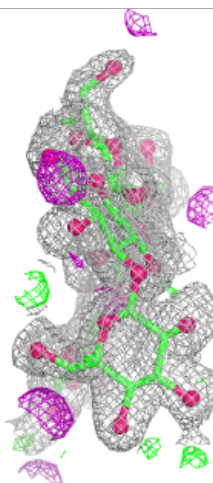
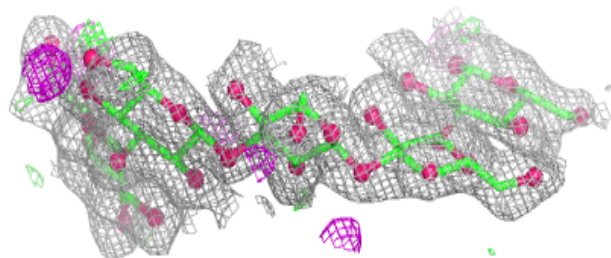
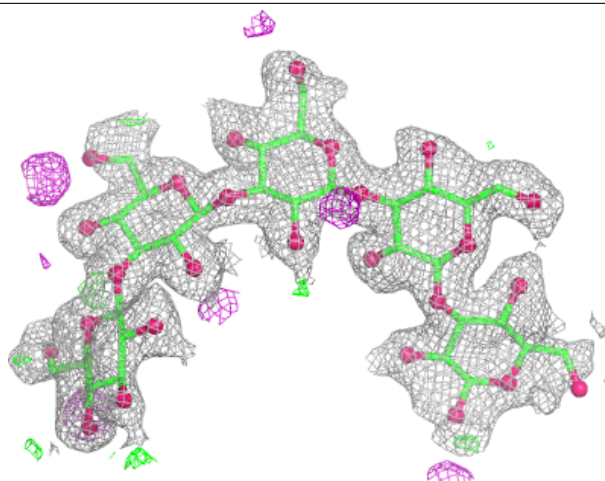
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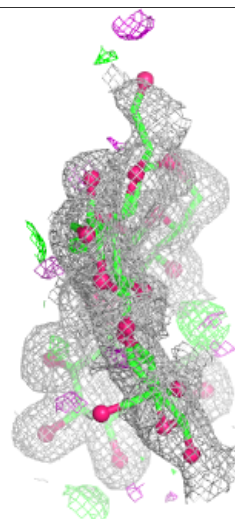
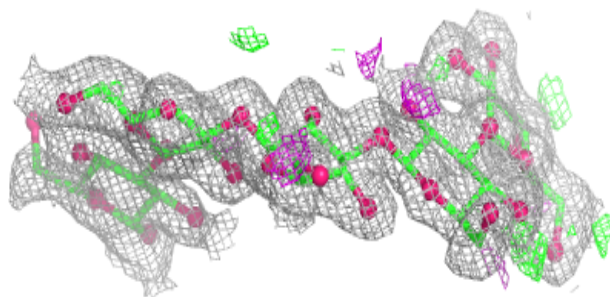
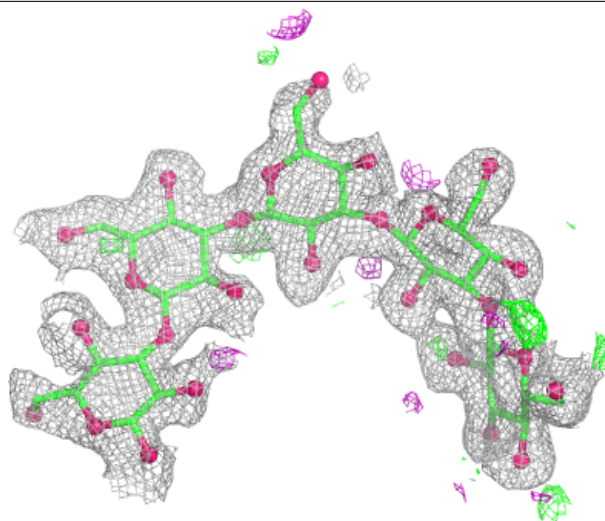
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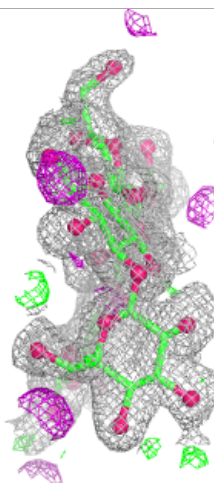
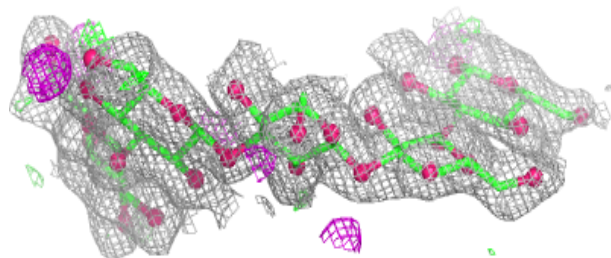
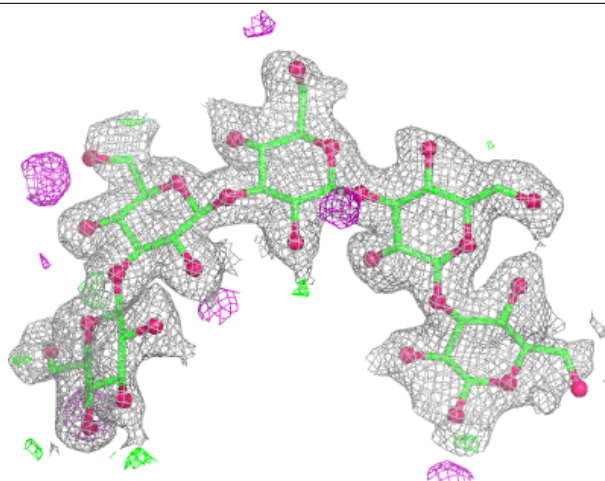
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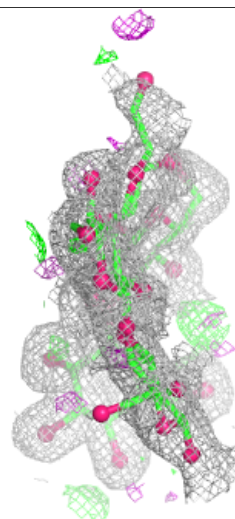
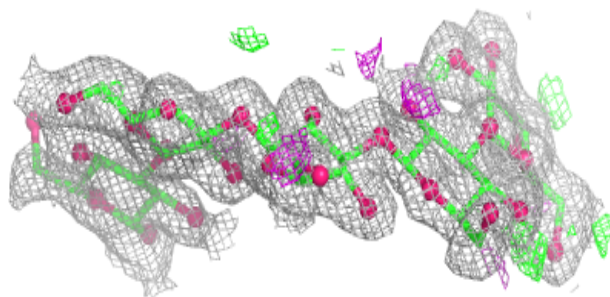
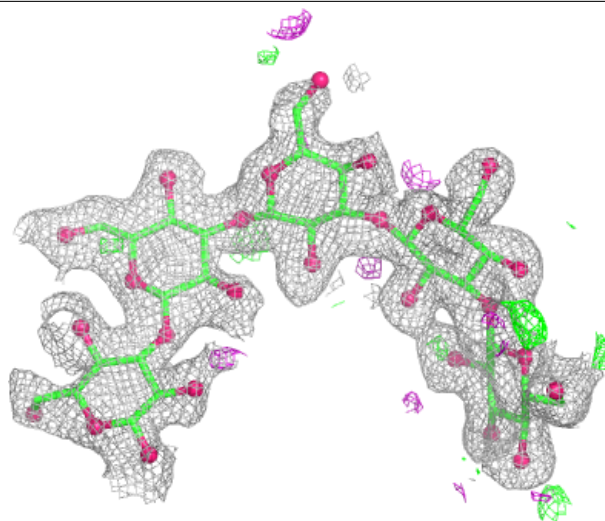
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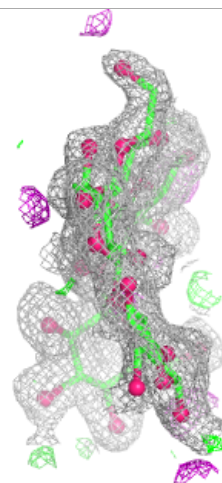
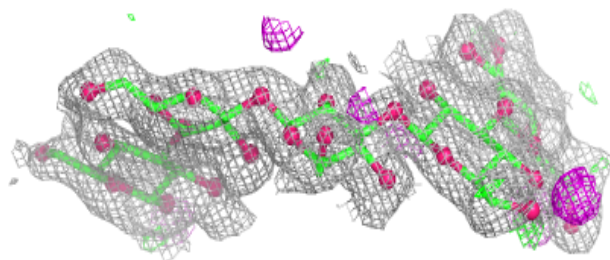
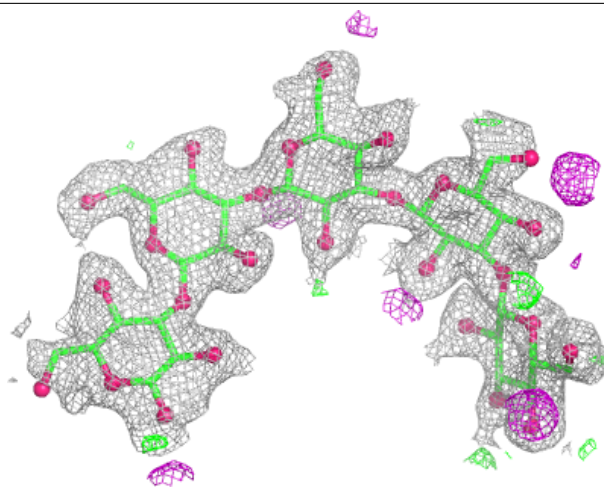
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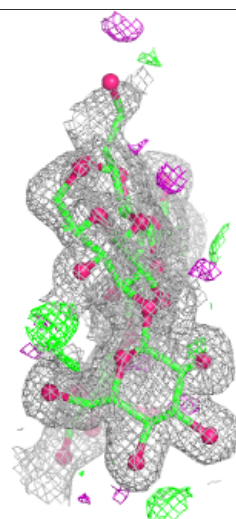
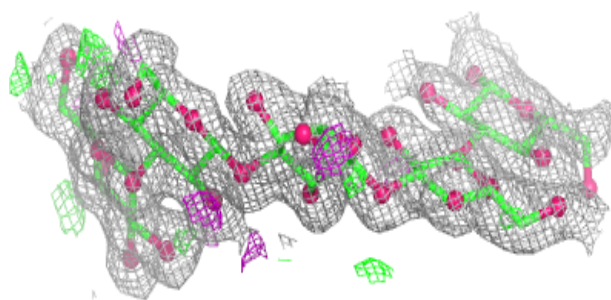
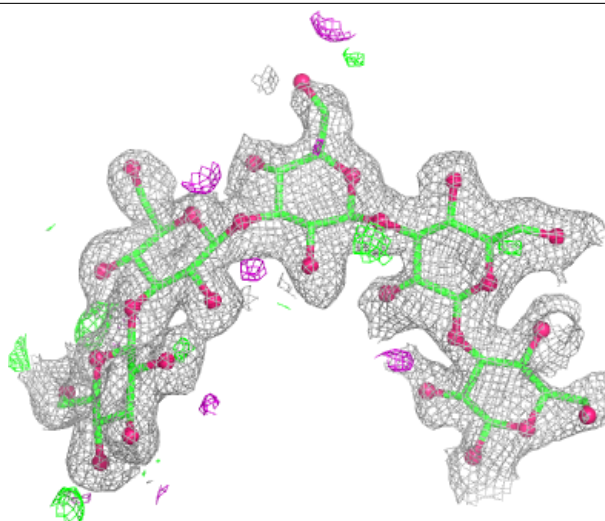
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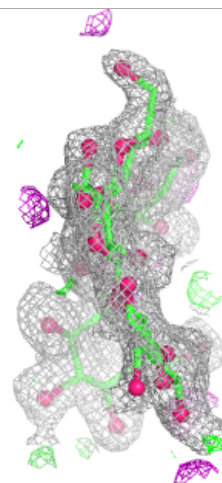
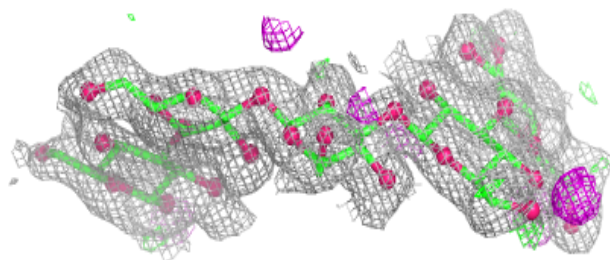
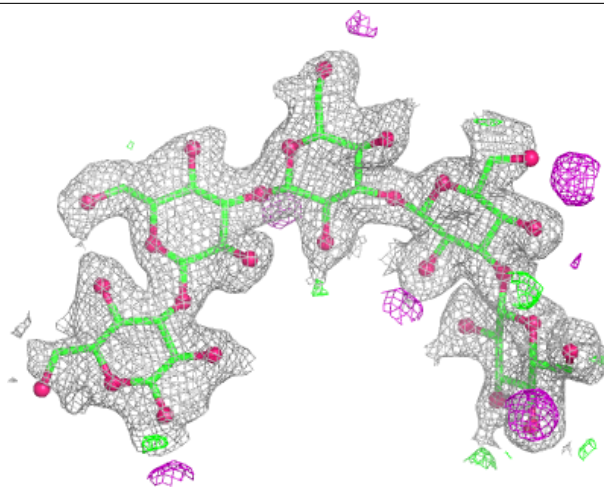
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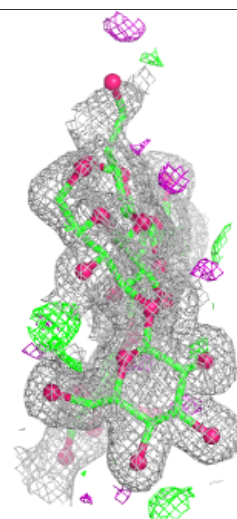
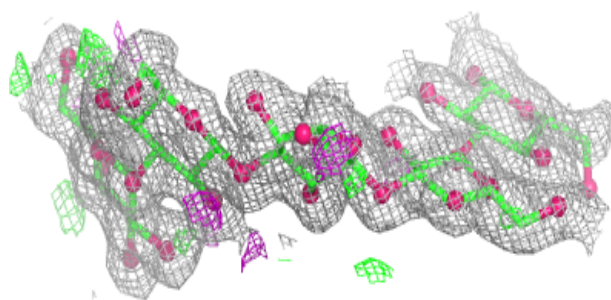
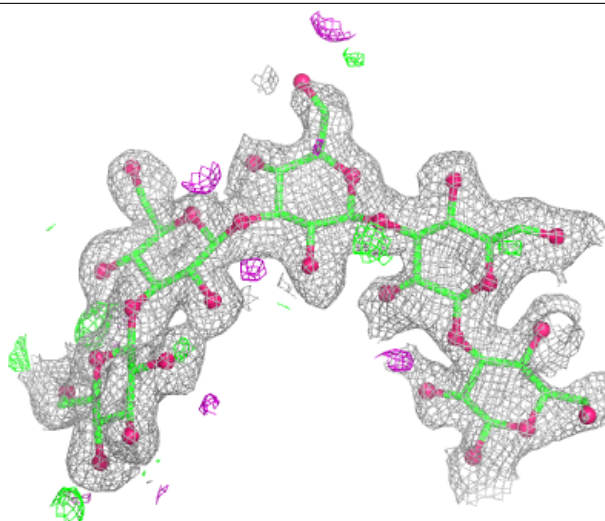
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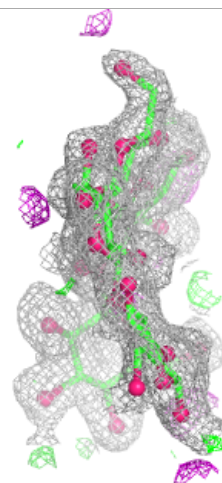
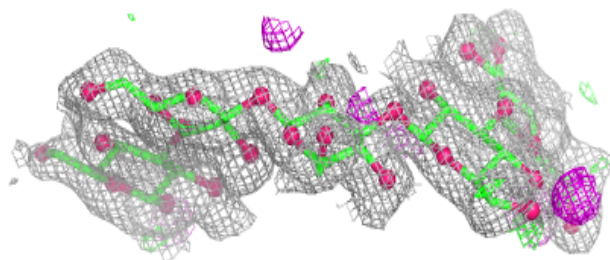
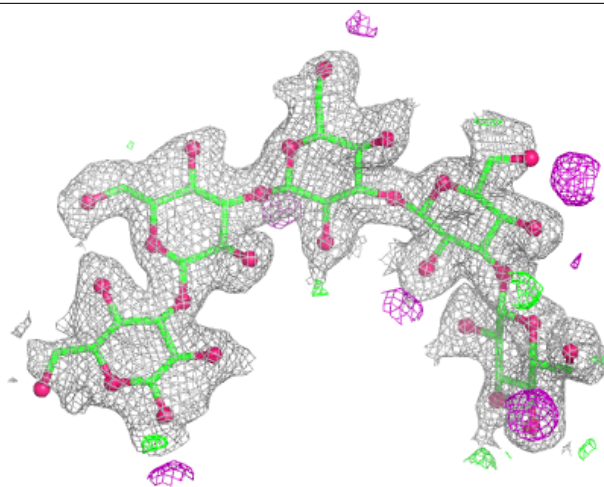
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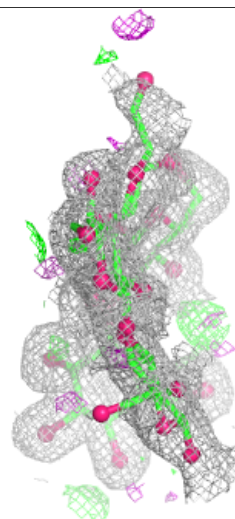
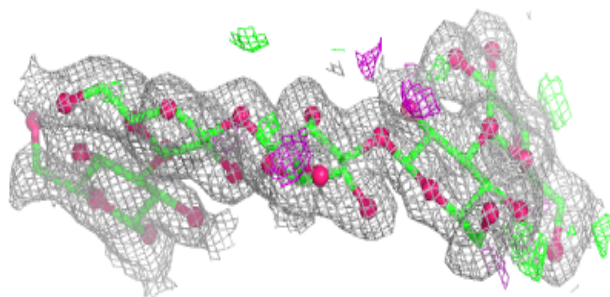
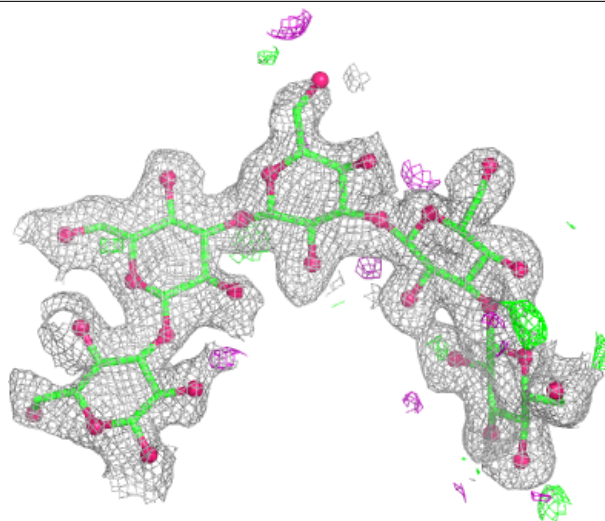
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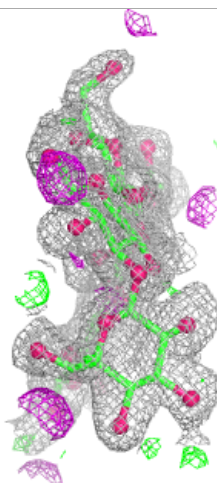
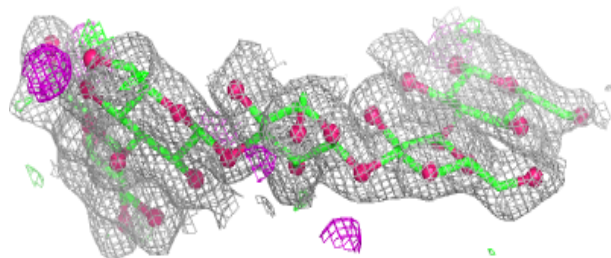
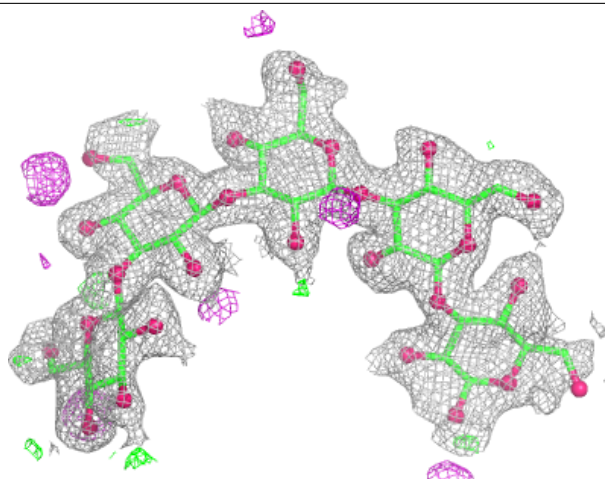
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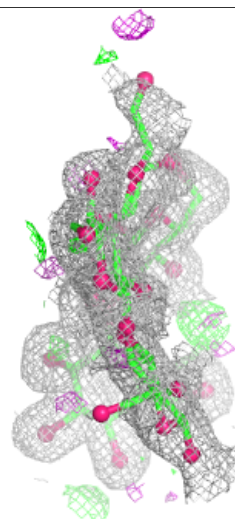
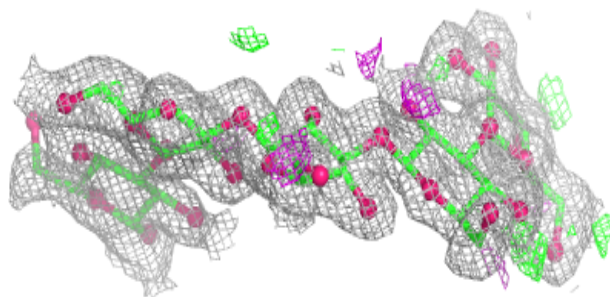
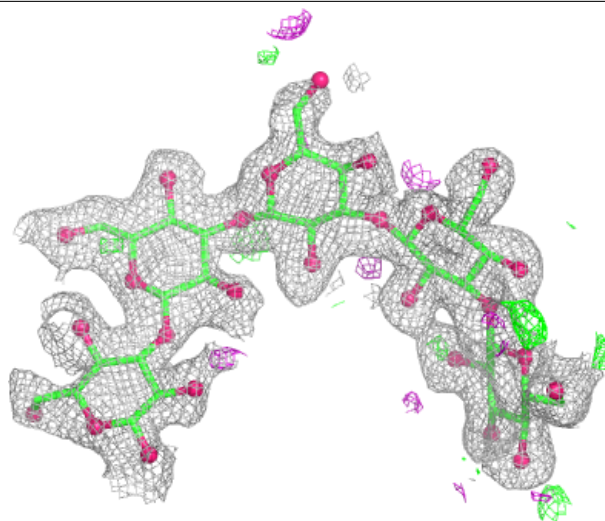
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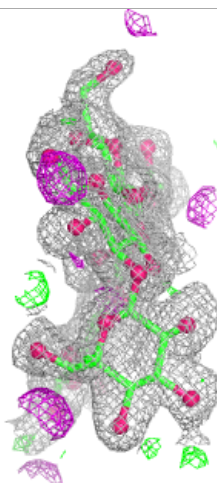
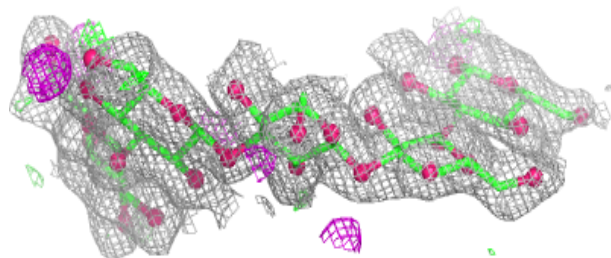
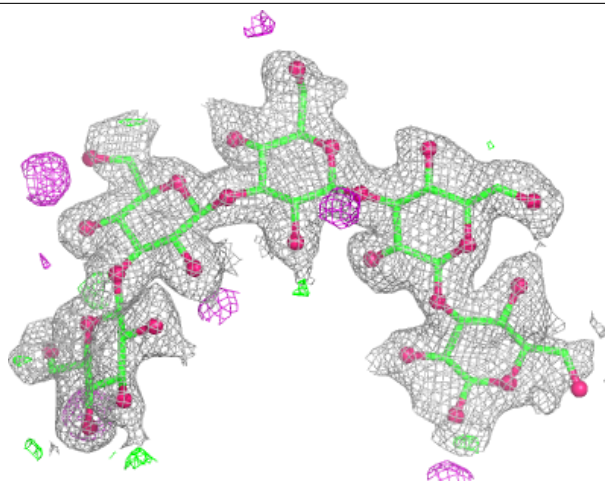
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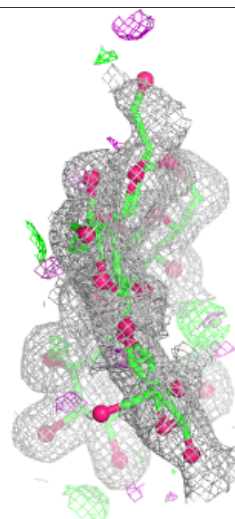
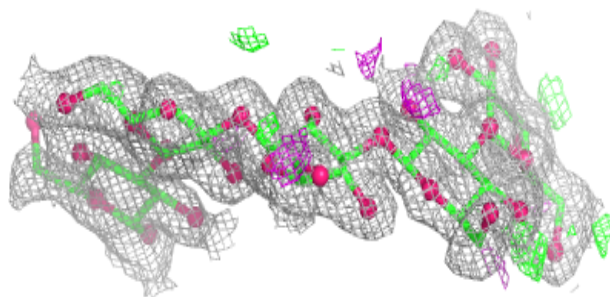
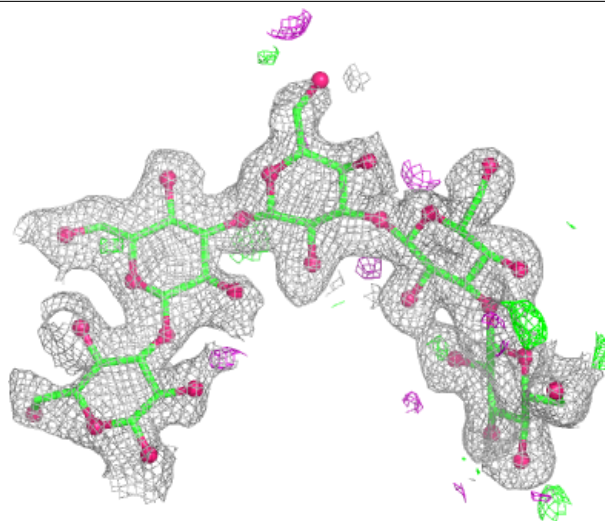
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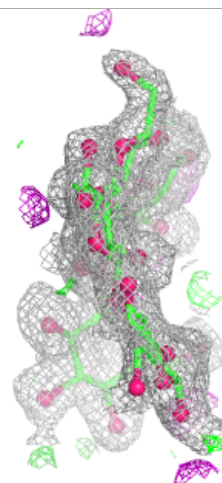
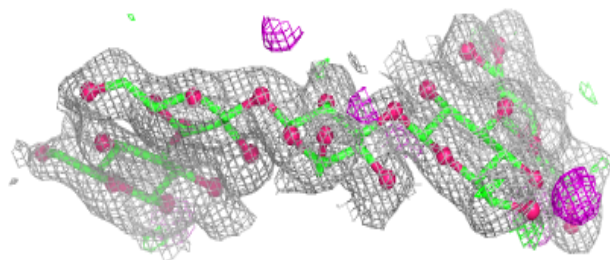
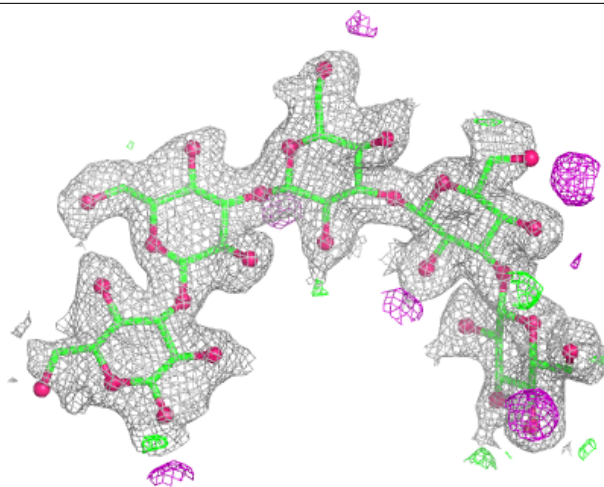
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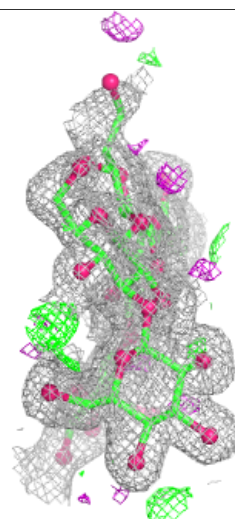
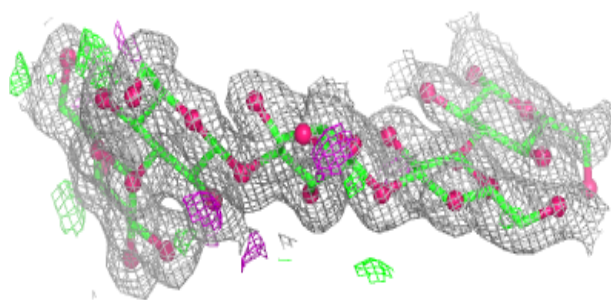
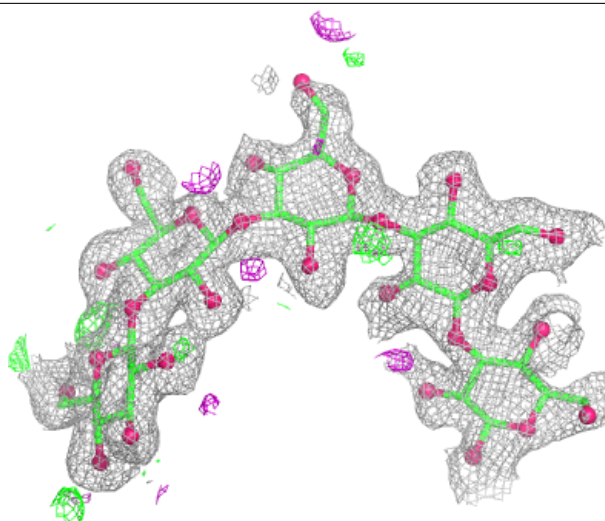
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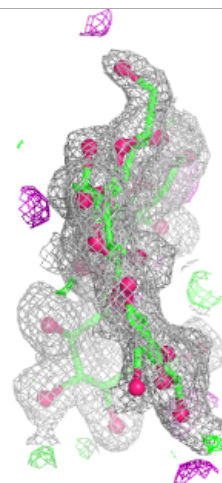
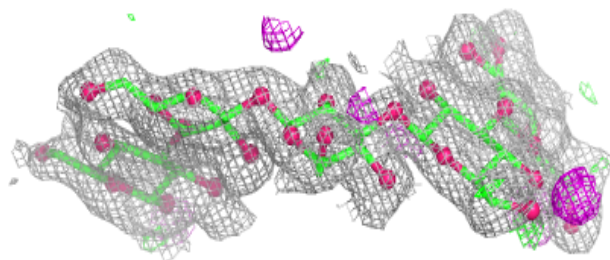
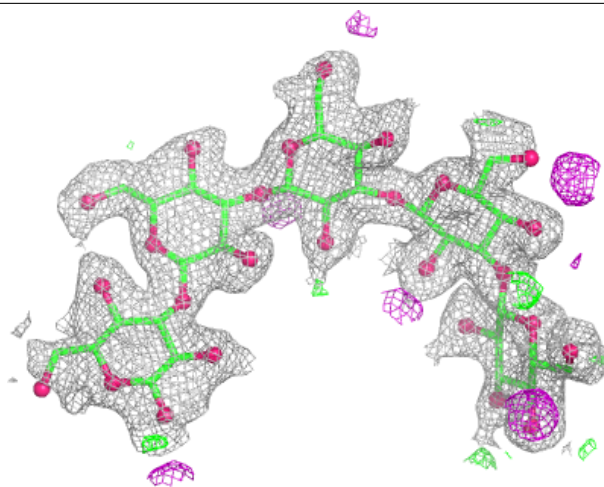
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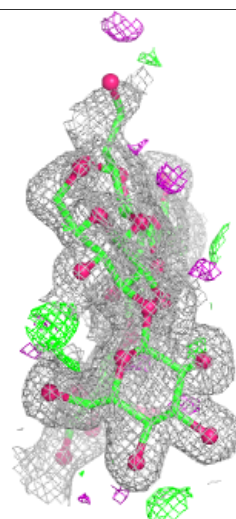
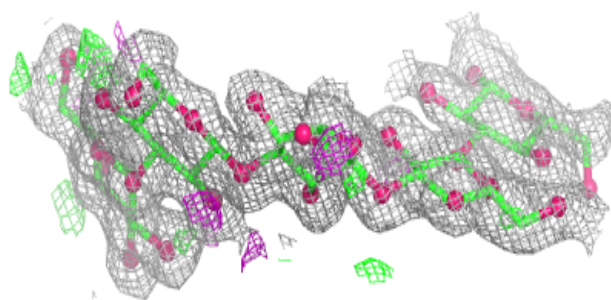
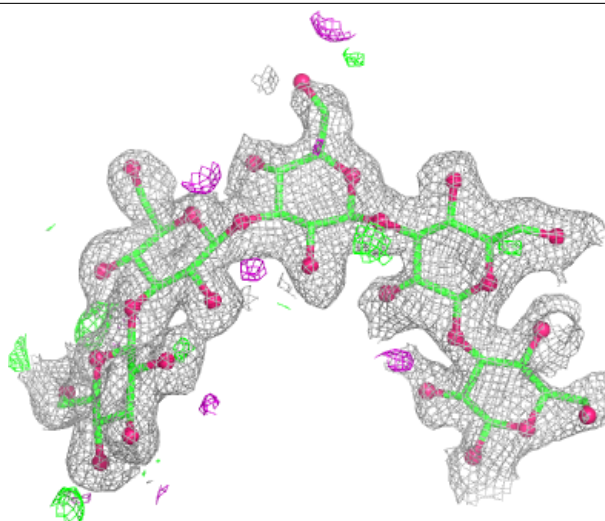
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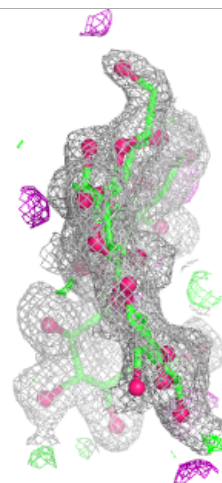
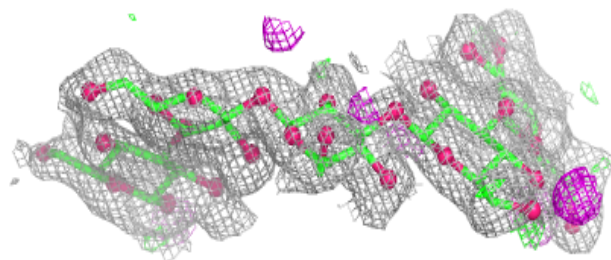
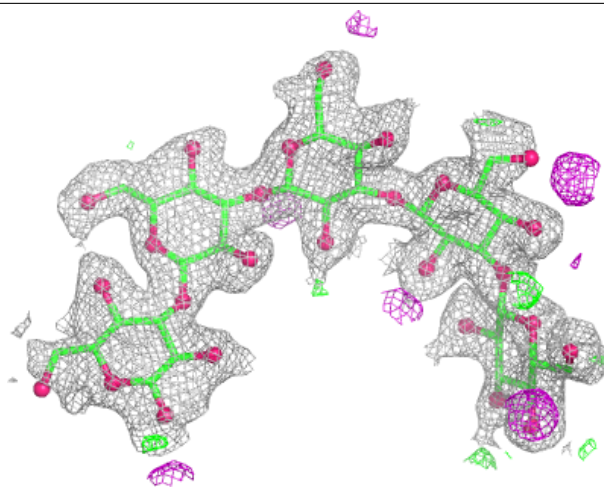
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and green (positive)



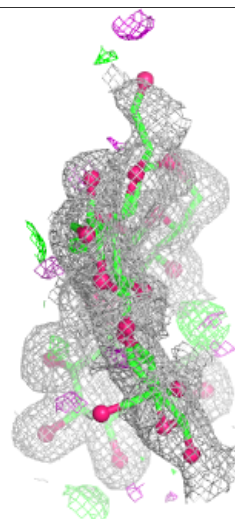
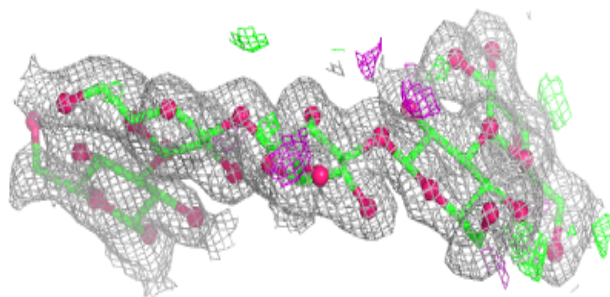
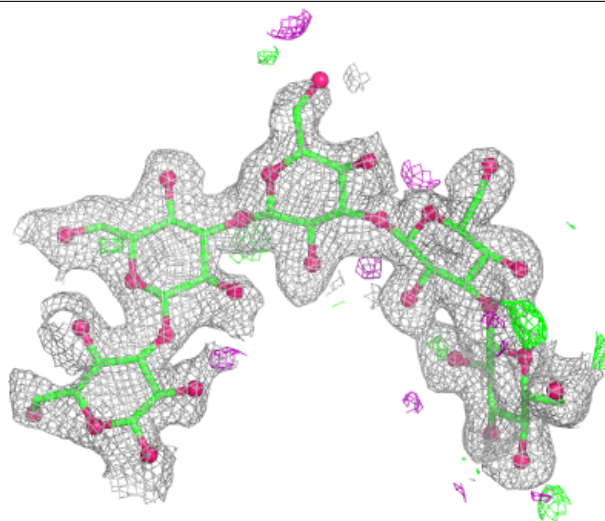
Electron density around Chain D:

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



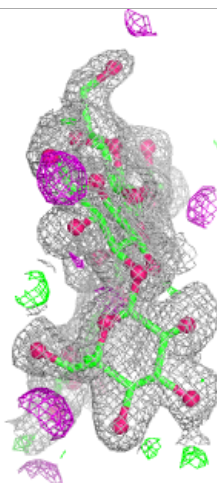
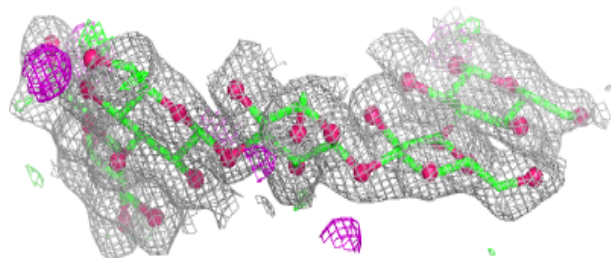
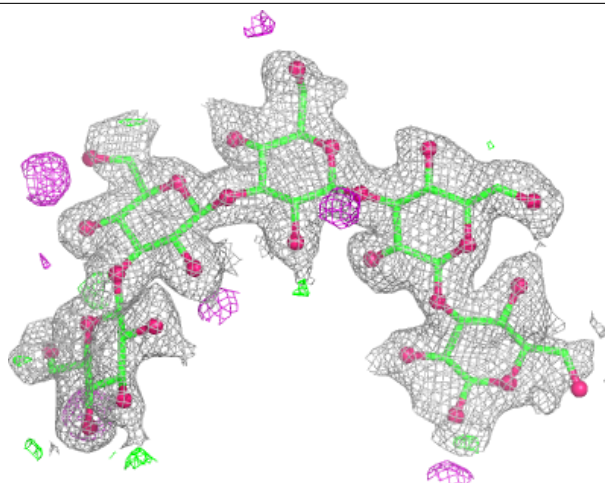
Electron density around Chain F:

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



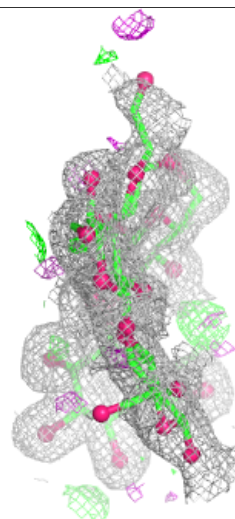
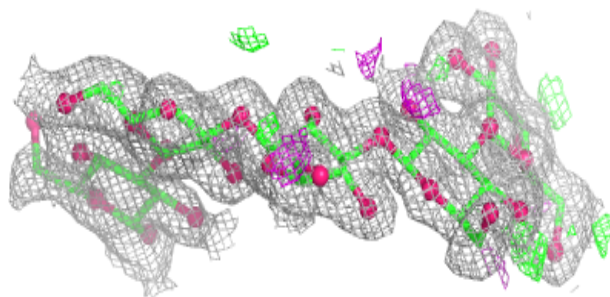
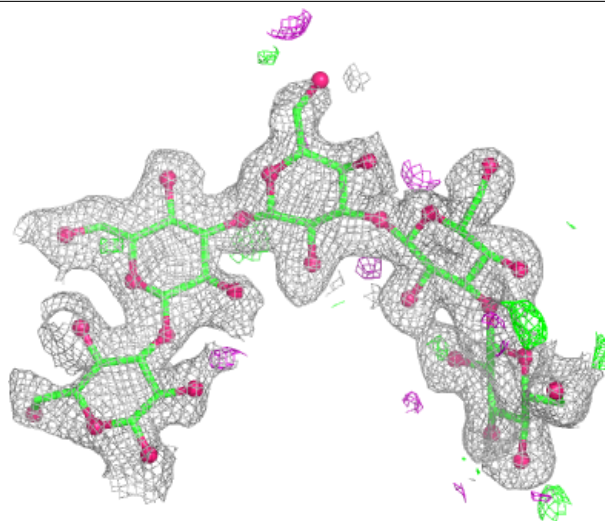
Electron density around Chain D:

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



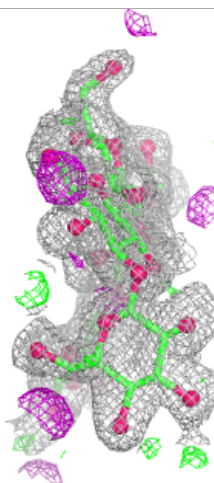
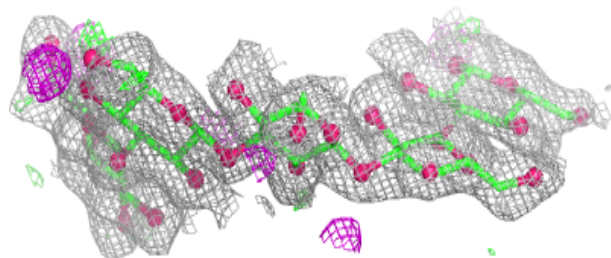
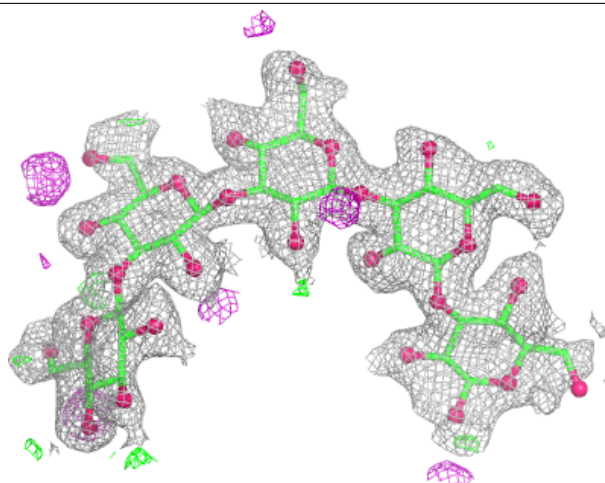
Electron density around Chain F:

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



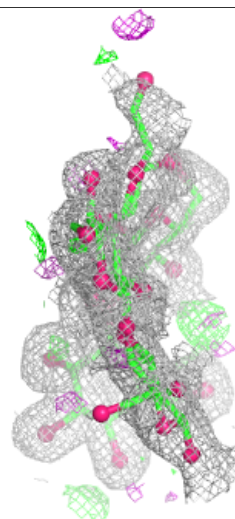
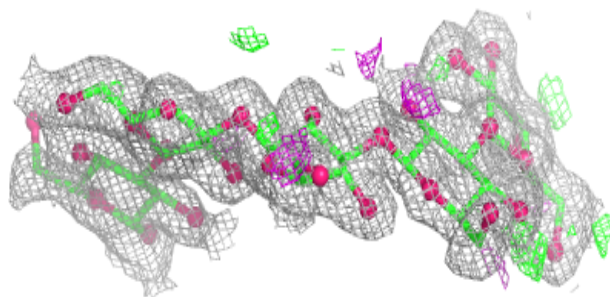
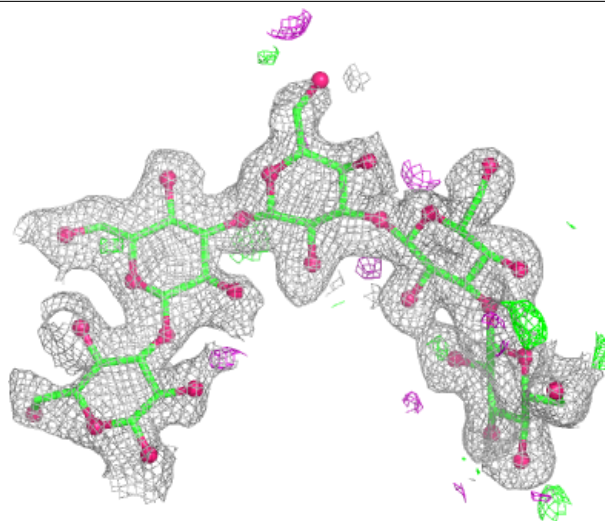
Electron density around Chain D:

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



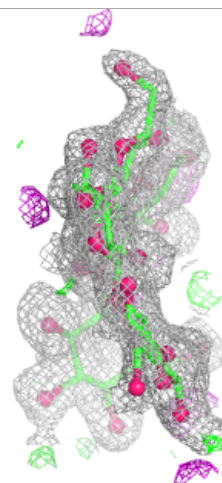
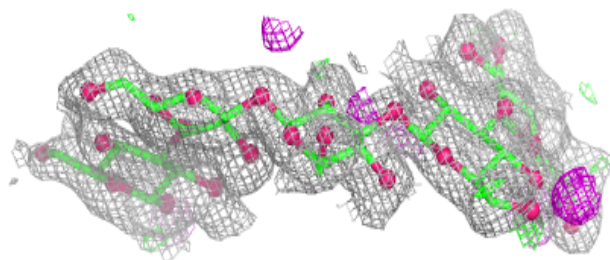
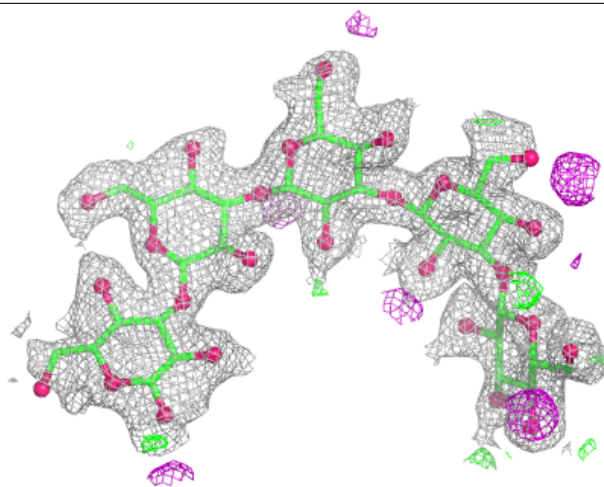
Electron density around Chain F:

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



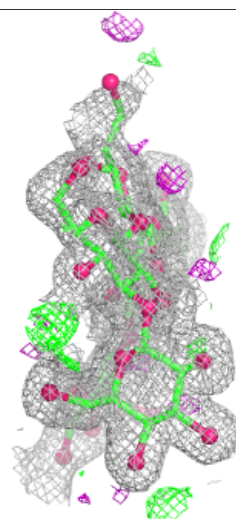
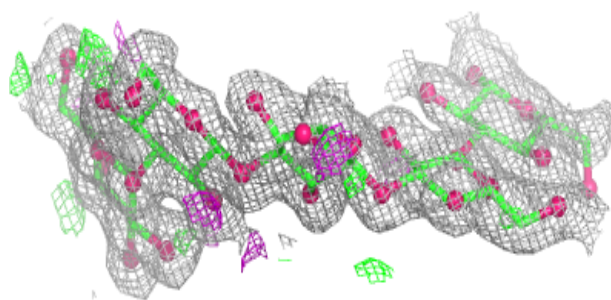
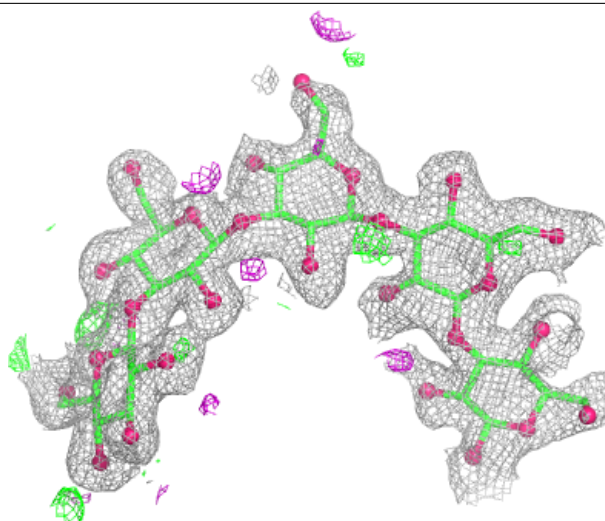
Electron density around Chain D:

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



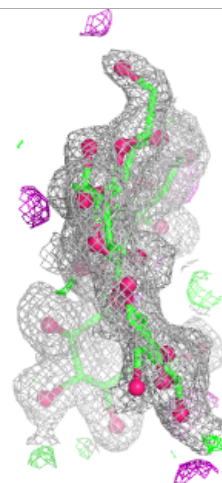
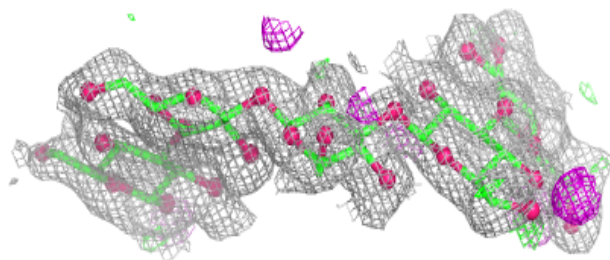
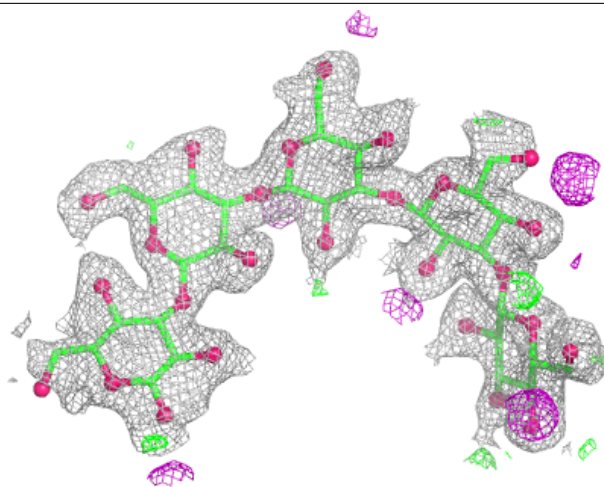
Electron density around Chain F:

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



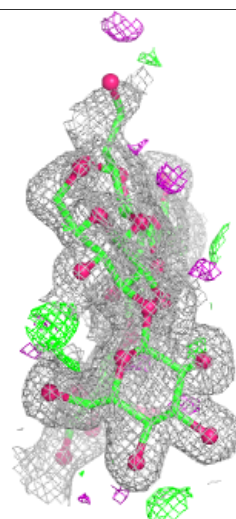
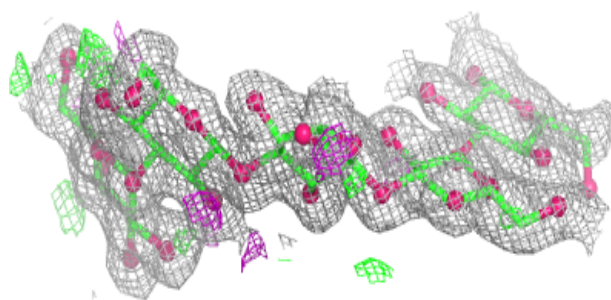
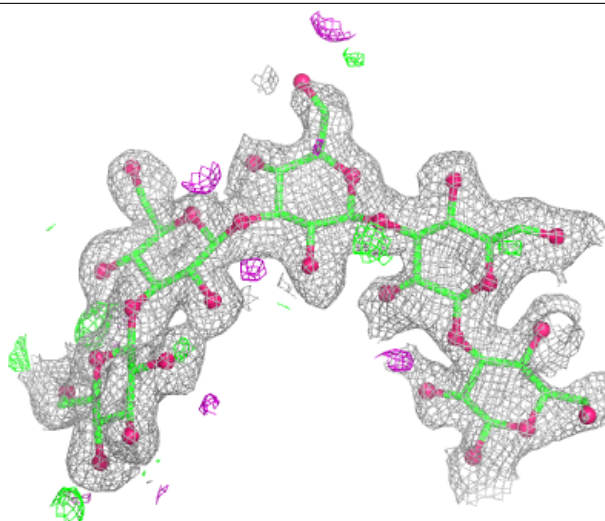
Electron density around Chain D:

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



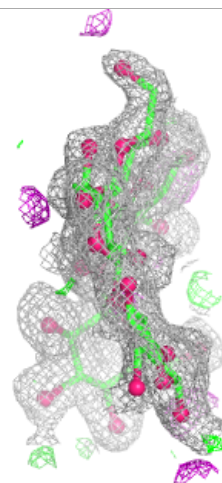
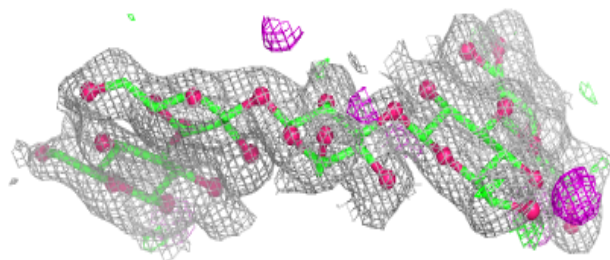
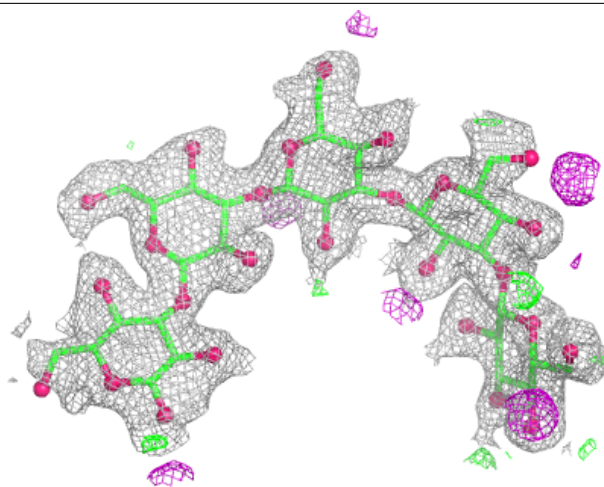
Electron density around Chain F:

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



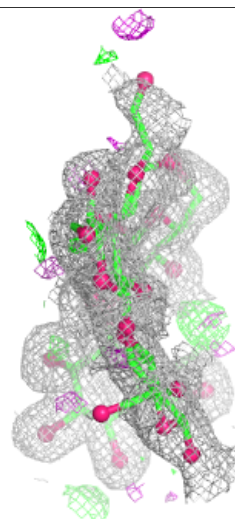
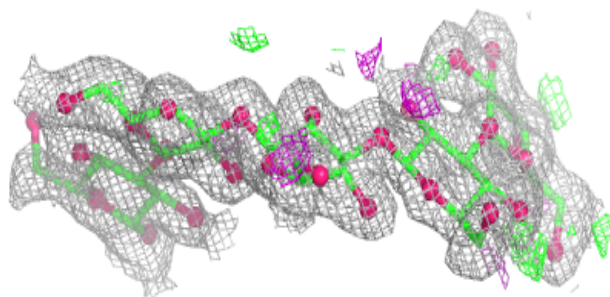
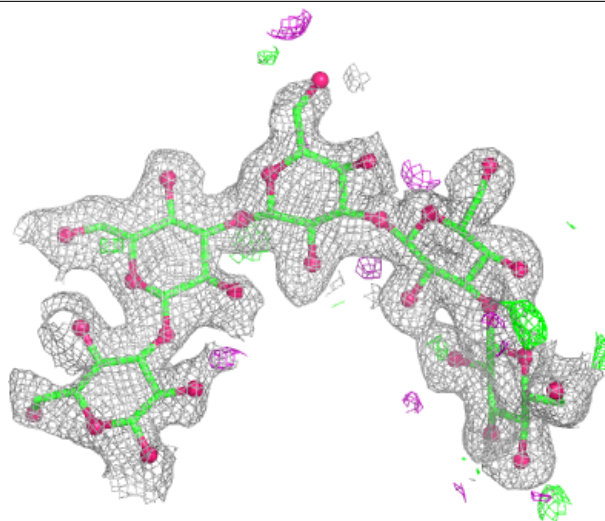
Electron density around Chain D:

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



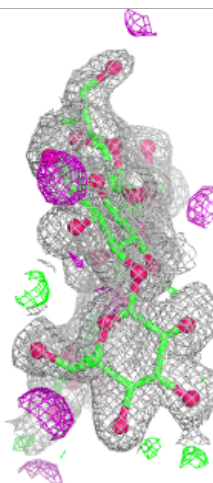
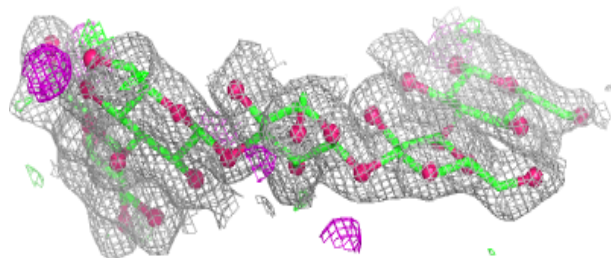
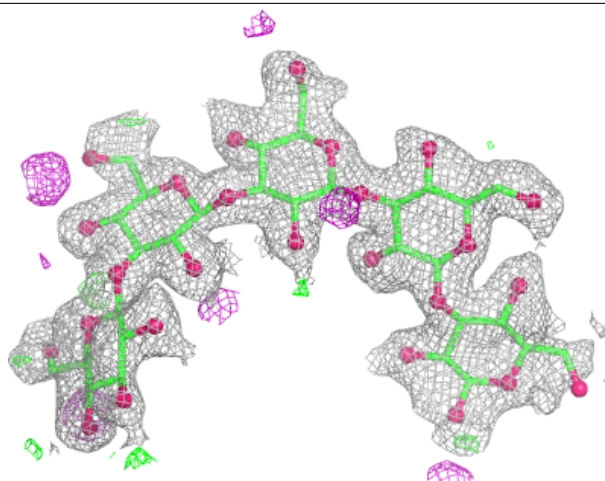
Electron density around Chain F:

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



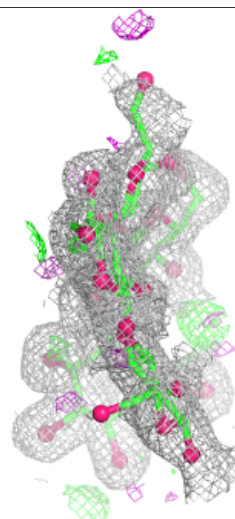
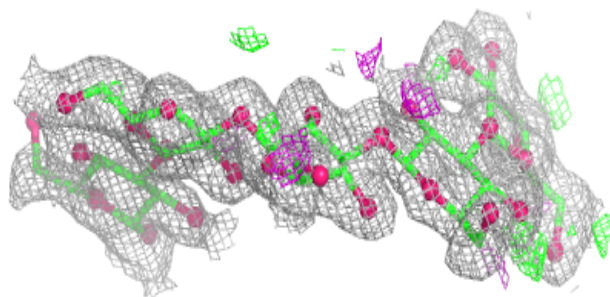
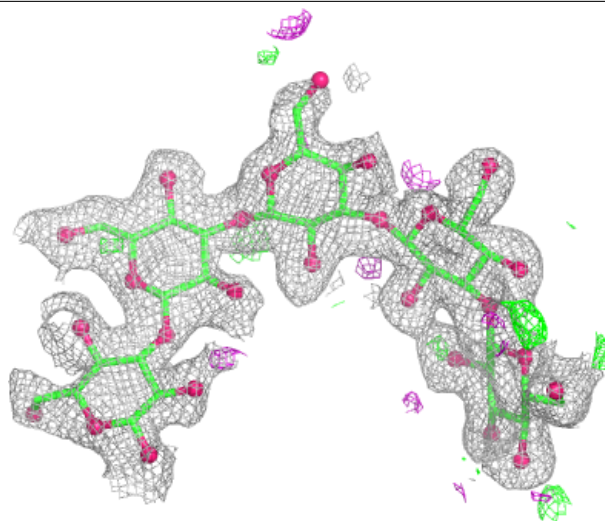
Electron density around Chain D:

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



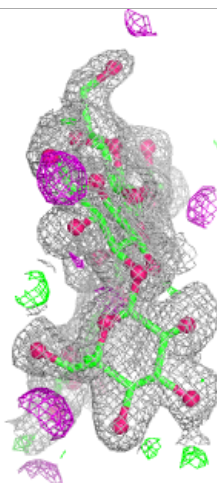
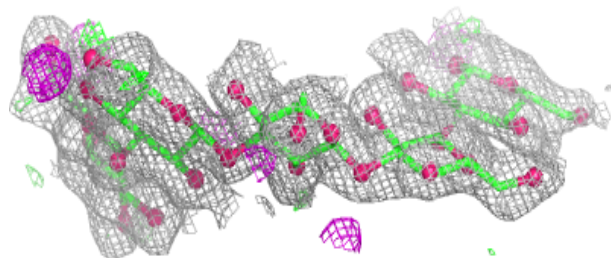
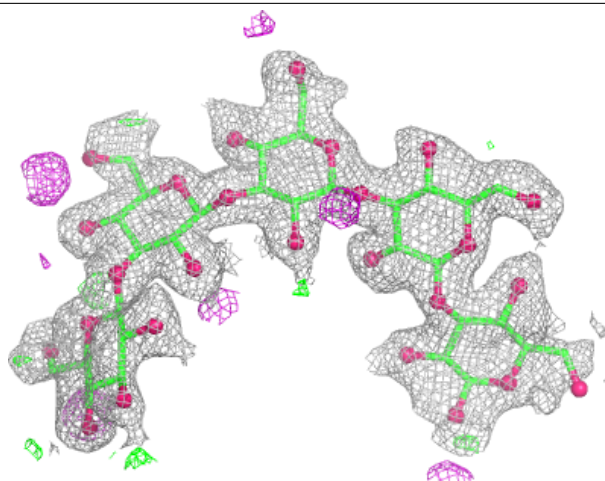
Electron density around Chain F:

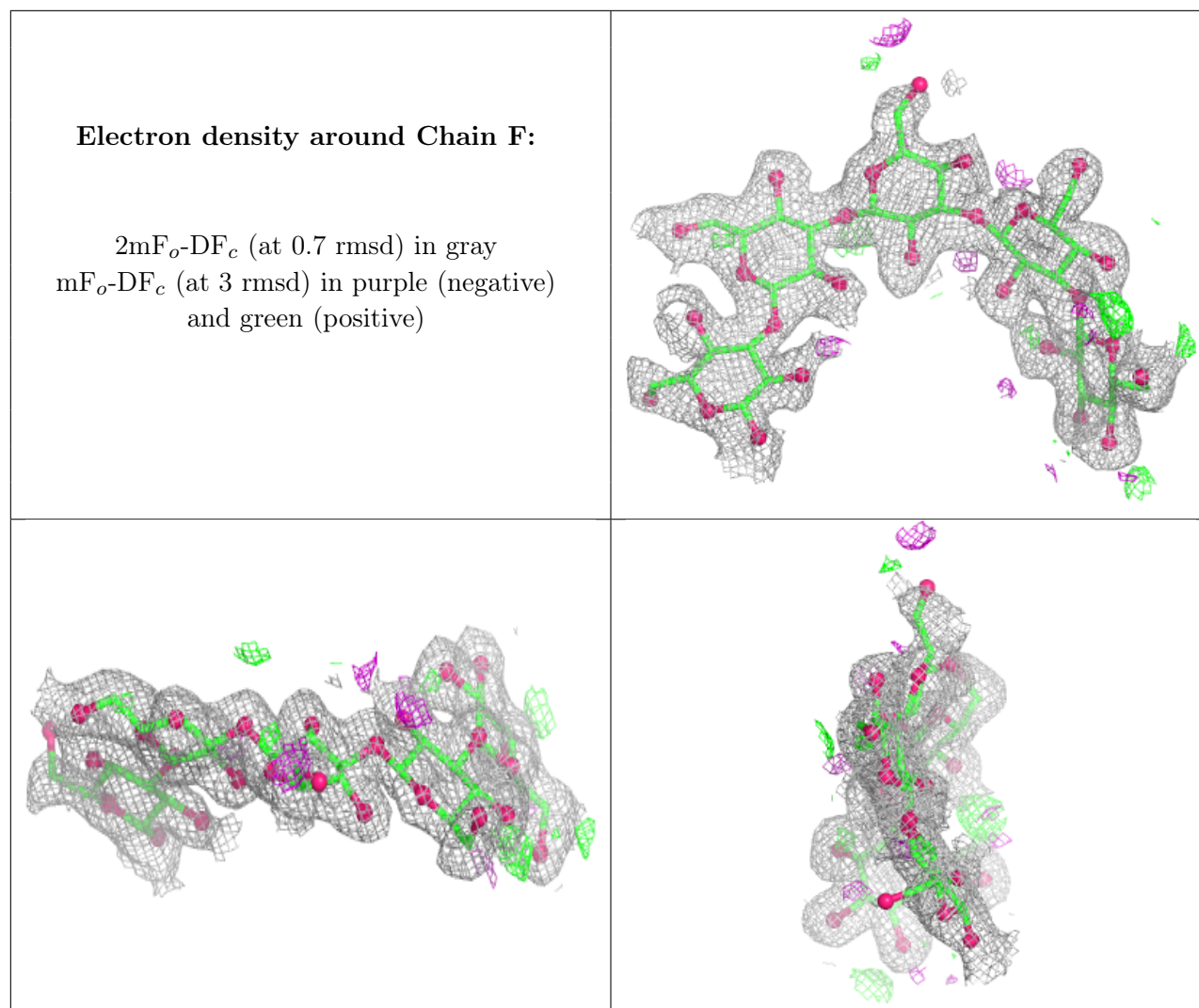
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

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





5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	1-B	701	4/4	0.46	0.27	13,21,21,22	10
4	EDO	2-A	701	4/4	-	-	13,13,19,19	10
4	EDO	3-A	701	4/4	-	-	13,13,19,19	10
4	EDO	4-A	701	4/4	-	-	13,13,19,19	10
4	EDO	5-A	701	4/4	-	-	13,13,19,19	10
4	EDO	6-A	701	4/4	-	-	13,13,19,19	10
4	EDO	7-A	701	4/4	-	-	13,13,19,19	10
4	EDO	8-A	701	4/4	-	-	13,13,19,19	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	9-A	701	4/4	-	-	13,13,19,19	10
4	EDO	10-A	701	4/4	-	-	13,13,19,19	10
4	EDO	11-A	701	4/4	-	-	13,13,19,19	10
4	EDO	12-A	701	4/4	-	-	13,13,19,19	10
4	EDO	13-A	701	4/4	-	-	13,13,19,19	10
4	EDO	14-A	701	4/4	-	-	13,13,19,19	10
4	EDO	15-A	701	4/4	-	-	13,13,19,19	10
4	EDO	16-A	701	4/4	-	-	13,13,19,19	10
4	EDO	17-A	701	4/4	-	-	13,13,19,19	10
4	EDO	18-A	701	4/4	-	-	13,13,19,19	10
4	EDO	19-A	701	4/4	-	-	13,13,19,19	10
4	EDO	20-A	701	4/4	-	-	13,13,19,19	10
4	EDO	21-A	701	4/4	-	-	13,13,19,19	10
4	EDO	22-A	701	4/4	-	-	13,13,19,19	10
4	EDO	23-A	701	4/4	-	-	13,13,19,19	10
4	EDO	24-A	701	4/4	-	-	13,13,19,19	10
4	EDO	25-A	701	4/4	-	-	13,13,19,19	10
4	EDO	1-A	701	4/4	0.70	0.19	13,13,19,19	10
4	EDO	2-B	701	4/4	-	-	13,21,21,22	10
4	EDO	3-B	701	4/4	-	-	13,21,21,22	10
4	EDO	4-B	701	4/4	-	-	13,21,21,22	10
4	EDO	5-B	701	4/4	-	-	13,21,21,22	10
4	EDO	6-B	701	4/4	-	-	13,21,21,22	10
4	EDO	7-B	701	4/4	-	-	13,21,21,22	10
4	EDO	8-B	701	4/4	-	-	13,21,21,22	10
4	EDO	9-B	701	4/4	-	-	13,21,21,22	10
4	EDO	10-B	701	4/4	-	-	13,21,21,22	10
4	EDO	11-B	701	4/4	-	-	13,21,21,22	10
4	EDO	12-B	701	4/4	-	-	13,21,21,22	10
4	EDO	13-B	701	4/4	-	-	13,21,21,22	10
4	EDO	14-B	701	4/4	-	-	13,21,21,22	10
4	EDO	15-B	701	4/4	-	-	13,21,21,22	10
4	EDO	16-B	701	4/4	-	-	13,21,21,22	10
4	EDO	17-B	701	4/4	-	-	13,21,21,22	10
4	EDO	18-B	701	4/4	-	-	13,21,21,22	10
4	EDO	19-B	701	4/4	-	-	13,21,21,22	10
4	EDO	20-B	701	4/4	-	-	13,21,21,22	10
4	EDO	21-B	701	4/4	-	-	13,21,21,22	10
4	EDO	22-B	701	4/4	-	-	13,21,21,22	10
4	EDO	23-B	701	4/4	-	-	13,21,21,22	10
4	EDO	24-B	701	4/4	-	-	13,21,21,22	10
4	EDO	25-B	701	4/4	-	-	13,21,21,22	10

5.5 Other polymers ⓘ

There are no such residues in this entry.