wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 07:32 AM EDT

PDB ID	:	4TZ5
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

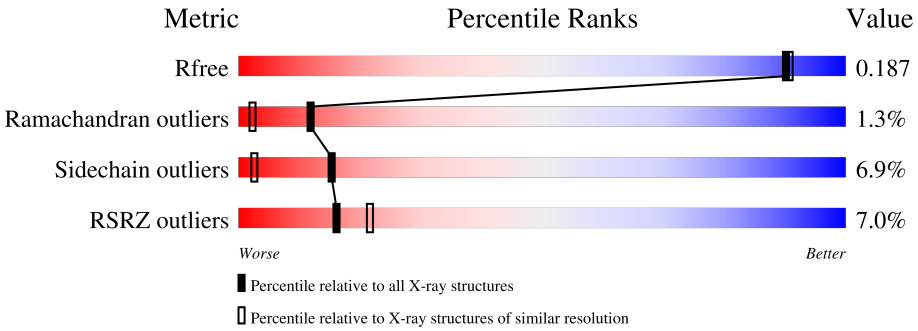
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2340 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	549	7% 91% 9%
1	1-B	549	8% 92% 7% •
1	10-A	549	7% 92% 7% •
1	10-B	549	8% 92% 6% •
1	11-A	549	7% 94% 5% •
1	11-B	549	8% 93% 7% •

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Mol	Chain	Length	Quality of chain
1	12-A	549	7% 91% 9%
1	12-B	549	8% 93% 6%
1	13-A	549	7% 91% 8%
1	13-B	549	8% 92% 7%
1	14-A	549	7% 90% 8%
1	14-B	549	8% 91% 7%
1	15-A	549	7% 90% 8%
1	15-B	549	8% 90% 9%
1	16-A	549	7% 91% 9%
1	16-B	549	8% 92% 8%
1	17-A	549	7% 90% 7%
1	17-B	549	8% 91% 8%
1	18-A	549	7% 91% 7%
1	18-B	549	8% 93% 6%
1	19-A	549	7% 91% 8%
1	19-B	549	8% 92% 7%
1	2-A	549	7% 93% 6%
1	2-B	549	8% 91% 7%
1	20-A	549	7% 93% 6%
1	20-B	549	8% 91% 7%
1	21-A	549	7% 91% 7%
1	21-B	549	8% 92% 7%
1	22-A	549	7% 90% 8%
1	22-B	549	8% 91% 7%
1	23-A	549	7% 90% 9%

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Mol	Chain	Length	Quality of chain
1	23-B	549	8% 90% 8%
1	24-A	549	7% 92% 6%
1	24-B	549	8% 93% 7%
1	25-A	549	7% 90% 9%
1	25-B	549	8% 92% 7%
1	3-A	549	7% 94% 5%
1	3-B	549	8% 91% 7%
1	4-A	549	7% 91% 8%
1	4-B	549	8% 93% 7%
1	5-A	549	7% 90% 7%
1	5-B	549	8% 92% 7%
1	6-A	549	7% 91% 8%
1	6-B	549	8% 91% 7%
1	7-A	549	7% 93% 6%
1	7-B	549	8% 93% 7%
1	8-A	549	7% 92% 7%
1	8-B	549	8% 90% 7%
1	9-A	549	7% 92% 7%
1	9-B	549	8% 93% 5%
2	1-C	6	100%
2	1-E	6	100%
2	10-C	6	100%
2	10-E	6	100%
2	11-C	6	100%
2	11-E	6	100%

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Mol	Chain	Length	Quality of chain
2	12-C	6	100%
2	12-E	6	100%
2	13-C	6	100%
2	13-E	6	100%
2	14-C	6	100%
2	14-E	6	100%
2	15-C	6	100%
2	15-E	6	100%
2	16-C	6	100%
2	16-E	6	100%
2	17-C	6	100%
2	17-E	6	100%
2	18-C	6	100%
2	18-E	6	100%
2	19-C	6	100%
2	19-E	6	100%
2	2-C	6	100%
2	2-E	6	100%
2	20-C	6	100%
2	20-E	6	100%
2	21-C	6	100%
2	21-E	6	100%
2	22-C	6	100%
2	22-E	6	100%
2	23-C	6	100%

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Mol	Chain	Length	Quality of chain
2	23-E	6	100%
2	24-C	6	100%
2	24-E	6	100%
2	25-C	6	100%
2	25-E	6	100%
2	3-C	6	100%
2	3-E	6	100%
2	4-C	6	100%
2	4-E	6	100%
2	5-C	6	100%
2	5-E	6	100%
2	6-C	6	100%
2	6-E	6	100%
2	7-C	6	100%
2	7-E	6	100%
2	8-C	6	100%
2	8-E	6	100%
2	9-C	6	100%
2	9-E	6	100%
3	1-D	5	100%
3	1-F	5	100%
3	10-D	5	100%
3	10-F	5	100%
3	11-D	5	100%
3	11-F	5	100%

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Mol	Chain	Length	Quality of chain
3	12-D	5	100%
3	12-F	5	100%
3	13-D	5	100%
3	13-F	5	100%
3	14-D	5	100%
3	14-F	5	100%
3	15-D	5	100%
3	15-F	5	100%
3	16-D	5	100%
3	16-F	5	100%
3	17-D	5	100%
3	17-F	5	100%
3	18-D	5	100%
3	18-F	5	100%
3	19-D	5	100%
3	19-F	5	100%
3	2-D	5	100%
3	2-F	5	100%
3	20-D	5	100%
3	20-F	5	100%
3	21-D	5	100%
3	21-F	5	100%
3	22-D	5	100%
3	22-F	5	100%
3	23-D	5	100%

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Mol	Chain	Length	Quality of chain
3	23-F	5	100%
3	24-D	5	100%
3	24-F	5	100%
3	25-D	5	100%
3	25-F	5	100%
3	3-D	5	100%
3	3-F	5	100%
3	4-D	5	100%
3	4-F	5	100%
3	5-D	5	100%
3	5-F	5	100%
3	6-D	5	100%
3	6-F	5	100%
3	7-D	5	100%
3	7-F	5	100%
3	8-D	5	100%
3	8-F	5	100%
3	9-D	5	100%
3	9-F	5	100%

2 Entry composition (i)

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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	18-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	19-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	20-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	21-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	22-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	23-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	24-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	25-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	1-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	2-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	3-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	4-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	5-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	6-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	7-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	8-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	9-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	10-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	11-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	12-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			

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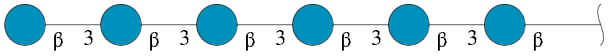
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	13-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	14-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	15-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	16-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	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-(1-3)-beta-D-glucopyranose.



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

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

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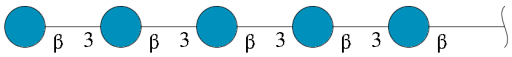
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	19-E	6	Total C O 67 36 31	0	0	0
2	20-E	6	Total C O 67 36 31	0	0	0
2	21-E	6	Total C O 67 36 31	0	0	0
2	22-E	6	Total C O 67 36 31	0	0	0
2	23-E	6	Total C O 67 36 31	0	0	0
2	24-E	6	Total C O 67 36 31	0	0	0
2	25-E	6	Total C O 67 36 31	0	0	0

- 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 56 30 26	0	0	0
3	2-D	5	Total C O 56 30 26	0	0	0
3	3-D	5	Total C O 56 30 26	0	0	0
3	4-D	5	Total C O 56 30 26	0	0	0
3	5-D	5	Total C O 56 30 26	0	0	0
3	6-D	5	Total C O 56 30 26	0	0	0
3	7-D	5	Total C O 56 30 26	0	0	0
3	8-D	5	Total C O 56 30 26	0	0	0
3	9-D	5	Total C O 56 30 26	0	0	0
3	10-D	5	Total C O 56 30 26	0	0	0

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

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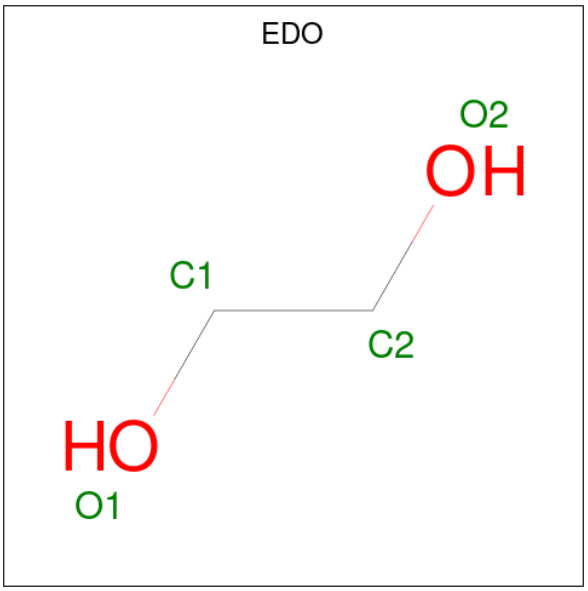
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	7-F	5	Total C O 56 30 26	0	0	0
3	8-F	5	Total C O 56 30 26	0	0	0
3	9-F	5	Total C O 56 30 26	0	0	0
3	10-F	5	Total C O 56 30 26	0	0	0
3	11-F	5	Total C O 56 30 26	0	0	0
3	12-F	5	Total C O 56 30 26	0	0	0
3	13-F	5	Total C O 56 30 26	0	0	0
3	14-F	5	Total C O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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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 10 2 6 2	0	0
4	12-B	1	Total C H O 10 2 6 2	0	0
4	13-B	1	Total C H O 10 2 6 2	0	0
4	14-B	1	Total C H O 10 2 6 2	0	0
4	15-B	1	Total C H O 10 2 6 2	0	0
4	16-B	1	Total C H O 10 2 6 2	0	0
4	17-B	1	Total C H O 10 2 6 2	0	0
4	18-B	1	Total C H O 10 2 6 2	0	0
4	19-B	1	Total C H O 10 2 6 2	0	0
4	20-B	1	Total C H O 10 2 6 2	0	0
4	21-B	1	Total C H O 10 2 6 2	0	0
4	22-B	1	Total C H O 10 2 6 2	0	0
4	23-B	1	Total C H O 10 2 6 2	0	0
4	24-B	1	Total C H O 10 2 6 2	0	0
4	25-B	1	Total C H O 10 2 6 2	0	0

- Molecule 5 is water.

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

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

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

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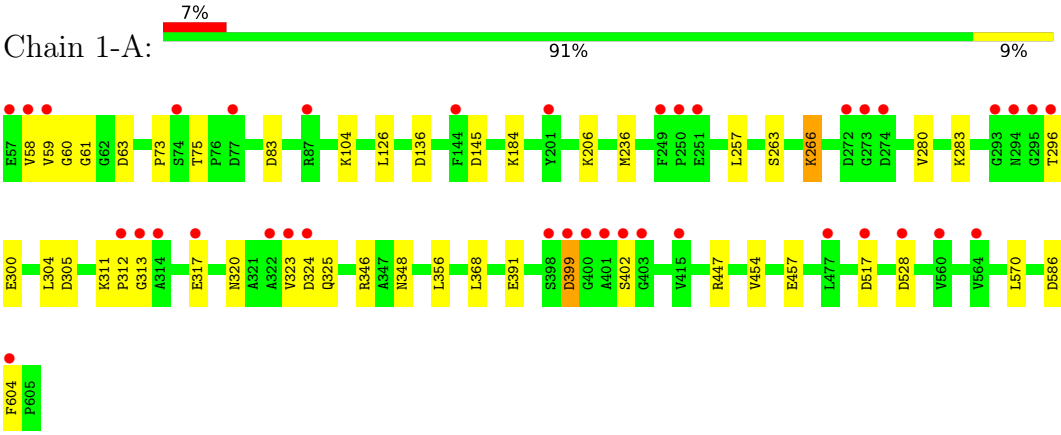
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	22-B	386	Total O 386 386	0	0
5	23-B	332	Total O 332 332	0	0
5	24-B	360	Total O 360 360	0	0
5	25-B	372	Total O 372 372	0	0

3 Residue-property plots (i)

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

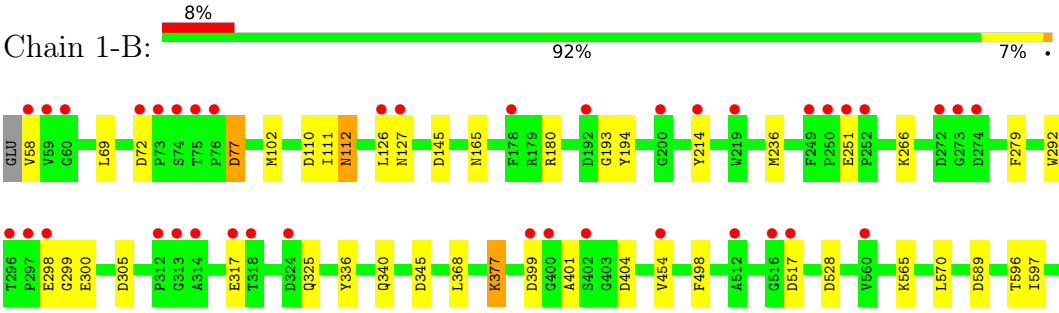
• Molecule 1: Putative secreted protein

Chain 1-A:



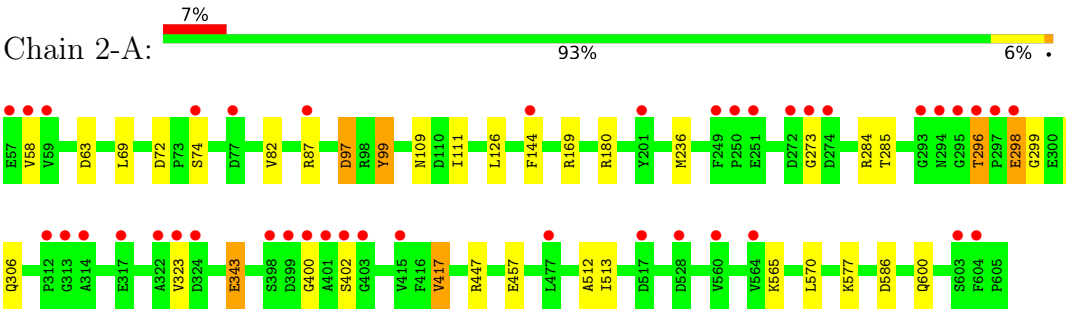
• Molecule 1: Putative secreted protein

Chain 1-B:



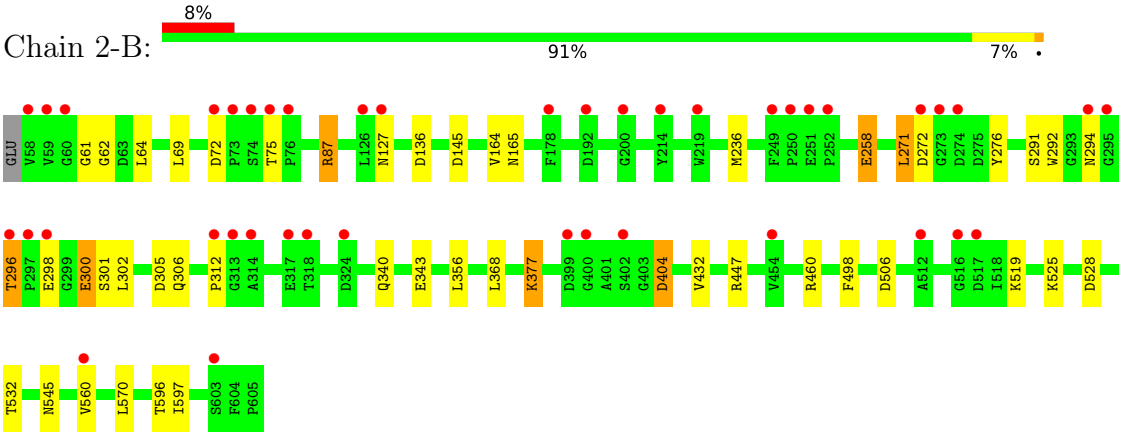
• Molecule 1: Putative secreted protein

Chain 2-A:



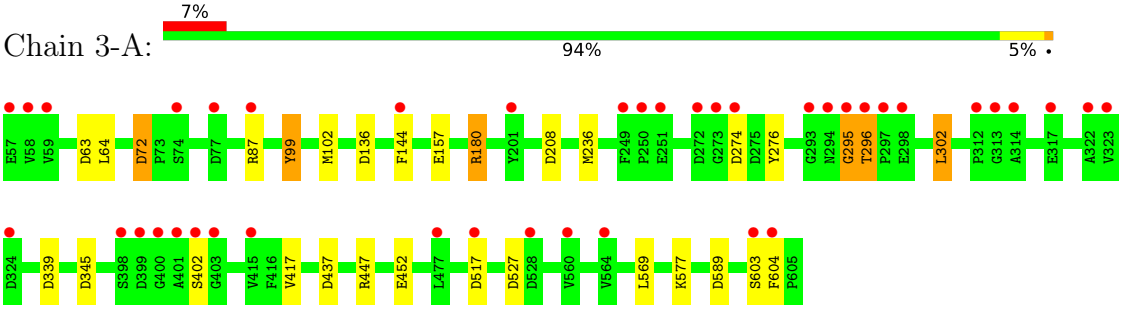
• Molecule 1: Putative secreted protein

Chain 2-B:



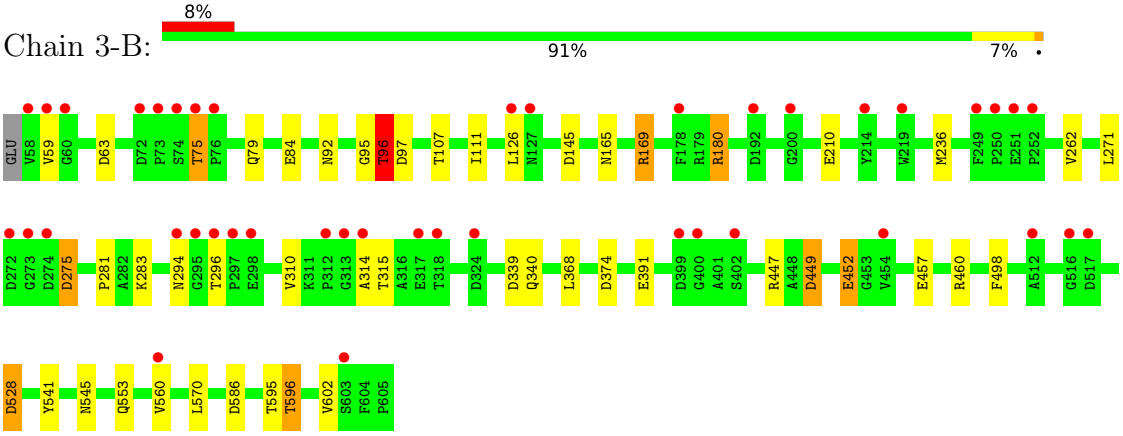
• Molecule 1: Putative secreted protein

Chain 3-A:



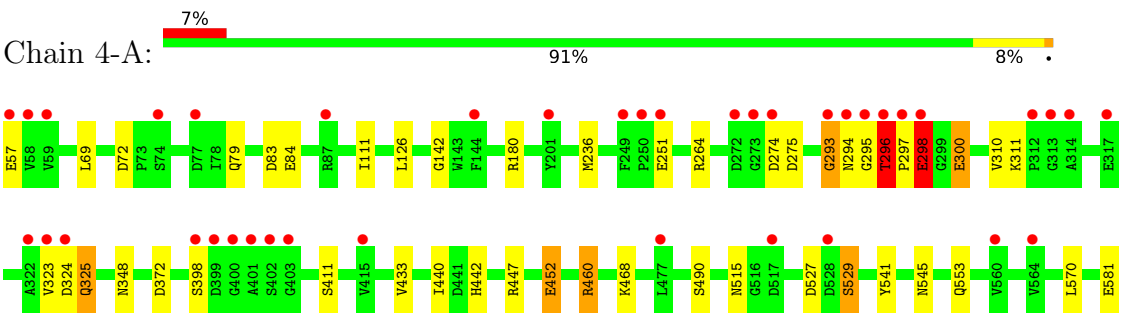
• Molecule 1: Putative secreted protein

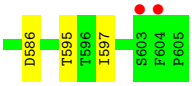
Chain 3-B:



• Molecule 1: Putative secreted protein

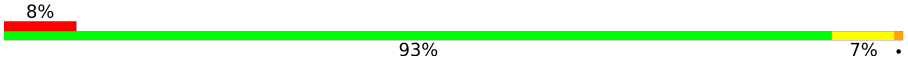
Chain 4-A:

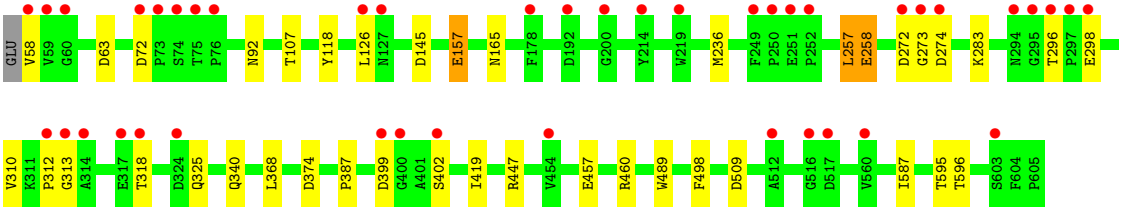




• Molecule 1: Putative secreted protein

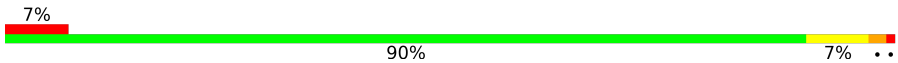
Chain 4-B:

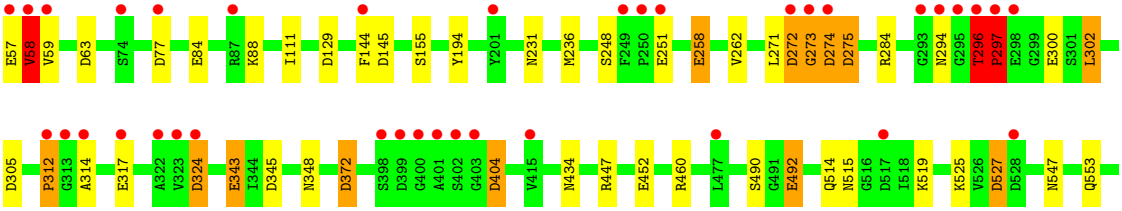




• Molecule 1: Putative secreted protein

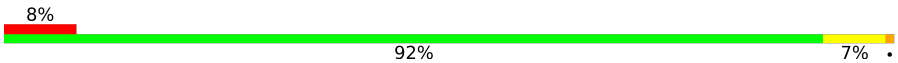
Chain 5-A:

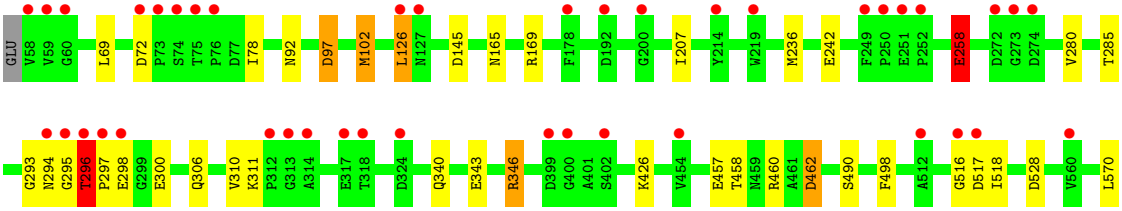




• Molecule 1: Putative secreted protein

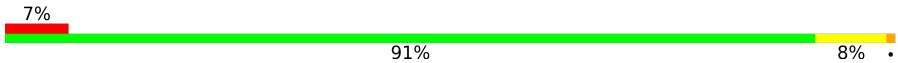
Chain 5-B:

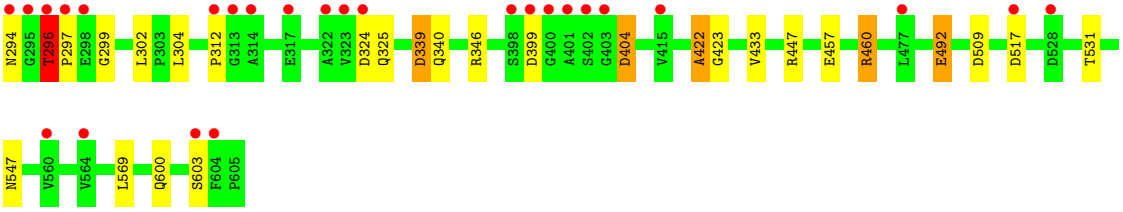




• Molecule 1: Putative secreted protein

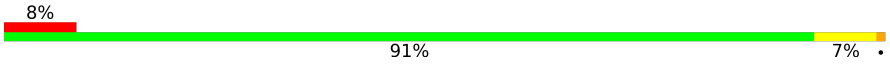
Chain 6-A:

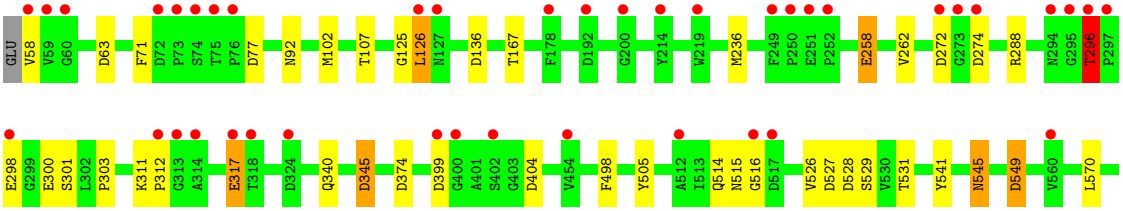




• Molecule 1: Putative secreted protein

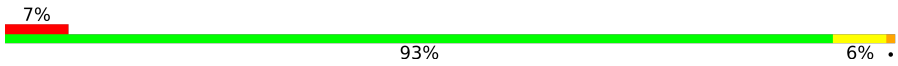
Chain 6-B:

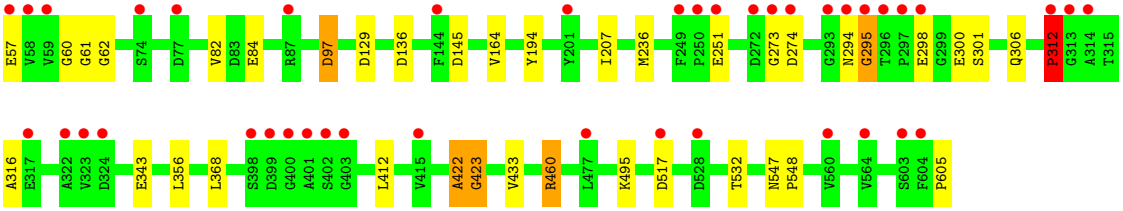




• Molecule 1: Putative secreted protein

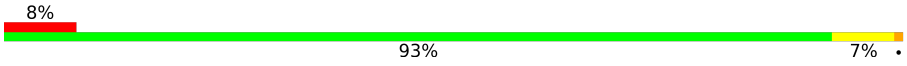
Chain 7-A:

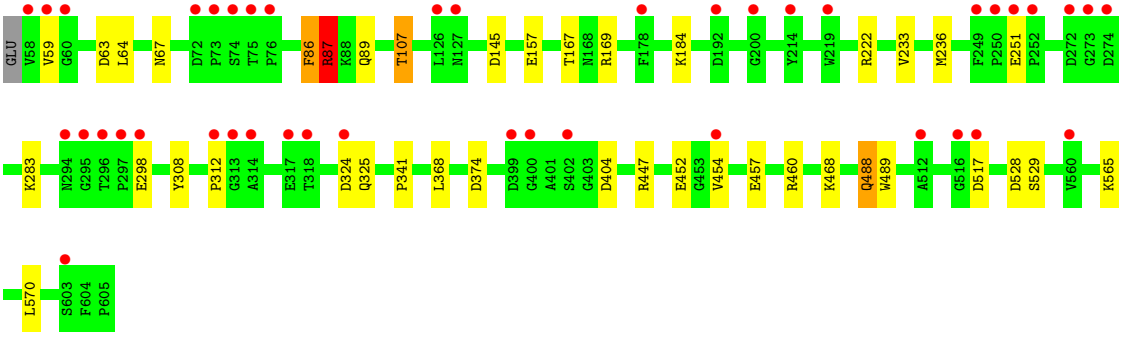




• Molecule 1: Putative secreted protein

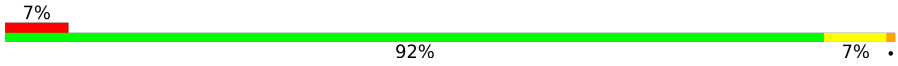
Chain 7-B:

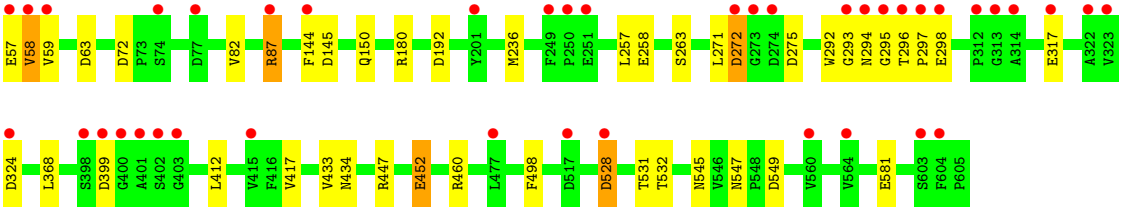




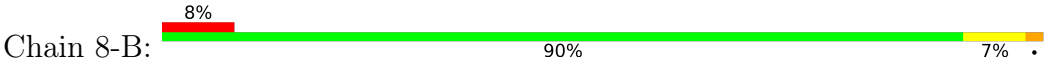
• Molecule 1: Putative secreted protein

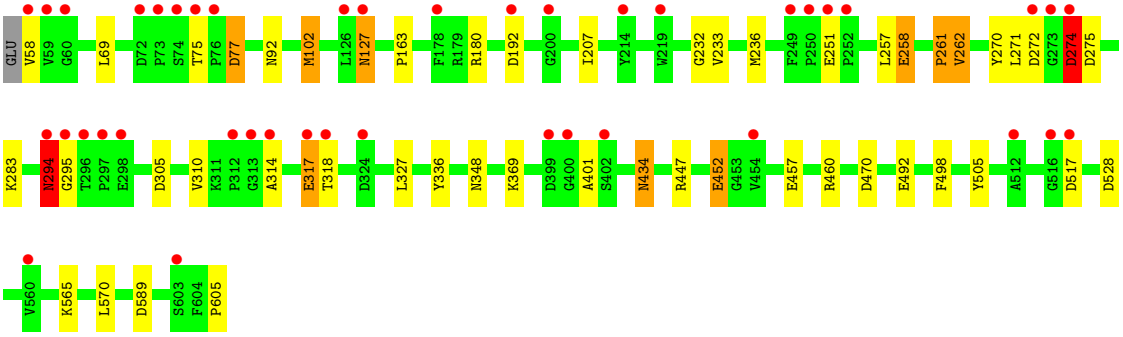
Chain 8-A:



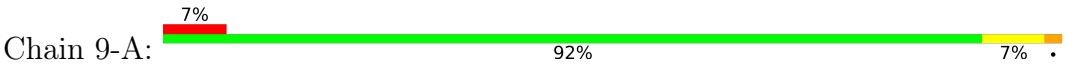


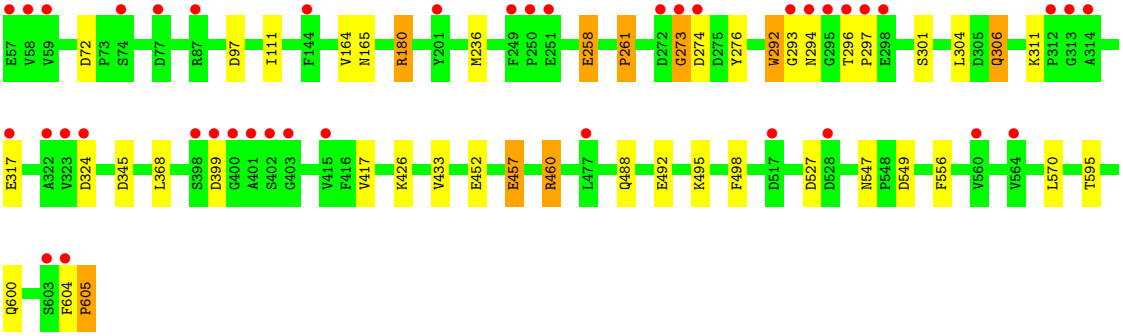
• Molecule 1: Putative secreted protein



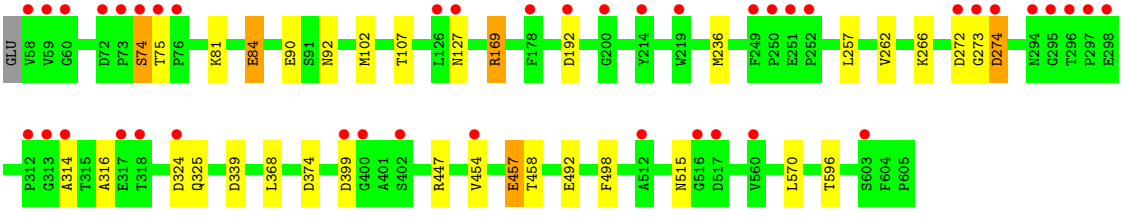


• Molecule 1: Putative secreted protein

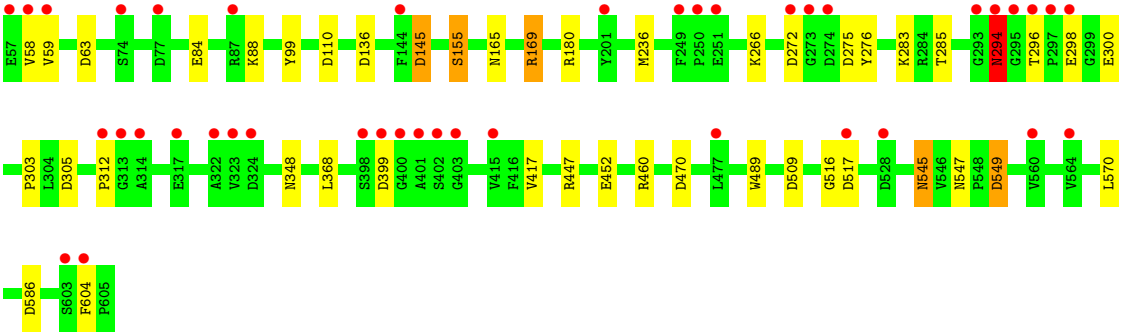




• Molecule 1: Putative secreted protein

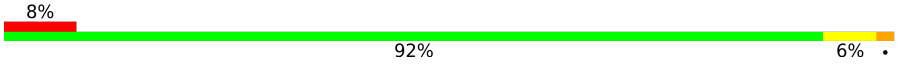


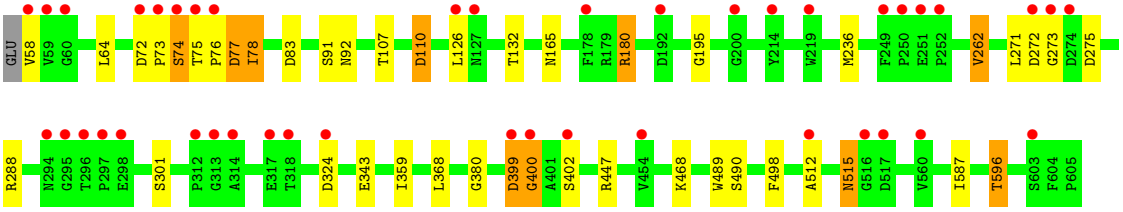
• Molecule 1: Putative secreted protein



• Molecule 1: Putative secreted protein

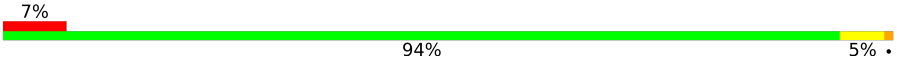
Chain 10-B:

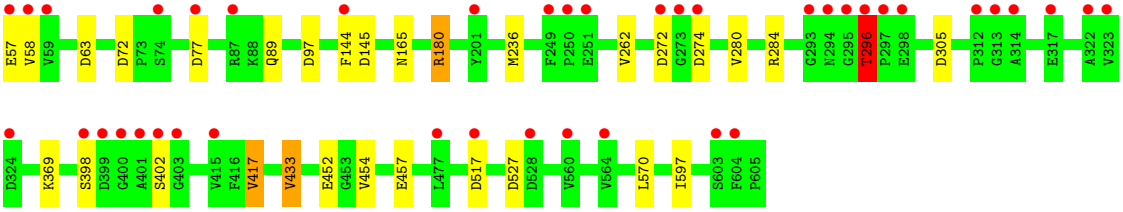




• Molecule 1: Putative secreted protein

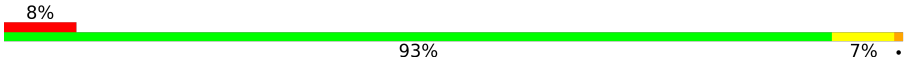
Chain 11-A:

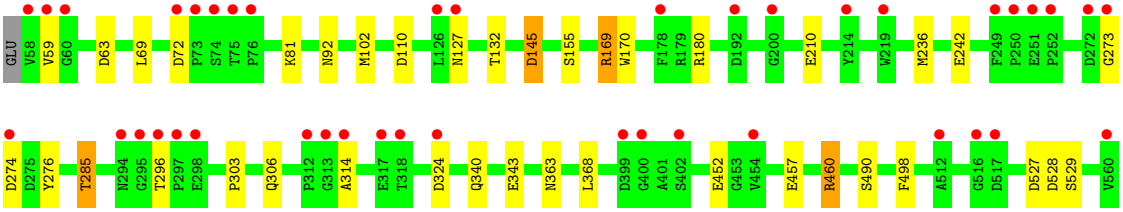




• Molecule 1: Putative secreted protein

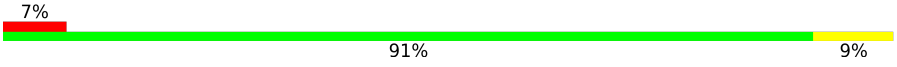
Chain 11-B:

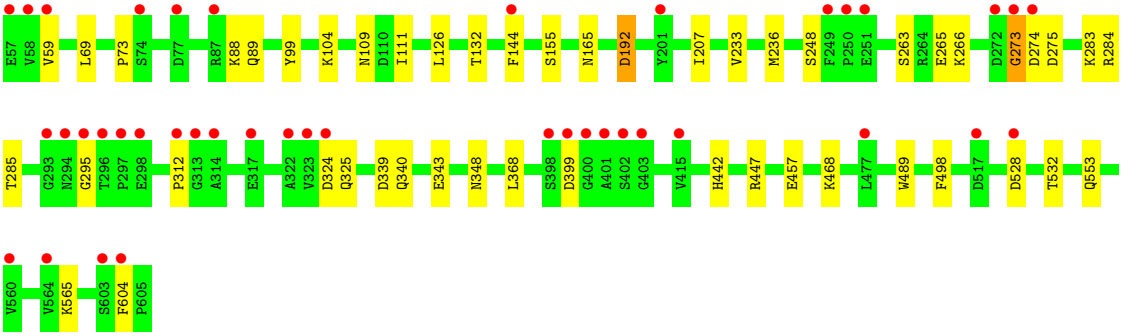




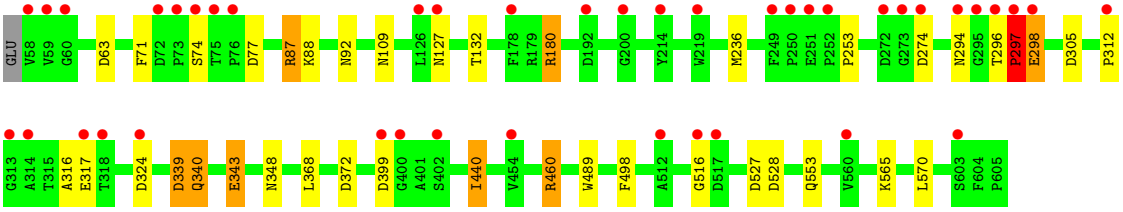
• Molecule 1: Putative secreted protein

Chain 12-A:

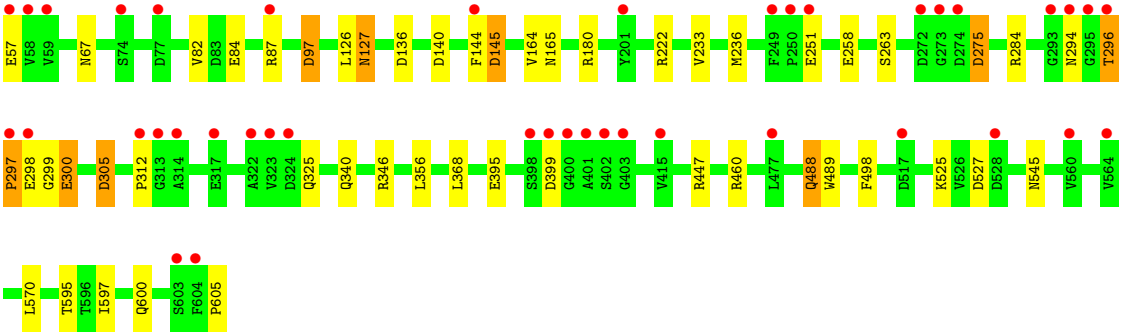




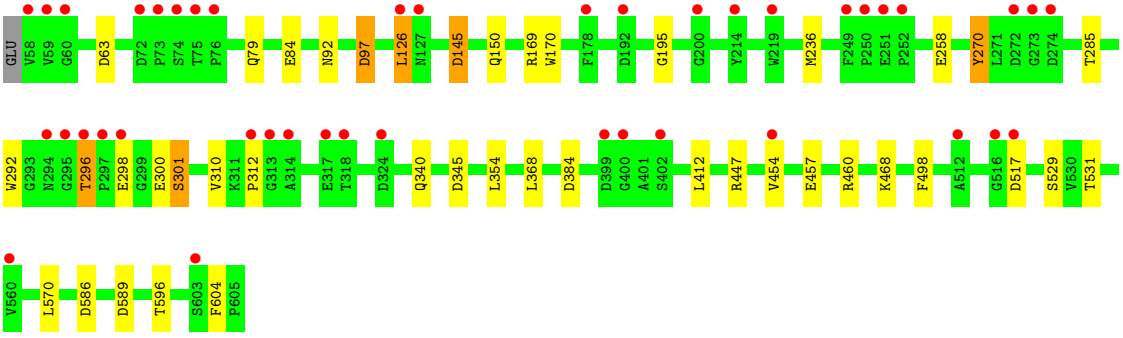
• Molecule 1: Putative secreted protein



• Molecule 1: Putative secreted protein

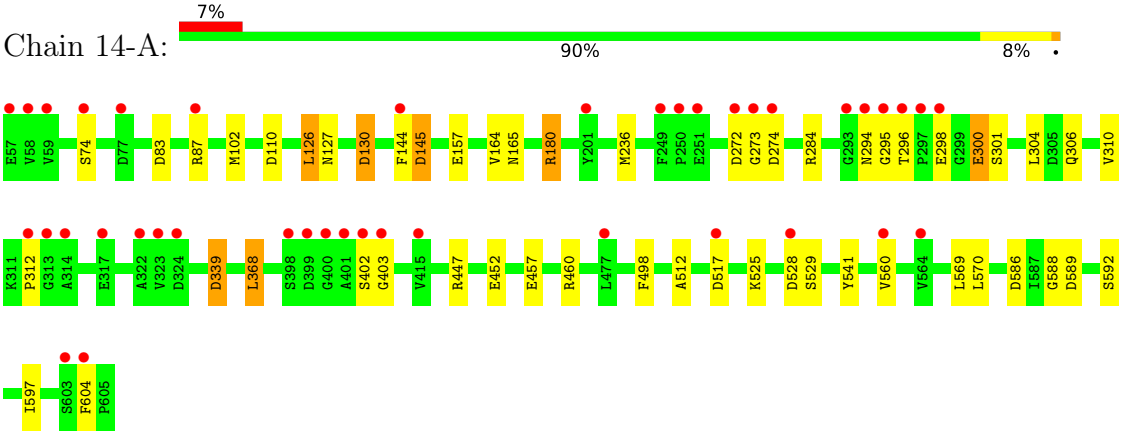


• Molecule 1: Putative secreted protein



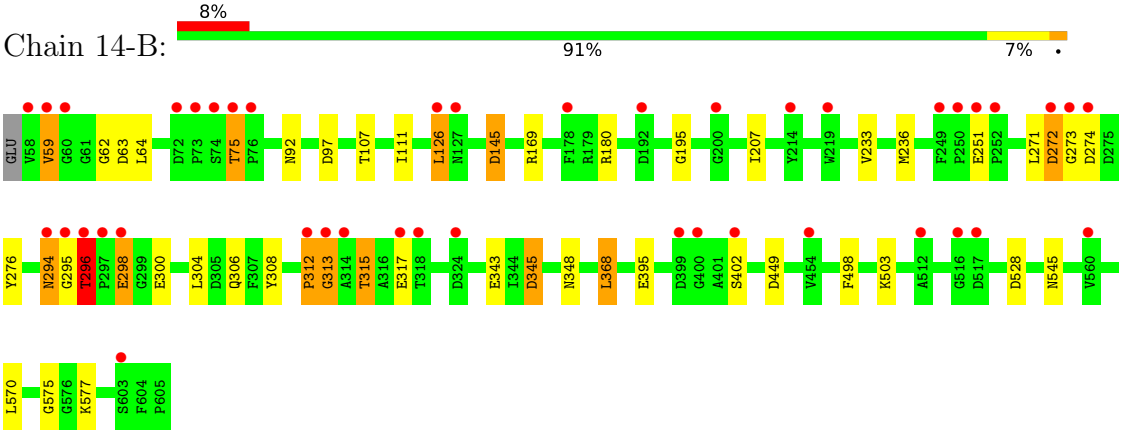
• Molecule 1: Putative secreted protein

Chain 14-A:



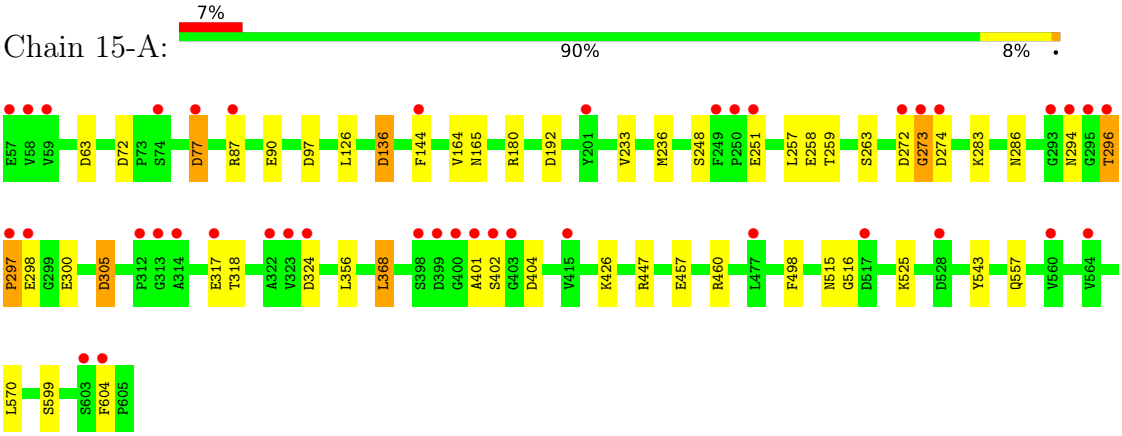
• Molecule 1: Putative secreted protein

Chain 14-B:



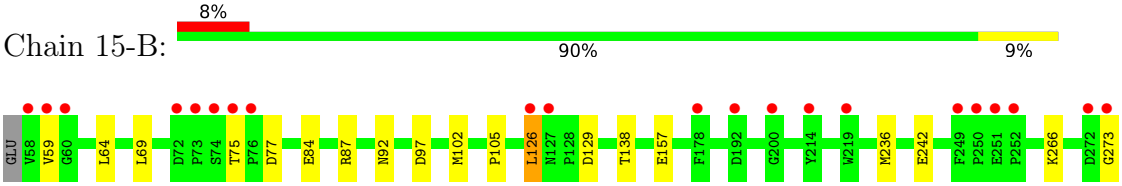
• Molecule 1: Putative secreted protein

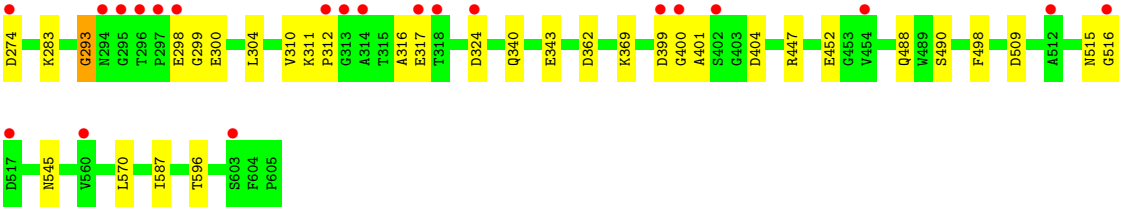
Chain 15-A:



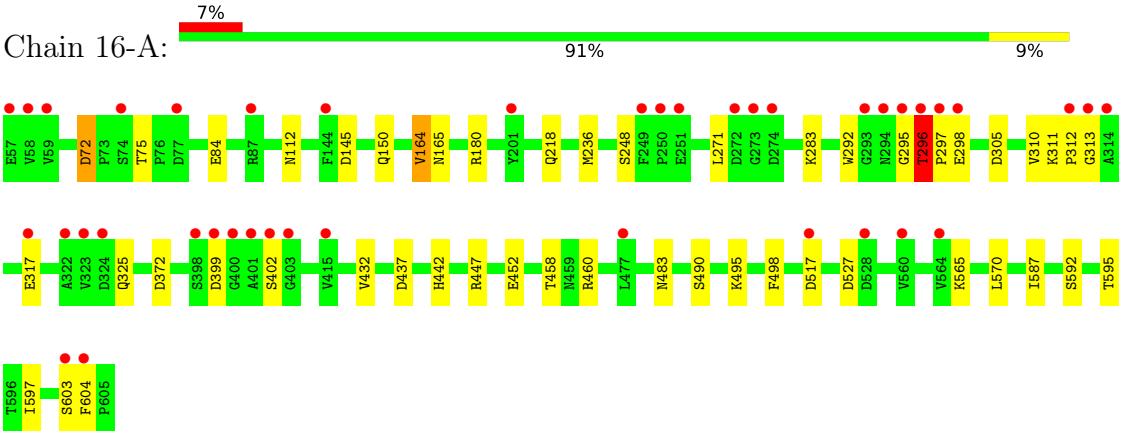
• Molecule 1: Putative secreted protein

Chain 15-B:

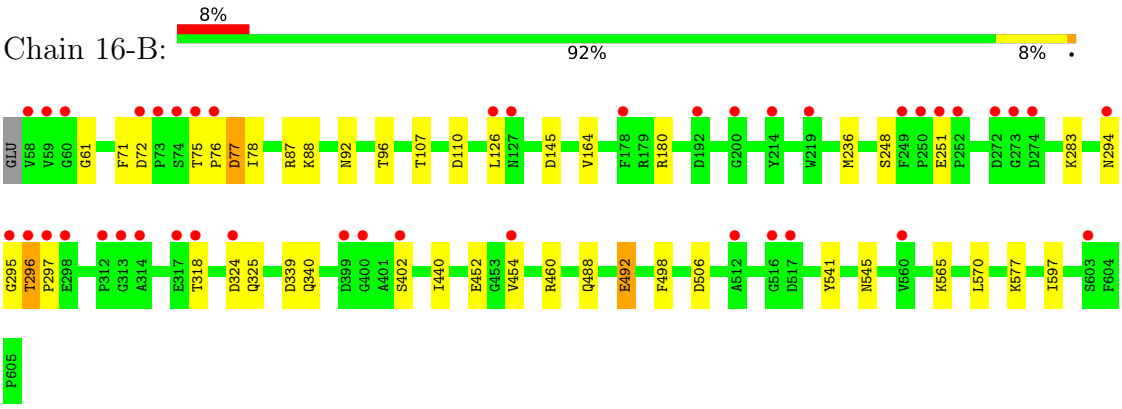




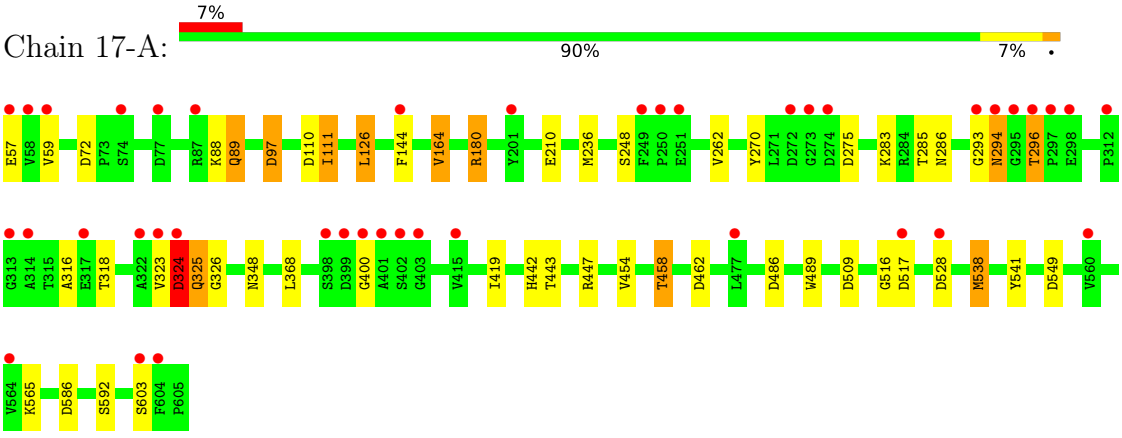
• Molecule 1: Putative secreted protein



• Molecule 1: Putative secreted protein

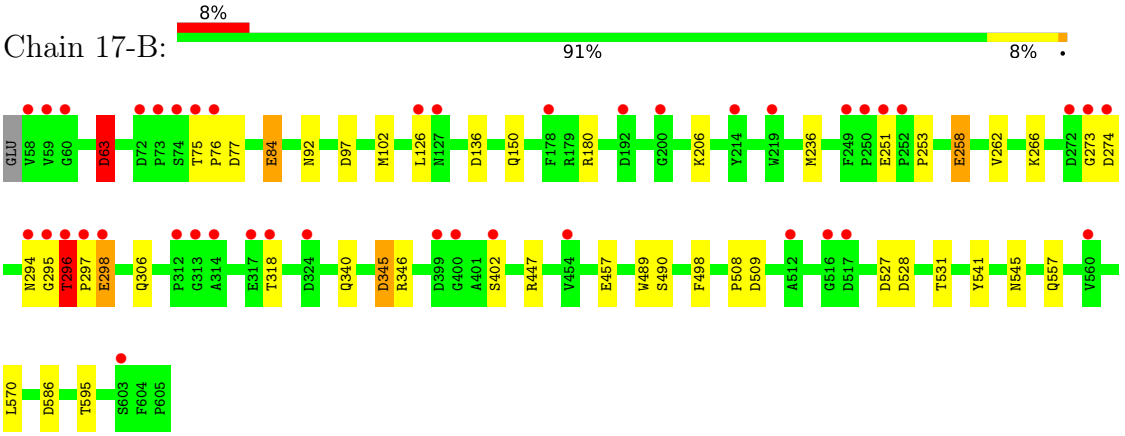


• Molecule 1: Putative secreted protein



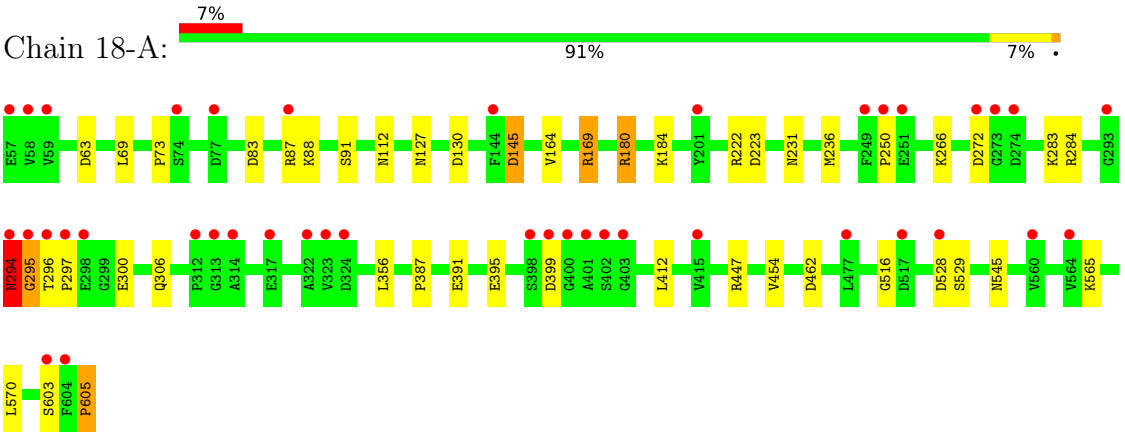
• Molecule 1: Putative secreted protein

Chain 17-B:



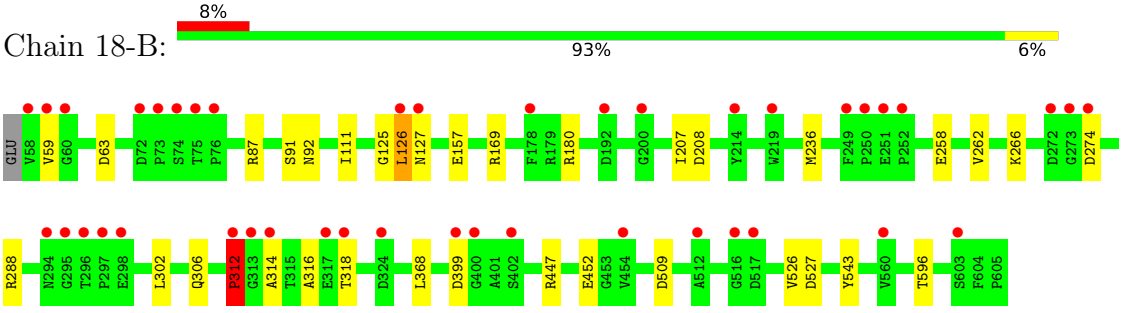
• Molecule 1: Putative secreted protein

Chain 18-A:



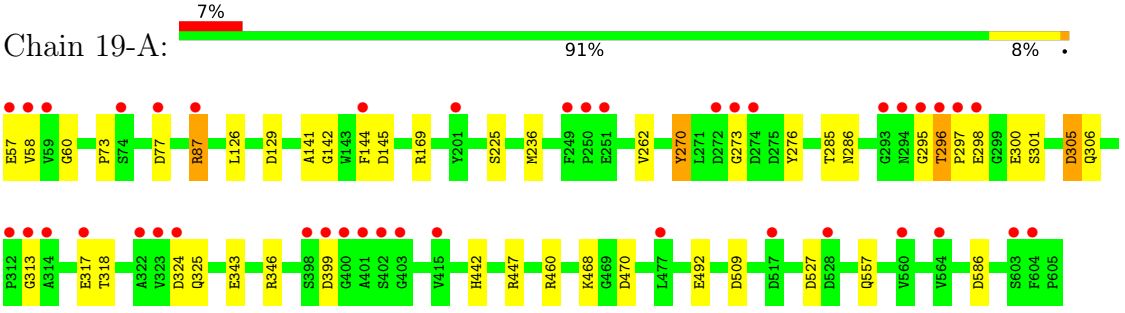
• Molecule 1: Putative secreted protein

Chain 18-B:



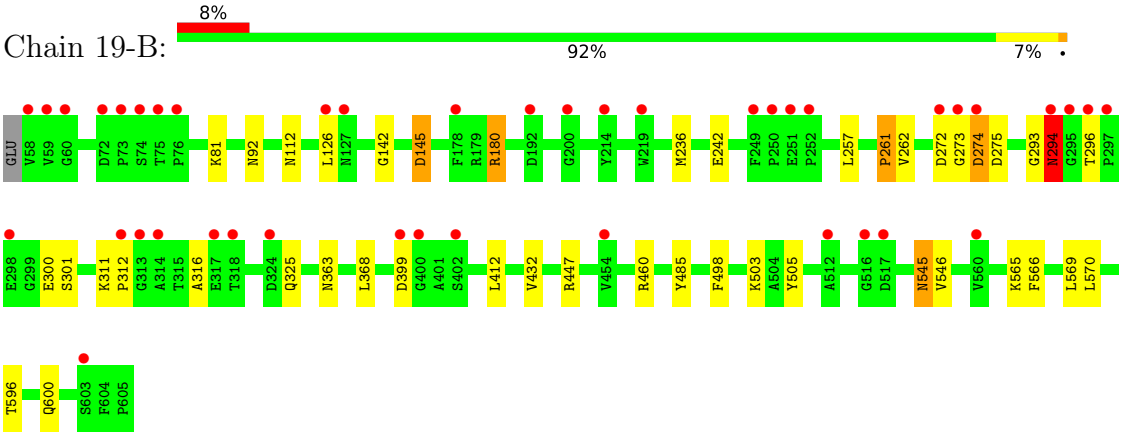
• Molecule 1: Putative secreted protein

Chain 19-A:



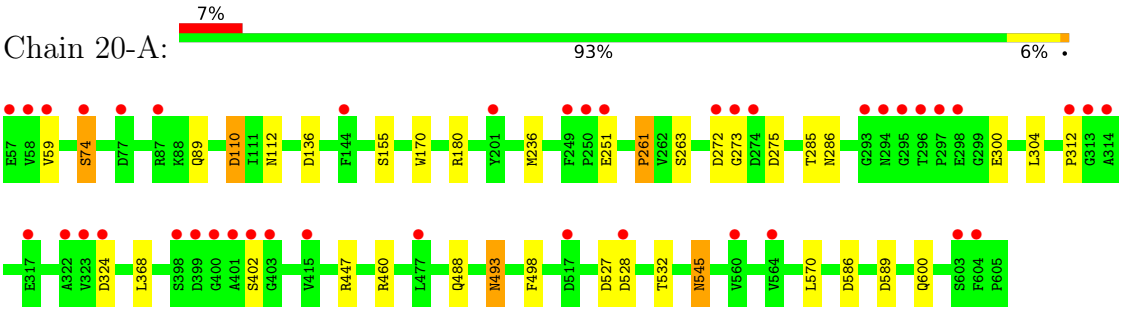
• Molecule 1: Putative secreted protein

Chain 19-B:



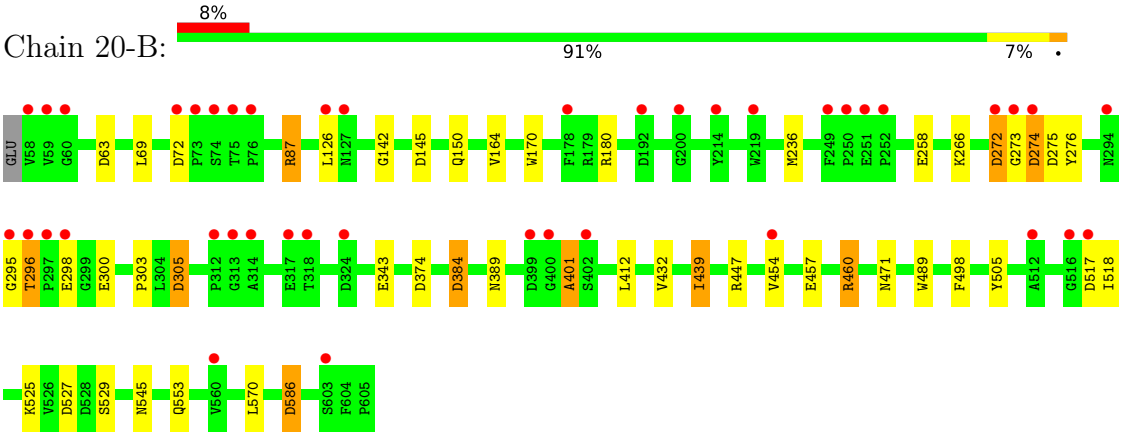
• Molecule 1: Putative secreted protein

Chain 20-A:



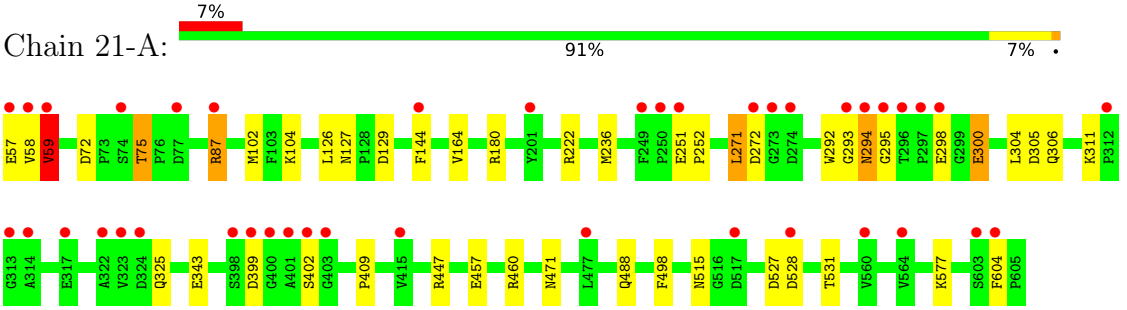
• Molecule 1: Putative secreted protein

Chain 20-B:



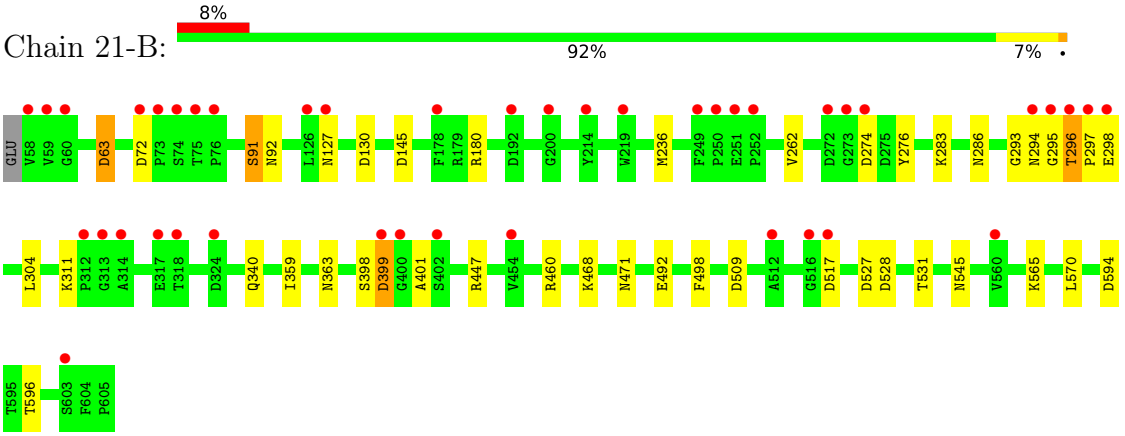
• Molecule 1: Putative secreted protein

Chain 21-A:



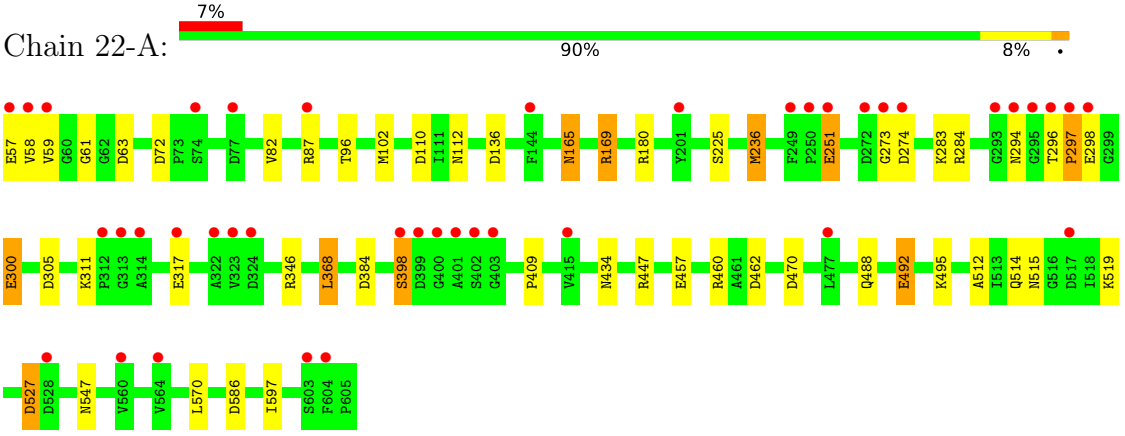
• Molecule 1: Putative secreted protein

Chain 21-B:



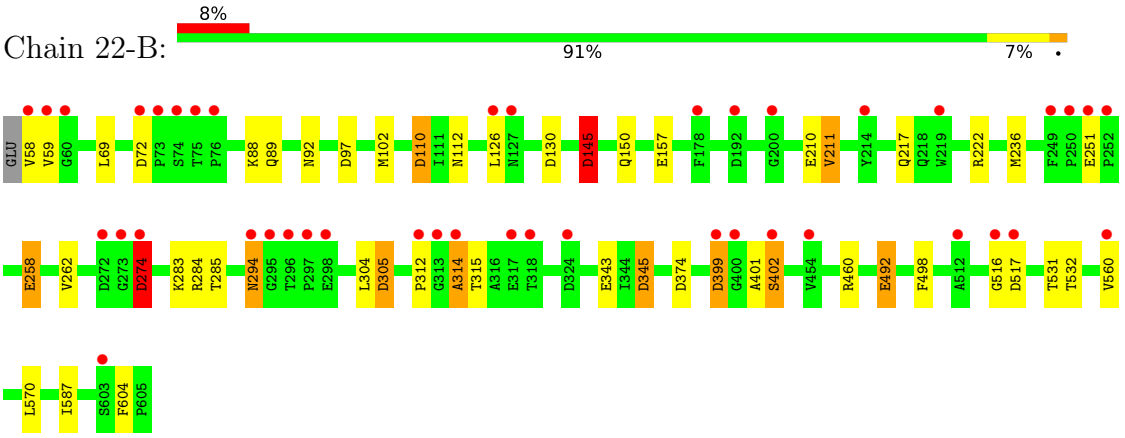
• Molecule 1: Putative secreted protein

Chain 22-A:



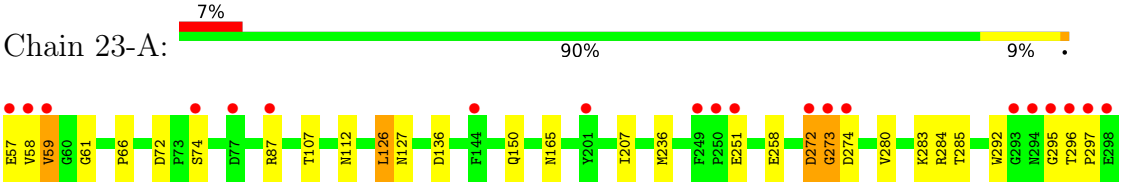
• Molecule 1: Putative secreted protein

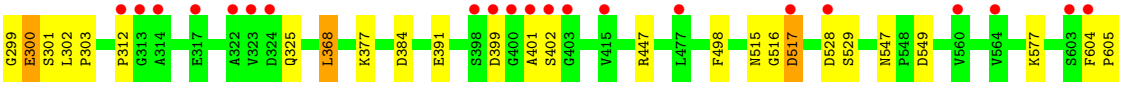
Chain 22-B:



• Molecule 1: Putative secreted protein

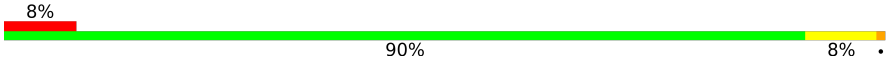
Chain 23-A:

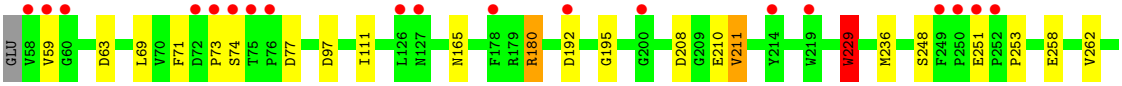


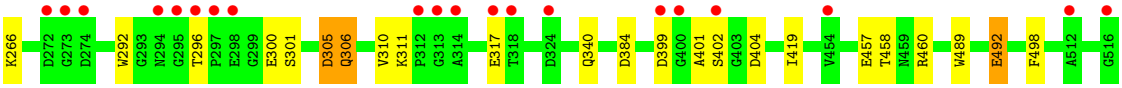


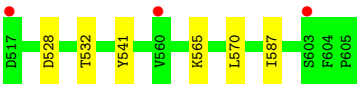
• Molecule 1: Putative secreted protein

Chain 23-B:



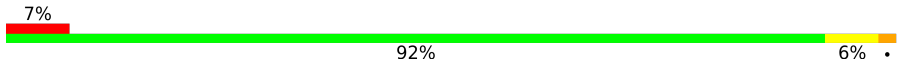


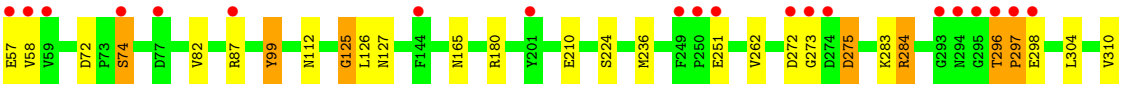


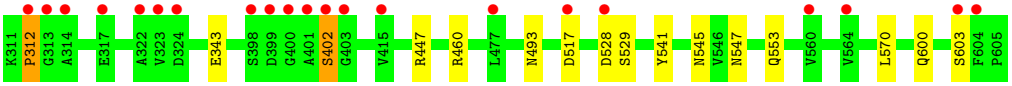


• Molecule 1: Putative secreted protein

Chain 24-A:

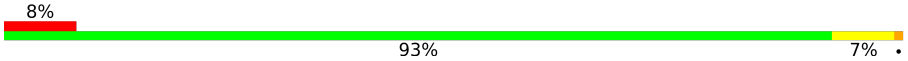


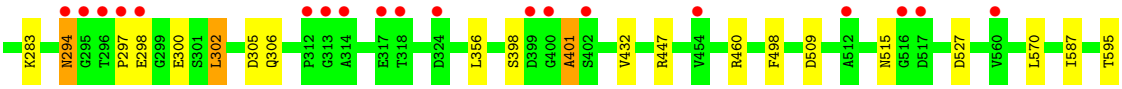




• Molecule 1: Putative secreted protein

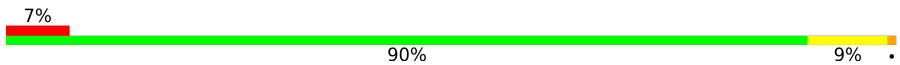
Chain 24-B:

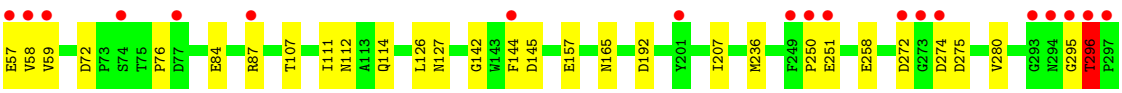


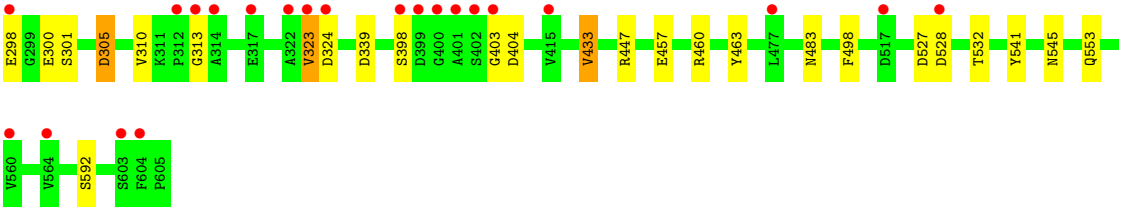


• Molecule 1: Putative secreted protein

Chain 25-A:

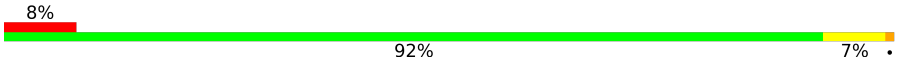


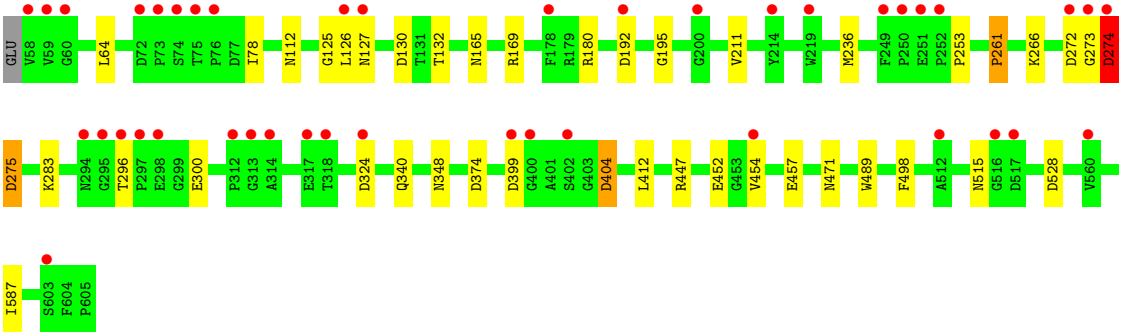




• Molecule 1: Putative secreted protein

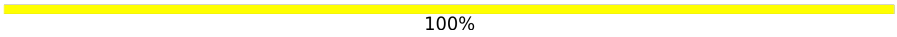
Chain 25-B:





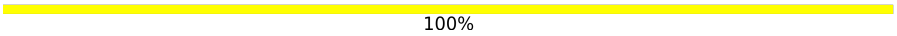
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 1-C:



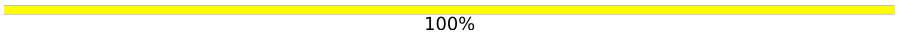
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 1-E:



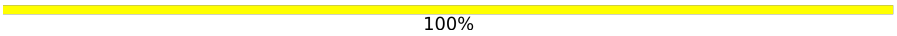
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 2-C:



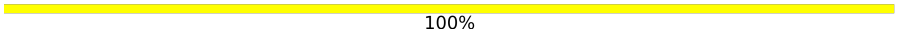
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 2-E:



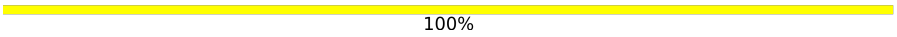
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 3-C:



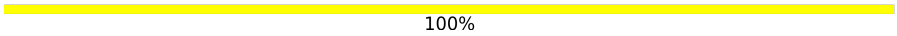
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 3-E:



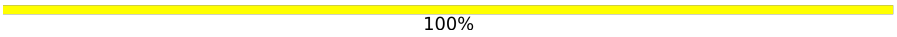
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 4-C:



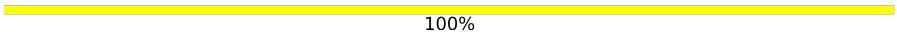
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 4-E:



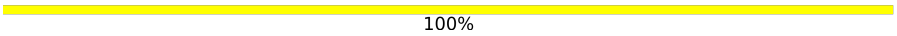
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 5-C:



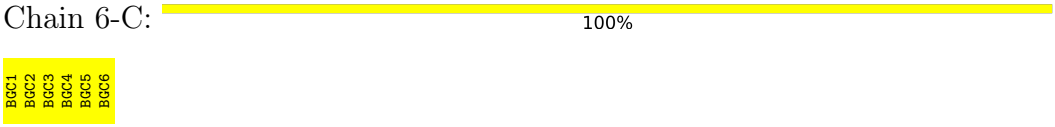
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 5-E:



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

Chain 6-C:



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

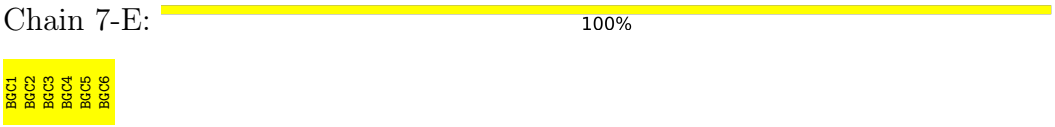
Chain 6-E:

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

Chain 7-C:

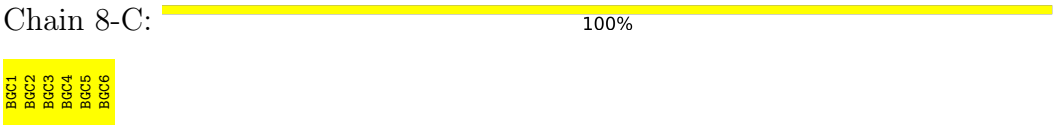
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 7-E:



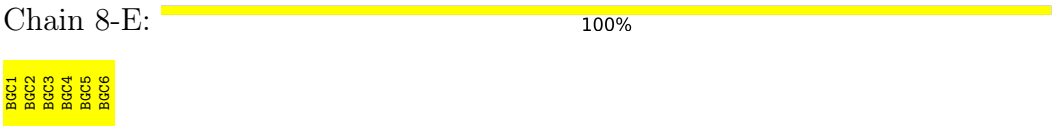
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 8-C:



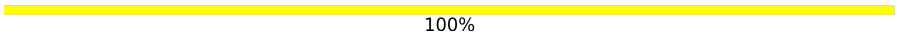
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 8-E:



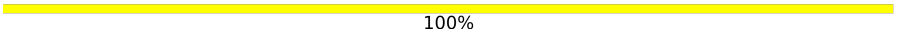
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-C:



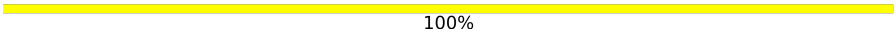
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-E:



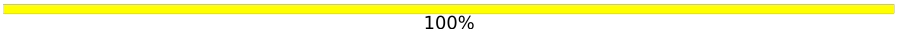
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-C:



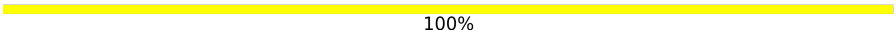
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-E:



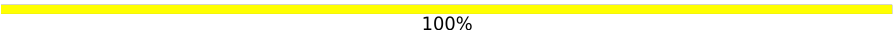
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 11-C:



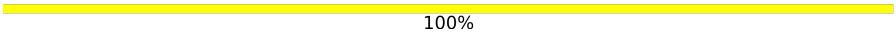
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 11-E:



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

Chain 12-C:



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

Chain 12-E:

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

Chain 13-C:

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

Chain 13-E:

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

Chain 14-C:

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

Chain 14-E:

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

Chain 15-C:

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

Chain 15-E:

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

Chain 16-C:

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

Chain 16-E:

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

Chain 17-C:

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

Chain 17-E:

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

Chain 18-C:

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

Chain 18-E:

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

Chain 19-C:

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

Chain 19-E:

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

Chain 20-C:

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

Chain 20-E:

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

Chain 21-C:

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

Chain 21-E:

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

Chain 22-C:

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

Chain 22-E:

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

Chain 23-C:

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

Chain 23-E:

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

Chain 24-C:

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

Chain 24-E:

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

Chain 25-C:

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

Chain 25-E: 100%

BGC1 BGC2 BGC3 BGC4 BGC5 BGC6

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 1-D: 100%

BGC1 BGC2 BGC3 BGC4 BGC5

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 1-F: 100%

BGC1 BGC2 BGC3 BGC4 BGC5

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 2-D: 100%

BGC1 BGC2 BGC3 BGC4 BGC5

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 2-F: 100%

BGC1 BGC2 BGC3 BGC4 BGC5

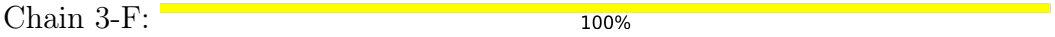
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 3-D: 100%

BGC1 BGC2 BGC3 BGC4 BGC5

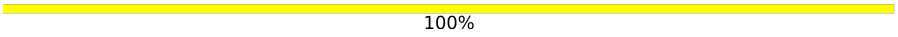
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 3-F:



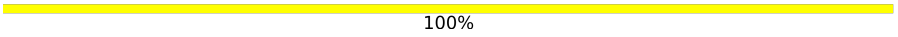
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 4-D:



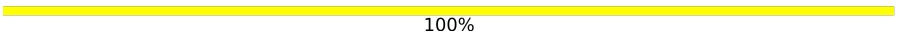
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 4-F:



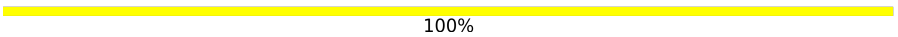
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 5-D:



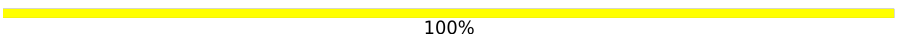
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 5-F:



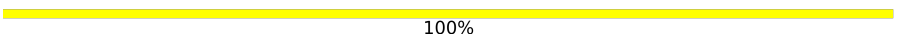
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 6-D:



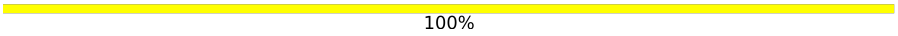
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 6-F:



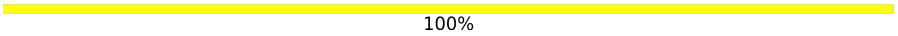
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 7-D:



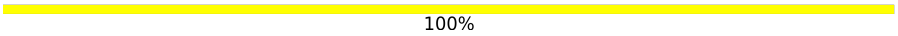
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 7-F:



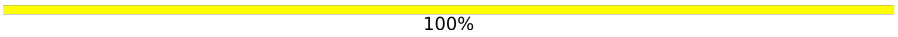
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 8-D:



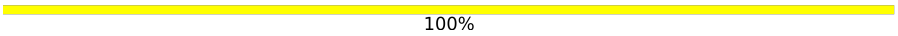
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 8-F:



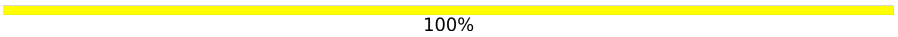
• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-D:



• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-F:



• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 11-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

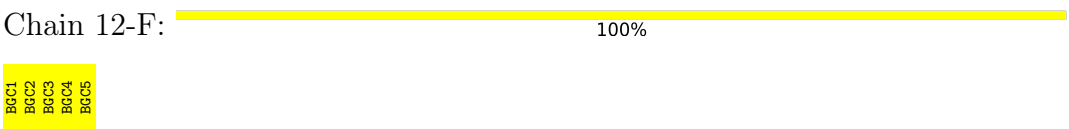
Chain 11-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 12-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 12-F:



• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 13-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 13-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 14-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 14-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 15-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 15-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 16-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 16-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 17-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

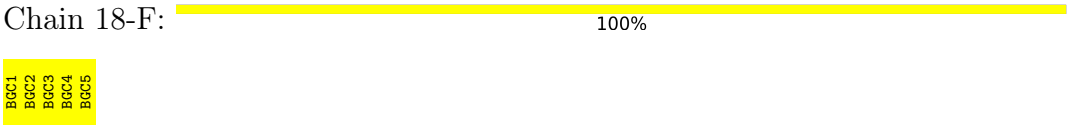
Chain 17-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 18-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 18-F:



• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 19-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 19-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 20-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 20-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 21-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 21-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 22-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 22-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 23-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 23-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 24-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

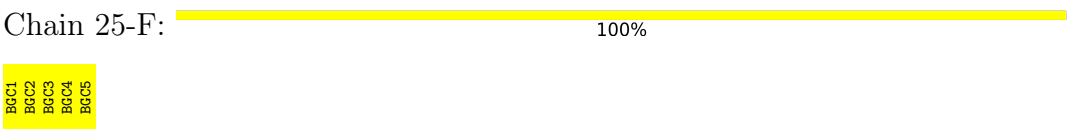
Chain 24-F:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 25-D:

• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 25-F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 0.187	Depositor DCC
R_{free} test set	5640 reflections (5.03%)	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)	0.28 , 229.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	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	0.97	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, BGC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1-A	0.86	3/4280 (0.1%)	0.95	14/5848 (0.2%)
1	1-B	0.87	7/4271 (0.2%)	0.92	6/5836 (0.1%)
1	2-A	0.88	7/4280 (0.2%)	0.96	13/5848 (0.2%)
1	2-B	0.87	6/4271 (0.1%)	0.95	12/5836 (0.2%)
1	3-A	0.86	3/4280 (0.1%)	0.93	11/5848 (0.2%)
1	3-B	0.89	9/4271 (0.2%)	0.97	12/5836 (0.2%)
1	4-A	0.84	4/4280 (0.1%)	0.96	12/5848 (0.2%)
1	4-B	0.86	4/4271 (0.1%)	0.91	5/5836 (0.1%)
1	5-A	0.95	12/4280 (0.3%)	1.03	26/5848 (0.4%)
1	5-B	0.87	5/4271 (0.1%)	0.97	16/5836 (0.3%)
1	6-A	0.89	8/4280 (0.2%)	1.00	14/5848 (0.2%)
1	6-B	0.89	8/4271 (0.2%)	0.97	13/5836 (0.2%)
1	7-A	0.87	7/4280 (0.2%)	0.97	11/5848 (0.2%)
1	7-B	0.83	4/4271 (0.1%)	0.92	6/5836 (0.1%)
1	8-A	0.88	8/4280 (0.2%)	0.98	11/5848 (0.2%)
1	8-B	0.89	11/4271 (0.3%)	0.98	15/5836 (0.3%)
1	9-A	0.90	7/4280 (0.2%)	0.95	10/5848 (0.2%)
1	9-B	0.86	6/4271 (0.1%)	0.90	8/5836 (0.1%)
1	10-A	0.91	9/4280 (0.2%)	0.99	14/5848 (0.2%)
1	10-B	0.88	4/4271 (0.1%)	1.01	14/5836 (0.2%)
1	11-A	0.84	4/4280 (0.1%)	0.94	7/5848 (0.1%)
1	11-B	0.83	3/4271 (0.1%)	0.93	9/5836 (0.2%)
1	12-A	0.89	7/4280 (0.2%)	0.93	8/5848 (0.1%)
1	12-B	0.88	9/4271 (0.2%)	0.98	13/5836 (0.2%)
1	13-A	0.89	7/4280 (0.2%)	0.97	13/5848 (0.2%)
1	13-B	0.84	3/4271 (0.1%)	0.96	17/5836 (0.3%)
1	14-A	0.88	7/4280 (0.2%)	1.00	17/5848 (0.3%)
1	14-B	0.88	5/4271 (0.1%)	0.96	8/5836 (0.1%)
1	15-A	0.88	9/4280 (0.2%)	0.94	13/5848 (0.2%)
1	15-B	0.87	7/4271 (0.2%)	0.98	14/5836 (0.2%)
1	16-A	0.87	5/4280 (0.1%)	0.95	12/5848 (0.2%)
1	16-B	0.85	2/4271 (0.0%)	0.94	11/5836 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	17-A	0.86	2/4280 (0.0%)	0.98	14/5848 (0.2%)
1	17-B	0.87	6/4271 (0.1%)	0.95	10/5836 (0.2%)
1	18-A	0.91	6/4280 (0.1%)	0.98	16/5848 (0.3%)
1	18-B	0.87	5/4271 (0.1%)	0.95	11/5836 (0.2%)
1	19-A	0.86	5/4280 (0.1%)	0.96	17/5848 (0.3%)
1	19-B	0.83	7/4271 (0.2%)	0.93	11/5836 (0.2%)
1	20-A	0.88	4/4280 (0.1%)	0.95	11/5848 (0.2%)
1	20-B	0.84	6/4271 (0.1%)	0.98	16/5836 (0.3%)
1	21-A	0.85	5/4280 (0.1%)	0.94	12/5848 (0.2%)
1	21-B	0.81	4/4271 (0.1%)	0.91	8/5836 (0.1%)
1	22-A	0.89	8/4280 (0.2%)	1.02	21/5848 (0.4%)
1	22-B	0.87	6/4271 (0.1%)	0.95	13/5836 (0.2%)
1	23-A	0.89	4/4280 (0.1%)	0.98	15/5848 (0.3%)
1	23-B	0.88	8/4271 (0.2%)	0.98	8/5836 (0.1%)
1	24-A	0.85	2/4280 (0.0%)	0.95	12/5848 (0.2%)
1	24-B	0.85	5/4271 (0.1%)	0.95	8/5836 (0.1%)
1	25-A	0.86	3/4280 (0.1%)	0.99	14/5848 (0.2%)
1	25-B	0.85	4/4271 (0.1%)	0.95	8/5836 (0.1%)
All	All	0.87	290/213775 (0.1%)	0.96	610/292100 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	1-B	0	4
1	2-A	0	3
1	2-B	0	2
1	3-A	0	1
1	3-B	0	2
1	4-A	0	2
1	4-B	0	1
1	5-A	0	2
1	5-B	0	1
1	6-A	0	5
1	6-B	0	1
1	7-A	0	3
1	7-B	0	1
1	8-A	0	3
1	8-B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	9-A	0	3
1	9-B	0	1
1	10-A	0	1
1	10-B	0	4
1	11-A	0	1
1	12-A	0	2
1	12-B	0	2
1	13-A	0	4
1	13-B	0	1
1	14-A	0	1
1	14-B	0	5
1	15-A	0	1
1	15-B	0	2
1	16-A	0	2
1	16-B	0	2
1	17-A	0	4
1	17-B	1	1
1	18-A	0	1
1	18-B	0	2
1	19-A	0	1
1	19-B	0	3
1	20-A	0	1
1	20-B	0	2
1	21-A	0	1
1	21-B	0	3
1	22-A	0	4
1	22-B	0	1
1	23-A	0	3
1	23-B	0	3
1	24-A	0	2
1	24-B	0	2
1	25-A	0	4
1	25-B	0	2
All	All	1	105

The worst 5 of 290 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	457	GLU	CB-CG	10.83	1.72	1.52
1	24-B	211	VAL	CB-CG2	-10.77	1.30	1.52
1	20-A	170	TRP	CB-CG	-10.53	1.31	1.50
1	10-A	417	VAL	CB-CG2	-10.53	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-B	452	GLU	CB-CG	9.69	1.70	1.52

The worst 5 of 610 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	14-A	460	ARG	NE-CZ-NH2	14.57	127.59	120.30
1	10-B	180	ARG	NE-CZ-NH1	13.36	126.98	120.30
1	24-B	460	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	17-A	538	MET	CG-SD-CE	-12.78	79.76	100.20
1	5-B	97	ASP	CB-CG-OD1	-12.62	106.94	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	17-B	345	ASP	CA

5 of 105 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	73	PRO	Peptide
1	1-B	193	GLY	Peptide
1	1-B	292	TRP	Peptide
1	1-B	299	GLY	Peptide
1	1-B	401	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	4167	3907	3919	0	0
1	1-B	4158	3901	3913	0	0
1	2-A	4167	3907	3919	0	0
1	2-B	4158	3901	3913	0	0
1	3-A	4167	3907	3919	0	0
1	3-B	4158	3901	3913	0	0
1	4-A	4167	3907	3919	0	0
1	4-B	4158	3901	3913	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5-A	4167	3907	3919	0	0
1	5-B	4158	3901	3913	0	0
1	6-A	4167	3907	3919	0	0
1	6-B	4158	3901	3913	0	0
1	7-A	4167	3907	3919	0	0
1	7-B	4158	3901	3913	0	0
1	8-A	4167	3907	3919	0	0
1	8-B	4158	3901	3913	0	0
1	9-A	4167	3907	3919	0	0
1	9-B	4158	3901	3913	0	0
1	10-A	4167	3907	3919	0	0
1	10-B	4158	3901	3913	0	0
1	11-A	4167	3907	3919	0	0
1	11-B	4158	3901	3913	0	0
1	12-A	4167	3907	3919	0	0
1	12-B	4158	3901	3913	0	0
1	13-A	4167	3907	3919	0	0
1	13-B	4158	3901	3913	0	0
1	14-A	4167	3907	3919	0	0
1	14-B	4158	3901	3913	0	0
1	15-A	4167	3907	3919	0	0
1	15-B	4158	3901	3913	0	0
1	16-A	4167	3907	3919	0	0
1	16-B	4158	3901	3913	0	0
1	17-A	4167	3907	3919	0	0
1	17-B	4158	3901	3913	0	0
1	18-A	4167	3907	3919	0	0
1	18-B	4158	3901	3913	0	0
1	19-A	4167	3907	3919	0	0
1	19-B	4158	3901	3913	0	0
1	20-A	4167	3907	3919	0	0
1	20-B	4158	3901	3913	0	0
1	21-A	4167	3907	3919	0	0
1	21-B	4158	3901	3913	0	0
1	22-A	4167	3907	3919	0	0
1	22-B	4158	3901	3913	0	0
1	23-A	4167	3907	3918	0	0
1	23-B	4158	3901	3913	0	0
1	24-A	4167	3907	3919	0	0
1	24-B	4158	3901	3913	0	0
1	25-A	4167	3907	3919	0	0
1	25-B	4158	3901	3913	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1-C	67	0	56	0	0
2	1-E	67	0	56	0	0
2	2-C	67	0	56	0	0
2	2-E	67	0	56	0	0
2	3-C	67	0	56	0	0
2	3-E	67	0	56	0	0
2	4-C	67	0	55	0	0
2	4-E	67	0	56	0	0
2	5-C	67	0	56	0	0
2	5-E	67	0	56	0	0
2	6-C	67	0	56	0	0
2	6-E	67	0	56	0	0
2	7-C	67	0	56	0	0
2	7-E	67	0	56	0	0
2	8-C	67	0	56	0	0
2	8-E	67	0	56	0	0
2	9-C	67	0	56	0	0
2	9-E	67	0	56	0	0
2	10-C	67	0	56	0	0
2	10-E	67	0	56	0	0
2	11-C	67	0	56	0	0
2	11-E	67	0	56	0	0
2	12-C	67	0	56	0	0
2	12-E	67	0	56	0	0
2	13-C	67	0	56	0	0
2	13-E	67	0	56	0	0
2	14-C	67	0	56	0	0
2	14-E	67	0	56	0	0
2	15-C	67	0	56	0	0
2	15-E	67	0	56	0	0
2	16-C	67	0	56	0	0
2	16-E	67	0	56	0	0
2	17-C	67	0	56	0	0
2	17-E	67	0	55	0	0
2	18-C	67	0	56	0	0
2	18-E	67	0	56	0	0
2	19-C	67	0	56	0	0
2	19-E	67	0	55	0	0
2	20-C	67	0	56	0	0
2	20-E	67	0	56	0	0
2	21-C	67	0	56	0	0
2	21-E	67	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	22-C	67	0	56	0	0
2	22-E	67	0	55	0	0
2	23-C	67	0	56	0	0
2	23-E	67	0	56	0	0
2	24-C	67	0	55	0	0
2	24-E	67	0	56	0	0
2	25-C	67	0	56	0	0
2	25-E	67	0	56	0	0
3	1-D	56	0	47	0	0
3	1-F	56	0	47	0	0
3	2-D	56	0	47	0	0
3	2-F	56	0	47	0	0
3	3-D	56	0	47	0	0
3	3-F	56	0	47	0	0
3	4-D	56	0	47	0	0
3	4-F	56	0	47	0	0
3	5-D	56	0	47	0	0
3	5-F	56	0	47	0	0
3	6-D	56	0	47	0	0
3	6-F	56	0	47	0	0
3	7-D	56	0	47	0	0
3	7-F	56	0	47	0	0
3	8-D	56	0	47	0	0
3	8-F	56	0	47	0	0
3	9-D	56	0	47	0	0
3	9-F	56	0	47	0	0
3	10-D	56	0	47	0	0
3	10-F	56	0	47	0	0
3	11-D	56	0	47	0	0
3	11-F	56	0	47	0	0
3	12-D	56	0	47	0	0
3	12-F	56	0	47	0	0
3	13-D	56	0	47	0	0
3	13-F	56	0	47	0	0
3	14-D	56	0	47	0	0
3	14-F	56	0	47	0	0
3	15-D	56	0	47	0	0
3	15-F	56	0	47	0	0
3	16-D	56	0	47	0	0
3	16-F	56	0	47	0	0
3	17-D	56	0	47	0	0
3	17-F	56	0	47	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	18-D	56	0	47	0	0
3	18-F	56	0	47	0	0
3	19-D	56	0	47	0	0
3	19-F	56	0	47	0	0
3	20-D	56	0	47	0	0
3	20-F	56	0	47	0	0
3	21-D	56	0	47	0	0
3	21-F	56	0	47	0	0
3	22-D	56	0	47	0	0
3	22-F	56	0	47	0	0
3	23-D	56	0	47	0	0
3	23-F	56	0	47	0	0
3	24-D	56	0	47	0	0
3	24-F	56	0	47	0	0
3	25-D	56	0	47	0	0
3	25-F	56	0	47	0	0
4	1-A	4	6	6	0	0
4	1-B	4	6	6	0	0
4	2-A	4	6	6	0	0
4	2-B	4	6	6	0	0
4	3-A	4	6	6	0	0
4	3-B	4	6	6	0	0
4	4-A	4	6	6	0	0
4	4-B	4	6	6	0	0
4	5-A	4	6	6	0	0
4	5-B	4	6	6	0	0
4	6-A	4	6	6	0	0
4	6-B	4	6	6	0	0
4	7-A	4	6	6	0	0
4	7-B	4	6	6	0	0
4	8-A	4	6	6	0	0
4	8-B	4	6	6	0	0
4	9-A	4	6	6	0	0
4	9-B	4	6	6	0	0
4	10-A	4	6	6	0	0
4	10-B	4	6	6	0	0
4	11-A	4	6	6	0	0
4	11-B	4	6	6	0	0
4	12-A	4	6	6	0	0
4	12-B	4	6	6	0	0
4	13-A	4	6	6	0	0
4	13-B	4	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	14-A	4	6	6	0	0
4	14-B	4	6	6	0	0
4	15-A	4	6	6	0	0
4	15-B	4	6	6	0	0
4	16-A	4	6	6	0	0
4	16-B	4	6	6	0	0
4	17-A	4	6	6	0	0
4	17-B	4	6	6	0	0
4	18-A	4	6	6	0	0
4	18-B	4	6	6	0	0
4	19-A	4	6	6	0	0
4	19-B	4	6	6	0	0
4	20-A	4	6	6	0	0
4	20-B	4	6	6	0	0
4	21-A	4	6	6	0	0
4	21-B	4	6	6	0	0
4	22-A	4	6	6	0	0
4	22-B	4	6	6	0	0
4	23-A	4	6	6	0	0
4	23-B	4	6	6	0	0
4	24-A	4	6	6	0	0
4	24-B	4	6	6	0	0
4	25-A	4	6	6	0	0
4	25-B	4	6	6	0	0
5	1-A	355	0	0	0	0
5	1-B	381	0	0	0	0
5	2-A	362	0	0	0	0
5	2-B	369	0	0	0	0
5	3-A	360	0	0	0	0
5	3-B	348	0	0	0	0
5	4-A	370	0	0	0	0
5	4-B	377	0	0	0	0
5	5-A	364	0	0	0	0
5	5-B	350	0	0	0	0
5	6-A	356	0	0	0	0
5	6-B	364	0	0	0	0
5	7-A	325	0	0	0	0
5	7-B	377	0	0	0	0
5	8-A	356	0	0	0	0
5	8-B	372	0	0	0	0
5	9-A	327	0	0	0	0
5	9-B	353	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	10-A	365	0	0	0	0
5	10-B	367	0	0	0	0
5	11-A	361	0	0	0	0
5	11-B	357	0	0	0	0
5	12-A	360	0	0	0	0
5	12-B	379	0	0	0	0
5	13-A	335	0	0	0	0
5	13-B	360	0	0	0	0
5	14-A	359	0	0	0	0
5	14-B	392	0	0	0	0
5	15-A	348	0	0	0	0
5	15-B	373	0	0	0	0
5	16-A	369	0	0	0	0
5	16-B	361	0	0	0	0
5	17-A	351	0	0	0	0
5	17-B	377	0	0	0	0
5	18-A	349	0	0	0	0
5	18-B	373	0	0	0	0
5	19-A	346	0	0	0	0
5	19-B	355	0	0	0	0
5	20-A	324	0	0	0	0
5	20-B	372	0	0	0	0
5	21-A	347	0	0	0	0
5	21-B	370	0	0	0	0
5	22-A	338	0	0	0	0
5	22-B	386	0	0	0	0
5	23-A	366	0	0	0	0
5	23-B	332	0	0	0	0
5	24-A	364	0	0	0	0
5	24-B	360	0	0	0	0
5	25-A	359	0	0	0	0
5	25-B	372	0	0	0	0
All	All	232468	195500	201244	0	0

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1-A	547/549 (100%)	500 (91%)	38 (7%)	9 (2%)	9 1
1	1-B	546/549 (100%)	515 (94%)	28 (5%)	3 (0%)	29 12
1	2-A	547/549 (100%)	509 (93%)	35 (6%)	3 (0%)	29 12
1	2-B	546/549 (100%)	510 (93%)	31 (6%)	5 (1%)	17 5
1	3-A	547/549 (100%)	511 (93%)	34 (6%)	2 (0%)	34 17
1	3-B	546/549 (100%)	506 (93%)	34 (6%)	6 (1%)	14 3
1	4-A	547/549 (100%)	505 (92%)	32 (6%)	10 (2%)	8 1
1	4-B	546/549 (100%)	509 (93%)	36 (7%)	1 (0%)	47 29
1	5-A	547/549 (100%)	510 (93%)	29 (5%)	8 (2%)	10 2
1	5-B	546/549 (100%)	509 (93%)	29 (5%)	8 (2%)	10 2
1	6-A	547/549 (100%)	505 (92%)	36 (7%)	6 (1%)	14 3
1	6-B	546/549 (100%)	513 (94%)	27 (5%)	6 (1%)	14 3
1	7-A	547/549 (100%)	511 (93%)	30 (6%)	6 (1%)	14 3
1	7-B	546/549 (100%)	511 (94%)	29 (5%)	6 (1%)	14 3
1	8-A	547/549 (100%)	511 (93%)	29 (5%)	7 (1%)	12 2
1	8-B	546/549 (100%)	510 (93%)	28 (5%)	8 (2%)	10 2
1	9-A	547/549 (100%)	507 (93%)	32 (6%)	8 (2%)	10 2
1	9-B	546/549 (100%)	511 (94%)	32 (6%)	3 (0%)	29 12
1	10-A	547/549 (100%)	507 (93%)	34 (6%)	6 (1%)	14 3
1	10-B	546/549 (100%)	504 (92%)	31 (6%)	11 (2%)	7 1
1	11-A	547/549 (100%)	514 (94%)	33 (6%)	0	100 100
1	11-B	546/549 (100%)	507 (93%)	35 (6%)	4 (1%)	22 8
1	12-A	547/549 (100%)	509 (93%)	30 (6%)	8 (2%)	10 2
1	12-B	546/549 (100%)	507 (93%)	31 (6%)	8 (2%)	10 2
1	13-A	547/549 (100%)	510 (93%)	30 (6%)	7 (1%)	12 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13-B	546/549 (100%)	506 (93%)	34 (6%)	6 (1%)	14	3
1	14-A	547/549 (100%)	509 (93%)	28 (5%)	10 (2%)	8	1
1	14-B	546/549 (100%)	504 (92%)	29 (5%)	13 (2%)	6	1
1	15-A	547/549 (100%)	510 (93%)	28 (5%)	9 (2%)	9	1
1	15-B	546/549 (100%)	506 (93%)	33 (6%)	7 (1%)	12	2
1	16-A	547/549 (100%)	514 (94%)	27 (5%)	6 (1%)	14	3
1	16-B	546/549 (100%)	511 (94%)	28 (5%)	7 (1%)	12	2
1	17-A	547/549 (100%)	505 (92%)	29 (5%)	13 (2%)	6	1
1	17-B	546/549 (100%)	509 (93%)	28 (5%)	9 (2%)	9	1
1	18-A	547/549 (100%)	507 (93%)	34 (6%)	6 (1%)	14	3
1	18-B	546/549 (100%)	509 (93%)	33 (6%)	4 (1%)	22	8
1	19-A	547/549 (100%)	505 (92%)	34 (6%)	8 (2%)	10	2
1	19-B	546/549 (100%)	506 (93%)	32 (6%)	8 (2%)	10	2
1	20-A	547/549 (100%)	515 (94%)	26 (5%)	6 (1%)	14	3
1	20-B	546/549 (100%)	506 (93%)	33 (6%)	7 (1%)	12	2
1	21-A	547/549 (100%)	508 (93%)	30 (6%)	9 (2%)	9	1
1	21-B	546/549 (100%)	514 (94%)	26 (5%)	6 (1%)	14	3
1	22-A	547/549 (100%)	510 (93%)	34 (6%)	3 (0%)	29	12
1	22-B	546/549 (100%)	501 (92%)	33 (6%)	12 (2%)	6	1
1	23-A	547/549 (100%)	496 (91%)	37 (7%)	14 (3%)	5	0
1	23-B	546/549 (100%)	510 (93%)	29 (5%)	7 (1%)	12	2
1	24-A	547/549 (100%)	504 (92%)	34 (6%)	9 (2%)	9	1
1	24-B	546/549 (100%)	514 (94%)	27 (5%)	5 (1%)	17	5
1	25-A	547/549 (100%)	501 (92%)	36 (7%)	10 (2%)	8	1
1	25-B	546/549 (100%)	508 (93%)	32 (6%)	6 (1%)	14	3
All	All	27325/27450 (100%)	25409 (93%)	1567 (6%)	349 (1%)	12	2

5 of 349 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	58	VAL
1	1-A	59	VAL
1	1-A	61	GLY

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Mol	Chain	Res	Type
1	1-A	63	ASP
1	1-A	75	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1-A	436/436 (100%)	407 (93%)	29 (7%)	16 3
1	1-B	435/436 (100%)	404 (93%)	31 (7%)	14 2
1	2-A	436/436 (100%)	409 (94%)	27 (6%)	18 4
1	2-B	435/436 (100%)	401 (92%)	34 (8%)	12 2
1	3-A	436/436 (100%)	413 (95%)	23 (5%)	22 5
1	3-B	435/436 (100%)	401 (92%)	34 (8%)	12 2
1	4-A	436/436 (100%)	401 (92%)	35 (8%)	12 1
1	4-B	435/436 (100%)	402 (92%)	33 (8%)	13 2
1	5-A	436/436 (100%)	397 (91%)	39 (9%)	9 1
1	5-B	435/436 (100%)	405 (93%)	30 (7%)	15 2
1	6-A	436/436 (100%)	402 (92%)	34 (8%)	12 2
1	6-B	435/436 (100%)	405 (93%)	30 (7%)	15 2
1	7-A	436/436 (100%)	411 (94%)	25 (6%)	20 5
1	7-B	435/436 (100%)	407 (94%)	28 (6%)	17 3
1	8-A	436/436 (100%)	411 (94%)	25 (6%)	20 5
1	8-B	435/436 (100%)	400 (92%)	35 (8%)	12 1
1	9-A	436/436 (100%)	405 (93%)	31 (7%)	14 2
1	9-B	435/436 (100%)	412 (95%)	23 (5%)	22 5
1	10-A	436/436 (100%)	407 (93%)	29 (7%)	16 3
1	10-B	435/436 (100%)	409 (94%)	26 (6%)	19 4
1	11-A	436/436 (100%)	411 (94%)	25 (6%)	20 5
1	11-B	435/436 (100%)	406 (93%)	29 (7%)	16 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	12-A	436/436 (100%)	405 (93%)	31 (7%)	14 2
1	12-B	435/436 (100%)	411 (94%)	24 (6%)	21 5
1	13-A	436/436 (100%)	403 (92%)	33 (8%)	13 2
1	13-B	435/436 (100%)	410 (94%)	25 (6%)	20 5
1	14-A	436/436 (100%)	404 (93%)	32 (7%)	14 2
1	14-B	435/436 (100%)	403 (93%)	32 (7%)	13 2
1	15-A	436/436 (100%)	403 (92%)	33 (8%)	13 2
1	15-B	435/436 (100%)	406 (93%)	29 (7%)	16 3
1	16-A	436/436 (100%)	404 (93%)	32 (7%)	14 2
1	16-B	435/436 (100%)	405 (93%)	30 (7%)	15 2
1	17-A	436/436 (100%)	400 (92%)	36 (8%)	11 1
1	17-B	435/436 (100%)	403 (93%)	32 (7%)	13 2
1	18-A	436/436 (100%)	405 (93%)	31 (7%)	14 2
1	18-B	435/436 (100%)	415 (95%)	20 (5%)	27 8
1	19-A	436/436 (100%)	412 (94%)	24 (6%)	21 5
1	19-B	435/436 (100%)	409 (94%)	26 (6%)	19 4
1	20-A	436/436 (100%)	411 (94%)	25 (6%)	20 5
1	20-B	435/436 (100%)	401 (92%)	34 (8%)	12 2
1	21-A	436/436 (100%)	406 (93%)	30 (7%)	15 2
1	21-B	435/436 (100%)	407 (94%)	28 (6%)	17 3
1	22-A	436/436 (100%)	400 (92%)	36 (8%)	11 1
1	22-B	435/436 (100%)	400 (92%)	35 (8%)	12 1
1	23-A	436/436 (100%)	402 (92%)	34 (8%)	12 2
1	23-B	435/436 (100%)	398 (92%)	37 (8%)	10 1
1	24-A	436/436 (100%)	406 (93%)	30 (7%)	15 2
1	24-B	435/436 (100%)	407 (94%)	28 (6%)	17 3
1	25-A	436/436 (100%)	402 (92%)	34 (8%)	12 2
1	25-B	435/436 (100%)	406 (93%)	29 (7%)	16 3
All	All	21775/21800 (100%)	20270 (93%)	1505 (7%)	15 2

5 of 1505 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	16-B	71	PHE
1	20-A	570	LEU
1	16-B	570	LEU
1	16-A	603	SER
1	18-A	283	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 451 such sidechains are listed below:

Mol	Chain	Res	Type
1	14-B	340	GLN
1	25-B	112	ASN
1	17-B	306	GLN
1	25-A	483	ASN
1	23-B	127	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	1.59	3 (25%)	17,17,17	1.36	2 (11%)
2	BGC	1-C	2	2	11,11,12	1.41	3 (27%)	15,15,17	1.43	2 (13%)
2	BGC	1-C	3	2	11,11,12	1.51	3 (27%)	15,15,17	1.32	1 (6%)
2	BGC	1-C	4	2	11,11,12	0.99	1 (9%)	15,15,17	1.69	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	1-C	5	2	11,11,12	1.15	1 (9%)	15,15,17	1.44	2 (13%)
2	BGC	1-C	6	2	11,11,12	1.34	2 (18%)	15,15,17	1.37	3 (20%)
3	BGC	1-D	1	3	12,12,12	1.29	1 (8%)	17,17,17	1.08	0
3	BGC	1-D	2	3	11,11,12	1.46	1 (9%)	15,15,17	1.55	1 (6%)
3	BGC	1-D	3	3	11,11,12	1.28	1 (9%)	15,15,17	1.53	3 (20%)
3	BGC	1-D	4	3	11,11,12	1.34	2 (18%)	15,15,17	1.23	1 (6%)
3	BGC	1-D	5	3	11,11,12	1.56	1 (9%)	15,15,17	1.12	1 (6%)
2	BGC	1-E	1	2	12,12,12	1.57	3 (25%)	17,17,17	1.08	0
2	BGC	1-E	2	2	11,11,12	1.49	3 (27%)	15,15,17	1.29	2 (13%)
2	BGC	1-E	3	2	11,11,12	1.38	1 (9%)	15,15,17	1.36	2 (13%)
2	BGC	1-E	4	2	11,11,12	0.84	1 (9%)	15,15,17	1.43	2 (13%)
2	BGC	1-E	5	2	11,11,12	1.29	2 (18%)	15,15,17	2.09	2 (13%)
2	BGC	1-E	6	2	11,11,12	1.42	3 (27%)	15,15,17	1.07	1 (6%)
3	BGC	1-F	1	3	12,12,12	1.32	2 (16%)	17,17,17	1.00	1 (5%)
3	BGC	1-F	2	3	11,11,12	1.57	1 (9%)	15,15,17	1.68	3 (20%)
3	BGC	1-F	3	3	11,11,12	1.33	1 (9%)	15,15,17	2.83	3 (20%)
3	BGC	1-F	4	3	11,11,12	1.20	2 (18%)	15,15,17	0.95	1 (6%)
3	BGC	1-F	5	3	11,11,12	1.75	1 (9%)	15,15,17	0.86	0
2	BGC	10-C	1	2	12,12,12	1.65	3 (25%)	17,17,17	1.08	1 (5%)
2	BGC	10-C	2	2	11,11,12	1.37	3 (27%)	15,15,17	1.49	3 (20%)
2	BGC	10-C	3	2	11,11,12	1.37	3 (27%)	15,15,17	1.26	2 (13%)
2	BGC	10-C	4	2	11,11,12	0.89	0	15,15,17	1.16	1 (6%)
2	BGC	10-C	5	2	11,11,12	1.23	1 (9%)	15,15,17	1.58	2 (13%)
2	BGC	10-C	6	2	11,11,12	1.35	3 (27%)	15,15,17	1.04	1 (6%)
3	BGC	10-D	1	3	12,12,12	1.30	1 (8%)	17,17,17	1.21	0
3	BGC	10-D	2	3	11,11,12	1.45	1 (9%)	15,15,17	1.68	2 (13%)
3	BGC	10-D	3	3	11,11,12	1.29	2 (18%)	15,15,17	1.51	2 (13%)
3	BGC	10-D	4	3	11,11,12	1.23	2 (18%)	15,15,17	1.27	2 (13%)
3	BGC	10-D	5	3	11,11,12	1.60	1 (9%)	15,15,17	1.34	2 (13%)
2	BGC	10-E	1	2	12,12,12	1.68	3 (25%)	17,17,17	1.02	1 (5%)
2	BGC	10-E	2	2	11,11,12	1.57	3 (27%)	15,15,17	1.15	2 (13%)
2	BGC	10-E	3	2	11,11,12	1.38	2 (18%)	15,15,17	1.17	1 (6%)
2	BGC	10-E	4	2	11,11,12	0.83	1 (9%)	15,15,17	1.44	2 (13%)
2	BGC	10-E	5	2	11,11,12	1.37	3 (27%)	15,15,17	1.38	3 (20%)
2	BGC	10-E	6	2	11,11,12	1.46	2 (18%)	15,15,17	2.10	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	10-F	1	3	12,12,12	1.34	2 (16%)	17,17,17	1.02	0
3	BGC	10-F	2	3	11,11,12	1.58	2 (18%)	15,15,17	1.50	3 (20%)
3	BGC	10-F	3	3	11,11,12	1.09	1 (9%)	15,15,17	1.47	3 (20%)
3	BGC	10-F	4	3	11,11,12	1.43	2 (18%)	15,15,17	1.11	1 (6%)
3	BGC	10-F	5	3	11,11,12	1.63	1 (9%)	15,15,17	0.91	0
2	BGC	11-C	1	2	12,12,12	1.67	3 (25%)	17,17,17	1.04	2 (11%)
2	BGC	11-C	2	2	11,11,12	1.49	3 (27%)	15,15,17	1.82	3 (20%)
2	BGC	11-C	3	2	11,11,12	1.34	3 (27%)	15,15,17	1.27	2 (13%)
2	BGC	11-C	4	2	11,11,12	1.01	0	15,15,17	1.28	1 (6%)
2	BGC	11-C	5	2	11,11,12	1.27	1 (9%)	15,15,17	1.59	1 (6%)
2	BGC	11-C	6	2	11,11,12	1.36	2 (18%)	15,15,17	1.50	5 (33%)
3	BGC	11-D	1	3	12,12,12	1.29	1 (8%)	17,17,17	1.39	2 (11%)
3	BGC	11-D	2	3	11,11,12	1.31	1 (9%)	15,15,17	1.56	3 (20%)
3	BGC	11-D	3	3	11,11,12	1.35	1 (9%)	15,15,17	1.69	4 (26%)
3	BGC	11-D	4	3	11,11,12	1.58	2 (18%)	15,15,17	2.35	7 (46%)
3	BGC	11-D	5	3	11,11,12	1.71	1 (9%)	15,15,17	1.67	2 (13%)
2	BGC	11-E	1	2	12,12,12	1.69	3 (25%)	17,17,17	1.46	4 (23%)
2	BGC	11-E	2	2	11,11,12	1.53	3 (27%)	15,15,17	1.03	1 (6%)
2	BGC	11-E	3	2	11,11,12	1.30	1 (9%)	15,15,17	1.47	2 (13%)
2	BGC	11-E	4	2	11,11,12	0.96	1 (9%)	15,15,17	1.22	2 (13%)
2	BGC	11-E	5	2	11,11,12	1.21	1 (9%)	15,15,17	1.64	2 (13%)
2	BGC	11-E	6	2	11,11,12	1.43	3 (27%)	15,15,17	1.34	3 (20%)
3	BGC	11-F	1	3	12,12,12	1.35	2 (16%)	17,17,17	1.28	3 (17%)
3	BGC	11-F	2	3	11,11,12	1.65	2 (18%)	15,15,17	1.57	2 (13%)
3	BGC	11-F	3	3	11,11,12	1.39	2 (18%)	15,15,17	2.04	4 (26%)
3	BGC	11-F	4	3	11,11,12	1.11	1 (9%)	15,15,17	0.96	0
3	BGC	11-F	5	3	11,11,12	1.59	1 (9%)	15,15,17	0.94	1 (6%)
2	BGC	12-C	1	2	12,12,12	1.75	3 (25%)	17,17,17	1.63	5 (29%)
2	BGC	12-C	2	2	11,11,12	1.42	3 (27%)	15,15,17	1.47	3 (20%)
2	BGC	12-C	3	2	11,11,12	1.43	3 (27%)	15,15,17	1.54	4 (26%)
2	BGC	12-C	4	2	11,11,12	0.88	0	15,15,17	1.33	3 (20%)
2	BGC	12-C	5	2	11,11,12	1.33	1 (9%)	15,15,17	1.29	1 (6%)
2	BGC	12-C	6	2	11,11,12	1.45	2 (18%)	15,15,17	1.66	5 (33%)
3	BGC	12-D	1	3	12,12,12	1.33	2 (16%)	17,17,17	1.37	4 (23%)
3	BGC	12-D	2	3	11,11,12	1.57	2 (18%)	15,15,17	2.07	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	12-D	3	3	11,11,12	1.45	1 (9%)	15,15,17	1.59	3 (20%)
3	BGC	12-D	4	3	11,11,12	1.27	1 (9%)	15,15,17	1.32	3 (20%)
3	BGC	12-D	5	3	11,11,12	1.63	1 (9%)	15,15,17	1.30	3 (20%)
2	BGC	12-E	1	2	12,12,12	1.69	3 (25%)	17,17,17	1.32	3 (17%)
2	BGC	12-E	2	2	11,11,12	1.41	3 (27%)	15,15,17	1.26	1 (6%)
2	BGC	12-E	3	2	11,11,12	1.25	1 (9%)	15,15,17	1.33	2 (13%)
2	BGC	12-E	4	2	11,11,12	0.68	0	15,15,17	1.45	4 (26%)
2	BGC	12-E	5	2	11,11,12	1.50	3 (27%)	15,15,17	1.91	3 (20%)
2	BGC	12-E	6	2	11,11,12	1.47	2 (18%)	15,15,17	1.26	2 (13%)
3	BGC	12-F	1	3	12,12,12	1.29	2 (16%)	17,17,17	0.99	1 (5%)
3	BGC	12-F	2	3	11,11,12	1.57	2 (18%)	15,15,17	1.57	2 (13%)
3	BGC	12-F	3	3	11,11,12	1.22	1 (9%)	15,15,17	1.25	2 (13%)
3	BGC	12-F	4	3	11,11,12	1.36	2 (18%)	15,15,17	1.07	0
3	BGC	12-F	5	3	11,11,12	1.73	1 (9%)	15,15,17	0.79	1 (6%)
2	BGC	13-C	1	2	12,12,12	1.75	3 (25%)	17,17,17	1.65	2 (11%)
2	BGC	13-C	2	2	11,11,12	1.43	3 (27%)	15,15,17	1.44	3 (20%)
2	BGC	13-C	3	2	11,11,12	1.64	3 (27%)	15,15,17	1.46	2 (13%)
2	BGC	13-C	4	2	11,11,12	1.00	1 (9%)	15,15,17	1.95	4 (26%)
2	BGC	13-C	5	2	11,11,12	1.32	1 (9%)	15,15,17	1.22	2 (13%)
2	BGC	13-C	6	2	11,11,12	1.38	1 (9%)	15,15,17	2.32	5 (33%)
3	BGC	13-D	1	3	12,12,12	1.29	1 (8%)	17,17,17	1.23	1 (5%)
3	BGC	13-D	2	3	11,11,12	1.38	1 (9%)	15,15,17	1.89	3 (20%)
3	BGC	13-D	3	3	11,11,12	1.45	2 (18%)	15,15,17	1.61	4 (26%)
3	BGC	13-D	4	3	11,11,12	1.44	2 (18%)	15,15,17	2.26	3 (20%)
3	BGC	13-D	5	3	11,11,12	1.43	1 (9%)	15,15,17	2.05	6 (40%)
2	BGC	13-E	1	2	12,12,12	1.65	3 (25%)	17,17,17	1.17	3 (17%)
2	BGC	13-E	2	2	11,11,12	1.31	2 (18%)	15,15,17	1.19	1 (6%)
2	BGC	13-E	3	2	11,11,12	1.40	1 (9%)	15,15,17	1.35	3 (20%)
2	BGC	13-E	4	2	11,11,12	0.72	0	15,15,17	1.44	2 (13%)
2	BGC	13-E	5	2	11,11,12	1.18	1 (9%)	15,15,17	2.50	3 (20%)
2	BGC	13-E	6	2	11,11,12	1.43	2 (18%)	15,15,17	1.30	2 (13%)
3	BGC	13-F	1	3	12,12,12	1.33	2 (16%)	17,17,17	1.21	2 (11%)
3	BGC	13-F	2	3	11,11,12	1.51	1 (9%)	15,15,17	1.56	2 (13%)
3	BGC	13-F	3	3	11,11,12	1.32	2 (18%)	15,15,17	1.21	2 (13%)
3	BGC	13-F	4	3	11,11,12	1.49	2 (18%)	15,15,17	1.18	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	13-F	5	3	11,11,12	1.49	1 (9%)	15,15,17	1.00	1 (6%)
2	BGC	14-C	1	2	12,12,12	1.71	3 (25%)	17,17,17	1.07	2 (11%)
2	BGC	14-C	2	2	11,11,12	1.38	3 (27%)	15,15,17	1.59	3 (20%)
2	BGC	14-C	3	2	11,11,12	1.38	3 (27%)	15,15,17	1.40	1 (6%)
2	BGC	14-C	4	2	11,11,12	0.92	1 (9%)	15,15,17	1.35	2 (13%)
2	BGC	14-C	5	2	11,11,12	1.28	1 (9%)	15,15,17	1.60	3 (20%)
2	BGC	14-C	6	2	11,11,12	1.32	1 (9%)	15,15,17	1.31	2 (13%)
3	BGC	14-D	1	3	12,12,12	1.31	1 (8%)	17,17,17	1.42	3 (17%)
3	BGC	14-D	2	3	11,11,12	1.58	1 (9%)	15,15,17	1.50	3 (20%)
3	BGC	14-D	3	3	11,11,12	1.32	1 (9%)	15,15,17	1.69	4 (26%)
3	BGC	14-D	4	3	11,11,12	1.39	2 (18%)	15,15,17	1.59	3 (20%)
3	BGC	14-D	5	3	11,11,12	1.58	1 (9%)	15,15,17	1.03	1 (6%)
2	BGC	14-E	1	2	12,12,12	1.77	3 (25%)	17,17,17	1.68	2 (11%)
2	BGC	14-E	2	2	11,11,12	1.69	3 (27%)	15,15,17	1.34	2 (13%)
2	BGC	14-E	3	2	11,11,12	1.41	2 (18%)	15,15,17	1.55	3 (20%)
2	BGC	14-E	4	2	11,11,12	0.62	0	15,15,17	1.21	1 (6%)
2	BGC	14-E	5	2	11,11,12	1.33	3 (27%)	15,15,17	1.39	2 (13%)
2	BGC	14-E	6	2	11,11,12	1.49	2 (18%)	15,15,17	1.36	3 (20%)
3	BGC	14-F	1	3	12,12,12	1.33	2 (16%)	17,17,17	1.16	1 (5%)
3	BGC	14-F	2	3	11,11,12	1.65	2 (18%)	15,15,17	1.57	2 (13%)
3	BGC	14-F	3	3	11,11,12	1.32	2 (18%)	15,15,17	1.44	1 (6%)
3	BGC	14-F	4	3	11,11,12	1.24	1 (9%)	15,15,17	0.60	0
3	BGC	14-F	5	3	11,11,12	1.60	1 (9%)	15,15,17	0.83	0
2	BGC	15-C	1	2	12,12,12	1.69	3 (25%)	17,17,17	1.25	3 (17%)
2	BGC	15-C	2	2	11,11,12	1.57	3 (27%)	15,15,17	1.88	3 (20%)
2	BGC	15-C	3	2	11,11,12	1.33	2 (18%)	15,15,17	1.29	2 (13%)
2	BGC	15-C	4	2	11,11,12	0.98	1 (9%)	15,15,17	1.37	2 (13%)
2	BGC	15-C	5	2	11,11,12	1.27	1 (9%)	15,15,17	1.38	1 (6%)
2	BGC	15-C	6	2	11,11,12	1.41	2 (18%)	15,15,17	1.14	1 (6%)
3	BGC	15-D	1	3	12,12,12	1.44	2 (16%)	17,17,17	1.56	4 (23%)
3	BGC	15-D	2	3	11,11,12	1.29	1 (9%)	15,15,17	2.34	4 (26%)
3	BGC	15-D	3	3	11,11,12	1.49	2 (18%)	15,15,17	1.53	1 (6%)
3	BGC	15-D	4	3	11,11,12	1.36	2 (18%)	15,15,17	1.35	2 (13%)
3	BGC	15-D	5	3	11,11,12	1.56	1 (9%)	15,15,17	1.56	2 (13%)
2	BGC	15-E	1	2	12,12,12	1.60	3 (25%)	17,17,17	1.71	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	15-E	2	2	11,11,12	1.49	3 (27%)	15,15,17	1.43	2 (13%)
2	BGC	15-E	3	2	11,11,12	1.24	2 (18%)	15,15,17	1.49	3 (20%)
2	BGC	15-E	4	2	11,11,12	0.89	1 (9%)	15,15,17	1.42	2 (13%)
2	BGC	15-E	5	2	11,11,12	1.34	2 (18%)	15,15,17	1.89	4 (26%)
2	BGC	15-E	6	2	11,11,12	1.53	3 (27%)	15,15,17	1.35	1 (6%)
3	BGC	15-F	1	3	12,12,12	1.43	2 (16%)	17,17,17	1.06	0
3	BGC	15-F	2	3	11,11,12	1.59	2 (18%)	15,15,17	1.63	2 (13%)
3	BGC	15-F	3	3	11,11,12	1.35	1 (9%)	15,15,17	1.11	0
3	BGC	15-F	4	3	11,11,12	1.29	2 (18%)	15,15,17	1.05	0
3	BGC	15-F	5	3	11,11,12	1.64	1 (9%)	15,15,17	0.89	1 (6%)
2	BGC	16-C	1	2	12,12,12	1.66	3 (25%)	17,17,17	1.13	0
2	BGC	16-C	2	2	11,11,12	1.36	3 (27%)	15,15,17	1.35	3 (20%)
2	BGC	16-C	3	2	11,11,12	1.43	3 (27%)	15,15,17	1.18	2 (13%)
2	BGC	16-C	4	2	11,11,12	0.91	0	15,15,17	1.29	2 (13%)
2	BGC	16-C	5	2	11,11,12	1.31	1 (9%)	15,15,17	1.59	2 (13%)
2	BGC	16-C	6	2	11,11,12	1.55	2 (18%)	15,15,17	1.29	2 (13%)
3	BGC	16-D	1	3	12,12,12	1.33	1 (8%)	17,17,17	1.02	1 (5%)
3	BGC	16-D	2	3	11,11,12	1.43	1 (9%)	15,15,17	1.96	3 (20%)
3	BGC	16-D	3	3	11,11,12	1.32	2 (18%)	15,15,17	1.75	4 (26%)
3	BGC	16-D	4	3	11,11,12	1.17	1 (9%)	15,15,17	1.48	3 (20%)
3	BGC	16-D	5	3	11,11,12	1.62	1 (9%)	15,15,17	0.81	0
2	BGC	16-E	1	2	12,12,12	1.53	3 (25%)	17,17,17	1.19	2 (11%)
2	BGC	16-E	2	2	11,11,12	1.48	2 (18%)	15,15,17	1.20	2 (13%)
2	BGC	16-E	3	2	11,11,12	1.41	2 (18%)	15,15,17	1.43	2 (13%)
2	BGC	16-E	4	2	11,11,12	0.73	0	15,15,17	1.28	2 (13%)
2	BGC	16-E	5	2	11,11,12	1.45	2 (18%)	15,15,17	1.93	3 (20%)
2	BGC	16-E	6	2	11,11,12	1.51	2 (18%)	15,15,17	2.92	4 (26%)
3	BGC	16-F	1	3	12,12,12	1.27	2 (16%)	17,17,17	1.01	1 (5%)
3	BGC	16-F	2	3	11,11,12	1.57	2 (18%)	15,15,17	1.67	3 (20%)
3	BGC	16-F	3	3	11,11,12	1.32	2 (18%)	15,15,17	1.33	2 (13%)
3	BGC	16-F	4	3	11,11,12	1.19	1 (9%)	15,15,17	0.80	0
3	BGC	16-F	5	3	11,11,12	1.67	1 (9%)	15,15,17	0.79	1 (6%)
2	BGC	17-C	1	2	12,12,12	1.69	4 (33%)	17,17,17	1.42	2 (11%)
2	BGC	17-C	2	2	11,11,12	1.37	3 (27%)	15,15,17	1.51	2 (13%)
2	BGC	17-C	3	2	11,11,12	1.46	3 (27%)	15,15,17	1.25	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	17-C	4	2	11,11,12	0.86	0	15,15,17	1.38	2 (13%)
2	BGC	17-C	5	2	11,11,12	1.30	1 (9%)	15,15,17	1.48	2 (13%)
2	BGC	17-C	6	2	11,11,12	1.41	3 (27%)	15,15,17	1.43	4 (26%)
3	BGC	17-D	1	3	12,12,12	1.29	1 (8%)	17,17,17	1.54	4 (23%)
3	BGC	17-D	2	3	11,11,12	1.38	1 (9%)	15,15,17	2.00	3 (20%)
3	BGC	17-D	3	3	11,11,12	1.31	1 (9%)	15,15,17	1.26	3 (20%)
3	BGC	17-D	4	3	11,11,12	1.37	2 (18%)	15,15,17	1.22	3 (20%)
3	BGC	17-D	5	3	11,11,12	1.53	1 (9%)	15,15,17	1.05	1 (6%)
2	BGC	17-E	1	2	12,12,12	1.61	3 (25%)	17,17,17	1.35	3 (17%)
2	BGC	17-E	2	2	11,11,12	1.42	3 (27%)	15,15,17	1.33	1 (6%)
2	BGC	17-E	3	2	11,11,12	1.39	2 (18%)	15,15,17	1.34	2 (13%)
2	BGC	17-E	4	2	11,11,12	0.73	0	15,15,17	1.10	2 (13%)
2	BGC	17-E	5	2	11,11,12	1.30	2 (18%)	15,15,17	1.40	3 (20%)
2	BGC	17-E	6	2	11,11,12	1.86	3 (27%)	15,15,17	2.71	5 (33%)
3	BGC	17-F	1	3	12,12,12	1.46	3 (25%)	17,17,17	1.89	4 (23%)
3	BGC	17-F	2	3	11,11,12	1.69	1 (9%)	15,15,17	1.70	2 (13%)
3	BGC	17-F	3	3	11,11,12	1.23	1 (9%)	15,15,17	1.25	2 (13%)
3	BGC	17-F	4	3	11,11,12	1.23	2 (18%)	15,15,17	1.32	1 (6%)
3	BGC	17-F	5	3	11,11,12	1.64	1 (9%)	15,15,17	0.99	1 (6%)
2	BGC	18-C	1	2	12,12,12	1.68	3 (25%)	17,17,17	1.07	1 (5%)
2	BGC	18-C	2	2	11,11,12	1.35	3 (27%)	15,15,17	1.56	3 (20%)
2	BGC	18-C	3	2	11,11,12	1.49	3 (27%)	15,15,17	1.60	3 (20%)
2	BGC	18-C	4	2	11,11,12	0.87	0	15,15,17	1.25	2 (13%)
2	BGC	18-C	5	2	11,11,12	1.42	2 (18%)	15,15,17	1.51	1 (6%)
2	BGC	18-C	6	2	11,11,12	1.38	2 (18%)	15,15,17	1.75	5 (33%)
3	BGC	18-D	1	3	12,12,12	1.41	2 (16%)	17,17,17	1.52	5 (29%)
3	BGC	18-D	2	3	11,11,12	1.26	1 (9%)	15,15,17	2.05	4 (26%)
3	BGC	18-D	3	3	11,11,12	1.33	1 (9%)	15,15,17	1.68	2 (13%)
3	BGC	18-D	4	3	11,11,12	1.16	1 (9%)	15,15,17	1.30	2 (13%)
3	BGC	18-D	5	3	11,11,12	1.49	1 (9%)	15,15,17	1.71	5 (33%)
2	BGC	18-E	1	2	12,12,12	1.52	3 (25%)	17,17,17	1.04	0
2	BGC	18-E	2	2	11,11,12	1.47	2 (18%)	15,15,17	1.53	4 (26%)
2	BGC	18-E	3	2	11,11,12	1.34	2 (18%)	15,15,17	1.97	4 (26%)
2	BGC	18-E	4	2	11,11,12	0.76	0	15,15,17	1.41	2 (13%)
2	BGC	18-E	5	2	11,11,12	1.26	2 (18%)	15,15,17	1.47	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	18-E	6	2	11,11,12	1.36	2 (18%)	15,15,17	1.52	5 (33%)
3	BGC	18-F	1	3	12,12,12	1.36	2 (16%)	17,17,17	1.14	1 (5%)
3	BGC	18-F	2	3	11,11,12	1.70	1 (9%)	15,15,17	1.79	2 (13%)
3	BGC	18-F	3	3	11,11,12	1.22	2 (18%)	15,15,17	1.22	2 (13%)
3	BGC	18-F	4	3	11,11,12	1.36	2 (18%)	15,15,17	1.03	0
3	BGC	18-F	5	3	11,11,12	1.69	1 (9%)	15,15,17	0.93	1 (6%)
2	BGC	19-C	1	2	12,12,12	1.74	3 (25%)	17,17,17	1.81	6 (35%)
2	BGC	19-C	2	2	11,11,12	1.42	2 (18%)	15,15,17	1.92	4 (26%)
2	BGC	19-C	3	2	11,11,12	1.31	2 (18%)	15,15,17	1.22	3 (20%)
2	BGC	19-C	4	2	11,11,12	1.17	1 (9%)	15,15,17	1.65	3 (20%)
2	BGC	19-C	5	2	11,11,12	1.30	2 (18%)	15,15,17	1.54	3 (20%)
2	BGC	19-C	6	2	11,11,12	1.39	2 (18%)	15,15,17	1.22	2 (13%)
3	BGC	19-D	1	3	12,12,12	1.24	1 (8%)	17,17,17	1.17	2 (11%)
3	BGC	19-D	2	3	11,11,12	1.37	1 (9%)	15,15,17	2.41	6 (40%)
3	BGC	19-D	3	3	11,11,12	1.31	2 (18%)	15,15,17	2.11	5 (33%)
3	BGC	19-D	4	3	11,11,12	1.36	2 (18%)	15,15,17	1.26	1 (6%)
3	BGC	19-D	5	3	11,11,12	1.50	1 (9%)	15,15,17	1.32	3 (20%)
2	BGC	19-E	1	2	12,12,12	1.58	3 (25%)	17,17,17	1.05	2 (11%)
2	BGC	19-E	2	2	11,11,12	1.44	3 (27%)	15,15,17	1.51	2 (13%)
2	BGC	19-E	3	2	11,11,12	1.32	2 (18%)	15,15,17	1.33	1 (6%)
2	BGC	19-E	4	2	11,11,12	0.65	0	15,15,17	1.10	1 (6%)
2	BGC	19-E	5	2	11,11,12	1.36	3 (27%)	15,15,17	1.34	1 (6%)
2	BGC	19-E	6	2	11,11,12	1.43	3 (27%)	15,15,17	2.15	4 (26%)
3	BGC	19-F	1	3	12,12,12	1.32	1 (8%)	17,17,17	1.15	2 (11%)
3	BGC	19-F	2	3	11,11,12	1.46	1 (9%)	15,15,17	1.73	3 (20%)
3	BGC	19-F	3	3	11,11,12	1.28	1 (9%)	15,15,17	1.39	3 (20%)
3	BGC	19-F	4	3	11,11,12	1.32	2 (18%)	15,15,17	0.88	0
3	BGC	19-F	5	3	11,11,12	1.60	1 (9%)	15,15,17	0.97	2 (13%)
2	BGC	2-C	1	2	12,12,12	1.60	3 (25%)	17,17,17	0.88	0
2	BGC	2-C	2	2	11,11,12	1.30	3 (27%)	15,15,17	1.74	3 (20%)
2	BGC	2-C	3	2	11,11,12	1.35	2 (18%)	15,15,17	1.25	1 (6%)
2	BGC	2-C	4	2	11,11,12	0.80	0	15,15,17	1.61	3 (20%)
2	BGC	2-C	5	2	11,11,12	1.34	1 (9%)	15,15,17	1.53	3 (20%)
2	BGC	2-C	6	2	11,11,12	1.55	2 (18%)	15,15,17	1.58	4 (26%)
3	BGC	2-D	1	3	12,12,12	1.34	2 (16%)	17,17,17	1.40	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	2-D	2	3	11,11,12	1.26	0	15,15,17	1.63	1 (6%)
3	BGC	2-D	3	3	11,11,12	1.33	2 (18%)	15,15,17	1.55	4 (26%)
3	BGC	2-D	4	3	11,11,12	1.32	2 (18%)	15,15,17	1.21	2 (13%)
3	BGC	2-D	5	3	11,11,12	1.66	1 (9%)	15,15,17	1.28	3 (20%)
2	BGC	2-E	1	2	12,12,12	1.64	3 (25%)	17,17,17	0.95	0
2	BGC	2-E	2	2	11,11,12	1.37	3 (27%)	15,15,17	1.51	2 (13%)
2	BGC	2-E	3	2	11,11,12	1.24	1 (9%)	15,15,17	1.25	1 (6%)
2	BGC	2-E	4	2	11,11,12	0.53	0	15,15,17	1.13	1 (6%)
2	BGC	2-E	5	2	11,11,12	1.37	2 (18%)	15,15,17	1.55	3 (20%)
2	BGC	2-E	6	2	11,11,12	1.48	2 (18%)	15,15,17	1.44	4 (26%)
3	BGC	2-F	1	3	12,12,12	1.38	2 (16%)	17,17,17	1.18	1 (5%)
3	BGC	2-F	2	3	11,11,12	1.67	1 (9%)	15,15,17	1.99	4 (26%)
3	BGC	2-F	3	3	11,11,12	1.28	1 (9%)	15,15,17	1.14	1 (6%)
3	BGC	2-F	4	3	11,11,12	1.21	2 (18%)	15,15,17	1.00	0
3	BGC	2-F	5	3	11,11,12	1.59	1 (9%)	15,15,17	0.88	1 (6%)
2	BGC	20-C	1	2	12,12,12	1.71	3 (25%)	17,17,17	1.05	1 (5%)
2	BGC	20-C	2	2	11,11,12	1.43	3 (27%)	15,15,17	1.90	3 (20%)
2	BGC	20-C	3	2	11,11,12	1.33	3 (27%)	15,15,17	1.41	1 (6%)
2	BGC	20-C	4	2	11,11,12	1.01	1 (9%)	15,15,17	1.41	2 (13%)
2	BGC	20-C	5	2	11,11,12	1.42	2 (18%)	15,15,17	1.50	2 (13%)
2	BGC	20-C	6	2	11,11,12	1.29	2 (18%)	15,15,17	1.50	3 (20%)
3	BGC	20-D	1	3	12,12,12	1.29	1 (8%)	17,17,17	1.21	2 (11%)
3	BGC	20-D	2	3	11,11,12	1.53	1 (9%)	15,15,17	1.71	2 (13%)
3	BGC	20-D	3	3	11,11,12	1.43	1 (9%)	15,15,17	1.53	3 (20%)
3	BGC	20-D	4	3	11,11,12	1.31	1 (9%)	15,15,17	0.99	0
3	BGC	20-D	5	3	11,11,12	1.57	1 (9%)	15,15,17	1.16	2 (13%)
2	BGC	20-E	1	2	12,12,12	1.65	3 (25%)	17,17,17	0.96	1 (5%)
2	BGC	20-E	2	2	11,11,12	1.47	3 (27%)	15,15,17	1.33	1 (6%)
2	BGC	20-E	3	2	11,11,12	1.31	1 (9%)	15,15,17	1.57	2 (13%)
2	BGC	20-E	4	2	11,11,12	0.60	0	15,15,17	1.29	2 (13%)
2	BGC	20-E	5	2	11,11,12	1.38	2 (18%)	15,15,17	1.52	2 (13%)
2	BGC	20-E	6	2	11,11,12	1.37	3 (27%)	15,15,17	1.09	1 (6%)
3	BGC	20-F	1	3	12,12,12	1.30	2 (16%)	17,17,17	1.14	1 (5%)
3	BGC	20-F	2	3	11,11,12	1.67	3 (27%)	15,15,17	1.83	2 (13%)
3	BGC	20-F	3	3	11,11,12	1.30	2 (18%)	15,15,17	1.24	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	20-F	4	3	11,11,12	1.39	2 (18%)	15,15,17	0.93	0
3	BGC	20-F	5	3	11,11,12	1.68	1 (9%)	15,15,17	0.78	0
2	BGC	21-C	1	2	12,12,12	1.72	3 (25%)	17,17,17	1.23	1 (5%)
2	BGC	21-C	2	2	11,11,12	1.71	3 (27%)	15,15,17	1.96	5 (33%)
2	BGC	21-C	3	2	11,11,12	1.43	3 (27%)	15,15,17	1.40	3 (20%)
2	BGC	21-C	4	2	11,11,12	0.94	1 (9%)	15,15,17	1.19	1 (6%)
2	BGC	21-C	5	2	11,11,12	1.37	1 (9%)	15,15,17	1.64	3 (20%)
2	BGC	21-C	6	2	11,11,12	1.44	2 (18%)	15,15,17	1.16	0
3	BGC	21-D	1	3	12,12,12	1.36	2 (16%)	17,17,17	1.31	2 (11%)
3	BGC	21-D	2	3	11,11,12	1.38	2 (18%)	15,15,17	2.12	2 (13%)
3	BGC	21-D	3	3	11,11,12	1.29	2 (18%)	15,15,17	1.34	3 (20%)
3	BGC	21-D	4	3	11,11,12	1.34	2 (18%)	15,15,17	1.29	3 (20%)
3	BGC	21-D	5	3	11,11,12	1.65	1 (9%)	15,15,17	1.13	2 (13%)
2	BGC	21-E	1	2	12,12,12	1.87	3 (25%)	17,17,17	1.51	3 (17%)
2	BGC	21-E	2	2	11,11,12	1.54	3 (27%)	15,15,17	1.53	2 (13%)
2	BGC	21-E	3	2	11,11,12	1.37	2 (18%)	15,15,17	1.22	2 (13%)
2	BGC	21-E	4	2	11,11,12	0.90	1 (9%)	15,15,17	1.65	4 (26%)
2	BGC	21-E	5	2	11,11,12	1.45	3 (27%)	15,15,17	1.91	5 (33%)
2	BGC	21-E	6	2	11,11,12	1.36	3 (27%)	15,15,17	1.49	2 (13%)
3	BGC	21-F	1	3	12,12,12	1.26	2 (16%)	17,17,17	0.94	0
3	BGC	21-F	2	3	11,11,12	1.67	2 (18%)	15,15,17	1.73	2 (13%)
3	BGC	21-F	3	3	11,11,12	1.34	2 (18%)	15,15,17	1.42	3 (20%)
3	BGC	21-F	4	3	11,11,12	1.22	2 (18%)	15,15,17	1.04	0
3	BGC	21-F	5	3	11,11,12	1.73	1 (9%)	15,15,17	0.79	0
2	BGC	22-C	1	2	12,12,12	1.60	3 (25%)	17,17,17	1.05	0
2	BGC	22-C	2	2	11,11,12	1.45	3 (27%)	15,15,17	1.68	4 (26%)
2	BGC	22-C	3	2	11,11,12	1.27	2 (18%)	15,15,17	1.46	2 (13%)
2	BGC	22-C	4	2	11,11,12	1.09	1 (9%)	15,15,17	1.24	1 (6%)
2	BGC	22-C	5	2	11,11,12	1.50	2 (18%)	15,15,17	1.57	1 (6%)
2	BGC	22-C	6	2	11,11,12	1.42	1 (9%)	15,15,17	2.08	5 (33%)
3	BGC	22-D	1	3	12,12,12	1.29	1 (8%)	17,17,17	1.91	5 (29%)
3	BGC	22-D	2	3	11,11,12	1.35	1 (9%)	15,15,17	1.87	4 (26%)
3	BGC	22-D	3	3	11,11,12	1.31	2 (18%)	15,15,17	1.69	4 (26%)
3	BGC	22-D	4	3	11,11,12	1.25	2 (18%)	15,15,17	1.14	1 (6%)
3	BGC	22-D	5	3	11,11,12	1.38	1 (9%)	15,15,17	1.51	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	22-E	1	2	12,12,12	1.55	3 (25%)	17,17,17	1.29	2 (11%)
2	BGC	22-E	2	2	11,11,12	1.48	3 (27%)	15,15,17	1.37	2 (13%)
2	BGC	22-E	3	2	11,11,12	1.23	1 (9%)	15,15,17	1.32	1 (6%)
2	BGC	22-E	4	2	11,11,12	0.79	0	15,15,17	1.56	2 (13%)
2	BGC	22-E	5	2	11,11,12	1.49	2 (18%)	15,15,17	1.35	2 (13%)
2	BGC	22-E	6	2	11,11,12	1.53	2 (18%)	15,15,17	1.05	1 (6%)
3	BGC	22-F	1	3	12,12,12	1.31	1 (8%)	17,17,17	1.28	2 (11%)
3	BGC	22-F	2	3	11,11,12	1.43	2 (18%)	15,15,17	1.43	1 (6%)
3	BGC	22-F	3	3	11,11,12	1.28	1 (9%)	15,15,17	1.26	3 (20%)
3	BGC	22-F	4	3	11,11,12	1.43	2 (18%)	15,15,17	1.12	1 (6%)
3	BGC	22-F	5	3	11,11,12	1.57	1 (9%)	15,15,17	0.76	0
2	BGC	23-C	1	2	12,12,12	1.63	3 (25%)	17,17,17	1.56	3 (17%)
2	BGC	23-C	2	2	11,11,12	1.47	3 (27%)	15,15,17	1.69	3 (20%)
2	BGC	23-C	3	2	11,11,12	1.33	3 (27%)	15,15,17	1.31	2 (13%)
2	BGC	23-C	4	2	11,11,12	0.82	0	15,15,17	1.99	5 (33%)
2	BGC	23-C	5	2	11,11,12	1.22	1 (9%)	15,15,17	1.39	2 (13%)
2	BGC	23-C	6	2	11,11,12	1.52	2 (18%)	15,15,17	1.70	4 (26%)
3	BGC	23-D	1	3	12,12,12	1.34	2 (16%)	17,17,17	1.63	5 (29%)
3	BGC	23-D	2	3	11,11,12	1.44	1 (9%)	15,15,17	1.55	1 (6%)
3	BGC	23-D	3	3	11,11,12	1.34	2 (18%)	15,15,17	1.60	2 (13%)
3	BGC	23-D	4	3	11,11,12	1.32	2 (18%)	15,15,17	1.35	4 (26%)
3	BGC	23-D	5	3	11,11,12	1.54	1 (9%)	15,15,17	1.28	2 (13%)
2	BGC	23-E	1	2	12,12,12	1.55	3 (25%)	17,17,17	1.12	2 (11%)
2	BGC	23-E	2	2	11,11,12	1.42	2 (18%)	15,15,17	1.22	2 (13%)
2	BGC	23-E	3	2	11,11,12	1.40	1 (9%)	15,15,17	1.60	2 (13%)
2	BGC	23-E	4	2	11,11,12	0.88	1 (9%)	15,15,17	1.87	2 (13%)
2	BGC	23-E	5	2	11,11,12	1.28	3 (27%)	15,15,17	1.35	2 (13%)
2	BGC	23-E	6	2	11,11,12	1.43	2 (18%)	15,15,17	1.87	3 (20%)
3	BGC	23-F	1	3	12,12,12	1.45	2 (16%)	17,17,17	1.78	6 (35%)
3	BGC	23-F	2	3	11,11,12	1.46	2 (18%)	15,15,17	1.47	3 (20%)
3	BGC	23-F	3	3	11,11,12	1.14	1 (9%)	15,15,17	1.42	2 (13%)
3	BGC	23-F	4	3	11,11,12	1.38	2 (18%)	15,15,17	1.16	1 (6%)
3	BGC	23-F	5	3	11,11,12	1.61	1 (9%)	15,15,17	1.86	3 (20%)
2	BGC	24-C	1	2	12,12,12	1.53	3 (25%)	17,17,17	1.44	3 (17%)
2	BGC	24-C	2	2	11,11,12	1.52	3 (27%)	15,15,17	1.51	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	24-C	3	2	11,11,12	1.46	2 (18%)	15,15,17	1.33	2 (13%)
2	BGC	24-C	4	2	11,11,12	0.94	0	15,15,17	1.40	2 (13%)
2	BGC	24-C	5	2	11,11,12	1.24	1 (9%)	15,15,17	1.56	2 (13%)
2	BGC	24-C	6	2	11,11,12	1.39	2 (18%)	15,15,17	2.25	3 (20%)
3	BGC	24-D	1	3	12,12,12	1.31	1 (8%)	17,17,17	1.35	2 (11%)
3	BGC	24-D	2	3	11,11,12	1.23	1 (9%)	15,15,17	1.64	1 (6%)
3	BGC	24-D	3	3	11,11,12	1.37	2 (18%)	15,15,17	1.39	3 (20%)
3	BGC	24-D	4	3	11,11,12	1.34	2 (18%)	15,15,17	1.36	3 (20%)
3	BGC	24-D	5	3	11,11,12	1.64	1 (9%)	15,15,17	1.21	1 (6%)
2	BGC	24-E	1	2	12,12,12	1.58	3 (25%)	17,17,17	1.37	2 (11%)
2	BGC	24-E	2	2	11,11,12	1.60	2 (18%)	15,15,17	0.94	0
2	BGC	24-E	3	2	11,11,12	1.28	1 (9%)	15,15,17	1.22	1 (6%)
2	BGC	24-E	4	2	11,11,12	0.85	1 (9%)	15,15,17	1.41	2 (13%)
2	BGC	24-E	5	2	11,11,12	1.39	2 (18%)	15,15,17	1.53	2 (13%)
2	BGC	24-E	6	2	11,11,12	1.50	2 (18%)	15,15,17	1.60	5 (33%)
3	BGC	24-F	1	3	12,12,12	1.35	2 (16%)	17,17,17	1.11	1 (5%)
3	BGC	24-F	2	3	11,11,12	1.58	1 (9%)	15,15,17	1.74	4 (26%)
3	BGC	24-F	3	3	11,11,12	1.24	1 (9%)	15,15,17	1.50	2 (13%)
3	BGC	24-F	4	3	11,11,12	1.32	2 (18%)	15,15,17	1.12	0
3	BGC	24-F	5	3	11,11,12	1.67	1 (9%)	15,15,17	0.84	0
2	BGC	25-C	1	2	12,12,12	1.62	3 (25%)	17,17,17	1.03	0
2	BGC	25-C	2	2	11,11,12	1.40	3 (27%)	15,15,17	1.46	2 (13%)
2	BGC	25-C	3	2	11,11,12	1.30	3 (27%)	15,15,17	1.40	3 (20%)
2	BGC	25-C	4	2	11,11,12	0.82	0	15,15,17	1.45	4 (26%)
2	BGC	25-C	5	2	11,11,12	1.37	1 (9%)	15,15,17	1.52	3 (20%)
2	BGC	25-C	6	2	11,11,12	1.25	1 (9%)	15,15,17	1.81	3 (20%)
3	BGC	25-D	1	3	12,12,12	1.34	2 (16%)	17,17,17	1.41	2 (11%)
3	BGC	25-D	2	3	11,11,12	1.39	1 (9%)	15,15,17	2.05	4 (26%)
3	BGC	25-D	3	3	11,11,12	1.35	1 (9%)	15,15,17	1.56	2 (13%)
3	BGC	25-D	4	3	11,11,12	1.38	2 (18%)	15,15,17	1.36	3 (20%)
3	BGC	25-D	5	3	11,11,12	1.59	1 (9%)	15,15,17	1.15	2 (13%)
2	BGC	25-E	1	2	12,12,12	1.66	3 (25%)	17,17,17	1.58	5 (29%)
2	BGC	25-E	2	2	11,11,12	1.39	3 (27%)	15,15,17	1.49	2 (13%)
2	BGC	25-E	3	2	11,11,12	1.30	1 (9%)	15,15,17	1.43	3 (20%)
2	BGC	25-E	4	2	11,11,12	0.71	1 (9%)	15,15,17	1.60	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	25-E	5	2	11,11,12	1.31	3 (27%)	15,15,17	1.39	2 (13%)
2	BGC	25-E	6	2	11,11,12	1.33	2 (18%)	15,15,17	1.04	0
3	BGC	25-F	1	3	12,12,12	1.35	2 (16%)	17,17,17	1.10	0
3	BGC	25-F	2	3	11,11,12	1.58	3 (27%)	15,15,17	2.08	3 (20%)
3	BGC	25-F	3	3	11,11,12	1.46	2 (18%)	15,15,17	1.97	5 (33%)
3	BGC	25-F	4	3	11,11,12	1.28	2 (18%)	15,15,17	1.77	2 (13%)
3	BGC	25-F	5	3	11,11,12	1.52	1 (9%)	15,15,17	1.03	1 (6%)
2	BGC	3-C	1	2	12,12,12	1.66	3 (25%)	17,17,17	1.05	1 (5%)
2	BGC	3-C	2	2	11,11,12	1.40	3 (27%)	15,15,17	1.66	3 (20%)
2	BGC	3-C	3	2	11,11,12	1.39	2 (18%)	15,15,17	1.10	1 (6%)
2	BGC	3-C	4	2	11,11,12	0.95	1 (9%)	15,15,17	1.33	2 (13%)
2	BGC	3-C	5	2	11,11,12	1.34	1 (9%)	15,15,17	2.13	5 (33%)
2	BGC	3-C	6	2	11,11,12	1.36	2 (18%)	15,15,17	1.34	1 (6%)
3	BGC	3-D	1	3	12,12,12	1.34	1 (8%)	17,17,17	1.46	4 (23%)
3	BGC	3-D	2	3	11,11,12	1.41	1 (9%)	15,15,17	1.71	3 (20%)
3	BGC	3-D	3	3	11,11,12	1.35	2 (18%)	15,15,17	1.56	2 (13%)
3	BGC	3-D	4	3	11,11,12	1.19	1 (9%)	15,15,17	1.56	3 (20%)
3	BGC	3-D	5	3	11,11,12	1.73	1 (9%)	15,15,17	1.22	1 (6%)
2	BGC	3-E	1	2	12,12,12	1.69	4 (33%)	17,17,17	0.99	1 (5%)
2	BGC	3-E	2	2	11,11,12	1.49	3 (27%)	15,15,17	1.49	2 (13%)
2	BGC	3-E	3	2	11,11,12	1.57	3 (27%)	15,15,17	1.24	1 (6%)
2	BGC	3-E	4	2	11,11,12	1.00	1 (9%)	15,15,17	3.84	7 (46%)
2	BGC	3-E	5	2	11,11,12	1.23	2 (18%)	15,15,17	1.31	2 (13%)
2	BGC	3-E	6	2	11,11,12	1.45	2 (18%)	15,15,17	1.65	3 (20%)
3	BGC	3-F	1	3	12,12,12	1.32	2 (16%)	17,17,17	1.00	0
3	BGC	3-F	2	3	11,11,12	1.49	1 (9%)	15,15,17	1.79	2 (13%)
3	BGC	3-F	3	3	11,11,12	1.40	2 (18%)	15,15,17	1.26	2 (13%)
3	BGC	3-F	4	3	11,11,12	1.29	2 (18%)	15,15,17	1.06	1 (6%)
3	BGC	3-F	5	3	11,11,12	1.64	1 (9%)	15,15,17	0.84	0
2	BGC	4-C	1	2	12,12,12	1.72	3 (25%)	17,17,17	1.22	2 (11%)
2	BGC	4-C	2	2	11,11,12	1.46	3 (27%)	15,15,17	1.57	4 (26%)
2	BGC	4-C	3	2	11,11,12	1.52	3 (27%)	15,15,17	1.41	4 (26%)
2	BGC	4-C	4	2	11,11,12	0.90	0	15,15,17	1.09	1 (6%)
2	BGC	4-C	5	2	11,11,12	1.46	1 (9%)	15,15,17	1.38	1 (6%)
2	BGC	4-C	6	2	11,11,12	1.60	2 (18%)	15,15,17	1.69	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	4-D	1	3	12,12,12	1.28	1 (8%)	17,17,17	1.24	3 (17%)
3	BGC	4-D	2	3	11,11,12	1.43	1 (9%)	15,15,17	1.91	4 (26%)
3	BGC	4-D	3	3	11,11,12	1.47	2 (18%)	15,15,17	1.97	4 (26%)
3	BGC	4-D	4	3	11,11,12	1.71	2 (18%)	15,15,17	1.53	4 (26%)
3	BGC	4-D	5	3	11,11,12	1.65	1 (9%)	15,15,17	1.29	2 (13%)
2	BGC	4-E	1	2	12,12,12	1.63	3 (25%)	17,17,17	1.22	3 (17%)
2	BGC	4-E	2	2	11,11,12	1.49	2 (18%)	15,15,17	1.32	3 (20%)
2	BGC	4-E	3	2	11,11,12	1.37	1 (9%)	15,15,17	1.22	2 (13%)
2	BGC	4-E	4	2	11,11,12	0.81	0	15,15,17	1.38	3 (20%)
2	BGC	4-E	5	2	11,11,12	1.26	2 (18%)	15,15,17	1.08	2 (13%)
2	BGC	4-E	6	2	11,11,12	1.47	3 (27%)	15,15,17	1.57	2 (13%)
3	BGC	4-F	1	3	12,12,12	1.33	1 (8%)	17,17,17	0.91	0
3	BGC	4-F	2	3	11,11,12	1.45	1 (9%)	15,15,17	1.68	2 (13%)
3	BGC	4-F	3	3	11,11,12	1.43	2 (18%)	15,15,17	1.29	2 (13%)
3	BGC	4-F	4	3	11,11,12	1.29	2 (18%)	15,15,17	1.06	0
3	BGC	4-F	5	3	11,11,12	1.59	1 (9%)	15,15,17	1.28	2 (13%)
2	BGC	5-C	1	2	12,12,12	1.70	3 (25%)	17,17,17	1.69	5 (29%)
2	BGC	5-C	2	2	11,11,12	1.51	3 (27%)	15,15,17	1.75	4 (26%)
2	BGC	5-C	3	2	11,11,12	1.45	3 (27%)	15,15,17	1.43	1 (6%)
2	BGC	5-C	4	2	11,11,12	0.90	0	15,15,17	1.34	2 (13%)
2	BGC	5-C	5	2	11,11,12	1.44	2 (18%)	15,15,17	1.33	1 (6%)
2	BGC	5-C	6	2	11,11,12	1.59	2 (18%)	15,15,17	1.31	2 (13%)
3	BGC	5-D	1	3	12,12,12	1.34	1 (8%)	17,17,17	1.42	1 (5%)
3	BGC	5-D	2	3	11,11,12	1.35	1 (9%)	15,15,17	1.82	4 (26%)
3	BGC	5-D	3	3	11,11,12	1.45	2 (18%)	15,15,17	1.84	5 (33%)
3	BGC	5-D	4	3	11,11,12	1.24	1 (9%)	15,15,17	1.39	4 (26%)
3	BGC	5-D	5	3	11,11,12	1.57	1 (9%)	15,15,17	0.94	0
2	BGC	5-E	1	2	12,12,12	1.56	3 (25%)	17,17,17	1.06	1 (5%)
2	BGC	5-E	2	2	11,11,12	1.67	3 (27%)	15,15,17	0.89	0
2	BGC	5-E	3	2	11,11,12	1.42	2 (18%)	15,15,17	1.33	1 (6%)
2	BGC	5-E	4	2	11,11,12	0.91	1 (9%)	15,15,17	1.65	2 (13%)
2	BGC	5-E	5	2	11,11,12	1.37	2 (18%)	15,15,17	1.37	2 (13%)
2	BGC	5-E	6	2	11,11,12	1.42	2 (18%)	15,15,17	1.55	4 (26%)
3	BGC	5-F	1	3	12,12,12	1.44	3 (25%)	17,17,17	1.82	4 (23%)
3	BGC	5-F	2	3	11,11,12	1.74	1 (9%)	15,15,17	1.84	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	5-F	3	3	11,11,12	1.34	2 (18%)	15,15,17	1.12	0
3	BGC	5-F	4	3	11,11,12	1.41	2 (18%)	15,15,17	1.28	1 (6%)
3	BGC	5-F	5	3	11,11,12	1.67	1 (9%)	15,15,17	1.12	2 (13%)
2	BGC	6-C	1	2	12,12,12	1.59	3 (25%)	17,17,17	1.19	2 (11%)
2	BGC	6-C	2	2	11,11,12	1.43	3 (27%)	15,15,17	1.69	4 (26%)
2	BGC	6-C	3	2	11,11,12	1.37	3 (27%)	15,15,17	1.69	3 (20%)
2	BGC	6-C	4	2	11,11,12	0.80	0	15,15,17	1.13	2 (13%)
2	BGC	6-C	5	2	11,11,12	1.41	2 (18%)	15,15,17	1.43	2 (13%)
2	BGC	6-C	6	2	11,11,12	1.38	1 (9%)	15,15,17	1.51	3 (20%)
3	BGC	6-D	1	3	12,12,12	1.34	1 (8%)	17,17,17	2.01	6 (35%)
3	BGC	6-D	2	3	11,11,12	1.80	2 (18%)	15,15,17	2.53	6 (40%)
3	BGC	6-D	3	3	11,11,12	1.27	2 (18%)	15,15,17	1.62	5 (33%)
3	BGC	6-D	4	3	11,11,12	1.24	1 (9%)	15,15,17	1.18	2 (13%)
3	BGC	6-D	5	3	11,11,12	1.43	1 (9%)	15,15,17	1.64	3 (20%)
2	BGC	6-E	1	2	12,12,12	1.65	3 (25%)	17,17,17	1.42	1 (5%)
2	BGC	6-E	2	2	11,11,12	1.54	3 (27%)	15,15,17	1.23	2 (13%)
2	BGC	6-E	3	2	11,11,12	1.20	1 (9%)	15,15,17	1.52	2 (13%)
2	BGC	6-E	4	2	11,11,12	0.86	1 (9%)	15,15,17	1.31	2 (13%)
2	BGC	6-E	5	2	11,11,12	1.24	2 (18%)	15,15,17	1.38	2 (13%)
2	BGC	6-E	6	2	11,11,12	1.33	2 (18%)	15,15,17	1.17	1 (6%)
3	BGC	6-F	1	3	12,12,12	1.28	1 (8%)	17,17,17	0.89	0
3	BGC	6-F	2	3	11,11,12	1.59	1 (9%)	15,15,17	2.06	5 (33%)
3	BGC	6-F	3	3	11,11,12	1.42	3 (27%)	15,15,17	1.65	2 (13%)
3	BGC	6-F	4	3	11,11,12	1.29	2 (18%)	15,15,17	0.75	0
3	BGC	6-F	5	3	11,11,12	1.78	1 (9%)	15,15,17	0.91	0
2	BGC	7-C	1	2	12,12,12	1.66	3 (25%)	17,17,17	1.68	5 (29%)
2	BGC	7-C	2	2	11,11,12	1.61	3 (27%)	15,15,17	4.18	5 (33%)
2	BGC	7-C	3	2	11,11,12	1.46	2 (18%)	15,15,17	1.31	2 (13%)
2	BGC	7-C	4	2	11,11,12	1.02	1 (9%)	15,15,17	1.35	2 (13%)
2	BGC	7-C	5	2	11,11,12	1.50	2 (18%)	15,15,17	1.45	3 (20%)
2	BGC	7-C	6	2	11,11,12	1.40	2 (18%)	15,15,17	1.07	0
3	BGC	7-D	1	3	12,12,12	1.25	1 (8%)	17,17,17	1.24	2 (11%)
3	BGC	7-D	2	3	11,11,12	1.46	1 (9%)	15,15,17	1.75	1 (6%)
3	BGC	7-D	3	3	11,11,12	1.32	2 (18%)	15,15,17	1.63	5 (33%)
3	BGC	7-D	4	3	11,11,12	1.41	2 (18%)	15,15,17	1.35	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	7-D	5	3	11,11,12	1.47	1 (9%)	15,15,17	1.44	2 (13%)
2	BGC	7-E	1	2	12,12,12	1.57	3 (25%)	17,17,17	1.07	2 (11%)
2	BGC	7-E	2	2	11,11,12	1.38	2 (18%)	15,15,17	1.29	1 (6%)
2	BGC	7-E	3	2	11,11,12	1.29	1 (9%)	15,15,17	1.38	2 (13%)
2	BGC	7-E	4	2	11,11,12	0.76	0	15,15,17	1.31	1 (6%)
2	BGC	7-E	5	2	11,11,12	1.31	3 (27%)	15,15,17	1.44	2 (13%)
2	BGC	7-E	6	2	11,11,12	1.44	3 (27%)	15,15,17	1.29	2 (13%)
3	BGC	7-F	1	3	12,12,12	1.23	1 (8%)	17,17,17	1.17	1 (5%)
3	BGC	7-F	2	3	11,11,12	1.50	3 (27%)	15,15,17	1.88	3 (20%)
3	BGC	7-F	3	3	11,11,12	1.26	2 (18%)	15,15,17	1.41	4 (26%)
3	BGC	7-F	4	3	11,11,12	1.49	2 (18%)	15,15,17	1.10	1 (6%)
3	BGC	7-F	5	3	11,11,12	1.63	1 (9%)	15,15,17	0.82	0
2	BGC	8-C	1	2	12,12,12	1.70	3 (25%)	17,17,17	1.37	3 (17%)
2	BGC	8-C	2	2	11,11,12	1.46	3 (27%)	15,15,17	1.49	3 (20%)
2	BGC	8-C	3	2	11,11,12	1.44	2 (18%)	15,15,17	1.29	2 (13%)
2	BGC	8-C	4	2	11,11,12	1.08	1 (9%)	15,15,17	1.52	3 (20%)
2	BGC	8-C	5	2	11,11,12	1.22	1 (9%)	15,15,17	1.00	0
2	BGC	8-C	6	2	11,11,12	1.41	2 (18%)	15,15,17	1.75	3 (20%)
3	BGC	8-D	1	3	12,12,12	1.26	2 (16%)	17,17,17	1.29	1 (5%)
3	BGC	8-D	2	3	11,11,12	1.47	1 (9%)	15,15,17	1.70	2 (13%)
3	BGC	8-D	3	3	11,11,12	1.30	1 (9%)	15,15,17	1.43	1 (6%)
3	BGC	8-D	4	3	11,11,12	1.23	1 (9%)	15,15,17	1.31	2 (13%)
3	BGC	8-D	5	3	11,11,12	1.68	1 (9%)	15,15,17	1.59	2 (13%)
2	BGC	8-E	1	2	12,12,12	1.66	3 (25%)	17,17,17	1.39	3 (17%)
2	BGC	8-E	2	2	11,11,12	1.58	2 (18%)	15,15,17	2.17	5 (33%)
2	BGC	8-E	3	2	11,11,12	1.38	2 (18%)	15,15,17	1.65	3 (20%)
2	BGC	8-E	4	2	11,11,12	0.77	1 (9%)	15,15,17	1.50	3 (20%)
2	BGC	8-E	5	2	11,11,12	1.49	2 (18%)	15,15,17	1.45	2 (13%)
2	BGC	8-E	6	2	11,11,12	1.32	2 (18%)	15,15,17	1.09	0
3	BGC	8-F	1	3	12,12,12	1.33	1 (8%)	17,17,17	0.96	1 (5%)
3	BGC	8-F	2	3	11,11,12	1.54	2 (18%)	15,15,17	2.03	2 (13%)
3	BGC	8-F	3	3	11,11,12	1.31	2 (18%)	15,15,17	1.34	2 (13%)
3	BGC	8-F	4	3	11,11,12	1.34	2 (18%)	15,15,17	1.18	0
3	BGC	8-F	5	3	11,11,12	1.70	2 (18%)	15,15,17	0.88	1 (6%)
2	BGC	9-C	1	2	12,12,12	1.74	3 (25%)	17,17,17	1.60	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	9-C	2	2	11,11,12	1.42	3 (27%)	15,15,17	1.89	4 (26%)
2	BGC	9-C	3	2	11,11,12	1.36	2 (18%)	15,15,17	1.17	1 (6%)
2	BGC	9-C	4	2	11,11,12	0.89	0	15,15,17	1.19	1 (6%)
2	BGC	9-C	5	2	11,11,12	1.41	1 (9%)	15,15,17	1.37	1 (6%)
2	BGC	9-C	6	2	11,11,12	1.32	2 (18%)	15,15,17	1.70	3 (20%)
3	BGC	9-D	1	3	12,12,12	1.34	1 (8%)	17,17,17	1.35	4 (23%)
3	BGC	9-D	2	3	11,11,12	1.30	1 (9%)	15,15,17	1.87	2 (13%)
3	BGC	9-D	3	3	11,11,12	1.19	2 (18%)	15,15,17	1.77	3 (20%)
3	BGC	9-D	4	3	11,11,12	1.19	1 (9%)	15,15,17	1.28	2 (13%)
3	BGC	9-D	5	3	11,11,12	1.66	1 (9%)	15,15,17	1.05	2 (13%)
2	BGC	9-E	1	2	12,12,12	1.74	3 (25%)	17,17,17	1.40	2 (11%)
2	BGC	9-E	2	2	11,11,12	1.44	2 (18%)	15,15,17	2.04	4 (26%)
2	BGC	9-E	3	2	11,11,12	1.37	1 (9%)	15,15,17	1.20	1 (6%)
2	BGC	9-E	4	2	11,11,12	0.76	0	15,15,17	1.14	2 (13%)
2	BGC	9-E	5	2	11,11,12	1.28	3 (27%)	15,15,17	1.73	4 (26%)
2	BGC	9-E	6	2	11,11,12	1.48	2 (18%)	15,15,17	1.44	3 (20%)
3	BGC	9-F	1	3	12,12,12	1.30	2 (16%)	17,17,17	0.99	0
3	BGC	9-F	2	3	11,11,12	1.55	2 (18%)	15,15,17	1.51	2 (13%)
3	BGC	9-F	3	3	11,11,12	1.21	1 (9%)	15,15,17	1.49	3 (20%)
3	BGC	9-F	4	3	11,11,12	1.21	2 (18%)	15,15,17	1.13	0
3	BGC	9-F	5	3	11,11,12	1.98	1 (9%)	15,15,17	1.07	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
2	BGC	18-E	2	2	-	0/2/19/22	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
2	BGC	23-C	3	2	-	2/2/19/22	0/1/1/1
2	BGC	23-C	4	2	-	1/2/19/22	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/2/22/22	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

The worst 5 of 981 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-F	5	BGC	C2-C3	-5.86	1.43	1.52
3	3-D	5	BGC	C2-C3	-5.12	1.45	1.52
3	6-F	5	BGC	C2-C3	-5.04	1.45	1.52
3	9-D	5	BGC	C2-C3	-4.99	1.45	1.52
3	8-D	5	BGC	C2-C3	-4.91	1.45	1.52

The worst 5 of 1223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3-E	4	BGC	O5-C5-C6	-11.51	89.16	107.20
2	7-C	2	BGC	O5-C5-C6	10.11	123.05	107.20
3	1-F	3	BGC	C1-O5-C5	9.37	124.88	112.19
2	7-C	2	BGC	C1-O5-C5	-8.29	100.96	112.19
2	17-E	6	BGC	C6-C5-C4	-8.18	93.84	113.00

There are no chirality outliers.

5 of 248 torsion outliers are listed below:

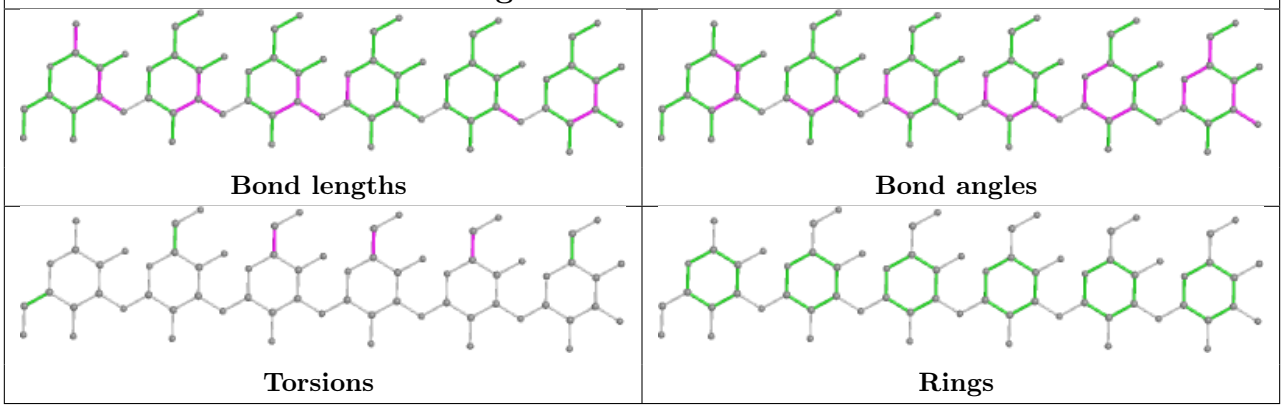
Mol	Chain	Res	Type	Atoms
3	18-D	1	BGC	C4-C5-C6-O6
2	6-C	2	BGC	C4-C5-C6-O6
2	9-C	6	BGC	C4-C5-C6-O6
3	9-D	4	BGC	C4-C5-C6-O6
2	21-E	1	BGC	O5-C5-C6-O6

There are no ring outliers.

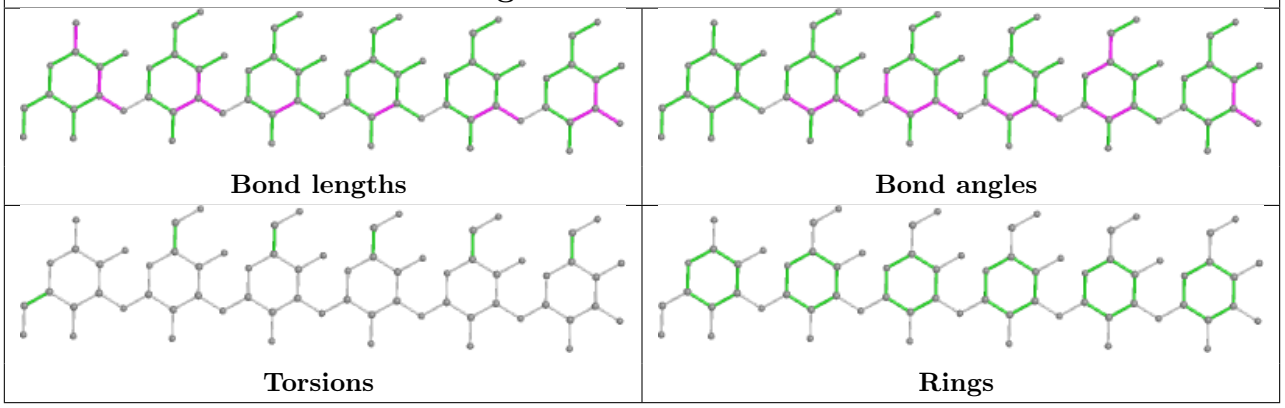
No monomer is involved in short contacts.

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

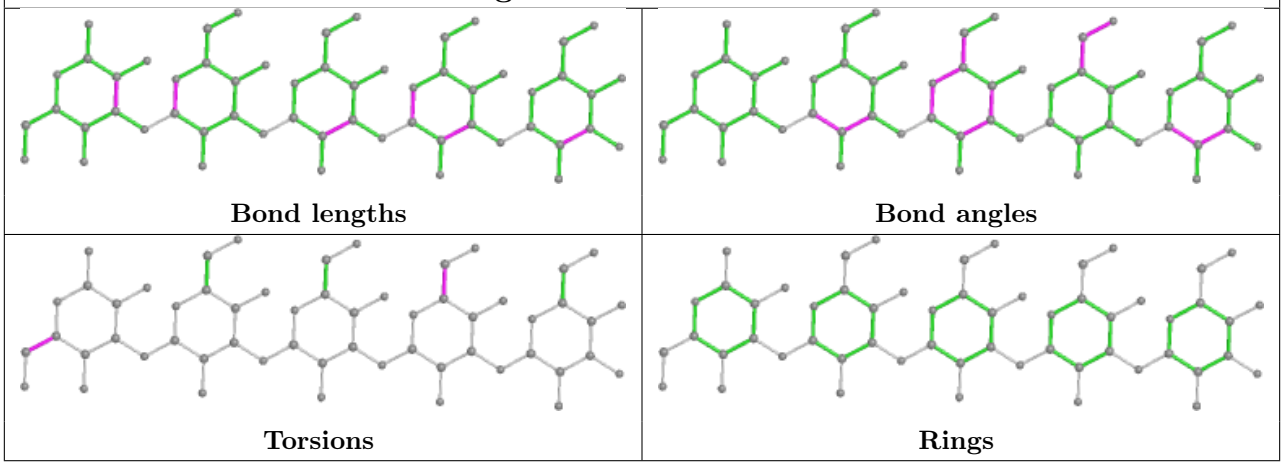
Oligosaccharide Chain C

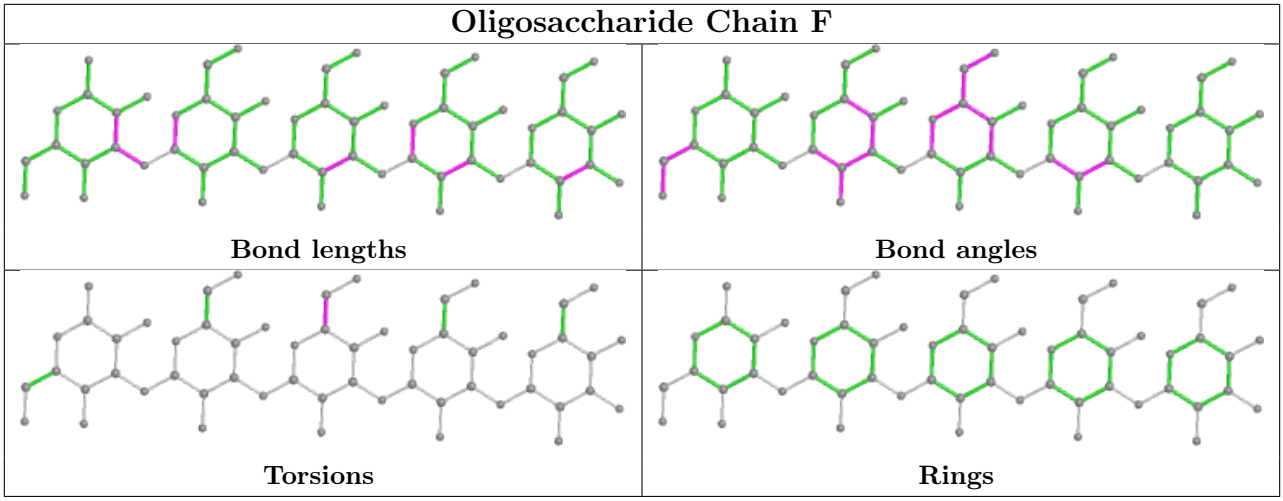


Oligosaccharide Chain E



Oligosaccharide Chain D





5.6 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	15-B	701	-	3,3,3	0.53	0	2,2,2	0.38	0
4	EDO	9-A	701	-	3,3,3	0.39	0	2,2,2	0.30	0
4	EDO	11-A	701	-	3,3,3	0.43	0	2,2,2	0.27	0
4	EDO	24-B	701	-	3,3,3	0.71	0	2,2,2	1.30	0
4	EDO	13-B	701	-	3,3,3	0.56	0	2,2,2	0.27	0
4	EDO	23-B	701	-	3,3,3	0.80	0	2,2,2	0.46	0
4	EDO	25-B	701	-	3,3,3	0.46	0	2,2,2	0.49	0
4	EDO	6-A	701	-	3,3,3	0.44	0	2,2,2	0.56	0
4	EDO	11-B	701	-	3,3,3	0.37	0	2,2,2	0.22	0
4	EDO	7-B	701	-	3,3,3	0.44	0	2,2,2	0.18	0
4	EDO	15-A	701	-	3,3,3	0.45	0	2,2,2	0.31	0
4	EDO	2-A	701	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	21-A	701	-	3,3,3	0.49	0	2,2,2	0.45	0
4	EDO	16-B	701	-	3,3,3	0.78	0	2,2,2	0.33	0
4	EDO	7-A	701	-	3,3,3	0.59	0	2,2,2	0.32	0
4	EDO	6-B	701	-	3,3,3	0.50	0	2,2,2	1.70	1 (50%)
4	EDO	19-B	701	-	3,3,3	0.61	0	2,2,2	0.32	0
4	EDO	16-A	701	-	3,3,3	0.58	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	19-A	701	-	3,3,3	0.44	0	2,2,2	0.19	0
4	EDO	25-A	701	-	3,3,3	0.50	0	2,2,2	0.21	0
4	EDO	10-B	701	-	3,3,3	0.79	0	2,2,2	0.78	0
4	EDO	14-A	701	-	3,3,3	0.52	0	2,2,2	0.16	0
4	EDO	12-B	701	-	3,3,3	0.57	0	2,2,2	0.28	0
4	EDO	20-A	701	-	3,3,3	0.43	0	2,2,2	0.56	0
4	EDO	3-B	701	-	3,3,3	0.39	0	2,2,2	0.51	0
4	EDO	22-A	701	-	3,3,3	0.57	0	2,2,2	0.39	0
4	EDO	5-A	701	-	3,3,3	0.78	0	2,2,2	0.23	0
4	EDO	4-A	701	-	3,3,3	0.48	0	2,2,2	0.15	0
4	EDO	21-B	701	-	3,3,3	0.42	0	2,2,2	0.31	0
4	EDO	1-A	701	-	3,3,3	0.53	0	2,2,2	0.20	0
4	EDO	10-A	701	-	3,3,3	0.42	0	2,2,2	0.40	0
4	EDO	18-A	701	-	3,3,3	0.47	0	2,2,2	0.23	0
4	EDO	12-A	701	-	3,3,3	0.60	0	2,2,2	0.28	0
4	EDO	17-B	701	-	3,3,3	0.40	0	2,2,2	1.11	0
4	EDO	3-A	701	-	3,3,3	0.25	0	2,2,2	0.98	0
4	EDO	8-A	701	-	3,3,3	0.49	0	2,2,2	0.76	0
4	EDO	24-A	701	-	3,3,3	0.43	0	2,2,2	0.51	0
4	EDO	20-B	701	-	3,3,3	0.68	0	2,2,2	0.52	0
4	EDO	13-A	701	-	3,3,3	0.52	0	2,2,2	0.16	0
4	EDO	23-A	701	-	3,3,3	0.42	0	2,2,2	0.46	0
4	EDO	22-B	701	-	3,3,3	0.40	0	2,2,2	0.30	0
4	EDO	9-B	701	-	3,3,3	0.49	0	2,2,2	0.07	0
4	EDO	5-B	701	-	3,3,3	0.50	0	2,2,2	0.66	0
4	EDO	4-B	701	-	3,3,3	0.69	0	2,2,2	0.43	0
4	EDO	17-A	701	-	3,3,3	0.46	0	2,2,2	0.74	0
4	EDO	14-B	701	-	3,3,3	0.40	0	2,2,2	0.56	0
4	EDO	2-B	701	-	3,3,3	0.66	0	2,2,2	0.46	0
4	EDO	1-B	701	-	3,3,3	0.62	0	2,2,2	0.74	0
4	EDO	18-B	701	-	3,3,3	0.41	0	2,2,2	0.30	0
4	EDO	8-B	701	-	3,3,3	0.34	0	2,2,2	0.75	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	15-B	701	-	-	0/1/1/1	-
4	EDO	9-A	701	-	-	0/1/1/1	-
4	EDO	11-A	701	-	-	0/1/1/1	-
4	EDO	24-B	701	-	-	0/1/1/1	-

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	2-B	701	-	-	1/1/1/1	-
4	EDO	1-B	701	-	-	1/1/1/1	-
4	EDO	18-B	701	-	-	0/1/1/1	-
4	EDO	8-B	701	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	6-B	701	EDO	O2-C2-C1	-2.32	95.20	111.91

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	5-A	701	EDO	O1-C1-C2-O2
4	8-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	14-B	701	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	1-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	2-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	2-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	3-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	3-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	4-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	4-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	5-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	5-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	6-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	6-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	7-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	7-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	8-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	8-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	9-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	9-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	10-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	10-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	11-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	11-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	12-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	12-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	13-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	13-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	14-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	14-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	15-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	15-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	16-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	16-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	17-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	17-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	18-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	18-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	19-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	19-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	20-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	20-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	21-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	21-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	22-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	22-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	23-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	23-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	24-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	24-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
1	25-A	549/549 (100%)	0.24	41 (7%)	14	19	13, 14, 15, 16	549 (100%)
1	25-B	548/549 (99%)	0.17	42 (7%)	13	18	13, 14, 15, 16	548 (100%)
All	All	27425/27450 (99%)	0.21	2075 (7%)	16	18	13, 14, 15, 16	27425 (100%)

The worst 5 of 2075 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	57	GLU	10.3
1	2-A	57	GLU	10.3

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Mol	Chain	Res	Type	RSRZ
1	3-A	57	GLU	10.3
1	4-A	57	GLU	10.3
1	5-A	57	GLU	10.3

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	0.83	0.29	35,43,47,53	12
3	BGC	2-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	3-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	4-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	5-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	6-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	7-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	8-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	9-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	10-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	11-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	12-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	13-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	14-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	15-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	16-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	17-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	18-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	19-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	20-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	21-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	22-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	23-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	24-D	1	12/12	0.83	0.29	35,43,47,53	12
3	BGC	25-D	1	12/12	0.83	0.29	35,43,47,53	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	1-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	2-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	3-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	4-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	5-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	6-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	7-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	8-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	9-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	10-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	11-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	12-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	13-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	14-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	15-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	16-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	17-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	18-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	19-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	20-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	21-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	22-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	23-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	24-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	25-F	1	12/12	0.90	0.29	27,35,46,66	12
3	BGC	1-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	2-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	3-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	4-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	5-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	6-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	7-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	8-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	9-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	10-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	11-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	12-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	13-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	14-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	15-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	16-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	17-D	4	11/12	0.92	0.20	18,20,25,28	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	18-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	19-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	20-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	21-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	22-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	23-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	24-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	25-D	4	11/12	0.92	0.20	18,20,25,28	11
3	BGC	1-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	2-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	3-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	4-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	5-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	6-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	7-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	8-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	9-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	10-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	11-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	12-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	13-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	14-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	15-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	16-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	17-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	18-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	19-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	20-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	21-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	22-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	23-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	24-D	2	11/12	0.93	0.22	21,28,33,36	11
3	BGC	25-D	2	11/12	0.93	0.22	21,28,33,36	11
2	BGC	1-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	2-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	3-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	4-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	5-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	6-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	7-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	8-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	9-E	1	12/12	0.93	0.23	17,20,30,39	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	10-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	11-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	12-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	13-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	14-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	15-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	16-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	17-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	18-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	19-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	20-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	21-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	22-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	23-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	24-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	25-E	1	12/12	0.93	0.23	17,20,30,39	12
2	BGC	1-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	2-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	3-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	4-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	5-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	6-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	7-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	8-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	9-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	10-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	11-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	12-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	13-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	14-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	15-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	16-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	17-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	18-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	19-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	20-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	21-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	22-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	23-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	24-C	1	12/12	0.93	0.18	20,24,32,37	12
2	BGC	25-C	1	12/12	0.93	0.18	20,24,32,37	12
3	BGC	1-F	3	11/12	0.93	0.17	19,23,30,35	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	2-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	3-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	4-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	5-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	6-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	7-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	8-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	9-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	10-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	11-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	12-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	13-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	14-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	15-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	16-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	17-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	18-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	19-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	20-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	21-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	22-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	23-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	24-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	25-F	3	11/12	0.93	0.17	19,23,30,35	11
3	BGC	1-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	2-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	3-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	4-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	5-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	6-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	7-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	8-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	9-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	10-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	11-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	12-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	13-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	14-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	15-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	16-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	17-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	18-F	2	11/12	0.95	0.27	24,27,30,33	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	19-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	20-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	21-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	22-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	23-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	24-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	25-F	2	11/12	0.95	0.27	24,27,30,33	11
3	BGC	1-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	2-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	3-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	4-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	5-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	6-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	7-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	8-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	9-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	10-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	11-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	12-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	13-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	14-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	15-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	16-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	17-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	18-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	19-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	20-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	21-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	22-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	23-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	24-D	3	11/12	0.95	0.19	21,25,31,42	11
3	BGC	25-D	3	11/12	0.95	0.19	21,25,31,42	11
2	BGC	1-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	2-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	3-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	4-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	5-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	6-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	7-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	8-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	9-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	10-C	2	11/12	0.96	0.13	13,17,24,24	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	11-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	12-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	13-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	14-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	15-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	16-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	17-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	18-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	19-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	20-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	21-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	22-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	23-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	24-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	25-C	2	11/12	0.96	0.13	13,17,24,24	11
2	BGC	1-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	2-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	3-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	4-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	5-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	6-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	7-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	8-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	9-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	10-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	11-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	12-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	13-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	14-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	15-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	16-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	17-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	18-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	19-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	20-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	21-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	22-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	23-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	24-E	3	11/12	0.96	0.11	11,14,19,23	11
2	BGC	25-E	3	11/12	0.96	0.11	11,14,19,23	11
3	BGC	1-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	2-D	5	11/12	0.96	0.15	16,19,23,27	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	3-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	4-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	5-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	6-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	7-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	8-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	9-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	10-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	11-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	12-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	13-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	14-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	15-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	16-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	17-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	18-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	19-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	20-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	21-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	22-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	23-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	24-D	5	11/12	0.96	0.15	16,19,23,27	11
3	BGC	25-D	5	11/12	0.96	0.15	16,19,23,27	11
2	BGC	1-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	2-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	3-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	4-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	5-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	6-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	7-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	8-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	9-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	10-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	11-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	12-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	13-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	14-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	15-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	16-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	17-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	18-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	19-E	5	11/12	0.96	0.08	11,13,18,20	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	20-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	21-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	22-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	23-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	24-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	25-E	5	11/12	0.96	0.08	11,13,18,20	11
2	BGC	1-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	2-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	3-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	4-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	5-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	6-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	7-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	8-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	9-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	10-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	11-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	12-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	13-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	14-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	15-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	16-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	17-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	18-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	19-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	20-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	21-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	22-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	23-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	24-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	25-C	3	11/12	0.96	0.12	12,13,18,26	11
2	BGC	1-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	2-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	3-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	4-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	5-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	6-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	7-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	8-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	9-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	10-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	11-C	5	11/12	0.96	0.07	10,12,18,22	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	12-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	13-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	14-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	15-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	16-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	17-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	18-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	19-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	20-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	21-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	22-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	23-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	24-C	5	11/12	0.96	0.07	10,12,18,22	11
2	BGC	25-C	5	11/12	0.96	0.07	10,12,18,22	11
3	BGC	1-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	2-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	3-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	4-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	5-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	6-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	7-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	8-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	9-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	10-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	11-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	12-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	13-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	14-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	15-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	16-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	17-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	18-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	19-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	20-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	21-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	22-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	23-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	24-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	25-F	4	11/12	0.96	0.21	15,19,22,29	11
3	BGC	1-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	2-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	3-F	5	11/12	0.96	0.10	15,17,22,25	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	4-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	5-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	6-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	7-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	8-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	9-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	10-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	11-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	12-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	13-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	14-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	15-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	16-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	17-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	18-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	19-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	20-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	21-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	22-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	23-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	24-F	5	11/12	0.96	0.10	15,17,22,25	11
3	BGC	25-F	5	11/12	0.96	0.10	15,17,22,25	11
2	BGC	1-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	2-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	3-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	4-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	5-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	6-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	7-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	8-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	9-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	10-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	11-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	12-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	13-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	14-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	15-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	16-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	17-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	18-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	19-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	20-E	2	11/12	0.97	0.08	15,17,23,23	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	21-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	22-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	23-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	24-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	25-E	2	11/12	0.97	0.08	15,17,23,23	11
2	BGC	1-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	2-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	3-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	4-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	5-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	6-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	7-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	8-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	9-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	10-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	11-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	12-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	13-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	14-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	15-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	16-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	17-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	18-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	19-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	20-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	21-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	22-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	23-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	24-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	25-E	6	11/12	0.97	0.08	10,12,13,14	11
2	BGC	1-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	2-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	3-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	4-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	5-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	6-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	7-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	8-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	9-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	10-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	11-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	12-C	4	11/12	0.97	0.10	11,12,16,17	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	13-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	14-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	15-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	16-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	17-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	18-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	19-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	20-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	21-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	22-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	23-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	24-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	25-C	4	11/12	0.97	0.10	11,12,16,17	11
2	BGC	1-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	2-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	3-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	4-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	5-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	6-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	7-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	8-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	9-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	10-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	11-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	12-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	13-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	14-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	15-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	16-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	17-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	18-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	19-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	20-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	21-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	22-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	23-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	24-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	25-E	4	11/12	0.97	0.07	11,12,17,18	11
2	BGC	1-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	2-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	3-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	4-C	6	11/12	0.98	0.07	9,12,14,14	11

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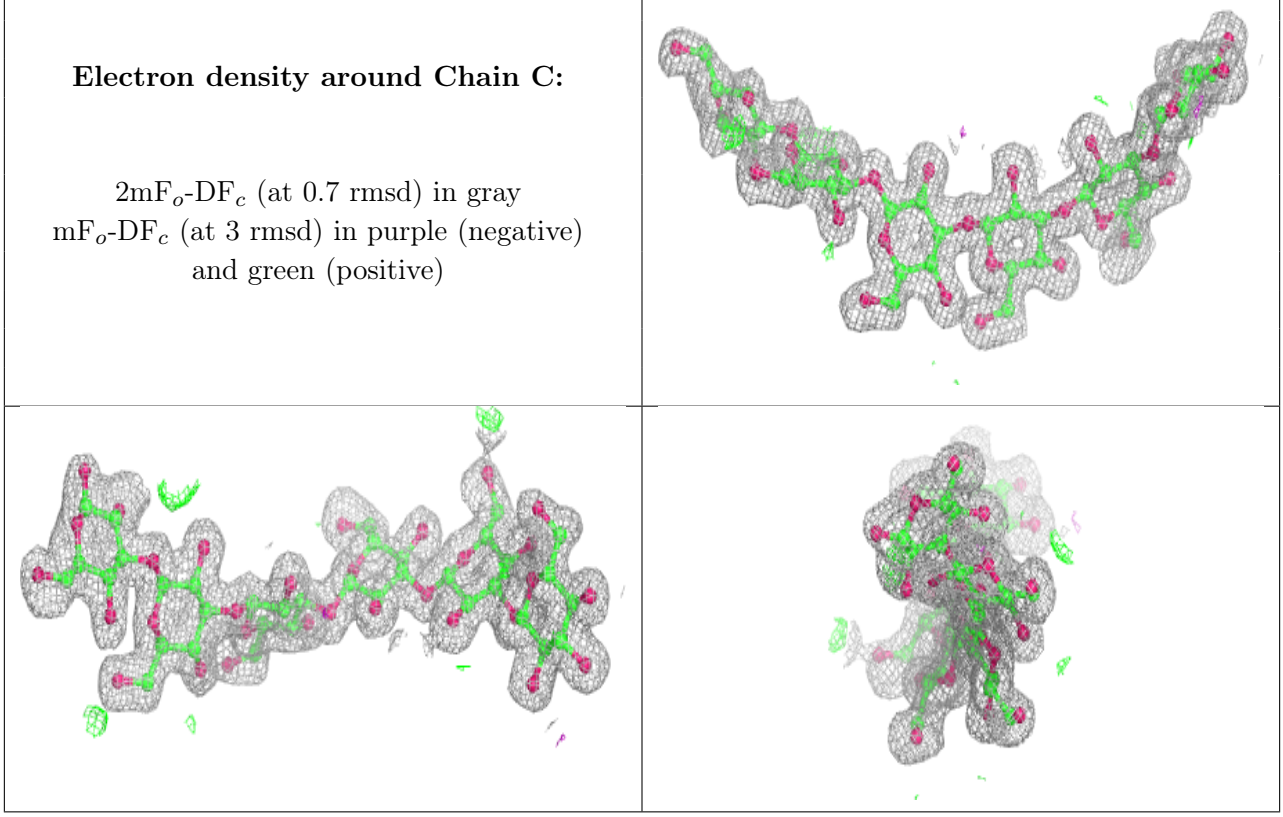
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	5-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	6-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	7-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	8-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	9-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	10-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	11-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	12-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	13-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	14-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	15-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	16-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	17-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	18-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	19-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	20-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	21-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	22-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	23-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	24-C	6	11/12	0.98	0.07	9,12,14,14	11
2	BGC	25-C	6	11/12	0.98	0.07	9,12,14,14	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.

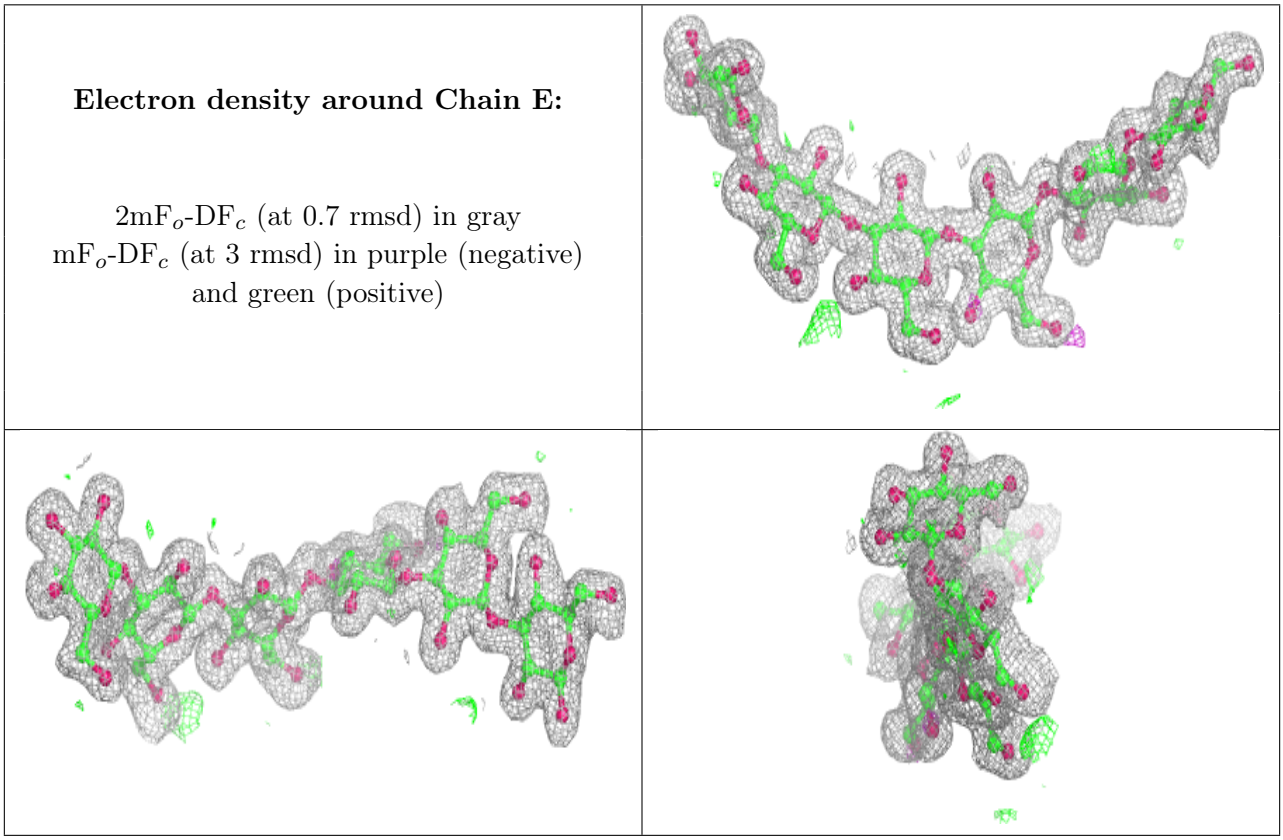
Electron density around Chain C:

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



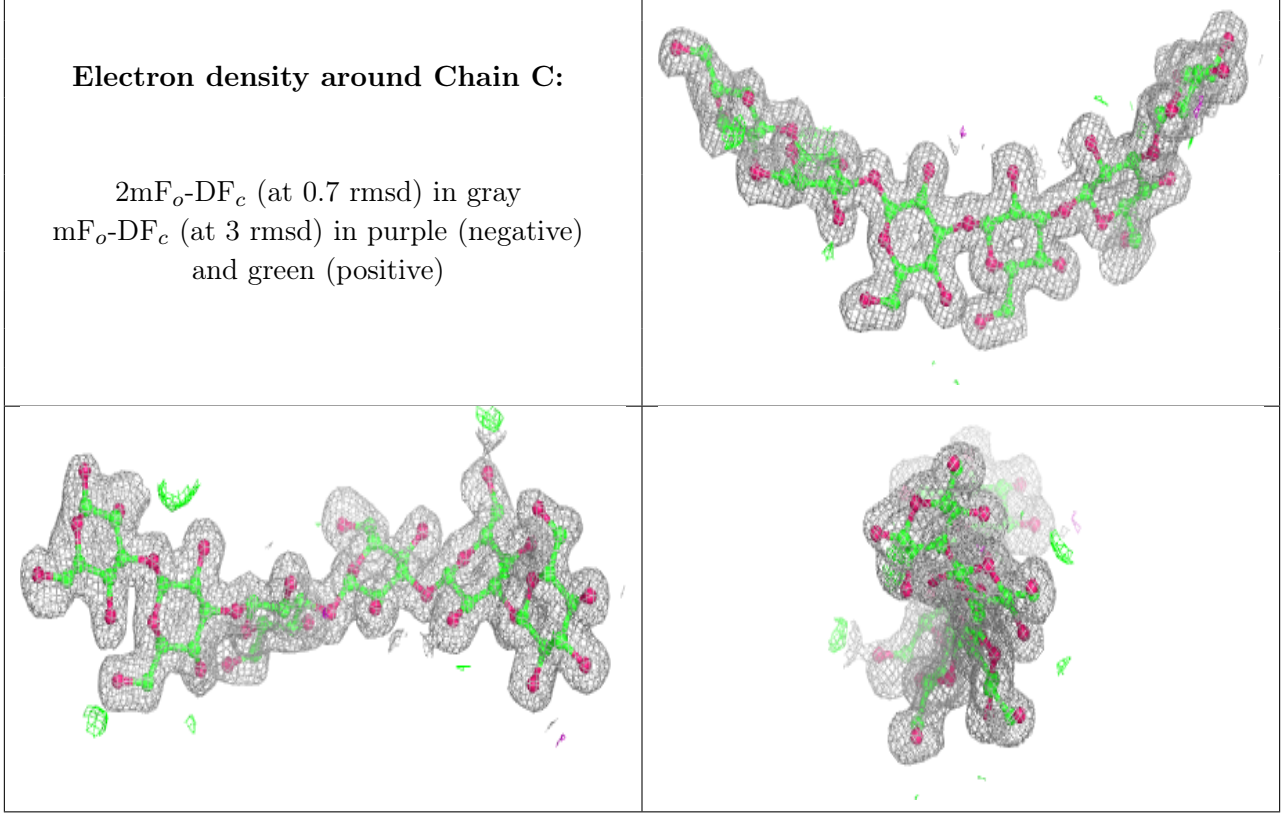
Electron density around Chain E:

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



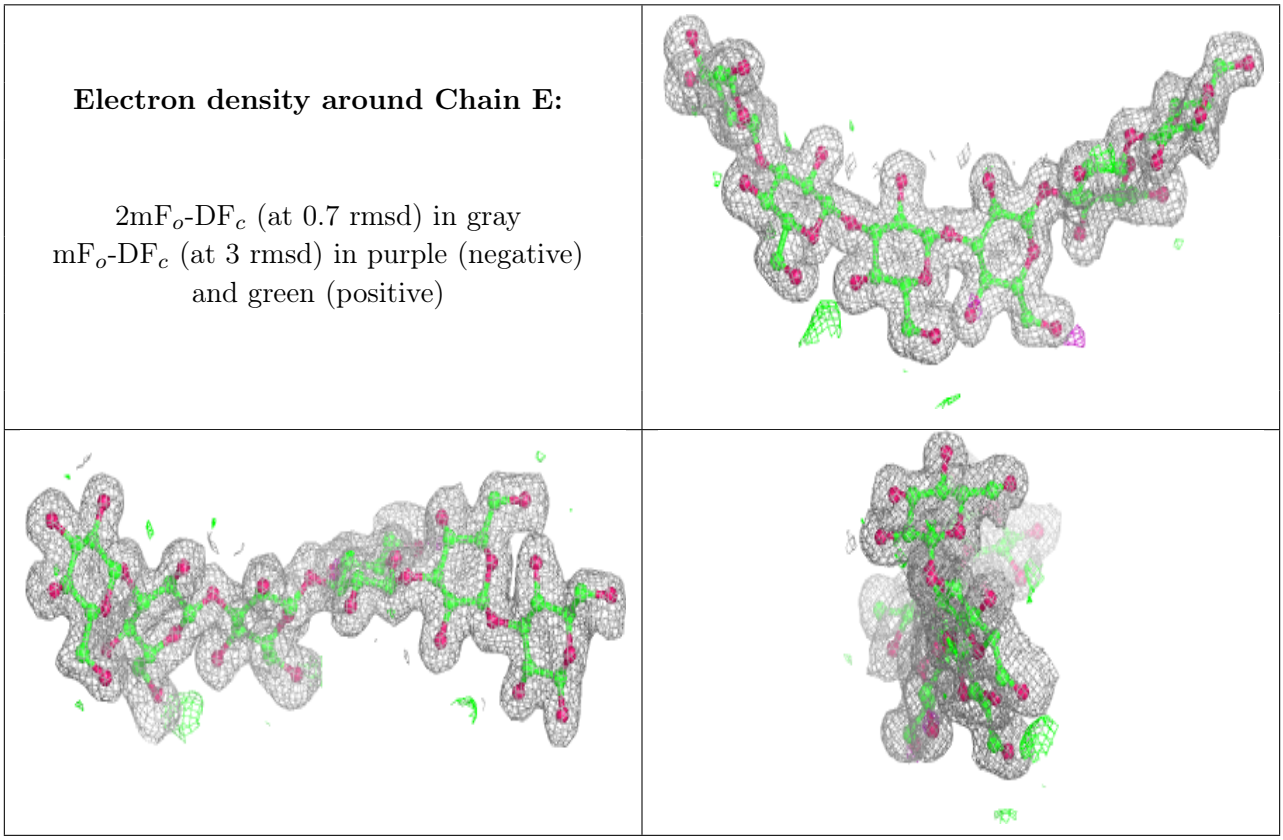
Electron density around Chain C:

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



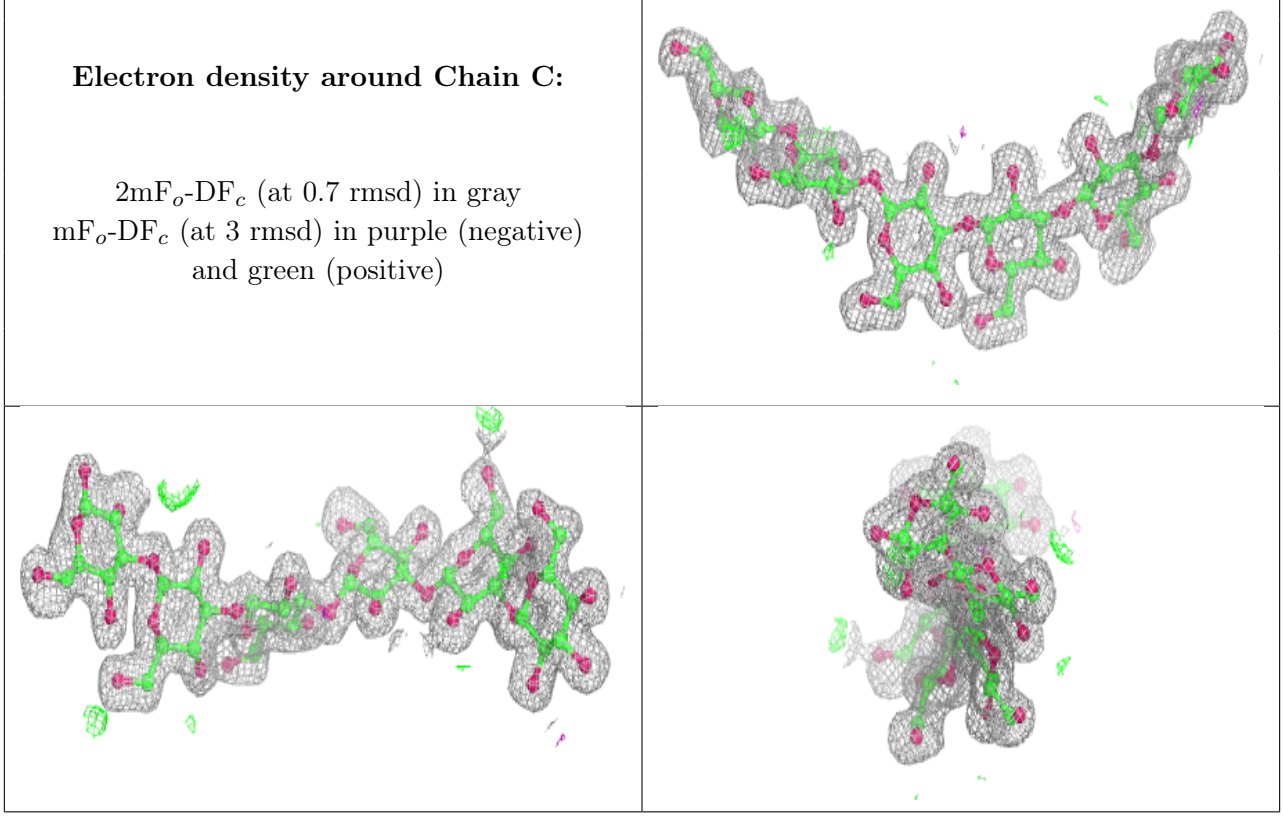
Electron density around Chain E:

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



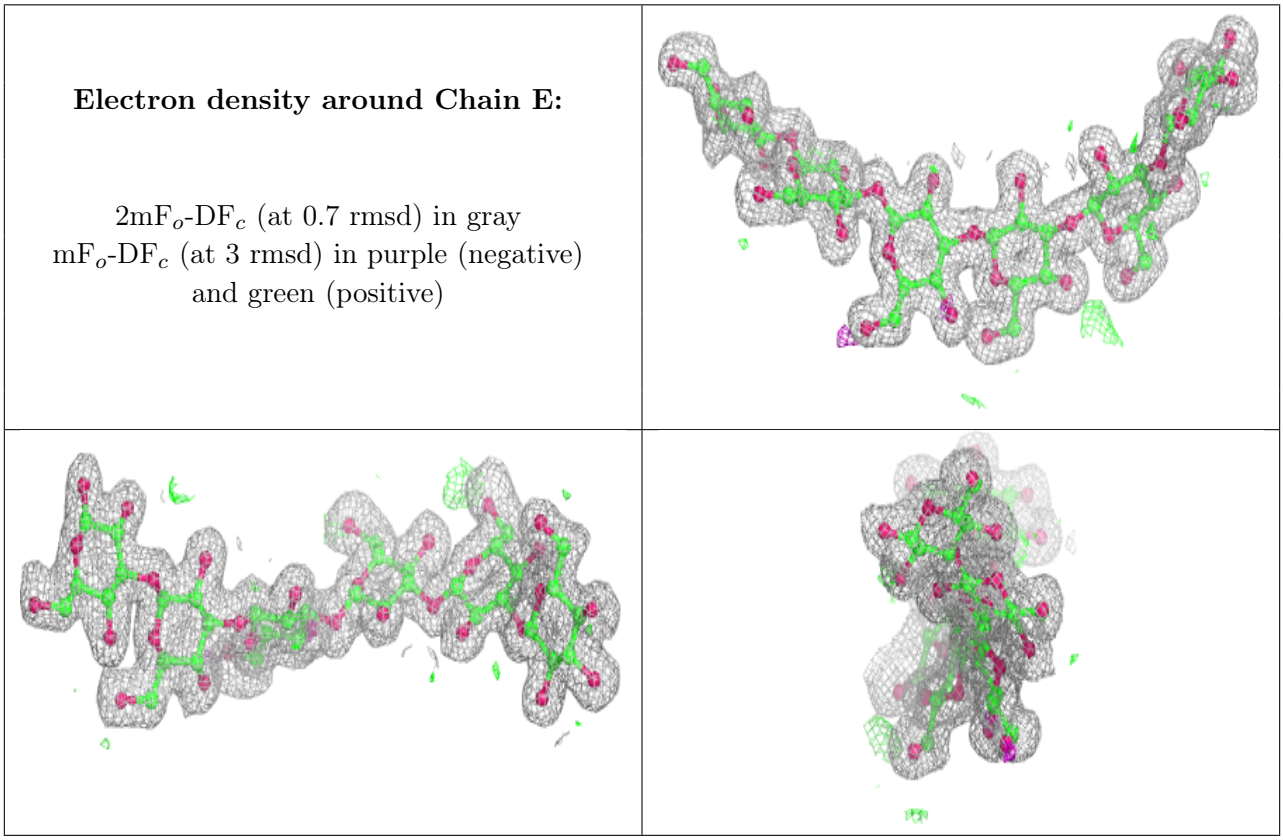
Electron density around Chain C:

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



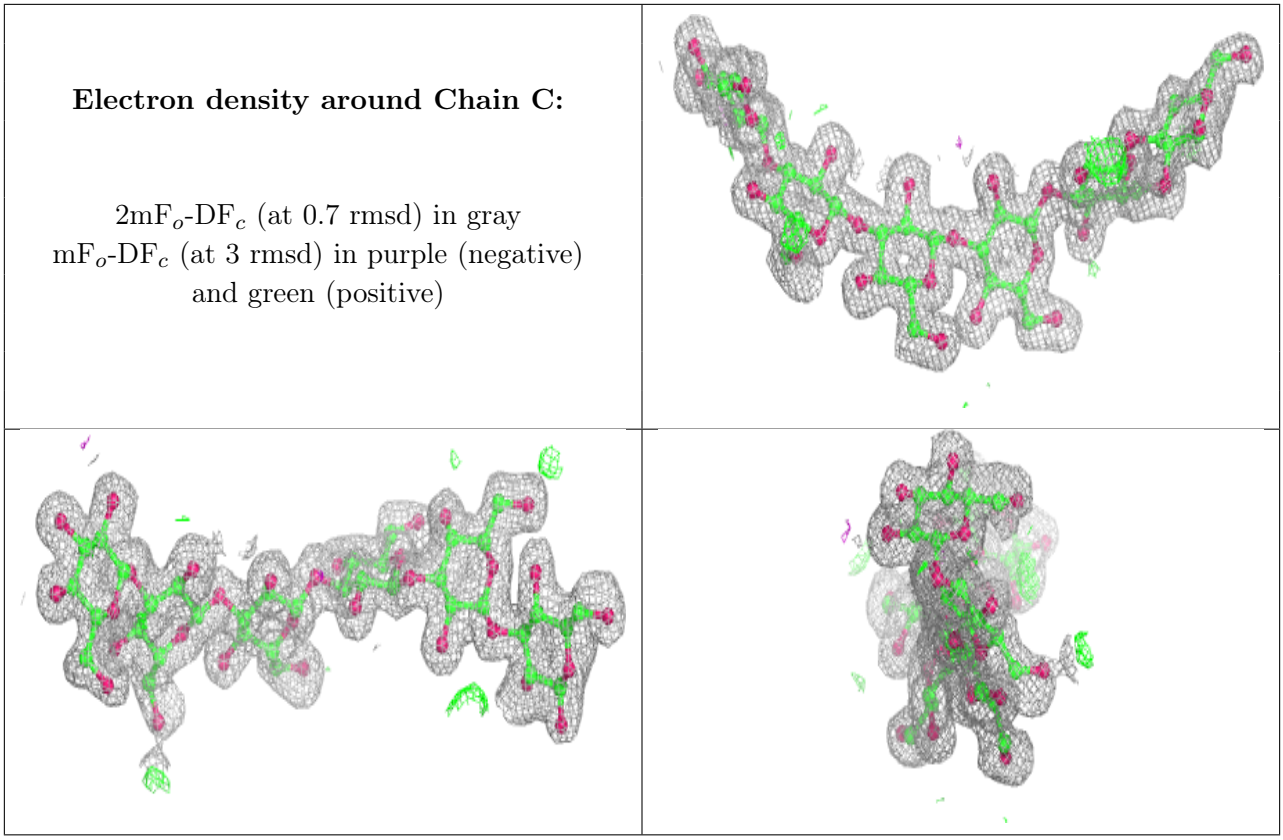
Electron density around Chain E:

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



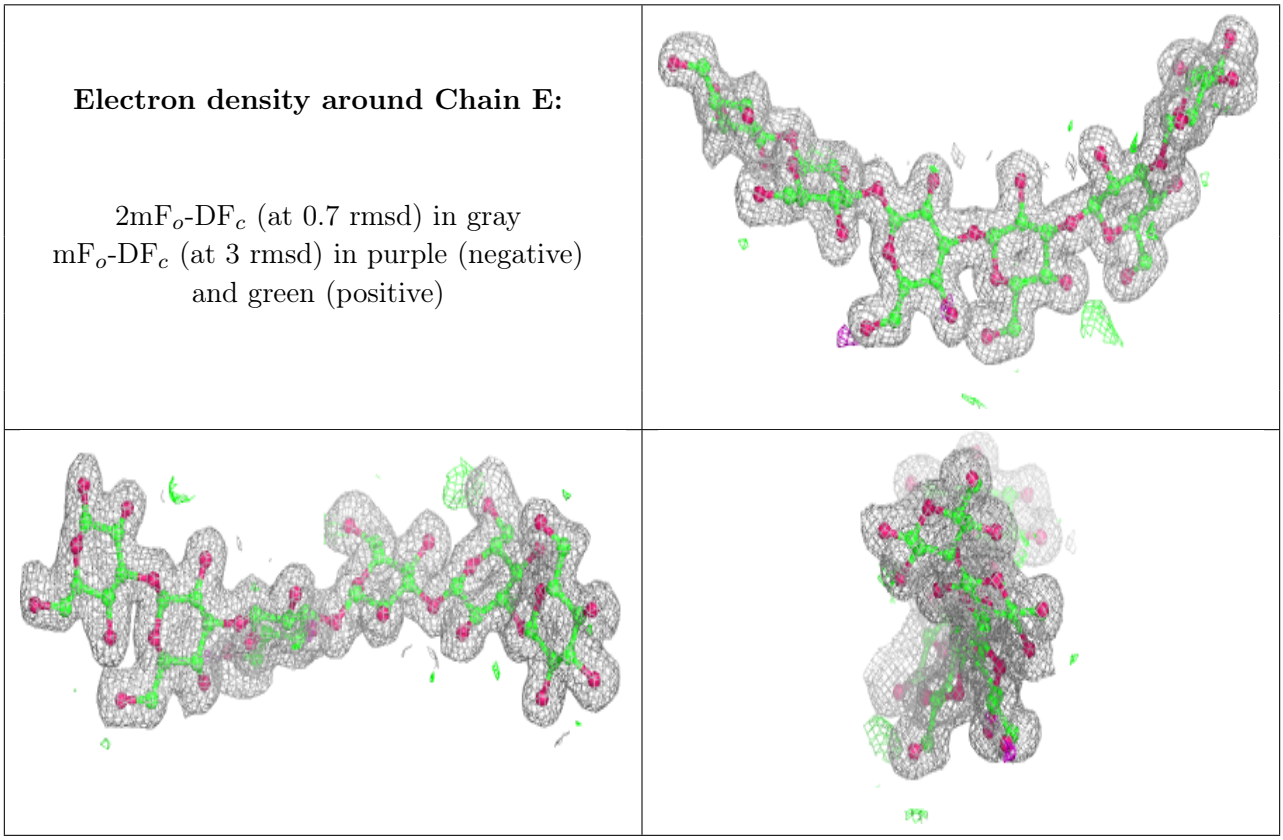
Electron density around Chain C:

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



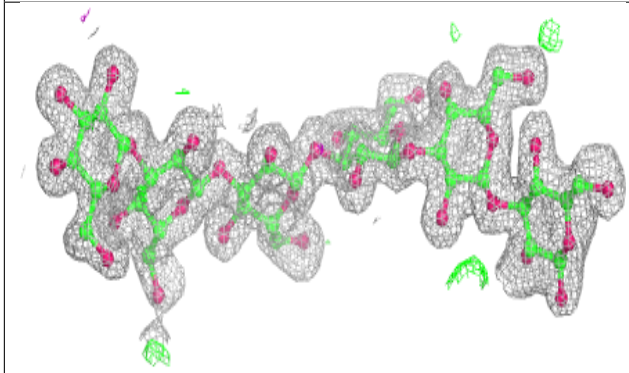
Electron density around Chain E:

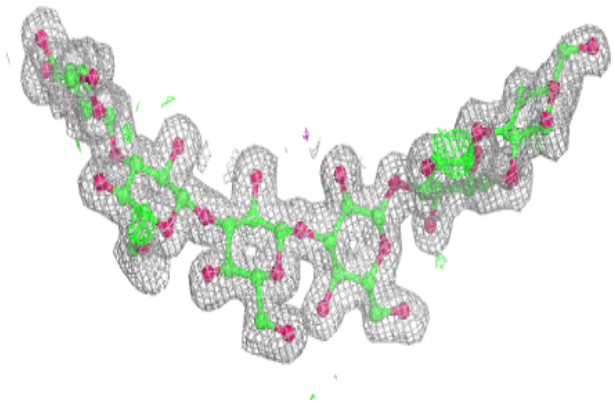
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

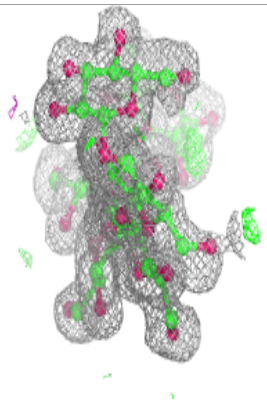


Electron density around Chain C:

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

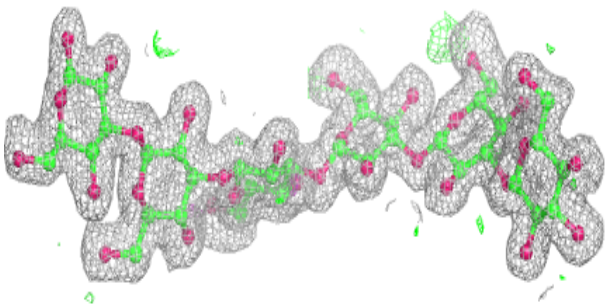


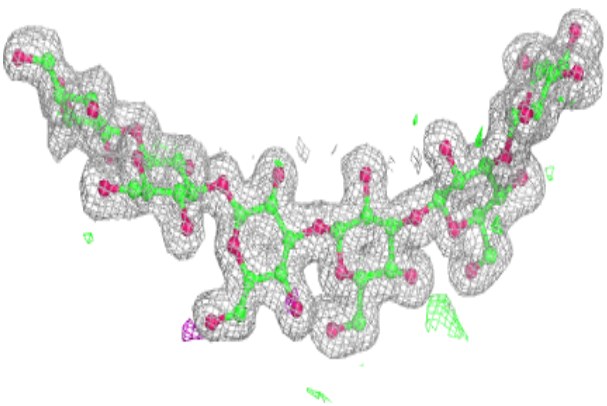


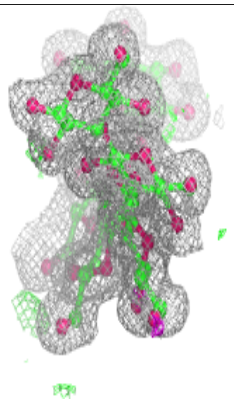


Electron density around Chain E:

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

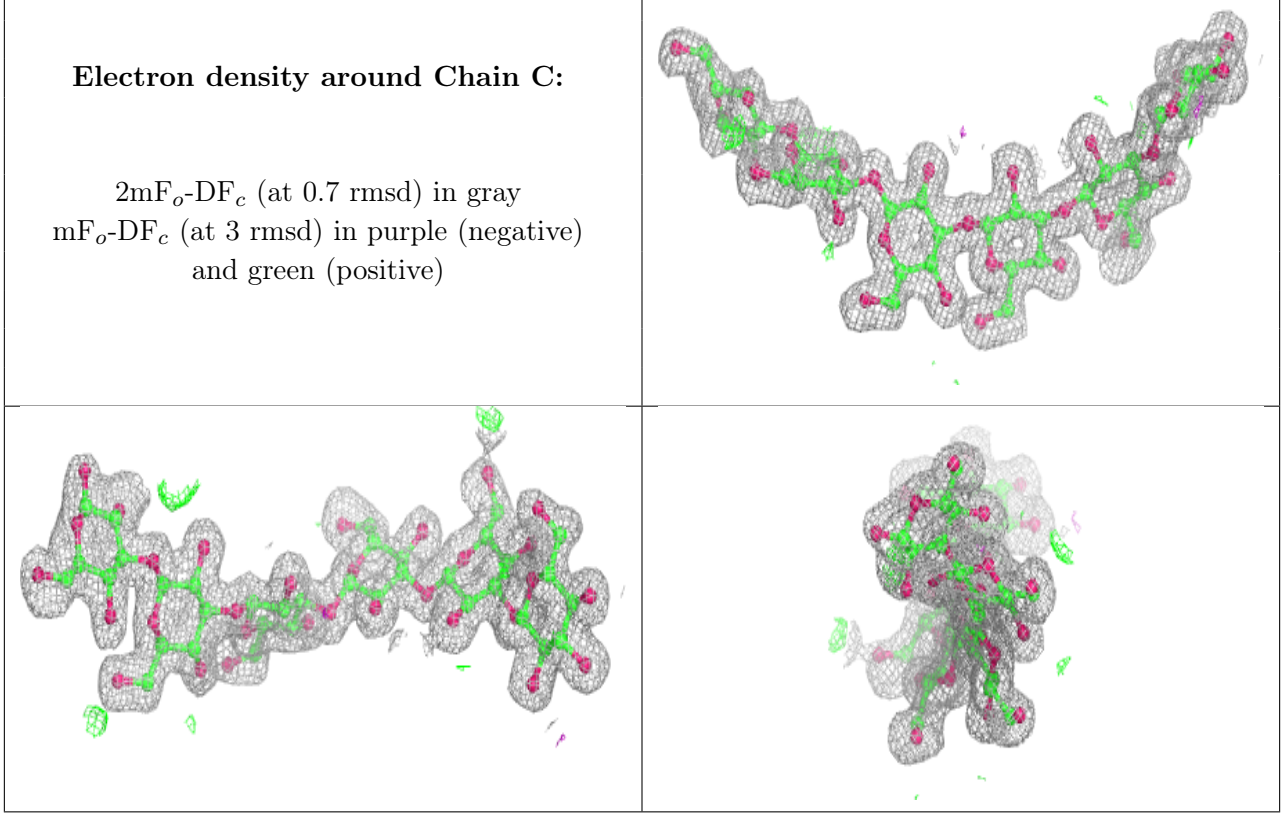






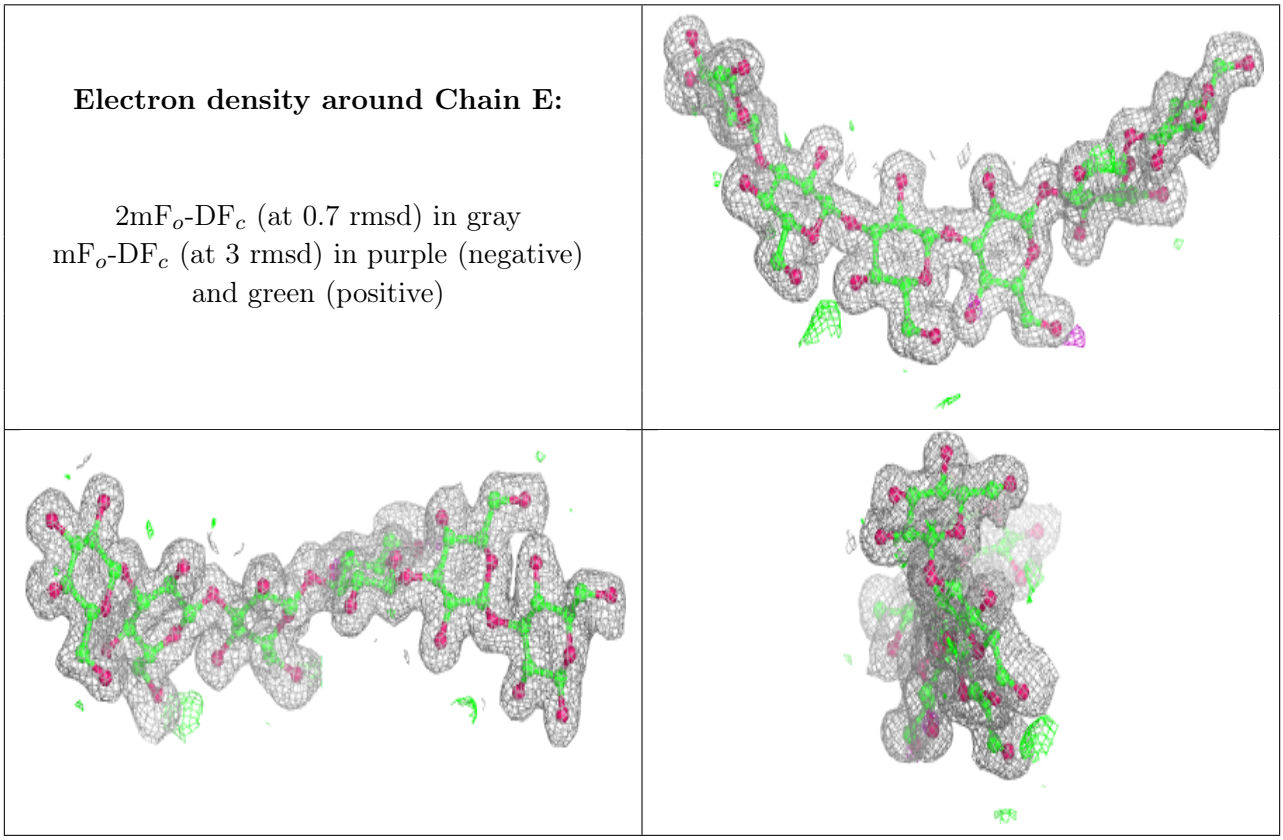
Electron density around Chain C:

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



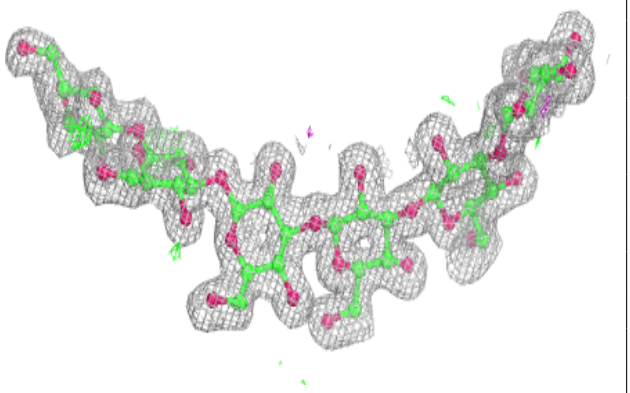
Electron density around Chain E:

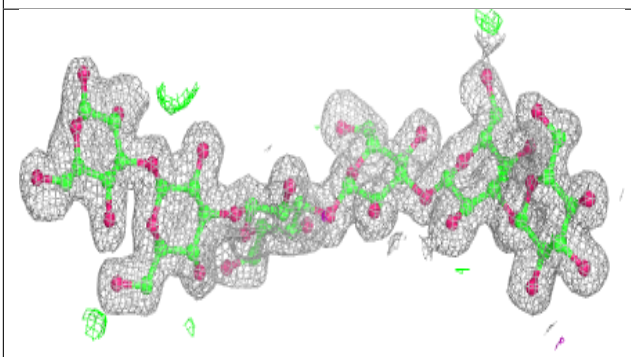
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

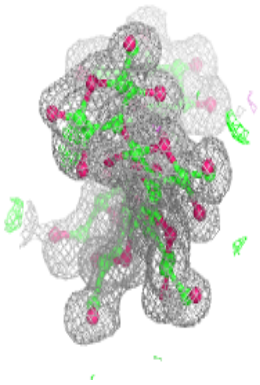


Electron density around Chain C:

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

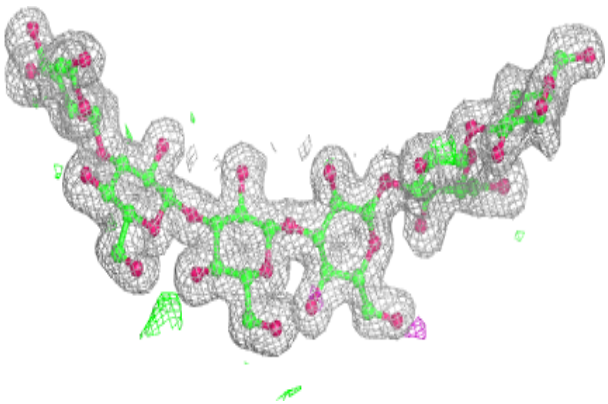


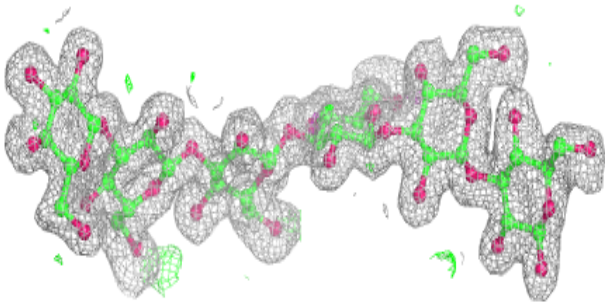


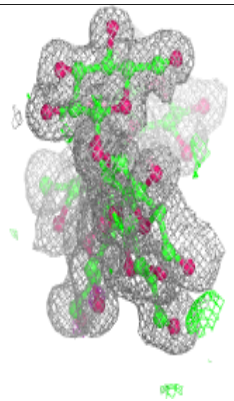


Electron density around Chain E:

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

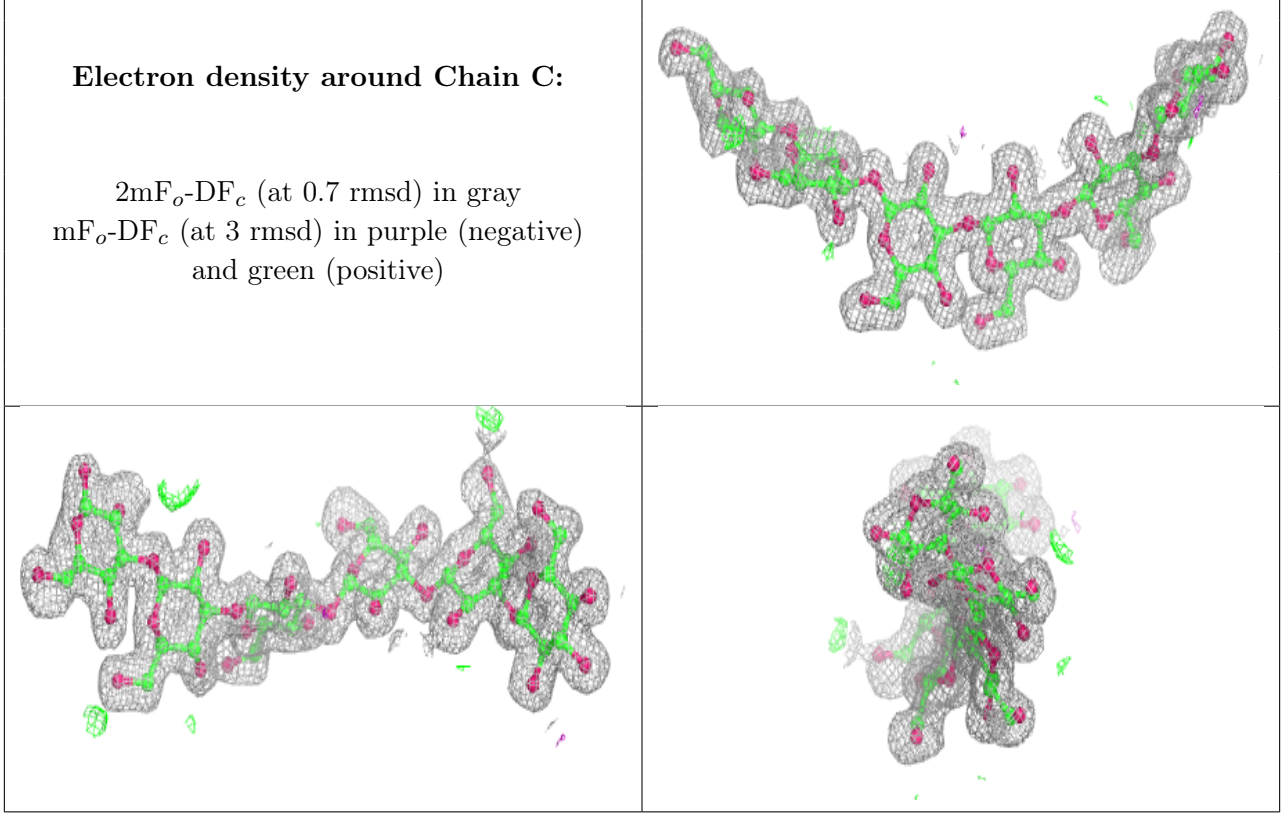






Electron density around Chain C:

$2mF_o$-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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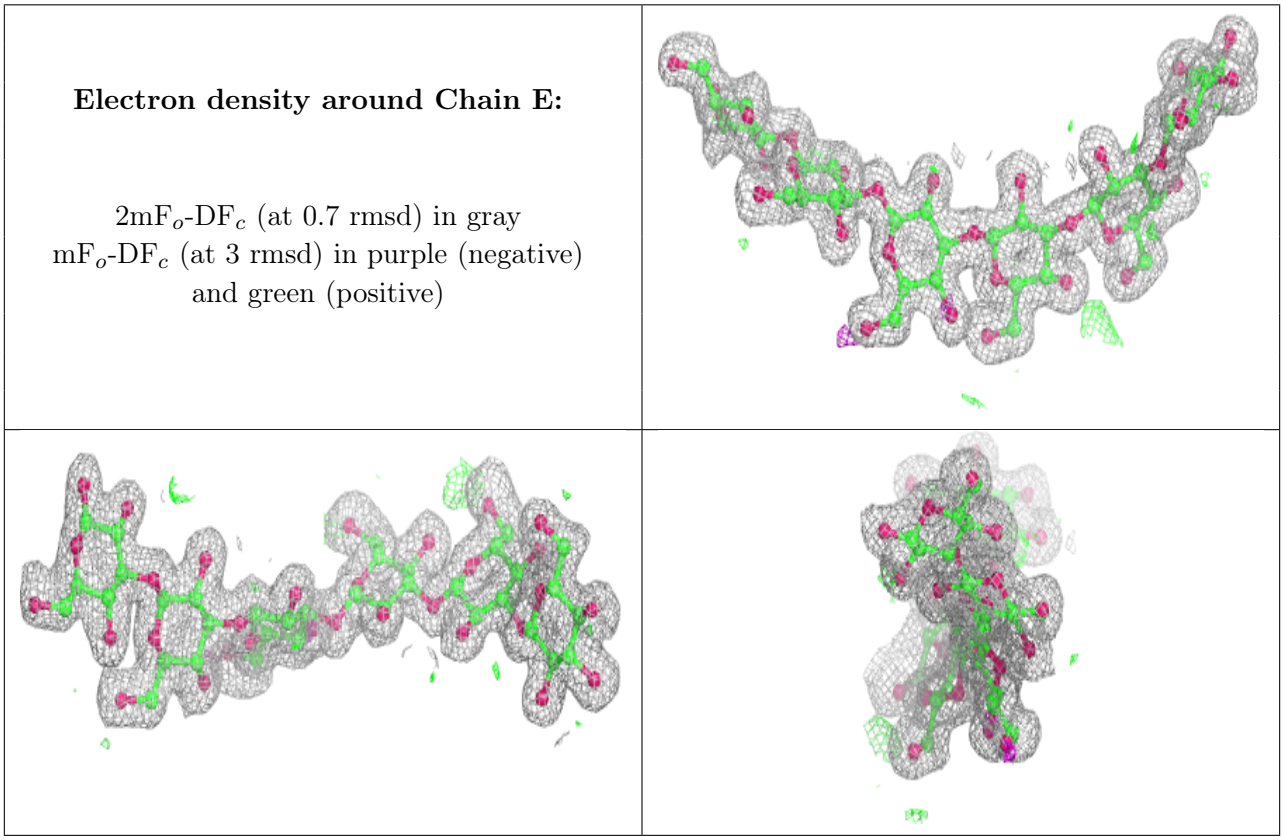

Electron density around Chain C:

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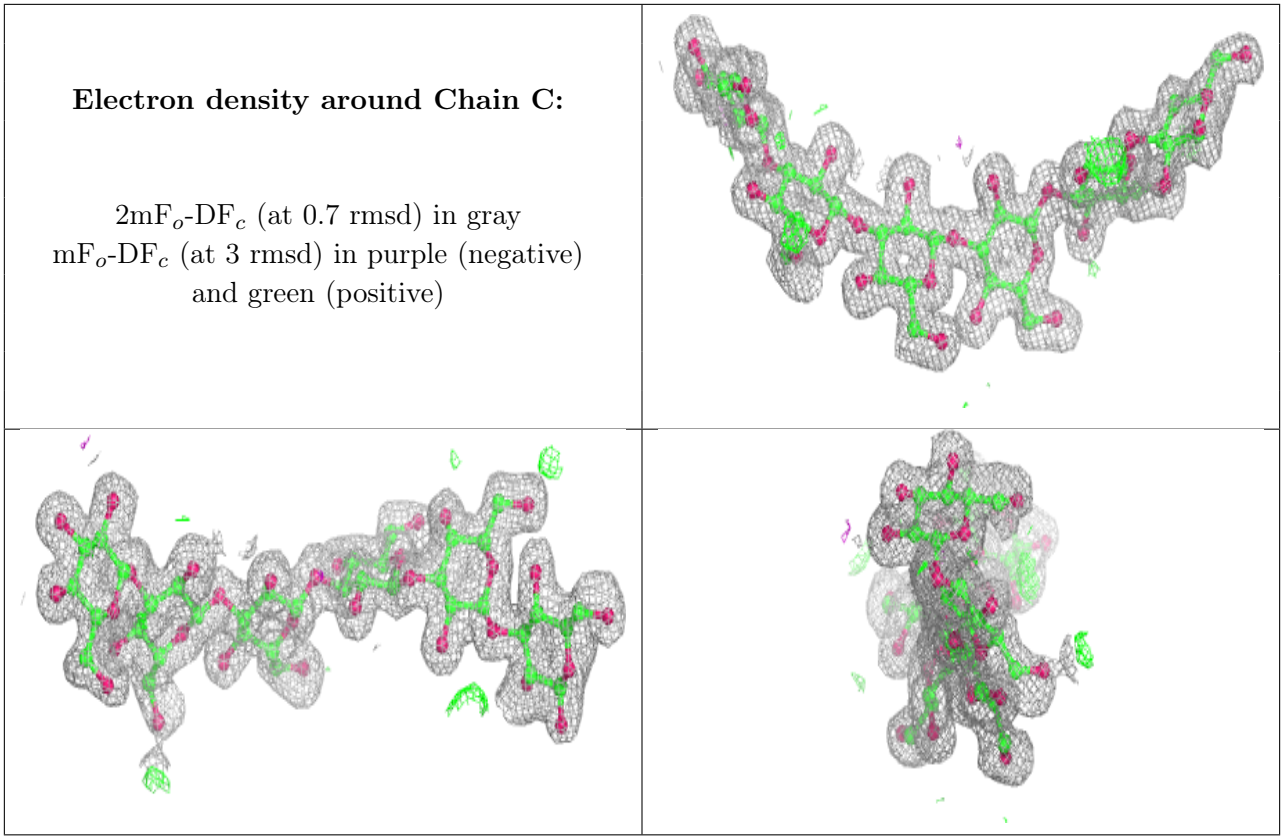

Electron density around Chain E:

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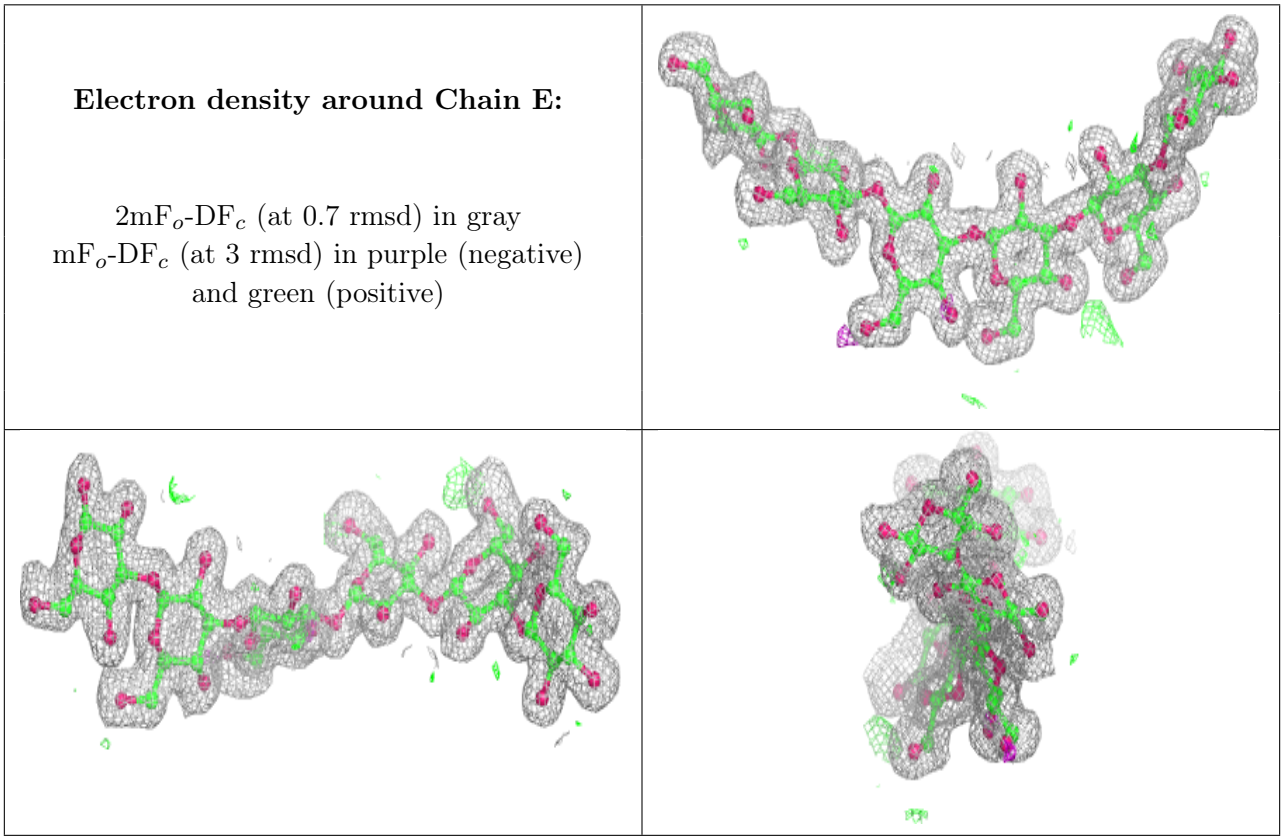

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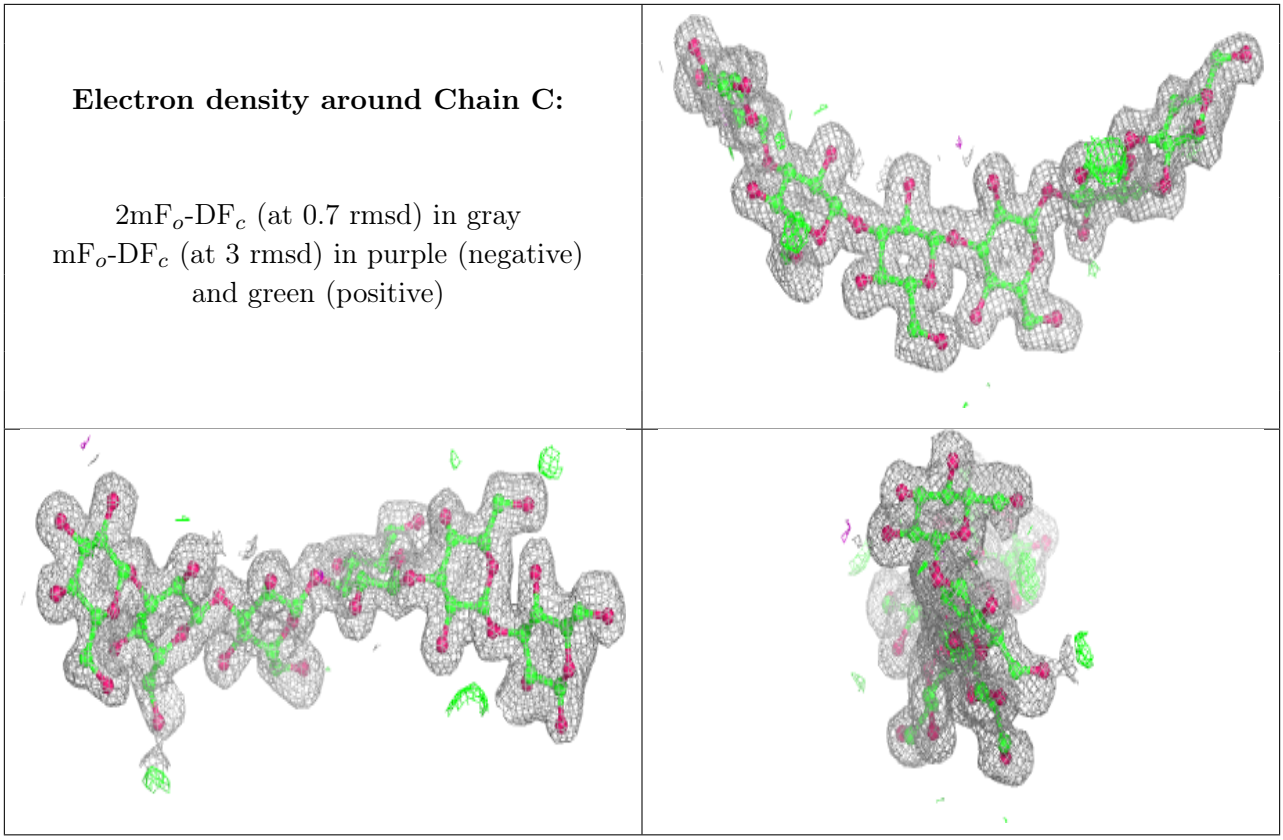

Electron density around Chain E:

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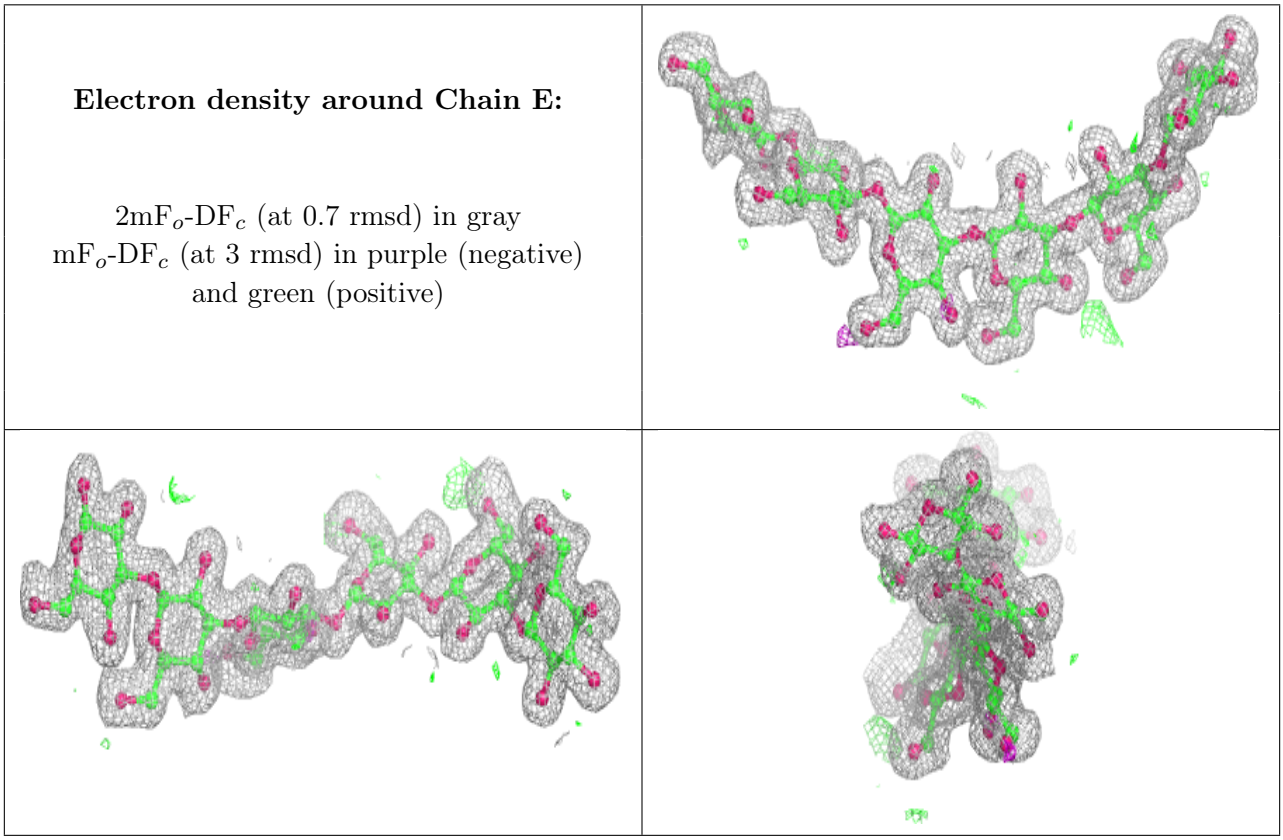

Electron density around Chain C:

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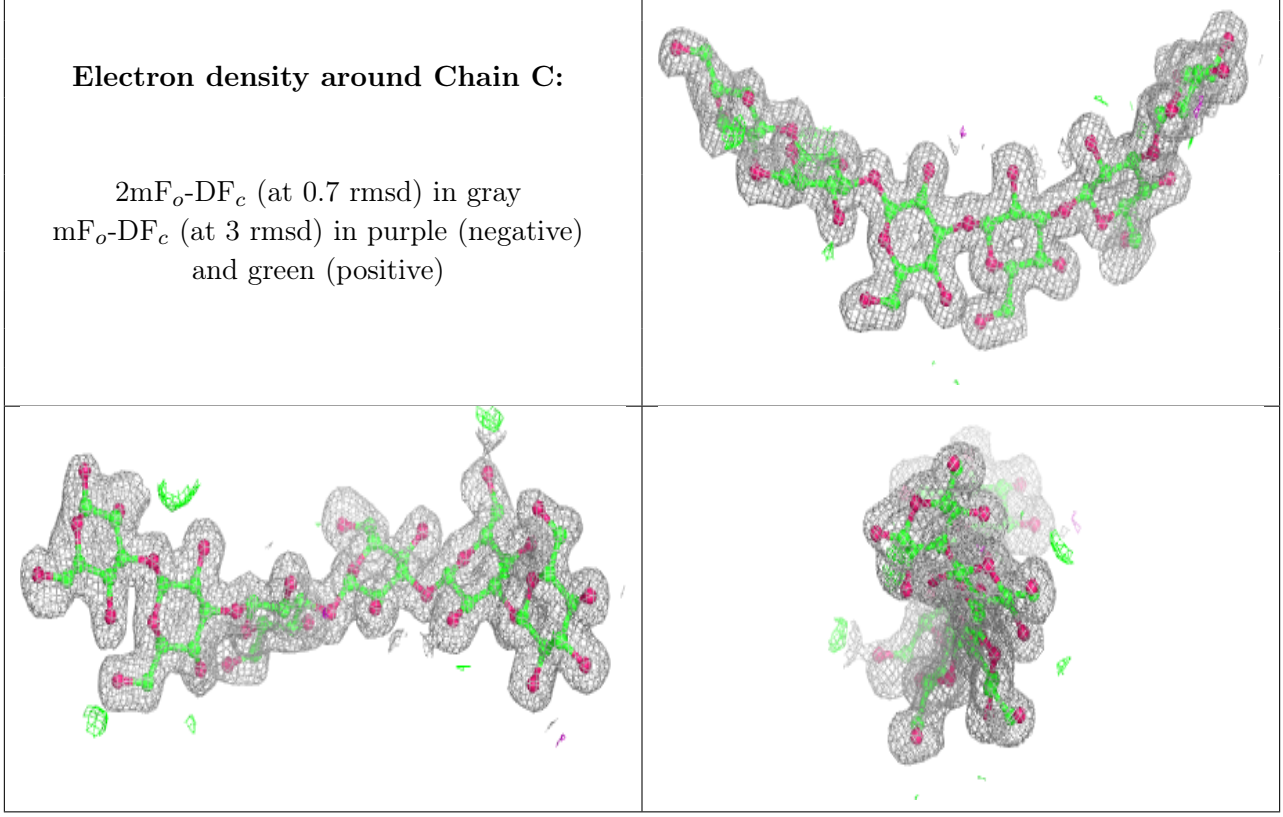
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain E:

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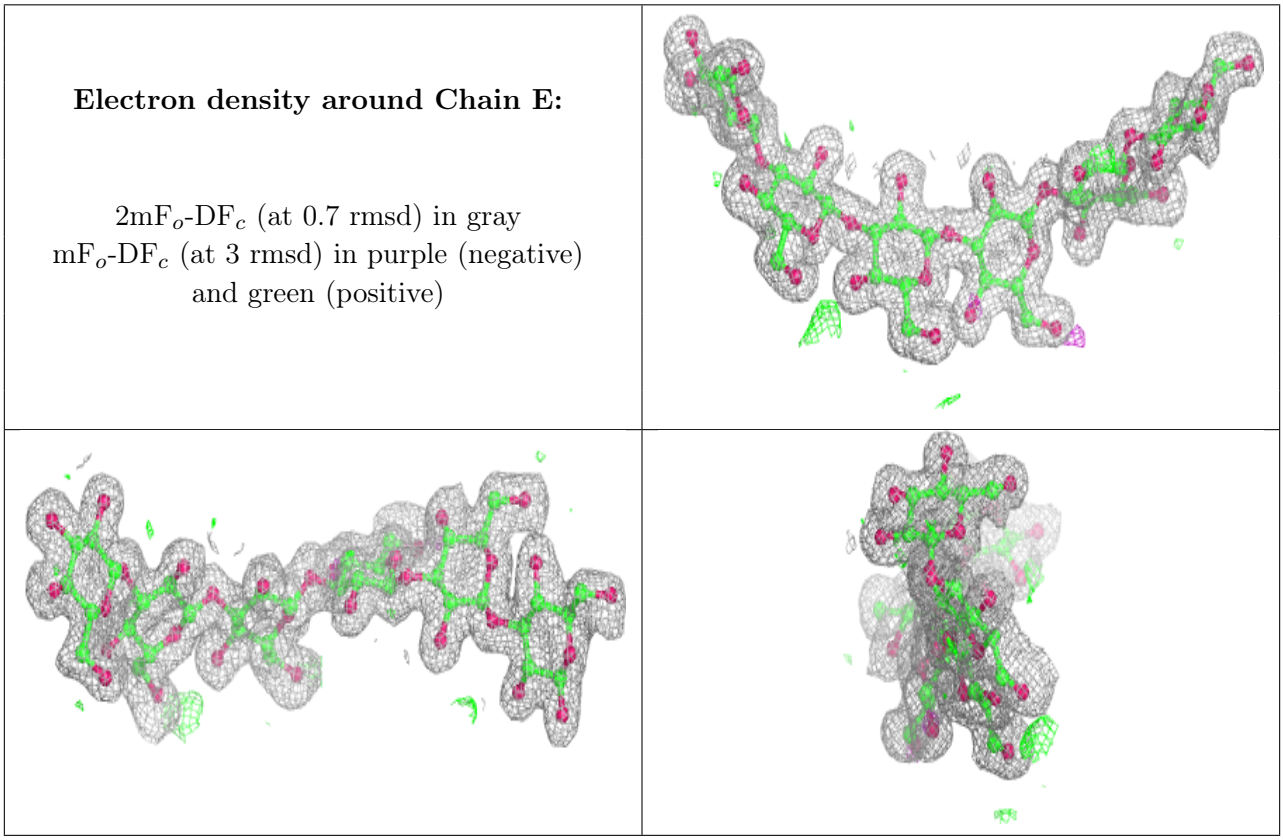
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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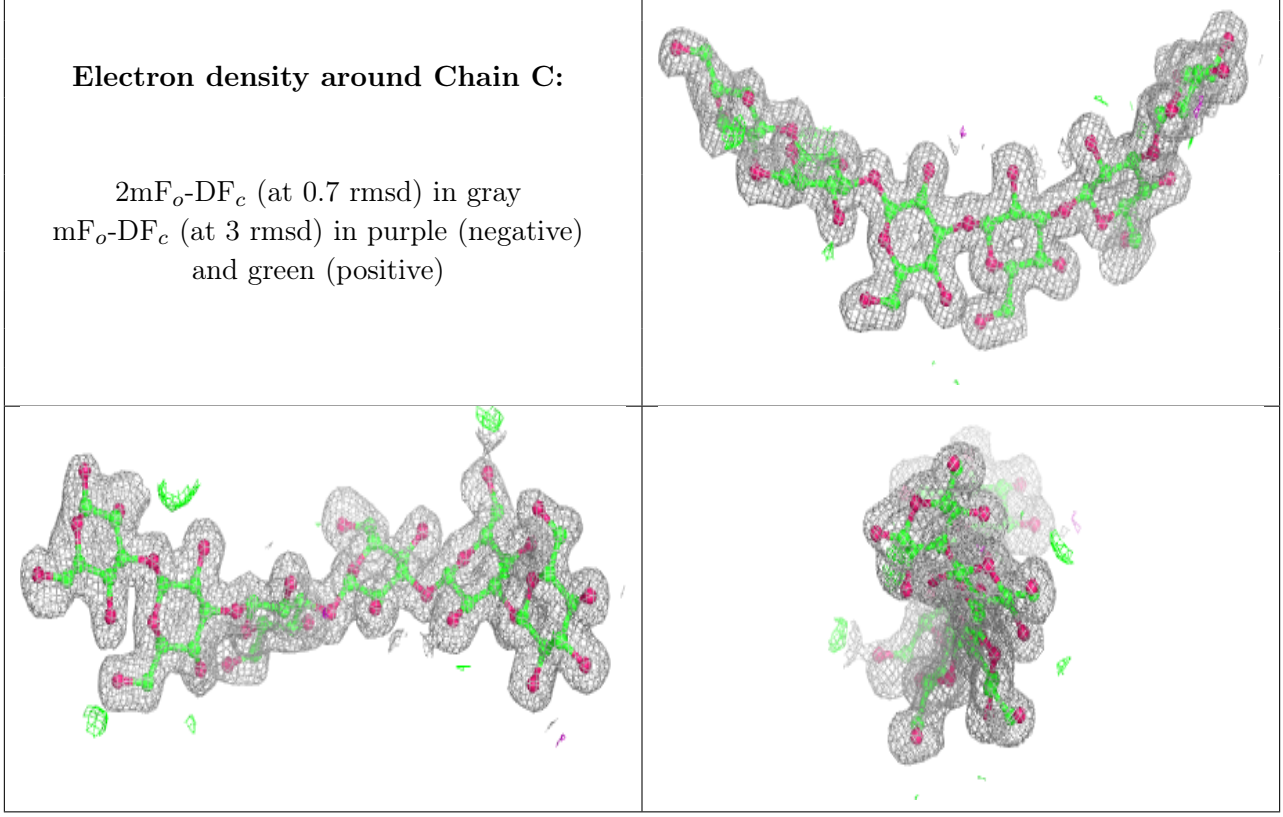

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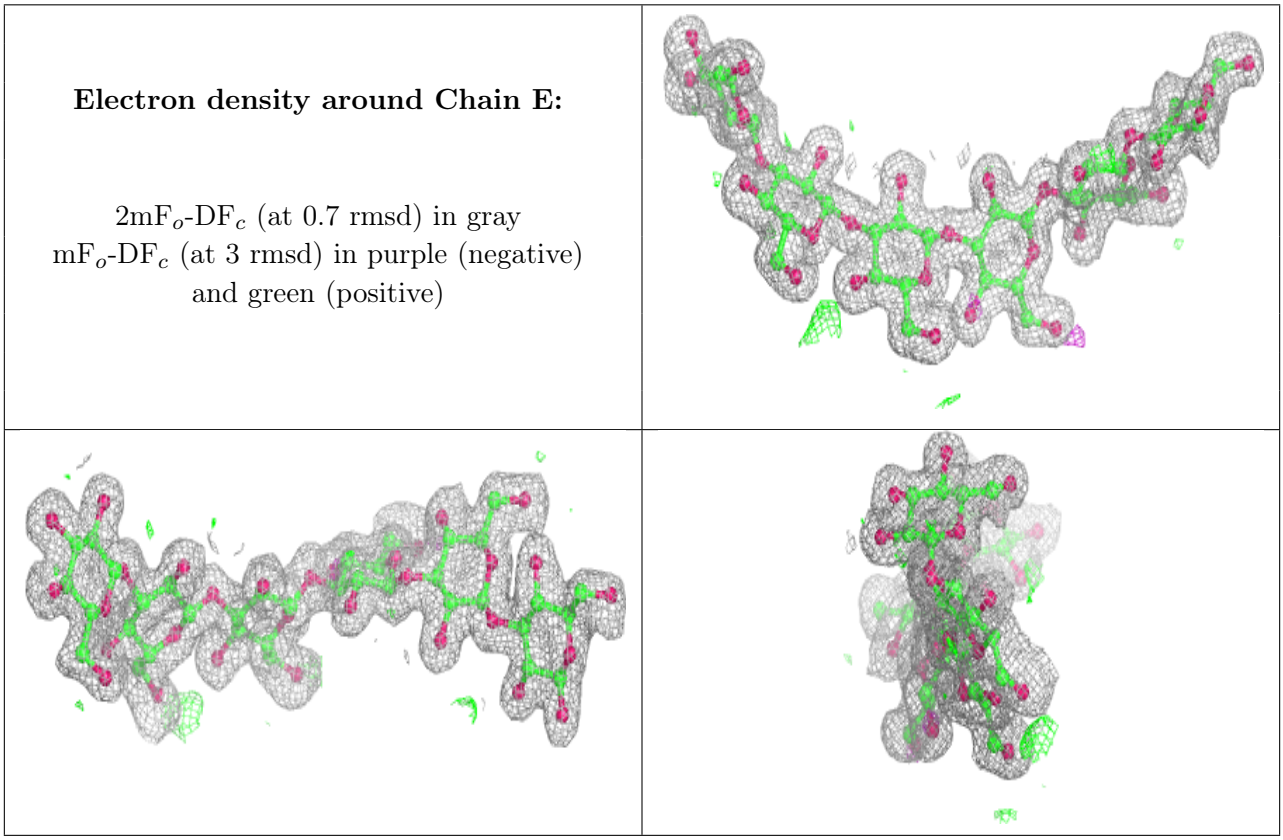

Electron density around Chain C:

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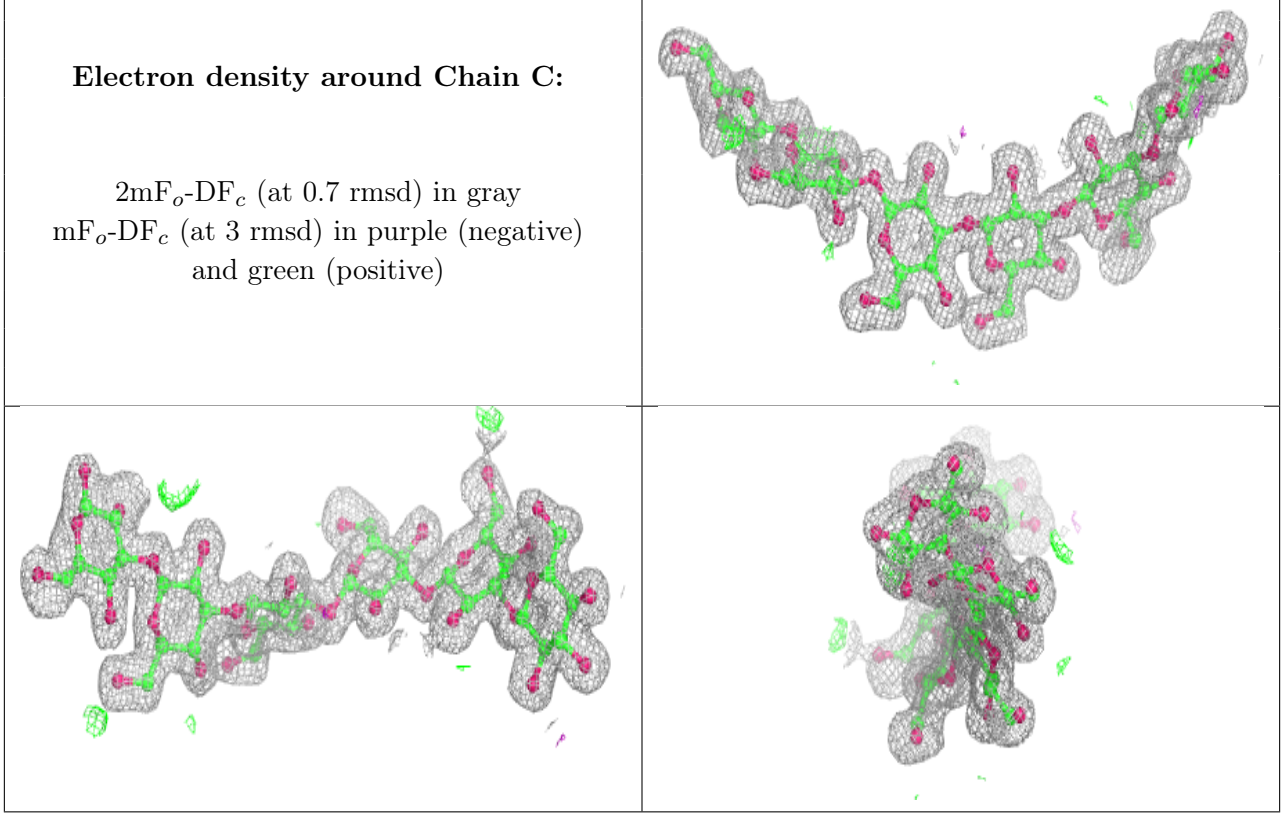

Electron density around Chain E:

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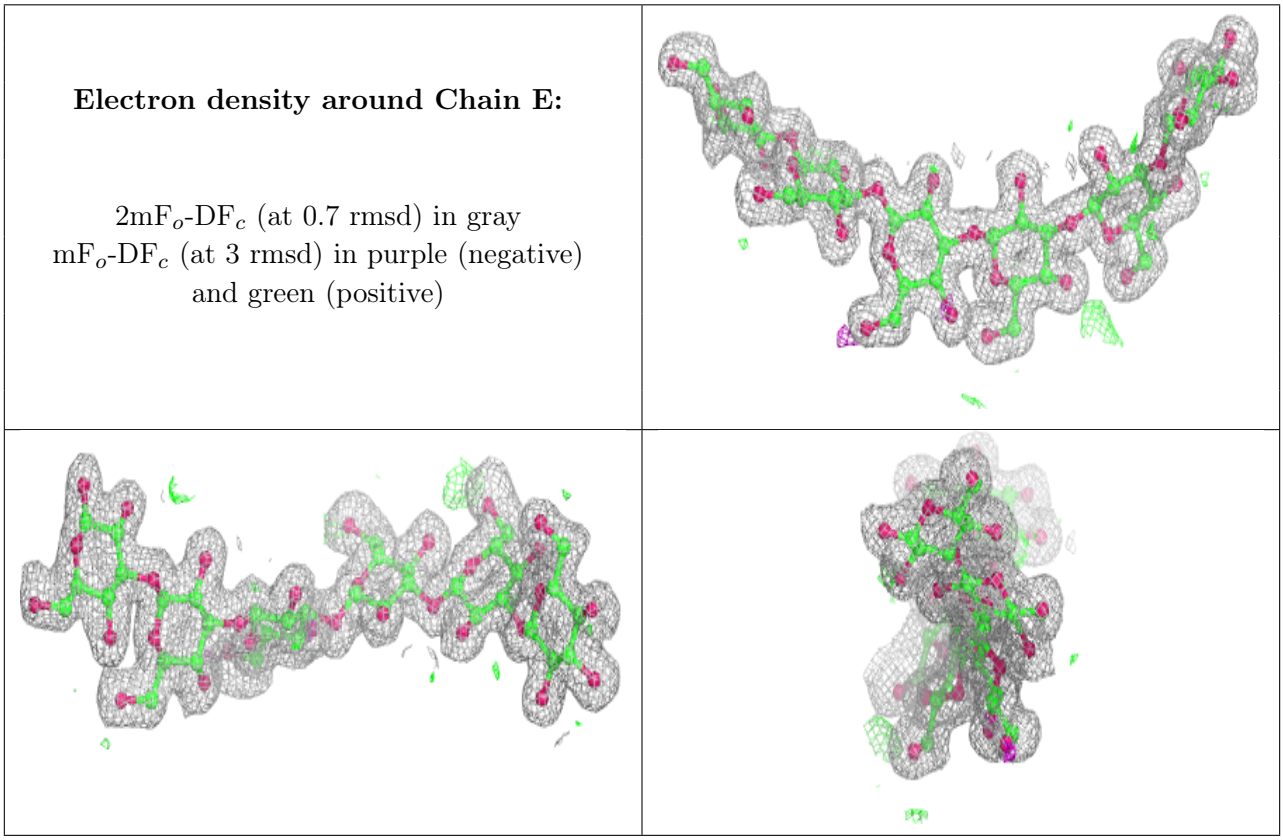

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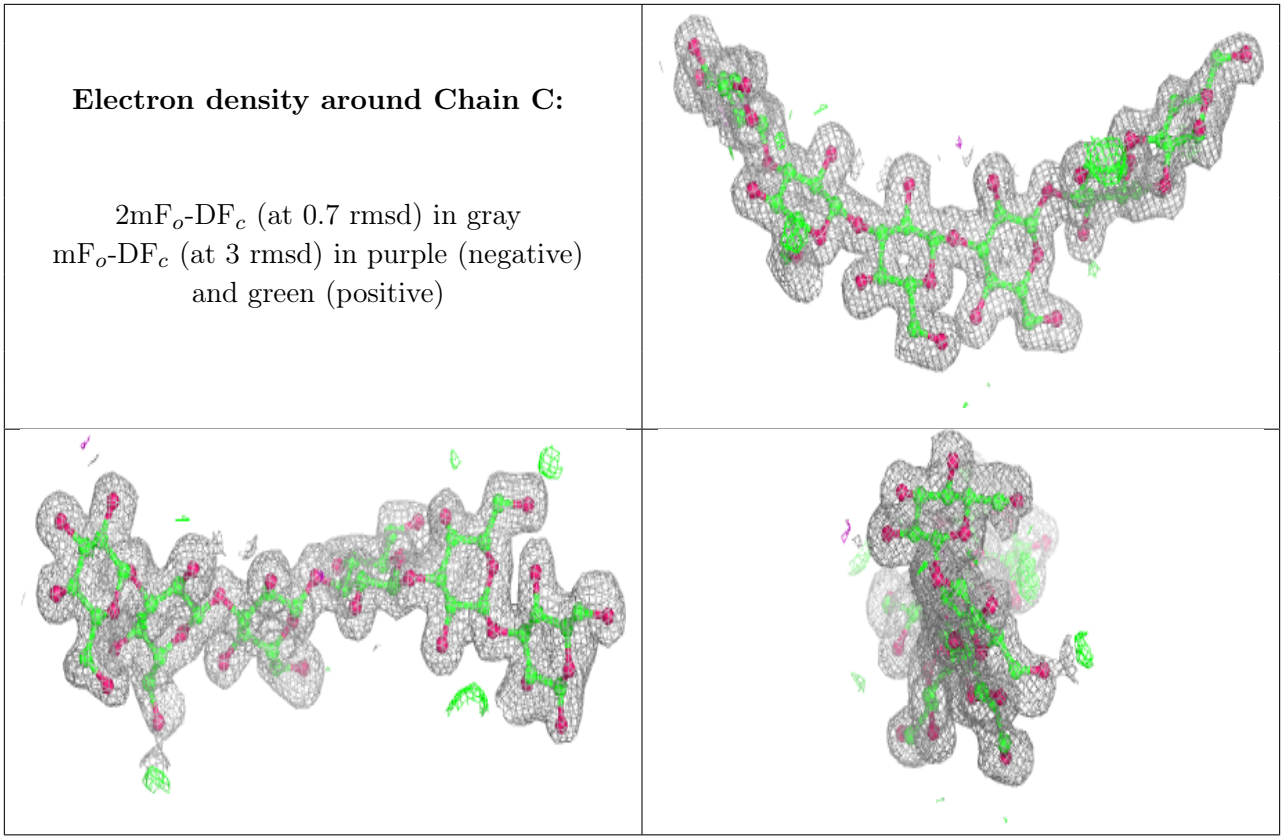

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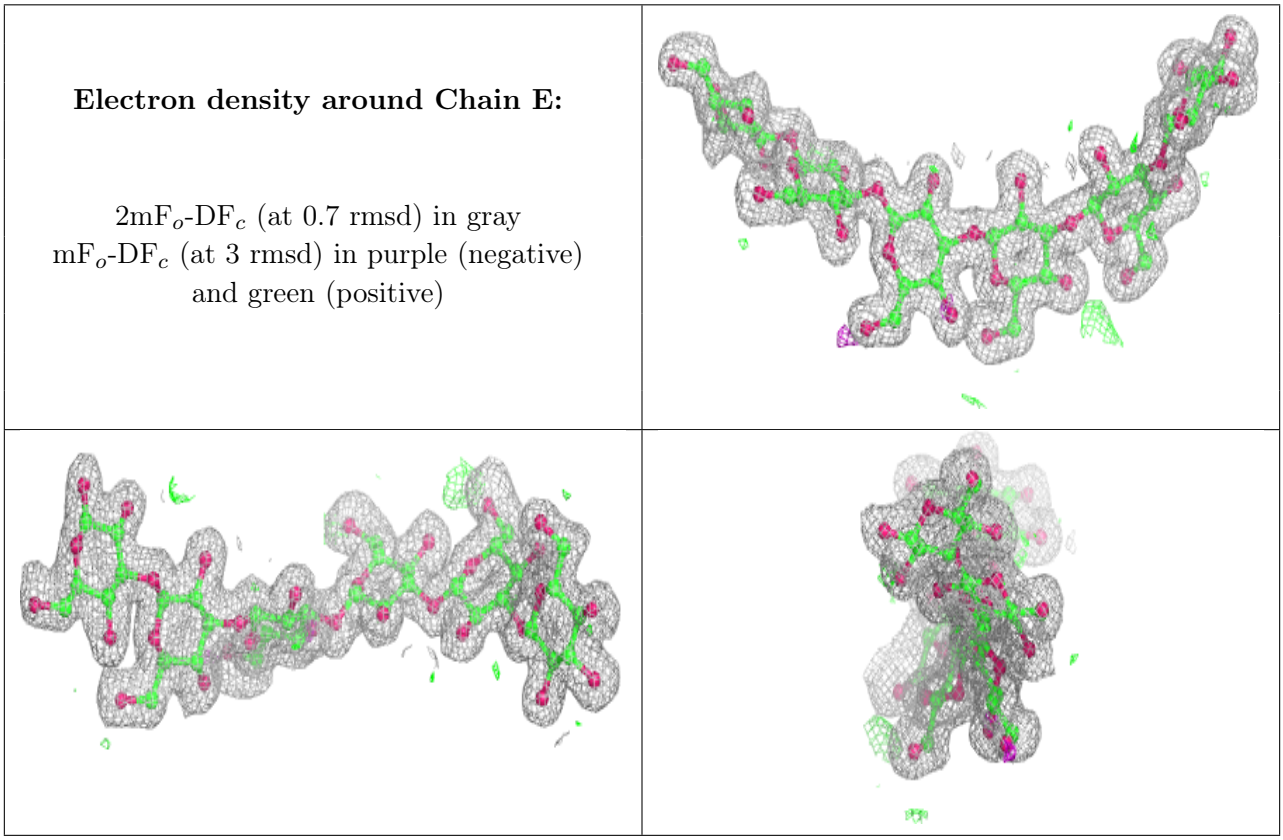

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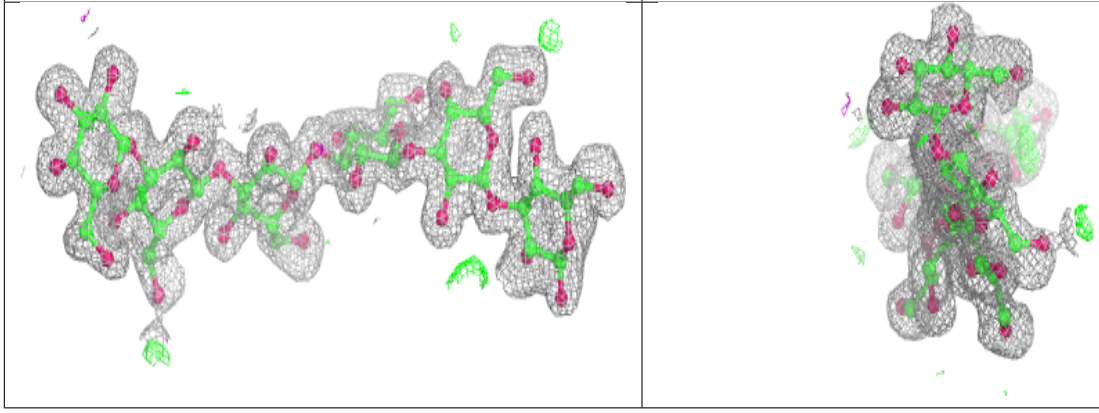

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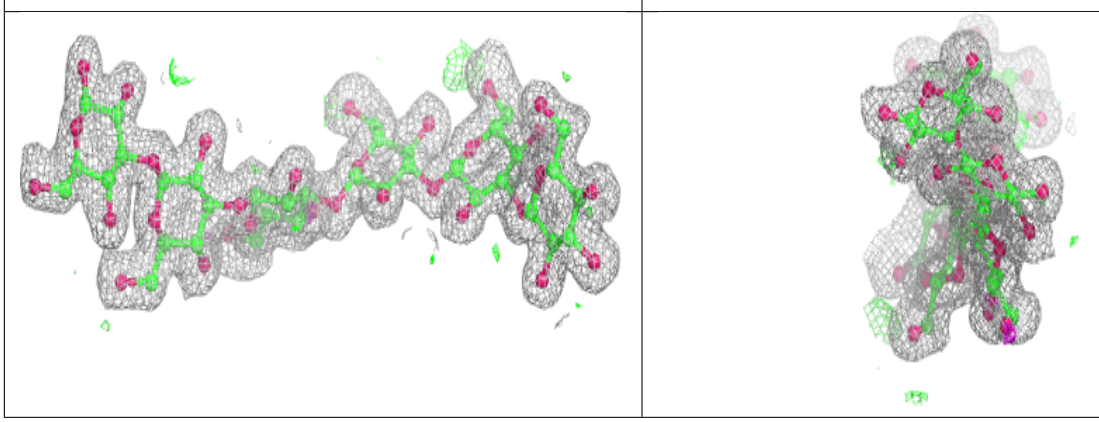

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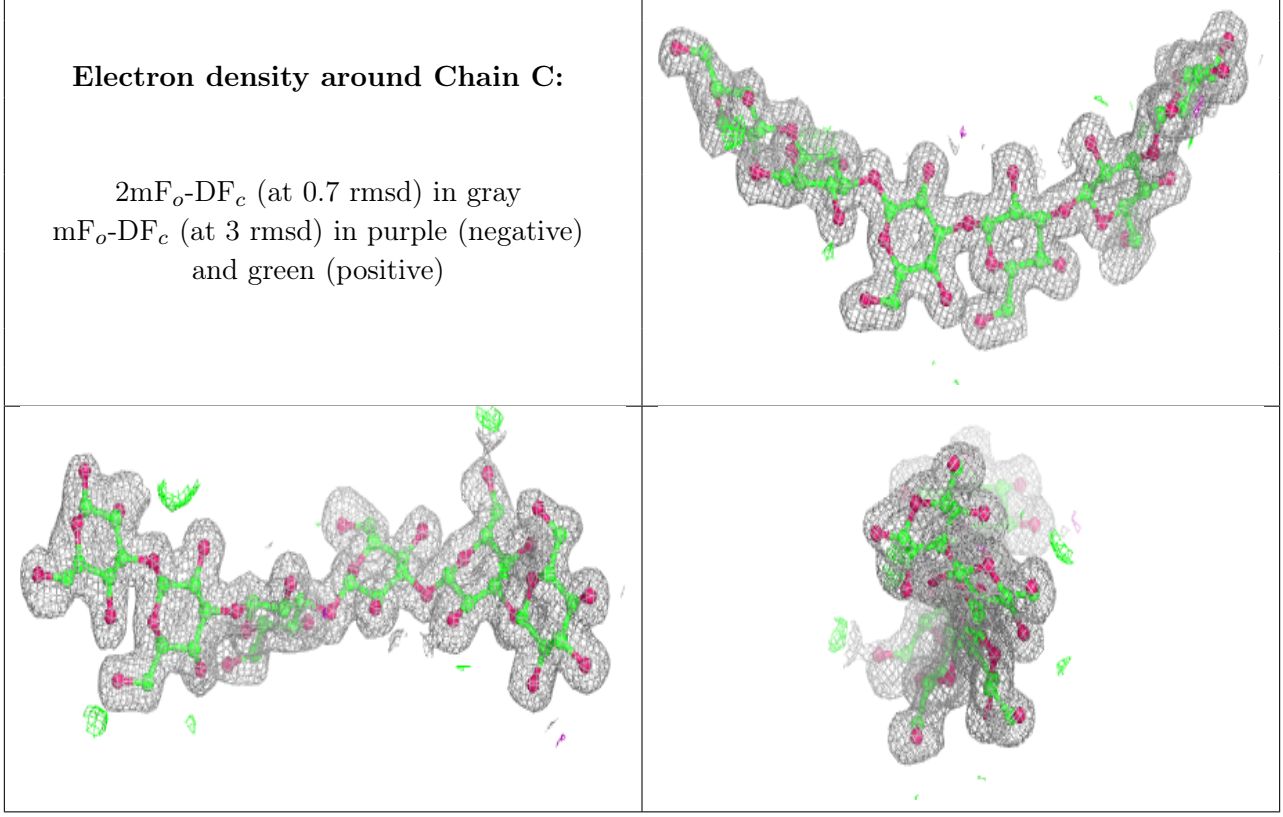

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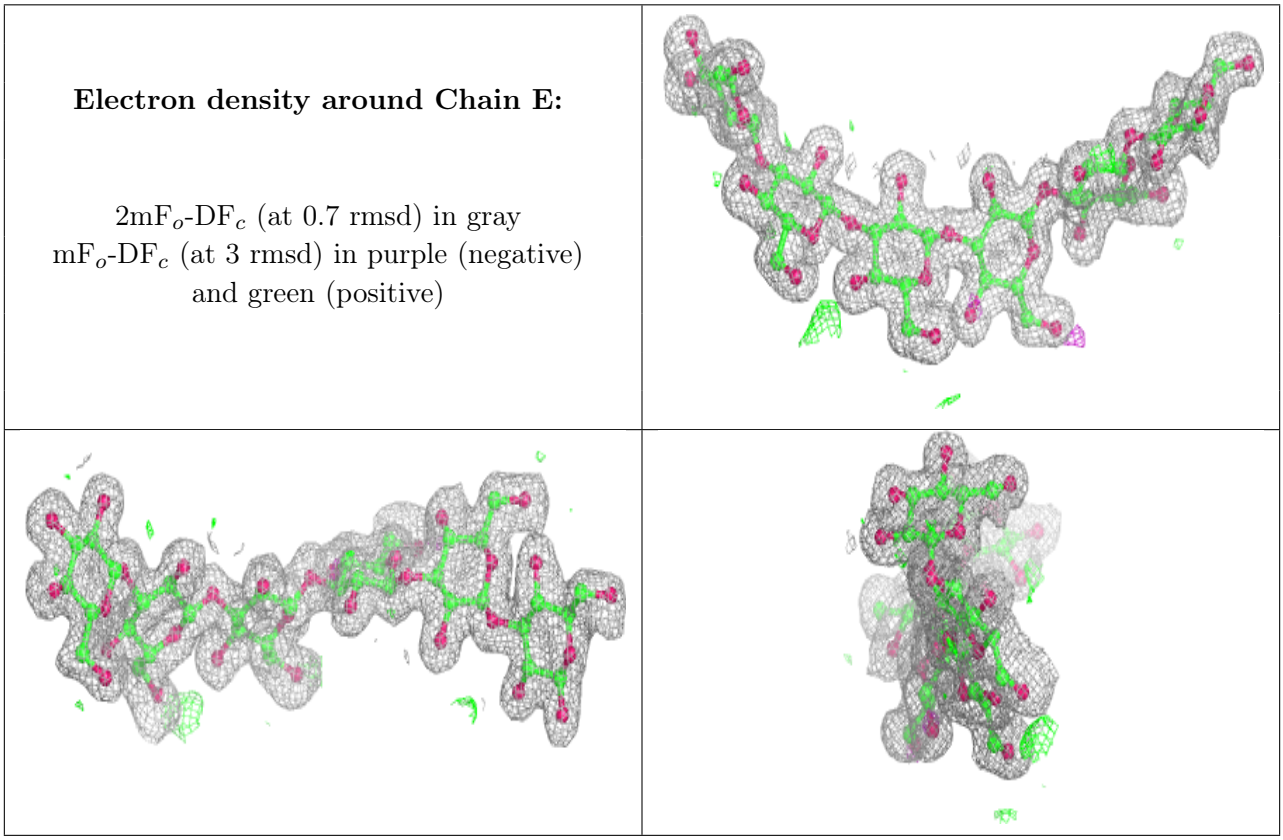

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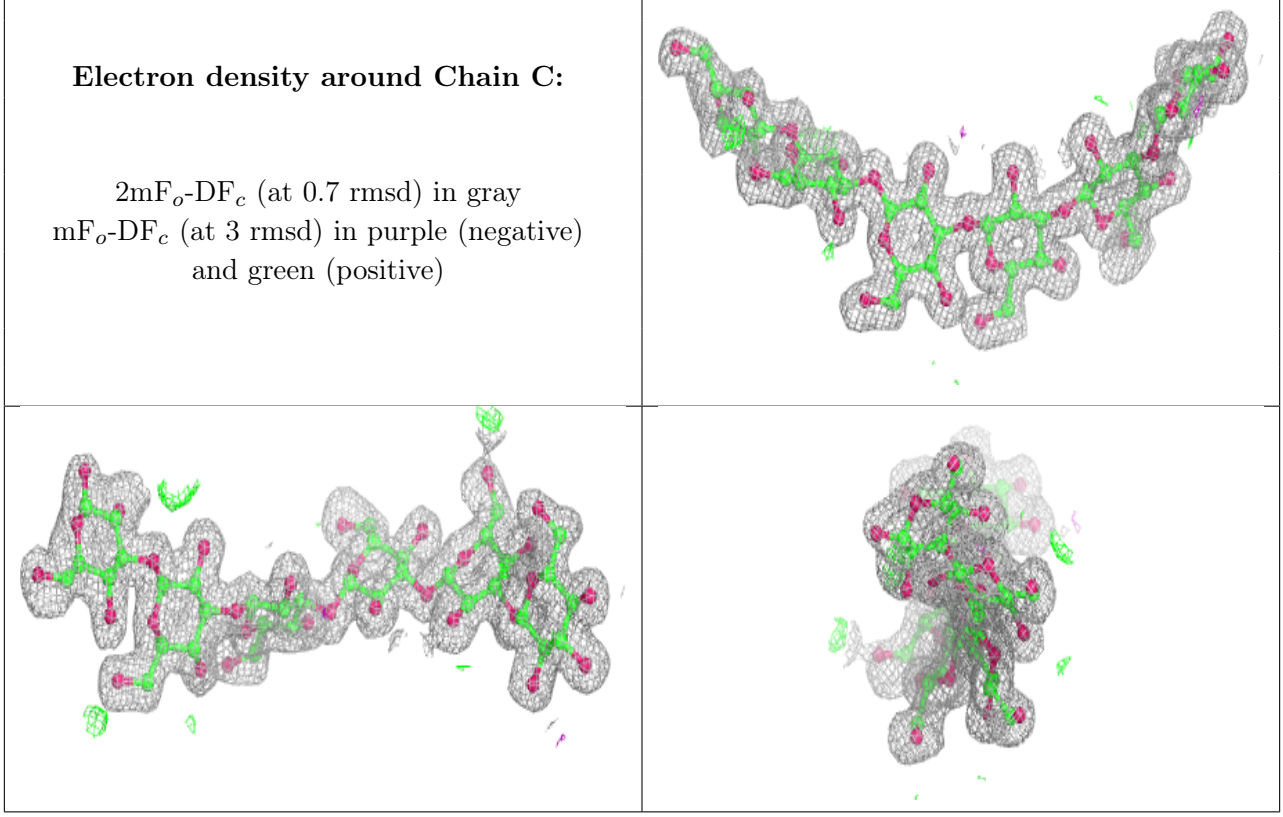

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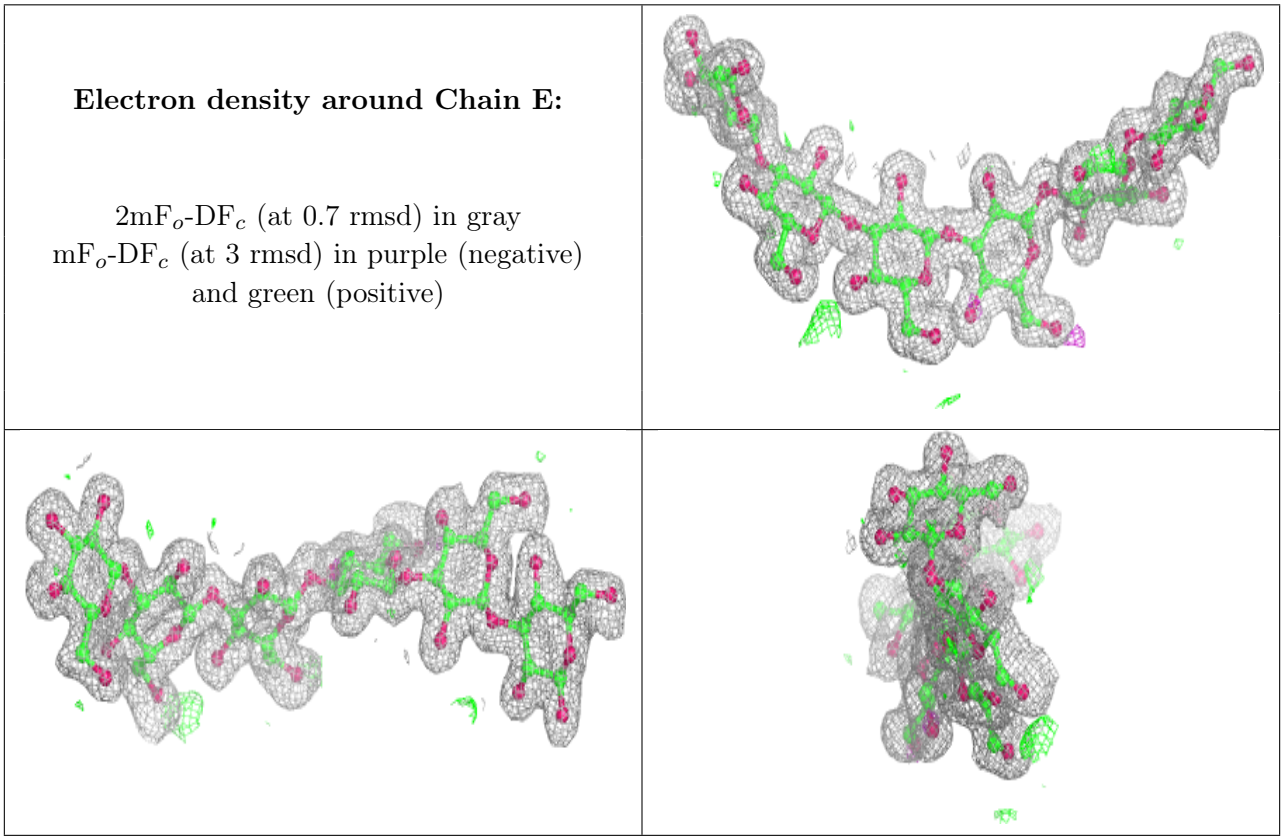

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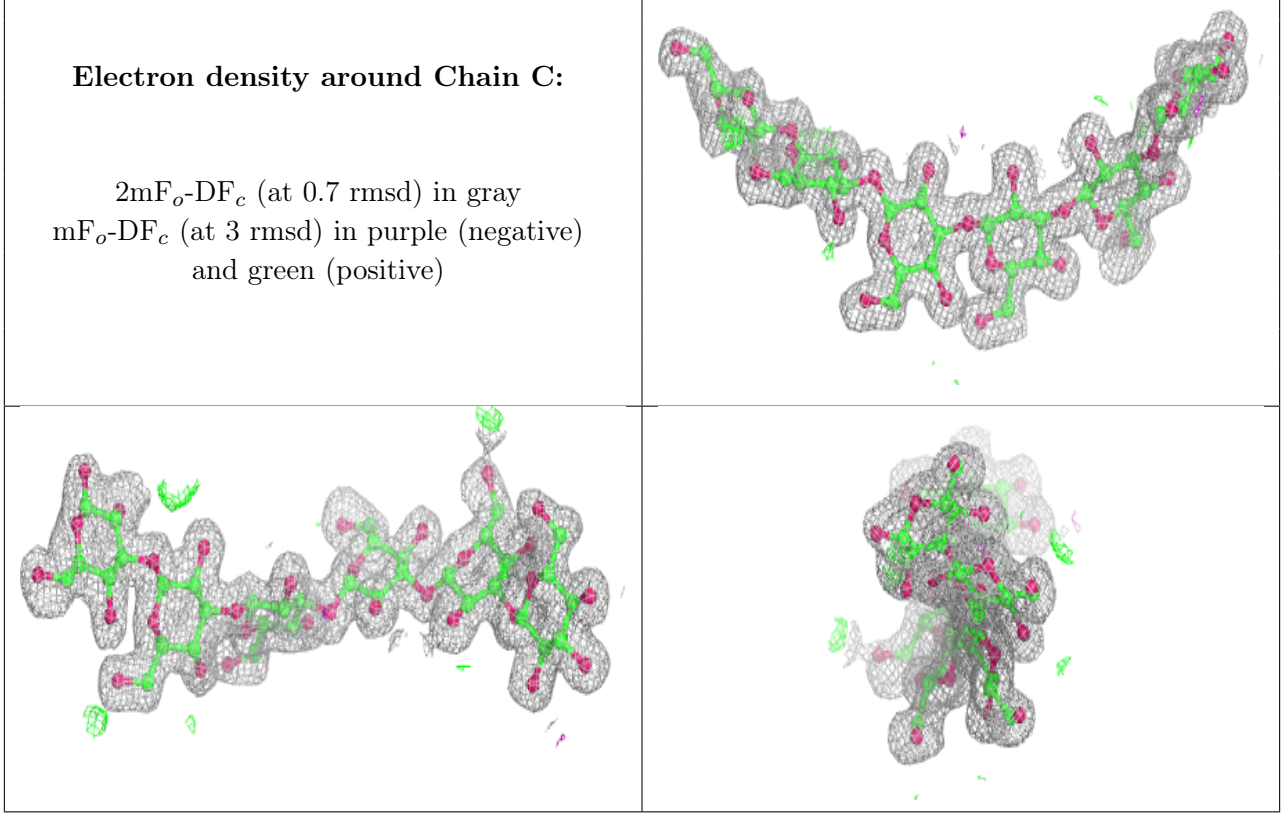

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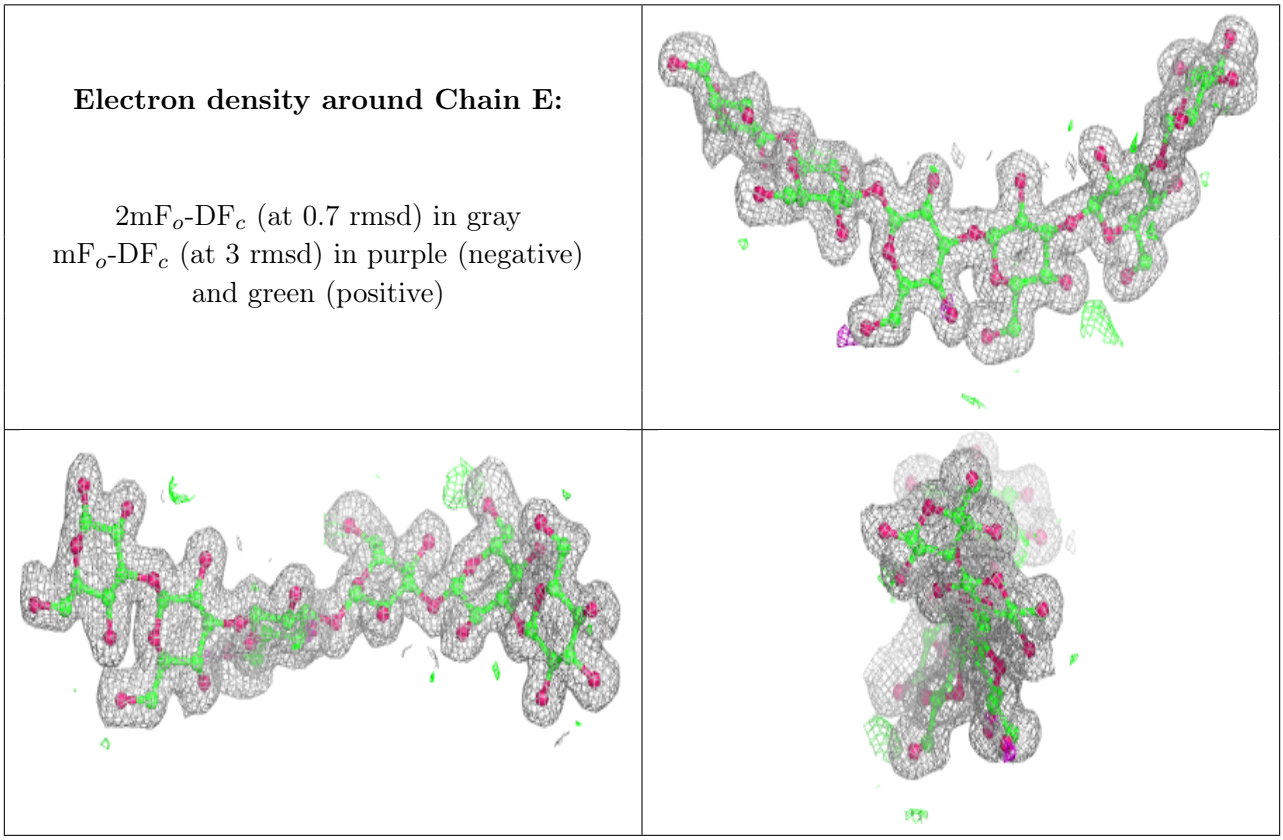

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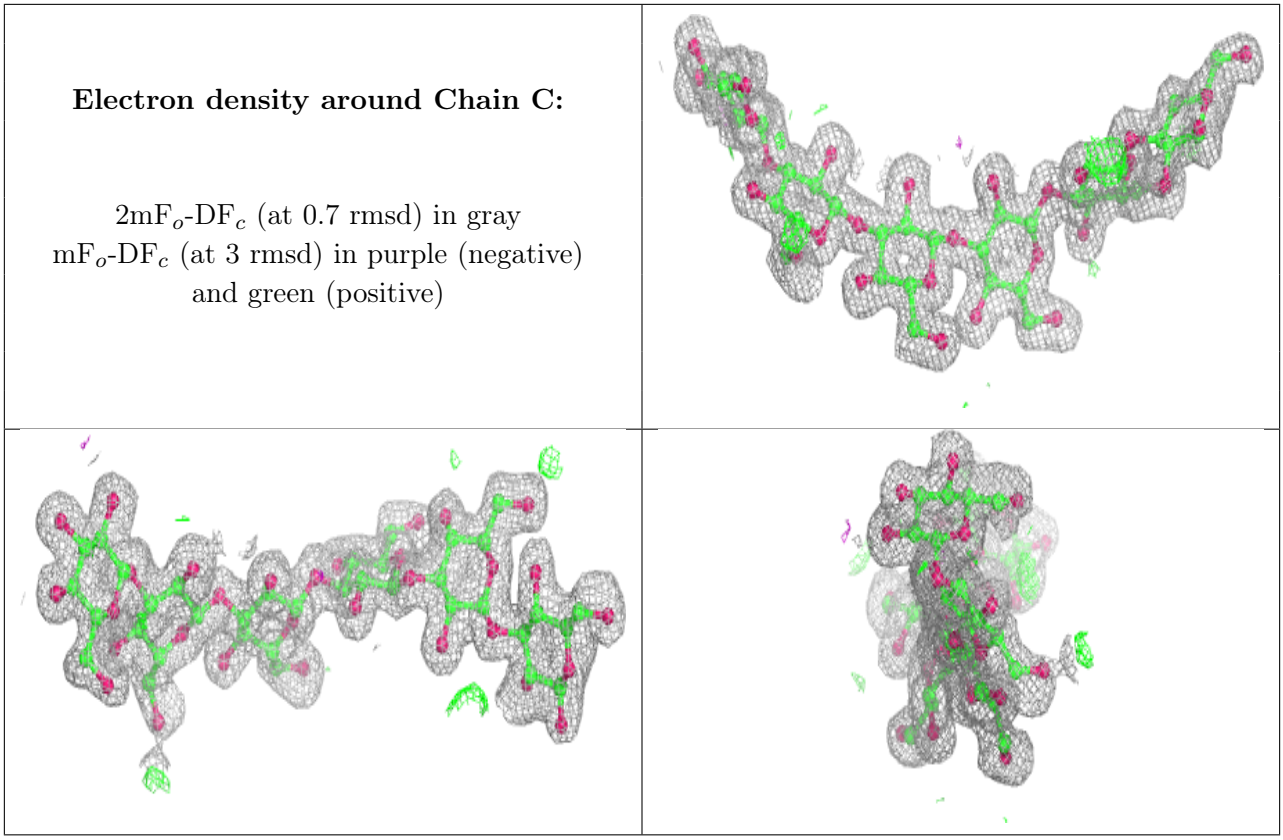

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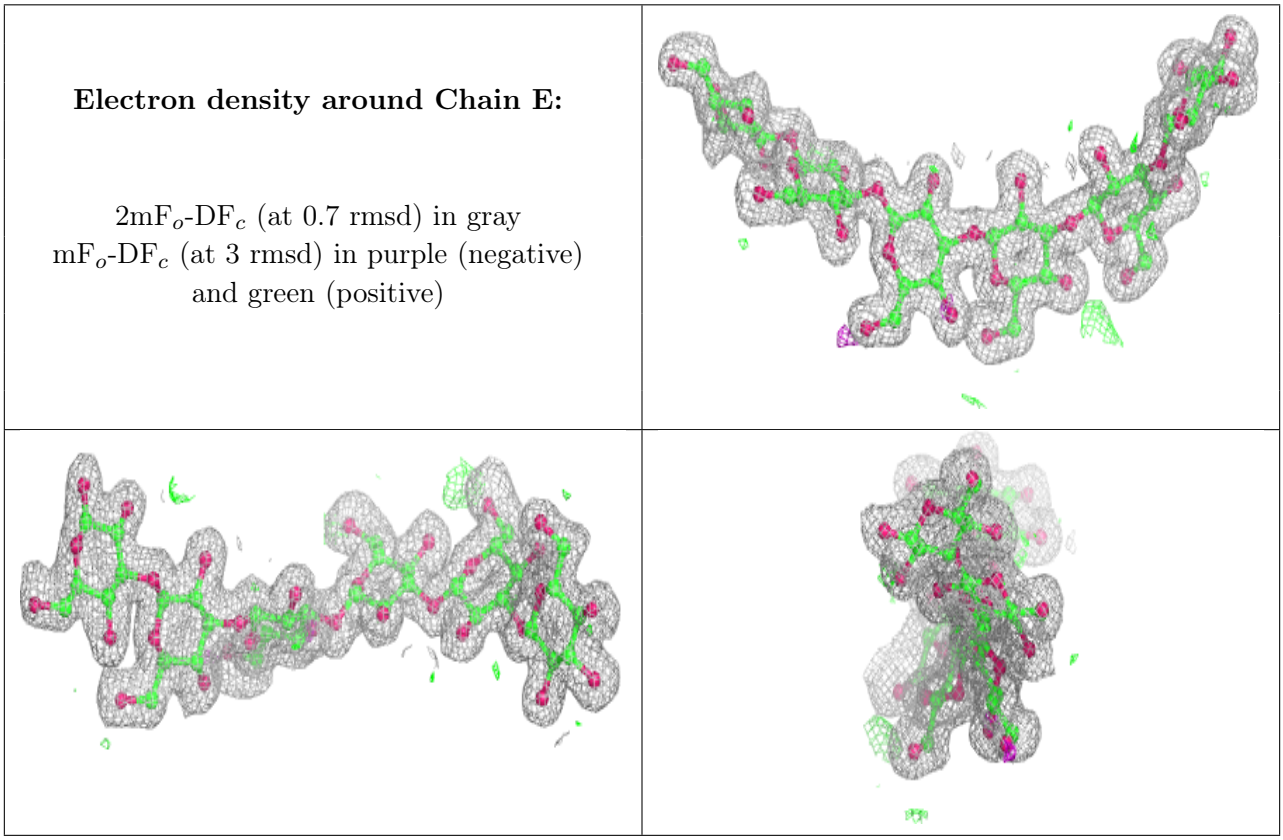

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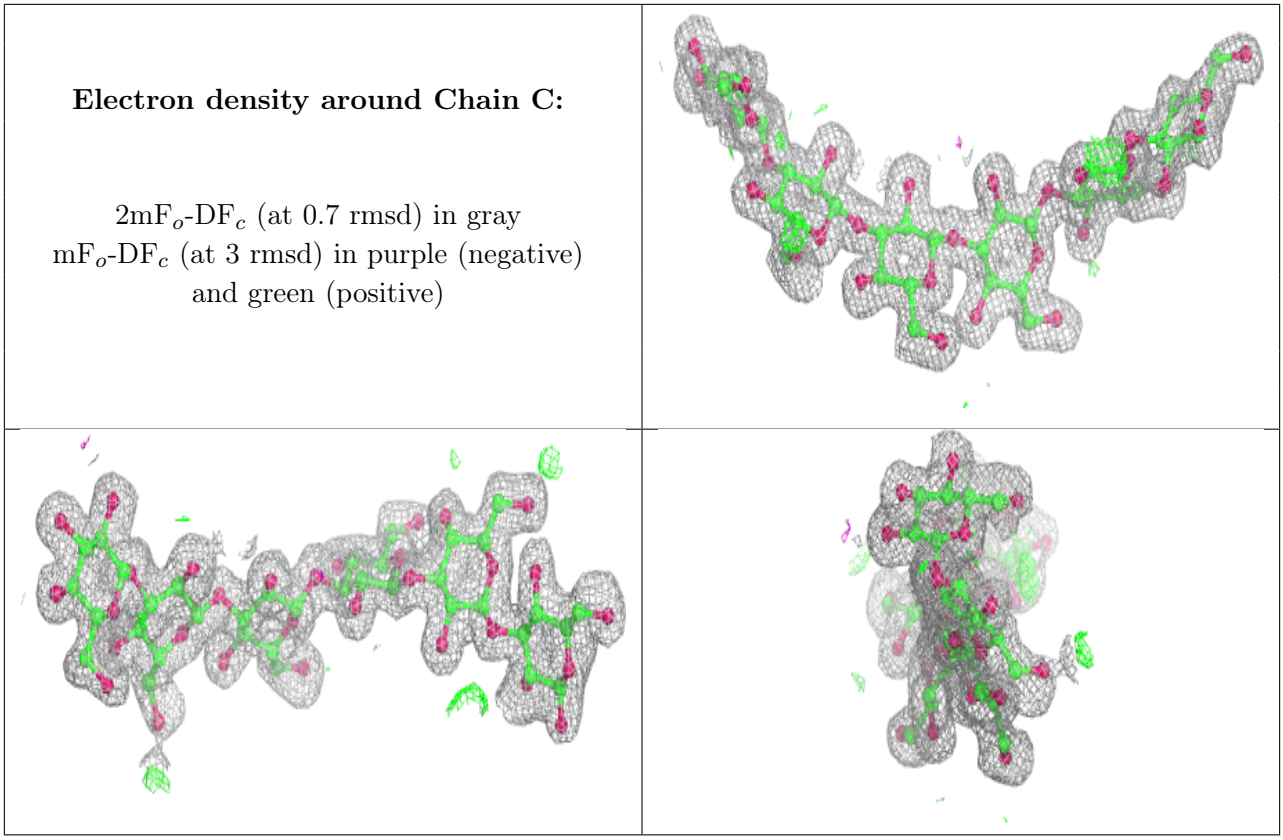

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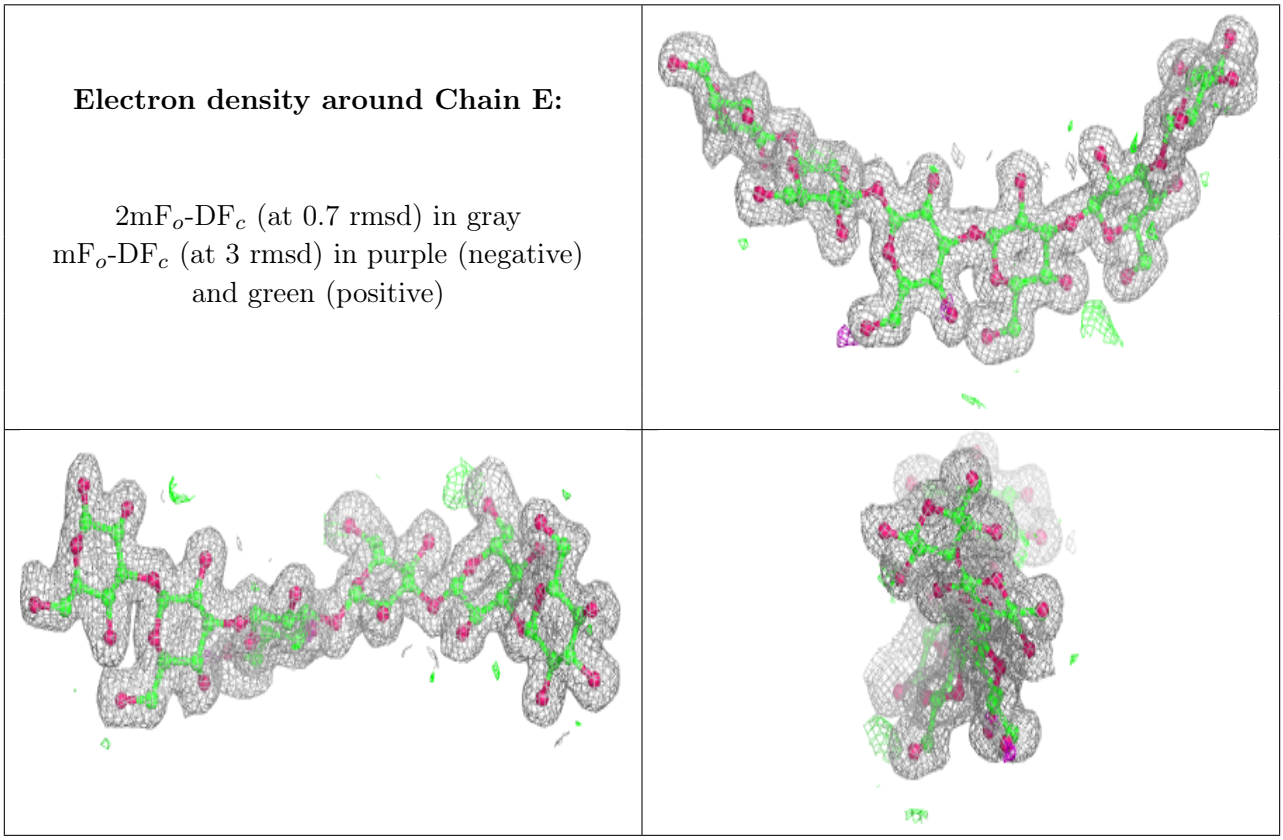

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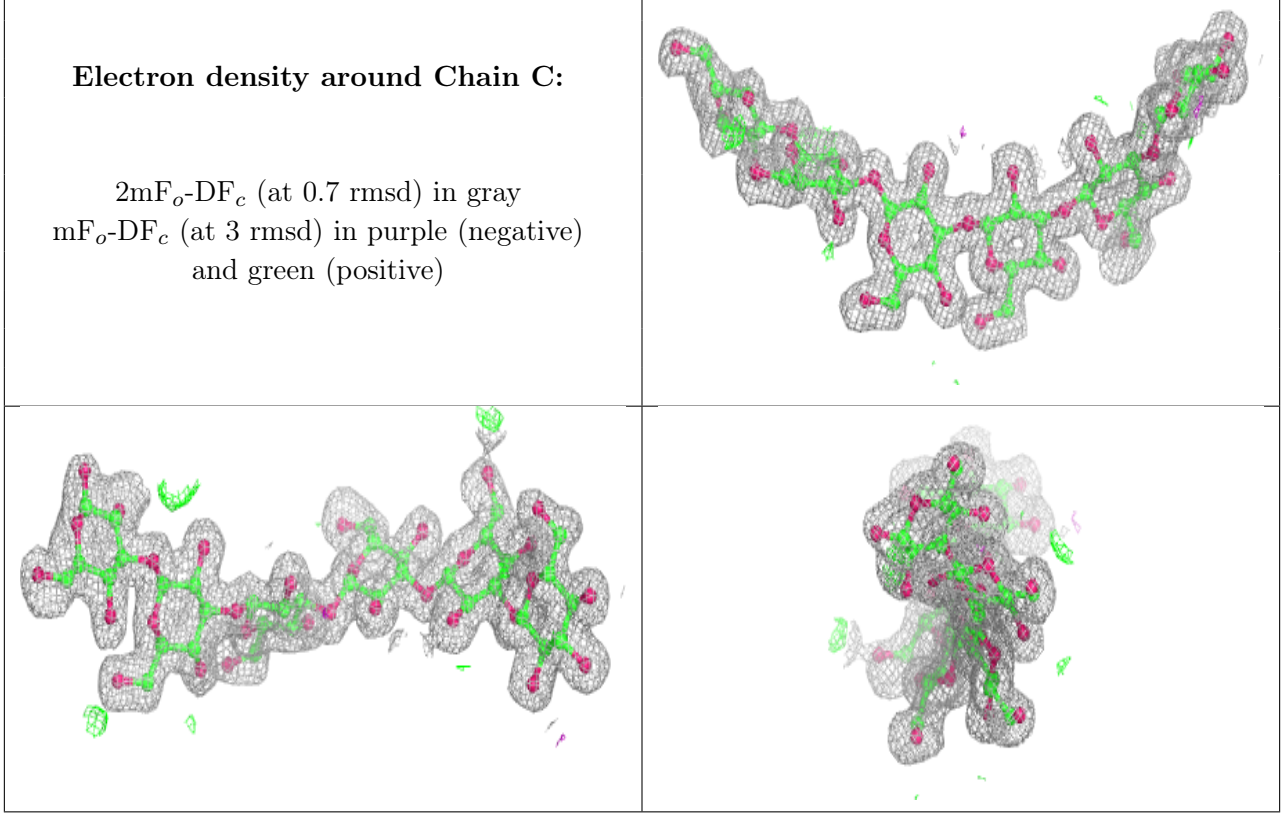

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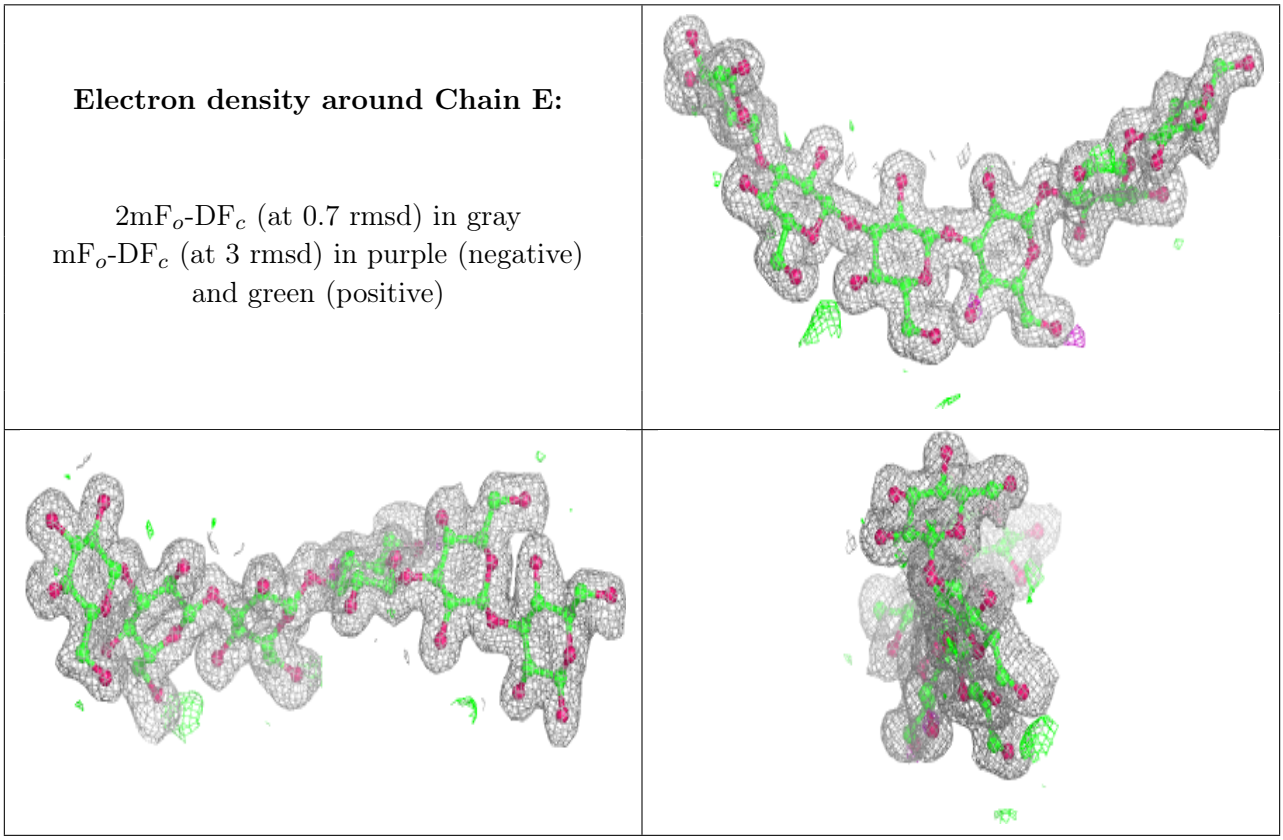

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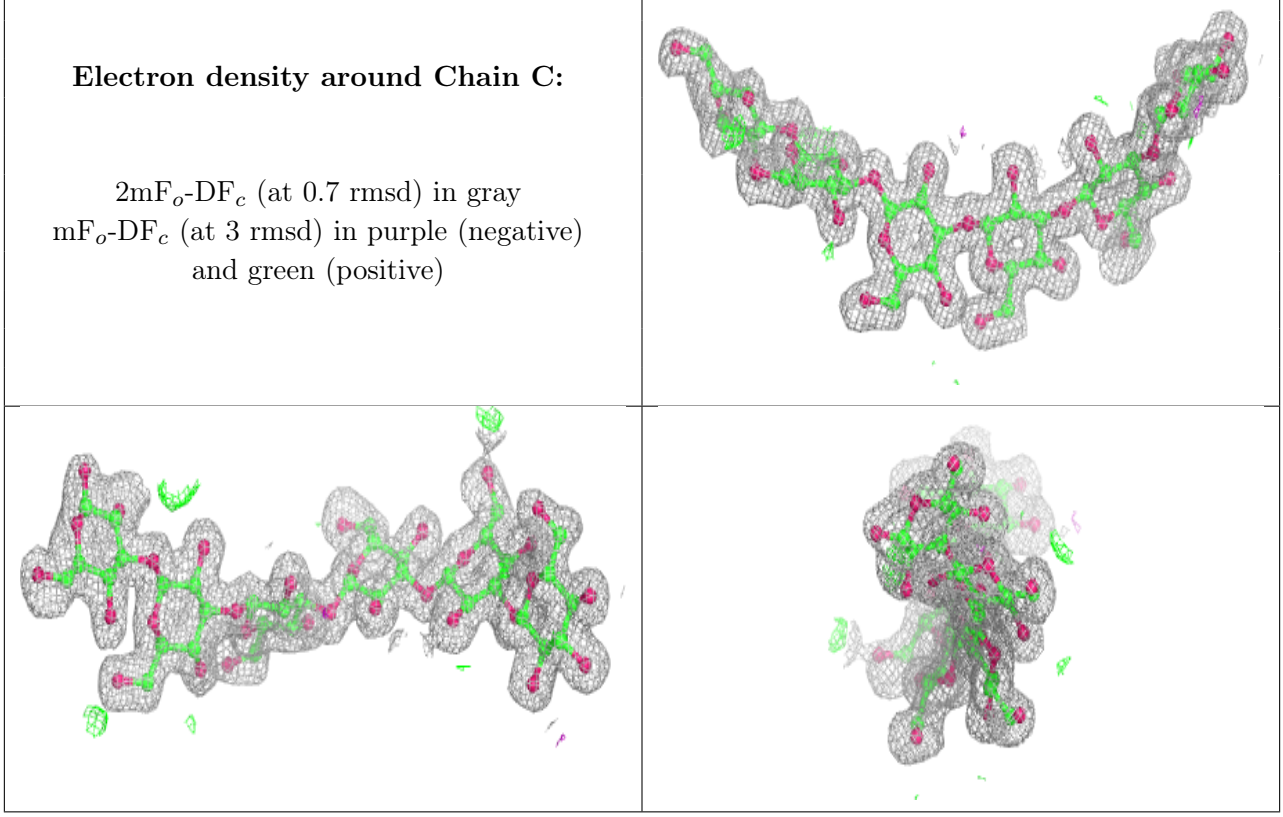

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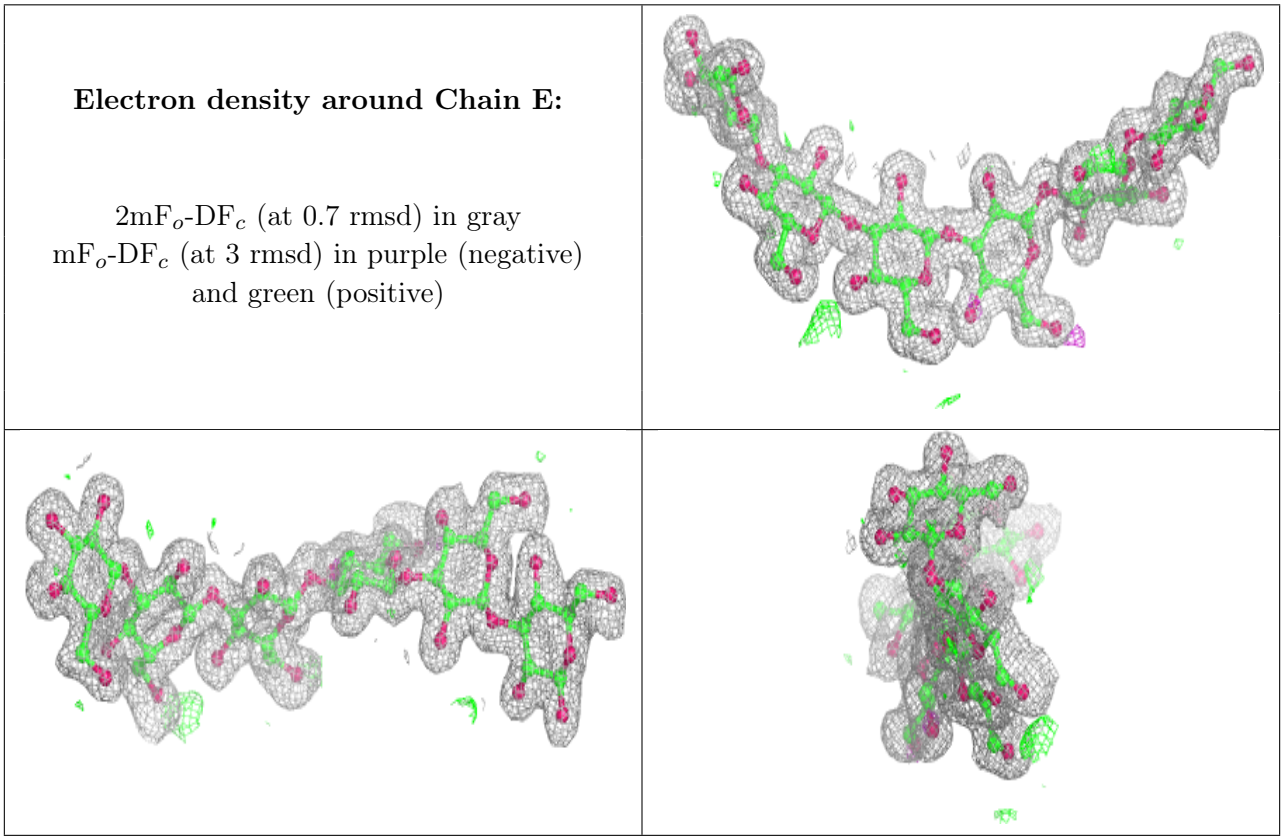

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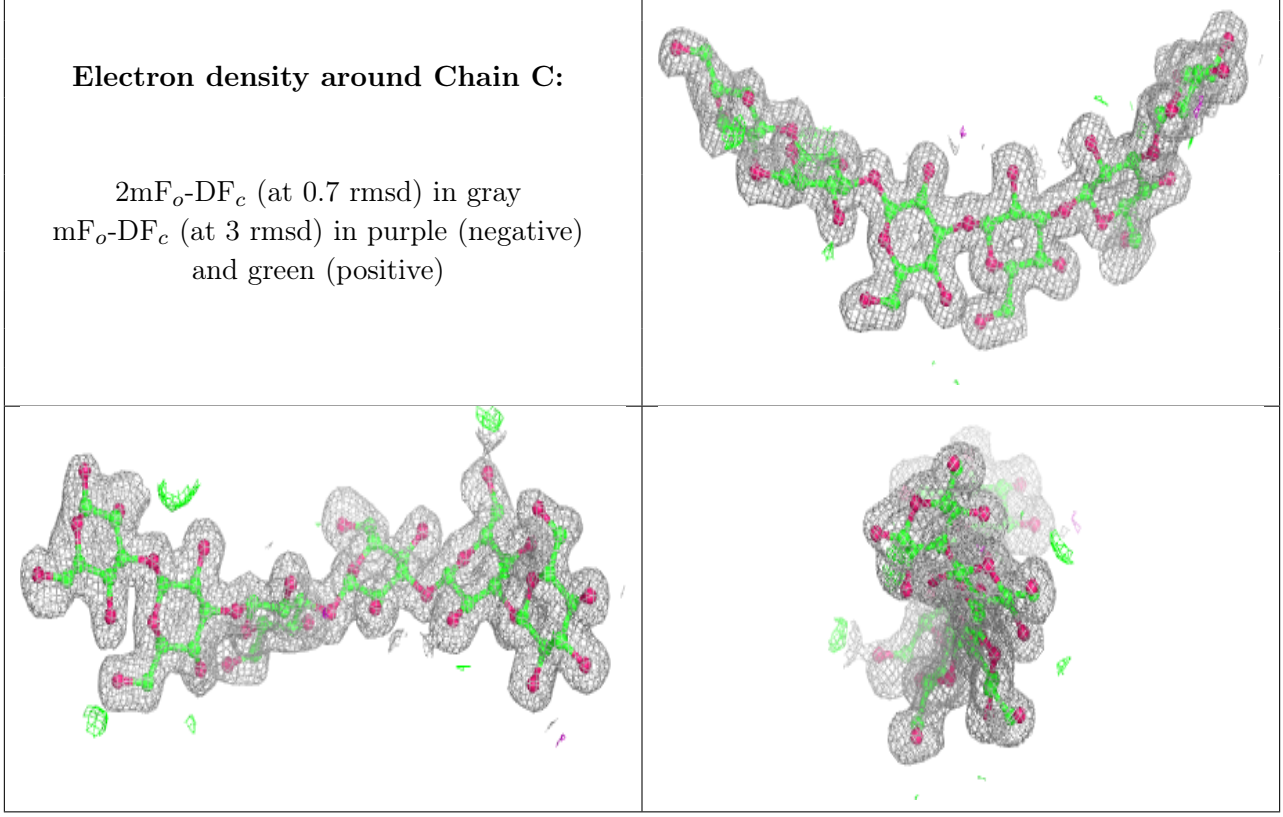

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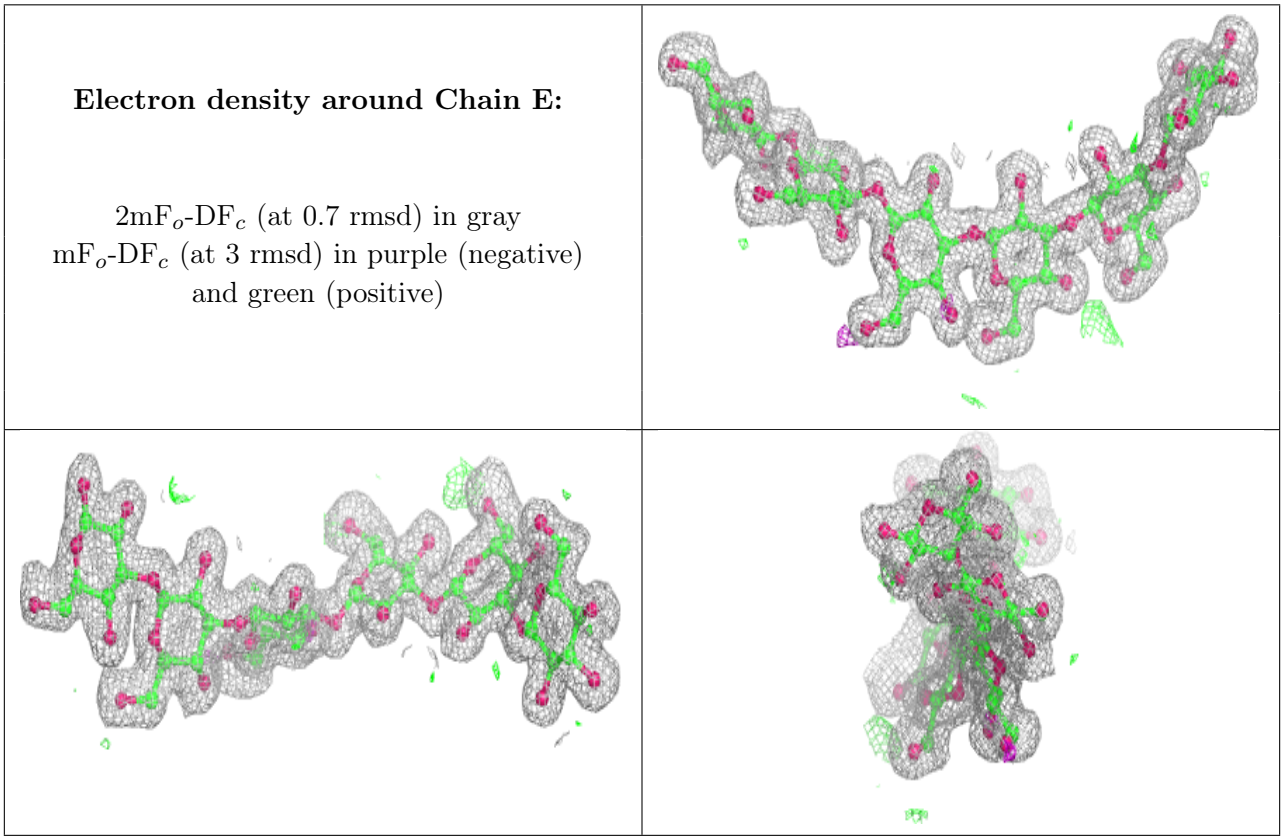

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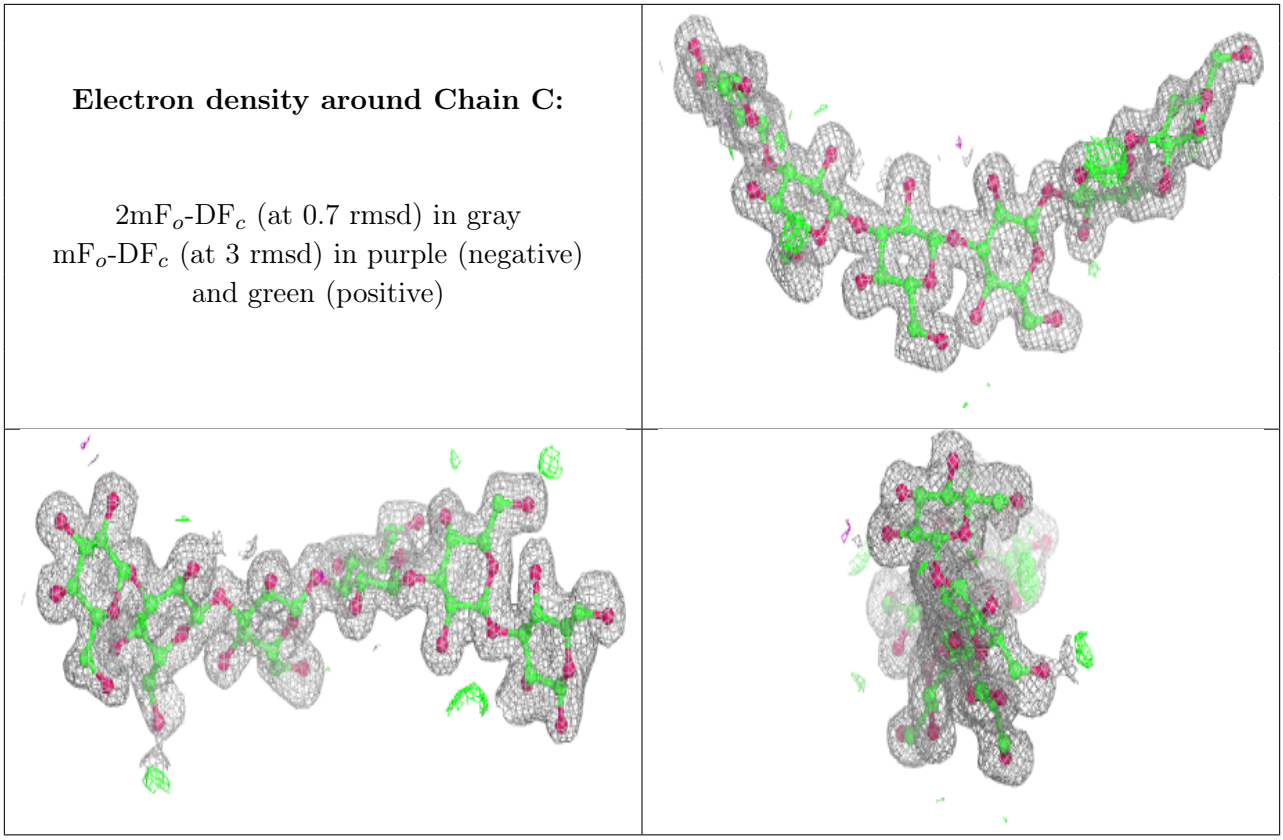

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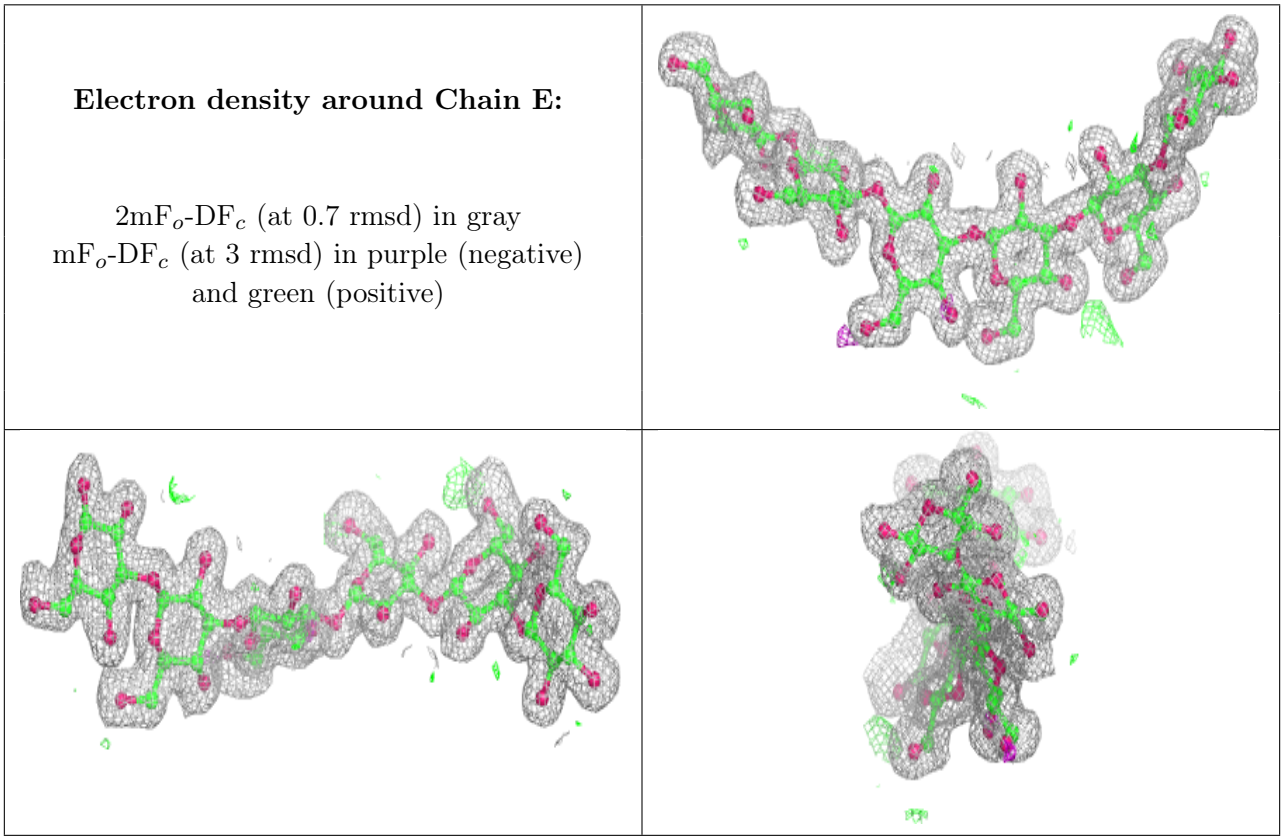

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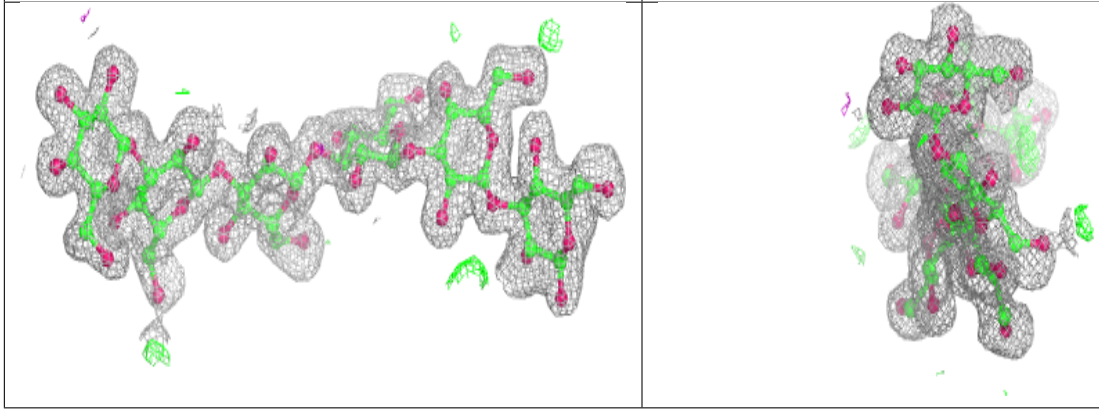
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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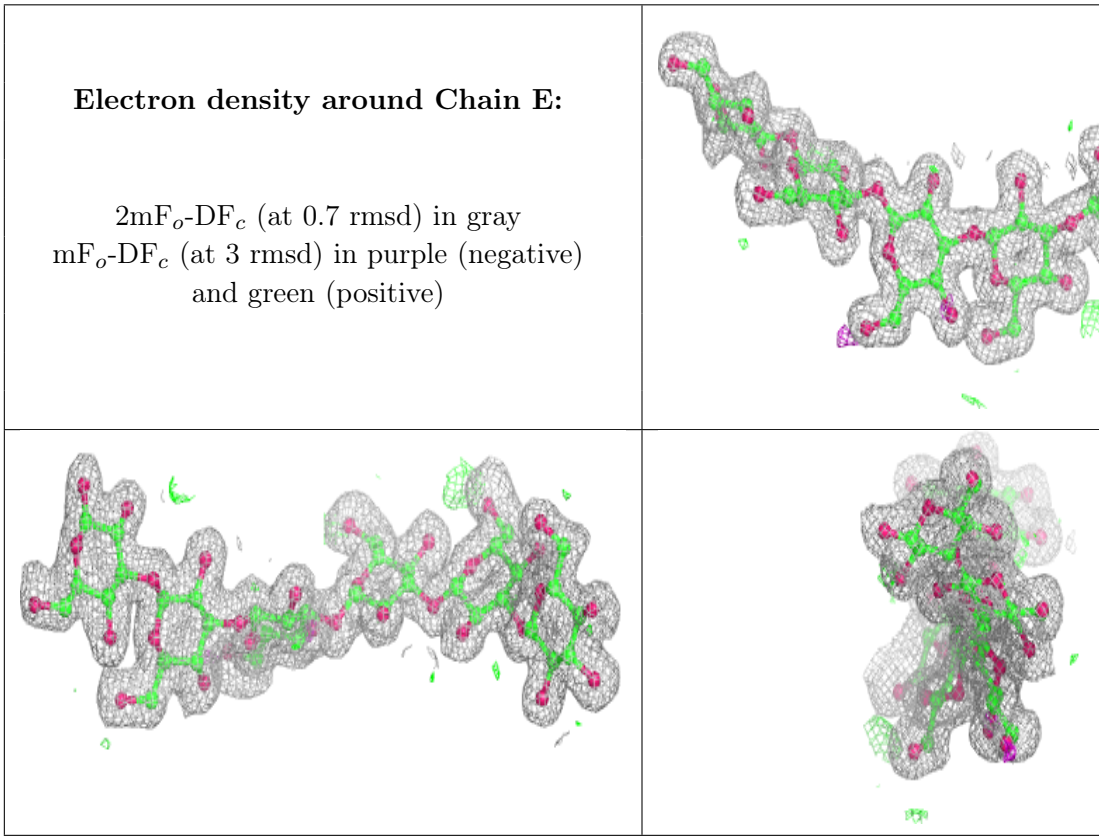
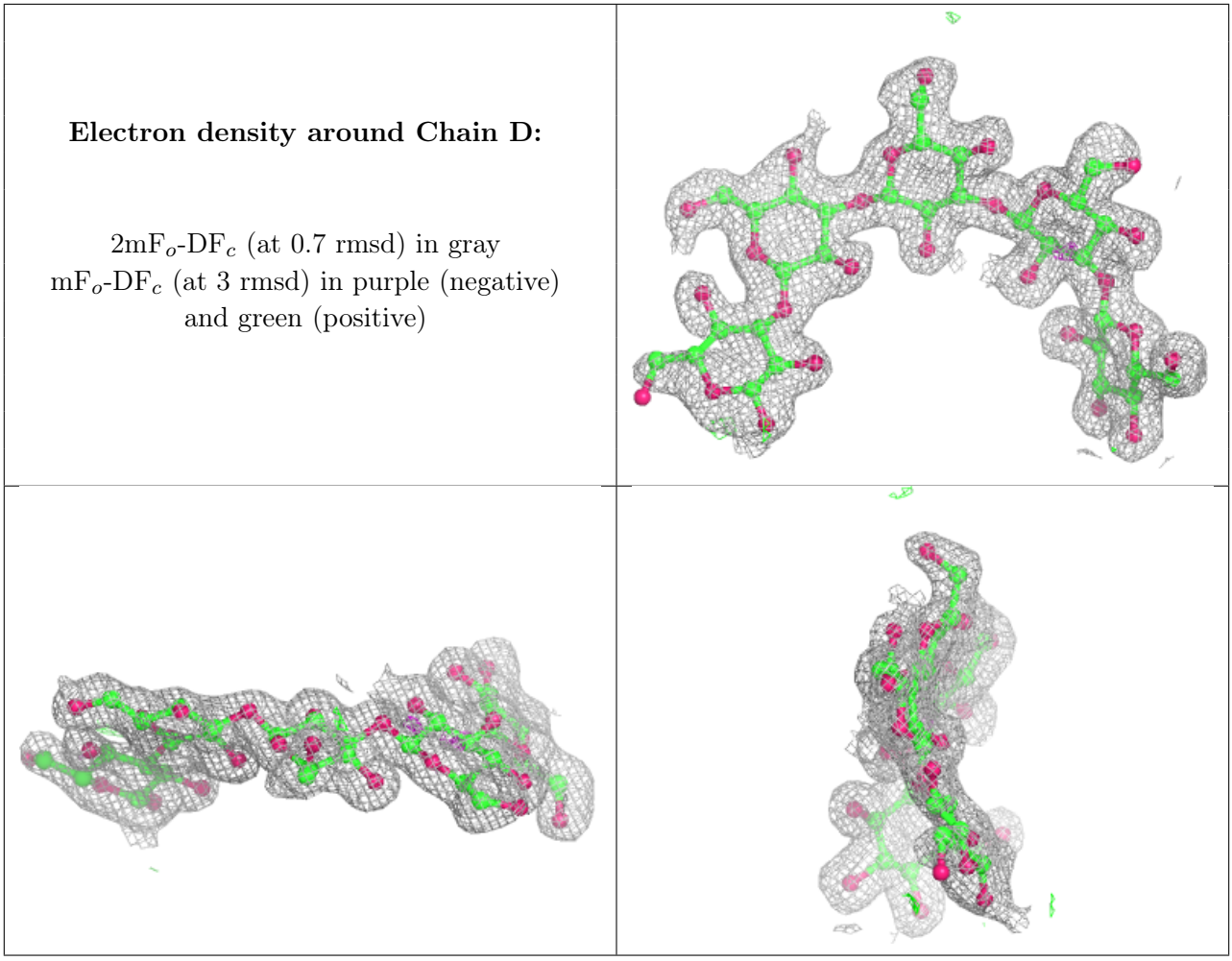
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



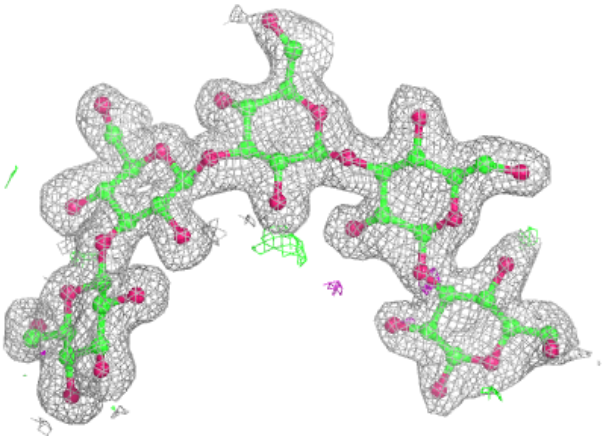
Electron density around Chain D:

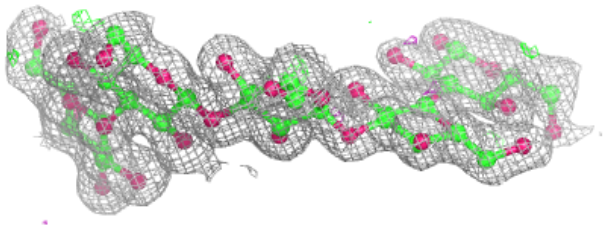
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

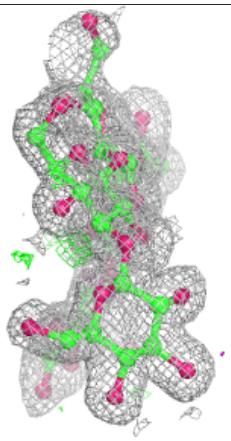


Electron density around Chain F:

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

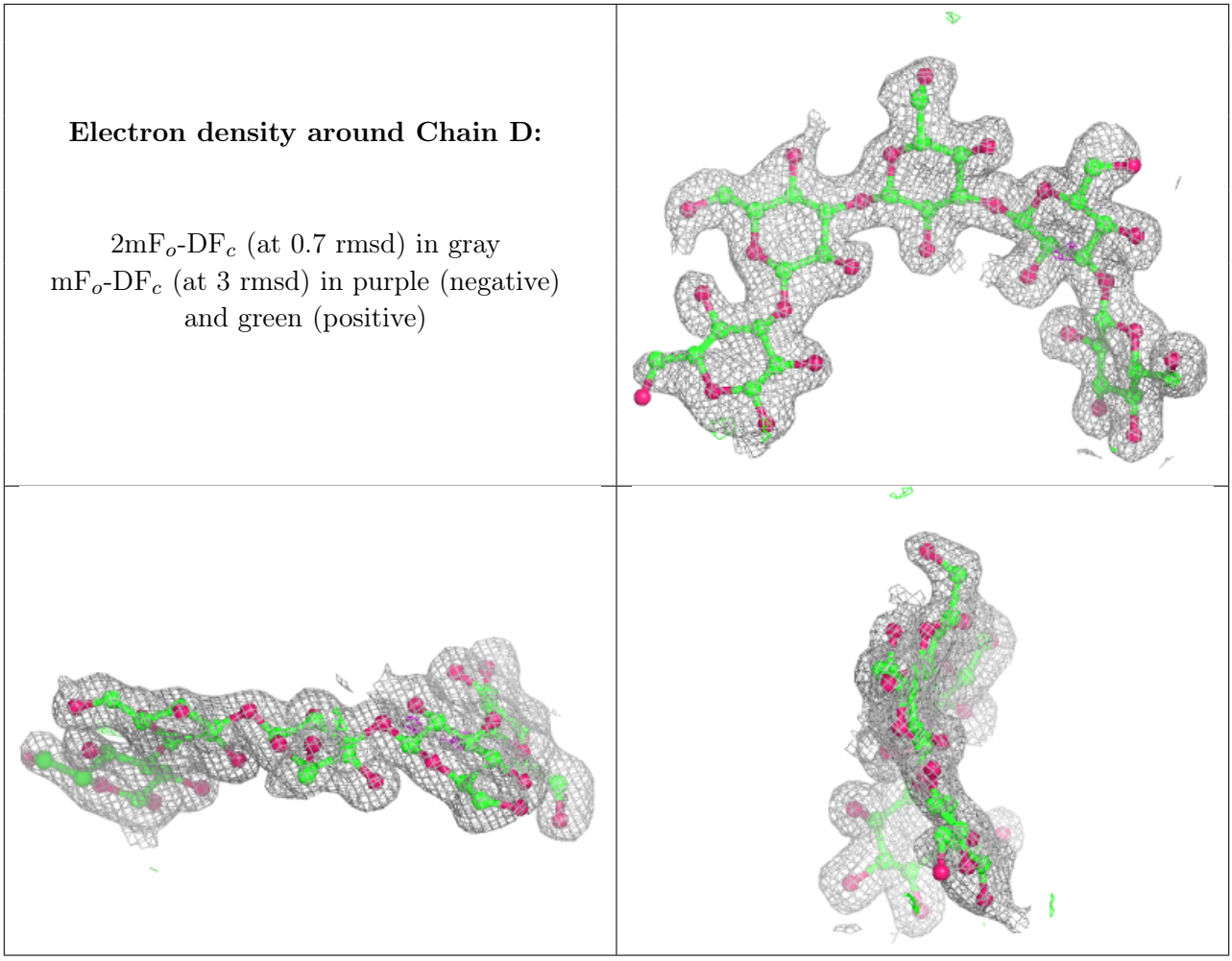






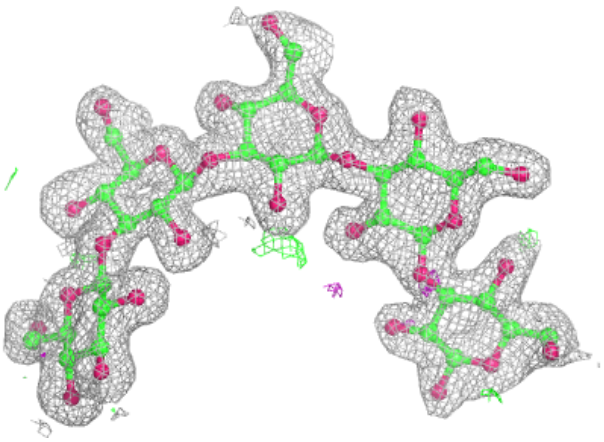
Electron density around Chain D:

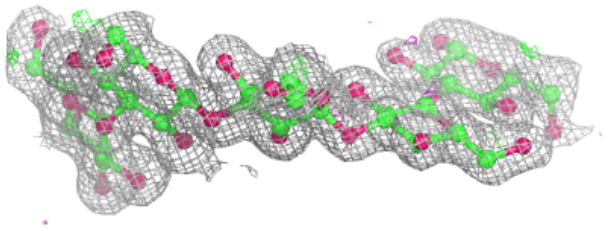
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

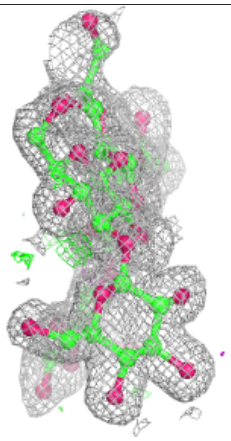


Electron density around Chain F:

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

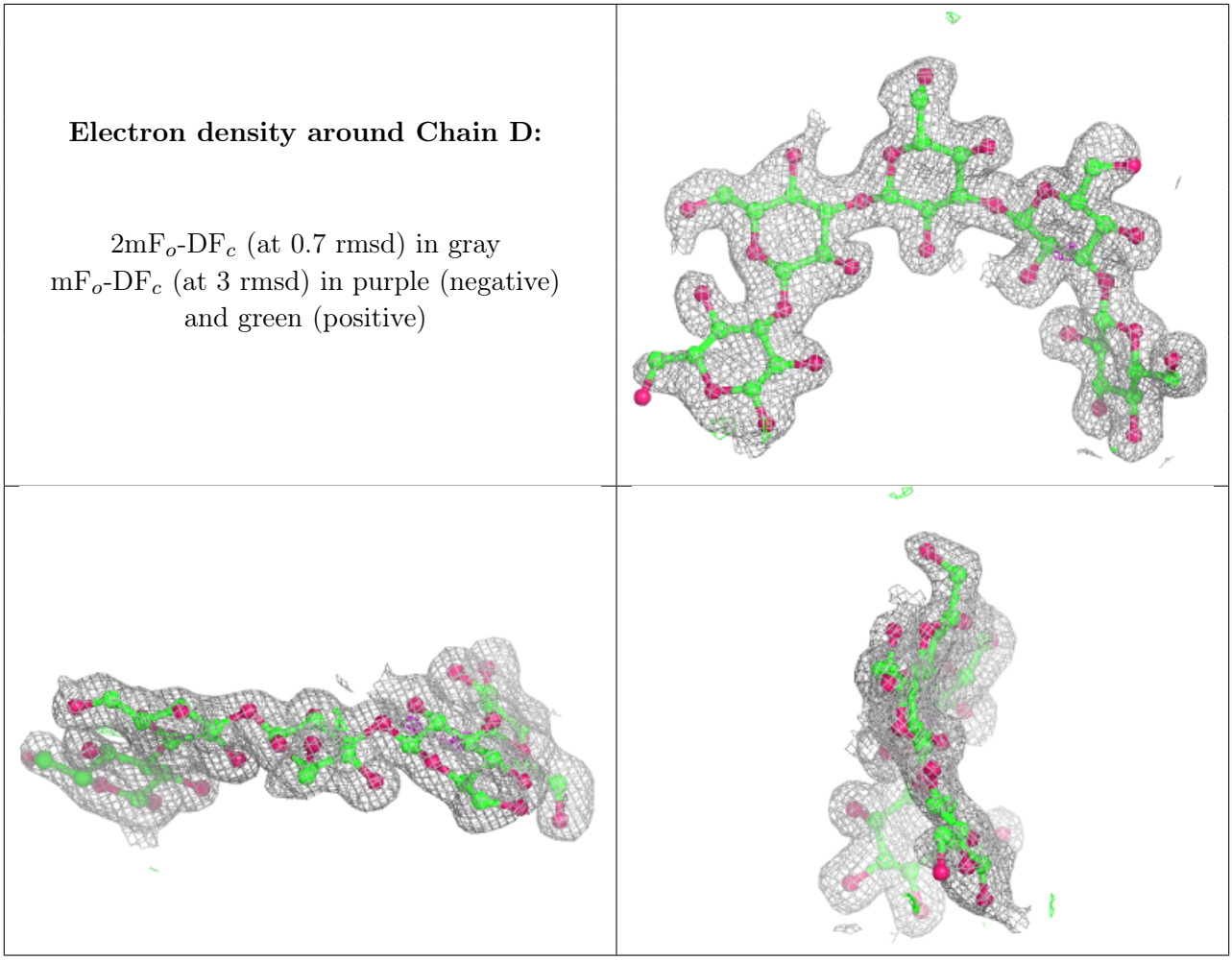






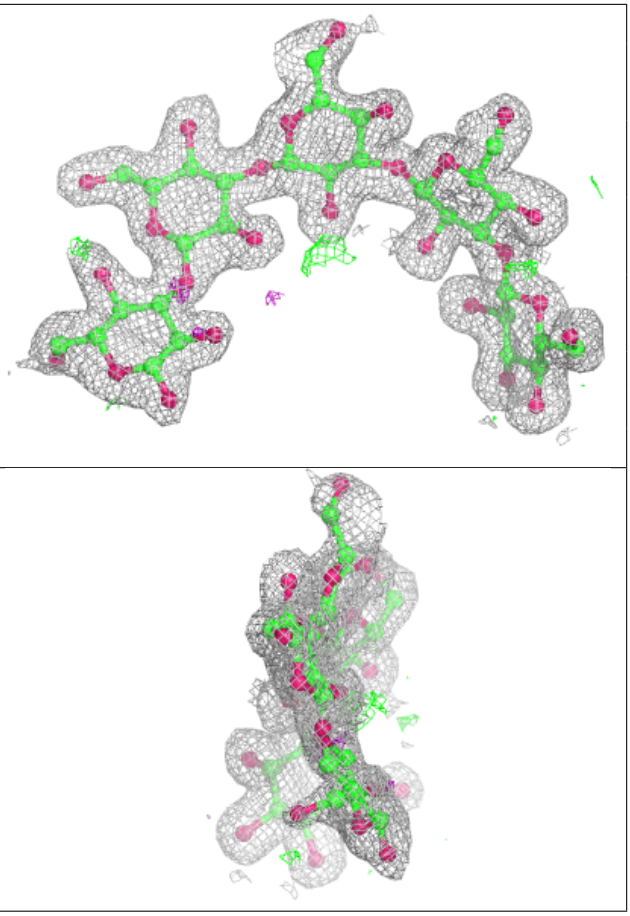
Electron density around Chain D:

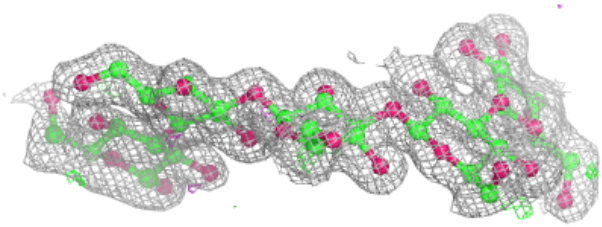
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain F:

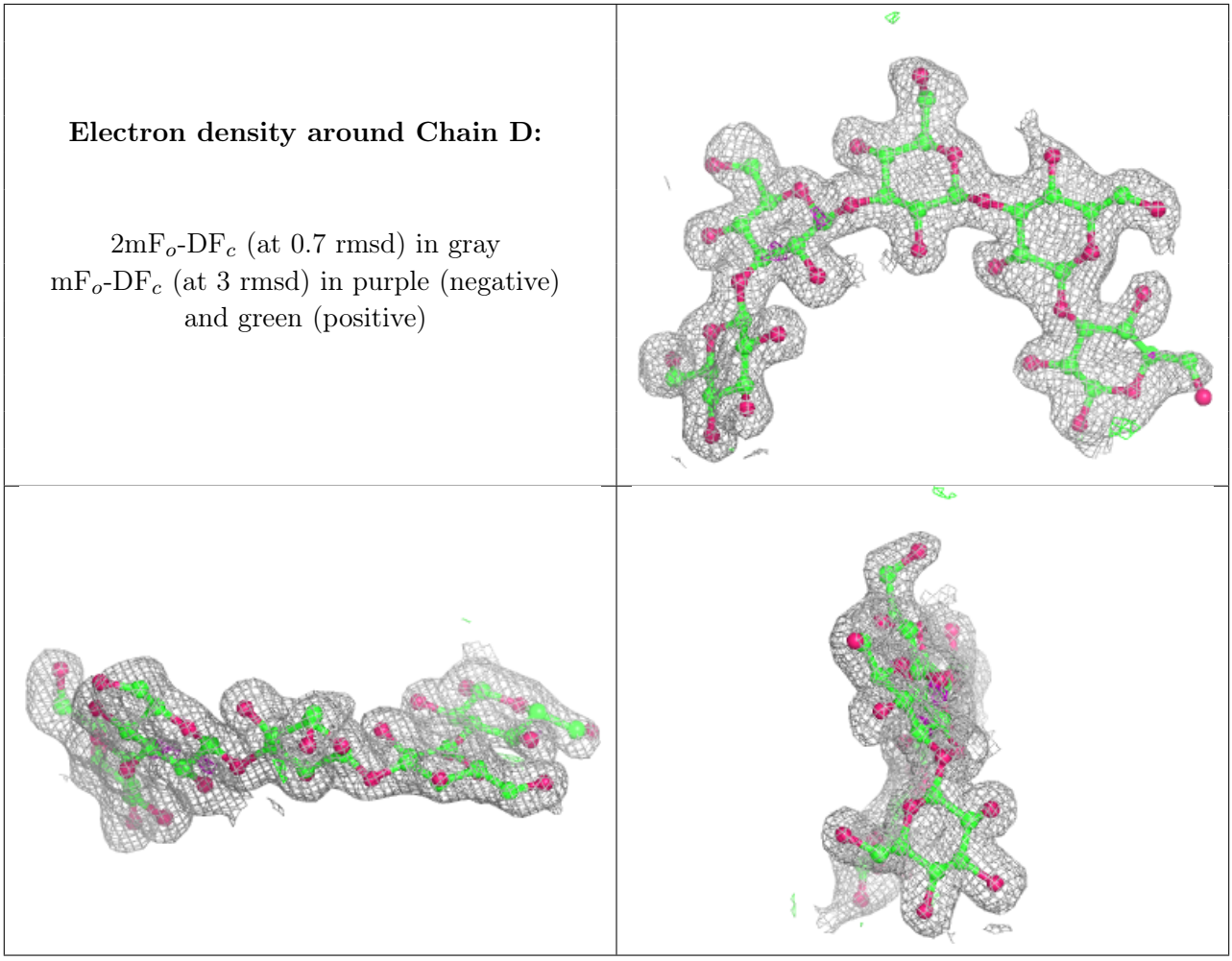
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





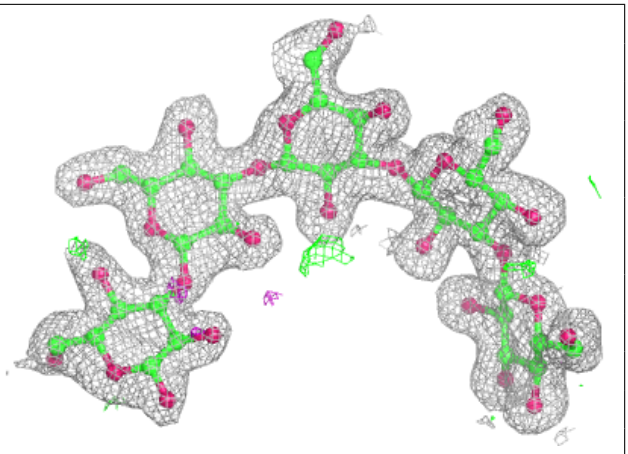
Electron density around Chain D:

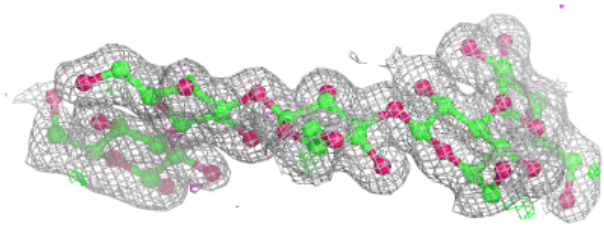
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

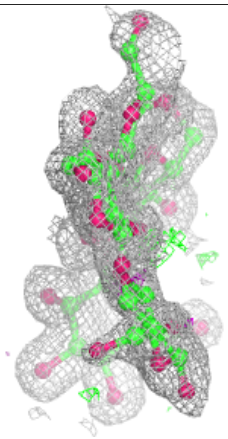


Electron density around Chain F:

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

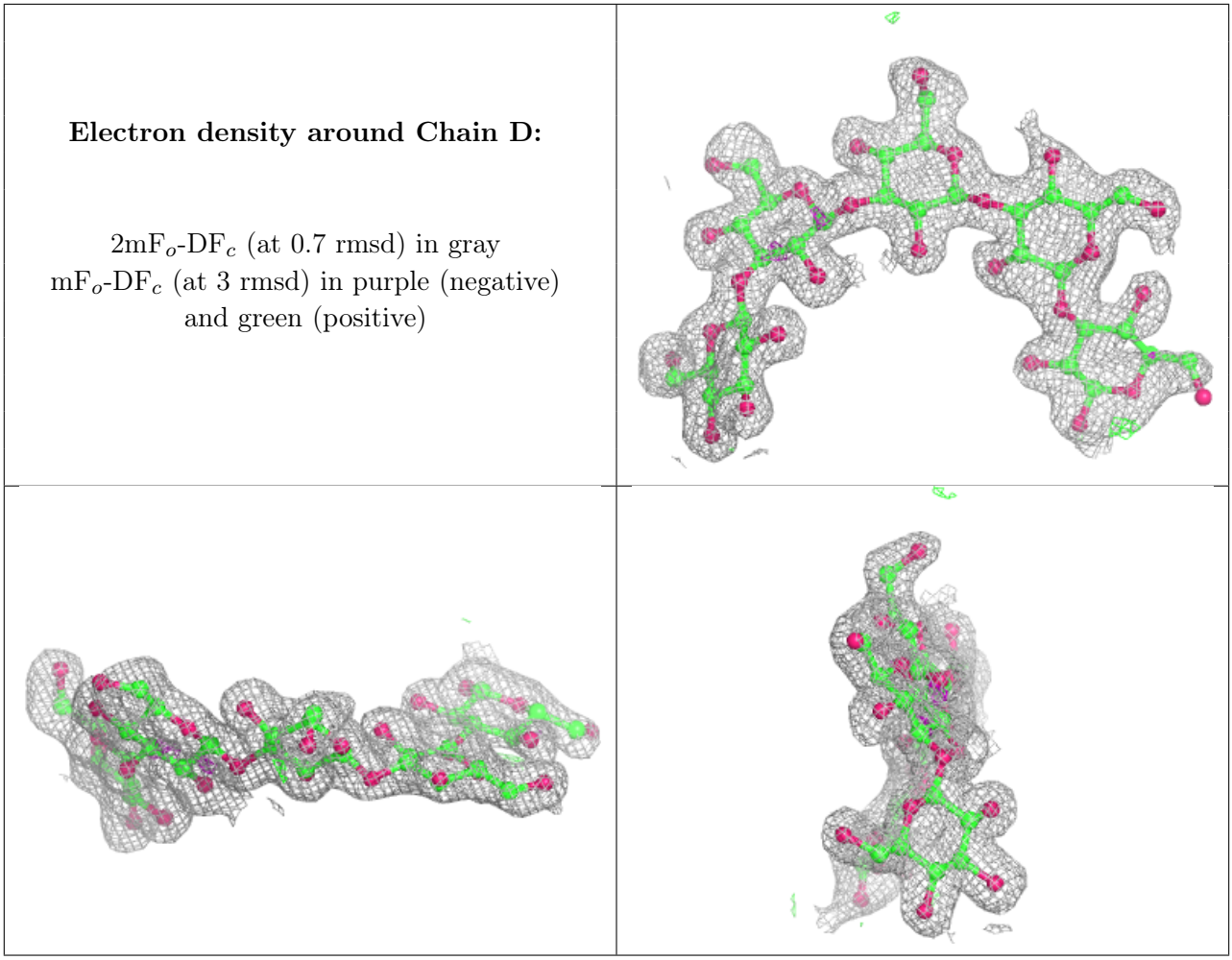






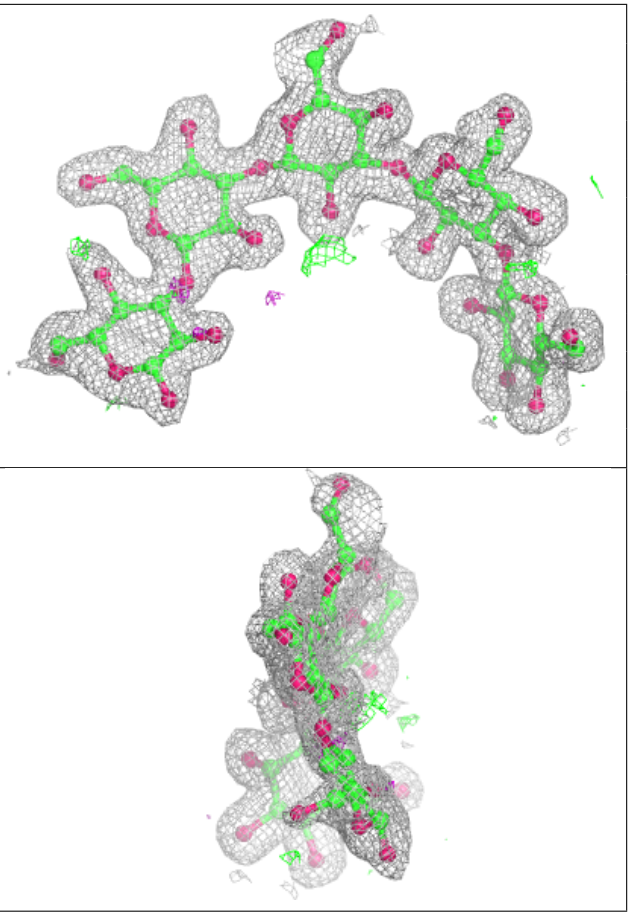
Electron density around Chain D:

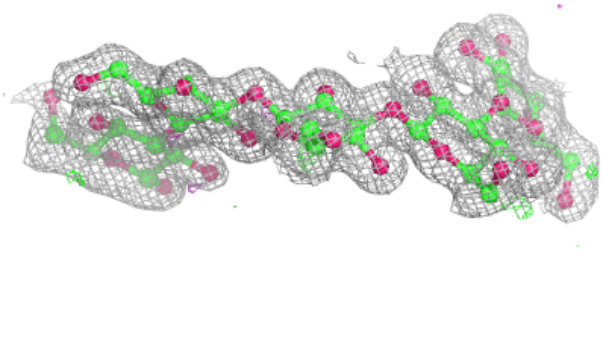
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain F:

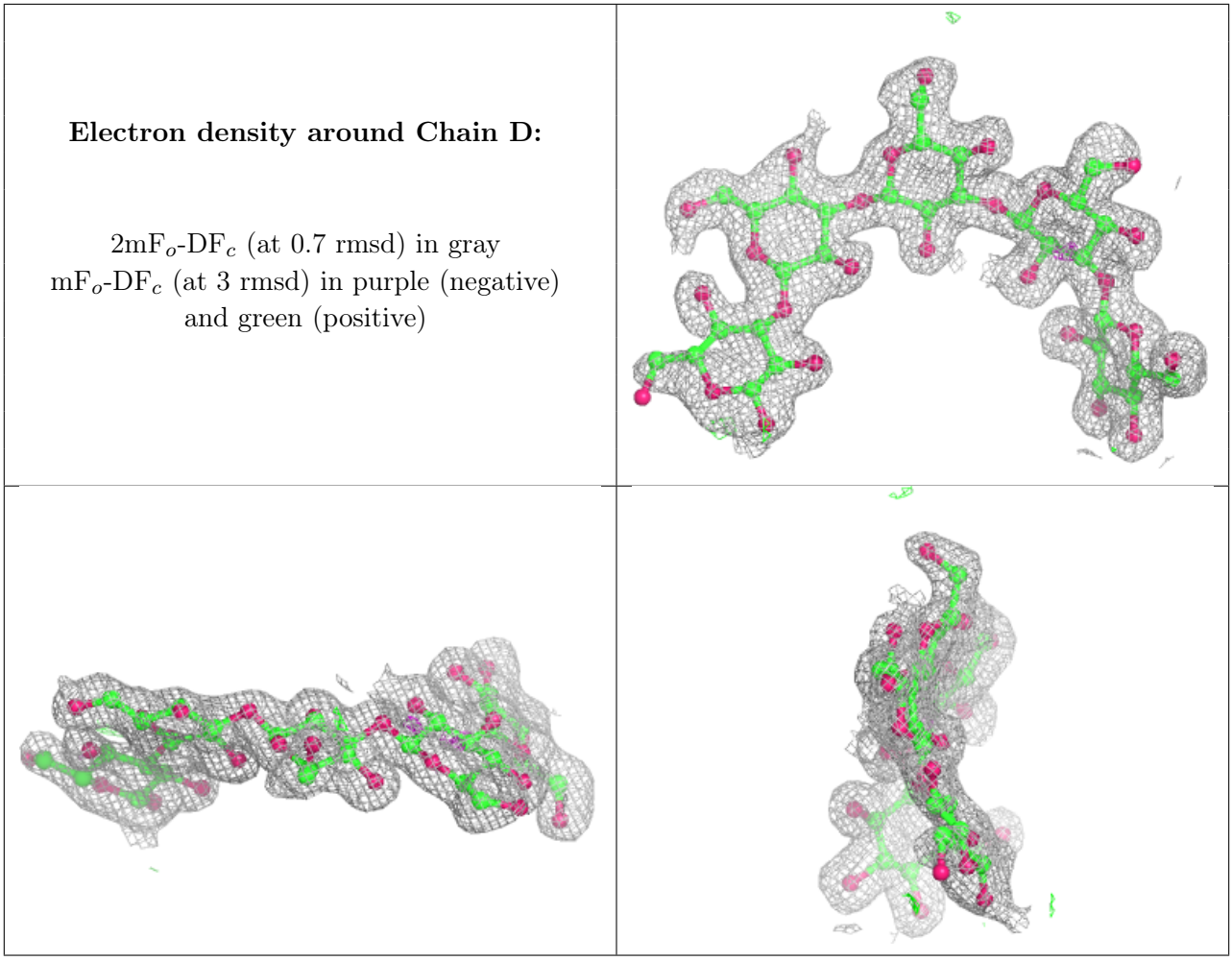
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





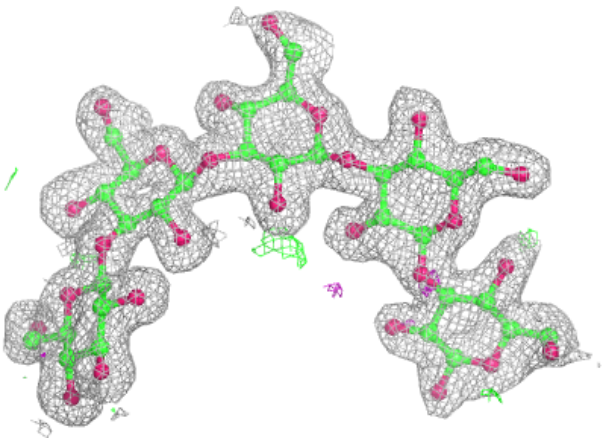
Electron density around Chain D:

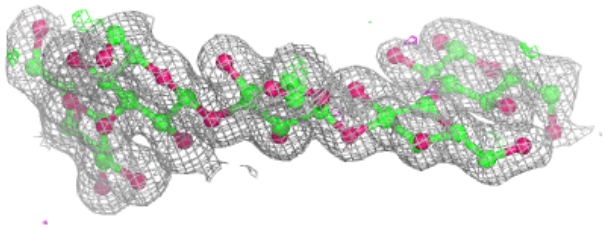
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

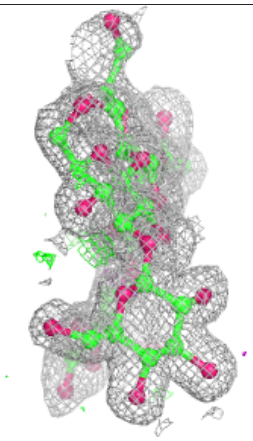


Electron density around Chain F:

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

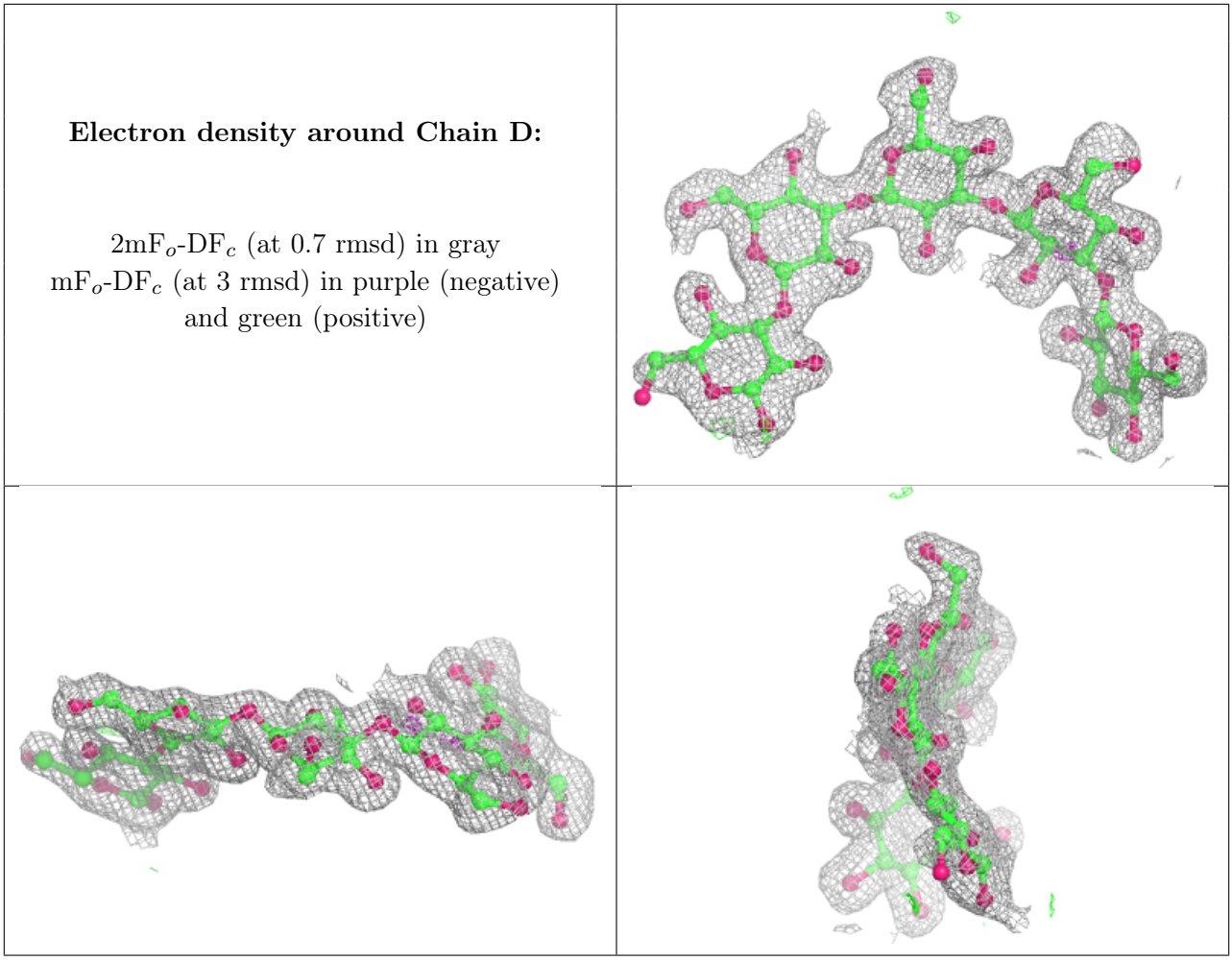






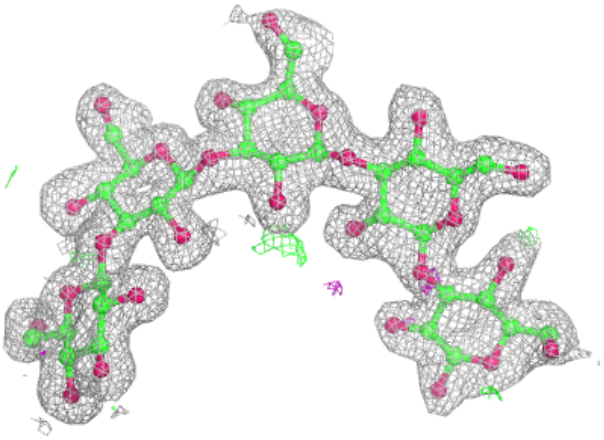
Electron density around Chain D:

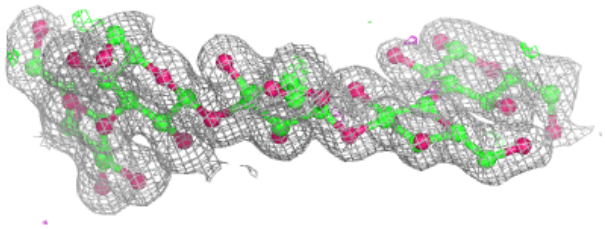
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

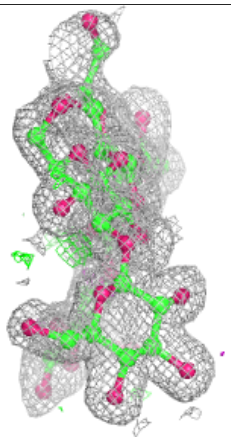


Electron density around Chain F:

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

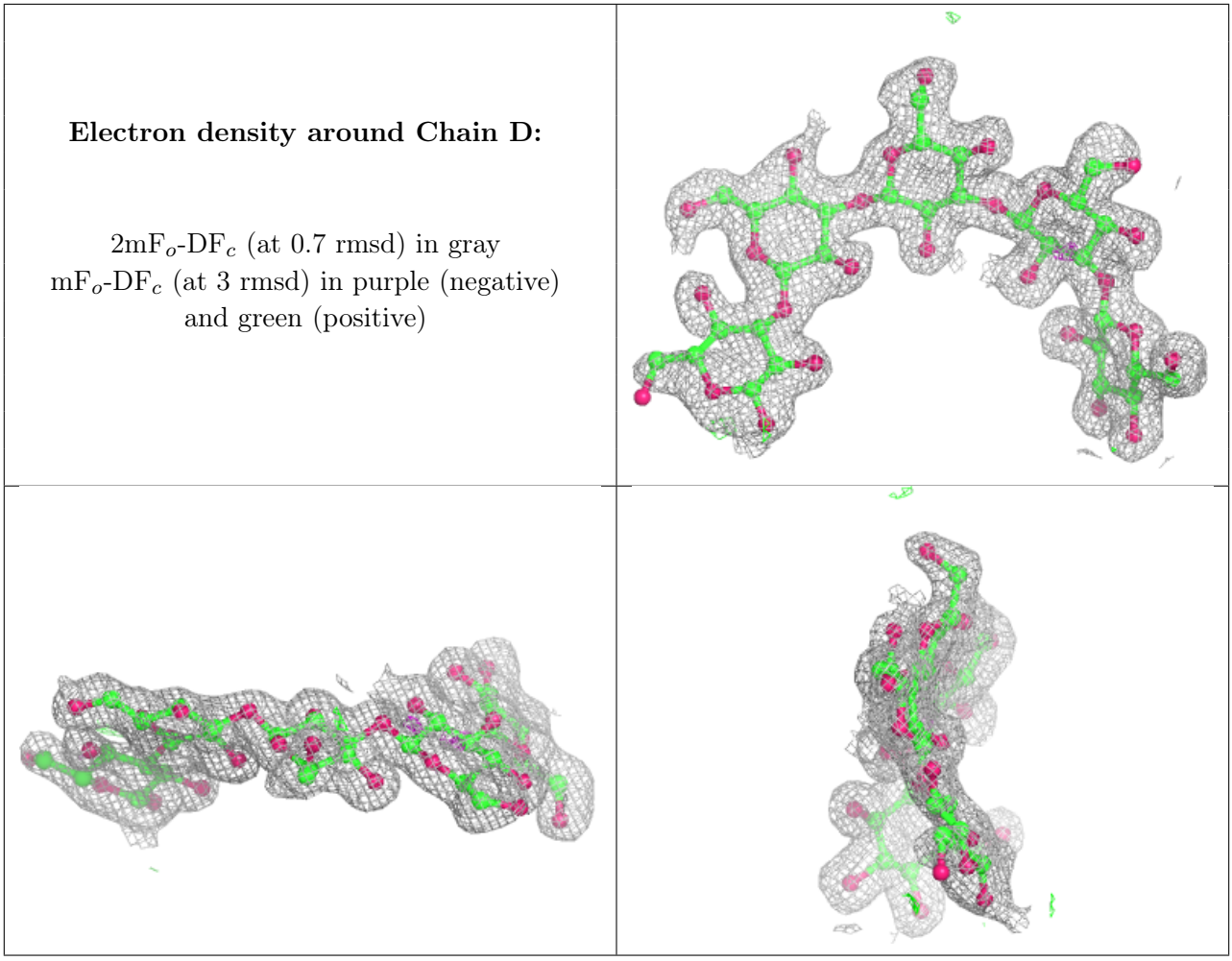






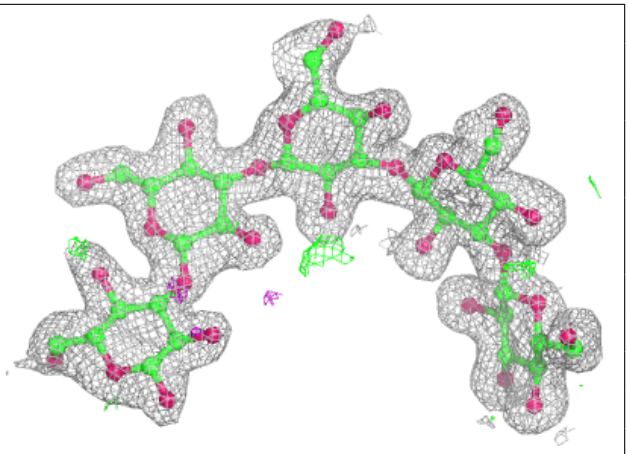
Electron density around Chain D:

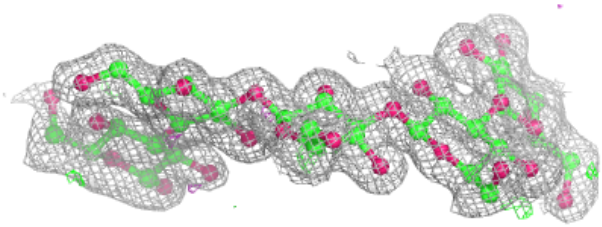
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

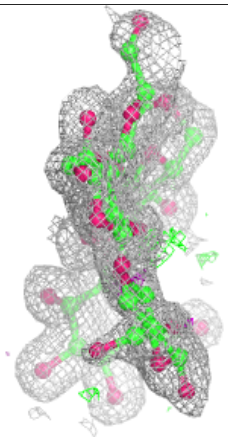


Electron density around Chain F:

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

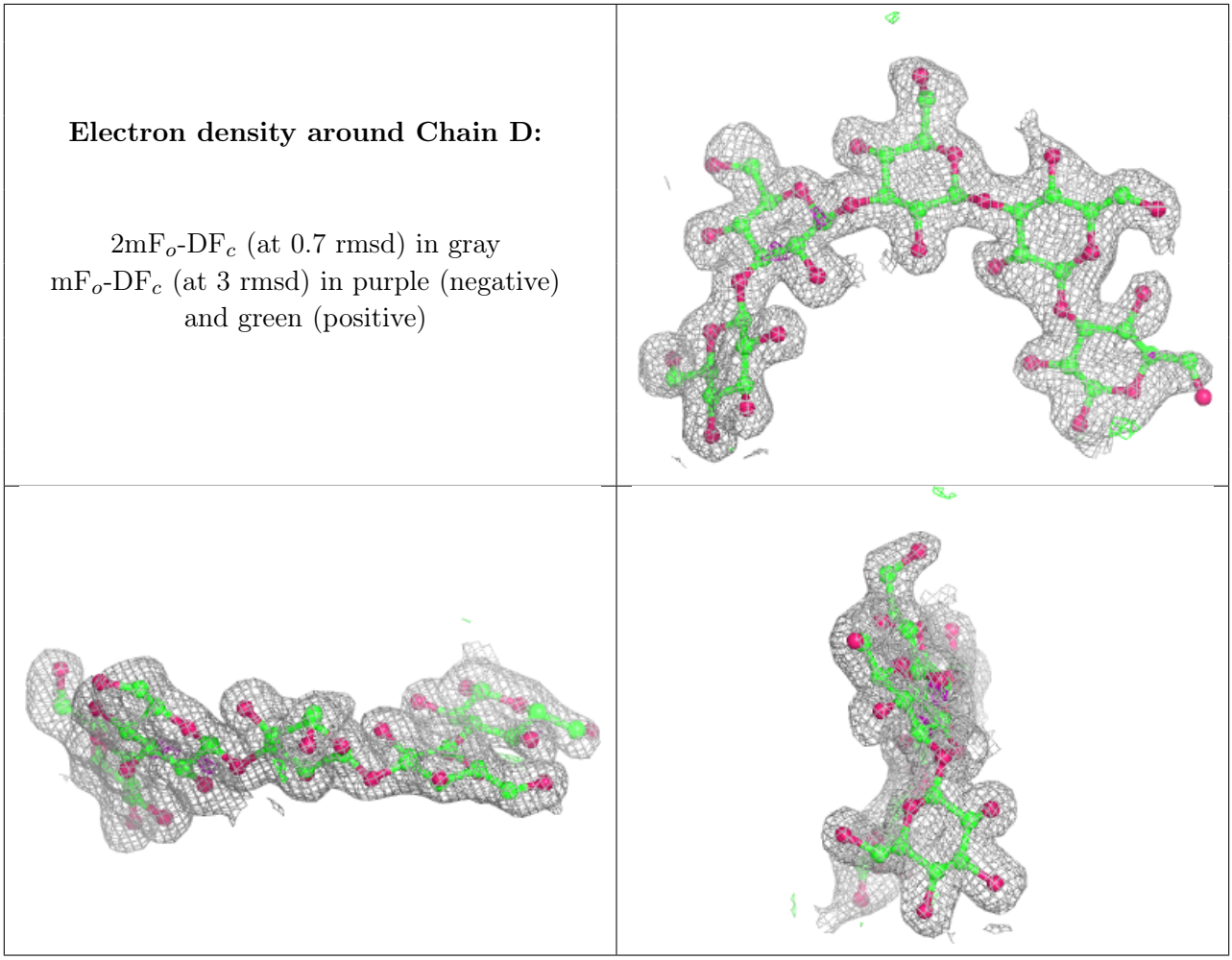






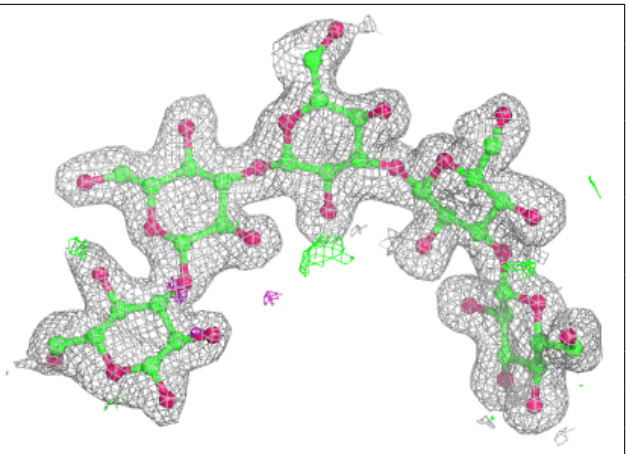
Electron density around Chain D:

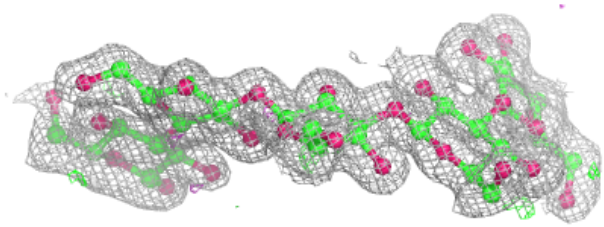
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

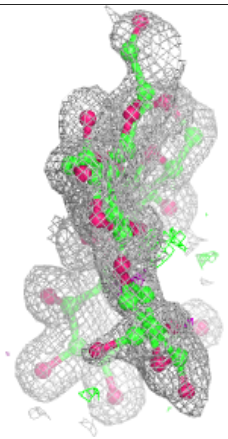


Electron density around Chain F:

$2mF_o$-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
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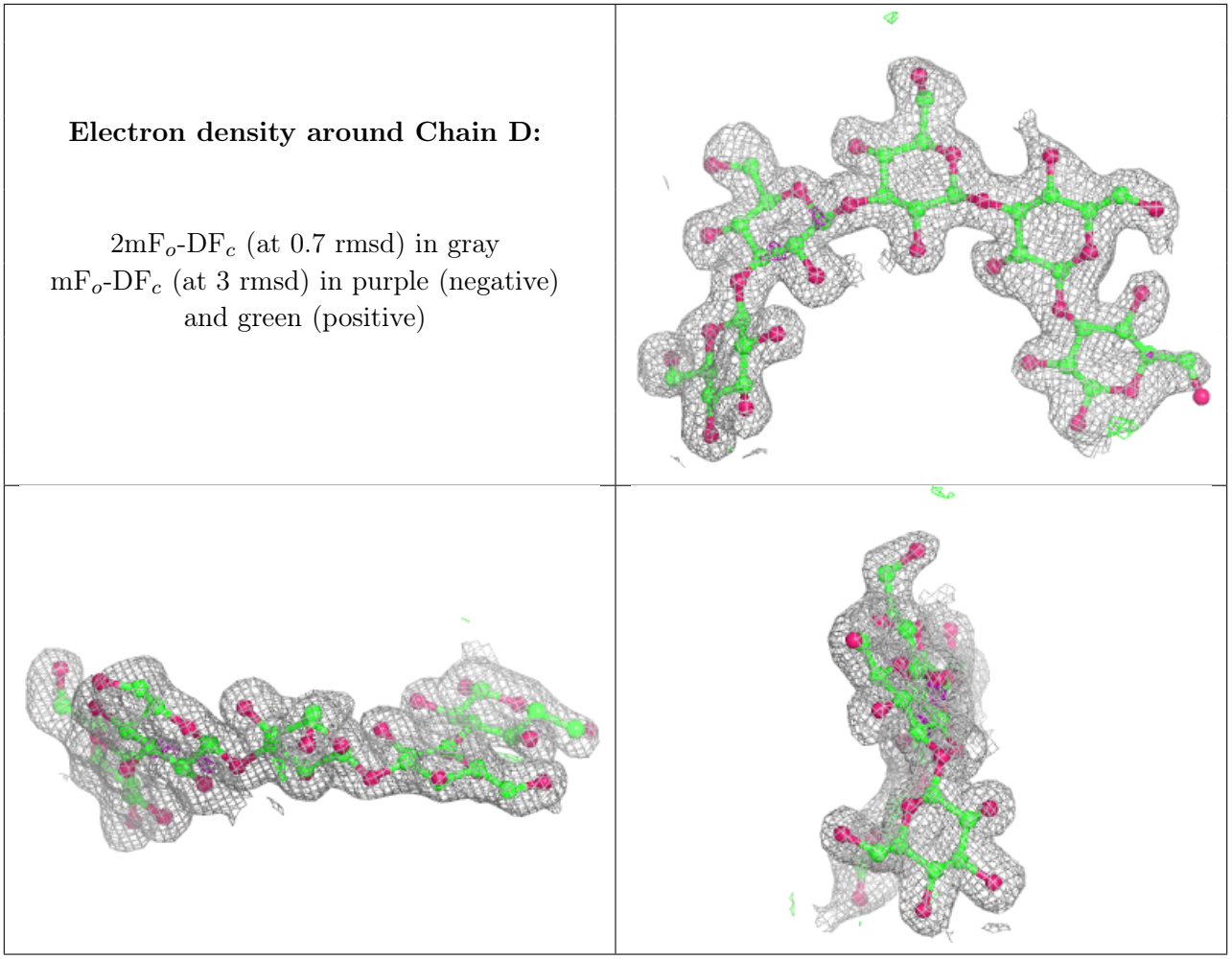

Electron density around Chain F:

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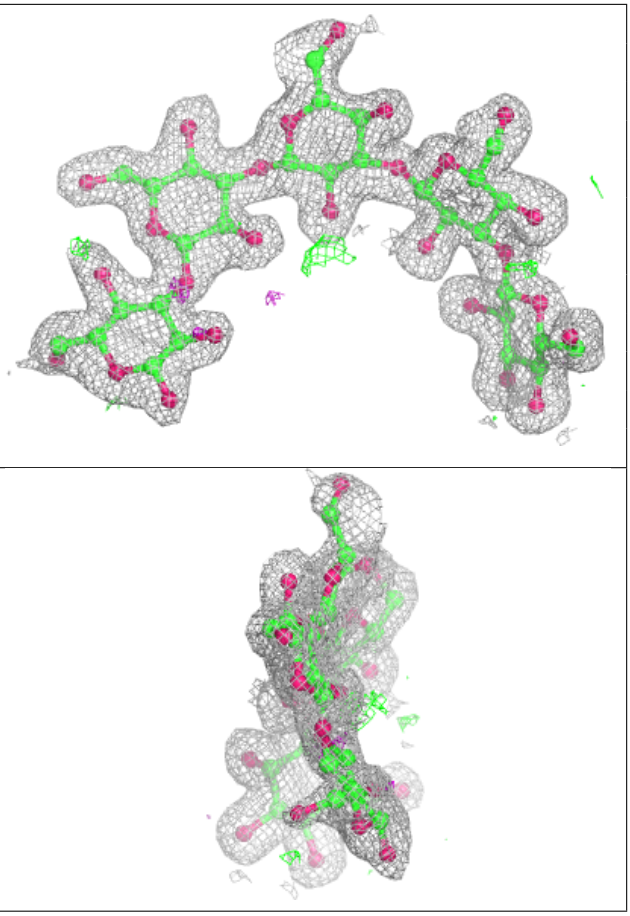
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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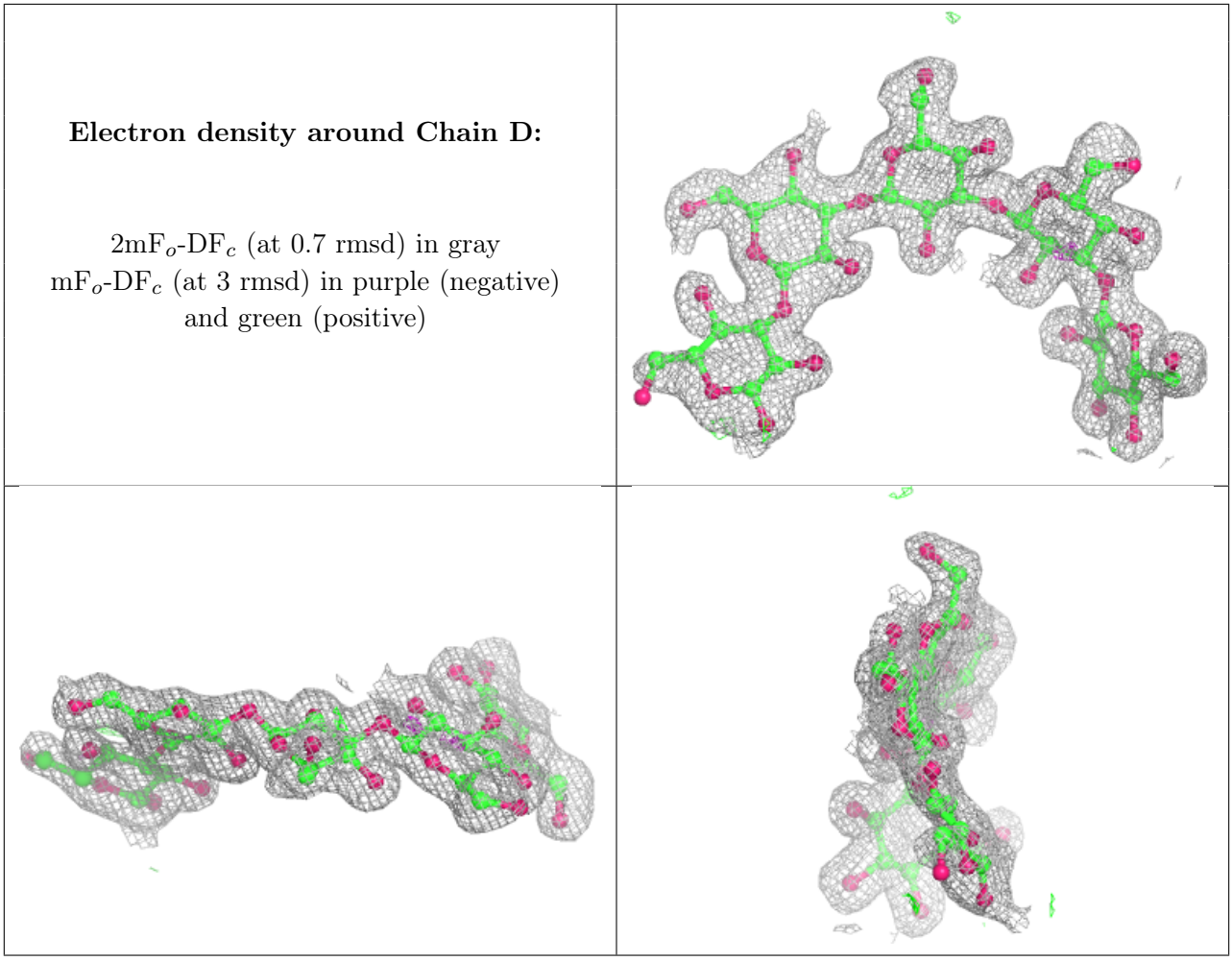

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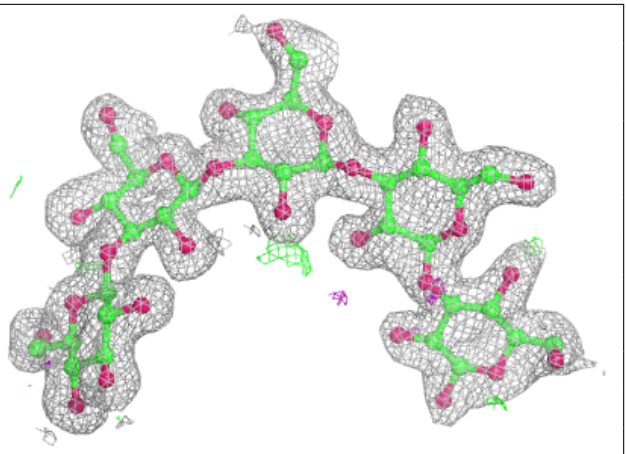

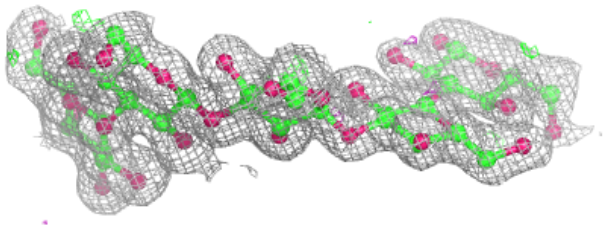

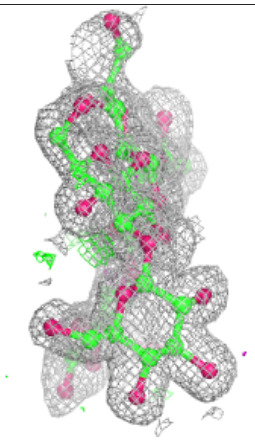

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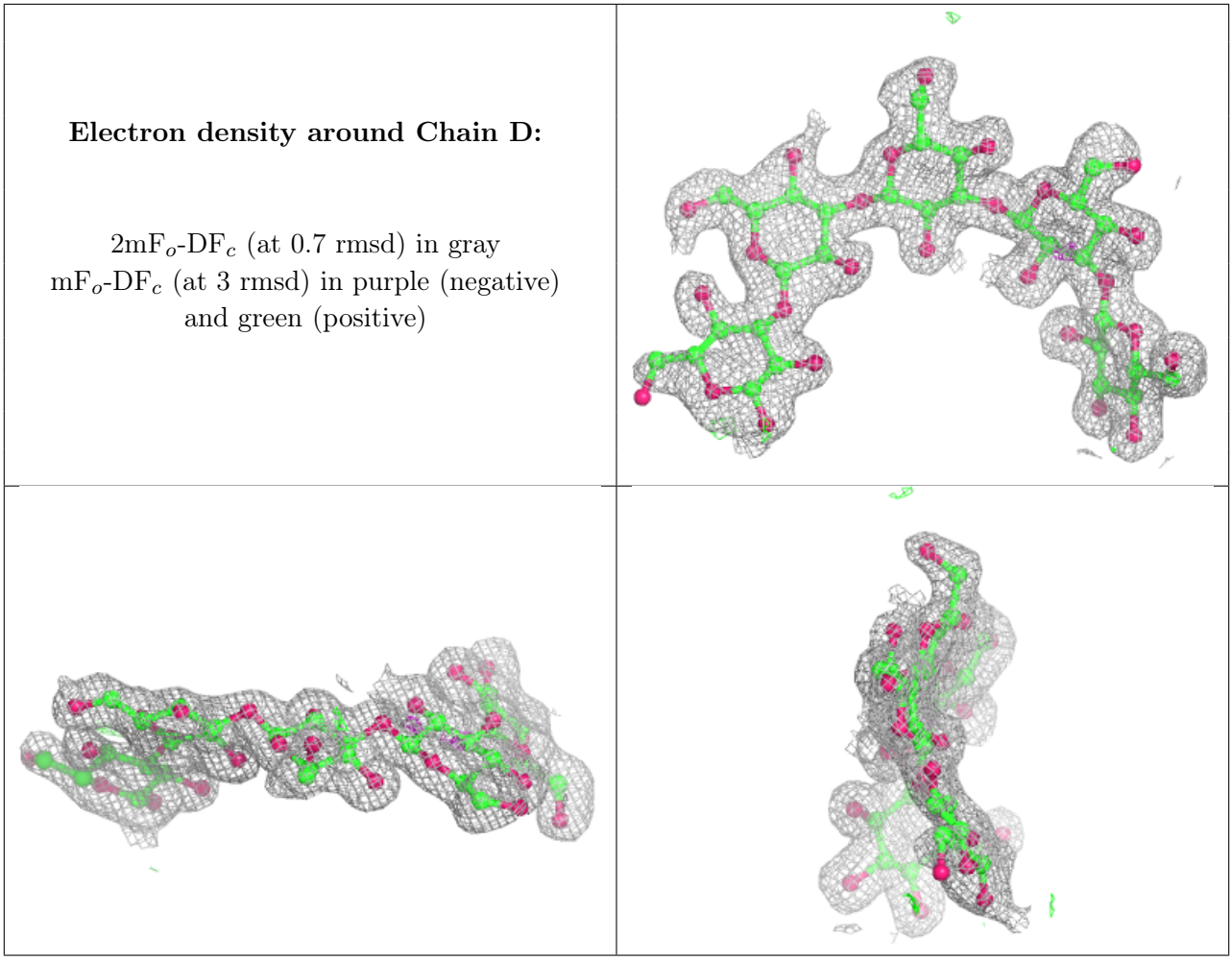
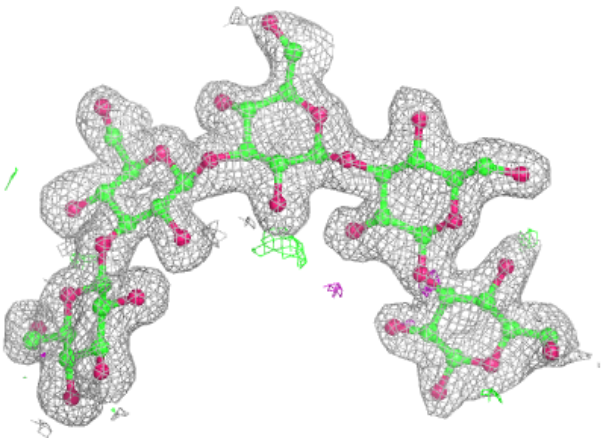
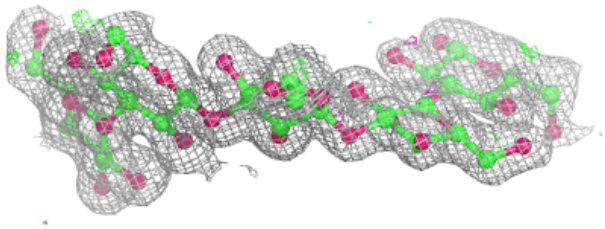
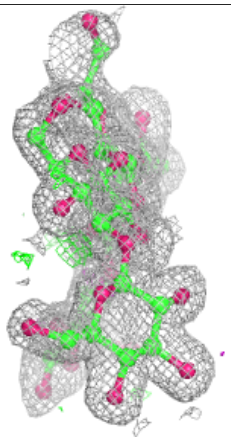


Electron density around Chain F:

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







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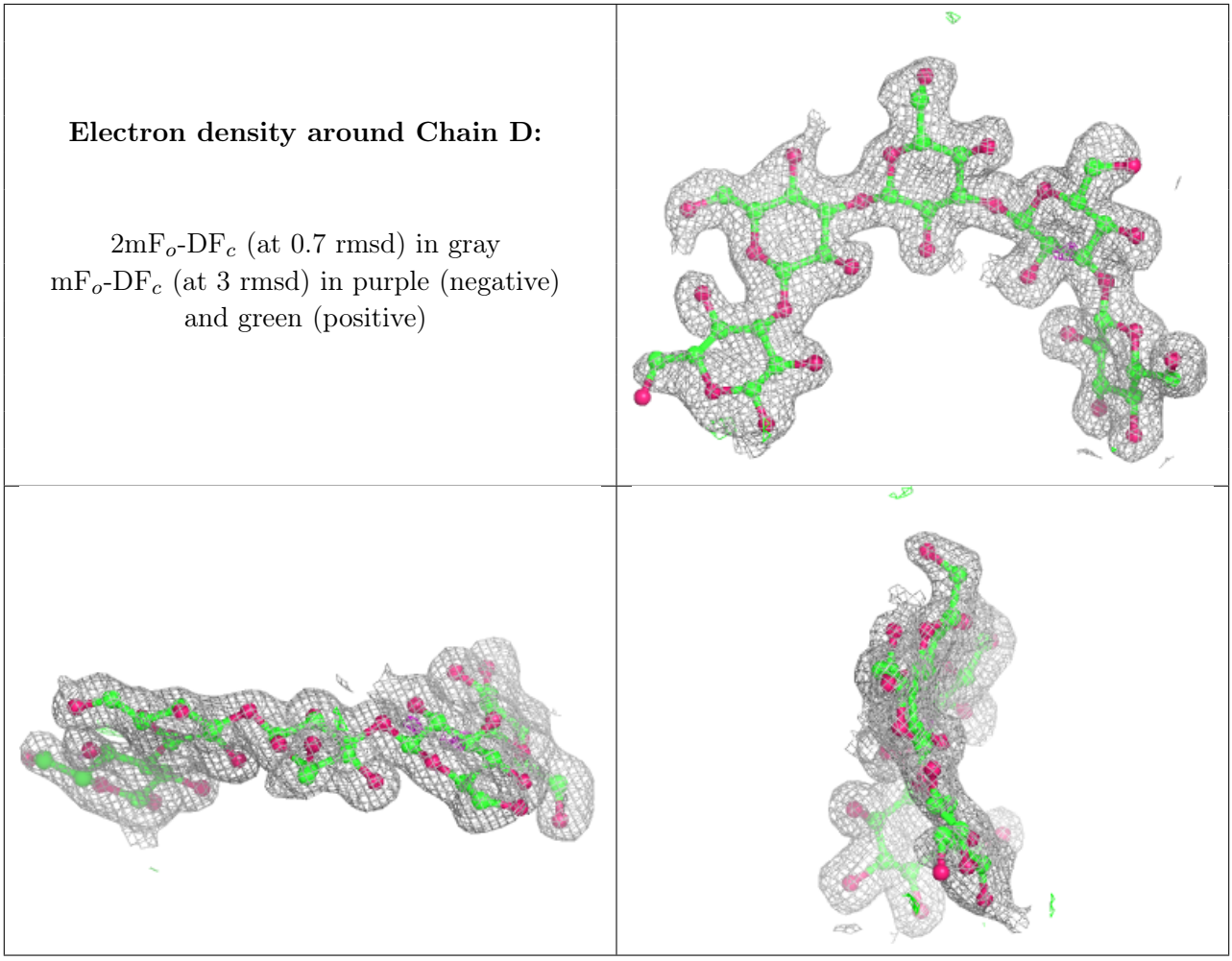
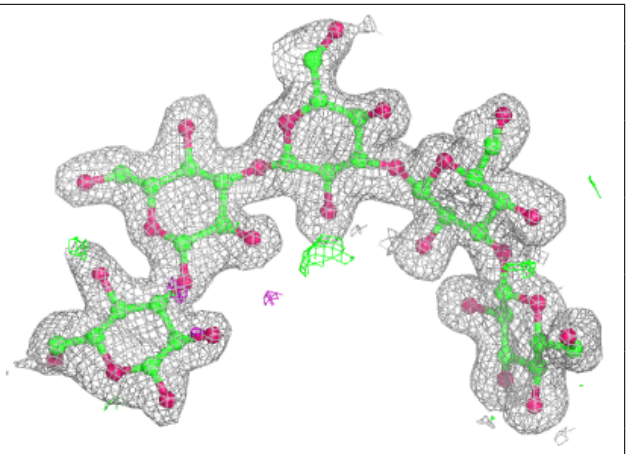
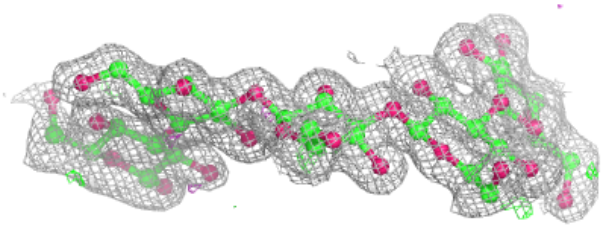
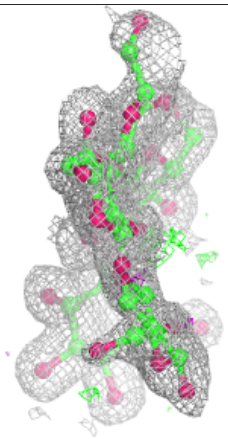


Electron density around Chain F:

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







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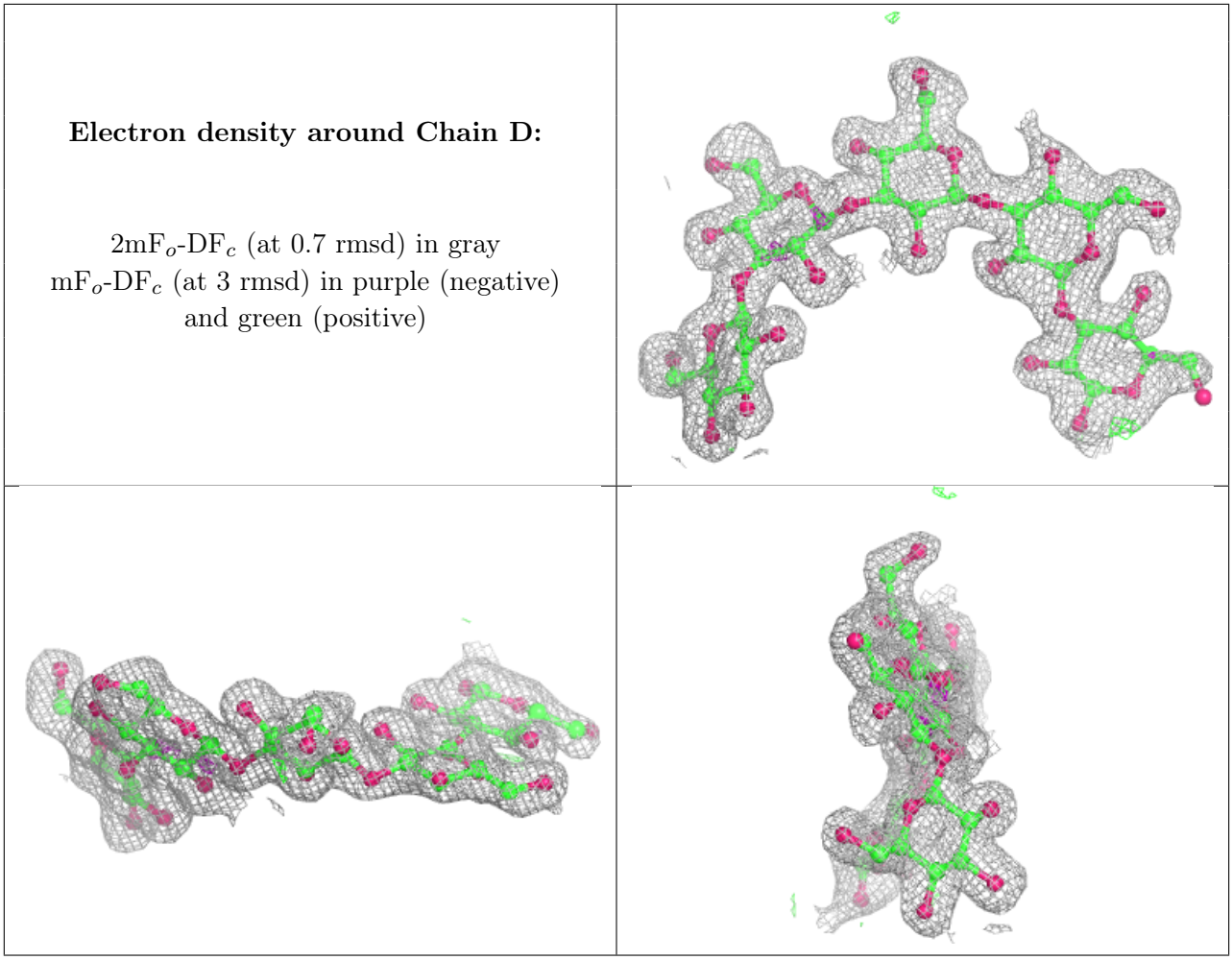

Electron density around Chain F:

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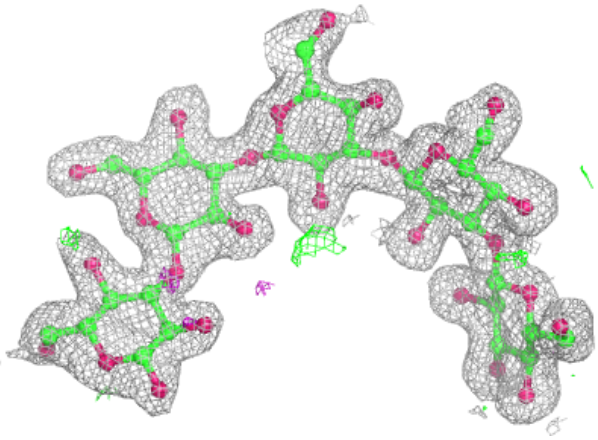
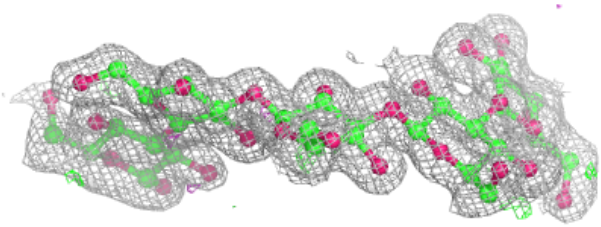
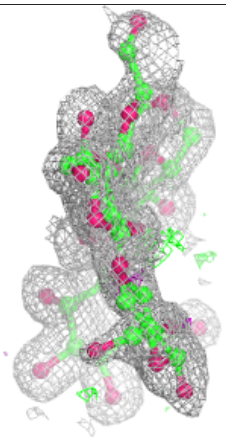
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







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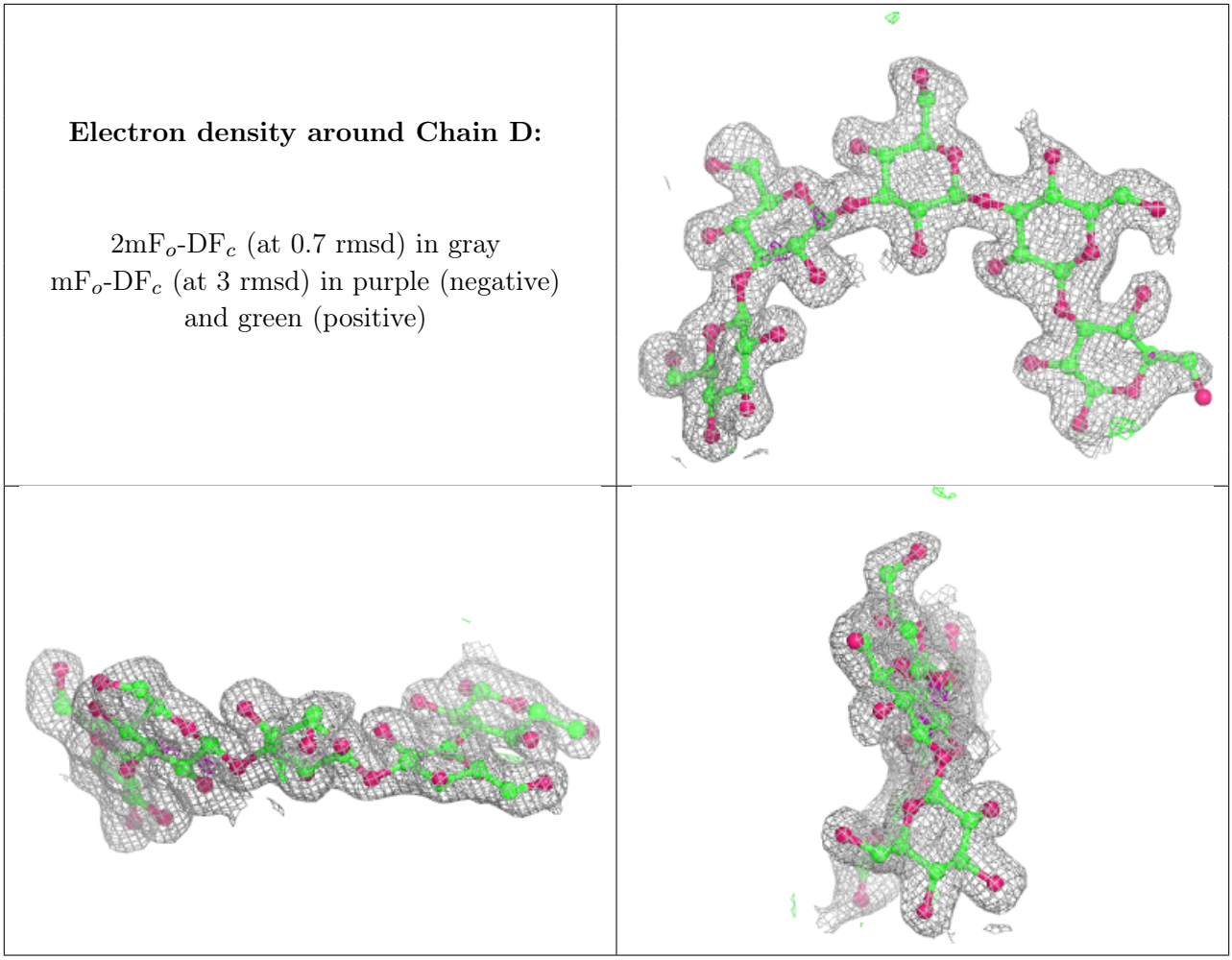

Electron density around Chain F:

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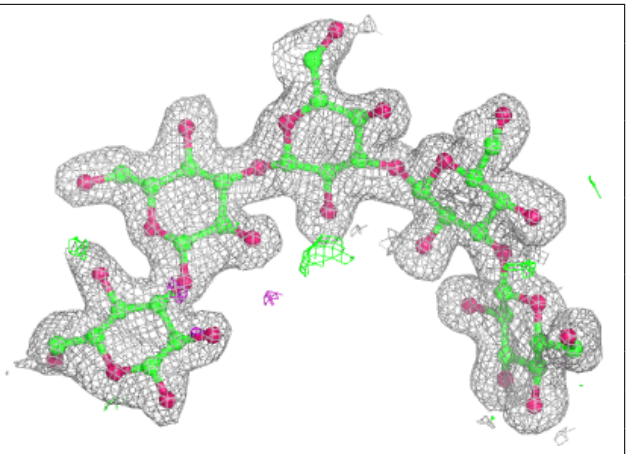
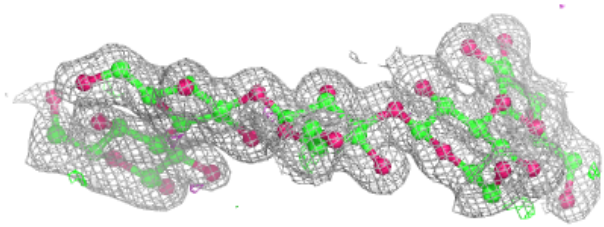
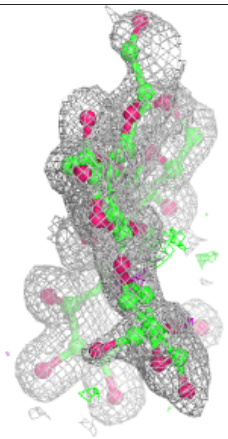
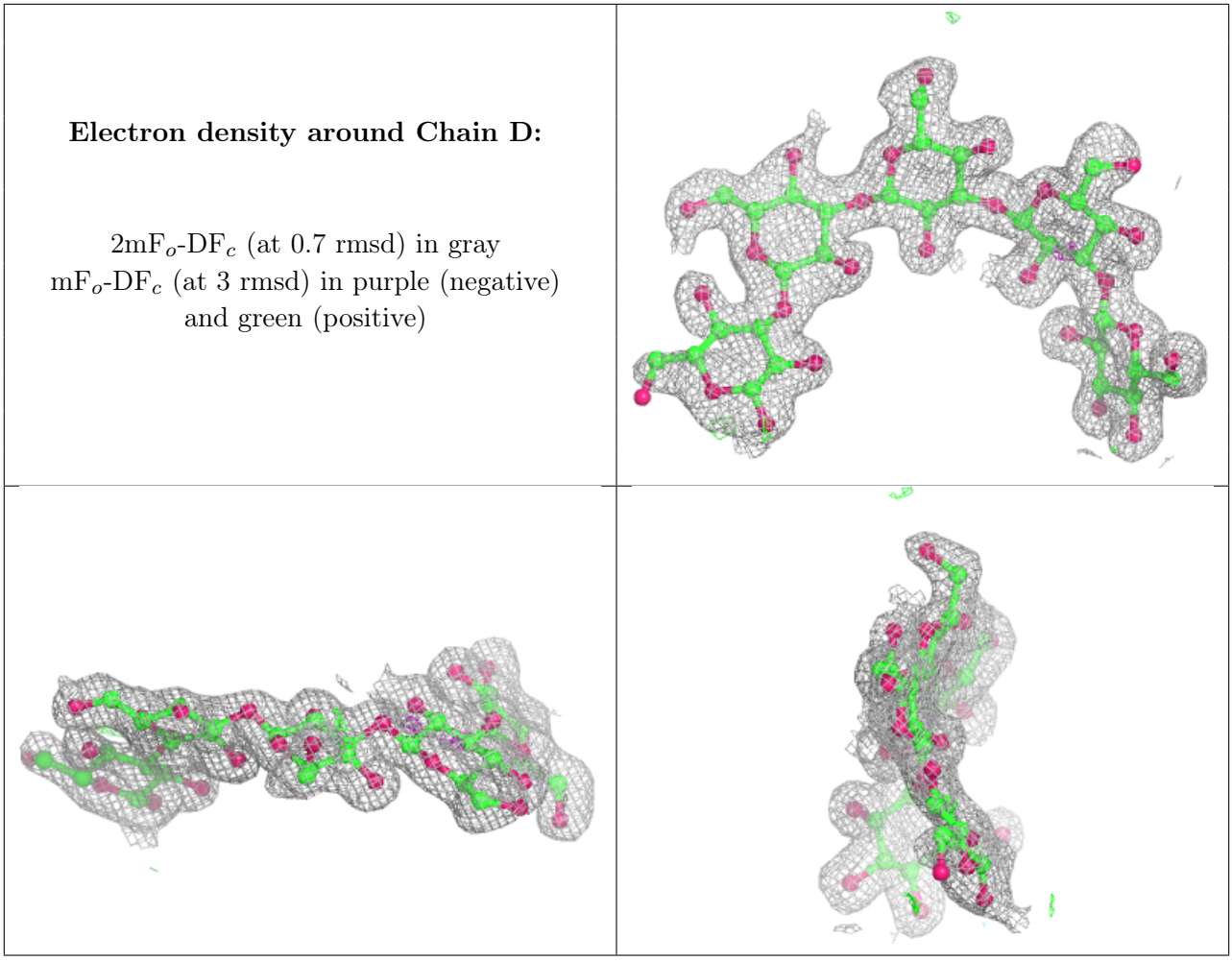






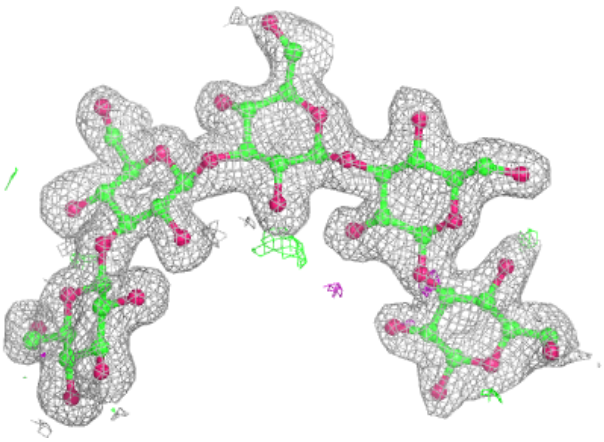
Electron density around Chain D:

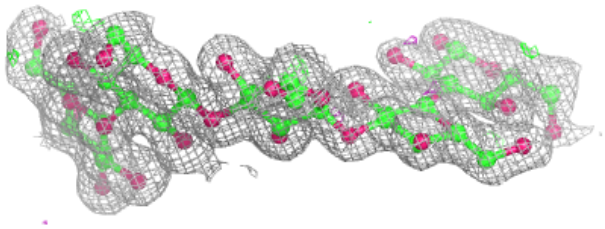
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

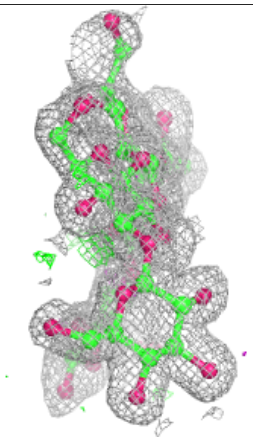


Electron density around Chain F:

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

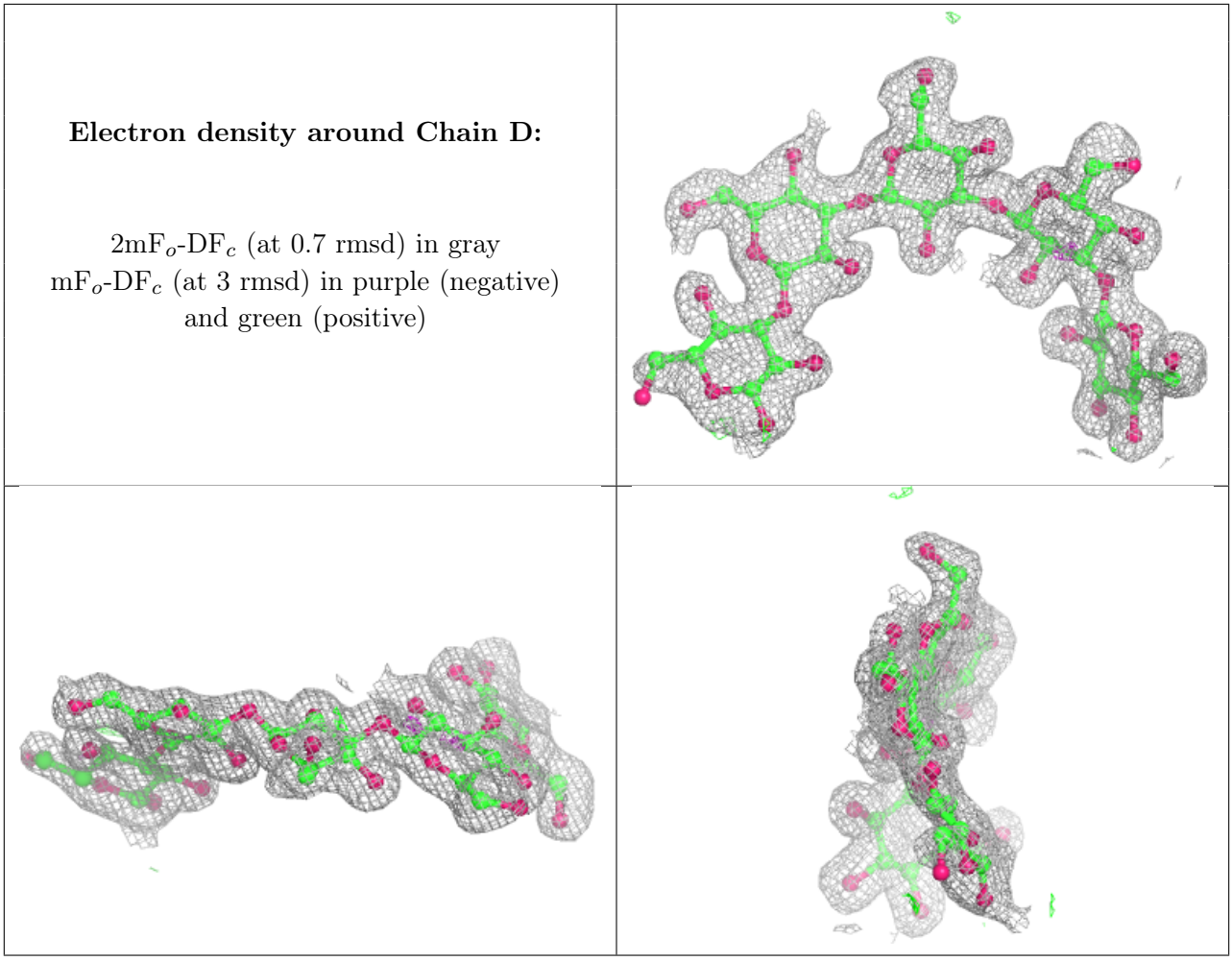






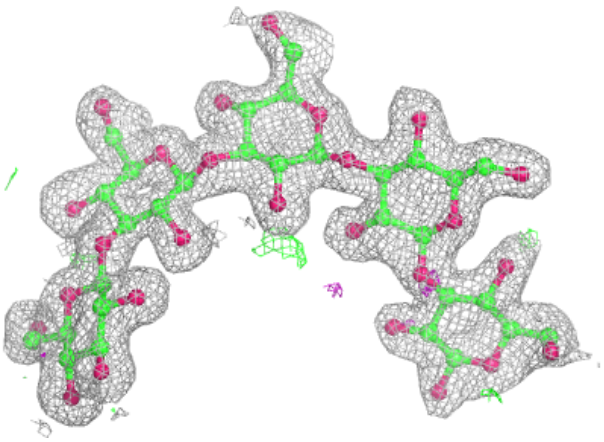
Electron density around Chain D:

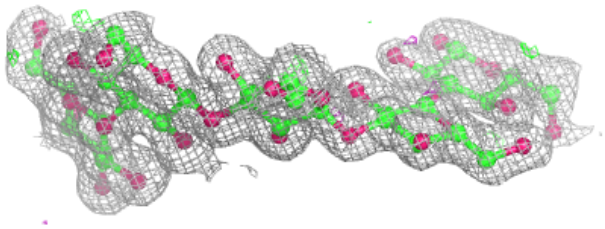
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

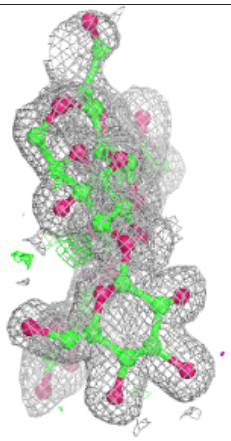


Electron density around Chain F:

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

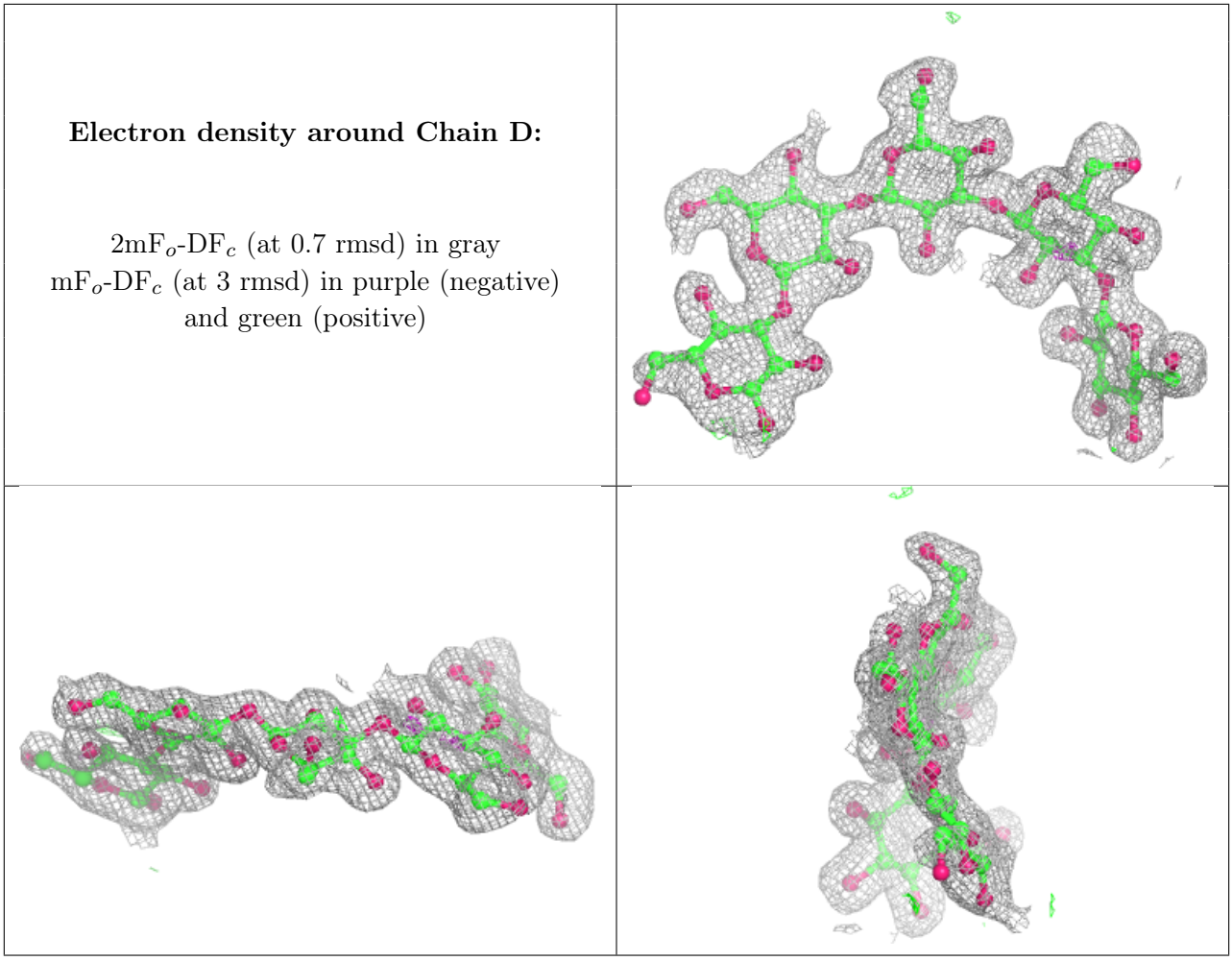






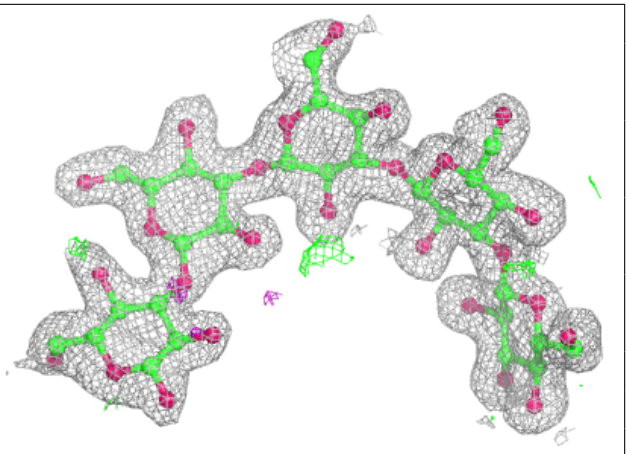
Electron density around Chain D:

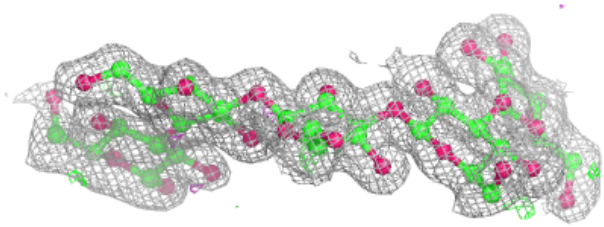
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

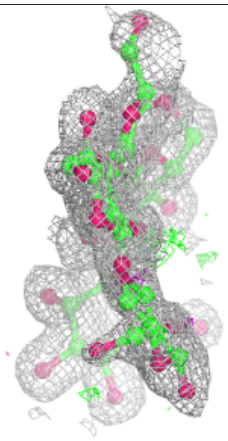


Electron density around Chain F:

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

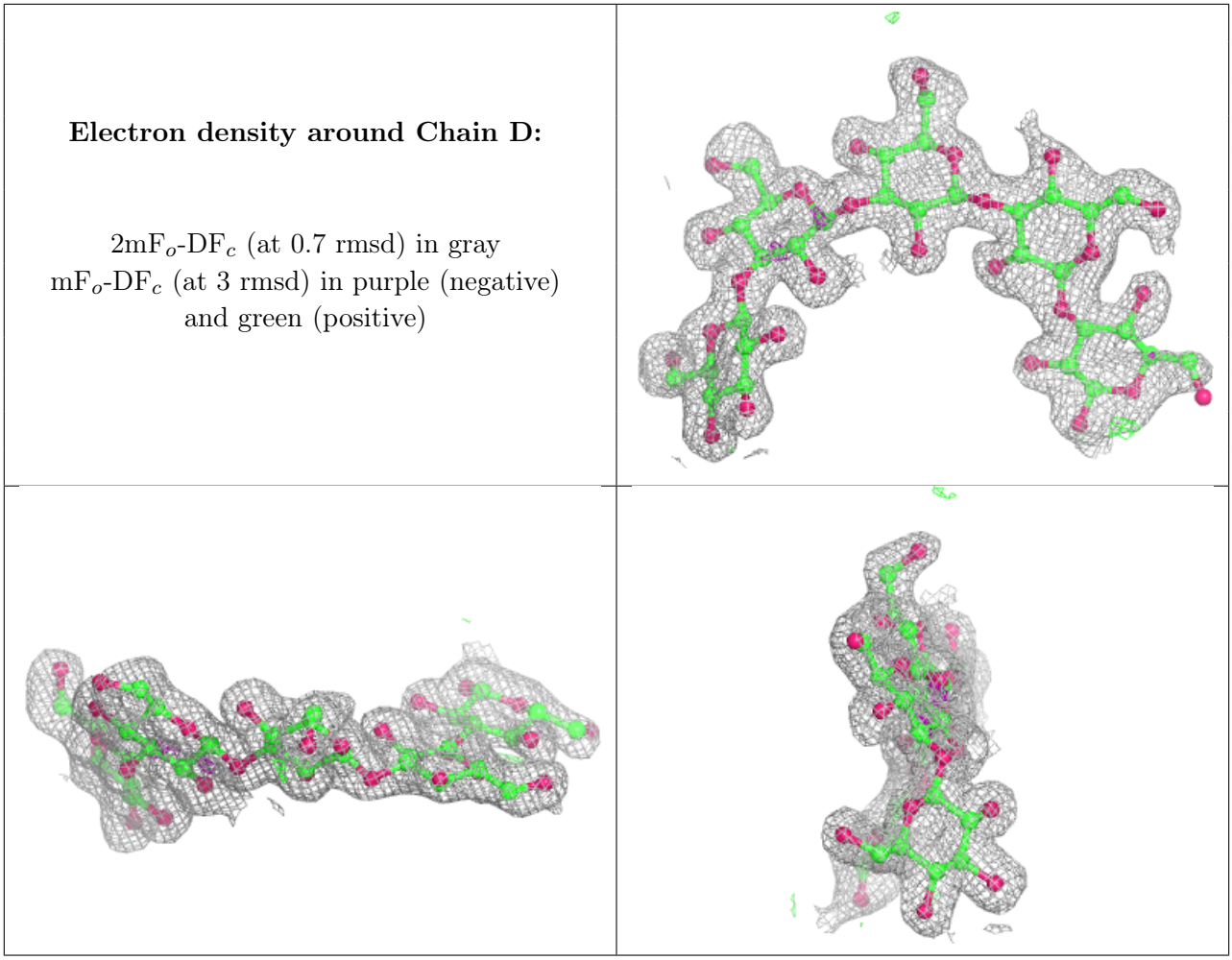






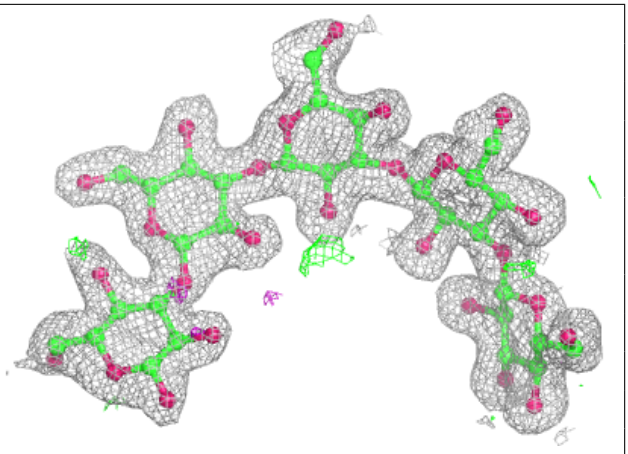
Electron density around Chain D:

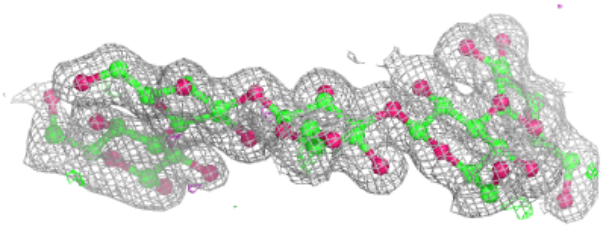
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

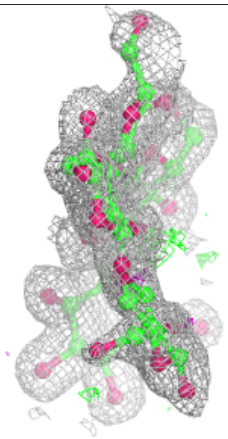


Electron density around Chain F:

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

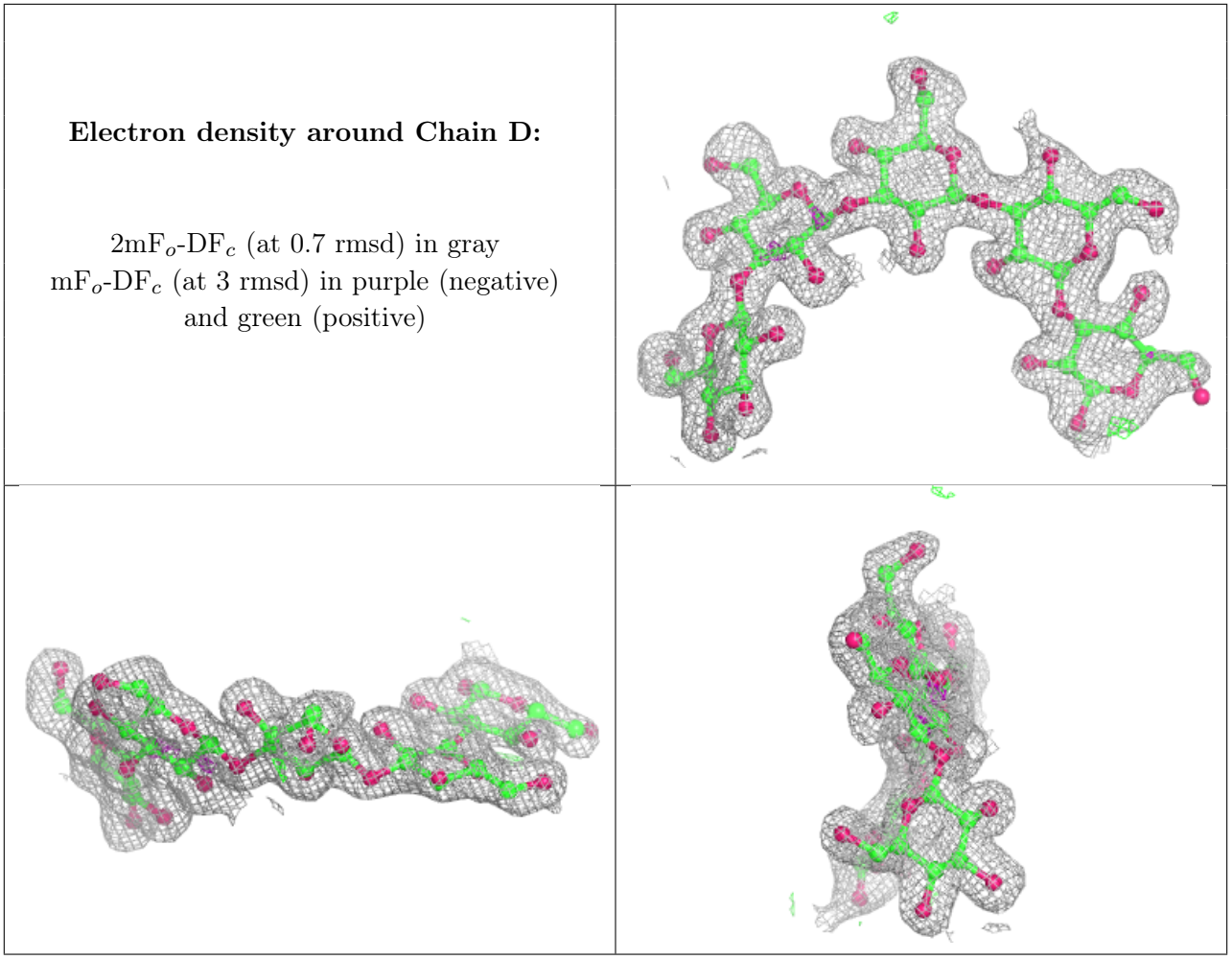






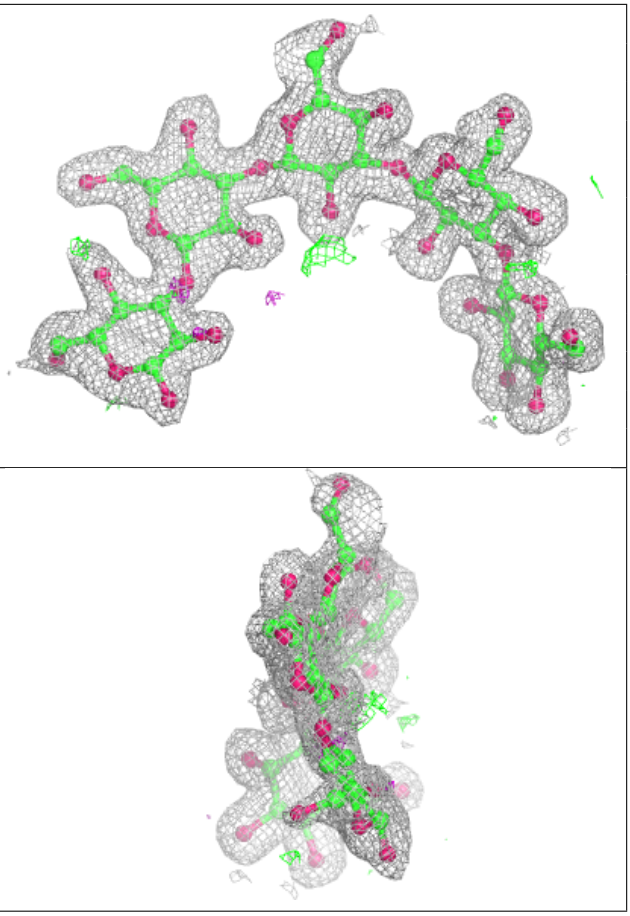
Electron density around Chain D:

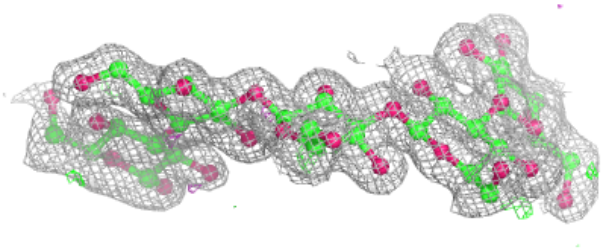
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain F:

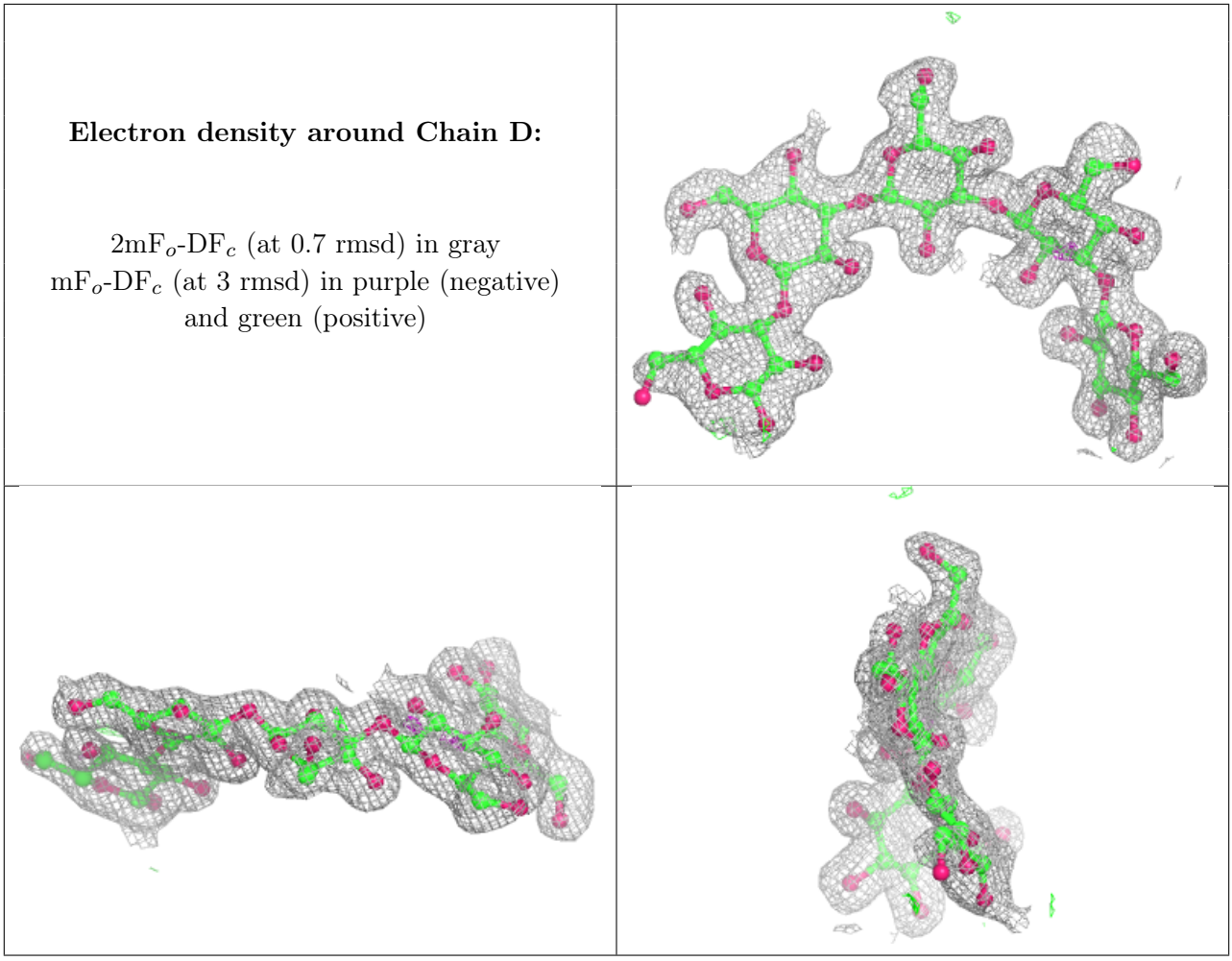
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





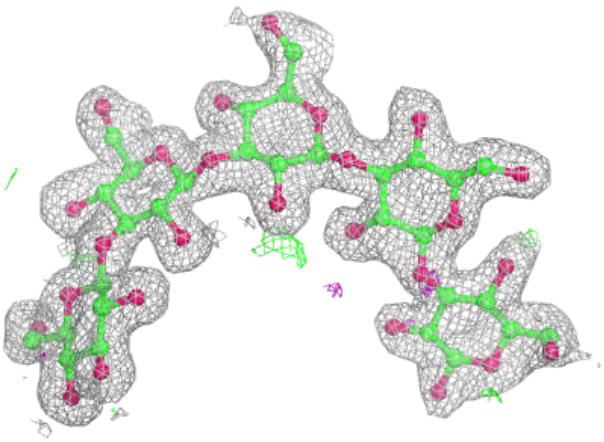
Electron density around Chain D:

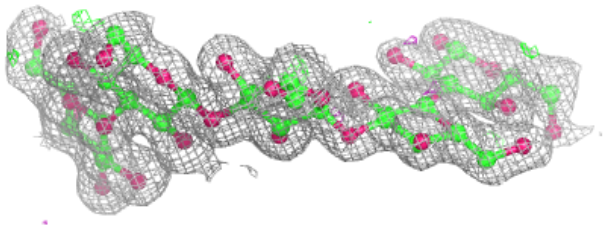
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

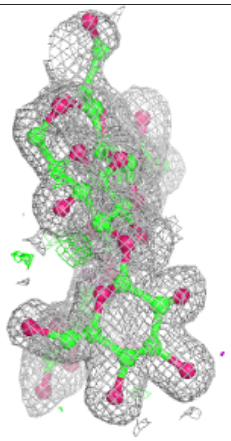


Electron density around Chain F:

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

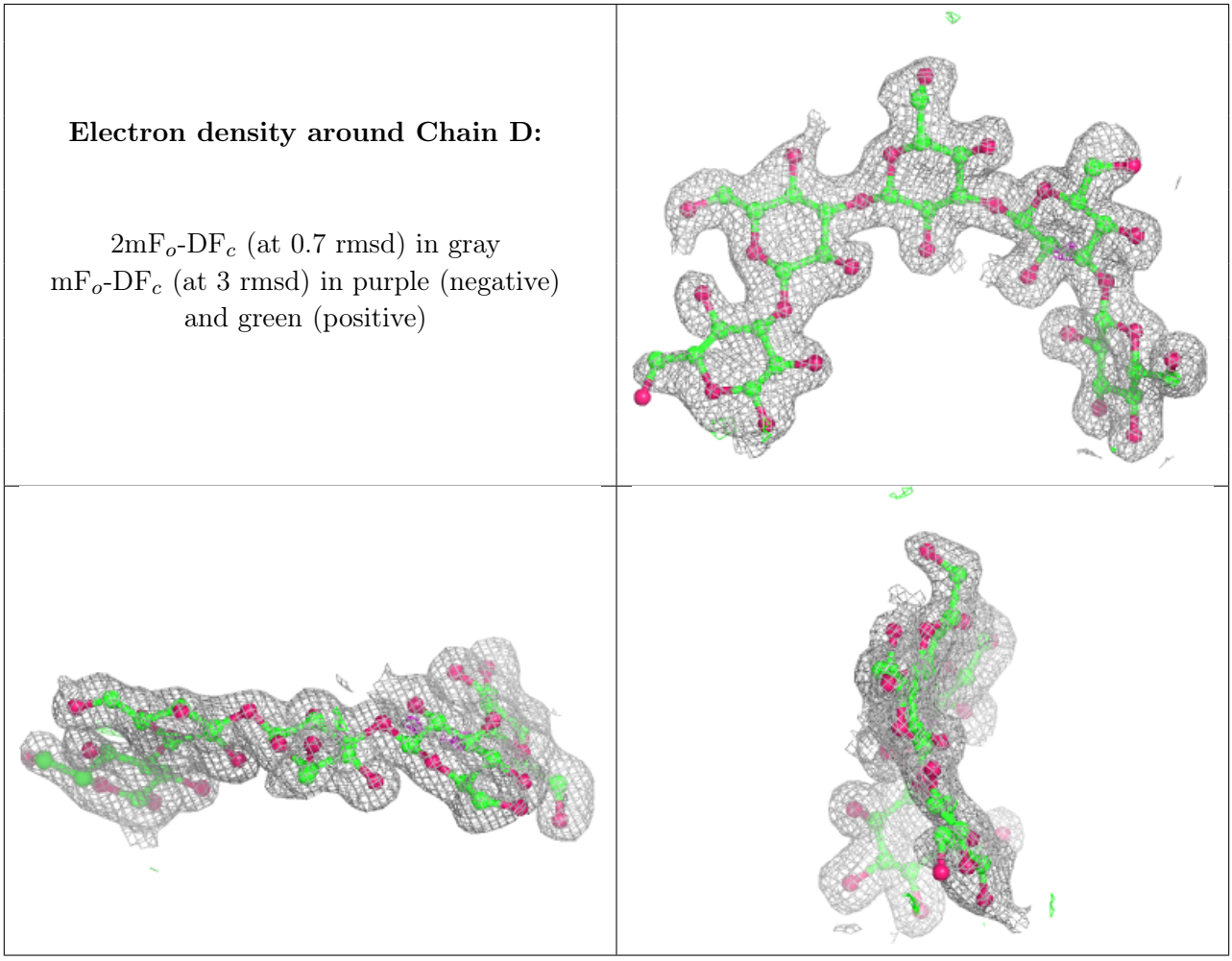






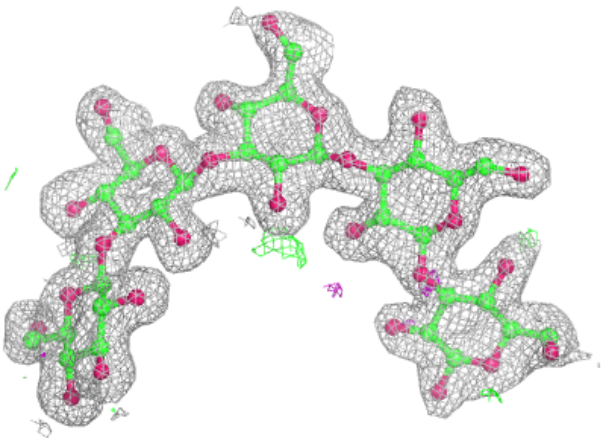
Electron density around Chain D:

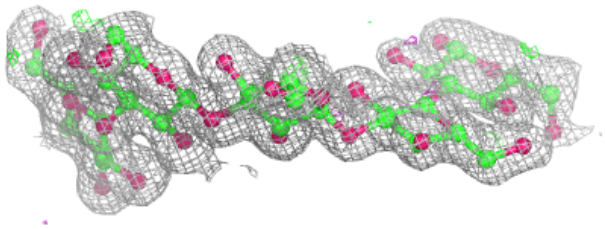
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

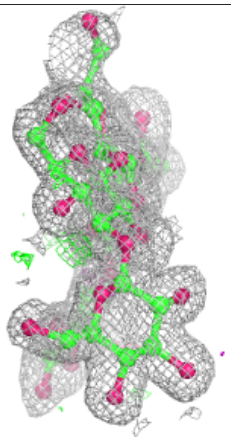


Electron density around Chain F:

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

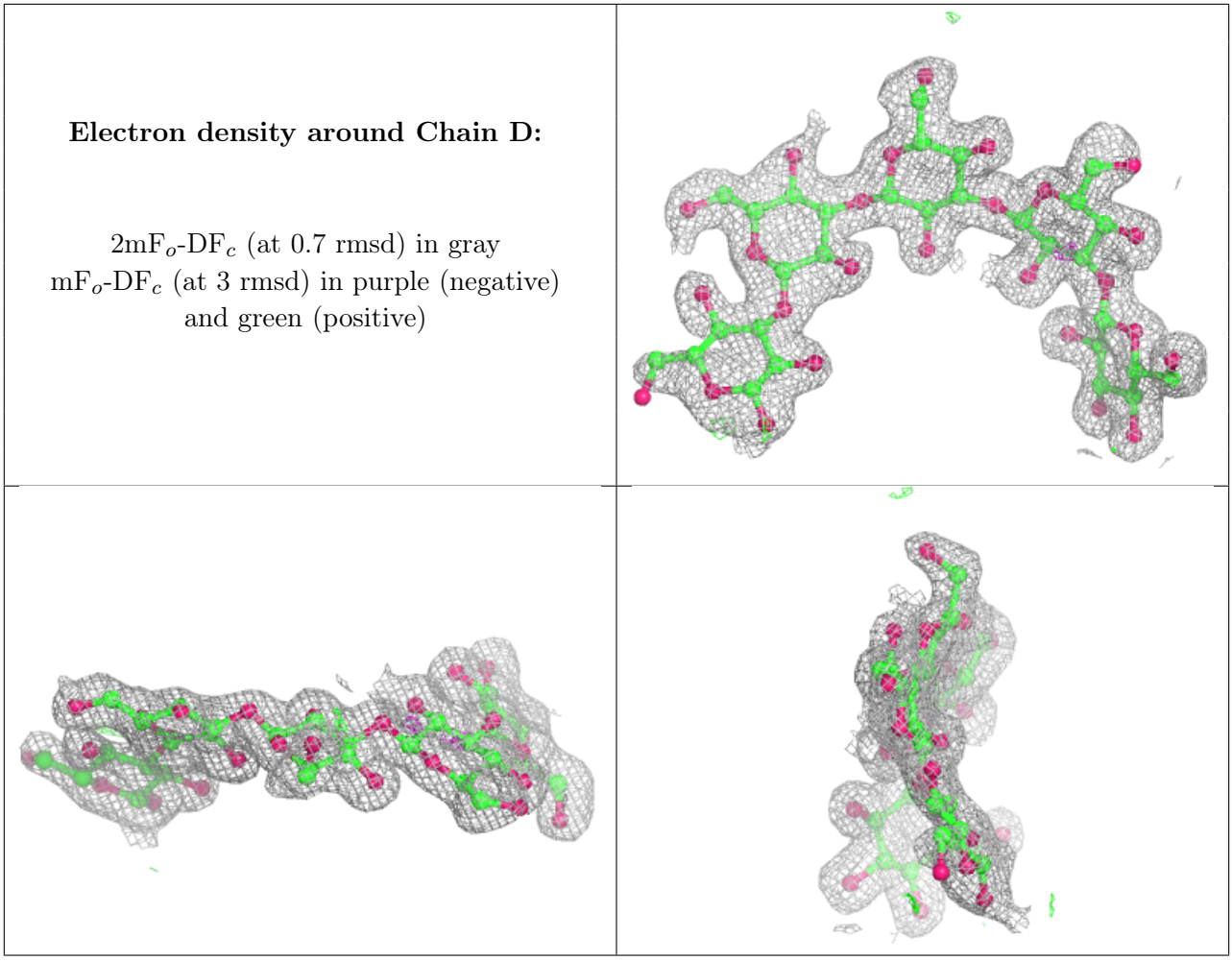






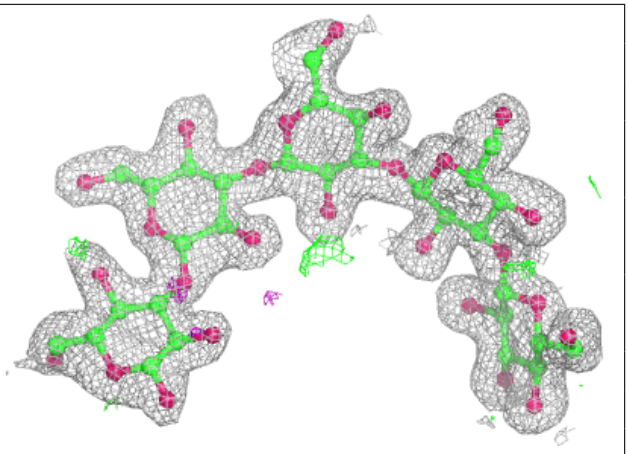
Electron density around Chain D:

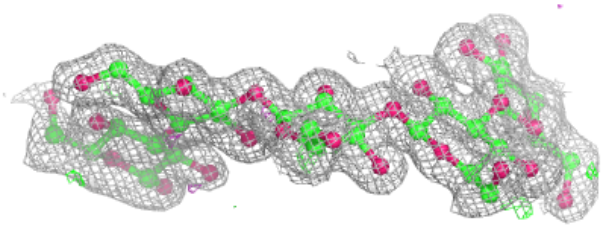
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

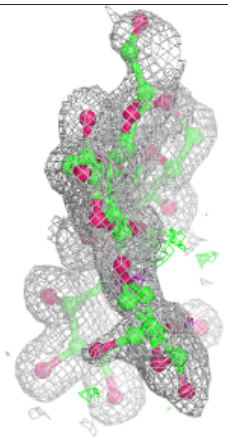


Electron density around Chain F:

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

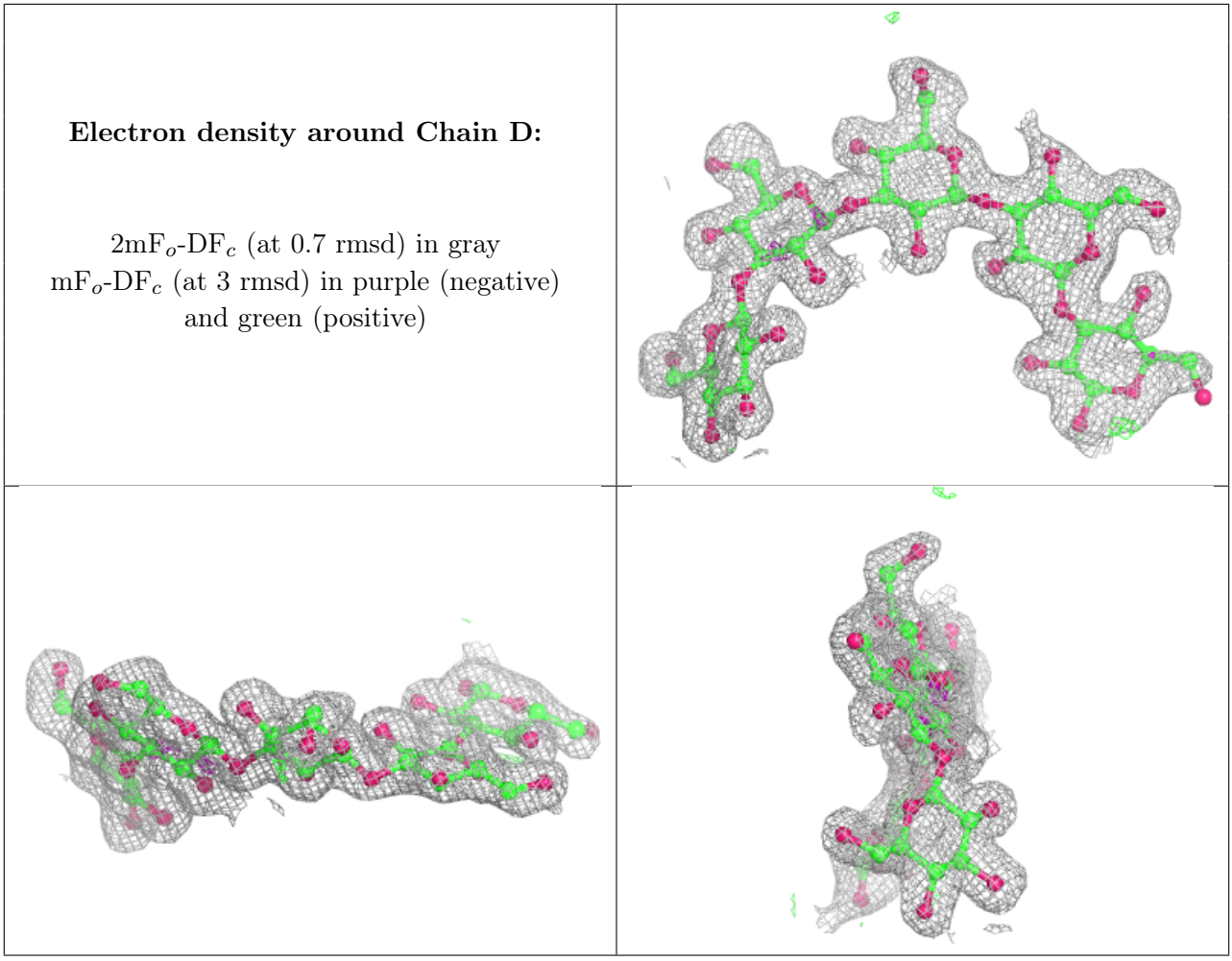






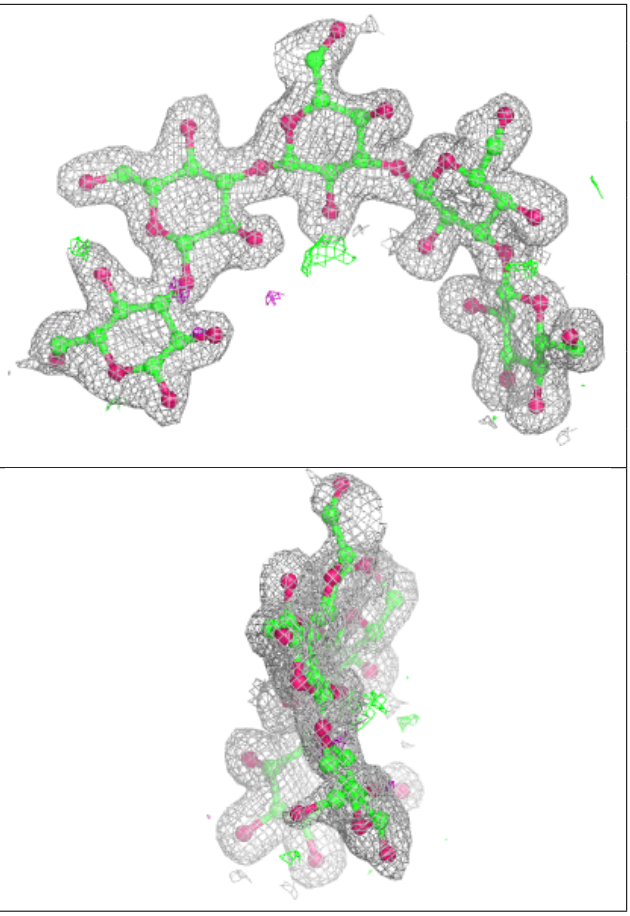
Electron density around Chain D:

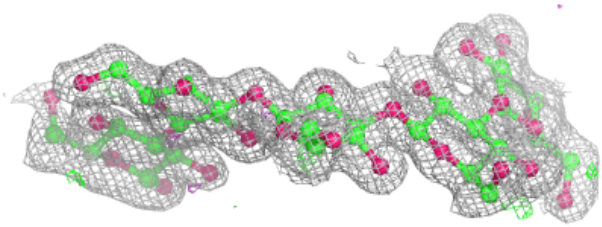
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain F:

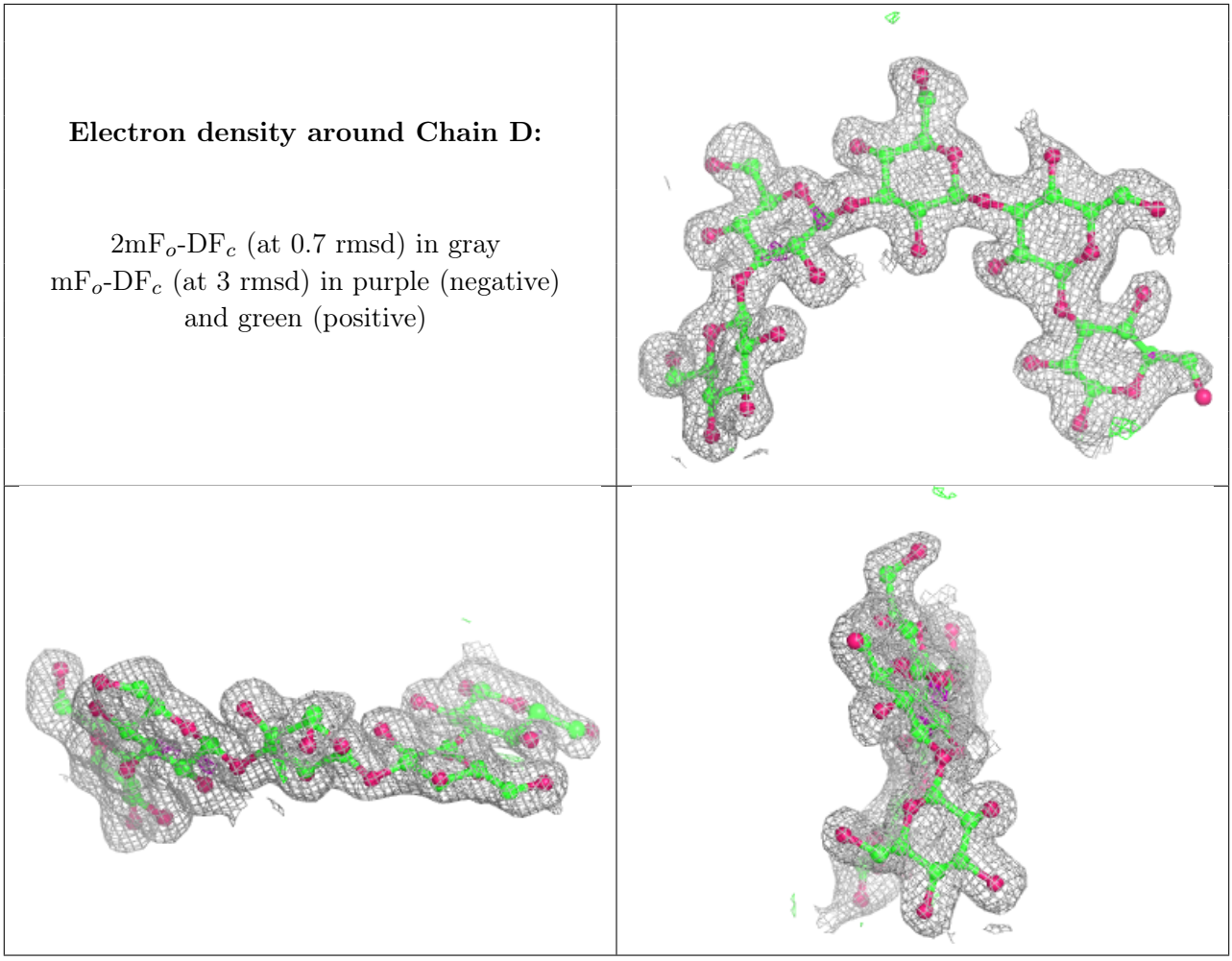
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





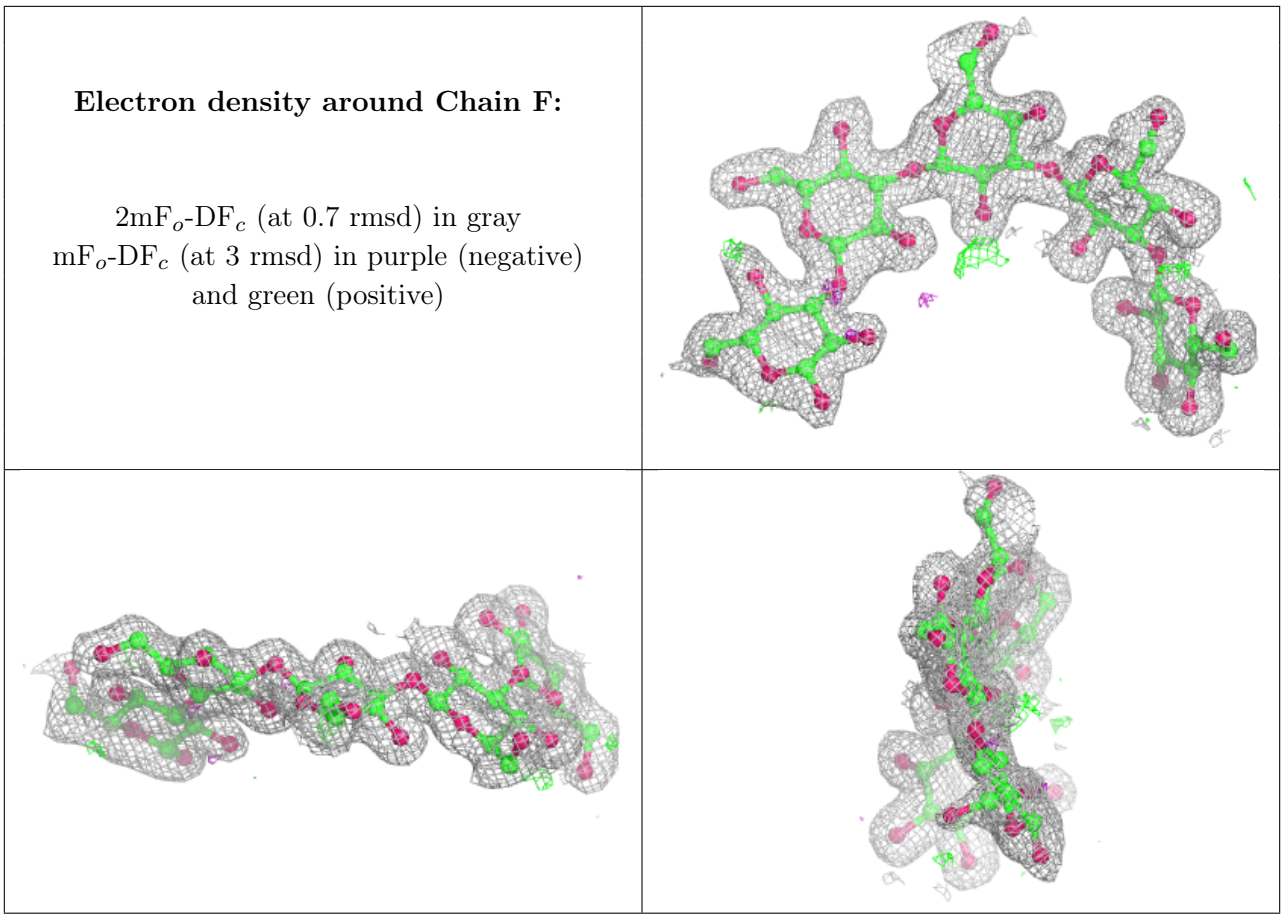
Electron density around Chain D:

$2mF_o$-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)



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	0.93	0.11	13,21,21,22	10
4	EDO	2-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	3-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	4-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	5-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	6-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	7-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	8-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	9-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	10-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	11-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	12-B	701	4/4	0.93	0.11	13,21,21,22	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	13-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	14-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	15-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	16-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	17-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	18-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	19-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	20-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	21-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	22-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	23-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	24-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	25-B	701	4/4	0.93	0.11	13,21,21,22	10
4	EDO	1-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	2-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	3-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	4-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	5-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	6-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	7-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	8-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	9-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	10-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	11-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	12-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	13-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	14-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	15-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	16-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	17-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	18-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	19-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	20-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	21-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	22-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	23-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	24-A	701	4/4	0.98	0.07	13,13,19,19	10
4	EDO	25-A	701	4/4	0.98	0.07	13,13,19,19	10

6.5 Other polymers (i)

There are no such residues in this entry.