Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 10:29 AM EDT

PDB ID	:	9C1V / pdb_00009c1v
Title	:	M. tuberculosis PKS13 acyltransferase (AT) domain in complex with SuFEx inhibitor CMX410
Authors	:	Krieger, I.K.; Tang, S.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2024-05-29
Resolution	:	2.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

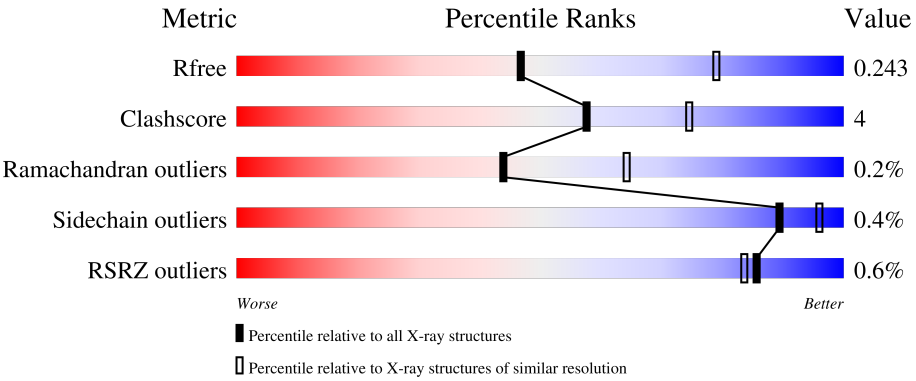
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.57 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}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	A	512	82% 9% 9%
1	B	512	% 81% 10% 9%
2	C	2	50% 50%
2	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	E	2	100%
2	F	2	50% 50%
2	G	2	50% 50%
2	H	2	50% 50%
2	I	2	50% 50%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7621 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Polyketide synthase Pks13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	2	0
			3564	2252	619	680	13			
1	B	468	Total	C	N	O	S	0	1	0
			3565	2252	621	680	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	MET	-	initiating methionine	UNP I6X8D2
A	553	HIS	-	expression tag	UNP I6X8D2
A	554	HIS	-	expression tag	UNP I6X8D2
A	555	HIS	-	expression tag	UNP I6X8D2
A	556	HIS	-	expression tag	UNP I6X8D2
A	557	HIS	-	expression tag	UNP I6X8D2
A	558	HIS	-	expression tag	UNP I6X8D2
A	559	SER	-	expression tag	UNP I6X8D2
A	560	SER	-	expression tag	UNP I6X8D2
A	561	GLY	-	expression tag	UNP I6X8D2
A	562	VAL	-	expression tag	UNP I6X8D2
A	563	ASP	-	expression tag	UNP I6X8D2
A	564	LEU	-	expression tag	UNP I6X8D2
A	565	GLY	-	expression tag	UNP I6X8D2
A	566	THR	-	expression tag	UNP I6X8D2
A	567	GLU	-	expression tag	UNP I6X8D2
A	568	ASN	-	expression tag	UNP I6X8D2
A	569	LEU	-	expression tag	UNP I6X8D2
A	570	TYR	-	expression tag	UNP I6X8D2
A	571	PHE	-	expression tag	UNP I6X8D2
A	572	GLN	-	expression tag	UNP I6X8D2
A	573	SER	-	expression tag	UNP I6X8D2
A	574	ASN	-	expression tag	UNP I6X8D2
A	575	ALA	-	expression tag	UNP I6X8D2
B	552	MET	-	initiating methionine	UNP I6X8D2

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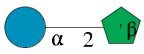
Chain	Residue	Modelled	Actual	Comment	Reference
B	553	HIS	-	expression tag	UNP I6X8D2
B	554	HIS	-	expression tag	UNP I6X8D2
B	555	HIS	-	expression tag	UNP I6X8D2
B	556	HIS	-	expression tag	UNP I6X8D2
B	557	HIS	-	expression tag	UNP I6X8D2
B	558	HIS	-	expression tag	UNP I6X8D2
B	559	SER	-	expression tag	UNP I6X8D2
B	560	SER	-	expression tag	UNP I6X8D2
B	561	GLY	-	expression tag	UNP I6X8D2
B	562	VAL	-	expression tag	UNP I6X8D2
B	563	ASP	-	expression tag	UNP I6X8D2
B	564	LEU	-	expression tag	UNP I6X8D2
B	565	GLY	-	expression tag	UNP I6X8D2
B	566	THR	-	expression tag	UNP I6X8D2
B	567	GLU	-	expression tag	UNP I6X8D2
B	568	ASN	-	expression tag	UNP I6X8D2
B	569	LEU	-	expression tag	UNP I6X8D2
B	570	TYR	-	expression tag	UNP I6X8D2
B	571	PHE	-	expression tag	UNP I6X8D2
B	572	GLN	-	expression tag	UNP I6X8D2
B	573	SER	-	expression tag	UNP I6X8D2
B	574	ASN	-	expression tag	UNP I6X8D2
B	575	ALA	-	expression tag	UNP I6X8D2

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	2	Total C O 23 12 11	0	0	0
2	D	2	Total C O 23 12 11	0	0	0
2	E	2	Total C O 23 12 11	0	0	0
2	F	2	Total C O 23 12 11	0	0	0
2	G	2	Total C O 23 12 11	0	0	0

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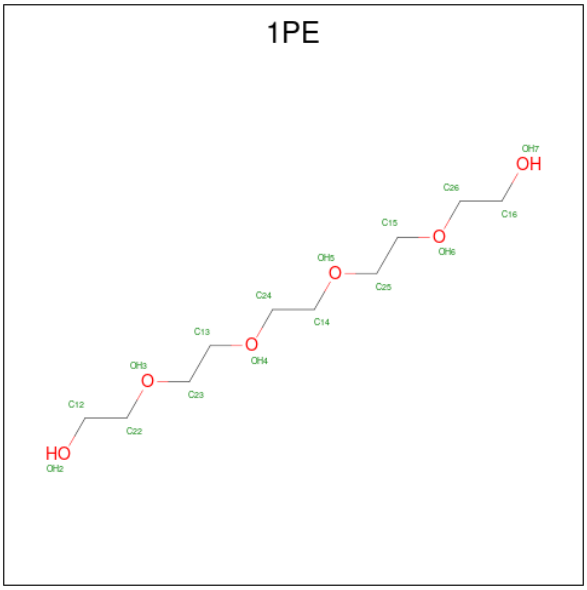
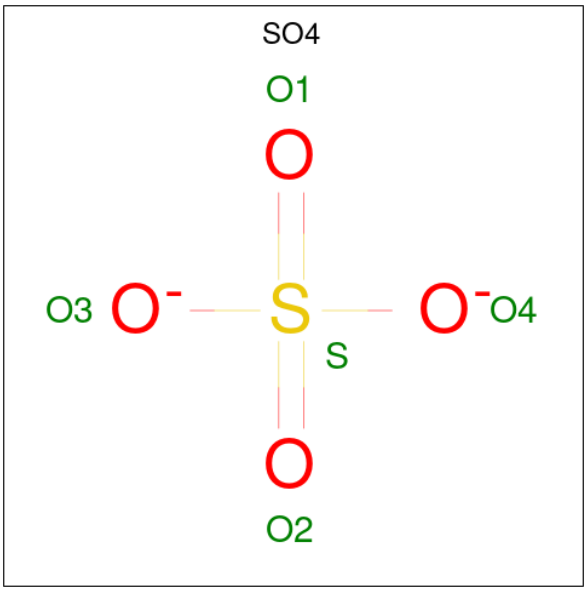
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	2	Total C O 23 12 11	0	0	0
2	I	2	Total C O 23 12 11	0	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



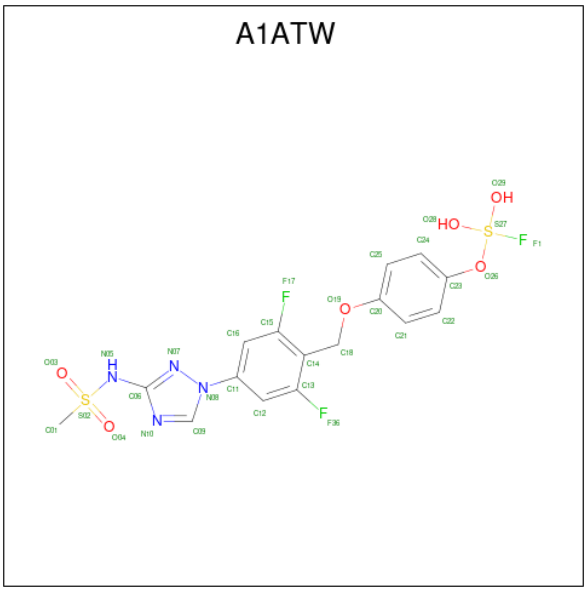
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 13 8 5	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is N-(1-{3,5-difluoro-4-[(4-{[fluorodi(hydroxy)-lambda 4 -sulfanyl]oxy}phenoxy)methyl]phenyl}-1H-1,2,4-triazol-3-yl)methanesulfonamide (CCD ID: A1ATW) (formula: $C_{16}H_{15}F_3N_4O_6S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C F N O S 30 16 2 4 6 2	0	0

- Molecule 6 is water.

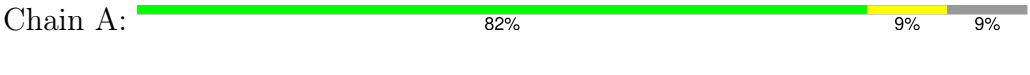
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	132	Total O 132 132	0	0
6	B	96	Total O 96 96	0	0

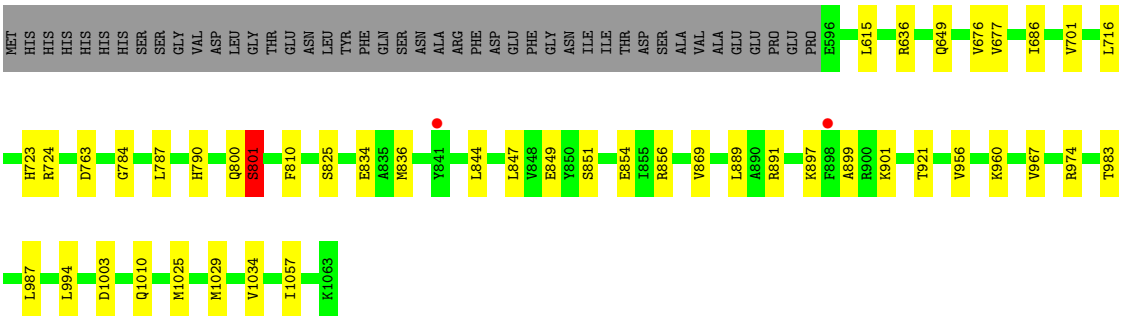
3 Residue-property plots (i)

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: Polyketide synthase Pks13

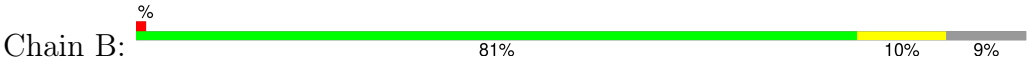
Chain A:

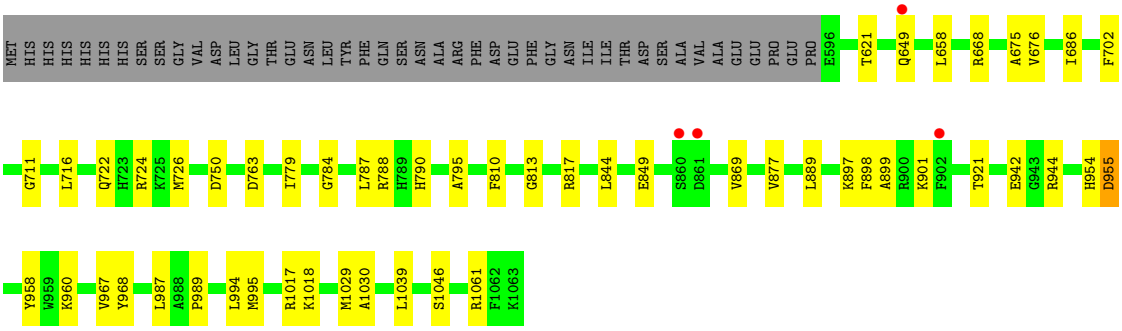




• Molecule 1: Polyketide synthase Pks13

Chain B:





• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

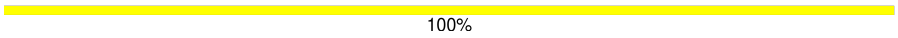
Chain C:

• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain D:

• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E:



• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain F:

• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain G:

• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain H:

• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.53Å 106.53Å 259.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.57 49.26 – 2.57	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.26-2.57) 99.9 (49.26-2.57)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.194 , 0.238 0.202 , 0.243	Depositor DCC
R_{free} test set	2398 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7621	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1ATW, 1PE, SO4, FRU, GLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.42	2/3644 (0.1%)	0.90	4/4947 (0.1%)
1	B	0.38	0/3642	0.56	0/4944
All	All	0.40	2/7286 (0.0%)	0.75	4/9891 (0.0%)

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	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	801	SER	C-N	7.76	1.43	1.33
1	A	800	GLN	C-N	7.00	1.43	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	801	SER	O-C-N	-32.53	79.33	122.59
1	A	801	SER	CA-C-N	26.93	164.01	121.19
1	A	801	SER	C-N-CA	26.93	164.01	121.19
1	A	1057	ILE	N-CA-C	-5.55	102.74	109.01

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	801	SER	Peptide,Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3564	0	3536	27	0
1	B	3565	0	3540	38	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
2	E	23	0	21	0	0
2	F	23	0	21	1	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
2	I	23	0	21	0	0
3	A	33	0	43	0	0
4	A	25	0	0	0	0
4	B	15	0	0	1	0
5	A	30	0	0	0	0
6	A	132	0	0	3	0
6	B	96	0	0	4	0
All	All	7621	0	7266	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:LEU:HD23	1:B:1029:MET:HE3	1.55	0.86
1:A:889:LEU:HD22	1:A:899:ALA:HB1	1.62	0.80
1:A:787:LEU:HD23	1:A:1029:MET:HE3	1.63	0.79
1:B:722:GLN:HA	1:B:726:MET:HE1	1.68	0.74
1:A:649:GLN:HG3	1:A:686:ILE:HD13	1.72	0.71
1:B:722:GLN:HA	1:B:726:MET:CE	2.25	0.66
1:B:898:PHE:HE2	1:B:995:MET:HE1	1.61	0.66
1:B:750:ASP:OD2	1:B:817:ARG:NH2	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:MET:HE2	1:B:989:PRO:HG3	1.79	0.62
1:A:844:LEU:HD13	1:A:901:LYS:HD3	1.83	0.61
1:A:724:ARG:HD2	1:A:763:ASP:O	2.01	0.60
1:A:891:ARG:NH1	6:A:1202:HOH:O	2.26	0.58
1:A:849:GLU:HB3	1:A:897:LYS:HB3	1.86	0.57
1:B:790:HIS:CD2	1:B:1029:MET:HE1	2.40	0.56
1:A:834:GLU:OE1	6:A:1201:HOH:O	2.18	0.56
1:B:649:GLN:HG3	1:B:686:ILE:HD13	1.88	0.55
1:B:921:THR:OG1	1:B:960:LYS:HD2	2.06	0.55
1:B:1017:ARG:O	1:B:1018:LYS:HG2	2.06	0.54
1:A:677:VAL:HG22	1:A:701:VAL:HG22	1.90	0.53
1:A:974:ARG:NH2	1:A:1003:ASP:OD2	2.39	0.53
1:B:716:LEU:HD11	1:B:987:LEU:HD12	1.90	0.53
1:A:921:THR:OG1	1:A:960:LYS:HD2	2.09	0.52
1:B:788:ARG:NH2	6:B:1202:HOH:O	2.40	0.52
1:B:724:ARG:HD3	1:B:763:ASP:O	2.10	0.51
1:B:1029:MET:HB3	1:B:1039:LEU:HD11	1.93	0.50
1:B:1046:SER:HB3	2:F:1:GLC:H61	1.93	0.49
1:A:856:ARG:HH11	1:A:856:ARG:HG2	1.77	0.49
1:A:956:VAL:O	1:A:960:LYS:HG3	2.13	0.48
1:A:1025:MET:O	1:A:1029:MET:HG3	2.14	0.48
1:B:1061:ARG:HG3	6:B:1230:HOH:O	2.13	0.47
1:B:621:THR:HG22	6:B:1285:HOH:O	2.15	0.46
1:B:898:PHE:CE2	1:B:995:MET:HE1	2.46	0.46
1:B:955:ASP:CB	1:B:958:TYR:H	2.28	0.46
1:A:723:HIS:HD2	6:A:1206:HOH:O	1.99	0.46
1:A:869:VAL:HG22	1:A:967:VAL:HB	1.98	0.46
1:A:847:LEU:O	1:A:899:ALA:HA	2.16	0.46
1:A:983:THR:HA	1:A:1010:GLN:HB2	1.98	0.45
1:A:851:SER:OG	1:A:854:GLU:HG3	2.15	0.45
1:B:711:GLY:HA3	1:B:795:ALA:HB2	1.98	0.45
1:A:790:HIS:HB2	1:A:1029:MET:CE	2.47	0.45
1:B:942:GLU:HA	1:B:968:TYR:CD2	2.52	0.44
1:A:994:LEU:HD23	1:A:994:LEU:HA	1.68	0.44
1:B:668:ARG:HA	4:B:1101:SO4:O4	2.18	0.44
1:A:790:HIS:HB2	1:A:1029:MET:HE1	2.00	0.44
1:B:849:GLU:HB3	1:B:897:LYS:HB3	1.99	0.44
1:B:944:ARG:HD2	6:B:1284:HOH:O	2.17	0.44
1:B:726:MET:HG3	1:B:779:ILE:CD1	2.48	0.43
1:A:615:LEU:HD12	1:A:615:LEU:HA	1.81	0.43
1:B:869:VAL:HG22	1:B:967:VAL:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:869:VAL:HB	1:B:877:VAL:HB	2.00	0.43
1:B:726:MET:CE	1:B:989:PRO:HG3	2.48	0.42
1:A:676:VAL:HG23	1:A:1034:VAL:HG22	2.02	0.42
1:B:658:LEU:HD23	1:B:658:LEU:HA	1.82	0.42
1:B:898:PHE:CD1	1:B:899:ALA:N	2.87	0.42
1:B:994:LEU:HD12	1:B:994:LEU:HA	1.90	0.41
1:A:790:HIS:CG	1:A:1029:MET:HE1	2.56	0.41
1:B:675:ALA:HA	1:B:702:PHE:O	2.20	0.41
1:A:784:GLY:HA3	1:A:810:PHE:CZ	2.55	0.41
1:B:726:MET:HG3	1:B:779:ILE:HD11	2.03	0.41
1:B:784:GLY:HA3	1:B:810:PHE:CZ	2.57	0.40
1:A:716:LEU:HD11	1:A:987:LEU:HD12	2.04	0.40
1:B:844:LEU:HD13	1:B:901:LYS:HD2	2.03	0.40
1:B:676:VAL:HG11	1:B:1030:ALA:HB1	2.03	0.40
1:B:813:GLY:HA3	1:B:954:HIS:ND1	2.36	0.40
1:B:889:LEU:HD21	1:B:901:LYS:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	468/512 (91%)	460 (98%)	7 (2%)	1 (0%)	44	64
1	B	467/512 (91%)	454 (97%)	12 (3%)	1 (0%)	44	64
All	All	935/1024 (91%)	914 (98%)	19 (2%)	2 (0%)	44	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	801	SER
1	B	955	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	369/406 (91%)	365 (99%)	4 (1%)	70 86
1	B	369/406 (91%)	369 (100%)	0	100 100
All	All	738/812 (91%)	734 (100%)	4 (0%)	89 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	636	ARG
1	A	825	SER
1	A	836[A]	MET
1	A	836[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	669	ASN
1	A	780	GLN
1	A	800	GLN
1	A	965	HIS
1	A	971	HIS
1	A	975	ASN
1	B	680	HIS
1	B	723	HIS
1	B	925	GLN
1	B	1019	GLN

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)

14 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	GLC	C	1	2	11,11,12	0.58	0	15,15,17	0.94	2 (13%)
2	FRU	C	2	2	11,12,12	0.39	0	10,18,18	0.65	0
2	GLC	D	1	2	11,11,12	0.52	0	15,15,17	1.15	2 (13%)
2	FRU	D	2	2	11,12,12	0.48	0	10,18,18	0.61	0
2	GLC	E	1	2	11,11,12	1.29	2 (18%)	15,15,17	0.98	1 (6%)
2	FRU	E	2	2	11,12,12	0.56	0	10,18,18	1.10	1 (10%)
2	GLC	F	1	2	11,11,12	0.57	0	15,15,17	0.67	0
2	FRU	F	2	2	11,12,12	0.45	0	10,18,18	0.92	0
2	GLC	G	1	2	11,11,12	0.71	0	15,15,17	0.78	1 (6%)
2	FRU	G	2	2	11,12,12	0.44	0	10,18,18	0.45	0
2	GLC	H	1	2	11,11,12	0.64	0	15,15,17	0.96	1 (6%)
2	FRU	H	2	2	11,12,12	0.39	0	10,18,18	0.61	0
2	GLC	I	1	2	11,11,12	0.63	0	15,15,17	1.09	2 (13%)
2	FRU	I	2	2	11,12,12	0.47	0	10,18,18	0.74	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	GLC	C	1	2	-	0/2/19/22	0/1/1/1
2	FRU	C	2	2	-	2/5/24/24	0/1/1/1
2	GLC	D	1	2	-	0/2/19/22	0/1/1/1
2	FRU	D	2	2	-	0/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	1	2	-	1/2/19/22	0/1/1/1
2	FRU	E	2	2	-	0/5/24/24	0/1/1/1
2	GLC	F	1	2	-	2/2/19/22	0/1/1/1
2	FRU	F	2	2	-	0/5/24/24	0/1/1/1
2	GLC	G	1	2	-	0/2/19/22	0/1/1/1
2	FRU	G	2	2	-	0/5/24/24	0/1/1/1
2	GLC	H	1	2	-	0/2/19/22	0/1/1/1
2	FRU	H	2	2	-	0/5/24/24	0/1/1/1
2	GLC	I	1	2	-	1/2/19/22	0/1/1/1
2	FRU	I	2	2	-	0/5/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	GLC	O5-C5	2.87	1.49	1.43
2	E	1	GLC	C2-C3	2.56	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1	GLC	C1-O5-C5	3.08	116.32	112.19
2	D	1	GLC	C1-O5-C5	3.06	116.28	112.19
2	H	1	GLC	C1-O5-C5	2.70	115.81	112.19
2	E	1	GLC	C1-O5-C5	2.43	115.45	112.19
2	E	2	FRU	O1-C1-C2	2.35	116.86	111.67
2	G	1	GLC	C1-O5-C5	2.28	115.24	112.19
2	I	1	GLC	C1-C2-C3	2.17	112.81	109.64
2	C	1	GLC	C1-O5-C5	2.06	114.95	112.19
2	D	1	GLC	C1-C2-C3	2.04	112.62	109.64
2	C	1	GLC	O3-C3-C2	-2.02	105.94	110.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	FRU	C4-C5-C6-O6
2	C	2	FRU	O5-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6

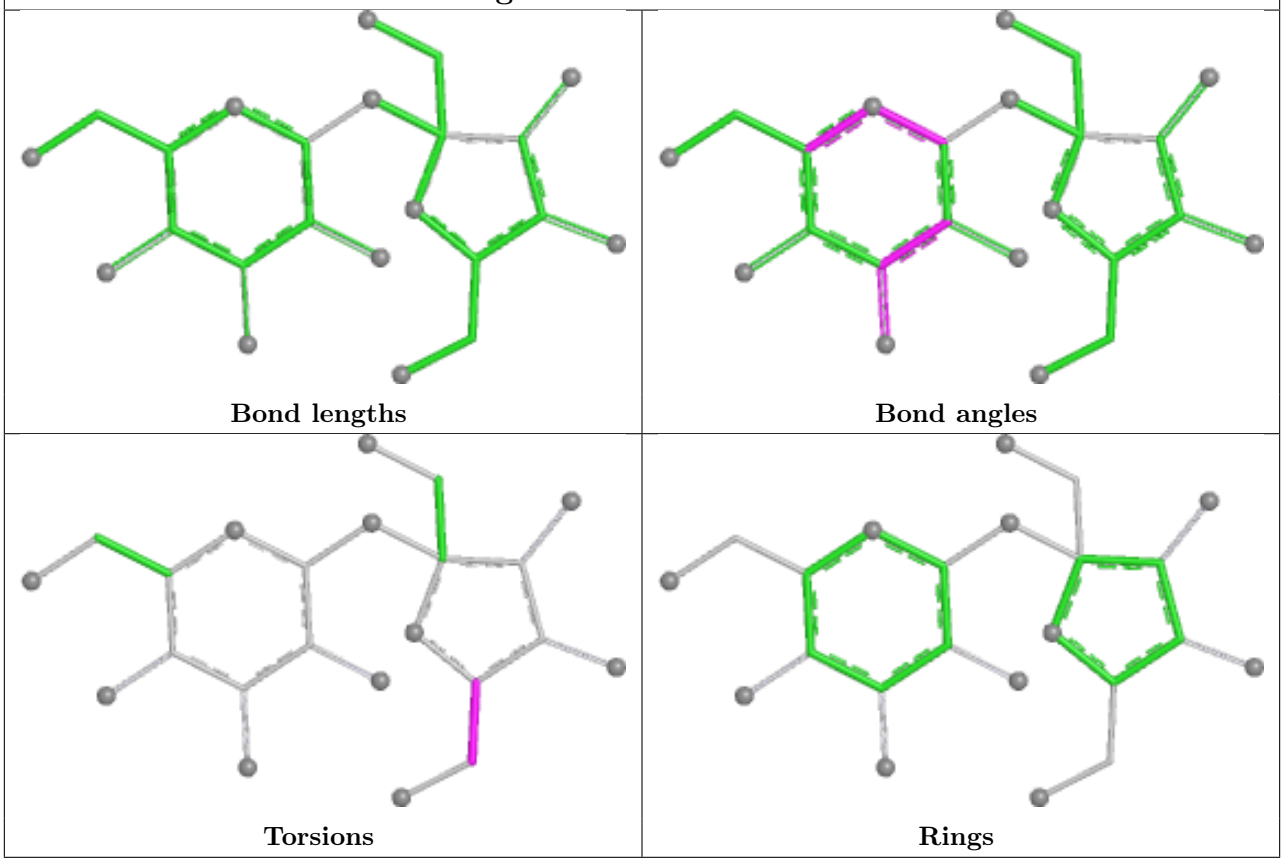
There are no ring outliers.

1 monomer is involved in 1 short contact:

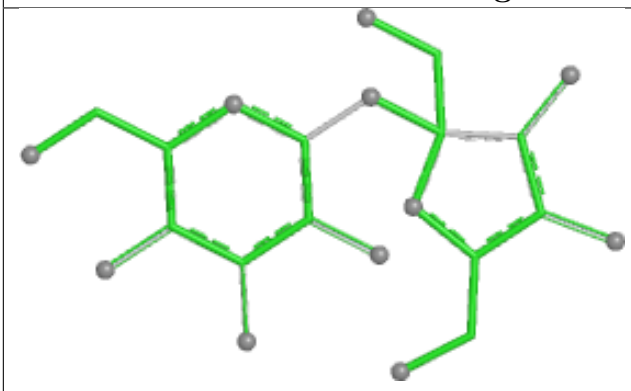
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	GLC	1	0

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

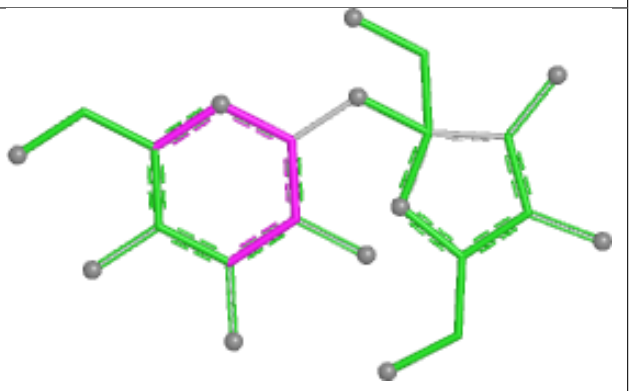
Oligosaccharide Chain C



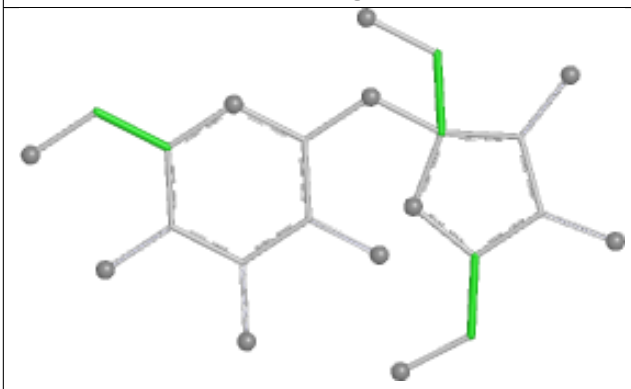
Oligosaccharide Chain D



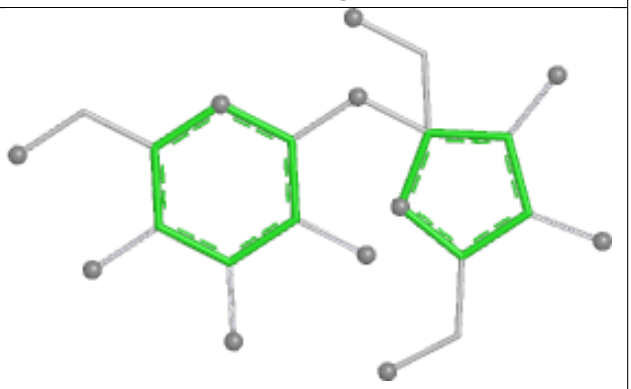
Bond lengths



Bond angles

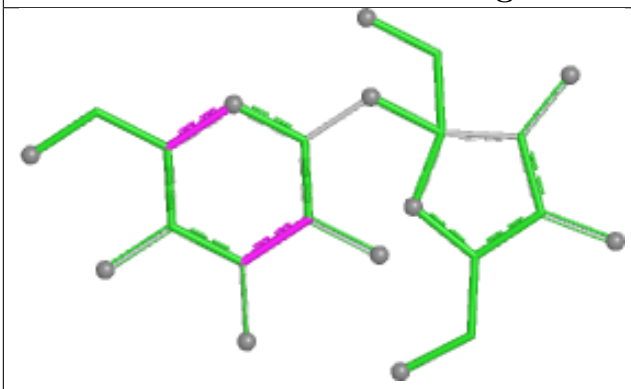


Torsions

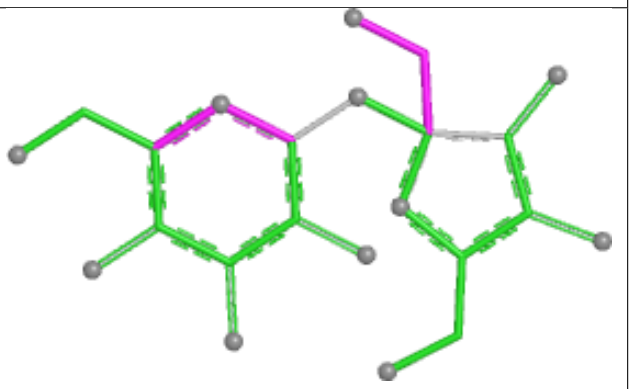


Rings

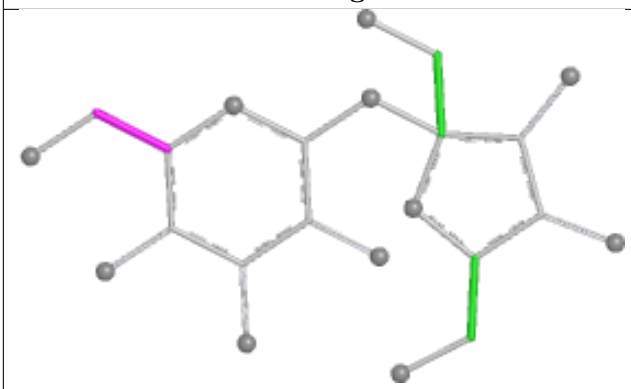
Oligosaccharide Chain E



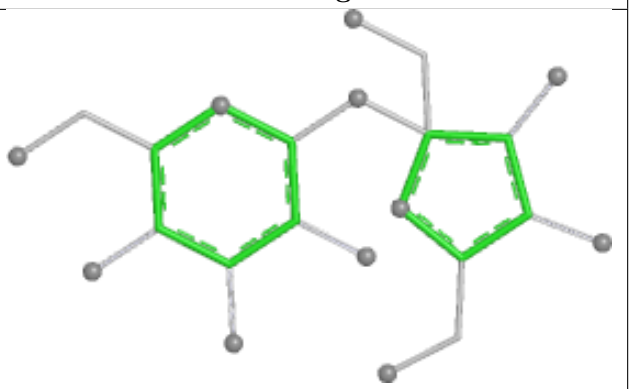
Bond lengths



Bond angles

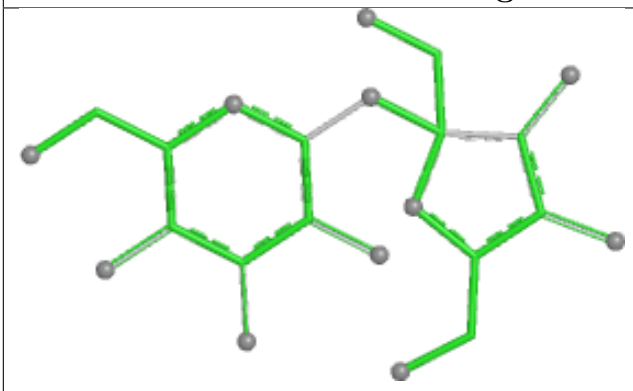


Torsions

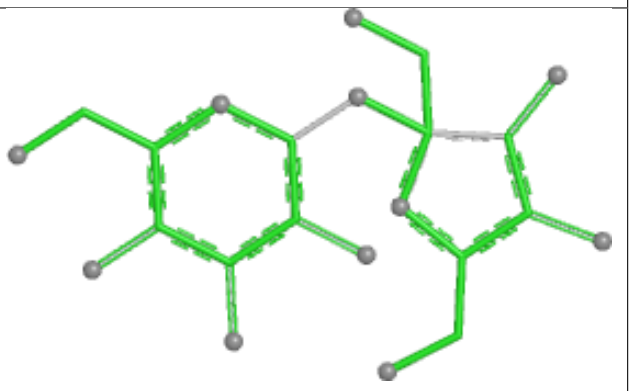


Rings

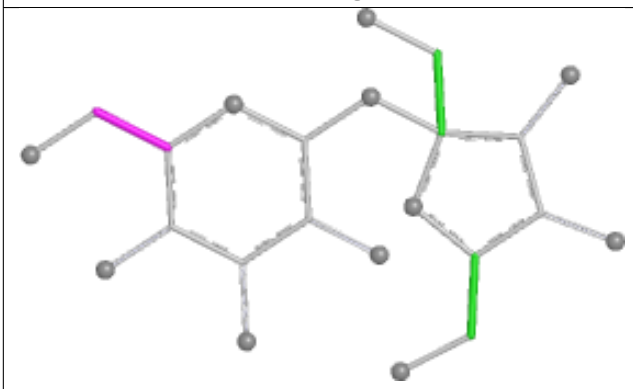
Oligosaccharide Chain F



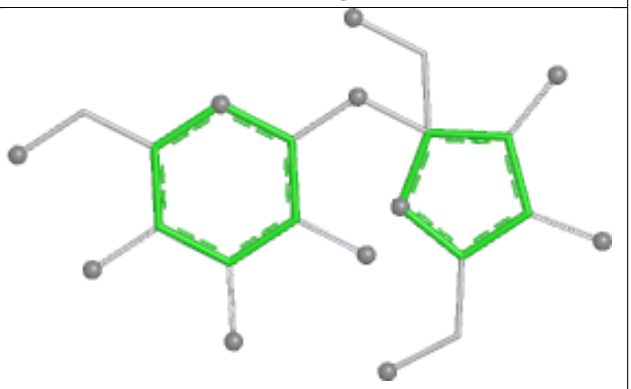
Bond lengths



Bond angles

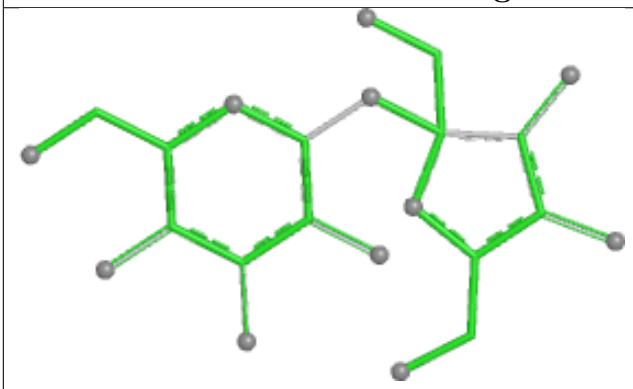


Torsions

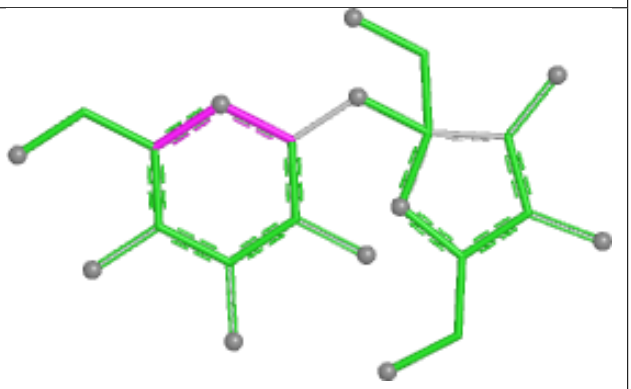


Rings

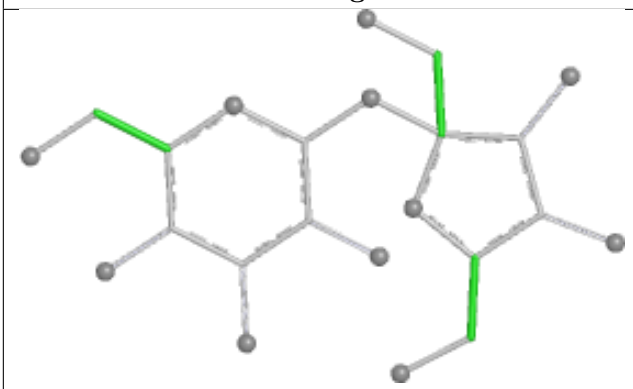
Oligosaccharide Chain G



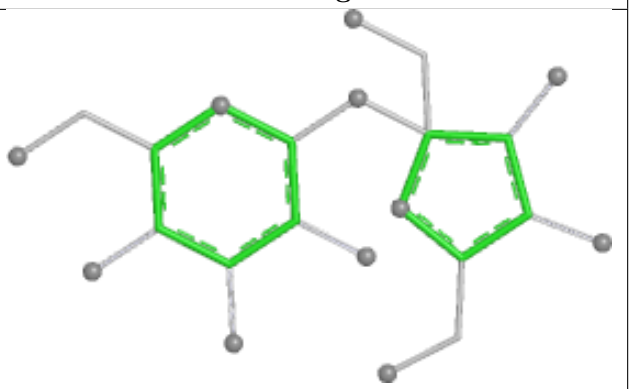
Bond lengths



Bond angles

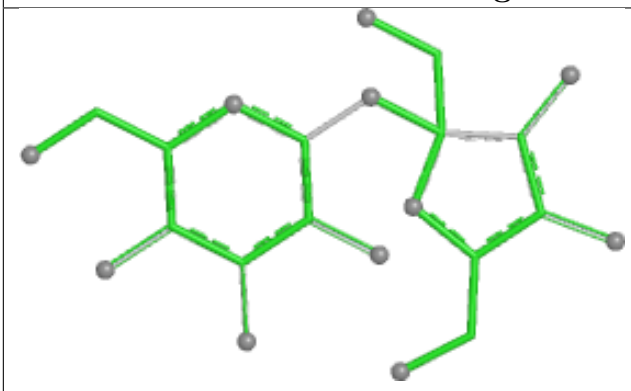


Torsions

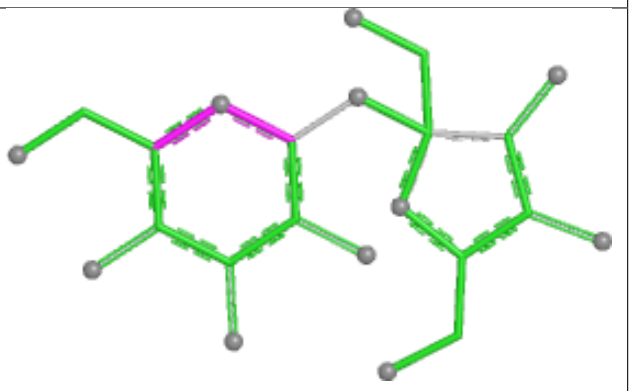


Rings

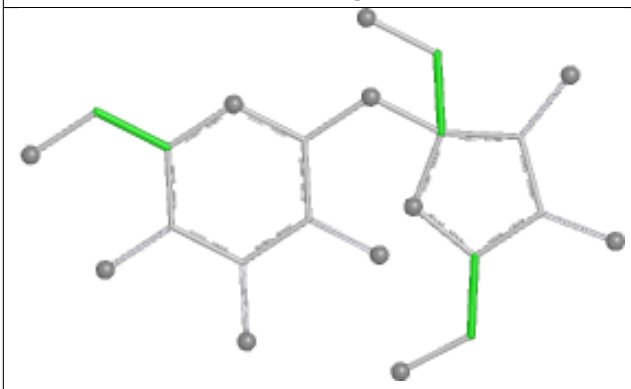
Oligosaccharide Chain H



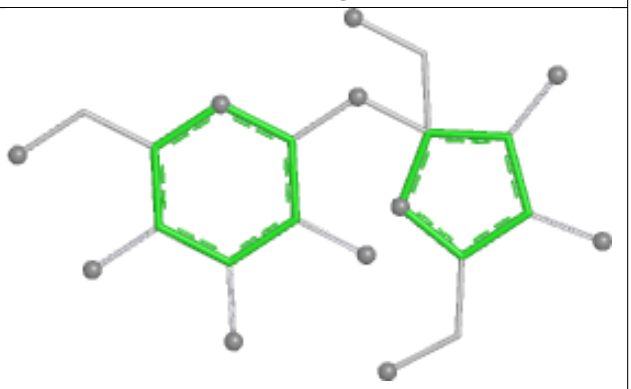
Bond lengths



Bond angles

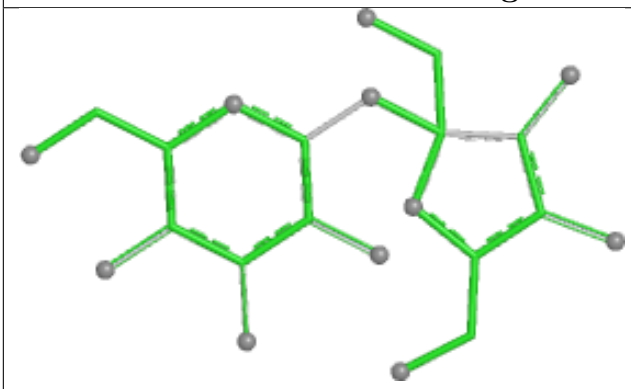


Torsions

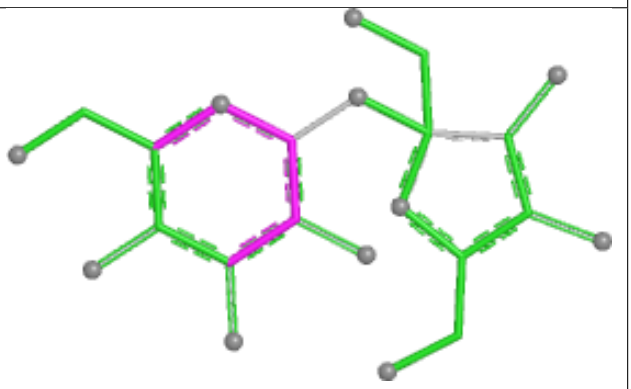


Rings

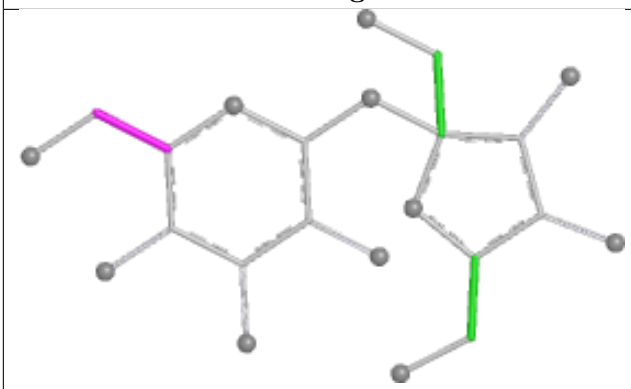
Oligosaccharide Chain I



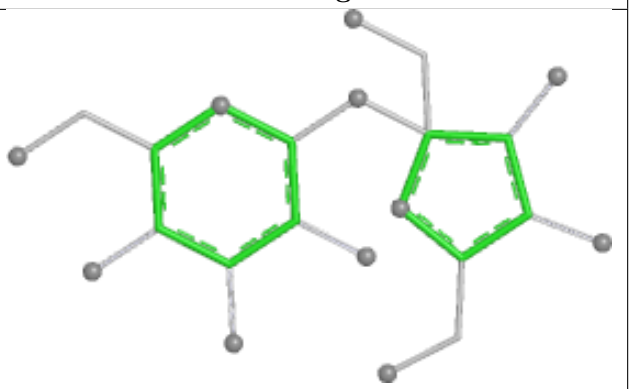
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
3	1PE	A	1101	-	12,12,15	0.24	0	11,11,14	0.22	0
3	1PE	A	1103	-	12,12,15	0.28	0	11,11,14	0.24	0
4	SO4	B	1101	-	4,4,4	0.26	0	6,6,6	0.13	0
4	SO4	A	1106	-	4,4,4	0.26	0	6,6,6	0.19	0
4	SO4	A	1107	-	4,4,4	0.22	0	6,6,6	0.21	0
4	SO4	A	1105	-	4,4,4	0.28	0	6,6,6	0.38	0
4	SO4	A	1108	-	4,4,4	0.42	0	6,6,6	0.33	0
4	SO4	B	1103	-	4,4,4	0.44	0	6,6,6	0.34	0
4	SO4	B	1102	-	4,4,4	0.24	0	6,6,6	0.09	0
3	1PE	A	1102	-	6,6,15	0.11	0	5,5,14	0.19	0
5	A1ATW	A	1109	1	26,32,33	2.44	7 (26%)	33,46,49	3.37	13 (39%)
4	SO4	A	1104	-	4,4,4	0.28	0	6,6,6	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	1102	-	-	3/4/4/13	-
3	1PE	A	1103	-	-	4/10/10/13	-
5	A1ATW	A	1109	1	-	5/14/18/19	0/3/3/3
3	1PE	A	1101	-	-	5/10/10/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1109	A1ATW	C06-N05	7.63	1.47	1.39
5	A	1109	A1ATW	S02-N05	7.04	1.72	1.63
5	A	1109	A1ATW	C01-S02	3.24	1.82	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1109	A1ATW	O04-S02	2.71	1.48	1.43
5	A	1109	A1ATW	N07-N08	-2.38	1.34	1.39
5	A	1109	A1ATW	O19-C20	2.21	1.42	1.37
5	A	1109	A1ATW	O03-S02	2.15	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1109	A1ATW	O04-S02-O03	-14.53	99.40	118.87
5	A	1109	A1ATW	C16-C15-C14	-5.55	120.33	124.45
5	A	1109	A1ATW	C12-C13-C14	-5.26	120.54	124.45
5	A	1109	A1ATW	O04-S02-C01	4.53	115.42	108.26
5	A	1109	A1ATW	C15-C14-C13	3.29	118.98	114.54
5	A	1109	A1ATW	O04-S02-N05	3.03	113.15	107.10
5	A	1109	A1ATW	C18-C14-C13	-2.86	120.39	122.51
5	A	1109	A1ATW	F36-C13-C14	2.62	120.91	117.64
5	A	1109	A1ATW	C18-C14-C15	-2.52	120.64	122.51
5	A	1109	A1ATW	C16-C11-C12	-2.51	118.64	121.68
5	A	1109	A1ATW	O26-C23-C22	2.44	123.50	118.70
5	A	1109	A1ATW	F17-C15-C14	2.39	120.62	117.64
5	A	1109	A1ATW	O03-S02-N05	2.04	111.16	107.10

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1103	1PE	C25-C15-OH6-C26
3	A	1103	1PE	OH6-C15-C25-OH5
3	A	1102	1PE	OH4-C13-C23-OH3
3	A	1101	1PE	OH6-C15-C25-OH5
5	A	1109	A1ATW	C25-C20-O19-C18
5	A	1109	A1ATW	C21-C20-O19-C18
3	A	1102	1PE	OH2-C12-C22-OH3
3	A	1101	1PE	OH7-C16-C26-OH6
3	A	1101	1PE	OH4-C13-C23-OH3
5	A	1109	A1ATW	C06-N05-S02-O03
3	A	1101	1PE	OH5-C14-C24-OH4
3	A	1102	1PE	C13-C23-OH3-C22
3	A	1103	1PE	C14-C24-OH4-C13
5	A	1109	A1ATW	C12-C11-N08-N07
3	A	1103	1PE	C16-C26-OH6-C15
3	A	1101	1PE	C16-C26-OH6-C15

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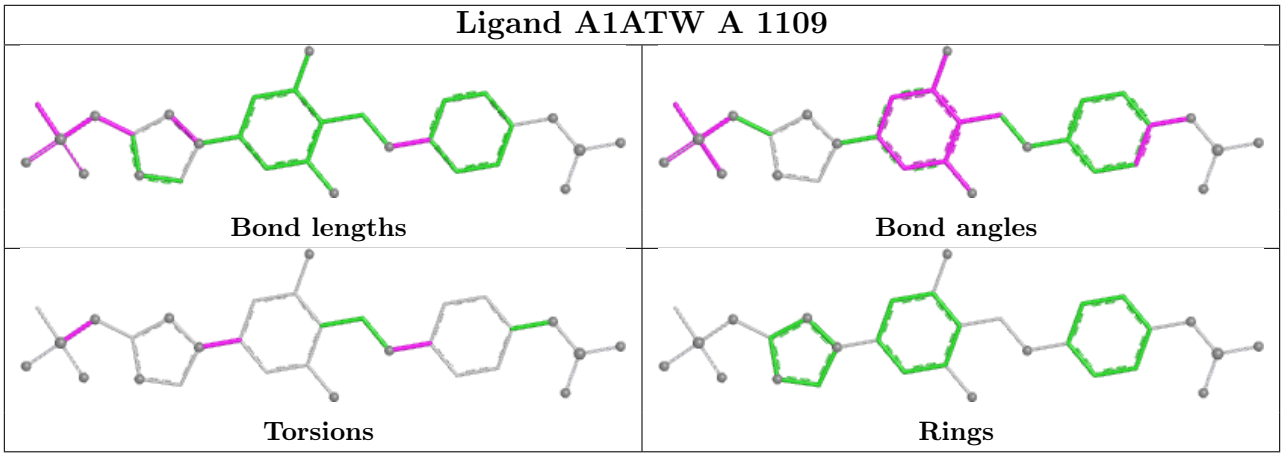
Mol	Chain	Res	Type	Atoms
5	A	1109	A1ATW	C06-N05-S02-C01

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1101	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	A	468/512 (91%)	-0.33	2 (0%)	89	87	40, 50, 66, 89	2 (0%)
1	B	468/512 (91%)	-0.18	4 (0%)	81	78	29, 51, 71, 91	1 (0%)
All	All	936/1024 (91%)	-0.26	6 (0%)	85	83	29, 51, 69, 91	3 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	902	PHE	2.9
1	A	898	PHE	2.4
1	B	861	ASP	2.2
1	A	841	TYR	2.1
1	B	649	GLN	2.1
1	B	860	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	FRU	G	2	12/12	0.55	0.19	42,60,72,81	0
2	FRU	H	2	12/12	0.64	0.18	41,59,71,75	0
2	GLC	G	1	11/12	0.66	0.17	34,47,55,57	0

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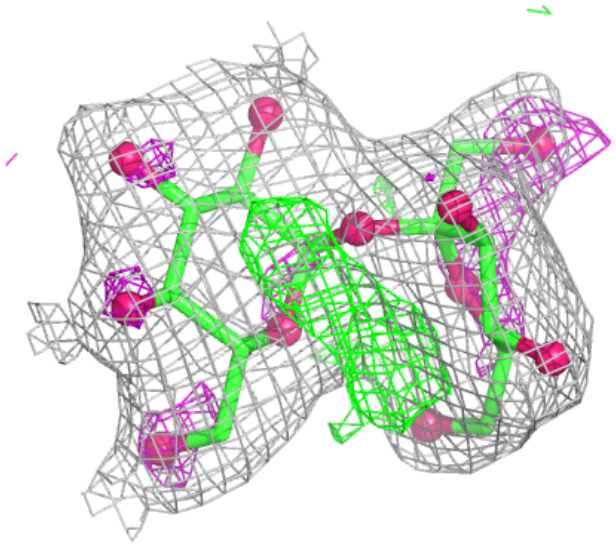
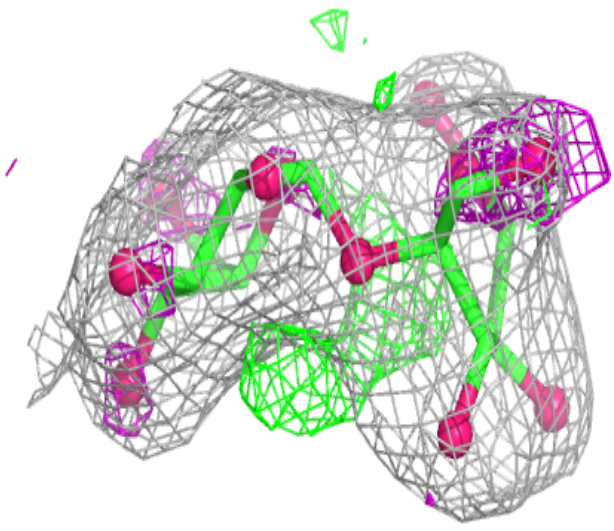
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRU	E	2	12/12	0.70	0.17	26,46,58,64	0
2	GLC	E	1	11/12	0.74	0.14	24,38,45,45	0
2	GLC	H	1	11/12	0.77	0.15	31,42,51,56	0
2	GLC	F	1	11/12	0.79	0.12	39,42,48,49	0
2	GLC	D	1	11/12	0.84	0.12	27,34,45,61	0
2	FRU	C	2	12/12	0.87	0.13	31,40,54,60	0
2	FRU	F	2	12/12	0.89	0.11	28,41,48,54	0
2	FRU	I	2	12/12	0.89	0.11	19,22,24,26	0
2	FRU	D	2	12/12	0.90	0.08	26,30,32,33	0
2	GLC	I	1	11/12	0.91	0.10	21,25,35,48	0
2	GLC	C	1	11/12	0.93	0.08	25,29,30,31	0

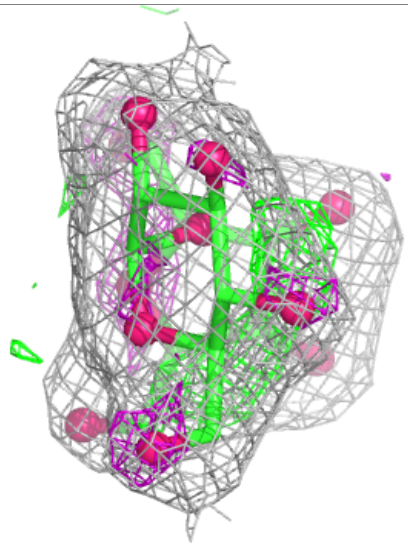
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

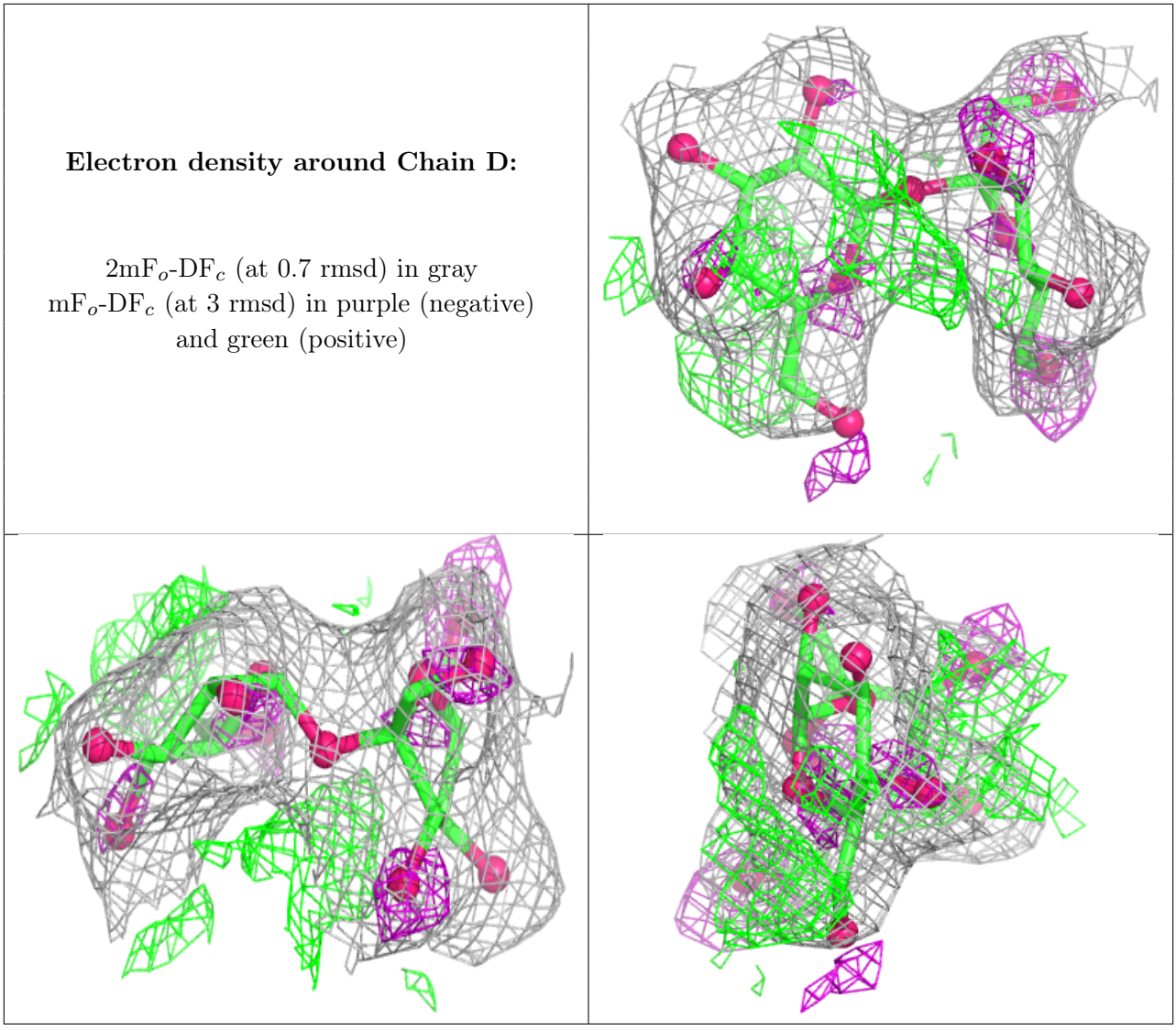






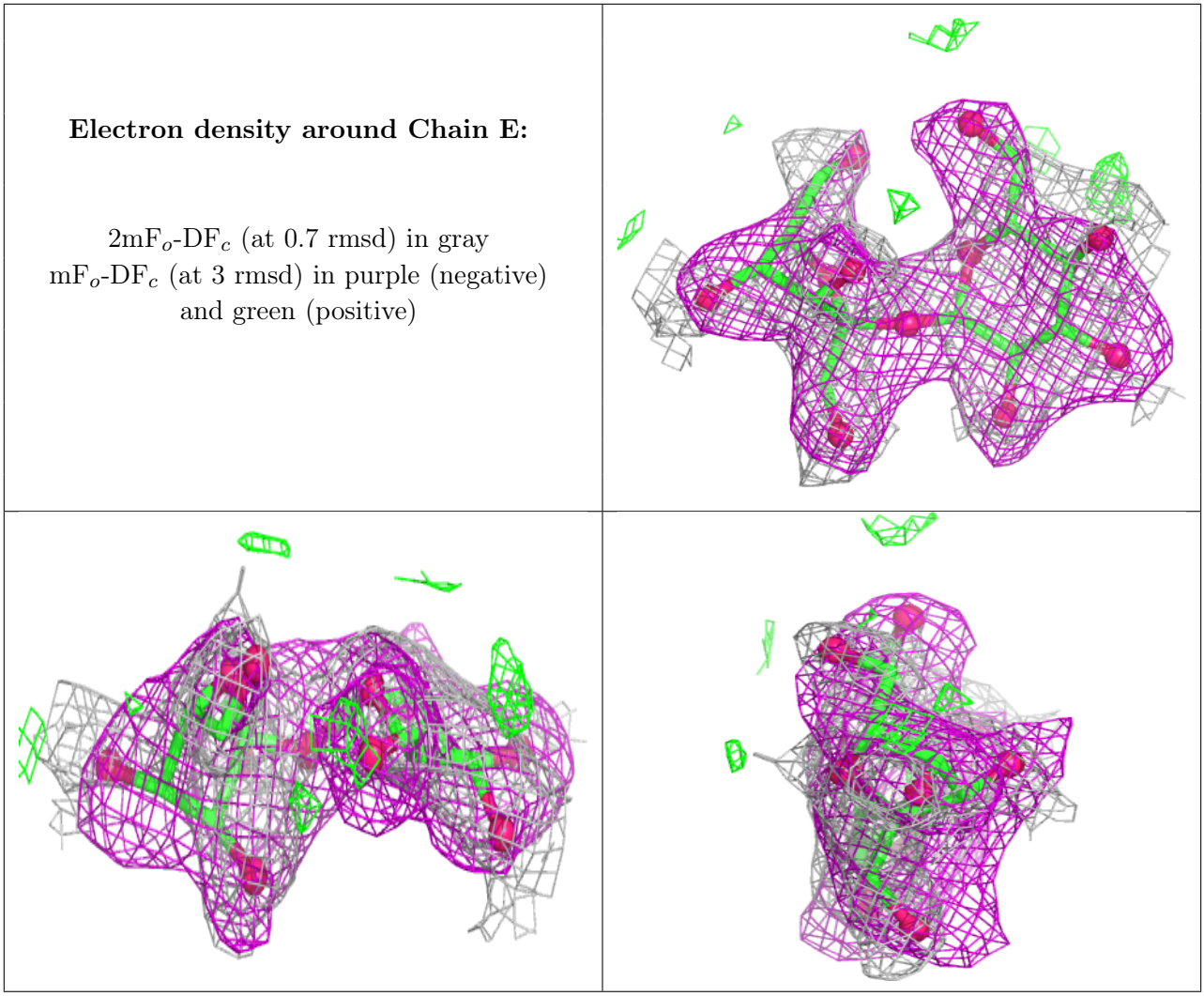
Electron density around Chain D:

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



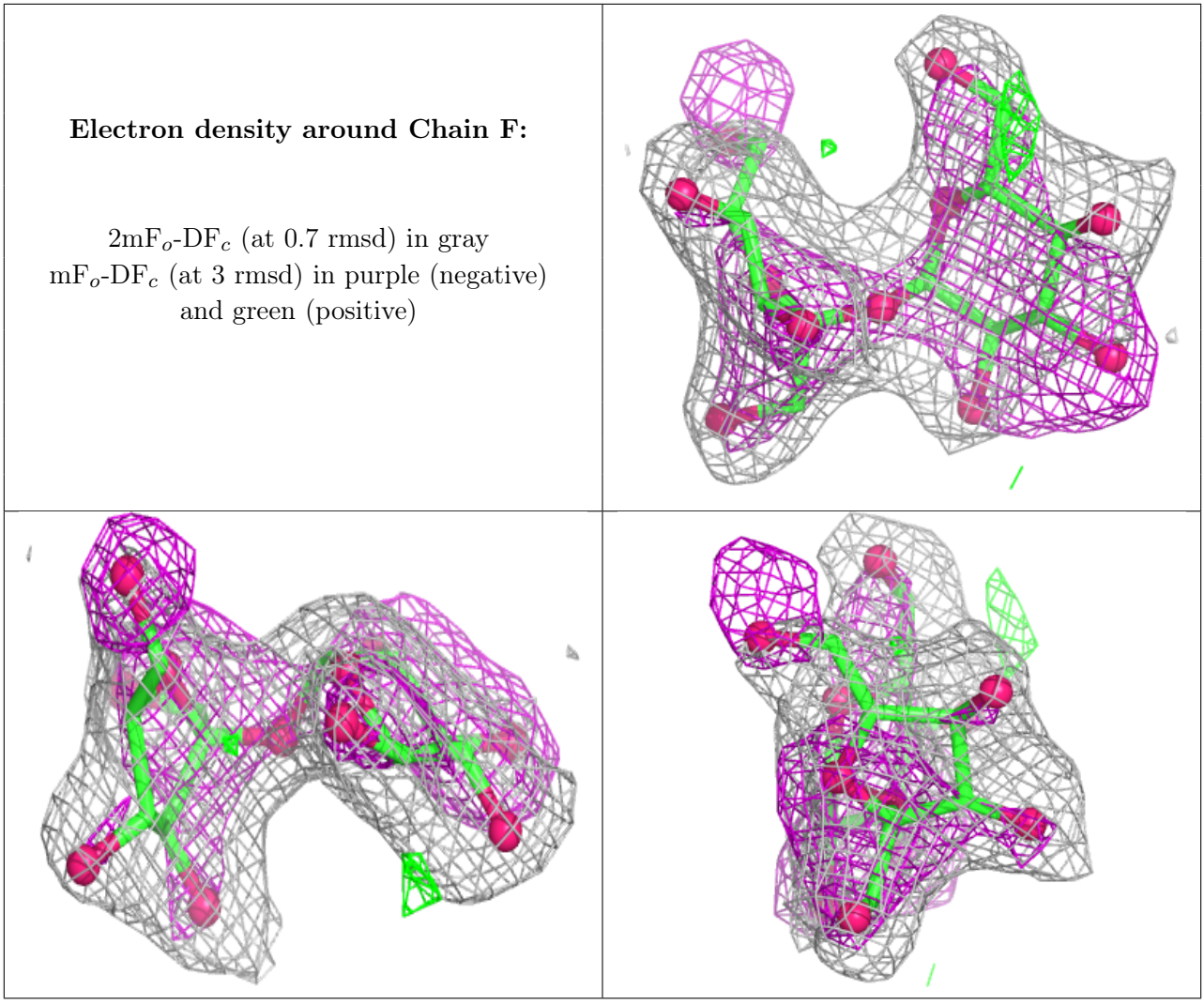
Electron density around Chain E:

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



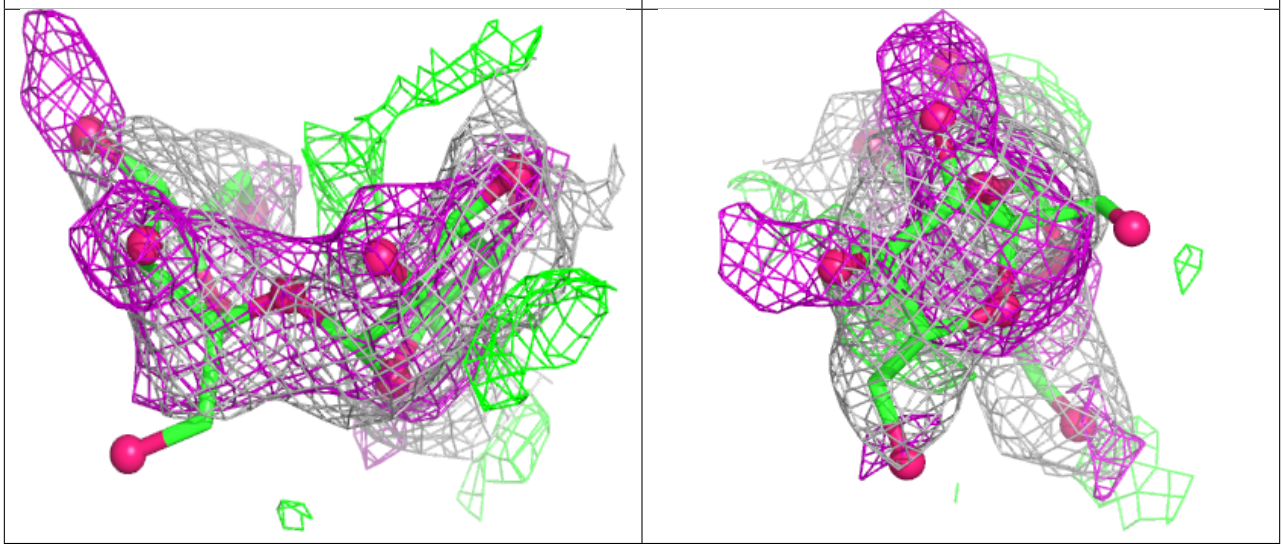
Electron density around Chain F:

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



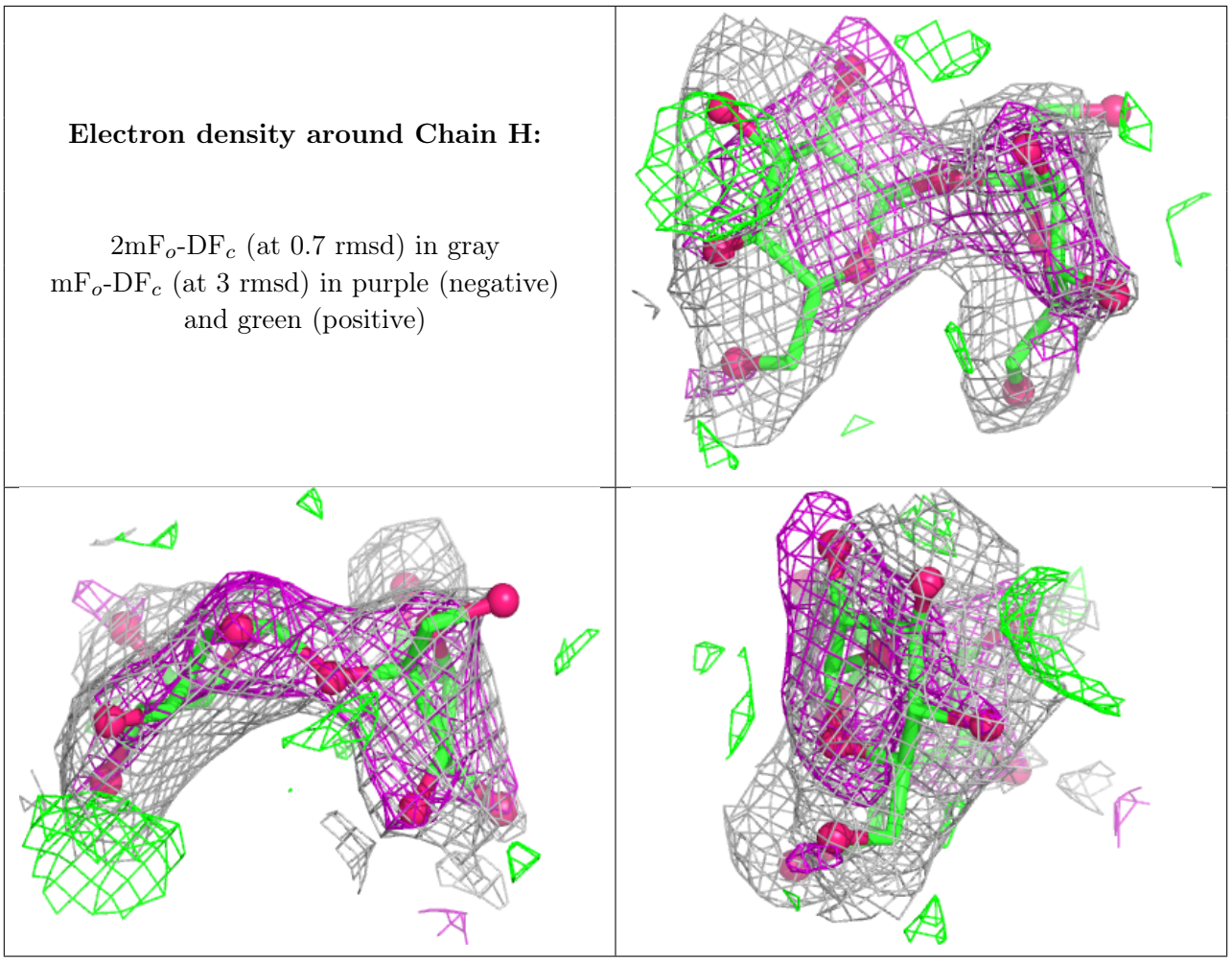
Electron density around Chain G:

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



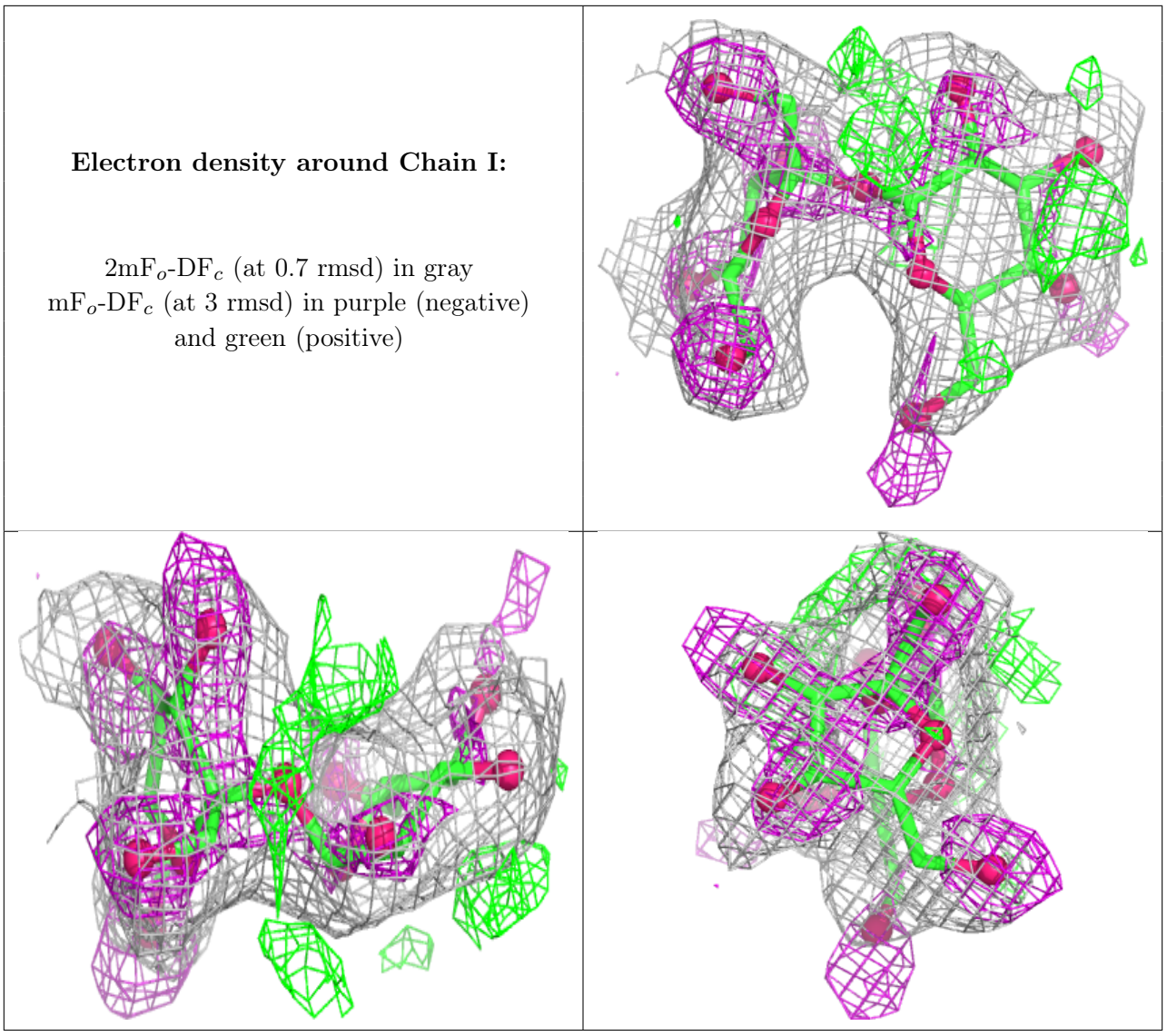
Electron density around Chain H:

$2mF_o$-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 I:

$2mF_o$-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	SO4	A	1106	5/5	0.67	0.13	121,121,123,127	0
4	SO4	B	1103	5/5	0.68	0.14	94,95,118,126	0
4	SO4	B	1102	5/5	0.69	0.11	149,151,159,161	0
4	SO4	A	1105	5/5	0.74	0.17	94,94,103,108	0
3	1PE	A	1103	13/16	0.74	0.23	66,74,78,81	0
4	SO4	A	1108	5/5	0.82	0.33	85,86,92,101	0
4	SO4	A	1107	5/5	0.83	0.11	112,112,118,124	0

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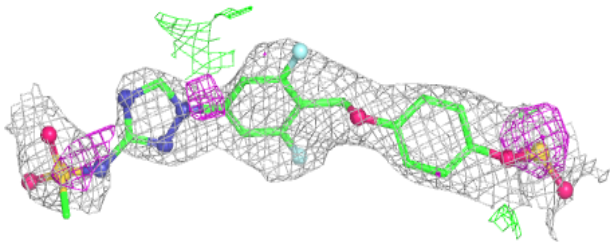
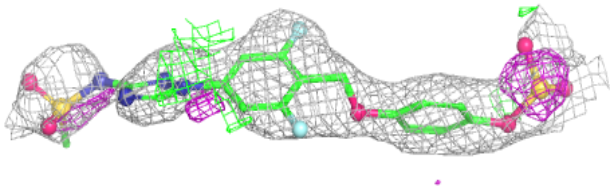
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	A1ATW	A	1109	30/31	0.84	0.15	72,84,119,126	0
3	1PE	A	1102	7/16	0.88	0.19	69,78,83,86	0
4	SO4	A	1104	5/5	0.89	0.14	95,99,103,114	0
3	1PE	A	1101	13/16	0.92	0.15	65,68,74,75	0
4	SO4	B	1101	5/5	0.99	0.07	48,49,51,51	5

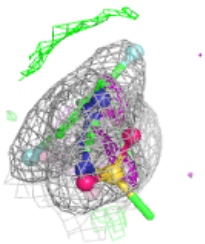
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1ATW A 1109:

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







6.5 Other polymers

There are no such residues in this entry.