wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 10:14 PM EDT

PDB ID	:	8E0P
Title	:	Crystal structure of mouse APCDD1 in fusion with engineered MBP
Authors	:	Hsieh, F.L.; Chang, T.H.; Gabelli, S.B.; Nathans, J.
Deposited on	:	2022-08-09
Resolution	:	2.33 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:

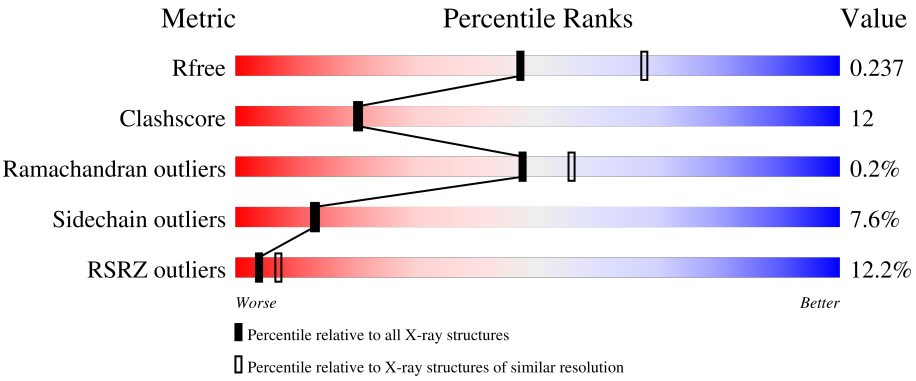
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	818	11% 71% 22% 5%
1	B	818	26% 62% 29% 6%
1	C	818	6% 73% 20%
1	D	818	5% 75% 18%
2	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	G	2	
2	H	2	
2	I	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	DMX	D	905	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 25921 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 Maltodextrin-binding protein, Protein APCDD1 complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	778	Total	C	N	O	S	0	3	0
			6184	3943	1076	1139	26			
1	B	789	Total	C	N	O	S	0	2	0
			6242	3975	1086	1153	28			
1	C	782	Total	C	N	O	S	0	4	0
			6221	3967	1078	1150	26			
1	D	784	Total	C	N	O	S	0	6	0
			6251	3978	1088	1159	26			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP C3SHQ8
A	2	THR	-	expression tag	UNP C3SHQ8
A	3	GLY	-	expression tag	UNP C3SHQ8
A	4	LYS	-	expression tag	UNP C3SHQ8
A	5	THR	-	expression tag	UNP C3SHQ8
A	85	ALA	ASP	engineered mutation	UNP C3SHQ8
A	86	ALA	LYS	engineered mutation	UNP C3SHQ8
A	175	ALA	GLU	engineered mutation	UNP C3SHQ8
A	176	ALA	ASN	engineered mutation	UNP C3SHQ8
A	218	HIS	ALA	engineered mutation	UNP C3SHQ8
A	222	HIS	LYS	engineered mutation	UNP C3SHQ8
A	242	ALA	LYS	engineered mutation	UNP C3SHQ8
A	315	VAL	ALA	engineered mutation	UNP C3SHQ8
A	320	VAL	ILE	engineered mutation	UNP C3SHQ8
A	362	ALA	GLU	engineered mutation	UNP C3SHQ8
A	365	ALA	LYS	engineered mutation	UNP C3SHQ8
A	366	ALA	ASP	engineered mutation	UNP C3SHQ8
A	370	ASN	-	linker	UNP C3SHQ8
A	371	ALA	-	linker	UNP C3SHQ8
A	372	ALA	-	linker	UNP C3SHQ8
A	810	THR	-	expression tag	UNP Q3U128

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Chain	Residue	Modelled	Actual	Comment	Reference
A	811	HIS	-	expression tag	UNP Q3U128
A	812	HIS	-	expression tag	UNP Q3U128
A	813	HIS	-	expression tag	UNP Q3U128
A	814	HIS	-	expression tag	UNP Q3U128
A	815	HIS	-	expression tag	UNP Q3U128
A	816	HIS	-	expression tag	UNP Q3U128
A	817	HIS	-	expression tag	UNP Q3U128
A	818	HIS	-	expression tag	UNP Q3U128
B	1	GLU	-	expression tag	UNP C3SHQ8
B	2	THR	-	expression tag	UNP C3SHQ8
B	3	GLY	-	expression tag	UNP C3SHQ8
B	4	LYS	-	expression tag	UNP C3SHQ8
B	5	THR	-	expression tag	UNP C3SHQ8
B	85	ALA	ASP	engineered mutation	UNP C3SHQ8
B	86	ALA	LYS	engineered mutation	UNP C3SHQ8
B	175	ALA	GLU	engineered mutation	UNP C3SHQ8
B	176	ALA	ASN	engineered mutation	UNP C3SHQ8
B	218	HIS	ALA	engineered mutation	UNP C3SHQ8
B	222	HIS	LYS	engineered mutation	UNP C3SHQ8
B	242	ALA	LYS	engineered mutation	UNP C3SHQ8
B	315	VAL	ALA	engineered mutation	UNP C3SHQ8
B	320	VAL	ILE	engineered mutation	UNP C3SHQ8
B	362	ALA	GLU	engineered mutation	UNP C3SHQ8
B	365	ALA	LYS	engineered mutation	UNP C3SHQ8
B	366	ALA	ASP	engineered mutation	UNP C3SHQ8
B	370	ASN	-	linker	UNP C3SHQ8
B	371	ALA	-	linker	UNP C3SHQ8
B	372	ALA	-	linker	UNP C3SHQ8
B	810	THR	-	expression tag	UNP Q3U128
B	811	HIS	-	expression tag	UNP Q3U128
B	812	HIS	-	expression tag	UNP Q3U128
B	813	HIS	-	expression tag	UNP Q3U128
B	814	HIS	-	expression tag	UNP Q3U128
B	815	HIS	-	expression tag	UNP Q3U128
B	816	HIS	-	expression tag	UNP Q3U128
B	817	HIS	-	expression tag	UNP Q3U128
B	818	HIS	-	expression tag	UNP Q3U128
C	1	GLU	-	expression tag	UNP C3SHQ8
C	2	THR	-	expression tag	UNP C3SHQ8
C	3	GLY	-	expression tag	UNP C3SHQ8
C	4	LYS	-	expression tag	UNP C3SHQ8
C	5	THR	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	85	ALA	ASP	engineered mutation	UNP C3SHQ8
C	86	ALA	LYS	engineered mutation	UNP C3SHQ8
C	175	ALA	GLU	engineered mutation	UNP C3SHQ8
C	176	ALA	ASN	engineered mutation	UNP C3SHQ8
C	218	HIS	ALA	engineered mutation	UNP C3SHQ8
C	222	HIS	LYS	engineered mutation	UNP C3SHQ8
C	242	ALA	LYS	engineered mutation	UNP C3SHQ8
C	315	VAL	ALA	engineered mutation	UNP C3SHQ8
C	320	VAL	ILE	engineered mutation	UNP C3SHQ8
C	362	ALA	GLU	engineered mutation	UNP C3SHQ8
C	365	ALA	LYS	engineered mutation	UNP C3SHQ8
C	366	ALA	ASP	engineered mutation	UNP C3SHQ8
C	370	ASN	-	linker	UNP C3SHQ8
C	371	ALA	-	linker	UNP C3SHQ8
C	372	ALA	-	linker	UNP C3SHQ8
C	810	THR	-	expression tag	UNP Q3U128
C	811	HIS	-	expression tag	UNP Q3U128
C	812	HIS	-	expression tag	UNP Q3U128
C	813	HIS	-	expression tag	UNP Q3U128
C	814	HIS	-	expression tag	UNP Q3U128
C	815	HIS	-	expression tag	UNP Q3U128
C	816	HIS	-	expression tag	UNP Q3U128
C	817	HIS	-	expression tag	UNP Q3U128
C	818	HIS	-	expression tag	UNP Q3U128
D	1	GLU	-	expression tag	UNP C3SHQ8
D	2	THR	-	expression tag	UNP C3SHQ8
D	3	GLY	-	expression tag	UNP C3SHQ8
D	4	LYS	-	expression tag	UNP C3SHQ8
D	5	THR	-	expression tag	UNP C3SHQ8
D	85	ALA	ASP	engineered mutation	UNP C3SHQ8
D	86	ALA	LYS	engineered mutation	UNP C3SHQ8
D	175	ALA	GLU	engineered mutation	UNP C3SHQ8
D	176	ALA	ASN	engineered mutation	UNP C3SHQ8
D	218	HIS	ALA	engineered mutation	UNP C3SHQ8
D	222	HIS	LYS	engineered mutation	UNP C3SHQ8
D	242	ALA	LYS	engineered mutation	UNP C3SHQ8
D	315	VAL	ALA	engineered mutation	UNP C3SHQ8
D	320	VAL	ILE	engineered mutation	UNP C3SHQ8
D	362	ALA	GLU	engineered mutation	UNP C3SHQ8
D	365	ALA	LYS	engineered mutation	UNP C3SHQ8
D	366	ALA	ASP	engineered mutation	UNP C3SHQ8
D	370	ASN	-	linker	UNP C3SHQ8

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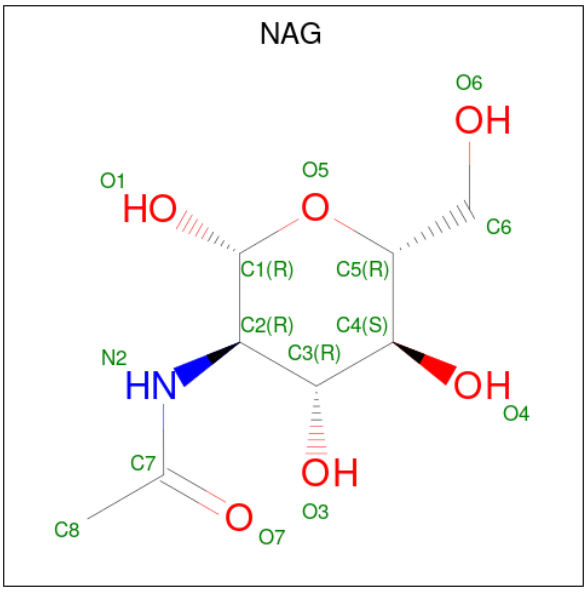
Chain	Residue	Modelled	Actual	Comment	Reference
D	371	ALA	-	linker	UNP C3SHQ8
D	372	ALA	-	linker	UNP C3SHQ8
D	810	THR	-	expression tag	UNP Q3U128
D	811	HIS	-	expression tag	UNP Q3U128
D	812	HIS	-	expression tag	UNP Q3U128
D	813	HIS	-	expression tag	UNP Q3U128
D	814	HIS	-	expression tag	UNP Q3U128
D	815	HIS	-	expression tag	UNP Q3U128
D	816	HIS	-	expression tag	UNP Q3U128
D	817	HIS	-	expression tag	UNP Q3U128
D	818	HIS	-	expression tag	UNP Q3U128

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

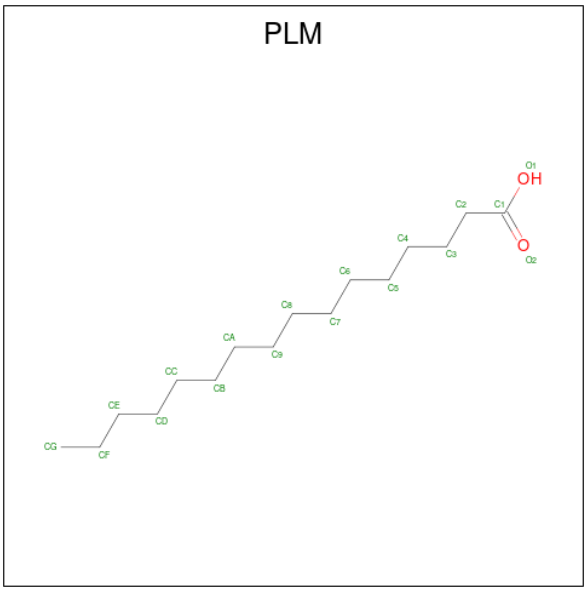
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



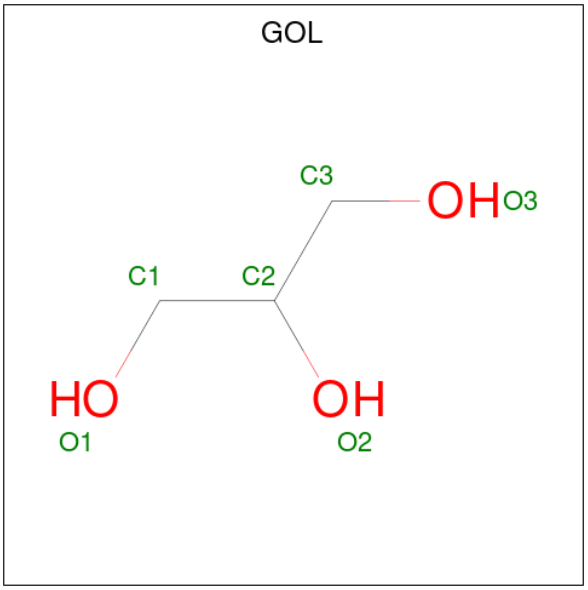
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 18 16 2	0	0
4	C	1	Total C O 18 16 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

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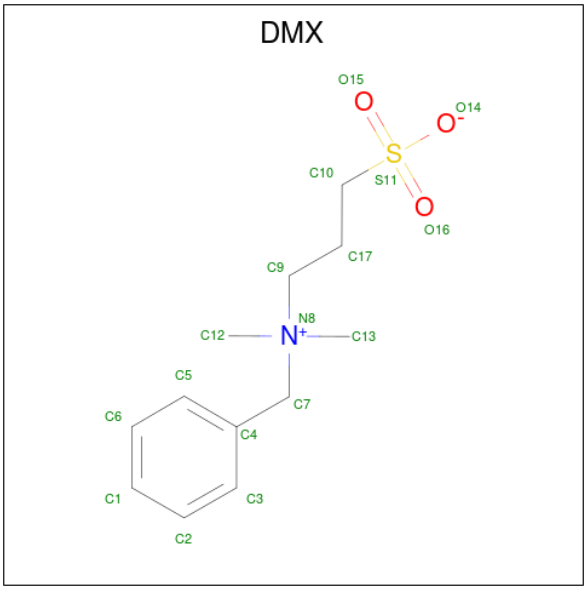
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0
6	D	1	Total Cl 1 1	0	0

- Molecule 7 is 3-[BENZYL(DIMETHYL)AMMONIO]PROPANE-1-SULFONATE (three-letter code: DMX) (formula: $C_{12}H_{19}NO_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C N O S 17 12 1 3 1	0	0
7	C	1	Total C N O S 17 12 1 3 1	0	0
7	D	1	Total C N O S 17 12 1 3 1	0	0

- Molecule 8 is water.

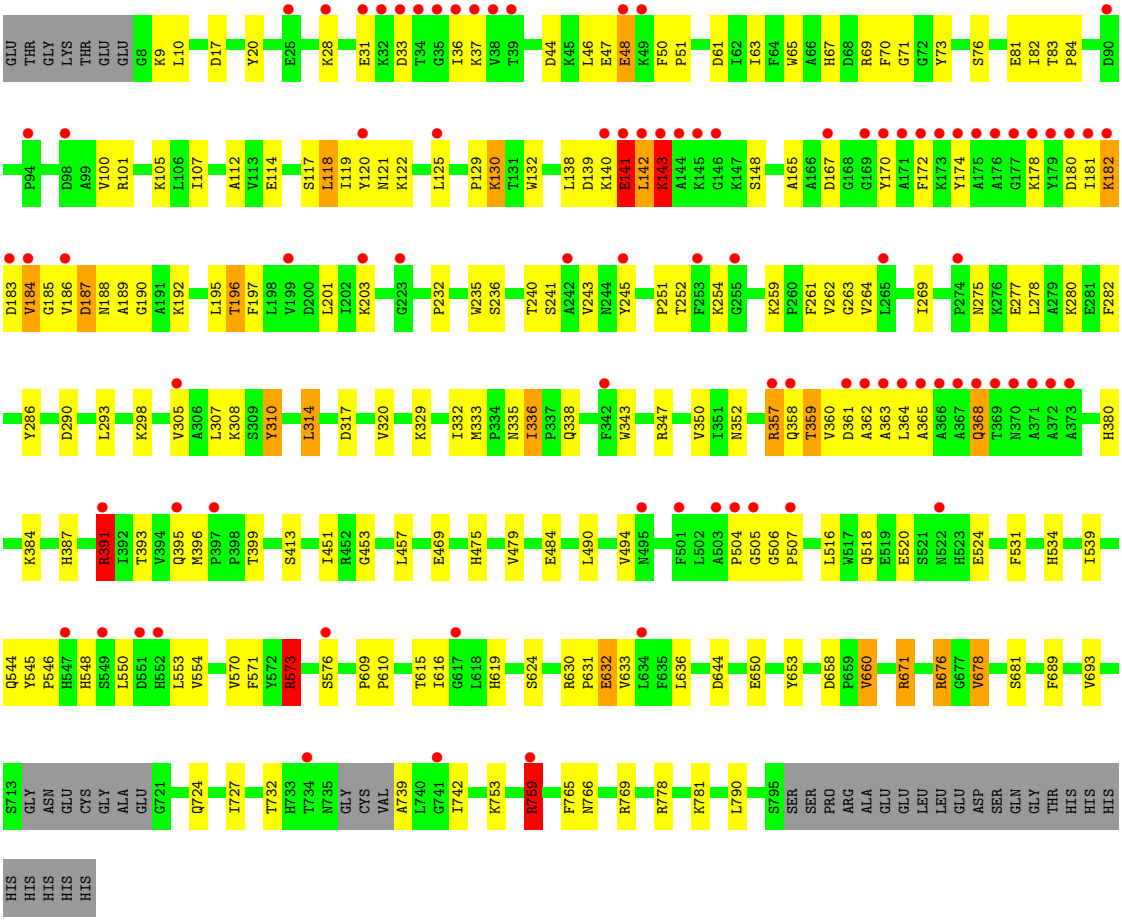
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	160	Total O 160 160	0	0
8	B	79	Total O 79 79	0	0
8	C	184	Total O 184 184	0	0
8	D	220	Total O 220 220	0	0

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.

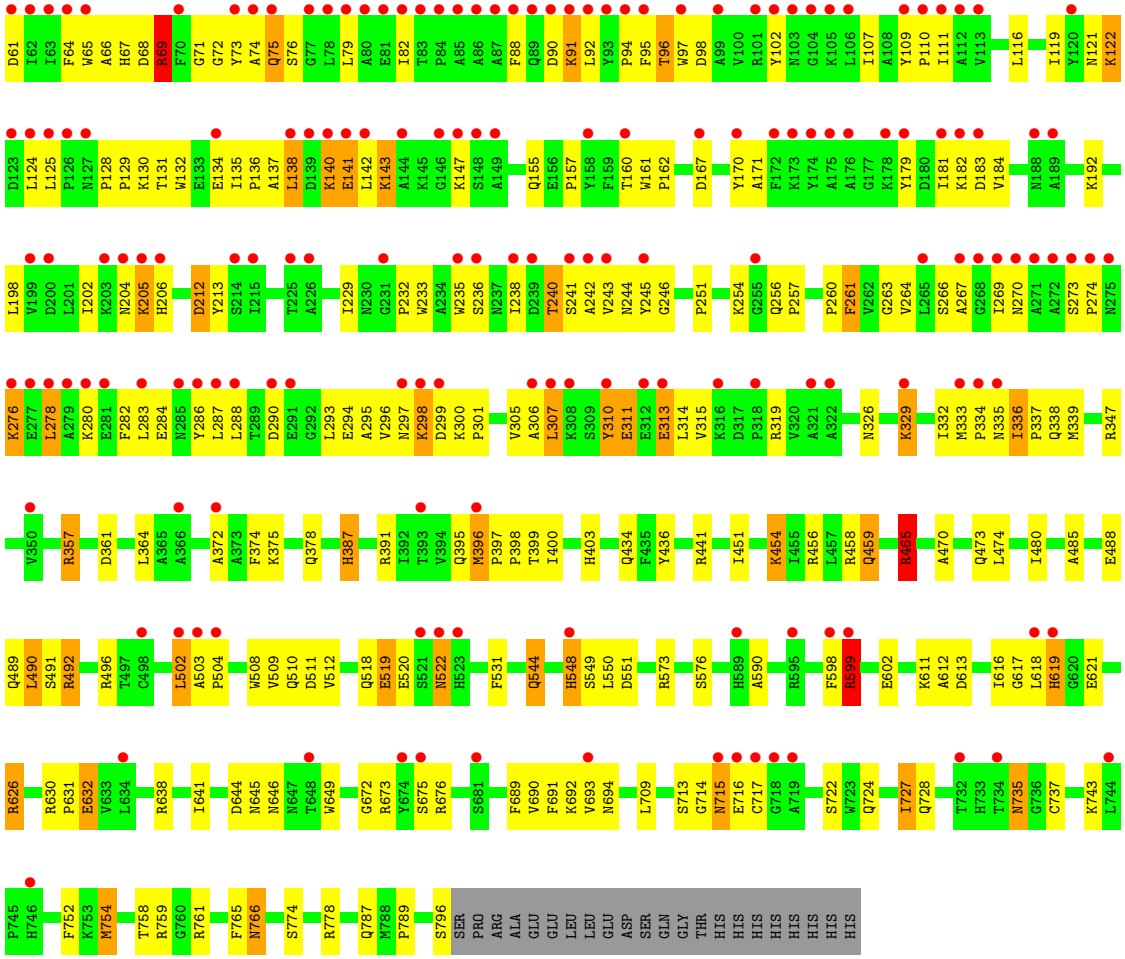
• Molecule 1: Maltodextrin-binding protein, Protein APCDD1 complex

Chain A:



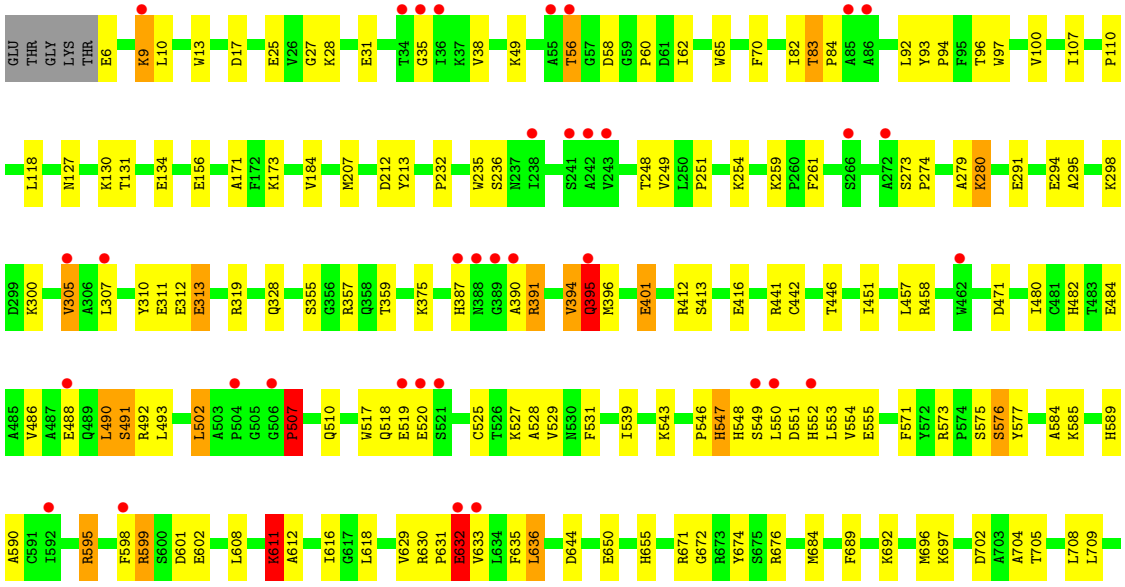
• Molecule 1: Maltodextrin-binding protein, Protein APCDD1 complex

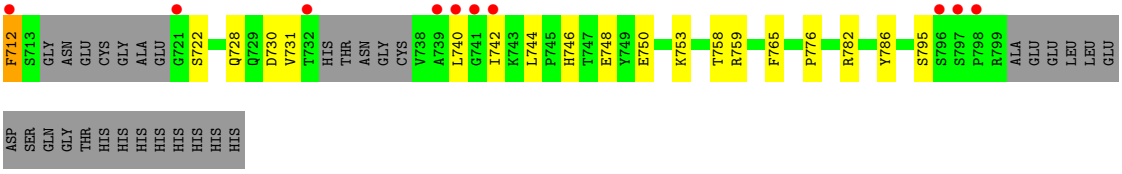
Chain B:



• Molecule 1: Maltodextrin-binding protein, Protein APCDD1 complex

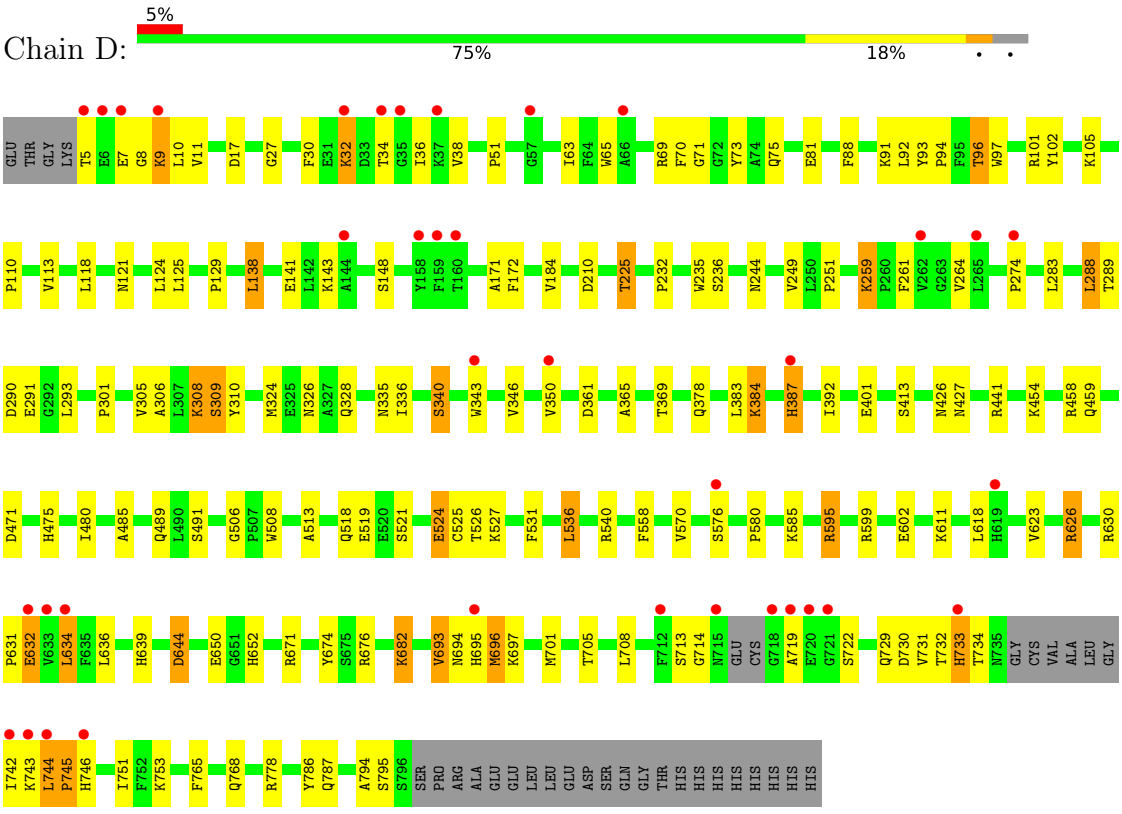
Chain C:





• Molecule 1: Maltodextrin-binding protein, Protein APCDD1 complex

Chain D:

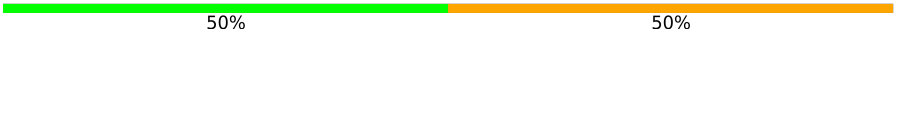


• Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F:

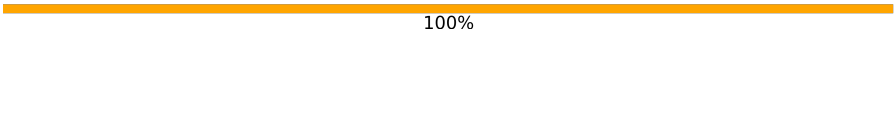
• Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G:



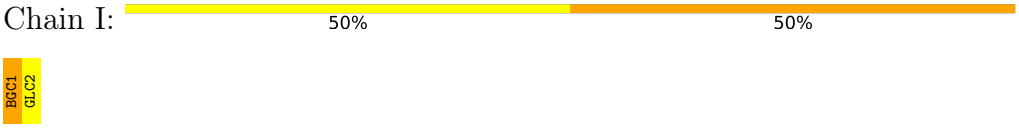
• Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain H:



• Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	123.91Å 98.36Å 156.51Å 90.00° 109.73° 90.00°	Depositor
Resolution (Å)	39.67 – 2.33 39.67 – 2.31	Depositor EDS
% Data completeness (in resolution range)	87.7 (39.67-2.33) 86.3 (39.67-2.31)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.192 , 0.239 0.206 , 0.237	Depositor DCC
R_{free} test set	1990 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25921	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% 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: CL, GLC, NAG, GOL, DMX, BGC, PLM

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	0.41	1/6356 (0.0%)	0.74	20/8638 (0.2%)
1	B	0.42	0/6417	0.65	9/8724 (0.1%)
1	C	0.52	11/6394 (0.2%)	0.94	32/8690 (0.4%)
1	D	0.40	1/6427 (0.0%)	0.63	9/8734 (0.1%)
All	All	0.44	13/25594 (0.1%)	0.75	70/34786 (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	A	0	5
1	B	0	4
1	C	0	4
1	D	0	6
All	All	0	19

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	611	LYS	CE-NZ	16.22	1.89	1.49
1	D	32	LYS	CD-CE	8.03	1.71	1.51
1	C	488	GLU	CD-OE1	7.69	1.34	1.25
1	C	759	ARG	CG-CD	7.04	1.69	1.51
1	C	313	GLU	CB-CG	6.62	1.64	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	488	GLU	OE1-CD-OE2	-30.45	86.76	123.30
1	C	488	GLU	CG-CD-OE1	21.91	162.12	118.30
1	C	488	GLU	CG-CD-OE2	-19.70	78.89	118.30
1	A	391	ARG	CA-CB-CG	16.64	150.02	113.40
1	A	391	ARG	CB-CG-CD	-16.64	68.33	111.60

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	141	GLU	Peptide
1	A	391	ARG	Sidechain
1	A	573	ARG	Sidechain
1	A	759	ARG	Sidechain

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	6184	0	5991	135	1
1	B	6242	0	6036	225	1
1	C	6221	0	6018	142	1
1	D	6251	0	6034	121	1
2	F	23	0	21	2	0
2	G	23	0	21	1	0
2	H	23	0	21	3	0
2	I	23	0	21	2	0
3	A	42	0	39	1	0
3	B	42	0	39	1	0
3	C	42	0	39	0	0
3	D	42	0	39	0	0
4	A	18	0	31	6	0
4	C	18	0	31	4	0
5	A	6	0	8	0	0
5	B	12	0	16	1	0
5	C	6	0	8	1	0
5	D	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	1	0
6	D	1	0	0	1	0
7	C	34	0	38	8	0
7	D	17	0	19	5	0
8	A	160	0	0	6	1
8	B	79	0	0	3	1
8	C	184	0	0	3	0
8	D	220	0	0	3	2
All	All	25921	0	24478	618	4

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 12.

The worst 5 of 618 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:C:611:LYS:CE	1:C:611:LYS:NZ	1.89	1.36
1:C:611:LYS:NZ	1:C:611:LYS:CD	2.22	1.01
1:C:6:GLU:HB2	1:C:9:LYS:HD3	1.44	0.98
1:D:387:HIS:CD2	1:D:626:ARG:HE	1.83	0.97
1:D:731:VAL:HG23	1:D:744:LEU:HD11	1.51	0.92

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NH1	1:C:482:HIS:O[2_546]	1.42	0.78
1:B:313:GLU:OE1	1:D:244:ASN:ND2[2_555]	1.98	0.22
8:A:1002:HOH:O	8:D:1006:HOH:O[2_646]	1.99	0.21
8:B:1071:HOH:O	8:D:1159:HOH:O[2_656]	2.17	0.03

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	775/818 (95%)	746 (96%)	27 (4%)	2 (0%)	41	47
1	B	789/818 (96%)	754 (96%)	34 (4%)	1 (0%)	51	62
1	C	780/818 (95%)	758 (97%)	20 (3%)	2 (0%)	41	47
1	D	784/818 (96%)	755 (96%)	27 (3%)	2 (0%)	41	47
All	All	3128/3272 (96%)	3013 (96%)	108 (4%)	7 (0%)	47	55

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	632	GLU
1	C	507	PRO
1	D	632	GLU
1	A	632	GLU
1	B	632	GLU

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	651/681 (96%)	598 (92%)	53 (8%)	11	11
1	B	657/681 (96%)	585 (89%)	72 (11%)	6	5
1	C	656/681 (96%)	620 (94%)	36 (6%)	21	25
1	D	659/681 (97%)	616 (94%)	43 (6%)	17	19
All	All	2623/2724 (96%)	2419 (92%)	204 (8%)	13	12

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	722	SER
1	C	490	LEU
1	D	743	LYS

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Mol	Chain	Res	Type
1	B	754	MET
1	C	130	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	459	GLN
1	D	489	GLN
1	B	547	HIS
1	B	475	HIS
1	D	518	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)

8 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	F	1	2	12,12,12	0.64	0	17,17,17	1.96	3 (17%)
2	GLC	F	2	2	11,11,12	0.61	0	15,15,17	0.86	0
2	BGC	G	1	2	12,12,12	0.68	0	17,17,17	2.15	6 (35%)
2	GLC	G	2	2	11,11,12	0.74	0	15,15,17	0.93	0
2	BGC	H	1	2	12,12,12	0.59	0	17,17,17	1.84	3 (17%)
2	GLC	H	2	2	11,11,12	1.38	1 (9%)	15,15,17	1.34	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	I	1	2	12,12,12	0.61	0	17,17,17	2.08	4 (23%)
2	GLC	I	2	2	11,11,12	0.63	0	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	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	BGC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	GLC	O5-C1	-4.10	1.37	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	BGC	C1-O5-C5	-5.62	103.06	113.66
2	F	1	BGC	C1-O5-C5	-5.46	103.35	113.66
2	I	1	BGC	C1-O5-C5	-5.45	103.39	113.66
2	H	1	BGC	C1-O5-C5	-4.90	104.42	113.66
2	G	1	BGC	C1-C2-C3	-3.82	102.40	110.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	BGC	1	0
2	I	2	GLC	1	0

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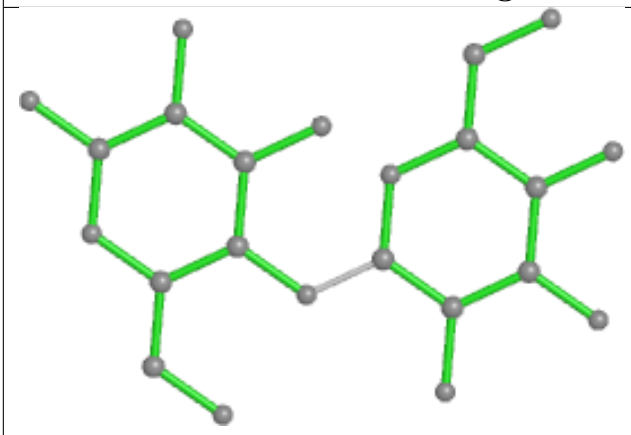
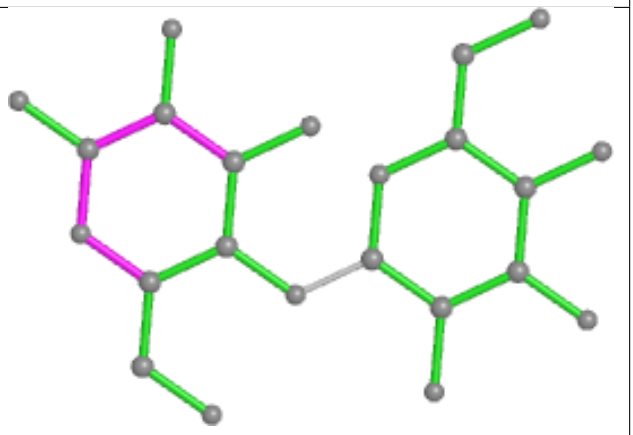
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	BGC	1	0
2	F	2	GLC	1	0
2	H	2	GLC	2	0
2	F	1	BGC	1	0
2	G	1	BGC	1	0

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

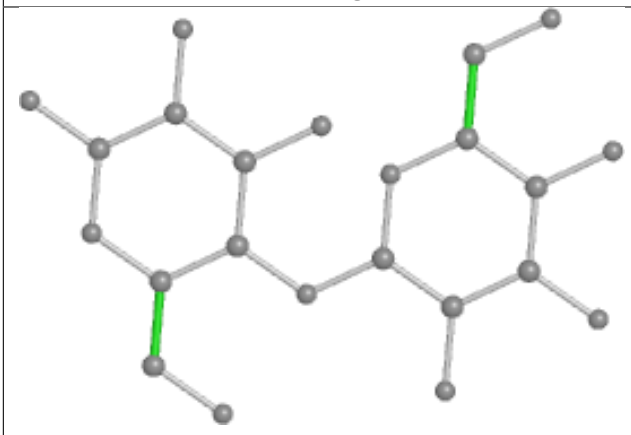
Oligosaccharide Chain F



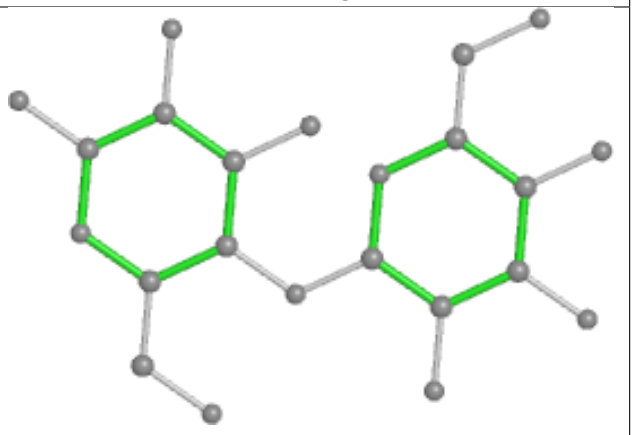
Bond lengths



Bond angles

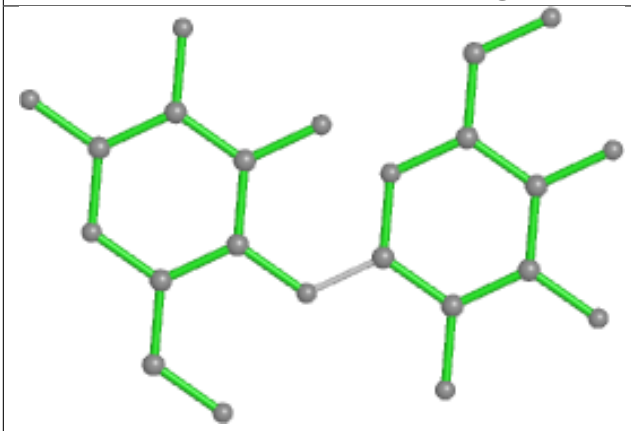


Torsions

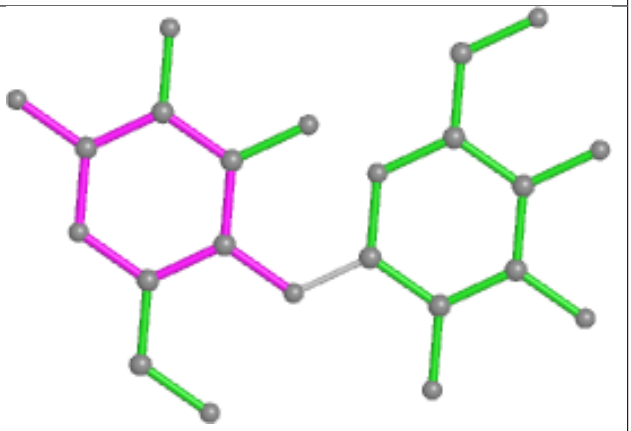


Rings

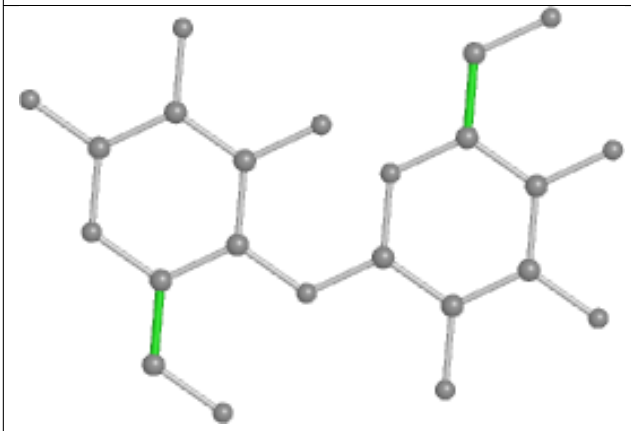
Oligosaccharide Chain G



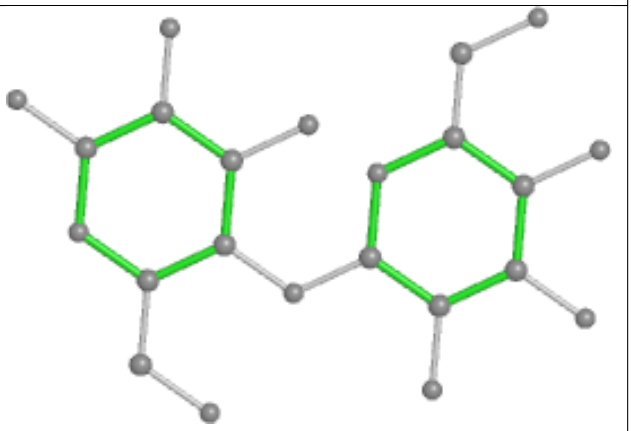
Bond lengths



Bond angles

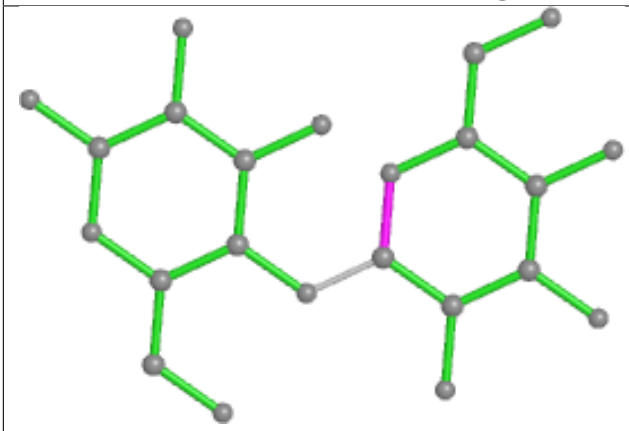


Torsions

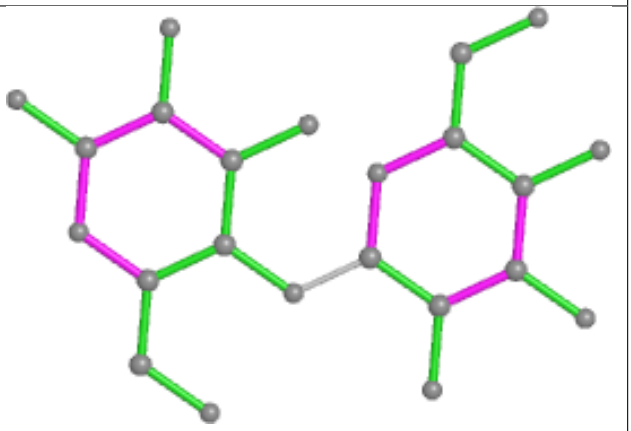


Rings

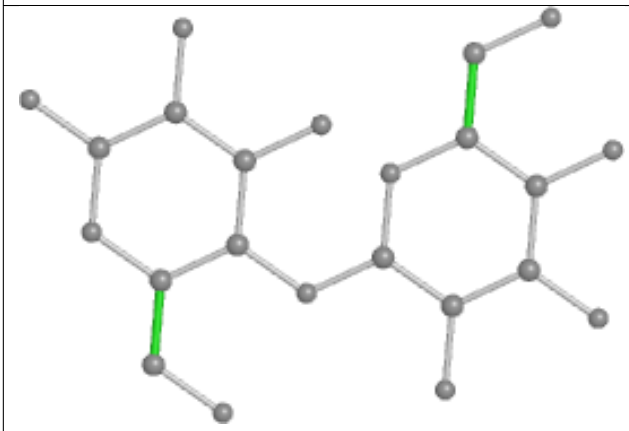
Oligosaccharide Chain H



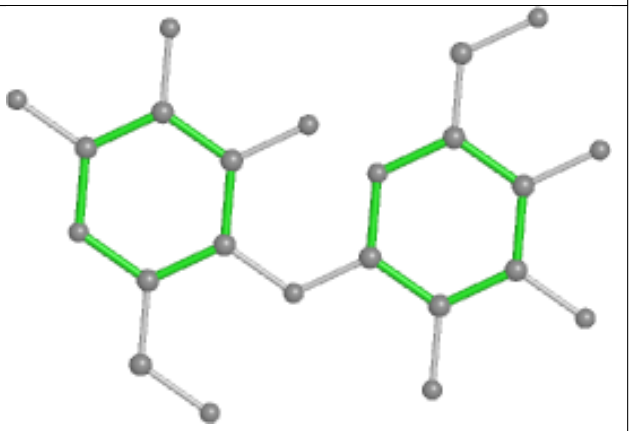
Bond lengths



Bond angles

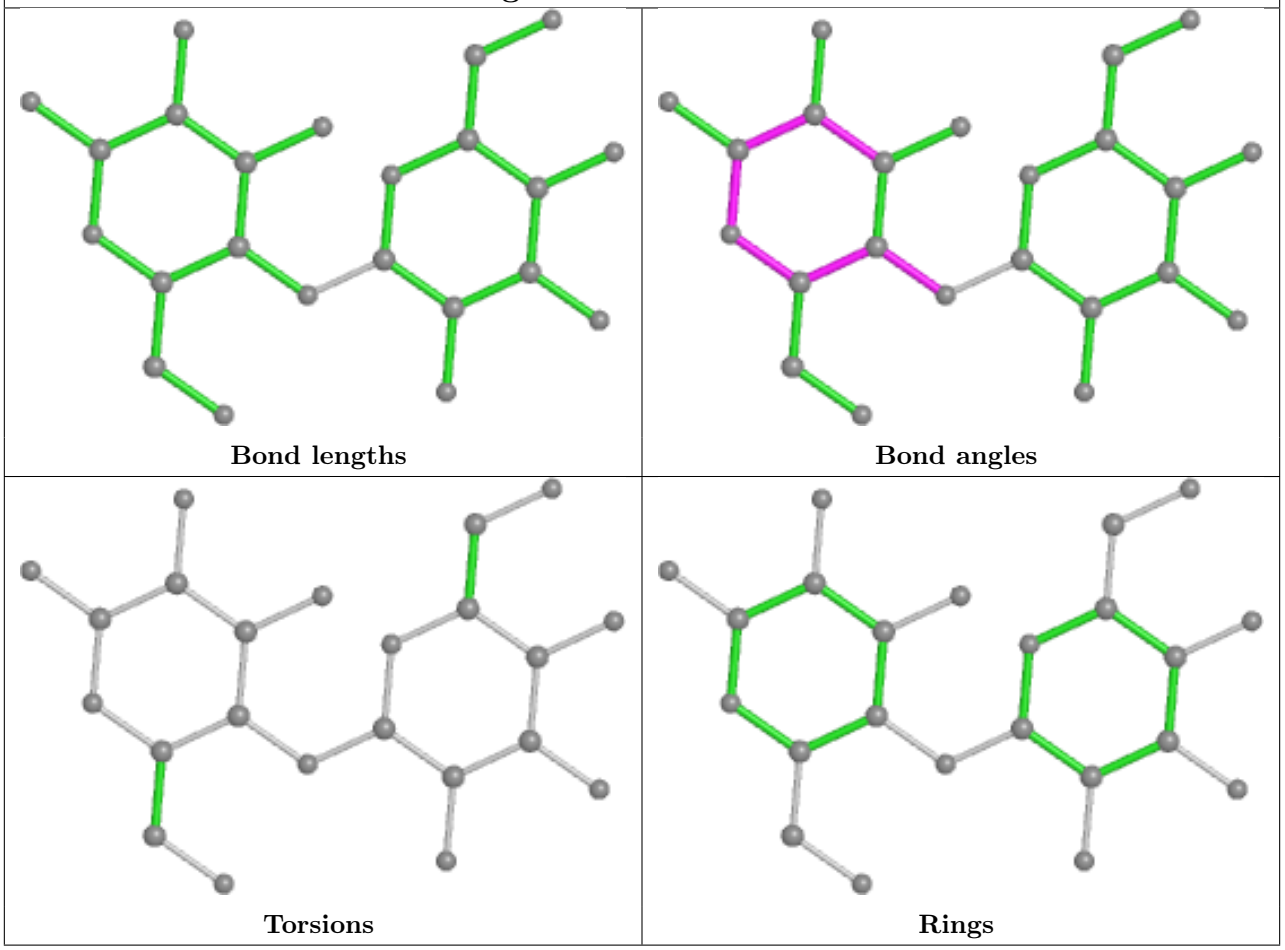


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 for Mogul analysis.

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	$\#\|Z\| > 2$
5	GOL	C	904	-	5,5,5	0.92	0	5,5,5	0.91	0
5	GOL	B	905	-	5,5,5	0.91	0	5,5,5	0.98	0
5	GOL	A	905	-	5,5,5	1.06	0	5,5,5	0.97	0
3	NAG	A	903	1	14,14,15	0.27	0	17,19,21	0.43	0
7	DMX	C	905	-	17,17,17	1.55	2 (11%)	23,24,24	1.76	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PLM	A	904	-	17,17,17	0.38	0	17,17,17	0.90	1 (5%)
3	NAG	B	902	1	14,14,15	0.43	0	17,19,21	0.58	0
3	NAG	C	901	1	14,14,15	0.18	0	17,19,21	0.40	0
3	NAG	B	901	1	14,14,15	0.33	0	17,19,21	0.40	0
7	DMX	D	905	-	17,17,17	1.34	2 (11%)	23,24,24	1.76	8 (34%)
3	NAG	D	903	1	14,14,15	0.39	0	17,19,21	0.35	0
3	NAG	A	901	1	14,14,15	0.28	0	17,19,21	0.47	0
5	GOL	D	904	-	5,5,5	0.92	0	5,5,5	1.01	0
3	NAG	D	901	1	14,14,15	0.27	0	17,19,21	0.38	0
3	NAG	B	903	1	14,14,15	0.42	0	17,19,21	0.86	0
5	GOL	B	904	-	5,5,5	0.89	0	5,5,5	0.93	0
3	NAG	A	902	1	14,14,15	0.34	0	17,19,21	0.66	0
4	PLM	C	907	-	17,17,17	0.31	0	17,17,17	0.82	0
3	NAG	D	902	1	14,14,15	0.31	0	17,19,21	0.82	0
3	NAG	C	902	1	14,14,15	0.44	0	17,19,21	0.68	0
7	DMX	C	906	-	17,17,17	1.50	1 (5%)	23,24,24	1.54	3 (13%)
3	NAG	C	903	1	14,14,15	0.39	0	17,19,21	0.56	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
5	GOL	C	904	-	-	0/4/4/4	-
5	GOL	B	905	-	-	4/4/4/4	-
5	GOL	A	905	-	-	2/4/4/4	-
3	NAG	A	903	1	-	2/6/23/26	0/1/1/1
7	DMX	C	905	-	-	6/13/13/13	0/1/1/1
4	PLM	A	904	-	-	14/15/15/15	-
3	NAG	B	902	1	-	2/6/23/26	0/1/1/1
3	NAG	C	901	1	-	2/6/23/26	0/1/1/1
3	NAG	B	901	1	-	2/6/23/26	0/1/1/1
7	DMX	D	905	-	-	13/13/13/13	0/1/1/1
3	NAG	D	903	1	-	1/6/23/26	0/1/1/1
3	NAG	A	901	1	-	0/6/23/26	0/1/1/1
5	GOL	D	904	-	-	3/4/4/4	-
3	NAG	D	901	1	-	0/6/23/26	0/1/1/1
3	NAG	B	903	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	904	-	-	2/4/4/4	-
3	NAG	A	902	1	-	2/6/23/26	0/1/1/1
4	PLM	C	907	-	-	11/15/15/15	-
3	NAG	D	902	1	-	2/6/23/26	0/1/1/1
3	NAG	C	902	1	-	2/6/23/26	0/1/1/1
7	DMX	C	906	-	-	10/13/13/13	0/1/1/1
3	NAG	C	903	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	906	DMX	C10-S11	5.29	1.85	1.77
7	C	905	DMX	C10-S11	4.96	1.84	1.77
7	D	905	DMX	C10-S11	4.12	1.83	1.77
7	C	905	DMX	C9-N8	2.64	1.57	1.52
7	D	905	DMX	C7-N8	2.04	1.59	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	905	DMX	O15-S11-C10	-5.31	100.52	106.92
7	C	906	DMX	O15-S11-C10	-4.36	101.67	106.92
7	D	905	DMX	O16-S11-C10	-3.73	102.42	106.92
7	D	905	DMX	O15-S11-C10	-3.57	102.61	106.92
7	C	906	DMX	O16-S11-C10	-2.92	103.40	106.92

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	904	GOL	C1-C2-C3-O3
5	B	905	GOL	C1-C2-C3-O3
7	C	905	DMX	C10-C17-C9-N8
7	C	905	DMX	C17-C10-S11-O14
7	C	905	DMX	C17-C10-S11-O15

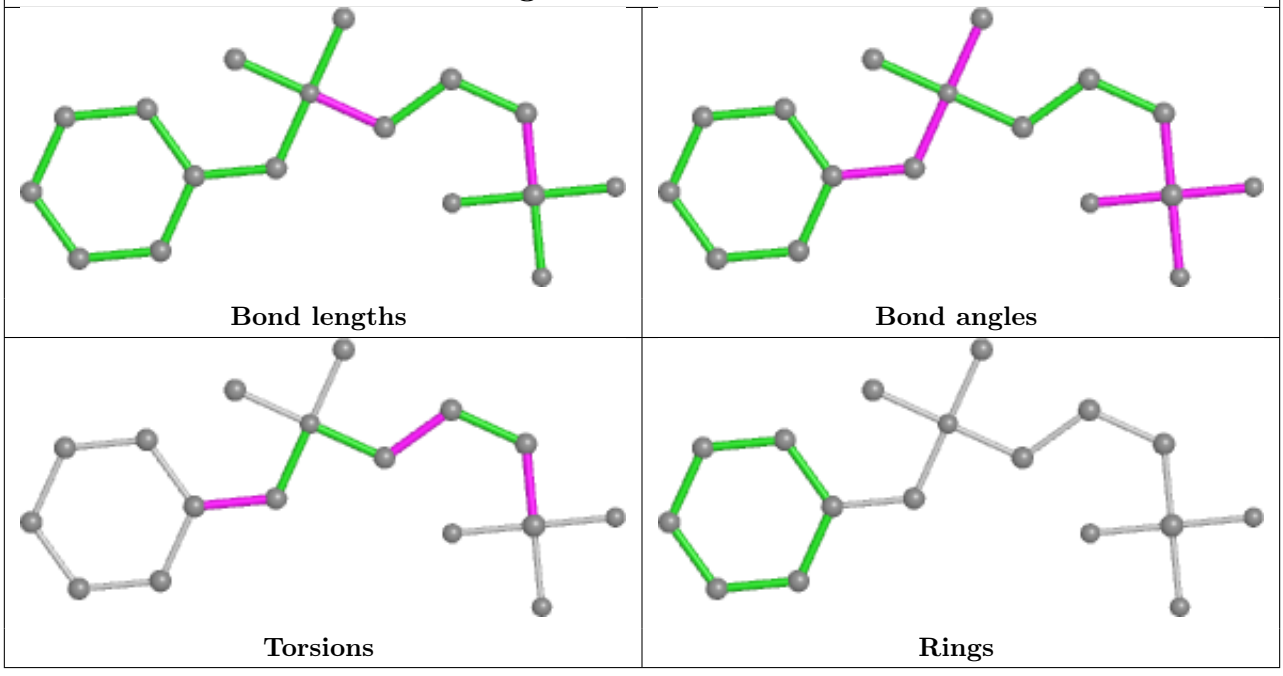
There are no ring outliers.

9 monomers are involved in 27 short contacts:

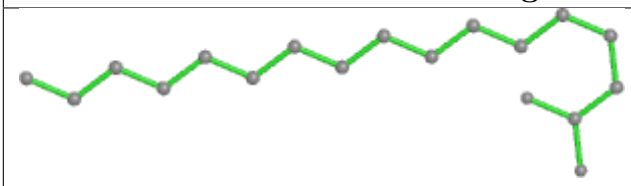
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	904	GOL	1	0
5	B	905	GOL	1	0
3	A	903	NAG	1	0
7	C	905	DMX	4	0
4	A	904	PLM	6	0
3	B	902	NAG	1	0
7	D	905	DMX	5	0
4	C	907	PLM	4	0
7	C	906	DMX	4	0

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.

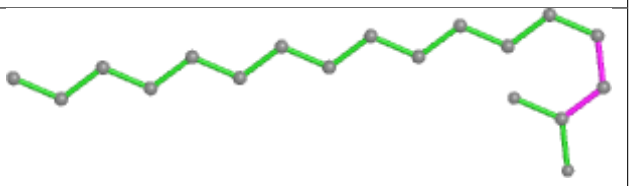
Ligand DMX C 905



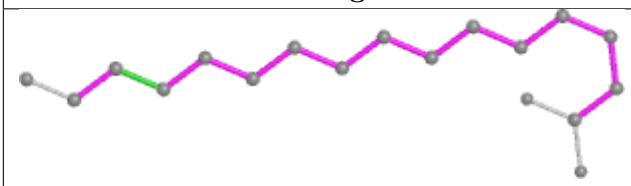
Ligand PLM A 904



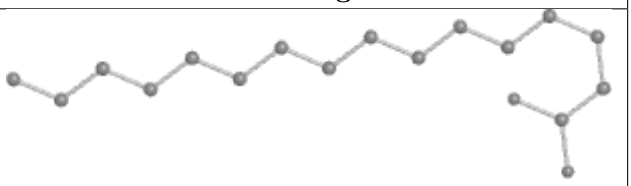
Bond lengths



Bond angles

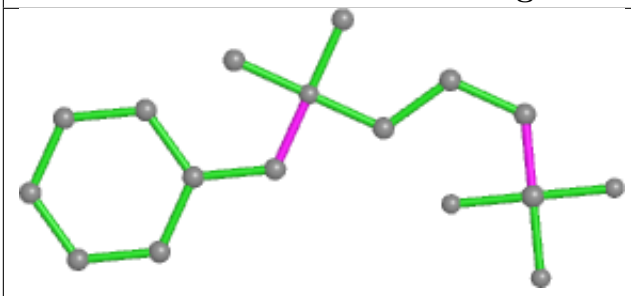


Torsions

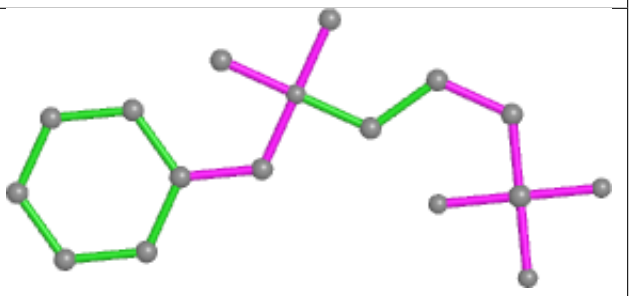


Rings

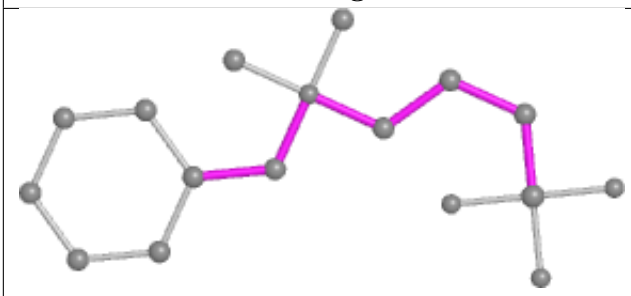
Ligand DMX D 905



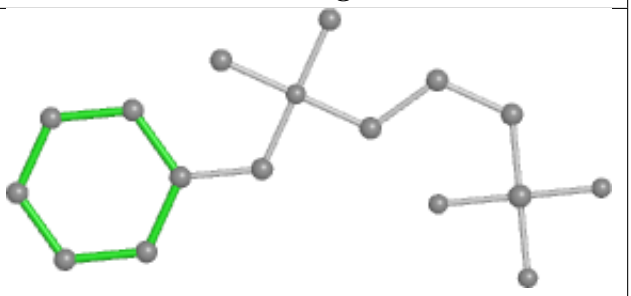
Bond lengths



Bond angles

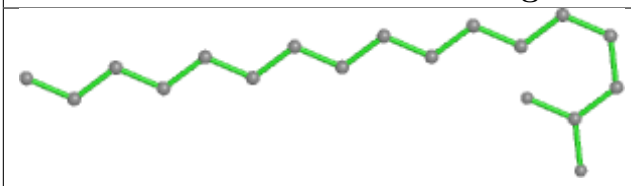


Torsions

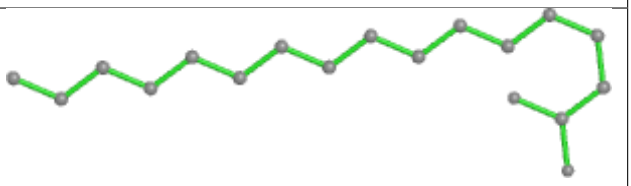


Rings

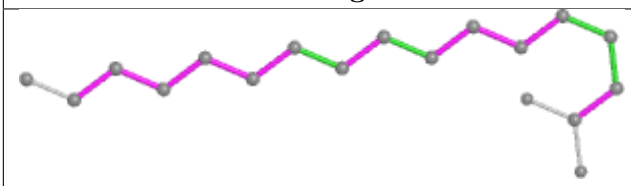
Ligand PLM C 907



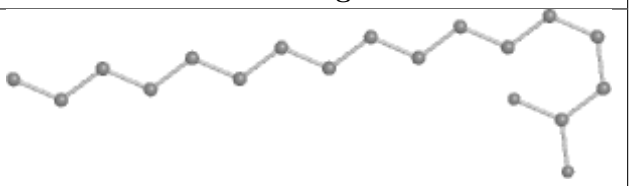
Bond lengths



Bond angles

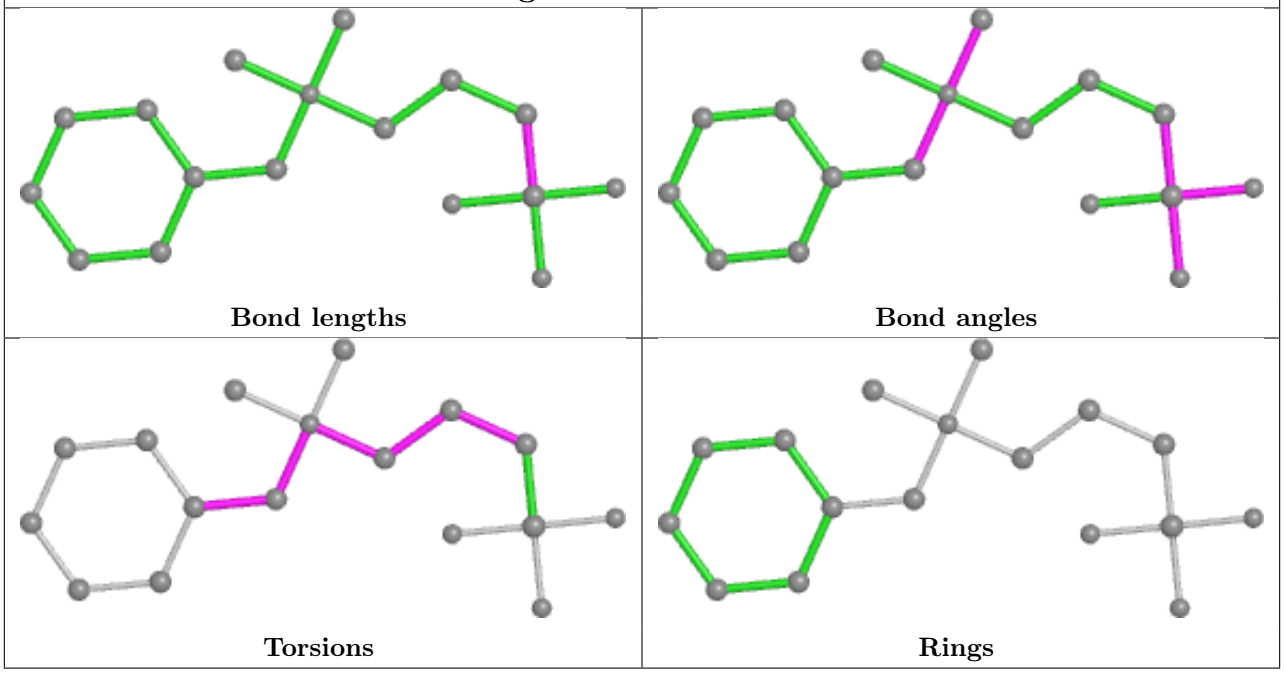


Torsions



Rings

Ligand DMX C 906



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	778/818 (95%)	0.77	89 (11%) 5 8	25, 69, 119, 200	0
1	B	789/818 (96%)	1.47	212 (26%) 0 0	36, 84, 181, 238	0
1	C	782/818 (95%)	0.41	45 (5%) 23 32	30, 58, 102, 185	0
1	D	784/818 (95%)	0.37	37 (4%) 31 42	32, 51, 89, 165	0
All	All	3133/3272 (95%)	0.76	383 (12%) 4 7	25, 63, 138, 238	0

The worst 5 of 383 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	GLY	12.6
1	B	274	PRO	10.8
1	B	87	ALA	10.1
1	B	53	VAL	9.9
1	B	94	PRO	9.8

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	GLC	G	2	11/12	0.75	0.21	78,95,104,105	0
2	BGC	G	1	12/12	0.80	0.24	76,97,108,113	0

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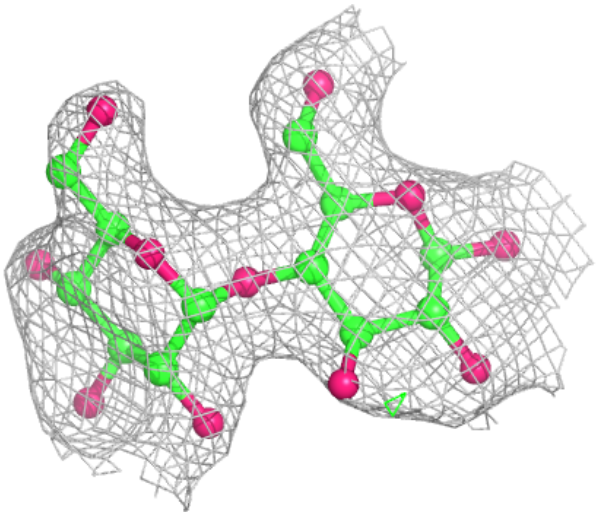
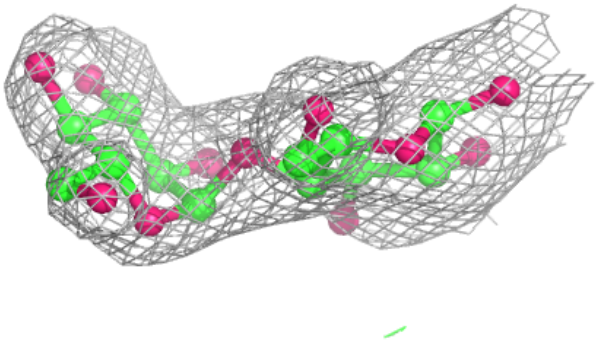
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	F	1	12/12	0.90	0.17	48,64,69,73	0
2	BGC	I	1	12/12	0.91	0.22	34,43,48,52	0
2	GLC	H	2	11/12	0.93	0.17	44,47,51,53	0
2	GLC	F	2	11/12	0.95	0.14	52,65,69,71	0
2	BGC	H	1	12/12	0.95	0.16	37,47,53,56	0
2	GLC	I	2	11/12	0.97	0.19	29,33,40,44	0

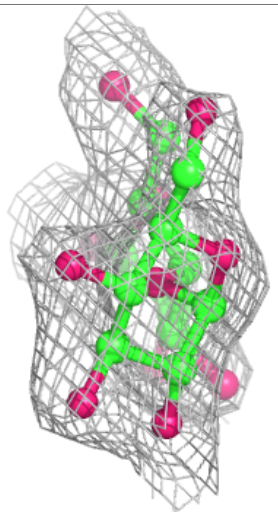
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F:

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

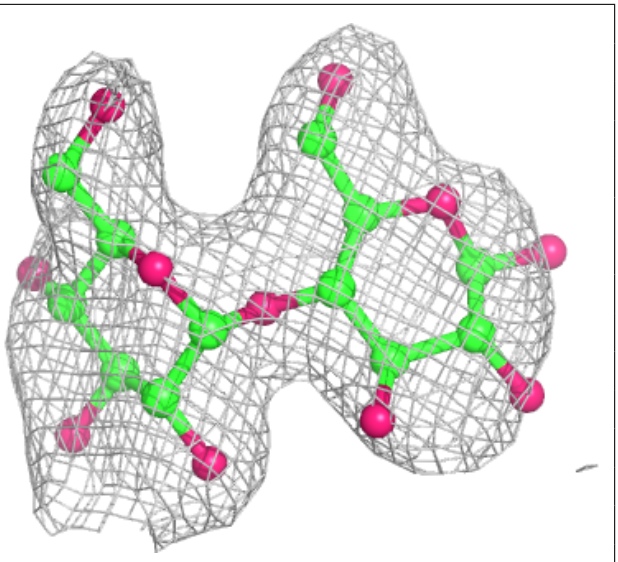


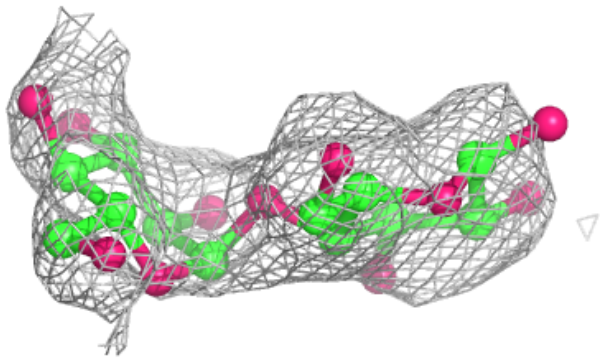


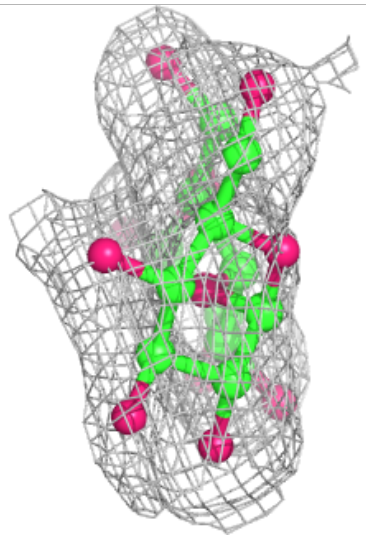


Electron density around Chain G:

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

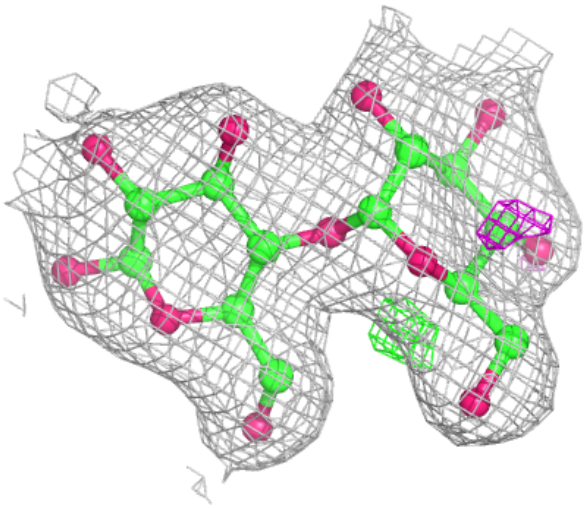


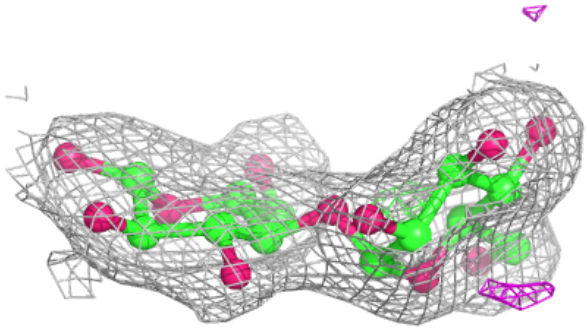


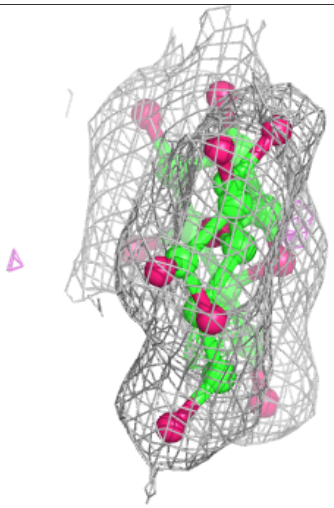


Electron density around Chain H:

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

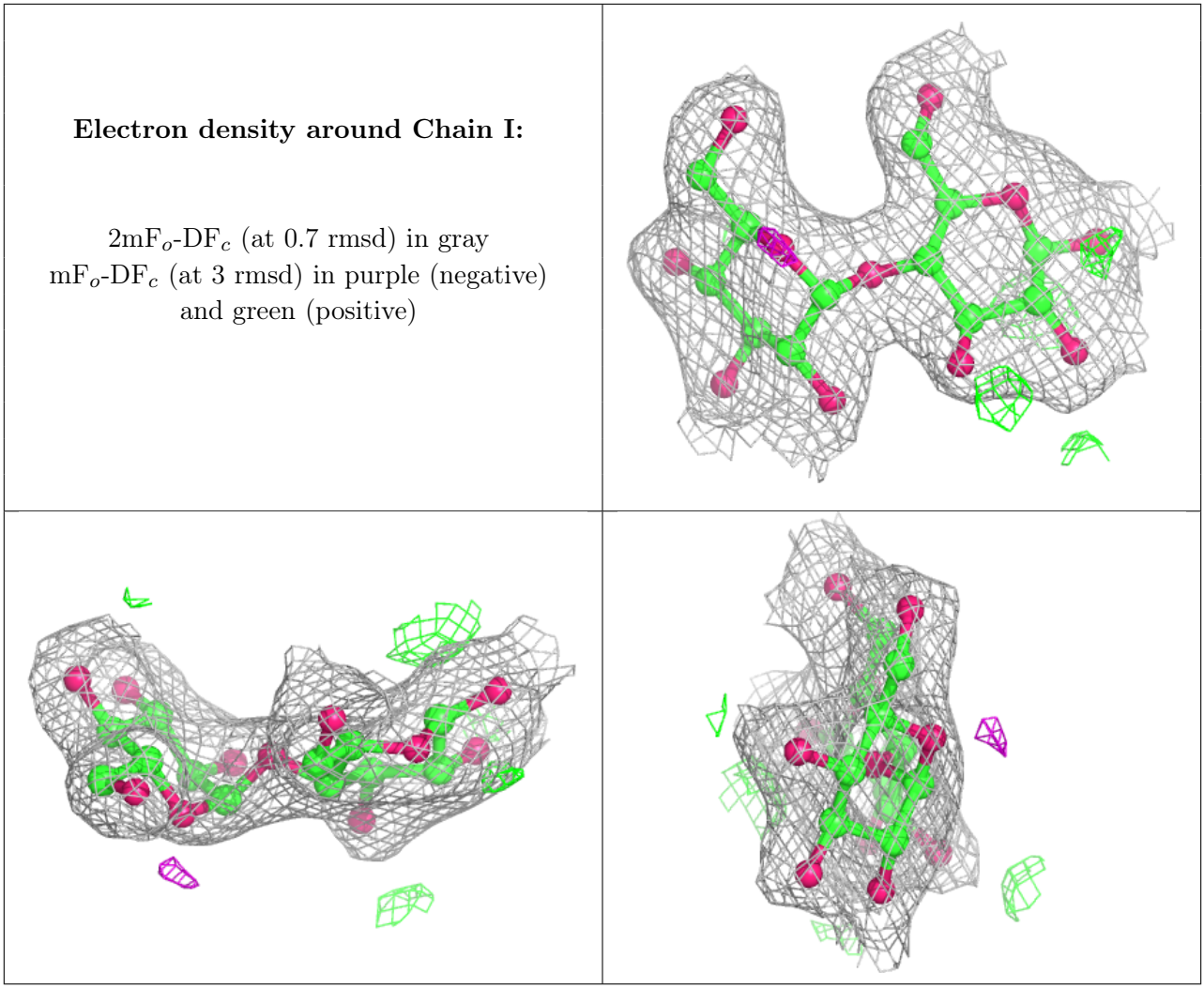






Electron density around Chain I:

$2mF_o$-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
3	NAG	B	902	14/15	0.71	0.32	82,92,104,106	0
5	GOL	B	905	6/6	0.72	0.25	68,76,80,82	0
7	DMX	C	906	17/17	0.73	0.39	68,84,120,187	0
3	NAG	A	902	14/15	0.77	0.22	81,93,101,102	0
7	DMX	D	905	17/17	0.77	0.28	85,120,133,196	0
4	PLM	A	904	18/18	0.79	0.31	48,61,75,76	0
3	NAG	D	901	14/15	0.79	0.29	79,93,100,108	0
3	NAG	B	901	14/15	0.80	0.33	74,85,96,98	0
7	DMX	C	905	17/17	0.81	0.25	71,93,101,158	0

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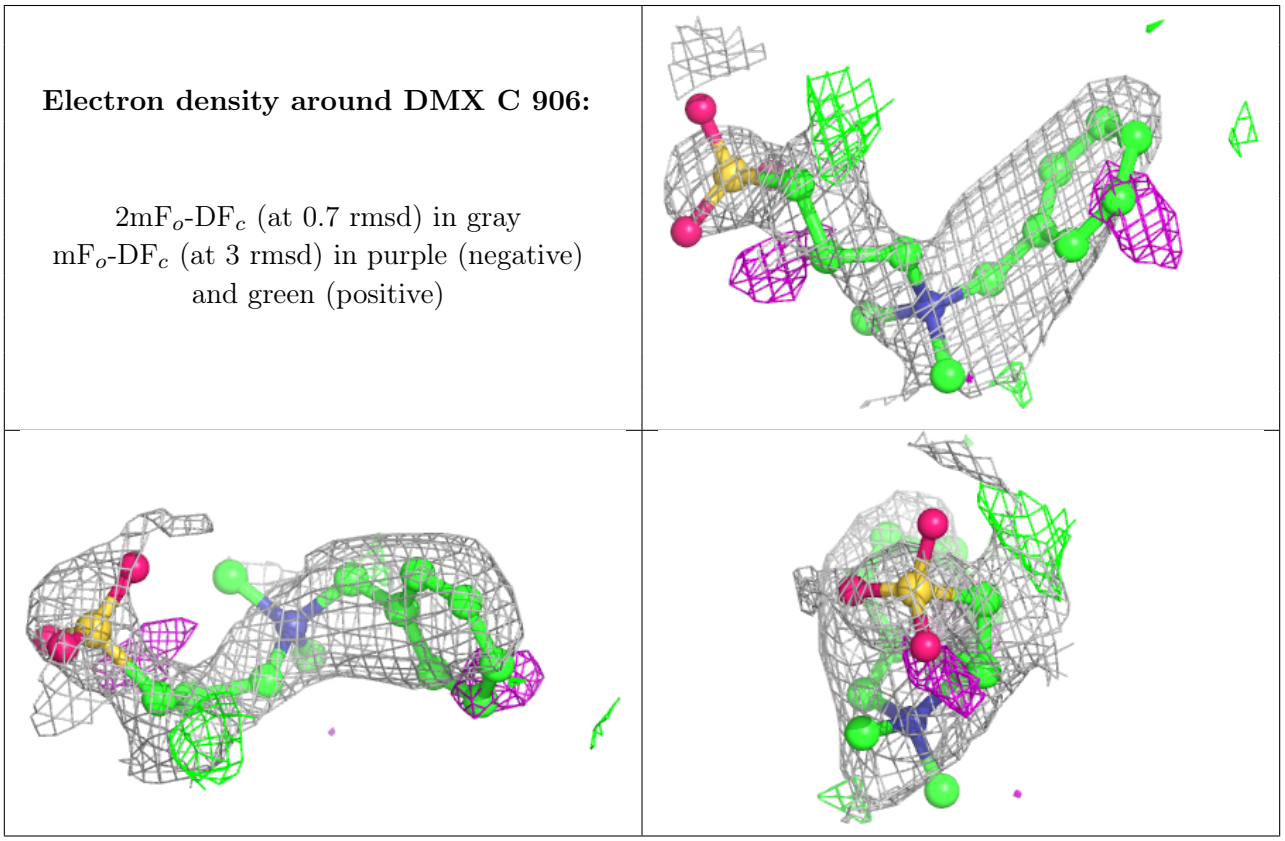
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PLM	C	907	18/18	0.81	0.29	49,63,73,75	0
3	NAG	D	902	14/15	0.81	0.15	68,87,96,114	0
3	NAG	B	903	14/15	0.84	0.21	79,90,101,106	0
3	NAG	C	902	14/15	0.87	0.22	54,63,76,76	0
5	GOL	B	904	6/6	0.87	0.24	67,71,79,82	0
5	GOL	A	905	6/6	0.91	0.22	69,79,83,105	0
5	GOL	D	904	6/6	0.91	0.24	64,69,70,70	0
6	CL	A	906	1/1	0.91	0.08	82,82,82,82	0
3	NAG	C	903	14/15	0.92	0.19	48,53,62,64	0
3	NAG	A	901	14/15	0.92	0.15	55,62,78,79	0
6	CL	D	906	1/1	0.92	0.25	63,63,63,63	0
3	NAG	C	901	14/15	0.93	0.14	36,57,63,70	0
3	NAG	A	903	14/15	0.93	0.15	66,77,86,93	0
5	GOL	C	904	6/6	0.93	0.47	64,69,70,78	0
3	NAG	D	903	14/15	0.94	0.20	53,68,81,87	0
6	CL	B	906	1/1	0.95	0.32	68,68,68,68	0

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.

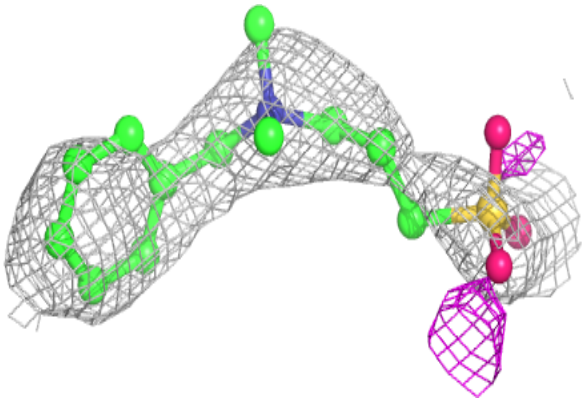
Electron density around DMX C 906:

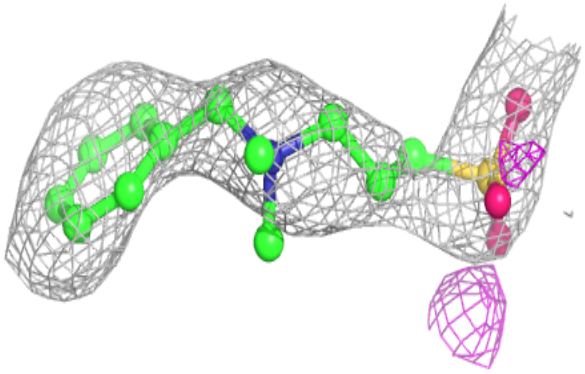
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

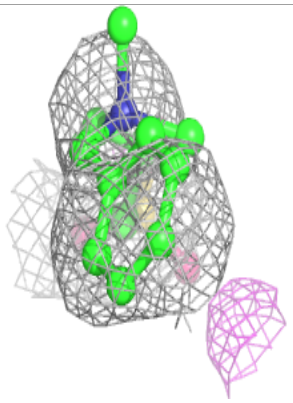


Electron density around DMX D 905:

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

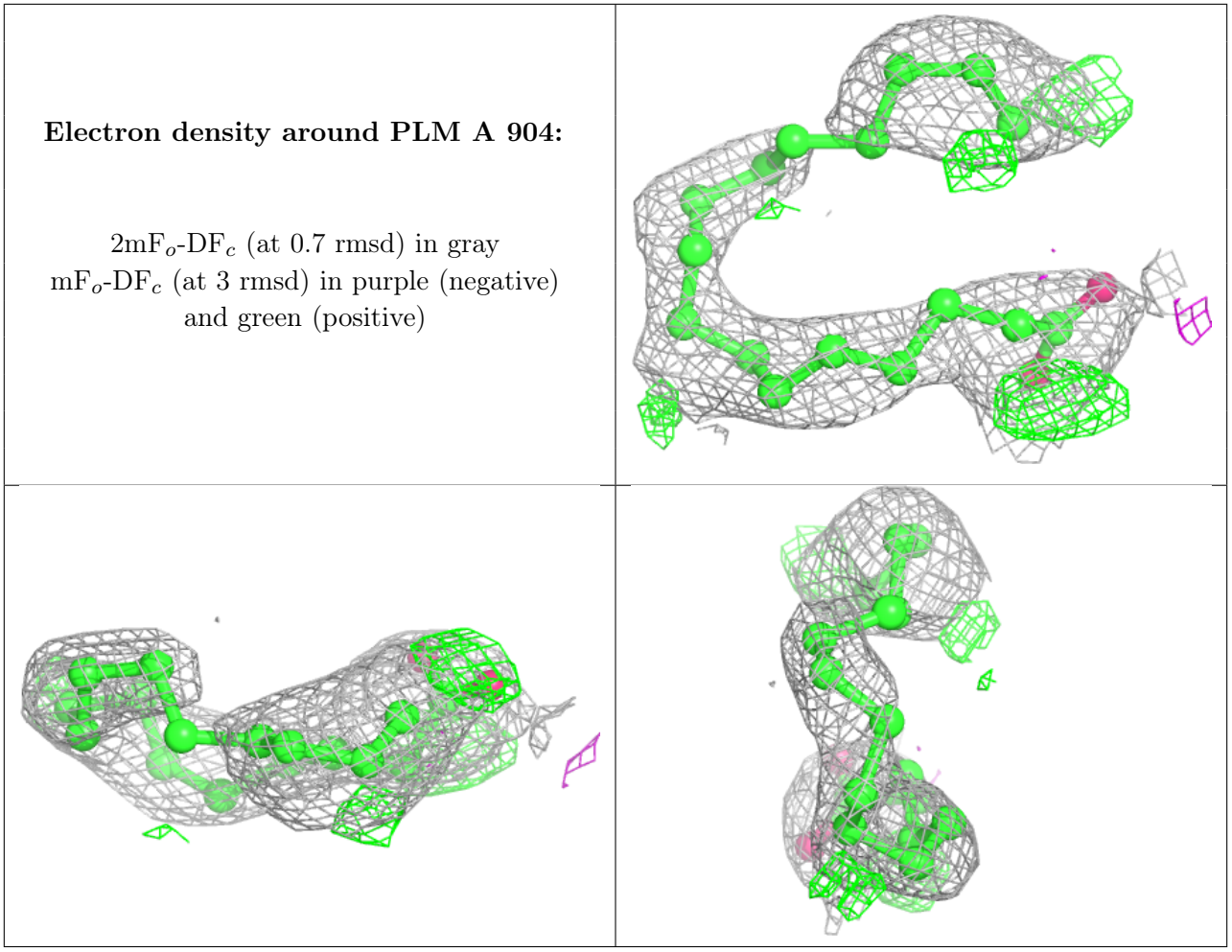






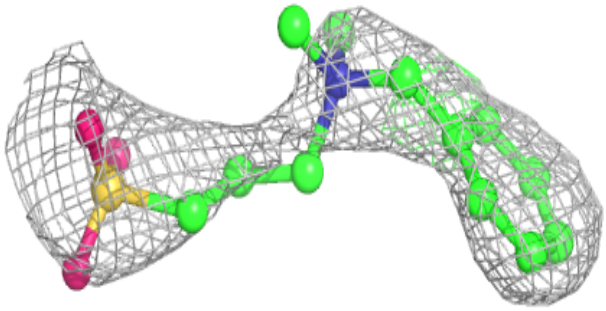
Electron density around PLM A 904:

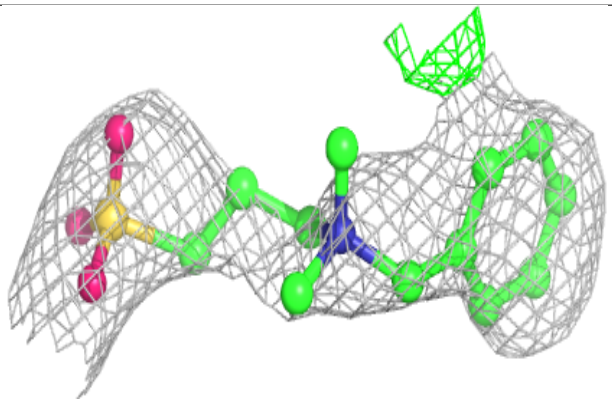
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

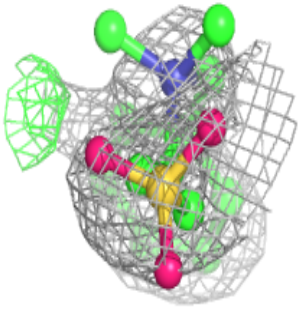


Electron density around DMX C 905:

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

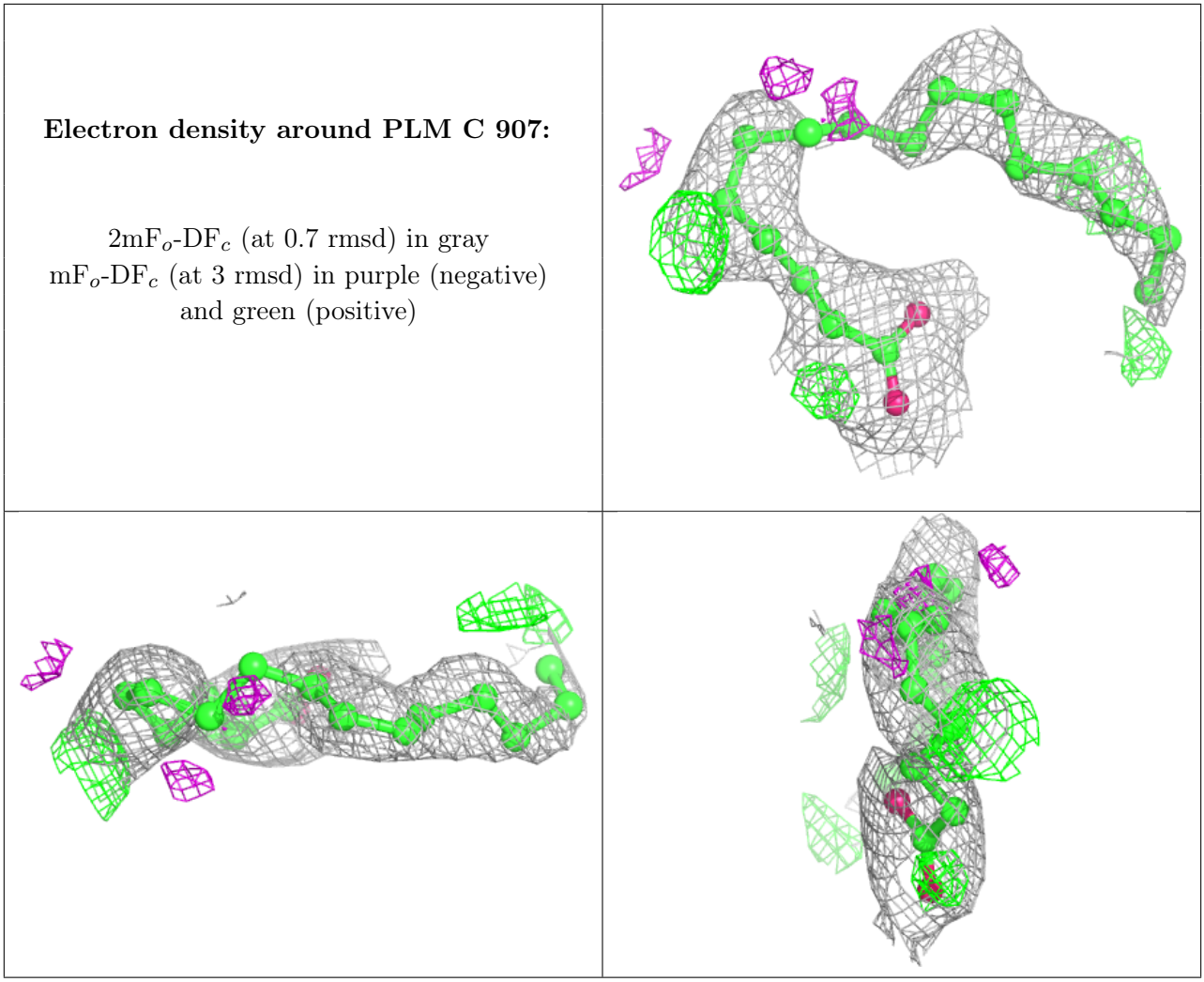






Electron density around PLM C 907:

$2mF_o$-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.