wwPDB X-ray Structure Validation Summary Report (i)

Apr 12, 2022 – 08:06 AM EDT

PDB ID	:	2QJR
Title	:	dipepdyl peptidase IV in complex with inhibitor PZF
Authors	:	Shenping, L.
Deposited on	:	2007-07-09
Resolution	:	2.20 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 following versions of software and data (see references (i)) were used in the production of this report:

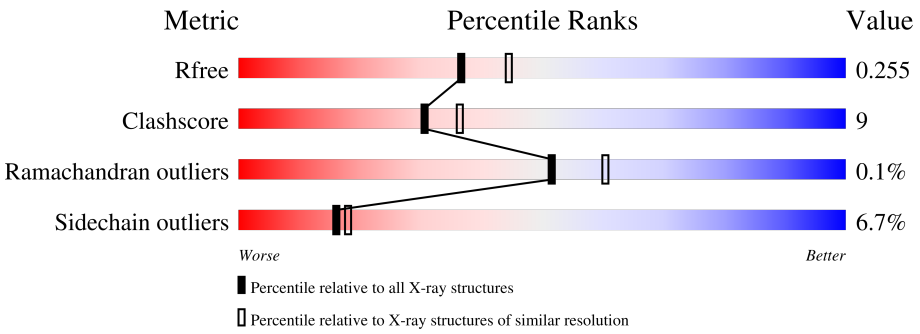
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Mol	Chain	Length	Quality of chain
1	A	748	75% 20% • •
1	B	748	69% 23% 5% •
2	C	2	100%
2	E	2	100%
2	F	2	50% 50%
2	G	2	100%
2	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	D	4	100%

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
2	NAG	G	1	X	-	-	-
2	NAG	H	1	X	-	-	-
3	LGU	D	3	X	-	-	-
6	LGU	A	803	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12532 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 Dipeptidyl peptidase 4 membrane form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5957	3825	980	1126	26	0	0	0
1	B	728	5957	3825	980	1126	26	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	LEU	-	expression tag	UNP P27487
A	768	VAL	-	expression tag	UNP P27487
A	769	PRO	-	expression tag	UNP P27487
A	770	ARG	-	expression tag	UNP P27487
A	771	GLY	-	expression tag	UNP P27487
A	772	SER	-	expression tag	UNP P27487
A	773	HIS	-	expression tag	UNP P27487
A	774	HIS	-	expression tag	UNP P27487
A	775	HIS	-	expression tag	UNP P27487
A	776	HIS	-	expression tag	UNP P27487
A	777	HIS	-	expression tag	UNP P27487
A	778	HIS	-	expression tag	UNP P27487
B	767	LEU	-	expression tag	UNP P27487
B	768	VAL	-	expression tag	UNP P27487
B	769	PRO	-	expression tag	UNP P27487
B	770	ARG	-	expression tag	UNP P27487
B	771	GLY	-	expression tag	UNP P27487
B	772	SER	-	expression tag	UNP P27487
B	773	HIS	-	expression tag	UNP P27487
B	774	HIS	-	expression tag	UNP P27487
B	775	HIS	-	expression tag	UNP P27487
B	776	HIS	-	expression tag	UNP P27487
B	777	HIS	-	expression tag	UNP P27487
B	778	HIS	-	expression tag	UNP P27487

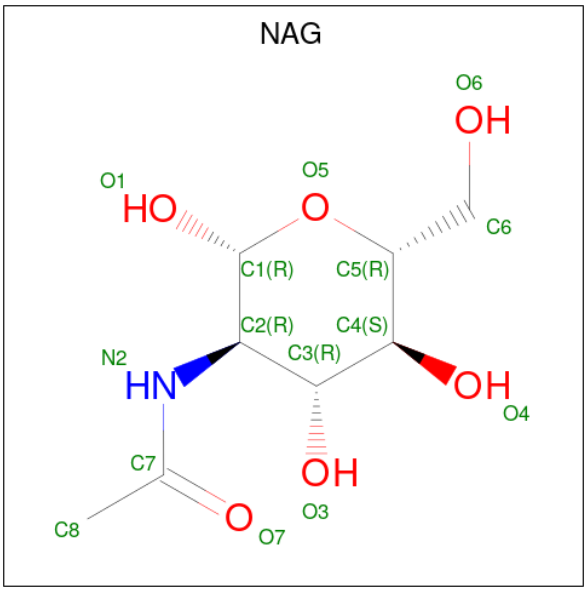
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0
2	G	2	28	16	2	10	0	0	0
2	H	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-L-gulopyranuronic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

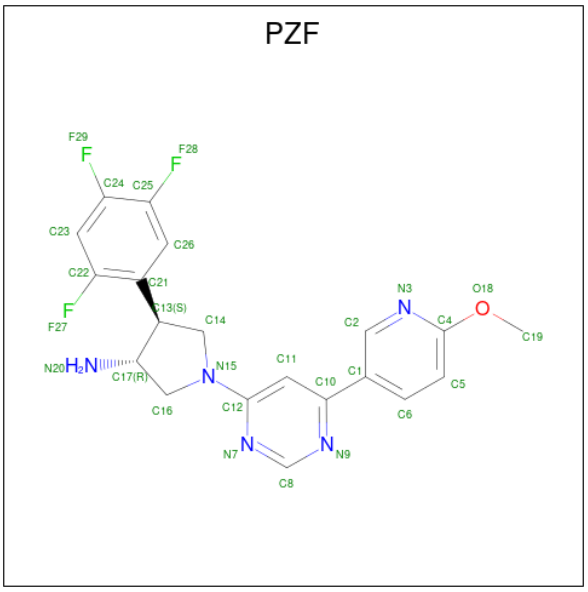
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	4	50	28	2	20	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is (3R,4S)-1-[6-(6-METHOXYPYRIDIN-3-YL)PYRIMIDIN-4-YL]-4-(2,4,5-TRIFLUOROPHENYL)PYRROLIDIN-3-AMINE (three-letter code: PZF) (formula: $C_{20}H_{18}F_3N_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
5	A	1	29	20	3	5	1	0	0

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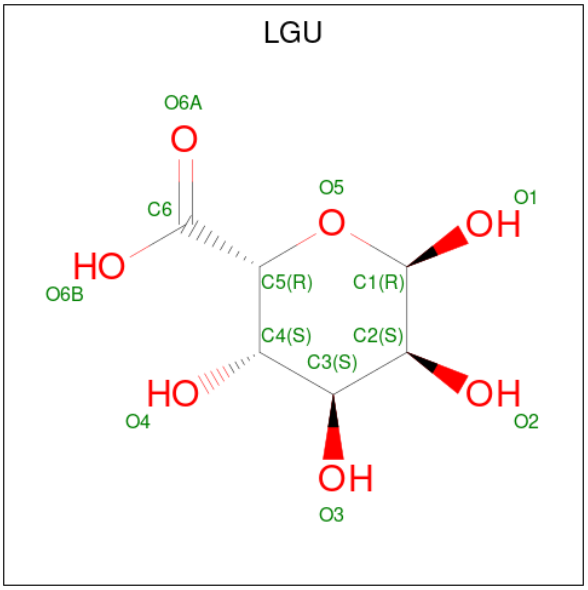
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
5	B	1	29	20	3	5	1	0	0

- Molecule 6 is alpha-L-gulopyranuronic acid (three-letter code: LGU) (formula: $C_6H_{10}O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	O				
6	A	1	11	6	5			0	0

- Molecule 7 is water.

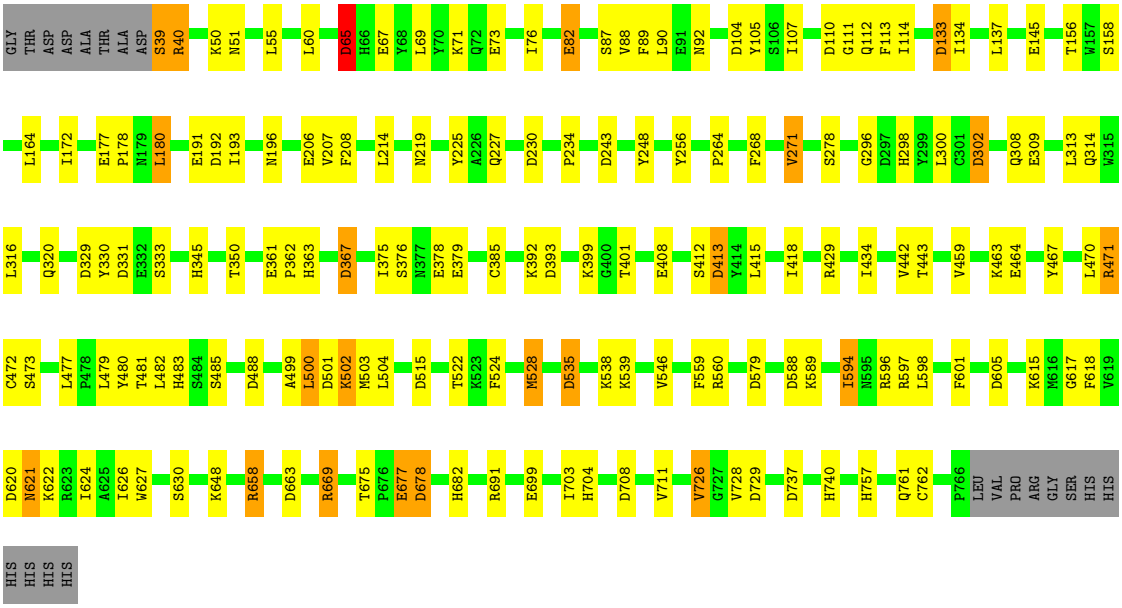
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	O					
7	A	105	105	105				0	0
			Total	O					
7	B	226	226	226				0	0

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. 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. 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.

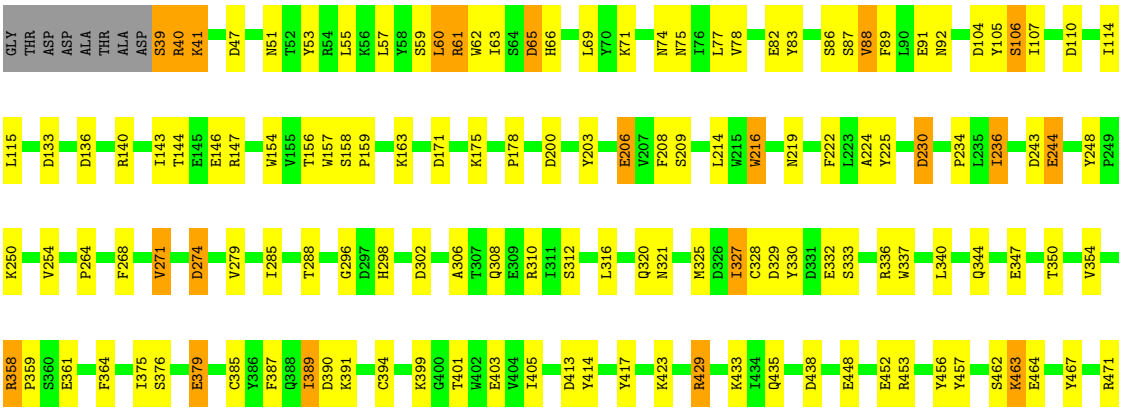
- Molecule 1: Dipeptidyl peptidase 4 membrane form

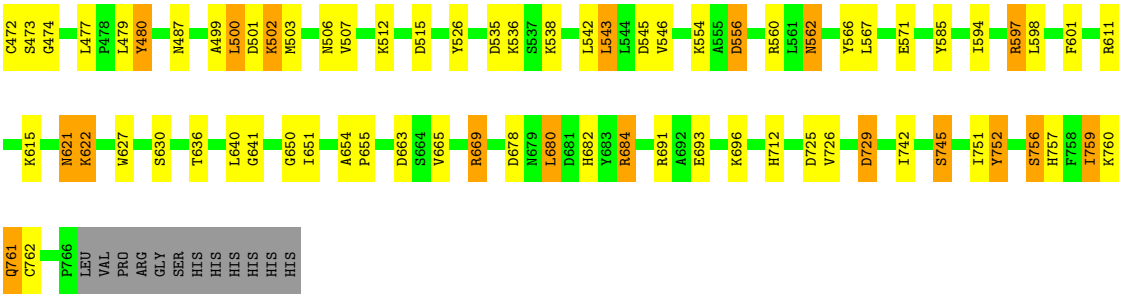
Chain A:



- Molecule 1: Dipeptidyl peptidase 4 membrane form

Chain B:



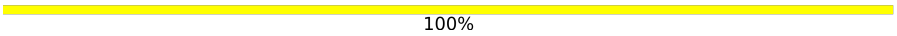


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

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

Chain E:



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

Chain F:

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

Chain G:

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

Chain H:

• Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-L-gulopyranuronic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1
NAG2
LGU3
MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.47Å 68.80Å 422.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.90 – 2.20 41.90 – 2.19	Depositor EDS
% Data completeness (in resolution range)	85.7 (41.90-2.20) 85.4 (41.90-2.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.191 , 0.253 0.200 , 0.255	Depositor DCC
R_{free} test set	4280 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.929	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12532	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LGU, PZF, NAG, MAN

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	1.12	6/6129 (0.1%)	1.09	33/8336 (0.4%)
1	B	1.43	42/6129 (0.7%)	1.24	43/8336 (0.5%)
All	All	1.29	48/12258 (0.4%)	1.17	76/16672 (0.5%)

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	385	CYS	CB-SG	-8.03	1.68	1.82
1	B	250	LYS	CD-CE	6.76	1.68	1.51
1	B	244	GLU	CD-OE1	6.63	1.32	1.25
1	B	83	TYR	CE1-CZ	6.46	1.47	1.38
1	B	82	GLU	CD-OE1	6.43	1.32	1.25

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	669	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	A	669	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	B	453	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	B	61	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	A	658	ARG	NE-CZ-NH1	10.27	125.44	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5957	0	5672	94	0
1	B	5957	0	5672	125	0
2	C	28	0	25	1	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	2	0
2	H	28	0	25	1	0
3	D	50	0	40	0	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
5	A	29	0	18	1	0
5	B	29	0	18	0	0
6	A	11	0	7	0	0
7	A	105	0	0	10	0
7	B	226	0	0	22	0
All	All	12532	0	11578	219	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 9.

The worst 5 of 219 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:A:39:SER:O	1:A:40:ARG:CZ	1.79	1.29
1:B:40:ARG:N	1:B:40:ARG:HD3	1.64	1.12
1:B:39:SER:HB2	1:B:40:ARG:HD2	1.31	1.08
1:B:597:ARG:HD3	7:B:992:HOH:O	1.56	1.02
1:A:621:ASN:C	1:A:621:ASN:HD22	1.64	0.99

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	726/748 (97%)	694 (96%)	31 (4%)	1 (0%)	51	60
1	B	726/748 (97%)	689 (95%)	36 (5%)	1 (0%)	51	60
All	All	1452/1496 (97%)	1383 (95%)	67 (5%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	630	SER

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	651/669 (97%)	610 (94%)	41 (6%)	18	20
1	B	651/669 (97%)	605 (93%)	46 (7%)	14	16
All	All	1302/1338 (97%)	1215 (93%)	87 (7%)	16	18

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	271	VAL
1	B	500	LEU
1	B	288	THR
1	B	361	GLU
1	B	542	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	75	ASN

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Mol	Chain	Res	Type
1	B	263	ASN
1	B	682	HIS
1	B	169	ASN
1	B	298	HIS

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	NAG	C	1	2,1	14,14,15	1.50	3 (21%)	17,19,21	1.64	4 (23%)
2	NAG	C	2	2	14,14,15	0.86	0	17,19,21	1.94	6 (35%)
3	NAG	D	1	3,1	14,14,15	1.30	2 (14%)	17,19,21	2.20	9 (52%)
3	NAG	D	2	3	14,14,15	0.91	0	17,19,21	1.15	1 (5%)
3	LGU	D	3	3,6	11,11,13	0.84	1 (9%)	15,15,19	2.44	6 (40%)
3	MAN	D	4	3	11,11,12	1.10	1 (9%)	15,15,17	1.77	1 (6%)
2	NAG	E	1	2,1	14,14,15	0.73	0	17,19,21	2.60	6 (35%)
2	NAG	E	2	2	14,14,15	0.81	1 (7%)	17,19,21	1.37	2 (11%)
2	NAG	F	1	2,1	14,14,15	1.21	1 (7%)	17,19,21	2.24	4 (23%)
2	NAG	F	2	2	14,14,15	1.21	1 (7%)	17,19,21	1.72	5 (29%)
2	NAG	G	1	2,1	14,14,15	1.13	1 (7%)	17,19,21	1.88	4 (23%)
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	1.53	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	H	1	2,1	14,14,15	0.90	1 (7%)	17,19,21	1.77	2 (11%)
2	NAG	H	2	2	14,14,15	0.65	0	17,19,21	1.81	5 (29%)

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	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	LGU	D	3	3,6	1/1/4/6	2/2/19/24	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2,1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2,1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	O5-C1	-3.60	1.38	1.43
3	D	1	NAG	O5-C1	-3.55	1.38	1.43
2	C	1	NAG	O5-C1	-3.19	1.38	1.43
2	C	1	NAG	C2-N2	-3.18	1.40	1.46
2	H	1	NAG	O5-C1	-2.74	1.39	1.43

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C1-O5-C5	6.95	121.60	112.19
2	F	1	NAG	O5-C1-C2	-6.83	100.50	111.29
3	D	4	MAN	O5-C1-C2	-5.73	101.93	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3	LGU	C1-O5-C5	5.22	119.27	112.19
2	E	1	NAG	O5-C1-C2	5.11	119.35	111.29

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NAG	C1
2	H	1	NAG	C1
3	D	3	LGU	C5

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3	LGU	C4-C5-C6-O6B
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	D	3	LGU	O5-C5-C6-O6B
3	D	1	NAG	C4-C5-C6-O6

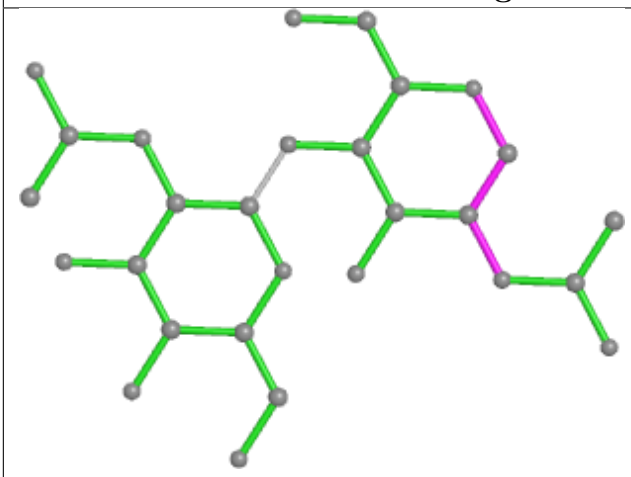
There are no ring outliers.

6 monomers are involved in 5 short contacts:

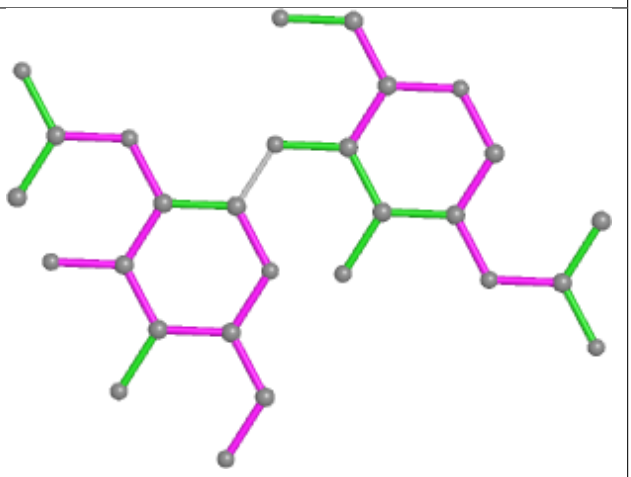
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	C	1	NAG	1	0
2	G	2	NAG	1	0
2	C	2	NAG	1	0
2	H	1	NAG	1	0
2	F	1	NAG	1	0

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

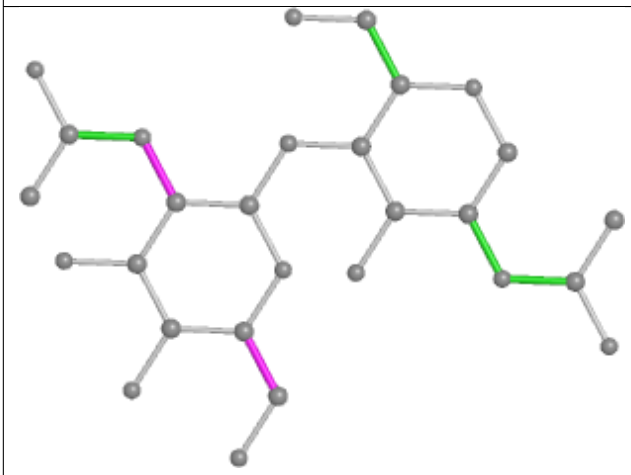
Oligosaccharide Chain C



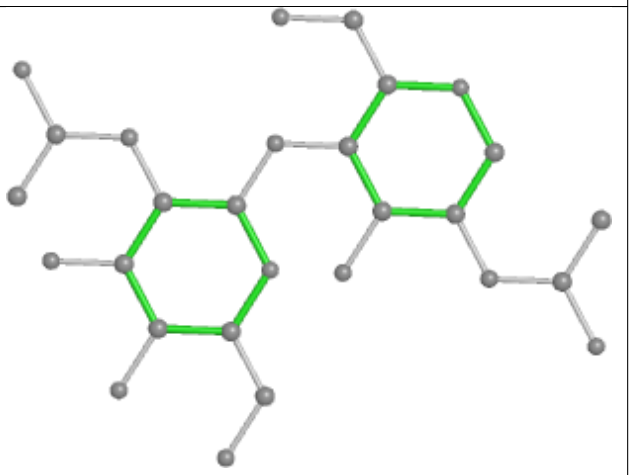
Bond lengths



Bond angles

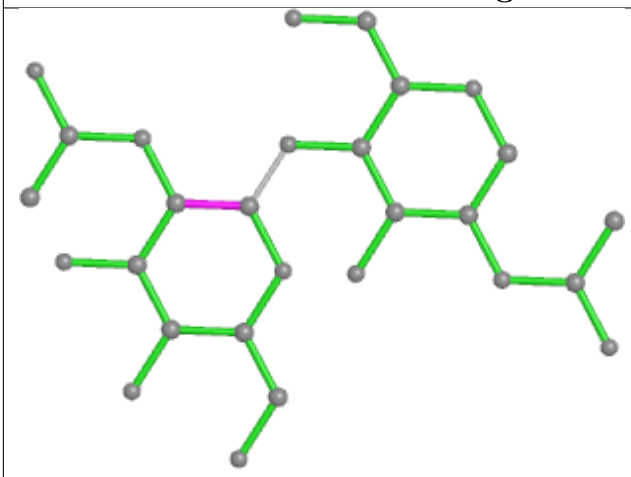


Torsions

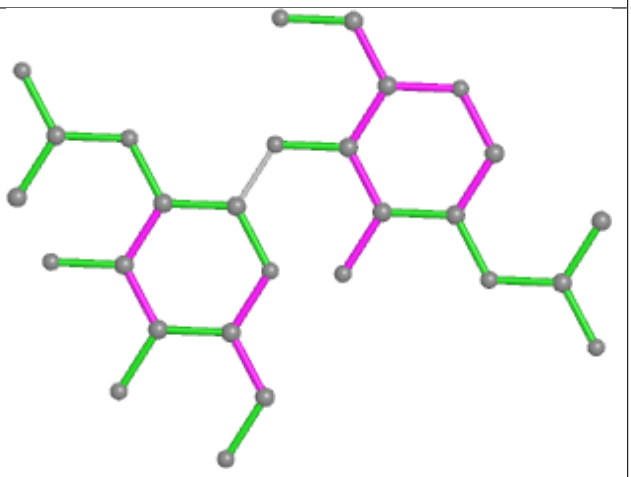


Rings

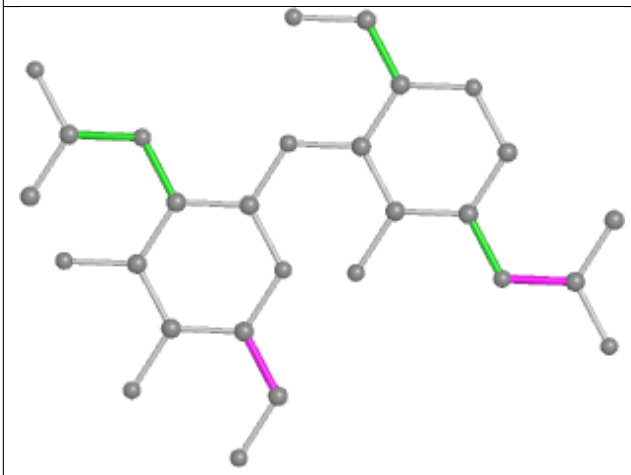
Oligosaccharide Chain E



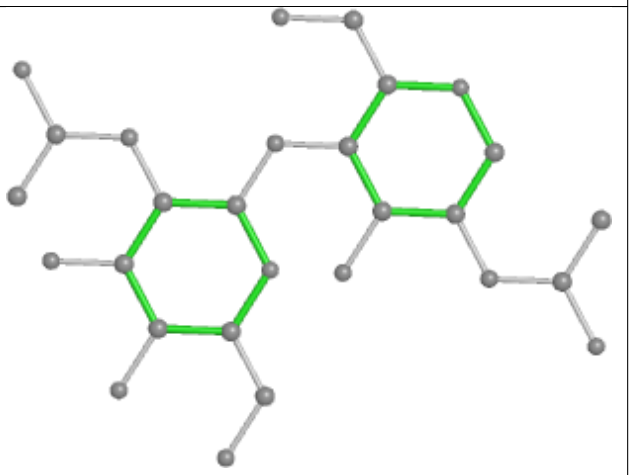
Bond lengths



Bond angles

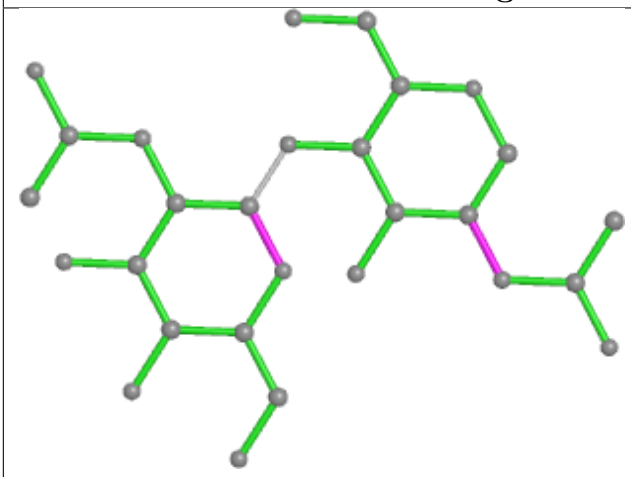


Torsions

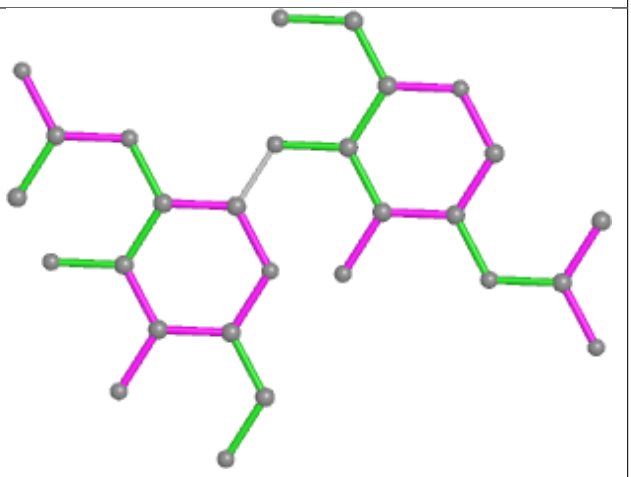


Rings

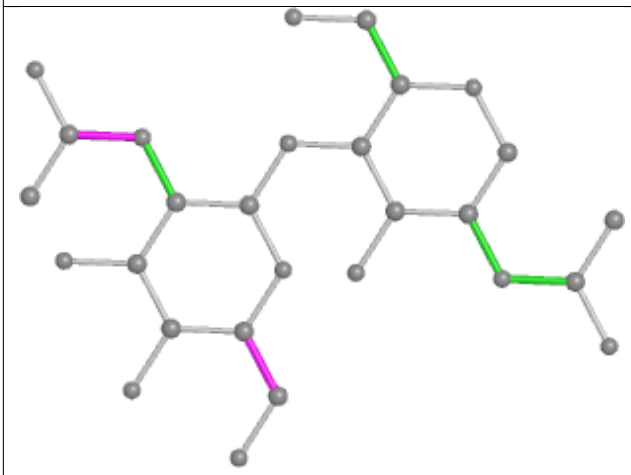
Oligosaccharide Chain F



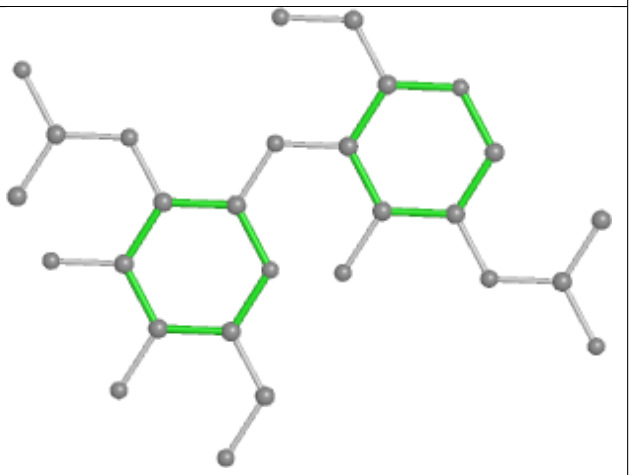
Bond lengths



Bond angles

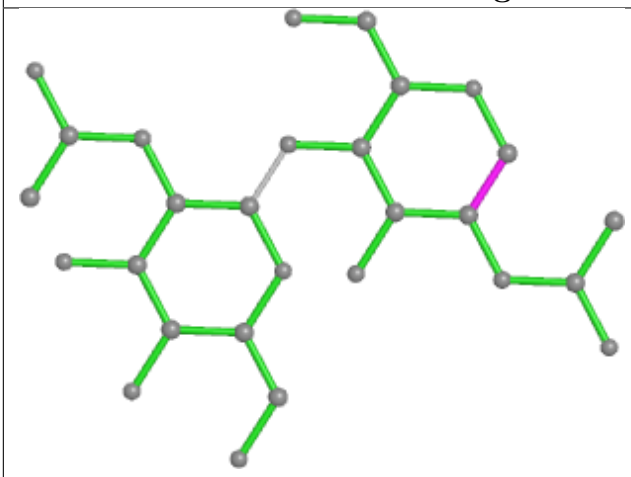


Torsions

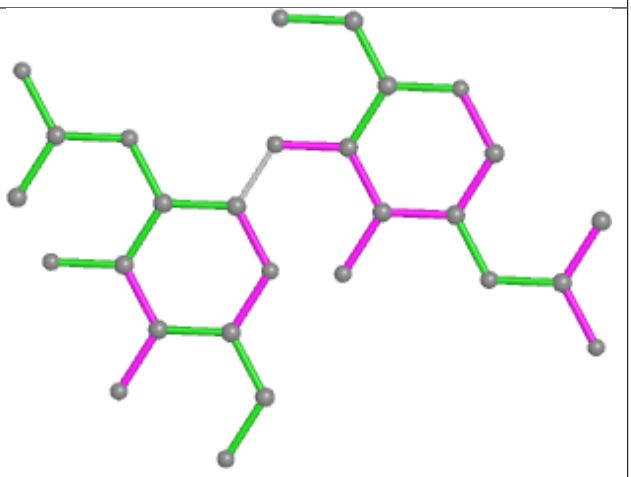


Rings

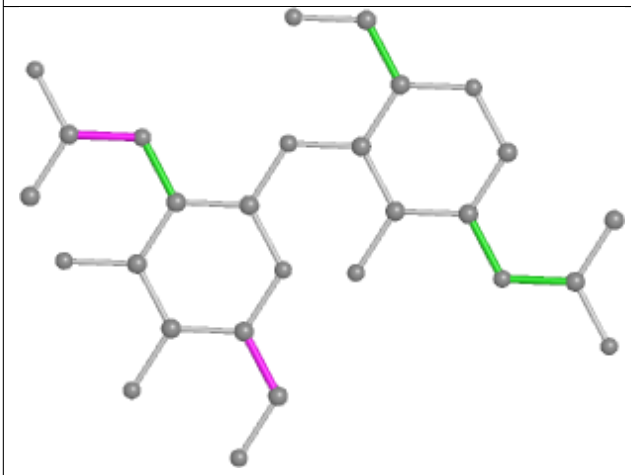
Oligosaccharide Chain G



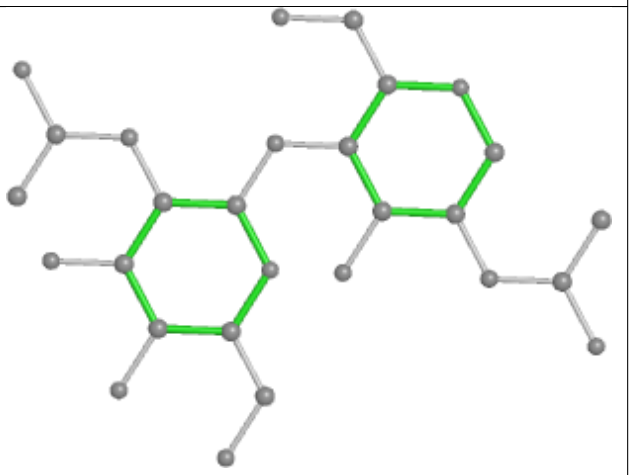
Bond lengths



Bond angles

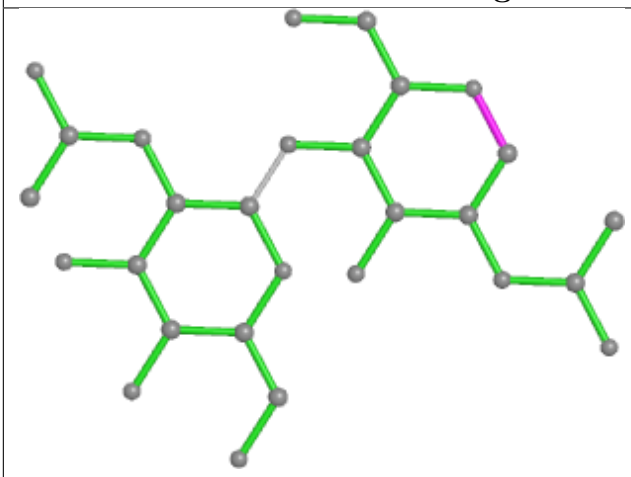


Torsions

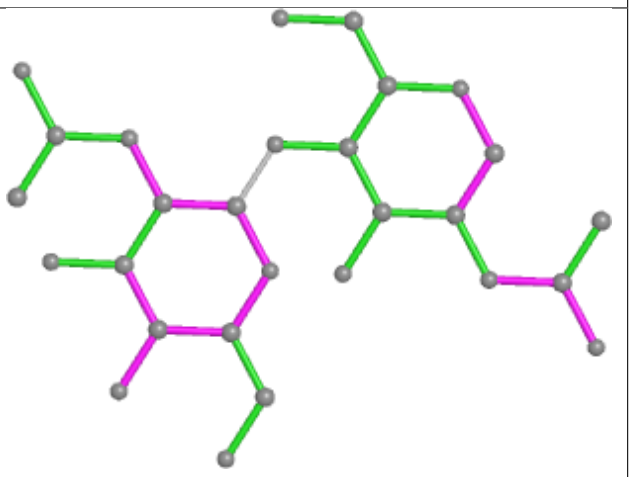


Rings

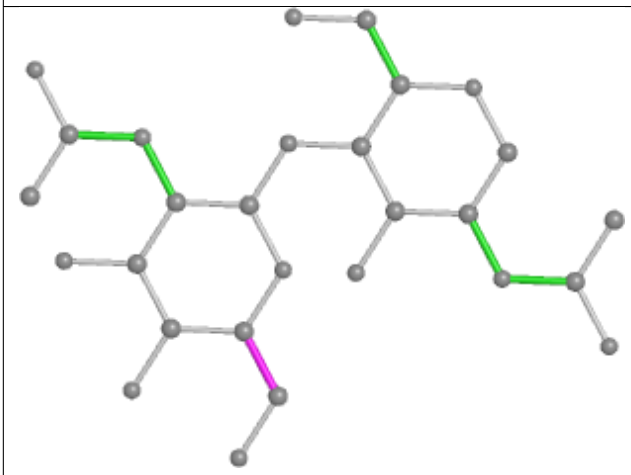
Oligosaccharide Chain H



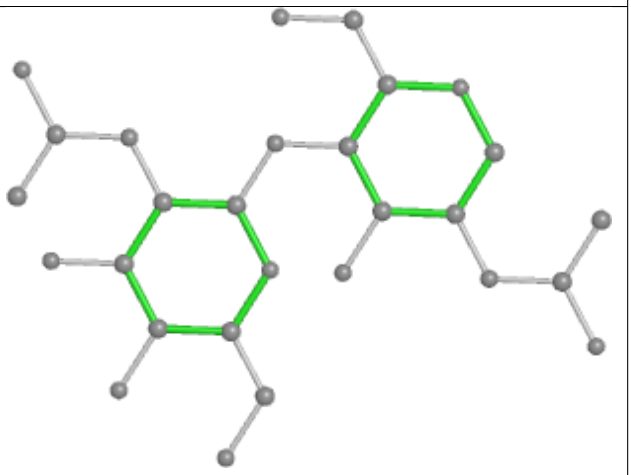
Bond lengths



Bond angles

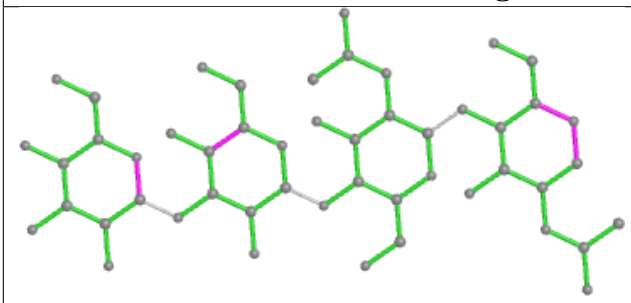


Torsions

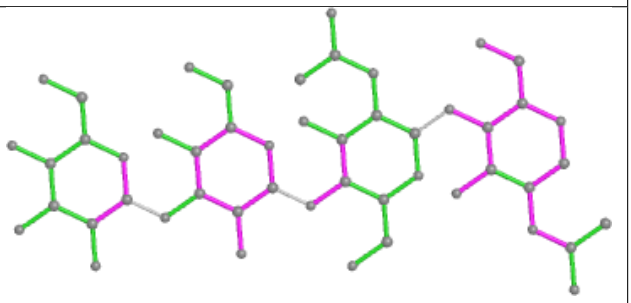


Rings

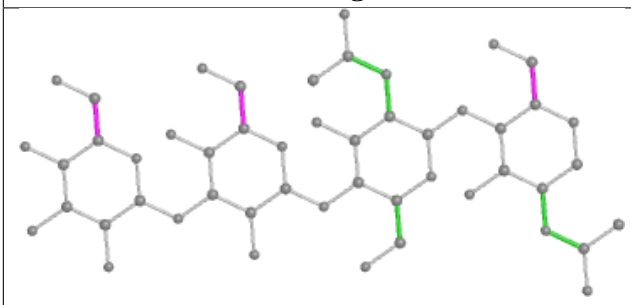
Oligosaccharide Chain D



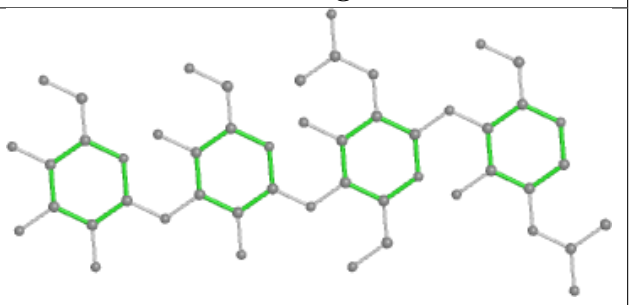
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	801	1	14,14,15	0.92	1 (7%)	17,19,21	1.50	3 (17%)
5	PZF	A	802	-	32,32,32	0.99	1 (3%)	40,46,46	2.36	16 (40%)
4	NAG	B	801	1	14,14,15	1.16	1 (7%)	17,19,21	2.39	7 (41%)
6	LGU	A	803	3	11,11,13	0.87	0	15,15,19	1.98	5 (33%)
5	PZF	B	802	-	32,32,32	1.50	8 (25%)	40,46,46	2.60	15 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	801	1	-	4/6/23/26	0/1/1/1
5	PZF	A	802	-	-	0/14/26/26	0/4/4/4
4	NAG	B	801	1	-	2/6/23/26	0/1/1/1
6	LGU	A	803	3	1/1/4/6	2/2/19/24	0/1/1/1
5	PZF	B	802	-	-	0/14/26/26	0/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	NAG	O5-C1	-3.60	1.38	1.43
5	B	802	PZF	C26-C21	-3.33	1.34	1.39
5	B	802	PZF	F29-C24	-2.75	1.28	1.35
5	B	802	PZF	C4-N3	2.57	1.36	1.32
5	B	802	PZF	C14-N15	2.54	1.49	1.46

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	802	PZF	C8-N7-C12	8.15	122.06	114.94
5	B	802	PZF	C10-C11-C12	6.69	121.42	117.03
5	A	802	PZF	C8-N7-C12	5.90	120.09	114.94
5	A	802	PZF	C8-N9-C10	5.82	123.63	115.74
5	A	802	PZF	N9-C8-N7	-5.34	120.25	128.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	803	LGU	C5

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2
6	A	803	LGU	O5-C5-C6-O6B
6	A	803	LGU	C4-C5-C6-O6B
4	B	801	NAG	C4-C5-C6-O6

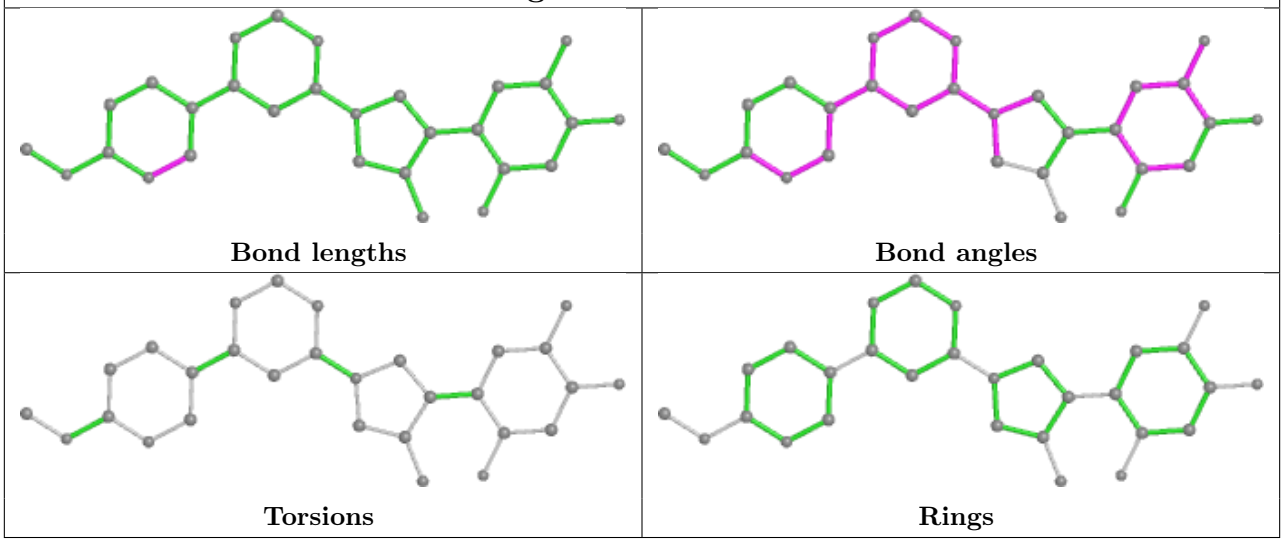
There are no ring outliers.

2 monomers are involved in 2 short contacts:

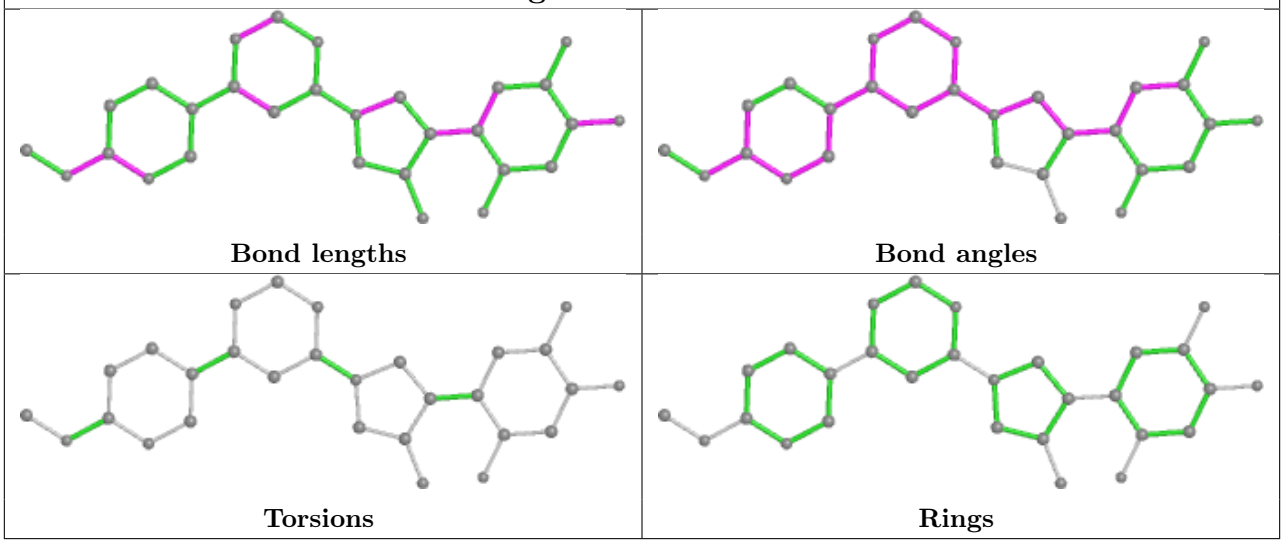
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	802	PZF	1	0
4	B	801	NAG	1	0

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.

Ligand PZF A 802



Ligand PZF B 802



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

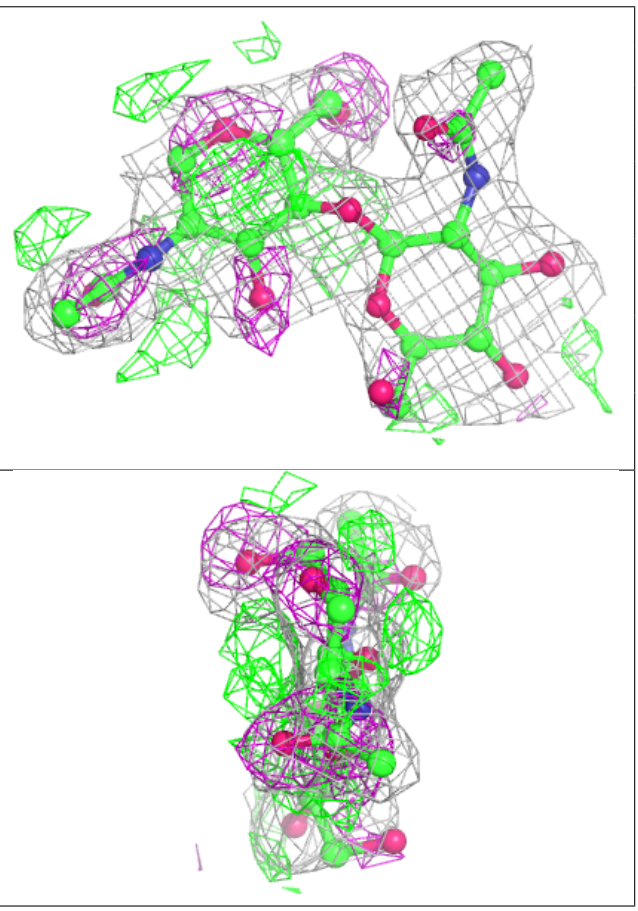
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

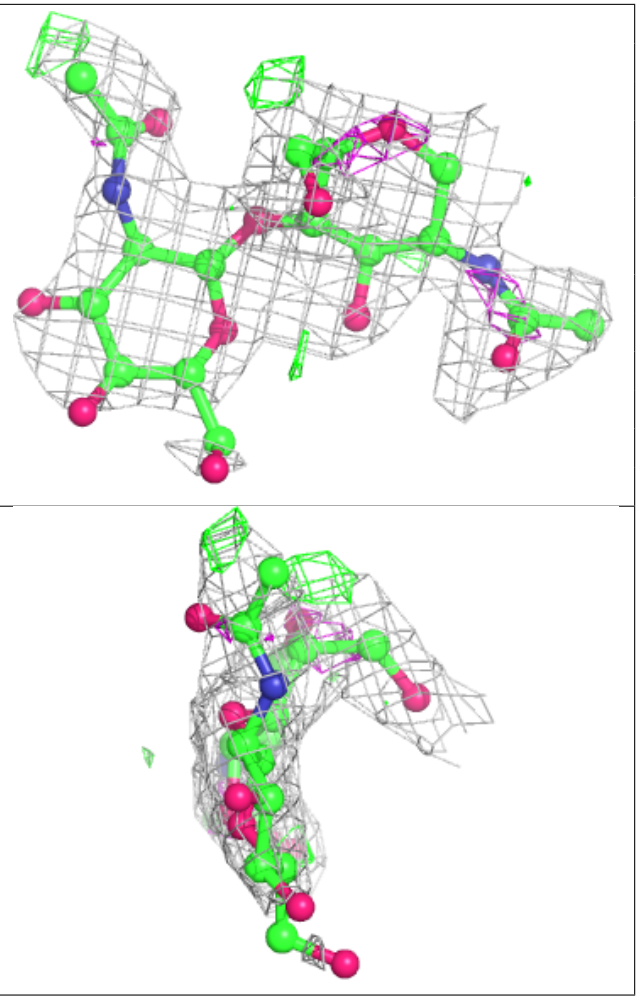
Electron density around Chain C:

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



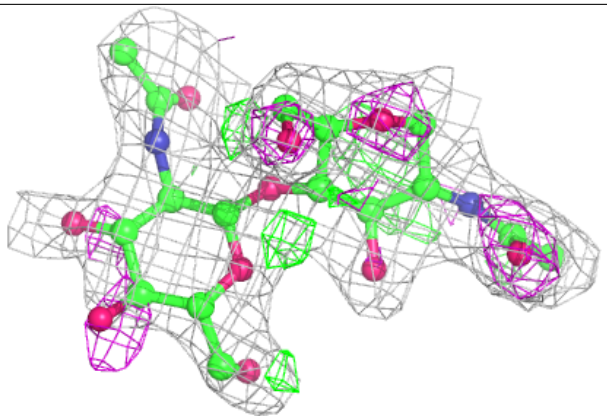
Electron density around Chain E:

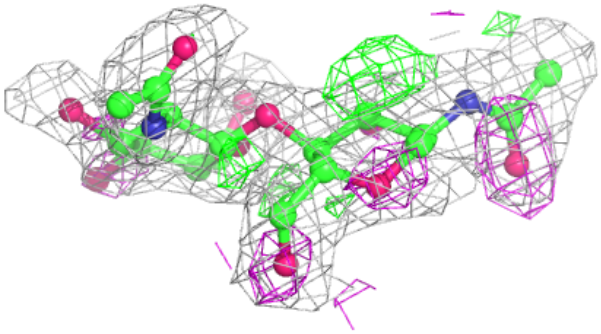
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

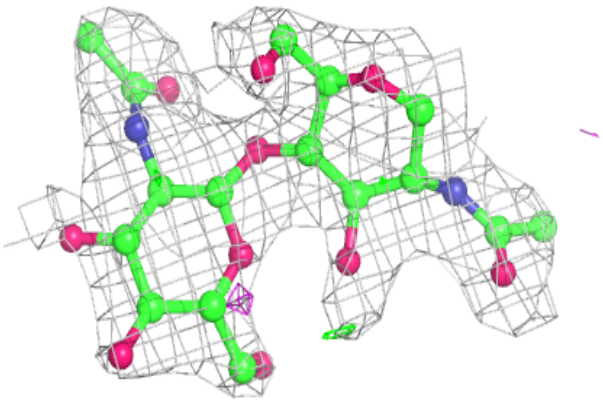
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

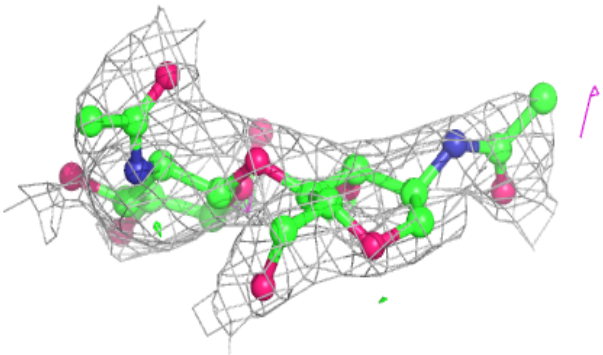


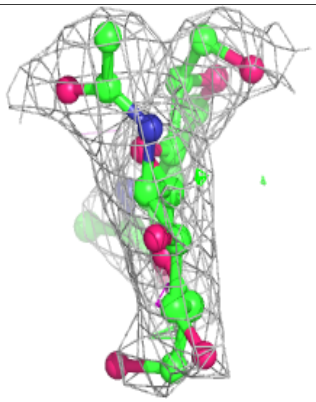


Electron density around Chain G:

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

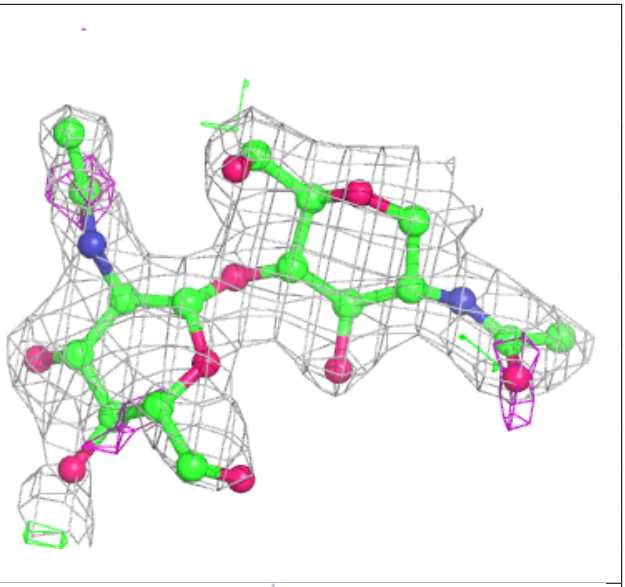


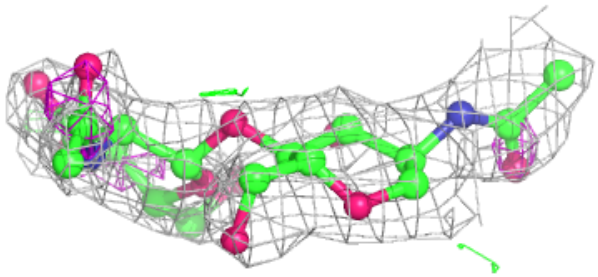


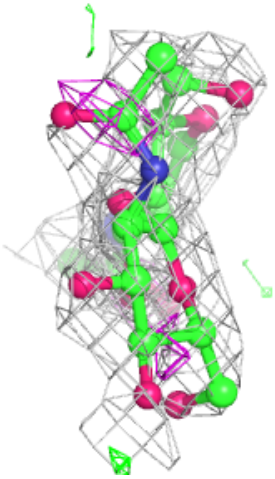


Electron density around Chain H:

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

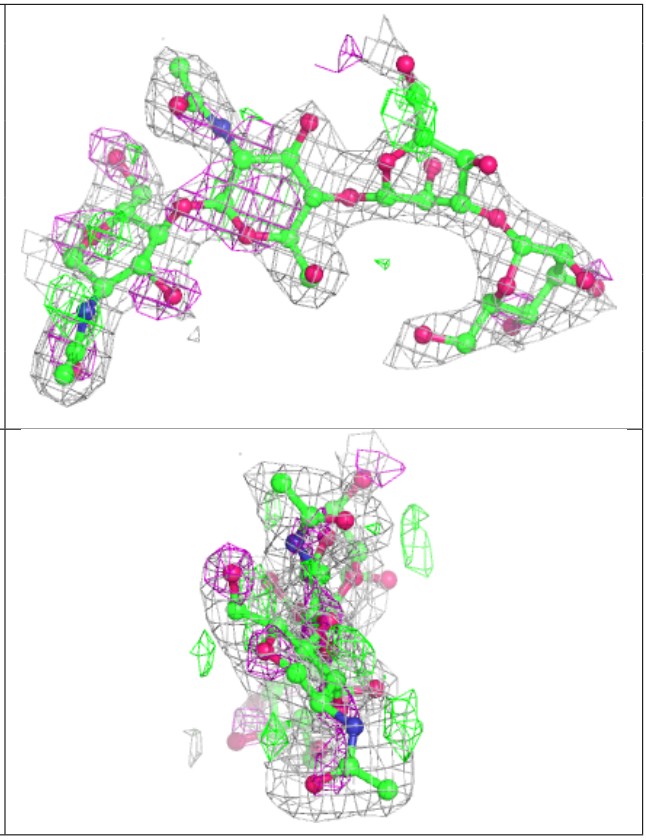






Electron density around Chain D:

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



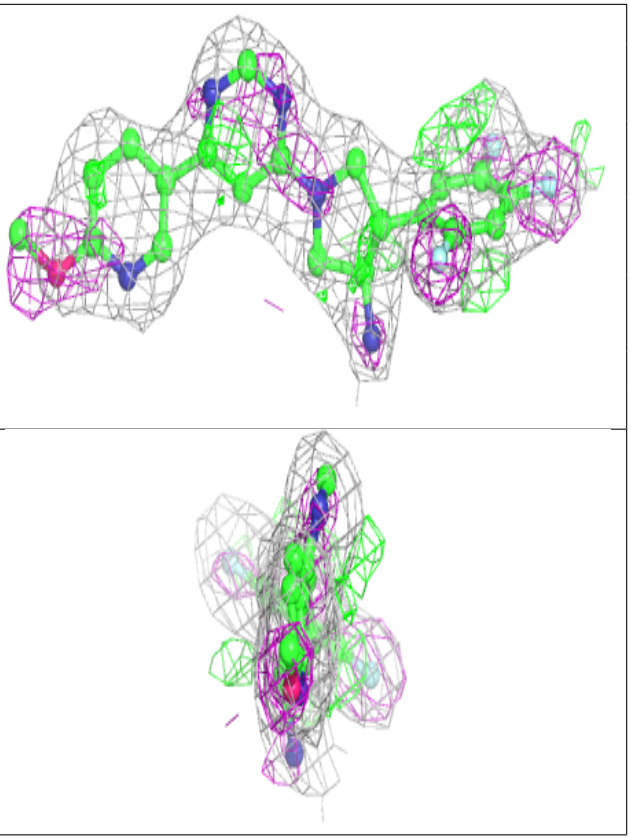
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

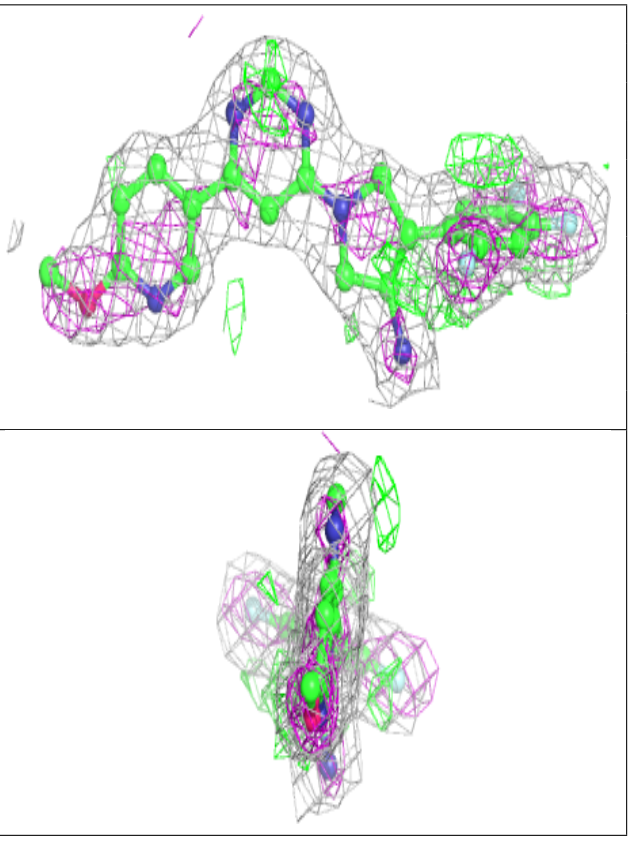
Electron density around PZF A 802:

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



Electron density around PZF B 802:

$2mF_o$-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 (i)

Unable to reproduce the depositors R factor - this section is therefore empty.