Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 12:05 PM EDT

PDB ID	:	6TRH
Title	:	Structure of E70A mutant of Rex8A from Paenibacillus barcinonensis complexed with 3(3)-alpha-L-arabinofuranosyl-xylotetraose.
Authors	:	Jimenez-Ortega, E.; Ramirez-Escudero, M.; Sanz-Aparicio, J.
Deposited on	:	2019-12-18
Resolution	:	1.86 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 (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:

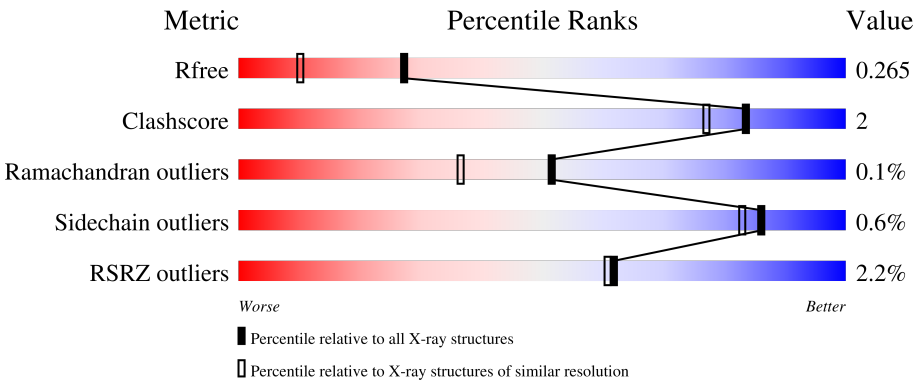
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	385	% 93% 6% •
1	B	385	4% 91% 7% •
1	C	385	2% 92% 8% •
1	D	385	2% 95% • •
2	E	5	100%

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Mol	Chain	Length	Quality of chain
2	F	5	100%
2	G	5	100%
2	H	5	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12933 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 Reducing-end xylose-releasing exo-oligoxylanase Rex8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	3128	1995	536	582	15	0	0	0
1	B	380	3132	1998	538	581	15	0	1	0
1	C	385	3173	2023	545	589	16	0	2	0
1	D	380	3124	1993	535	581	15	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	ALA	GLU	engineered mutation	UNP A0A0S2UQQ5
A	381	GLN	-	expression tag	UNP A0A0S2UQQ5
A	382	GLN	-	expression tag	UNP A0A0S2UQQ5
A	383	ALA	-	expression tag	UNP A0A0S2UQQ5
A	384	ALA	-	expression tag	UNP A0A0S2UQQ5
A	385	ALA	-	expression tag	UNP A0A0S2UQQ5
B	70	ALA	GLU	engineered mutation	UNP A0A0S2UQQ5
B	381	GLN	-	expression tag	UNP A0A0S2UQQ5
B	382	GLN	-	expression tag	UNP A0A0S2UQQ5
B	383	ALA	-	expression tag	UNP A0A0S2UQQ5
B	384	ALA	-	expression tag	UNP A0A0S2UQQ5
B	385	ALA	-	expression tag	UNP A0A0S2UQQ5
C	70	ALA	GLU	engineered mutation	UNP A0A0S2UQQ5
C	381	GLN	-	expression tag	UNP A0A0S2UQQ5
C	382	GLN	-	expression tag	UNP A0A0S2UQQ5
C	383	ALA	-	expression tag	UNP A0A0S2UQQ5
C	384	ALA	-	expression tag	UNP A0A0S2UQQ5
C	385	ALA	-	expression tag	UNP A0A0S2UQQ5
D	70	ALA	GLU	engineered mutation	UNP A0A0S2UQQ5
D	381	GLN	-	expression tag	UNP A0A0S2UQQ5
D	382	GLN	-	expression tag	UNP A0A0S2UQQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	383	ALA	-	expression tag	UNP A0A0S2UQQ5
D	384	ALA	-	expression tag	UNP A0A0S2UQQ5
D	385	ALA	-	expression tag	UNP A0A0S2UQQ5

- Molecule 2 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	5	46	25	21	0	0	0
2	F	5	46	25	21	0	0	0
2	G	5	46	25	21	0	0	0
2	H	5	46	25	21	0	0	0

- Molecule 3 is water.

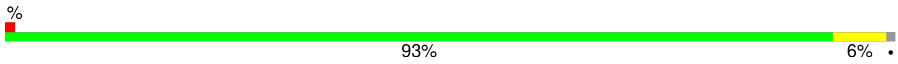
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	50	50	50	0	0
3	B	46	46	46	0	0
3	C	41	41	41	0	0
3	D	55	55	55	0	0

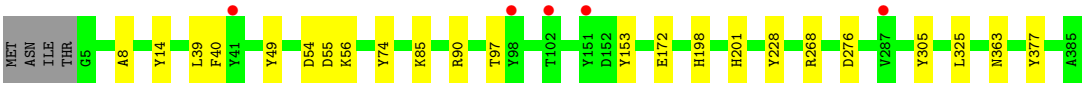
3 Residue-property plots (i)

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: Reducing-end xylose-releasing exo-oligoxylanase Rex8A

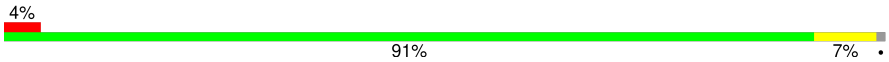
Chain A:

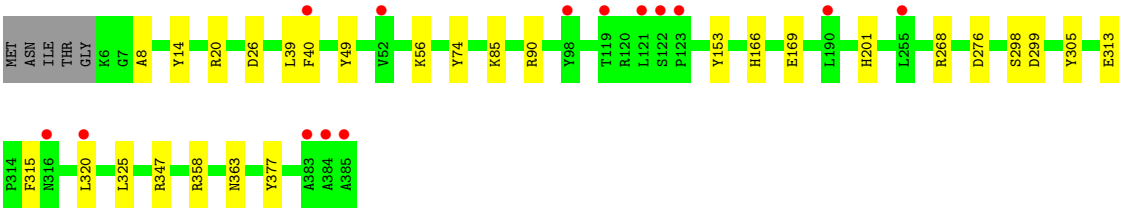




• Molecule 1: Reducing-end xylose-releasing exo-oligoxylanase Rex8A

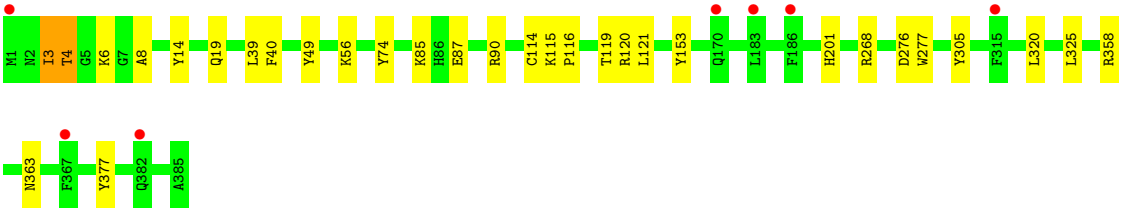
Chain B:





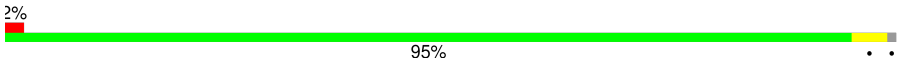
• Molecule 1: Reducing-end xylose-releasing exo-oligoxylanase Rex8A

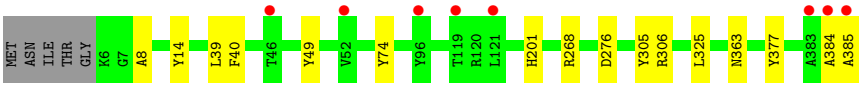
Chain C:



• Molecule 1: Reducing-end xylose-releasing exo-oligoxylanase Rex8A

Chain D:





• Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain E: 100%

XYP1
XYP2
XYP3
AHR4
XYP5

• Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain F: 100%

XYP1
XYP2
XYP3
AHR4
XYP5

• Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain G: 100%

XYP1
XYP2
XYP3
AHR4
XYP5

• Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain H: 100%

XYP1
XYP2
XYP3
AHR4
XYP5

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	82.30Å 82.72Å 465.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.62 – 1.86 46.62 – 1.86	Depositor EDS
% Data completeness (in resolution range)	95.7 (46.62-1.86) 95.7 (46.62-1.86)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.238 , 0.263 0.241 , 0.265	Depositor DCC
R_{free} test set	6472 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 13.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.428 for -k,-h,-l	Xtriage
Reported twinning fraction	0.520 for H, K, L 0.480 for -K, -H, -L	Depositor
Outliers	0 of 129753 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12933	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: AHR, XYP

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	0.65	0/3235	0.74	0/4394
1	B	0.65	0/3242	0.74	0/4403
1	C	0.65	0/3286	0.74	0/4462
1	D	0.65	0/3231	0.73	0/4389
All	All	0.65	0/12994	0.74	0/17648

There are no bond length outliers.

There are no bond angle outliers.

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	3128	0	2867	13	0
1	B	3132	0	2877	17	0
1	C	3173	0	2924	24	0
1	D	3124	0	2864	8	0
2	E	46	0	0	0	0
2	F	46	0	0	0	0
2	G	46	0	0	0	0
2	H	46	0	0	0	0
3	A	50	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	46	0	0	1	0
3	C	41	0	0	2	0
3	D	55	0	0	1	0
All	All	12933	0	11532	58	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 2.

All (58) 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:115:LYS:HG3	1:C:121:LEU:HD11	1.45	0.97
1:C:39:LEU:HD21	1:C:363:ASN:HB3	1.55	0.89
1:A:39:LEU:HD21	1:A:363:ASN:HB3	1.55	0.88
1:D:39:LEU:HD21	1:D:363:ASN:HB3	1.57	0.87
1:C:114:CYS:HA	1:C:121:LEU:HD13	1.57	0.86
1:B:39:LEU:HD21	1:B:363:ASN:HB3	1.58	0.84
1:B:320:LEU:HD11	1:B:358:ARG:HD3	1.73	0.71
1:B:320:LEU:HD11	1:B:358:ARG:CD	2.31	0.61
1:C:114:CYS:CA	1:C:121:LEU:HD13	2.31	0.59
1:D:40:PHE:HA	1:D:49:TYR:HB3	1.85	0.59
1:B:26:ASP:HB2	3:B:503:HOH:O	2.03	0.58
1:B:315:PHE:CZ	1:C:3:ILE:HG23	2.38	0.58
1:B:40:PHE:HA	1:B:49:TYR:HB3	1.85	0.58
1:C:40:PHE:HA	1:C:49:TYR:HB3	1.85	0.56
1:A:54:ASP:HB2	3:A:526:HOH:O	2.06	0.56
1:B:166:HIS:HB3	1:B:169:GLU:HG3	1.87	0.56
1:A:40:PHE:HA	1:A:49:TYR:HB3	1.86	0.56
1:B:315:PHE:CD2	1:C:3:ILE:HG22	2.41	0.55
1:B:315:PHE:CG	1:C:3:ILE:HG22	2.43	0.54
1:C:120:ARG:C	1:C:121:LEU:HD12	2.32	0.50
1:C:19:GLN:HG2	3:C:515:HOH:O	2.11	0.50
1:A:201:HIS:HB3	1:A:276:ASP:HA	1.94	0.50
1:B:201:HIS:HB3	1:B:276:ASP:HA	1.94	0.49
1:D:201:HIS:HB3	1:D:276:ASP:HA	1.94	0.49
1:C:201:HIS:HB3	1:C:276:ASP:HA	1.94	0.49
1:C:87:GLU:N	1:C:87:GLU:OE1	2.43	0.48
1:D:384:ALA:O	1:D:385:ALA:HB3	2.13	0.48
1:A:56:LYS:NZ	1:A:97:THR:HG21	2.29	0.48
1:B:8:ALA:HB1	1:B:14:TYR:CE1	2.49	0.47
1:A:55:ASP:HB3	3:A:526:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:TYR:OH	1:B:268:ARG:NH1	2.39	0.46
1:C:8:ALA:HB1	1:C:14:TYR:CE1	2.50	0.46
1:D:8:ALA:HB1	1:D:14:TYR:CE1	2.50	0.46
1:A:8:ALA:HB1	1:A:14:TYR:CE1	2.51	0.46
1:D:306:ARG:NH1	3:D:504:HOH:O	2.48	0.46
1:A:74:TYR:OH	1:A:268:ARG:NH1	2.37	0.46
1:D:74:TYR:OH	1:D:268:ARG:NH1	2.39	0.45
1:C:74:TYR:OH	1:C:268:ARG:NH1	2.38	0.45
1:C:119:THR:O	1:C:121:LEU:CD1	2.64	0.45
1:C:56:LYS:O	1:C:90:ARG:NH1	2.48	0.44
1:A:56:LYS:HZ3	1:A:97:THR:HG21	1.81	0.43
1:B:56:LYS:O	1:B:90:ARG:NH1	2.48	0.43
1:C:305:TYR:CD2	1:C:325:LEU:HD23	2.53	0.43
1:B:305:TYR:CD2	1:B:325:LEU:HD23	2.53	0.43
1:B:313:GLU:HB3	1:C:3:ILE:CD1	2.49	0.43
1:A:305:TYR:CD2	1:A:325:LEU:HD23	2.54	0.43
1:D:305:TYR:CD2	1:D:325:LEU:HD23	2.54	0.42
1:B:85:LYS:NZ	1:B:153:TYR:OH	2.50	0.42
1:C:4:THR:HG21	1:C:277:TRP:CH2	2.55	0.42
1:A:56:LYS:O	1:A:90:ARG:NH1	2.48	0.42
1:C:121:LEU:HD12	1:C:121:LEU:N	2.35	0.42
1:B:298:SER:O	1:B:347:ARG:NH2	2.51	0.41
1:A:85:LYS:NZ	1:A:153:TYR:OH	2.52	0.41
1:C:116:PRO:HD2	3:C:531:HOH:O	2.21	0.41
1:A:198:HIS:CE1	1:A:228:TYR:CD2	3.09	0.41
1:C:121:LEU:CD1	1:C:121:LEU:N	2.83	0.41
1:C:320:LEU:HD11	1:C:358:ARG:CZ	2.51	0.41
1:C:85:LYS:NZ	1:C:153:TYR:OH	2.52	0.41

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	379/385 (98%)	366 (97%)	13 (3%)	0	100	100
1	B	379/385 (98%)	365 (96%)	14 (4%)	0	100	100
1	C	385/385 (100%)	371 (96%)	12 (3%)	2 (0%)	29	15
1	D	378/385 (98%)	366 (97%)	12 (3%)	0	100	100
All	All	1521/1540 (99%)	1468 (96%)	51 (3%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	ILE
1	C	6	LYS

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	314/318 (99%)	312 (99%)	2 (1%)	86	83
1	B	315/318 (99%)	312 (99%)	3 (1%)	76	69
1	C	320/318 (101%)	318 (99%)	2 (1%)	86	83
1	D	314/318 (99%)	313 (100%)	1 (0%)	92	91
All	All	1263/1272 (99%)	1255 (99%)	8 (1%)	86	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	GLU
1	A	377	TYR
1	B	20	ARG
1	B	299	ASP
1	B	377	TYR
1	C	4	THR
1	C	377	TYR
1	D	377	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	350	ASN
1	D	316	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

20 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	XYP	E	1	2	10,10,10	1.32	2 (20%)	14,14,14	1.46	2 (14%)
2	XYP	E	2	2	9,9,10	1.61	2 (22%)	10,12,14	2.42	4 (40%)
2	XYP	E	3	2	9,9,10	1.96	3 (33%)	10,12,14	2.02	3 (30%)
2	AHR	E	4	2	9,9,10	1.84	3 (33%)	11,12,14	1.62	3 (27%)
2	XYP	E	5	2	9,9,10	2.09	2 (22%)	10,12,14	3.74	5 (50%)
2	XYP	F	1	2	10,10,10	1.49	2 (20%)	14,14,14	1.29	2 (14%)
2	XYP	F	2	2	9,9,10	1.46	2 (22%)	10,12,14	2.50	4 (40%)
2	XYP	F	3	2	9,9,10	1.89	3 (33%)	10,12,14	2.20	3 (30%)
2	AHR	F	4	2	9,9,10	1.98	3 (33%)	11,12,14	1.35	2 (18%)
2	XYP	F	5	2	9,9,10	2.10	4 (44%)	10,12,14	3.60	6 (60%)
2	XYP	G	1	2	10,10,10	1.62	2 (20%)	14,14,14	1.25	2 (14%)
2	XYP	G	2	2	9,9,10	1.64	3 (33%)	10,12,14	2.52	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	XYP	G	3	2	9,9,10	2.26	3 (33%)	10,12,14	2.11	3 (30%)
2	AHR	G	4	2	9,9,10	2.18	2 (22%)	11,12,14	1.44	2 (18%)
2	XYP	G	5	2	9,9,10	1.85	2 (22%)	10,12,14	3.82	5 (50%)
2	XYP	H	1	2	10,10,10	1.49	3 (30%)	14,14,14	1.26	2 (14%)
2	XYP	H	2	2	9,9,10	1.54	2 (22%)	10,12,14	2.43	3 (30%)
2	XYP	H	3	2	9,9,10	1.97	3 (33%)	10,12,14	2.23	3 (30%)
2	AHR	H	4	2	9,9,10	2.03	3 (33%)	11,12,14	1.38	1 (9%)
2	XYP	H	5	2	9,9,10	1.78	3 (33%)	10,12,14	3.93	5 (50%)

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	XYP	E	1	2	-	-	0/1/1/1
2	XYP	E	2	2	-	-	0/1/1/1
2	XYP	E	3	2	-	-	0/1/1/1
2	AHR	E	4	2	-	0/2/15/18	0/1/1/1
2	XYP	E	5	2	-	-	0/1/1/1
2	XYP	F	1	2	-	-	0/1/1/1
2	XYP	F	2	2	-	-	0/1/1/1
2	XYP	F	3	2	-	-	0/1/1/1
2	AHR	F	4	2	-	0/2/15/18	0/1/1/1
2	XYP	F	5	2	-	-	0/1/1/1
2	XYP	G	1	2	-	-	0/1/1/1
2	XYP	G	2	2	-	-	0/1/1/1
2	XYP	G	3	2	-	-	0/1/1/1
2	AHR	G	4	2	-	0/2/15/18	0/1/1/1
2	XYP	G	5	2	-	-	0/1/1/1
2	XYP	H	1	2	-	-	0/1/1/1
2	XYP	H	2	2	-	-	0/1/1/1
2	XYP	H	3	2	-	-	0/1/1/1
2	AHR	H	4	2	-	0/2/15/18	0/1/1/1
2	XYP	H	5	2	-	-	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	XYP	C2-C3	4.98	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	XYP	O5-C5	-4.73	1.34	1.43
2	G	4	AHR	C1-C2	4.44	1.59	1.51
2	H	4	AHR	C1-C2	4.43	1.59	1.51
2	G	5	XYP	O5-C5	-4.01	1.35	1.43
2	F	4	AHR	C1-C2	3.86	1.58	1.51
2	G	4	AHR	C2-C3	-3.78	1.47	1.53
2	F	5	XYP	O5-C5	-3.77	1.35	1.43
2	G	3	XYP	O3-C3	3.67	1.52	1.43
2	H	3	XYP	C2-C3	3.49	1.57	1.52
2	E	4	AHR	C1-C2	3.49	1.57	1.51
2	E	3	XYP	O3-C3	3.43	1.51	1.43
2	H	5	XYP	O5-C5	-3.39	1.36	1.43
2	E	2	XYP	C4-C3	3.31	1.57	1.52
2	F	5	XYP	O5-C1	-3.25	1.36	1.43
2	F	4	AHR	C2-C3	-3.23	1.48	1.53
2	E	3	XYP	C4-C3	3.22	1.57	1.52
2	E	3	XYP	C2-C3	3.17	1.57	1.52
2	H	3	XYP	O3-C3	3.10	1.50	1.43
2	F	3	XYP	C4-C3	3.03	1.57	1.52
2	E	4	AHR	C2-C3	-2.99	1.48	1.53
2	F	3	XYP	C2-C3	2.96	1.57	1.52
2	H	3	XYP	C4-C3	2.90	1.56	1.52
2	F	3	XYP	O3-C3	2.85	1.50	1.43
2	G	2	XYP	C4-C3	2.78	1.56	1.52
2	G	5	XYP	O5-C1	-2.76	1.37	1.43
2	G	1	XYP	C5-C4	-2.69	1.45	1.52
2	G	2	XYP	O2-C2	2.66	1.48	1.43
2	H	5	XYP	O3-C3	-2.64	1.36	1.43
2	F	1	XYP	O5-C1	2.56	1.47	1.43
2	E	2	XYP	O2-C2	2.54	1.48	1.43
2	F	2	XYP	C4-C3	2.53	1.56	1.52
2	H	2	XYP	C4-C3	2.53	1.56	1.52
2	G	1	XYP	O5-C1	2.51	1.47	1.43
2	E	5	XYP	O5-C1	-2.50	1.38	1.43
2	H	4	AHR	O3-C3	2.48	1.49	1.43
2	H	1	XYP	O5-C5	2.44	1.47	1.43
2	F	4	AHR	O2-C2	2.31	1.48	1.43
2	E	1	XYP	O1-C1	2.30	1.46	1.39
2	F	5	XYP	C4-C3	2.27	1.56	1.52
2	F	5	XYP	O3-C3	-2.23	1.37	1.43
2	H	2	XYP	O2-C2	2.22	1.48	1.43
2	H	4	AHR	C2-C3	-2.22	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	XYP	O3-C3	-2.19	1.37	1.43
2	E	4	AHR	O3-C3	2.16	1.48	1.43
2	F	1	XYP	C5-C4	-2.15	1.47	1.52
2	F	2	XYP	O2-C2	2.12	1.47	1.43
2	H	5	XYP	C1-C2	-2.08	1.47	1.52
2	H	1	XYP	C5-C4	-2.06	1.47	1.52
2	G	3	XYP	C4-C3	2.04	1.55	1.52
2	G	2	XYP	O5-C5	2.02	1.46	1.43
2	H	1	XYP	O5-C1	2.02	1.46	1.43

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	5	XYP	C5-O5-C1	-8.49	97.71	111.42
2	G	5	XYP	C5-O5-C1	-8.47	97.74	111.42
2	E	5	XYP	C5-O5-C1	-7.80	98.82	111.42
2	F	5	XYP	C5-O5-C1	-7.23	99.75	111.42
2	E	5	XYP	C1-C2-C3	-6.96	99.51	109.64
2	G	5	XYP	C1-C2-C3	-6.83	99.70	109.64
2	F	5	XYP	C1-C2-C3	-6.66	99.95	109.64
2	H	5	XYP	C1-C2-C3	-6.63	99.99	109.64
2	F	2	XYP	C4-C3-C2	5.04	116.90	110.92
2	E	2	XYP	C4-C3-C2	4.81	116.64	110.92
2	G	2	XYP	C4-C3-C2	4.73	116.54	110.92
2	H	2	XYP	C4-C3-C2	4.71	116.52	110.92
2	F	3	XYP	C4-C3-C2	-4.58	105.48	110.92
2	H	2	XYP	C5-C4-C3	4.38	116.03	109.64
2	G	2	XYP	C5-C4-C3	4.31	115.93	109.64
2	H	3	XYP	O4-C4-C3	4.10	118.64	110.15
2	F	2	XYP	C5-C4-C3	4.00	115.47	109.64
2	H	3	XYP	C4-C3-C2	-3.90	106.28	110.92
2	E	2	XYP	C5-C4-C3	3.88	115.29	109.64
2	H	5	XYP	C5-C4-C3	3.87	115.28	109.64
2	G	3	XYP	C4-C3-C2	-3.83	106.37	110.92
2	G	3	XYP	O4-C4-C3	3.66	117.73	110.15
2	E	1	XYP	O5-C5-C4	-3.62	102.16	110.79
2	E	3	XYP	O4-C4-C3	3.58	117.56	110.15
2	E	3	XYP	C4-C3-C2	-3.58	106.67	110.92
2	G	2	XYP	C5-O5-C1	-3.57	105.65	111.42
2	G	3	XYP	O4-C4-C5	-3.44	101.34	109.22
2	H	5	XYP	O3-C3-C4	-3.42	103.07	110.05
2	G	5	XYP	C5-C4-C3	3.42	114.62	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	XYP	O5-C5-C4	-3.41	102.66	110.79
2	E	4	AHR	O2-C2-C3	-3.39	104.75	111.43
2	F	1	XYP	O5-C5-C4	-3.39	102.71	110.79
2	F	5	XYP	C5-C4-C3	3.38	114.57	109.64
2	E	2	XYP	C5-O5-C1	-3.34	106.02	111.42
2	F	2	XYP	C5-O5-C1	-3.34	106.03	111.42
2	H	3	XYP	O4-C4-C5	-3.31	101.63	109.22
2	H	1	XYP	O5-C5-C4	-3.30	102.91	110.79
2	H	4	AHR	O2-C2-C3	-3.30	104.94	111.43
2	F	3	XYP	O4-C4-C3	3.27	116.92	110.15
2	E	5	XYP	C5-C4-C3	3.25	114.38	109.64
2	E	3	XYP	O4-C4-C5	-3.21	101.88	109.22
2	H	2	XYP	C5-O5-C1	-3.15	106.33	111.42
2	E	5	XYP	O3-C3-C4	-3.12	103.69	110.05
2	F	3	XYP	O4-C4-C5	-3.09	102.14	109.22
2	E	1	XYP	C5-C4-C3	-2.92	105.39	109.64
2	F	5	XYP	O3-C3-C4	-2.84	104.26	110.05
2	F	5	XYP	O2-C2-C1	2.80	115.64	109.22
2	F	4	AHR	O2-C2-C3	-2.79	105.93	111.43
2	G	4	AHR	O2-C2-C3	-2.67	106.16	111.43
2	G	5	XYP	O3-C3-C4	-2.66	104.64	110.05
2	H	5	XYP	O2-C2-C1	2.64	115.27	109.22
2	G	5	XYP	O2-C2-C1	2.44	114.82	109.22
2	F	2	XYP	O3-C3-C2	-2.43	105.10	110.05
2	F	1	XYP	C5-C4-C3	-2.39	106.17	109.64
2	H	1	XYP	C5-C4-C3	-2.39	106.17	109.64
2	G	2	XYP	O3-C3-C2	-2.37	105.21	110.05
2	E	5	XYP	O2-C2-C1	2.35	114.60	109.22
2	G	4	AHR	C1-C2-C3	2.27	105.25	101.63
2	G	1	XYP	C5-C4-C3	-2.22	106.41	109.64
2	E	4	AHR	C5-C4-C3	-2.17	109.98	115.10
2	E	4	AHR	C1-C2-C3	2.10	104.99	101.63
2	E	2	XYP	O3-C3-C2	-2.07	105.83	110.05
2	F	5	XYP	O2-C2-C3	-2.06	105.89	110.15
2	F	4	AHR	C1-C2-C3	2.04	104.89	101.63

There are no chirality outliers.

There are no torsion outliers.

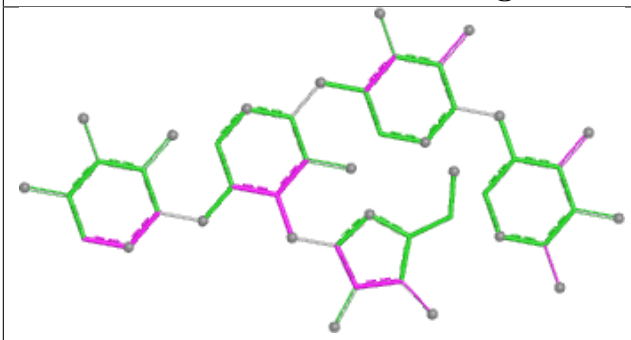
There are no ring outliers.

No monomer is involved in short contacts.

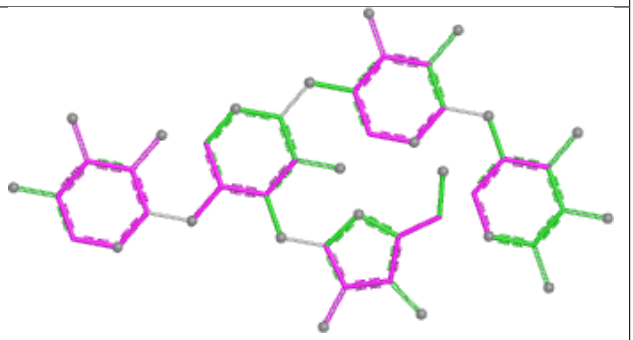
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

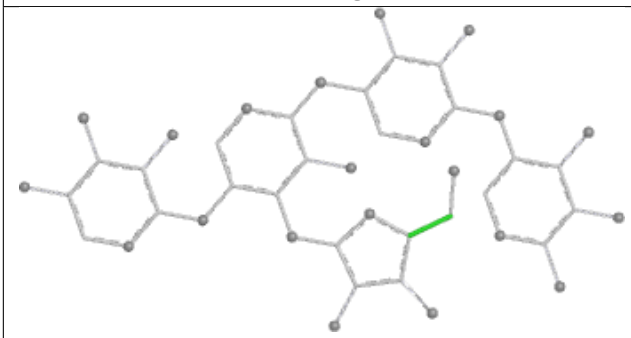
Oligosaccharide Chain E



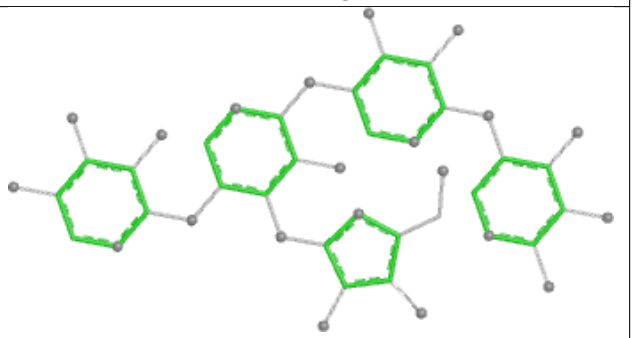
Bond lengths



Bond angles

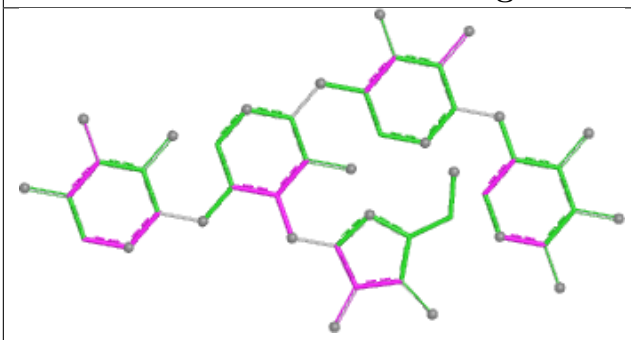


Torsions

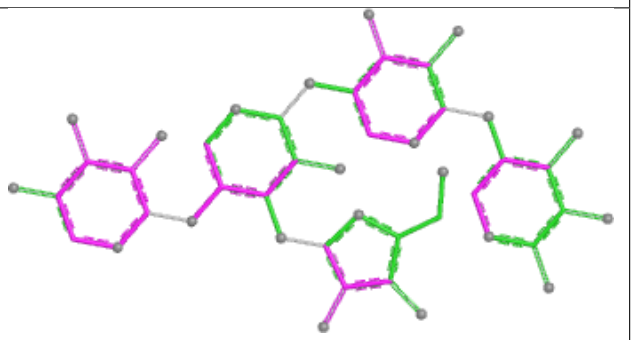


Rings

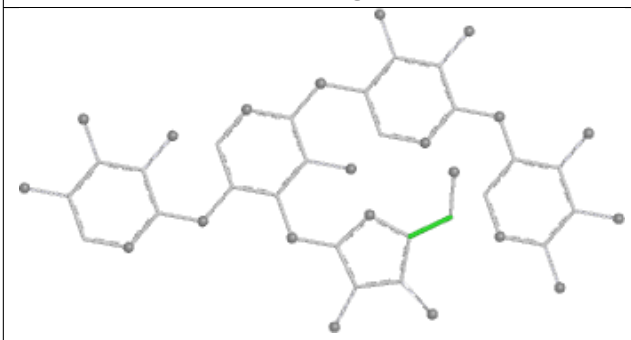
Oligosaccharide Chain F



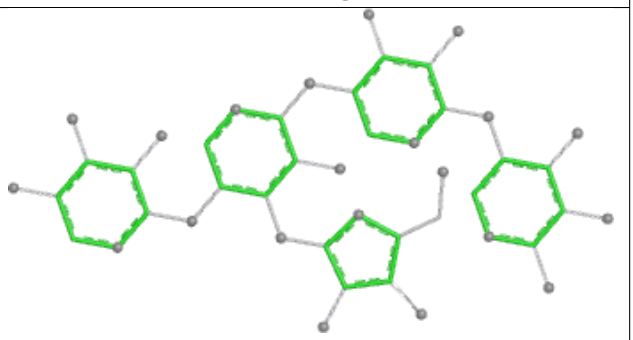
Bond lengths



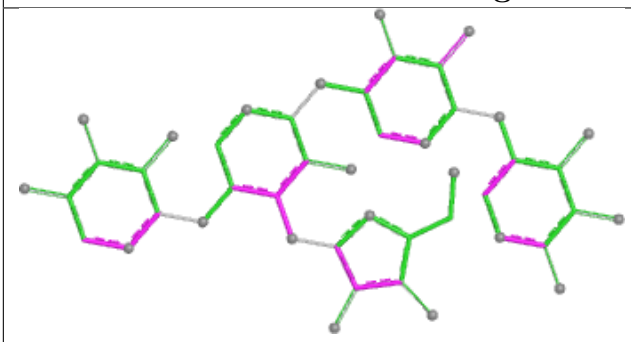
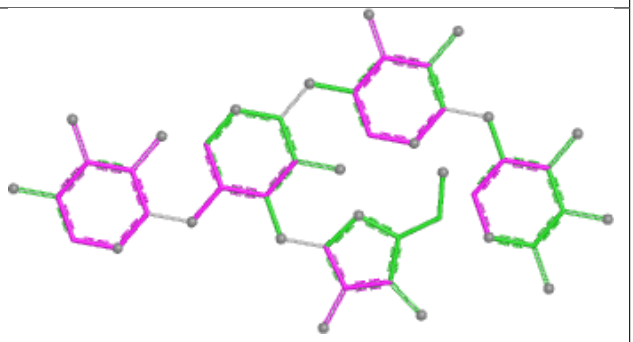
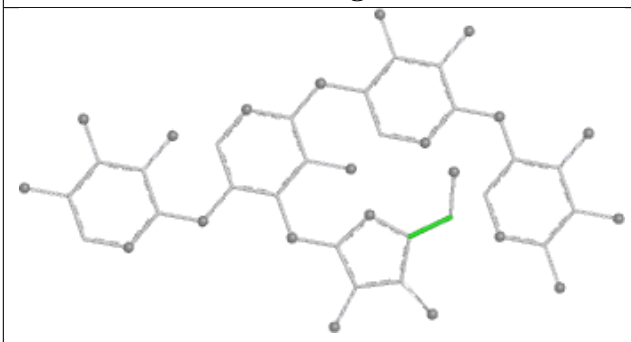
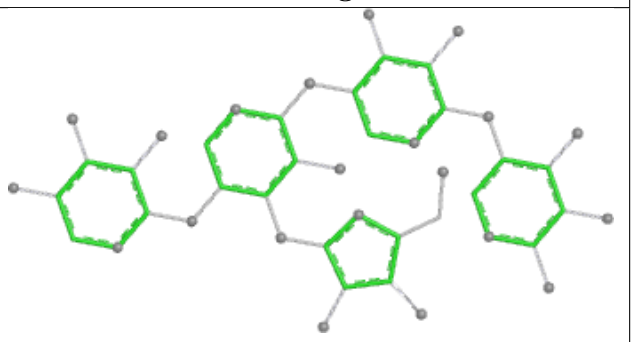
Bond angles

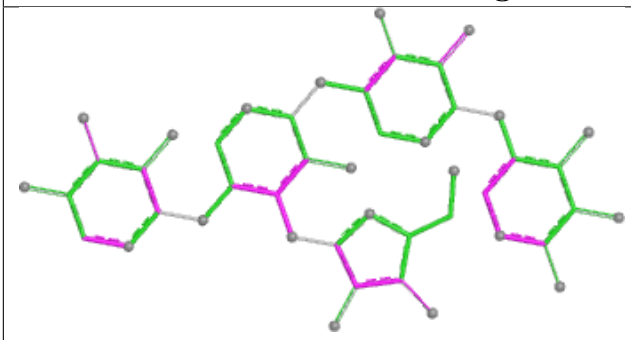
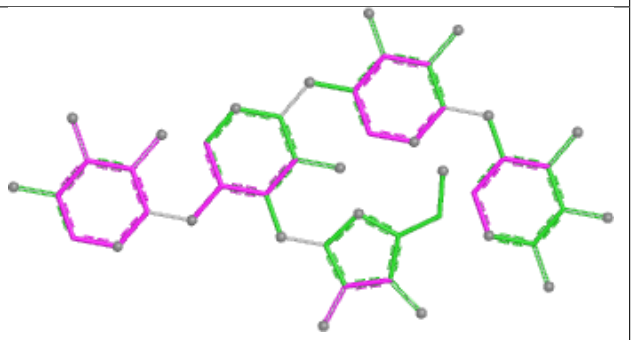
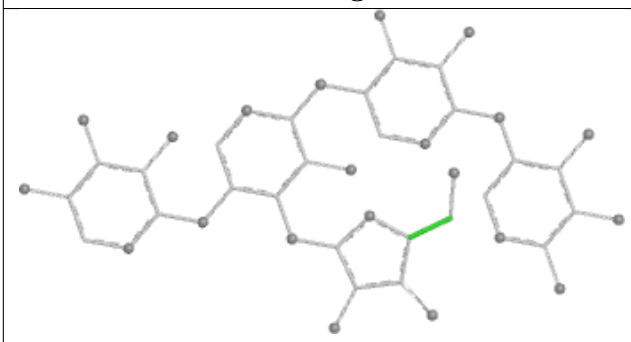
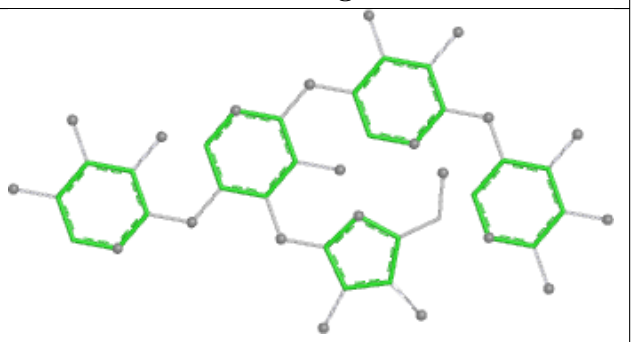


Torsions



Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	381/385 (98%)	0.34	5 (1%)	77	78	21, 35, 52, 62	0
1	B	380/385 (98%)	0.50	14 (3%)	41	39	23, 35, 54, 61	0
1	C	385/385 (100%)	0.44	7 (1%)	68	68	21, 37, 51, 59	0
1	D	380/385 (98%)	0.48	8 (2%)	63	63	21, 35, 52, 62	0
All	All	1526/1540 (99%)	0.44	34 (2%)	62	61	21, 35, 52, 62	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	384	ALA	4.1
1	D	121	LEU	3.7
1	B	384	ALA	3.5
1	B	121	LEU	3.2
1	D	96	TYR	3.0
1	A	98	TYR	2.9
1	B	119	THR	2.9
1	B	190	LEU	2.9
1	C	170	GLN	2.8
1	C	186	PHE	2.8
1	B	385	ALA	2.6
1	C	183	LEU	2.6
1	B	52	VAL	2.5
1	B	316	ASN	2.5
1	D	46	THR	2.4
1	C	315	PHE	2.4
1	A	102	THR	2.4
1	A	41	TYR	2.4
1	D	119	THR	2.4
1	D	385	ALA	2.3
1	B	320	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	52	VAL	2.3
1	A	151	TYR	2.2
1	B	122	SER	2.2
1	C	367	PHE	2.2
1	D	383	ALA	2.2
1	C	1	MET	2.1
1	B	40	PHE	2.1
1	C	382	GLN	2.1
1	B	383	ALA	2.1
1	B	255	LEU	2.1
1	B	98	TYR	2.1
1	A	287	VAL	2.0
1	B	123	PRO	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AHR	F	4	9/10	0.82	0.38	20,21,22,22	0
2	AHR	E	4	9/10	0.84	0.34	20,21,22,22	0
2	XYP	F	5	9/10	0.84	0.30	21,21,22,22	0
2	XYP	F	2	9/10	0.85	0.20	20,20,21,21	0
2	XYP	G	5	9/10	0.85	0.39	21,21,22,22	0
2	XYP	H	2	9/10	0.86	0.18	21,21,21,21	0
2	XYP	F	3	9/10	0.88	0.19	21,21,22,22	0
2	AHR	G	4	9/10	0.88	0.28	20,21,21,22	0
2	XYP	E	3	9/10	0.89	0.22	20,21,21,22	0
2	XYP	H	3	9/10	0.89	0.23	21,21,22,22	0
2	AHR	H	4	9/10	0.89	0.32	20,21,21,22	0
2	XYP	G	3	9/10	0.90	0.19	21,21,21,22	0
2	XYP	G	2	9/10	0.90	0.14	20,21,21,22	0
2	XYP	H	5	9/10	0.90	0.30	21,22,22,22	0
2	XYP	F	1	10/10	0.91	0.16	21,21,21,22	0

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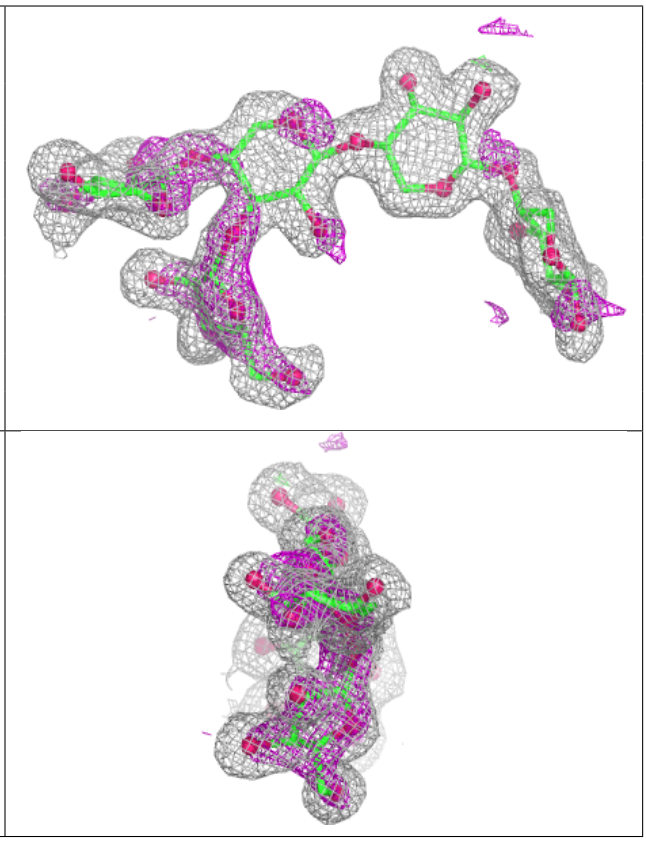
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XYP	G	1	10/10	0.92	0.12	21,21,21,22	0
2	XYP	H	1	10/10	0.92	0.16	20,21,21,21	0
2	XYP	E	2	9/10	0.92	0.10	20,20,21,21	0
2	XYP	E	5	9/10	0.93	0.23	20,21,21,21	0
2	XYP	E	1	10/10	0.93	0.14	20,21,21,21	0

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.

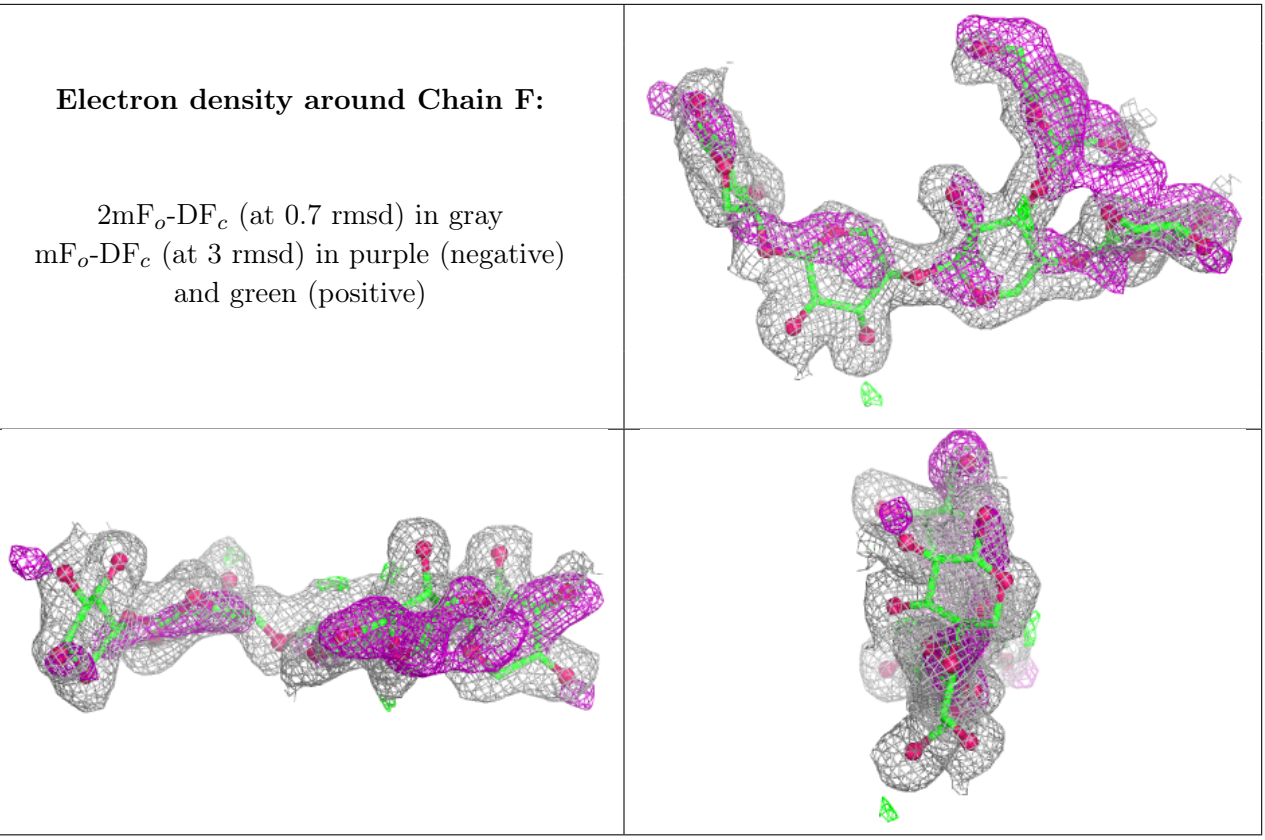
Electron density around Chain E:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



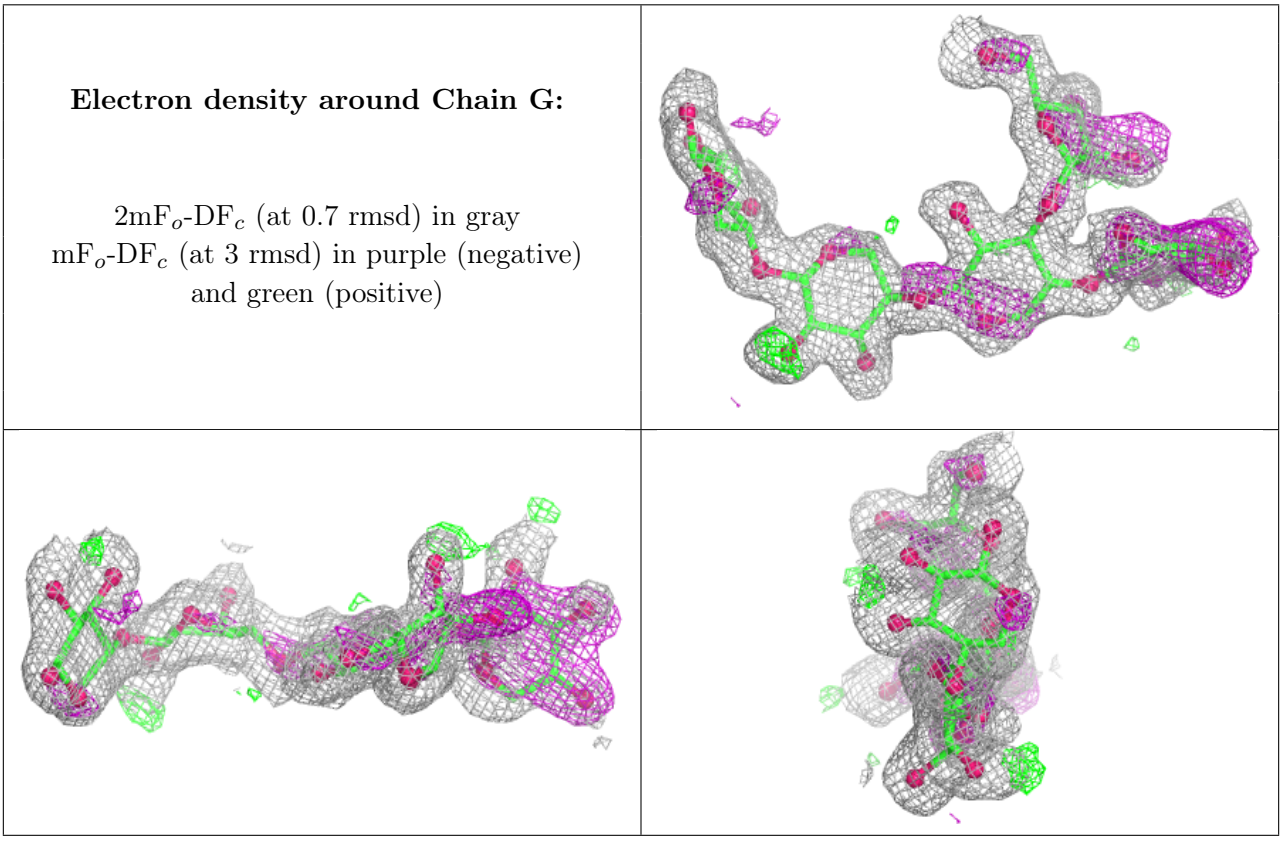
Electron density around Chain F:

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



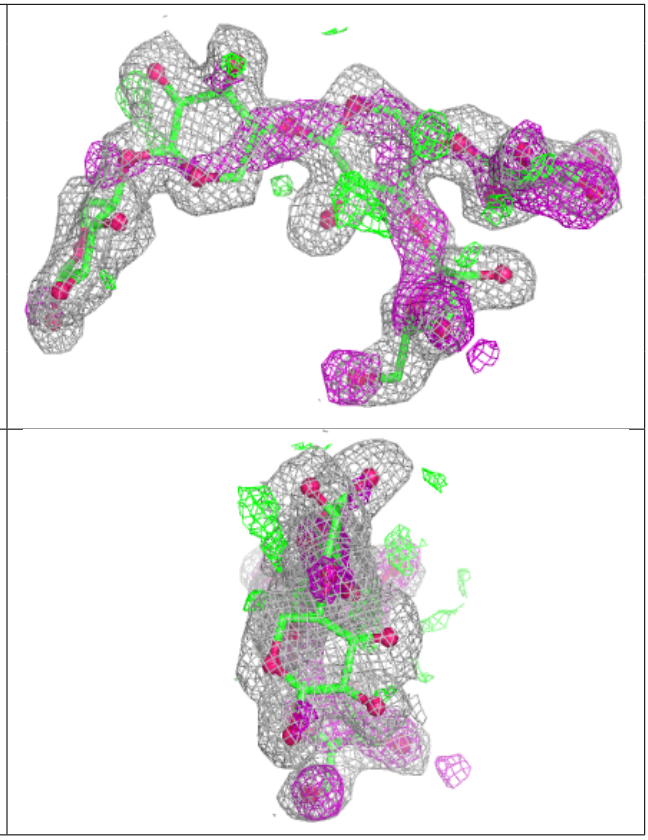
Electron density around Chain G:

$2mF_o$-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)



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.