



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:09 AM BST

PDB ID : 2CDP
Title : Structure of a CBM6 in complex with neoagarohexaose
Authors : Henshaw, J.; Horne, A.; Van Bueren, A.L.; Money, V.A.; Bolam, D.N.; Czjzek, M.; Weiner, R.M.; Hutcheson, S.W.; Davies, G.J.; Boraston, A.B.; Gilbert, H.J.
Deposited on : 2006-01-26
Resolution : 1.59 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

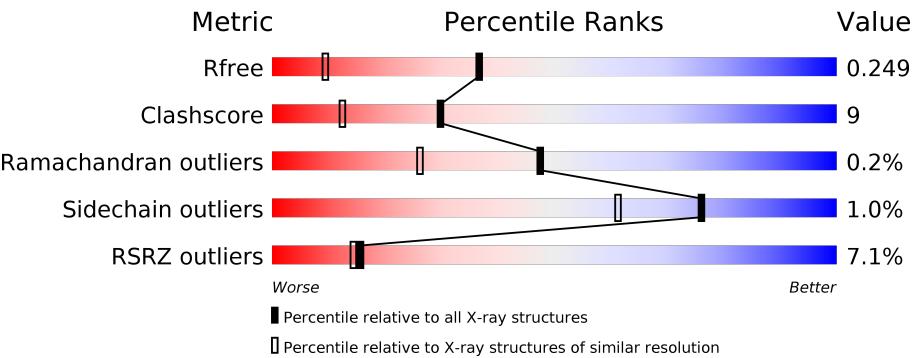
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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.



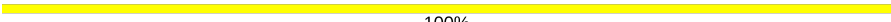
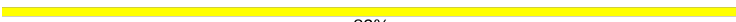

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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 $\leq 5\%$. 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	160	<div><div>6%</div><div><div></div><div>74%</div><div>13%</div><div>14%</div></div></div>
1	B	160	<div><div>3%</div><div><div></div><div>69%</div><div>11%</div><div>20%</div></div></div>
1	C	160	<div><div>4%</div><div><div></div><div>71%</div><div>9%</div><div>21%</div></div></div>
1	D	160	<div><div>10%</div><div><div></div><div>62%</div><div>18%</div><div>•</div><div>19%</div></div></div>
2	E	6	<div><div></div><div><div>17%</div><div>83%</div></div></div>
2	F	6	<div><div></div><div><div>100%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	6	 100%
2	H	6	 83%  17%

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	GAL	E	1	X	-	-	-
2	GAL	F	1	X	-	-	-
2	GAL	G	1	X	-	-	-
2	GAL	H	1	X	-	-	-
4	EDO	A	1141	-	-	X	-

2 Entry composition [i](#)

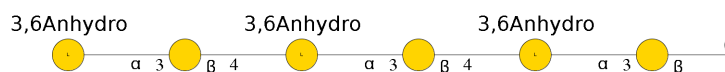
There are 6 unique types of molecules in this entry. The entry contains 4877 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-AGARASE 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	0	4	0
			1041	648	177	216			
1	B	128	Total	C	N	O	0	5	0
			977	613	166	198			
1	C	127	Total	C	N	O	0	7	0
			978	613	165	200			
1	D	130	Total	C	N	O	0	9	0
			1012	638	170	204			

- Molecule 2 is an oligosaccharide called 3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	6	Total	C	O	0	0	0
			64	36	28			
2	F	6	Total	C	O	0	0	0
			64	36	28			
2	G	6	Total	C	O	0	0	0
			64	36	28			
2	H	6	Total	C	O	0	0	0
			64	36	28			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total 3	Cl 3	0	0
5	A	3	Total 3	Cl 3	0	0
5	D	1	Total 1	Cl 1	0	0
5	C	2	Total 2	Cl 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total 156	O 156	0	0
6	B	140	Total 140	O 140	0	0
6	C	136	Total 136	O 136	0	0
6	D	140	Total 140	O 140	0	0

- Molecule 1: BETA-AGARASE 1





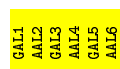
- Molecule 2: 3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose

Chain E: 17% 83%



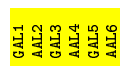
- Molecule 2: 3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose

Chain F: 100%



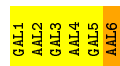
- Molecule 2: 3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose

Chain G: 100%



- Molecule 2: 3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose

Chain H: 83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.72Å 55.00Å 195.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.62 – 1.59 19.61 – 1.59	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.62-1.59) 98.3 (19.61-1.59)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.253 0.206 , 0.249	Depositor DCC
R_{free} test set	3905 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4877	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: AAL, CA, GAL, EDO, CL

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	0.92	0/1077	0.81	1/1474 (0.1%)
1	B	0.95	0/1014	0.76	0/1386
1	C	0.96	0/1021	0.79	0/1396
1	D	0.90	0/1062	0.82	1/1453 (0.1%)
All	All	0.93	0/4174	0.80	2/5709 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	45	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	118	ARG	NE-CZ-NH2	-5.65	117.48	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	42	ASN	Peptide

5.2 Too-close contacts ⓘ

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	1041	0	963	16	0
1	B	977	0	916	15	0
1	C	978	0	916	11	0
1	D	1012	0	955	36	0
2	E	64	0	51	0	0
2	F	64	0	51	0	0
2	G	64	0	51	0	0
2	H	64	0	51	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	4	0	6	4	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	12	0	18	3	0
5	A	3	0	0	1	0
5	B	3	0	0	1	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	156	0	0	5	0
6	B	140	0	0	5	0
6	C	136	0	0	1	2
6	D	140	0	0	8	2
All	All	4877	0	3990	78	2

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.

All (78) 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:D:19:PHE:CE1	1:D:126[B]:ASN:OD1	1.82	1.30
1:D:51[A]:ILE:HD12	1:D:117[A]:VAL:HG21	1.24	1.09
1:D:13[A]:ASN:ND2	6:D:2014:HOH:O	1.75	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51[A]:ILE:HD12	1:D:117[A]:VAL:CG2	1.95	0.94
1:D:13[B]:ASN:ND2	6:D:2013:HOH:O	1.99	0.88
1:D:11:ASN:HB3	6:D:2007:HOH:O	1.75	0.86
1:D:58[B]:ASN:ND2	4:D:1142:EDO:H21	1.90	0.84
1:D:51[A]:ILE:CD1	1:D:117[A]:VAL:HG21	2.06	0.84
1:A:89:VAL:O	4:A:1141:EDO:H22	1.87	0.74
1:D:19:PHE:CD1	1:D:126[B]:ASN:OD1	2.40	0.74
1:D:19:PHE:CZ	1:D:126[B]:ASN:ND2	2.57	0.71
1:D:19:PHE:HZ	1:D:126[B]:ASN:HD21	1.39	0.69
1:D:19:PHE:CE1	1:D:126[B]:ASN:CG	2.64	0.69
1:C:73:SER:H	1:C:128:GLN:HE22	1.40	0.69
1:C:75:GLU:OE1	1:C:120:HIS:HD2	1.76	0.68
1:D:19:PHE:CZ	1:D:126[B]:ASN:OD1	2.45	0.67
1:D:58[B]:ASN:OD1	6:D:2055:HOH:O	2.12	0.67
1:D:111:SER:O	1:D:115:HIS:HE1	1.79	0.65
1:C:111:SER:O	1:C:115:HIS:HE1	1.80	0.64
1:A:75:GLU:OE1	1:A:120:HIS:HD2	1.81	0.61
1:B:75:GLU:OE1	1:B:120:HIS:HD2	1.85	0.60
1:B:111:SER:O	1:B:115:HIS:HE1	1.86	0.59
1:D:49:TYR:HB2	1:D:117[B]:VAL:HG23	1.83	0.59
1:A:111:SER:O	1:A:115:HIS:HE1	1.88	0.57
1:D:58[B]:ASN:ND2	4:D:1142:EDO:C2	2.63	0.57
1:C:73:SER:H	1:C:128:GLN:NE2	2.04	0.56
1:D:73:SER:H	1:D:128:GLN:HE22	1.52	0.56
1:D:75:GLU:OE1	1:D:120:HIS:HD2	1.88	0.55
1:A:115:HIS:HD2	6:A:2030:HOH:O	1.88	0.55
1:D:44:GLY:HA2	1:D:120:HIS:HE1	1.72	0.55
1:D:19:PHE:HB2	6:D:2041:HOH:O	2.06	0.55
1:B:115:HIS:HD2	6:B:2057:HOH:O	1.91	0.54
1:D:73:SER:H	1:D:128:GLN:NE2	2.05	0.53
1:C:31[A]:THR:HG23	1:C:35:ASN:O	2.09	0.53
1:D:44:GLY:HA2	1:D:120:HIS:CE1	2.43	0.53
1:A:89:VAL:O	4:A:1141:EDO:C2	2.57	0.52
1:B:135[B]:THR:HG21	6:B:2124:HOH:O	2.08	0.52
1:A:120:HIS:HE1	6:A:2124:HOH:O	1.94	0.51
1:C:74:ILE:HG12	1:C:129:TRP:CE2	2.45	0.50
1:D:58[B]:ASN:HD22	4:D:1142:EDO:H21	1.72	0.50
1:A:70:THR:HG23	6:A:2072:HOH:O	2.12	0.50
1:D:138:ASN:HB2	6:D:2124:HOH:O	2.12	0.50
1:D:115:HIS:HD2	6:D:2068:HOH:O	1.95	0.50
1:D:19:PHE:CZ	1:D:126[B]:ASN:CG	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:TYR:HB2	1:D:117[B]:VAL:CG2	2.43	0.49
1:D:97:TRP:CG	2:H:6:AAL:H5	2.48	0.48
1:B:73:SER:H	1:B:128:GLN:NE2	2.12	0.47
1:B:73:SER:H	1:B:128:GLN:HE22	1.61	0.47
1:C:75:GLU:OE1	1:C:120:HIS:CD2	2.63	0.47
1:D:133:LYS:HD3	6:D:2005:HOH:O	2.14	0.47
1:B:123:GLY:H	1:B:128:GLN:NE2	2.12	0.47
1:B:44:GLY:HA2	1:B:120:HIS:HE1	1.80	0.47
1:B:92:VAL:O	5:B:1142:CL:CL	2.70	0.47
1:A:58:ASN:HB2	1:C:13:ASN:HD22	1.80	0.46
1:B:60[B]:THR:OG1	1:B:137:SER:HB2	2.16	0.46
4:A:1141:EDO:C1	5:A:1142:CL:CL	3.02	0.45
1:A:89:VAL:O	4:A:1141:EDO:H12	2.17	0.45
1:A:125:ASN:HB3	1:A:127:TRP:O	2.16	0.45
1:B:26:PRO:N	6:B:2011:HOH:O	2.50	0.44
1:D:5:ILE:HG21	1:D:51[A]:ILE:HG23	1.99	0.44
1:C:120:HIS:HE1	6:C:2112:HOH:O	2.02	0.43
1:C:133:LYS:HB3	1:C:133:LYS:HE2	1.85	0.43
1:B:60[A]:THR:HG23	6:B:2096:HOH:O	2.19	0.42
1:D:12:PHE:CD1	1:D:15:VAL:HG13	2.54	0.42
1:A:16:GLY:HA3	1:A:46:TYR:CZ	2.54	0.42
1:D:74:ILE:HG12	1:D:129:TRP:CE2	2.54	0.42
1:A:74:ILE:HG12	1:A:129:TRP:CE2	2.54	0.42
1:A:25:GLN:HG3	6:A:2025:HOH:O	2.19	0.42
1:D:125:ASN:HB3	1:D:127:TRP:O	2.20	0.42
1:A:12:PHE:CD1	1:A:15:VAL:HG13	2.54	0.42
1:A:17:GLY:HA3	1:A:45:ASP:OD1	2.20	0.42
1:D:123:GLY:H	1:D:128:GLN:NE2	2.19	0.41
1:B:125:ASN:HB3	1:B:127:TRP:O	2.20	0.41
1:A:1:SER:N	6:A:2002:HOH:O	2.37	0.41
1:D:17:GLY:HA3	1:D:45:ASP:OD1	2.20	0.41
1:B:135[B]:THR:CG2	6:B:2124:HOH:O	2.66	0.41
1:C:123:GLY:H	1:C:128:GLN:NE2	2.19	0.41
1:B:74:ILE:HG12	1:B:129:TRP:CE2	2.56	0.41

All (2) 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)
6:C:2053:HOH:O	6:D:2111:HOH:O[1_455]	2.12	0.08
6:C:2054:HOH:O	6:D:2111:HOH:O[1_455]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	140/160 (88%)	137 (98%)	3 (2%)	0	100	100
1	B	129/160 (81%)	126 (98%)	3 (2%)	0	100	100
1	C	130/160 (81%)	126 (97%)	4 (3%)	0	100	100
1	D	135/160 (84%)	130 (96%)	4 (3%)	1 (1%)	22	7
All	All	534/640 (83%)	519 (97%)	14 (3%)	1 (0%)	47	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	43	GLN

5.3.2 Protein sidechains

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	110/124 (89%)	110 (100%)	0	100	100
1	B	103/124 (83%)	102 (99%)	1 (1%)	76	61
1	C	105/124 (85%)	104 (99%)	1 (1%)	76	61
1	D	109/124 (88%)	107 (98%)	2 (2%)	59	36
All	All	427/496 (86%)	423 (99%)	4 (1%)	76	65

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

Mol	Chain	Res	Type
1	B	83	SER
1	C	32	VAL
1	D	18	THR
1	D	133	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	116	GLN
1	A	120	HIS
1	B	81	ASN
1	B	115	HIS
1	B	116	GLN
1	B	120	HIS
1	B	128	GLN
1	B	138	ASN
1	C	13	ASN
1	C	81	ASN
1	C	115	HIS
1	C	120	HIS
1	C	128	GLN
1	D	33	ASN
1	D	64	GLN
1	D	115	HIS
1	D	120	HIS
1	D	128	GLN
1	D	138	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](#)

24 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	GAL	E	1	2	12,12,12	0.82	0	17,17,17	0.95	0
2	AAL	E	2	2	11,11,12	0.70	0	15,16,18	1.14	2 (13%)
2	GAL	E	3	2	11,11,12	0.56	0	15,15,17	2.07	4 (26%)
2	AAL	E	4	2	11,11,12	0.87	0	15,16,18	1.89	4 (26%)
2	GAL	E	5	2	11,11,12	0.73	0	15,15,17	1.12	1 (6%)
2	AAL	E	6	2	11,11,12	0.81	0	15,16,18	1.27	2 (13%)
2	GAL	F	1	2	12,12,12	0.99	0	17,17,17	1.22	3 (17%)
2	AAL	F	2	2	11,11,12	0.86	0	15,16,18	1.45	2 (13%)
2	GAL	F	3	2	11,11,12	0.72	0	15,15,17	1.81	3 (20%)
2	AAL	F	4	2	11,11,12	1.10	0	15,16,18	1.68	3 (20%)
2	GAL	F	5	2	11,11,12	1.00	0	15,15,17	1.26	1 (6%)
2	AAL	F	6	2	11,11,12	0.97	0	15,16,18	1.46	2 (13%)
2	GAL	G	1	2	12,12,12	0.67	0	17,17,17	2.26	7 (41%)
2	AAL	G	2	2	11,11,12	0.74	0	15,16,18	1.29	2 (13%)
2	GAL	G	3	2	11,11,12	0.57	0	15,15,17	1.22	1 (6%)
2	AAL	G	4	2	11,11,12	0.82	0	15,16,18	1.60	4 (26%)
2	GAL	G	5	2	11,11,12	0.79	0	15,15,17	1.57	2 (13%)
2	AAL	G	6	2	11,11,12	0.92	0	15,16,18	1.57	1 (6%)
2	GAL	H	1	2	12,12,12	0.88	0	17,17,17	2.65	7 (41%)
2	AAL	H	2	2	11,11,12	0.69	0	15,16,18	1.81	5 (33%)
2	GAL	H	3	2	11,11,12	0.60	0	15,15,17	1.27	2 (13%)
2	AAL	H	4	2	11,11,12	1.50	2 (18%)	15,16,18	1.49	5 (33%)
2	GAL	H	5	2	11,11,12	0.63	0	15,15,17	1.49	1 (6%)
2	AAL	H	6	2	11,11,12	1.08	1 (9%)	15,16,18	1.55	2 (13%)

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	GAL	E	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	AAL	E	2	2	-	-	0/3/2/2
2	GAL	E	3	2	-	0/2/19/22	0/1/1/1
2	AAL	E	4	2	-	-	0/3/2/2
2	GAL	E	5	2	-	0/2/19/22	0/1/1/1
2	AAL	E	6	2	-	-	0/3/2/2
2	GAL	F	1	2	1/1/5/5	1/2/22/22	0/1/1/1
2	AAL	F	2	2	-	-	0/3/2/2
2	GAL	F	3	2	-	0/2/19/22	0/1/1/1
2	AAL	F	4	2	-	-	0/3/2/2
2	GAL	F	5	2	-	0/2/19/22	0/1/1/1
2	AAL	F	6	2	-	-	0/3/2/2
2	GAL	G	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	AAL	G	2	2	-	-	0/3/2/2
2	GAL	G	3	2	-	0/2/19/22	0/1/1/1
2	AAL	G	4	2	-	-	0/3/2/2
2	GAL	G	5	2	-	0/2/19/22	0/1/1/1
2	AAL	G	6	2	-	-	0/3/2/2
2	GAL	H	1	2	1/1/5/5	1/2/22/22	0/1/1/1
2	AAL	H	2	2	-	-	0/3/2/2
2	GAL	H	3	2	-	0/2/19/22	0/1/1/1
2	AAL	H	4	2	-	-	0/3/2/2
2	GAL	H	5	2	-	0/2/19/22	0/1/1/1
2	AAL	H	6	2	-	-	0/3/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	4	AAL	O5-C1	3.09	1.48	1.43
2	H	4	AAL	O3-C6	2.55	1.49	1.43
2	H	6	AAL	C1-C2	2.02	1.56	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	GAL	O4-C4-C3	-5.35	97.97	110.35
2	H	1	GAL	O3-C3-C2	5.00	121.91	110.35
2	E	3	GAL	O5-C5-C6	4.90	114.88	107.20
2	G	5	GAL	O3-C3-C2	-4.76	100.89	109.99
2	G	1	GAL	C3-C4-C5	4.75	118.71	110.24
2	F	3	GAL	O5-C5-C6	4.73	114.62	107.20
2	H	1	GAL	C3-C4-C5	4.71	118.65	110.24
2	F	4	AAL	C1-O5-C5	4.56	118.38	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	6	AAL	C1-O5-C5	4.54	118.34	112.19
2	H	1	GAL	C4-C3-C2	4.43	118.56	110.82
2	E	4	AAL	C1-O5-C5	4.43	118.19	112.19
2	H	2	AAL	C1-O5-C5	4.00	117.61	112.19
2	H	5	GAL	O3-C3-C2	-3.82	102.67	109.99
2	H	6	AAL	C1-O5-C5	3.77	117.30	112.19
2	F	6	AAL	C1-O5-C5	3.55	117.01	112.19
2	E	3	GAL	O3-C3-C2	-3.51	103.27	109.99
2	H	1	GAL	O5-C5-C4	3.48	116.01	109.69
2	F	6	AAL	C2-C3-C4	-3.35	105.55	113.85
2	H	1	GAL	O2-C2-C3	3.35	118.09	110.35
2	F	3	GAL	O3-C3-C2	-3.31	103.65	109.99
2	F	5	GAL	O3-C3-C2	-3.12	104.03	109.99
2	H	1	GAL	C1-O5-C5	3.05	119.42	113.66
2	F	2	AAL	C1-C2-C3	3.02	112.83	109.17
2	E	3	GAL	O2-C2-C1	3.01	115.31	109.15
2	G	4	AAL	C1-C2-C3	2.92	112.70	109.17
2	E	3	GAL	C1-O5-C5	2.90	116.12	112.19
2	E	5	GAL	O3-C3-C2	-2.80	104.64	109.99
2	E	4	AAL	O4-C4-C5	-2.76	103.07	111.05
2	H	1	GAL	O4-C4-C3	-2.75	104.00	110.35
2	E	2	AAL	C1-O5-C5	2.75	115.91	112.19
2	E	6	AAL	C1-C2-C3	2.72	112.46	109.17
2	G	1	GAL	C1-C2-C3	2.71	115.94	110.31
2	E	4	AAL	O5-C5-C6	-2.70	109.32	113.33
2	G	1	GAL	C4-C3-C2	2.66	115.47	110.82
2	H	2	AAL	C2-C3-C4	-2.61	107.38	113.85
2	G	1	GAL	O1-C1-C2	-2.57	101.80	109.03
2	E	4	AAL	C3-C4-C5	-2.52	96.53	101.99
2	F	1	GAL	C3-C4-C5	2.52	114.73	110.24
2	G	4	AAL	O5-C5-C6	-2.51	109.61	113.33
2	H	4	AAL	O5-C5-C6	-2.49	109.63	113.33
2	H	2	AAL	O2-C2-C3	-2.48	104.19	110.07
2	G	1	GAL	O3-C3-C4	2.47	116.05	110.35
2	H	3	GAL	C1-O5-C5	2.40	115.44	112.19
2	F	4	AAL	C2-C3-C4	-2.36	108.02	113.85
2	H	4	AAL	C2-C3-C4	-2.35	108.03	113.85
2	G	5	GAL	C1-O5-C5	2.35	115.37	112.19
2	H	3	GAL	O5-C1-C2	-2.33	107.17	110.77
2	E	2	AAL	C2-C3-C4	-2.31	108.14	113.85
2	G	2	AAL	O4-C4-C3	-2.29	104.66	111.17
2	H	2	AAL	O5-C5-C6	-2.29	109.93	113.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	GAL	O2-C2-C3	2.27	114.68	110.14
2	H	6	AAL	C2-C3-C4	-2.26	108.25	113.85
2	G	3	GAL	O5-C5-C6	2.26	110.75	107.20
2	G	2	AAL	C2-C3-C4	-2.26	108.26	113.85
2	H	2	AAL	O2-C2-C1	2.25	113.76	109.15
2	H	4	AAL	O5-C1-C2	2.22	114.20	110.77
2	E	6	AAL	C1-O5-C5	2.19	115.16	112.19
2	G	4	AAL	O2-C2-C1	-2.18	104.69	109.15
2	F	1	GAL	C4-C3-C2	2.15	114.58	110.82
2	H	4	AAL	C1-O5-C5	2.15	115.10	112.19
2	G	4	AAL	C3-C4-C5	-2.13	97.37	101.99
2	F	1	GAL	C1-O5-C5	-2.09	109.71	113.66
2	H	4	AAL	O4-C4-C5	-2.09	105.00	111.05
2	F	4	AAL	O3-C3-C4	2.08	107.31	103.59
2	F	2	AAL	C2-C3-C4	-2.07	108.72	113.85
2	G	1	GAL	O2-C2-C3	2.03	115.04	110.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	GAL	C3
2	G	1	GAL	C3
2	E	1	GAL	C3
2	H	1	GAL	C3

All (2) torsion outliers are listed below:

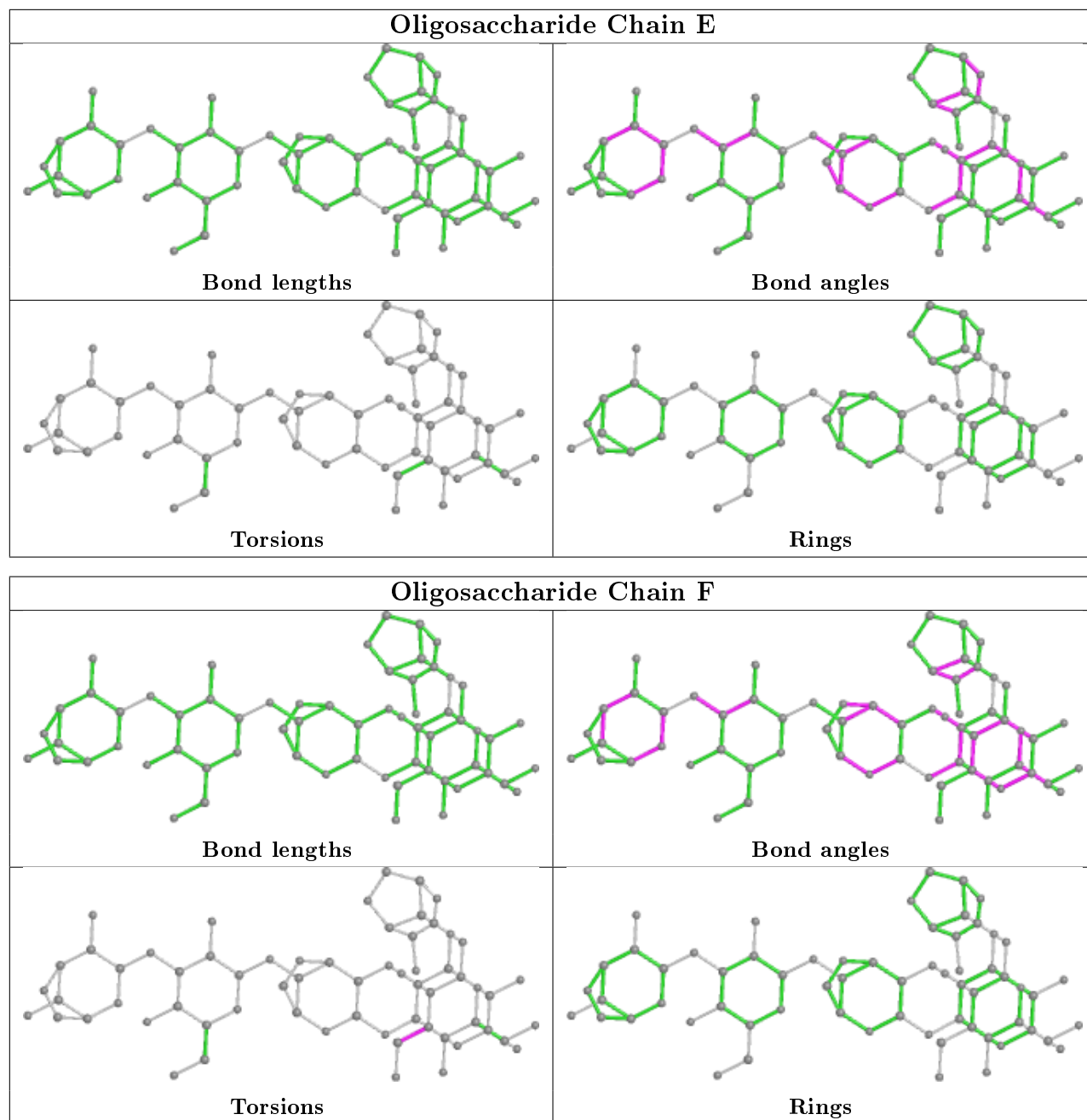
Mol	Chain	Res	Type	Atoms
2	H	1	GAL	C4-C5-C6-O6
2	F	1	GAL	C4-C5-C6-O6

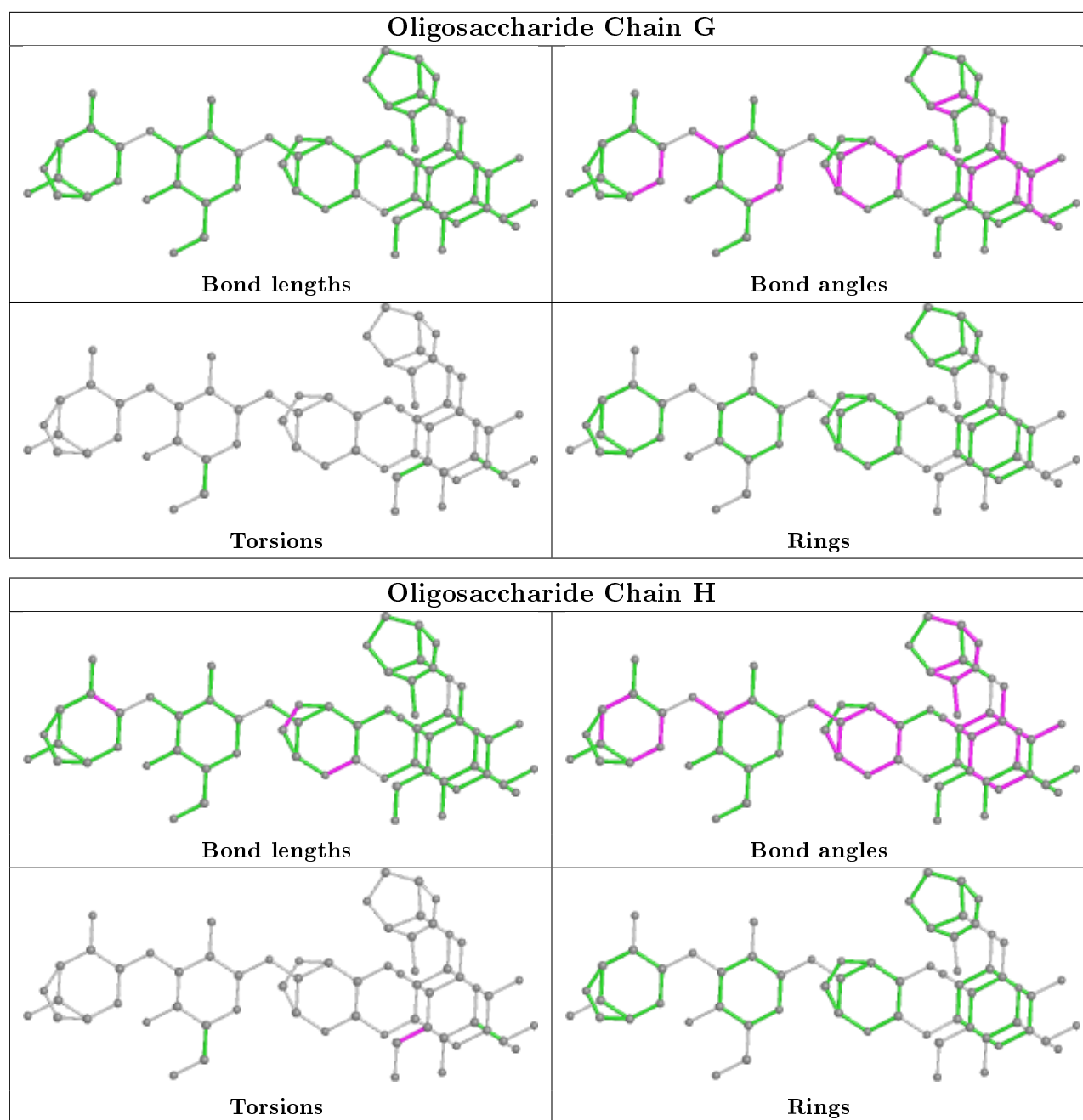
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	6	AAL	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.





5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 17 are monoatomic - leaving 6 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
4	EDO	D	1143	-	3,3,3	0.75	0	2,2,2	0.18	0
4	EDO	D	1142	-	3,3,3	0.62	0	2,2,2	0.40	0
4	EDO	A	1141	-	3,3,3	0.95	0	2,2,2	1.27	0
4	EDO	B	1141	-	3,3,3	0.50	0	2,2,2	0.23	0
4	EDO	C	1141	-	3,3,3	0.59	0	2,2,2	0.33	0
4	EDO	D	1144	-	3,3,3	0.76	0	2,2,2	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	1143	-	-	0/1/1/1	-
4	EDO	D	1142	-	-	0/1/1/1	-
4	EDO	A	1141	-	-	1/1/1/1	-
4	EDO	B	1141	-	-	0/1/1/1	-
4	EDO	C	1141	-	-	0/1/1/1	-
4	EDO	D	1144	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1141	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1142	EDO	3	0
4	A	1141	EDO	4	0

5.7 Other polymers [\(i\)](#)

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, 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	138/160 (86%)	0.47	10 (7%) 15 14	14, 19, 32, 36	0
1	B	128/160 (80%)	0.25	4 (3%) 49 46	14, 18, 27, 36	0
1	C	127/160 (79%)	0.47	7 (5%) 25 22	14, 19, 29, 36	0
1	D	130/160 (81%)	0.66	16 (12%) 4 3	13, 21, 32, 38	2 (1%)
All	All	523/640 (81%)	0.47	37 (7%) 16 14	13, 19, 31, 38	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	THR	8.0
1	A	24	ALA	8.0
1	C	34	GLY	6.4
1	B	3	ALA	5.9
1	D	34	GLY	4.4
1	D	19	PHE	4.2
1	A	20	SER	4.2
1	C	26	PRO	4.1
1	A	81	ASN	4.0
1	A	22	GLY	4.0
1	A	25	GLN	3.7
1	D	82	GLY	3.4
1	A	19	PHE	3.4
1	A	18	THR	3.3
1	C	138	ASN	3.3
1	A	2	THR	3.2
1	D	81[A]	ASN	3.1
1	D	138	ASN	3.1
1	D	26	PRO	3.0
1	A	1	SER	3.0
1	C	17	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	55	GLN	2.9
1	D	129	TRP	2.9
1	D	17	GLY	2.8
1	B	129	TRP	2.8
1	D	33	ASN	2.7
1	C	55[A]	GLN	2.5
1	D	131	LEU	2.4
1	D	31	THR	2.3
1	A	21	ASP	2.3
1	B	138	ASN	2.3
1	D	32	VAL	2.3
1	C	33	ASN	2.2
1	D	38	ILE	2.1
1	D	102	PRO	2.1
1	C	119	LEU	2.1
1	D	41	VAL	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.

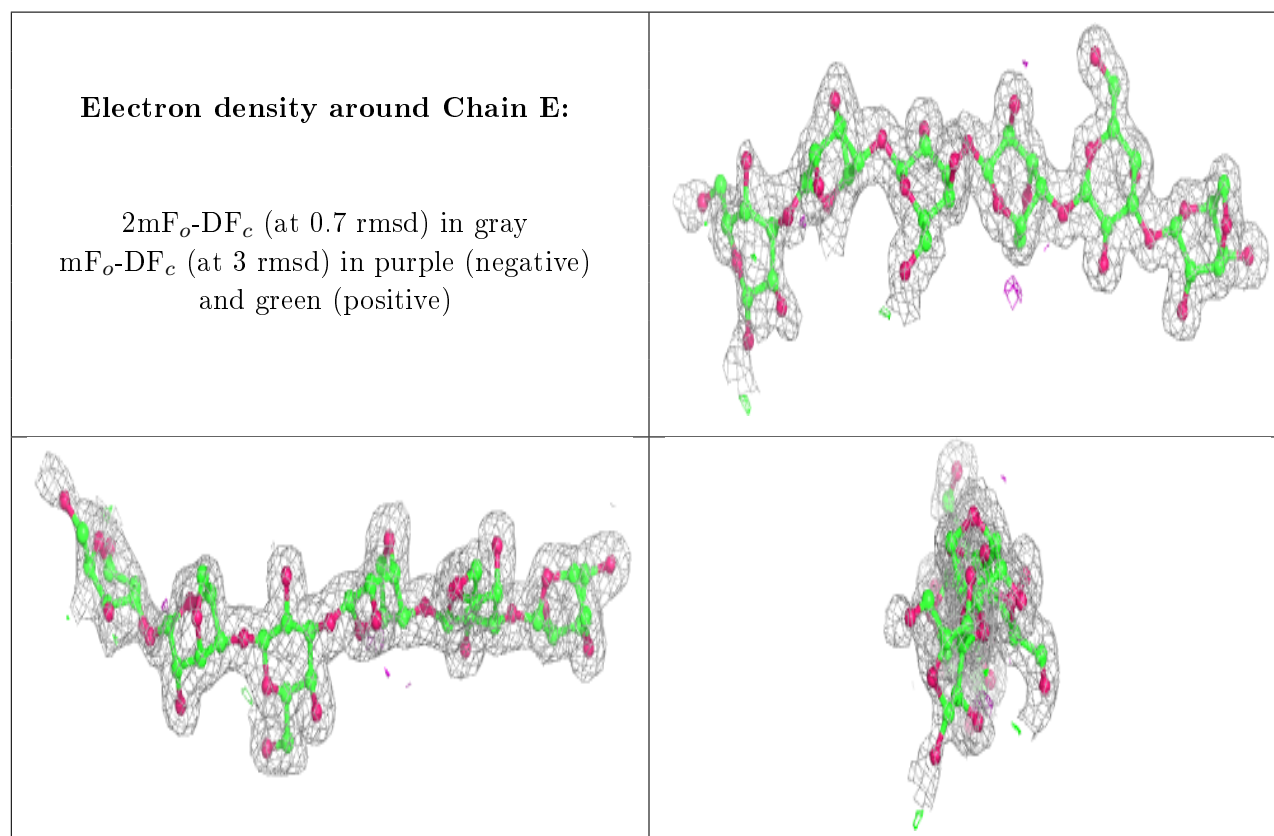
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	H	1	12/12	0.57	0.24	40,45,48,50	0
2	GAL	F	1	12/12	0.62	0.26	45,54,56,56	0
2	GAL	E	1	12/12	0.65	0.33	48,57,60,61	0
2	GAL	G	1	12/12	0.86	0.17	29,31,34,36	0
2	AAL	H	2	10/11	0.88	0.16	24,30,34,35	0
2	AAL	F	2	10/11	0.89	0.12	24,30,35,38	0
2	AAL	E	2	10/11	0.90	0.20	25,33,37,41	0
2	GAL	F	3	11/12	0.91	0.12	17,20,24,28	0
2	GAL	G	5	11/12	0.91	0.09	16,18,19,20	0
2	GAL	G	3	11/12	0.91	0.12	19,21,28,29	0
2	AAL	G	6	10/11	0.92	0.09	19,21,23,23	0
2	AAL	G	2	10/11	0.93	0.11	22,25,26,27	0

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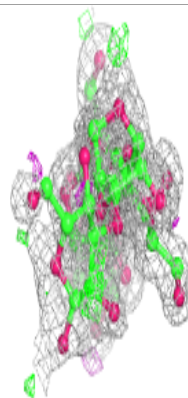
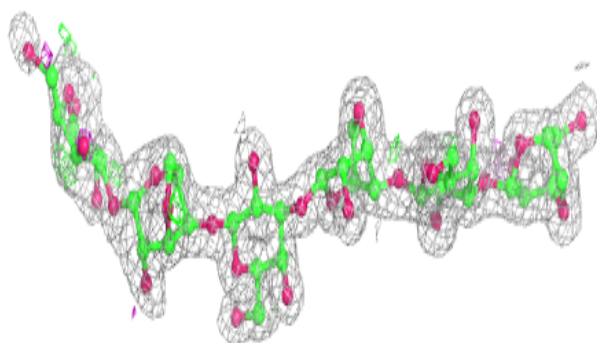
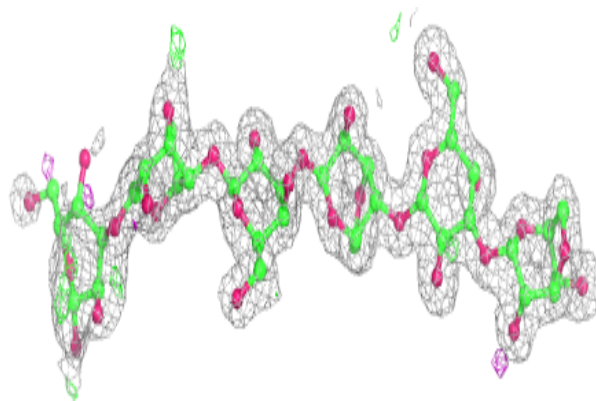
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AAL	F	4	10/11	0.94	0.09	15,17,18,19	0
2	AAL	H	6	10/11	0.94	0.09	19,22,24,25	0
2	GAL	H	3	11/12	0.95	0.08	18,23,28,29	0
2	AAL	G	4	10/11	0.95	0.07	17,19,19,20	0
2	GAL	E	3	11/12	0.95	0.07	17,22,27,31	0
2	AAL	E	4	10/11	0.95	0.07	16,17,19,20	0
2	AAL	F	6	10/11	0.96	0.08	14,16,17,17	0
2	GAL	H	5	11/12	0.96	0.07	16,18,21,22	0
2	AAL	H	4	10/11	0.96	0.06	15,18,18,19	0
2	GAL	E	5	11/12	0.97	0.07	15,16,17,18	0
2	AAL	E	6	10/11	0.97	0.06	15,16,19,19	0
2	GAL	F	5	11/12	0.98	0.08	11,16,18,20	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.

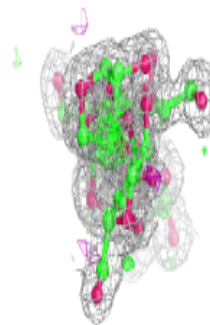
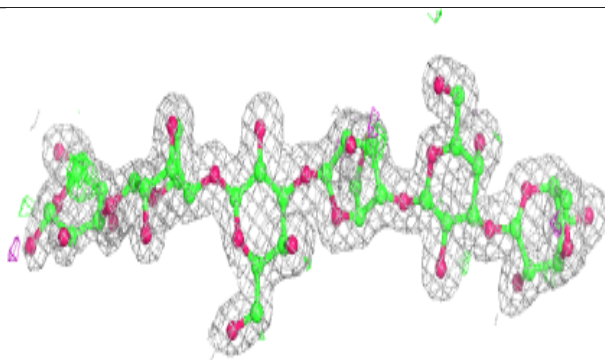
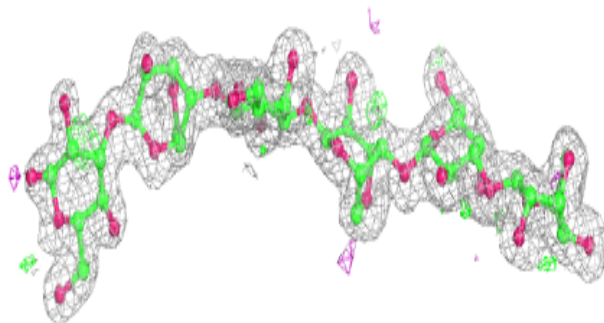


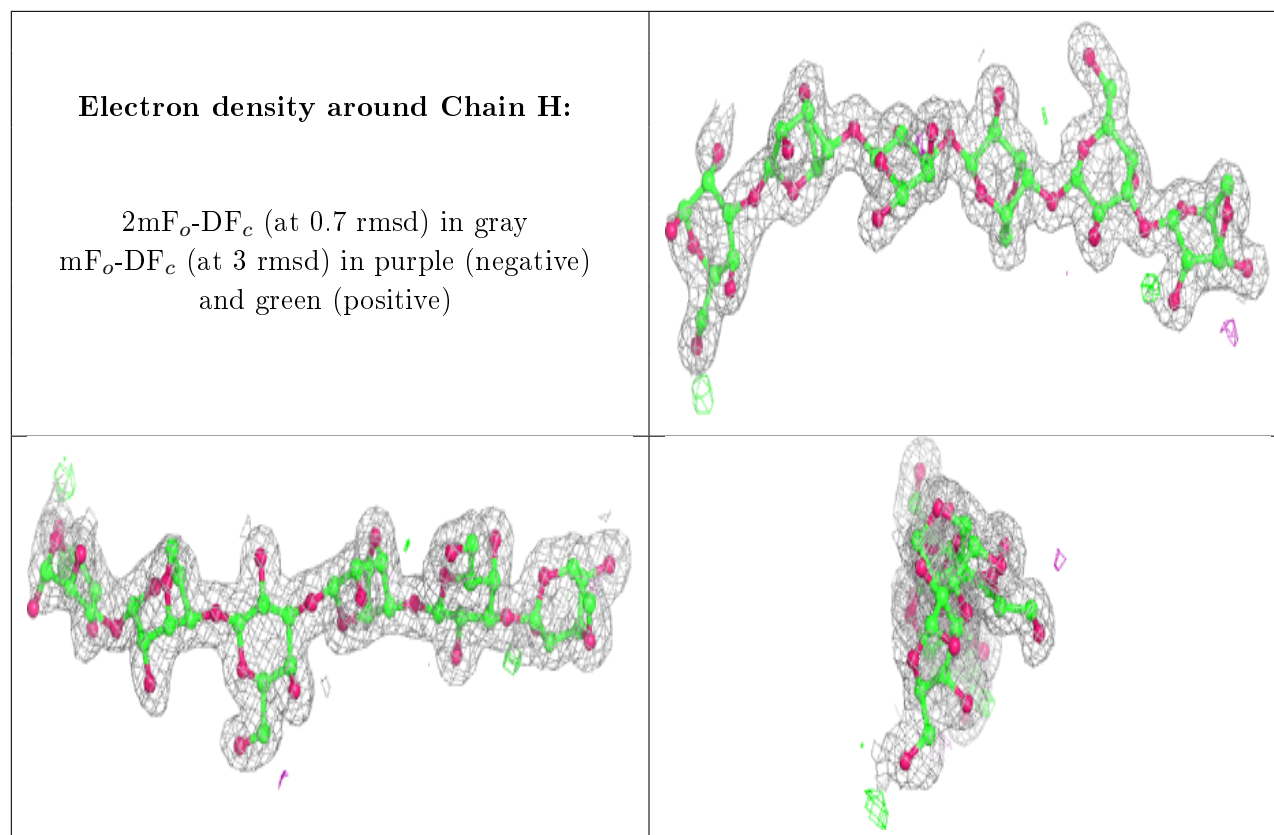
Electron density around Chain F:

$2mF_o-DF_c$ (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)





6.4 Ligands [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
4	EDO	D	1144	4/4	0.80	0.14	34,36,36,36	0
4	EDO	D	1143	4/4	0.85	0.12	28,28,29,31	0
4	EDO	D	1142	4/4	0.87	0.11	33,35,35,35	0
4	EDO	A	1141	4/4	0.87	0.15	21,23,25,28	0
5	CL	C	1143	1/1	0.97	0.05	30,30,30,30	0
4	EDO	B	1141	4/4	0.97	0.09	19,22,23,23	0
3	CA	C	1140	1/1	0.97	0.07	24,24,24,24	0
3	CA	A	1139	1/1	0.98	0.05	24,24,24,24	0
3	CA	C	1139	1/1	0.98	0.04	27,27,27,27	0
3	CA	D	1139	1/1	0.98	0.05	30,30,30,30	0
5	CL	B	1142	1/1	0.98	0.08	27,27,27,27	0
4	EDO	C	1141	4/4	0.98	0.11	17,17,19,19	0
5	CL	C	1142	1/1	0.98	0.08	26,26,26,26	1
5	CL	A	1143	1/1	0.98	0.08	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CL	B	1143	1/1	0.98	0.03	23,23,23,23	0
5	CL	D	1141	1/1	0.98	0.07	32,32,32,32	0
5	CL	B	1144	1/1	0.99	0.07	26,26,26,26	1
3	CA	A	1140	1/1	0.99	0.04	21,21,21,21	0
5	CL	A	1144	1/1	0.99	0.04	27,27,27,27	0
3	CA	B	1140	1/1	0.99	0.20	17,17,17,17	0
3	CA	B	1139	1/1	0.99	0.05	23,23,23,23	0
3	CA	D	1140	1/1	0.99	0.21	17,17,17,17	0
5	CL	A	1142	1/1	1.00	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.