Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2020 – 09:14 AM BST

PDB ID	:	6SZ6
Title	:	Chaetomium thermophilum beta-glucosidase
Authors	:	Mohsin, I.; Poudel, N.; Papageorgiou, A.C.
Deposited on	:	2019-10-02
Resolution	:	2.99 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:

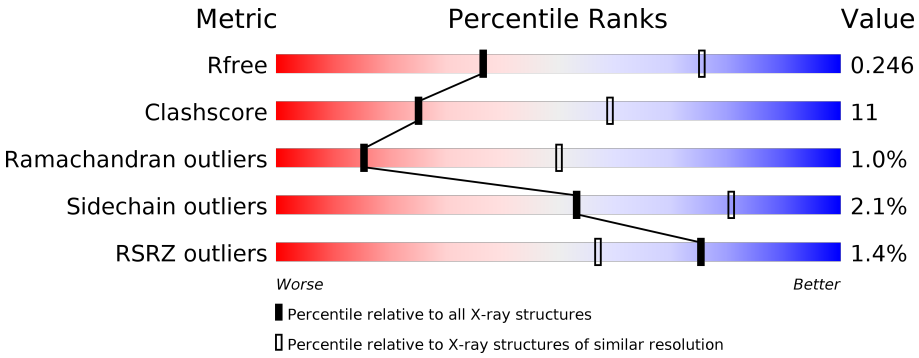
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.99 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 <=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	836	% 76% 23%
2	B	3	100%
2	C	3	33% 67%
2	H	3	67% 33%
3	D	2	50% 50%
3	G	2	50% 50%

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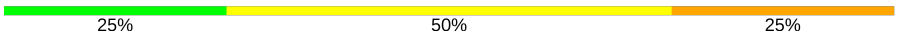
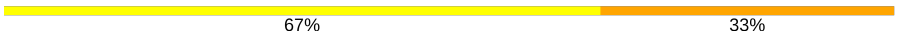
Mol	Chain	Length	Quality of chain
4	E	4	
5	F	3	

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	H	2	-	-	-	X
7	NAG	A	923	-	-	-	X
8	BMA	A	918	-	-	-	X

2 Entry composition

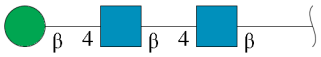
There are 10 unique types of molecules in this entry. The entry contains 6820 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	0	0
			6457	4082	1114	1236	25			

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(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
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

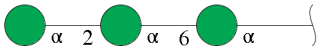
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos

e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.

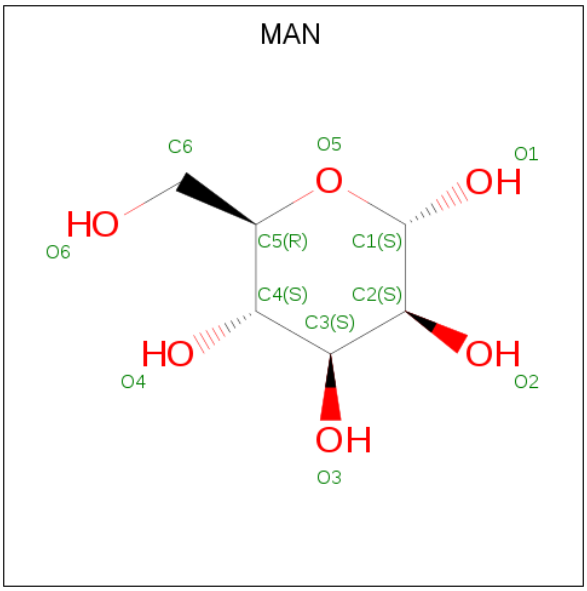
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-6)-alpha-D-mannopyranose.



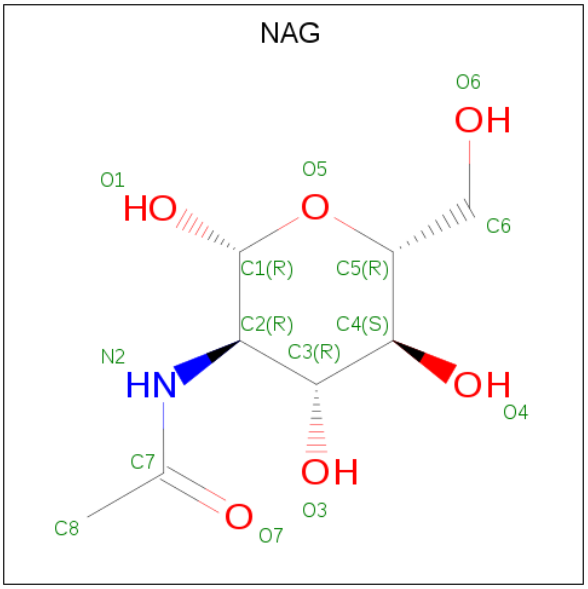
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	O		0	0	0
			33	18	15				

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



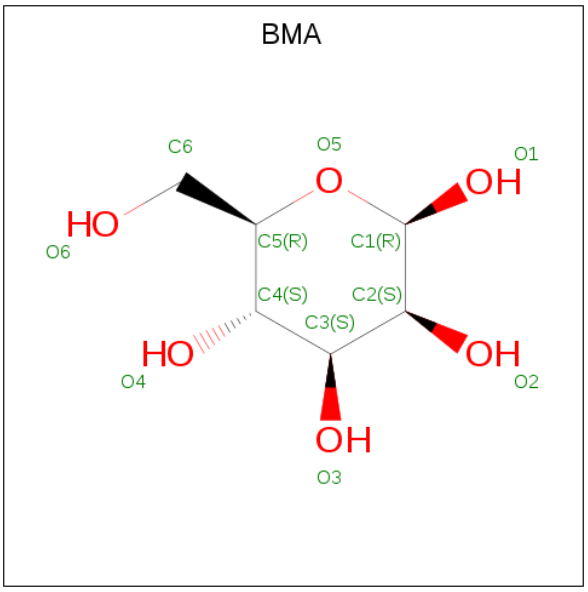
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			11	6	5			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



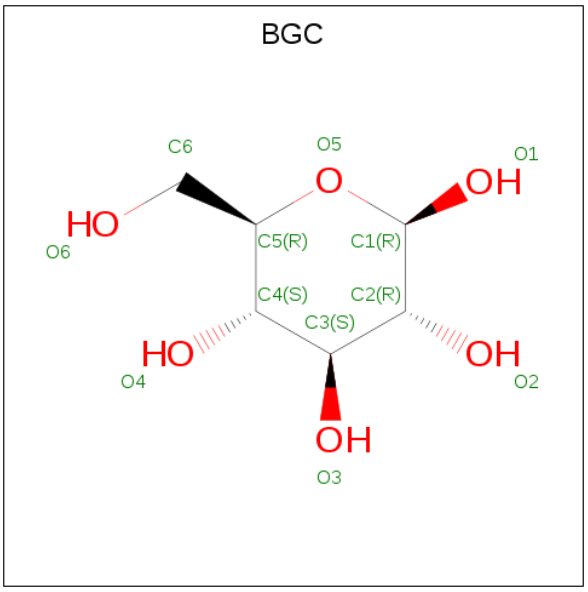
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 9 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 12 6 6	0	0

- Molecule 10 is water.

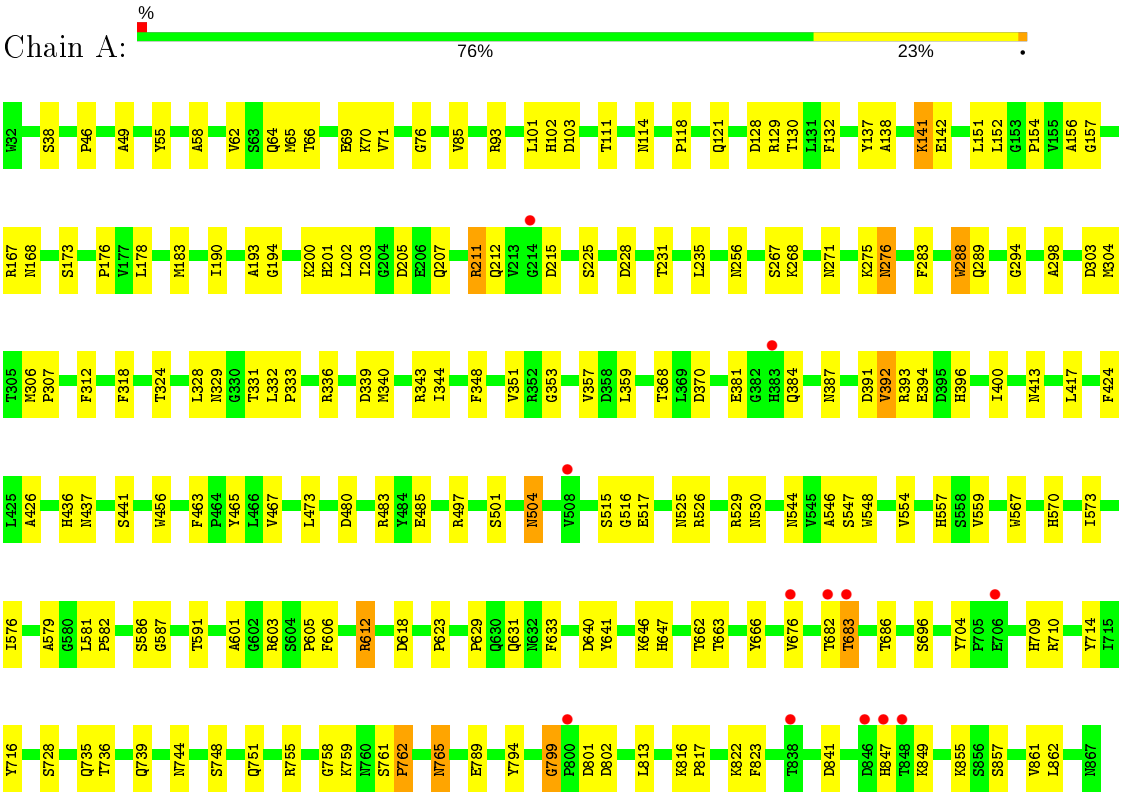
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	6	Total O 6 6	0	0

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.

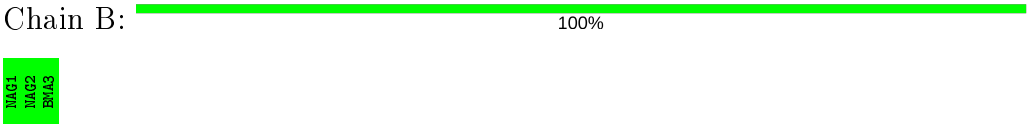
• Molecule 1: Beta-glucosidase

Chain A:



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

Chain B:



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

Chain C:

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

Chain H:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

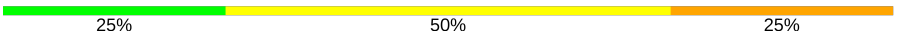
Chain D:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

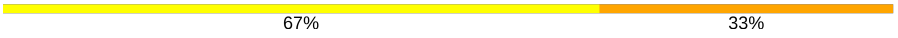
• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	121.86Å 121.86Å 264.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.99 19.83 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.83-2.99) 99.6 (19.83-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.98Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.201 , 0.249 0.201 , 0.246	Depositor DCC
R_{free} test set	2049 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6820	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, BMA, 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	0.36	0/6627	0.56	0/9033

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	LEU	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	6457	0	6165	139	2
2	B	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	39	0	34	1	0
2	H	39	0	34	0	0
3	D	28	0	25	1	0
3	G	28	0	25	0	0
4	E	50	0	43	1	0
5	F	33	0	28	2	0
6	A	11	0	10	2	0
7	A	56	0	52	7	0
8	A	22	0	20	0	0
9	A	12	0	11	1	0
10	A	6	0	0	0	0
All	All	6820	0	6481	142	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 11.

All (142) 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:744:ASN:HD21	7:A:924:NAG:C1	1.76	0.97
1:A:744:ASN:ND2	7:A:924:NAG:C1	2.36	0.89
1:A:582:PRO:HG2	1:A:586:SER:HB2	1.55	0.88
1:A:118:PRO:HD3	1:A:400:ILE:HG23	1.58	0.84
1:A:62:VAL:HA	1:A:65:MET:HG3	1.62	0.80
1:A:683:THR:HG21	1:A:759:LYS:HE2	1.70	0.74
1:A:85:VAL:H	1:A:102:HIS:HD2	1.38	0.71
1:A:303:ASP:OD1	1:A:336:ARG:NH2	2.23	0.71
1:A:504:ASN:CG	7:A:923:NAG:C1	2.60	0.70
1:A:207:GLN:HE22	1:A:631:GLN:HE22	1.38	0.69
1:A:176:PRO:HG3	1:A:235:LEU:HD12	1.73	0.69
1:A:138:ALA:HB1	1:A:396:HIS:CD2	2.29	0.68
1:A:215:ASP:OD2	1:A:526:ARG:NH2	2.28	0.67
1:A:413:ASN:HD21	1:A:417:LEU:H	1.43	0.66
1:A:207:GLN:NE2	1:A:631:GLN:HE22	1.94	0.66
1:A:71:VAL:HG21	1:A:324:THR:HG22	1.78	0.65
1:A:271:ASN:O	1:A:276:ASN:HB2	1.97	0.64
1:A:391:ASP:O	1:A:393:ARG:N	2.30	0.64
1:A:156:ALA:HB2	1:A:183:MET:SD	2.38	0.63
1:A:682:THR:HA	1:A:683:THR:HB	1.81	0.63
1:A:141:LYS:NZ	1:A:394:GLU:OE2	2.32	0.63
1:A:298:ALA:HB1	1:A:340:MET:HE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2:NAG:H3	3:D:2:NAG:H83	1.82	0.61
1:A:525:ASN:ND2	1:A:530:ASN:H	1.99	0.60
1:A:46:PRO:HB3	1:A:55:TYR:CE2	2.37	0.60
1:A:504:ASN:ND2	7:A:923:NAG:C1	2.65	0.59
1:A:704:TYR:OH	1:A:710:ARG:NH1	2.35	0.59
1:A:758:GLY:HA3	1:A:761:SER:OG	2.03	0.59
1:A:683:THR:HG23	1:A:759:LYS:NZ	2.18	0.58
1:A:351:VAL:O	1:A:353:GLY:N	2.36	0.58
1:A:755:ARG:HD3	1:A:841:ASP:HB2	1.86	0.58
1:A:275:LYS:HD3	1:A:343:ARG:CZ	2.33	0.57
1:A:66:THR:HG23	1:A:69:GLU:H	1.69	0.57
1:A:329:ASN:OD1	1:A:331:THR:HG22	2.05	0.57
1:A:497:ARG:HG3	1:A:548:TRP:CD2	2.41	0.56
1:A:288:TRP:CH2	1:A:306:MET:HG2	2.41	0.56
1:A:306:MET:HG3	1:A:307:PRO:HA	1.88	0.55
1:A:704:TYR:CE2	1:A:710:ARG:HD3	2.40	0.55
1:A:682:THR:HG23	1:A:683:THR:HG22	1.89	0.55
1:A:332:LEU:HD12	1:A:333:PRO:HD2	1.88	0.54
1:A:646:LYS:HD3	1:A:647:HIS:CE1	2.43	0.54
1:A:85:VAL:H	1:A:102:HIS:CD2	2.22	0.54
1:A:268:LYS:HE2	2:C:2:NAG:O6	2.08	0.54
1:A:467:VAL:HG12	1:A:587:GLY:HA3	1.90	0.54
1:A:666:TYR:HB2	1:A:861:VAL:HG21	1.91	0.53
1:A:582:PRO:HG2	1:A:586:SER:CB	2.35	0.53
1:A:283:PHE:CD1	1:A:344:ILE:HA	2.44	0.52
1:A:339:ASP:OD2	1:A:343:ARG:NH1	2.42	0.52
1:A:526:ARG:HH11	1:A:526:ARG:HB3	1.74	0.52
1:A:58:ALA:O	1:A:62:VAL:HG22	2.10	0.52
1:A:686:THR:HG22	1:A:751:GLN:H	1.75	0.52
1:A:525:ASN:HD22	1:A:530:ASN:H	1.56	0.52
1:A:682:THR:HA	1:A:683:THR:CB	2.39	0.51
1:A:799:GLY:HA3	1:A:802:ASP:OD1	2.10	0.51
1:A:861:VAL:HG23	1:A:862:LEU:HG	1.92	0.51
1:A:515:SER:HB3	1:A:529:ARG:HG3	1.92	0.51
1:A:473:LEU:HD23	1:A:591:THR:HG23	1.92	0.51
1:A:157:GLY:O	1:A:201:HIS:HB2	2.10	0.51
1:A:138:ALA:HB1	1:A:396:HIS:HD2	1.75	0.51
1:A:603:ARG:NH1	1:A:855:LYS:O	2.44	0.51
1:A:142:GLU:HA	1:A:392:VAL:HG22	1.93	0.50
1:A:559:VAL:HG12	1:A:581:LEU:HD11	1.92	0.50
1:A:103:ASP:OD2	9:A:928:BGC:H6C1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ASN:HD22	1:A:765:ASN:C	2.15	0.49
1:A:816:LYS:HB3	1:A:817:PRO:HD2	1.95	0.49
1:A:173:SER:HB2	1:A:178:LEU:HD23	1.95	0.48
1:A:137:TYR:CE2	1:A:141:LYS:HD3	2.47	0.48
1:A:736:THR:HG23	1:A:739:GLN:HG3	1.95	0.48
1:A:129:ARG:HA	1:A:132:PHE:CD2	2.49	0.48
1:A:339:ASP:O	1:A:343:ARG:HG3	2.14	0.48
1:A:128:ASP:OD2	1:A:130:THR:HB	2.14	0.47
1:A:336:ARG:HG3	1:A:340:MET:HE3	1.96	0.47
1:A:744:ASN:CG	7:A:924:NAG:C1	2.82	0.47
1:A:847:HIS:O	1:A:849:LYS:HG3	2.14	0.47
1:A:152:LEU:O	1:A:200:LYS:HD2	2.15	0.47
1:A:193:ALA:N	1:A:194:GLY:HA2	2.30	0.47
1:A:504:ASN:OD1	7:A:923:NAG:C1	2.63	0.47
1:A:735:GLN:HG3	4:E:2:NAG:O6	2.15	0.46
1:A:497:ARG:O	1:A:501:SER:OG	2.27	0.46
1:A:294:GLY:HA2	1:A:318:PHE:HB3	1.97	0.46
1:A:394:GLU:HB2	1:A:396:HIS:ND1	2.31	0.45
1:A:426:ALA:HA	1:A:485:GLU:O	2.16	0.45
1:A:683:THR:CG2	1:A:759:LYS:NZ	2.79	0.45
1:A:424:PHE:CD1	1:A:483:ARG:HG2	2.52	0.45
1:A:437:ASN:O	1:A:441:SER:HB3	2.16	0.45
1:A:64:GLN:O	1:A:93:ARG:NH2	2.45	0.45
1:A:151:LEU:HD23	1:A:190:ILE:HD13	1.98	0.45
1:A:111:THR:HG23	1:A:114:ASN:HD22	1.82	0.45
1:A:394:GLU:HB2	1:A:396:HIS:HD1	1.80	0.45
1:A:167:ARG:HD2	1:A:517:GLU:HG3	1.98	0.45
1:A:370:ASP:O	1:A:387:ASN:HB2	2.17	0.45
1:A:557:HIS:CD2	1:A:579:ALA:HB3	2.52	0.45
1:A:275:LYS:NZ	1:A:303:ASP:OD2	2.49	0.44
1:A:154:PRO:HB2	1:A:183:MET:HE3	2.00	0.44
1:A:497:ARG:HG3	1:A:548:TRP:CE2	2.53	0.44
1:A:168:ASN:N	1:A:168:ASN:HD22	2.14	0.44
1:A:683:THR:HG23	1:A:759:LYS:HZ3	1.82	0.44
1:A:463:PHE:HB3	1:A:465:TYR:O	2.18	0.44
1:A:554:VAL:HB	1:A:576:ILE:HG23	1.99	0.44
1:A:211:ARG:HG2	1:A:212:GLN:N	2.33	0.44
1:A:225:SER:HB2	1:A:633:PHE:CE1	2.52	0.44
1:A:640:ASP:OD1	1:A:641:TYR:N	2.51	0.43
1:A:686:THR:CG2	1:A:751:GLN:H	2.32	0.43
1:A:118:PRO:HB3	1:A:582:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:THR:HG21	1:A:759:LYS:CE	2.44	0.43
1:A:396:HIS:O	1:A:400:ILE:HG13	2.19	0.43
1:A:381:GLU:OE2	1:A:709:HIS:HE1	2.01	0.43
1:A:205:ASP:HB2	1:A:256:ASN:OD1	2.19	0.43
1:A:456:TRP:CD1	1:A:516:GLY:HA3	2.54	0.43
1:A:623:PRO:HB3	1:A:629:PRO:HG3	1.99	0.43
1:A:121:GLN:HE22	1:A:559:VAL:C	2.23	0.43
1:A:646:LYS:HD3	1:A:647:HIS:NE2	2.34	0.43
1:A:813:LEU:HD11	1:A:823:PHE:HB2	2.00	0.43
6:A:916:MAN:C1	5:F:1:MAN:HO3	2.26	0.43
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.89	0.42
1:A:605:PRO:HG2	1:A:606:PHE:CD2	2.54	0.42
1:A:228:ASP:OD2	1:A:231:THR:OG1	2.28	0.42
1:A:544:ASN:O	1:A:547:SER:HB3	2.19	0.42
1:A:612:ARG:NE	1:A:618:ASP:OD2	2.52	0.42
1:A:794:TYR:CZ	1:A:857:SER:HA	2.55	0.42
1:A:714:TYR:HB3	1:A:716:TYR:CE2	2.54	0.42
1:A:348:PHE:HZ	1:A:359:LEU:HD21	1.85	0.41
1:A:662:THR:OG1	1:A:663:THR:N	2.52	0.41
1:A:744:ASN:ND2	7:A:924:NAG:N2	2.68	0.41
1:A:141:LYS:HB3	1:A:141:LYS:HE2	1.59	0.41
1:A:38:SER:H	1:A:267:SER:CB	2.33	0.41
1:A:861:VAL:O	1:A:862:LEU:HD23	2.21	0.41
6:A:916:MAN:O5	5:F:1:MAN:O3	2.24	0.41
1:A:66:THR:O	1:A:70:LYS:HG3	2.21	0.41
1:A:101:LEU:HD11	1:A:304:MET:HE1	2.02	0.41
1:A:348:PHE:CZ	1:A:359:LEU:HD21	2.55	0.41
1:A:289:GLN:NE2	1:A:312:PHE:H	2.18	0.41
1:A:437:ASN:HA	1:A:437:ASN:HD22	1.73	0.41
1:A:546:ALA:HB1	1:A:570:HIS:CE1	2.56	0.41
1:A:603:ARG:NH2	1:A:789:GLU:OE1	2.54	0.41
1:A:368:THR:HG23	1:A:370:ASP:H	1.86	0.40
1:A:368:THR:HG23	1:A:370:ASP:N	2.36	0.40
1:A:567:TRP:O	1:A:573:ILE:HD12	2.21	0.40
1:A:49:ALA:HB2	1:A:762:PRO:HD2	2.03	0.40
1:A:141:LYS:HZ3	1:A:394:GLU:CD	2.24	0.40
1:A:76:GLY:HA3	1:A:306:MET:HE3	2.03	0.40
1:A:735:GLN:HB3	1:A:739:GLN:HB2	2.03	0.40

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)
1:A:436:HIS:NE2	1:A:436:HIS:NE2[8_554]	1.67	0.53
1:A:436:HIS:CE1	1:A:436:HIS:CE1[8_554]	2.18	0.02

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	834/836 (100%)	774 (93%)	52 (6%)	8 (1%)	15 50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	676	VAL
1	A	683	THR
1	A	203	ILE
1	A	357	VAL
1	A	392	VAL
1	A	601	ALA
1	A	799	GLY
1	A	762	PRO

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	680/684 (99%)	666 (98%)	14 (2%)	53 80

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LYS
1	A	211	ARG
1	A	276	ASN
1	A	288	TRP
1	A	384	GLN
1	A	480	ASP
1	A	504	ASN
1	A	612	ARG
1	A	696	SER
1	A	728	SER
1	A	748	SER
1	A	765	ASN
1	A	801	ASP
1	A	822	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	102	HIS
1	A	114	ASN
1	A	121	GLN
1	A	168	ASN
1	A	207	GLN
1	A	289	GLN
1	A	291	GLN
1	A	413	ASN
1	A	437	ASN
1	A	502	GLN
1	A	504	ASN
1	A	525	ASN
1	A	648	ASN
1	A	709	HIS
1	A	744	ASN
1	A	765	ASN
1	A	767	GLN

5.3.3 RNA

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	NAG	B	1	1,2	14,14,15	0.45	0	17,19,21	0.60	0
2	NAG	B	2	2	14,14,15	0.21	0	17,19,21	0.67	0
2	BMA	B	3	2	11,11,12	0.62	0	15,15,17	0.80	0
2	NAG	C	1	1,2	14,14,15	0.22	0	17,19,21	0.70	0
2	NAG	C	2	2	14,14,15	0.23	0	17,19,21	0.51	0
2	BMA	C	3	2	11,11,12	1.20	1 (9%)	15,15,17	1.72	5 (33%)
3	NAG	D	1	1,3	14,14,15	0.18	0	17,19,21	0.52	0
3	NAG	D	2	3	14,14,15	0.56	0	17,19,21	1.22	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.40	0	17,19,21	0.45	0
4	NAG	E	2	4	14,14,15	0.73	1 (7%)	17,19,21	0.40	0
4	BMA	E	3	4	11,11,12	1.04	0	15,15,17	1.11	1 (6%)
4	MAN	E	4	4	11,11,12	1.80	3 (27%)	15,15,17	0.99	1 (6%)
5	MAN	F	1	5	11,11,12	1.07	0	15,15,17	1.46	1 (6%)
5	MAN	F	2	5	11,11,12	1.08	1 (9%)	15,15,17	0.82	0
5	MAN	F	3	5	11,11,12	0.87	1 (9%)	15,15,17	1.13	2 (13%)
3	NAG	G	1	1,3	14,14,15	0.34	0	17,19,21	0.85	1 (5%)
3	NAG	G	2	3	14,14,15	0.26	0	17,19,21	0.56	0
2	NAG	H	1	1,2	14,14,15	0.56	0	17,19,21	0.63	0
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.40	0
2	BMA	H	3	2	11,11,12	1.14	1 (9%)	15,15,17	1.63	3 (20%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4	MAN	C2-C3	3.60	1.57	1.52
2	H	3	BMA	C1-C2	3.31	1.59	1.52
4	E	2	NAG	O5-C1	-2.61	1.39	1.43
4	E	4	MAN	O5-C5	2.56	1.48	1.43
5	F	2	MAN	O5-C1	-2.40	1.39	1.43
2	C	3	BMA	C6-C5	2.24	1.59	1.51
4	E	4	MAN	C4-C5	2.16	1.57	1.53
5	F	3	MAN	O5-C1	-2.08	1.40	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1	MAN	C1-O5-C5	4.10	117.75	112.19
3	D	2	NAG	C2-N2-C7	4.01	128.62	122.90
2	H	3	BMA	O5-C1-C2	3.63	116.37	110.77
2	C	3	BMA	O5-C1-C2	3.10	115.56	110.77
3	G	1	NAG	C1-O5-C5	3.03	116.30	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	BMA	O5-C5-C4	-2.98	103.58	110.83
5	F	3	MAN	O2-C2-C3	-2.71	104.72	110.14
2	H	3	BMA	C1-O5-C5	2.69	115.84	112.19
2	C	3	BMA	C1-C2-C3	2.62	112.89	109.67
2	H	3	BMA	C1-C2-C3	2.60	112.86	109.67
4	E	4	MAN	O3-C3-C2	2.35	114.50	109.99
2	C	3	BMA	C2-C3-C4	2.33	114.92	110.89
4	E	3	BMA	O2-C2-C3	-2.27	105.58	110.14
5	F	3	MAN	C1-O5-C5	2.16	115.12	112.19
2	C	3	BMA	O5-C5-C6	2.09	110.48	107.20

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
5	F	1	MAN	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C3-C2-N2-C7

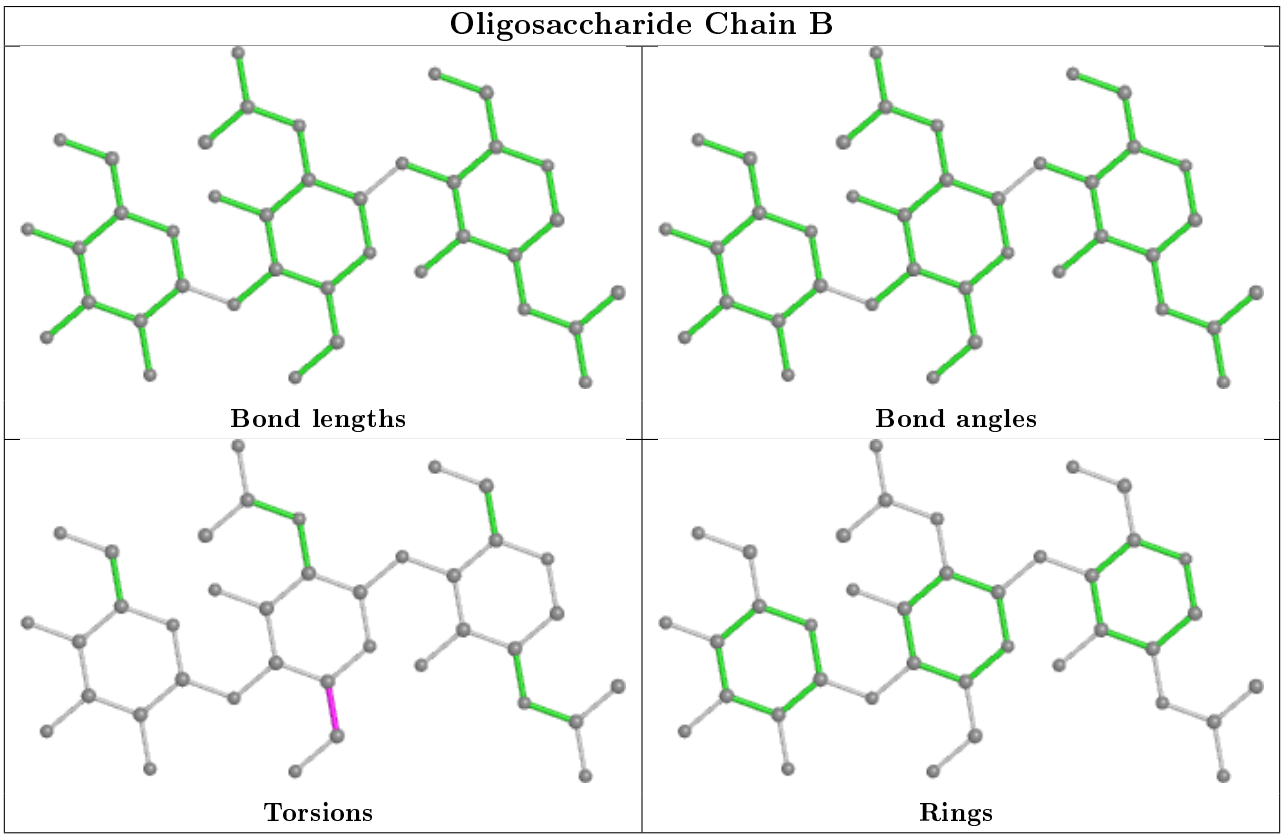
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1	MAN	C1-C2-C3-C4-C5-O5

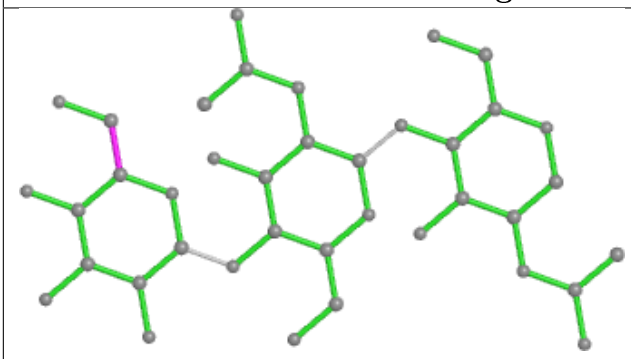
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
5	F	1	MAN	2	0
4	E	2	NAG	1	0
2	C	2	NAG	1	0

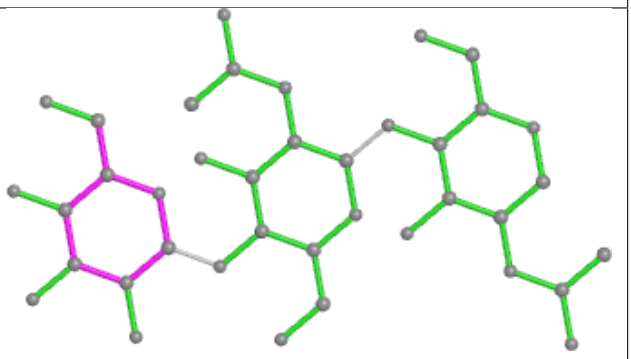
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



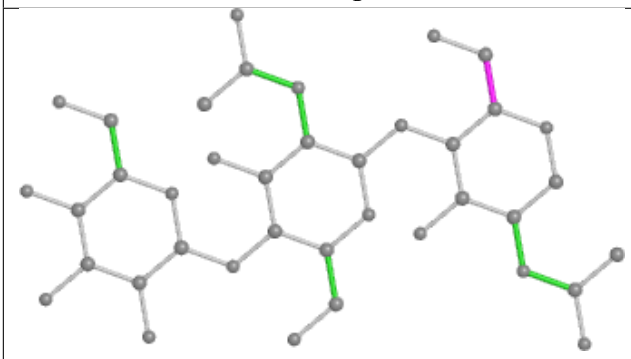
Oligosaccharide Chain C



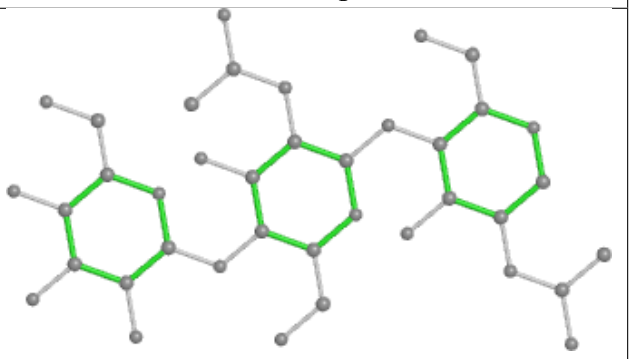
Bond lengths



Bond angles

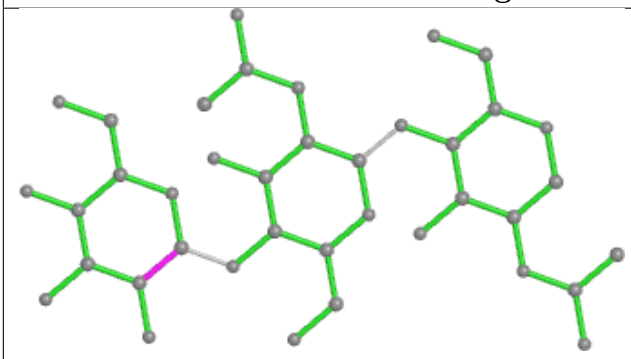


Torsions

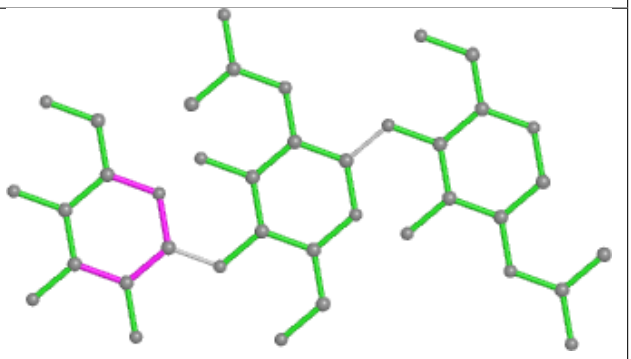


Rings

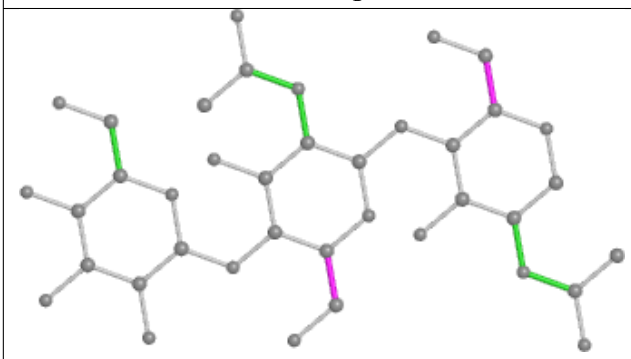
Oligosaccharide Chain H



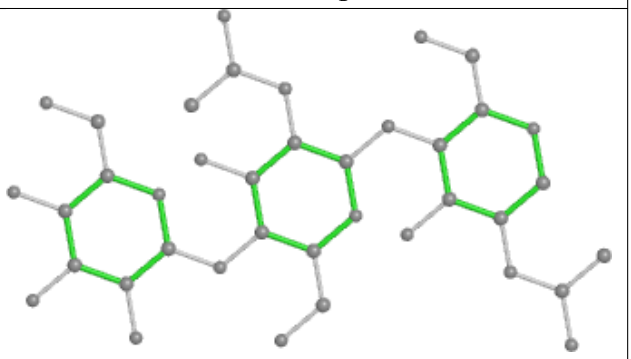
Bond lengths



Bond angles

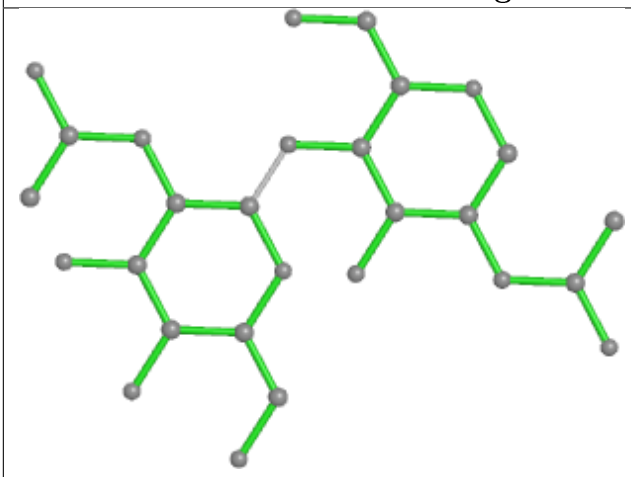


Torsions

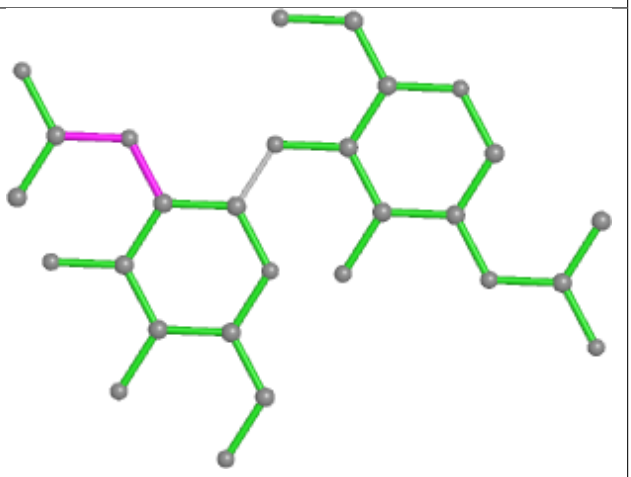


Rings

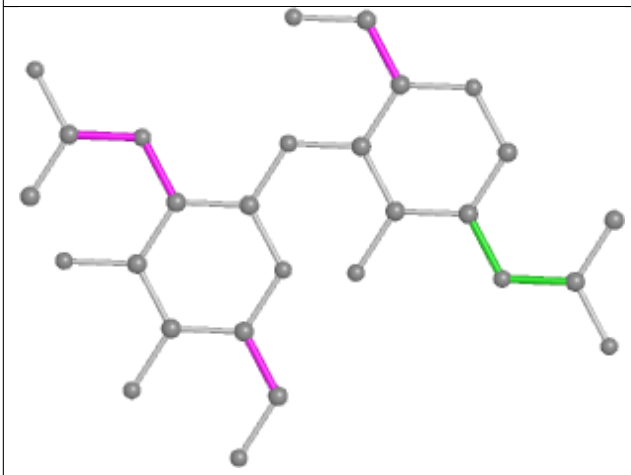
Oligosaccharide Chain D



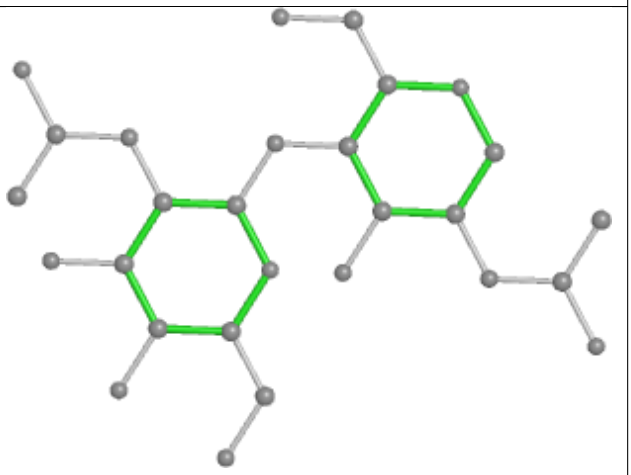
Bond lengths



Bond angles

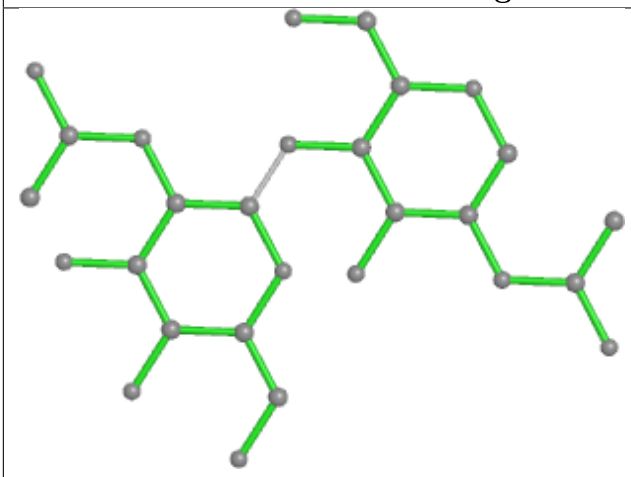


Torsions

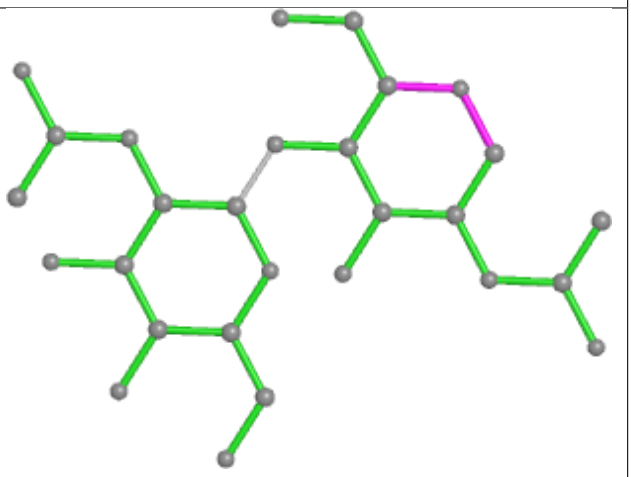


Rings

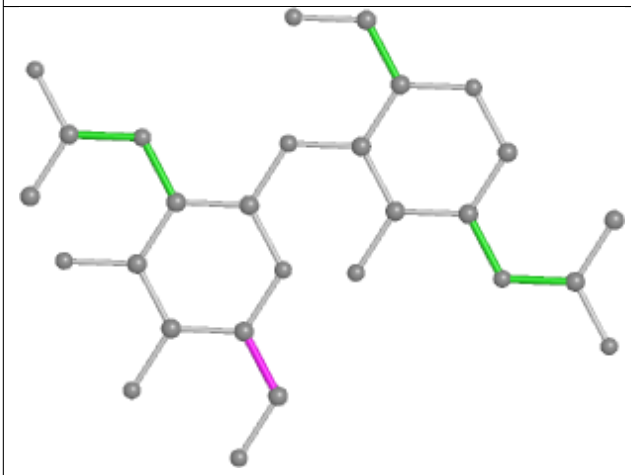
Oligosaccharide Chain G



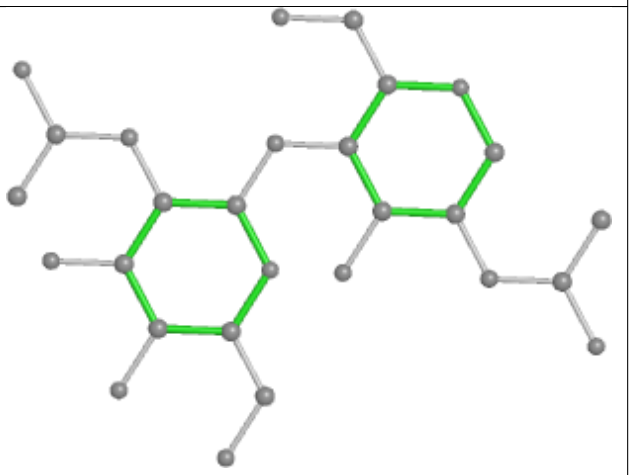
Bond lengths



Bond angles

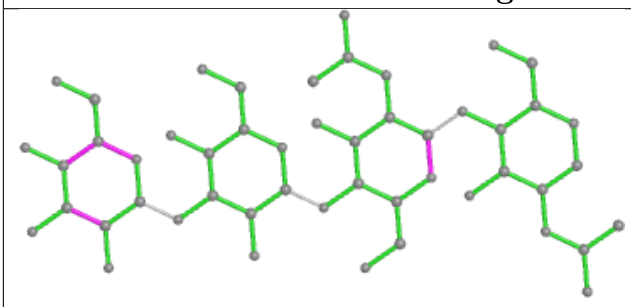


Torsions

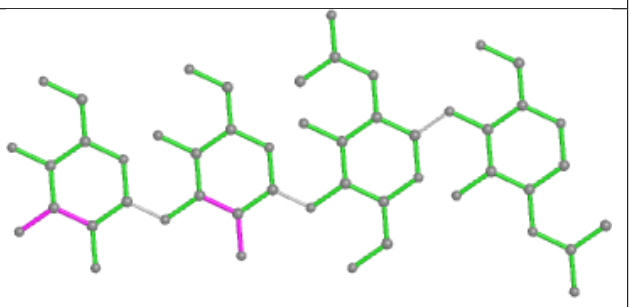


Rings

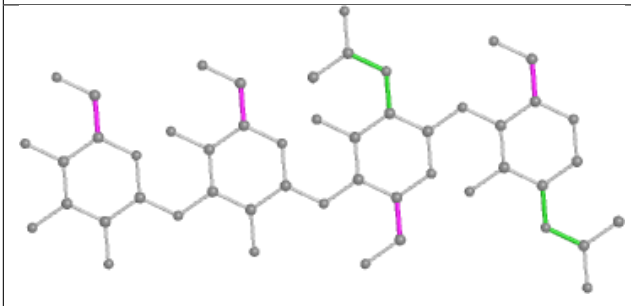
Oligosaccharide Chain E



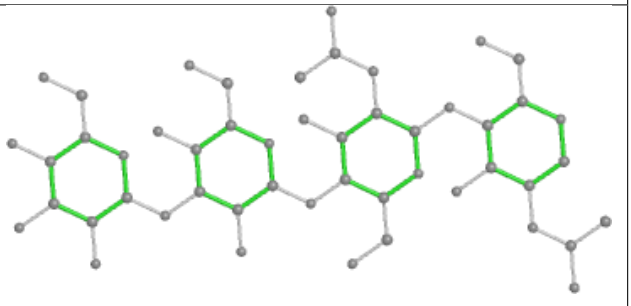
Bond lengths



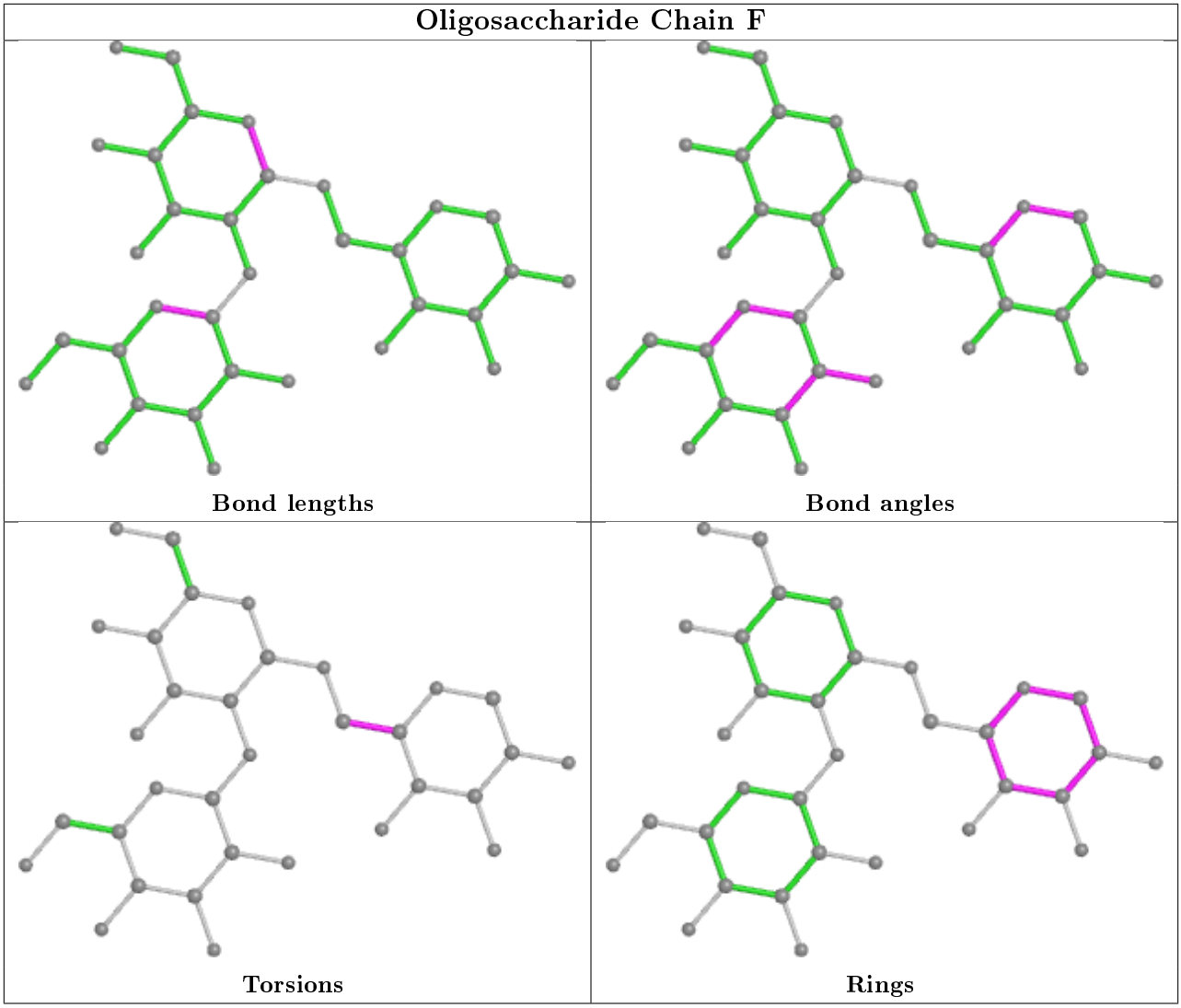
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
7	NAG	A	917	-	14,14,15	0.36	0	17,19,21	0.45	0
7	NAG	A	922	1	14,14,15	0.90	1 (7%)	17,19,21	0.66	0
8	BMA	A	921	-	11,11,12	1.18	1 (9%)	15,15,17	1.24	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BGC	A	928	-	12,12,12	2.18	5 (41%)	17,17,17	1.15	2 (11%)
6	MAN	A	916	-	11,11,12	1.21	2 (18%)	15,15,17	1.01	1 (6%)
8	BMA	A	918	-	11,11,12	1.47	2 (18%)	15,15,17	1.36	3 (20%)
7	NAG	A	924	-	14,14,15	0.45	0	17,19,21	0.45	0
7	NAG	A	923	-	14,14,15	0.40	0	17,19,21	0.41	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
7	NAG	A	917	-	-	1/6/23/26	0/1/1/1
7	NAG	A	922	1	-	2/6/23/26	0/1/1/1
8	BMA	A	921	-	-	0/2/19/22	0/1/1/1
9	BGC	A	928	-	-	2/2/22/22	0/1/1/1
6	MAN	A	916	-	-	0/2/19/22	0/1/1/1
8	BMA	A	918	-	-	0/2/19/22	0/1/1/1
7	NAG	A	924	-	-	2/6/23/26	0/1/1/1
7	NAG	A	923	-	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	928	BGC	O5-C1	5.13	1.55	1.42
8	A	918	BMA	C2-C3	3.23	1.57	1.52
6	A	916	MAN	C2-C3	2.81	1.56	1.52
7	A	922	NAG	O5-C1	2.67	1.48	1.43
8	A	921	BMA	C4-C3	2.65	1.59	1.52
8	A	918	BMA	C4-C3	2.60	1.59	1.52
9	A	928	BGC	O1-C1	-2.47	1.31	1.39
6	A	916	MAN	O5-C1	-2.45	1.39	1.43
9	A	928	BGC	O3-C3	2.19	1.48	1.43
9	A	928	BGC	C4-C5	-2.18	1.48	1.53
9	A	928	BGC	C4-C3	-2.12	1.46	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	928	BGC	C1-O5-C5	2.74	118.83	113.66
6	A	916	MAN	C1-O5-C5	2.72	115.88	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	921	BMA	O5-C5-C4	-2.71	104.23	110.83
8	A	918	BMA	O5-C1-C2	2.57	114.73	110.77
8	A	918	BMA	C2-C3-C4	2.56	115.33	110.89
8	A	918	BMA	C1-C2-C3	2.53	112.78	109.67
8	A	921	BMA	O5-C1-C2	2.41	114.49	110.77
9	A	928	BGC	O5-C5-C4	2.30	113.88	109.69

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	922	NAG	O5-C5-C6-O6
7	A	924	NAG	O5-C5-C6-O6
7	A	922	NAG	C4-C5-C6-O6
9	A	928	BGC	C4-C5-C6-O6
9	A	928	BGC	O5-C5-C6-O6
7	A	924	NAG	C4-C5-C6-O6
7	A	917	NAG	C3-C2-N2-C7

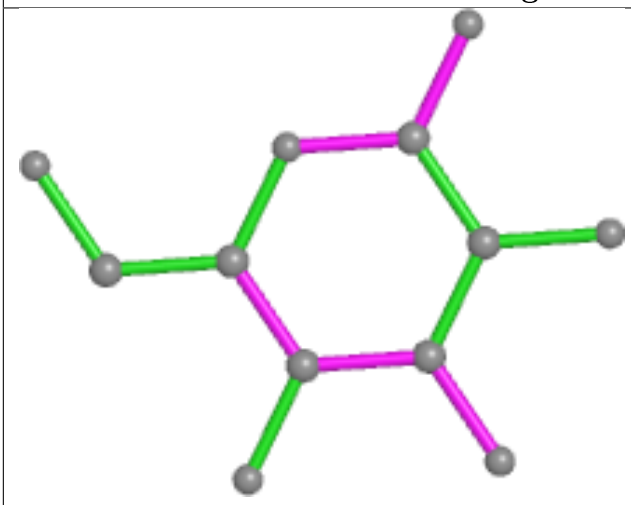
There are no ring outliers.

4 monomers are involved in 10 short contacts:

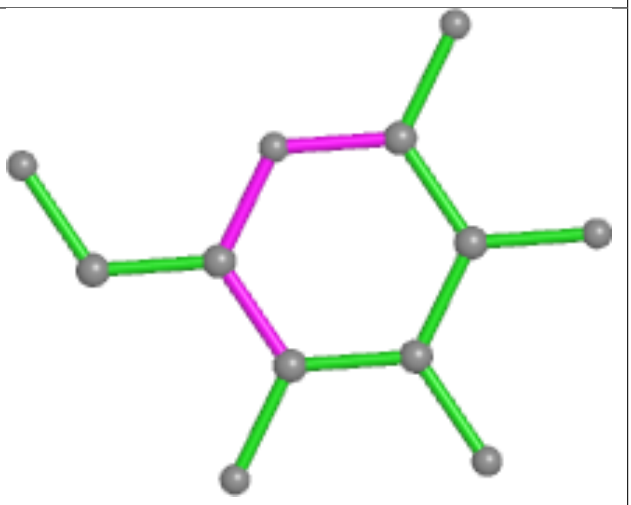
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	928	BGC	1	0
6	A	916	MAN	2	0
7	A	924	NAG	4	0
7	A	923	NAG	3	0

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.

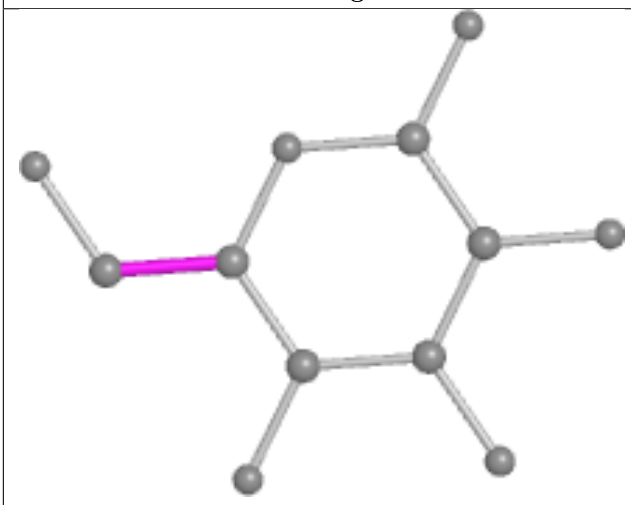
Ligand BGC A 928



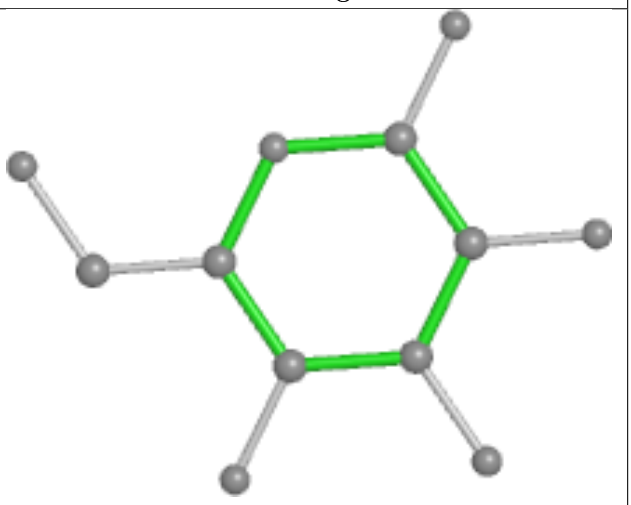
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	836/836 (100%)	-0.41	12 (1%) 75 57	28, 48, 72, 124	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	GLY	3.0
1	A	846	ASP	3.0
1	A	838	THR	2.8
1	A	383	HIS	2.6
1	A	847	HIS	2.4
1	A	508	VAL	2.4
1	A	683	THR	2.4
1	A	706	GLU	2.2
1	A	800	PRO	2.2
1	A	676	VAL	2.1
1	A	848	THR	2.1
1	A	682	THR	2.0

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

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

6.3 Carbohydrates

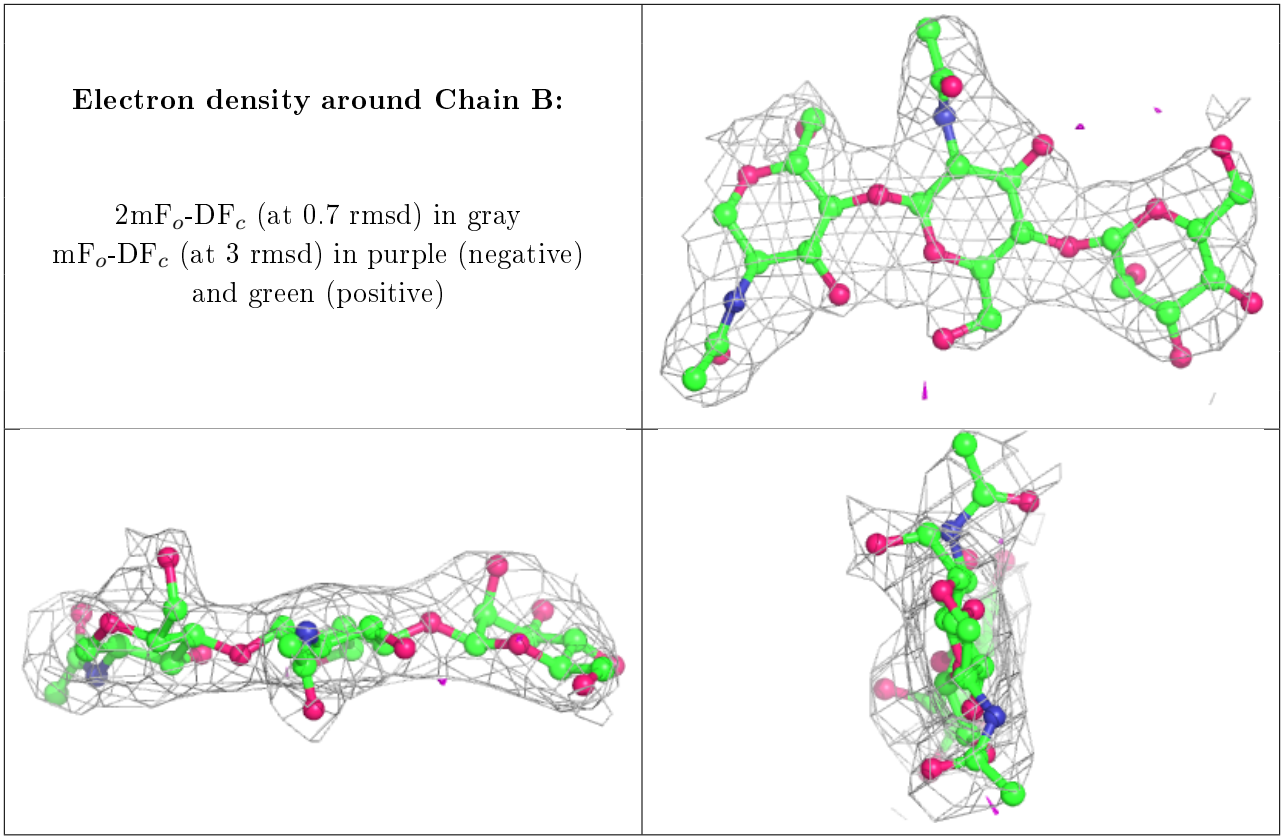
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	H	2	14/15	0.74	0.59	104,117,125,134	0
2	BMA	H	3	11/12	0.80	0.64	130,139,146,146	0
3	NAG	G	2	14/15	0.84	0.42	63,78,93,96	0
4	MAN	E	4	11/12	0.87	0.17	59,81,85,89	0
2	NAG	H	1	14/15	0.88	0.38	78,95,104,106	0
3	NAG	D	2	14/15	0.89	0.26	46,60,85,92	0
2	BMA	C	3	11/12	0.91	0.31	58,59,65,65	0
4	BMA	E	3	11/12	0.92	0.14	46,55,68,79	0
5	MAN	F	1	11/12	0.94	0.13	40,50,58,65	0
2	BMA	B	3	11/12	0.94	0.34	70,77,89,90	0
4	NAG	E	2	14/15	0.94	0.16	45,54,60,61	0
4	NAG	E	1	14/15	0.95	0.14	44,47,53,54	0
5	MAN	F	2	11/12	0.95	0.15	46,54,56,59	0
2	NAG	C	1	14/15	0.95	0.14	43,47,52,56	0
3	NAG	D	1	14/15	0.95	0.15	37,49,53,54	0
2	NAG	B	2	14/15	0.95	0.21	38,55,60,67	0
2	NAG	C	2	14/15	0.96	0.31	46,53,65,66	0
3	NAG	G	1	14/15	0.97	0.31	35,43,53,66	0
2	NAG	B	1	14/15	0.97	0.16	40,49,59,62	0
5	MAN	F	3	11/12	0.97	0.29	51,58,62,65	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.

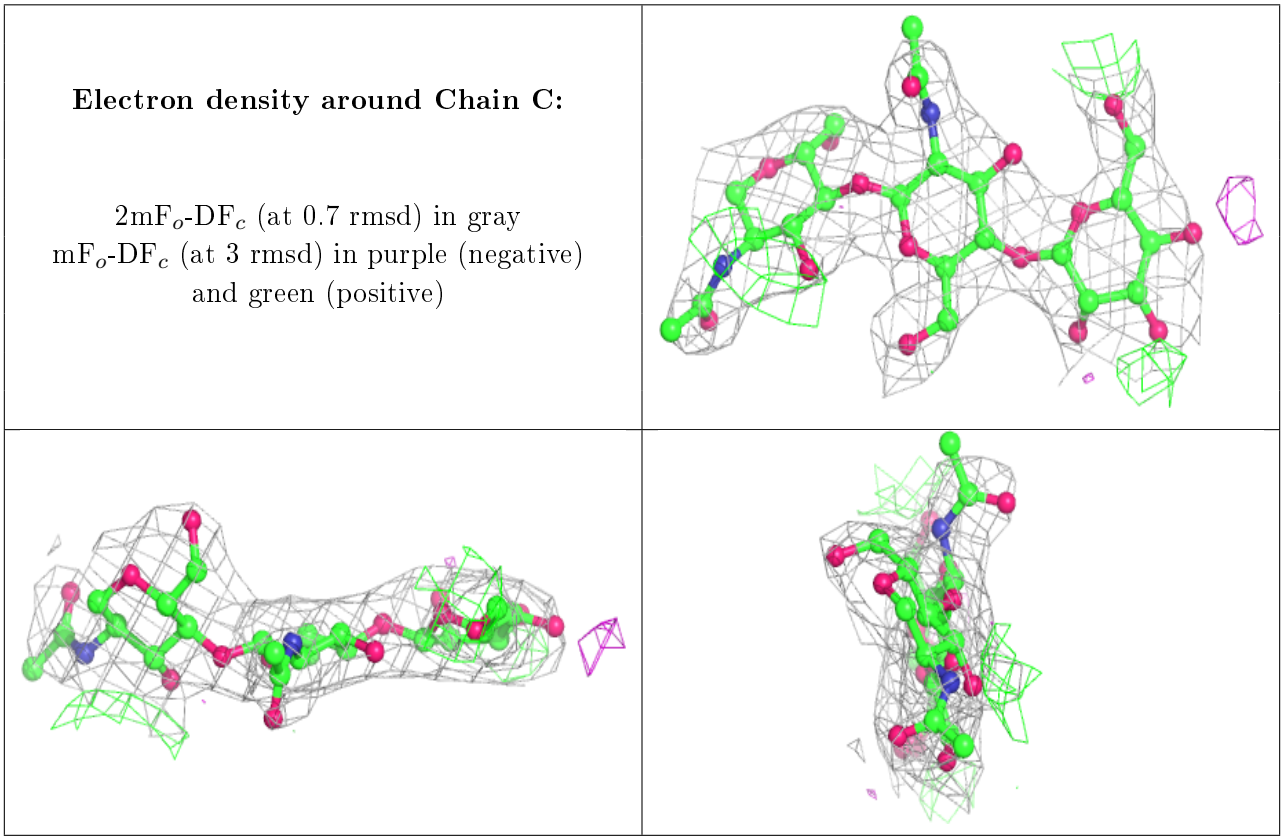
Electron density around Chain B:

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



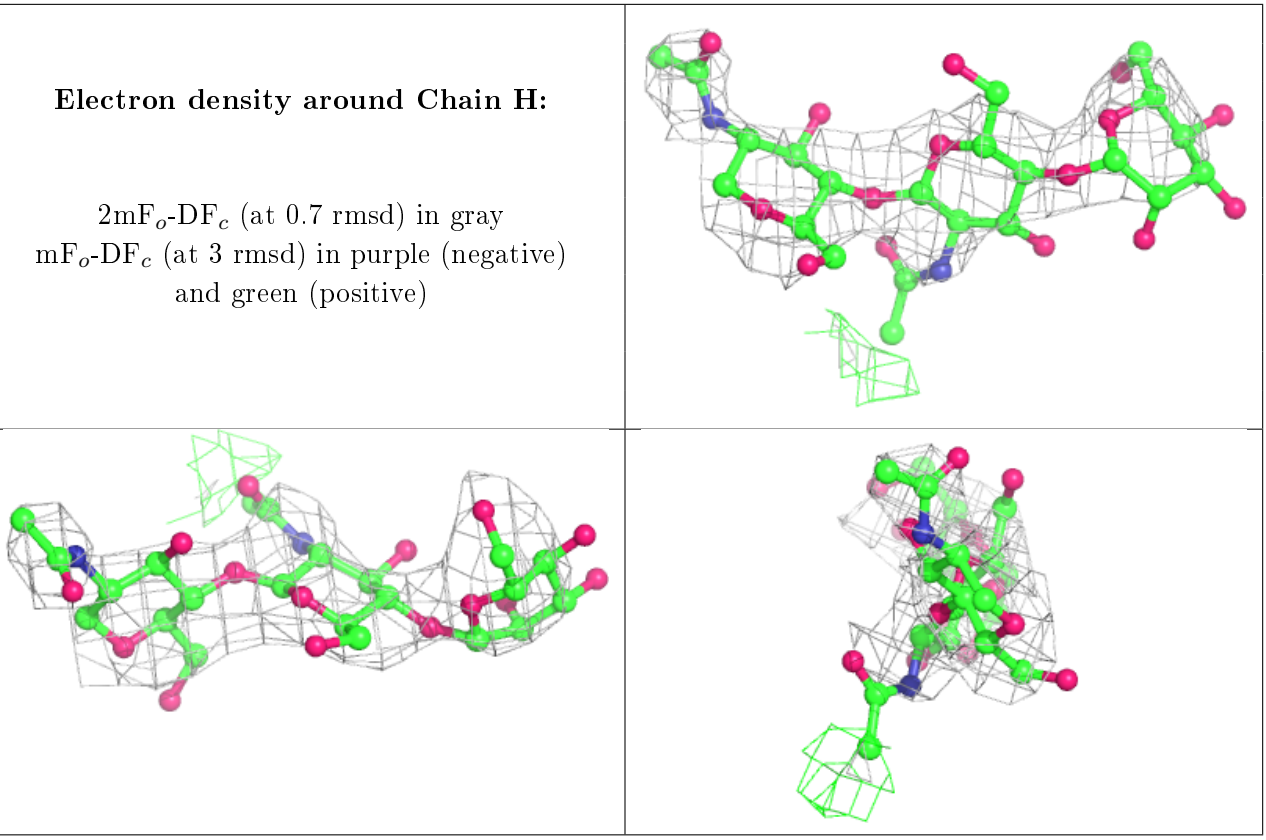
Electron density around Chain C:

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



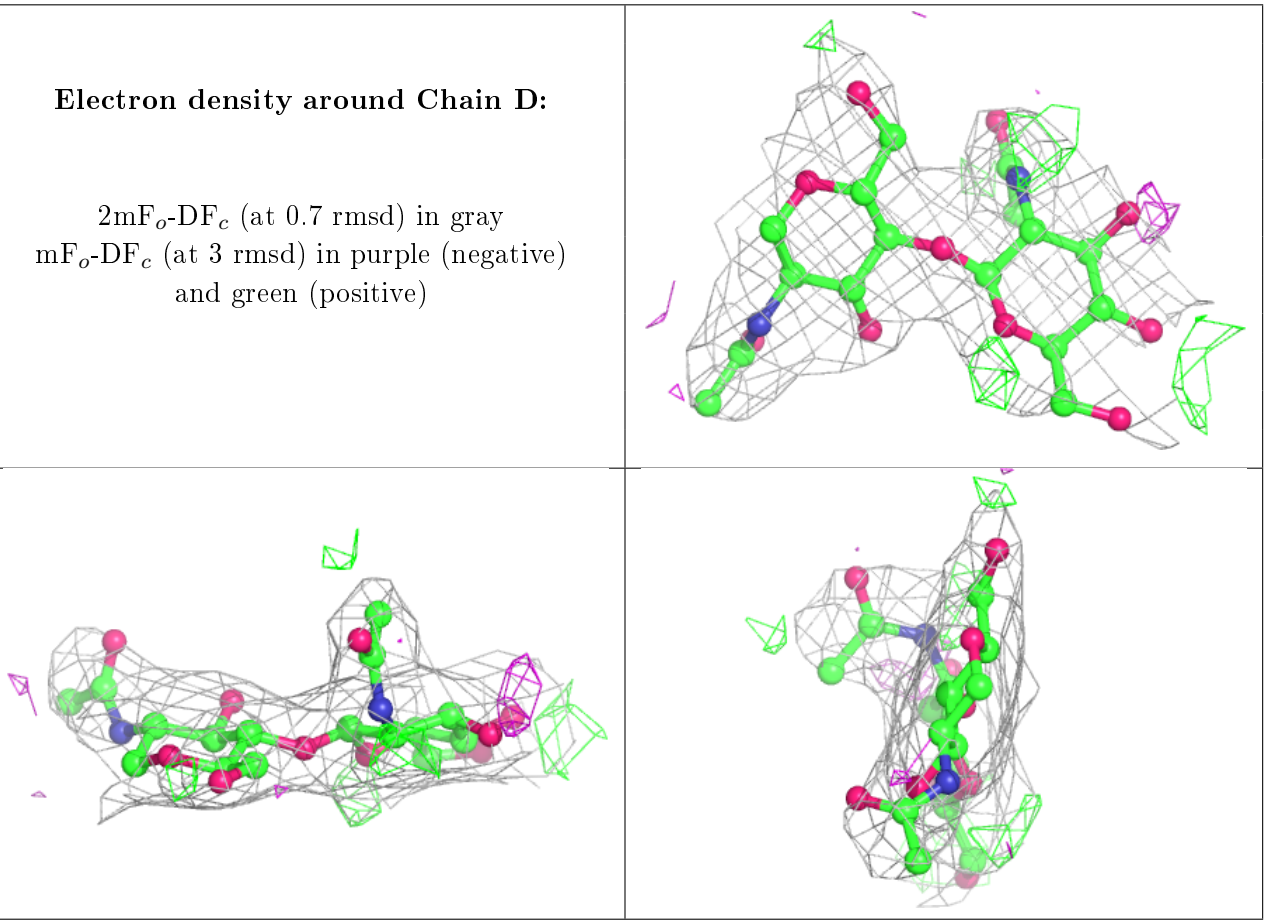
Electron density around Chain H:

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



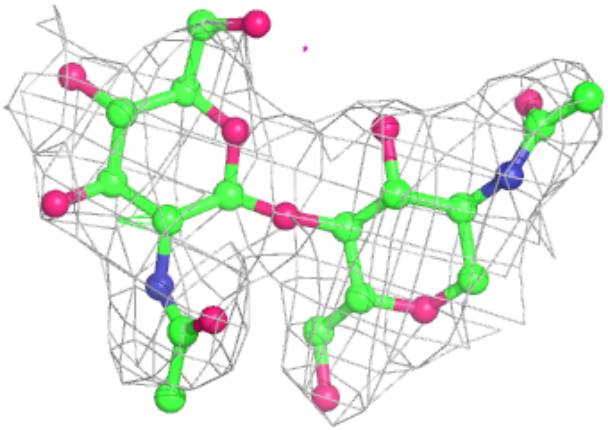
Electron density around Chain D:

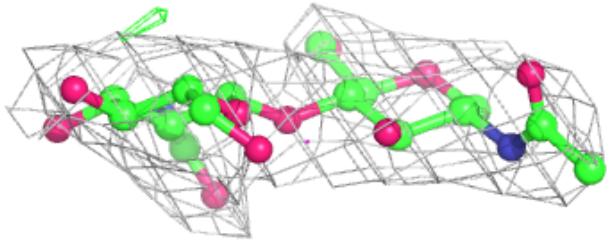
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

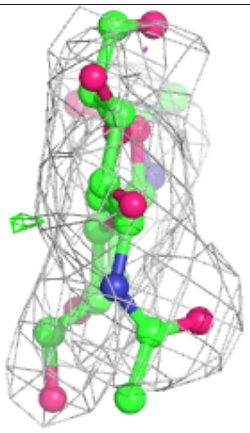


Electron density around Chain G:

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

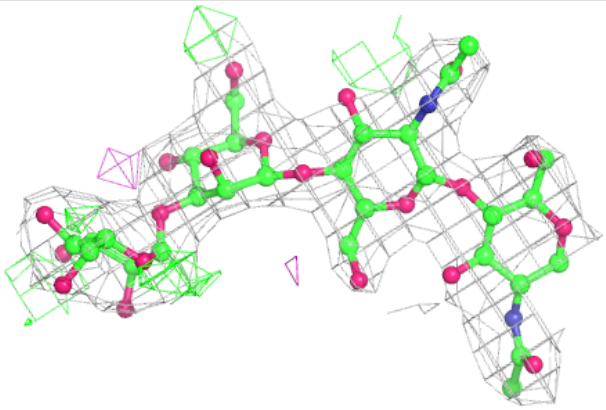


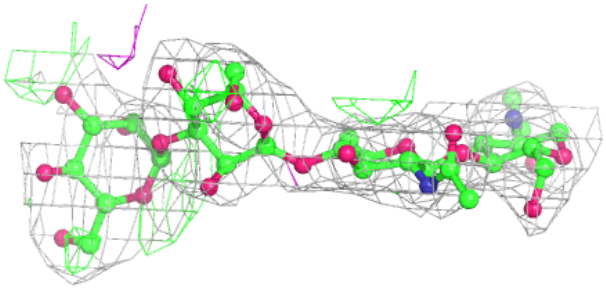


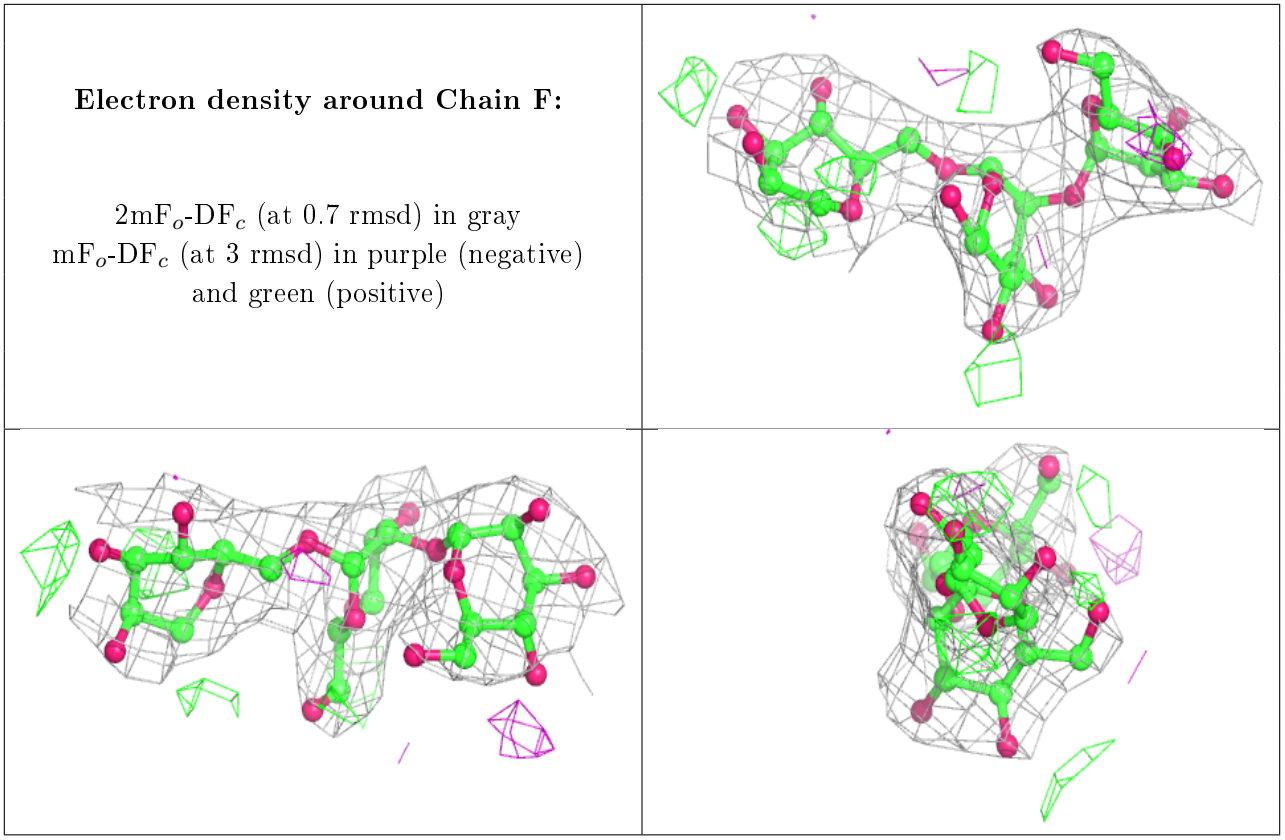


Electron density around Chain E:

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







6.4 Ligands

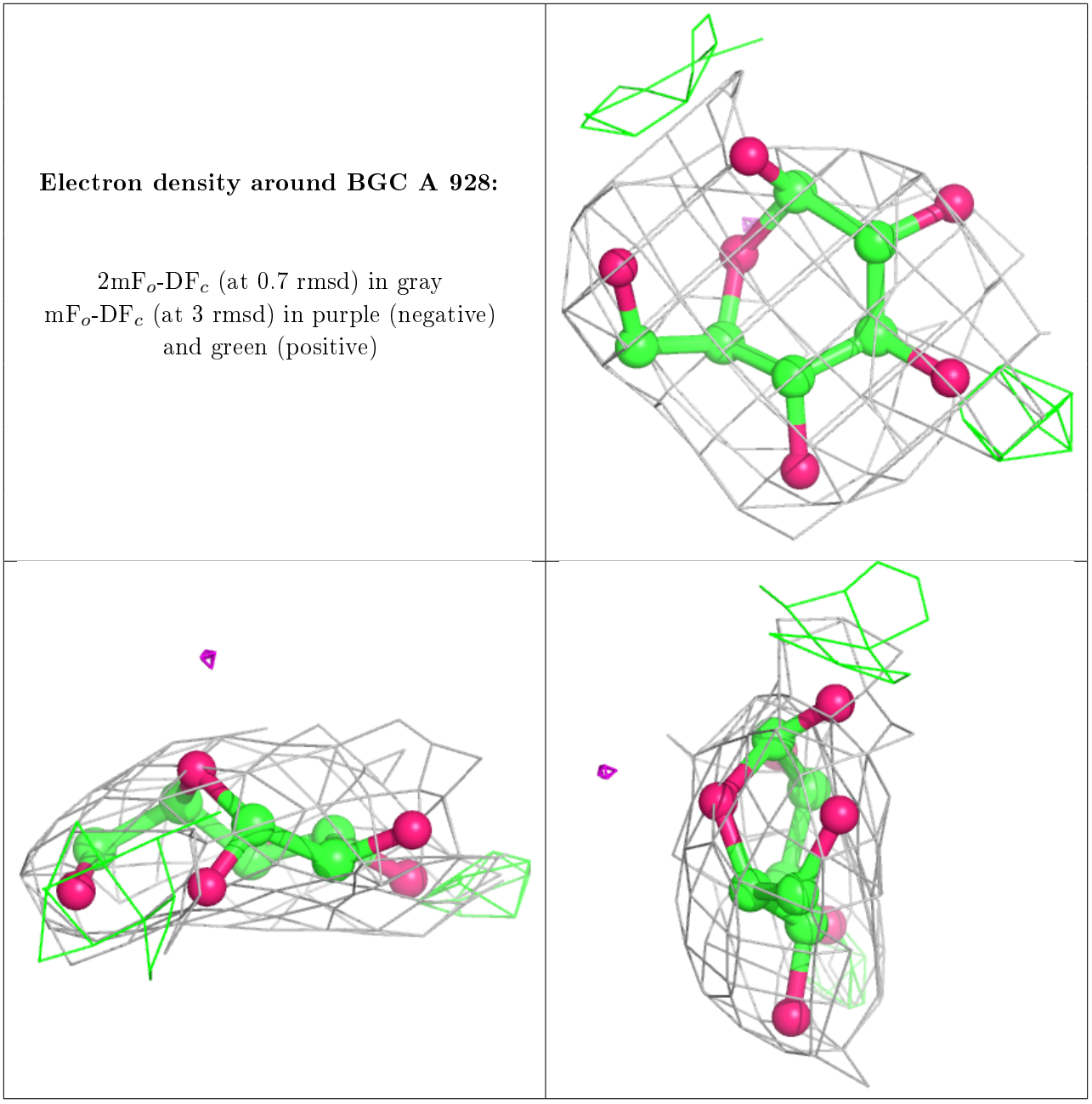
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	BMA	A	918	11/12	0.69	0.59	102,112,115,115	0
7	NAG	A	923	14/15	0.74	0.48	84,99,104,104	0
7	NAG	A	924	14/15	0.76	0.37	89,97,100,101	0
8	BMA	A	921	11/12	0.82	0.22	58,78,85,96	0
7	NAG	A	922	14/15	0.88	0.36	73,83,87,88	0
7	NAG	A	917	14/15	0.88	0.33	92,94,105,111	0
9	BGC	A	928	12/12	0.88	0.23	54,64,82,86	0
6	MAN	A	916	11/12	0.89	0.21	42,51,57,58	0

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

Electron density around BGC A 928:

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



6.5 Other polymers

There are no such residues in this entry.