Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 08:32 AM EDT

PDB ID	:	6E6B
Title	:	Crystal structure of the Protocadherin GammaB4 extracellular domain
Authors	:	Goodman, K.M.; Mannepalli, S.; Bahna, F.; Honig, B.; Shapiro, L.
Deposited on	:	2018-07-24
Resolution	:	4.52 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:

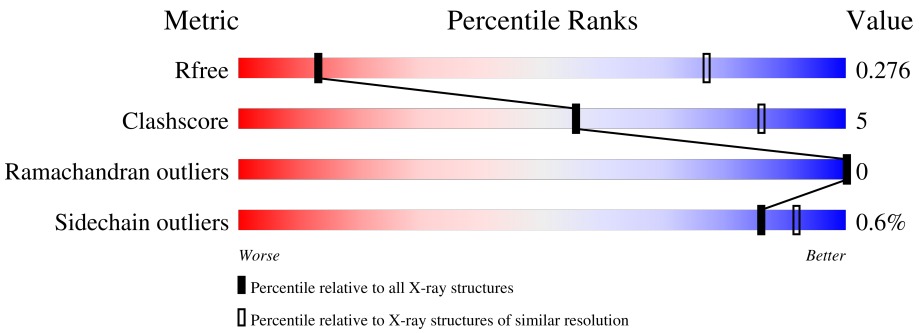
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 4.52 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	1056 (5.22-3.80)
Clashscore	141614	1124 (5.22-3.80)
Ramachandran outliers	138981	1070 (5.22-3.80)
Sidechain outliers	138945	1051 (5.22-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	646	87% 11% .
1	B	646	82% 15% .
2	C	2	50% 50%
3	D	6	67% 17% 17%
4	E	3	67% 33%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9742 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 Protocadherin gamma B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	633	4746	2958	807	973	8	0	0	0
1	B	625	4743	2972	794	966	11	0	0	0

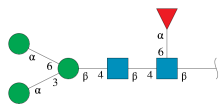
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	639	HIS	-	expression tag	UNP Q91XX6
A	640	HIS	-	expression tag	UNP Q91XX6
A	641	HIS	-	expression tag	UNP Q91XX6
A	642	HIS	-	expression tag	UNP Q91XX6
A	643	HIS	-	expression tag	UNP Q91XX6
A	644	HIS	-	expression tag	UNP Q91XX6
A	645	HIS	-	expression tag	UNP Q91XX6
A	646	HIS	-	expression tag	UNP Q91XX6
B	639	HIS	-	expression tag	UNP Q91XX6
B	640	HIS	-	expression tag	UNP Q91XX6
B	641	HIS	-	expression tag	UNP Q91XX6
B	642	HIS	-	expression tag	UNP Q91XX6
B	643	HIS	-	expression tag	UNP Q91XX6
B	644	HIS	-	expression tag	UNP Q91XX6
B	645	HIS	-	expression tag	UNP Q91XX6
B	646	HIS	-	expression tag	UNP Q91XX6

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

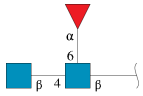
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	6	71	40	2	29	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

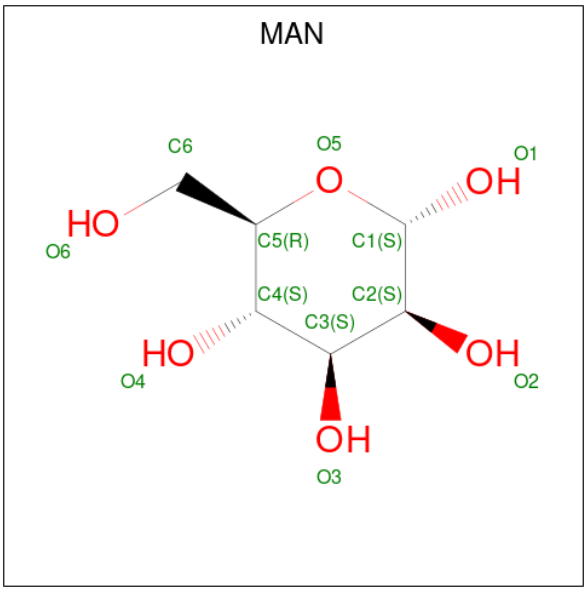


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	3	38	22	2	14	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

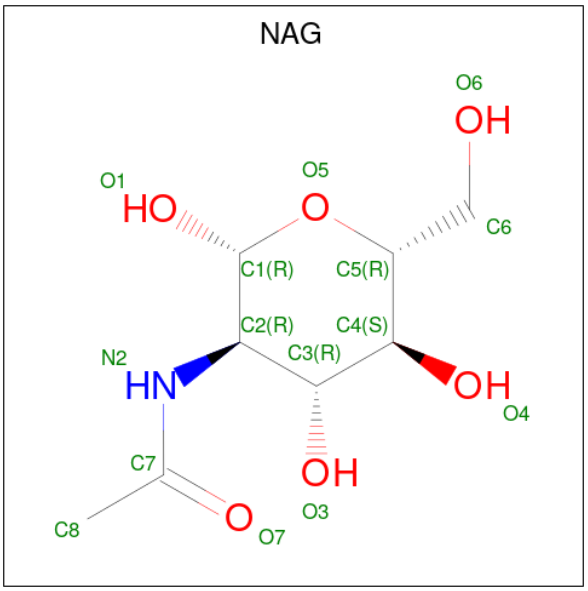
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	15	15	15	0	0
5	B	15	15	15	0	0

- 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			
6	A	1	Total	C	O		0	0
			11	6	5			
6	B	1	Total	C	O		0	0
			11	6	5			
6	B	1	Total	C	O		0	0
			11	6	5			

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



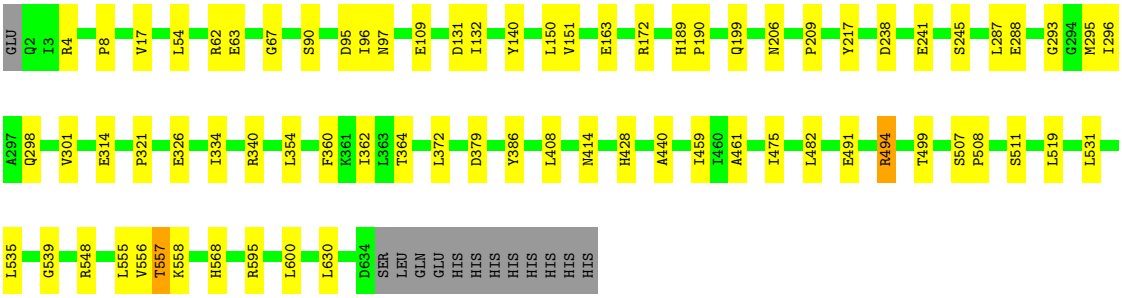
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
			Total	C	N	O		
7	B	1	14	8	1	5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

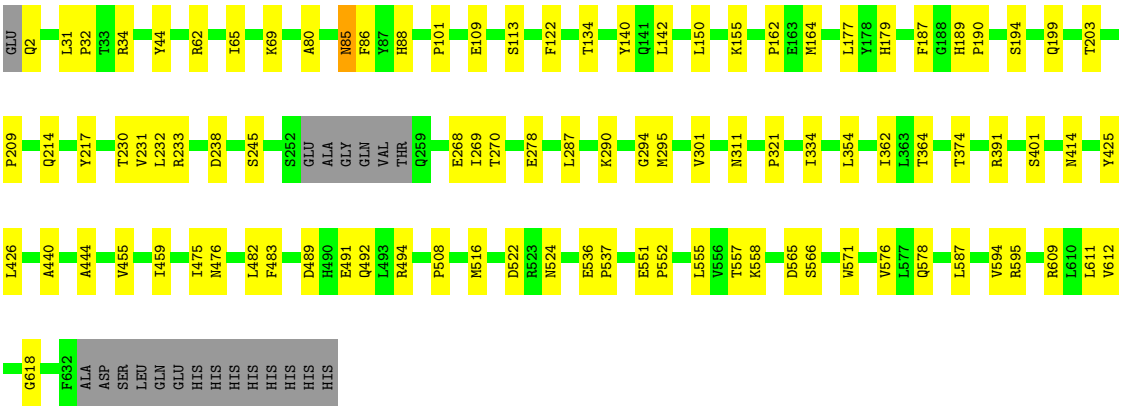
• Molecule 1: Protocadherin gamma B4

Chain A:



• Molecule 1: Protocadherin gamma B4

Chain B:



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

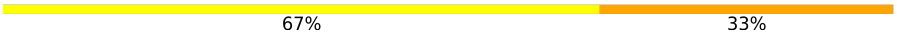
Chain C:

• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamid

o-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.73Å 87.58Å 149.33Å 90.00° 109.94° 90.00°	Depositor
Resolution (Å)	38.29 – 4.52 38.29 – 4.52	Depositor EDS
% Data completeness (in resolution range)	93.4 (38.29-4.52) 47.0 (38.29-4.52)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.69 (at 4.44Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.231 , 0.277 0.231 , 0.276	Depositor DCC
R_{free} test set	448 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	9742	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: CA, MAN, FUC, BMA, NAG

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	0.24	0/4837	0.45	0/6611
1	B	0.24	0/4836	0.44	0/6598
All	All	0.24	0/9673	0.44	0/13209

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	4746	0	4492	41	0
1	B	4743	0	4555	56	0
2	C	28	0	25	1	0
3	D	71	0	61	1	0
4	E	38	0	34	1	0
5	A	15	0	0	0	0
5	B	15	0	0	0	0
6	A	22	0	20	0	0
6	B	22	0	20	0	0
7	A	28	0	26	0	0
7	B	14	0	13	0	0
All	All	9742	0	9246	97	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 5.

All (97) 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:B:354:LEU:HD23	1:B:362:ILE:HG23	1.67	0.77
1:B:522:ASP:OD2	1:B:566:SER:N	2.25	0.69
1:B:230:THR:HA	1:B:270:THR:HG22	1.73	0.68
1:B:142:LEU:H	1:B:150:LEU:HD22	1.58	0.68
1:B:555:LEU:HA	1:B:595:ARG:HG2	1.78	0.66
1:B:278:GLU:OE2	1:B:311:ASN:ND2	2.30	0.64
1:B:217:TYR:HB2	1:B:301:VAL:HG12	1.78	0.64
1:B:578:GLN:HG2	1:B:611:LEU:HB3	1.79	0.64
1:A:461:ALA:HB3	1:A:499:THR:HB	1.81	0.63
1:B:62:ARG:NH2	1:B:69:LYS:O	2.33	0.61
1:B:444:ALA:HB3	1:B:455:VAL:HG11	1.82	0.61
1:A:62:ARG:NH1	1:A:67:GLY:O	2.34	0.60
1:A:209:PRO:HB3	1:A:295:MET:HG3	1.84	0.59
1:A:440:ALA:HB3	1:A:482:LEU:HD12	1.84	0.58
1:A:8:PRO:HB3	1:A:96:ILE:HD11	1.87	0.57
1:A:535:LEU:HB3	1:A:539:GLY:HA2	1.88	0.56
1:B:2:GLN:HB3	1:B:88:HIS:CE1	2.42	0.55
1:B:122:PHE:HB2	1:B:164:MET:HG3	1.89	0.55
1:B:34:ARG:HB3	1:B:80:ALA:HB1	1.90	0.54
1:B:134:THR:OG1	1:B:187:PHE:O	2.25	0.54
1:B:551:GLU:HG2	1:B:552:PRO:HD2	1.90	0.54
1:A:140:TYR:HB3	1:A:150:LEU:HD21	1.90	0.53
3:D:1:NAG:H61	3:D:2:NAG:H82	1.90	0.53
1:A:172:ARG:NH2	1:A:241:GLU:OE2	2.43	0.52
1:A:428:HIS:CE1	1:A:519:LEU:HD12	2.44	0.52
1:B:233:ARG:HD3	1:B:268:GLU:HB3	1.91	0.52
1:A:511:SER:OG	2:C:1:NAG:O7	2.28	0.52
1:A:288:GLU:HG3	1:A:296:ILE:HG23	1.92	0.52
1:B:85:ASN:HD22	1:B:86:PHE:H	1.58	0.52
1:B:414:ASN:ND2	1:B:508:PRO:O	2.43	0.51
1:A:95:ASP:OD2	1:A:132:ILE:HG13	2.11	0.51
1:B:290:LYS:HE2	1:B:294:GLY:HA2	1.93	0.51
1:B:476:ASN:HB2	1:B:483:PHE:HE2	1.74	0.51
1:A:17:VAL:HB	1:A:54:LEU:HD23	1.91	0.51
1:A:459:ILE:HD11	1:A:475:ILE:HG13	1.93	0.50
1:B:113:SER:HA	1:B:203:THR:HB	1.93	0.50
1:A:217:TYR:HD2	1:A:301:VAL:HG22	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:PHE:HB3	1:A:372:LEU:HD11	1.95	0.49
1:A:491:GLU:OE1	1:A:491:GLU:N	2.45	0.49
1:A:557:THR:HG22	1:A:558:LYS:H	1.78	0.49
1:A:555:LEU:HA	1:A:595:ARG:HG2	1.94	0.48
1:A:238:ASP:OD2	1:A:245:SER:HA	2.14	0.48
1:A:494:ARG:HD2	1:A:494:ARG:H	1.79	0.48
1:A:321:PRO:HG3	1:A:334:ILE:HG22	1.96	0.47
4:E:2:NAG:H62	4:E:3:FUC:O3	2.13	0.47
1:B:536:GLU:HG3	1:B:537:PRO:HD2	1.96	0.47
1:B:209:PRO:HB3	1:B:295:MET:HB3	1.97	0.47
1:B:494:ARG:HD2	1:B:494:ARG:H	1.80	0.47
1:A:531:LEU:HB3	1:B:571:TRP:CE3	2.50	0.47
1:A:556:VAL:HG11	1:A:630:LEU:HD13	1.96	0.47
1:B:140:TYR:CD1	1:B:162:PRO:HG3	2.50	0.47
1:A:63:GLU:HA	1:A:67:GLY:HA2	1.97	0.46
1:A:314:GLU:OE1	1:A:340:ARG:NH1	2.49	0.46
1:B:238:ASP:OD2	1:B:245:SER:HA	2.15	0.46
1:B:576:VAL:HG23	1:B:587:LEU:HD13	1.98	0.46
1:B:578:GLN:OE1	1:B:609:ARG:NH2	2.40	0.46
1:B:85:ASN:HD22	1:B:86:PHE:N	2.13	0.45
1:A:4:ARG:HA	1:A:90:SER:O	2.17	0.45
1:B:391:ARG:HD2	1:B:401:SER:HB2	1.98	0.45
1:A:386:TYR:HB2	1:A:408:LEU:HG	1.98	0.45
1:B:489:ASP:OD2	1:B:492:GLN:HG3	2.16	0.45
1:B:321:PRO:HG3	1:B:334:ILE:HG22	1.98	0.44
1:B:189:HIS:HA	1:B:190:PRO:HA	1.87	0.44
1:B:557:THR:OG1	1:B:558:LYS:N	2.50	0.44
1:B:459:ILE:HD11	1:B:475:ILE:HG13	2.00	0.44
1:B:44:TYR:OH	1:B:65:ILE:HD11	2.17	0.43
1:A:206:ASN:HD22	1:A:293:GLY:HA3	1.83	0.43
1:A:287:LEU:O	1:A:298:GLN:HA	2.19	0.43
1:B:491:GLU:OE1	1:B:491:GLU:N	2.48	0.43
1:A:62:ARG:CZ	1:A:132:ILE:HG12	2.48	0.43
1:B:231:VAL:HG12	1:B:232:LEU:HD23	2.00	0.43
1:A:326:GLU:HG3	1:A:379:ASP:HA	2.00	0.43
1:A:151:VAL:HG23	1:A:163:GLU:HG3	2.01	0.43
1:B:155:LYS:HE3	1:B:155:LYS:HB2	1.84	0.42
1:A:97:ASN:HA	1:A:131:ASP:OD2	2.20	0.42
1:A:568:HIS:CE1	1:B:426:LEU:HG	2.54	0.42
1:B:524:ASN:HA	1:B:565:ASP:OD2	2.19	0.42
1:B:536:GLU:CG	1:B:537:PRO:HD2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HB3	1:B:32:PRO:HD3	2.02	0.42
1:A:354:LEU:HD11	1:A:362:ILE:HG13	2.01	0.41
1:A:548:ARG:HG3	1:A:600:LEU:HD23	2.02	0.41
1:B:177:LEU:HD13	1:B:179:HIS:NE2	2.35	0.41
1:A:189:HIS:HA	1:A:190:PRO:HA	1.86	0.41
1:A:414:ASN:ND2	1:A:508:PRO:O	2.53	0.41
1:B:214:GLN:HB2	1:B:217:TYR:CE1	2.56	0.41
1:B:101:PRO:O	1:B:194:SER:HB2	2.19	0.41
1:B:269:ILE:HD11	1:B:287:LEU:HD11	2.02	0.41
1:B:425:TYR:O	1:B:516:MET:HA	2.21	0.41
1:B:109:GLU:HG2	1:B:199:GLN:HB2	2.01	0.41
1:B:334:ILE:HD11	1:B:374:THR:HG23	2.02	0.41
1:A:109:GLU:HG3	1:A:199:GLN:O	2.21	0.41
1:B:65:ILE:HD13	1:B:65:ILE:HA	1.88	0.40
1:B:440:ALA:HB3	1:B:482:LEU:HD12	2.03	0.40
1:B:576:VAL:HA	1:B:612:VAL:HG12	2.03	0.40
1:A:507:SER:HA	1:A:508:PRO:HA	1.91	0.40
1:B:269:ILE:HD11	1:B:287:LEU:HD21	2.04	0.40
1:B:524:ASN:ND2	1:B:618:GLY:HA3	2.37	0.40

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	631/646 (98%)	610 (97%)	21 (3%)	0	100	100
1	B	621/646 (96%)	604 (97%)	17 (3%)	0	100	100
All	All	1252/1292 (97%)	1214 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	515/560 (92%)	512 (99%)	3 (1%)	86 92
1	B	526/560 (94%)	523 (99%)	3 (1%)	86 92
All	All	1041/1120 (93%)	1035 (99%)	6 (1%)	86 92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	THR
1	A	494	ARG
1	A	557	THR
1	B	85	ASN
1	B	364	THR
1	B	594	VAL

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

Mol	Chain	Res	Type
1	B	311	ASN
1	B	497	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

11 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.74	0	17,19,21	0.74	1 (5%)
2	NAG	C	2	2	14,14,15	0.64	0	17,19,21	0.45	0
3	NAG	D	1	1,3	14,14,15	0.84	0	17,19,21	1.03	2 (11%)
3	NAG	D	2	3	14,14,15	0.67	0	17,19,21	0.41	0
3	BMA	D	3	3	11,11,12	1.17	0	15,15,17	1.03	0
3	MAN	D	4	3	11,11,12	1.14	0	15,15,17	0.97	0
3	MAN	D	5	3	11,11,12	0.90	0	15,15,17	0.89	0
3	FUC	D	6	3	10,10,11	1.14	0	14,14,16	0.79	0
4	NAG	E	1	1,4	14,14,15	1.08	1 (7%)	17,19,21	1.81	6 (35%)
4	NAG	E	2	4	14,14,15	0.67	0	17,19,21	0.63	0
4	FUC	E	3	4	10,10,11	1.52	2 (20%)	14,14,16	1.02	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
3	FUC	D	6	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	FUC	E	3	4	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C4-C5	2.55	1.58	1.53
4	E	3	FUC	O3-C3	-2.40	1.37	1.43
4	E	3	FUC	C4-C5	2.18	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	NAG	O5-C5-C6	-3.70	101.40	107.20
3	D	1	NAG	C3-C4-C5	2.94	115.48	110.24
4	E	1	NAG	O4-C4-C3	-2.63	104.27	110.35
4	E	1	NAG	C3-C4-C5	2.62	114.91	110.24
4	E	1	NAG	C2-N2-C7	2.60	126.60	122.90
4	E	1	NAG	C1-O5-C5	2.54	115.63	112.19
2	C	1	NAG	C2-N2-C7	2.29	126.17	122.90
4	E	1	NAG	C4-C3-C2	2.11	114.10	111.02
3	D	1	NAG	O5-C1-C2	-2.00	108.12	111.29

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
4	E	2	NAG	1	0

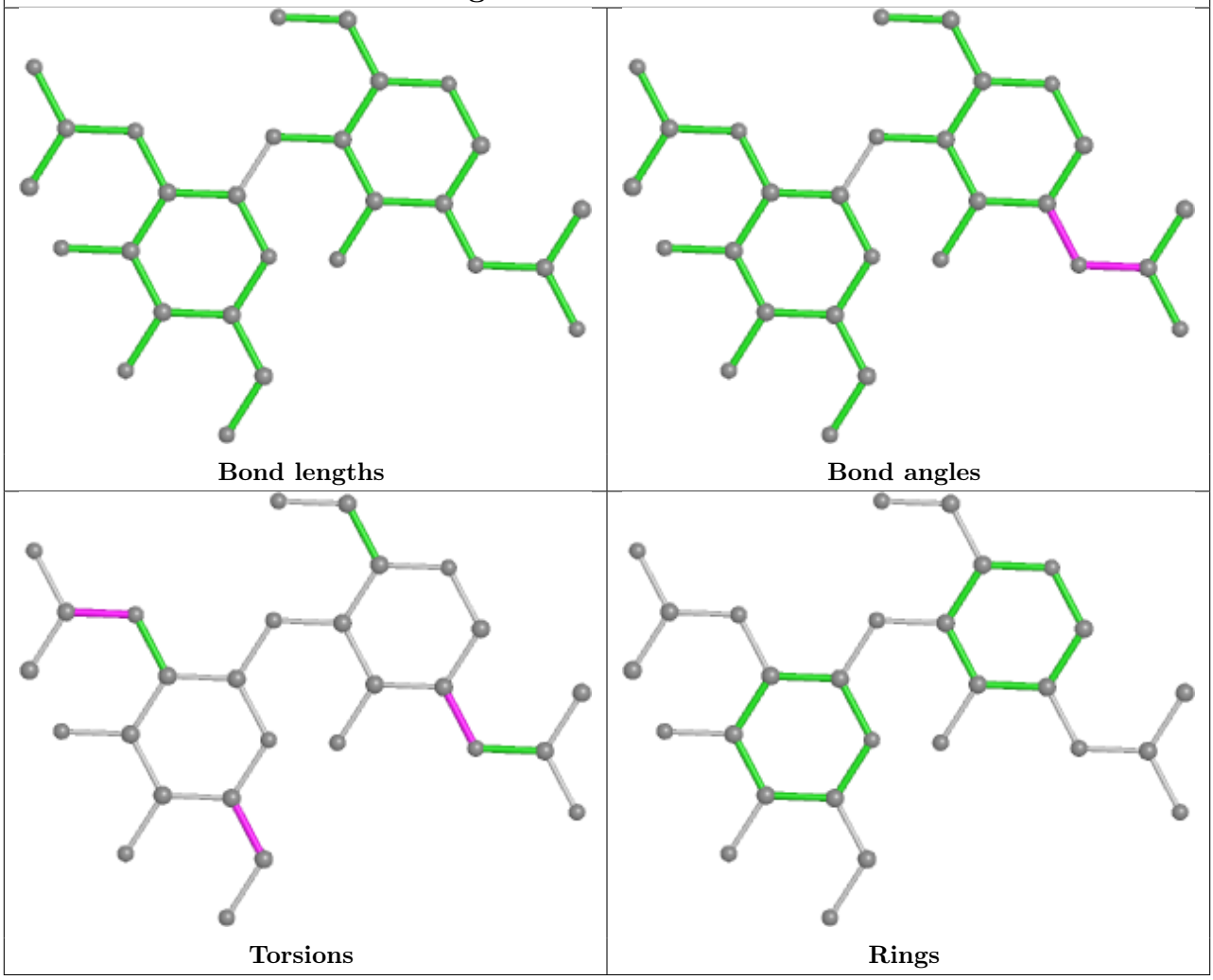
Continued on next page...

Continued from previous page...

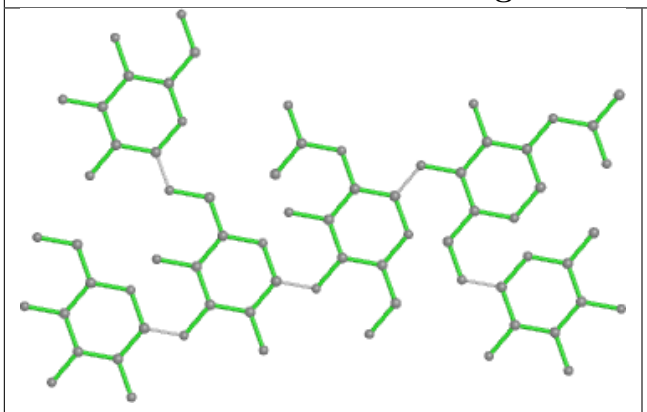
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
4	E	3	FUC	1	0
3	D	2	NAG	1	0

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

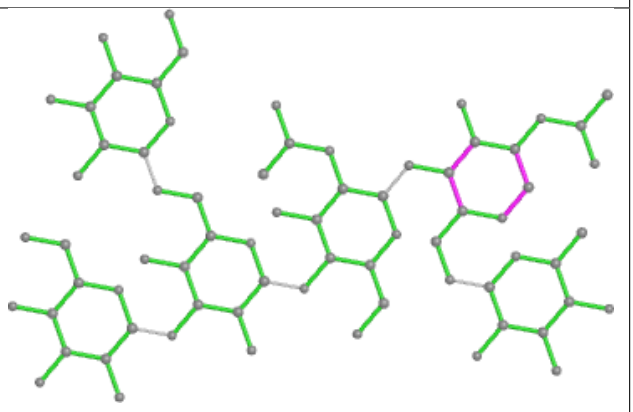
Oligosaccharide Chain C



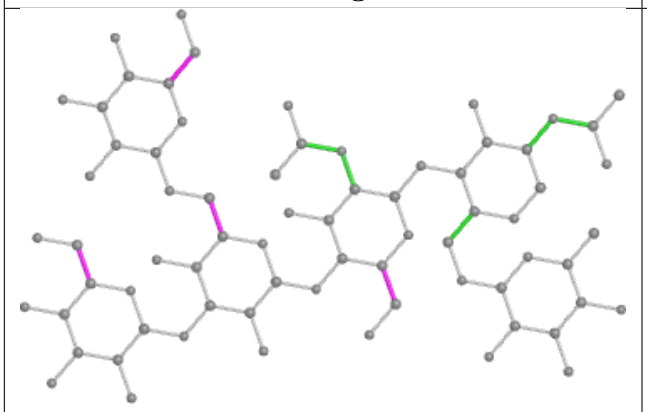
Oligosaccharide Chain D



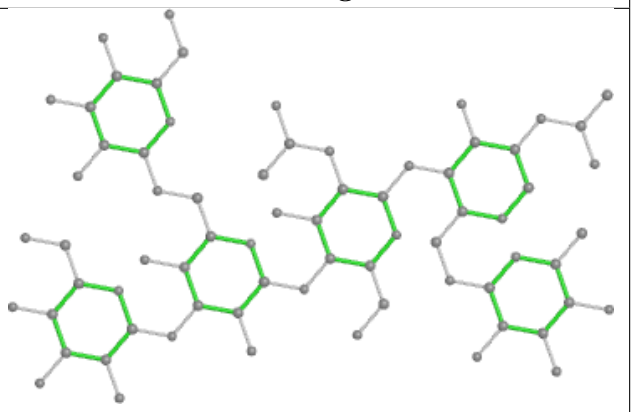
Bond lengths



Bond angles

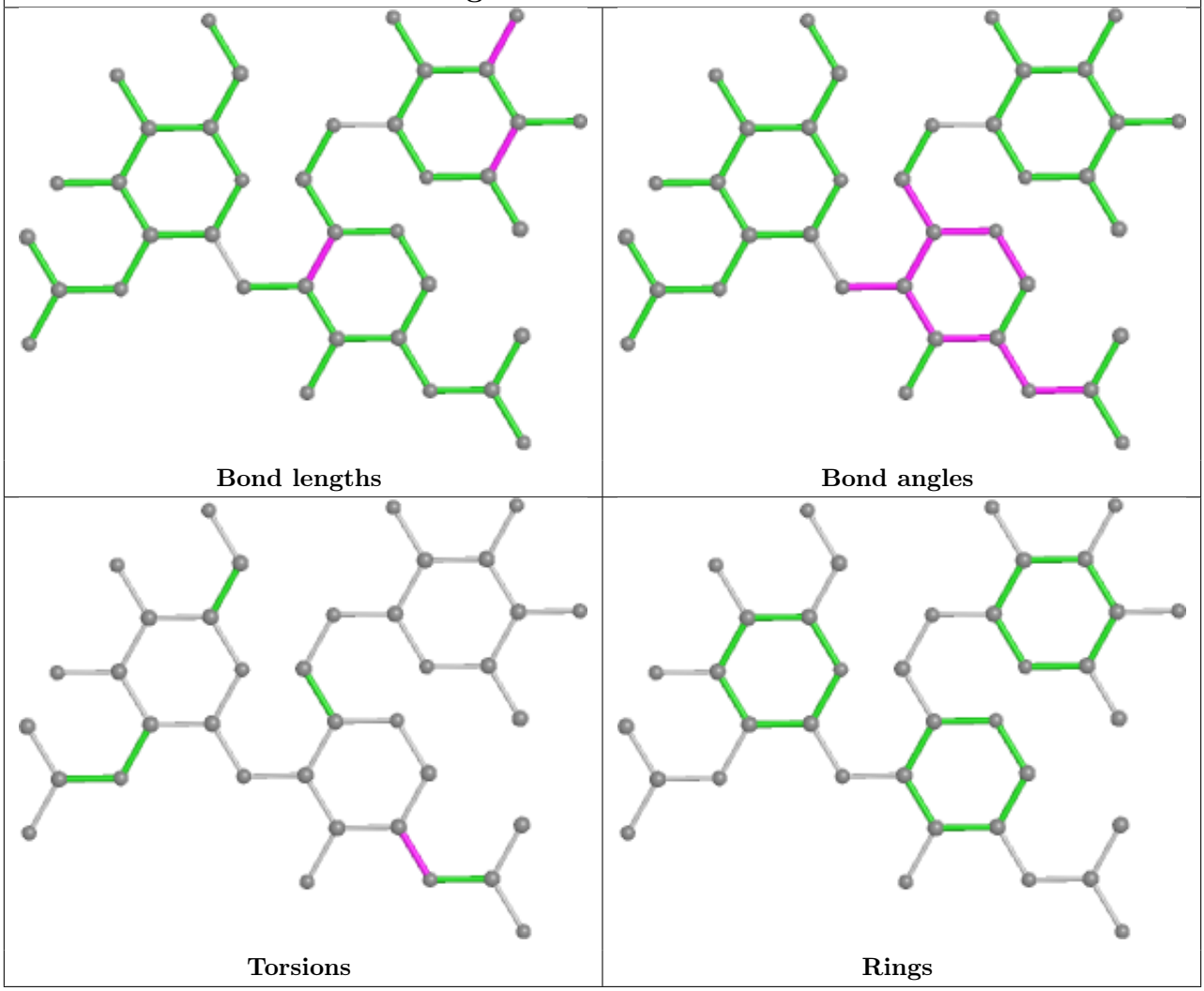


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 30 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
7	NAG	A	718	1	14,14,15	0.63	0	17,19,21	0.44	0
6	MAN	A	717	1	11,11,12	0.90	0	15,15,17	0.86	0
6	MAN	B	716	1	11,11,12	0.80	0	15,15,17	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	A	719	1	14,14,15	0.66	0	17,19,21	0.45	0
6	MAN	B	724	1	11,11,12	0.72	0	15,15,17	0.96	0
7	NAG	B	723	1	14,14,15	0.86	1 (7%)	17,19,21	0.39	0
6	MAN	A	716	1	11,11,12	0.97	0	15,15,17	0.86	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	718	1	-	2/6/23/26	0/1/1/1
6	MAN	A	717	1	-	2/2/19/22	0/1/1/1
6	MAN	B	716	1	-	1/2/19/22	0/1/1/1
7	NAG	A	719	1	-	2/6/23/26	0/1/1/1
6	MAN	B	724	1	-	2/2/19/22	0/1/1/1
7	NAG	B	723	1	-	3/6/23/26	0/1/1/1
6	MAN	A	716	1	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	723	NAG	C1-C2	2.29	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	724	MAN	O5-C5-C6-O6
7	A	719	NAG	C4-C5-C6-O6
7	B	723	NAG	O5-C5-C6-O6
6	B	724	MAN	C4-C5-C6-O6
7	B	723	NAG	C4-C5-C6-O6
7	A	719	NAG	O5-C5-C6-O6
6	B	716	MAN	O5-C5-C6-O6
7	A	718	NAG	C4-C5-C6-O6
7	A	718	NAG	O5-C5-C6-O6
7	B	723	NAG	C1-C2-N2-C7
6	A	717	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	717	MAN	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

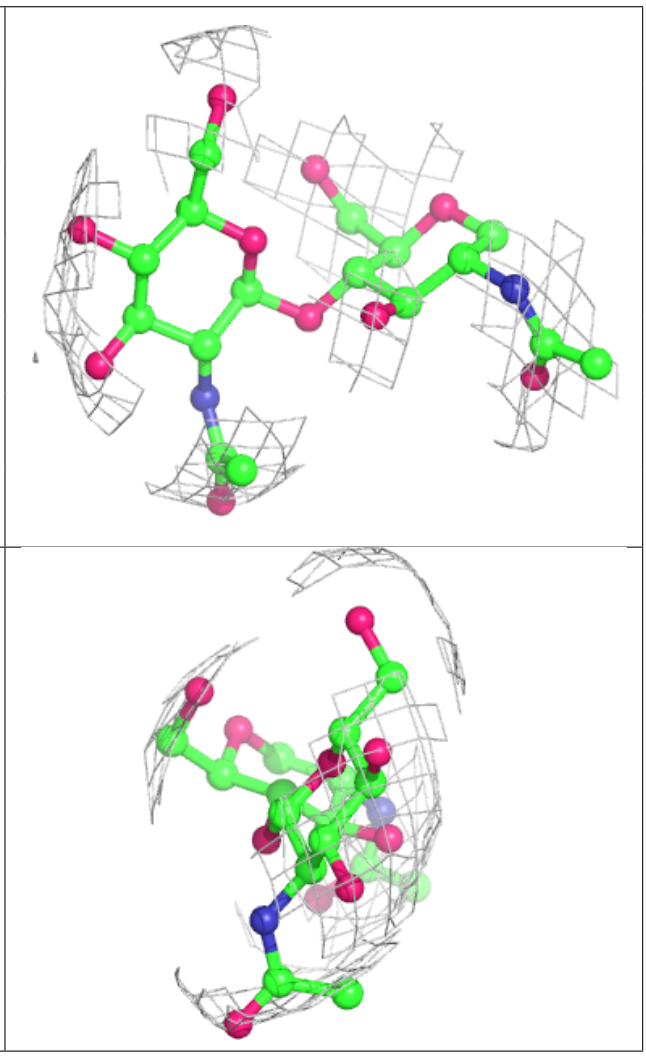
6.3 Carbohydrates (i)

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

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

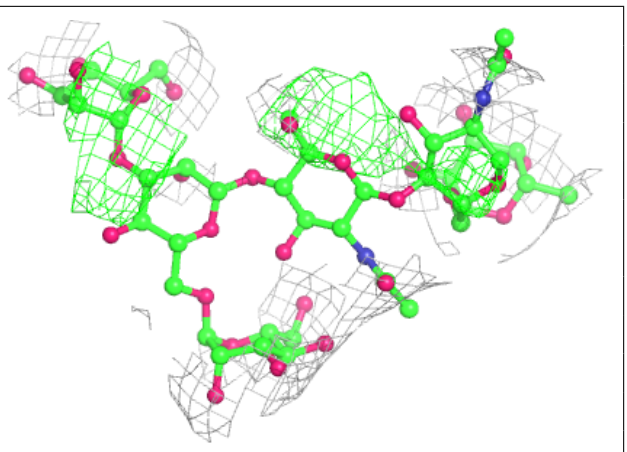
Electron density around Chain C:

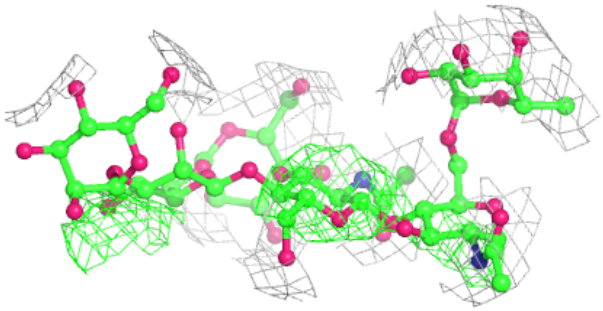
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

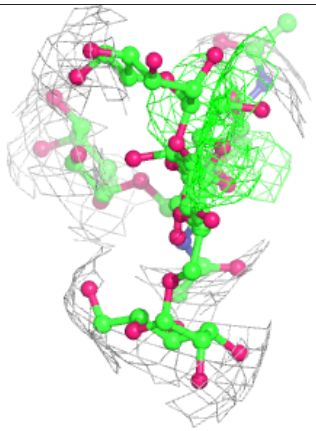


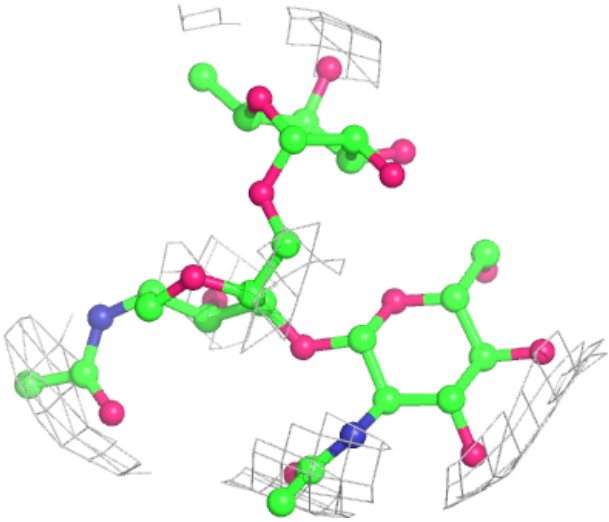
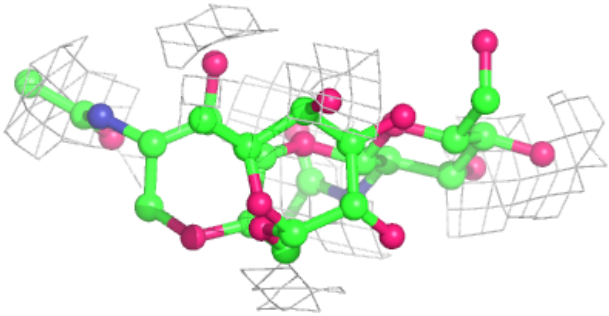
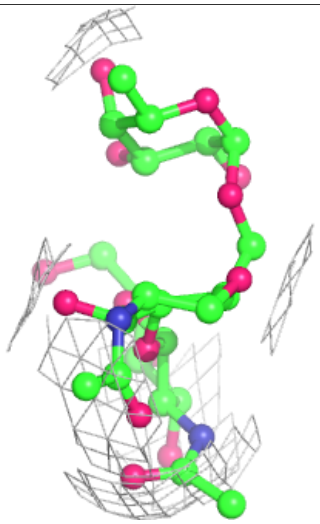
Electron density around Chain D:

$2mF_o$-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 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 (i)

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

6.5 Other polymers (i)

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