Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 03:56 AM EDT

PDB ID	:	3B2D
Title	:	Crystal structure of human RP105/MD-1 complex
Authors	:	Ohto, U.; Shimizu, T.
Deposited on	:	2011-07-29
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

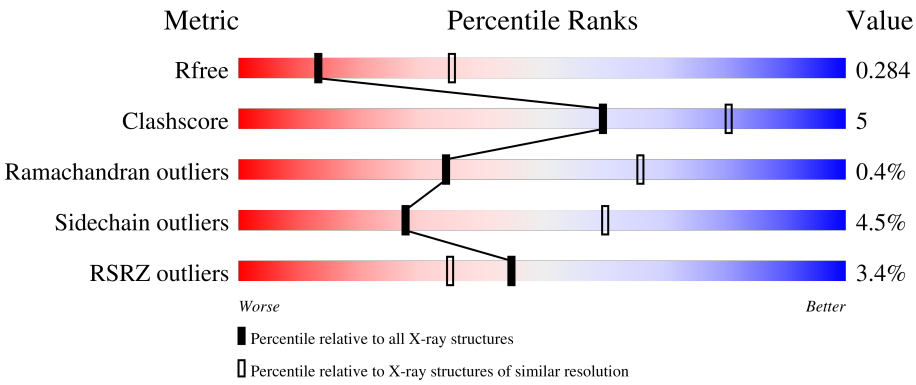
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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% 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	603	4% 86% 12% •
1	B	603	% 85% 12% •
2	C	144	7% 85% 11% •
2	D	144	7% 82% 11% • • •
3	E	9	33% 56% 11%

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Mol	Chain	Length	Quality of chain
4	F	2	50% 50%
4	H	2	50% 50%
5	G	8	25% 62% 12%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12165 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 CD180 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	601	4718	2984	806	903	25	0	0	0
1	B	601	4718	2984	806	903	25	0	0	0

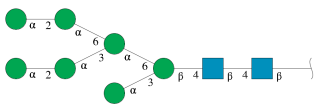
- Molecule 2 is a protein called Lymphocyte antigen 86.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	139	1095	701	177	208	9	0	0	0
2	D	139	1095	701	177	208	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	163	GLU	-	expression tag	UNP O95711
C	164	PHE	-	expression tag	UNP O95711
D	163	GLU	-	expression tag	UNP O95711
D	164	PHE	-	expression tag	UNP O95711

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.

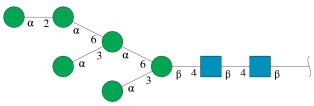


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	9	105	58	2	45	0	0	0

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

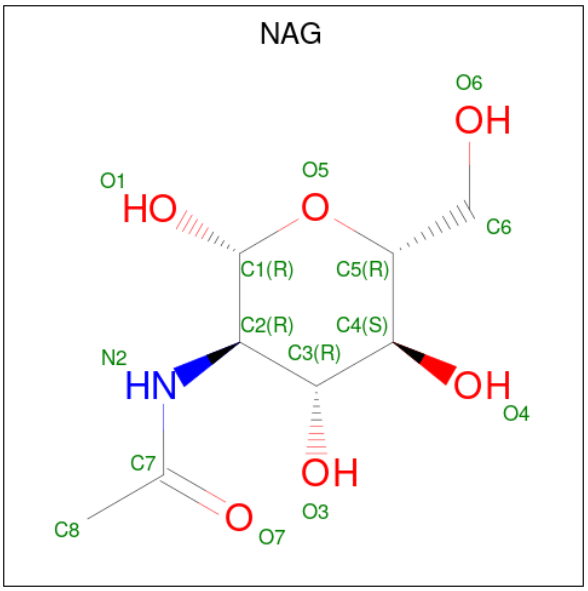
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	2	28	16	2	10	0	0	0
			Total	C	N	O			
4	H	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	G	8	94	52	2	40	0	0	0

- Molecule 6 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		
6	B	1	14	8	1	5	0	0

- Molecule 7 is water.

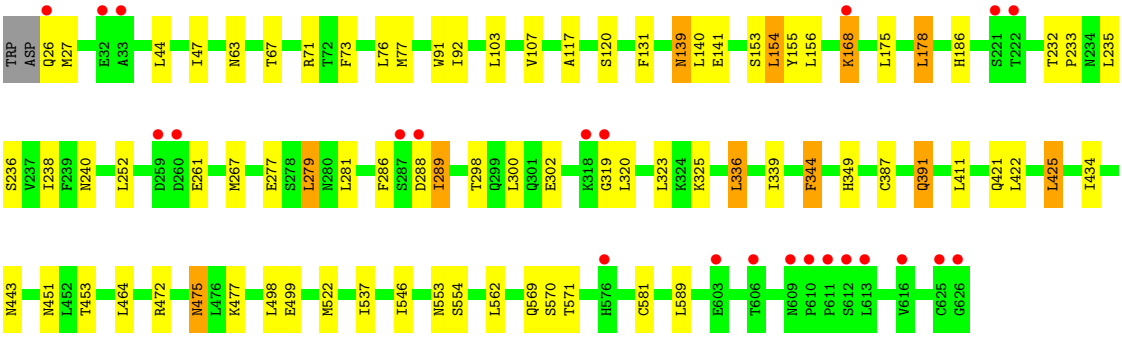
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	102	102	102	0	0
			Total	O		
7	B	118	118	118	0	0
			Total	O		
7	C	26	26	26	0	0
			Total	O		
7	D	24	24	24	0	0

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.

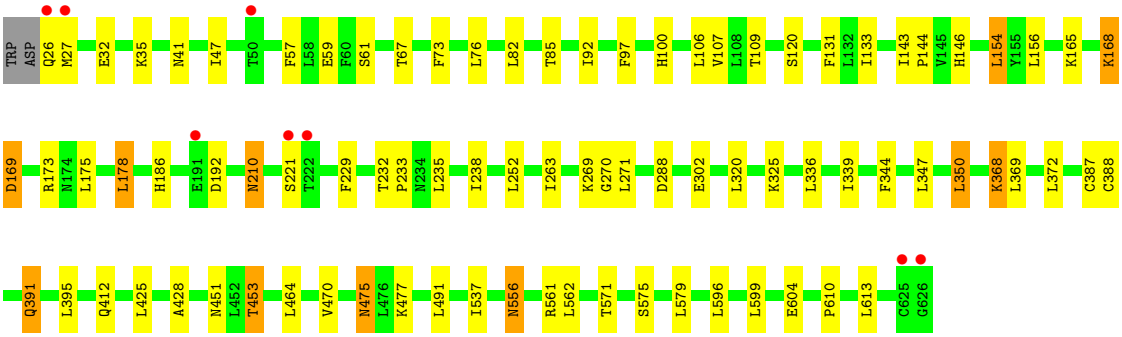
• Molecule 1: CD180 antigen

Chain A:



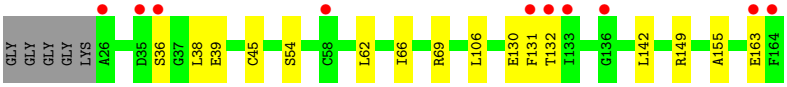
• Molecule 1: CD180 antigen

Chain B:



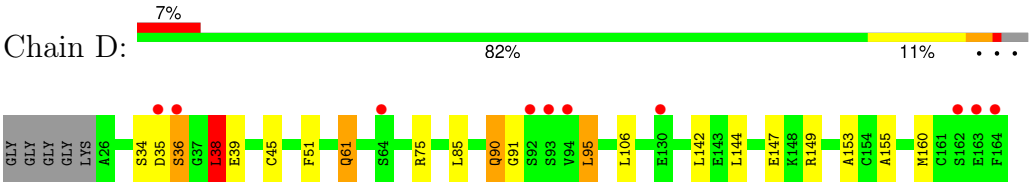
• Molecule 2: Lymphocyte antigen 86

Chain C:



• Molecule 2: Lymphocyte antigen 86

Chain D:



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

Chain F:

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

Chain H:

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[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 G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	204.00Å 66.44Å 119.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 2.80 30.02 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.9 (30.02-2.80) 86.0 (30.02-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	12.21 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.218 , 0.284 0.218 , 0.284	Depositor DCC
R_{free} test set	1744 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12165	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: MAN, NAG, BMA

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	0.42	1/4811 (0.0%)	0.51	0/6527
1	B	0.43	0/4811	0.51	0/6527
2	C	0.37	0/1119	0.52	0/1514
2	D	0.37	0/1119	0.57	2/1514 (0.1%)
All	All	0.41	1/11860 (0.0%)	0.52	2/16082 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	TRP	CD2-CE2	5.09	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	95	LEU	CA-CB-CG	5.36	127.62	115.30
2	D	38	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4718	0	4681	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4718	0	4682	52	0
2	C	1095	0	1070	4	0
2	D	1095	0	1070	10	0
3	E	105	0	88	1	0
4	F	28	0	25	1	0
4	H	28	0	25	1	0
5	G	94	0	79	1	0
6	B	14	0	13	0	0
7	A	102	0	0	0	0
7	B	118	0	0	1	0
7	C	26	0	0	1	0
7	D	24	0	0	0	0
All	All	12165	0	11733	108	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 (108) 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:391:GLN:H	1:A:391:GLN:HE21	1.32	0.78
1:B:168:LYS:O	1:B:169:ASP:HB2	1.82	0.78
1:B:451:ASN:OD1	1:B:453:THR:HG22	1.88	0.74
1:B:47:ILE:HD11	1:B:73:PHE:HD2	1.54	0.73
1:B:391:GLN:HE21	1:B:391:GLN:H	1.41	0.67
1:A:537:ILE:HB	1:A:562:LEU:HD22	1.78	0.66
1:B:368:LYS:H	1:B:368:LYS:HD2	1.62	0.64
1:A:47:ILE:HD11	1:A:73:PHE:HD2	1.66	0.60
1:B:575:SER:HB2	1:B:604:GLU:HB2	1.84	0.60
1:B:451:ASN:OD1	1:B:453:THR:CG2	2.50	0.60
1:A:47:ILE:HD11	1:A:73:PHE:CD2	2.39	0.58
1:B:238:ILE:HG21	1:B:252:LEU:HD21	1.85	0.58
1:A:236:SER:O	1:A:240:ASN:HB2	2.04	0.58
1:B:168:LYS:O	1:B:169:ASP:CB	2.52	0.57
1:B:154:LEU:HD22	1:B:156:LEU:HG	1.87	0.57
1:A:44:LEU:H	1:A:63:ASN:HD22	1.52	0.56
1:B:336:LEU:O	1:B:339:ILE:HG12	2.05	0.56
2:C:54:SER:HB3	2:C:69:ARG:HB2	1.90	0.54
2:C:62:LEU:O	2:C:130:GLU:HG3	2.08	0.53
1:B:175:LEU:HD21	1:B:178:LEU:HG	1.91	0.53
1:A:139:ASN:HD22	1:A:140:LEU:N	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASN:HD22	1:B:233:PRO:HG3	1.73	0.53
1:B:453:THR:HB	1:B:477:LYS:HB3	1.91	0.52
1:B:41:ASN:OD1	2:D:75:ARG:NH2	2.43	0.52
1:B:344:PHE:HB3	1:B:347:LEU:HG	1.91	0.52
1:A:320:LEU:HD22	1:A:323:LEU:HD22	1.92	0.52
1:B:165:LYS:HB2	1:B:192:ASP:OD1	2.09	0.52
1:A:391:GLN:HE21	1:A:391:GLN:N	2.05	0.52
1:A:422:LEU:HD21	1:A:425:LEU:HG	1.92	0.52
1:A:387:CYS:HB3	1:A:411:LEU:HD23	1.91	0.52
1:B:210:ASN:ND2	1:B:233:PRO:HG3	2.26	0.51
1:B:596:LEU:HA	1:B:599:LEU:HD12	1.93	0.51
2:D:85:LEU:CD2	2:D:142:LEU:HG	2.41	0.51
2:D:85:LEU:HD21	2:D:142:LEU:HG	1.93	0.50
1:A:238:ILE:HG21	1:A:252:LEU:HD21	1.94	0.50
1:B:92:ILE:HG22	1:B:120:SER:HB2	1.92	0.49
1:B:235:LEU:HD12	1:B:263:ILE:HD12	1.94	0.49
2:C:132:THR:HA	7:C:170:HOH:O	2.12	0.49
1:B:107:VAL:HA	1:B:131:PHE:HB2	1.94	0.49
1:A:325:LYS:HG2	1:A:349:HIS:HB2	1.95	0.48
1:A:475:ASN:HD22	1:A:477:LYS:H	1.61	0.48
1:A:320:LEU:HD13	1:A:344:PHE:HE1	1.77	0.48
1:A:472:ARG:HA	1:A:498:LEU:HA	1.95	0.48
1:B:350:LEU:HB2	1:B:372:LEU:HD11	1.96	0.48
1:B:610:PRO:HD2	1:B:613:LEU:HD12	1.96	0.48
1:A:302:GLU:HG2	1:A:325:LYS:HB2	1.96	0.47
1:B:391:GLN:HE21	1:B:391:GLN:N	2.11	0.47
1:B:428:ALA:HB3	4:H:1:NAG:H82	1.96	0.47
1:B:229:PHE:HB2	1:B:252:LEU:HD23	1.96	0.47
2:C:142:LEU:HB2	2:C:155:ALA:HB3	1.97	0.46
1:A:107:VAL:HA	1:A:131:PHE:HB2	1.98	0.46
1:B:475:ASN:ND2	1:B:477:LYS:H	2.14	0.45
1:B:320:LEU:HD13	1:B:344:PHE:HE1	1.81	0.45
1:B:453:THR:HA	1:B:477:LYS:O	2.16	0.45
1:B:143:ILE:HD11	1:B:156:LEU:HD21	1.99	0.45
2:D:51:PHE:HZ	2:D:155:ALA:HB2	1.81	0.45
1:A:44:LEU:H	1:A:63:ASN:ND2	2.15	0.45
1:A:139:ASN:ND2	1:A:141:GLU:H	2.16	0.44
1:A:154:LEU:HD22	1:A:156:LEU:HG	1.99	0.44
1:A:279:LEU:HB2	1:A:300:LEU:HD11	2.00	0.44
1:B:57:PHE:HD1	7:B:681:HOH:O	2.00	0.44
1:B:537:ILE:HB	1:B:562:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LYS:HD2	1:B:168:LYS:H	1.83	0.44
1:A:47:ILE:HD13	1:A:76:LEU:HD12	1.99	0.44
1:A:92:ILE:HG22	1:A:120:SER:HB2	2.00	0.44
1:A:581:CYS:HA	1:A:589:LEU:HD11	1.99	0.43
1:B:47:ILE:HD13	1:B:76:LEU:HD12	2.00	0.43
1:A:26:GLN:HA	1:A:27:MET:HA	1.60	0.43
1:A:336:LEU:O	1:A:339:ILE:HG12	2.19	0.43
1:B:387:CYS:HA	1:B:388:CYS:HA	1.84	0.43
1:A:434:ILE:HD13	1:A:464:LEU:HD11	1.99	0.43
1:B:61:SER:HB2	1:B:85:THR:HB	2.00	0.43
1:B:97:PHE:HA	1:B:100:HIS:HD2	1.83	0.43
1:A:186:HIS:HB2	1:B:186:HIS:CD2	2.54	0.43
1:A:235:LEU:HD22	1:A:252:LEU:HD22	2.00	0.43
1:A:279:LEU:HD12	1:A:281:LEU:HG	1.99	0.42
1:B:32:GLU:HB3	1:B:35:LYS:HB3	2.01	0.42
1:B:302:GLU:HG2	1:B:325:LYS:HB2	2.01	0.42
1:A:286:PHE:HB3	1:A:289:ILE:HB	2.02	0.42
1:B:475:ASN:HD22	1:B:477:LYS:H	1.68	0.42
2:D:38:LEU:HA	2:D:160:MET:O	2.20	0.42
2:D:144:LEU:HD12	2:D:153:ALA:HB3	2.02	0.42
1:B:109:THR:HG23	1:B:133:ILE:HB	2.02	0.42
2:D:34:SER:HA	2:D:39:GLU:HG2	2.01	0.41
5:G:1:NAG:H61	5:G:2:NAG:C7	2.50	0.41
2:D:35:ASP:O	2:D:36:SER:C	2.59	0.41
1:B:387:CYS:O	1:B:412:GLN:HG2	2.20	0.41
1:A:168:LYS:CD	1:A:168:LYS:H	2.34	0.41
1:A:153:SER:HB3	1:A:155:TYR:CE2	2.55	0.41
1:A:499:GLU:HA	1:A:522:MET:HA	2.03	0.41
1:A:546:ILE:HG12	1:A:569:GLN:OE1	2.21	0.41
1:A:298:THR:HG22	1:A:319:GLY:HA2	2.02	0.41
1:B:26:GLN:HA	1:B:27:MET:HA	1.59	0.41
1:A:553:ASN:HB3	1:A:554:SER:H	1.78	0.41
1:B:269:LYS:HG3	1:B:270:GLY:N	2.36	0.41
1:B:470:VAL:HG12	1:B:470:VAL:O	2.20	0.41
1:B:556:ASN:HA	1:B:579:LEU:HA	2.03	0.41
1:A:451:ASN:OD1	1:A:453:THR:HG22	2.20	0.40
3:E:2:NAG:H62	4:F:2:NAG:O6	2.21	0.40
2:D:61:GLN:H	2:D:61:GLN:HG2	1.75	0.40
1:A:175:LEU:HD21	1:A:178:LEU:HG	2.02	0.40
1:A:232:THR:HA	1:A:233:PRO:HD3	1.96	0.40
1:B:47:ILE:HD12	1:B:73:PHE:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HB3	1:A:120:SER:HB3	2.04	0.40
1:B:143:ILE:HA	1:B:144:PRO:HD3	1.96	0.40
1:B:464:LEU:HB3	1:B:491:LEU:HD21	2.04	0.40
1:B:229:PHE:O	1:B:232:THR:HB	2.22	0.40
2:D:90:GLN:HB2	2:D:91:GLY:H	1.62	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	599/603 (99%)	567 (95%)	31 (5%)	1 (0%)	47	78
1	B	599/603 (99%)	565 (94%)	32 (5%)	2 (0%)	41	72
2	C	137/144 (95%)	130 (95%)	6 (4%)	1 (1%)	22	53
2	D	137/144 (95%)	127 (93%)	8 (6%)	2 (2%)	10	33
All	All	1472/1494 (98%)	1389 (94%)	77 (5%)	6 (0%)	34	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ILE
2	C	36	SER
1	B	221	SER
2	D	36	SER
1	B	288	ASP
2	D	90	GLN

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	551/553 (100%)	529 (96%)	22 (4%)	31	65
1	B	551/553 (100%)	528 (96%)	23 (4%)	30	63
2	C	123/124 (99%)	115 (94%)	8 (6%)	17	44
2	D	123/124 (99%)	116 (94%)	7 (6%)	20	50
All	All	1348/1354 (100%)	1288 (96%)	60 (4%)	27	60

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	71	ARG
1	A	77	MET
1	A	103	LEU
1	A	139	ASN
1	A	154	LEU
1	A	168	LYS
1	A	178	LEU
1	A	261	GLU
1	A	267	MET
1	A	277	GLU
1	A	279	LEU
1	A	288	ASP
1	A	336	LEU
1	A	344	PHE
1	A	391	GLN
1	A	421	GLN
1	A	425	LEU
1	A	443	ASN
1	A	475	ASN
1	A	570	SER
1	A	571	THR
1	B	59	GLU
1	B	67	THR

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Mol	Chain	Res	Type
1	B	82	LEU
1	B	106	LEU
1	B	146	HIS
1	B	154	LEU
1	B	168	LYS
1	B	169	ASP
1	B	173	ARG
1	B	178	LEU
1	B	210	ASN
1	B	271	LEU
1	B	350	LEU
1	B	368	LYS
1	B	369	LEU
1	B	391	GLN
1	B	395	LEU
1	B	425	LEU
1	B	453	THR
1	B	475	ASN
1	B	556	ASN
1	B	561	ARG
1	B	571	THR
2	C	38	LEU
2	C	39	GLU
2	C	45	CYS
2	C	66	ILE
2	C	106	LEU
2	C	131	PHE
2	C	149	ARG
2	C	163	GLU
2	D	38	LEU
2	D	45	CYS
2	D	61	GLN
2	D	95	LEU
2	D	106	LEU
2	D	147	GLU
2	D	149	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	139	ASN

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Mol	Chain	Res	Type
1	A	147	ASN
1	A	181	GLN
1	A	321	ASN
1	A	349	HIS
1	A	391	GLN
1	A	421	GLN
1	A	462	GLN
1	A	475	ASN
1	A	568	GLN
1	B	63	ASN
1	B	69	HIS
1	B	93	HIS
1	B	100	HIS
1	B	150	ASN
1	B	210	ASN
1	B	349	HIS
1	B	391	GLN
1	B	414	GLN
1	B	421	GLN
1	B	442	GLN
1	B	448	GLN
1	B	462	GLN
1	B	473	HIS
1	B	475	ASN
1	B	493	GLN
1	B	517	HIS
1	B	568	GLN
2	D	119	GLN
2	D	135	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)

21 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	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.49	0	17,19,21	0.90	1 (5%)
3	NAG	E	2	3	14,14,15	0.62	0	17,19,21	1.29	2 (11%)
3	BMA	E	3	3	11,11,12	0.49	0	15,15,17	0.92	1 (6%)
3	MAN	E	4	3	11,11,12	0.64	0	15,15,17	0.58	0
3	MAN	E	5	3	11,11,12	0.48	0	15,15,17	1.19	1 (6%)
3	MAN	E	6	3	11,11,12	0.55	0	15,15,17	0.73	1 (6%)
3	MAN	E	7	3	11,11,12	0.58	0	15,15,17	0.66	0
3	MAN	E	8	3	11,11,12	0.53	0	15,15,17	1.08	1 (6%)
3	MAN	E	9	3	11,11,12	0.62	0	15,15,17	0.86	0
4	NAG	F	1	1,4	14,14,15	0.52	0	17,19,21	0.71	0
4	NAG	F	2	4	14,14,15	0.59	0	17,19,21	1.24	2 (11%)
5	NAG	G	1	1,5	14,14,15	0.57	0	17,19,21	0.80	0
5	NAG	G	2	5	14,14,15	0.63	0	17,19,21	1.11	1 (5%)
5	BMA	G	3	5	11,11,12	0.31	0	15,15,17	1.15	2 (13%)
5	MAN	G	4	5	11,11,12	0.62	0	15,15,17	0.69	1 (6%)
5	MAN	G	5	5	11,11,12	0.56	0	15,15,17	0.86	0
5	MAN	G	6	5	11,11,12	0.58	0	15,15,17	0.86	1 (6%)
5	MAN	G	7	5	11,11,12	0.46	0	15,15,17	1.24	1 (6%)
5	MAN	G	8	5	11,11,12	0.60	0	15,15,17	0.96	0
4	NAG	H	1	1,4	14,14,15	0.54	0	17,19,21	0.97	1 (5%)
4	NAG	H	2	4	14,14,15	0.45	0	17,19,21	1.75	2 (11%)

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
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	0/2/19/22	0/1/1/1
3	MAN	E	8	3	-	1/2/19/22	0/1/1/1
3	MAN	E	9	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1
5	MAN	G	6	5	-	2/2/19/22	0/1/1/1
5	MAN	G	7	5	-	1/2/19/22	0/1/1/1
5	MAN	G	8	5	-	0/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	2	NAG	C1-O5-C5	6.01	120.24	112.19
3	E	5	MAN	C1-O5-C5	4.26	117.90	112.19
5	G	7	MAN	C1-O5-C5	4.24	117.86	112.19
3	E	8	MAN	C1-O5-C5	3.56	116.96	112.19
5	G	3	BMA	C1-O5-C5	3.08	116.32	112.19
4	F	2	NAG	C1-O5-C5	3.01	116.22	112.19
3	E	2	NAG	C4-C3-C2	2.95	115.34	111.02
5	G	6	MAN	C1-O5-C5	2.93	116.11	112.19
5	G	2	NAG	C1-O5-C5	2.66	115.75	112.19
3	E	2	NAG	C1-C2-N2	-2.37	106.70	110.43
5	G	3	BMA	C1-C2-C3	2.28	112.96	109.64
4	F	2	NAG	C3-C4-C5	-2.17	106.29	110.23
3	E	1	NAG	O5-C5-C6	2.16	111.86	107.66
5	G	4	MAN	C1-O5-C5	2.13	115.05	112.19
4	H	1	NAG	C1-O5-C5	2.12	115.02	112.19
3	E	3	BMA	C1-C2-C3	2.07	112.66	109.64
3	E	6	MAN	C1-O5-C5	2.06	114.94	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	2	NAG	C3-C4-C5	2.05	113.95	110.23

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
5	G	6	MAN	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
5	G	6	MAN	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
5	G	5	MAN	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
5	G	7	MAN	C4-C5-C6-O6
3	E	8	MAN	C4-C5-C6-O6

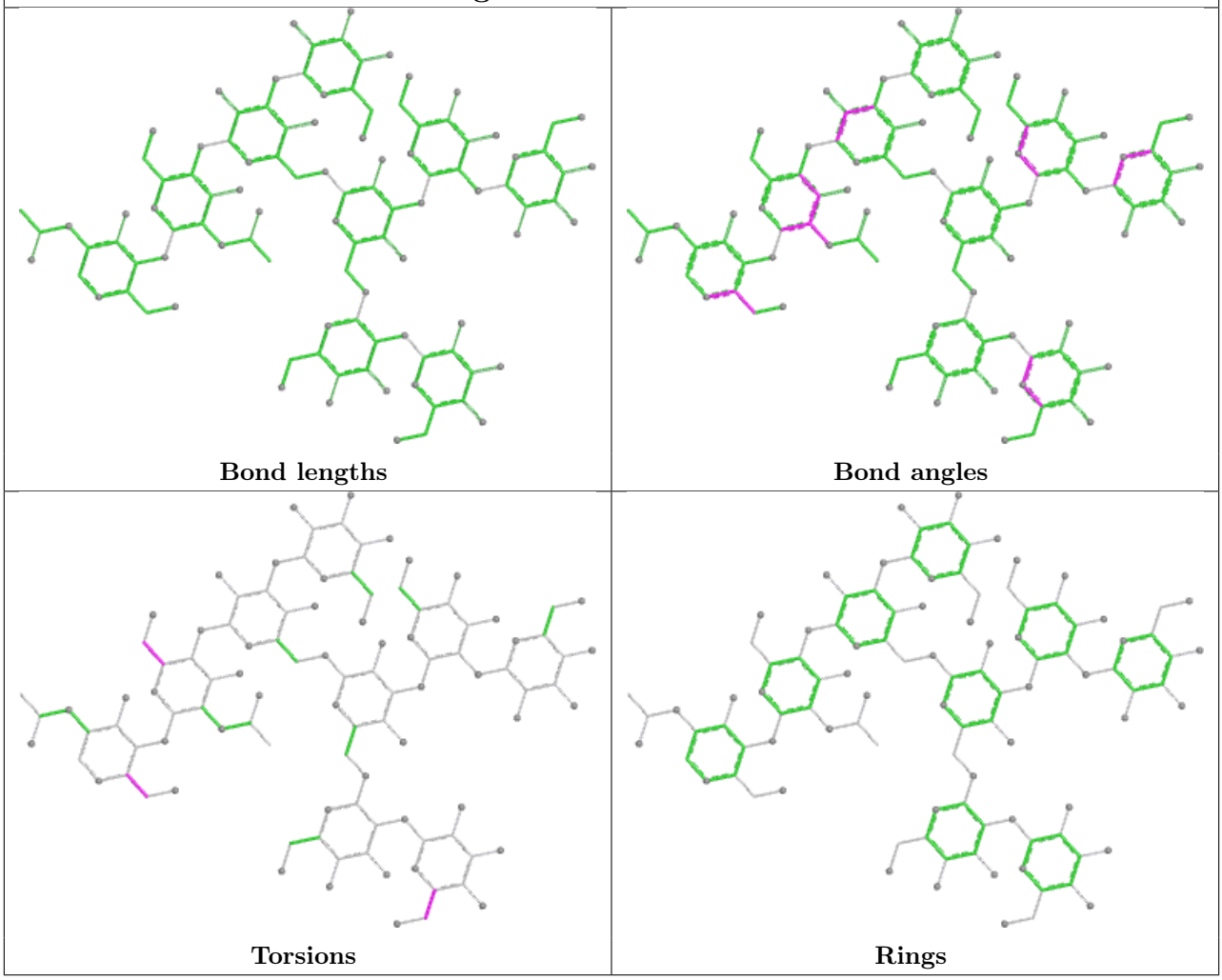
There are no ring outliers.

5 monomers are involved in 3 short contacts:

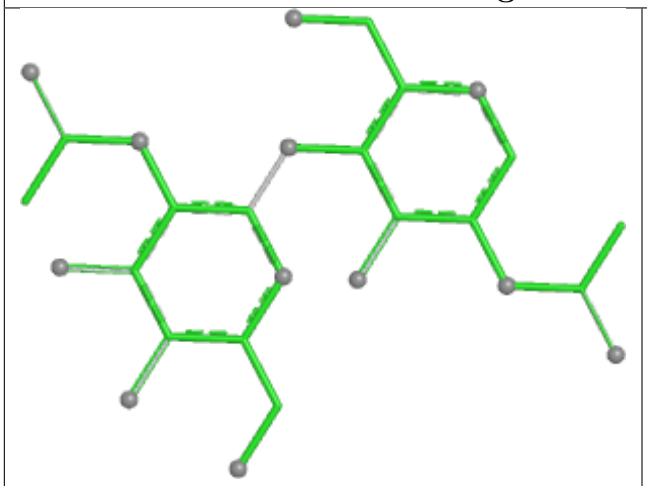
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
5	G	2	NAG	1	0
3	E	2	NAG	1	0
5	G	1	NAG	1	0
4	H	1	NAG	1	0

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

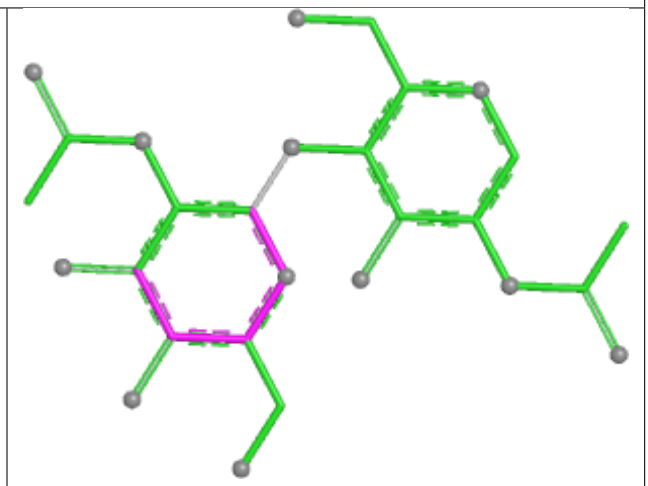
Oligosaccharide Chain E



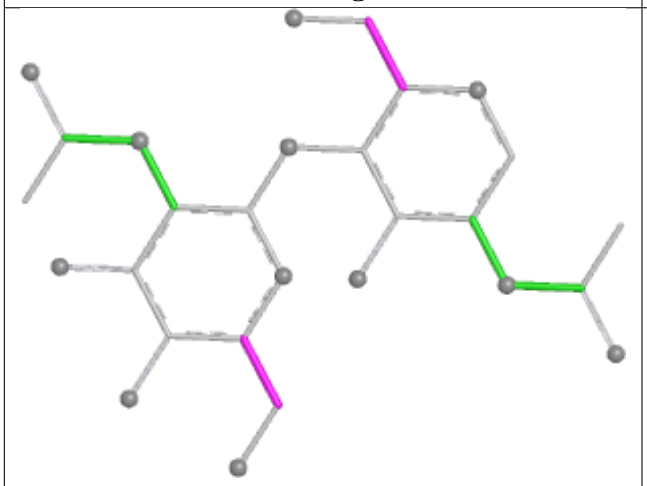
Oligosaccharide Chain F



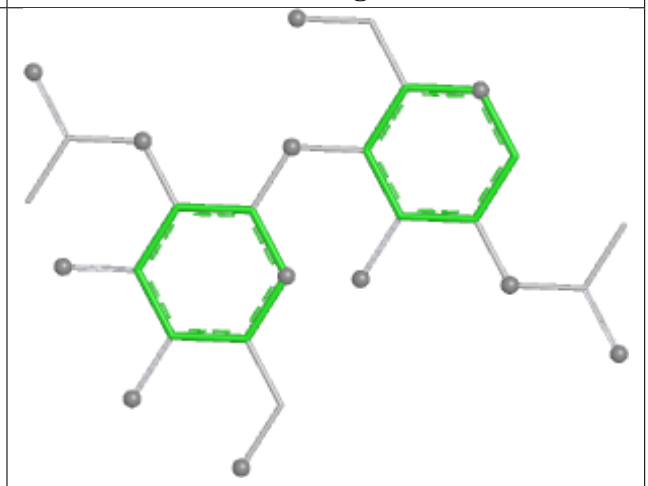
Bond lengths



Bond angles

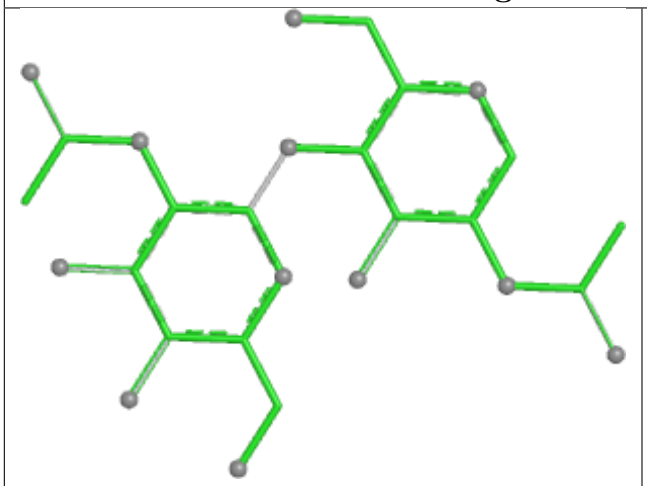


Torsions

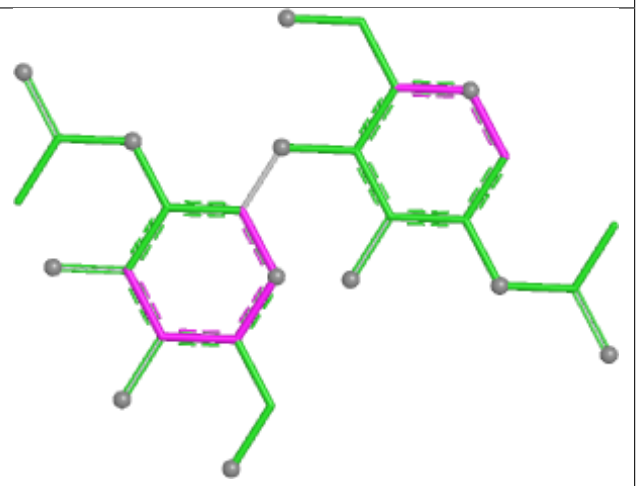


Rings

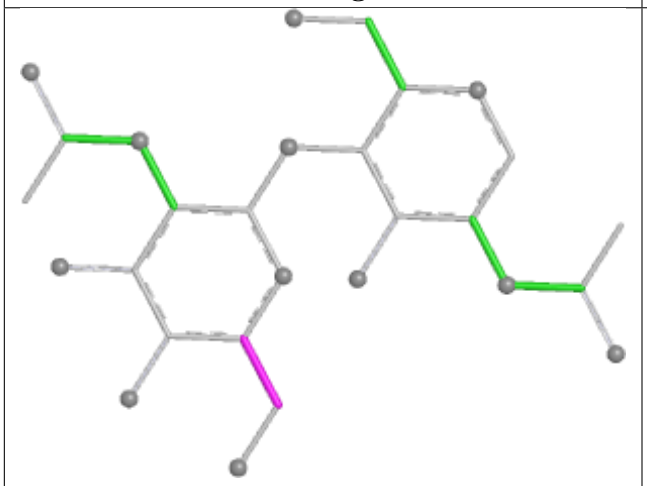
Oligosaccharide Chain H



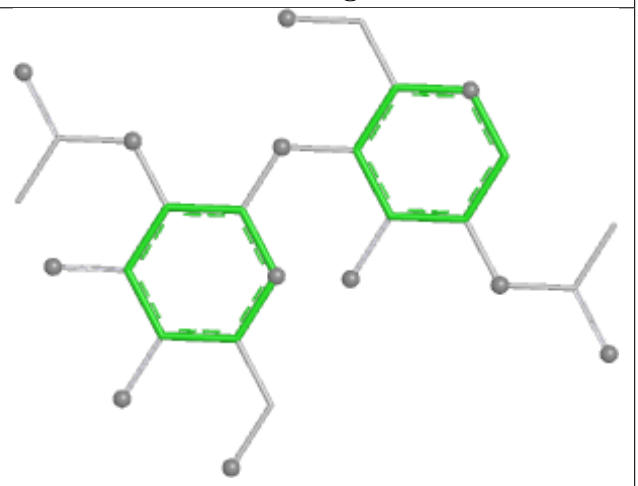
Bond lengths



Bond angles

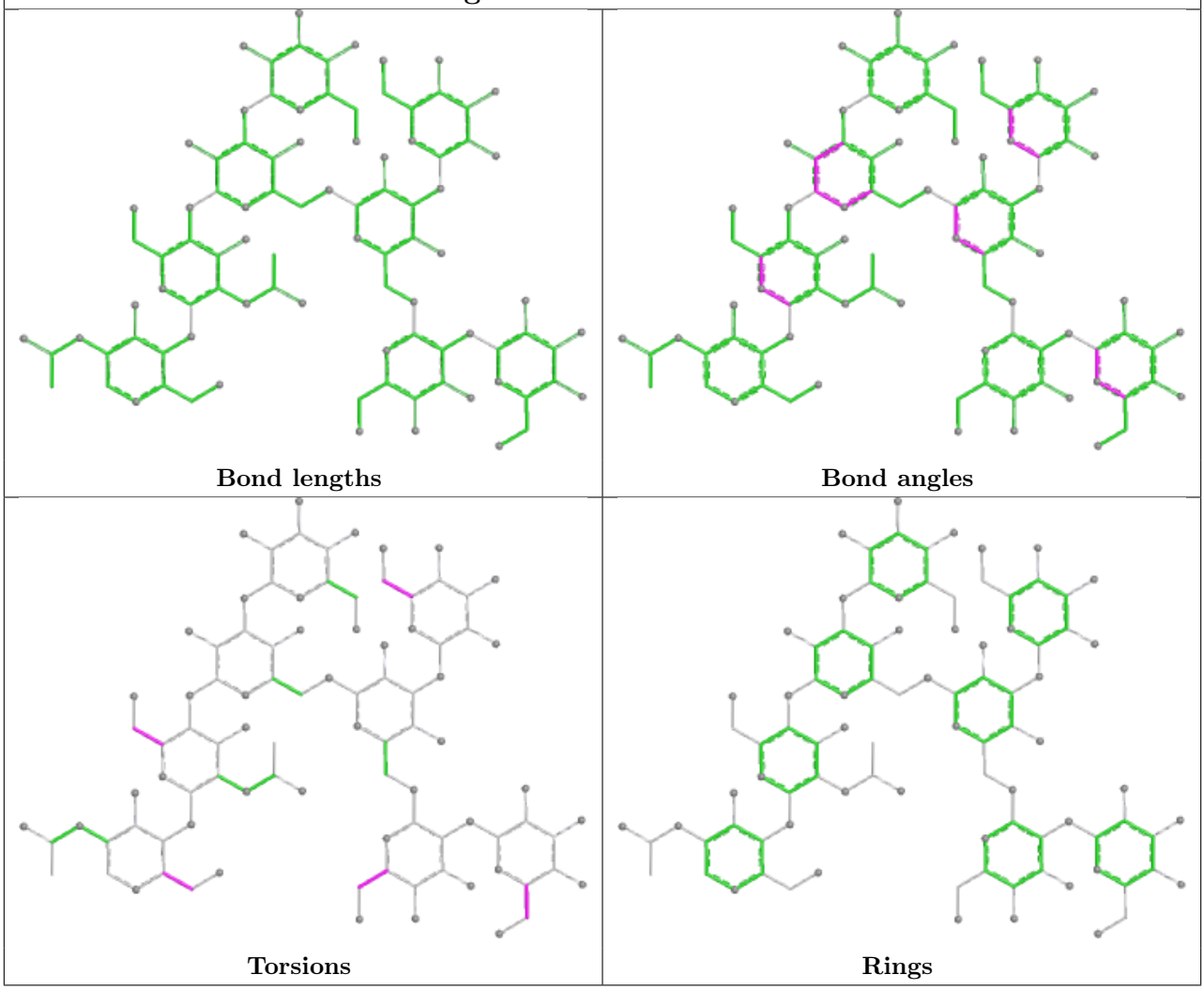


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
6	NAG	B	704	1	14,14,15	0.46	0	17,19,21	0.66	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
6	NAG	B	704	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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)

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	601/603 (99%)	0.04	23 (3%)	40	30	26, 47, 83, 139	2 (0%)
1	B	601/603 (99%)	-0.19	8 (1%)	77	72	25, 42, 68, 103	3 (0%)
2	C	139/144 (96%)	0.19	10 (7%)	15	8	30, 47, 97, 137	1 (0%)
2	D	139/144 (96%)	0.17	10 (7%)	15	8	27, 40, 87, 126	0
All	All	1480/1494 (99%)	-0.03	51 (3%)	45	35	25, 45, 81, 139	6 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	164	PHE	6.6
1	A	613	LEU	5.9
2	C	163	GLU	5.6
2	D	164	PHE	5.6
1	A	612	SER	5.5
1	A	625	CYS	5.3
1	B	26	GLN	5.2
1	B	626	GLY	5.1
1	A	626	GLY	4.8
2	C	132	THR	4.6
1	A	611	PRO	4.6
2	D	162	SER	4.4
1	A	610	PRO	4.4
1	B	625	CYS	4.3
2	C	133	ILE	4.3
2	C	58	CYS	3.9
2	D	36	SER	3.7
1	A	603	GLU	3.5
1	B	221	SER	3.4
2	D	35	ASP	3.4
1	A	319	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	288	ASP	3.3
2	D	163	GLU	3.3
1	A	260	ASP	3.3
1	B	222	THR	2.9
1	A	33	ALA	2.8
1	B	27	MET	2.8
1	A	287	SER	2.8
1	A	616	VAL	2.7
1	B	50	THR	2.6
2	C	26	ALA	2.6
2	D	94	VAL	2.6
2	C	131	PHE	2.6
1	A	26	GLN	2.5
1	A	318	LYS	2.5
2	D	130	GLU	2.5
2	D	93	SER	2.4
2	C	136	GLY	2.3
1	B	191	GLU	2.3
1	A	609	ASN	2.2
2	D	92	SER	2.2
1	A	221	SER	2.2
2	D	64	SER	2.2
1	A	222	THR	2.2
1	A	576	HIS	2.1
1	A	168	LYS	2.1
1	A	259	ASP	2.1
1	A	606	THR	2.1
1	A	32	GLU	2.1
2	C	36	SER	2.1
2	C	35	ASP	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)

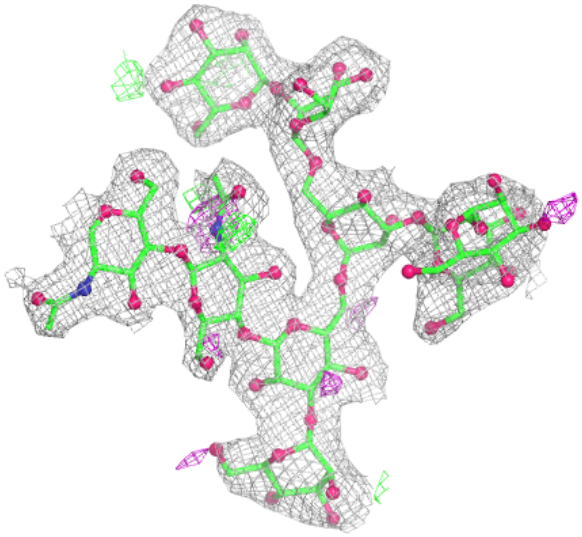
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

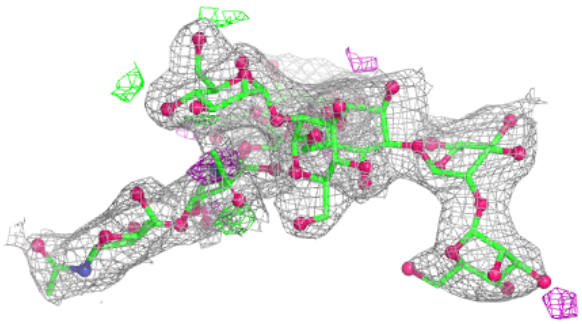
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	H	2	14/15	0.82	0.30	44,47,50,52	0
3	MAN	E	9	11/12	0.86	0.31	42,43,45,45	0
5	MAN	G	8	11/12	0.86	0.30	39,40,42,44	0
3	NAG	E	2	14/15	0.87	0.24	38,39,43,43	0
5	NAG	G	2	14/15	0.89	0.18	31,32,33,34	0
4	NAG	F	2	14/15	0.90	0.22	40,42,42,43	0
3	MAN	E	6	11/12	0.91	0.34	44,46,47,47	0
5	MAN	G	7	11/12	0.92	0.17	31,32,32,33	0
3	BMA	E	3	11/12	0.92	0.15	35,37,38,39	0
3	NAG	E	1	14/15	0.95	0.15	34,35,36,37	0
5	BMA	G	3	11/12	0.95	0.20	30,33,34,36	0
5	MAN	G	5	11/12	0.95	0.19	28,28,28,29	0
4	NAG	H	1	14/15	0.95	0.13	30,33,36,40	0
4	NAG	F	1	14/15	0.95	0.12	35,37,38,39	0
3	MAN	E	7	11/12	0.96	0.09	32,33,33,34	0
3	MAN	E	8	11/12	0.96	0.15	33,34,35,35	0
3	MAN	E	5	11/12	0.96	0.20	38,39,40,42	0
5	MAN	G	6	11/12	0.97	0.15	27,27,28,28	0
5	MAN	G	4	11/12	0.97	0.10	28,29,30,30	0
5	NAG	G	1	14/15	0.97	0.14	28,29,29,30	0
3	MAN	E	4	11/12	0.98	0.13	34,35,36,37	0

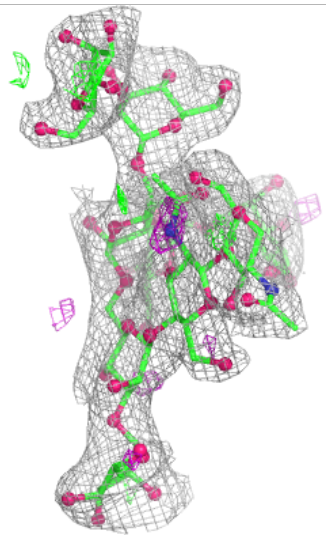
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

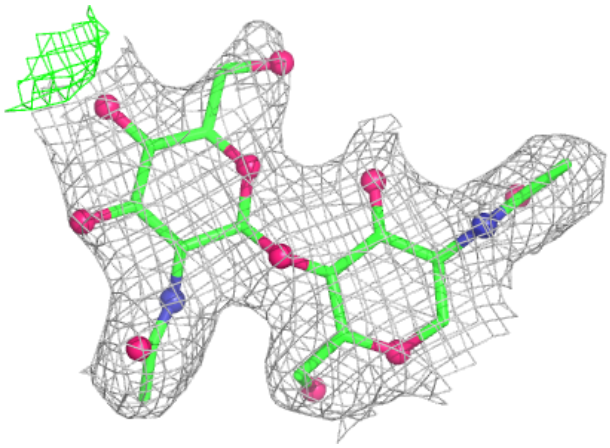


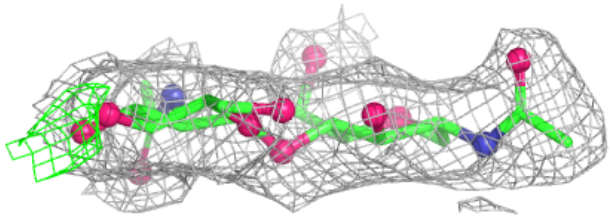


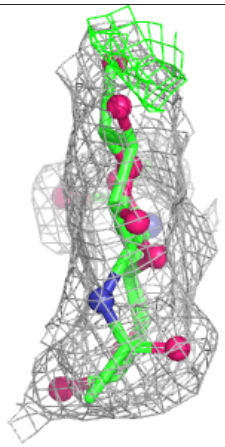


Electron density around Chain F:

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

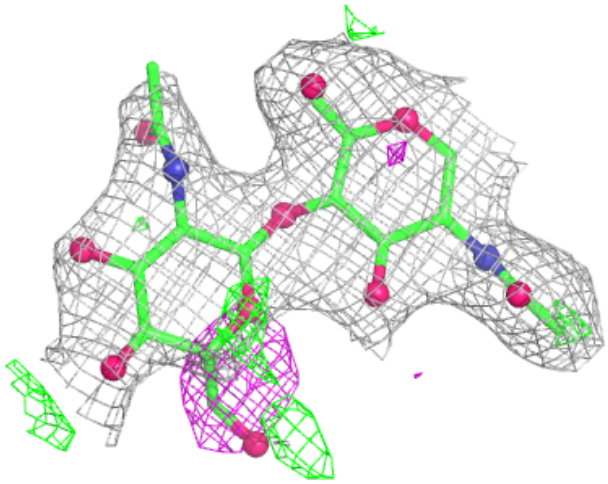


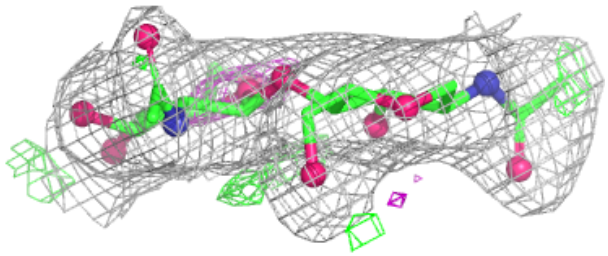


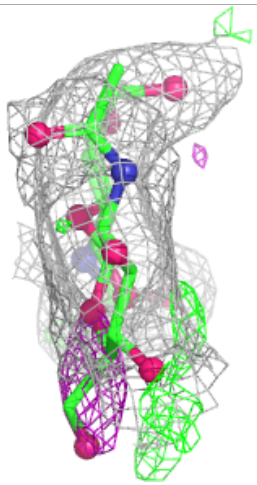


Electron density around Chain H:

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

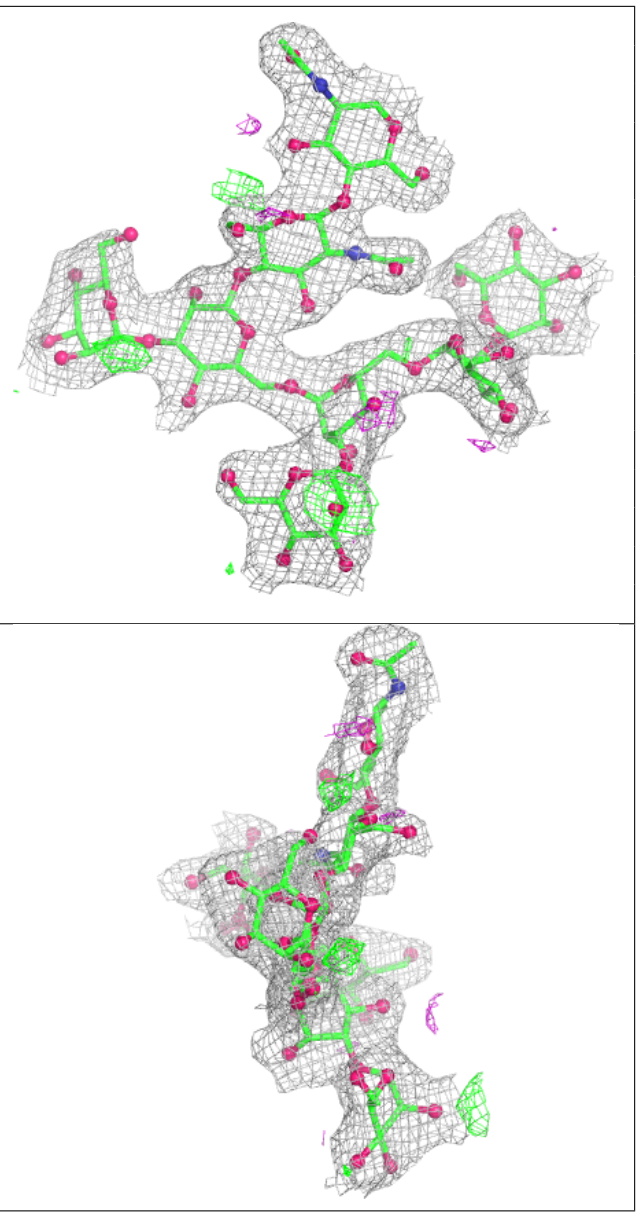






Electron density around Chain G:

$2mF_o$-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
6	NAG	B	704	14/15	0.91	0.17	49,51,52,53	0

6.5 Other polymers (i)

There are no such residues in this entry.