Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 02:43 PM EDT

PDB ID	:	5FFG
Title	:	Crystal structure of integrin alpha V beta 6 head
Authors	:	Dong, X.; Springer, T.A.
Deposited on	:	2015-12-18
Resolution	:	2.25 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:

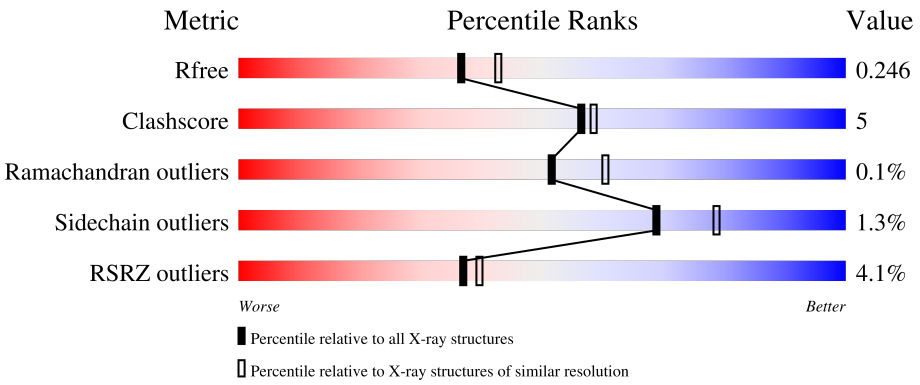
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	601	4%, 85%, 13%, •
2	B	257	4%, 84%, 12%, •
3	C	2	100%
4	D	3	100%
4	F	3	67%, 33%

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Mol	Chain	Length	Quality of chain
5	E	6	17% 83%
6	G	8	38% 62%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 7099 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	591	4580	2904	778	877	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	GLY	-	insertion	UNP P06756
A	401	CYS	MET	conflict	UNP P06756
A	597	THR	CYS	conflict	UNP P06756
A	599	GLY	-	expression tag	UNP P06756
A	600	LEU	-	expression tag	UNP P06756
A	601	GLU	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	248	1941	1240	311	379	11	0	0	0

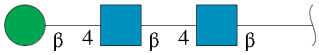
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	270	CYS	ILE	conflict	UNP P18564
B	362	HIS	-	expression tag	UNP P18564
B	363	HIS	-	expression tag	UNP P18564
B	364	HIS	-	expression tag	UNP P18564
B	365	HIS	-	expression tag	UNP P18564
B	366	HIS	-	expression tag	UNP P18564
B	367	HIS	-	expression tag	UNP P18564

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

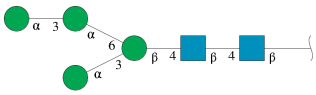
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

- Molecule 4 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.



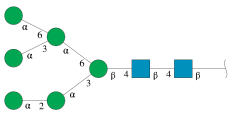
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	3	39	22	2	15	0	0	0
4	F	3	39	22	2	15	0	0	0

- Molecule 5 is an oligosaccharide called 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	E	6	72	40	2	30	0	0	0

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

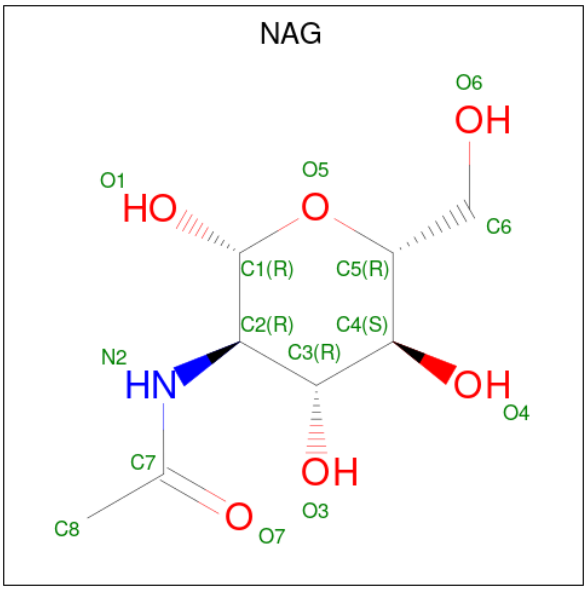


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	G	8	94	52	2	40	0	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

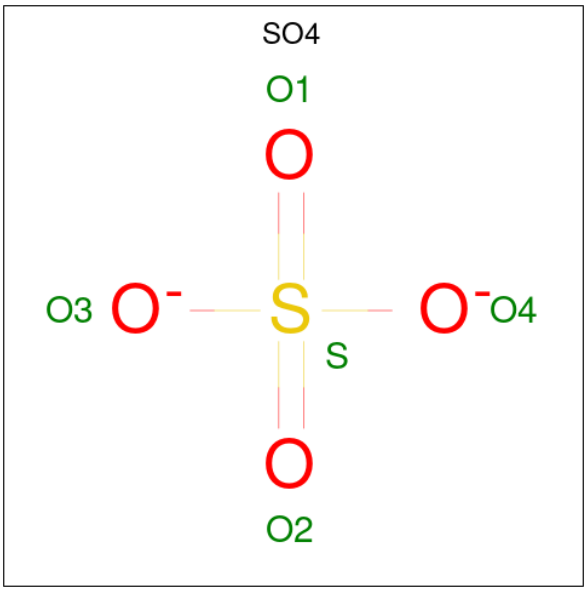
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	4	4	4	0	0
7	B	2	2	2	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



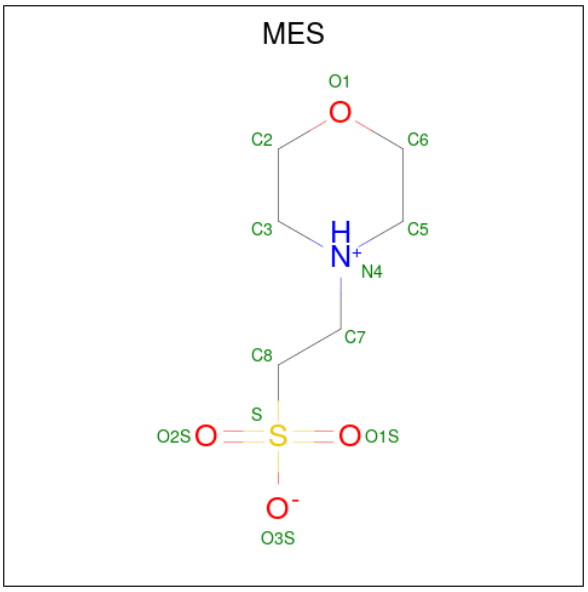
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	14	8	1	5	0	0
8	B	1	14	8	1	5	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



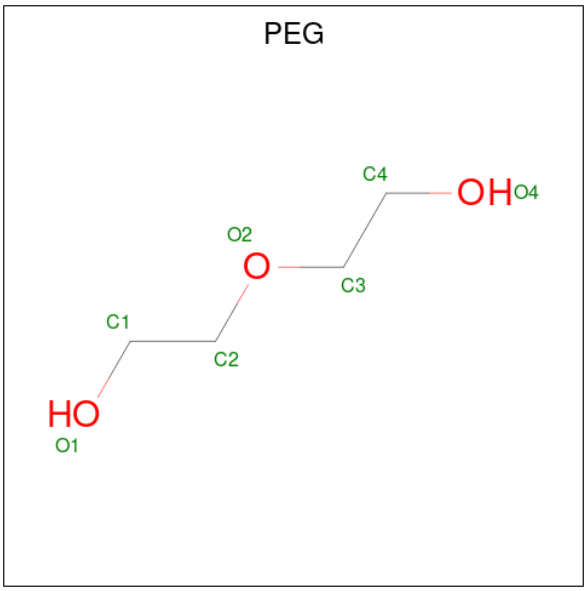
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
9	A	1	5	4	1	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	A	1	12	6	1	4	1	0	0

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	A	1	7	4	3	0	0
			Total	C	O		
11	B	1	7	4	3	0	0

- Molecule 12 is water.

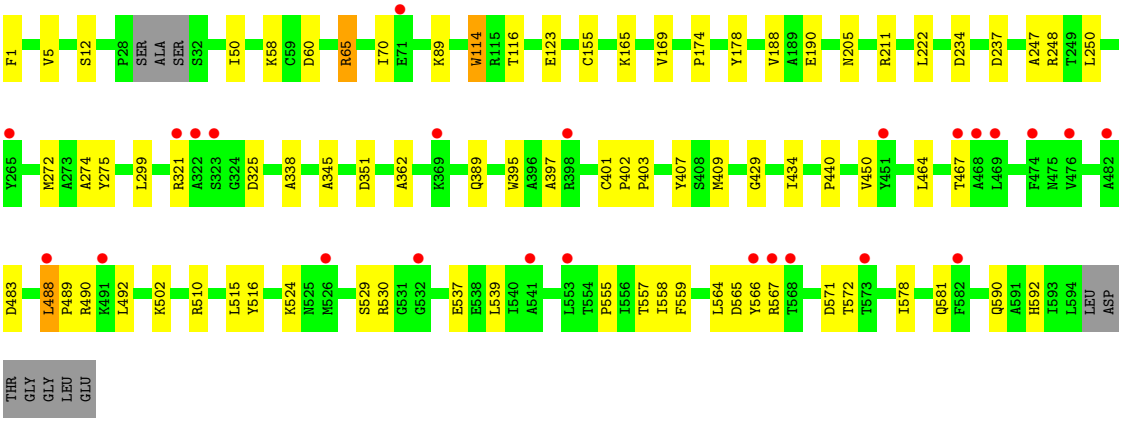
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	168	168	168	0	0
			Total	O		
12	B	73	73	73	0	0

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.

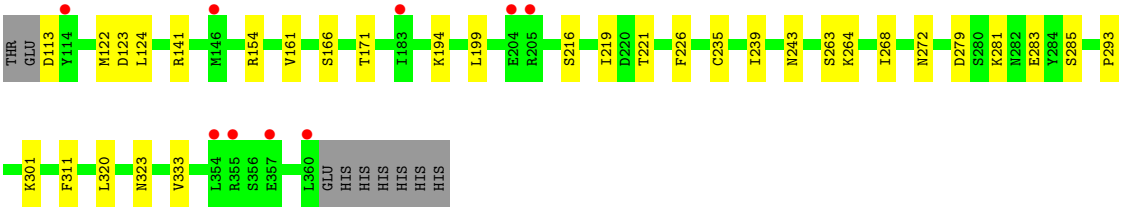
• Molecule 1: Integrin alpha-V

Chain A:



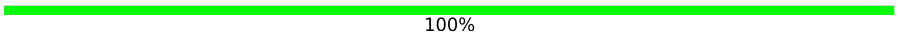
• Molecule 2: Integrin beta-6

Chain B:



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

Chain C:



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

Chain D: 100%

NAG1 NAG2 BMA3

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

Chain F: 67% 33%

NAG1 NAG2 BMA3

• Molecule 5: 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 E: 17% 83%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

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

Chain G: 38% 62%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN8

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	215.59Å 77.56Å 59.07Å 90.00° 101.46° 90.00°	Depositor
Resolution (Å)	46.99 – 2.25 46.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.99-2.25) 98.5 (46.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.208 , 0.246 0.208 , 0.246	Depositor DCC
R_{free} test set	905 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7099	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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, PEG, NAG, BMA, CA, MES, SO4

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	0.27	1/4683 (0.0%)	0.46	0/6338
2	B	0.26	0/1980	0.45	0/2685
All	All	0.27	1/6663 (0.0%)	0.46	0/9023

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	GLU	C-N	5.22	1.44	1.34

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	4580	0	4428	48	0
2	B	1941	0	1917	20	0
3	C	28	0	25	0	0
4	D	39	0	34	0	0
4	F	39	0	34	1	0
5	E	72	0	61	1	0
6	G	94	0	79	0	0
7	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	2	0	0	0	0
8	A	14	0	13	1	0
8	B	14	0	13	0	0
9	A	5	0	0	1	0
10	A	12	0	12	0	0
11	A	7	0	10	2	0
11	B	7	0	10	0	0
12	A	168	0	0	8	0
12	B	73	0	0	2	0
All	All	7099	0	6636	67	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 (67) 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)
2:B:141:ARG:NH1	12:B:2101:HOH:O	2.23	0.72
1:A:440:PRO:HB2	1:A:488:LEU:HD12	1.71	0.71
2:B:113:ASP:N	12:B:2102:HOH:O	2.27	0.68
1:A:397:ALA:HB2	1:A:403:PRO:HD3	1.76	0.67
1:A:488:LEU:HD21	1:A:492:LEU:HD21	1.78	0.66
1:A:165:LYS:NZ	1:A:237:ASP:OD1	2.29	0.63
1:A:321:ARG:HD3	1:A:325:ASP:HB2	1.81	0.63
1:A:211:ARG:NH1	12:A:2110:HOH:O	2.36	0.59
2:B:263:SER:HB2	2:B:268:ILE:HB	1.85	0.58
1:A:450:VAL:HG21	1:A:558:ILE:HD13	1.87	0.57
1:A:524:LYS:NZ	1:A:537:GLU:OE1	2.32	0.57
2:B:161:VAL:HG21	2:B:216:SER:HB3	1.87	0.57
1:A:467:THR:OG1	12:A:2101:HOH:O	2.17	0.56
1:A:248:ARG:HE	2:B:320:LEU:HB2	1.70	0.55
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.91	0.53
1:A:58:LYS:HB2	1:A:70:ILE:HD11	1.91	0.52
1:A:50:ILE:HD12	1:A:89:LYS:HB2	1.92	0.52
1:A:407:TYR:OH	2:B:264:LYS:NZ	2.32	0.51
2:B:154:ARG:HE	2:B:199:LEU:HD12	1.77	0.50
1:A:539:LEU:HD11	11:A:2030:PEG:H32	1.93	0.50
1:A:169:VAL:HG23	1:A:188:VAL:HG12	1.92	0.50
1:A:488:LEU:HG	1:A:489:PRO:HD2	1.92	0.50
2:B:279:ASP:O	2:B:281:LYS:N	2.37	0.49
2:B:279:ASP:HB3	2:B:285:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:LEU:HD23	1:A:515:LEU:HD12	1.95	0.48
1:A:566:TYR:CE1	1:A:578:ILE:HA	2.48	0.48
1:A:114:TRP:CZ2	1:A:116:THR:HA	2.49	0.48
2:B:194:LYS:HG2	2:B:283:GLU:HG2	1.96	0.48
1:A:1:PHE:CD1	1:A:581:GLN:HG2	2.49	0.48
1:A:190:GLU:OE1	1:A:205:ASN:N	2.36	0.47
1:A:345:ALA:HB2	1:A:409:MET:HG3	1.94	0.47
2:B:226:PHE:HB3	2:B:293:PRO:HG2	1.96	0.47
1:A:395:TRP:CH2	1:A:434:ILE:HG12	2.50	0.47
2:B:166:SER:HB2	2:B:171:THR:HG21	1.96	0.47
2:B:235:CYS:HB2	2:B:239:ILE:HD13	1.97	0.46
2:B:272:ASN:HD22	2:B:293:PRO:HD3	1.80	0.46
2:B:311:PHE:HB2	2:B:333:VAL:HG22	1.97	0.46
1:A:338:ALA:HB1	1:A:362:ALA:HB1	1.97	0.46
1:A:502:LYS:N	12:A:2104:HOH:O	2.48	0.46
1:A:234:ASP:CG	12:A:2102:HOH:O	2.54	0.45
1:A:272:MET:HG3	2:B:323:ASN:HB3	1.98	0.45
1:A:571:ASP:OD1	1:A:572:THR:N	2.45	0.45
1:A:488:LEU:HD23	1:A:489:PRO:O	2.16	0.45
12:A:2152:HOH:O	5:E:2:NAG:H81	2.17	0.45
1:A:567:ARG:NH2	12:A:2114:HOH:O	2.40	0.45
1:A:557:THR:HA	1:A:590:GLN:HA	1.99	0.44
1:A:559:PHE:CE1	8:A:2027:NAG:H82	2.53	0.44
1:A:274:ALA:HA	1:A:299:LEU:HB2	2.00	0.43
2:B:219:ILE:HG22	2:B:221:THR:H	1.84	0.43
1:A:351:ASP:OD1	1:A:351:ASP:N	2.52	0.42
1:A:557:THR:HB	12:A:2104:HOH:O	2.19	0.42
1:A:247:ALA:O	1:A:250:LEU:HB2	2.19	0.42
1:A:490:ARG:O	1:A:529:SER:HA	2.19	0.42
2:B:124:LEU:HD23	2:B:124:LEU:HA	1.80	0.42
12:A:2247:HOH:O	4:F:1:NAG:H83	2.20	0.42
1:A:174:PRO:HA	1:A:222:LEU:O	2.20	0.42
1:A:1:PHE:CE1	1:A:581:GLN:HG2	2.55	0.41
2:B:301:LYS:HD3	2:B:301:LYS:HA	1.88	0.41
2:B:122:MET:HG2	2:B:123:ASP:O	2.20	0.41
1:A:402:PRO:O	1:A:429:GLY:HA3	2.19	0.41
1:A:564:LEU:HB3	1:A:566:TYR:CE1	2.56	0.41
1:A:510:ARG:NH2	9:A:2028:SO4:O2	2.41	0.41
1:A:516:TYR:HB2	11:A:2030:PEG:H22	2.02	0.41
1:A:483:ASP:HA	1:A:530:ARG:HB2	2.03	0.41
1:A:565:ASP:C	1:A:567:ARG:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:PRO:HB3	1:A:592:HIS:CE1	2.56	0.40
1:A:12:SER:H	1:A:65:ARG:HE	1.70	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	587/601 (98%)	565 (96%)	21 (4%)	1 (0%)	47	55
2	B	246/257 (96%)	234 (95%)	12 (5%)	0	100	100
All	All	833/858 (97%)	799 (96%)	33 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ARG

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	484/491 (99%)	476 (98%)	8 (2%)	60	71
2	B	221/230 (96%)	220 (100%)	1 (0%)	88	92
All	All	705/721 (98%)	696 (99%)	9 (1%)	69	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	60	ASP
1	A	114	TRP
1	A	155	CYS
1	A	178	TYR
1	A	275	TYR
1	A	401	CYS
1	A	488	LEU
2	B	243	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

22 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	C	1	1,3	14,14,15	0.54	0	17,19,21	0.50	0
3	NAG	C	2	3	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	D	1	1,4	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.37	0
4	BMA	D	3	4	11,11,12	0.62	0	15,15,17	0.81	0
5	NAG	E	1	1,5	14,14,15	0.30	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	E	2	5	14,14,15	0.36	0	17,19,21	0.39	0
5	BMA	E	3	5	11,11,12	0.81	1 (9%)	15,15,17	0.87	0
5	MAN	E	4	5	11,11,12	1.01	1 (9%)	15,15,17	0.90	0
5	MAN	E	5	5	11,11,12	0.77	0	15,15,17	1.00	2 (13%)
5	MAN	E	6	5	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
4	NAG	F	1	1,4	14,14,15	0.32	0	17,19,21	0.43	0
4	NAG	F	2	4	14,14,15	0.26	0	17,19,21	0.43	0
4	BMA	F	3	4	11,11,12	0.62	0	15,15,17	0.89	0
6	NAG	G	1	1,6	14,14,15	0.26	0	17,19,21	0.55	0
6	NAG	G	2	6	14,14,15	0.32	0	17,19,21	0.49	0
6	BMA	G	3	6	11,11,12	0.84	0	15,15,17	0.72	0
6	MAN	G	4	6	11,11,12	2.09	4 (36%)	15,15,17	2.09	5 (33%)
6	MAN	G	5	6	11,11,12	0.92	1 (9%)	15,15,17	1.61	4 (26%)
6	MAN	G	6	6	11,11,12	0.86	0	15,15,17	1.10	2 (13%)
6	MAN	G	7	6	11,11,12	0.78	0	15,15,17	1.10	2 (13%)
6	MAN	G	8	6	11,11,12	0.65	0	15,15,17	1.11	2 (13%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	G	3	6	-	2/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	2/2/19/22	0/1/1/1
6	MAN	G	6	6	-	2/2/19/22	0/1/1/1
6	MAN	G	7	6	-	0/2/19/22	0/1/1/1
6	MAN	G	8	6	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	4	MAN	C2-C3	4.34	1.58	1.52
6	G	4	MAN	O2-C2	3.76	1.51	1.43
6	G	4	MAN	C1-C2	2.75	1.58	1.52
5	E	4	MAN	O5-C1	-2.39	1.39	1.43
6	G	5	MAN	C1-C2	2.35	1.57	1.52
5	E	3	BMA	O5-C1	-2.19	1.40	1.43
6	G	4	MAN	O5-C5	2.07	1.47	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	4	MAN	C1-O5-C5	5.45	119.58	112.19
6	G	4	MAN	O5-C1-C2	3.47	116.13	110.77
6	G	5	MAN	C1-O5-C5	3.01	116.27	112.19
6	G	5	MAN	O5-C1-C2	3.00	115.41	110.77
6	G	5	MAN	C1-C2-C3	2.91	113.24	109.67
6	G	8	MAN	C1-O5-C5	2.60	115.72	112.19
5	E	6	MAN	C1-O5-C5	2.55	115.65	112.19
5	E	6	MAN	O2-C2-C3	-2.51	105.12	110.14
6	G	4	MAN	O2-C2-C1	2.45	114.16	109.15
6	G	4	MAN	C1-C2-C3	2.44	112.67	109.67
6	G	6	MAN	C1-O5-C5	2.40	115.44	112.19
6	G	8	MAN	O2-C2-C3	-2.39	105.35	110.14
6	G	7	MAN	C1-O5-C5	2.30	115.31	112.19
6	G	4	MAN	O3-C3-C2	2.22	114.25	109.99
6	G	5	MAN	O2-C2-C3	-2.21	105.71	110.14
6	G	7	MAN	O2-C2-C3	-2.20	105.73	110.14
5	E	5	MAN	C1-O5-C5	2.06	114.98	112.19
6	G	6	MAN	O2-C2-C3	-2.04	106.05	110.14
5	E	5	MAN	O2-C2-C3	-2.03	106.08	110.14

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	3	BMA	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
6	G	6	MAN	C4-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
6	G	3	BMA	C4-C5-C6-O6
6	G	6	MAN	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
6	G	1	NAG	C4-C5-C6-O6
6	G	5	MAN	C4-C5-C6-O6
6	G	5	MAN	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6

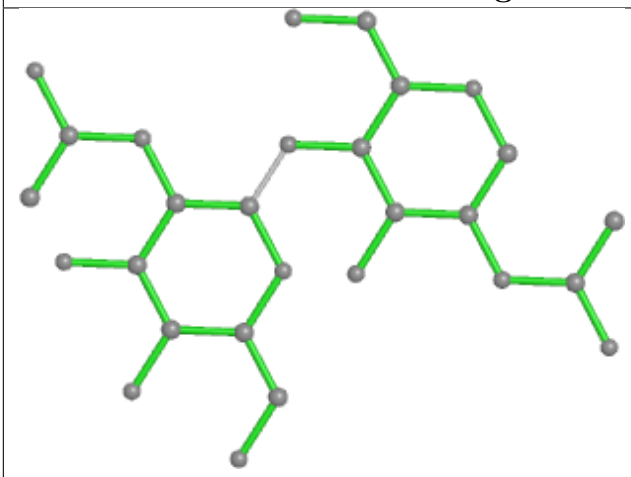
There are no ring outliers.

2 monomers are involved in 2 short contacts:

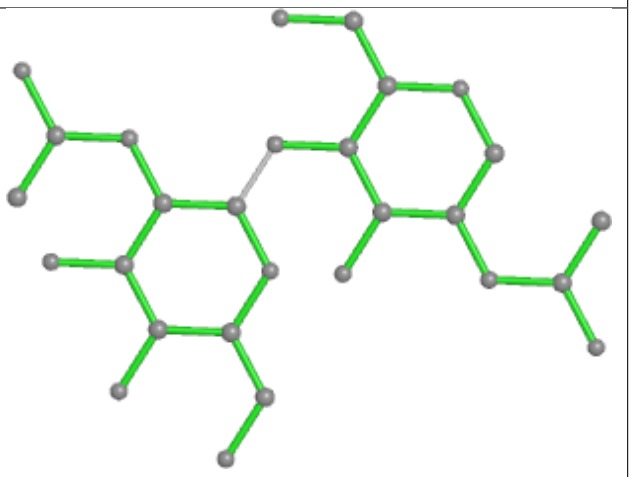
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0
5	E	2	NAG	1	0

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

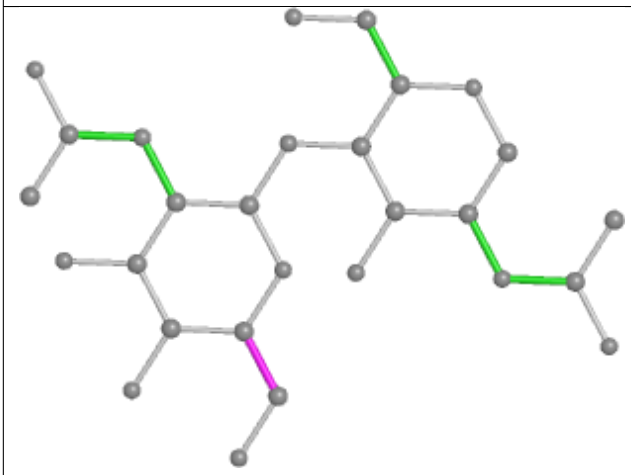
Oligosaccharide Chain C



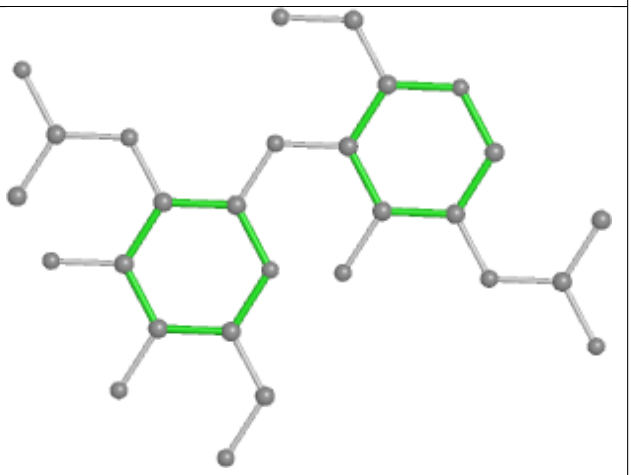
Bond lengths



Bond angles

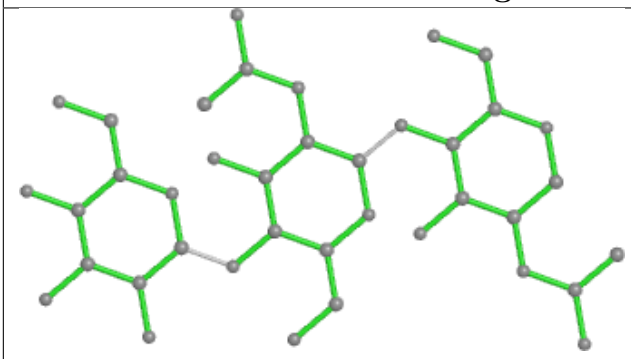


Torsions

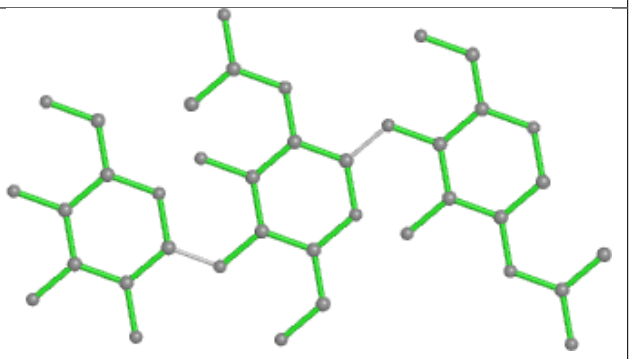


Rings

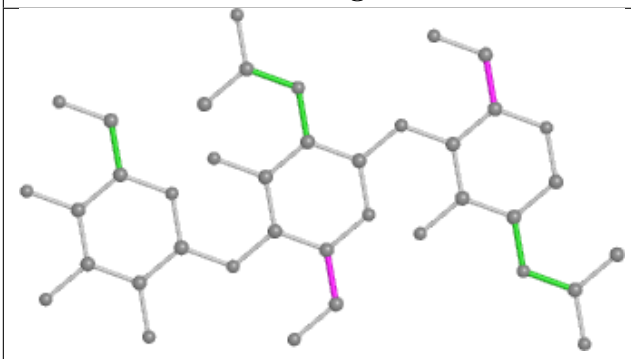
Oligosaccharide Chain D



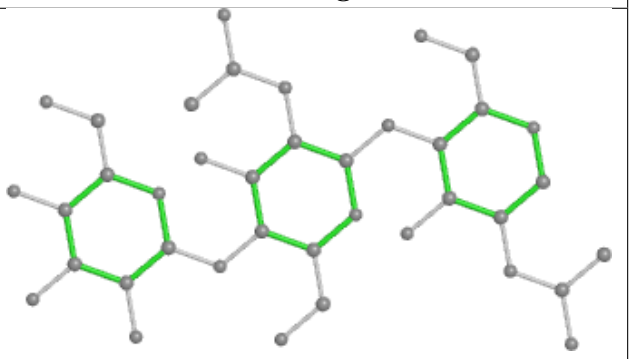
Bond lengths



Bond angles

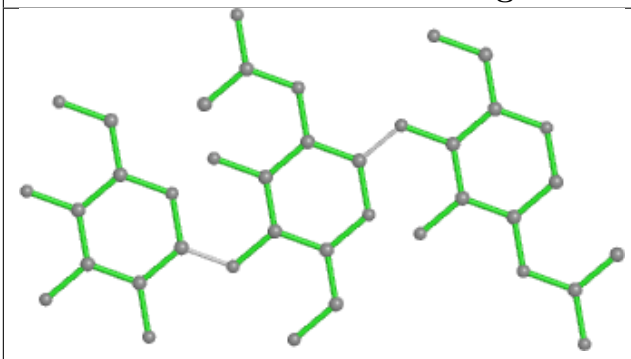


Torsions

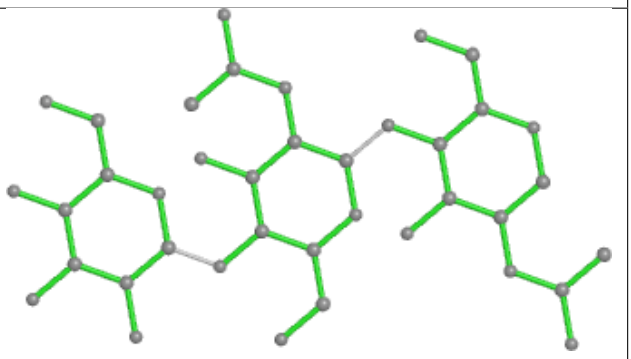


Rings

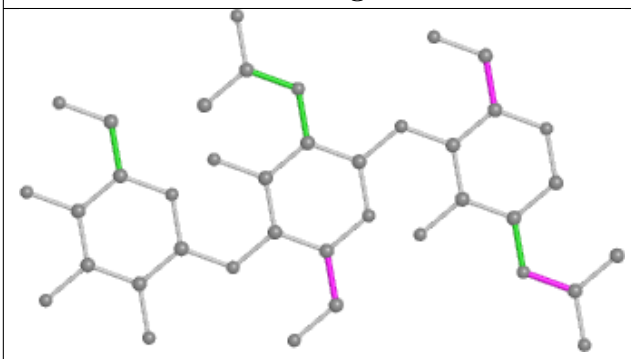
Oligosaccharide Chain F



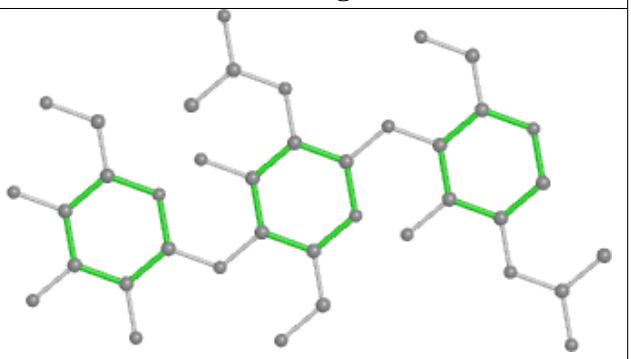
Bond lengths



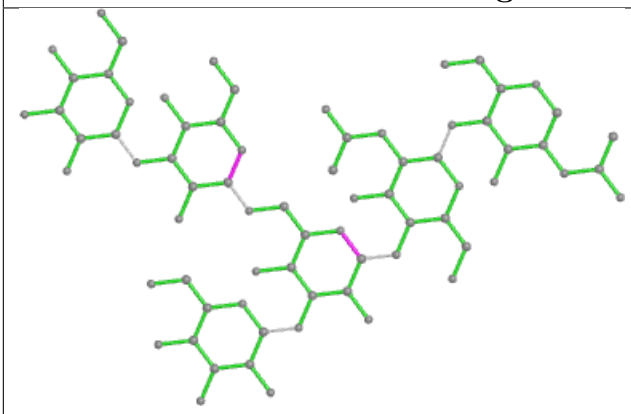
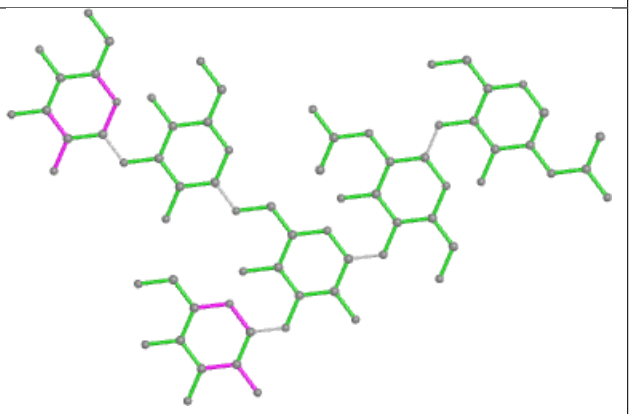
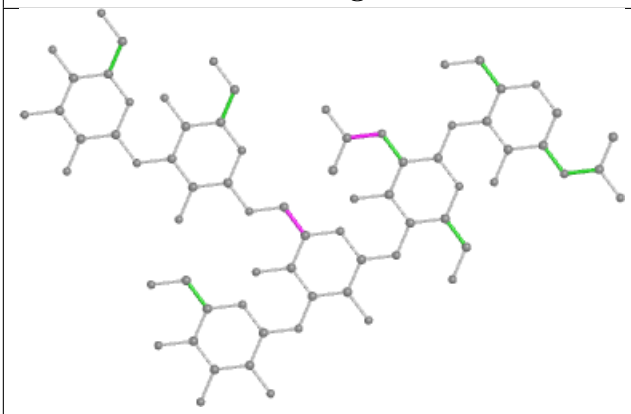
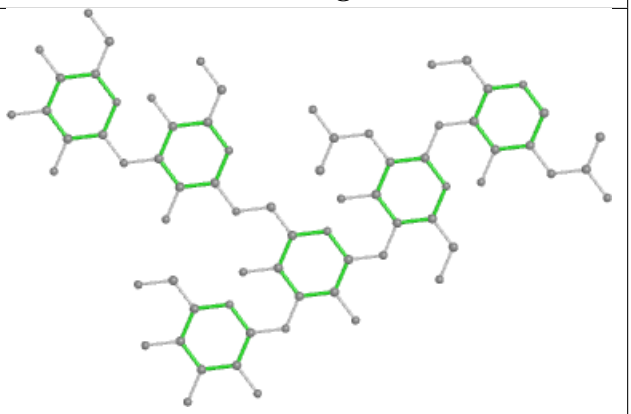
Bond angles



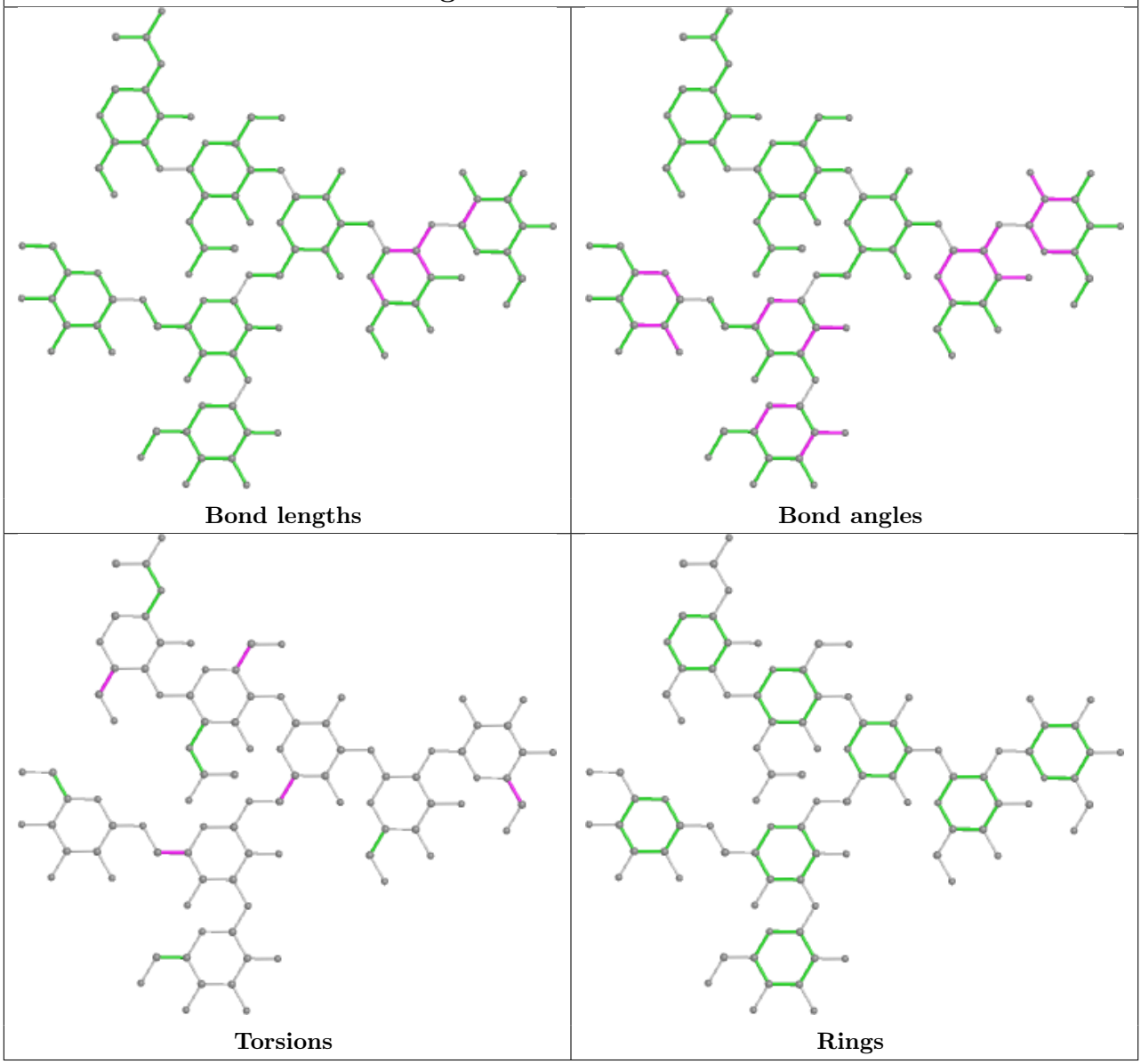
Torsions



Rings

Oligosaccharide Chain E	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	PEG	A	2030	-	6,6,6	0.63	0	5,5,5	0.68	0
10	MES	A	2029	-	12,12,12	2.25	1 (8%)	14,16,16	2.01	6 (42%)
8	NAG	B	2003	2	14,14,15	0.23	0	17,19,21	0.42	0
11	PEG	B	2004	-	6,6,6	0.64	0	5,5,5	0.67	0
9	SO4	A	2028	-	4,4,4	0.14	0	6,6,6	0.07	0
8	NAG	A	2027	1	14,14,15	0.31	0	17,19,21	0.37	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
11	PEG	A	2030	-	-	2/4/4/4	-
11	PEG	B	2004	-	-	0/4/4/4	-
10	MES	A	2029	-	-	4/6/14/14	0/1/1/1
8	NAG	B	2003	2	-	0/6/23/26	0/1/1/1
8	NAG	A	2027	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2029	MES	C8-S	-7.53	1.66	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2029	MES	C5-N4-C3	4.22	118.34	108.83
10	A	2029	MES	C6-C5-N4	-2.76	105.92	110.10
10	A	2029	MES	O2S-S-C8	2.51	109.93	106.92
10	A	2029	MES	C7-N4-C5	2.31	117.15	111.23
10	A	2029	MES	O1S-S-C8	2.29	109.67	106.92
10	A	2029	MES	O3S-S-C8	2.04	109.07	105.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2029	MES	C7-C8-S-O3S
8	A	2027	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	2027	NAG	O5-C5-C6-O6
11	A	2030	PEG	O1-C1-C2-O2
11	A	2030	PEG	O2-C3-C4-O4
10	A	2029	MES	C7-C8-S-O1S
10	A	2029	MES	C7-C8-S-O2S
10	A	2029	MES	C8-C7-N4-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	2030	PEG	2	0
9	A	2028	SO4	1	0
8	A	2027	NAG	1	0

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	591/601 (98%)	0.44	25 (4%)	36	38	32, 68, 100, 158	0
2	B	248/257 (96%)	0.29	9 (3%)	42	44	29, 51, 89, 138	0
All	All	839/858 (97%)	0.40	34 (4%)	37	40	29, 63, 100, 158	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	566	TYR	8.4
1	A	488	LEU	6.7
1	A	582	PHE	6.2
1	A	469	LEU	5.8
1	A	553	LEU	4.9
1	A	568	THR	4.6
1	A	567	ARG	4.5
1	A	451	TYR	4.0
1	A	468	ALA	3.5
1	A	398	ARG	3.3
2	B	114	TYR	3.1
1	A	491	LYS	3.0
1	A	265	TYR	2.9
2	B	360	LEU	2.7
1	A	541	ALA	2.7
2	B	183	ILE	2.6
1	A	482	ALA	2.6
1	A	321	ARG	2.5
1	A	467	THR	2.5
1	A	532	GLY	2.5
1	A	322	ALA	2.4
1	A	476	VAL	2.4
2	B	205	ARG	2.3
2	B	354	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	71	GLU	2.2
1	A	369	LYS	2.2
1	A	474	PHE	2.2
1	A	526	MET	2.1
2	B	204	GLU	2.1
1	A	323	SER	2.1
1	A	573	THR	2.0
2	B	357	GLU	2.0
2	B	146	MET	2.0
2	B	355	ARG	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
6	MAN	G	5	11/12	0.31	0.34	116,127,139,142	0
6	MAN	G	4	11/12	0.59	0.34	140,145,150,152	0
4	BMA	D	3	11/12	0.69	0.28	99,115,119,121	0
4	BMA	F	3	11/12	0.72	0.20	96,105,109,110	0
5	MAN	E	5	11/12	0.73	0.30	108,112,122,123	0
6	MAN	G	6	11/12	0.82	0.14	80,92,96,104	0
5	MAN	E	4	11/12	0.84	0.20	91,98,106,107	0
3	NAG	C	2	14/15	0.85	0.18	86,98,101,106	0
6	BMA	G	3	11/12	0.88	0.21	100,107,118,130	0
6	MAN	G	7	11/12	0.88	0.27	113,117,125,127	0
6	NAG	G	1	14/15	0.89	0.20	57,75,90,96	0
4	NAG	D	2	14/15	0.90	0.22	84,98,109,115	0
4	NAG	F	1	14/15	0.91	0.17	51,67,97,101	0
6	NAG	G	2	14/15	0.92	0.22	88,96,99,100	0
4	NAG	D	1	14/15	0.92	0.16	62,80,91,92	0
4	NAG	F	2	14/15	0.92	0.19	76,87,100,102	0
6	MAN	G	8	11/12	0.92	0.22	74,83,96,101	0
3	NAG	C	1	14/15	0.93	0.15	39,61,73,75	0

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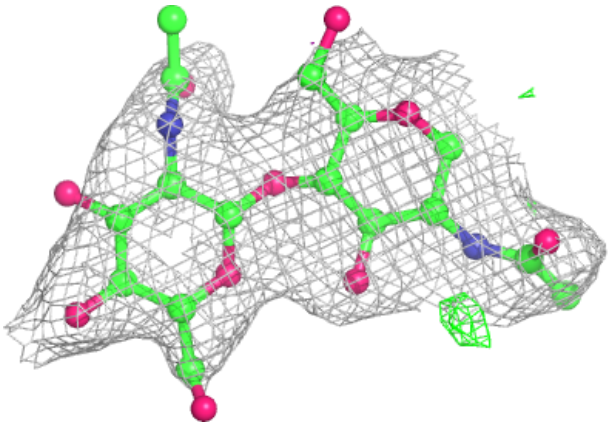
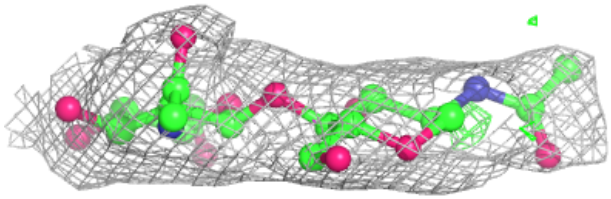
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	E	6	11/12	0.93	0.12	67,75,85,86	0
5	BMA	E	3	11/12	0.94	0.12	47,57,76,90	0
5	NAG	E	1	14/15	0.94	0.14	35,48,59,62	0
5	NAG	E	2	14/15	0.97	0.12	30,43,48,54	0

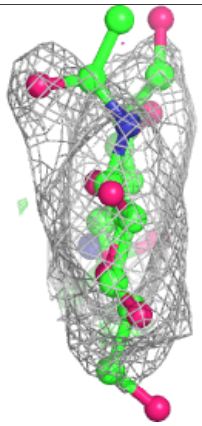
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

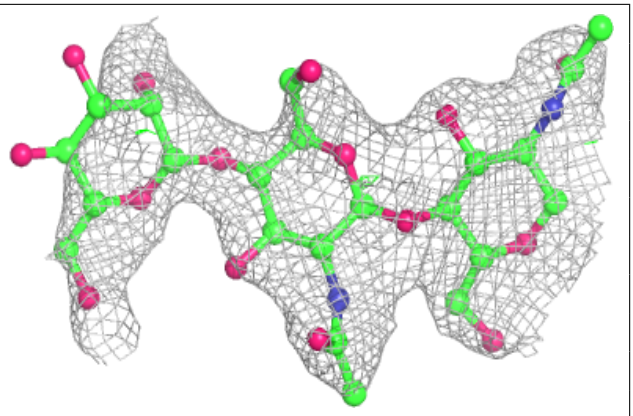


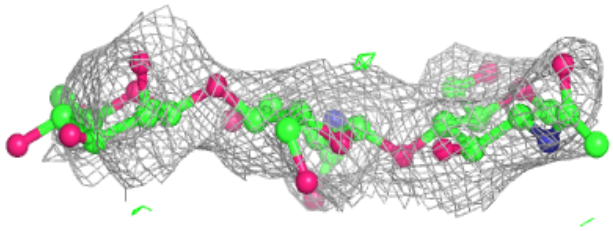


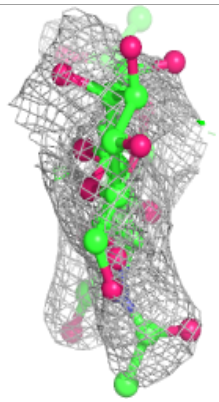


Electron density around Chain D:

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

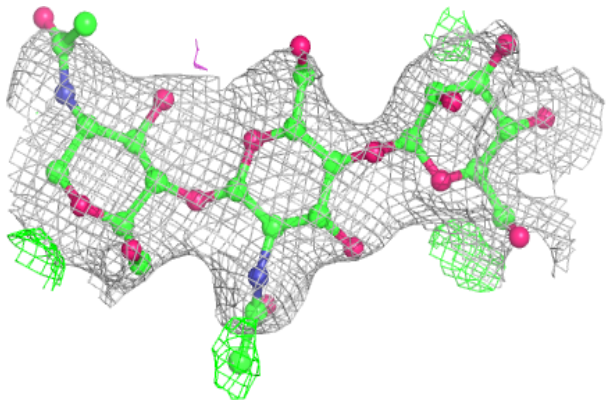


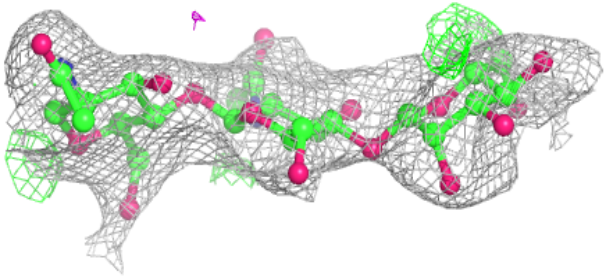


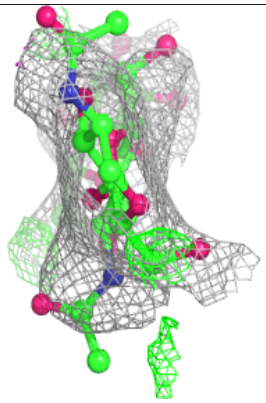


Electron density around Chain F:

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

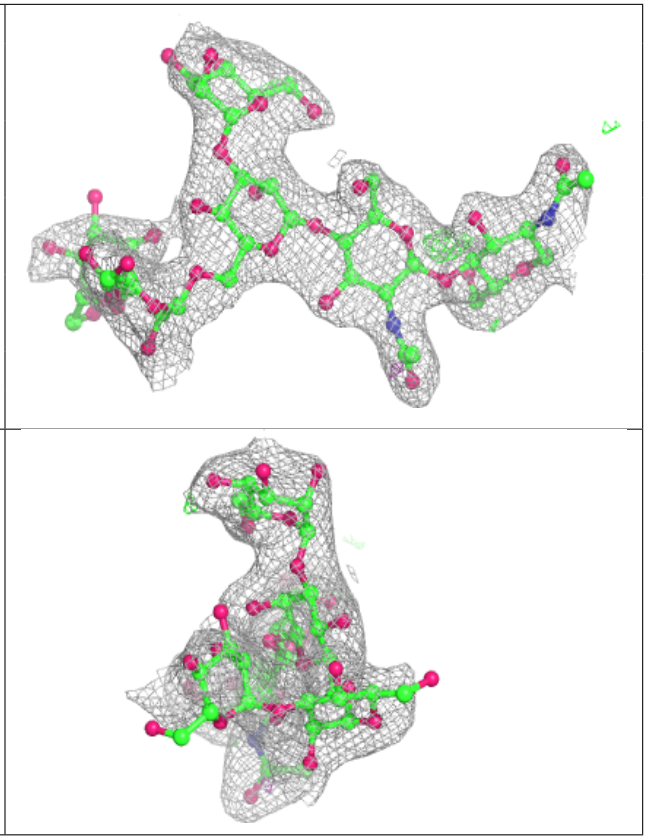






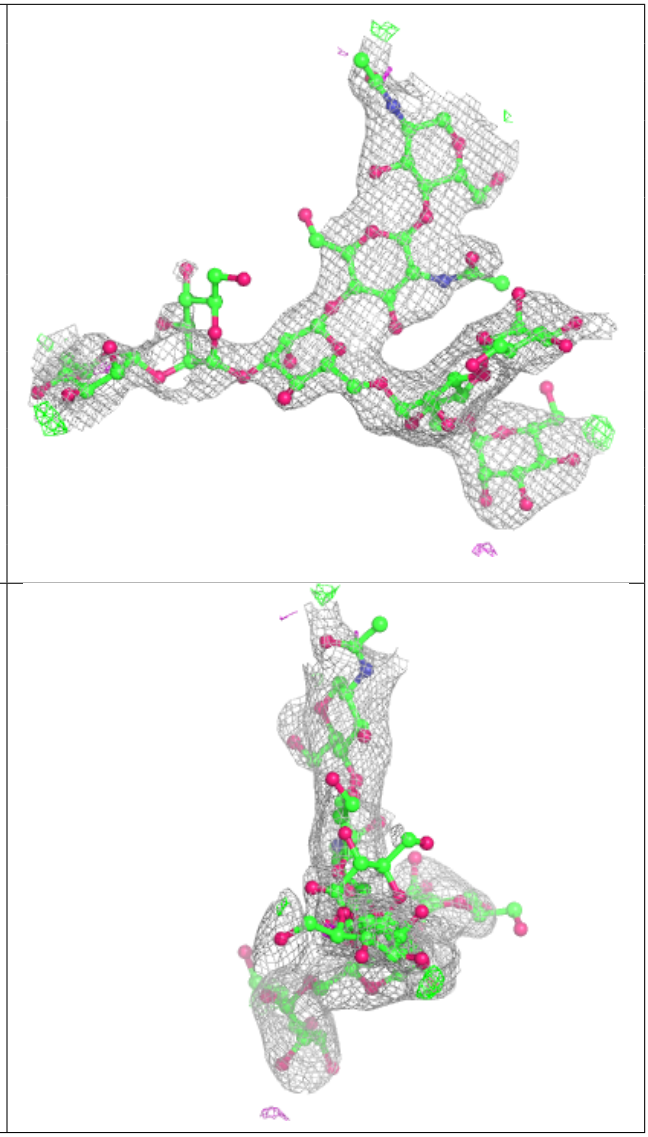
Electron density around Chain E:

$2mF_o$-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 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
11	PEG	A	2030	7/7	0.69	0.22	63,71,80,83	0
8	NAG	B	2003	14/15	0.77	0.26	78,94,99,103	0
8	NAG	A	2027	14/15	0.83	0.20	73,92,96,100	0
7	CA	A	2003	1/1	0.86	0.06	55,55,55,55	0
11	PEG	B	2004	7/7	0.86	0.27	82,84,88,89	0
7	CA	A	2002	1/1	0.88	0.09	58,58,58,58	0
7	CA	A	2004	1/1	0.92	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	MES	A	2029	12/12	0.94	0.22	51,79,98,98	0
7	CA	A	2001	1/1	0.95	0.06	49,49,49,49	0
9	SO4	A	2028	5/5	0.97	0.10	61,65,68,68	5
7	CA	B	2002	1/1	0.97	0.07	53,53,53,53	1
7	CA	B	2001	1/1	0.99	0.08	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.