Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 07:43 AM EDT

PDB ID	:	6DBS
Title	:	Fusion surface structure, function, and dynamics of gamete fusogen HAP2
Authors	:	Feng, J.; Dong, X.; Springer, T.A.
Deposited on	:	2018-05-03
Resolution	:	2.60 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:

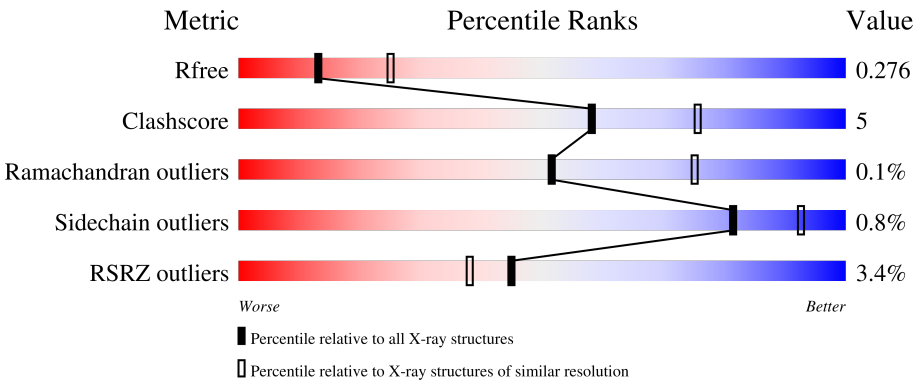
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	565	3%, 80%, 11%, • 9%
1	B	565	3%, 80%, 12%, 9%
1	C	565	4%, 79%, 12%, 9%
2	D	3	100%
3	E	4	75%, 25%

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Mol	Chain	Length	Quality of chain
3	F	4	75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	C	606	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11975 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 Hapless 2.

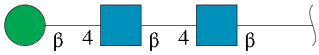
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	3875	2424	664	758	29	0	0	0
1	C	515	3870	2421	663	757	29	0	0	0
1	B	515	3870	2421	663	757	29	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP A4GRC6
A	583	HIS	-	expression tag	UNP A4GRC6
A	584	HIS	-	expression tag	UNP A4GRC6
A	585	HIS	-	expression tag	UNP A4GRC6
A	586	HIS	-	expression tag	UNP A4GRC6
A	587	HIS	-	expression tag	UNP A4GRC6
A	588	HIS	-	expression tag	UNP A4GRC6
C	?	-	THR	deletion	UNP A4GRC6
C	583	HIS	-	expression tag	UNP A4GRC6
C	584	HIS	-	expression tag	UNP A4GRC6
C	585	HIS	-	expression tag	UNP A4GRC6
C	586	HIS	-	expression tag	UNP A4GRC6
C	587	HIS	-	expression tag	UNP A4GRC6
C	588	HIS	-	expression tag	UNP A4GRC6
B	?	-	THR	deletion	UNP A4GRC6
B	583	HIS	-	expression tag	UNP A4GRC6
B	584	HIS	-	expression tag	UNP A4GRC6
B	585	HIS	-	expression tag	UNP A4GRC6
B	586	HIS	-	expression tag	UNP A4GRC6
B	587	HIS	-	expression tag	UNP A4GRC6
B	588	HIS	-	expression tag	UNP A4GRC6

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

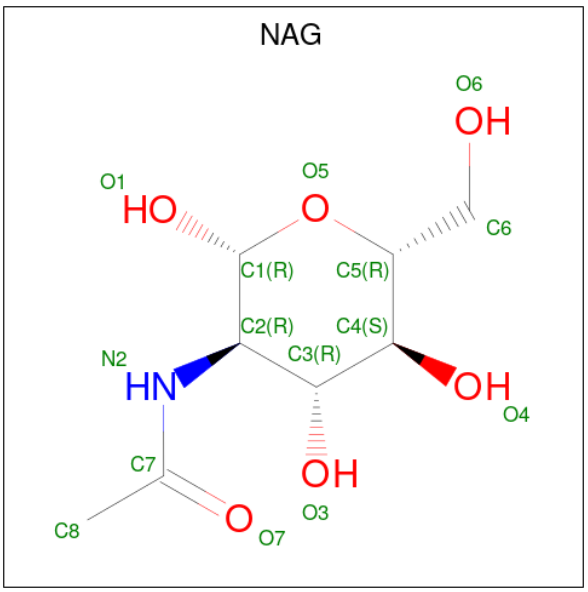


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called 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			
3	E	4	50	28	2	20	0	0	0
3	F	4	50	28	2	20	0	0	0

- Molecule 4 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		
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	C	1	14	8	1	5	0	0
4	C	1	14	8	1	5	0	0
4	C	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

- Molecule 5 is water.

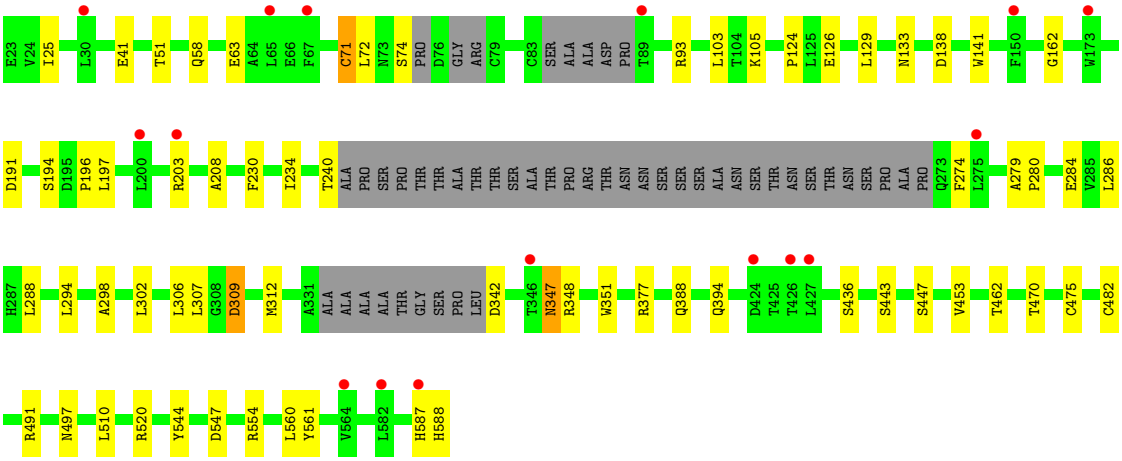
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	31	31	31	0	0
5	C	31	31	31	0	0
5	B	33	33	33	0	0

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.

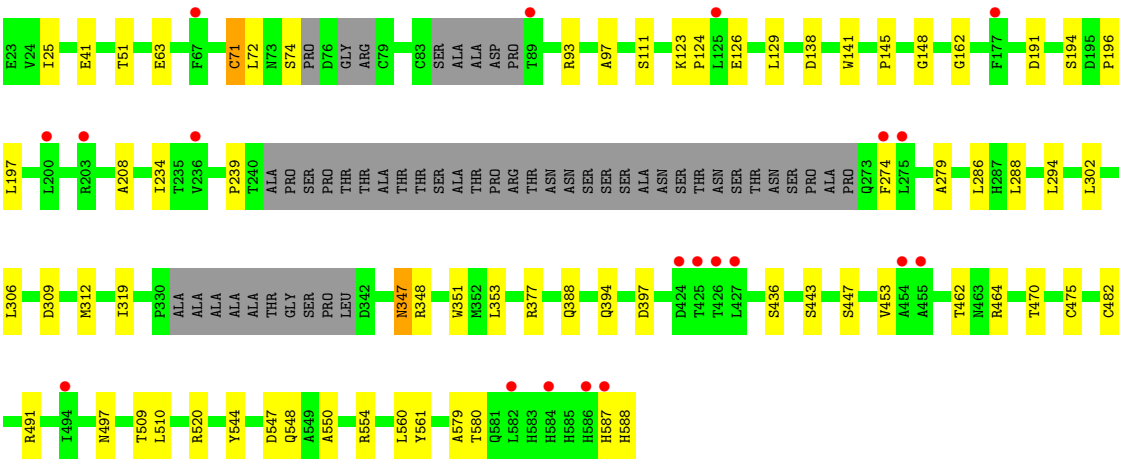
• Molecule 1: Hapless 2

Chain A: 3% 80% 11% • 9%



• Molecule 1: Hapless 2

Chain C: 4% 79% 12% 9%



• Molecule 1: Hapless 2

Chain B: 3% 80% 12% 9%

E23 V24 I25 G37 E41 T51 E63 C71 L72 N73 S74 PRO D76 GLY ARG C79 P80 C83 SER ALA ALA ASP PRO T89 R93 D94 K105 S111 P124 L129 N133 D138 W141 G162 D191 S194 D195 P196 L197 L200 R203

A208 L211 F230 I234 T235 V236 T240 ALA PRO SER PRO THR THR ALA THR THR SER ALA THR PRO ARG THR ASN ASN SER SER SER ALA ASN SER THR ASN SER THR ASN SER PRO ALA PRO Q273 F274 L275 S276 P277 P278 A279 P280 S281 L286 L294 L301 L302

D309 P330 ALA ALA ALA ALA ALA THR GLY SER PRO LEU D342 N347 R348 W351 R377 Q394 D424 L427 S436 S447 S452 V453 T462 T470 C475 C482 R491 N497 T509 L510 C515 L537 Y544 D547 A550

R554 L560 Y561 V564 T577 N578 A579 L582 H583 H584 H587 H588

• Molecule 2: 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 3: 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 E: 75% 25%

NAG1 NAG2 BMA3 MAN4

• Molecule 3: 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 F: 75% 25%

NAG1 NAG2 BMA3 MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	198.22Å 117.60Å 115.21Å 90.00° 123.79° 90.00°	Depositor
Resolution (Å)	48.99 – 2.60 48.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.99-2.60) 97.1 (48.99-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.61Å)	Xtriage
Refinement program	PHENIX V1.0	Depositor
R, R_{free}	0.237 , 0.276 0.237 , 0.276	Depositor DCC
R_{free} test set	1840 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å^2)	88.7	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 79.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h+3/2*k-l,1/2*h+1/2*k+l,1/2*h-1/2*k 0.000 for 1/2*h-1/2*k+2*l,-1/2*h+1/2*k,-1/2*h-1/2*k-l 0.000 for -h-k-l,l,k 0.000 for -h+k-l,-l,-k 0.000 for -1/2*h-3/2*k-l,-1/2*h+1/2*k-l,1/2*h+1/2*k 0.000 for 1/2*h+1/2*k+2*l,1/2*h+1/2*k,-1/2*h+1/2*k-l 0.460 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.468 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.000 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11975	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

[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.

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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: NAG, BMA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.25	0/3955	0.46	0/5387
1	B	0.25	0/3950	0.46	0/5380
1	C	0.25	0/3950	0.45	0/5380
All	All	0.25	0/11855	0.46	0/16147

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	ALA	Peptide
1	B	279	ALA	Peptide
1	C	279	ALA	Peptide

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	3875	0	3757	43	0
1	B	3870	0	3752	42	0
1	C	3870	0	3752	44	0
2	D	39	0	34	0	0
3	E	50	0	43	0	0
3	F	50	0	43	0	0
4	A	42	0	39	0	0
4	B	42	0	39	0	0
4	C	42	0	39	0	0
5	A	31	0	0	3	0
5	B	33	0	0	1	0
5	C	31	0	0	2	0
All	All	11975	0	11498	113	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 (113) 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:C:348:ARG:NH1	1:C:436:SER:O	2.14	0.79
1:A:348:ARG:NH1	1:A:436:SER:O	2.17	0.76
1:B:348:ARG:NH1	1:B:436:SER:O	2.18	0.75
1:B:129:LEU:HB2	1:B:208:ALA:HB3	1.68	0.74
1:B:515:CYS:SG	5:B:701:HOH:O	2.48	0.72
1:A:129:LEU:HB2	1:A:208:ALA:HB3	1.72	0.71
1:B:162:GLY:O	1:B:377:ARG:NH1	2.26	0.69
1:C:129:LEU:HB2	1:C:208:ALA:HB3	1.75	0.68
1:A:162:GLY:O	1:A:377:ARG:NH1	2.28	0.67
1:A:280:PRO:O	5:A:701:HOH:O	2.13	0.66
1:C:162:GLY:O	1:C:377:ARG:NH1	2.30	0.64
1:B:138:ASP:HB2	1:B:377:ARG:HH12	1.61	0.64
1:B:302:LEU:HD13	1:B:453:VAL:HG22	1.82	0.62
1:A:138:ASP:HB2	1:A:377:ARG:HH12	1.63	0.61
1:C:138:ASP:HB2	1:C:377:ARG:HH12	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:MET:HE3	1:C:443:SER:HB3	1.83	0.61
1:C:302:LEU:HD13	1:C:453:VAL:HG22	1.84	0.58
1:A:274:PHE:HB3	1:C:41:GLU:HG3	1.84	0.58
1:A:133:ASN:O	1:A:203:ARG:NH2	2.31	0.58
1:A:312:MET:HE3	1:A:443:SER:HB3	1.85	0.56
1:B:234:ILE:HB	1:B:286:LEU:HB2	1.88	0.55
1:B:196:PRO:HG2	1:B:197:LEU:HD12	1.88	0.55
1:A:510:LEU:HD13	1:A:560:LEU:HD13	1.88	0.55
1:A:63:GLU:HG2	1:A:462:THR:HG23	1.89	0.54
1:C:274:PHE:HB3	1:B:41:GLU:HG3	1.88	0.54
1:A:196:PRO:HG2	1:A:197:LEU:HD12	1.89	0.54
1:C:234:ILE:HB	1:C:286:LEU:HB2	1.89	0.53
1:A:342:ASP:N	5:A:704:HOH:O	2.41	0.53
1:A:41:GLU:HG3	1:B:274:PHE:HB3	1.90	0.53
1:C:510:LEU:HD13	1:C:560:LEU:HD13	1.91	0.53
1:C:196:PRO:HG2	1:C:197:LEU:HD12	1.90	0.52
1:A:191:ASP:O	1:A:194:SER:OG	2.25	0.51
1:B:63:GLU:HG2	1:B:462:THR:HG23	1.92	0.51
1:C:63:GLU:HG2	1:C:462:THR:HG23	1.92	0.51
1:B:510:LEU:HD13	1:B:560:LEU:HD13	1.92	0.51
1:B:547:ASP:OD2	1:B:554:ARG:NH2	2.43	0.51
1:A:74:SER:HB2	1:A:93:ARG:HE	1.76	0.51
1:C:74:SER:HB2	1:C:93:ARG:HE	1.77	0.50
1:C:124:PRO:HD2	1:C:394:GLN:HG3	1.94	0.50
1:A:274:PHE:HB2	1:C:41:GLU:HA	1.94	0.50
1:C:123:LYS:NZ	1:C:397:ASP:OD2	2.44	0.50
1:A:25:ILE:HG23	1:C:51:THR:HG21	1.94	0.49
1:A:309:ASP:HA	1:A:447:SER:HA	1.95	0.49
1:C:274:PHE:HB2	1:B:41:GLU:HA	1.94	0.49
1:A:41:GLU:HA	1:B:274:PHE:HB2	1.95	0.48
1:A:51:THR:HG21	1:B:25:ILE:HG23	1.95	0.48
1:A:284:GLU:OE2	1:A:298:ALA:N	2.47	0.48
1:C:191:ASP:O	1:C:194:SER:OG	2.27	0.48
1:A:302:LEU:HD13	1:A:453:VAL:HG22	1.96	0.48
1:A:547:ASP:OD2	1:A:554:ARG:NH2	2.47	0.48
1:C:72:LEU:O	1:C:93:ARG:HB3	2.14	0.48
1:A:348:ARG:HA	1:A:351:TRP:CD1	2.50	0.47
1:C:580:THR:N	5:C:701:HOH:O	2.31	0.47
1:A:240:THR:HG22	5:A:701:HOH:O	2.15	0.47
1:C:547:ASP:OD2	1:C:554:ARG:NH2	2.47	0.47
1:B:124:PRO:HD2	1:B:394:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:HD2	1:A:394:GLN:HG3	1.95	0.47
1:C:548:GLN:O	5:C:701:HOH:O	2.20	0.46
1:B:309:ASP:HA	1:B:447:SER:HA	1.98	0.46
1:A:491:ARG:HD3	1:A:544:TYR:CE2	2.51	0.46
1:B:133:ASN:O	1:B:203:ARG:NH2	2.37	0.46
1:C:288:LEU:HD23	1:C:306:LEU:HB2	1.97	0.46
1:A:520:ARG:NH2	1:C:111:SER:O	2.49	0.46
1:B:470:THR:N	1:B:497:ASN:O	2.47	0.46
1:B:191:ASP:O	1:B:194:SER:OG	2.27	0.45
1:B:72:LEU:O	1:B:93:ARG:HB3	2.17	0.45
1:A:561:TYR:CD2	1:C:294:LEU:HD11	2.51	0.45
1:C:97:ALA:HB1	1:C:239:PRO:HG2	1.98	0.45
1:A:470:THR:N	1:A:497:ASN:O	2.50	0.44
1:C:587:HIS:O	1:C:588:HIS:ND1	2.51	0.44
1:C:348:ARG:HA	1:C:351:TRP:CD1	2.52	0.44
1:B:79:CYS:HB3	1:B:80:PRO:HD3	1.99	0.44
1:A:105:LYS:HE3	1:A:230:PHE:CD2	2.53	0.44
1:A:491:ARG:HD3	1:A:544:TYR:CZ	2.52	0.44
1:A:475:CYS:HA	1:A:482:CYS:HA	2.00	0.44
1:C:309:ASP:HA	1:C:447:SER:HA	2.00	0.44
1:C:470:THR:N	1:C:497:ASN:O	2.48	0.44
1:B:509:THR:HB	1:B:561:TYR:HB2	1.99	0.44
1:A:72:LEU:O	1:A:93:ARG:HB3	2.17	0.44
1:A:234:ILE:HB	1:A:286:LEU:HB2	1.99	0.43
1:C:491:ARG:HD3	1:C:544:TYR:CE2	2.53	0.43
1:B:72:LEU:HB2	1:B:94:ASP:HB2	2.01	0.43
1:C:561:TYR:CD2	1:B:294:LEU:HD11	2.53	0.43
1:A:288:LEU:HD23	1:A:306:LEU:HB2	2.00	0.43
1:C:520:ARG:NH2	1:B:111:SER:O	2.52	0.43
1:A:587:HIS:O	1:A:588:HIS:ND1	2.52	0.43
1:B:475:CYS:HA	1:B:482:CYS:HA	2.00	0.43
1:B:587:HIS:O	1:B:588:HIS:ND1	2.52	0.42
1:A:294:LEU:HD11	1:B:561:TYR:CD2	2.54	0.42
1:C:319:ILE:HB	1:C:353:LEU:HD21	2.02	0.42
1:B:348:ARG:HA	1:B:351:TRP:CD1	2.54	0.42
1:C:126:GLU:HB3	1:C:388:GLN:OE1	2.20	0.42
1:C:475:CYS:HA	1:C:482:CYS:HA	2.00	0.42
1:B:491:ARG:HD3	1:B:544:TYR:CZ	2.54	0.42
1:B:550:ALA:HB2	1:B:579:ALA:HB2	2.01	0.42
1:B:554:ARG:HH11	1:B:577:THR:HG21	1.85	0.42
1:A:347:ASN:HB3	1:A:348:ARG:H	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:ALA:HB2	1:C:579:ALA:HB2	2.02	0.41
1:C:464:ARG:O	1:B:37:GLY:N	2.43	0.41
1:B:236:VAL:HG21	1:B:302:LEU:HD23	2.02	0.41
1:C:491:ARG:HD3	1:C:544:TYR:CZ	2.56	0.41
1:B:491:ARG:HD3	1:B:544:TYR:CE2	2.55	0.41
1:C:509:THR:HB	1:C:561:TYR:HB2	2.02	0.41
1:C:25:ILE:HG23	1:B:51:THR:HG21	2.02	0.41
1:C:145:PRO:HG2	1:C:148:GLY:H	1.86	0.41
1:C:347:ASN:HB3	1:C:348:ARG:H	1.45	0.41
1:B:74:SER:HB2	1:B:93:ARG:HE	1.85	0.41
1:A:58:GLN:NE2	1:A:103:LEU:O	2.54	0.40
1:A:126:GLU:HB3	1:A:388:GLN:OE1	2.21	0.40
1:A:307:LEU:HD21	1:B:23:GLU:HG2	2.03	0.40
1:A:309:ASP:OD1	1:A:447:SER:HB3	2.21	0.40
1:B:277:PRO:HA	1:B:278:PRO:HD3	1.97	0.40
1:B:105:LYS:HE3	1:B:230:PHE:CD2	2.56	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	505/565 (89%)	477 (94%)	27 (5%)	1 (0%)	47 71
1	B	504/565 (89%)	476 (94%)	28 (6%)	0	100 100
1	C	504/565 (89%)	476 (94%)	27 (5%)	1 (0%)	47 71
All	All	1513/1695 (89%)	1429 (94%)	82 (5%)	2 (0%)	51 75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	CYS

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Mol	Chain	Res	Type
1	C	71	CYS

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	430/466 (92%)	426 (99%)	4 (1%)	78	91
1	B	430/466 (92%)	427 (99%)	3 (1%)	84	94
1	C	430/466 (92%)	427 (99%)	3 (1%)	84	94
All	All	1290/1398 (92%)	1280 (99%)	10 (1%)	81	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	CYS
1	A	141	TRP
1	A	309	ASP
1	A	347	ASN
1	C	71	CYS
1	C	141	TRP
1	C	347	ASN
1	B	71	CYS
1	B	141	TRP
1	B	347	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)

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	D	1	2,1	14,14,15	0.29	0	17,19,21	0.42	0
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	BMA	D	3	2	11,11,12	0.57	0	15,15,17	0.74	0
3	NAG	E	1	1,3	14,14,15	0.31	0	17,19,21	0.41	0
3	NAG	E	2	3	14,14,15	0.26	0	17,19,21	0.46	0
3	BMA	E	3	3	11,11,12	0.58	0	15,15,17	0.89	0
3	MAN	E	4	3	11,11,12	0.74	0	15,15,17	1.19	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.29	0	17,19,21	0.42	0
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.42	0
3	BMA	F	3	3	11,11,12	0.58	0	15,15,17	0.90	0
3	MAN	F	4	3	11,11,12	0.76	0	15,15,17	1.20	2 (13%)

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

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	4	MAN	C1-O5-C5	3.50	116.93	112.19
3	E	4	MAN	C1-O5-C5	3.45	116.87	112.19
3	E	4	MAN	O2-C2-C3	-2.21	105.72	110.14
3	F	4	MAN	O2-C2-C3	-2.18	105.77	110.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	3	BMA	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6

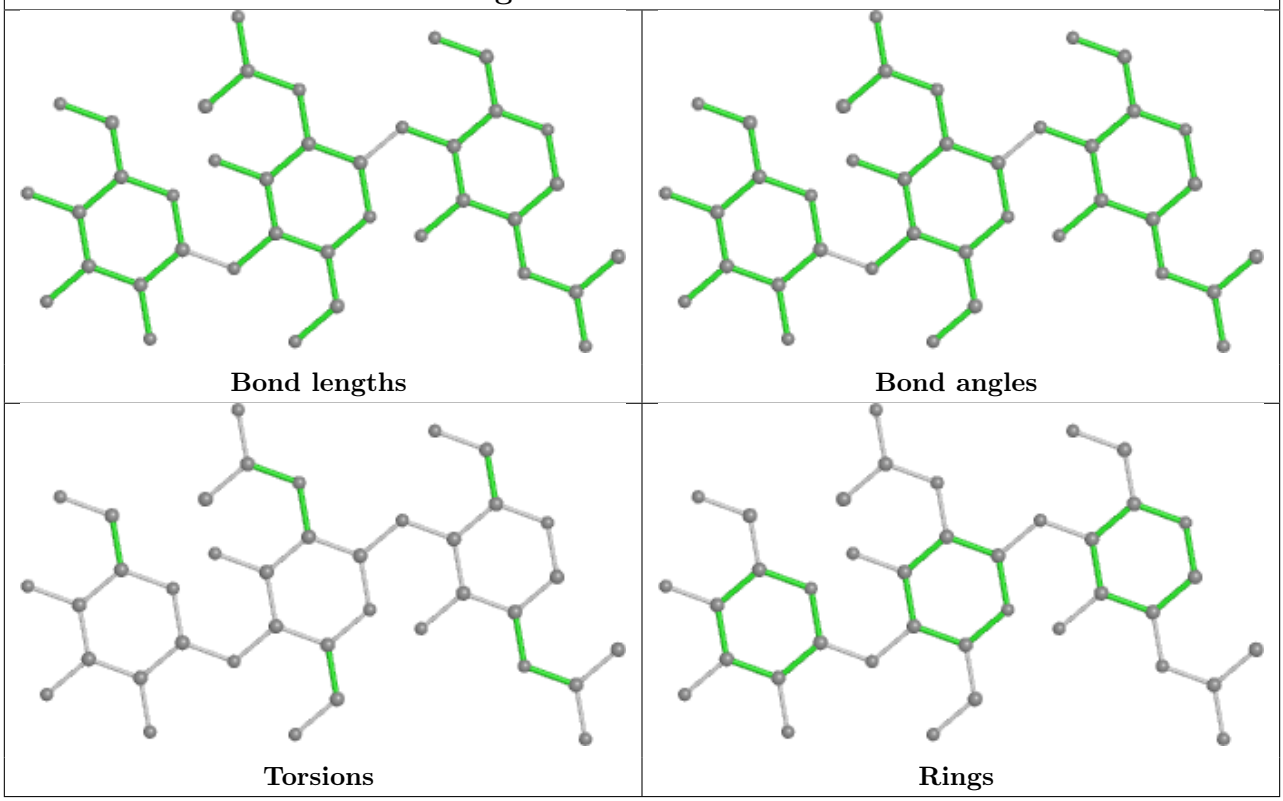
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	4	MAN	C1-C2-C3-C4-C5-O5
3	E	4	MAN	C1-C2-C3-C4-C5-O5

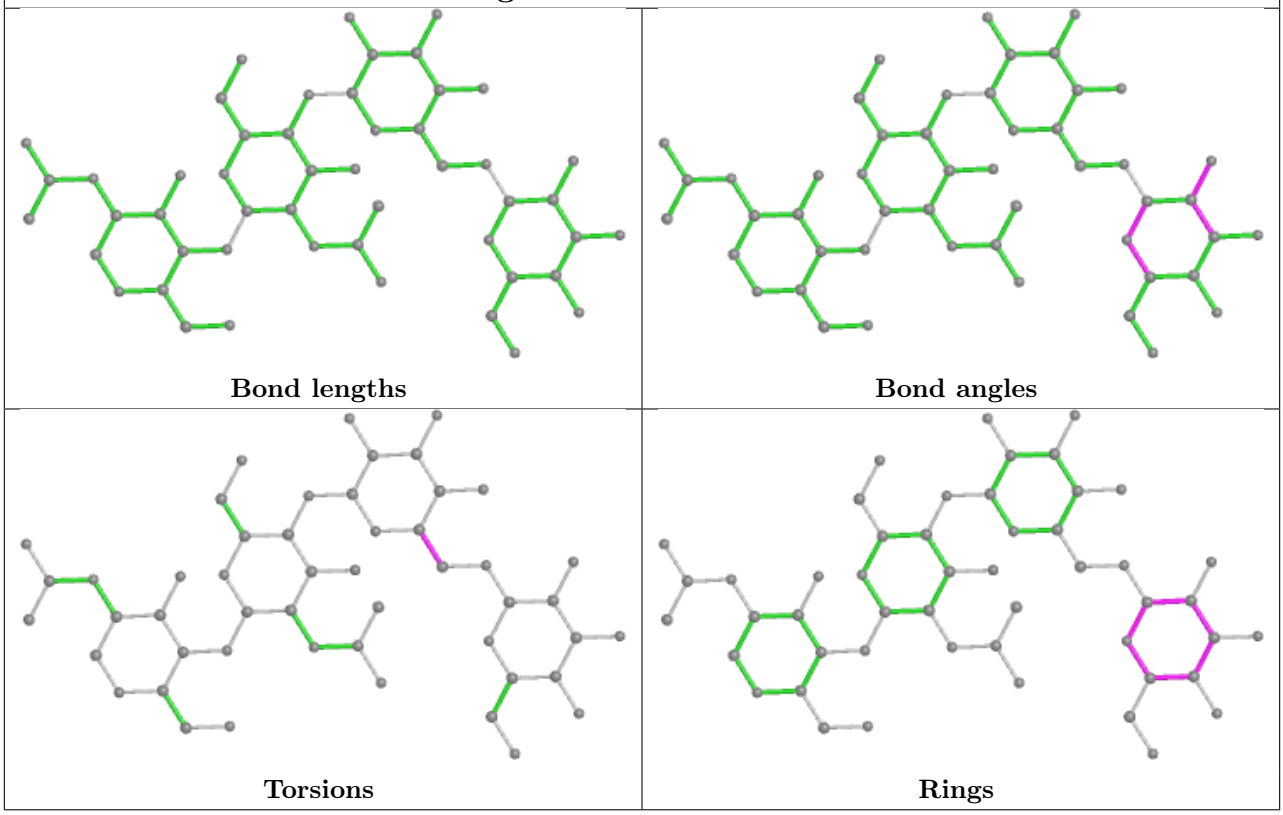
No monomer is involved in short contacts.

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

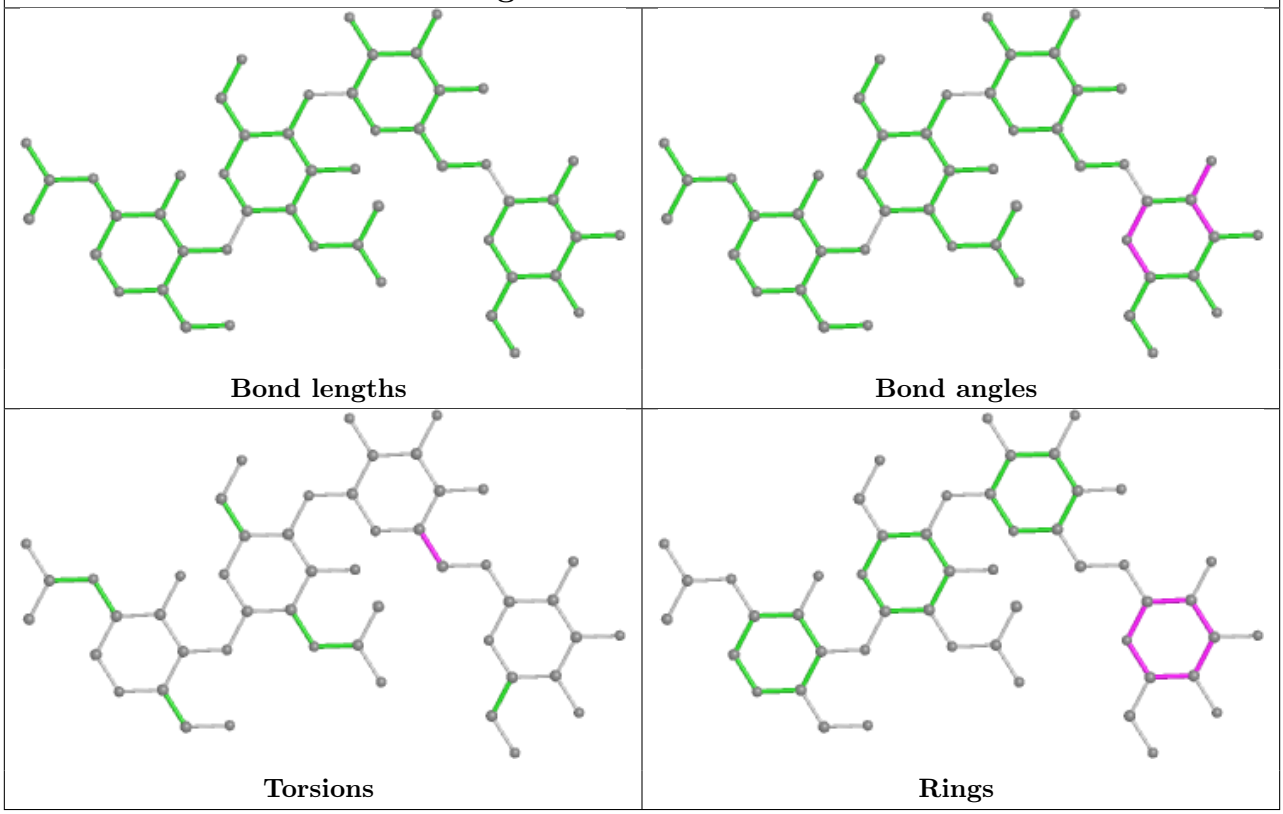
Oligosaccharide Chain D



Oligosaccharide Chain E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	601	1	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	C	605	1	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	C	607	1	14,14,15	0.44	0	17,19,21	0.52	0
4	NAG	A	604	1	14,14,15	0.26	0	17,19,21	0.33	0
4	NAG	B	607	1	14,14,15	0.40	0	17,19,21	0.49	0
4	NAG	C	606	1	14,14,15	0.35	0	17,19,21	0.45	0
4	NAG	A	606	1	14,14,15	0.46	0	17,19,21	0.50	0
4	NAG	B	606	1	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	A	605	1	14,14,15	0.28	0	17,19,21	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	C	605	1	-	2/6/23/26	0/1/1/1
4	NAG	C	607	1	-	3/6/23/26	0/1/1/1
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	NAG	B	607	1	-	2/6/23/26	0/1/1/1
4	NAG	C	606	1	-	1/6/23/26	0/1/1/1
4	NAG	A	606	1	-	2/6/23/26	0/1/1/1
4	NAG	B	606	1	-	0/6/23/26	0/1/1/1
4	NAG	A	605	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	605	NAG	C4-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
4	A	606	NAG	C1-C2-N2-C7
4	A	605	NAG	O5-C5-C6-O6
4	C	605	NAG	O5-C5-C6-O6
4	C	607	NAG	C1-C2-N2-C7
4	B	607	NAG	C1-C2-N2-C7
4	A	604	NAG	C4-C5-C6-O6
4	C	606	NAG	O5-C5-C6-O6
4	B	601	NAG	C4-C5-C6-O6
4	A	605	NAG	C4-C5-C6-O6
4	A	604	NAG	O5-C5-C6-O6
4	C	607	NAG	O5-C5-C6-O6
4	C	607	NAG	C3-C2-N2-C7
4	B	607	NAG	C3-C2-N2-C7
4	A	606	NAG	C3-C2-N2-C7

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	516/565 (91%)	0.07	16 (3%)	49	42	77, 110, 189, 270	0
1	B	515/565 (91%)	0.05	17 (3%)	46	39	78, 110, 189, 291	0
1	C	515/565 (91%)	0.11	20 (3%)	39	32	80, 110, 186, 277	0
All	All	1546/1695 (91%)	0.08	53 (3%)	45	38	77, 110, 189, 291	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	275	LEU	8.6
1	B	274	PHE	8.2
1	A	275	LEU	7.6
1	C	274	PHE	7.2
1	B	275	LEU	6.9
1	B	424	ASP	5.5
1	C	424	ASP	5.3
1	A	200	LEU	5.0
1	A	582	LEU	4.9
1	B	452	SER	4.8
1	C	200	LEU	4.7
1	C	89	THR	4.5
1	C	426	THR	4.3
1	C	454	ALA	4.3
1	C	584	HIS	3.8
1	C	587	HIS	3.6
1	C	427	LEU	3.4
1	B	211	LEU	3.4
1	C	67	PHE	3.3
1	B	587	HIS	3.3
1	C	582	LEU	3.2
1	A	424	ASP	3.1
1	C	455	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	67	PHE	2.9
1	C	425	THR	2.8
1	A	587	HIS	2.6
1	B	582	LEU	2.6
1	A	89	THR	2.6
1	C	125	LEU	2.6
1	A	564	VAL	2.5
1	A	346	THR	2.5
1	B	427	LEU	2.4
1	A	203	ARG	2.4
1	C	586	HIS	2.4
1	B	301	LEU	2.4
1	B	203	ARG	2.3
1	A	426	THR	2.3
1	A	173	TRP	2.3
1	B	200	LEU	2.3
1	A	30	LEU	2.3
1	A	427	LEU	2.2
1	B	564	VAL	2.2
1	B	584	HIS	2.2
1	B	74	SER	2.1
1	A	150	PHE	2.1
1	C	494	ILE	2.1
1	A	65	LEU	2.1
1	B	537	LEU	2.1
1	B	281	SER	2.1
1	C	236	VAL	2.0
1	C	177	PHE	2.0
1	C	203	ARG	2.0
1	B	377	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)

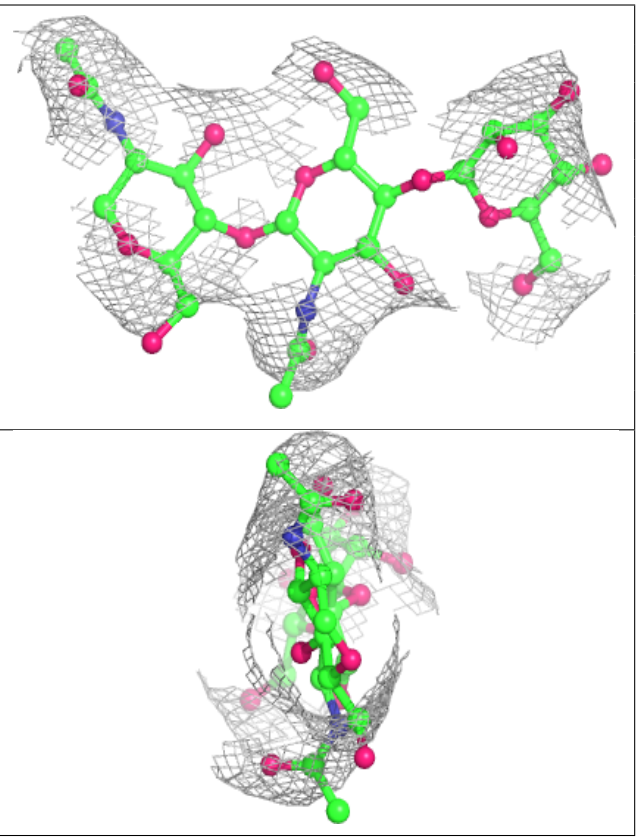
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	F	4	11/12	0.81	0.22	221,227,230,232	0
2	BMA	D	3	11/12	0.87	0.14	175,186,198,199	0
3	MAN	E	4	11/12	0.90	0.23	237,243,246,246	0
3	NAG	F	2	14/15	0.91	0.14	132,161,171,186	0
2	NAG	D	2	14/15	0.91	0.17	132,160,165,173	0
3	BMA	F	3	11/12	0.92	0.10	199,206,216,219	0
3	NAG	E	2	14/15	0.92	0.15	136,164,174,189	0
3	NAG	F	1	14/15	0.93	0.15	84,117,150,151	0
3	BMA	E	3	11/12	0.93	0.11	204,213,222,230	0
2	NAG	D	1	14/15	0.94	0.13	90,122,150,152	0
3	NAG	E	1	14/15	0.97	0.11	79,113,154,158	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.

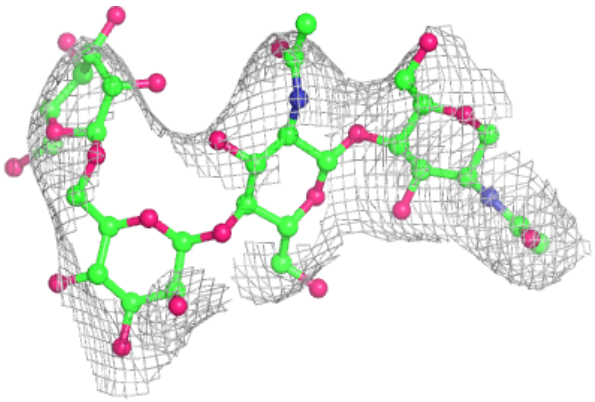
Electron density around Chain D:

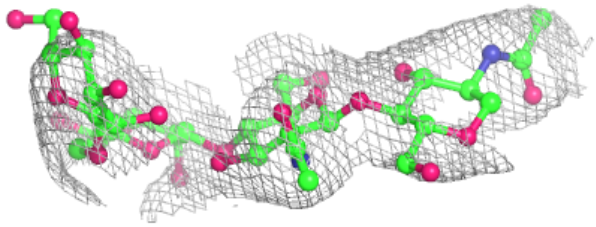
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

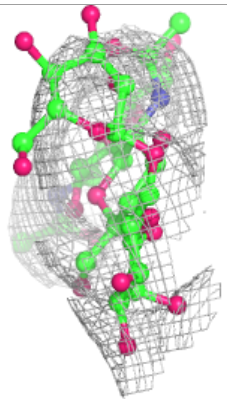


Electron density around Chain E:

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

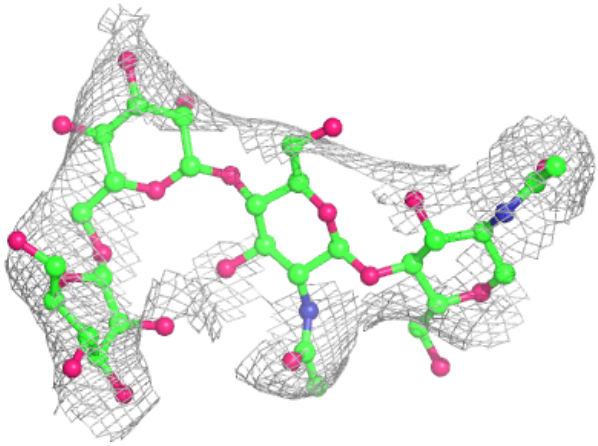


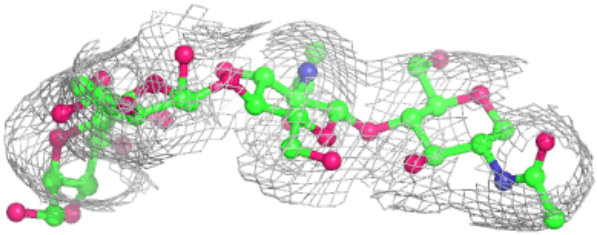


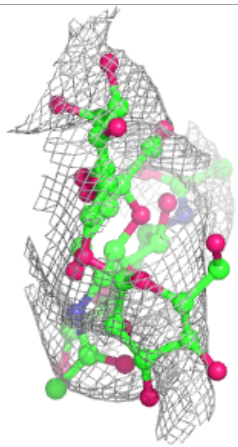


Electron density around Chain F:

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







6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	604	14/15	0.56	0.26	129,157,178,181	0
4	NAG	A	605	14/15	0.70	0.38	150,177,207,208	0
4	NAG	C	606	14/15	0.75	0.43	139,181,195,195	0
4	NAG	C	605	14/15	0.80	0.13	127,151,162,164	0
4	NAG	C	607	14/15	0.81	0.16	113,131,150,153	0
4	NAG	B	601	14/15	0.82	0.30	136,164,190,193	0
4	NAG	B	607	14/15	0.82	0.16	109,126,140,141	0
4	NAG	B	606	14/15	0.85	0.20	142,160,172,174	0
4	NAG	A	606	14/15	0.87	0.17	106,128,147,148	0

6.5 Other polymers (i)

There are no such residues in this entry.