Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:04 PM BST

PDB ID	:	2WR2
Title	:	structure of influenza H2 avian hemagglutinin with avian receptor
Authors	:	Liu, J.; Stevens, D.J.; Haire, L.F.; Walker, P.A.; Coombs, P.J.; Russell, R.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on	:	2009-08-29
Resolution	:	2.40 Å(reported)

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

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

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

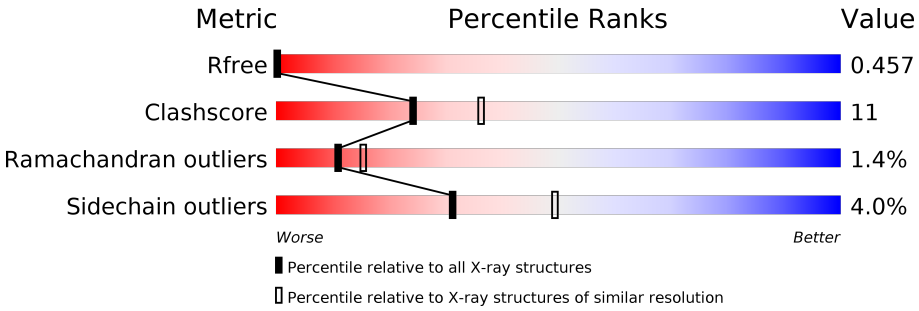
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	509	77% 18%
1	B	509	72% 22%
1	C	509	76% 17% 5%
2	D	3	100%
2	E	3	100%

2 Entry composition

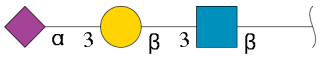
There are 4 unique types of molecules in this entry. The entry contains 12274 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEMAGGLUTININ.

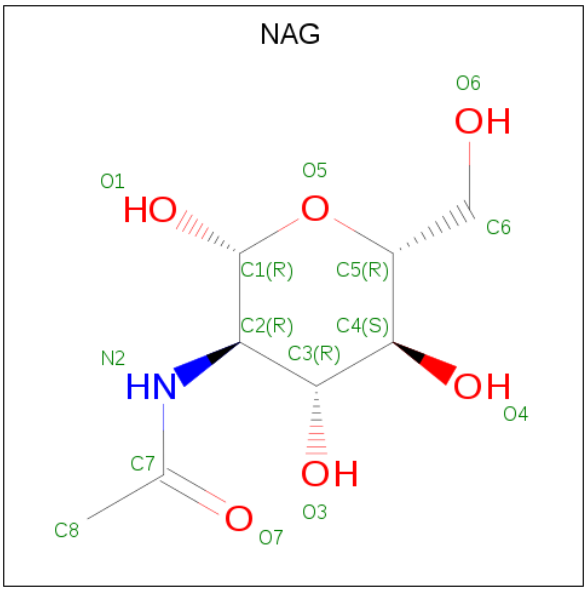
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	4	0	0
			3882	2436	671	753	22			
1	B	490	Total	C	N	O	S	0	1	0
			3887	2438	672	755	22			
1	C	485	Total	C	N	O	S	0	0	0
			3844	2413	664	745	22			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	E	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 13 8 1 4	0	0
3	C	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is water.

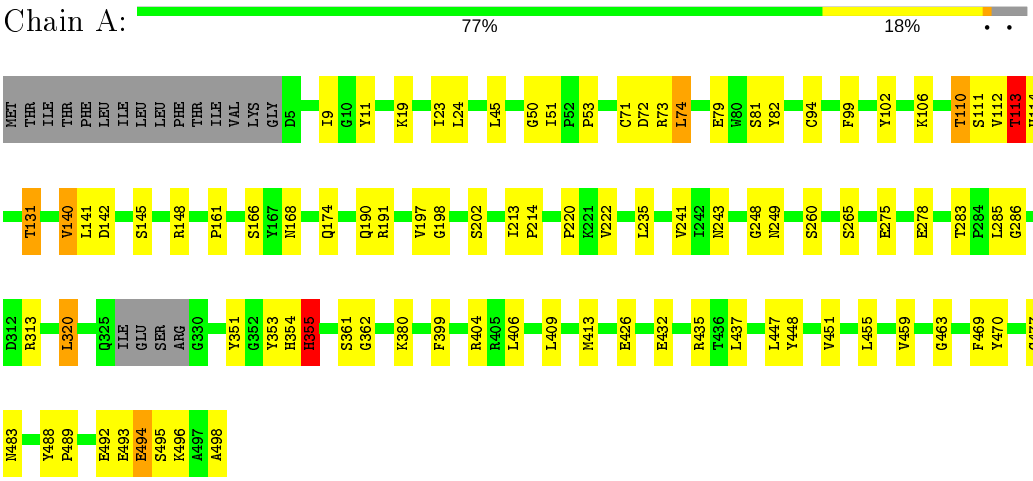
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	185	Total O 185 185	0	0
4	B	169	Total O 169 169	0	0
4	C	174	Total O 174 174	0	0

3 Residue-property plots (i)

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

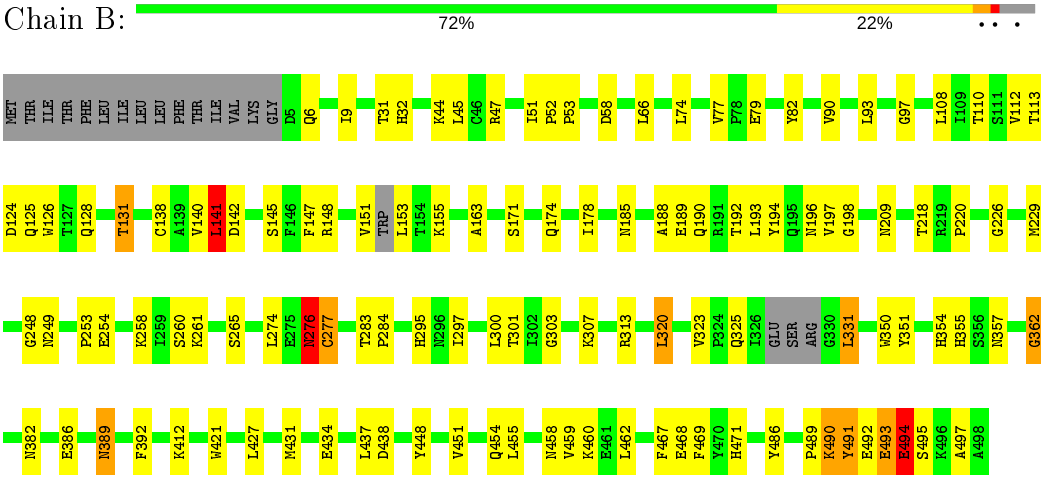
- Molecule 1: HEMAGGLUTININ

Chain A:



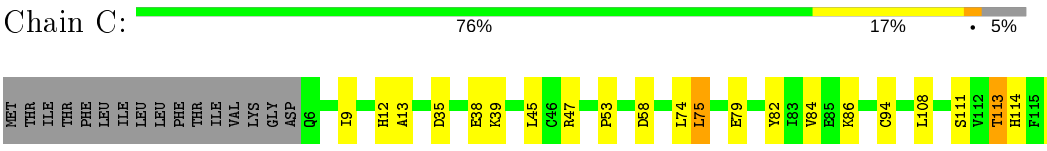
- Molecule 1: HEMAGGLUTININ

Chain B:



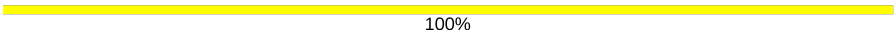
- Molecule 1: HEMAGGLUTININ

Chain C:



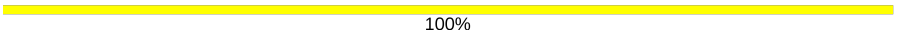
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.88Å 142.72Å 199.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.40 29.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.94-2.40) 99.9 (29.94-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.210 , 0.248 0.446 , 0.457	Depositor DCC
R_{free} test set	3956 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	50.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	12274	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.33	0/3968	0.51	0/5372
1	B	0.33	0/3970	0.53	0/5372
1	C	0.33	0/3927	0.51	0/5313
All	All	0.33	0/11865	0.52	0/16057

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3882	0	3742	85	2
1	B	3887	0	3756	109	2
1	C	3844	0	3718	67	0
2	D	46	0	40	2	0
2	E	46	0	40	0	0
3	A	27	0	25	7	0
3	C	14	0	13	3	0
4	A	185	0	0	5	0
4	B	169	0	0	9	0
4	C	174	0	0	2	0
All	All	12274	0	11334	254	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLN:NE2	4:B:2109:HOH:O	1.62	1.27
1:A:283:THR:HG22	1:A:285:LEU:H	1.18	1.05
1:A:148:ARG:HG2	1:A:148:ARG:HH11	1.32	0.94
1:B:325:GLN:HB3	4:B:2110:HOH:O	1.65	0.93
1:A:361:SER:HB3	1:A:362:GLY:HA3	1.49	0.92
1:C:114:HIS:H	1:C:260:SER:HB2	1.35	0.91
1:B:140:VAL:O	1:B:141:LEU:HB2	1.72	0.89
1:B:459:VAL:HG22	1:B:469:PHE:HA	1.55	0.89
1:B:276:ASN:HA	1:B:277:CYS:O	1.73	0.89
1:A:110:THR:CG2	1:A:265:SER:H	1.86	0.88
1:B:459:VAL:HG11	1:B:467:PHE:HB3	1.54	0.88
1:C:168:ASN:HD21	3:C:1500:NAG:C1	1.89	0.84
1:B:47:ARG:HE	1:B:276:ASN:HB2	1.42	0.84
1:C:141:LEU:N	1:C:142:ASP:HA	1.95	0.82
1:A:110:THR:HG21	1:A:265:SER:H	1.44	0.82
1:B:141:LEU:N	1:B:142:ASP:HA	1.97	0.79
1:A:114:HIS:H	1:A:260:SER:HB2	1.45	0.79
1:B:110:THR:CG2	1:B:265:SER:H	1.95	0.78
1:B:32:HIS:CD2	4:B:2124:HOH:O	2.37	0.78
1:C:114:HIS:N	1:C:260:SER:HB2	1.98	0.77
1:A:479:ASN:HB3	3:A:1499:NAG:H81	1.64	0.77
1:A:168:ASN:HD21	3:A:1500:NAG:C5	1.97	0.77
1:B:113:THR:HB	1:B:114:HIS:HB3	1.66	0.77
1:A:190:GLN:HE22	1:A:249:ASN:HD21	1.33	0.77
1:A:174:GLN:HE21	1:A:235:LEU:HD13	1.51	0.76
1:B:455:LEU:HD13	1:B:459:VAL:HG21	1.66	0.75
1:B:458:ASN:OD1	1:B:494:GLU:HG2	1.86	0.74
1:A:493:GLU:O	1:A:494:GLU:HB3	1.88	0.73
1:A:174:GLN:NE2	1:A:235:LEU:HD13	2.04	0.73
1:C:190:GLN:HE22	1:C:249:ASN:HD21	1.36	0.73
1:A:283:THR:HG22	1:A:285:LEU:N	1.99	0.73
1:A:320:LEU:H	1:A:320:LEU:HD23	1.53	0.72
1:A:166:SER:HB3	1:A:243:ASN:ND2	2.05	0.72
1:A:283:THR:HB	1:A:286:GLY:O	1.89	0.72
1:B:354:HIS:HA	1:B:362:GLY:O	1.90	0.72
1:B:140:VAL:HG12	1:B:141:LEU:HD23	1.73	0.70
1:C:74:LEU:O	1:C:75:LEU:HB2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:THR:HG23	1:B:265:SER:H	1.57	0.69
1:A:313:ARG:HA	4:A:2015:HOH:O	1.93	0.69
1:A:380:LYS:HE3	1:A:432:GLU:OE1	1.93	0.68
1:C:320:LEU:HD23	1:C:320:LEU:H	1.58	0.68
1:A:493:GLU:O	1:A:494:GLU:CB	2.43	0.67
1:A:168:ASN:ND2	3:A:1500:NAG:C1	2.58	0.66
1:B:490:LYS:O	1:B:490:LYS:HG2	1.93	0.66
1:B:188:ALA:O	1:B:192:THR:HG22	1.95	0.66
1:B:295:HIS:HD2	1:B:297:ILE:H	1.44	0.66
1:C:354:HIS:HA	1:C:362:GLY:O	1.94	0.66
1:A:114:HIS:N	1:A:260:SER:HB2	2.09	0.65
1:C:275:GLU:O	1:C:276:ASN:HB3	1.96	0.65
1:B:459:VAL:HG13	1:B:468:GLU:O	1.96	0.65
1:C:79:GLU:HG3	1:C:113:THR:HB	1.78	0.64
1:C:357:ASN:HB3	1:C:359:GLN:H	1.62	0.64
1:C:262:ARG:HG3	1:C:263:GLY:H	1.63	0.64
1:C:168:ASN:ND2	3:C:1500:NAG:C1	2.59	0.63
1:A:168:ASN:HD21	3:A:1500:NAG:C1	2.12	0.63
1:C:459:VAL:HG23	1:C:469:PHE:HA	1.80	0.62
1:A:283:THR:CG2	1:A:285:LEU:H	2.05	0.62
1:B:350:TRP:NE1	4:B:2124:HOH:O	2.27	0.62
1:B:113:THR:HB	1:B:114:HIS:CB	2.29	0.61
1:A:140:VAL:HG23	1:A:145:SER:HB2	1.81	0.61
1:A:455:LEU:HD23	1:A:459:VAL:HG21	1.81	0.61
1:A:50:GLY:HA2	1:A:278:GLU:OE2	2.00	0.61
1:C:111:SER:HB2	1:C:265:SER:HB2	1.83	0.61
1:A:191:ARG:HD2	4:A:2085:HOH:O	2.00	0.61
1:A:248:GLY:C	1:A:249:ASN:HD22	2.04	0.60
1:A:470:TYR:HB3	1:A:495:SER:HA	1.83	0.60
1:A:353:TYR:OH	1:A:447:LEU:HD11	2.01	0.60
1:B:320:LEU:HD23	1:B:320:LEU:H	1.66	0.60
1:A:435:ARG:NH1	1:C:435:ARG:NH1	2.49	0.60
1:C:459:VAL:HG21	1:C:467:PHE:HB3	1.84	0.59
1:B:190:GLN:HE22	1:B:249:ASN:HD21	1.49	0.59
1:B:454:GLN:NE2	1:B:486:TYR:H	2.00	0.58
1:A:72:ASP:OD1	1:A:73:ARG:N	2.36	0.58
1:B:123:ARG:HB2	1:B:254:GLU:OE2	2.03	0.58
1:B:171:SER:HB2	1:B:258:LYS:HD2	1.85	0.58
1:B:492:GLU:HA	1:B:493:GLU:C	2.23	0.58
1:B:325:GLN:CB	4:B:2110:HOH:O	2.38	0.57
1:C:58:ASP:HB3	1:C:86:LYS:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:THR:HG23	1:C:113:THR:O	2.03	0.57
1:B:110:THR:HG21	1:B:265:SER:H	1.68	0.57
1:A:111:SER:HB2	1:A:265:SER:HB2	1.85	0.57
1:A:148:ARG:CG	1:A:148:ARG:HH11	2.10	0.56
1:C:488:TYR:HB3	1:C:489:PRO:HD3	1.87	0.56
1:C:53:PRO:HG3	1:C:82:TYR:CZ	2.41	0.56
1:B:112:VAL:HG11	1:B:115:PHE:HB2	1.86	0.56
1:B:493:GLU:O	1:B:494:GLU:HB2	2.05	0.56
1:A:298:HIS:ND1	1:A:299:PRO:HD2	2.20	0.56
1:A:9:ILE:HD11	1:A:451:VAL:HG21	1.88	0.56
1:B:44:LYS:HD3	1:B:277:CYS:SG	2.46	0.56
1:B:140:VAL:C	1:B:142:ASP:HA	2.25	0.56
1:C:179:TRP:CE2	1:C:203:VAL:HG21	2.41	0.56
1:A:11:TYR:HB2	1:A:320:LEU:HD11	1.87	0.55
1:C:283:THR:HG22	1:C:301:THR:HG22	1.87	0.55
1:B:492:GLU:OE2	1:B:495:SER:N	2.39	0.55
1:C:47:ARG:O	1:C:279:THR:HG22	2.06	0.55
1:B:193:LEU:HD21	2:D:3:SIA:O10	2.06	0.55
1:C:493:GLU:C	1:C:494:GLU:HG3	2.27	0.55
1:C:114:HIS:H	1:C:260:SER:CB	2.14	0.55
1:C:45:LEU:HD21	1:C:84:VAL:HG21	1.88	0.54
1:A:72:ASP:OD2	1:A:148:ARG:HD2	2.07	0.54
1:B:283:THR:HG22	1:B:301:THR:HG22	1.89	0.54
1:B:382:ASN:O	1:B:386:GLU:HG2	2.07	0.54
1:B:9:ILE:HD11	1:B:451:VAL:HG21	1.89	0.54
1:A:148:ARG:NH1	1:A:148:ARG:HG2	2.11	0.54
1:A:110:THR:HG23	1:A:265:SER:HB3	1.90	0.54
1:B:138:CYS:O	1:B:145:SER:HB3	2.08	0.53
1:C:114:HIS:CE1	1:C:116:GLU:HB2	2.43	0.53
1:B:124:ASP:OD1	1:B:125:GLN:HG3	2.08	0.53
1:C:424:ASN:ND2	4:C:2149:HOH:O	2.42	0.53
1:B:492:GLU:CD	1:B:495:SER:H	2.12	0.52
1:A:110:THR:CG2	1:A:265:SER:N	2.66	0.52
1:B:53:PRO:HG3	1:B:82:TYR:CZ	2.45	0.52
1:B:355:HIS:CE1	1:B:362:GLY:HA2	2.44	0.52
1:C:357:ASN:OD1	1:C:473:CYS:O	2.28	0.52
1:B:490:LYS:HB2	4:B:2167:HOH:O	2.09	0.52
1:C:262:ARG:HG3	1:C:263:GLY:N	2.24	0.52
1:A:495:SER:HB2	4:A:2177:HOH:O	2.10	0.52
1:C:304:GLU:HB3	1:C:390:THR:HG22	1.90	0.51
1:B:490:LYS:C	1:B:492:GLU:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:SER:CB	1:A:362:GLY:HA3	2.29	0.51
1:B:491:TYR:O	1:B:494:GLU:HB2	2.09	0.51
1:A:19:LYS:O	1:A:313:ARG:NH2	2.44	0.51
1:B:126:TRP:HZ3	1:B:163:ALA:HB1	1.76	0.51
1:A:113:THR:O	1:A:113:THR:HG23	2.10	0.51
1:B:490:LYS:C	1:B:492:GLU:N	2.63	0.51
1:A:355:HIS:CE1	1:A:361:SER:HB2	2.46	0.50
1:B:492:GLU:OE1	1:B:492:GLU:HA	2.11	0.50
1:C:143:ASN:N	1:C:143:ASN:HD22	2.10	0.50
1:C:492:GLU:O	1:C:492:GLU:HG2	2.11	0.50
1:C:262:ARG:NH1	4:C:2029:HOH:O	2.44	0.50
1:A:213:ILE:HD12	1:A:214:PRO:O	2.12	0.50
1:A:141:LEU:O	1:A:141:LEU:HG	2.12	0.49
1:B:53:PRO:HD2	1:B:274:LEU:HD22	1.94	0.49
1:B:491:TYR:O	1:B:494:GLU:CB	2.61	0.49
1:B:357:ASN:HB2	4:B:2126:HOH:O	2.12	0.49
1:B:495:SER:C	1:B:497:ALA:N	2.65	0.49
1:A:140:VAL:HG12	1:A:141:LEU:HD22	1.93	0.49
1:A:413:MET:HE1	1:B:412:LYS:HE3	1.93	0.49
1:A:479:ASN:O	1:A:483:ASN:HB2	2.13	0.49
1:B:31:THR:C	1:B:32:HIS:CD2	2.86	0.49
1:B:126:TRP:CZ3	1:B:163:ALA:HB1	2.48	0.49
1:B:113:THR:HG22	1:B:114:HIS:HB2	1.96	0.48
1:C:248:GLY:O	1:C:249:ASN:HB2	2.13	0.48
1:B:123:ARG:HG2	1:B:131:THR:HG21	1.94	0.48
1:C:160:TYR:CZ	1:C:248:GLY:HA2	2.48	0.48
1:C:168:ASN:HD21	3:C:1500:NAG:C2	2.26	0.48
1:A:361:SER:HB3	1:A:362:GLY:CA	2.33	0.48
1:C:113:THR:C	1:C:260:SER:HB2	2.34	0.48
1:A:51:ILE:HB	1:A:81:SER:HB3	1.96	0.47
1:B:31:THR:OG1	1:B:32:HIS:HD2	1.98	0.47
1:A:354:HIS:O	1:A:355:HIS:CD2	2.67	0.47
1:B:471:HIS:HD2	1:B:494:GLU:OE2	1.98	0.47
1:A:102:TYR:CZ	1:A:106:LYS:HD3	2.50	0.47
1:B:331:LEU:HD22	1:B:438:ASP:OD2	2.14	0.47
1:B:459:VAL:CG1	1:B:460:LYS:N	2.77	0.47
1:B:218:THR:HA	4:B:2072:HOH:O	2.14	0.46
1:A:248:GLY:O	1:A:249:ASN:HB2	2.16	0.46
1:A:399:PHE:CE1	1:A:406:LEU:HG	2.51	0.46
1:B:189:GLU:HA	1:B:192:THR:HG22	1.97	0.46
1:B:459:VAL:HG12	1:B:460:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ALA:HB2	1:C:342:GLY:HA3	1.96	0.46
2:D:3:SIA:H6	2:D:3:SIA:O1A	2.16	0.46
1:B:491:TYR:C	1:B:494:GLU:HB2	2.36	0.46
1:C:480:SER:HA	1:C:483:ASN:OD1	2.16	0.46
1:B:155:LYS:HE2	1:B:192:THR:O	2.16	0.45
1:C:9:ILE:HG13	1:C:448:TYR:HA	1.98	0.45
3:A:1500:NAG:C1	3:A:1500:NAG:C5	2.95	0.45
1:A:220:PRO:HD3	1:C:243:ASN:HD22	1.81	0.45
1:C:12:HIS:HD2	1:C:346:MET:O	1.99	0.45
1:C:455:LEU:HD23	1:C:459:VAL:HG11	1.99	0.45
1:B:51:ILE:HG23	1:B:79:GLU:HG2	1.99	0.45
1:B:276:ASN:HA	1:B:277:CYS:C	2.35	0.45
1:A:9:ILE:HG13	1:A:448:TYR:HA	1.98	0.45
1:B:114:HIS:HB3	1:B:260:SER:HB2	1.98	0.45
1:A:498:ALA:C	4:A:2177:HOH:O	2.55	0.44
1:B:459:VAL:CG1	1:B:467:PHE:HB3	2.38	0.44
1:B:197:VAL:HG22	1:B:198:GLY:H	1.82	0.44
1:B:248:GLY:O	1:B:249:ASN:HB2	2.17	0.44
1:B:178:ILE:O	1:B:253:PRO:HG3	2.18	0.44
1:B:174:GLN:OE1	1:B:235:LEU:HD13	2.18	0.44
1:C:140:VAL:C	1:C:142:ASP:HA	2.38	0.44
1:C:182:HIS:CD2	1:C:194:TYR:OH	2.70	0.44
1:A:128:GLN:HB3	1:A:161:PRO:HG2	1.99	0.44
1:B:108:LEU:HD11	1:B:261:LYS:HE2	1.99	0.44
1:C:390:THR:O	1:C:390:THR:HG22	2.17	0.44
1:B:131:THR:HG23	1:B:131:THR:O	2.18	0.44
1:C:38:GLU:HB2	1:C:292:LEU:HD12	2.00	0.44
1:A:99:PHE:HB3	1:A:102:TYR:HB2	1.99	0.44
1:B:303:GLY:HA2	1:B:392:PHE:CE1	2.53	0.44
1:B:295:HIS:CD2	1:B:297:ILE:H	2.32	0.43
1:A:123:ARG:HG2	1:A:131:THR:HG21	2.00	0.43
1:A:220:PRO:HD3	1:C:243:ASN:ND2	2.34	0.43
1:B:113:THR:HB	1:B:260:SER:HB2	2.00	0.43
1:B:66:LEU:O	1:B:147:PHE:HB3	2.18	0.43
1:B:151:VAL:HG12	1:B:153:LEU:HD12	1.99	0.43
1:B:389:ASN:HD22	1:B:389:ASN:HA	1.68	0.43
1:A:71:CYS:O	1:A:74:LEU:HB2	2.18	0.43
1:B:112:VAL:CG1	1:B:115:PHE:HB2	2.48	0.43
1:B:493:GLU:O	1:B:494:GLU:CB	2.66	0.43
1:B:9:ILE:HG13	1:B:448:TYR:HA	2.01	0.43
1:C:9:ILE:HD11	1:C:451:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:SER:HA	1:A:483:ASN:HB3	2.01	0.43
1:A:74:LEU:O	1:A:74:LEU:HD13	2.18	0.43
1:B:458:ASN:OD1	1:B:491:TYR:HA	2.19	0.43
1:C:494:GLU:OE2	1:C:495:SER:N	2.42	0.43
1:A:23:ILE:HG23	1:A:24:LEU:HG	2.01	0.43
1:B:185[B]:ASN:OD1	1:B:226:GLY:C	2.56	0.43
1:B:194:TYR:O	1:B:196:ASN:N	2.47	0.43
1:A:112:VAL:C	1:A:113:THR:HG22	2.39	0.43
1:B:209:ASN:OD1	1:C:219:ARG:NH1	2.50	0.42
1:B:307:LYS:HA	1:B:307:LYS:HD3	1.90	0.42
1:C:320:LEU:HD23	1:C:320:LEU:N	2.30	0.42
1:A:197:VAL:HG12	1:A:198:GLY:N	2.33	0.42
1:A:110:THR:HG23	1:A:265:SER:H	1.77	0.42
1:B:189:GLU:HA	1:B:192:THR:CG2	2.48	0.42
1:A:492:GLU:O	4:A:2177:HOH:O	2.22	0.42
1:B:320:LEU:N	1:B:320:LEU:HD23	2.33	0.42
1:A:140:VAL:HG23	1:A:145:SER:CB	2.48	0.42
1:C:108:LEU:O	1:C:261:LYS:HD2	2.18	0.42
1:B:471:HIS:CD2	1:B:494:GLU:OE2	2.72	0.42
1:C:178:ILE:O	1:C:253:PRO:HG3	2.19	0.42
1:C:399:PHE:CE1	1:C:406:LEU:HG	2.55	0.42
1:A:311:SER:HB3	1:A:426:GLU:OE1	2.20	0.42
1:A:463:GLY:HA2	1:C:453:MET:CE	2.49	0.42
1:C:293:PRO:HG2	1:C:294:PHE:CD2	2.55	0.42
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.55	0.42
1:B:307:LYS:HE2	1:B:421:TRP:NE1	2.35	0.42
1:B:459:VAL:HG13	1:B:468:GLU:C	2.39	0.41
1:B:458:ASN:HA	1:B:494:GLU:CG	2.49	0.41
1:A:409:LEU:HD21	1:C:409:LEU:HD22	2.02	0.41
1:A:488:TYR:N	1:A:489:PRO:CD	2.83	0.41
1:C:388:MET:HE2	1:C:388:MET:HB2	1.85	0.41
1:B:367:LYS:HA	1:B:367:LYS:HD3	1.64	0.41
1:A:459:VAL:HG12	1:A:469:PHE:HA	2.02	0.41
1:B:52:PRO:HA	1:B:53:PRO:HD3	1.86	0.41
1:C:298:HIS:ND1	1:C:299:PRO:HD2	2.35	0.41
1:A:141:LEU:O	1:A:141:LEU:CG	2.68	0.41
1:B:163:ALA:O	1:B:245:GLU:HA	2.21	0.41
1:A:79:GLU:HG3	1:A:113:THR:HA	2.02	0.41
1:A:241:VAL:HG23	3:A:1500:NAG:H61	2.03	0.41
1:B:113:THR:CB	1:B:114:HIS:CB	2.98	0.41
1:B:323:VAL:HG12	4:B:2108:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:LEU:O	1:B:431:MET:HG3	2.20	0.41
1:B:97:GLY:HA3	1:B:229:MET:O	2.21	0.41
1:C:143:ASN:N	1:C:143:ASN:ND2	2.69	0.41
1:C:382:ASN:O	1:C:386:GLU:HB2	2.21	0.41
1:A:222:VAL:HG22	1:C:206:SER:HB2	2.03	0.41
1:B:495:SER:C	1:B:497:ALA:H	2.24	0.40
1:C:35:ASP:OD2	1:C:39:LYS:NZ	2.54	0.40
1:A:241:VAL:HB	1:B:220:PRO:HG3	2.03	0.40
1:C:372:LYS:HA	1:C:372:LYS:HD2	1.91	0.40
1:A:168:ASN:ND2	3:A:1500:NAG:C5	2.75	0.40
1:B:284:PRO:HD3	1:B:300:LEU:O	2.21	0.40
1:B:6:GLN:HB2	1:B:467:PHE:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:CD2	1:B:128:GLN:OE1[1_655]	1.82	0.38
1:A:141:LEU:CD1	1:B:128:GLN:OE1[1_655]	2.03	0.17

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	486/509 (96%)	459 (94%)	21 (4%)	6 (1%)	13 19
1	B	485/509 (95%)	456 (94%)	20 (4%)	9 (2%)	8 10
1	C	479/509 (94%)	457 (95%)	16 (3%)	6 (1%)	12 17
All	All	1450/1527 (95%)	1372 (95%)	57 (4%)	21 (1%)	11 15

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	A	494	GLU
1	B	277	CYS
1	B	490	LYS
1	B	494	GLU
1	C	113	THR
1	B	114	HIS
1	B	141	LEU
1	B	276	ASN
1	C	276	ASN
1	B	362	GLY
1	C	362	GLY
1	C	492	GLU
1	C	494	GLU
1	A	496	LYS
1	B	489	PRO
1	C	75	LEU
1	A	140	VAL
1	B	313	ARG
1	A	74	LEU
1	A	355	HIS

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	427/447 (96%)	413 (97%)	14 (3%)	38 57
1	B	429/447 (96%)	408 (95%)	21 (5%)	25 40
1	C	425/447 (95%)	409 (96%)	16 (4%)	33 51
All	All	1281/1341 (96%)	1230 (96%)	51 (4%)	31 49

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	94	CYS

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Mol	Chain	Res	Type
1	A	110	THR
1	A	113	THR
1	A	131	THR
1	A	142	ASP
1	A	202	SER
1	A	275	GLU
1	A	320	LEU
1	A	351	TYR
1	A	355	HIS
1	A	404	ARG
1	A	437	LEU
1	A	477	CYS
1	B	45	LEU
1	B	58	ASP
1	B	74	LEU
1	B	77	VAL
1	B	90	VAL
1	B	93	LEU
1	B	131	THR
1	B	141	LEU
1	B	148	ARG
1	B	276	ASN
1	B	320	LEU
1	B	331	LEU
1	B	351	TYR
1	B	377	ILE
1	B	389	ASN
1	B	434	GLU
1	B	437	LEU
1	B	462	LEU
1	B	491	TYR
1	B	493	GLU
1	B	494	GLU
1	C	94	CYS
1	C	136	ARG
1	C	186	ASP
1	C	196	ASN
1	C	208	LEU
1	C	264	SER
1	C	283	THR
1	C	320	LEU
1	C	347	VAL

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Mol	Chain	Res	Type
1	C	356	SER
1	C	389	ASN
1	C	455	LEU
1	C	459	VAL
1	C	462	LEU
1	C	493	GLU
1	C	494	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	114	HIS
1	A	168	ASN
1	A	174	GLN
1	A	182	HIS
1	A	243	ASN
1	A	249	ASN
1	A	295	HIS
1	A	483	ASN
1	B	27	ASN
1	B	32	HIS
1	B	114	HIS
1	B	182	HIS
1	B	249	ASN
1	B	295	HIS
1	B	382	ASN
1	B	391	GLN
1	B	408	ASN
1	B	454	GLN
1	C	12	HIS
1	C	15	ASN
1	C	32	HIS
1	C	91	ASN
1	C	100	ASN
1	C	114	HIS
1	C	125	GLN
1	C	143	ASN
1	C	168	ASN
1	C	174	GLN
1	C	182	HIS
1	C	243	ASN

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Mol	Chain	Res	Type
1	C	249	ASN
1	C	389	ASN
1	C	408	ASN
1	C	454	GLN
1	C	479	ASN

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)

6 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	15,15,15	0.91	1 (6%)	21,21,21	0.73	0
2	GAL	D	2	2	11,11,12	0.75	0	15,15,17	0.73	1 (6%)
2	SIA	D	3	2	17,20,21	0.67	0	21,28,31	0.75	0
2	NAG	E	1	2	15,15,15	0.89	0	21,21,21	1.10	2 (9%)
2	GAL	E	2	2	11,11,12	0.61	0	15,15,17	1.11	1 (6%)
2	SIA	E	3	2	17,20,21	0.85	1 (5%)	21,28,31	0.88	1 (4%)

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	-	2/6/26/26	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	SIA	D	3	2	-	0/14/34/38	0/1/1/1
2	NAG	E	1	2	-	1/6/26/26	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	SIA	E	3	2	-	0/14/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	SIA	C4-C5	2.29	1.55	1.53
2	D	1	NAG	C1-C2	2.04	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	GAL	C1-C2-C3	3.56	114.05	109.67
2	E	1	NAG	C3-C4-C5	2.76	115.16	110.24
2	E	3	SIA	C6-O6-C2	2.35	116.38	111.34
2	D	2	GAL	C1-C2-C3	2.12	112.27	109.67
2	E	1	NAG	O5-C5-C4	2.05	113.41	109.69

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	GAL	C4-C5-C6-O6
2	D	2	GAL	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

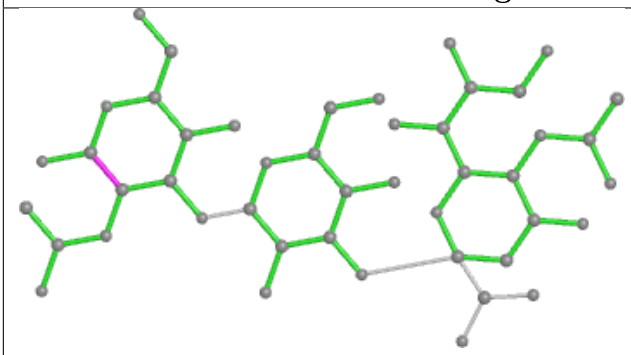
There are no ring outliers.

1 monomer is involved in 2 short contacts:

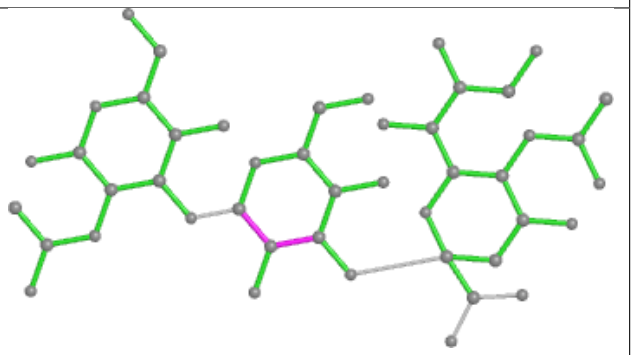
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	SIA	2	0

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

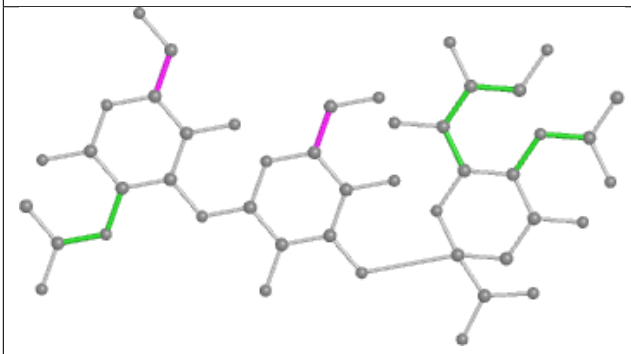
Oligosaccharide Chain D



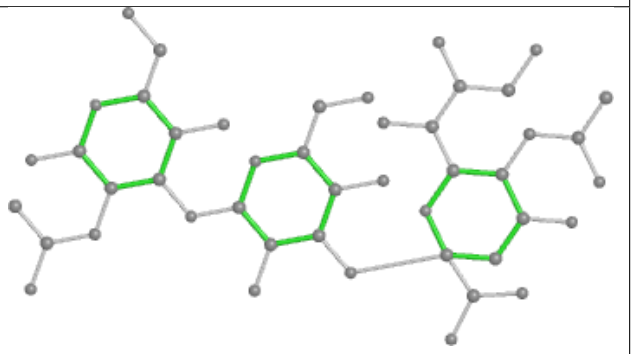
Bond lengths



Bond angles

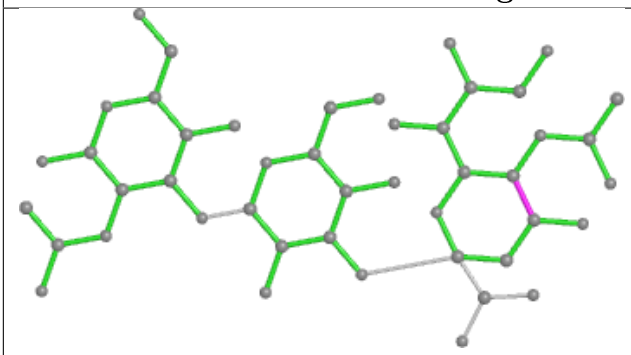


Torsions

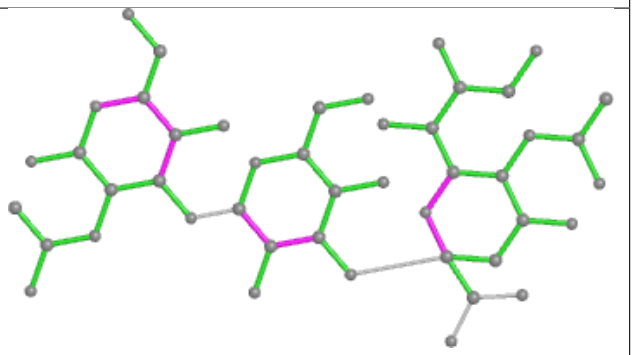


Rings

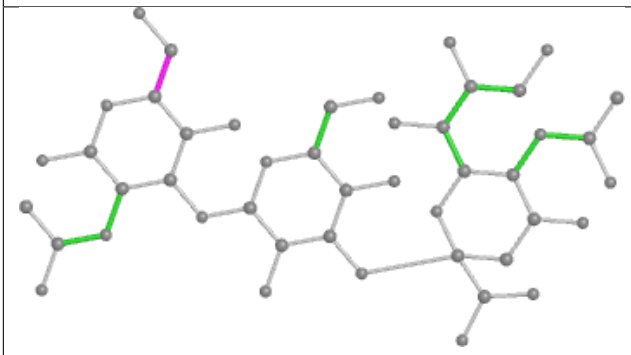
Oligosaccharide Chain E



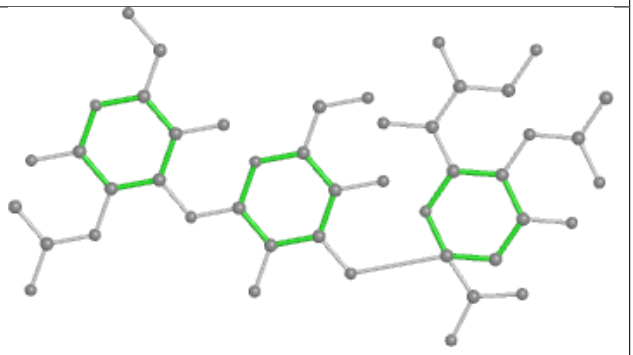
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
3	NAG	C	1500	-	14,14,15	0.58	0	17,19,21	0.89	0
3	NAG	A	1500	-	12,12,15	0.44	0	13,15,21	0.88	0
3	NAG	A	1499	-	14,14,15	0.47	0	17,19,21	0.78	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
3	NAG	C	1500	-	-	4/6/23/26	0/1/1/1
3	NAG	A	1500	-	-	6/15/15/26	-
3	NAG	A	1499	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1500	NAG	C1-C2-N2-C7
3	A	1500	NAG	O4-C4-C5-C6
3	A	1500	NAG	C8-C7-N2-C2
3	A	1500	NAG	O7-C7-N2-C2
3	A	1499	NAG	C1-C2-N2-C7
3	A	1499	NAG	C8-C7-N2-C2
3	A	1499	NAG	O7-C7-N2-C2
3	C	1500	NAG	O5-C5-C6-O6
3	A	1500	NAG	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	C	1500	NAG	C4-C5-C6-O6
3	A	1499	NAG	O5-C5-C6-O6
3	A	1500	NAG	C4-C5-C6-O6
3	C	1500	NAG	C8-C7-N2-C2
3	C	1500	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1500	NAG	3	0
3	A	1500	NAG	6	0
3	A	1499	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

6.1 Protein, DNA and RNA chains

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

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

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

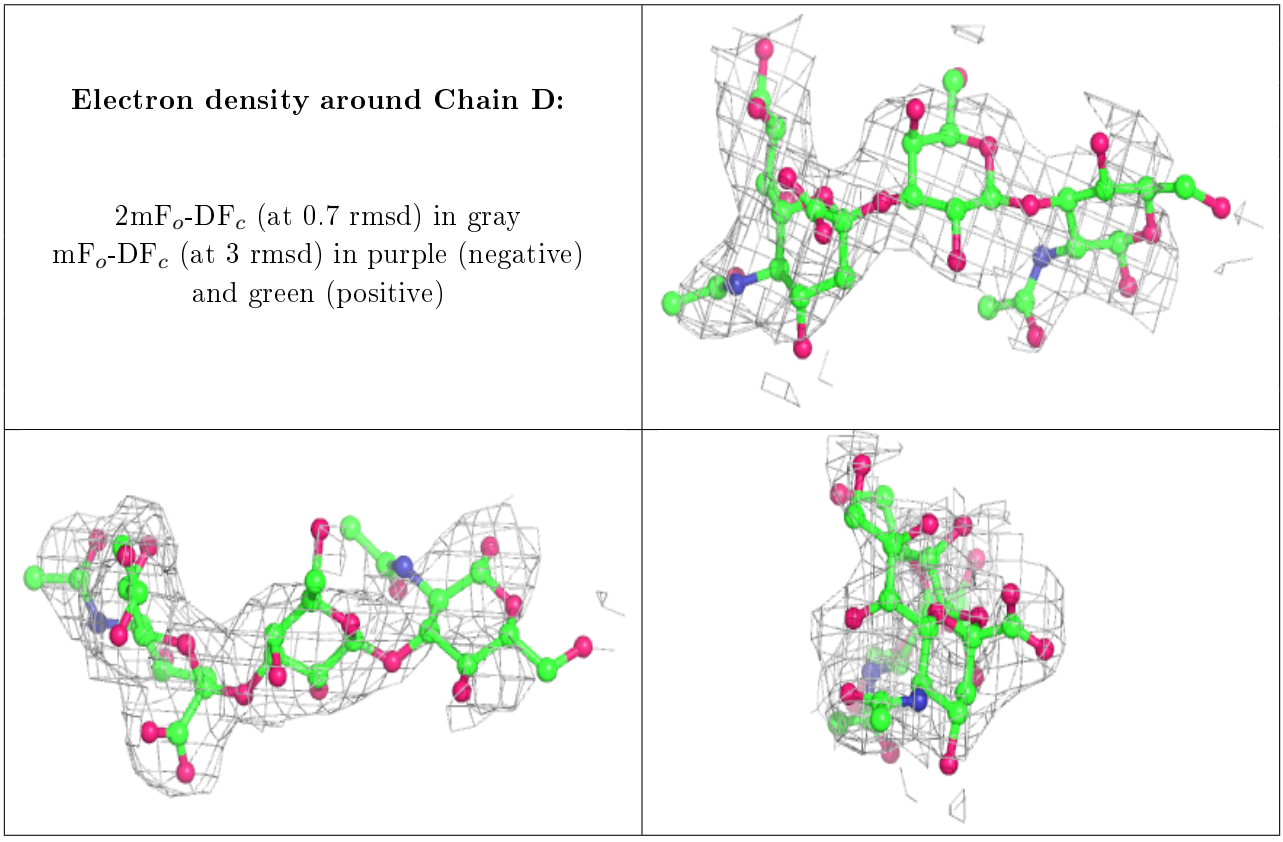
6.3 Carbohydrates

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

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

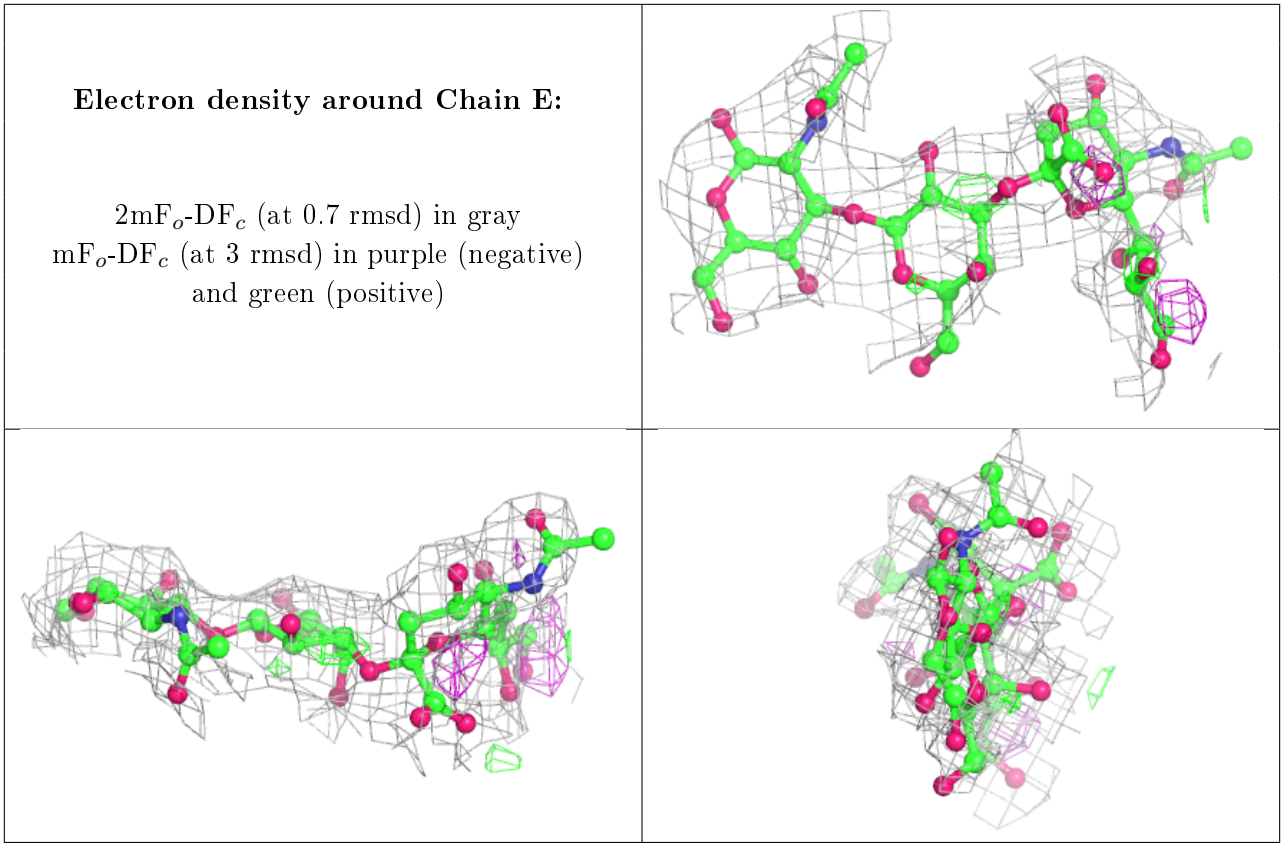
Electron density around Chain D:

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



Electron density around Chain E:

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



6.4 Ligands

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

6.5 Other polymers

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