



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:51 PM BST

PDB ID : 4DLO
Title : Crystal structure of the GAIN and HormR domains of brain angiogenesis inhibitor 3 (BAI3)
Authors : Arac, D.; Boucard, A.A.; Bolliger, M.F.; Nguyen, J.; Soltis, M.; Sudhof, T.C.; Brunger, A.T.
Deposited on : 2012-02-06
Resolution : 2.30 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

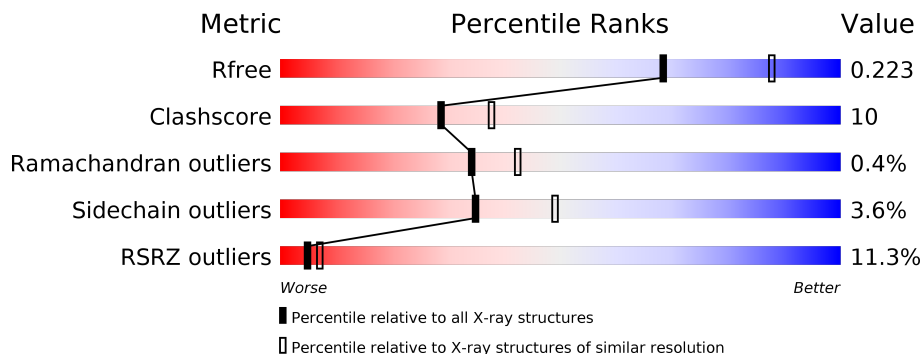
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. 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	382	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	B	382	<div style="display: flex; align-items: center;"> <div style="width: 16%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
2	C	3	<div style="width: 100%; height: 10px; background-color: yellow;"></div>
2	E	3	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div>
3	D	2	<div style="width: 100%; height: 10px; background-color: yellow;"></div>

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
2	NAG	C	3	-	-	-	X
3	NAG	D	2	-	-	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 5755 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.

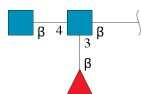
- Molecule 1 is a protein called Brain-specific angiogenesis inhibitor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2761	1753	464	524	20	0	0	0
1	B	337	2656	1688	449	498	21	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	ALA	-	expression tag	UNP O60242
A	496	ASP	-	expression tag	UNP O60242
A	497	PRO	-	expression tag	UNP O60242
A	503	SER	ASN	conflict	UNP O60242
A	869	HIS	-	expression tag	UNP O60242
A	870	HIS	-	expression tag	UNP O60242
A	871	HIS	-	expression tag	UNP O60242
A	872	HIS	-	expression tag	UNP O60242
A	873	HIS	-	expression tag	UNP O60242
A	874	HIS	-	expression tag	UNP O60242
A	875	HIS	-	expression tag	UNP O60242
A	876	HIS	-	expression tag	UNP O60242
B	495	ALA	-	expression tag	UNP O60242
B	496	ASP	-	expression tag	UNP O60242
B	497	PRO	-	expression tag	UNP O60242
B	503	SER	ASN	conflict	UNP O60242
B	869	HIS	-	expression tag	UNP O60242
B	870	HIS	-	expression tag	UNP O60242
B	871	HIS	-	expression tag	UNP O60242
B	872	HIS	-	expression tag	UNP O60242
B	873	HIS	-	expression tag	UNP O60242
B	874	HIS	-	expression tag	UNP O60242
B	875	HIS	-	expression tag	UNP O60242
B	876	HIS	-	expression tag	UNP O60242

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



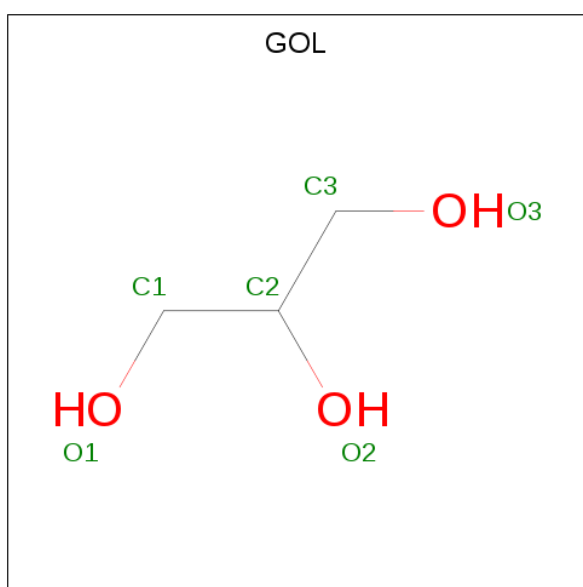
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	38	22	2	14	0	0	0
2	E	3	38	22	2	14	0	0	0

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



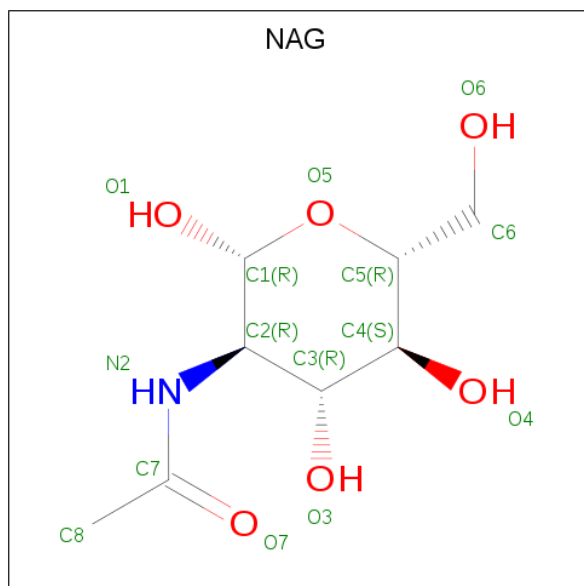
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

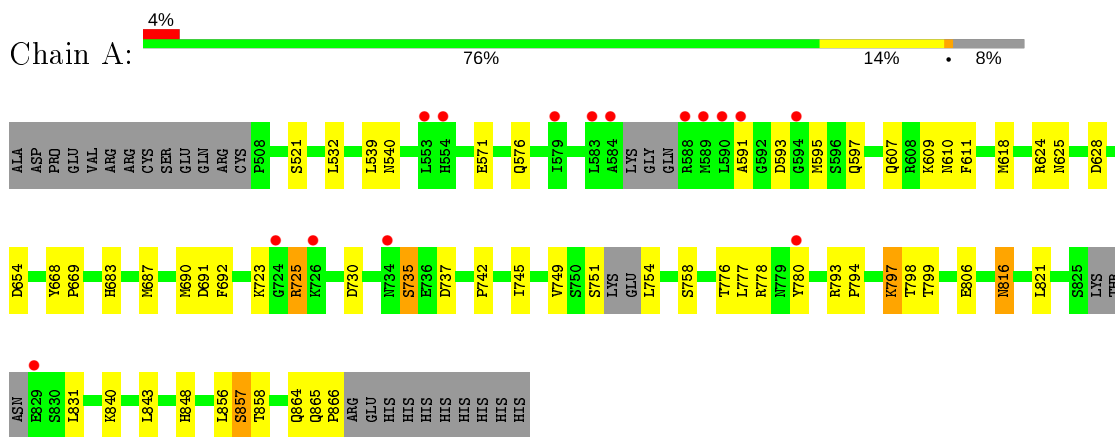
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total 106	O 106	0	0
6	B	60	Total 60	O 60	0	0

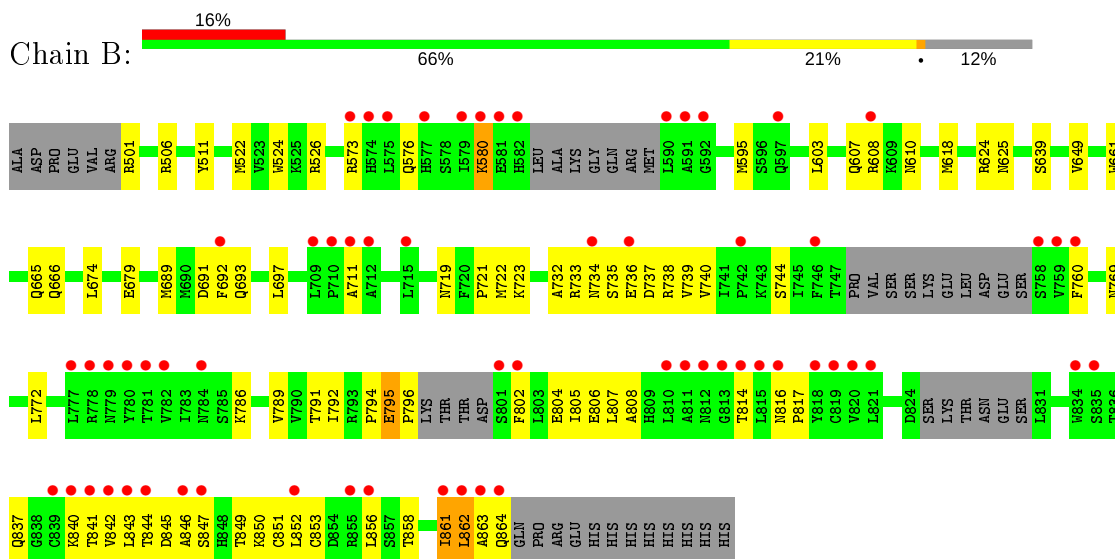
3 Residue-property plots [i](#)

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.

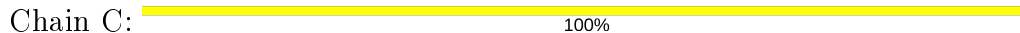
- Molecule 1: Brain-specific angiogenesis inhibitor 3



- Molecule 1: Brain-specific angiogenesis inhibitor 3



- Molecule 2: beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
FOL2
MAG3

- Molecule 2: beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%

MAG1
FOL2
MAG3

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

Chain D:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	123.36Å 128.01Å 160.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.40 – 2.30 44.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.40-2.30) 99.7 (44.41-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.186 , 0.228 0.181 , 0.223	Depositor DCC
R_{free} test set	2903 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtrriage
Anisotropy	0.289	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5755	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, FUL, 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	0.46	0/2817	0.58	0/3822
1	B	0.40	0/2709	0.53	0/3673
All	All	0.44	0/5526	0.56	0/7495

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	2761	0	2735	45	0
1	B	2656	0	2623	63	0
2	C	38	0	34	1	0
2	E	38	0	34	3	0
3	D	28	0	25	1	0
4	A	30	0	40	1	0
4	B	24	0	32	3	0
5	B	14	0	13	1	0
6	A	106	0	0	1	0
6	B	60	0	0	6	0
All	All	5755	0	5536	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:THR:HB	1:B:863:ALA:HB1	1.52	0.90
1:B:736:GLU:HB2	1:B:808:ALA:HB2	1.60	0.83
1:A:797:LYS:HE3	1:A:799:THR:HB	1.60	0.82
1:B:732:ALA:O	1:B:735:SER:HB3	1.87	0.74
1:A:865:GLN:N	1:A:866:PRO:HD2	2.07	0.69
1:A:865:GLN:N	1:A:866:PRO:CD	2.58	0.66
1:B:721:PRO:O	1:B:723:LYS:HD2	1.95	0.66
1:B:807:LEU:HD12	1:B:861:ILE:HD13	1.80	0.64
1:A:754:LEU:HA	1:A:758:SER:OG	1.99	0.61
1:A:725:ARG:N	1:A:725:ARG:HD2	2.15	0.61
1:A:864:GLN:HB3	1:A:866:PRO:HD2	1.82	0.60
1:B:526:ARG:NE	6:B:1034:HOH:O	1.98	0.60
1:A:749:VAL:HG12	1:A:751:SER:H	1.67	0.59
1:A:776:THR:O	1:A:778:ARG:HD2	2.02	0.59
1:B:852:LEU:HG	6:B:1059:HOH:O	2.03	0.59
1:A:840:LYS:HD3	1:B:722:MET:HE2	1.85	0.58
1:A:840:LYS:HD3	1:B:722:MET:CE	2.32	0.58
1:B:802:PHE:HA	1:B:853:CYS:O	2.04	0.58
1:B:723:LYS:HZ2	1:B:735:SER:CB	2.17	0.57
1:A:571:GLU:H	1:A:571:GLU:CD	2.07	0.57
1:A:856:LEU:O	1:A:857:SER:HB2	2.05	0.56
1:B:737:ASP:OD1	1:B:786:LYS:HD2	2.06	0.56
1:B:679:GLU:CD	1:B:791:THR:HG21	2.25	0.56
1:A:609:LYS:HA	1:A:611:PHE:CE2	2.41	0.56
1:A:624:ARG:O	1:A:624:ARG:HD3	2.06	0.55
1:A:816:ASN:O	1:A:816:ASN:CG	2.45	0.55
1:B:816:ASN:N	1:B:817:PRO:HD3	2.22	0.55
1:A:777:LEU:O	1:A:778:ARG:HG3	2.07	0.55
1:B:814:THR:CB	1:B:863:ALA:HB1	2.31	0.53
1:A:793:ARG:HA	1:A:794:PRO:C	2.29	0.52
1:B:666:GLN:OE1	4:B:908:GOL:H11	2.09	0.52
1:A:848:HIS:HB3	6:A:1104:HOH:O	2.09	0.51
1:A:624:ARG:HD3	1:A:624:ARG:C	2.31	0.51
1:B:624:ARG:HD3	1:B:624:ARG:O	2.10	0.51
1:B:526:ARG:NH2	6:B:1034:HOH:O	2.38	0.51
1:A:749:VAL:H	1:A:754:LEU:HB2	1.76	0.50
1:B:625:ASN:OD1	5:B:904:NAG:C7	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:817:PRO:HD2	1:B:843:LEU:HD21	1.94	0.50
1:B:719:ASN:OD1	1:B:740:VAL:HG22	2.12	0.50
1:A:532:LEU:HD21	4:A:906:GOL:H32	1.94	0.50
1:A:798:THR:HG21	1:A:856:LEU:HG	1.94	0.49
1:B:814:THR:HA	1:B:864:GLN:O	2.13	0.49
1:A:683:HIS:O	1:A:687:MET:HG2	2.12	0.49
1:A:625:ASN:OD1	3:D:1:NAG:O5	2.25	0.49
2:E:1:NAG:H3	2:E:2:FUL:O2	2.13	0.49
1:B:845:ASP:OD1	1:B:846:ALA:N	2.46	0.48
1:B:576:GLN:HG3	1:B:618:MET:SD	2.54	0.48
1:B:789:VAL:HG22	1:B:858:THR:HG23	1.94	0.48
1:B:522:MET:HE3	1:B:524:TRP:CZ2	2.49	0.48
1:B:691:ASP:O	1:B:692:PHE:HB2	2.14	0.47
1:A:725:ARG:N	1:A:725:ARG:CD	2.77	0.47
1:A:864:GLN:C	1:A:866:PRO:HD2	2.33	0.47
1:B:723:LYS:NZ	1:B:735:SER:HB2	2.29	0.47
1:A:624:ARG:HD2	1:A:628:ASP:OD2	2.15	0.47
1:B:845:ASP:CG	1:B:847:SER:H	2.18	0.47
1:A:865:GLN:O	1:A:866:PRO:C	2.52	0.47
4:B:908:GOL:HO3	4:B:908:GOL:HO1	1.62	0.47
1:B:733:ARG:O	1:B:735:SER:N	2.48	0.46
1:B:769:ASN:HB2	1:B:772:LEU:HD12	1.97	0.46
1:A:725:ARG:H	1:A:725:ARG:HD2	1.80	0.46
1:A:843:LEU:HD12	1:B:697:LEU:HD22	1.98	0.46
1:B:607:GLN:HA	1:B:607:GLN:OE1	2.15	0.46
1:B:738:ARG:HD2	1:B:806:GLU:OE2	2.15	0.46
1:B:711:ALA:HB2	1:B:760:PHE:HE1	1.80	0.46
1:B:845:ASP:OD2	1:B:847:SER:HB2	2.15	0.46
1:A:691:ASP:O	1:A:692:PHE:HB2	2.17	0.45
1:A:668:TYR:CG	1:A:669:PRO:HD2	2.52	0.45
1:B:817:PRO:HA	1:B:862:LEU:O	2.17	0.45
1:A:843:LEU:HD12	1:B:697:LEU:CD2	2.47	0.44
1:A:780:TYR:HB3	1:A:866:PRO:HD3	1.98	0.44
1:A:737:ASP:HA	1:A:806:GLU:O	2.18	0.44
1:B:792:ILE:N	1:B:792:ILE:HD12	2.32	0.44
2:E:1:NAG:N2	2:E:2:FUL:C1	2.80	0.44
1:A:742:PRO:HG2	1:A:745:ILE:HG23	2.00	0.44
1:A:591:ALA:O	1:A:595:MET:HG2	2.18	0.43
1:B:841:THR:HG22	1:B:842:VAL:N	2.33	0.43
1:A:539:LEU:O	1:A:540:ASN:HB2	2.17	0.43
1:B:804:GLU:CG	1:B:850:LYS:HD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:NAG:H62	2:C:3:NAG:C7	2.49	0.43
1:B:580:LYS:H	1:B:580:LYS:HG2	1.40	0.43
1:B:723:LYS:CG	1:B:735:SER:OG	2.67	0.43
1:B:760:PHE:CD2	1:B:794:PRO:HD2	2.54	0.43
1:B:805:ILE:HD12	1:B:805:ILE:N	2.34	0.42
1:B:610:ASN:OD1	2:E:2:FUL:H4	2.20	0.42
1:B:649:VAL:HG22	1:B:674:LEU:HD11	2.02	0.42
1:A:821:LEU:HD12	1:A:821:LEU:C	2.40	0.42
1:B:851:CYS:SG	1:B:861:ILE:HD11	2.58	0.42
1:B:739:VAL:HG13	1:B:739:VAL:O	2.20	0.42
1:A:576:GLN:HG3	1:A:618:MET:SD	2.60	0.42
1:B:769:ASN:HB2	1:B:772:LEU:CD1	2.50	0.42
1:B:506:ARG:NH2	6:B:1043:HOH:O	2.42	0.41
1:B:501:ARG:N	6:B:1044:HOH:O	2.52	0.41
1:B:689:MET:HE2	1:B:693:GLN:HB3	2.03	0.41
1:B:850:LYS:HG2	6:B:1059:HOH:O	2.20	0.41
1:B:603:LEU:O	1:B:607:GLN:HG2	2.21	0.41
1:B:689:MET:CE	1:B:693:GLN:HB3	2.51	0.41
1:B:849:THR:CG2	1:B:850:LYS:N	2.83	0.41
1:A:821:LEU:HA	1:A:858:THR:O	2.20	0.41
1:B:795:GLU:HA	1:B:796:PRO:HD3	1.69	0.41
1:A:821:LEU:HD12	1:A:821:LEU:O	2.21	0.41
1:B:856:LEU:N	1:B:856:LEU:HD22	2.36	0.41
1:A:797:LYS:HE3	1:A:799:THR:CB	2.42	0.41
1:A:669:PRO:HG2	1:A:831:LEU:HG	2.03	0.40
1:A:593:ASP:O	1:A:597:GLN:HG3	2.21	0.40
1:B:661:TRP:O	1:B:665:GLN:HG3	2.22	0.40
1:B:723:LYS:HG3	1:B:735:SER:OG	2.21	0.40
1:B:595:MET:HA	1:B:595:MET:HE2	2.04	0.40
1:B:511:TYR:HA	4:B:907:GOL:H12	2.03	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	343/382 (90%)	334 (97%)	7 (2%)	2 (1%)	25	31
1	B	327/382 (86%)	316 (97%)	10 (3%)	1 (0%)	41	50
All	All	670/764 (88%)	650 (97%)	17 (2%)	3 (0%)	34	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	857	SER
1	A	735	SER
1	B	734	ASN

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	312/341 (92%)	301 (96%)	11 (4%)	36	50
1	B	298/341 (87%)	287 (96%)	11 (4%)	34	48
All	All	610/682 (89%)	588 (96%)	22 (4%)	35	49

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	521	SER
1	A	607	GLN
1	A	610	ASN
1	A	654	ASP
1	A	690	MET
1	A	723	LYS
1	A	725	ARG
1	A	730	ASP
1	A	735	SER
1	A	797	LYS

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Mol	Chain	Res	Type
1	A	816	ASN
1	B	573	ARG
1	B	580	LYS
1	B	608	ARG
1	B	639	SER
1	B	744	SER
1	B	795	GLU
1	B	837	GLN
1	B	840	LYS
1	B	844	THR
1	B	861	ILE
1	B	862	LEU

Some 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](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.61	0	17,19,21	0.88	0
2	FUL	C	2	2	10,10,11	0.64	0	14,14,16	0.84	1 (7%)
2	NAG	C	3	2	14,14,15	0.58	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	1	1,3	14,14,15	0.49	0	17,19,21	0.85	0
3	NAG	D	2	3	14,14,15	0.49	0	17,19,21	1.05	2 (11%)
2	NAG	E	1	1,2	14,14,15	0.50	0	17,19,21	1.66	3 (17%)
2	FUL	E	2	2	10,10,11	0.68	0	14,14,16	0.94	1 (7%)
2	NAG	E	3	2	14,14,15	0.49	0	17,19,21	1.39	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	FUL	C	2	2	-	-	0/1/1/1
2	NAG	C	3	2	-	1/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	FUL	E	2	2	-	-	0/1/1/1
2	NAG	E	3	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	NAG	C1-O5-C5	4.87	118.80	112.19
2	E	1	NAG	C4-C3-C2	-3.81	105.43	111.02
2	E	1	NAG	O4-C4-C3	3.34	118.07	110.35
2	E	1	NAG	O5-C5-C6	3.10	112.06	107.20
3	D	2	NAG	C1-O5-C5	3.07	116.35	112.19
2	E	2	FUL	C1-C2-C3	2.27	112.46	109.67
3	D	2	NAG	O5-C5-C6	2.19	110.64	107.20
2	C	2	FUL	C1-C2-C3	2.10	112.25	109.67

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2

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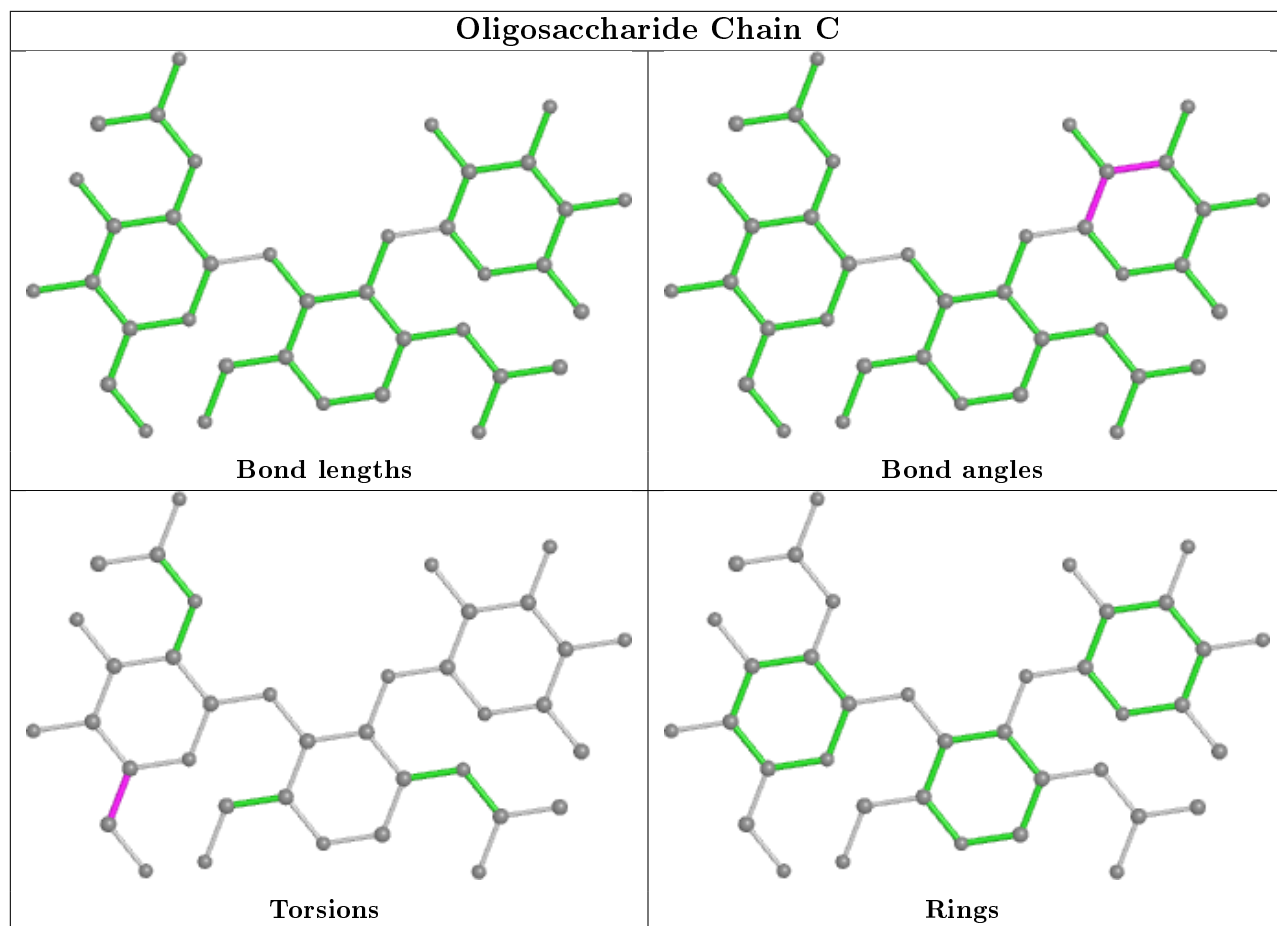
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	3	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

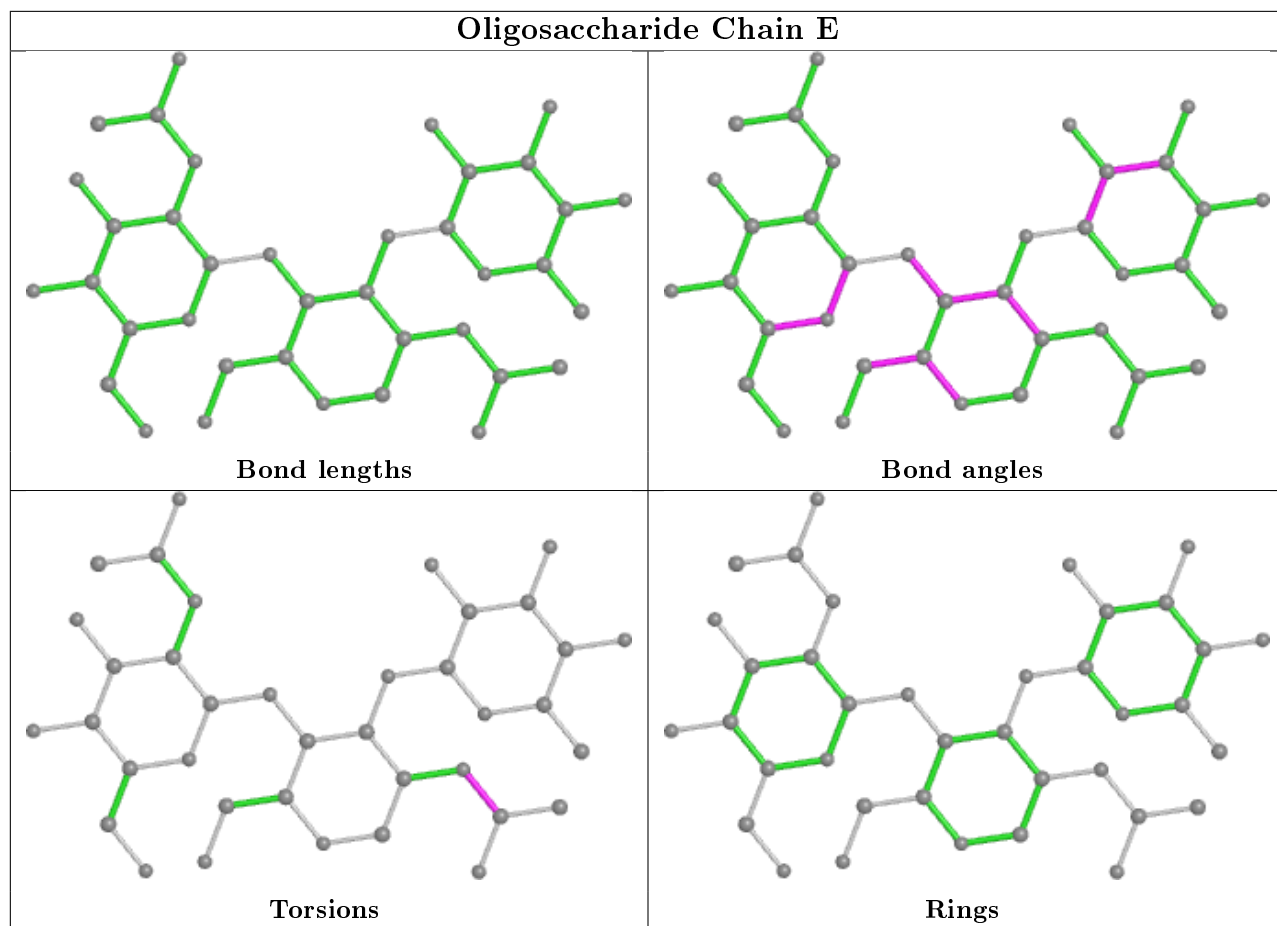
There are no ring outliers.

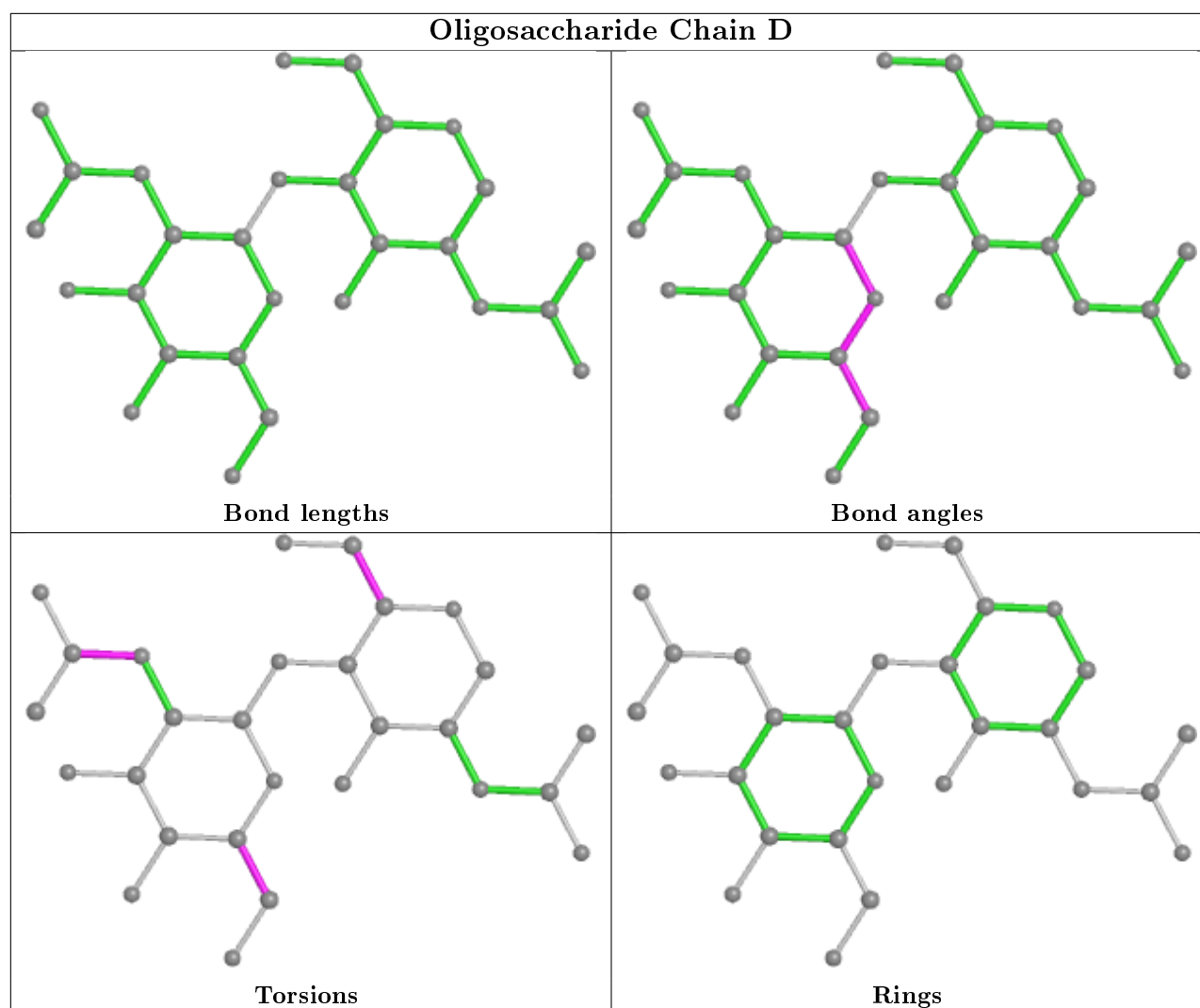
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	2	0
2	C	1	NAG	1	0
3	D	1	NAG	1	0
2	C	3	NAG	1	0
2	E	2	FUL	3	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.







5.6 Ligand geometry [i](#)

10 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	GOL	A	908	-	5,5,5	0.30	0	5,5,5	0.35	0
4	GOL	B	907	-	5,5,5	0.28	0	5,5,5	0.71	0
5	NAG	B	904	1	14,14,15	0.44	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	909	-	5,5,5	0.36	0	5,5,5	0.72	0
4	GOL	A	906	-	5,5,5	0.44	0	5,5,5	0.25	0
4	GOL	B	906	-	5,5,5	0.36	0	5,5,5	1.00	0
4	GOL	A	910	-	5,5,5	0.36	0	5,5,5	0.74	0
4	GOL	B	908	-	5,5,5	0.33	0	5,5,5	0.60	0
4	GOL	B	905	-	5,5,5	0.42	0	5,5,5	0.87	0
4	GOL	A	907	-	5,5,5	0.28	0	5,5,5	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	GOL	A	908	-	-	2/4/4/4	-
4	GOL	B	907	-	-	1/4/4/4	-
5	NAG	B	904	1	-	1/6/23/26	0/1/1/1
4	GOL	A	909	-	-	2/4/4/4	-
4	GOL	A	906	-	-	4/4/4/4	-
4	GOL	B	906	-	-	4/4/4/4	-
4	GOL	A	910	-	-	2/4/4/4	-
4	GOL	B	908	-	-	3/4/4/4	-
4	GOL	B	905	-	-	2/4/4/4	-
4	GOL	A	907	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	904	NAG	C1-O5-C5	2.33	115.34	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	906	GOL	O1-C1-C2-C3
4	A	906	GOL	C1-C2-C3-O3
4	B	906	GOL	O1-C1-C2-C3
4	A	907	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	908	GOL	O1-C1-C2-C3
4	A	909	GOL	C1-C2-C3-O3
4	B	906	GOL	C1-C2-C3-O3
4	A	910	GOL	C1-C2-C3-O3
4	B	908	GOL	O1-C1-C2-C3
4	B	905	GOL	O1-C1-C2-C3
4	A	908	GOL	O1-C1-C2-O2
4	A	906	GOL	O2-C2-C3-O3
4	B	906	GOL	O2-C2-C3-O3
4	A	907	GOL	O1-C1-C2-O2
4	B	906	GOL	O1-C1-C2-O2
4	B	908	GOL	O1-C1-C2-O2
4	A	906	GOL	O1-C1-C2-O2
4	A	910	GOL	O2-C2-C3-O3
5	B	904	NAG	C3-C2-N2-C7
4	B	905	GOL	O1-C1-C2-O2
4	B	908	GOL	C1-C2-C3-O3
4	B	907	GOL	O2-C2-C3-O3
4	A	909	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	907	GOL	1	0
5	B	904	NAG	1	0
4	A	906	GOL	1	0
4	B	908	GOL	2	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

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	351/382 (91%)	0.25	15 (4%) 35 42	29, 44, 95, 137	0
1	B	337/382 (88%)	0.91	63 (18%) 1 1	27, 70, 161, 192	0
All	All	688/764 (90%)	0.58	78 (11%) 5 7	27, 52, 144, 192	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	584	ALA	12.3
1	B	780	TYR	11.4
1	B	863	ALA	9.2
1	B	846	ALA	8.7
1	B	811	ALA	7.4
1	B	864	GLN	7.3
1	B	814	THR	6.9
1	B	819	CYS	6.7
1	A	590	LEU	6.7
1	B	758	SER	6.5
1	B	862	LEU	6.1
1	B	590	LEU	6.0
1	B	580	LYS	5.9
1	B	843	LEU	5.9
1	B	781	THR	5.7
1	A	589	MET	5.1
1	B	818	TYR	5.0
1	B	712	ALA	5.0
1	B	760	PHE	4.9
1	A	588	ARG	4.9
1	B	777	LEU	4.7
1	B	746	PHE	4.7
1	B	847	SER	4.6
1	B	582	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	780	TYR	4.5
1	A	553	LEU	4.4
1	B	710	PRO	4.4
1	B	736	GLU	4.3
1	B	711	ALA	4.2
1	B	835	SER	4.1
1	B	782	VAL	4.0
1	B	816	ASN	4.0
1	B	579	ILE	3.9
1	B	779	ASN	3.9
1	B	591	ALA	3.9
1	B	778	ARG	3.7
1	B	815	LEU	3.7
1	A	591	ALA	3.6
1	B	801	SER	3.6
1	B	861	ILE	3.6
1	B	759	VAL	3.6
1	B	802	PHE	3.5
1	B	812	ASN	3.5
1	B	842	VAL	3.2
1	B	810	LEU	3.1
1	B	742	PRO	3.1
1	B	840	LYS	3.1
1	B	856	LEU	3.1
1	B	577	HIS	3.0
1	B	784	ASN	3.0
1	B	834	TRP	3.0
1	B	813	GLY	2.9
1	A	734	ASN	2.9
1	B	575	LEU	2.9
1	B	820	VAL	2.8
1	B	839	CYS	2.8
1	B	709	LEU	2.7
1	B	855	ARG	2.7
1	A	579	ILE	2.7
1	B	821	LEU	2.7
1	A	724	GLY	2.6
1	B	692	PHE	2.6
1	B	852	LEU	2.6
1	B	597	GLN	2.6
1	B	581	GLU	2.6
1	B	592	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	583	LEU	2.5
1	A	829	GLU	2.5
1	A	726	LYS	2.5
1	B	841	THR	2.5
1	B	844	THR	2.5
1	A	554	HIS	2.4
1	B	715	LEU	2.3
1	B	608	ARG	2.2
1	B	573	ARG	2.1
1	B	574	HIS	2.1
1	A	594	GLY	2.1
1	B	734	ASN	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](#)

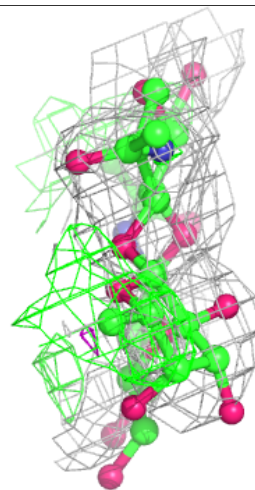
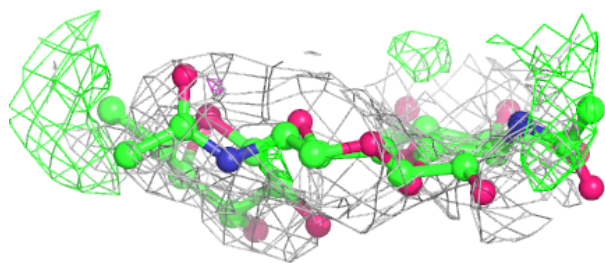
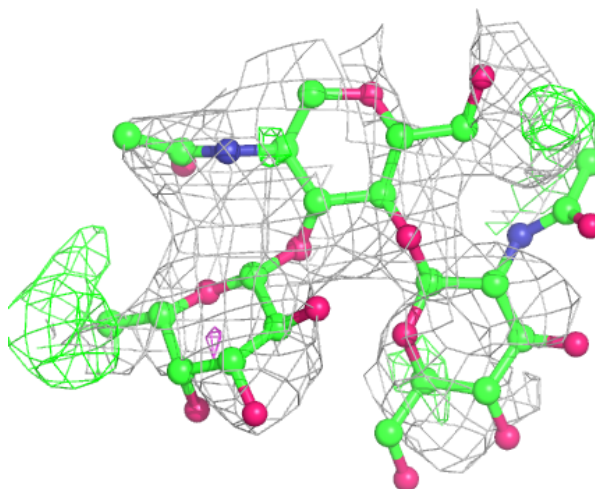
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	3	14/15	0.52	0.52	159,172,176,176	0
3	NAG	D	2	14/15	0.69	0.50	156,171,174,177	0
2	NAG	E	3	14/15	0.71	0.39	141,153,160,161	0
2	NAG	E	1	14/15	0.73	0.27	89,98,123,135	0
2	FUL	C	2	10/11	0.75	0.39	137,140,144,148	0
2	FUL	E	2	10/11	0.78	0.30	121,127,128,130	0
2	NAG	C	1	14/15	0.80	0.20	93,110,132,146	0
3	NAG	D	1	14/15	0.90	0.15	76,96,119,139	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.

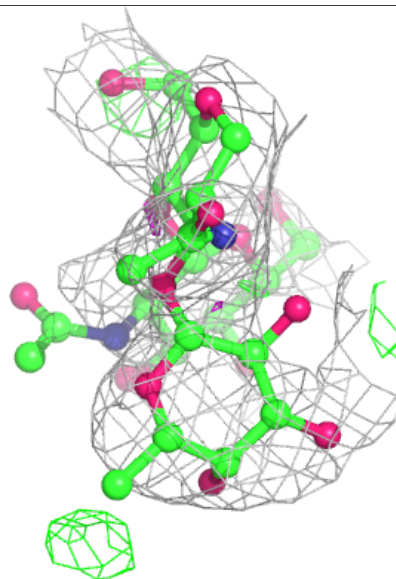
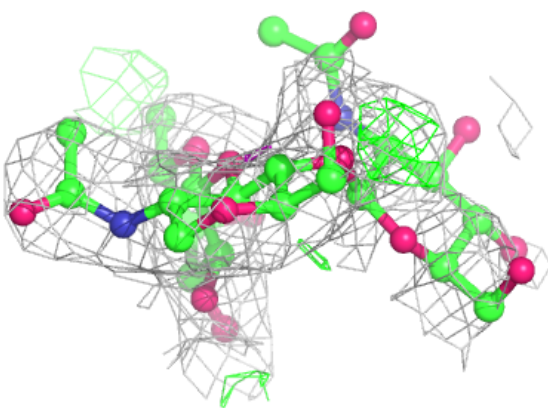
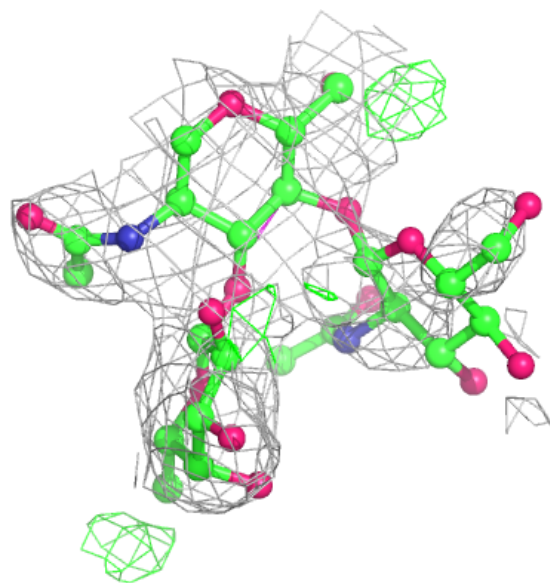
Electron density around Chain C:

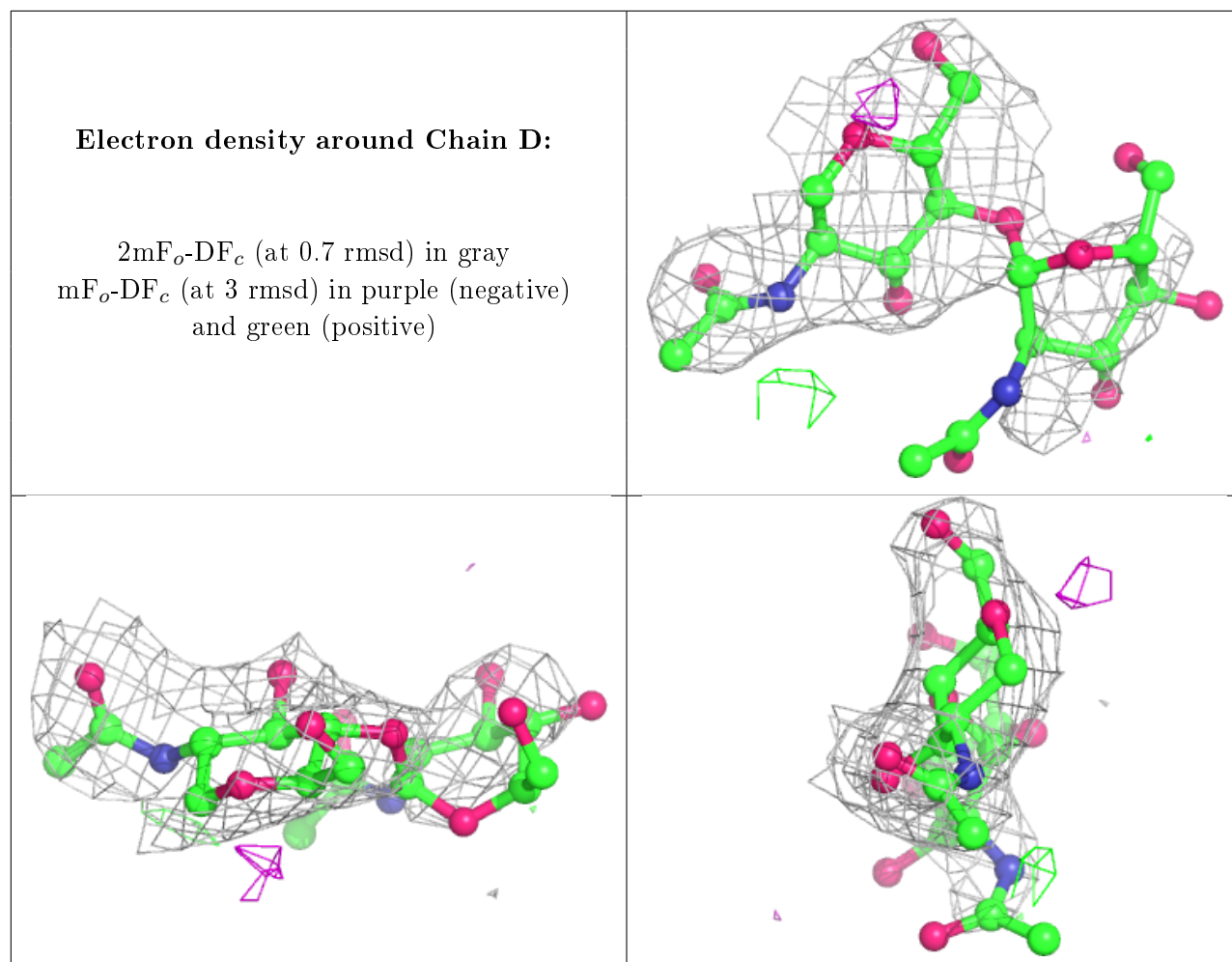
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands [i](#)

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	GOL	A	906	6/6	0.68	0.39	65,93,98,99	0
4	GOL	A	909	6/6	0.77	0.35	88,93,95,97	0
4	GOL	A	908	6/6	0.81	0.50	48,69,78,85	0
4	GOL	B	906	6/6	0.82	0.24	55,78,87,87	0
4	GOL	B	908	6/6	0.82	0.33	95,98,102,105	0
5	NAG	B	904	14/15	0.83	0.27	93,110,122,129	0
4	GOL	B	907	6/6	0.84	0.26	79,83,88,92	0
4	GOL	A	910	6/6	0.85	0.23	44,77,83,87	0
4	GOL	B	905	6/6	0.92	0.22	53,67,75,83	0
4	GOL	A	907	6/6	0.93	0.14	62,71,74,81	0

6.5 Other polymers

There are no such residues in this entry.