



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:18 AM UTC

PDB ID : 4DLO / pdb_00004dlo
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

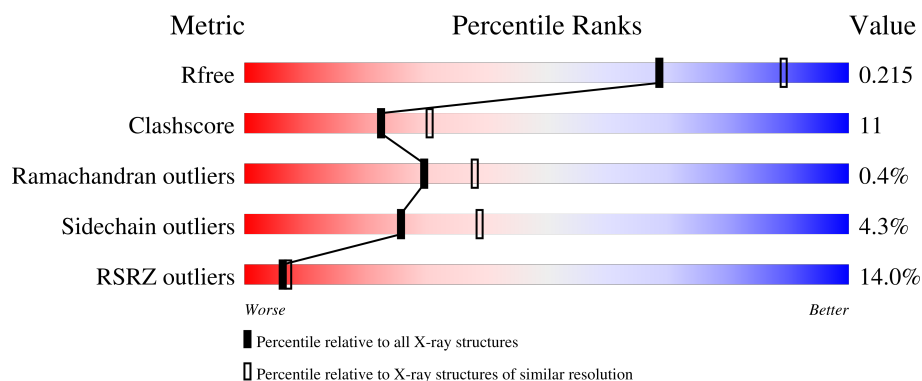
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	7% 75% 15% • 8%
1	B	382	18% 65% 22% • 12%
2	C	3	33% 67%
2	E	3	67% 33%
3	D	2	100%

2 Entry composition

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.

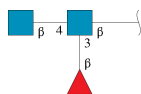
- Molecule 1 is a protein called Brain-specific angiogenesis inhibitor 3.

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

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.



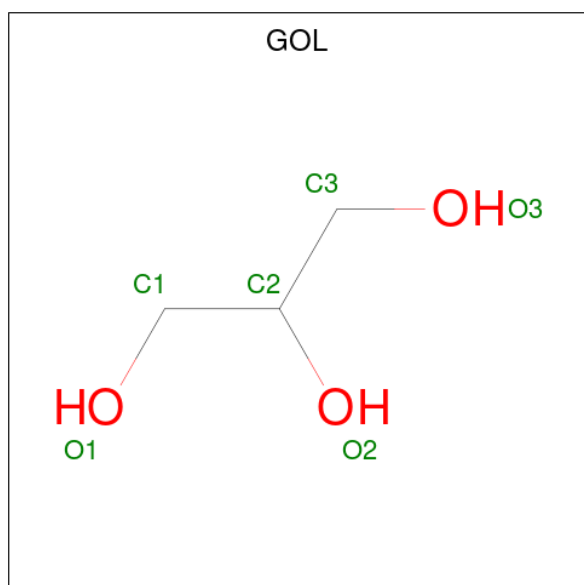
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



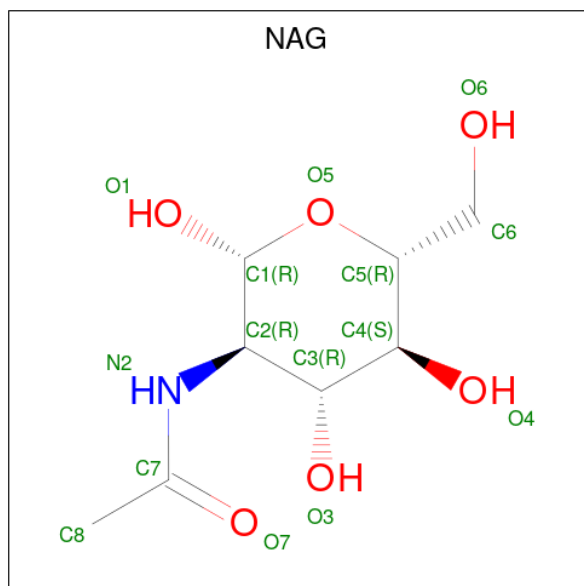
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is GLYCEROL (CCD ID: 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	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		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		

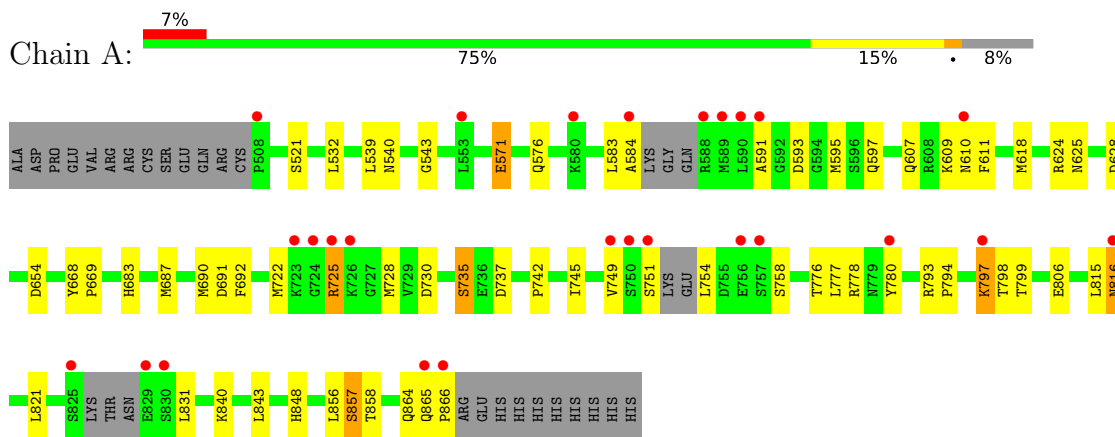
- Molecule 6 is water.

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

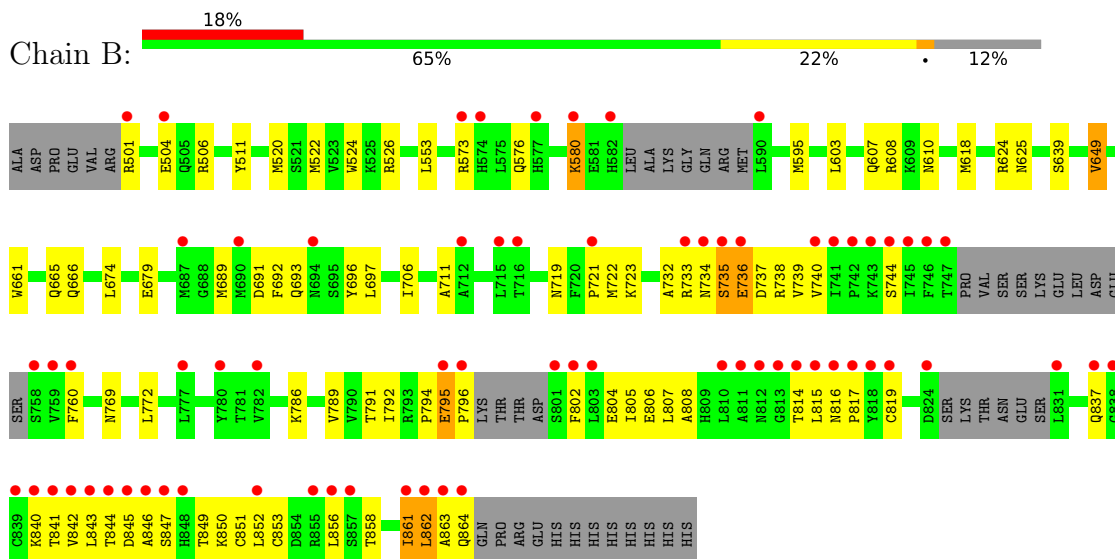
3 Residue-property plots

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.

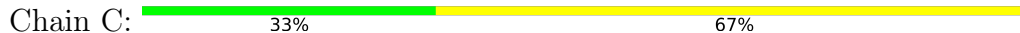
- Molecule 1: Brain-specific angiogenesis inhibitor 3



- 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





- 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:  67% 33%



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

Chain D:  100%



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 44.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.40-2.30) 99.8 (44.40-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.186 , 0.228 (Not available) , 0.215	Depositor DCC
R_{free} test set	2906 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
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

Xtriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.58	0/2817	0.81	1/3822 (0.0%)
1	B	0.50	0/2709	0.79	1/3673 (0.0%)
All	All	0.54	0/5526	0.80	2/7495 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	736	GLU	N-CA-C	-8.01	103.52	112.57
1	A	543	GLY	N-CA-C	-5.52	105.98	111.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2761	0	2735	48	0
1	B	2656	0	2623	70	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	13	1	0
6	A	106	0	0	1	0
6	B	60	0	0	8	0
All	All	5755	0	5536	117	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 11.

All (117) 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:A:840:LYS:HD3	1:B:722:MET:HE1	1.62	0.81
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:571:GLU:H	1:A:571:GLU:CD	2.07	0.62
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:B:679:GLU:CD	1:B:791:THR:HG21	2.25	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:816:ASN:CG	1:A:816:ASN:O	2.45	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: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:840:LYS:HD3	1:B:722:MET:CE	2.32	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:A:793:ARG:HA	1:A:794:PRO:C	2.29	0.56
1:A:624:ARG:HD3	1:A:624:ARG:C	2.31	0.56
1:A:609:LYS:HA	1:A:611:PHE:CE2	2.41	0.56
1:A:624:ARG:HD3	1:A:624:ARG:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:MET:HA	1:B:595:MET:HE2	1.89	0.55
1:B:696:TYR:CE1	1:B:722:MET:HE3	2.42	0.55
1:B:814:THR:CB	1:B:863:ALA:HB1	2.31	0.53
1:B:666:GLN:OE1	4:B:908:GOL:H11	2.09	0.52
1:A:864:GLN:C	1:A:866:PRO:HD2	2.33	0.52
1:B:845:ASP:CG	1:B:847:SER:H	2.18	0.51
1:A:848:HIS:HB3	6:A:1104:HOH:O	2.09	0.51
1:A:865:GLN:O	1:A:866:PRO:C	2.52	0.51
1:B:624:ARG:O	1:B:624:ARG:HD3	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
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: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: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:A:821:LEU:C	1:A:821:LEU:HD12	2.40	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:HD2	1:A:725:ARG:H	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:B:522:MET:HE3	1:B:524:TRP:CZ2	2.52	0.45
1:A:668:TYR:CG	1:A:669:PRO:HD2	2.52	0.45
1:B:520:MET:HE2	1:B:522:MET:HE2	1.99	0.45
1:B:817:PRO:HA	1:B:862:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:B:792:ILE:N	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:B:804:GLU:CG	1:B:850:LYS:HD2	2.49	0.43
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:A:539:LEU:O	1:A:540:ASN:HB2	2.17	0.42
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:777:LEU:C	1:A:778:ARG:HG3	2.45	0.42
1:B:851:CYS:SG	1:B:861:ILE:HD11	2.58	0.42
1:B:739:VAL:O	1:B:739:VAL:HG13	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:595:MET:HE2	1:B:595:MET:CA	2.50	0.41
1:A:583:LEU:O	1:A:584:ALA:C	2.63	0.41
1:B:689:MET:HE1	1:B:706:ILE:O	2.20	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:733:ARG:C	1:B:735:SER:N	2.78	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:B:819:CYS:C	6:B:1060:HOH:O	2.64	0.41
1:A:722:MET:O	1:A:728:MET:HE3	2.20	0.41
1:A:821:LEU:HD12	1:A:821:LEU:O	2.21	0.41
1:B:856:LEU:HD22	1:B:856:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:504:GLU:CD	6:B:1036:HOH:O	2.64	0.40
1:B:511:TYR:HA	4:B:907:GOL:H12	2.03	0.40
1:B:815:LEU:C	1:B:817:PRO:HD3	2.46	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%)	21	27
1	B	327/382 (86%)	316 (97%)	10 (3%)	1 (0%)	36	46
All	All	670/764 (88%)	650 (97%)	17 (2%)	3 (0%)	30	38

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%)	300 (96%)	12 (4%)	29	44
1	B	298/341 (87%)	284 (95%)	14 (5%)	23	35
All	All	610/682 (89%)	584 (96%)	26 (4%)	26	39

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	521	SER
1	A	571	GLU
1	A	607	GLN
1	A	610	ASN
1	A	654	ASP
1	A	690	MET
1	A	725	ARG
1	A	730	ASP
1	A	735	SER
1	A	797	LYS
1	A	815	LEU
1	A	816	ASN
1	B	553	LEU
1	B	573	ARG
1	B	580	LYS
1	B	608	ARG
1	B	639	SER
1	B	649	VAL
1	B	735	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	607	GLN
1	A	647	GLN
1	A	651	ASN
1	A	676	GLN

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Mol	Chain	Res	Type
1	A	701	ASN
1	B	577	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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	0.59	0	17,19,21	0.83	0
2	FUL	C	2	2	10,10,11	0.63	0	14,14,16	0.78	0
2	NAG	C	3	2	14,14,15	0.58	0	17,19,21	0.72	0
3	NAG	D	1	3,1	14,14,15	0.47	0	17,19,21	0.83	0
3	NAG	D	2	3	14,14,15	0.49	0	17,19,21	0.99	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.51	0	17,19,21	1.59	3 (17%)
2	FUL	E	2	2	10,10,11	0.68	0	14,14,16	0.85	0
2	NAG	E	3	2	14,14,15	0.49	0	17,19,21	1.40	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	3,1	-	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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	NAG	C1-O5-C5	4.93	118.80	112.19
2	E	1	NAG	C4-C3-C2	-3.81	105.43	111.02
2	E	1	NAG	O4-C4-C3	3.26	118.07	110.38
3	D	2	NAG	C1-O5-C5	3.11	116.35	112.19
2	E	1	NAG	O5-C5-C6	2.26	112.06	107.66

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
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:

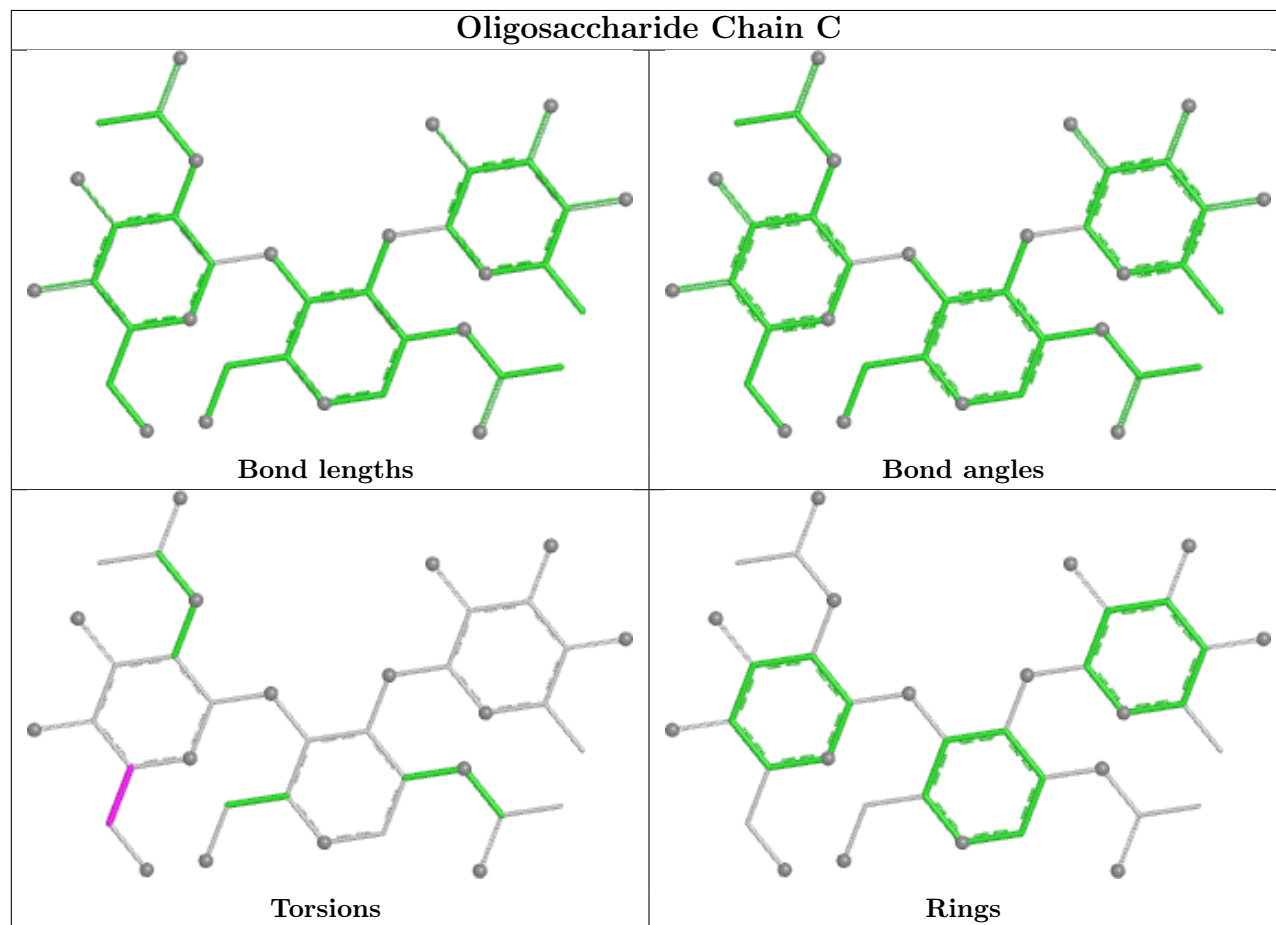
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
3	D	1	NAG	1	0
2	E	1	NAG	2	0
2	C	3	NAG	1	0

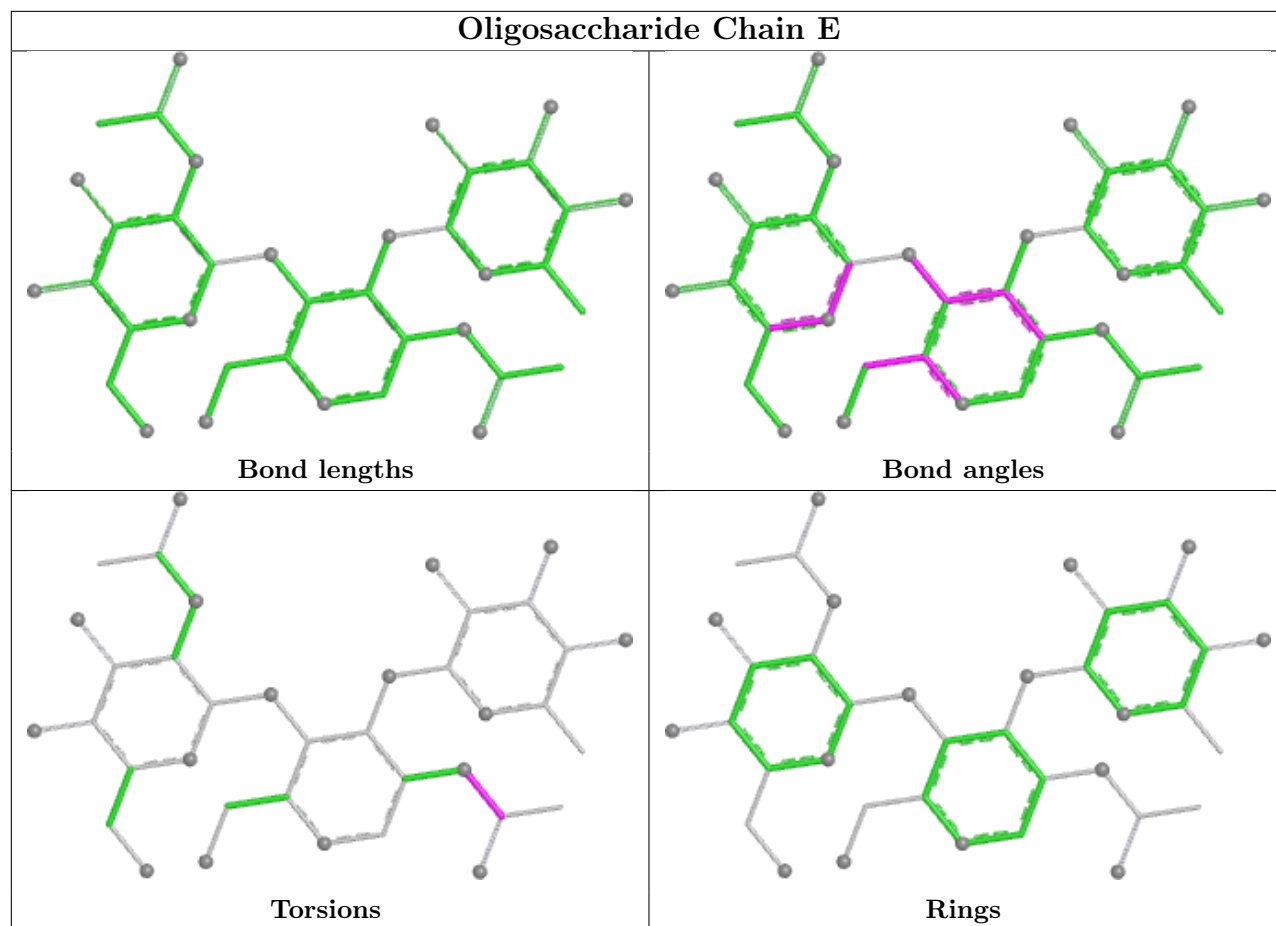
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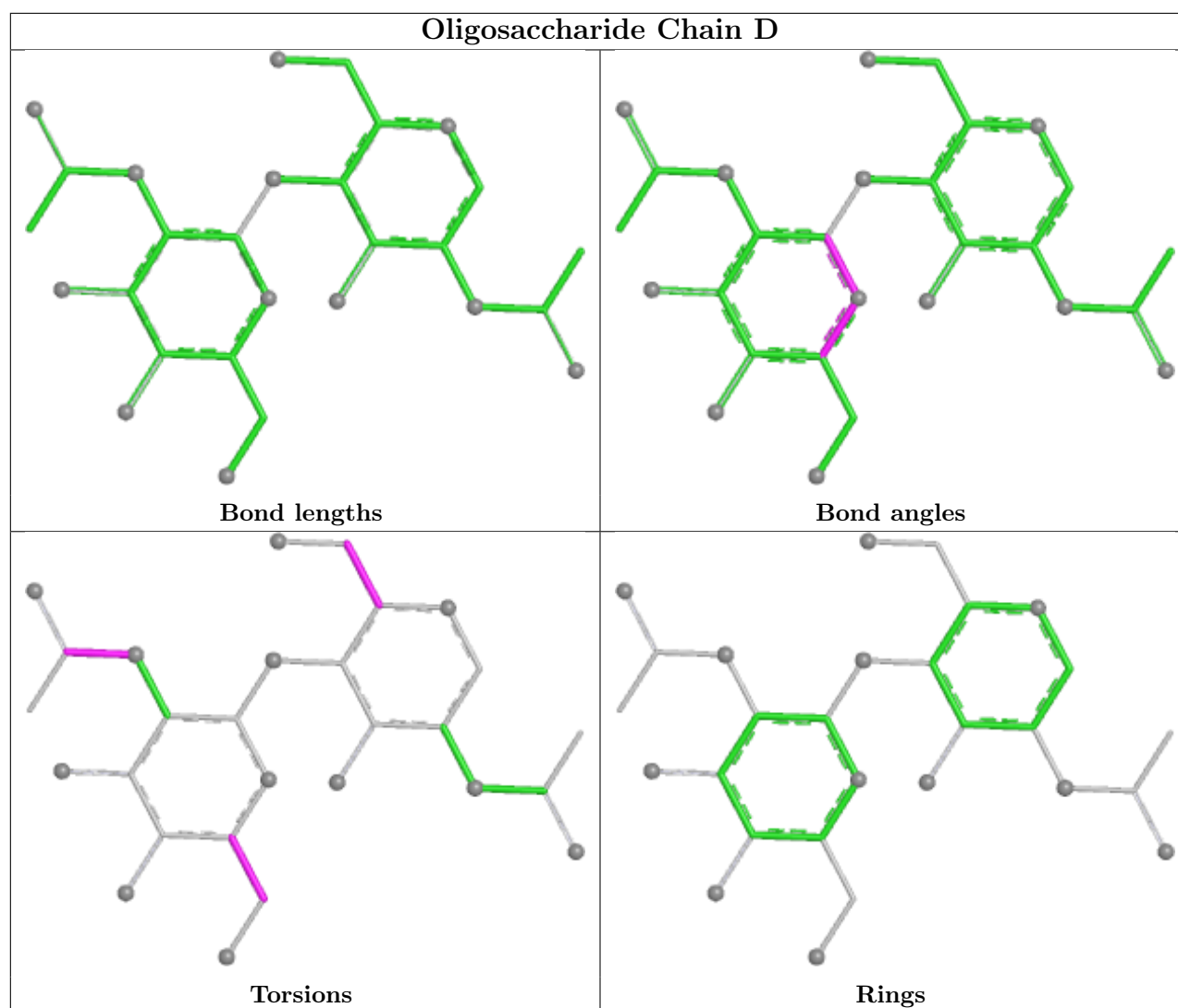
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	FUL	3	0

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	B	907	-	5,5,5	0.28	0	5,5,5	0.78	0
5	NAG	B	904	1	14,14,15	0.44	0	17,19,21	0.85	1 (5%)
4	GOL	A	910	-	5,5,5	0.36	0	5,5,5	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	907	-	5,5,5	0.29	0	5,5,5	0.51	0
4	GOL	B	908	-	5,5,5	0.34	0	5,5,5	0.66	0
4	GOL	A	909	-	5,5,5	0.36	0	5,5,5	0.78	0
4	GOL	B	906	-	5,5,5	0.37	0	5,5,5	1.06	0
4	GOL	A	906	-	5,5,5	0.44	0	5,5,5	0.29	0
4	GOL	B	905	-	5,5,5	0.43	0	5,5,5	0.94	0
4	GOL	A	908	-	5,5,5	0.31	0	5,5,5	0.38	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	B	907	-	-	1/4/4/4	-
5	NAG	B	904	1	-	2/6/23/26	0/1/1/1
4	GOL	A	910	-	-	2/4/4/4	-
4	GOL	A	907	-	-	2/4/4/4	-
4	GOL	B	908	-	-	3/4/4/4	-
4	GOL	A	909	-	-	3/4/4/4	-
4	GOL	B	906	-	-	4/4/4/4	-
4	GOL	A	906	-	-	4/4/4/4	-
4	GOL	B	905	-	-	2/4/4/4	-
4	GOL	A	908	-	-	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	2.36	115.34	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

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

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

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%)	0.04	26 (7%) 20 22	29, 44, 95, 137	0
1	B	337/382 (88%)	0.84	70 (20%) 2 3	27, 70, 161, 192	0
All	All	688/764 (90%)	0.43	96 (13%) 6 7	27, 52, 144, 192	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	747	THR	6.6
1	A	584	ALA	6.4
1	A	590	LEU	6.3
1	B	815	LEU	6.2
1	B	843	LEU	6.1
1	B	846	ALA	6.1
1	B	844	THR	5.6
1	B	801	SER	5.5
1	A	866	PRO	5.2
1	B	590	LEU	4.9
1	B	802	PHE	4.8
1	B	796	PRO	4.7
1	B	694	ASN	4.6
1	B	864	GLN	4.5
1	B	819	CYS	4.4
1	A	749	VAL	4.2
1	B	817	PRO	4.2
1	B	813	GLY	4.1
1	A	757	SER	4.1
1	B	824	ASP	4.1
1	B	840	LYS	4.1
1	A	508	PRO	4.1
1	B	780	TYR	4.0
1	A	750	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	742	PRO	3.9
1	A	553	LEU	3.9
1	B	734	ASN	3.8
1	B	582	HIS	3.7
1	A	830	SER	3.6
1	B	838	GLY	3.6
1	B	504	GLU	3.6
1	B	501	ARG	3.5
1	B	842	VAL	3.5
1	A	589	MET	3.5
1	B	580	LYS	3.5
1	A	588	ARG	3.5
1	B	812	ASN	3.4
1	B	856	LEU	3.4
1	B	863	ALA	3.3
1	B	855	ARG	3.3
1	B	831	LEU	3.2
1	B	816	ASN	3.2
1	B	852	LEU	3.2
1	A	797	LYS	3.2
1	B	736	GLU	3.1
1	B	733	ARG	3.1
1	B	746	PHE	3.1
1	B	759	VAL	3.1
1	A	725	ARG	3.1
1	B	743	LYS	3.1
1	B	814	THR	3.1
1	A	751	SER	3.1
1	A	825	SER	3.1
1	B	811	ALA	3.1
1	B	777	LEU	3.1
1	A	756	GLU	2.9
1	A	726	LYS	2.9
1	B	740	VAL	2.9
1	B	839	CYS	2.9
1	B	712	ALA	2.8
1	A	580	LYS	2.7
1	B	574	HIS	2.7
1	A	829	GLU	2.7
1	B	690	MET	2.7
1	B	721	PRO	2.7
1	B	857	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	758	SER	2.7
1	B	837	GLN	2.6
1	B	760	PHE	2.6
1	B	577	HIS	2.6
1	B	715	LEU	2.5
1	B	818	TYR	2.5
1	B	841	THR	2.5
1	B	847	SER	2.5
1	B	810	LEU	2.5
1	A	591	ALA	2.5
1	A	610	ASN	2.5
1	B	573	ARG	2.5
1	B	782	VAL	2.5
1	B	741	ILE	2.4
1	A	780	TYR	2.4
1	A	865	GLN	2.3
1	A	724	GLY	2.3
1	B	848	HIS	2.3
1	B	745	ILE	2.3
1	B	862	LEU	2.2
1	B	845	ASP	2.2
1	B	716	THR	2.2
1	B	861	ILE	2.2
1	B	803	LEU	2.2
1	A	816	ASN	2.2
1	B	744	SER	2.2
1	A	723	LYS	2.1
1	B	735	SER	2.1
1	B	795	GLU	2.1
1	B	687	MET	2.0

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

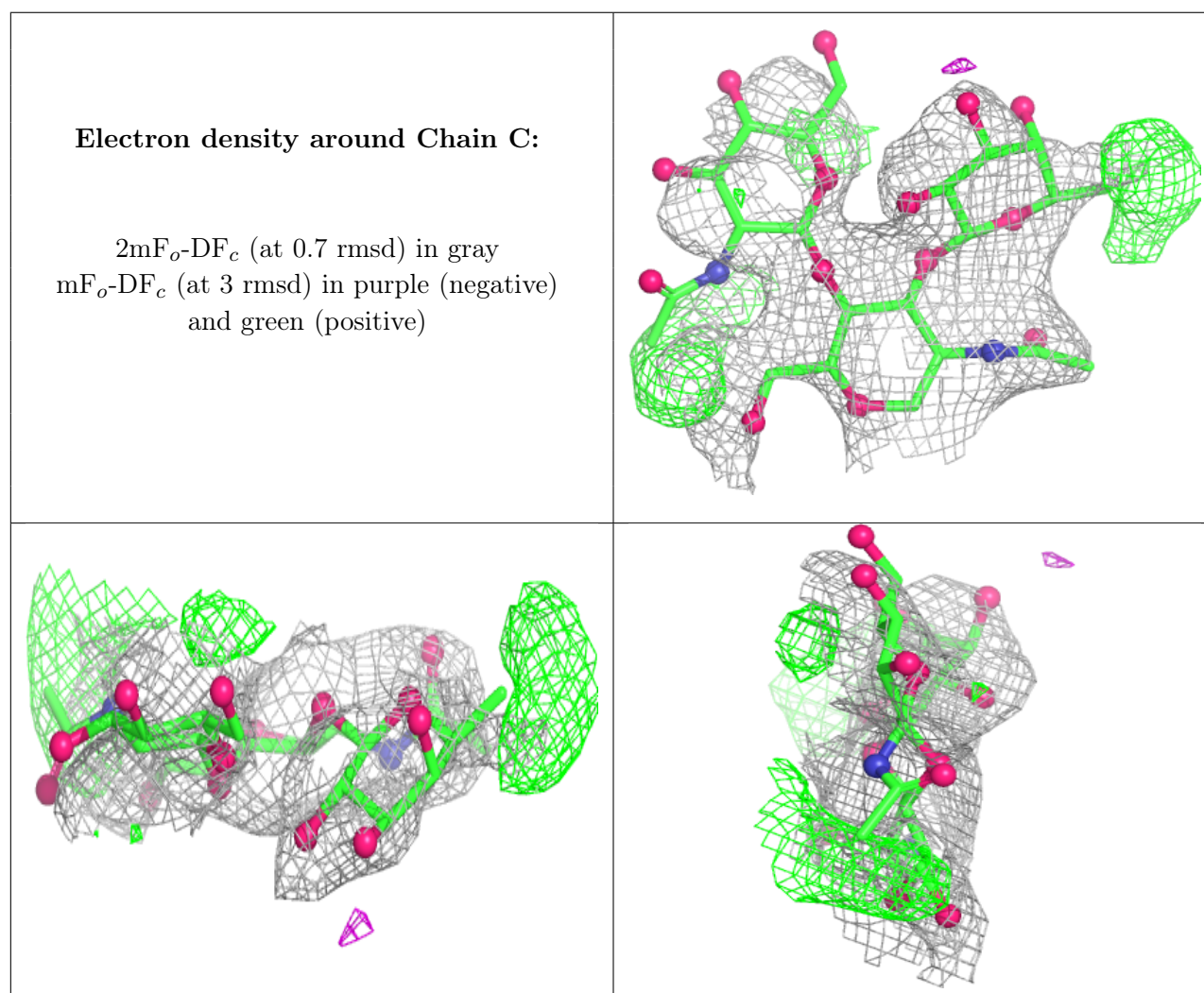
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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.

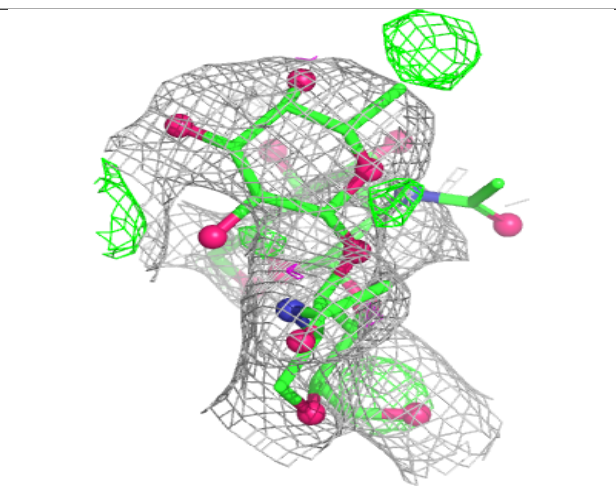
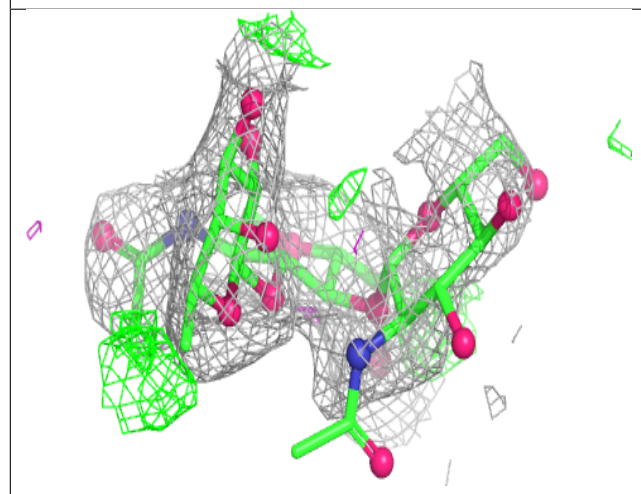
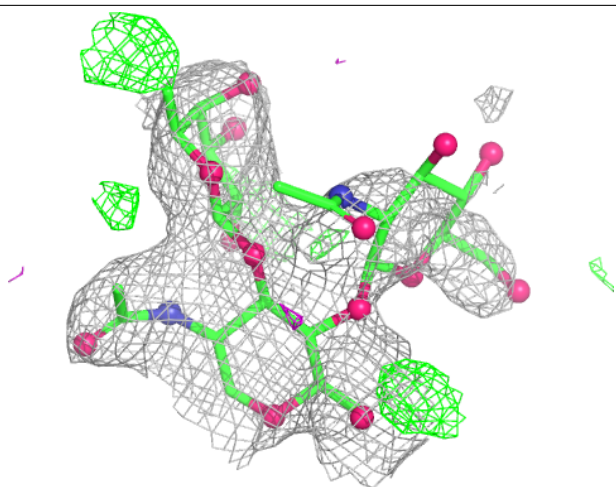
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUL	C	2	10/11	0.25	0.27	137,140,144,148	0
2	NAG	C	3	14/15	0.26	0.22	159,172,176,176	0
3	NAG	D	2	14/15	0.40	0.23	156,171,174,177	0
2	FUL	E	2	10/11	0.44	0.23	121,127,128,130	0
2	NAG	E	3	14/15	0.70	0.19	141,153,160,161	0
2	NAG	E	1	14/15	0.75	0.17	89,98,123,135	0
2	NAG	C	1	14/15	0.81	0.14	93,110,132,146	0
3	NAG	D	1	14/15	0.88	0.14	76,96,119,139	0

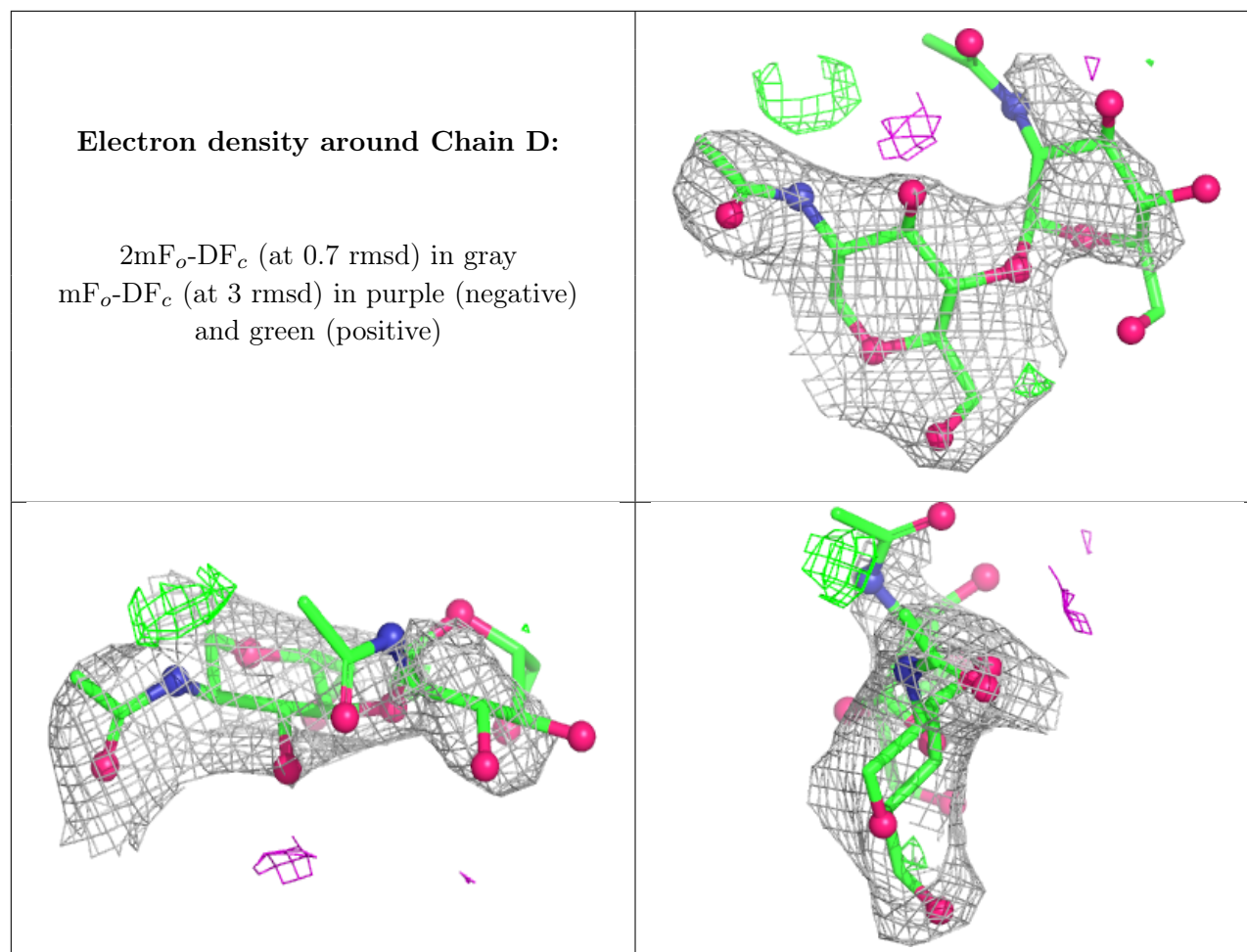
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain 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 ⓘ

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($\text{\AA}^2$)	Q<0.9
5	NAG	B	904	14/15	0.74	0.19	93,110,122,129	0
4	GOL	B	906	6/6	0.81	0.23	55,78,87,87	0
4	GOL	A	906	6/6	0.81	0.29	65,93,98,99	0
4	GOL	A	909	6/6	0.84	0.24	88,93,95,97	0
4	GOL	A	908	6/6	0.85	0.17	48,69,78,85	0
4	GOL	A	910	6/6	0.85	0.19	44,77,83,87	0
4	GOL	B	908	6/6	0.86	0.23	95,98,102,105	0
4	GOL	B	907	6/6	0.88	0.23	79,83,88,92	0
4	GOL	B	905	6/6	0.91	0.17	53,67,75,83	0
4	GOL	A	907	6/6	0.94	0.11	62,71,74,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.