



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2026 – 06:17 PM EDT

PDB ID : 9YO6 / pdb_00009yo6
Title : Crystal structure of integrin α 4b1 headpiece in complex with DS 13g (Mn)
Authors : Monroy, M.F.; Lin, F.Y.; Qiao, Q.
Deposited on : 2025-10-13
Resolution : 2.22 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 Phenix2.2
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.2
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

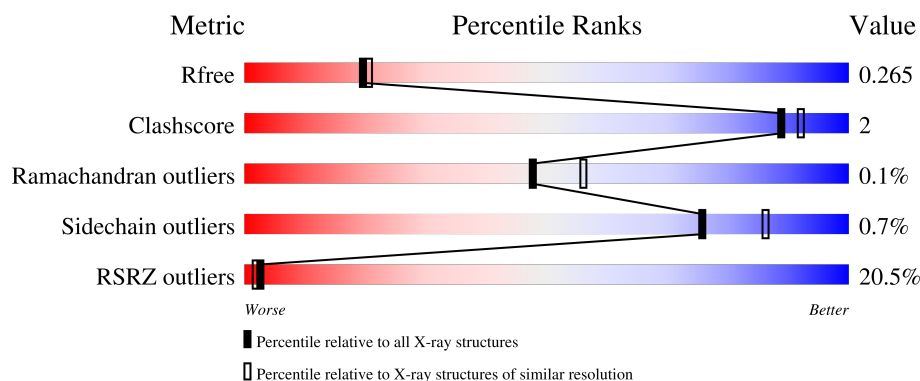
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	597	8% 95% ..
2	B	490	34% 87% • 8%
3	C	3	100%
3	E	3	67% 33%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16196 atoms, of which 7869 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Integrin α 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	588	Total	C	H	N	O	S	0	0	0
			8966	2858	4435	785	866	22			

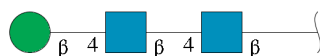
- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	449	Total	C	H	N	O	S	0	0	0
			6783	2155	3323	581	694	30			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	HIS	THR	conflict	UNP P05556
B	195	THR	SER	conflict	UNP P05556
B	482	GLY	-	expression tag	UNP P05556
B	483	GLY	-	expression tag	UNP P05556
B	484	SER	-	expression tag	UNP P05556
B	485	GLU	-	expression tag	UNP P05556
B	486	ASN	-	expression tag	UNP P05556
B	487	LEU	-	expression tag	UNP P05556
B	488	TYR	-	expression tag	UNP P05556
B	489	PHE	-	expression tag	UNP P05556
B	490	GLN	-	expression tag	UNP P05556

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

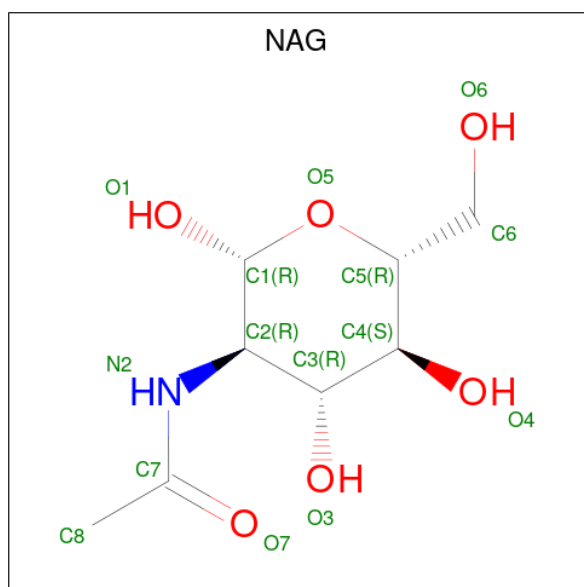


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	3	Total	C	H	N	O	0	0	0
			63	22	24	2	15			
3	E	3	Total	C	H	N	O	0	0	0
			62	22	23	2	15			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

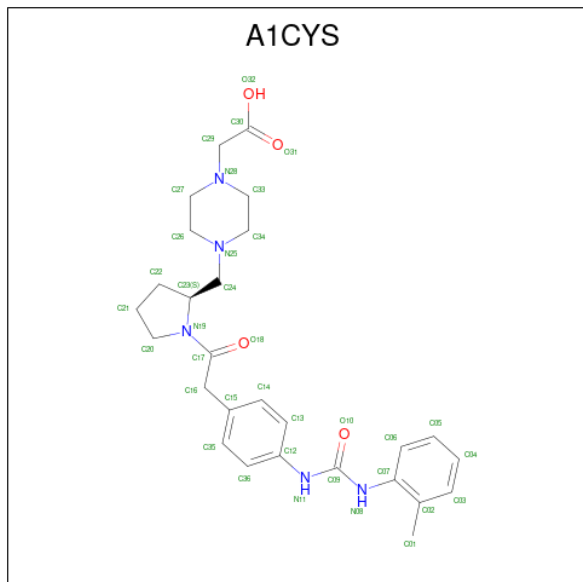
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mn	0	0
			3	3		
4	B	3	Total	Mn	0	0
			3	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			24	8	10	1	5		
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	H	N	O	0	0
			24	8	10	1	5		
5	A	1	Total	C	H	N	O	0	0
			24	8	10	1	5		
5	B	1	Total	C	N	O		0	0
			14	8	1	5			

- Molecule 6 is (4-{[(2S)-1-({4-[(2-methylphenyl)carbamamido]phenyl}acetyl)pyrrolidin-2-yl]methyl}piperazin-1-yl)acetic acid (CCD ID: A1CYS) (formula: $C_{27}H_{35}N_5O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	0	0
			70	27	34	5	4		

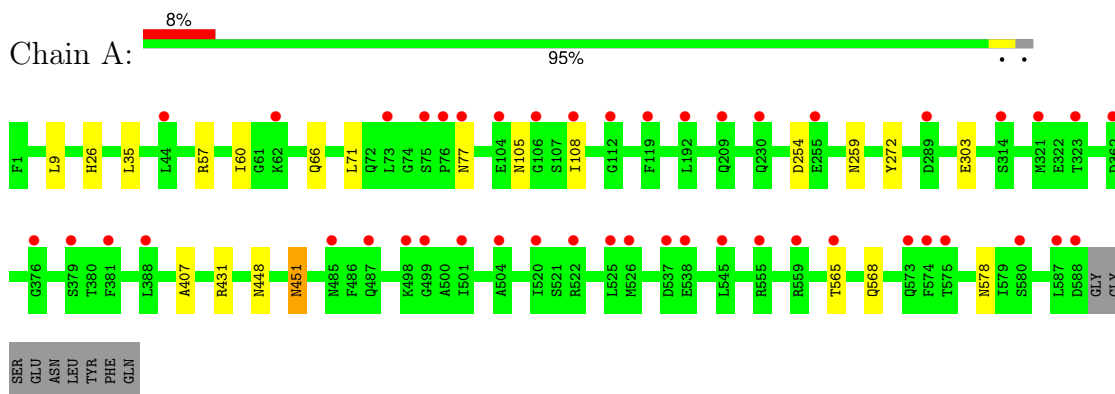
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	106	Total	O	0	0
			106	106		
7	B	40	Total	O	0	0
			40	40		

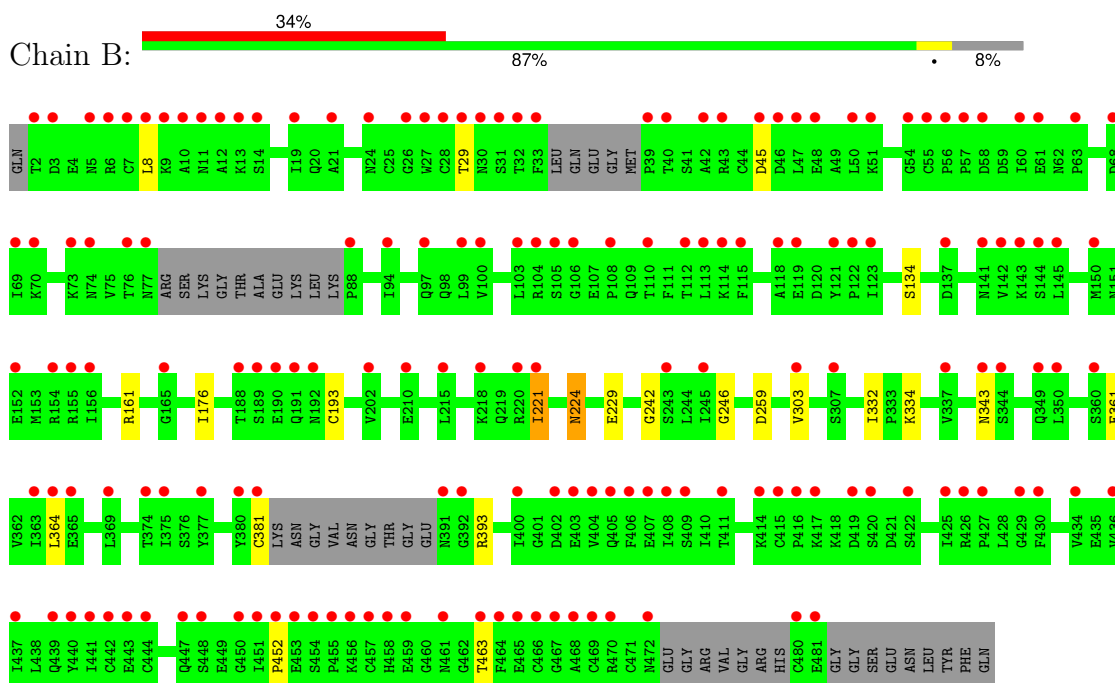
3 Residue-property plots

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: Integrin α 4



- Molecule 2: Integrin beta-1



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

Chain C:  100%

MAG1
MAG2
BMA3

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

Chain E:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.46Å 109.64Å 125.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.52 – 2.22 82.52 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.5 (82.52-2.22) 99.9 (82.52-2.22)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, R_{free}	0.233 , 0.258 0.239 , 0.265	Depositor DCC
R_{free} test set	2810 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16196	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: A1CYS, BMA, MN, 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	0.12	0/4624	0.34	0/6259
2	B	0.11	0/3520	0.30	0/4756
All	All	0.12	0/8144	0.33	0/11015

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	4531	4435	4436	17	0
2	B	3460	3323	3321	11	0
3	C	39	24	34	0	0
3	E	39	23	34	2	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	56	30	52	4	0
5	B	14	0	13	0	0
6	B	36	34	0	0	0
7	A	106	0	0	1	0
7	B	40	0	0	0	0
All	All	8327	7869	7890	30	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 2.

All (30) 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:A:77:ASN:HA	5:A:605:NAG:H83	1.59	0.81
1:A:35:LEU:CD1	1:A:108:ILE:HD13	2.28	0.62
1:A:451:ASN:OD1	3:E:1:NAG:C1	2.50	0.59
5:A:605:NAG:H82	5:A:605:NAG:O3	2.03	0.59
1:A:35:LEU:HD11	1:A:108:ILE:HD13	1.86	0.57
2:B:8:LEU:HD21	2:B:45:ASP:OD1	2.07	0.55
1:A:105:ASN:HD21	5:A:606:NAG:C1	2.19	0.55
1:A:9:LEU:HD22	1:A:66:GLN:NE2	2.22	0.54
2:B:303:VAL:HG22	2:B:332:ILE:HG12	1.89	0.53
2:B:161:ARG:NH2	2:B:246:GLY:O	2.43	0.51
2:B:452:PRO:HA	2:B:463:THR:HG22	1.92	0.50
1:A:26:HIS:CG	1:A:108:ILE:HD11	2.47	0.49
2:B:134:SER:OG	2:B:259:ASP:OD2	2.20	0.49
2:B:334:LYS:NZ	2:B:361:GLU:O	2.45	0.49
1:A:431:ARG:HD2	1:A:568:GLN:O	2.13	0.48
2:B:364:LEU:O	2:B:393:ARG:HD3	2.14	0.48
1:A:303:GLU:OE1	7:A:701:HOH:O	2.20	0.46
1:A:254:ASP:OD2	1:A:259:ASN:ND2	2.44	0.46
1:A:578:ASN:OD1	5:A:607:NAG:C1	2.63	0.46
3:E:2:NAG:O3	3:E:3:BMA:H2	2.17	0.45
1:A:60:ILE:HG21	1:A:407:ALA:HB1	1.99	0.45
1:A:9:LEU:HD22	1:A:66:GLN:HE21	1.81	0.44
2:B:176:ILE:HG22	2:B:224:ASN:HB2	2.00	0.43
1:A:565:THR:HG22	1:A:565:THR:O	2.18	0.43
1:A:57:ARG:HD3	1:A:71:LEU:HD21	2.01	0.42
2:B:29:THR:O	2:B:29:THR:OG1	2.37	0.42
1:A:26:HIS:ND1	1:A:108:ILE:HD11	2.35	0.42
2:B:229:GLU:OE1	2:B:229:GLU:HA	2.20	0.41
2:B:193:CYS:SG	2:B:221:ILE:HG22	2.61	0.41
1:A:448:ASN:HB3	1:A:451:ASN:HB3	2.04	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	586/597 (98%)	569 (97%)	17 (3%)	0	100	100
2	B	439/490 (90%)	416 (95%)	22 (5%)	1 (0%)	43	50
All	All	1025/1087 (94%)	985 (96%)	39 (4%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	242	GLY

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	487/496 (98%)	485 (100%)	2 (0%)	84	91
2	B	394/431 (91%)	390 (99%)	4 (1%)	68	80
All	All	881/927 (95%)	875 (99%)	6 (1%)	76	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	TYR
1	A	451	ASN
2	B	221	ILE
2	B	224	ASN
2	B	343	ASN

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Mol	Chain	Res	Type
2	B	381	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	72	GLN
1	A	105	ASN
1	A	123	ASN
1	A	209	GLN
1	A	437	ASN
2	B	249	ASN

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 ⓘ

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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.27	0	17,19,21	0.57	0
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.47	0
3	BMA	C	3	3	11,11,12	0.61	0	15,15,17	0.77	0
3	NAG	E	1	3	14,14,15	0.74	1 (7%)	17,19,21	0.48	0
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	0.58	0
3	BMA	E	3	3	11,11,12	0.87	0	15,15,17	0.84	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	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-2.65	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

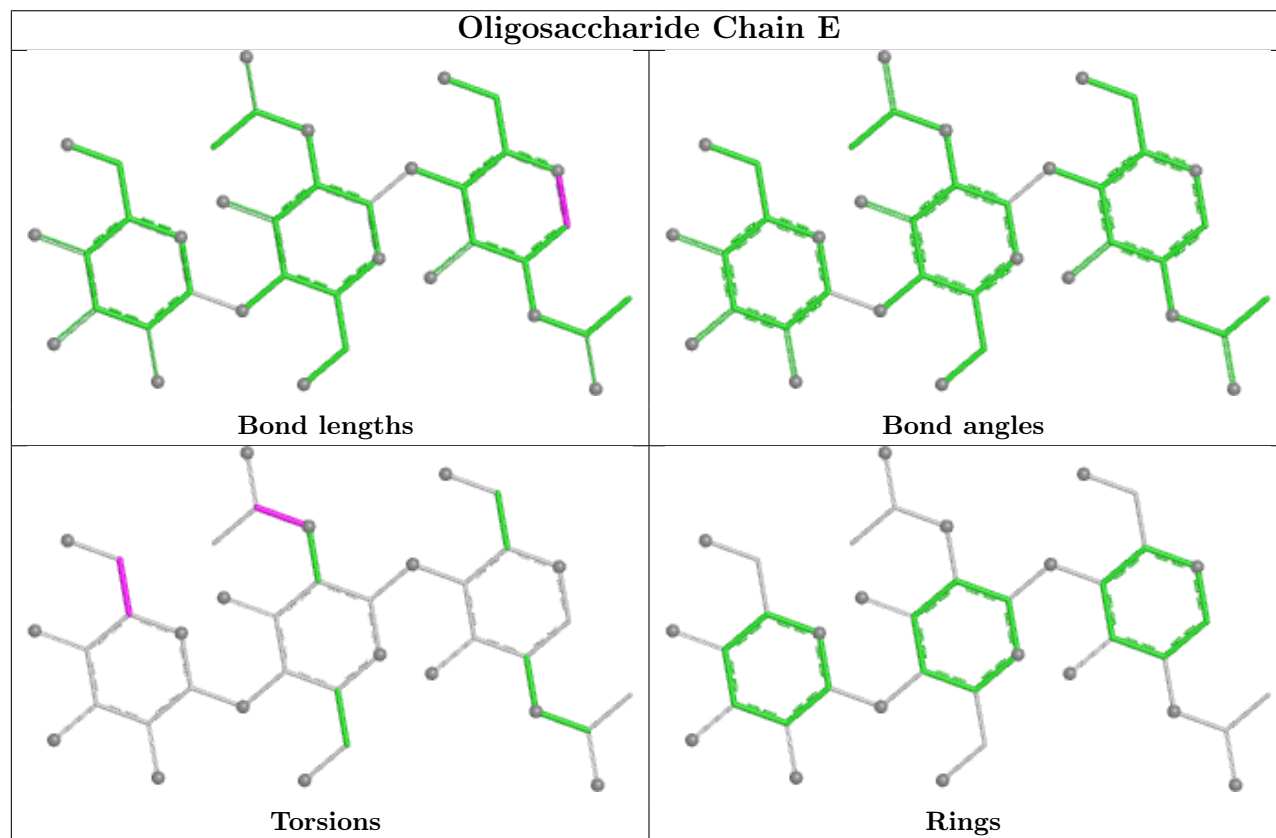
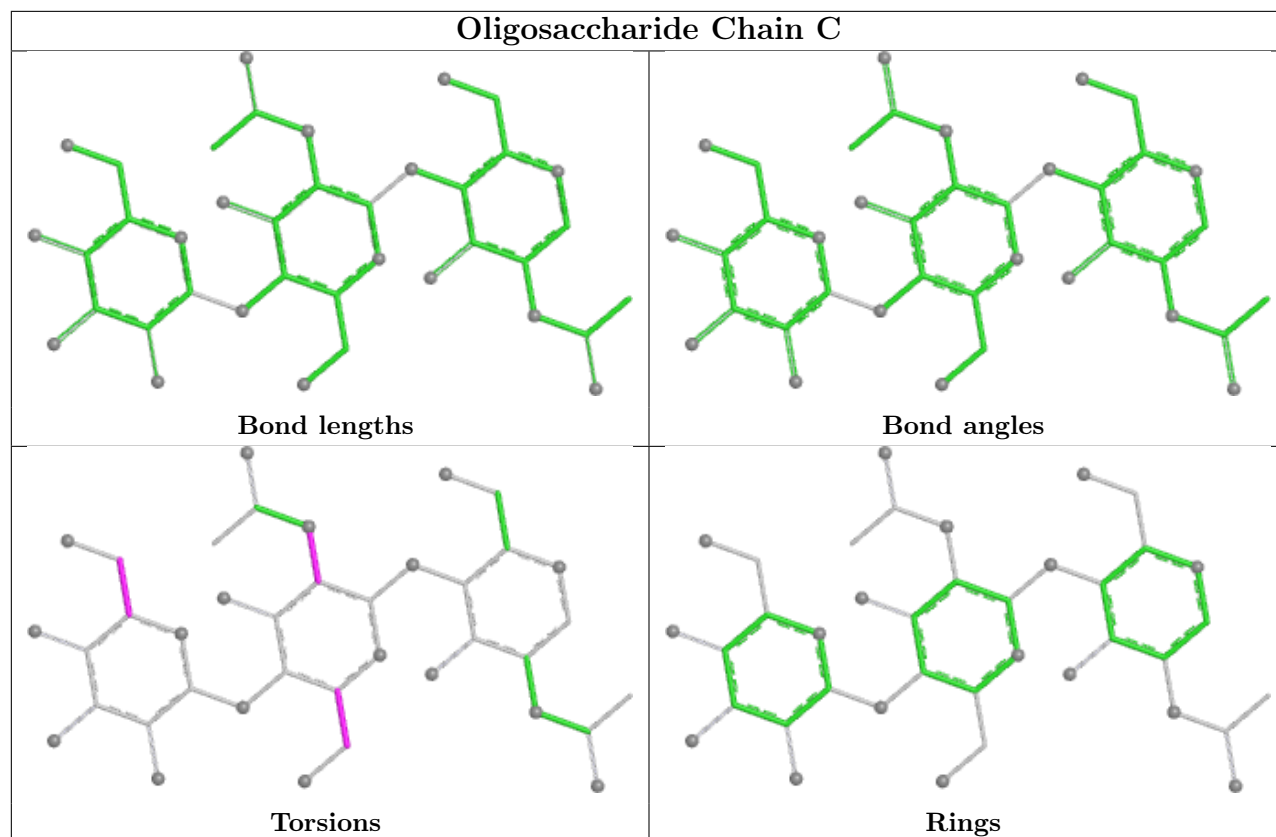
Mol	Chain	Res	Type	Atoms
3	C	3	BMA	O5-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	C	3	BMA	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 2 short contacts:

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

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



5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	2004	2	14,14,15	0.35	0	17,19,21	0.47	0
6	A1CYS	B	2005	4	39,39,39	2.75	11 (28%)	53,53,53	1.31	8 (15%)
5	NAG	A	606	-	14,14,15	0.57	0	17,19,21	0.94	1 (5%)
5	NAG	A	605	1	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	A	604	1	14,14,15	0.44	0	17,19,21	0.51	0
5	NAG	A	607	-	14,14,15	0.44	0	17,19,21	0.42	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
5	NAG	B	2004	2	-	2/6/23/26	0/1/1/1
6	A1CYS	B	2005	4	-	1/24/44/44	0/4/4/4
5	NAG	A	606	-	-	0/6/23/26	0/1/1/1
5	NAG	A	605	1	-	4/6/23/26	0/1/1/1
5	NAG	A	604	1	-	2/6/23/26	0/1/1/1
5	NAG	A	607	-	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2005	A1CYS	C23-N19	7.98	1.60	1.47
6	B	2005	A1CYS	C20-N19	-7.12	1.33	1.47
6	B	2005	A1CYS	C22-C23	-6.78	1.36	1.53
6	B	2005	A1CYS	C09-N11	4.89	1.48	1.37
6	B	2005	A1CYS	C17-N19	4.84	1.49	1.35
6	B	2005	A1CYS	C09-N08	4.40	1.47	1.37
6	B	2005	A1CYS	C12-N11	4.20	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2005	A1CYS	C29-C30	2.76	1.57	1.51
6	B	2005	A1CYS	C16-C15	2.69	1.56	1.51
6	B	2005	A1CYS	O10-C09	-2.55	1.17	1.23
6	B	2005	A1CYS	C01-C02	2.13	1.55	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2005	A1CYS	C03-C02-C07	2.57	119.91	117.50
6	B	2005	A1CYS	C34-N25-C26	2.28	113.75	108.84
6	B	2005	A1CYS	C21-C20-N19	2.28	107.16	103.24
5	A	606	NAG	C1-O5-C5	2.27	115.23	112.19
6	B	2005	A1CYS	C29-N28-C33	-2.26	107.63	111.14
6	B	2005	A1CYS	C22-C23-N19	2.24	106.73	102.85
6	B	2005	A1CYS	C01-C02-C07	-2.20	118.73	121.23
6	B	2005	A1CYS	C33-N28-C27	2.15	113.48	108.84
6	B	2005	A1CYS	C27-C26-N25	2.03	114.74	110.65

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	605	NAG	O5-C5-C6-O6
5	B	2004	NAG	O5-C5-C6-O6
5	A	605	NAG	C4-C5-C6-O6
5	A	604	NAG	O5-C5-C6-O6
5	B	2004	NAG	C4-C5-C6-O6
5	A	605	NAG	C8-C7-N2-C2
5	A	605	NAG	O7-C7-N2-C2
5	A	604	NAG	C4-C5-C6-O6
6	B	2005	A1CYS	N28-C29-C30-O31

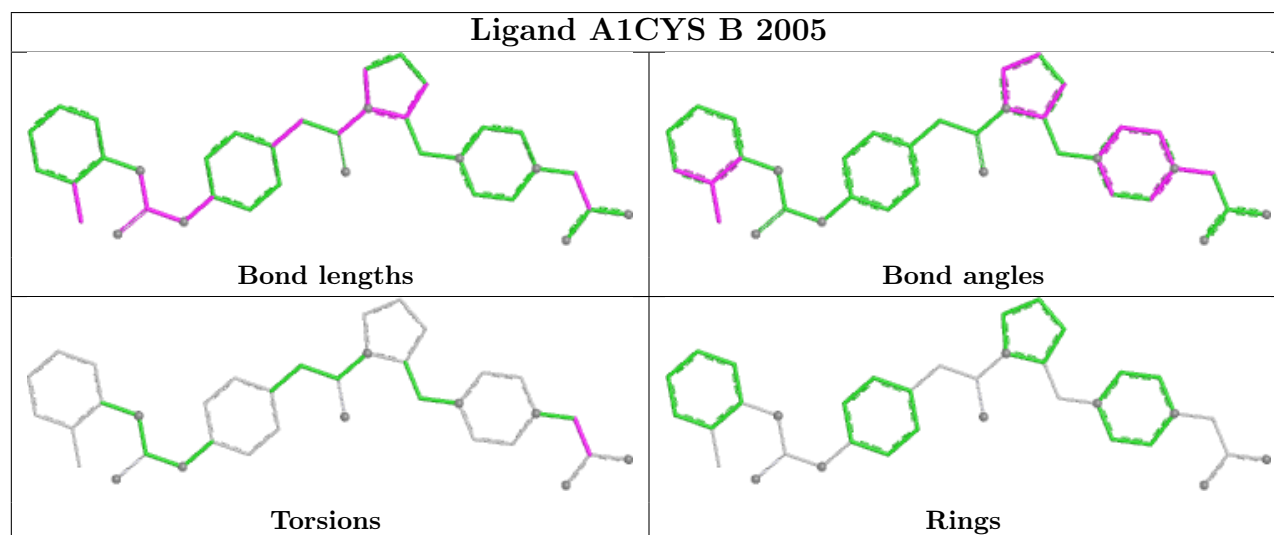
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	NAG	1	0
5	A	605	NAG	2	0
5	A	607	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	588/597 (98%)	0.64	46 (7%)	19 16	29, 51, 90, 150	0
2	B	449/490 (91%)	1.68	167 (37%)	1 0	32, 84, 134, 155	0
All	All	1037/1087 (95%)	1.09	213 (20%)	2 2	29, 58, 121, 155	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	60	ILE	8.9
2	B	468	ALA	7.5
2	B	57	PRO	6.5
2	B	469	CYS	6.4
2	B	47	LEU	6.2
2	B	464	PHE	5.9
2	B	451	ILE	5.8
2	B	50	LEU	5.6
2	B	369	LEU	5.1
2	B	427	PRO	4.9
2	B	150	MET	4.8
2	B	5	ASN	4.7
2	B	452	PRO	4.7
2	B	188	THR	4.7
1	A	538	GLU	4.5
2	B	404	VAL	4.4
2	B	88	PRO	4.4
2	B	142	VAL	4.2
2	B	27	TRP	4.1
2	B	414	LYS	4.1
2	B	31	SER	4.1
2	B	457	CYS	4.1
1	A	498	LYS	4.1
2	B	100	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	447	GLN	4.0
2	B	381	CYS	4.0
2	B	42	ALA	3.9
1	A	555	ARG	3.9
2	B	400	ILE	3.8
1	A	574	PHE	3.8
2	B	189	SER	3.8
2	B	408	ILE	3.8
2	B	39	PRO	3.7
2	B	54	GLY	3.7
2	B	364	LEU	3.7
2	B	156	ILE	3.7
2	B	55	CYS	3.7
2	B	458	HIS	3.6
2	B	45	ASP	3.6
2	B	380	TYR	3.6
2	B	40	THR	3.6
2	B	112	THR	3.6
2	B	110	THR	3.6
2	B	465	GLU	3.6
2	B	94	ILE	3.5
2	B	113	LEU	3.5
2	B	415	CYS	3.5
2	B	425	ILE	3.5
1	A	525	LEU	3.5
2	B	68	ASP	3.5
1	A	487	GLN	3.5
2	B	434	VAL	3.5
2	B	33	PHE	3.5
1	A	76	PRO	3.4
2	B	6	ARG	3.4
2	B	73	LYS	3.4
2	B	363	ILE	3.4
2	B	430	PHE	3.4
2	B	2	THR	3.4
2	B	463	THR	3.4
1	A	104	GLU	3.4
2	B	375	ILE	3.3
1	A	75	SER	3.3
2	B	12	ALA	3.3
2	B	343	ASN	3.3
2	B	119	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	453	GLU	3.2
2	B	76	THR	3.2
2	B	115	PHE	3.2
2	B	154	ARG	3.2
2	B	417	LYS	3.2
2	B	436	VAL	3.2
2	B	56	PRO	3.1
2	B	99	LEU	3.1
2	B	349	GLN	3.1
2	B	70	LYS	3.1
2	B	360	SER	3.1
2	B	405	GLN	3.1
2	B	190	GLU	3.1
2	B	406	PHE	3.1
2	B	429	GLY	3.1
1	A	73	LEU	3.1
1	A	545	LEU	3.1
2	B	14	SER	3.0
2	B	481	GLU	3.0
2	B	470	ARG	3.0
1	A	588	ASP	3.0
1	A	522	ARG	3.0
2	B	9	LYS	3.0
2	B	422	SER	3.0
2	B	77	ASN	3.0
2	B	32	THR	3.0
2	B	467	GLY	3.0
1	A	501	ILE	2.9
2	B	30	ASN	2.9
1	A	381	PHE	2.9
2	B	392	GLY	2.9
2	B	51	LYS	2.9
2	B	455	PRO	2.9
2	B	472	ASN	2.9
1	A	526	MET	2.8
2	B	377	TYR	2.8
2	B	21	ALA	2.8
2	B	440	TYR	2.8
2	B	456	LYS	2.8
2	B	103	LEU	2.7
2	B	350	LEU	2.7
2	B	137	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	580	SER	2.7
2	B	307	SER	2.7
2	B	454	SER	2.7
2	B	108	PRO	2.7
2	B	61	GLU	2.7
2	B	480	CYS	2.7
2	B	3	ASP	2.7
2	B	13	LYS	2.7
2	B	118	ALA	2.6
2	B	459	GLU	2.6
1	A	575	THR	2.6
2	B	411	THR	2.6
2	B	145	LEU	2.6
2	B	202	VAL	2.6
2	B	420	SER	2.6
1	A	321	MET	2.6
2	B	441	ILE	2.6
2	B	26	GLY	2.5
2	B	437	ILE	2.5
1	A	379	SER	2.5
2	B	344	SER	2.5
2	B	391	ASN	2.5
2	B	450	GLY	2.5
1	A	565	THR	2.5
1	A	119	PHE	2.5
2	B	403	GLU	2.5
1	A	230	GLN	2.5
1	A	499	GLY	2.5
2	B	106	GLY	2.5
2	B	29	THR	2.4
2	B	365	GLU	2.4
2	B	443	GLU	2.4
2	B	215	LEU	2.4
2	B	24	ASN	2.4
1	A	323	THR	2.4
2	B	448	SER	2.4
2	B	245	ILE	2.4
2	B	402	ASP	2.4
1	A	520	ILE	2.4
2	B	69	ILE	2.4
2	B	220	ARG	2.4
2	B	11	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	8	LEU	2.4
2	B	407	GLU	2.4
1	A	362	ASP	2.3
2	B	46	ASP	2.3
1	A	559	ARG	2.3
2	B	444	CYS	2.3
1	A	587	LEU	2.3
1	A	255	GLU	2.3
2	B	416	PRO	2.3
2	B	10	ALA	2.3
2	B	74	ASN	2.3
2	B	63	PRO	2.3
2	B	43	ARG	2.3
2	B	409	SER	2.3
1	A	192	LEU	2.3
1	A	106	GLY	2.3
2	B	155	ARG	2.3
2	B	374	THR	2.3
1	A	209	GLN	2.3
2	B	210	GLU	2.3
2	B	439	GLN	2.3
1	A	112	GLY	2.2
2	B	152	GLU	2.2
1	A	314	SER	2.2
2	B	419	ASP	2.2
1	A	376	GLY	2.2
1	A	388	LEU	2.2
2	B	303	VAL	2.2
2	B	192	ASN	2.2
2	B	165	GLY	2.2
2	B	48	GLU	2.2
2	B	143	LYS	2.2
2	B	105	SER	2.2
2	B	19	ILE	2.2
2	B	426	ARG	2.2
1	A	77	ASN	2.2
1	A	485	ASN	2.2
2	B	104	ARG	2.1
1	A	573	GLN	2.1
2	B	466	CYS	2.1
1	A	504	ALA	2.1
1	A	108	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	58	ASP	2.1
2	B	337	VAL	2.1
2	B	97	GLN	2.1
2	B	144	SER	2.1
1	A	44	LEU	2.1
2	B	221	ILE	2.1
2	B	191	GLN	2.1
2	B	28	CYS	2.1
2	B	218	LYS	2.1
2	B	121	TYR	2.1
2	B	243	SER	2.0
2	B	442	CYS	2.0
2	B	141	ASN	2.0
2	B	461	ASN	2.0
2	B	123	ILE	2.0
2	B	122	PRO	2.0
1	A	62	LYS	2.0
2	B	7	CYS	2.0
1	A	289	ASP	2.0
1	A	537	ASP	2.0
2	B	114	LYS	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 ⓘ

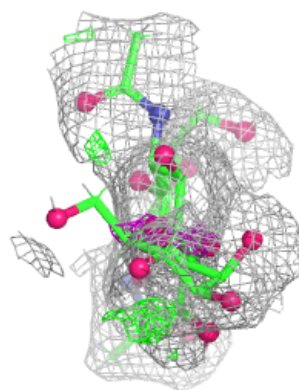
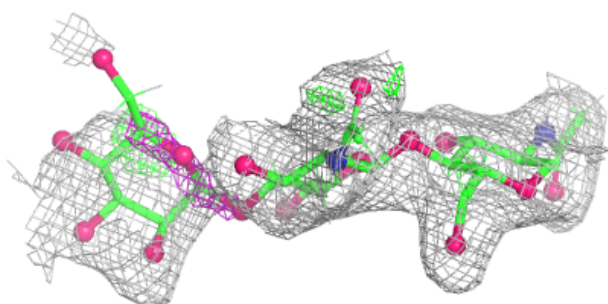
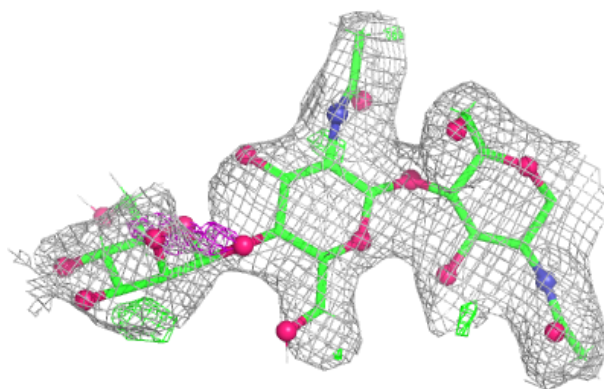
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	BMA	C	3	11/12	0.35	0.18	75,78,95,96	0
3	NAG	C	2	14/15	0.55	0.16	59,71,86,88	0
3	NAG	C	1	14/15	0.84	0.10	43,51,62,63	0
3	NAG	E	1	14/15	-	-	49,59,74,74	0
3	NAG	E	2	14/15	-	-	52,63,79,79	0
3	BMA	E	3	11/12	-	-	61,70,84,84	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.

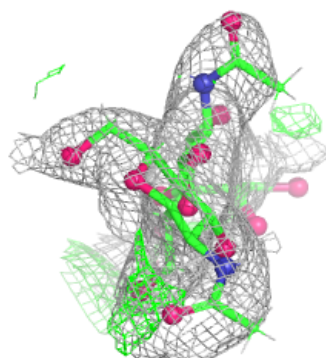
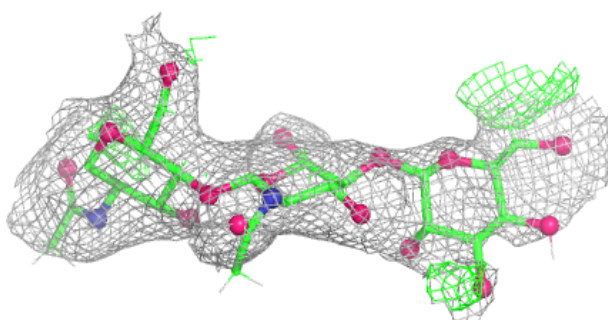
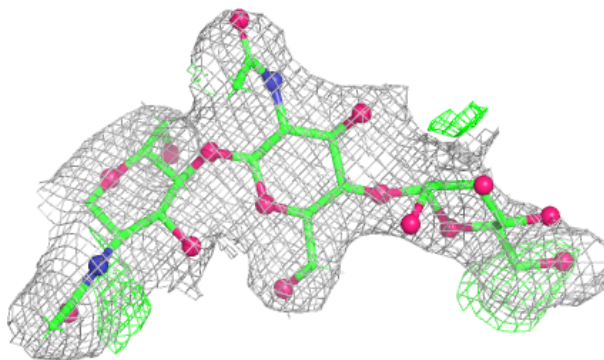
Electron density around Chain C:

$2mF_o-DF_c$ (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

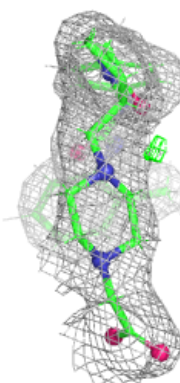
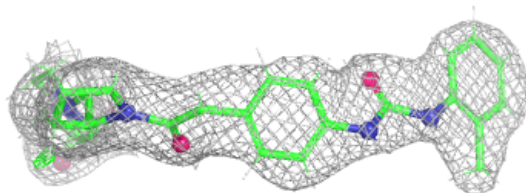
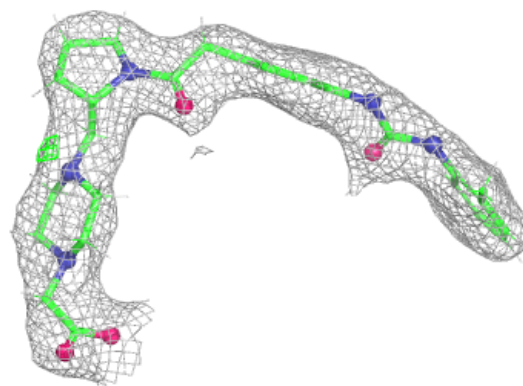
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	604	14/15	0.41	0.18	61,67,81,81	0
5	NAG	B	2004	14/15	0.58	0.19	56,58,62,65	0
5	NAG	A	606	14/15	0.60	0.20	72,77,91,92	0
5	NAG	A	607	14/15	0.61	0.19	69,72,88,89	0
5	NAG	A	605	14/15	0.64	0.16	62,64,69,70	0
4	MN	B	2003	1/1	0.89	0.12	69,69,69,69	0
6	A1CYS	B	2005	36/36	0.91	0.11	39,44,52,52	0
4	MN	A	602	1/1	0.95	0.12	53,53,53,53	0
4	MN	A	603	1/1	0.96	0.12	53,53,53,53	0
4	MN	B	2002	1/1	0.98	0.06	37,37,37,37	0
4	MN	A	601	1/1	0.98	0.07	52,52,52,52	0
4	MN	B	2001	1/1	0.99	0.02	38,38,38,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1CYS B 2005:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.