



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 12:05 AM EDT

PDB ID : 3BN3
Title : crystal structure of ICAM-5 in complex with aL I domain
Authors : Zhang, H.; Springer, T.A.; Wang, J.-h.
Deposited on : 2007-12-13
Resolution : 2.10 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 : 2.23.2
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) : 2.23.2

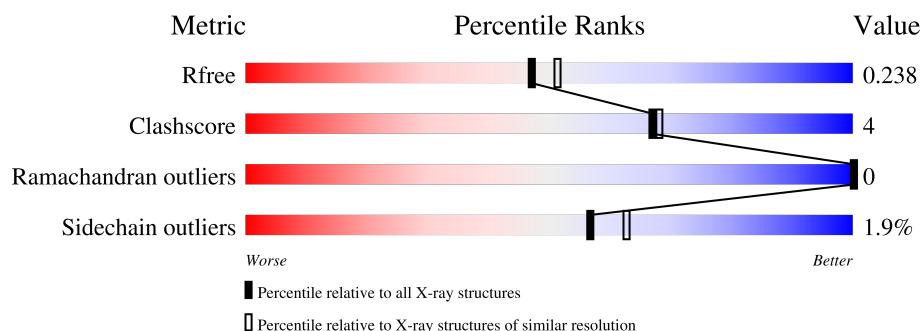
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	180	
2	B	196	
3	C	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3323 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 Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1446	933	230	278	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	MET	-	initiating methionine	UNP P20701
A	189	TRP	ARG	variant	UNP P20701
A	265	SER	PHE	engineered mutation	UNP P20701
A	292	GLY	PHE	engineered mutation	UNP P20701

- Molecule 2 is a protein called Intercellular adhesion molecule 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1554	968	308	271	7			

- 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	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- 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		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

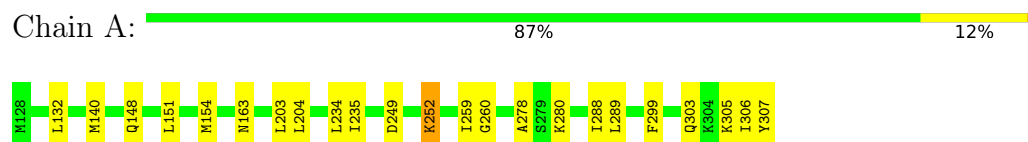
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total	O	0	0
			102	102		
7	B	124	Total	O	0	0
			124	124		

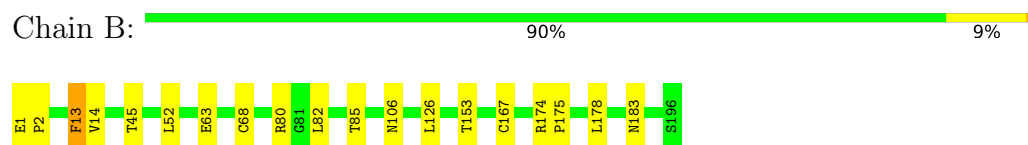
3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Integrin alpha-L



- Molecule 2: Intercellular adhesion molecule 5



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.79Å 71.51Å 143.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.98 – 2.10 39.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (71.98-2.10) 98.1 (39.20-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.3.0026	Depositor
R, R_{free}	0.191 , 0.235 0.201 , 0.238	Depositor DCC
R_{free} test set	1863 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3323	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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, NAG, MG

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	0.45	0/1474	0.58	0/1983
2	B	0.43	0/1590	0.67	0/2155
All	All	0.44	0/3064	0.63	0/4138

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	1446	0	1448	13	0
2	B	1554	0	1554	11	0
3	C	28	0	25	0	0
4	A	1	0	0	0	0
5	B	56	0	52	1	0
6	B	12	0	16	0	0
7	A	102	0	0	2	0
7	B	124	0	0	0	0
All	All	3323	0	3095	24	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 4.

All (24) 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:132:LEU:HD21	1:A:235:ILE:HD12	1.68	0.74
2:B:63:GLU:HG3	2:B:82:LEU:HD11	1.74	0.69
1:A:259:ILE:HG23	1:A:289:LEU:HD13	1.80	0.64
2:B:1:GLU:N	2:B:2:PRO:CD	2.65	0.60
1:A:260:GLY:HA3	1:A:288:ILE:HD13	1.87	0.56
1:A:259:ILE:CG2	1:A:289:LEU:HD13	2.40	0.51
1:A:148:GLN:NE2	7:A:359:HOH:O	2.42	0.51
2:B:13:PHE:HB3	2:B:178:LEU:HD11	1.91	0.51
1:A:163:ASN:O	7:A:344:HOH:O	2.19	0.51
1:A:140:MET:HE2	1:A:203:LEU:HB3	1.92	0.50
2:B:1:GLU:H3	2:B:2:PRO:CD	2.24	0.50
5:B:201:NAG:O3	5:B:201:NAG:H83	2.11	0.50
1:A:306:ILE:O	1:A:307:TYR:HB2	2.11	0.49
2:B:1:GLU:H3	2:B:2:PRO:HD3	1.78	0.48
2:B:14:VAL:O	2:B:85:THR:HA	2.15	0.46
1:A:299:PHE:O	1:A:303:GLN:HG2	2.17	0.45
1:A:204:LEU:HD23	2:B:80:ARG:HH12	1.82	0.44
1:A:151:LEU:HD23	1:A:154:MET:CE	2.47	0.44
1:A:278:ALA:O	1:A:280:LYS:NZ	2.52	0.43
2:B:126:LEU:HD23	2:B:167:CYS:HB3	1.99	0.43
2:B:45:THR:HG23	2:B:52:LEU:HD11	2.00	0.43
2:B:106:ASN:HB3	2:B:153:THR:CG2	2.50	0.42
2:B:174:ARG:N	2:B:175:PRO:CD	2.83	0.42
1:A:249:ASP:O	1:A:252:LYS:HD2	2.20	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	178/180 (99%)	171 (96%)	7 (4%)	0	100	100
2	B	194/196 (99%)	191 (98%)	3 (2%)	0	100	100
All	All	372/376 (99%)	362 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	160/160 (100%)	157 (98%)	3 (2%)	57	63
2	B	164/164 (100%)	161 (98%)	3 (2%)	59	65
All	All	324/324 (100%)	318 (98%)	6 (2%)	57	63

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

Mol	Chain	Res	Type
1	A	234	LEU
1	A	252	LYS
1	A	305	LYS
2	B	13	PHE
2	B	68	CYS
2	B	183	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates

2 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	2,3	14,14,15	0.46	0	17,19,21	2.14	4 (23%)
3	NAG	C	2	3	14,14,15	0.68	0	17,19,21	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	2,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	5.27	119.33	112.19
3	C	1	NAG	O4-C4-C5	4.24	119.83	109.30
3	C	1	NAG	C4-C3-C2	-3.43	105.99	111.02
3	C	1	NAG	C1-C2-N2	2.06	114.00	110.49

There are no chirality outliers.

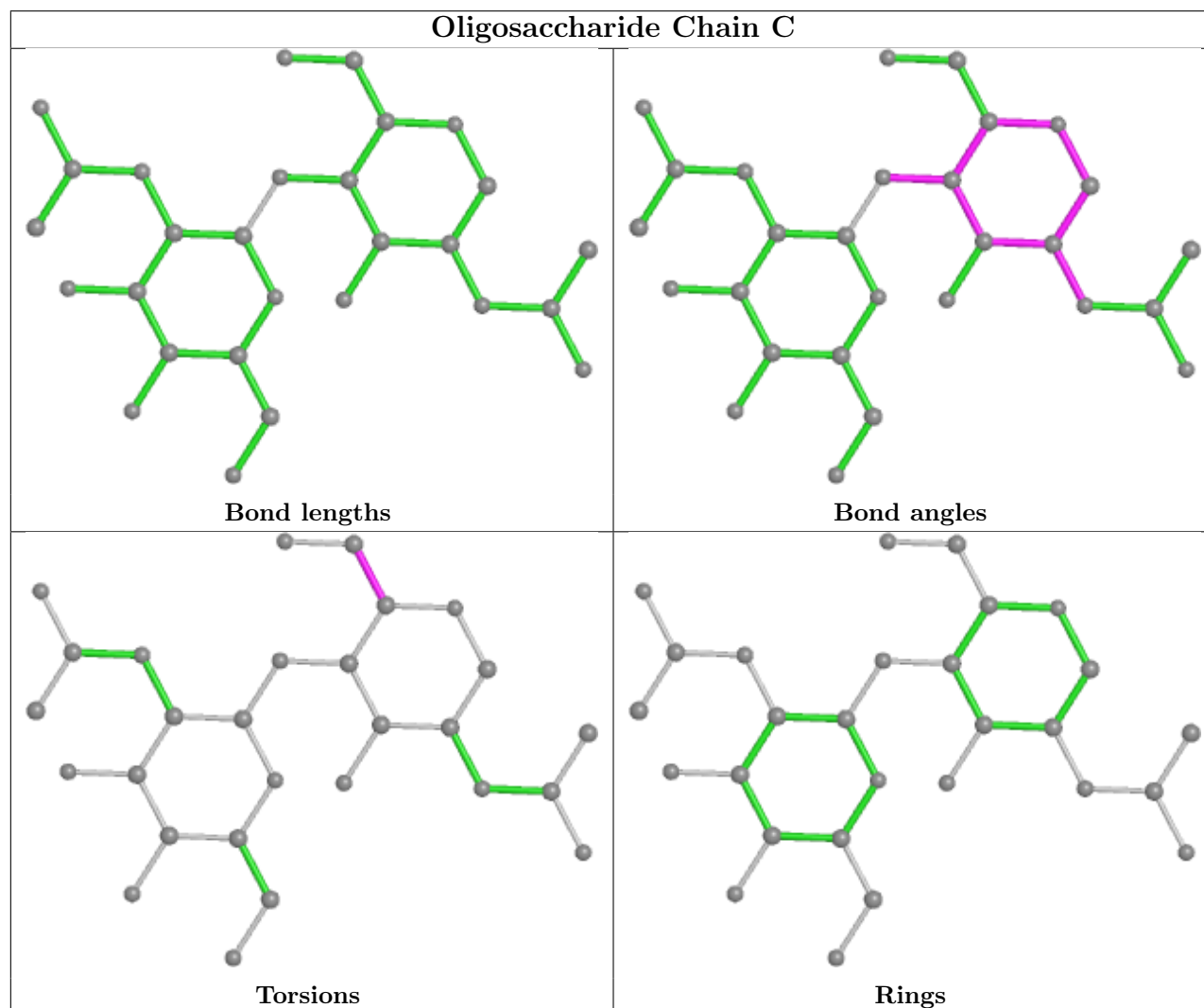
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is 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	201	2	14,14,15	0.56	0	17,19,21	1.24	2 (11%)
5	NAG	B	199	2	14,14,15	0.55	0	17,19,21	0.79	0
6	GOL	B	204	-	5,5,5	0.46	0	5,5,5	0.22	0
6	GOL	B	203	-	5,5,5	0.42	0	5,5,5	0.20	0
5	NAG	B	202	2	14,14,15	0.52	0	17,19,21	1.45	1 (5%)
5	NAG	B	200	2	14,14,15	0.60	0	17,19,21	0.98	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
5	NAG	B	201	2	-	4/6/23/26	0/1/1/1
5	NAG	B	199	2	-	1/6/23/26	0/1/1/1
6	GOL	B	204	-	-	4/4/4/4	-
6	GOL	B	203	-	-	1/4/4/4	-
5	NAG	B	202	2	-	0/6/23/26	0/1/1/1
5	NAG	B	200	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	202	NAG	C1-O5-C5	4.83	118.74	112.19
5	B	201	NAG	C1-O5-C5	3.66	117.15	112.19
5	B	200	NAG	C1-O5-C5	3.12	116.42	112.19
5	B	201	NAG	O5-C5-C6	2.05	110.42	107.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	201	NAG	C8-C7-N2-C2
5	B	201	NAG	O7-C7-N2-C2
6	B	204	GOL	O1-C1-C2-C3
6	B	204	GOL	C1-C2-C3-O3
5	B	201	NAG	O5-C5-C6-O6
5	B	201	NAG	C4-C5-C6-O6
6	B	204	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	203	GOL	O1-C1-C2-O2
6	B	204	GOL	O2-C2-C3-O3
5	B	199	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	201	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

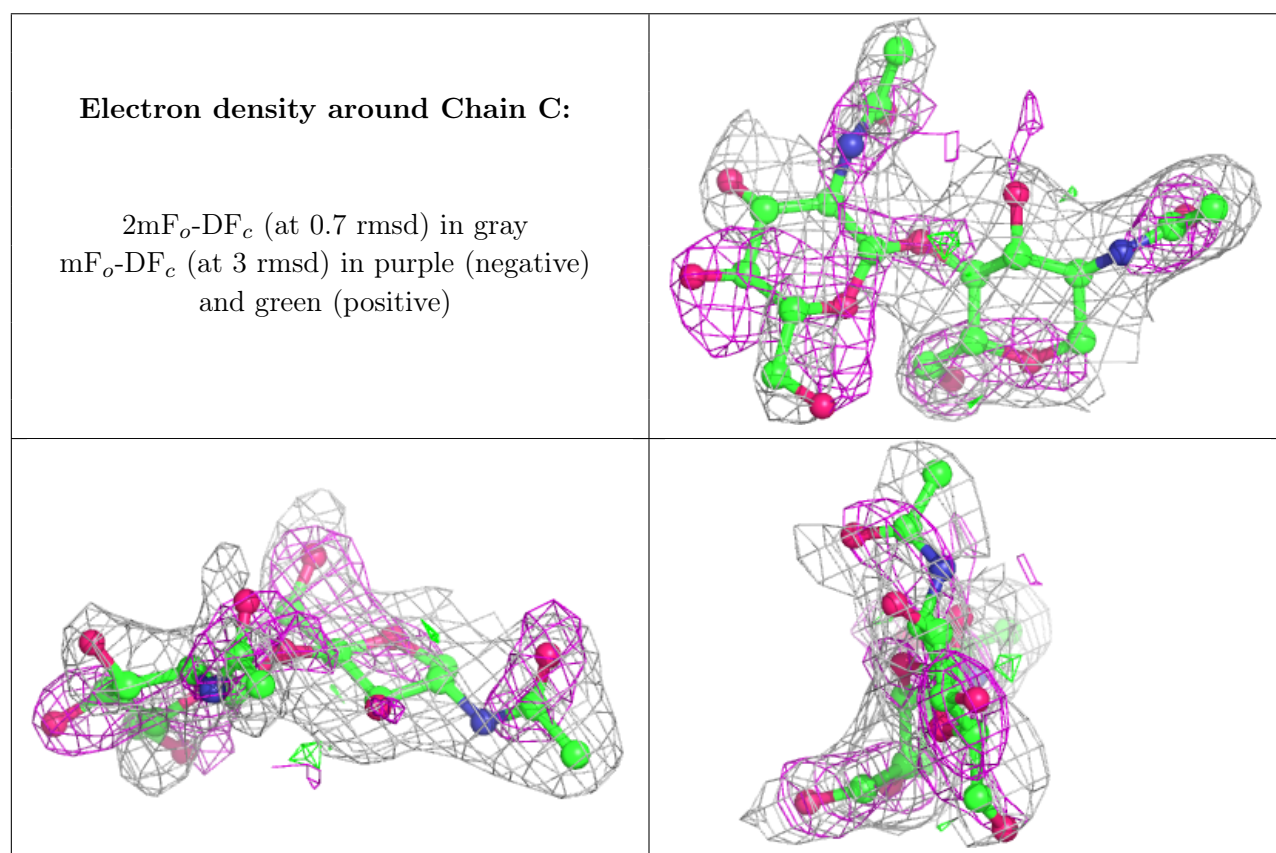
6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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

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



6.4 Ligands ⓘ

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

6.5 Other polymers [i](#)

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