



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2024 – 08:33 AM EDT

PDB ID : 4L1R
Title : Glycoprotein B from Herpes Simplex Virus type 1, A549T Rate-of-Entry mutant, low-pH
Authors : Stampfer, S.D.; Heldwein, E.E.
Deposited on : 2013-06-03
Resolution : 3.03 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

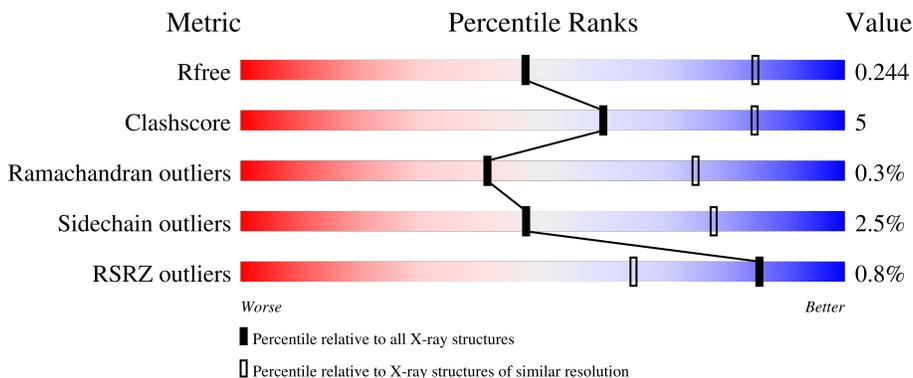
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	703	
1	B	703	
2	C	2	
2	D	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9943 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	608	4871	3073	857	919	22	0	0	0
1	B	608	4900	3090	861	927	22	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASP	-	expression tag	UNP P06437
A	29	PRO	-	expression tag	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437
A	313	SER	THR	SEE REMARK 999	UNP P06437
A	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	549	THR	ALA	engineered mutation	UNP P06437
B	28	ASP	-	expression tag	UNP P06437
B	29	PRO	-	expression tag	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
B	549	THR	ALA	engineered mutation	UNP P06437

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



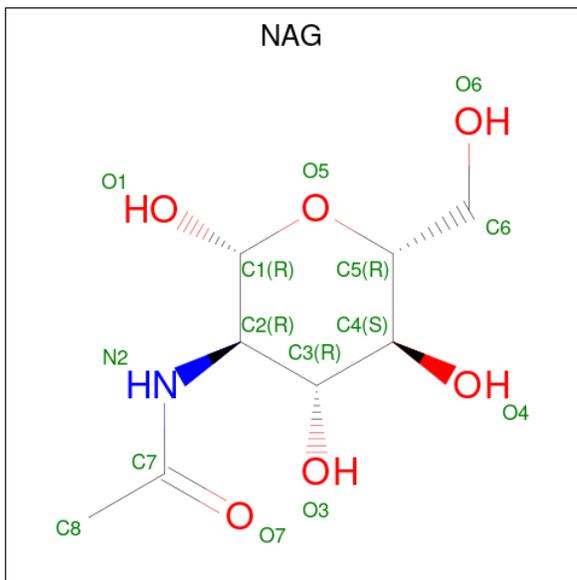
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0

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

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



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total 10	O 10	0	0
5	B	21	Total 21	O 21	0	0

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

Chain C:  100%

MAG1
MAG2

- Molecule 2: 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	P 3	Depositor
Cell constants a, b, c, α , β , γ	117.43Å 117.43Å 160.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.47 – 3.03 48.47 – 3.03	Depositor EDS
% Data completeness (in resolution range)	93.1 (48.47-3.03) 93.1 (48.47-3.03)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtrriage
Refinement program	PHENIX dev_1391	Depositor
R, R_{free}	0.201 , 0.243 0.204 , 0.244	Depositor DCC
R_{free} test set	2427 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.026 for -h,-k,l 0.479 for h,-h-k,-l 0.029 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9943	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: NAG, CL

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	0.34	0/4992	0.49	0/6791
1	B	0.34	0/5022	0.48	0/6830
All	All	0.34	0/10014	0.49	0/13621

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	4871	0	4646	51	0
1	B	4900	0	4679	36	0
2	C	28	0	25	0	0
2	D	28	0	25	2	0
3	A	28	0	26	0	0
3	B	56	0	52	0	0
4	A	1	0	0	0	0
5	A	10	0	0	1	0
5	B	21	0	0	2	0
All	All	9943	0	9453	89	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 5.

The worst 5 of 89 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:192:VAL:HG11	1:B:201:ILE:HD11	1.72	0.71
1:A:543:ARG:HD2	1:A:568:MET:HE3	1.74	0.70
1:A:314:TYR:HB3	1:A:318:ARG:HD2	1.73	0.68
1:A:176:GLY:O	1:A:258:ARG:NH2	2.28	0.67
1:A:207:CYS:HB3	1:A:249:THR:HG21	1.78	0.64

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	604/703 (86%)	580 (96%)	21 (4%)	3 (0%)	29 66
1	B	605/703 (86%)	574 (95%)	30 (5%)	1 (0%)	47 81
All	All	1209/1406 (86%)	1154 (96%)	51 (4%)	4 (0%)	41 75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	629	ALA
1	A	629	ALA
1	A	637	HIS
1	A	201	ILE

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	520/594 (88%)	505 (97%)	15 (3%)	42	75
1	B	526/594 (89%)	515 (98%)	11 (2%)	53	81
All	All	1046/1188 (88%)	1020 (98%)	26 (2%)	47	78

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	634	THR
1	B	228	HIS
1	B	519	ASP
1	B	170	VAL
1	B	262	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	584	GLN

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](#)

4 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	0.42	0	17,19,21	0.41	0
2	NAG	C	2	2	14,14,15	0.39	0	17,19,21	0.45	0
2	NAG	D	1	1,2	14,14,15	0.73	1 (7%)	17,19,21	0.91	1 (5%)
2	NAG	D	2	2	14,14,15	0.95	1 (7%)	17,19,21	0.71	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	3.27	1.56	1.52
2	D	1	NAG	O5-C1	2.44	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	2.96	116.15	112.19

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

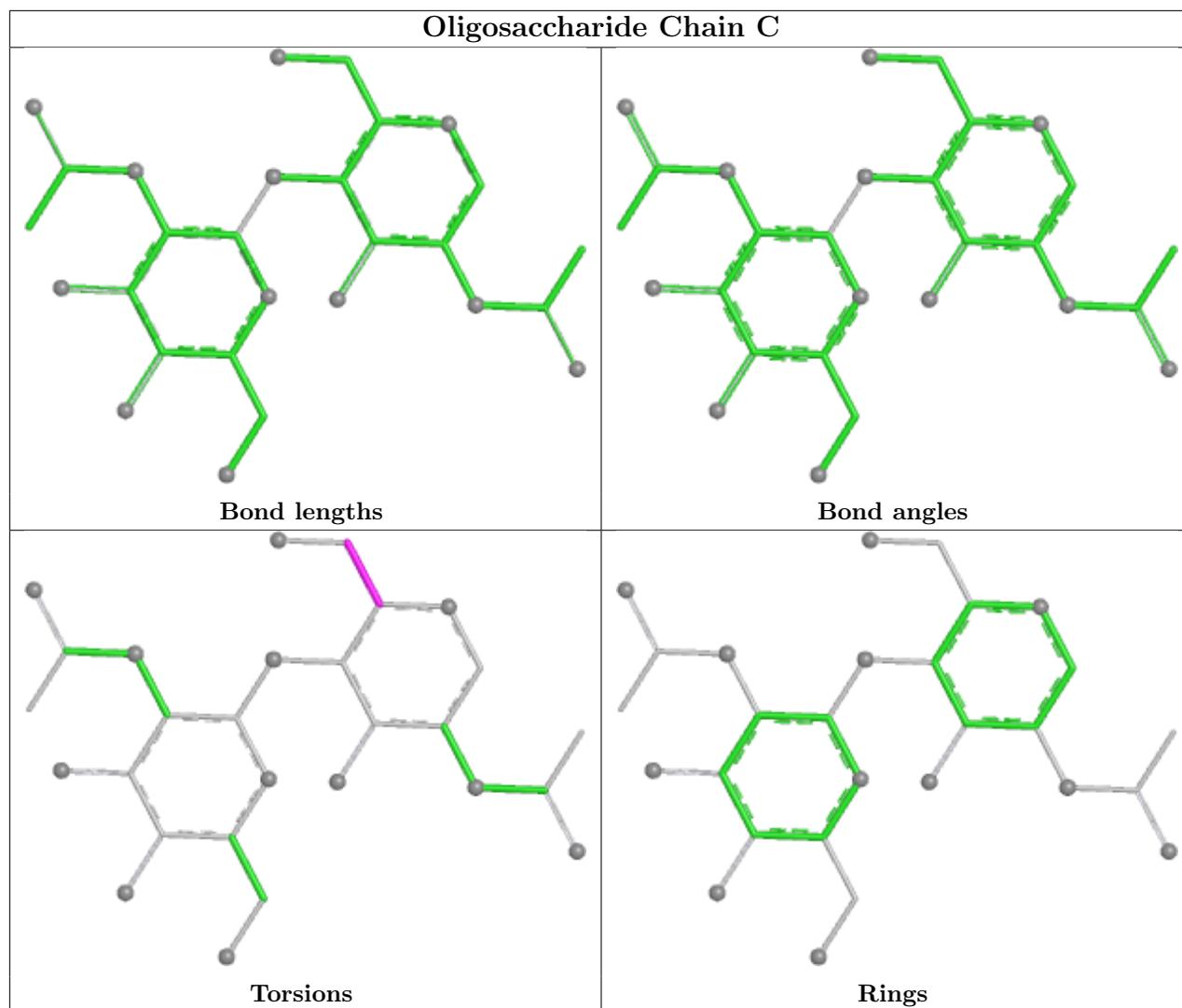
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2

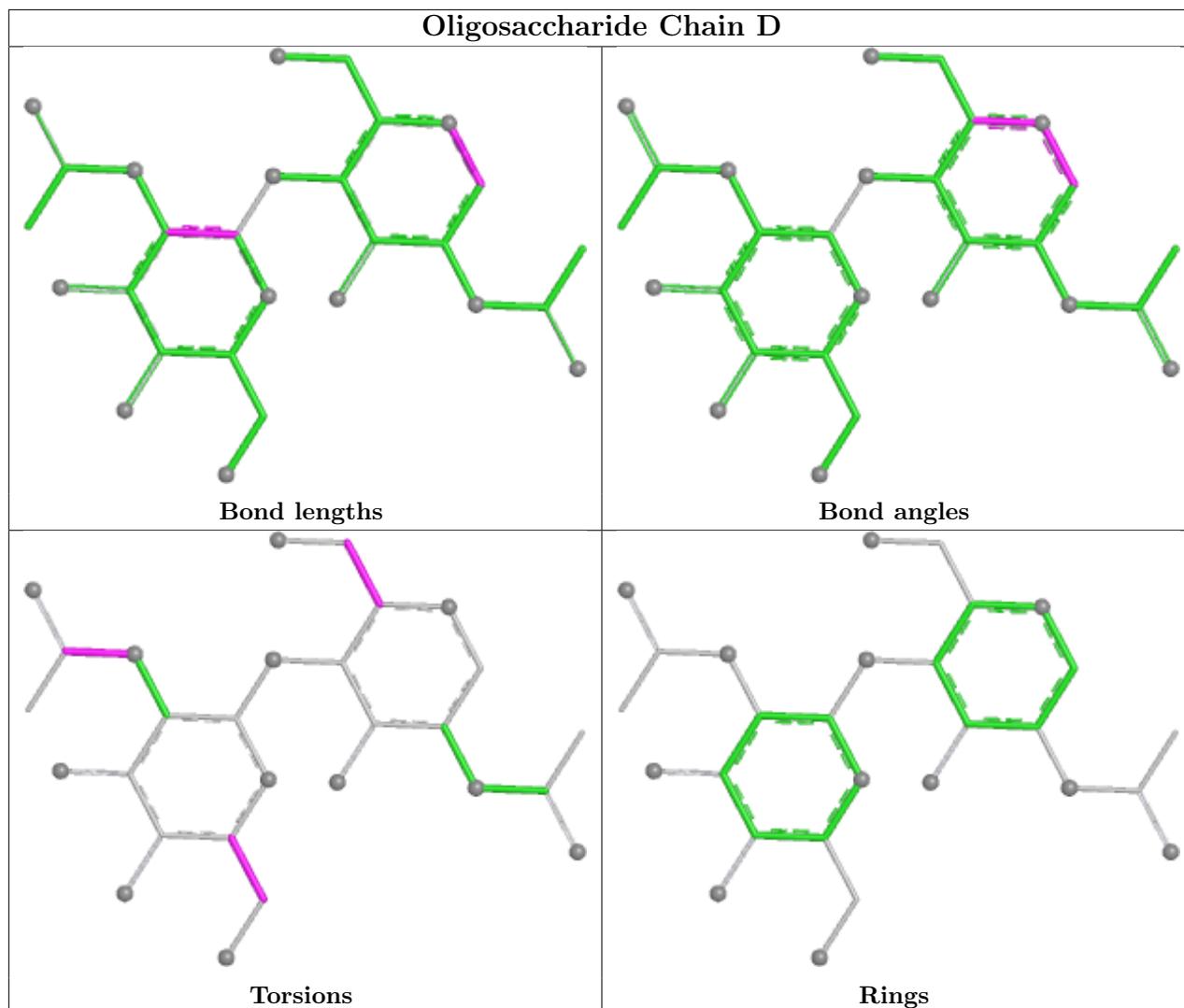
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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





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	$\# Z > 2$
3	NAG	B	1141	1	14,14,15	0.26	0	17,19,21	0.40	0
3	NAG	B	1398	1	14,14,15	0.25	0	17,19,21	0.35	0
3	NAG	A	1674	1	14,14,15	0.26	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1430	1	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	B	1674	1	14,14,15	0.38	0	17,19,21	0.50	0
3	NAG	A	1141	1	14,14,15	0.37	0	17,19,21	0.40	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	B	1141	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1398	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1674	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1430	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1674	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1141	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1674	NAG	C4-C5-C6-O6
3	A	1674	NAG	O5-C5-C6-O6
3	B	1674	NAG	O5-C5-C6-O6
3	B	1398	NAG	O5-C5-C6-O6
3	A	1674	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	608/703 (86%)	0.12	1 (0%) 95 87	40, 95, 154, 193	0
1	B	608/703 (86%)	0.18	9 (1%) 73 46	38, 96, 157, 203	0
All	All	1216/1406 (86%)	0.15	10 (0%) 86 65	38, 95, 156, 203	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	TYR	6.8
1	B	476	PRO	3.3
1	B	477	PRO	3.2
1	B	321	GLN	3.0
1	B	492	VAL	2.8

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

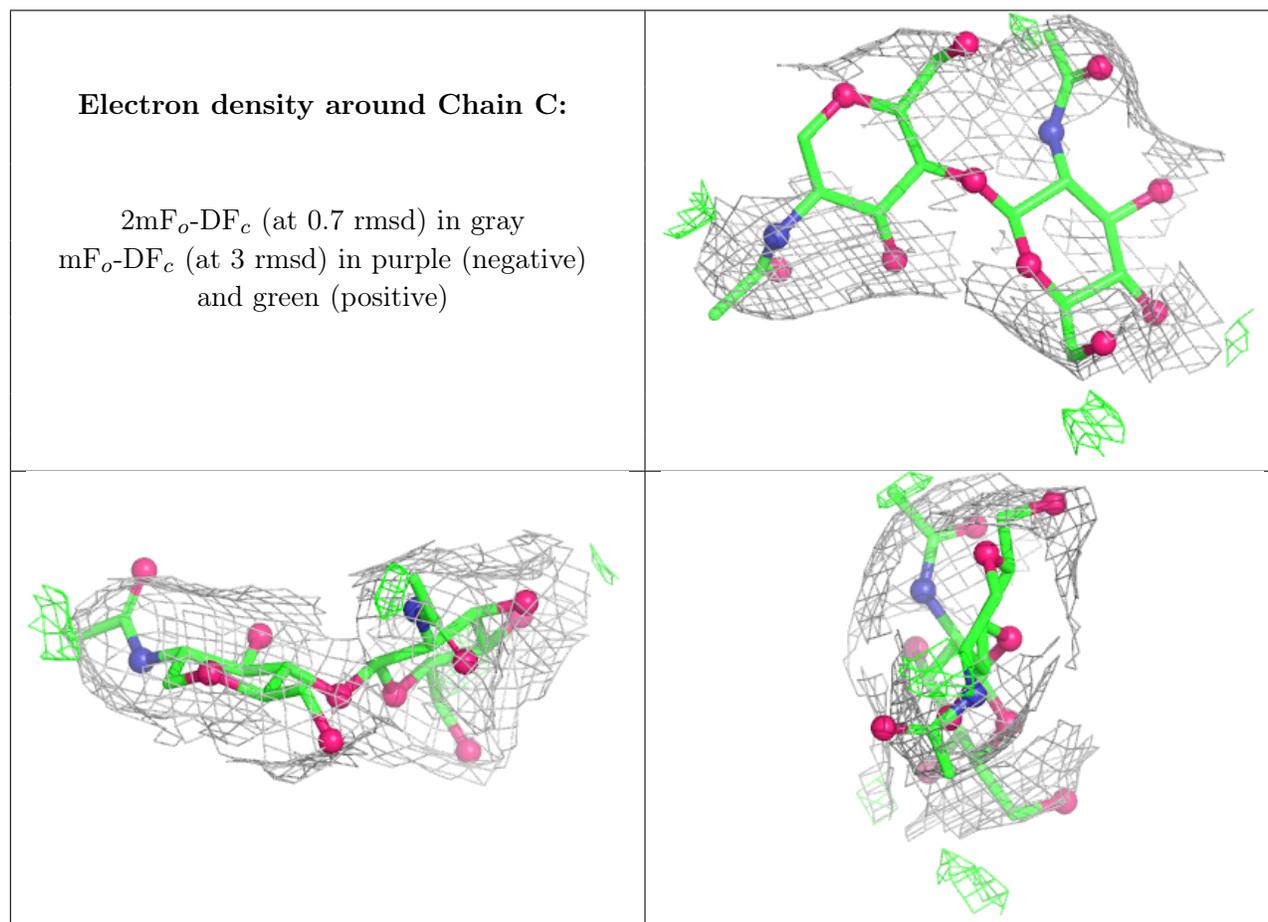
There are no non-standard protein/DNA/RNA residues in this entry.

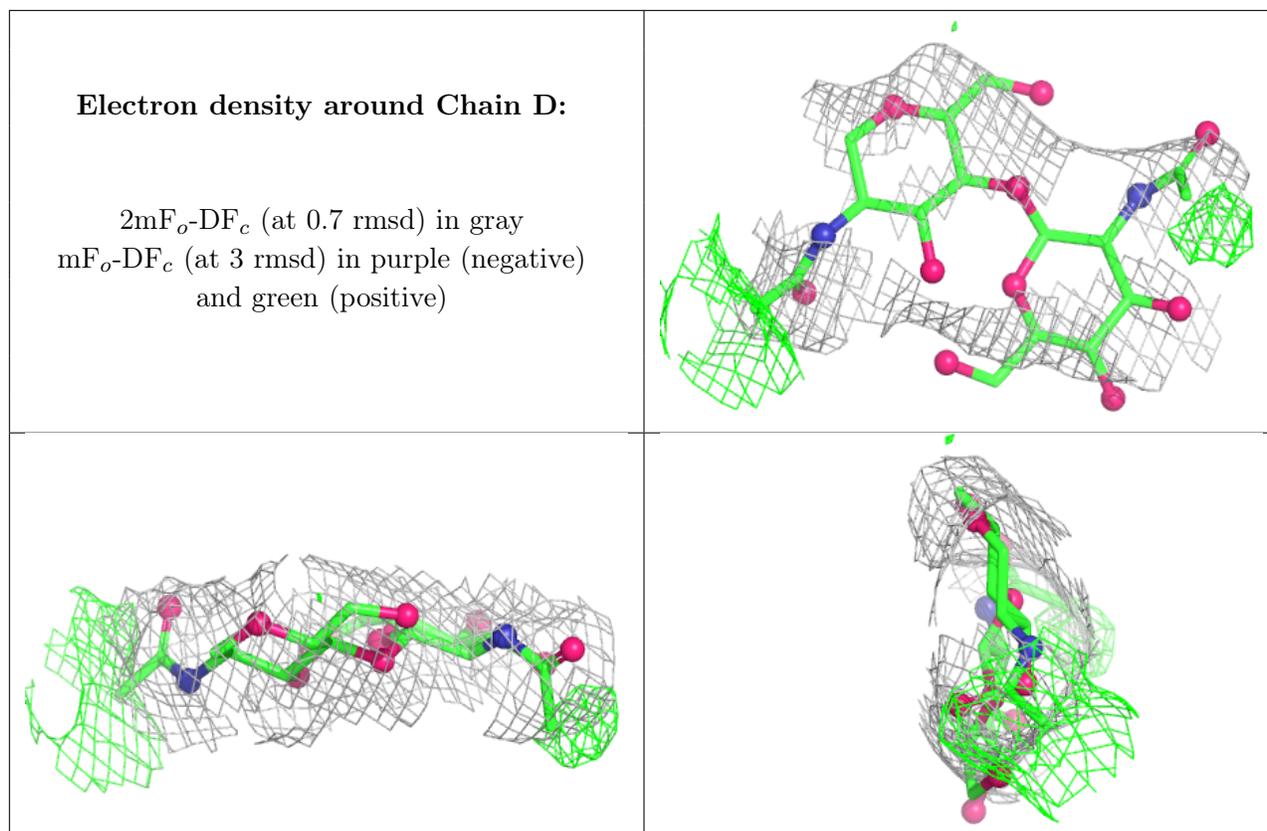
6.3 Carbohydrates [i](#)

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	D	2	14/15	0.84	0.18	176,176,176,176	0
2	NAG	D	1	14/15	0.90	0.12	175,175,175,175	0
2	NAG	C	2	14/15	0.91	0.11	173,173,173,173	0
2	NAG	C	1	14/15	0.94	0.15	156,156,156,156	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.





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(\AA^2)	Q<0.9
3	NAG	A	1674	14/15	0.72	0.25	149,149,149,149	0
3	NAG	A	1141	14/15	0.80	0.31	172,172,172,172	0
3	NAG	B	1674	14/15	0.85	0.16	130,130,130,130	0
3	NAG	B	1430	14/15	0.88	0.19	167,167,167,167	0
3	NAG	B	1141	14/15	0.89	0.24	177,177,177,177	0
3	NAG	B	1398	14/15	0.90	0.13	131,147,159,163	0
4	CL	A	801	1/1	0.92	0.13	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.