wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2021 – 06:16 PM EDT

PDB ID	:	1RZJ
Title	:	HIV-1 HXBC2 GP120 ENVELOPE GLYCOPROTEIN COMPLEXED WITH CD4 AND INDUCED NEUTRALIZING ANTIBODY 17B
Authors	:	Huang, C.C.; Venturi, M.; Majeed, S.; Moore, M.J.; Phogat, S.; Zhang, M.-Y.; Dimitrov, D.S.; Hendrickson, W.A.; Robinson, J.; Sodroski, J.; Wyatt, R.; Choe, H.; Farzan, M.; Kwong, P.D.
Deposited on	:	2003-12-24
Resolution	:	2.20 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 (i) symbol.

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

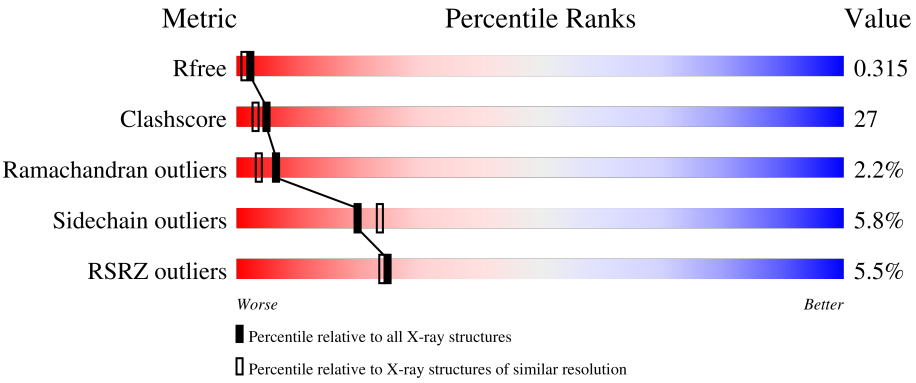
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	G	321	9% 47% 44% • • 5%
2	C	185	4% 47% 45% 5% •
3	L	214	2% 59% 37% •
4	H	229	4% 65% 32% •
5	A	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	B	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FUC	A	2	-	-	-	X
5	NAG	B	1	-	-	-	X
5	FUC	B	2	-	-	-	X
6	NAG	G	588	X	-	-	-
6	NAG	G	697	-	-	-	X
6	NAG	G	730	X	-	X	X
6	NAG	G	741	X	-	-	-
6	NAG	G	789	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7947 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 GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	305	Total	C	N	O	S	0	0	0
			2360	1480	411	449	20			

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	79	GLY	-	insertion	UNP P04578
G	80	ALA	-	insertion	UNP P04578
G	81	ARG	-	insertion	UNP P04578
G	82	SER	-	insertion	UNP P04578
G	83	GLU	-	insertion	UNP P04578
G	84	VAL	-	insertion	UNP P04578
G	85	VAL	-	insertion	UNP P04578
G	86	LEU	-	insertion	UNP P04578
G	87	VAL	-	insertion	UNP P04578
G	88	ASN	-	insertion	UNP P04578
G	89	VAL	-	insertion	UNP P04578
G	90	THR	-	insertion	UNP P04578
G	91	GLU	-	insertion	UNP P04578
G	92	ASN	-	insertion	UNP P04578
G	93	PHE	-	insertion	UNP P04578
G	94	ASN	-	insertion	UNP P04578
G	95	MET	-	insertion	UNP P04578
G	96	TRP	-	insertion	UNP P04578
G	97	LYS	-	insertion	UNP P04578
G	98	ASN	-	insertion	UNP P04578
G	99	ASP	-	insertion	UNP P04578
G	100	MET	-	insertion	UNP P04578
G	101	VAL	-	insertion	UNP P04578
G	102	GLU	-	insertion	UNP P04578
G	103	GLN	-	insertion	UNP P04578
G	104	MET	-	insertion	UNP P04578
G	105	HIS	-	insertion	UNP P04578

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Chain	Residue	Modelled	Actual	Comment	Reference
G	106	GLU	-	insertion	UNP P04578
G	107	ASP	-	insertion	UNP P04578
G	108	ILE	-	insertion	UNP P04578
G	109	ILE	-	insertion	UNP P04578
G	110	SER	-	insertion	UNP P04578
G	111	LEU	-	insertion	UNP P04578
G	112	TRP	-	insertion	UNP P04578
G	113	ASP	-	insertion	UNP P04578
G	114	GLN	-	insertion	UNP P04578
G	115	SER	-	insertion	UNP P04578
G	116	LEU	-	insertion	UNP P04578
G	117	LYS	-	insertion	UNP P04578
G	118	PRO	-	insertion	UNP P04578
G	119	CYS	-	insertion	UNP P04578
G	120	VAL	-	insertion	UNP P04578
G	121	LYS	-	insertion	UNP P04578
G	122	LEU	-	insertion	UNP P04578
G	123	THR	-	insertion	UNP P04578
G	124	PRO	-	insertion	UNP P04578
G	125	LEU	-	insertion	UNP P04578
G	126	CYS	-	insertion	UNP P04578
G	127	VAL	-	insertion	UNP P04578
G	128	GLY	-	insertion	UNP P04578
G	129	ALA	-	insertion	UNP P04578
G	194	GLY	-	insertion	UNP P04578
G	?	-	ARG	deletion	UNP P04578
G	?	-	PRO	deletion	UNP P04578
G	?	-	ASN	deletion	UNP P04578
G	?	-	ASN	deletion	UNP P04578
G	?	-	ASN	deletion	UNP P04578
G	?	-	THR	deletion	UNP P04578
G	?	-	ARG	deletion	UNP P04578
G	?	-	LYS	deletion	UNP P04578
G	?	-	ARG	deletion	UNP P04578
G	?	-	ILE	deletion	UNP P04578
G	?	-	ARG	deletion	UNP P04578
G	?	-	ILE	deletion	UNP P04578
G	?	-	GLN	deletion	UNP P04578
G	?	-	ARG	deletion	UNP P04578
G	?	-	GLY	deletion	UNP P04578
G	?	-	PRO	deletion	UNP P04578
G	?	-	ARG	deletion	UNP P04578

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	PHE	deletion	UNP P04578
G	?	-	VAL	deletion	UNP P04578
G	?	-	THR	deletion	UNP P04578
G	?	-	ILE	deletion	UNP P04578
G	?	-	GLY	deletion	UNP P04578
G	?	-	LYS	deletion	UNP P04578
G	?	-	ILE	deletion	UNP P04578
G	?	-	ASN	deletion	UNP P04578
G	?	-	MET	deletion	UNP P04578
G	?	-	ARG	deletion	UNP P04578
G	?	-	GLN	deletion	UNP P04578
G	?	-	ALA	deletion	UNP P04578

- Molecule 2 is a protein called T-CELL SURFACE GLYCOPROTEIN CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	181	Total	C	N	O	S	0	0	0
			1412	885	247	276	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	184	ASN	SER	engineered mutation	UNP P01730
C	185	THR	ILE	engineered mutation	UNP P01730

- Molecule 3 is a protein called ANTIBODY 17B, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1647	1028	282	332	5			

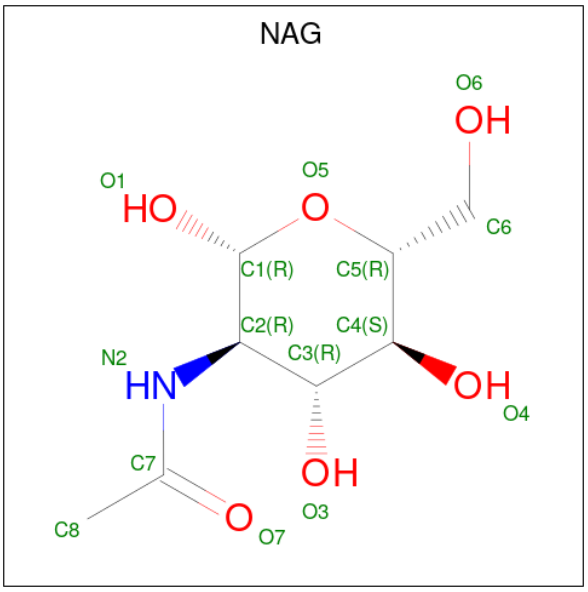
- Molecule 4 is a protein called ANTIBODY 17B, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	229	Total	C	N	O	S	0	0	0
			1722	1086	289	342	5			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	A	2	Total C N O 24 14 1 9	0	0	0
5	B	2	Total C N O 24 14 1 9	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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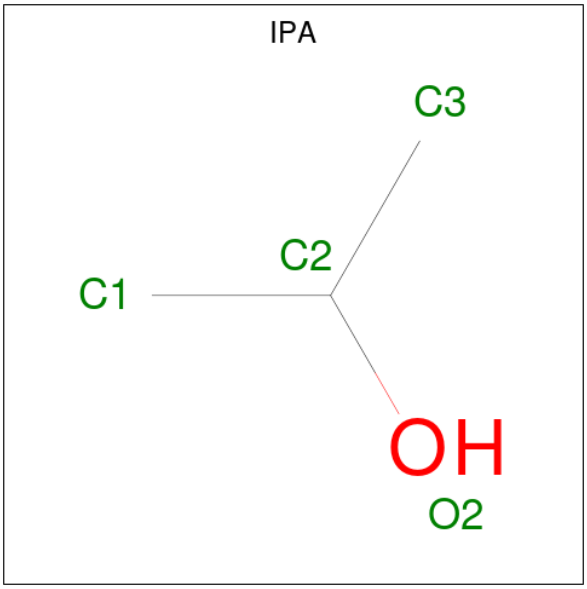
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total C O 4 3 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	201	Total O 201 201	0	0
8	C	91	Total O 91 91	0	0
8	L	140	Total O 140 140	0	0

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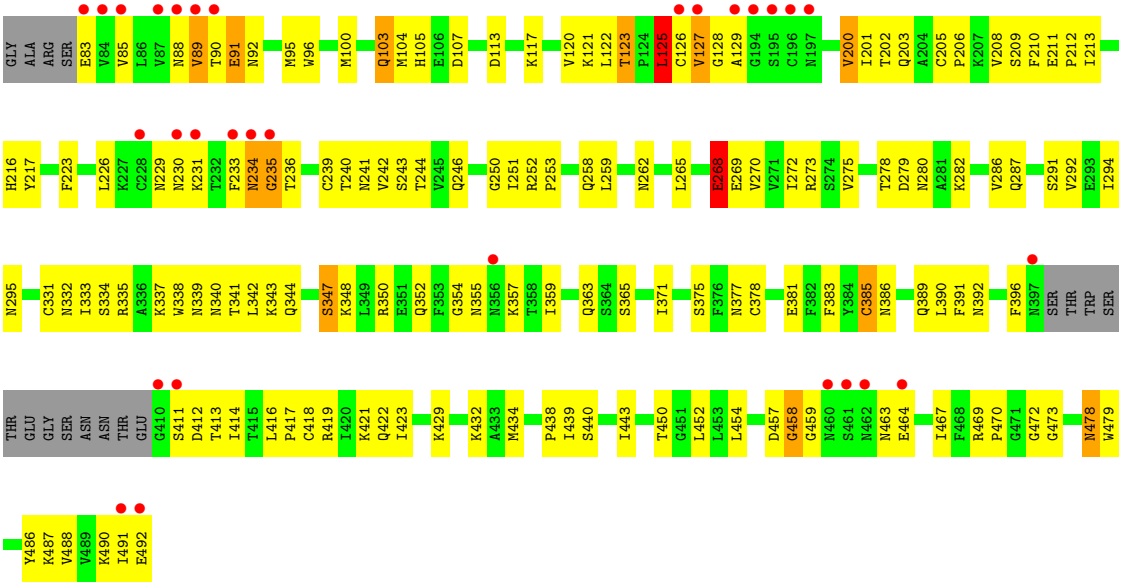
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	154	Total 154	O 154	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

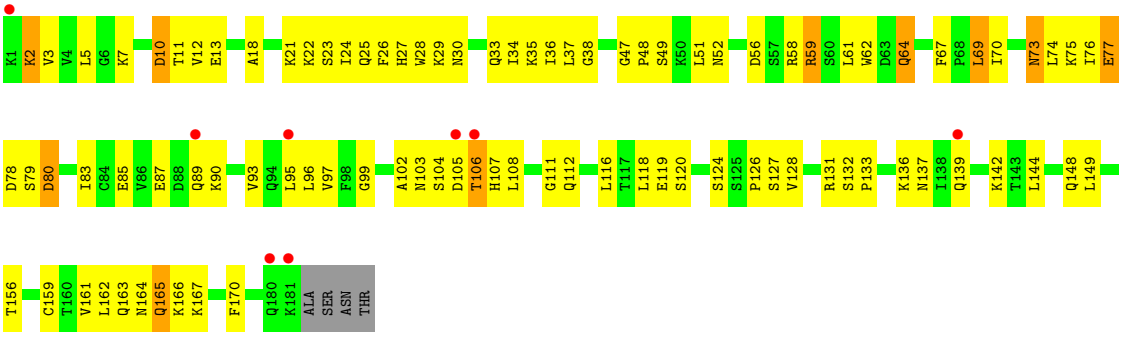
• Molecule 1: ENVELOPE GLYCOPROTEIN GP120

Chain G:



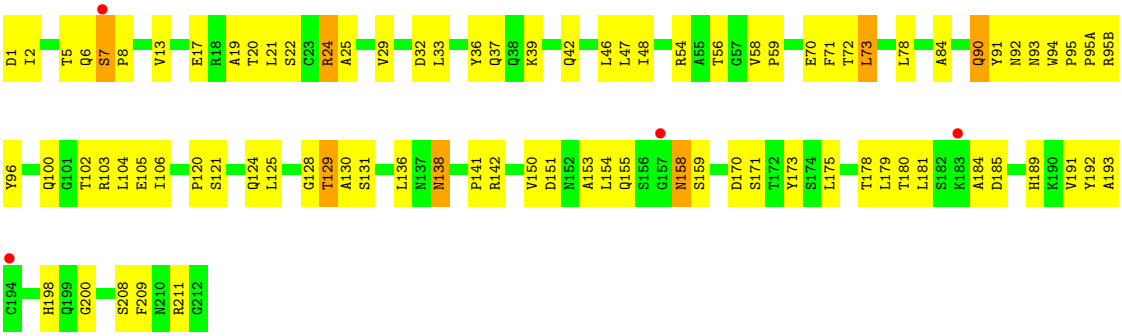
• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4

Chain C:

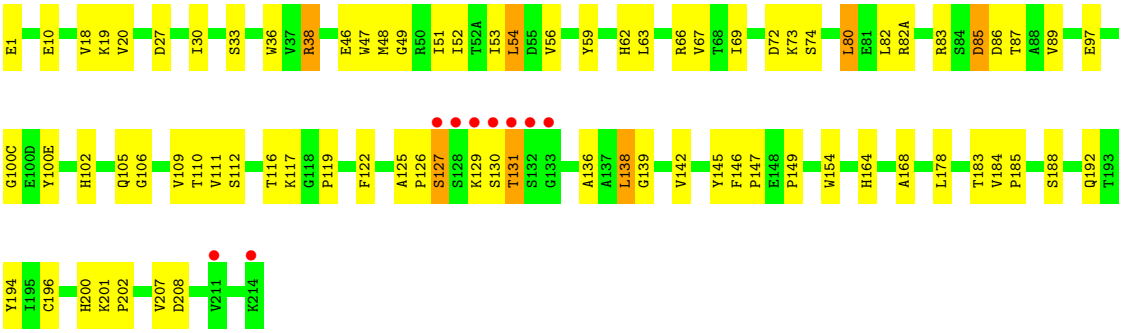


• Molecule 3: ANTIBODY 17B, LIGHT CHAIN

Chain L:



• Molecule 4: ANTIBODY 17B, HEAVY CHAIN



• Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	71.25Å 88.11Å 196.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.20 19.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.6 (19.81-2.20) 87.7 (19.81-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.83 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.323 0.256 , 0.315	Depositor DCC
R_{free} test set	3946 reflections (7.07%)	wwPDB-VP
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.871	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	7947	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: IPA, NAG, FUC

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	G	0.38	0/2406	0.63	0/3262
2	C	0.35	0/1432	0.64	0/1930
3	L	0.41	0/1684	0.67	0/2288
4	H	0.42	0/1762	0.64	0/2399
All	All	0.39	0/7284	0.64	0/9879

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	G	2360	0	2301	161	0
2	C	1412	0	1444	87	0
3	L	1647	0	1593	91	0
4	H	1722	0	1691	62	0
5	A	24	0	22	1	0
5	B	24	0	22	2	0
6	G	168	0	156	32	0
7	G	4	0	8	0	0
8	C	91	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	201	0	0	11	0
8	H	154	0	0	2	0
8	L	140	0	0	7	0
All	All	7947	0	7237	400	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 27.

The worst 5 of 400 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:G:280:ASN:HD22	1:G:458:GLY:HA3	1.28	0.97
2:C:13:GLU:HG3	2:C:70:ILE:HG12	1.47	0.94
2:C:131:ARG:NH1	2:C:137:ASN:HD21	1.66	0.94
2:C:131:ARG:HH11	2:C:137:ASN:HD21	1.11	0.92
3:L:78:LEU:HD21	3:L:104:LEU:HD21	1.52	0.92

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	G	301/321 (94%)	262 (87%)	32 (11%)	7 (2%)	6 3
2	C	179/185 (97%)	158 (88%)	14 (8%)	7 (4%)	3 1
3	L	212/214 (99%)	192 (91%)	16 (8%)	4 (2%)	8 5
4	H	227/229 (99%)	205 (90%)	20 (9%)	2 (1%)	17 16
All	All	919/949 (97%)	817 (89%)	82 (9%)	20 (2%)	6 4

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	235	GLY
2	C	106	THR
2	C	107	HIS
1	G	127	VAL
1	G	129	ALA

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	G	270/283 (95%)	251 (93%)	19 (7%)	15	16
2	C	164/167 (98%)	152 (93%)	12 (7%)	14	15
3	L	184/184 (100%)	179 (97%)	5 (3%)	44	57
4	H	193/193 (100%)	182 (94%)	11 (6%)	20	24
All	All	811/827 (98%)	764 (94%)	47 (6%)	20	23

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	104	SER
3	L	158	ASN
2	C	139	GLN
3	L	73	LEU
4	H	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	137	ASN
3	L	138	ASN
4	H	102	HIS
3	L	124	GLN
3	L	152	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

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	$\#\|Z\| > 2$
5	NAG	A	1	5,1	14,14,15	0.60	0	17,19,21	0.65	0
5	FUC	A	2	5	10,10,11	0.76	0	14,14,16	0.49	0
5	NAG	B	1	5,1	14,14,15	0.76	0	17,19,21	0.73	0
5	FUC	B	2	5	10,10,11	0.55	0	14,14,16	0.51	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	A	1	5,1	-	6/6/23/26	0/1/1/1
5	FUC	A	2	5	-	-	0/1/1/1
5	NAG	B	1	5,1	-	4/6/23/26	0/1/1/1
5	FUC	B	2	5	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

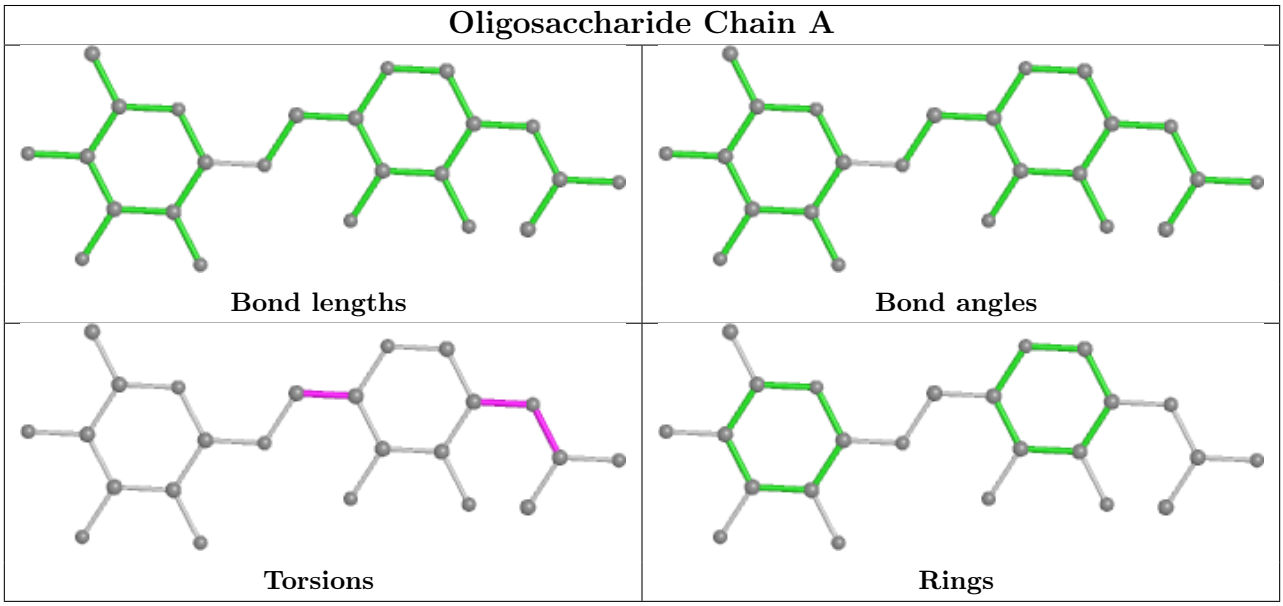
Mol	Chain	Res	Type	Atoms
5	A	1	NAG	C8-C7-N2-C2
5	A	1	NAG	O7-C7-N2-C2
5	B	1	NAG	C8-C7-N2-C2
5	B	1	NAG	O7-C7-N2-C2
5	A	1	NAG	C1-C2-N2-C7

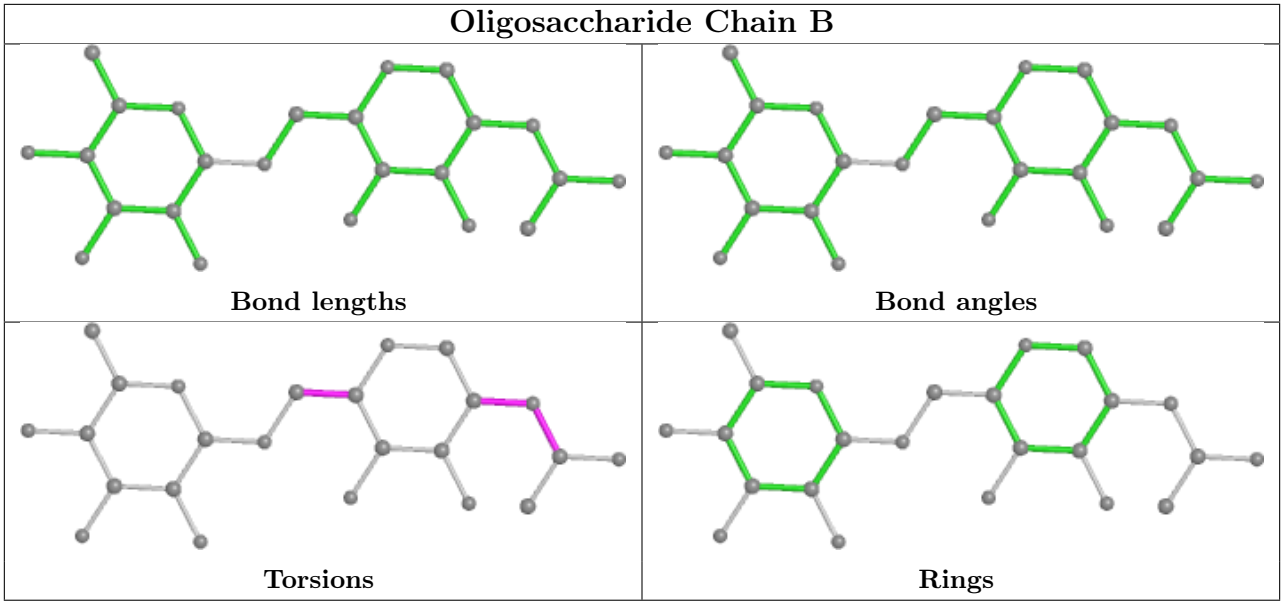
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1	NAG	2	0
5	A	1	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 oligosaccharide.





5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
7	IPA	G	1000	-	3,3,3	0.73	0	3,3,3	0.28	0
6	NAG	G	730	1	14,14,15	0.57	0	17,19,21	0.55	0
6	NAG	G	741	1	14,14,15	0.54	0	17,19,21	0.65	1 (5%)
6	NAG	G	697	1	14,14,15	0.62	0	17,19,21	0.61	0
6	NAG	G	734	1	14,14,15	0.54	0	17,19,21	0.61	0
6	NAG	G	886	1	14,14,15	0.57	0	17,19,21	0.80	1 (5%)
6	NAG	G	839	1	14,14,15	0.65	0	17,19,21	0.74	0
6	NAG	G	892	1	14,14,15	0.53	0	17,19,21	0.63	0
6	NAG	G	789	1	14,14,15	0.61	0	17,19,21	0.61	0
6	NAG	G	948	1	14,14,15	0.77	1 (7%)	17,19,21	0.65	0
6	NAG	G	588	1	14,14,15	0.49	0	17,19,21	0.78	1 (5%)
6	NAG	G	762	1	14,14,15	0.72	1 (7%)	17,19,21	0.73	0
6	NAG	G	776	1	14,14,15	0.61	0	17,19,21	0.77	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
6	NAG	G	730	1	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	G	741	1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	G	697	1	-	4/6/23/26	0/1/1/1
6	NAG	G	734	1	-	5/6/23/26	0/1/1/1
6	NAG	G	886	1	-	4/6/23/26	0/1/1/1
6	NAG	G	839	1	-	2/6/23/26	0/1/1/1
6	NAG	G	892	1	-	3/6/23/26	0/1/1/1
6	NAG	G	789	1	-	4/6/23/26	0/1/1/1
6	NAG	G	948	1	-	3/6/23/26	0/1/1/1
6	NAG	G	588	1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	G	762	1	-	4/6/23/26	0/1/1/1
6	NAG	G	776	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	948	NAG	C1-C2	2.27	1.55	1.52
6	G	762	NAG	C1-C2	2.01	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	776	NAG	C2-N2-C7	-2.50	119.34	122.90
6	G	886	NAG	C2-N2-C7	-2.32	119.59	122.90
6	G	588	NAG	C2-N2-C7	-2.17	119.81	122.90
6	G	741	NAG	C2-N2-C7	-2.03	120.02	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	G	588	NAG	C1
6	G	730	NAG	C1
6	G	741	NAG	C1

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	588	NAG	C8-C7-N2-C2
6	G	588	NAG	O7-C7-N2-C2
6	G	697	NAG	C8-C7-N2-C2
6	G	697	NAG	O7-C7-N2-C2
6	G	730	NAG	C3-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	730	NAG	8	0
6	G	734	NAG	1	0
6	G	886	NAG	2	0
6	G	839	NAG	5	0
6	G	892	NAG	1	0
6	G	789	NAG	7	0
6	G	948	NAG	4	0
6	G	588	NAG	2	0
6	G	762	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	G	305/321 (95%)	0.43	30 (9%)	7	6	5, 26, 81, 101	0
2	C	181/185 (97%)	0.42	8 (4%)	34	32	7, 33, 60, 78	0
3	L	214/214 (100%)	0.11	4 (1%)	66	65	2, 22, 53, 60	0
4	H	229/229 (100%)	0.07	9 (3%)	39	37	3, 15, 61, 101	0
All	All	929/949 (97%)	0.27	51 (5%)	25	24	2, 24, 64, 101	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	131	THR	8.5
4	H	130	SER	8.2
4	H	133	GLY	7.0
2	C	106	THR	5.6
1	G	194	GLY	5.5

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, 95^{th} 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	B	1	14/15	0.33	0.60	114,118,122,125	0
5	FUC	B	2	10/11	0.45	0.59	127,129,129,130	0

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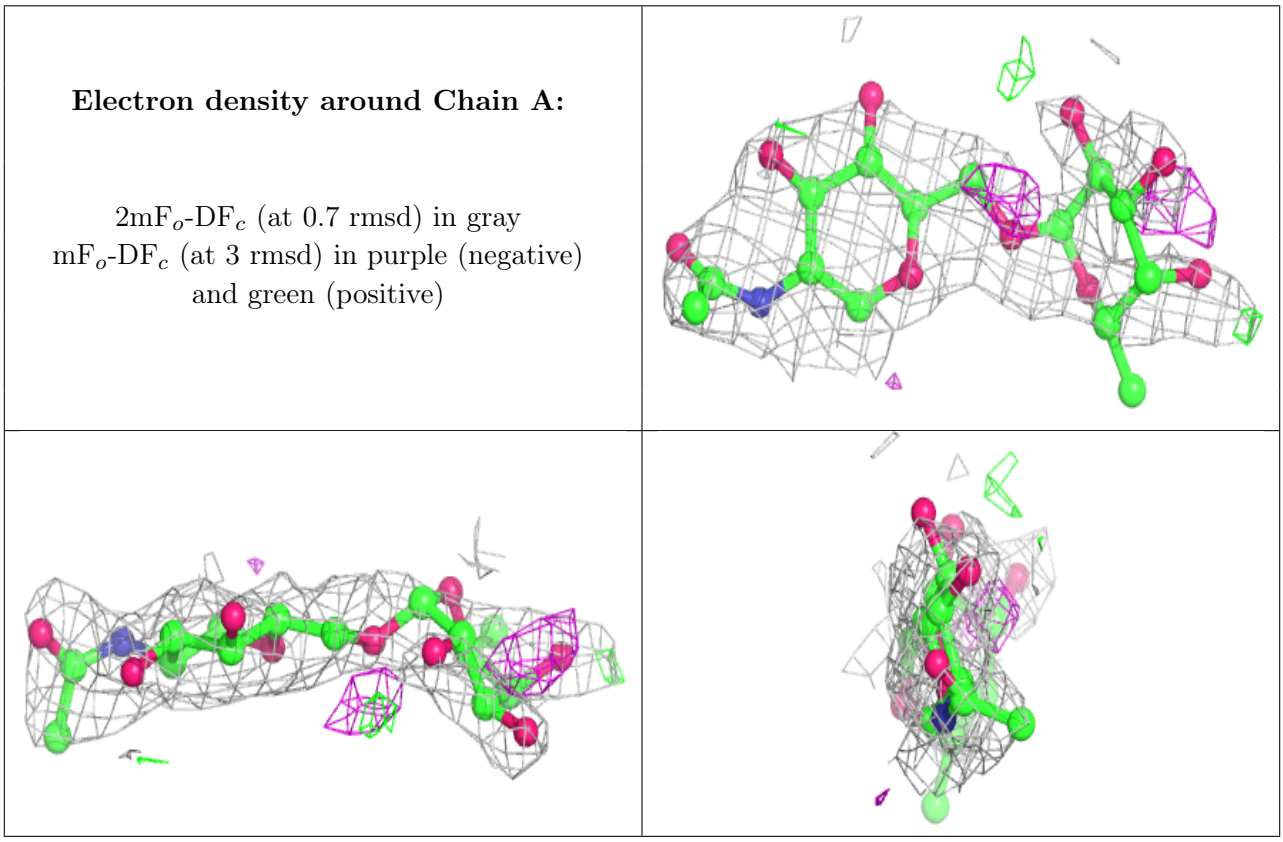
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FUC	A	2	10/11	0.61	0.41	63,64,66,66	0
5	NAG	A	1	14/15	0.81	0.23	49,50,57,61	0

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.

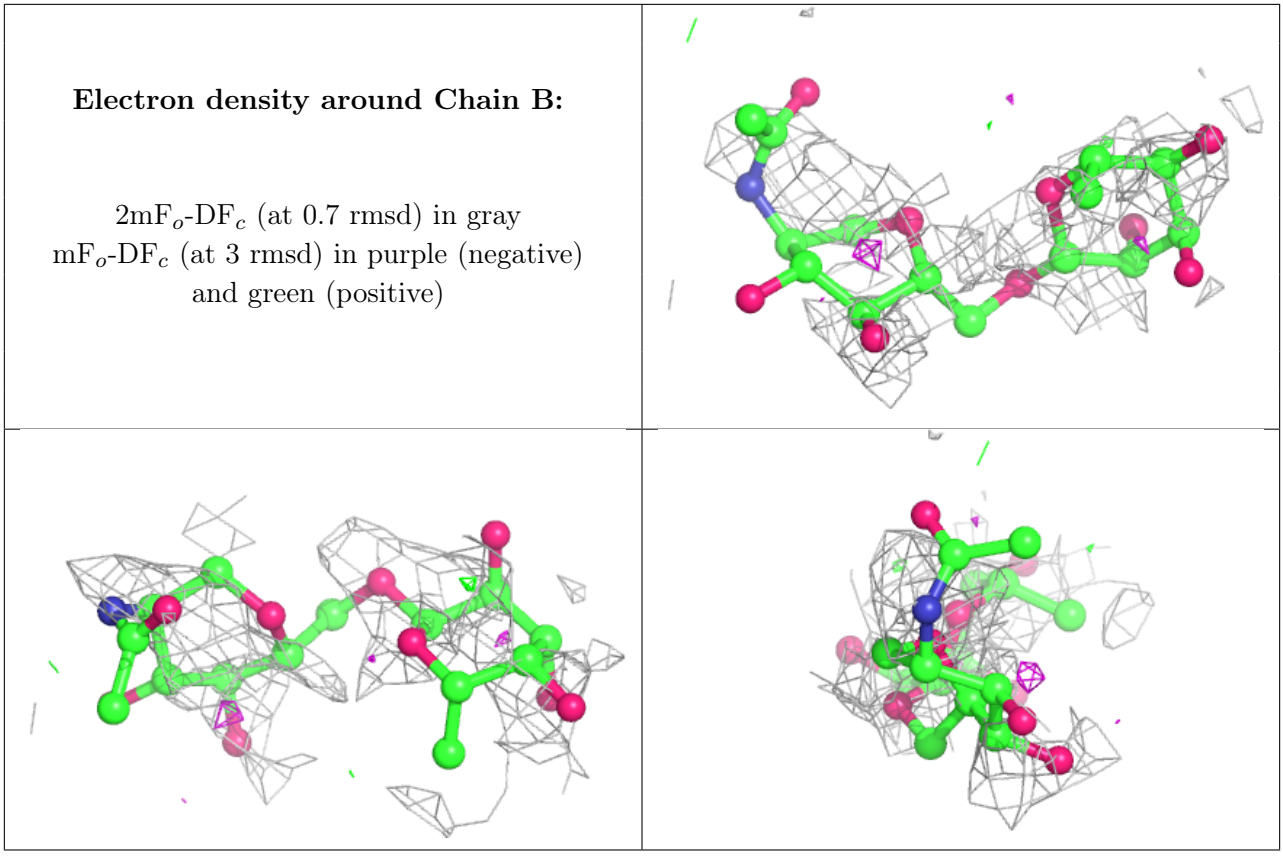
Electron density around Chain A:

$2mF_o$-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 B:

$2mF_o$-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, 95^{th} 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
6	NAG	G	697	14/15	0.49	0.50	100,104,105,106	0
6	NAG	G	839	14/15	0.49	0.38	62,66,67,67	0
6	NAG	G	892	14/15	0.52	0.37	63,66,68,69	0
6	NAG	G	741	14/15	0.55	0.35	69,72,73,74	0
6	NAG	G	730	14/15	0.58	0.52	82,84,85,86	0
6	NAG	G	588	14/15	0.64	0.28	97,98,100,100	0
6	NAG	G	734	14/15	0.65	0.25	60,63,65,65	0
6	NAG	G	948	14/15	0.65	0.34	49,54,55,57	0
6	NAG	G	776	14/15	0.78	0.20	40,42,45,45	0
6	NAG	G	789	14/15	0.80	0.20	41,44,46,48	0
6	NAG	G	886	14/15	0.82	0.19	30,33,37,38	0
6	NAG	G	762	14/15	0.90	0.16	10,22,32,34	0
7	IPA	G	1000	4/4	0.97	0.16	1,3,3,4	0

6.5 Other polymers (i)

There are no such residues in this entry.