Full wwPDB X-ray Structure Validation Report ⓘ

Apr 8, 2024 – 12:32 PM EDT

PDB ID	:	8SGN
Title	:	Crystal structure of Epstein-Barr virus glycoprotein 350 (gp350) in complex with Cy651H02, a monoclonal antibody isolated from macaques immunized with a gp350 nanoparticle vaccine
Authors	:	Joyce, M.G.; Jensen, J.L.; Chen, W.H.; Kanekiyo, M.
Deposited on	:	2023-04-12
Resolution	:	2.20 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:

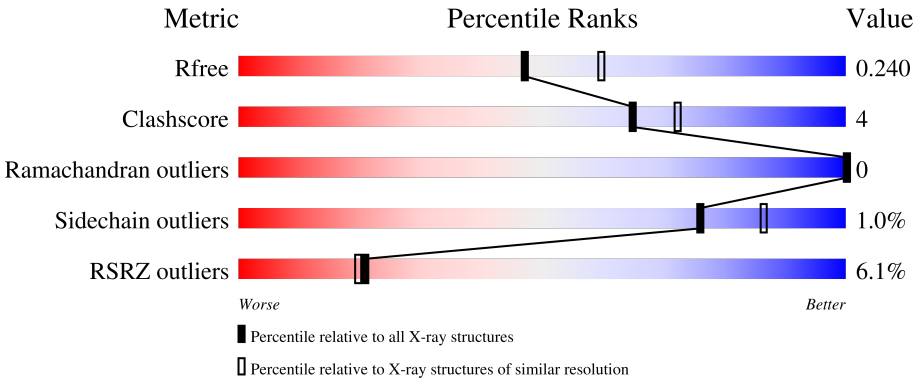
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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	L	214	2% 95% 5%
2	H	223	6% 88% 8% ·
3	G	431	8% 83% 11% 5%
4	K	2	100%

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
4	FUC	K	2	-	-	-	X
7	NAG	G	501	-	-	-	X
7	NAG	G	504	-	-	-	X
7	NAG	G	507	-	-	-	X
7	NAG	G	508	-	-	-	X
7	NAG	G	509	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6884 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 Cy651H02 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1581	986	263	327	5			

- Molecule 2 is a protein called Cy651H02 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1615	1026	272	313	4			

- Molecule 3 is a protein called Envelope glycoprotein gp350.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	408	Total	C	N	O	S	0	0	0
			3120	1970	506	627	17			

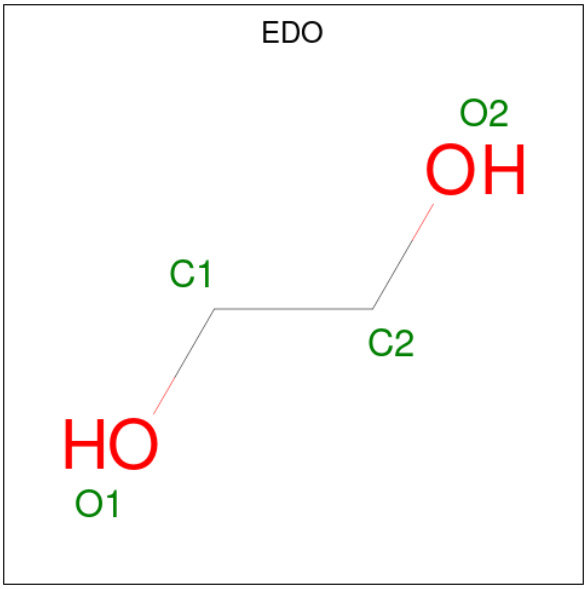
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	426	HIS	-	expression tag	UNP P03200
G	427	HIS	-	expression tag	UNP P03200
G	428	HIS	-	expression tag	UNP P03200
G	429	HIS	-	expression tag	UNP P03200
G	430	HIS	-	expression tag	UNP P03200
G	431	HIS	-	expression tag	UNP P03200

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	K	2	Total C N O 24 14 1 9	0	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

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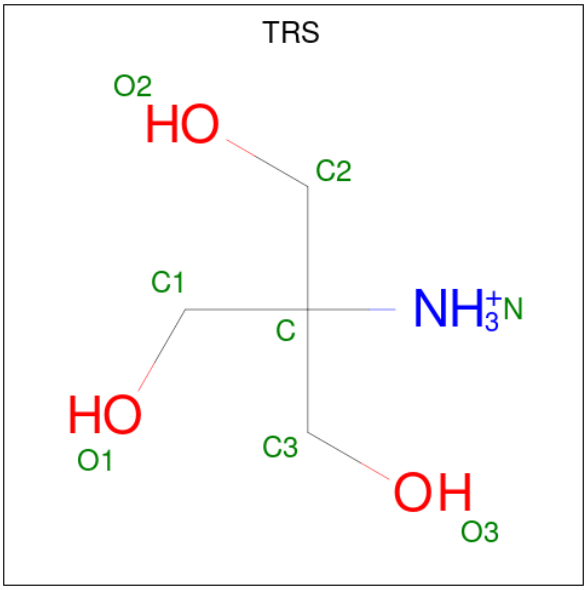
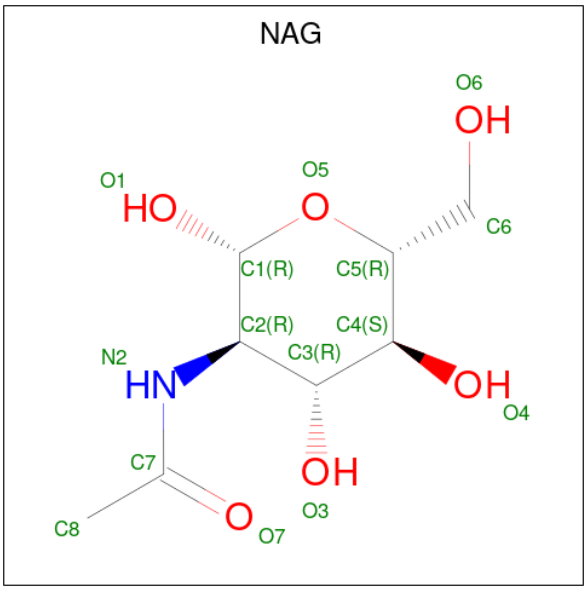
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C N O 8 4 1 3	0	0
6	L	1	Total C N O 8 4 1 3	0	0
6	L	1	Total C N O 8 4 1 3	0	0
6	H	1	Total C N O 8 4 1 3	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 8 is water.

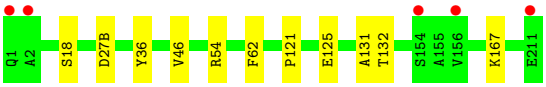
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	122	Total O 122 122	0	0
8	H	77	Total O 77 77	0	0
8	G	95	Total O 95 95	0	0

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.

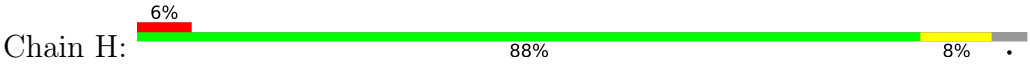
• Molecule 1: Cy651H02 Fab light chain

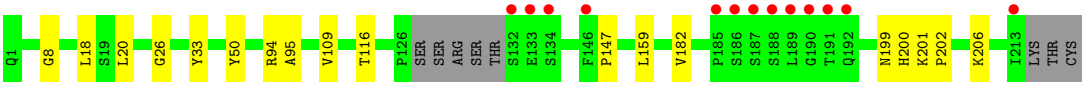
Chain L:



• Molecule 2: Cy651H02 Fab heavy chain

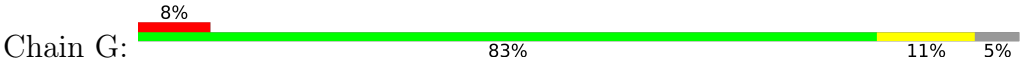
Chain H:

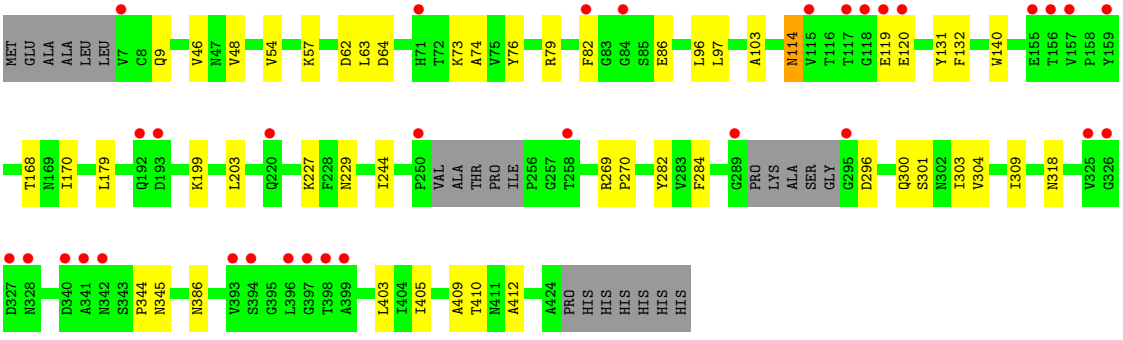




• Molecule 3: Envelope glycoprotein gp350

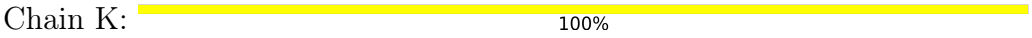
Chain G:





• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	139.15Å 139.15Å 172.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.92 – 2.20 40.57 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.0 (32.92-2.20) 88.0 (40.57-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.193 , 0.237 0.202 , 0.240	Depositor DCC
R_{free} test set	2951 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.009 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.010 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.011 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.011 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.019 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.023 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6884	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: EDO, TRS, FUC, 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	L	0.28	0/1618	0.50	0/2203
2	H	0.27	0/1656	0.53	0/2263
3	G	0.32	0/3193	0.54	0/4364
All	All	0.30	0/6467	0.53	0/8830

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	L	1581	0	1520	5	0
2	H	1615	0	1597	15	0
3	G	3120	0	2979	33	0
4	K	24	0	22	3	0
5	G	32	0	48	1	0
5	H	32	0	48	3	0
5	L	28	0	42	0	0
6	H	8	0	12	2	0
6	L	24	0	36	1	0
7	G	126	0	117	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	95	0	0	0	0
8	H	77	0	0	0	0
8	L	122	0	0	0	0
All	All	6884	0	6421	53	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 (53) 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)
3:G:62:ASP:HB3	4:K:2:FUC:H62	1.47	0.95
3:G:64:ASP:HB2	4:K:2:FUC:O5	1.96	0.64
1:L:18:SER:H	6:L:303:TRS:H31	1.67	0.59
3:G:345:ASN:HB2	3:G:410:THR:HG23	1.83	0.59
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.88	0.55
2:H:94:ARG:HH12	6:H:304:TRS:H21	1.70	0.55
3:G:9:GLN:HA	7:G:506:NAG:H61	1.91	0.53
2:H:199:ASN:HD21	2:H:206:LYS:HE3	1.74	0.52
3:G:179:LEU:HD12	3:G:303:ILE:HD12	1.92	0.52
3:G:64:ASP:O	3:G:79:ARG:N	2.44	0.51
3:G:318:ASN:HB2	5:G:517:EDO:H22	1.93	0.51
3:G:97:LEU:HD11	3:G:103:ALA:HB2	1.93	0.51
3:G:409:ALA:HB3	3:G:412:ALA:HB3	1.94	0.50
3:G:344:PRO:HG2	3:G:410:THR:HG21	1.95	0.48
1:L:125:GLU:OE2	1:L:132:THR:HG23	2.13	0.47
1:L:36:TYR:CE2	1:L:46:VAL:HG22	2.50	0.47
3:G:48:VAL:HG23	3:G:63:LEU:HB2	1.96	0.47
2:H:26:GLY:H	5:H:301:EDO:H12	1.79	0.46
3:G:344:PRO:HB2	7:G:506:NAG:H82	1.96	0.46
3:G:199:LYS:HB2	3:G:199:LYS:HE2	1.86	0.46
3:G:86:GLU:HG2	7:G:505:NAG:H81	1.98	0.46
3:G:168:THR:HG22	3:G:300:GLN:O	2.16	0.46
3:G:74:ALA:HB2	3:G:309:ILE:HG23	1.97	0.46
2:H:18:LEU:HD13	2:H:109:VAL:HG11	1.98	0.46
2:H:94:ARG:HH22	6:H:304:TRS:H12	1.81	0.46
1:L:54:ARG:HD3	1:L:62:PHE:O	2.16	0.45
3:G:170:ILE:O	3:G:301:SER:HB2	2.16	0.45
2:H:147:PRO:HD2	2:H:200:HIS:CE1	2.52	0.45
1:L:121:PRO:HG3	1:L:131:ALA:HB1	1.99	0.44
2:H:116:THR:H	5:H:303:EDO:H12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:54:VAL:CG1	3:G:120:GLU:HB3	2.46	0.44
2:H:116:THR:HG22	5:H:303:EDO:H12	1.98	0.44
3:G:403:LEU:HD23	3:G:405:ILE:HD11	1.99	0.44
3:G:63:LEU:C	4:K:2:FUC:H63	2.38	0.44
3:G:227:LYS:HG2	3:G:244:ILE:HG12	2.00	0.44
3:G:269:ARG:HB3	3:G:270:PRO:HD3	2.00	0.43
3:G:284:PHE:CE1	3:G:296:ASP:HB2	2.53	0.43
3:G:46:VAL:HA	3:G:131:TYR:O	2.19	0.43
3:G:203:LEU:HD12	3:G:282:TYR:HE2	1.84	0.43
3:G:304:VAL:HB	7:G:501:NAG:HN2	1.82	0.43
3:G:57:LYS:HD3	3:G:57:LYS:HA	1.72	0.43
3:G:73:LYS:HD3	3:G:76:TYR:CE2	2.52	0.43
2:H:20:LEU:HD21	2:H:109:VAL:HG21	2.00	0.43
2:H:33:TYR:HB2	2:H:95:ALA:HB3	2.00	0.43
3:G:114:ASN:OD1	3:G:114:ASN:N	2.49	0.42
2:H:8:GLY:HA3	2:H:20:LEU:HD23	2.02	0.42
2:H:147:PRO:HB2	2:H:202:PRO:HG2	2.02	0.41
3:G:119:GLU:O	3:G:120:GLU:HB2	2.20	0.41
3:G:132:PHE:HB3	3:G:140:TRP:HB2	2.02	0.41
3:G:74:ALA:HA	3:G:96:LEU:HD12	2.02	0.41
2:H:199:ASN:ND2	2:H:206:LYS:HE3	2.36	0.40
2:H:201:LYS:H	2:H:201:LYS:HG2	1.70	0.40
3:G:203:LEU:HD12	3:G:282:TYR:CE2	2.57	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	L	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
2	H	211/223 (95%)	207 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	G	402/431 (93%)	391 (97%)	11 (3%)	0	100 100
All	All	825/868 (95%)	801 (97%)	24 (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	L	175/175 (100%)	173 (99%)	2 (1%)	73 85
2	H	184/192 (96%)	183 (100%)	1 (0%)	88 94
3	G	355/373 (95%)	351 (99%)	4 (1%)	73 85
All	All	714/740 (96%)	707 (99%)	7 (1%)	76 86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	27(B)	ASP
1	L	167	LYS
2	H	50	TYR
3	G	82	PHE
3	G	114	ASN
3	G	229	ASN
3	G	386	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 (i)

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	$\#\|Z\| > 2$
4	NAG	K	1	4,3	14,14,15	0.31	0	17,19,21	1.21	3 (17%)
4	FUC	K	2	4	10,10,11	0.29	0	14,14,16	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	1	4,3	-	2/6/23/26	0/1/1/1
4	FUC	K	2	4	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	1	NAG	O5-C5-C6	2.65	111.36	107.20
4	K	1	NAG	C4-C3-C2	-2.49	107.37	111.02
4	K	1	NAG	C2-N2-C7	-2.36	119.54	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	NAG	C8-C7-N2-C2

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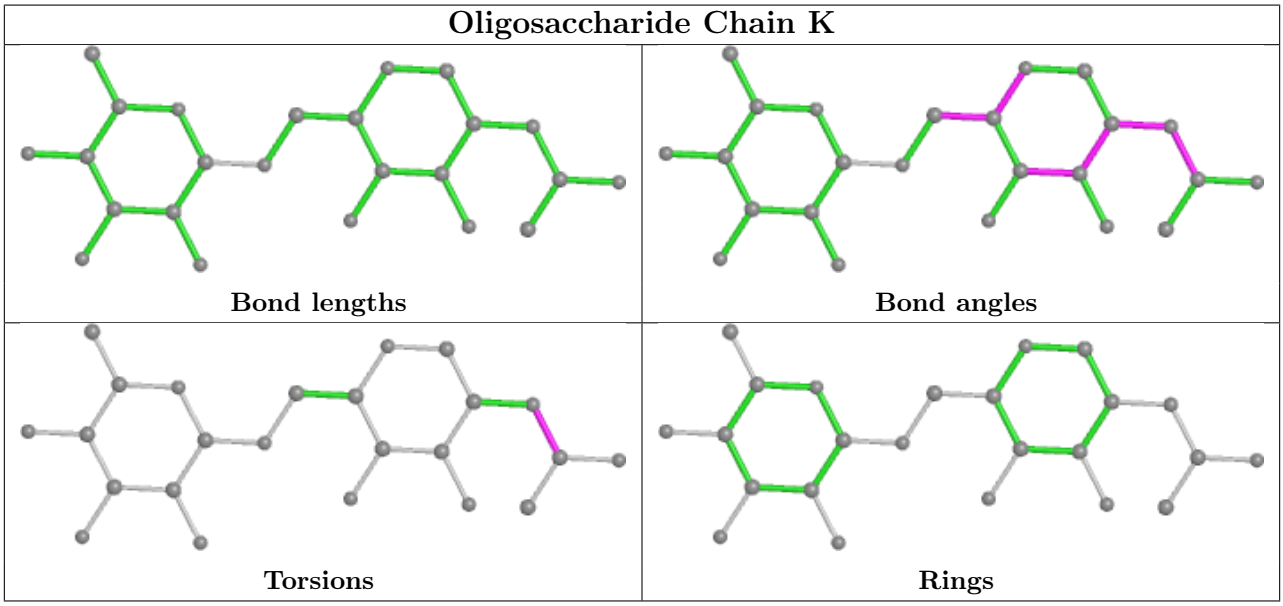
Mol	Chain	Res	Type	Atoms
4	K	1	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	2	FUC	3	0

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



5.6 Ligand geometry (i)

36 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	$\#\|Z\| > 2$
6	TRS	L	305	-	7,7,7	0.35	0	9,9,9	0.35	0
5	EDO	L	307	-	3,3,3	0.46	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	G	516	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	G	514	-	3,3,3	0.46	0	2,2,2	0.38	0
5	EDO	G	517	-	3,3,3	0.46	0	2,2,2	0.34	0
7	NAG	G	507	3	14,14,15	0.35	0	17,19,21	0.37	0
5	EDO	L	302	-	3,3,3	0.41	0	2,2,2	0.51	0
5	EDO	G	512	-	3,3,3	0.44	0	2,2,2	0.45	0
5	EDO	L	306	-	3,3,3	0.46	0	2,2,2	0.40	0
5	EDO	L	309	-	3,3,3	0.43	0	2,2,2	0.41	0
5	EDO	H	308	-	3,3,3	0.47	0	2,2,2	0.26	0
5	EDO	H	305	-	3,3,3	0.47	0	2,2,2	0.29	0
7	NAG	G	503	3	14,14,15	0.38	0	17,19,21	0.65	0
7	NAG	G	508	3	14,14,15	0.29	0	17,19,21	0.59	0
5	EDO	H	309	-	3,3,3	0.50	0	2,2,2	0.24	0
7	NAG	G	502	3	14,14,15	0.36	0	17,19,21	0.63	0
5	EDO	H	302	-	3,3,3	0.42	0	2,2,2	0.49	0
7	NAG	G	505	3	14,14,15	0.37	0	17,19,21	1.21	3 (17%)
5	EDO	G	515	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	G	513	-	3,3,3	0.45	0	2,2,2	0.39	0
7	NAG	G	509	3	14,14,15	0.37	0	17,19,21	0.81	0
6	TRS	L	303	-	7,7,7	0.33	0	9,9,9	0.29	0
5	EDO	G	510	-	3,3,3	0.44	0	2,2,2	0.51	0
5	EDO	H	303	-	3,3,3	0.44	0	2,2,2	0.32	0
5	EDO	H	301	-	3,3,3	0.47	0	2,2,2	0.37	0
5	EDO	L	301	-	3,3,3	0.41	0	2,2,2	0.51	0
5	EDO	L	310	-	3,3,3	0.48	0	2,2,2	0.26	0
5	EDO	H	307	-	3,3,3	0.47	0	2,2,2	0.35	0
7	NAG	G	501	3	14,14,15	0.29	0	17,19,21	1.16	2 (11%)
5	EDO	G	511	-	3,3,3	0.44	0	2,2,2	0.36	0
6	TRS	L	304	-	7,7,7	0.33	0	9,9,9	0.38	0
7	NAG	G	506	3	14,14,15	0.34	0	17,19,21	0.82	0
7	NAG	G	504	3	14,14,15	0.37	0	17,19,21	0.74	0
5	EDO	H	306	-	3,3,3	0.48	0	2,2,2	0.33	0
6	TRS	H	304	-	7,7,7	0.37	0	9,9,9	0.51	0
5	EDO	L	308	-	3,3,3	0.49	0	2,2,2	0.30	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
6	TRS	L	305	-	-	6/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	L	307	-	-	0/1/1/1	-
5	EDO	G	516	-	-	0/1/1/1	-
5	EDO	G	514	-	-	0/1/1/1	-
5	EDO	G	517	-	-	0/1/1/1	-
7	NAG	G	507	3	-	0/6/23/26	0/1/1/1
5	EDO	L	302	-	-	0/1/1/1	-
5	EDO	G	512	-	-	0/1/1/1	-
5	EDO	L	306	-	-	0/1/1/1	-
5	EDO	L	309	-	-	0/1/1/1	-
5	EDO	H	308	-	-	0/1/1/1	-
5	EDO	H	305	-	-	0/1/1/1	-
7	NAG	G	503	3	-	3/6/23/26	0/1/1/1
7	NAG	G	508	3	-	1/6/23/26	0/1/1/1
5	EDO	H	309	-	-	0/1/1/1	-
7	NAG	G	502	3	-	0/6/23/26	0/1/1/1
5	EDO	H	302	-	-	0/1/1/1	-
7	NAG	G	505	3	-	1/6/23/26	0/1/1/1
5	EDO	G	515	-	-	0/1/1/1	-
5	EDO	G	513	-	-	0/1/1/1	-
7	NAG	G	509	3	-	1/6/23/26	0/1/1/1
6	TRS	L	303	-	-	0/9/9/9	-
5	EDO	G	510	-	-	1/1/1/1	-
5	EDO	H	303	-	-	0/1/1/1	-
5	EDO	H	301	-	-	0/1/1/1	-
5	EDO	L	301	-	-	0/1/1/1	-
5	EDO	L	310	-	-	1/1/1/1	-
5	EDO	H	307	-	-	1/1/1/1	-
7	NAG	G	501	3	-	5/6/23/26	0/1/1/1
5	EDO	G	511	-	-	0/1/1/1	-
6	TRS	L	304	-	-	0/9/9/9	-
7	NAG	G	506	3	-	0/6/23/26	0/1/1/1
7	NAG	G	504	3	-	4/6/23/26	0/1/1/1
5	EDO	H	306	-	-	0/1/1/1	-
6	TRS	H	304	-	-	0/9/9/9	-
5	EDO	L	308	-	-	0/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	505	NAG	C1-O5-C5	3.55	117.01	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	501	NAG	C1-O5-C5	3.12	116.42	112.19
7	G	501	NAG	O5-C5-C6	2.55	111.19	107.20
7	G	505	NAG	C2-N2-C7	-2.17	119.81	122.90
7	G	505	NAG	C4-C3-C2	-2.04	108.03	111.02

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	305	TRS	C3-C-C1-O1
7	G	501	NAG	C3-C2-N2-C7
7	G	501	NAG	C8-C7-N2-C2
7	G	501	NAG	O7-C7-N2-C2
7	G	503	NAG	C3-C2-N2-C7
7	G	503	NAG	O7-C7-N2-C2
7	G	503	NAG	C8-C7-N2-C2
7	G	504	NAG	C8-C7-N2-C2
7	G	504	NAG	O7-C7-N2-C2
7	G	501	NAG	C4-C5-C6-O6
7	G	501	NAG	O5-C5-C6-O6
7	G	509	NAG	O5-C5-C6-O6
6	L	305	TRS	C2-C-C1-O1
7	G	508	NAG	O5-C5-C6-O6
7	G	505	NAG	O5-C5-C6-O6
6	L	305	TRS	C1-C-C2-O2
6	L	305	TRS	C3-C-C2-O2
7	G	504	NAG	C1-C2-N2-C7
5	L	310	EDO	O1-C1-C2-O2
5	G	510	EDO	O1-C1-C2-O2
6	L	305	TRS	N-C-C1-O1
6	L	305	TRS	N-C-C2-O2
7	G	504	NAG	C3-C2-N2-C7
5	H	307	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	517	EDO	1	0
7	G	505	NAG	1	0
6	L	303	TRS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	303	EDO	2	0
5	H	301	EDO	1	0
7	G	501	NAG	1	0
7	G	506	NAG	2	0
6	H	304	TRS	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	L	214/214 (100%)	-0.25	5 (2%)	60	58	29, 43, 73, 122	0
2	H	215/223 (96%)	-0.06	13 (6%)	21	20	27, 46, 100, 170	0
3	G	408/431 (94%)	0.23	33 (8%)	12	10	35, 64, 113, 179	0
All	All	837/868 (96%)	0.03	51 (6%)	21	20	27, 52, 106, 179	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	250	PRO	7.0
2	H	189	LEU	6.2
3	G	118	GLY	5.8
3	G	120	GLU	5.1
2	H	187	SER	4.7
3	G	156	THR	4.5
2	H	191	THR	4.5
3	G	82	PHE	4.4
3	G	192	GLN	4.4
3	G	119	GLU	4.3
3	G	326	GLY	4.2
3	G	398	THR	4.1
2	H	185	PRO	3.8
3	G	325	VAL	3.6
2	H	133	GLU	3.3
3	G	289	GLY	3.2
3	G	155	GLU	3.2
3	G	117	THR	3.1
3	G	258	THR	3.0
3	G	397	GLY	3.0
1	L	1	GLN	3.0
3	G	157	VAL	2.9
3	G	84	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	327	ASP	2.9
2	H	190	GLY	2.8
2	H	188	SER	2.8
3	G	220	GLN	2.7
2	H	134	SER	2.7
3	G	396	LEU	2.7
2	H	132	SER	2.7
2	H	146	PHE	2.6
1	L	154	SER	2.6
3	G	393	VAL	2.5
3	G	341	ALA	2.5
3	G	340	ASP	2.5
2	H	192	GLN	2.5
1	L	2	ALA	2.5
1	L	211	GLU	2.5
3	G	71	HIS	2.5
3	G	394	SER	2.4
3	G	295	GLY	2.4
3	G	159	TYR	2.3
3	G	7	VAL	2.3
3	G	115	VAL	2.2
2	H	186	SER	2.2
3	G	328	ASN	2.2
2	H	213	ILE	2.2
3	G	399	ALA	2.1
1	L	156	VAL	2.1
3	G	342	ASN	2.1
3	G	193	ASP	2.0

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

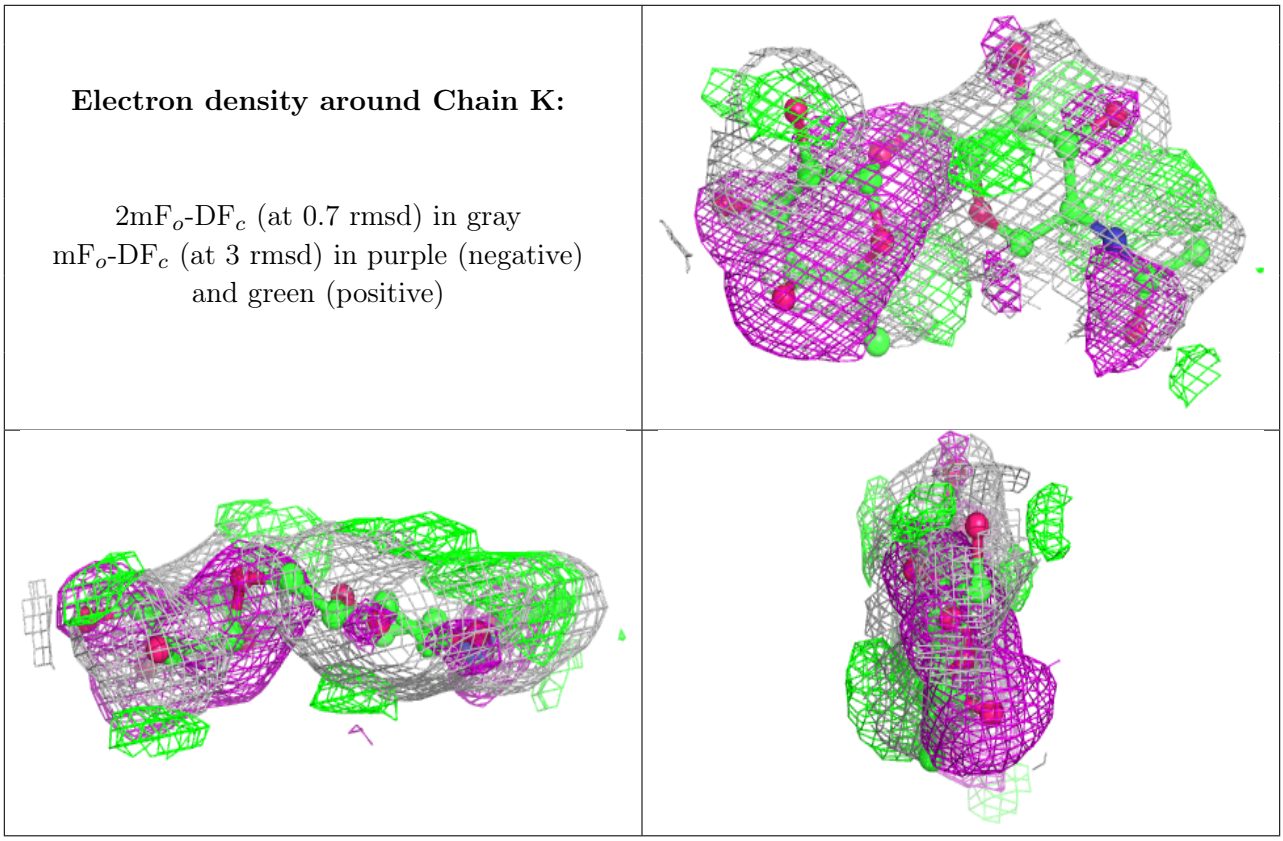
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
4	FUC	K	2	10/11	0.48	0.48	50,50,50,50	0
4	NAG	K	1	14/15	0.62	0.26	50,50,50,50	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

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
7	NAG	G	509	14/15	0.51	0.45	50,50,50,50	0
7	NAG	G	501	14/15	0.55	0.44	78,88,98,113	0
7	NAG	G	507	14/15	0.60	0.43	91,115,125,126	0
5	EDO	L	310	4/4	0.60	0.21	63,65,75,76	0
7	NAG	G	504	14/15	0.62	0.45	86,119,123,124	0
5	EDO	G	515	4/4	0.69	0.21	68,79,80,80	0
7	NAG	G	508	14/15	0.77	0.45	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	G	505	14/15	0.77	0.37	82,104,116,119	0
5	EDO	H	308	4/4	0.78	0.23	66,71,76,81	0
5	EDO	G	516	4/4	0.79	0.26	76,83,89,95	0
7	NAG	G	503	14/15	0.80	0.23	70,88,96,101	0
5	EDO	H	306	4/4	0.81	0.19	65,67,71,77	0
5	EDO	L	301	4/4	0.83	0.27	71,72,73,74	0
5	EDO	H	307	4/4	0.83	0.16	57,63,73,75	0
5	EDO	L	308	4/4	0.86	0.14	54,65,67,75	0
7	NAG	G	506	14/15	0.87	0.44	85,98,105,107	0
6	TRS	L	303	8/8	0.87	0.19	44,72,76,77	0
5	EDO	L	306	4/4	0.88	0.29	75,77,79,86	0
5	EDO	H	301	4/4	0.88	0.12	67,75,75,77	0
5	EDO	H	309	4/4	0.90	0.14	45,46,57,61	0
7	NAG	G	502	14/15	0.90	0.15	54,71,91,98	0
5	EDO	L	307	4/4	0.90	0.11	72,73,82,90	0
5	EDO	G	517	4/4	0.91	0.16	58,67,82,84	0
5	EDO	H	305	4/4	0.91	0.22	72,74,77,82	0
6	TRS	H	304	8/8	0.91	0.18	45,63,86,87	0
5	EDO	G	514	4/4	0.91	0.09	73,84,85,92	0
5	EDO	G	510	4/4	0.92	0.12	55,57,72,78	0
6	TRS	L	304	8/8	0.92	0.28	74,77,87,87	0
5	EDO	H	303	4/4	0.93	0.16	55,67,69,75	0
5	EDO	G	513	4/4	0.93	0.26	54,65,73,81	0
6	TRS	L	305	8/8	0.94	0.19	41,64,78,81	0
5	EDO	H	302	4/4	0.95	0.13	57,64,72,78	0
5	EDO	L	302	4/4	0.95	0.13	39,52,59,70	0
5	EDO	L	309	4/4	0.96	0.12	42,51,53,62	0
5	EDO	G	512	4/4	0.96	0.14	39,43,53,59	0
5	EDO	G	511	4/4	0.97	0.07	51,53,80,89	0

6.5 Other polymers (i)

There are no such residues in this entry.