



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:07 am GMT

PDB ID : 4MC5
Title : Crystal structure of a subtype H18 hemagglutinin homologue from A/flat-faced bat/Peru/033/2010 (H18N11)
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Guo, Z.; Stevens, J.
Deposited on : 2013-08-21
Resolution : 2.24 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

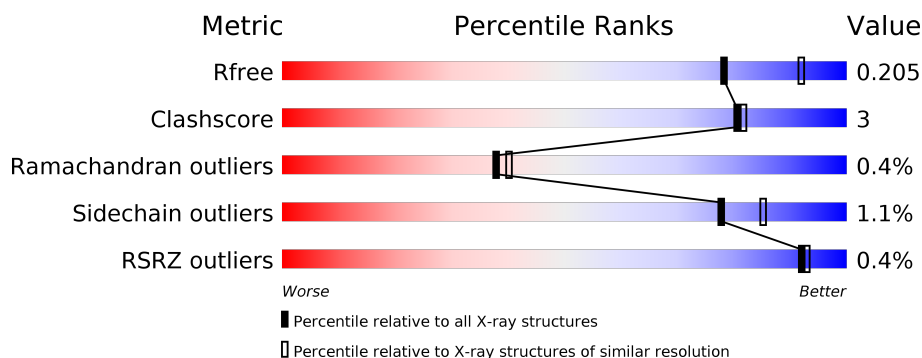
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	100719	1804 (2.26-2.22)
Clashscore	112137	1957 (2.26-2.22)
Ramachandran outliers	110173	1916 (2.26-2.22)
Sidechain outliers	110143	1917 (2.26-2.22)
RSRZ outliers	101464	1809 (2.26-2.22)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	510	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 91%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 91%; width: 8%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 99%; width: 1%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 91%; width: 8%; text-align: center;">91%</div> <div style="position: absolute; top: 0; left: 99%; width: 1%; text-align: center;">5%</div> <div style="position: absolute; top: 0; left: 99%; text-align: center;">•</div> </div> </div>
1	B	510	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 90%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 90%; width: 8%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 98%; width: 1%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 90%; width: 8%; text-align: center;">90%</div> <div style="position: absolute; top: 0; left: 98%; width: 1%; text-align: center;">6%</div> <div style="position: absolute; top: 0; left: 98%; text-align: center;">•</div> </div> </div>
1	C	510	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 91%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 91%; width: 8%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 99%; width: 1%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 91%; width: 8%; text-align: center;">91%</div> <div style="position: absolute; top: 0; left: 99%; width: 1%; text-align: center;">6%</div> <div style="position: absolute; top: 0; left: 99%; text-align: center;">•</div> </div> </div>

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
3	MAN	A	611	-	-	-	X
3	MAN	B	607	-	-	-	X
4	NAG	A	612	-	-	-	X
4	NAG	C	606	-	-	-	X
5	FUC	C	608	-	-	-	X
6	NAG	A	616	X	-	-	-
6	NAG	B	612	X	-	-	-
6	NAG	C	609	-	-	-	X
6	NAG	C	610	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13219 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3914	2459	660	777	18			
1	B	494	Total	C	N	O	S	0	0	0
			3914	2459	660	777	18			
1	C	497	Total	C	N	O	S	0	0	0
			3938	2476	664	780	18			

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			50	28	2	20		

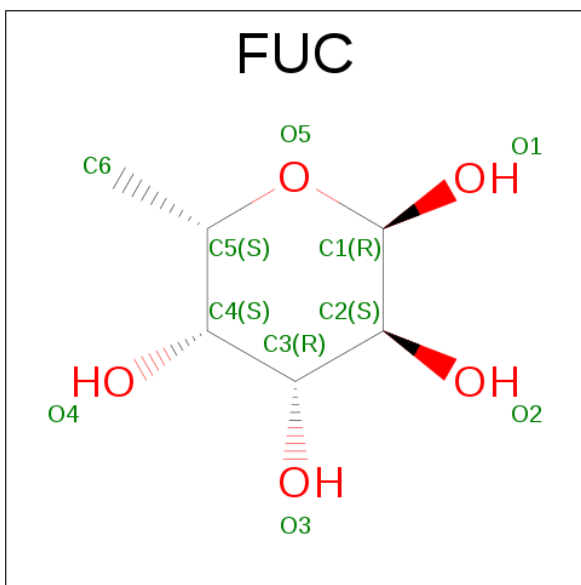
- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	7	Total	C	N	O	0	0
			81	46	2	33		
3	B	7	Total	C	N	O	0	0
			81	46	2	33		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

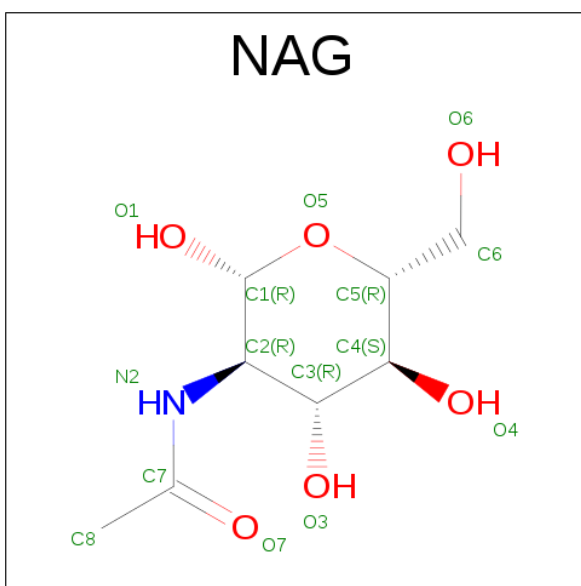
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	4	Total	C	N	O	0	0
			48	28	2	18		

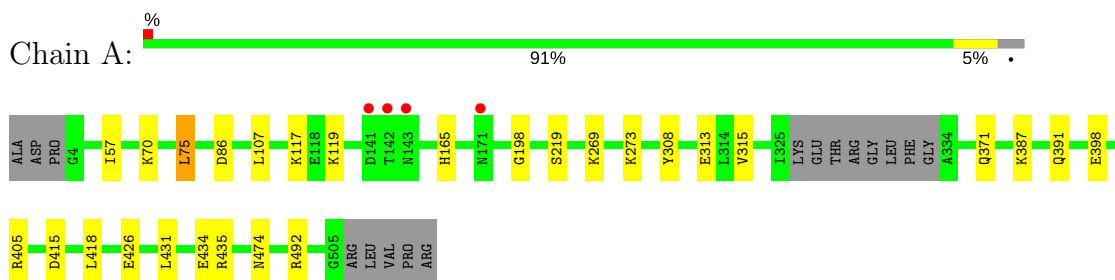
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	292	Total	O	0	0
			292	292		
8	B	343	Total	O	0	0
			343	343		
8	C	332	Total	O	0	0
			332	332		

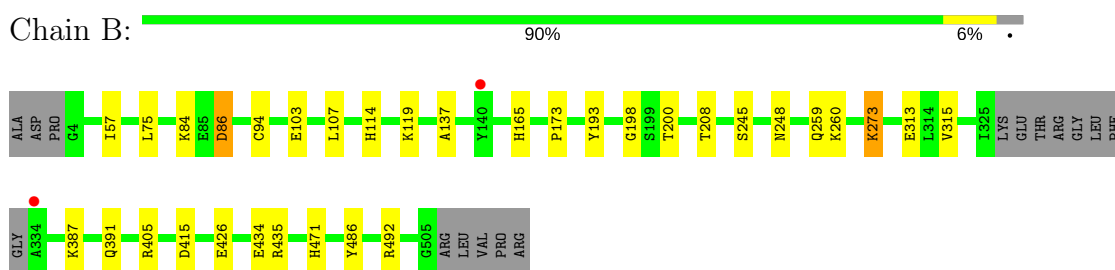
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

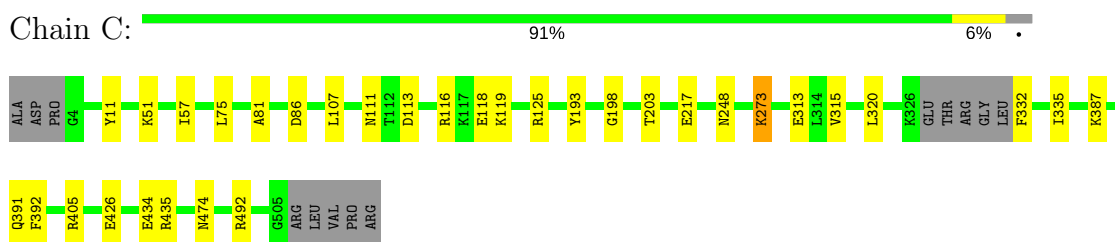
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	239.09Å 239.09Å 161.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 2.24 48.02 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.02-2.24) 95.7 (48.02-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.175 , 0.204 0.174 , 0.205	Depositor DCC
R_{free} test set	5564 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13219	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, FUL, BMA, 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	A	0.30	0/3998	0.46	0/5425
1	B	0.31	0/3998	0.47	0/5425
1	C	0.30	0/4023	0.46	0/5457
All	All	0.30	0/12019	0.46	0/16307

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 [i](#)

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	3914	0	3734	27	0
1	B	3914	0	3733	26	1
1	C	3938	0	3758	26	0
2	A	50	0	43	0	0
3	A	81	0	70	2	1
3	B	81	0	70	2	1
4	A	28	0	25	0	0
4	B	28	0	25	0	0
4	C	28	0	25	3	0
5	A	10	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	10	0	10	1	0
5	C	10	0	10	3	0
6	A	28	0	26	0	0
6	B	42	0	39	1	0
6	C	42	0	39	0	0
7	C	48	0	43	1	0
8	A	292	0	0	12	0
8	B	343	0	0	7	1
8	C	332	0	0	12	0
All	All	13219	0	11660	74	2

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 3.

All (74) 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:C:125:ARG:NH2	8:C:980:HOH:O	2.01	0.91
4:C:607:NAG:O4	8:C:997:HOH:O	1.91	0.87
1:C:113:ASP:OD2	8:C:927:HOH:O	1.96	0.82
1:C:474:ASN:OD1	8:C:811:HOH:O	1.99	0.80
1:A:474:ASN:OD1	8:A:812:HOH:O	2.01	0.78
1:B:119:LYS:NZ	8:B:811:HOH:O	2.15	0.77
1:C:217:GLU:OE1	8:C:897:HOH:O	2.04	0.76
1:C:111:ASN:ND2	8:C:903:HOH:O	2.17	0.75
1:A:371:GLN:OE1	8:A:899:HOH:O	2.04	0.75
1:B:208:THR:OG1	8:B:770:HOH:O	2.06	0.73
1:A:119:LYS:NZ	8:A:712:HOH:O	2.22	0.73
1:A:391:GLN:HB3	5:A:614:FUC:H61	1.70	0.73
3:A:607:BMA:O2	8:A:896:HOH:O	2.07	0.72
4:C:606:NAG:O3	8:C:981:HOH:O	2.07	0.71
1:C:203:THR:OG1	8:C:784:HOH:O	2.10	0.68
1:B:260:LYS:NZ	8:B:1024:HOH:O	2.26	0.67
1:B:391:GLN:HB3	5:B:610:FUC:H61	1.77	0.67
1:A:435:ARG:HH22	1:B:434:GLU:CD	1.98	0.67
1:A:434:GLU:CD	1:C:435:ARG:HH22	1.97	0.67
1:A:426:GLU:HG2	1:C:387:LYS:HD2	1.79	0.65
1:B:86:ASP:OD2	8:B:785:HOH:O	2.15	0.65
1:B:435:ARG:HH22	1:C:434:GLU:CD	2.00	0.65
1:B:313:GLU:HG3	1:B:315:VAL:HG23	1.79	0.65
1:A:387:LYS:HD2	1:B:426:GLU:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LYS:NZ	8:C:736:HOH:O	2.19	0.64
1:C:313:GLU:HG3	1:C:315:VAL:HG23	1.78	0.64
1:B:387:LYS:HD2	1:C:426:GLU:HG2	1.77	0.64
1:C:273:LYS:NZ	8:C:970:HOH:O	2.31	0.64
1:A:313:GLU:HG3	1:A:315:VAL:HG23	1.78	0.64
1:A:398:GLU:HG3	8:A:931:HOH:O	1.99	0.60
1:C:391:GLN:HB3	5:C:608:FUC:H61	1.83	0.60
1:A:117:LYS:NZ	8:A:807:HOH:O	2.18	0.57
1:A:165:HIS:HD2	8:A:922:HOH:O	1.88	0.56
1:A:165:HIS:CG	3:A:610:FUL:H5	2.41	0.55
1:B:103:GLU:OE2	8:B:842:HOH:O	2.18	0.55
1:A:70:LYS:NZ	8:A:945:HOH:O	2.41	0.53
1:B:165:HIS:CG	3:B:606:FUL:H5	2.43	0.53
1:B:165:HIS:CD2	3:B:606:FUL:H5	2.44	0.53
1:C:11:TYR:HB2	1:C:320:LEU:HD22	1.95	0.48
1:B:471:HIS:HE2	1:B:486:TYR:HH	1.62	0.48
1:C:313:GLU:CG	1:C:315:VAL:HG23	2.44	0.47
4:C:607:NAG:O3	8:C:850:HOH:O	2.18	0.47
6:B:611:NAG:O4	8:B:851:HOH:O	2.21	0.46
1:B:107:LEU:HD11	1:C:405:ARG:HA	1.98	0.46
1:A:405:ARG:HA	1:C:107:LEU:HD11	1.98	0.45
1:A:431:LEU:O	1:A:435:ARG:HG3	2.16	0.45
1:B:173:PRO:HG3	1:B:260:LYS:HE3	1.98	0.45
1:B:313:GLU:CG	1:B:315:VAL:HG23	2.46	0.44
1:B:387:LYS:CD	1:C:426:GLU:HG2	2.47	0.44
1:C:193:TYR:CZ	1:C:248:ASN:HA	2.52	0.44
1:A:435:ARG:NH2	8:A:834:HOH:O	2.41	0.44
1:A:308:TYR:CD2	1:A:418:LEU:HD13	2.53	0.44
1:A:107:LEU:HD11	1:B:405:ARG:HA	2.00	0.44
1:A:219:SER:OG	8:A:856:HOH:O	2.09	0.43
1:A:313:GLU:CG	1:A:315:VAL:HG23	2.46	0.43
1:A:435:ARG:NE	8:A:834:HOH:O	2.48	0.42
1:C:113:ASP:O	8:C:941:HOH:O	2.21	0.42
1:A:269:LYS:HE2	8:A:818:HOH:O	2.19	0.42
1:B:84:LYS:NZ	8:B:718:HOH:O	2.28	0.42
5:A:614:FUC:H62	1:B:415:ASP:OD2	2.20	0.42
1:B:193:TYR:CZ	1:B:248:ASN:HA	2.54	0.42
1:C:273:LYS:HA	1:C:273:LYS:HE3	2.01	0.42
1:C:474:ASN:N	1:C:474:ASN:OD1	2.52	0.41
7:C:603:NAG:O5	7:C:604:FUC:H3	2.19	0.41
1:A:474:ASN:OD1	1:A:474:ASN:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:CYS:HB2	1:B:137:ALA:O	2.20	0.41
1:A:75:LEU:HA	1:A:75:LEU:HD12	1.92	0.41
1:C:116:ARG:NH1	1:C:118:GLU:OE1	2.47	0.41
1:B:200:THR:HG23	1:B:245:SER:HB2	2.03	0.41
1:A:387:LYS:CD	1:B:426:GLU:HG2	2.48	0.41
1:B:114:HIS:ND1	1:B:259:GLN:OE1	2.54	0.40
1:A:415:ASP:OD2	5:C:608:FUC:H62	2.20	0.40
1:C:392:PHE:HB3	5:C:608:FUC:H63	2.03	0.40
1:C:51:LYS:HB3	1:C:81:ALA:HB2	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:608:MAN:O4	3:B:601:NAG:O7[3_755]	2.16	0.04
1:B:273:LYS:NZ	8:B:969:HOH:O[6_575]	2.18	0.02

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	490/510 (96%)	480 (98%)	8 (2%)	2 (0%)	38	40
1	B	490/510 (96%)	479 (98%)	9 (2%)	2 (0%)	38	40
1	C	493/510 (97%)	482 (98%)	9 (2%)	2 (0%)	38	40
All	All	1473/1530 (96%)	1441 (98%)	26 (2%)	6 (0%)	38	40

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	198	GLY

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Mol	Chain	Res	Type
1	B	57	ILE
1	C	57	ILE
1	C	198	GLY
1	B	198	GLY

5.3.2 Protein sidechains ⓘ

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	437/450 (97%)	433 (99%)	4 (1%)	82	88
1	B	437/450 (97%)	433 (99%)	4 (1%)	82	88
1	C	439/450 (98%)	433 (99%)	6 (1%)	71	80
All	All	1313/1350 (97%)	1299 (99%)	14 (1%)	78	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	86	ASP
1	A	273	LYS
1	A	492	ARG
1	B	75	LEU
1	B	86	ASP
1	B	273	LYS
1	B	492	ARG
1	C	75	LEU
1	C	86	ASP
1	C	273	LYS
1	C	332	PHE
1	C	335	ILE
1	C	492	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	165	HIS
1	C	133	ASN
1	C	161	GLN

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 ⓘ

28 carbohydrates 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	A	601	1,2	14,14,15	0.47	0	15,19,21	1.64	2 (13%)
2	NAG	A	602	2	14,14,15	0.56	0	15,19,21	0.96	0
2	BMA	A	603	2	11,11,12	0.62	0	13,15,17	0.88	1 (7%)
2	MAN	A	604	2	11,11,12	0.53	0	13,15,17	0.83	1 (7%)
3	NAG	A	605	1,3	14,14,15	0.55	0	15,19,21	0.85	0
3	NAG	A	606	3	14,14,15	0.47	0	15,19,21	0.72	0
3	BMA	A	607	3	11,11,12	0.58	0	13,15,17	1.26	1 (7%)
3	MAN	A	608	3	11,11,12	0.60	0	13,15,17	0.92	1 (7%)
3	FUC	A	609	3	9,10,11	0.83	0	13,14,16	0.80	0
3	FUL	A	610	3	9,10,11	1.19	1 (11%)	13,14,16	1.22	2 (15%)
3	MAN	A	611	3	11,11,12	0.53	0	13,15,17	1.22	1 (7%)
4	NAG	A	612	1,4	14,14,15	0.44	0	15,19,21	1.29	2 (13%)
4	NAG	A	613	4	14,14,15	0.51	0	15,19,21	1.86	2 (13%)
3	NAG	B	601	1,3	14,14,15	0.53	0	15,19,21	1.17	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	602	3	14,14,15	0.53	0	15,19,21	0.91	1 (6%)
3	BMA	B	603	3	11,11,12	0.64	0	13,15,17	0.99	0
3	MAN	B	604	3	11,11,12	0.48	0	13,15,17	2.22	2 (15%)
3	FUC	B	605	3	9,10,11	0.91	0	13,14,16	0.72	0
3	FUL	B	606	3	9,10,11	1.15	1 (11%)	13,14,16	1.32	2 (15%)
3	MAN	B	607	3	11,11,12	0.57	0	13,15,17	1.71	2 (15%)
4	NAG	B	608	1,4	14,14,15	0.52	0	15,19,21	1.03	0
4	NAG	B	609	4	14,14,15	0.44	0	15,19,21	2.31	3 (20%)
7	NAG	C	602	1,7	14,14,15	0.39	0	15,19,21	1.15	2 (13%)
7	NAG	C	603	7	14,14,15	0.57	0	15,19,21	1.35	2 (13%)
7	FUC	C	604	7	9,10,11	1.10	1 (11%)	13,14,16	1.46	2 (15%)
7	FUL	C	605	7	9,10,11	1.12	0	13,14,16	1.01	1 (7%)
4	NAG	C	606	1,4	14,14,15	0.46	0	15,19,21	1.02	2 (13%)
4	NAG	C	607	4	14,14,15	0.55	0	15,19,21	1.03	1 (6%)

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	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
2	BMA	A	603	2	-	0/2/19/22	0/1/1/1
2	MAN	A	604	2	-	0/2/19/22	0/1/1/1
3	NAG	A	605	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	606	3	-	0/6/23/26	0/1/1/1
3	BMA	A	607	3	-	0/2/19/22	0/1/1/1
3	MAN	A	608	3	-	0/2/19/22	1/1/1/1
3	FUC	A	609	3	-	0/0/17/20	0/1/1/1
3	FUL	A	610	3	-	0/0/17/20	0/1/1/1
3	MAN	A	611	3	-	0/2/19/22	0/1/1/1
4	NAG	A	612	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	613	4	-	0/6/23/26	0/1/1/1
3	NAG	B	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	602	3	-	0/6/23/26	0/1/1/1
3	BMA	B	603	3	-	0/2/19/22	0/1/1/1
3	MAN	B	604	3	-	0/2/19/22	0/1/1/1
3	FUC	B	605	3	-	0/0/17/20	0/1/1/1
3	FUL	B	606	3	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	B	607	3	-	0/2/19/22	0/1/1/1
4	NAG	B	608	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	609	4	-	0/6/23/26	0/1/1/1
7	NAG	C	602	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	603	7	-	0/6/23/26	0/1/1/1
7	FUC	C	604	7	-	0/0/17/20	0/1/1/1
7	FUL	C	605	7	-	0/0/17/20	0/1/1/1
4	NAG	C	606	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	607	4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	606	FUL	O5-C1	-2.23	1.40	1.43
7	C	604	FUC	C4-C5	2.37	1.57	1.53
3	A	610	FUL	C4-C5	2.40	1.57	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	609	NAG	C4-C3-C2	-3.73	105.56	111.02
7	C	603	NAG	O5-C1-C2	-3.64	106.41	111.47
4	A	612	NAG	O5-C1-C2	-3.33	106.85	111.47
3	B	601	NAG	C2-N2-C7	-3.24	118.22	122.94
3	A	611	MAN	C1-C2-C3	-3.10	105.72	109.65
3	A	607	BMA	C6-C5-C4	-2.99	106.01	113.00
4	B	609	NAG	C2-N2-C7	-2.73	118.96	122.94
4	A	612	NAG	C2-N2-C7	-2.53	119.25	122.94
3	B	604	MAN	C2-C3-C4	-2.46	106.58	110.88
2	A	601	NAG	O4-C4-C3	-2.40	105.14	110.36
4	C	607	NAG	O5-C1-C2	-2.33	108.23	111.47
3	B	602	NAG	C2-N2-C7	-2.26	119.64	122.94
4	C	606	NAG	O5-C1-C2	-2.20	108.42	111.47
7	C	602	NAG	O5-C1-C2	-2.16	108.47	111.47
2	A	604	MAN	O5-C1-C2	-2.01	107.65	110.79
7	C	605	FUL	O5-C5-C4	2.09	113.06	109.62
7	C	602	NAG	O3-C3-C2	2.09	113.87	109.39
3	B	606	FUL	O2-C2-C1	2.17	113.58	109.18
3	A	610	FUL	O2-C2-C1	2.23	113.72	109.18
3	A	610	FUL	O5-C5-C4	2.38	113.54	109.62
4	C	606	NAG	C1-O5-C5	2.44	115.53	112.17
7	C	603	NAG	C3-C4-C5	2.49	114.60	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	604	FUC	C1-O5-C5	2.68	118.31	112.39
3	A	608	MAN	C1-O5-C5	2.68	115.86	112.17
3	B	606	FUL	O5-C5-C4	2.80	114.23	109.62
2	A	603	BMA	C1-C2-C3	2.89	113.32	109.65
3	B	607	MAN	C3-C4-C5	2.90	115.33	110.22
7	C	604	FUC	O5-C5-C4	3.44	115.29	109.62
4	A	613	NAG	C3-C4-C5	3.48	116.36	110.22
3	B	607	MAN	C1-O5-C5	4.41	118.25	112.17
2	A	601	NAG	C1-O5-C5	4.87	118.88	112.17
4	A	613	NAG	C1-O5-C5	5.26	119.41	112.17
4	B	609	NAG	C1-O5-C5	7.07	121.91	112.17
3	B	604	MAN	C1-O5-C5	7.20	122.09	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	608	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	607	BMA	1	0
3	A	608	MAN	0	1
3	A	610	FUL	1	0
3	B	601	NAG	0	1
3	B	606	FUL	2	0
7	C	603	NAG	1	0
7	C	604	FUC	1	0
4	C	606	NAG	1	0
4	C	607	NAG	2	0

5.6 Ligand geometry

11 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$
5	FUC	A	614	-	9,10,11	0.55	0	13,14,16	2.28	3 (23%)
6	NAG	A	615	1	14,14,15	0.54	0	15,19,21	0.96	1 (6%)
6	NAG	A	616	1	14,14,15	0.49	0	15,19,21	0.93	1 (6%)
5	FUC	B	610	-	9,10,11	0.40	0	13,14,16	2.25	4 (30%)
6	NAG	B	611	1	14,14,15	0.55	0	15,19,21	0.80	0
6	NAG	B	612	1	14,14,15	0.46	0	15,19,21	0.96	1 (6%)
6	NAG	B	613	1	14,14,15	0.47	0	15,19,21	0.97	1 (6%)
6	NAG	C	601	1	14,14,15	0.38	0	15,19,21	2.17	4 (26%)
5	FUC	C	608	-	9,10,11	0.39	0	13,14,16	2.47	4 (30%)
6	NAG	C	609	1	14,14,15	0.57	0	15,19,21	0.77	0
6	NAG	C	610	1	14,14,15	0.55	0	15,19,21	0.78	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	FUC	A	614	-	-	0/0/17/20	0/1/1/1
6	NAG	A	615	1	-	0/6/23/26	0/1/1/1
6	NAG	A	616	1	1/1/5/7	0/6/23/26	0/1/1/1
5	FUC	B	610	-	-	0/0/17/20	0/1/1/1
6	NAG	B	611	1	-	0/6/23/26	0/1/1/1
6	NAG	B	612	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	B	613	1	-	0/6/23/26	0/1/1/1
6	NAG	C	601	1	-	0/6/23/26	0/1/1/1
5	FUC	C	608	-	-	0/0/17/20	0/1/1/1
6	NAG	C	609	1	-	0/6/23/26	0/1/1/1
6	NAG	C	610	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	NAG	C4-C3-C2	-3.66	105.66	111.02
5	B	610	FUC	C2-C3-C4	-2.03	107.34	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	NAG	C2-N2-C7	-2.00	120.02	122.94
6	A	615	NAG	C1-O5-C5	2.04	114.98	112.17
5	C	608	FUC	C1-C2-C3	2.08	112.29	109.65
6	A	616	NAG	C1-O5-C5	2.22	115.22	112.17
6	C	601	NAG	O5-C1-C2	2.37	114.77	111.47
6	B	612	NAG	C1-O5-C5	2.76	115.97	112.17
5	B	610	FUC	C1-O5-C5	2.85	118.69	112.39
5	A	614	FUC	C1-O5-C5	2.88	118.75	112.39
5	B	610	FUC	O5-C5-C4	3.07	114.68	109.62
6	B	613	NAG	C1-O5-C5	3.13	116.48	112.17
5	C	608	FUC	O5-C5-C4	3.17	114.85	109.62
5	C	608	FUC	C1-O5-C5	3.31	119.71	112.39
5	A	614	FUC	O5-C5-C4	3.50	115.39	109.62
5	B	610	FUC	O5-C1-C2	6.17	120.46	110.79
5	A	614	FUC	O5-C1-C2	6.22	120.53	110.79
6	C	601	NAG	C1-O5-C5	6.61	121.27	112.17
5	C	608	FUC	O5-C1-C2	6.86	121.54	110.79

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	610	NAG	C1
6	B	612	NAG	C1
6	A	616	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	614	FUC	2	0
5	B	610	FUC	1	0
6	B	611	NAG	1	0
5	C	608	FUC	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	494/510 (96%)	-0.31	4 (0%) 86 86	23, 39, 59, 110	0
1	B	494/510 (96%)	-0.48	2 (0%) 92 93	21, 34, 56, 86	0
1	C	497/510 (97%)	-0.51	0 100 100	22, 36, 56, 82	0
All	All	1485/1530 (97%)	-0.43	6 (0%) 92 93	21, 37, 57, 110	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	THR	7.5
1	A	143	ASN	7.1
1	A	171	ASN	2.9
1	B	334	ALA	2.5
1	B	140	TYR	2.3
1	A	141	ASP	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MAN	B	607	11/12	0.79	0.25	6.45	84,90,96,96	0
4	NAG	C	606	14/15	0.89	0.29	4.40	55,64,76,79	0
4	NAG	A	612	14/15	0.82	0.23	3.98	61,69,75,81	0
3	MAN	A	611	11/12	0.77	0.24	3.28	67,76,86,87	0
4	NAG	B	608	14/15	0.90	0.14	1.54	57,65,76,82	0
3	NAG	B	601	14/15	0.94	0.10	-1.12	37,47,57,66	0
7	FUC	C	604	10/11	0.85	0.43	-	102,104,105,106	0
3	NAG	B	602	14/15	0.93	0.11	-	52,59,63,63	0
3	MAN	A	608	11/12	0.84	0.23	-	82,88,94,94	0
3	FUL	B	606	10/11	0.80	0.18	-	63,73,84,85	0
4	NAG	A	613	14/15	0.81	0.20	-	72,74,80,81	0
4	NAG	B	609	14/15	0.78	0.21	-	66,73,86,86	0
3	NAG	A	605	14/15	0.94	0.17	-	42,52,62,69	0
2	NAG	A	602	14/15	0.89	0.29	-	78,80,82,83	0
3	BMA	A	607	11/12	0.88	0.16	-	65,69,75,75	0
7	FUL	C	605	10/11	0.62	0.36	-	93,106,135,135	0
7	NAG	C	603	14/15	0.57	0.32	-	104,114,120,120	0
3	FUC	A	609	10/11	0.94	0.14	-	52,58,63,65	0
3	FUC	B	605	10/11	0.96	0.13	-	52,55,59,60	0
7	NAG	C	602	14/15	0.82	0.24	-	80,87,100,108	0
2	NAG	A	601	14/15	0.83	0.28	-	73,79,85,85	0
2	BMA	A	603	11/12	0.76	0.31	-	66,72,77,80	0
4	NAG	C	607	14/15	0.71	0.34	-	73,84,90,90	0
2	MAN	A	604	11/12	0.75	0.48	-	82,87,91,91	0
3	FUL	A	610	10/11	0.82	0.22	-	58,68,71,72	0
3	NAG	A	606	14/15	0.91	0.19	-	53,58,63,65	0
3	BMA	B	603	11/12	0.73	0.20	-	74,82,89,92	0
3	MAN	B	604	11/12	0.60	0.43	-	103,109,114,114	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	FUC	C	608	10/11	0.56	0.32	6.49	86,89,92,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	C	609	14/15	0.83	0.21	3.17	58,68,71,73	0
6	NAG	B	611	14/15	0.85	0.19	1.91	63,68,73,75	0
6	NAG	B	612	14/15	0.88	0.18	0.98	83,91,92,93	0
6	NAG	A	615	14/15	0.84	0.15	0.80	64,73,75,76	0
6	NAG	B	613	14/15	0.76	0.39	-	85,90,93,95	0
5	FUC	B	610	10/11	0.60	0.38	-	81,86,87,87	0
6	NAG	C	601	14/15	0.78	0.20	-	95,103,107,108	0
6	NAG	A	616	14/15	0.88	0.23	-	82,89,91,92	0
6	NAG	C	610	14/15	0.82	0.23	-	81,88,89,90	0
5	FUC	A	614	10/11	0.65	0.24	-	75,83,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.