

wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 – 07:12 AM BST

PDB ID : 3M1C

> Title : Crystal structure of the conserved herpesvirus fusion regulator complex gH-gL

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2010-03-04 Deposited on

3.00 Å(reported) Resolution

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 (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.13.1

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

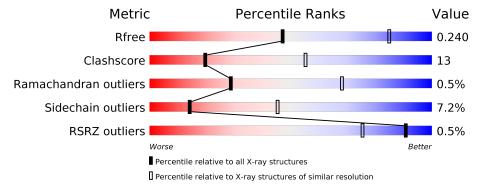
Validation Pipeline (wwPDB-VP) 2.13.1

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 3.00 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	Q	uality of chain			
1	A	762	70%			22%	• 6%
2	В	204	39%	31%	·	28%	
3	С	2		100%			



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6708 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 H.

Mol Chain Residues	Atoms			$\mathbf{AltConf}$	Trace
1 A 719 Total 5428 3	C N (3453 985 9'	O S 75 15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	804	HIS	_	expression tag	UNP P89445
A	805	HIS	-	expression tag	UNP P89445
A	806	HIS	_	expression tag	UNP P89445
A	807	HIS	_	expression tag	UNP P89445
A	808	HIS	_	expression tag	UNP P89445
A	809	HIS	-	expression tag	UNP P89445

• Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	146	Total 1162	C 729	N 218	O 210	S 5	0	0	0

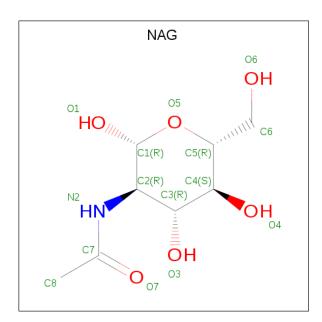
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



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

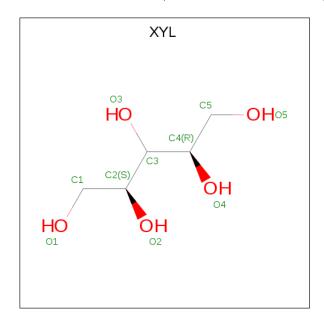
• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
1	Λ	1	Total	С	N	О	0	0	
4	Α	1	14	8	1	5	U	U	
4	Λ	1	Total	С	N	О	0	0	
4	А	1	14	8	1	5	0	0	

 \bullet Molecule 5 is Xylitol (three-letter code: XYL) (formula: $\mathrm{C_5H_{12}O_5}).$



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

 $\bullet\,$ Molecule 6 is water.



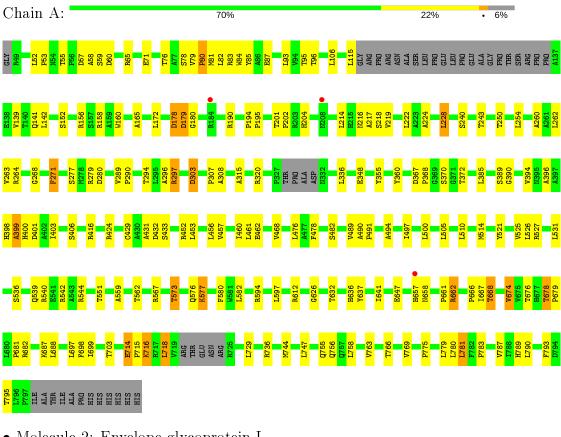
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	46	Total O 46 46	0	0
6	В	6	Total O 6 6	0	0



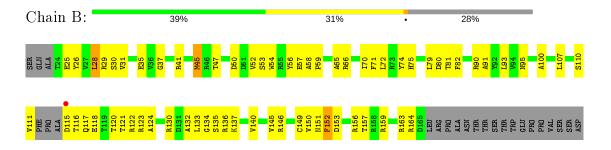
Residue-property plots (i) 3

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 H



• Molecule 2: Envelope glycoprotein L





ASP ALA ALA ALA ALA ALA ALA ALA ALA GLU LIEU LIEU PRO PRO PRO GLN THR GLN PRO PRO PRO	ALA ALA ARG ARG ARG ARG ARG ARG ARG ARG ARG AR
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 $\bullet \ \, \text{Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose} \\$

Chain C: 100%

NAG1 NAG2



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 41 21 2	Depositor	
Cell constants	88.25Å 88.25Å 333.41Å	Danagitan	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	39.20 - 3.00	Depositor	
resolution (A)	49.96 - 2.84	EDS	
% Data completeness	94.6 (39.20-3.00)	Depositor	
(in resolution range)	92.1 (49.96-2.84)	EDS	
R_{merge}	0.13	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.45 (at 2.86Å)	Xtriage	
Refinement program	PHENIX 1.4_175	Depositor	
D D.	0.170 , 0.242	Depositor	
R, R_{free}	0.172 , 0.240	DCC	
R_{free} test set	3107 reflections (9.63%)	wwPDB-VP	
Wilson B-factor (Å ²)	51.5	Xtriage	
Anisotropy	0.337	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 50.8	EDS	
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.94	EDS	
Total number of atoms	6708	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 3.32% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: XYL, 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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.45	0/5569	0.61	0/7616	
2	В	0.47	0/1186	0.61	0/1606	
All	All	0.45	0/6755	0.61	0/9222	

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	5428	0	5412	129	0
2	В	1162	0	1116	49	0
3	С	28	0	25	0	0
4	A	28	0	26	0	0
5	A	10	0	12	2	0
6	A	46	0	0	1	0
6	В	6	0	0	0	0
All	All	6708	0	6591	168	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 13.



The worst 5 of 168 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{\AA}) \end{array}$	Clash overlap (Å)
1:A:368:PRO:HG3	1:A:626:GLY:HA2	1.67	0.75
1:A:416:ARG:HB2	1:A:416:ARG:NH1	2.01	0.74
2:B:132:ALA:O	2:B:135:SER:HB3	1.86	0.74
1:A:279:ARG:HG2	1:A:280:ASP:OD2	1.88	0.73
1:A:576:GLN:HG3	1:A:577:LYS:HD3	1.71	0.73

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	Analysed Favoured Allowed		Outliers	Percentiles		
1	A	711/762 (93%)	660 (93%)	48 (7%)	3 (0%)	34	72	
2	В	140/204~(69%)	128 (91%)	11 (8%)	1 (1%)	22	60	
All	All	851/966 (88%)	788 (93%)	59 (7%)	4 (0%)	29	68	

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ALA
1	A	80	PRO
1	A	399	ALA
2	В	164	ARG

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	Rotameric Outliers		
1	A	551/587 (94%)	515 (94%)	36 (6%)	17 50	
2	В	119/176 (68%)	107 (90%)	12 (10%)	7 29	
All	All	670/763~(88%)	622 (93%)	48 (7%)	14 45	

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	${f Res}$	Type
1	A	540	ARG
1	A	647	GLU
2	В	130	ARG
1	A	567	ARG
1	A	577	LYS

Some 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		
			nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	С	1	1,3	14,14,15	0.53	0	17,19,21	1.62	1 (5%)



	Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	3	NAG	С	2	3	14,14,15	0.42	0	17,19,21	0.97	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
3	NAG	С	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	С	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
3	С	1	NAG	C1-O5-C5	5.31	119.39	112.19
3	С	2	NAG	C1-O5-C5	2.25	115.25	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

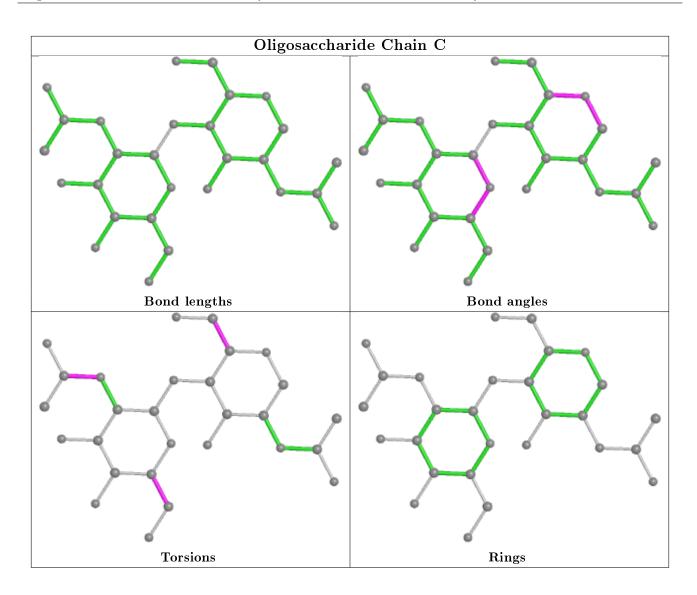
Mol	Chain	Res	Type	Atoms
3	С	2	NAG	O7-C7-N2-C2
3	С	2	NAG	C8-C7-N2-C2
3	С	2	NAG	O5-C5-C6-O6
3	С	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry (i)

3 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	Bo	Bond lengths			Bond angles		
MIOI	турс			LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	NAG	A	1670	1	14,14,15	0.85	1 (7%)	17,19,21	1.63	3 (17%)	
5	XYL	A	1	-	9,9,9	0.74	0	11,11,11	1.33	2 (18%)	
4	NAG	A	810	1	14,14,15	0.53	0	17,19,21	0.72	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	${ m Res}$	Link	Chirals	Torsions	Rings
4	NAG	A	1670	1	-	1/6/23/26	0/1/1/1
5	XYL	A	1	_	-	0/12/12/12	-
4	NAG	A	810	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${f Observed(\AA)}$	$\operatorname{Ideal}(ext{\AA})$
4	A	1670	NAG	C1-C2	2.11	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
4	A	1670	NAG	C1-O5-C5	4.85	118.77	112.19
4	A	1670	NAG	O5-C1-C2	2.84	115.77	111.29
5	A	1	XYL	C4-C3-C2	2.69	118.96	113.36
4	A	1670	NAG	C4-C3-C2	2.11	114.11	111.02
5	A	1	XYL	C1-C2-C3	2.11	116.99	112.41

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1670	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	XYL	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 (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, 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	${f Analysed}$			$OWAB(A^2)$	Q<0.9
1	A	719/762~(94%)	-0.48	3 (0%) 92 79	25, 52, 104, 146	0
2	В	146/204 (71%)	-0.51	1 (0%) 87 69	36, 57, 93, 149	0
All	All	865/966 (89%)	-0.48	4 (0%) 91 75	25, 53, 101, 149	0

All (4) RSRZ outliers are listed below:

Mol	Chain	${f Res}$	Type	RSRZ
1	A	184	ARG	3.5
1	A	657	HIS	2.6
2	В	115	ASP	2.4
1	A	208	ASN	2.2

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

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

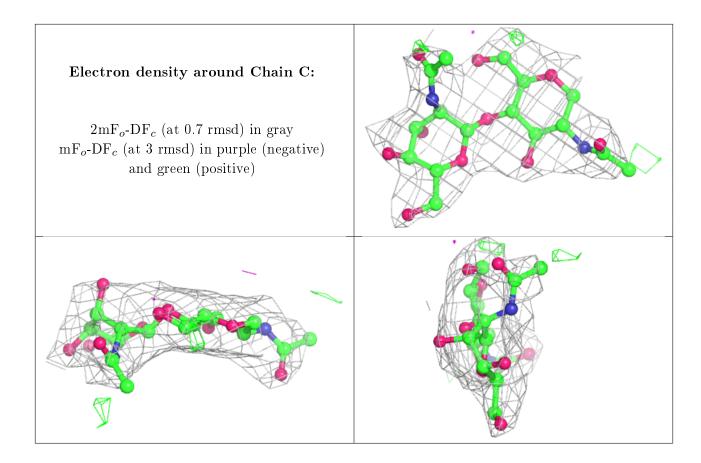
6.3 Carbohydrates (i)

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	${f B-factors}({f A}^2)$	Q<0.9
3	NAG	С	2	14/15	0.89	0.24	85,106,113,116	0
3	NAG	С	1	14/15	0.94	0.14	57,74,80,93	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, 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	$ m B ext{-}factors(\AA^2)$	Q<0.9
4	NAG	A	810	14/15	0.68	0.32	100,124,141,142	0
4	NAG	A	1670	14/15	0.79	0.28	81,118,137,145	0
5	XYL	A	1	10/10	0.81	0.39	65,74,126,126	0

6.5 Other polymers (i)

There are no such residues in this entry.

