



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:55 PM GMT

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

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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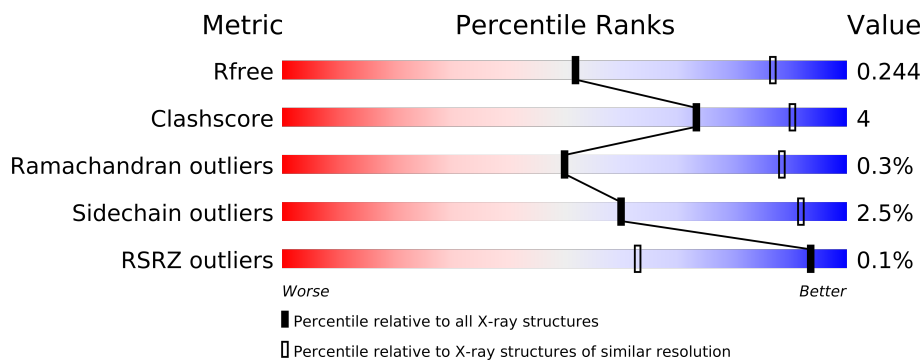
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 3.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1332 (3.04-3.00)
Clashscore	79885	1732 (3.04-3.00)
Ramachandran outliers	78287	1669 (3.04-3.00)
Sidechain outliers	78261	1672 (3.04-3.00)
RSRZ outliers	66119	1333 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	703	
1	B	703	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9943 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

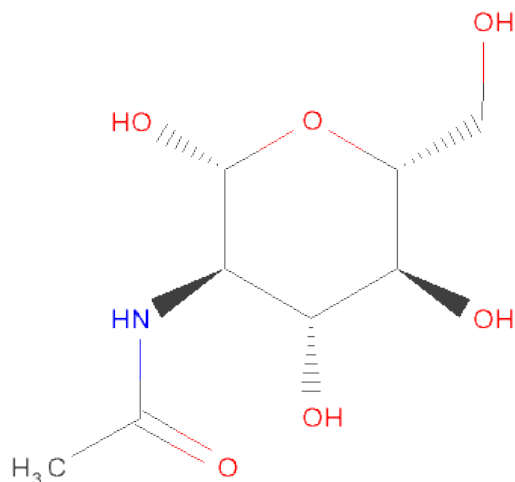
- Molecule 1 is a protein called Envelope glycoprotein B.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASP	-	EXPRESSION TAG	UNP P06437
A	29	PRO	-	EXPRESSION TAG	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437
A	313	SER	THR	SEE REMARK 999	UNP P06437
A	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	549	THR	ALA	ENGINEERED MUTATION	UNP P06437
B	28	ASP	-	EXPRESSION TAG	UNP P06437
B	29	PRO	-	EXPRESSION TAG	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
B	549	THR	ALA	ENGINEERED MUTATION	UNP P06437

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASP	-	EXPRESSION TAG	UNP P06437
A	29	PRO	-	EXPRESSION TAG	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437

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Chain	Residue	Modelled	Actual	Comment	Reference
A	313	SER	THR	SEE REMARK 999	UNP P06437
A	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	549	THR	ALA	ENGINEERED MUTATION	UNP P06437
A	28	ASP	-	EXPRESSION TAG	UNP P06437
A	29	PRO	-	EXPRESSION TAG	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437
A	313	SER	THR	SEE REMARK 999	UNP P06437
A	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	549	THR	ALA	ENGINEERED MUTATION	UNP P06437

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

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

- Molecule 5 is water.

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.43Å 117.43Å 160.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.47 – 3.03 48.47 – 3.03	Depositor EDS
% Data completeness (in resolution range)	93.1 (48.47-3.03) 93.1 (48.47-3.03)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1391)	Depositor
R, $R_{free}$	0.201 , 0.243 0.202 , 0.244	Depositor DCC
$R_{free}$ test set	2259 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.2	EDS
Estimated twinning fraction	0.026 for -h,-k,l 0.479 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 48077 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.34	0/4992	0.49	0/6791
1	B	0.34	0/5022	0.48	0/6830
All	All	0.34	0/10014	0.49	0/13621

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4871	0	0	22	0
1	B	4900	0	0	18	0
2	A	28	0	26	0	0
2	B	56	0	52	0	0
3	A	56	0	50	2	0
4	A	1	0	0	0	0
5	A	10	0	0	2	0
5	B	21	0	0	2	0
All	All	9943	0	128	42	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:562:ARG:NH2	5:B:927:HOH:O	2.23	0.70
1:A:176:GLY:O	1:A:258:ARG:NH2	2.28	0.67
1:A:245:ARG:NH2	1:A:275:GLU:OE1	2.29	0.66
1:A:245:ARG:NH1	1:A:329:ASP:OD2	2.28	0.65
1:A:304:ARG:NH1	1:A:323:ASP:OD2	2.33	0.61
3:A:1430:NAG:O3	3:A:1431:NAG:O5	2.19	0.60
1:A:166:LYS:NZ	1:A:210:THR:O	2.34	0.59
1:B:282:TYR:OH	1:B:408:ASP:OD2	2.22	0.57
1:B:589:ILE:O	1:B:591:SER:N	2.38	0.56
1:B:207:CYS:O	1:B:232:MET:N	2.39	0.56
1:A:359:LYS:N	5:A:902:HOH:O	2.39	0.56
1:B:304:ARG:NH1	5:B:903:HOH:O	2.39	0.55
1:A:248:HIS:NE2	1:A:251:ASP:OD1	2.41	0.53
1:A:318:ARG:NH1	1:A:346:THR:O	2.41	0.53
1:B:176:GLY:O	1:B:258:ARG:NH2	2.41	0.53
1:B:470:ARG:O	1:B:473:SER:OG	2.27	0.52
1:A:637:HIS:O	1:A:652:GLU:N	2.44	0.50
1:A:558:ARG:NH1	1:A:620:ASN:O	2.45	0.49
1:A:105:LYS:O	1:A:658:GLN:NE2	2.46	0.49
1:A:195:GLU:OE1	1:A:195:GLU:N	2.46	0.48
1:A:196:GLU:OE2	1:A:208:ARG:N	2.45	0.48
1:A:347:THR:N	1:A:350:PHE:O	2.46	0.48
1:A:110:ASP:OD1	1:A:110:ASP:N	2.47	0.47
1:A:440:GLN:OE1	1:A:442:TYR:OH	2.32	0.47
1:B:105:LYS:O	1:B:658:GLN:NE2	2.47	0.47
1:B:144:GLU:OE2	1:B:433:HIS:NE2	2.48	0.47
1:A:194:PHE:N	5:A:901:HOH:O	2.48	0.46
1:A:464:TYR:O	1:A:468:HIS:N	2.50	0.44
1:A:237:ALA:N	1:A:246:GLY:O	2.50	0.44
3:A:1430:NAG:O3	3:A:1431:NAG:O6	2.29	0.44
1:B:440:GLN:OE1	1:B:442:TYR:OH	2.36	0.43
1:B:604:PHE:O	1:B:613:VAL:N	2.52	0.43
1:B:377:ARG:NH2	1:B:471:GLU:OE2	2.52	0.43
1:B:250:THR:O	1:B:270:ASN:ND2	2.52	0.42
1:B:200:LYS:NZ	1:B:231:ASP:OD2	2.53	0.42
1:B:587:MET:O	1:B:597:TYR:N	2.53	0.41
1:A:643:PHE:N	1:A:646:GLY:O	2.53	0.41
1:B:110:ASP:OD1	1:B:110:ASP:N	2.53	0.41
1:A:200:LYS:NZ	1:A:231:ASP:OD2	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:718:ASP:OD2	1:B:721:THR:OG1	2.38	0.41
1:A:579:ASP:N	1:A:579:ASP:OD1	2.54	0.40
1:B:596:CYS:N	1:B:631:GLU:O	2.54	0.40

There are no symmetry-related clashes.

## 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	604/703 (86%)	580 (96%)	21 (4%)	3 (0%)	38	83
1	B	605/703 (86%)	574 (95%)	30 (5%)	1 (0%)	56	91
All	All	1209/1406 (86%)	1154 (96%)	51 (4%)	4 (0%)	50	88

All (4) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	520/594 (88%)	505 (97%)	15 (3%)	55	90
1	B	526/594 (89%)	515 (98%)	11 (2%)	66	94
All	All	1046/1188 (88%)	1020 (98%)	26 (2%)	60	92

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	THR
1	A	135	THR
1	A	199	ASP
1	A	228	HIS
1	A	244	SER
1	A	309	THR
1	A	352	VAL
1	A	384	PHE
1	A	387	SER
1	A	392	SER
1	A	432	THR
1	A	465	VAL
1	A	557	ARG
1	A	572	THR
1	A	634	THR
1	B	135	THR
1	B	170	VAL
1	B	228	HIS
1	B	262	PHE
1	B	340	THR
1	B	352	VAL
1	B	397	THR
1	B	405	SER
1	B	432	THR
1	B	519	ASP
1	B	588	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 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	$\# Z  > 2$
3	NAG	A	1398	1,3	12,14,15	0.31	0	15,19,21	0.31	0
3	NAG	A	1399	3	12,14,15	0.29	0	15,19,21	0.41	0
3	NAG	A	1430	1,3	12,14,15	0.25	0	15,19,21	0.45	0
3	NAG	A	1431	3	12,14,15	0.49	0	15,19,21	0.76	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
3	NAG	A	1398	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1399	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1430	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1431	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1431	NAG	O5-C5-C4	-2.31	107.73	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	1141	1	12,14,15	0.30	0	15,19,21	0.35	0
2	NAG	A	1674	1	12,14,15	0.26	0	15,19,21	0.36	0
2	NAG	B	1141	1	12,14,15	0.29	0	15,19,21	0.29	0
2	NAG	B	1398	1	12,14,15	0.30	0	15,19,21	0.29	0
2	NAG	B	1430	1	12,14,15	0.27	0	15,19,21	0.30	0
2	NAG	B	1674	1	12,14,15	0.27	0	15,19,21	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1141	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1674	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1141	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1398	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1430	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1674	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	608/703 (86%)	0.03	0	100   100	40, 95, 154, 193	0
1	B	608/703 (86%)	0.07	1 (0%)	93   53	38, 96, 157, 203	0
All	All	1216/1406 (86%)	0.05	1 (0%)	93   63	38, 95, 156, 203	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	TYR	4.2

### 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. 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	1398	14/15	0.15	-1.90	156,156,156,156	0
3	NAG	A	1430	14/15	0.12	-3.44	175,175,175,175	0
3	NAG	A	1399	14/15	0.11	-	173,173,173,173	0
3	NAG	A	1431	14/15	0.17	-	176,176,176,176	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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	1141	14/15	0.31	0.67	172,172,172,172	0
2	NAG	B	1141	14/15	0.24	0.10	177,177,177,177	0
2	NAG	A	1674	14/15	0.24	-0.17	149,149,149,149	0
2	NAG	B	1430	14/15	0.19	-0.56	167,167,167,167	0
2	NAG	B	1398	14/15	0.13	-2.07	131,147,159,163	0
2	NAG	B	1674	14/15	0.17	-4.91	130,130,130,130	0
4	CL	A	801	1/1	0.14	-5.79	85,85,85,85	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.