



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 08:39 AM BST

PDB ID : 6C5J  
Title : S25-23 Fab in complex with Chlamydiaceae LPS (Crystal form 1)  
Authors : Haji-Ghassemi, O.; Evans, S.V.  
Deposited on : 2018-01-16  
Resolution : 2.29 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
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  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

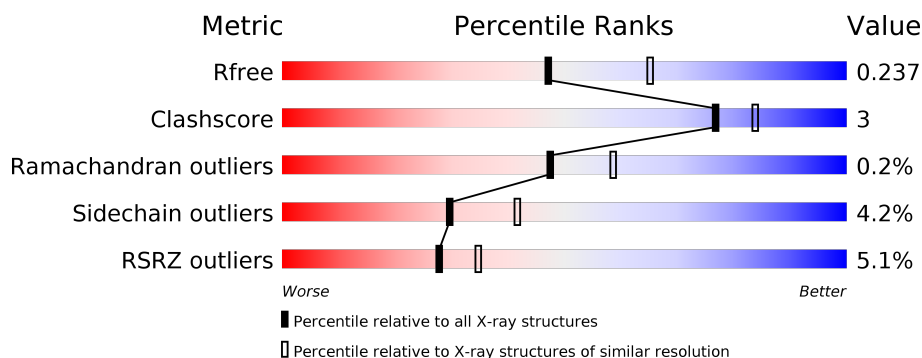
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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  $\leq 5\%$ . 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	H	218	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> <div>•</div> </div>
2	L	219	<div> <div>7%</div> <div> <div></div> <div>88%</div> <div>10%</div> </div> <div>••</div> </div>
3	A	5	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3456 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.

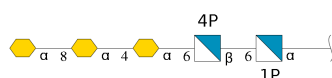
- Molecule 1 is a protein called IgG1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	0	0
			1648	1050	271	320	7			

- Molecule 2 is a protein called IgG1 Fab Light Chain (Kappa).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1684	1056	286	336	6			

- Molecule 3 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-8)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	5	Total	C	N	O	P	0	0	0
			76	36	2	36	2			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

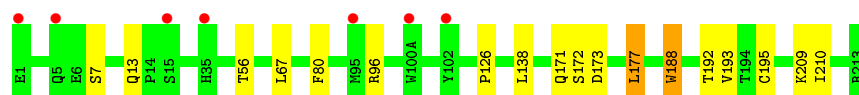
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	14	Total	O	0	0
			14	14		
5	L	20	Total	O	0	0
			20	20		

### 3 Residue-property plots


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.

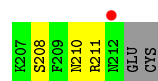
- Molecule 1: IgG1 Fab Heavy Chain

Chain H: 



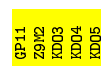
- Molecule 2: IgG1 Fab Light Chain (Kappa)

Chain L: 



- Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-8)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.23Å 45.45Å 75.67Å 90.00° 105.31° 90.00°	Depositor
Resolution (Å)	25.00 – 2.29 22.73 – 2.28	Depositor EDS
% Data completeness (in resolution range)	93.7 (25.00-2.29) 93.8 (22.73-2.28)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 2.28Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.193 , 0.239 0.198 , 0.237	Depositor DCC
$R_{free}$ test set	813 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3456	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: KDO, Z9M, NAG, GP1

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	H	0.50	0/1693	0.71	1/2321 (0.0%)
2	L	0.48	0/1723	0.69	0/2338
All	All	0.49	0/3416	0.70	1/4659 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	177	LEU	CA-CB-CG	5.60	128.18	115.30

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	H	1648	0	1615	8	0
2	L	1684	0	1634	14	0
3	A	76	0	40	1	0
4	H	14	0	13	0	0
5	H	14	0	0	0	0
5	L	20	0	0	2	0
All	All	3456	0	3302	20	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 3.

All (20) 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)
2:L:137:ASN:ND2	5:L:301:HOH:O	2.21	0.61
1:H:67:LEU:HD11	1:H:80:PHE:CE2	2.36	0.61
2:L:137:ASN:HB3	2:L:138:ASN:HD22	1.71	0.55
1:H:56:THR:OG1	3:A:3:KDO:O1B	2.26	0.53
2:L:138:ASN:HA	2:L:172:THR:CG2	2.40	0.52
2:L:170:ASP:OD1	2:L:172:THR:HG22	2.11	0.50
2:L:189:HIS:O	2:L:211:ARG:HD3	2.12	0.49
2:L:138:ASN:HA	2:L:172:THR:HG21	1.95	0.49
1:H:138:LEU:HD12	1:H:193:VAL:HG11	1.96	0.48
2:L:193:THR:OG1	2:L:208:SER:HB3	2.14	0.47
1:H:188:TRP:HA	1:H:188:TRP:CE3	2.50	0.47
2:L:114:THR:HG22	5:L:301:HOH:O	2.17	0.45
2:L:185:GLU:HA	2:L:188:ARG:HG3	1.99	0.44
1:H:172:SER:OG	1:H:173:ASP:N	2.50	0.43
2:L:155:ARG:HG2	2:L:179:LEU:HD21	2.02	0.42
1:H:96:ARG:HG3	2:L:91:GLY:HA3	2.01	0.42
1:H:210:ILE:HD12	1:H:210:ILE:N	2.35	0.42
2:L:28:ASN:HD22	2:L:30:ASN:H	1.66	0.42
2:L:137:ASN:HB3	2:L:138:ASN:ND2	2.36	0.40
1:H:171:GLN:HE22	2:L:180:THR:HG21	1.85	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	H	216/218 (99%)	205 (95%)	10 (5%)	1 (0%)	29 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	215/219 (98%)	210 (98%)	5 (2%)	0	100	100
All	All	431/437 (99%)	415 (96%)	15 (4%)	1 (0%)	47	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	126	PRO

### 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	H	189/190 (100%)	182 (96%)	7 (4%)	34	48
2	L	193/195 (99%)	184 (95%)	9 (5%)	26	37
All	All	382/385 (99%)	366 (96%)	16 (4%)	30	42

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	7	SER
1	H	13	GLN
1	H	177	LEU
1	H	188	TRP
1	H	192	THR
1	H	195	CYS
1	H	209	LYS
2	L	3	LEU
2	L	28	ASN
2	L	39	LYS
2	L	107	LYS
2	L	142	LYS
2	L	169	LYS
2	L	185	GLU
2	L	200	THR

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Mol	Chain	Res	Type
2	L	210	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	171	GLN
2	L	28	ASN
2	L	42	GLN
2	L	137	ASN
2	L	138	ASN
2	L	212	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

5 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	$\# Z  > 2$
3	GP1	A	1	3	15,16,16	1.40	2 (13%)	23,24,24	1.12	1 (4%)
3	Z9M	A	2	3	15,15,16	1.04	1 (6%)	18,22,24	1.51	2 (11%)
3	KDO	A	3	3	12,15,16	0.65	0	16,21,24	0.93	0
3	KDO	A	4	3	12,15,16	0.89	1 (8%)	16,21,24	1.35	3 (18%)
3	KDO	A	5	3	12,15,16	0.99	1 (8%)	16,21,24	1.59	4 (25%)

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	GP1	A	1	3	-	0/6/27/27	0/1/1/1
3	Z9M	A	2	3	-	0/7/24/27	0/1/1/1
3	KDO	A	3	3	-	2/6/26/30	0/1/1/1
3	KDO	A	4	3	-	1/6/26/30	0/1/1/1
3	KDO	A	5	3	-	0/6/26/30	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	GP1	P4B-O8B	3.30	1.61	1.50
3	A	1	GP1	P4B-O1	3.01	1.65	1.59
3	A	2	Z9M	P1-O9	2.90	1.59	1.50
3	A	4	KDO	C4-C5	2.41	1.56	1.52
3	A	5	KDO	C4-C5	-2.33	1.49	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	Z9M	O8-P1-O7	3.69	121.74	107.64
3	A	1	GP1	O9B-P4B-O7B	3.38	120.56	107.64
3	A	2	Z9M	C1-O5-C5	-2.85	108.32	112.19
3	A	5	KDO	C6-O6-C2	2.57	116.83	111.34
3	A	5	KDO	O6-C6-C5	2.47	111.34	107.87
3	A	4	KDO	C3-C2-C1	-2.27	106.97	111.93
3	A	5	KDO	C4-C3-C2	2.26	113.87	109.81
3	A	4	KDO	C3-C4-C5	2.26	113.97	110.69
3	A	5	KDO	O4-C4-C5	-2.19	105.75	110.14
3	A	4	KDO	O8-C8-C7	-2.12	106.45	111.07

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4	KDO	C5-C6-C7-C8
3	A	3	KDO	C6-C7-C8-O8
3	A	3	KDO	O7-C7-C8-O8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	KDO	1	0

## 5.6 Ligand geometry

1 ligand is 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	H	301	1	14,14,15	0.44	0	17,19,21	1.03	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
4	NAG	H	301	1	-	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	H	301	NAG	C4-C3-C2	-2.26	107.70	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	H	218/218 (100%)	0.15	7 (3%)	47	54	35, 50, 78, 111	0
2	L	217/219 (99%)	0.38	15 (6%)	16	22	35, 53, 81, 102	0
All	All	435/437 (99%)	0.26	22 (5%)	28	35	35, 52, 81, 111	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	152	GLY	3.4
2	L	201	SER	3.4
2	L	212	ASN	3.3
1	H	95	MET	3.3
1	H	15	SER	3.1
1	H	102	TYR	3.1
2	L	27(E)	LYS	3.0
2	L	133	VAL	2.8
2	L	204	PRO	2.7
2	L	158	GLY	2.5
2	L	9	LEU	2.4
1	H	1	GLU	2.3
2	L	202	THR	2.3
1	H	5	GLN	2.2
2	L	134	CYS	2.2
2	L	3	LEU	2.2
2	L	118	PHE	2.2
2	L	198	HIS	2.1
1	H	100(A)	TRP	2.1
2	L	206	VAL	2.1
2	L	135	PHE	2.1
1	H	35	HIS	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<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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GP1	A	1	16/16	0.81	0.30	68,95,120,120	0
3	KDO	A	4	15/16	0.91	0.11	42,44,61,63	0
3	Z9M	A	2	15/16	0.94	0.12	54,60,66,69	0
3	KDO	A	5	15/16	0.94	0.12	40,46,48,53	0
3	KDO	A	3	15/16	0.94	0.15	47,52,64,69	0

## 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<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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	H	301	14/15	0.76	0.31	83,87,94,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.