



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 02:24 PM GMT

PDB ID : 3VDF  
Title : Crystal Structure of C-lobe of Bovine lactoferrin Complexed with di-aminopimelic acid at 1.46 Å Resolution  
Authors : Shukla, P.K.; Gautam, L.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2012-01-05  
Resolution : 1.46 Å(reported)

This is a wwPDB validation summary 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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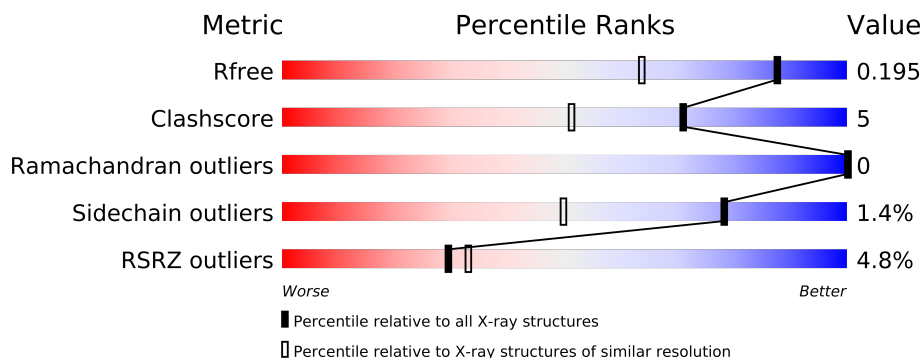
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.46 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	2476 (1.50-1.42)
Clashscore	79885	2834 (1.50-1.42)
Ramachandran outliers	78287	2769 (1.50-1.42)
Sidechain outliers	78261	2767 (1.50-1.42)
RSRZ outliers	66119	2477 (1.50-1.42)

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	335	
2	B	6	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
8	SO4	A	710	-	X
9	API	A	711	-	X

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 3154 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 Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2560	1593	448	499	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LYS	ASN	CONFLICT	UNP P24627
A	608	GLU	LYS	CONFLICT	UNP P24627

- Molecule 2 is a protein called C-TERMINAL PEPTIDE OF LACTOTRANSFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	6	44	29	6	8	1	0	0	0

- Molecule 3 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
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	A	2	Total	C	N	O	0	0
			28	16	2	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LYS	ASN	CONFLICT	UNP P24627
A	608	GLU	LYS	CONFLICT	UNP P24627
A	565	LYS	ASN	CONFLICT	UNP P24627
A	608	GLU	LYS	CONFLICT	UNP P24627

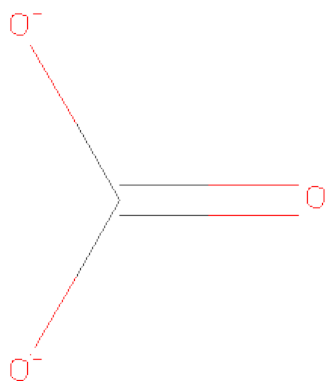
- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Fe	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Zn	0	0
			2	2		

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



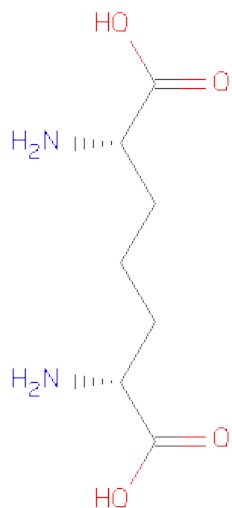
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is 2,6-DIAMINOPIMELIC ACID (three-letter code: API) (formula: C<sub>7</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			13	7	2	4		

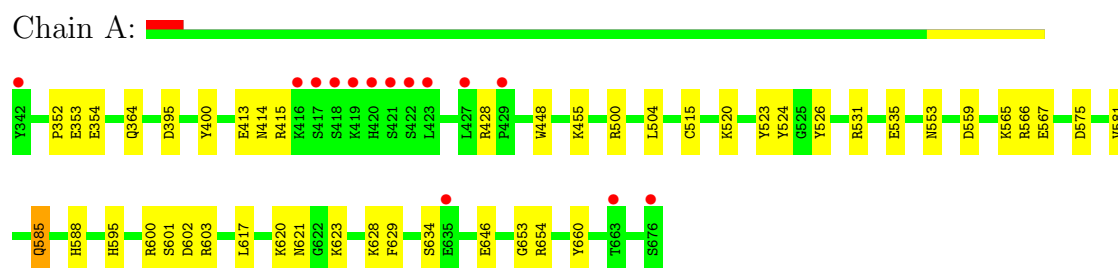
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	453	Total	O	0	0
			453	453		
10	B	2	Total	O	0	0
			2	2		

### 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 errors 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: Lactotransferrin



#### • Molecule 2: C-TERMINAL PEPTIDE OF LACTOTRANSFERRIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.21Å 50.02Å 65.21Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	37.87 – 1.46 37.87 – 1.46	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.87-1.46) 99.2 (37.87-1.46)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.160 , 0.194 0.163 , 0.195	Depositor DCC
$R_{free}$ test set	3356 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.5	EDS
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 66074 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: ZN, NAG, CO3, API, SO4, FE

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	1.45	14/2608 (0.5%)	1.29	9/3533 (0.3%)
2	B	1.11	0/44	1.14	0/58
All	All	1.44	14/2652 (0.5%)	1.29	9/3591 (0.3%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	601	SER	CB-OG	-8.15	1.31	1.42
1	A	413	GLU	CD-OE1	-7.28	1.17	1.25
1	A	448	TRP	CD2-CE2	7.12	1.49	1.41
1	A	400	TYR	CE1-CZ	-6.48	1.30	1.38
1	A	600	ARG	CD-NE	-5.93	1.36	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	531	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	600	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	575	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	500	ARG	NE-CZ-NH1	5.57	123.08	120.30

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	2560	0	2480	24	0
2	B	44	0	39	0	0
3	A	14	0	13	0	0
4	A	56	0	50	0	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
7	A	4	0	0	0	0
8	A	5	0	0	0	0
9	A	13	0	12	1	0
10	A	453	0	0	2	0
10	B	2	0	0	0	0
All	All	3154	0	2594	24	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 5.

The worst 5 of 24 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:565:LYS:HE3	1:A:567:GLU:CB	2.15	0.76
1:A:566:ARG:HG2	1:A:581:VAL:HG21	1.69	0.75
1:A:565:LYS:HD2	1:A:566:ARG:N	2.03	0.72
1:A:565:LYS:HE3	1:A:567:GLU:HB2	1.78	0.66
1:A:566:ARG:HG2	1:A:581:VAL:CG2	2.27	0.64

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	333/335 (99%)	321 (96%)	12 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	4/6 (67%)	4 (100%)	0	0	100	100
All	All	337/341 (99%)	325 (96%)	12 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	278/278 (100%)	275 (99%)	3 (1%)	84	60
2	B	4/4 (100%)	3 (75%)	1 (25%)	1	0
All	All	282/282 (100%)	278 (99%)	4 (1%)	78	50

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	515	CYS
1	A	585	GLN
1	A	602	ASP
2	B	682	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	489	GLN
1	A	551	ASN
1	A	585	GLN
1	A	624	ASN

### 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$
4	NAG	A	702	1,4	12,14,15	1.41	2 (16%)	15,19,21	1.69	5 (33%)
4	NAG	A	703	4	12,14,15	0.72	0	15,19,21	2.28	5 (33%)
4	NAG	A	704	1,4	12,14,15	1.28	1 (8%)	15,19,21	2.70	9 (60%)
4	NAG	A	705	4	12,14,15	0.82	1 (8%)	15,19,21	2.55	6 (40%)

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	A	702	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	703	4	-	0/6/23/26	0/1/1/1
4	NAG	A	704	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	705	4	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	NAG	O7-C7	2.84	1.29	1.23
4	A	704	NAG	C2-N2	2.79	1.49	1.46
4	A	702	NAG	C4-C3	2.12	1.58	1.52
4	A	705	NAG	C3-C2	2.04	1.56	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	705	NAG	C3-C4-C5	-7.03	97.65	110.20
4	A	703	NAG	O5-C5-C6	5.13	112.36	106.98
4	A	704	NAG	C2-N2-C7	-4.43	115.65	123.09
4	A	704	NAG	O5-C5-C4	-4.33	105.16	110.65
4	A	704	NAG	O5-C5-C6	4.06	111.24	106.98

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, 3 are monoatomic - leaving 4 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
3	NAG	A	701	1	12,14,15	1.06	1 (8%)	15,19,21	2.23	4 (26%)
7	CO3	A	709	5	0,3,3	0.00	-	0,3,3	0.00	-
8	SO4	A	710	-	4,4,4	1.12	0	6,6,6	0.83	0
9	API	A	711	6	12,12,12	0.89	1 (8%)	15,15,15	2.04	4 (26%)

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	701	1	-	0/6/23/26	0/1/1/1
7	CO3	A	709	5	-	0/0/0/0	0/0/0/0
8	SO4	A	710	-	-	0/0/0/0	0/0/0/0
9	API	A	711	6	-	0/14/14/14	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	NAG	O7-C7	2.56	1.28	1.23
9	A	711	API	O2-C1	-2.38	1.21	1.30

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAG	O5-C5-C6	6.93	114.25	106.98
9	A	711	API	O2-C1-C2	4.22	126.34	116.88
9	A	711	API	C1-C2-N2	-3.62	103.37	109.36
9	A	711	API	C3-C2-N2	3.30	118.20	110.14
9	A	711	API	C7-C6-N6	-2.64	105.00	109.36

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	335/335 (100%)	0.07	14 (4%) 35 38	8, 15, 40, 77	0
2	B	6/6 (100%)	5.84	2 (33%) 1 0	27, 31, 102, 110	0
All	All	341/341 (100%)	0.18	16 (4%) 29 33	8, 15, 40, 110	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	681	LEU	22.6
1	A	342	TYR	8.9
2	B	682	GLU	7.8
1	A	418	SER	5.6
1	A	422	SER	4.4

### 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
4	NAG	A	703	14/15	0.20	1.74	39,45,54,57	0
4	NAG	A	702	14/15	0.13	0.92	27,33,43,46	0
4	NAG	A	705	14/15	0.14	-0.44	27,32,40,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	704	14/15	0.06	-0.99	17,20,24,27	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( $\text{\AA}^2$ )	Q<0.9
8	SO4	A	710	5/5	0.14	7.32	33,35,38,45	0
9	API	A	711	13/13	0.26	5.12	19,37,47,51	13
3	NAG	A	701	14/15	0.17	0.46	25,35,41,47	0
7	CO3	A	709	4/4	0.11	0.18	8,9,9,9	0
6	ZN	A	707	1/1	0.04	-1.45	12,12,12,12	0
6	ZN	A	708	1/1	0.04	-2.39	16,16,16,16	0
5	FE	A	706	1/1	0.06	-3.75	8,8,8,8	0

## 6.5 Other polymers

There are no such residues in this entry.