



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 08:08 PM GMT

PDB ID : 1T26  
Title : Plasmodium falciparum lactate dehydrogenase complexed with NADH and 4-hydroxy-1,2,5-thiadiazole-3-carboxylic acid  
Authors : Cameron, A.; Read, J.; Tranter, R.; Winter, V.J.; Sessions, R.B.; Brady, R.L.; Vivas, L.; Easton, A.; Kendrick, H.; Croft, S.L.; Barros, D.; Lavandera, J.L.; Martin, J.J.; Risco, F.; Garcia-Ochoa, S.; Gamo, F.J.; Sanz, L.; Leon, L.; Ruiz, J.R.; Gabarro, R.; Mallo, A.; De Las Heras, F.G.  
Deposited on : 2004-04-20  
Resolution : 1.80 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>

---

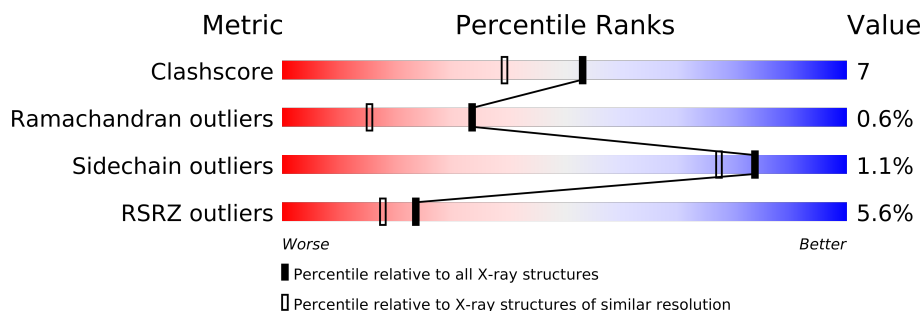
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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	322	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2717 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.

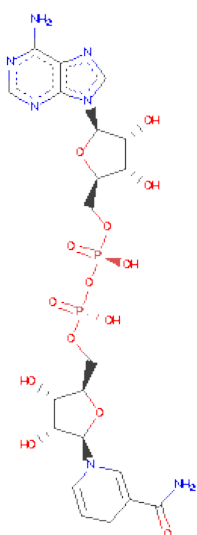
- Molecule 1 is a protein called L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2394	1523	410	448	13	99	2	0

There are 6 discrepancies between the modelled and reference sequences:

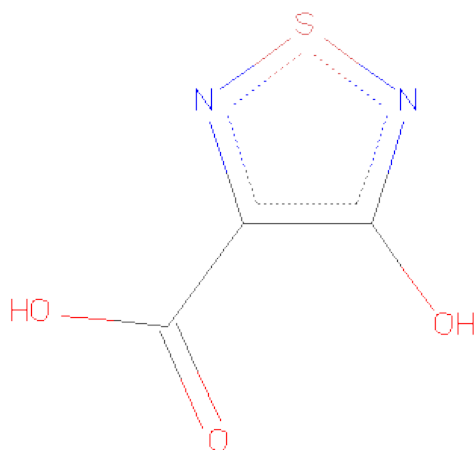
Chain	Residue	Modelled	Actual	Comment	Reference
A	330	HIS	-	EXPRESSION TAG	UNP Q27743
A	331	HIS	-	EXPRESSION TAG	UNP Q27743
A	332	HIS	-	EXPRESSION TAG	UNP Q27743
A	333	HIS	-	EXPRESSION TAG	UNP Q27743
A	334	HIS	-	EXPRESSION TAG	UNP Q27743
A	335	HIS	-	EXPRESSION TAG	UNP Q27743

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDEADENINE DINUCLEOTIDE (three-letter code: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 4-HYDROXY-1,2,5-THIADIAZOLE-3-CARBOXYLICACID (three-letter code: GBD) (formula:  $C_3H_2N_2O_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			9	3	2	3	1		

- Molecule 4 is water.

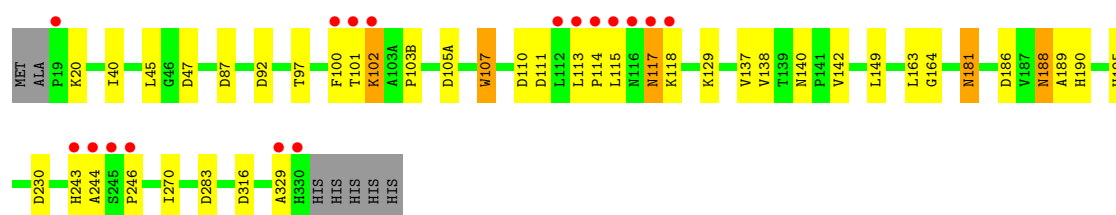
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	270	Total	O	0	0
			270	270		

### 3 Residue-property plots

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: L-lactate dehydrogenase

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.62Å 86.63Å 91.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 1.80 29.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.49-1.80) 97.2 (29.51-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.174 , 0.209 0.184 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29685 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: GBD, NAI

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	0.90	4/2442 (0.2%)	0.78	12/3307 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	TRP	C-N	-36.57	0.49	1.34
1	A	102	LYS	CA-CB	-12.29	1.26	1.53
1	A	102	LYS	C-N	5.78	1.47	1.34
1	A	129	LYS	CD-CE	5.49	1.65	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	TRP	O-C-N	-7.54	110.64	122.70
1	A	101	THR	CA-CB-CG2	-7.13	102.42	112.40
1	A	186	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	283	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	230[A]	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	230[B]	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	105(A)	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	87	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	92	ASP	CB-CG-OD2	5.21	122.99	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	LYS	CB-CA-C	5.16	120.71	110.40
1	A	316	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	110	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	LYS	Mainchain
1	A	107	TRP	Mainchain

## 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	2394	0	2472	33	0
2	A	44	0	27	3	0
3	A	9	0	1	2	0
4	A	270	0	0	3	2
All	All	2717	0	2500	33	2

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 7.

All (33) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:100:PHE:CD1	1:A:115:LEU:HB3	1.90	1.06
1:A:118:LYS:HD2	4:A:606:HOH:O	1.75	0.87
1:A:114:PRO:HG2	1:A:115:LEU:HD12	1.64	0.79
1:A:140:ASN:HD22	1:A:142:VAL:H	1.32	0.77
1:A:113:LEU:HD11	1:A:329:ALA:HB2	1.75	0.68
1:A:114:PRO:HG2	1:A:115:LEU:CD1	2.27	0.65
1:A:246:PRO:HD2	3:A:401:GBD:N2	2.14	0.61
1:A:181[A]:ASN:ND2	4:A:600:HOH:O	2.34	0.60
1:A:188:ASN:HD22	1:A:189:ALA:H	1.47	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:100:PHE:CG	1:A:115:LEU:HB3	2.35	0.59
1:A:113:LEU:HB3	1:A:114:PRO:HD3	1.88	0.54
1:A:115:LEU:N	1:A:115:LEU:HD12	2.22	0.54
1:A:140:ASN:HD22	1:A:142:VAL:N	2.04	0.52
1:A:138:VAL:O	2:A:416:NAI:H2N	2.12	0.50
1:A:100:PHE:CE1	1:A:115:LEU:O	2.65	0.49
1:A:20:LYS:HE3	1:A:47:ASP:OD1	2.13	0.49
1:A:188:ASN:HD22	1:A:189:ALA:N	2.10	0.48
1:A:117:ASN:HD22	1:A:117:ASN:H	1.61	0.48
1:A:140:ASN:ND2	1:A:142:VAL:H	2.06	0.47
1:A:190:HIS:CD2	1:A:270:ILE:HD11	2.50	0.46
1:A:113:LEU:HB3	1:A:114:PRO:CD	2.45	0.46
1:A:113:LEU:N	1:A:114:PRO:HD2	2.31	0.46
1:A:97:THR:HB	2:A:416:NAI:H51N	1.97	0.46
1:A:100:PHE:CD1	1:A:115:LEU:CB	2.80	0.44
1:A:100:PHE:CE1	1:A:115:LEU:HB3	2.46	0.43
1:A:118:LYS:CD	4:A:606:HOH:O	2.51	0.43
1:A:243:HIS:CG	1:A:244:ALA:N	2.85	0.43
1:A:163:LEU:HD23	2:A:416:NAI:C7N	2.47	0.43
1:A:40:ILE:HG23	1:A:45:LEU:HB2	2.01	0.42
1:A:195:HIS:NE2	3:A:401:GBD:O4	2.53	0.42
1:A:100:PHE:HE1	1:A:115:LEU:O	2.03	0.41
1:A:111:ASP:O	1:A:115:LEU:HD13	2.22	0.40
1:A:137:VAL:HG22	1:A:149:LEU:HD23	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	Distance(Å)	Clash(Å)
4:A:663:HOH:O	4:A:664:HOH:O[3_555]	1.93	0.27
4:A:641:HOH:O	4:A:670:HOH:O[3_655]	2.02	0.18

## 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	315/322 (98%)	303 (96%)	10 (3%)	2 (1%)	33	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103(B)	PRO
1	A	164	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	265/269 (98%)	261 (98%)	4 (2%)	76	66

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

Mol	Chain	Res	Type
1	A	117	ASN
1	A	181[A]	ASN
1	A	181[B]	ASN
1	A	188	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	117	ASN
1	A	132(B)	ASN
1	A	140	ASN
1	A	151	GLN
1	A	188	ASN
1	A	190	HIS
1	A	210(B)	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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$
3	GBD	A	401	-	9,9,9	2.72	4 (44%)	8,12,12	3.01	6 (75%)
2	NAI	A	416	-	48,48,48	1.70	7 (14%)	73,73,73	1.77	12 (16%)

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	GBD	A	401	-	-	0/3/4/4	0/0/1/1
2	NAI	A	416	-	-	0/30/72/72	0/3/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	416	NAI	O7N-C7N	6.54	1.41	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	416	NAI	C4N-C3N	-5.51	1.39	1.50
3	A	401	GBD	O4-C4	4.80	1.48	1.27
3	A	401	GBD	C3-C4	4.27	1.48	1.40
2	A	416	NAI	C4N-C5N	-4.16	1.40	1.49
3	A	401	GBD	O11-C1	3.23	1.33	1.23
2	A	416	NAI	C6N-C5N	3.13	1.39	1.33
2	A	416	NAI	C2A-N3A	2.97	1.38	1.32
3	A	401	GBD	O13-C1	-2.58	1.22	1.30
2	A	416	NAI	C2A-N1A	2.35	1.38	1.33
2	A	416	NAI	C2N-C3N	2.07	1.38	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	416	NAI	N3A-C2A-N1A	-10.72	119.75	128.71
3	A	401	GBD	C3-N2-S1	4.20	111.01	104.81
3	A	401	GBD	O4-C4-C3	-3.94	124.02	128.67
3	A	401	GBD	C4-C3-C1	-3.29	124.47	130.79
2	A	416	NAI	O4B-C1B-N9A	3.17	111.39	108.44
3	A	401	GBD	C1-C3-N2	2.94	126.89	120.12
3	A	401	GBD	N5-S1-N2	-2.91	97.23	100.42
2	A	416	NAI	C4A-C5A-N7A	-2.72	107.19	109.52
2	A	416	NAI	C5N-C4N-C3N	2.61	119.68	112.60
3	A	401	GBD	O13-C1-C3	2.60	121.52	114.39
2	A	416	NAI	N3A-C4A-N9A	2.54	130.02	125.43
2	A	416	NAI	C1B-N9A-C4A	-2.50	122.32	126.64
2	A	416	NAI	C8A-N9A-C1B	2.16	130.64	126.38
2	A	416	NAI	C4N-C3N-C2N	-2.15	119.06	121.68
2	A	416	NAI	C1D-N1N-C2N	-2.11	117.42	121.02
2	A	416	NAI	C4B-O4B-C1B	-2.09	107.48	109.75
2	A	416	NAI	C2A-N3A-C4A	2.02	119.76	114.01
2	A	416	NAI	N7A-C8A-N9A	-2.02	108.66	114.36

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	305/322 (94%)	-0.18	17 (5%) 24 18	12, 18, 31, 47	24 (7%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	ASN	5.8
1	A	100	PHE	5.4
1	A	243	HIS	5.3
1	A	246	PRO	5.2
1	A	115	LEU	5.2
1	A	113	LEU	4.8
1	A	114	PRO	4.1
1	A	116	ASN	4.0
1	A	19	PRO	3.7
1	A	245	SER	3.7
1	A	101	THR	3.4
1	A	112	LEU	3.3
1	A	330	HIS	3.2
1	A	244	ALA	3.0
1	A	118	LYS	2.8
1	A	329	ALA	2.4
1	A	102	LYS	2.3

### 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 ⓘ

There are no carbohydrates in this entry.

## 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
2	NAI	A	416	44/44	0.13	-	19,23,30,31	0
3	GBD	A	401	9/9	0.21	-	35,37,38,39	0

## 6.5 Other polymers

There are no such residues in this entry.