



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:33 PM GMT

PDB ID : 4YI5
Title : Crystal structure of Gpb in complex with 4b
Authors : Kantsadi, A.L.; Chatzileontiadou, D.S.M.; Stravodimos, G.A.; Leonidas, D.D.
Deposited on : 2015-02-27
Resolution : 1.80 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

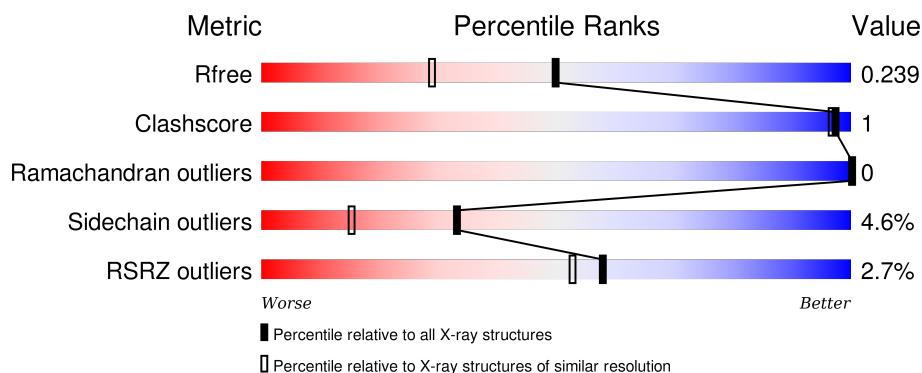
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

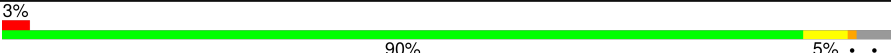
The reported resolution of this entry is 1.80 Å.

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))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	843	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IMP	A	903	X	-	-	-

2 Entry composition [i](#)

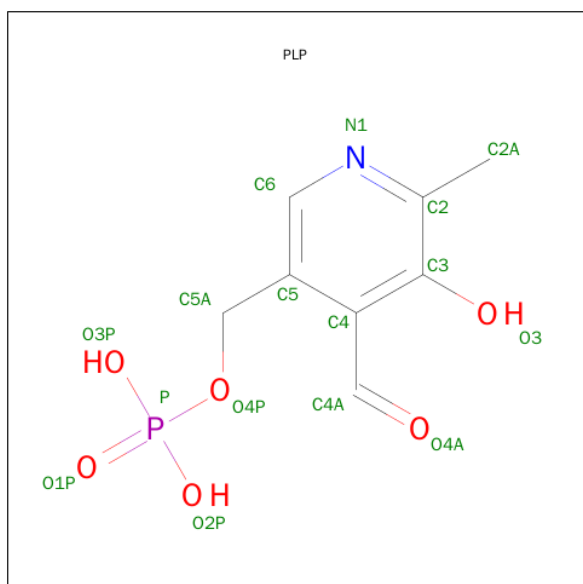
There are 5 unique types of molecules in this entry. The entry contains 7035 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen phosphorylase, muscle form.

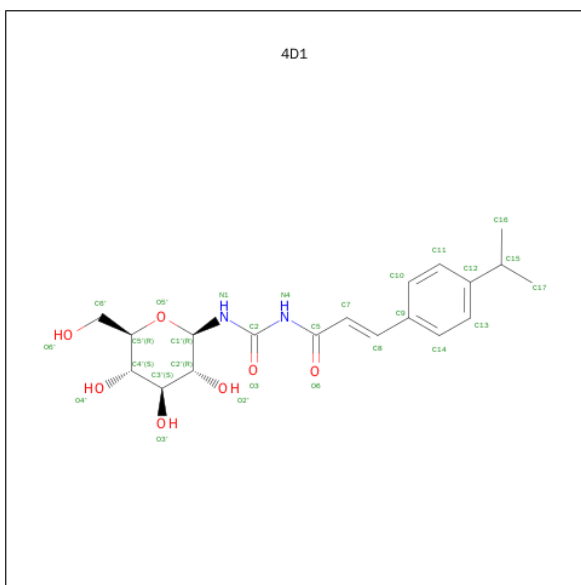
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	809	6585	4199	1159	1197	30	0	1	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



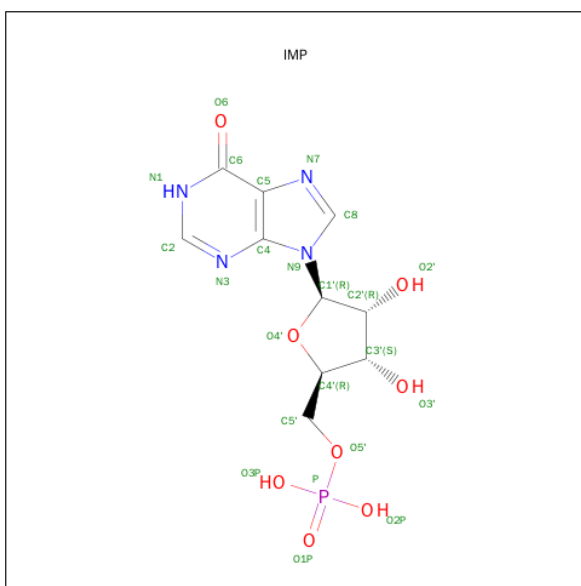
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0

- Molecule 3 is N-((2E)-3-[4-(propan-2-yl)phenyl]prop-2-enoyl}carbamoyl)-beta-D-glucopyranosylamine (three-letter code: 4D1) (formula: $C_{19}H_{26}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	2	7		

- Molecule 4 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



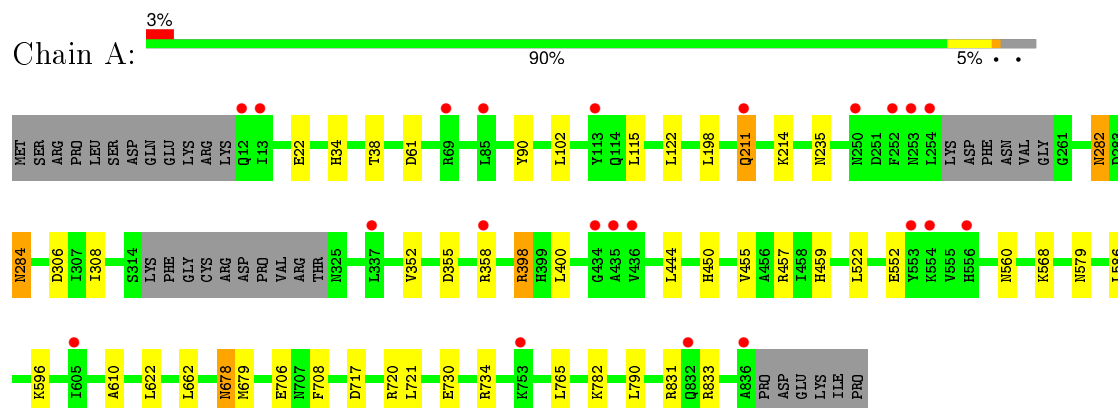
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	384	Total 384	O 384	0	0



- Molecule 1: Glycogen phosphorylase, muscle form



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.54Å 128.54Å 116.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.88 – 1.80 35.74 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.3 (38.88-1.80) 90.3 (35.74-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.194 , 0.230 0.204 , 0.239	Depositor DCC
R_{free} test set	4005 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 81770 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7035	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: IMP, 4D1, PLP

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	0.47	0/6735	0.72	4/9114 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	398	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	457	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	398	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	A	457	ARG	NE-CZ-NH2	5.01	122.81	120.30

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	A	6585	0	6531	16	0
2	A	15	0	7	0	0
3	A	28	0	26	0	0
4	A	23	0	11	0	0
5	A	384	0	0	1	1
All	All	7035	0	6575	16	1

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 1.

All (16) 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)
1:A:282:ASN:HD22	1:A:282:ASN:H	1.47	0.62
1:A:678:ASN:HD22	1:A:679:MET:H	1.49	0.61
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.93	0.52
1:A:455:VAL:H	1:A:459:HIS:HD2	1.58	0.51
1:A:282:ASN:ND2	1:A:282:ASN:H	2.10	0.48
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.97	0.47
1:A:730:GLU:O	1:A:734:ARG:HG3	2.14	0.46
1:A:717:ASP:OD1	1:A:720:ARG:NH1	2.47	0.46
1:A:282:ASN:HD22	1:A:282:ASN:N	2.13	0.46
1:A:308:ILE:HD13	1:A:352:VAL:HG11	2.01	0.43
1:A:450:HIS:HD2	5:A:1243:HOH:O	2.00	0.43
1:A:284:ASN:HD21	1:A:610:ALA:CB	2.32	0.42
1:A:355:ASP:OD2	1:A:398:ARG:HD3	2.20	0.41
1:A:211:GLN:O	1:A:358:ARG:NH1	2.53	0.41
1:A:678:ASN:HD22	1:A:679:MET:N	2.16	0.41
1:A:284:ASN:HD21	1:A:610:ALA:HB3	1.86	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
5:A:1046:HOH:O	5:A:1046:HOH:O[7_555]	1.50	0.70

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	Favoured	Allowed	Outliers	Percentiles	
1	A	804/843 (95%)	784 (98%)	20 (2%)	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	701/732 (96%)	669 (95%)	32 (5%)	33	15

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	90	TYR
1	A	102	LEU
1	A	115	LEU
1	A	122	LEU
1	A	198	LEU
1	A	211	GLN
1	A	214	LYS
1	A	235	ASN
1	A	282	ASN
1	A	284	ASN
1	A	306	ASP
1	A	400	LEU
1	A	444	LEU
1	A	522	LEU
1	A	552	GLU
1	A	560	ASN
1	A	568	LYS
1	A	579	ASN
1	A	586	LEU
1	A	596	LYS
1	A	622	LEU
1	A	662	LEU
1	A	678	ASN
1	A	706	GLU
1	A	708	PHE
1	A	721	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	765	LEU
1	A	782	LYS
1	A	790	LEU
1	A	831	ARG
1	A	833	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	211	GLN
1	A	235	ASN
1	A	264	GLN
1	A	270	ASN
1	A	282	ASN
1	A	284	ASN
1	A	412	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	571	HIS
1	A	579	ASN
1	A	678	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PLP	A	901	1	15,15,16	2.84	3 (20%)	21,22,23	1.65	4 (19%)
3	4D1	A	902	-	29,29,29	1.85	6 (20%)	40,40,40	1.42	6 (15%)
4	IMP	A	903	-	21,25,25	1.32	2 (9%)	22,38,38	2.28	4 (18%)

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	PLP	A	901	1	-	0/6/6/8	0/1/1/1
3	4D1	A	902	-	-	0/19/39/39	0/2/2/2
4	IMP	A	903	-	1/1/5/5	0/6/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	4D1	C12-C15	-3.67	1.43	1.53
3	A	902	4D1	C9-C8	-2.33	1.40	1.47
3	A	902	4D1	C4'-C5'	2.59	1.58	1.53
2	A	901	PLP	C3-C4	2.96	1.46	1.40
3	A	902	4D1	C7-C5	3.05	1.54	1.48
4	A	903	IMP	C5-C4	3.26	1.47	1.40
4	A	903	IMP	C6-C5	3.71	1.48	1.41
3	A	902	4D1	C1'-N1	3.80	1.47	1.43
3	A	902	4D1	C7-C8	6.00	1.49	1.32
2	A	901	PLP	C5-C4	6.76	1.48	1.40
2	A	901	PLP	C3-C2	7.28	1.45	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	IMP	N3-C2-N1	-7.89	122.68	128.87
3	A	902	4D1	C5-N4-C2	-5.31	122.34	128.07
2	A	901	PLP	C2A-C2-C3	-3.71	117.14	120.90
4	A	903	IMP	C6-C5-C4	-3.49	116.87	120.86
2	A	901	PLP	O4P-P-O1P	-3.40	98.53	107.08
4	A	903	IMP	C1'-N9-C4	-2.58	123.93	126.81
3	A	902	4D1	C3'-C2'-C1'	-2.38	106.26	110.07
3	A	902	4D1	O5'-C1'-C2'	-2.17	107.23	109.92
3	A	902	4D1	C5'-O5'-C1'	-2.08	109.40	112.45
2	A	901	PLP	C2A-C2-N1	2.09	122.57	117.96
2	A	901	PLP	O3P-P-O2P	2.12	115.22	107.44
3	A	902	4D1	O5'-C5'-C6'	2.13	111.89	106.38
3	A	902	4D1	O6-C5-N4	2.38	127.62	121.28
4	A	903	IMP	C2-N1-C6	3.58	122.29	116.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	903	IMP	C4'

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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 ²)	Q<0.9
1	A	809/843 (95%)	-0.05	22 (2%) 58 53	18, 30, 54, 90	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	PHE	7.5
1	A	253	ASN	4.1
1	A	211	GLN	4.0
1	A	254	LEU	3.3
1	A	836	ALA	3.1
1	A	435	ALA	3.0
1	A	556	HIS	2.8
1	A	12	GLN	2.8
1	A	434	GLY	2.7
1	A	85	LEU	2.6
1	A	554	LYS	2.5
1	A	553	TYR	2.4
1	A	436	VAL	2.3
1	A	113	TYR	2.2
1	A	13	ILE	2.2
1	A	605	ILE	2.2
1	A	250	ASN	2.2
1	A	358	ARG	2.2
1	A	69	ARG	2.1
1	A	753	LYS	2.1
1	A	832	GLN	2.0
1	A	337	LEU	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](#)

There are no carbohydrates in this entry.

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. 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, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
4	IMP	A	903	23/23	0.83	0.19	1.76	68,74,76,77	0
2	PLP	A	901	15/16	0.98	0.15	0.62	19,19,22,23	0
3	4D1	A	902	28/28	0.95	0.09	-0.65	18,21,25,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.