



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID : 2BMB
Title : X-RAY STRUCTURE OF THE BIFUNCTIONAL 6-HYDROXYMETHYL-7, 8-DIHYDROXYPTERIN PYROPHOSPHOKINASE DIHYDROPTEROATE SYNTHASE FROM SACCHAROMYCES CEREVISIAE
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Deposited on : 2005-03-11
Resolution : 2.30 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

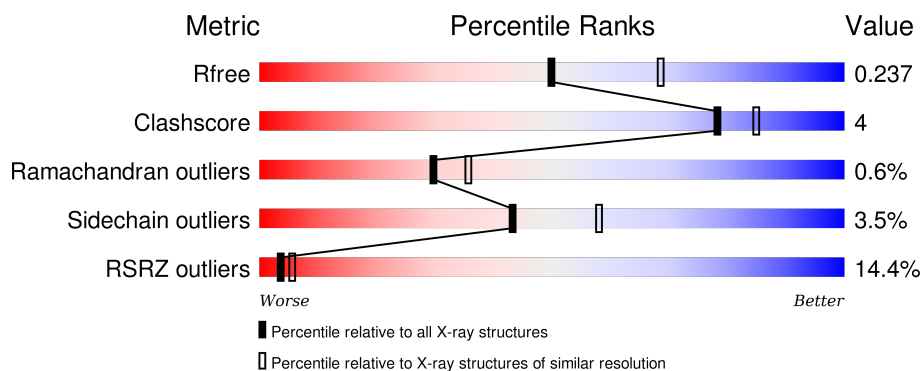
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 ≥ 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	545	

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
2	PMM	A	1866	-	-	-	X

2 Entry composition [i](#)

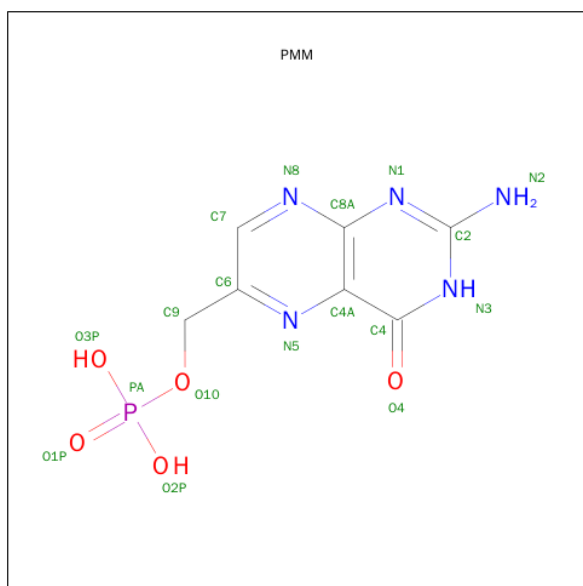
There are 3 unique types of molecules in this entry. The entry contains 4282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FOLIC ACID SYNTHESIS PROTEIN FOL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	8	0
			4122	2617	706	778	21			

- Molecule 2 is PTERIN-6-YL-METHYL-MONOPHOSPHATE (three-letter code: PMM) (formula: $C_7H_8N_5O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			18	7	5	5	1		
2	A	1	Total	C	N	O	P	0	0
			18	7	5	5	1		

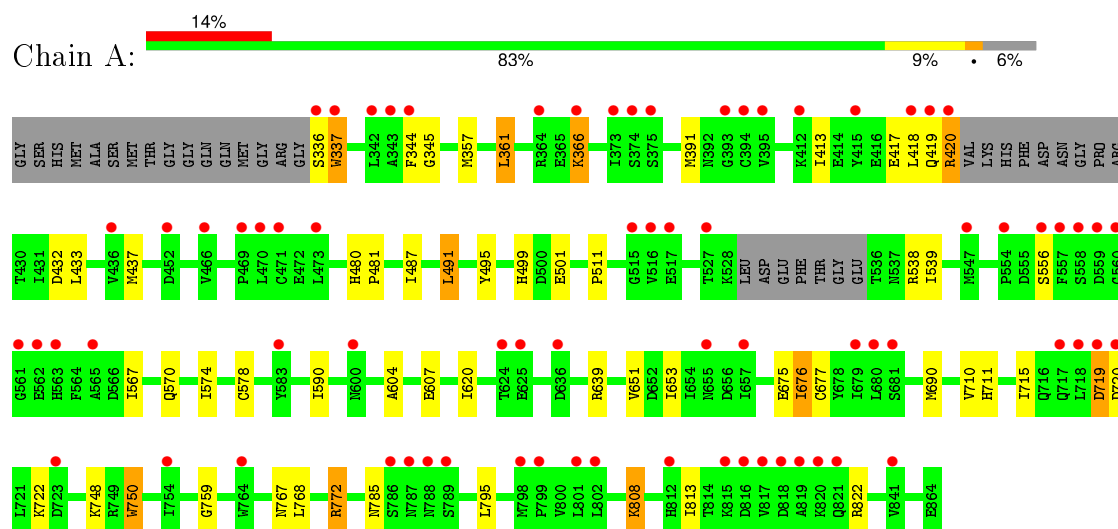
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total	O	0	0
			124	124		

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 ($\text{RSRZ} > 2$). 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: FOLIC ACID SYNTHESIS PROTEIN FOL1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.57Å 92.57Å 192.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 29.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-2.30) 99.2 (29.59-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.216 0.210 , 0.237	Depositor DCC
R_{free} test set	1877 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	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 37615 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4282	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: PMM

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	0.46	0/4241	0.57	2/5733 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	772	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	772	ARG	NE-CZ-NH2	-5.24	117.68	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	4122	0	4149	30	0
2	A	36	0	12	0	0
3	A	124	0	0	5	0
All	All	4282	0	4161	30	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 4.

All (30) 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:690:MET:CE	3:A:2075:HOH:O	2.22	0.86
1:A:604:ALA:O	1:A:639:ARG:NH2	2.14	0.81
1:A:690:MET:HE2	3:A:2075:HOH:O	1.81	0.80
1:A:808:LYS:HE2	1:A:822:ARG:HH12	1.52	0.72
1:A:366:LYS:HD2	1:A:366:LYS:H	1.58	0.67
1:A:759:GLY:H	1:A:767:ASN:HD21	1.46	0.62
1:A:690:MET:HE1	3:A:2075:HOH:O	1.92	0.59
1:A:715:ILE:HD12	1:A:722:LYS:HG3	1.87	0.55
1:A:578:CYS:SG	1:A:590:ILE:HD11	2.48	0.54
1:A:511:PRO:HG3	1:A:676:ILE:HD12	1.90	0.53
1:A:748:LYS:HD3	1:A:750:TRP:CZ2	2.45	0.52
1:A:538:ARG:HB3	3:A:2050:HOH:O	2.10	0.51
1:A:437:MET:HE3	1:A:487:ILE:HD11	1.92	0.50
1:A:419:GLN:HB2	1:A:420:ARG:HH21	1.77	0.50
1:A:491:LEU:HD22	1:A:495:TYR:CE2	2.46	0.50
1:A:336:SER:OG	1:A:337:TRP:N	2.45	0.50
1:A:567:ILE:HA	1:A:570:GLN:HE21	1.80	0.46
1:A:344:PHE:HA	1:A:432:ASP:O	2.16	0.45
1:A:357[B]:MET:SD	1:A:417:GLU:HG2	2.57	0.45
1:A:710:VAL:HG12	1:A:711[B]:HIS:CD2	2.52	0.44
1:A:574:ILE:HD13	1:A:620:ILE:HD11	2.01	0.43
1:A:361:LEU:HB3	1:A:413:ILE:HG12	2.01	0.43
1:A:759:GLY:H	1:A:767:ASN:ND2	2.16	0.42
1:A:499:HIS:HB3	1:A:501:GLU:OE1	2.21	0.41
1:A:768:LEU:HD11	1:A:813:ILE:HD11	2.03	0.41
1:A:772:ARG:NH2	3:A:2102:HOH:O	2.43	0.41
1:A:653:ILE:HG12	1:A:677:CYS:HB3	2.03	0.41
1:A:345:GLY:HA2	1:A:391:MET:O	2.21	0.40
1:A:480:HIS:HA	1:A:481:PRO:HD3	1.95	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	515/545 (94%)	503 (98%)	9 (2%)	3 (1%)	30	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	556	SER
1	A	337	TRP
1	A	719	ASP

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	470/486 (97%)	454 (97%)	16 (3%)	44	59

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

Mol	Chain	Res	Type
1	A	361	LEU
1	A	366	LYS
1	A	418	LEU
1	A	420	ARG
1	A	433	LEU
1	A	491	LEU
1	A	539	ILE
1	A	651	VAL
1	A	675	GLU
1	A	676	ILE
1	A	719	ASP
1	A	720	ASP
1	A	750	TRP
1	A	785	ASN
1	A	795	LEU
1	A	808	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	570	GLN
1	A	767	ASN
1	A	785	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	PMM	A	1865	-	18,19,19	3.44	4 (22%)	21,28,28	2.79	8 (38%)
2	PMM	A	1866	-	18,19,19	3.62	5 (27%)	21,28,28	2.45	8 (38%)

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	PMM	A	1865	-	-	0/6/6/6	0/2/2/2
2	PMM	A	1866	-	-	0/6/6/6	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1866	PMM	C6-N5	-2.51	1.26	1.32
2	A	1866	PMM	C4-C4A	2.90	1.47	1.41
2	A	1865	PMM	C4-C4A	3.57	1.48	1.41
2	A	1866	PMM	C4A-N5	7.58	1.45	1.33
2	A	1865	PMM	C7-C6	7.59	1.51	1.39
2	A	1865	PMM	C4A-N5	8.02	1.45	1.33
2	A	1865	PMM	C7-N8	8.23	1.45	1.31
2	A	1866	PMM	C7-C6	8.68	1.53	1.39
2	A	1866	PMM	C7-N8	9.02	1.47	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1865	PMM	C4-C4A-C8A	-5.16	116.64	119.94
2	A	1866	PMM	C4A-C4-N3	-4.25	117.78	123.59
2	A	1865	PMM	C4A-C4-N3	-3.76	118.45	123.59
2	A	1865	PMM	N1-C2-N3	-3.62	121.94	127.44
2	A	1866	PMM	C4-C4A-C8A	-3.23	117.88	119.94
2	A	1866	PMM	N1-C2-N3	-2.98	122.91	127.44
2	A	1866	PMM	C4A-C8A-N1	-2.35	118.18	122.18
2	A	1866	PMM	C6-N5-C4A	2.36	121.34	118.41
2	A	1865	PMM	C6-N5-C4A	3.07	122.22	118.41
2	A	1866	PMM	C7-N8-C8A	3.28	120.80	116.93
2	A	1865	PMM	N8-C8A-N1	3.99	121.85	116.14
2	A	1865	PMM	C4-N3-C2	4.64	122.37	115.94
2	A	1866	PMM	C4-N3-C2	4.70	122.46	115.94
2	A	1865	PMM	C7-N8-C8A	4.71	122.48	116.93
2	A	1865	PMM	C4-C4A-N5	4.77	124.51	118.72
2	A	1866	PMM	N8-C8A-N1	5.02	123.32	116.14

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, 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	513/545 (94%)	0.64	74 (14%) 3 5	14, 28, 60, 91	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	788	ASN	7.8
1	A	817	VAL	7.0
1	A	557	PHE	6.8
1	A	558	SER	5.8
1	A	515	GLY	5.6
1	A	818	ASP	5.3
1	A	560	GLY	5.2
1	A	394[A]	CYS	5.1
1	A	419	GLN	5.0
1	A	415	TYR	4.6
1	A	821	GLN	4.6
1	A	336	SER	4.5
1	A	787	ASN	4.5
1	A	561	GLY	4.3
1	A	718	LEU	4.3
1	A	819	ALA	4.2
1	A	719	ASP	4.2
1	A	717	GLN	4.1
1	A	720	ASP	4.0
1	A	559	ASP	3.9
1	A	816	ASP	3.9
1	A	366	LYS	3.8
1	A	516	VAL	3.7
1	A	679	ILE	3.7
1	A	562	GLU	3.6
1	A	393	GLY	3.6
1	A	420	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	556	SER	3.6
1	A	789	SER	3.4
1	A	469	PRO	3.3
1	A	820	LYS	3.2
1	A	342	LEU	3.0
1	A	418	LEU	3.0
1	A	436	VAL	2.9
1	A	625	GLU	2.9
1	A	802	LEU	2.9
1	A	517	GLU	2.9
1	A	547	MET	2.9
1	A	815	LYS	2.9
1	A	364	ARG	2.8
1	A	723	ASP	2.8
1	A	395	VAL	2.7
1	A	801	LEU	2.7
1	A	754	ILE	2.7
1	A	343	ALA	2.7
1	A	583	TYR	2.7
1	A	812	HIS	2.7
1	A	786	SER	2.6
1	A	764	TRP	2.6
1	A	375	SER	2.6
1	A	337	TRP	2.6
1	A	624	THR	2.6
1	A	412	LYS	2.5
1	A	554	PRO	2.4
1	A	473	LEU	2.4
1	A	471	CYS	2.4
1	A	841	VAL	2.4
1	A	470	LEU	2.4
1	A	680	LEU	2.4
1	A	636	ASP	2.3
1	A	452	ASP	2.3
1	A	374	SER	2.3
1	A	798	MET	2.2
1	A	373	ILE	2.2
1	A	657	ILE	2.2
1	A	600	ASN	2.2
1	A	563	HIS	2.2
1	A	466	VAL	2.2
1	A	565	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	527	THR	2.1
1	A	655	ASN	2.0
1	A	681	SER	2.0
1	A	799	PRO	2.0
1	A	344	PHE	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(Å ²)	Q<0.9
2	PMM	A	1866	18/18	0.85	0.28	2.68	43,48,88,89	0
2	PMM	A	1865	18/18	0.91	0.32	1.60	46,49,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.