



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2016 – 05:19 PM EDT

PDB ID : 5EE9  
Title : Complex structure of OSYCHF1 with GMP-PNP  
Authors : Li, X.; Chen, Z.  
Deposited on : 2015-10-22  
Resolution : 2.75 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

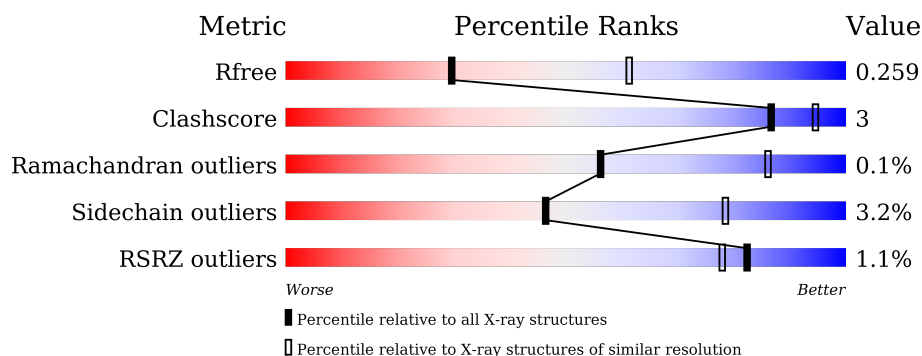
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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. 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	395	
1	B	395	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5729 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.

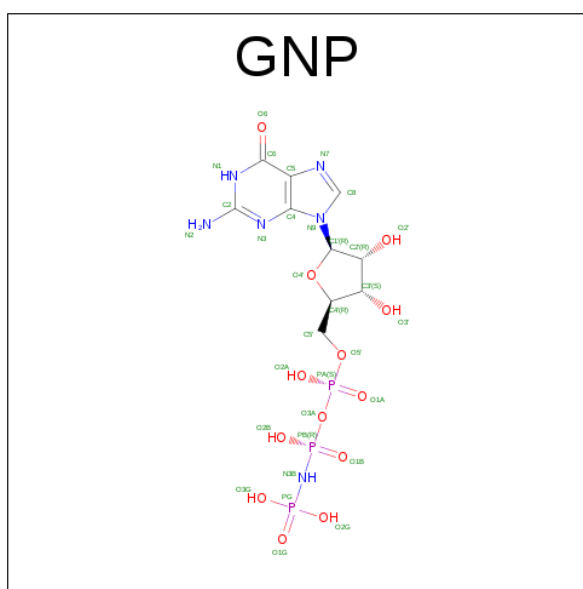
- Molecule 1 is a protein called Obg-like ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2717	1761	439	506	11			
1	B	359	Total	C	N	O	S	0	0	0
			2716	1756	442	507	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q6Z1J6
B	0	SER	-	expression tag	UNP Q6Z1J6

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



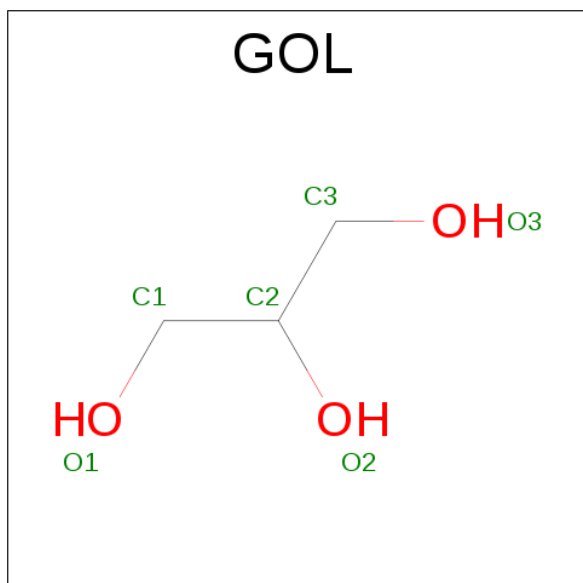
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		


- Molecule 6 is water.

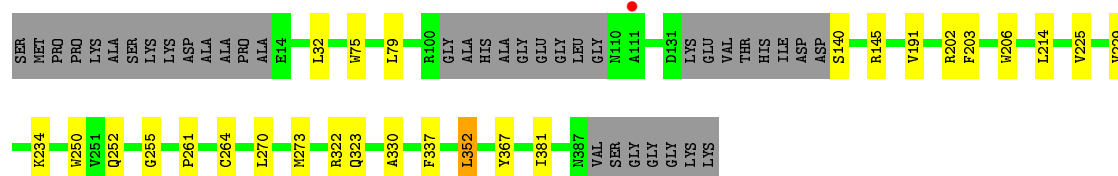
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	127	Total	O	0	0
			127	127		
6	B	129	Total	O	0	0
			129	129		

### 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.

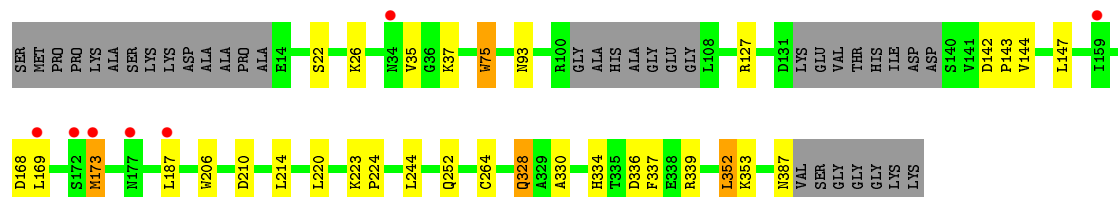
#### • Molecule 1: Obg-like ATPase 1

Chain A: 



#### • Molecule 1: Obg-like ATPase 1

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.45Å 112.06Å 115.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 41.53 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-2.75) 97.5 (41.53-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.229 , 0.262 0.229 , 0.259	Depositor DCC
$R_{free}$ test set	1133 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 18.7	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 23844 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5729	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.96 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.3882e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 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: K, GOL, MG, GNP

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	0.42	2/2777 (0.1%)	0.46	0/3767
1	B	0.43	2/2778 (0.1%)	0.48	0/3766
All	All	0.42	4/5555 (0.1%)	0.47	0/7533

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	TRP	CD2-CE2	5.10	1.47	1.41
1	A	206	TRP	CD2-CE2	5.06	1.47	1.41
1	B	75	TRP	CD2-CE2	5.06	1.47	1.41
1	B	206	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

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	2717	0	2551	11	0
1	B	2716	0	2501	17	0
2	A	32	0	13	0	0
3	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	8	1	0
6	A	127	0	0	0	0
6	B	129	0	0	0	0
All	All	5729	0	5073	28	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 (28) 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:B:328:GLN:H	1:B:328:GLN:HE21	1.25	0.83
1:B:328:GLN:HE21	1:B:328:GLN:N	1.93	0.65
1:B:334:HIS:HD2	1:B:336:ASP:H	1.47	0.62
1:B:75:TRP:CH2	1:B:353:LYS:HA	2.38	0.57
1:B:330:ALA:HB1	1:B:337:PHE:HB3	1.87	0.56
1:A:330:ALA:HB1	1:A:337:PHE:HB3	1.90	0.54
1:B:336:ASP:HA	1:B:339:ARG:HG2	1.90	0.53
1:A:229:VAL:HG13	1:A:261:PRO:HA	1.91	0.53
1:A:322:ARG:O	1:A:323:GLN:HB2	2.12	0.49
1:B:187:LEU:HD21	1:B:214:LEU:HG	1.93	0.49
1:A:352:LEU:HD12	1:A:381:ILE:HD13	1.94	0.49
1:B:37:LYS:HB2	5:B:402:GOL:H12	1.95	0.48
1:B:144:VAL:HA	1:B:147:LEU:HD12	1.95	0.48
1:B:169:LEU:O	1:B:173:MET:HB2	2.13	0.48
1:A:337:PHE:N	1:A:337:PHE:CD1	2.84	0.46
1:A:337:PHE:HD1	1:A:337:PHE:N	2.14	0.46
1:A:75:TRP:CZ3	1:A:79:LEU:HD22	2.52	0.45
1:A:191:VAL:HG21	1:A:214:LEU:HD21	1.98	0.44
1:B:35:VAL:HG12	1:B:127:ARG:HB2	2.00	0.43
1:B:187:LEU:HD13	1:B:210:ASP:HB3	2.01	0.42
1:B:26:LYS:HD3	1:B:93:ASN:ND2	2.34	0.42
1:B:142:ASP:HA	1:B:143:PRO:HD2	1.92	0.42
1:B:223:LYS:HA	1:B:224:PRO:HD3	1.96	0.42
1:A:270:LEU:HA	1:A:273:MET:HE3	2.01	0.41
1:A:203:PHE:CZ	1:A:255:GLY:HA3	2.56	0.41
1:B:26:LYS:HD3	1:B:93:ASN:HD21	1.85	0.41
1:B:75:TRP:HZ3	1:B:352:LEU:HD13	1.85	0.40
1:A:140:SER:HB2	1:A:145:ARG:NH2	2.37	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	351/395 (89%)	341 (97%)	9 (3%)	1 (0%)	46	77
1	B	353/395 (89%)	346 (98%)	7 (2%)	0	100	100
All	All	704/790 (89%)	687 (98%)	16 (2%)	1 (0%)	56	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	TYR

### 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	268/336 (80%)	261 (97%)	7 (3%)	54	84
1	B	257/336 (76%)	247 (96%)	10 (4%)	39	72
All	All	525/672 (78%)	508 (97%)	17 (3%)	46	78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	202	ARG
1	A	225	VAL
1	A	234	LYS
1	A	252	GLN

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Mol	Chain	Res	Type
1	A	264	CYS
1	A	352	LEU
1	B	22	SER
1	B	168	ASP
1	B	173	MET
1	B	220	LEU
1	B	244	LEU
1	B	252	GLN
1	B	264	CYS
1	B	328	GLN
1	B	352	LEU
1	B	387	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	194	HIS
1	A	285	ASN
1	A	323	GLN
1	A	387	ASN
1	B	164	ASN
1	B	194	HIS
1	B	328	GLN
1	B	334	HIS
1	B	369	GLN
1	B	387	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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
2	GNP	A	401	3	29,34,34	2.64	8 (27%)	28,54,54	1.27	3 (10%)
5	GOL	B	402	-	5,5,5	0.29	0	5,5,5	0.38	0

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	GNP	A	401	3	-	0/16/38/38	0/3/3/3
5	GOL	B	402	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GNP	C4-N9	-10.08	1.34	1.47
2	A	401	GNP	C8-N9	-3.74	1.35	1.47
2	A	401	GNP	C5-C6	-2.26	1.48	1.53
2	A	401	GNP	C2-N1	-2.04	1.35	1.44
2	A	401	GNP	PB-O1B	2.30	1.48	1.46
2	A	401	GNP	C1'-N9	3.73	1.49	1.42
2	A	401	GNP	PG-N3B	4.15	1.74	1.63
2	A	401	GNP	PB-N3B	4.26	1.75	1.63

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GNP	PA-O3A-PB	-3.16	121.24	132.71
2	A	401	GNP	C4-C5-N7	2.54	106.63	102.67
2	A	401	GNP	C8-N9-C4	3.03	108.24	104.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	GOL	1	0

## 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, 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	357/395 (90%)	0.03	1 (0%) 94 93	21, 42, 60, 78	0
1	B	359/395 (90%)	0.12	7 (1%) 70 64	18, 44, 69, 79	0
All	All	716/790 (90%)	0.08	8 (1%) 82 78	18, 43, 65, 79	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	MET	3.8
1	B	187	LEU	2.8
1	B	172	SER	2.7
1	B	34	ASN	2.7
1	B	169	LEU	2.6
1	B	159	ILE	2.3
1	B	177	ASN	2.2
1	A	111	ALA	2.2

### 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	402	6/6	0.86	0.23	0.42	49,52,53,53	0
2	GNP	A	401	32/32	0.94	0.16	-0.83	50,54,57,58	0
3	MG	A	402	1/1	0.92	0.29	-	46,46,46,46	0
4	K	B	401	1/1	0.89	0.09	-	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.