



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:13 AM GMT

PDB ID : 3L1V  
Title : Crystal structure of GmhB from E. coli in complex with calcium and phosphate.  
Authors : Sugiman-Marangos, S.N.; Junop, M.S.  
Deposited on : 2009-12-14  
Resolution : 1.95 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>

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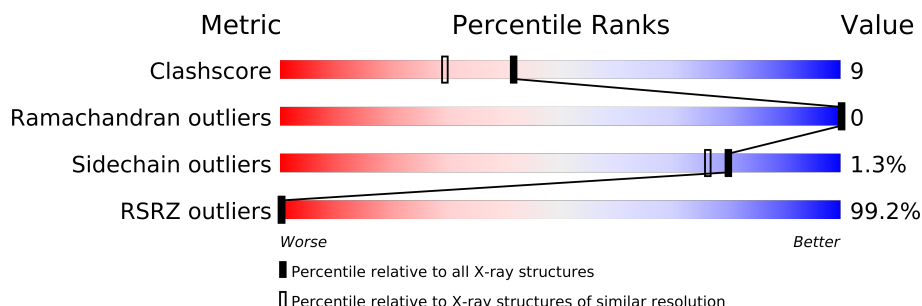
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.95 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	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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	211	
1	B	211	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	B	213	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3095 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 D,D-heptose 1,7-bisphosphate phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1415	893	240	272	10			
1	B	182	Total	C	N	O	S	0	0	0
			1415	893	240	272	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P63228
A	2	GLY	-	EXPRESSION TAG	UNP P63228
A	3	SER	-	EXPRESSION TAG	UNP P63228
A	4	SER	-	EXPRESSION TAG	UNP P63228
A	5	HIS	-	EXPRESSION TAG	UNP P63228
A	6	HIS	-	EXPRESSION TAG	UNP P63228
A	7	HIS	-	EXPRESSION TAG	UNP P63228
A	8	HIS	-	EXPRESSION TAG	UNP P63228
A	9	HIS	-	EXPRESSION TAG	UNP P63228
A	10	HIS	-	EXPRESSION TAG	UNP P63228
A	11	SER	-	EXPRESSION TAG	UNP P63228
A	12	SER	-	EXPRESSION TAG	UNP P63228
A	13	GLY	-	EXPRESSION TAG	UNP P63228
A	14	LEU	-	EXPRESSION TAG	UNP P63228
A	15	VAL	-	EXPRESSION TAG	UNP P63228
A	16	PRO	-	EXPRESSION TAG	UNP P63228
A	17	ARG	-	EXPRESSION TAG	UNP P63228
A	18	GLY	-	EXPRESSION TAG	UNP P63228
A	19	SER	-	EXPRESSION TAG	UNP P63228
A	20	HIS	-	EXPRESSION TAG	UNP P63228
B	1	MET	-	EXPRESSION TAG	UNP P63228
B	2	GLY	-	EXPRESSION TAG	UNP P63228
B	3	SER	-	EXPRESSION TAG	UNP P63228
B	4	SER	-	EXPRESSION TAG	UNP P63228
B	5	HIS	-	EXPRESSION TAG	UNP P63228

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	EXPRESSION TAG	UNP P63228
B	7	HIS	-	EXPRESSION TAG	UNP P63228
B	8	HIS	-	EXPRESSION TAG	UNP P63228
B	9	HIS	-	EXPRESSION TAG	UNP P63228
B	10	HIS	-	EXPRESSION TAG	UNP P63228
B	11	SER	-	EXPRESSION TAG	UNP P63228
B	12	SER	-	EXPRESSION TAG	UNP P63228
B	13	GLY	-	EXPRESSION TAG	UNP P63228
B	14	LEU	-	EXPRESSION TAG	UNP P63228
B	15	VAL	-	EXPRESSION TAG	UNP P63228
B	16	PRO	-	EXPRESSION TAG	UNP P63228
B	17	ARG	-	EXPRESSION TAG	UNP P63228
B	18	GLY	-	EXPRESSION TAG	UNP P63228
B	19	SER	-	EXPRESSION TAG	UNP P63228
B	20	HIS	-	EXPRESSION TAG	UNP P63228

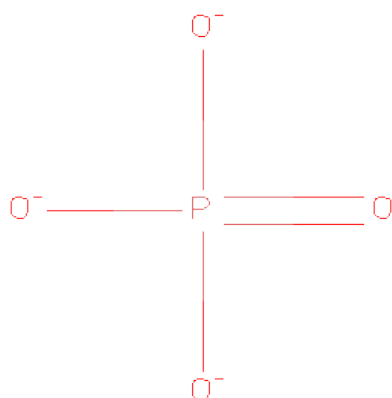
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

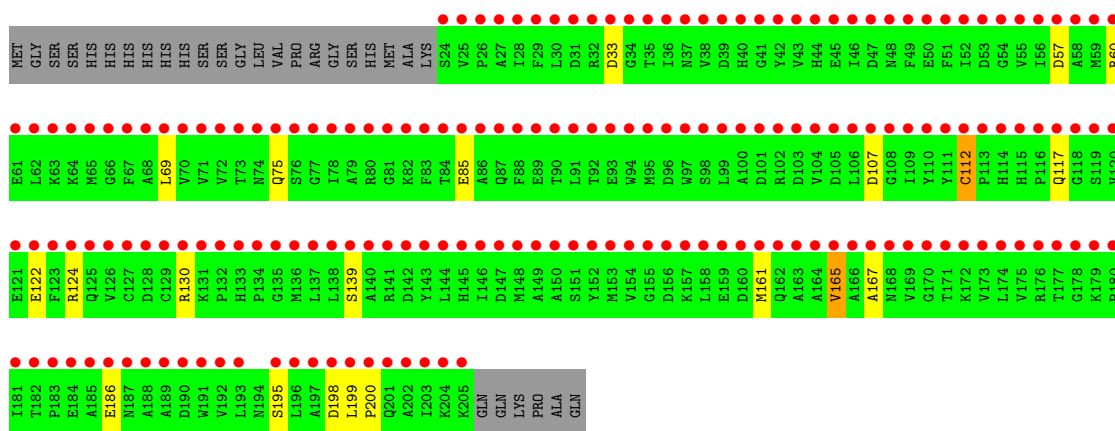
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total	O	0	0
			137	137		
5	B	114	Total	O	0	0
			114	114		

### 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.

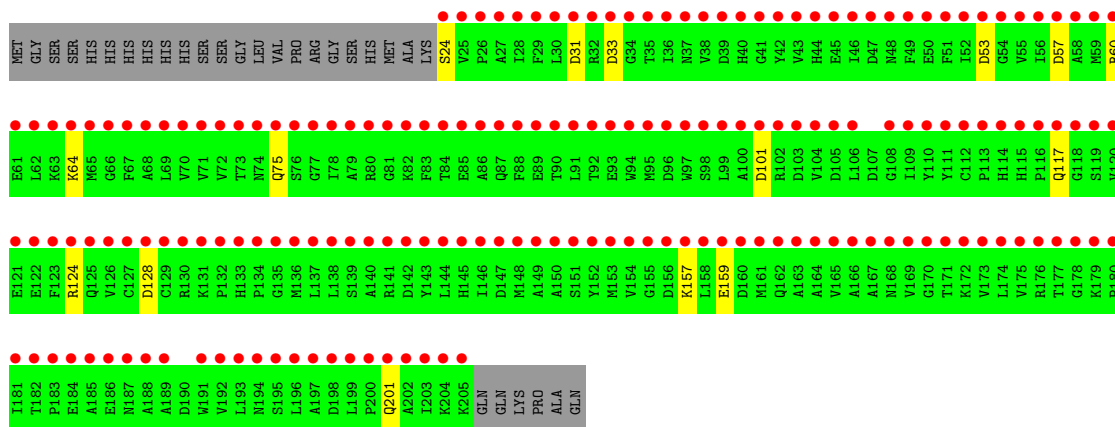
- Molecule 1: D,D-heptose 1,7-bisphosphate phosphatase

Chain A:



- Molecule 1: D,D-heptose 1,7-bisphosphate phosphatase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.58Å 64.31Å 104.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.14 – 1.95 45.51 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.1 (27.14-1.95) 94.7 (45.51-1.95)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.50 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5.2)	Depositor
R, $R_{free}$	0.246 , 0.284 0.246 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	12.9	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	9 of 24747 reflections (0.036%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 97.47 % 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 1.5452e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PO4, CA, ZN

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	0.65	0/1446	0.64	0/1965
1	B	0.68	0/1446	0.64	0/1965
All	All	0.66	0/2892	0.64	0/3930

There are no bond length outliers.

There are no bond angle outliers.

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	1415	0	0	11	3
1	B	1415	0	0	15	3
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
5	A	137	0	0	5	2
5	B	114	0	0	12	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3095	0	0	26	6

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 9.

All (26) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:57:ASP:OD1	1:B:60:ARG:NH2	1.56	1.34
1:A:57:ASP:OD1	1:A:60:ARG:NH2	1.94	1.00
1:A:130:ARG:NE	5:A:326:HOH:O	1.96	0.97
1:B:33:ASP:OD1	5:B:216:HOH:O	1.89	0.89
1:A:198:ASP:OD2	5:A:227:HOH:O	1.89	0.88
1:B:53:ASP:O	5:B:254:HOH:O	1.98	0.81
1:A:167:ALA:O	5:A:323:HOH:O	1.99	0.80
1:B:128:ASP:OD2	5:B:309:HOH:O	1.97	0.80
1:B:24:SER:N	5:B:298:HOH:O	2.14	0.79
1:A:85:GLU:OE2	5:A:331:HOH:O	2.03	0.75
1:B:24:SER:OG	5:B:316:HOH:O	2.09	0.70
1:A:122:GLU:O	5:A:322:HOH:O	2.09	0.70
1:B:101:ASP:OD1	5:B:284:HOH:O	2.13	0.66
1:B:33:ASP:CG	5:B:216:HOH:O	2.34	0.64
1:B:75:GLN:NE2	5:B:215:HOH:O	2.38	0.57
1:B:201:GLN:NE2	5:B:306:HOH:O	2.38	0.56
1:A:69:LEU:N	1:A:107:ASP:OD2	2.39	0.56
1:B:31:ASP:OD1	4:B:214:PO4:O2	2.29	0.49
1:B:64:LYS:NZ	5:B:290:HOH:O	2.48	0.46
1:B:24:SER:C	5:B:316:HOH:O	2.56	0.44
1:B:117:GLN:O	5:B:313:HOH:O	2.21	0.43
1:B:157:LYS:NZ	1:B:159:GLU:OE2	2.51	0.43
1:A:75:GLN:N	1:A:112:CYS:O	2.52	0.43
1:A:161:MET:O	1:A:165:VAL:CG1	2.69	0.41
1:A:199:LEU:N	1:A:200:PRO:CD	2.84	0.41
1:A:33:ASP:N	4:A:214:PO4:O2	2.54	0.40

All (6) 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)
1:B:124:ARG:NH1	5:B:284:HOH:O[4_455]	1.78	0.42
1:A:117:GLN:NE2	5:B:256:HOH:O[1_545]	1.85	0.35
5:A:222:HOH:O	5:B:324:HOH:O[4_445]	1.89	0.31
5:A:341:HOH:O	5:B:222:HOH:O[1_445]	1.92	0.28

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:186:GLU:O	1:B:64:LYS:NZ[3_644]	1.97	0.23
1:A:124:ARG:NH2	1:B:124:ARG:NH2[1_545]	2.01	0.19

## 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	180/211 (85%)	177 (98%)	3 (2%)	0	100	100
1	B	180/211 (85%)	175 (97%)	5 (3%)	0	100	100
All	All	360/422 (85%)	352 (98%)	8 (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	150/176 (85%)	146 (97%)	4 (3%)	57	45
1	B	150/176 (85%)	150 (100%)	0	100	100
All	All	300/352 (85%)	296 (99%)	4 (1%)	80	76

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

Mol	Chain	Res	Type
1	A	112	CYS
1	A	139	SER
1	A	165	VAL
1	A	195	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 6 ligands modelled in this entry, 4 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	$\# Z  > 2$
4	PO4	A	214	3	4,4,4	0.95	0	6,6,6	0.34	0
4	PO4	B	214	3	4,4,4	0.91	0	6,6,6	0.33	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
4	PO4	A	214	3	-	0/0/0/0	0/0/0/0
4	PO4	B	214	3	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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	182/211 (86%)	8.72	181 (99%) 0 0	18, 31, 47, 69	0
1	B	182/211 (86%)	9.04	180 (98%) 0 0	18, 31, 50, 68	0
All	All	364/422 (86%)	8.88	361 (99%) 0 0	18, 31, 50, 69	0

All (361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	VAL	32.9
1	A	70	VAL	29.7
1	B	69	LEU	26.5
1	B	30	LEU	25.8
1	B	36	ILE	24.5
1	A	69	LEU	23.3
1	A	30	LEU	23.2
1	B	88	PHE	22.7
1	B	183	PRO	22.4
1	B	29	PHE	22.2
1	A	175	VAL	20.5
1	A	36	ILE	20.2
1	B	137	LEU	20.2
1	A	29	PHE	19.8
1	B	65	MET	19.0
1	B	138	LEU	18.9
1	B	175	VAL	18.9
1	A	204	LYS	18.7
1	A	110	TYR	18.7
1	A	160	ASP	18.6
1	A	137	LEU	18.6
1	B	192	VAL	18.4
1	B	72	VAL	18.3
1	B	204	LYS	18.1

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Mol	Chain	Res	Type	RSRZ
1	A	88	PHE	18.0
1	A	183	PRO	17.8
1	A	138	LEU	17.4
1	A	93	GLU	17.3
1	B	84	THR	16.6
1	B	146	ILE	16.5
1	B	110	TYR	16.5
1	B	92	THR	16.3
1	A	28	ILE	16.2
1	B	28	ILE	15.9
1	A	146	ILE	15.7
1	A	205	LYS	15.7
1	B	153	MET	15.4
1	B	63	LYS	15.4
1	B	126	VAL	14.6
1	A	136	MET	14.6
1	B	93	GLU	14.6
1	B	199	LEU	14.6
1	A	199	LEU	14.6
1	A	72	VAL	14.5
1	B	160	ASP	14.2
1	B	94	TRP	14.2
1	A	92	THR	14.0
1	B	140	ALA	13.8
1	A	46	ILE	13.8
1	B	200	PRO	13.7
1	B	71	VAL	13.7
1	B	55	VAL	13.6
1	A	68	ALA	13.6
1	B	68	ALA	13.6
1	B	136	MET	13.5
1	A	153	MET	13.4
1	B	46	ILE	13.4
1	A	181	ILE	13.3
1	A	78	ILE	13.0
1	A	140	ALA	13.0
1	A	65	MET	12.9
1	A	192	VAL	12.8
1	A	111	TYR	12.6
1	B	154	VAL	12.6
1	B	174	LEU	12.5
1	B	87	GLN	12.5

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Mol	Chain	Res	Type	RSRZ
1	A	150	ALA	12.5
1	B	150	ALA	12.5
1	A	166	ALA	12.4
1	B	67	PHE	12.3
1	B	35	THR	12.3
1	B	166	ALA	12.3
1	B	41	GLY	12.3
1	A	81	GLY	12.3
1	B	181	ILE	12.2
1	A	94	TRP	12.0
1	A	66	GLY	12.0
1	A	71	VAL	11.8
1	A	116	PRO	11.7
1	B	149	ALA	11.7
1	A	200	PRO	11.6
1	B	62	LEU	11.6
1	B	58	ALA	11.6
1	A	84	THR	11.6
1	A	42	TYR	11.6
1	B	203	ILE	11.6
1	A	67	PHE	11.6
1	B	109	ILE	11.6
1	A	86	ALA	11.5
1	B	205	LYS	11.3
1	B	104	VAL	11.3
1	A	112	CYS	11.2
1	B	158	LEU	11.2
1	A	106	LEU	11.2
1	A	154	VAL	11.1
1	B	42	TYR	11.1
1	B	78	ILE	11.0
1	A	196	LEU	11.0
1	A	120	VAL	11.0
1	A	62	LEU	11.0
1	A	113	PRO	11.0
1	B	152	TYR	10.9
1	B	86	ALA	10.8
1	A	59	MET	10.8
1	B	96	ASP	10.7
1	B	180	PRO	10.7
1	A	126	VAL	10.7
1	A	123	PHE	10.6

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Mol	Chain	Res	Type	RSRZ
1	A	35	THR	10.6
1	A	87	GLN	10.6
1	A	203	ILE	10.5
1	A	104	VAL	10.5
1	A	158	LEU	10.4
1	B	111	TYR	10.4
1	B	91	LEU	10.4
1	B	113	PRO	10.4
1	A	95	MET	10.4
1	B	81	GLY	10.3
1	A	188	ALA	10.3
1	B	123	PHE	10.3
1	A	109	ILE	10.3
1	B	161	MET	10.2
1	B	188	ALA	10.2
1	B	173	VAL	10.2
1	A	91	LEU	10.2
1	B	66	GLY	10.2
1	A	56	ILE	10.1
1	A	55	VAL	10.1
1	B	106	LEU	10.1
1	B	141	ARG	9.9
1	B	76	SER	9.9
1	B	52	ILE	9.8
1	A	51	PHE	9.7
1	A	184	GLU	9.7
1	A	173	VAL	9.6
1	A	174	LEU	9.6
1	B	143	TYR	9.6
1	A	63	LYS	9.6
1	A	25	VAL	9.6
1	A	180	PRO	9.5
1	A	139	SER	9.4
1	B	25	VAL	9.4
1	A	191	TRP	9.3
1	B	165	VAL	9.2
1	A	96	ASP	9.2
1	B	38	VAL	9.1
1	B	59	MET	9.1
1	A	105	ASP	9.0
1	B	202	ALA	8.9
1	B	184	GLU	8.8

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Mol	Chain	Res	Type	RSRZ
1	A	189	ALA	8.8
1	A	149	ALA	8.7
1	A	161	MET	8.7
1	B	197	ALA	8.7
1	B	26	PRO	8.6
1	B	56	ILE	8.6
1	A	186	GLU	8.6
1	A	41	GLY	8.6
1	B	179	LYS	8.6
1	A	52	ILE	8.6
1	B	34	GLY	8.5
1	A	152	TYR	8.5
1	A	38	VAL	8.5
1	B	196	LEU	8.5
1	B	33	ASP	8.5
1	B	159	GLU	8.5
1	A	132	PRO	8.4
1	A	162	GLN	8.4
1	A	76	SER	8.3
1	A	164	ALA	8.2
1	A	131	LYS	8.2
1	B	145	HIS	8.2
1	B	90	THR	8.2
1	A	193	LEU	8.1
1	B	95	MET	8.1
1	B	187	ASN	8.0
1	B	191	TRP	7.9
1	A	79	ALA	7.9
1	B	116	PRO	7.9
1	B	99	LEU	7.9
1	A	145	HIS	7.8
1	A	31	ASP	7.8
1	B	162	GLN	7.7
1	B	32	ARG	7.7
1	A	26	PRO	7.7
1	B	127	CYS	7.6
1	B	51	PHE	7.6
1	A	127	CYS	7.6
1	A	165	VAL	7.6
1	A	119	SER	7.5
1	B	112	CYS	7.5
1	A	108	GLY	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	7.5
1	B	176	ARG	7.4
1	A	170	GLY	7.4
1	A	37	ASN	7.4
1	B	186	GLU	7.3
1	A	171	THR	7.3
1	B	64	LYS	7.1
1	A	151	SER	7.1
1	A	202	ALA	7.0
1	B	31	ASP	7.0
1	B	120	VAL	6.9
1	B	44	HIS	6.9
1	A	197	ALA	6.9
1	A	102	ARG	6.9
1	B	83	PHE	6.9
1	B	144	LEU	6.8
1	A	187	ASN	6.8
1	A	141	ARG	6.8
1	A	83	PHE	6.8
1	A	143	TYR	6.7
1	B	102	ARG	6.7
1	A	169	VAL	6.7
1	A	44	HIS	6.7
1	B	171	THR	6.6
1	A	176	ARG	6.6
1	A	99	LEU	6.6
1	A	58	ALA	6.5
1	B	105	ASP	6.5
1	B	189	ALA	6.5
1	B	119	SER	6.5
1	A	64	LYS	6.4
1	B	73	THR	6.4
1	B	89	GLU	6.4
1	B	167	ALA	6.4
1	A	133	HIS	6.4
1	B	193	LEU	6.4
1	A	159	GLU	6.3
1	B	43	VAL	6.3
1	A	34	GLY	6.3
1	B	198	ASP	6.3
1	B	169	VAL	6.3
1	B	37	ASN	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	129	CYS	6.2
1	A	117	GLN	6.2
1	B	129	CYS	6.2
1	A	179	LYS	6.2
1	B	114	HIS	6.1
1	B	170	GLY	6.1
1	B	142	ASP	6.0
1	A	195	SER	6.0
1	B	131	LYS	6.0
1	A	40	HIS	6.0
1	A	144	LEU	6.0
1	A	182	THR	5.9
1	A	90	THR	5.8
1	A	49	PHE	5.8
1	B	148	MET	5.8
1	B	128	ASP	5.8
1	B	132	PRO	5.7
1	A	39	ASP	5.7
1	B	40	HIS	5.7
1	B	108	GLY	5.7
1	B	133	HIS	5.6
1	B	97	TRP	5.6
1	B	139	SER	5.6
1	A	73	THR	5.6
1	B	151	SER	5.6
1	B	115	HIS	5.6
1	A	74	ASN	5.5
1	B	79	ALA	5.5
1	B	164	ALA	5.5
1	A	114	HIS	5.5
1	B	172	LYS	5.4
1	A	43	VAL	5.4
1	A	198	ASP	5.3
1	B	49	PHE	5.3
1	B	82	LYS	5.3
1	B	163	ALA	5.3
1	A	32	ARG	5.2
1	A	121	GLU	5.2
1	B	135	GLY	5.2
1	A	172	LYS	5.2
1	A	128	ASP	5.1
1	A	177	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	85	GLU	5.1
1	B	61	GLU	5.0
1	A	97	TRP	5.0
1	A	80	ARG	5.0
1	A	148	MET	5.0
1	B	122	GLU	5.0
1	B	39	ASP	5.0
1	A	115	HIS	5.0
1	A	75	GLN	4.9
1	A	82	LYS	4.9
1	B	168	ASN	4.9
1	B	134	PRO	4.8
1	A	61	GLU	4.8
1	B	60	ARG	4.8
1	B	195	SER	4.8
1	A	122	GLU	4.7
1	B	117	GLN	4.7
1	A	60	ARG	4.7
1	B	124	ARG	4.7
1	B	177	THR	4.7
1	B	74	ASN	4.7
1	A	167	ALA	4.6
1	A	185	ALA	4.6
1	A	89	GLU	4.6
1	A	125	GLN	4.5
1	B	125	GLN	4.5
1	B	121	GLU	4.5
1	A	135	GLY	4.5
1	A	168	ASN	4.5
1	A	134	PRO	4.4
1	A	142	ASP	4.4
1	B	47	ASP	4.4
1	B	155	GLY	4.4
1	B	85	GLU	4.4
1	B	130	ARG	4.3
1	B	157	LYS	4.3
1	A	33	ASP	4.3
1	A	124	ARG	4.2
1	B	178	GLY	4.2
1	A	100	ALA	4.1
1	B	54	GLY	4.1
1	B	182	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	118	GLY	4.1
1	A	101	ASP	4.0
1	B	156	ASP	4.0
1	A	24	SER	3.9
1	B	201	GLN	3.9
1	B	75	GLN	3.9
1	B	98	SER	3.9
1	B	100	ALA	3.9
1	A	130	ARG	3.9
1	A	54	GLY	3.8
1	A	155	GLY	3.8
1	A	53	ASP	3.8
1	A	156	ASP	3.8
1	B	103	ASP	3.6
1	A	201	GLN	3.5
1	B	53	ASP	3.5
1	A	50	GLU	3.5
1	B	45	GLU	3.4
1	A	178	GLY	3.4
1	B	48	ASN	3.3
1	A	45	GLU	3.3
1	A	103	ASP	3.3
1	A	27	ALA	3.3
1	B	24	SER	3.2
1	A	147	ASP	3.2
1	A	48	ASN	3.2
1	A	157	LYS	3.2
1	B	147	ASP	2.9
1	B	50	GLU	2.9
1	A	77	GLY	2.9
1	A	47	ASP	2.9
1	A	98	SER	2.9
1	B	80	ARG	2.8
1	B	101	ASP	2.7
1	B	27	ALA	2.7
1	B	57	ASP	2.7
1	B	194	ASN	2.7
1	A	107	ASP	2.6
1	A	118	GLY	2.6
1	B	77	GLY	2.3
1	A	57	ASP	2.3
1	B	185	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	190	ASP	2.2

## 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(Å <sup>2</sup> )	Q<0.9
3	CA	B	213	1/1	0.91	1.40	75,75,75,75	0
4	PO4	A	214	5/5	0.46	-0.57	31,31,36,37	0
3	CA	A	213	1/1	0.39	-0.62	28,28,28,28	0
4	PO4	B	214	5/5	0.33	-1.26	25,27,30,33	0
2	ZN	A	212	1/1	0.21	-2.36	28,28,28,28	0
2	ZN	B	212	1/1	0.19	-3.01	28,28,28,28	0

## 6.5 Other polymers

There are no such residues in this entry.