



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2018 – 07:55 AM EDT

PDB ID : 5LD1  
Title : Crystal Structure of Polyphosphate Kinase from *Meiothermus ruber* bound to ATP  
Authors : Gerhardt, S.; Einsle, O.; Kemper, F.; Schwarzer, N.  
Deposited on : 2016-06-23  
Resolution : 2.09 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030736

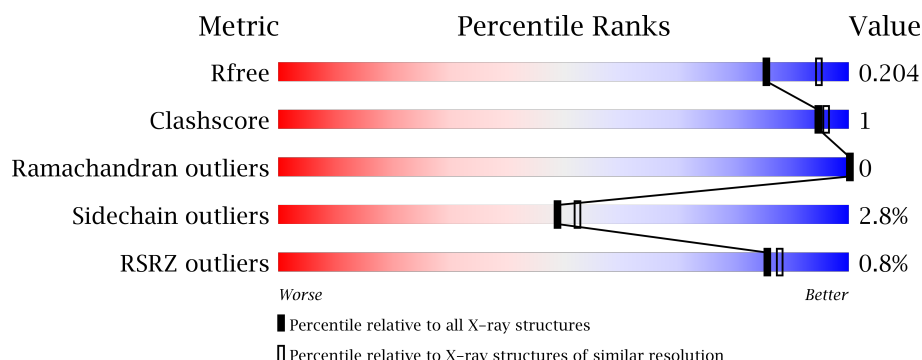
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	287	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 84%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>84%</span> <span>5%</span> <span>10%</span> </div> </div>
1	B	287	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 86%, yellow 5%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>86%</span> <span>5%</span> <span>9%</span> </div> </div>
1	C	287	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 83%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>83%</span> <span>8%</span> <span>9%</span> </div> </div>
1	D	287	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 86%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>86%</span> <span>5%</span> <span>9%</span> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	1007	-	-	-	X
5	GOL	B	1004	-	-	-	X
5	GOL	C	1004	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9900 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 Polyphosphate:AMP phosphotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	2	0
			2168	1380	398	385	5			
1	B	260	Total	C	N	O	S	0	0	0
			2179	1388	397	389	5			
1	C	261	Total	C	N	O	S	0	2	0
			2200	1405	399	391	5			
1	D	261	Total	C	N	O	S	0	1	0
			2192	1397	399	391	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A0S7ASE9
A	-18	GLY	-	expression tag	UNP A0A0S7ASE9
A	-17	SER	-	expression tag	UNP A0A0S7ASE9
A	-16	SER	-	expression tag	UNP A0A0S7ASE9
A	-15	HIS	-	expression tag	UNP A0A0S7ASE9
A	-14	HIS	-	expression tag	UNP A0A0S7ASE9
A	-13	HIS	-	expression tag	UNP A0A0S7ASE9
A	-12	HIS	-	expression tag	UNP A0A0S7ASE9
A	-11	HIS	-	expression tag	UNP A0A0S7ASE9
A	-10	HIS	-	expression tag	UNP A0A0S7ASE9
A	-9	SER	-	expression tag	UNP A0A0S7ASE9
A	-8	SER	-	expression tag	UNP A0A0S7ASE9
A	-7	GLY	-	expression tag	UNP A0A0S7ASE9
A	-6	LEU	-	expression tag	UNP A0A0S7ASE9
A	-5	VAL	-	expression tag	UNP A0A0S7ASE9
A	-4	PRO	-	expression tag	UNP A0A0S7ASE9
A	-3	ARG	-	expression tag	UNP A0A0S7ASE9
A	-2	GLY	-	expression tag	UNP A0A0S7ASE9
A	-1	SER	-	expression tag	UNP A0A0S7ASE9
A	0	HIS	-	expression tag	UNP A0A0S7ASE9
B	-19	MET	-	initiating methionine	UNP A0A0S7ASE9

*Continued on next page...*

*Continued from previous page...*

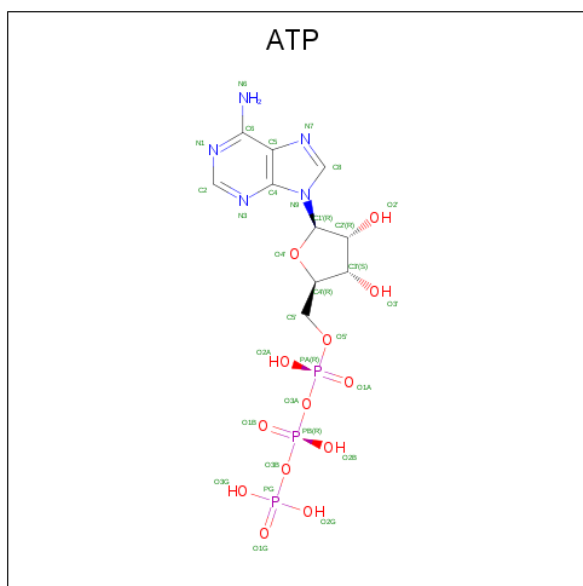
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A0S7ASE9
B	-17	SER	-	expression tag	UNP A0A0S7ASE9
B	-16	SER	-	expression tag	UNP A0A0S7ASE9
B	-15	HIS	-	expression tag	UNP A0A0S7ASE9
B	-14	HIS	-	expression tag	UNP A0A0S7ASE9
B	-13	HIS	-	expression tag	UNP A0A0S7ASE9
B	-12	HIS	-	expression tag	UNP A0A0S7ASE9
B	-11	HIS	-	expression tag	UNP A0A0S7ASE9
B	-10	HIS	-	expression tag	UNP A0A0S7ASE9
B	-9	SER	-	expression tag	UNP A0A0S7ASE9
B	-8	SER	-	expression tag	UNP A0A0S7ASE9
B	-7	GLY	-	expression tag	UNP A0A0S7ASE9
B	-6	LEU	-	expression tag	UNP A0A0S7ASE9
B	-5	VAL	-	expression tag	UNP A0A0S7ASE9
B	-4	PRO	-	expression tag	UNP A0A0S7ASE9
B	-3	ARG	-	expression tag	UNP A0A0S7ASE9
B	-2	GLY	-	expression tag	UNP A0A0S7ASE9
B	-1	SER	-	expression tag	UNP A0A0S7ASE9
B	0	HIS	-	expression tag	UNP A0A0S7ASE9
C	-19	MET	-	initiating methionine	UNP A0A0S7ASE9
C	-18	GLY	-	expression tag	UNP A0A0S7ASE9
C	-17	SER	-	expression tag	UNP A0A0S7ASE9
C	-16	SER	-	expression tag	UNP A0A0S7ASE9
C	-15	HIS	-	expression tag	UNP A0A0S7ASE9
C	-14	HIS	-	expression tag	UNP A0A0S7ASE9
C	-13	HIS	-	expression tag	UNP A0A0S7ASE9
C	-12	HIS	-	expression tag	UNP A0A0S7ASE9
C	-11	HIS	-	expression tag	UNP A0A0S7ASE9
C	-10	HIS	-	expression tag	UNP A0A0S7ASE9
C	-9	SER	-	expression tag	UNP A0A0S7ASE9
C	-8	SER	-	expression tag	UNP A0A0S7ASE9
C	-7	GLY	-	expression tag	UNP A0A0S7ASE9
C	-6	LEU	-	expression tag	UNP A0A0S7ASE9
C	-5	VAL	-	expression tag	UNP A0A0S7ASE9
C	-4	PRO	-	expression tag	UNP A0A0S7ASE9
C	-3	ARG	-	expression tag	UNP A0A0S7ASE9
C	-2	GLY	-	expression tag	UNP A0A0S7ASE9
C	-1	SER	-	expression tag	UNP A0A0S7ASE9
C	0	HIS	-	expression tag	UNP A0A0S7ASE9
D	-19	MET	-	initiating methionine	UNP A0A0S7ASE9
D	-18	GLY	-	expression tag	UNP A0A0S7ASE9
D	-17	SER	-	expression tag	UNP A0A0S7ASE9

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A0S7ASE9
D	-15	HIS	-	expression tag	UNP A0A0S7ASE9
D	-14	HIS	-	expression tag	UNP A0A0S7ASE9
D	-13	HIS	-	expression tag	UNP A0A0S7ASE9
D	-12	HIS	-	expression tag	UNP A0A0S7ASE9
D	-11	HIS	-	expression tag	UNP A0A0S7ASE9
D	-10	HIS	-	expression tag	UNP A0A0S7ASE9
D	-9	SER	-	expression tag	UNP A0A0S7ASE9
D	-8	SER	-	expression tag	UNP A0A0S7ASE9
D	-7	GLY	-	expression tag	UNP A0A0S7ASE9
D	-6	LEU	-	expression tag	UNP A0A0S7ASE9
D	-5	VAL	-	expression tag	UNP A0A0S7ASE9
D	-4	PRO	-	expression tag	UNP A0A0S7ASE9
D	-3	ARG	-	expression tag	UNP A0A0S7ASE9
D	-2	GLY	-	expression tag	UNP A0A0S7ASE9
D	-1	SER	-	expression tag	UNP A0A0S7ASE9
D	0	HIS	-	expression tag	UNP A0A0S7ASE9

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

Continued on next page...

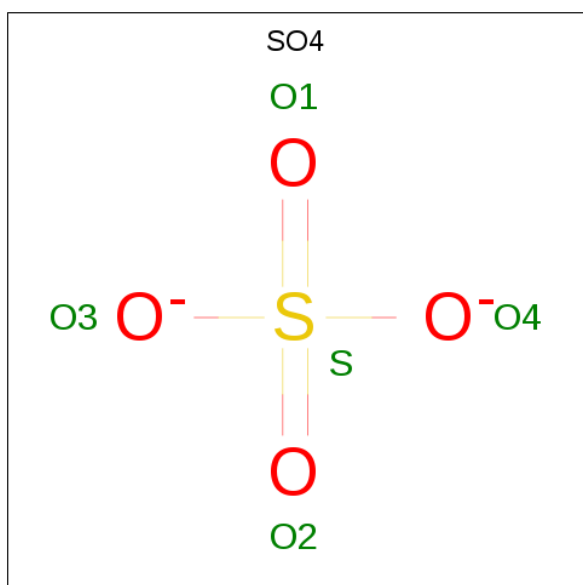
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

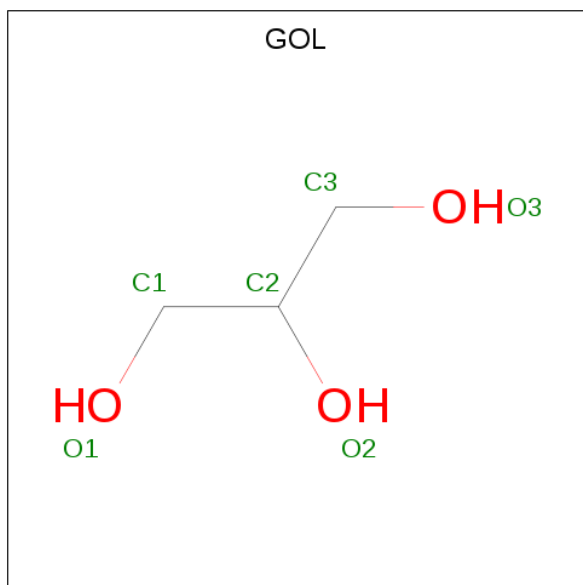
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

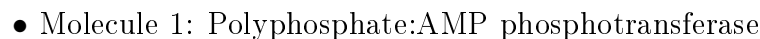
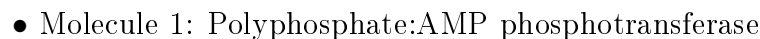
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	235	Total O 235 235	0	0
6	B	231	Total O 231 231	0	0
6	C	216	Total O 216 216	0	0
6	D	192	Total O 192 192	0	0





- Molecule 1: Polyphosphate:AMP phosphotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.01Å 168.01Å 95.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.80 – 2.09 118.80 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.5 (118.80-2.09) 100.0 (118.80-2.09)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	0.26	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.08Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.3	Depositor
R, $R_{free}$	0.163 , 0.202 0.168 , 0.204	Depositor DCC
$R_{free}$ test set	3972 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9900	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 37.95 % 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 3.9698e-04. 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, MG, SO4, ATP

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	0.53	0/2225	0.62	0/3005
1	B	0.55	0/2228	0.64	0/3008
1	C	0.52	0/2257	0.63	0/3048
1	D	0.51	0/2245	0.63	0/3032
All	All	0.53	0/8955	0.63	0/12093

There are no bond length outliers.

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	2168	0	2160	7	0
1	B	2179	0	2168	6	0
1	C	2200	0	2192	10	0
1	D	2192	0	2183	5	0
2	A	62	0	24	0	0
2	B	62	0	24	0	0
2	C	62	0	24	0	0
2	D	62	0	24	0	0
3	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
6	A	235	0	0	1	0
6	B	231	0	0	0	0
6	C	216	0	0	1	0
6	D	192	0	0	0	0
All	All	9900	0	8815	26	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 1.

All (26) 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:C:15:LYS:HG3	6:C:1112:HOH:O	1.84	0.76
1:B:183:LEU:HD21	1:C:264:ILE:HB	1.81	0.61
1:C:171:SER:H	1:C:230:ASN:HD21	1.49	0.60
1:C:179:LEU:HB3	1:C:192[B]:PHE:HZ	1.67	0.59
1:D:198:GLU:O	1:D:201:ARG:HG2	2.06	0.55
1:B:78:PHE:HA	1:B:81:VAL:HG22	1.89	0.54
1:D:78:PHE:HA	1:D:81:VAL:HG22	1.90	0.52
1:A:78:PHE:HA	1:A:81:VAL:HG22	1.90	0.52
1:D:101:ARG:HD3	1:D:105:TRP:CE2	2.45	0.52
1:B:265:VAL:HA	1:C:180:GLN:HE22	1.74	0.51
1:A:101:ARG:HD3	1:A:105:TRP:CE2	2.45	0.51
1:C:101:ARG:HD3	1:C:105:TRP:CE2	2.46	0.51
1:C:78:PHE:HA	1:C:81:VAL:HG22	1.92	0.50
1:D:101:ARG:HD3	1:D:105:TRP:CD2	2.47	0.50
1:C:192[A]:PHE:HZ	1:C:197:LEU:HG	1.77	0.49
1:B:101:ARG:HD3	1:B:105:TRP:CE2	2.48	0.49
1:A:192:PHE:HZ	1:A:197:LEU:HG	1.79	0.47
1:A:75:ARG:O	1:A:75:ARG:HD3	2.15	0.46
1:C:101:ARG:HD3	1:C:105:TRP:CD2	2.50	0.46
1:B:101:ARG:HD3	1:B:105:TRP:CD2	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:HD3	1:A:105:TRP:CD2	2.51	0.45
1:A:55:GLN:HG3	6:A:1322:HOH:O	2.18	0.44
1:A:8:PRO:HB3	1:A:219:THR:HA	2.00	0.44
1:C:8:PRO:HB3	1:C:219:THR:HA	2.00	0.44
1:B:8:PRO:HB3	1:B:219:THR:HA	2.00	0.43
1:D:8:PRO:HB3	1:D:219:THR:HA	2.00	0.43

There are no symmetry-related clashes.

## 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	257/287 (90%)	253 (98%)	4 (2%)	0	100	100
1	B	256/287 (89%)	252 (98%)	4 (2%)	0	100	100
1	C	259/287 (90%)	256 (99%)	3 (1%)	0	100	100
1	D	258/287 (90%)	255 (99%)	3 (1%)	0	100	100
All	All	1030/1148 (90%)	1016 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	228/252 (90%)	221 (97%)	7 (3%)	45	48
1	B	229/252 (91%)	224 (98%)	5 (2%)	57	62
1	C	232/252 (92%)	223 (96%)	9 (4%)	37	37
1	D	231/252 (92%)	226 (98%)	5 (2%)	57	62
All	All	920/1008 (91%)	894 (97%)	26 (3%)	49	52

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	16	ARG
1	A	75	ARG
1	A	76	VAL
1	A	121	ASN
1	A	199	ASP
1	B	1	MET
1	B	143	GLN
1	B	181	GLU
1	B	198	GLU
1	B	199	ASP
1	C	1	MET
1	C	3	LYS
1	C	11	ARG
1	C	22	THR
1	C	121	ASN
1	C	143	GLN
1	C	173	ASP
1	C	198	GLU
1	C	199	ASP
1	D	1	MET
1	D	26	GLU
1	D	140	GLN
1	D	194	MET
1	D	199	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	121	ASN
1	A	207	GLN
1	B	40	ASN
1	B	135	ASN
1	B	139	GLN
1	C	40	ASN
1	C	121	ASN
1	C	139	GLN
1	C	180	GLN
1	C	207	GLN
1	C	230	ASN
1	D	121	ASN
1	D	140	GLN

### 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](#)

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 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	ATP	A	1001	3	27,33,33	0.64	0	25,52,52	0.93	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ATP	A	1002	3	27,33,33	0.70	0	25,52,52	0.67	0
4	SO4	A	1004	-	4,4,4	0.30	0	6,6,6	0.28	0
2	ATP	B	1001	3	27,33,33	0.83	1 (3%)	25,52,52	0.95	1 (4%)
2	ATP	B	1002	3	27,33,33	0.68	0	25,52,52	0.69	0
5	GOL	B	1004	-	5,5,5	0.32	0	5,5,5	0.66	0
4	SO4	B	1007	-	4,4,4	0.50	0	6,6,6	0.45	0
2	ATP	C	1001	3	27,33,33	0.70	0	25,52,52	0.96	1 (4%)
2	ATP	C	1002	3	27,33,33	0.77	1 (3%)	25,52,52	0.64	0
5	GOL	C	1004	-	5,5,5	0.18	0	5,5,5	0.46	0
4	SO4	C	1006	-	4,4,4	0.36	0	6,6,6	0.23	0
2	ATP	D	1001	3	27,33,33	0.70	1 (3%)	25,52,52	0.92	1 (4%)
2	ATP	D	1002	3	27,33,33	0.71	0	25,52,52	0.61	0
4	SO4	D	1004	-	4,4,4	0.32	0	6,6,6	0.13	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	ATP	A	1001	3	-	0/18/38/38	0/3/3/3
2	ATP	A	1002	3	-	0/18/38/38	0/3/3/3
4	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
2	ATP	B	1001	3	-	0/18/38/38	0/3/3/3
2	ATP	B	1002	3	-	0/18/38/38	0/3/3/3
5	GOL	B	1004	-	-	0/4/4/4	0/0/0/0
4	SO4	B	1007	-	-	0/0/0/0	0/0/0/0
2	ATP	C	1001	3	-	0/18/38/38	0/3/3/3
2	ATP	C	1002	3	-	0/18/38/38	0/3/3/3
5	GOL	C	1004	-	-	0/4/4/4	0/0/0/0
4	SO4	C	1006	-	-	0/0/0/0	0/0/0/0
2	ATP	D	1001	3	-	0/18/38/38	0/3/3/3
2	ATP	D	1002	3	-	0/18/38/38	0/3/3/3
4	SO4	D	1004	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1002	ATP	PG-O3G	-2.17	1.45	1.54
2	D	1001	ATP	PG-O3G	-2.16	1.45	1.54
2	B	1001	ATP	PG-O1G	2.21	1.58	1.50



All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ATP	C4'-O4'-C1'	-2.66	106.94	109.77
2	C	1001	ATP	C4'-O4'-C1'	-2.49	107.12	109.77
2	B	1001	ATP	C4'-O4'-C1'	-2.45	107.16	109.77
2	D	1001	ATP	C4'-O4'-C1'	-2.34	107.27	109.77

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 [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	257/287 (89%)	-0.61	2 (0%) 86 88	15, 24, 61, 83	0
1	B	260/287 (90%)	-0.62	0 100 100	16, 24, 61, 99	0
1	C	261/287 (90%)	-0.53	4 (1%) 74 77	16, 29, 66, 92	0
1	D	261/287 (90%)	-0.57	2 (0%) 86 88	17, 29, 68, 103	0
All	All	1039/1148 (90%)	-0.58	8 (0%) 86 88	15, 26, 66, 103	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	MET	5.8
1	C	194	MET	4.9
1	C	26	GLU	3.8
1	A	198	GLU	2.5
1	C	1	MET	2.5
1	D	264	ILE	2.4
1	C	11	ARG	2.2
1	D	1	MET	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, 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(Å <sup>2</sup> )	Q<0.9
5	GOL	C	1004	6/6	0.85	0.16	6.79	48,51,52,52	0
5	GOL	B	1004	6/6	0.83	0.13	3.31	38,44,51,54	0
4	SO4	B	1007	5/5	0.91	0.14	3.03	45,54,56,61	0
2	ATP	A	1002	31/31	0.99	0.08	0.05	17,20,23,27	0
2	ATP	D	1001	31/31	0.99	0.08	-0.14	19,24,32,33	0
2	ATP	B	1002	31/31	0.99	0.08	-0.24	16,19,23,28	0
2	ATP	B	1001	31/31	0.99	0.08	-0.41	16,21,28,32	0
2	ATP	A	1001	31/31	0.99	0.07	-0.49	18,23,29,30	0
3	MG	C	1005	1/1	0.99	0.08	-0.61	26,26,26,26	0
2	ATP	C	1002	31/31	0.99	0.08	-0.62	16,23,28,29	0
2	ATP	C	1001	31/31	0.99	0.08	-0.76	20,26,30,33	0
2	ATP	D	1002	31/31	0.99	0.07	-0.84	16,23,27,29	0
3	MG	D	1003	1/1	0.99	0.07	-	26,26,26,26	0
3	MG	A	1003	1/1	0.96	0.08	-	20,20,20,20	0
3	MG	B	1005	1/1	0.99	0.14	-	31,31,31,31	0
4	SO4	D	1004	5/5	0.86	0.13	-	74,75,77,79	0
4	SO4	A	1004	5/5	0.92	0.15	-	48,53,59,61	0
3	MG	C	1003	1/1	0.99	0.06	-	25,25,25,25	0
4	SO4	C	1006	5/5	0.90	0.15	-	72,75,76,77	0
3	MG	B	1006	1/1	1.00	0.12	-	37,37,37,37	0
3	MG	B	1003	1/1	0.98	0.07	-	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.