



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:03 pm GMT

PDB ID : 2WWF  
Title : Plasmodium falciparum thymidylate kinase in complex with TMP and ADP  
Authors : Whittingham, J.L.; Carrero-Lerida, J.; Brannigan, J.A.; Ruiz-Perez, L.M.; Silva, A.P.G.; Fogg, M.J.; Wilkinson, A.J.; Gilbert, I.H.; Wilson, K.S.; Gonzalez-Pacanowska, D.  
Deposited on : 2009-10-23  
Resolution : 1.89 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	:	trunk28620
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)	:	recalc28949

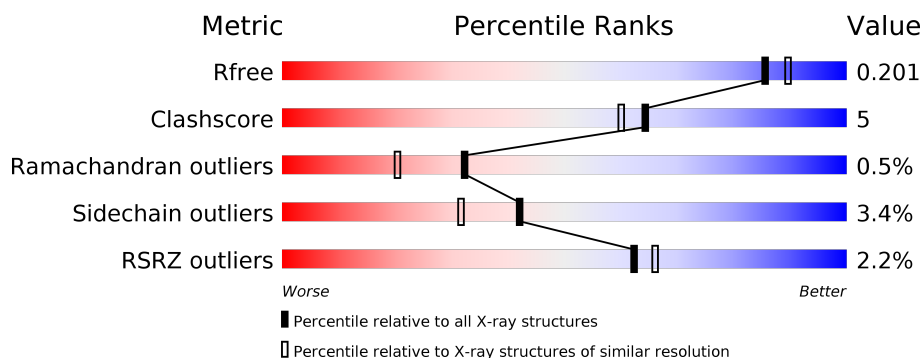
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	212	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 83%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>14% ..</span> </div> </div>
1	B	212	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 13%, green 84%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>84%</span> <span>13% ..</span> </div> </div>
1	C	212	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 10%, green 86%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>86%</span> <span>10% .</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	A	218	-	-	-	X
5	GOL	A	217	-	-	-	X
5	GOL	C	216	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5987 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.

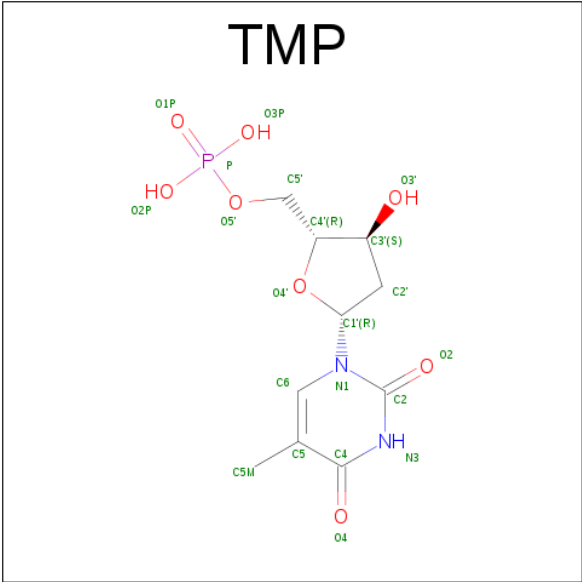
- Molecule 1 is a protein called THYMIDILATE KINASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	12	2	0
			1769	1133	295	334	7			
1	B	208	Total	C	N	O	S	27	4	0
			1750	1124	288	332	6			
1	C	212	Total	C	N	O	S	36	2	0
			1774	1135	296	336	7			

There are 6 discrepancies between the modelled and reference sequences:

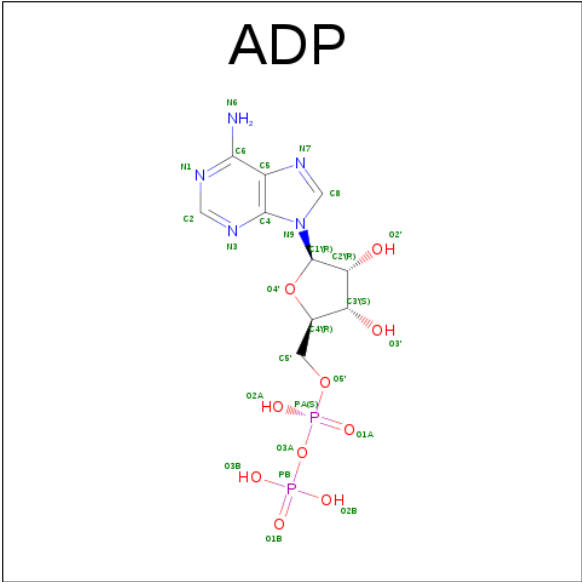
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8I4S1
A	-1	HIS	-	EXPRESSION TAG	UNP Q8I4S1
B	-2	SER	-	EXPRESSION TAG	UNP Q8I4S1
B	-1	HIS	-	EXPRESSION TAG	UNP Q8I4S1
C	-2	SER	-	EXPRESSION TAG	UNP Q8I4S1
C	-1	HIS	-	EXPRESSION TAG	UNP Q8I4S1

- Molecule 2 is THYMIDINE-5'-PHOSPHATE (three-letter code: TMP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

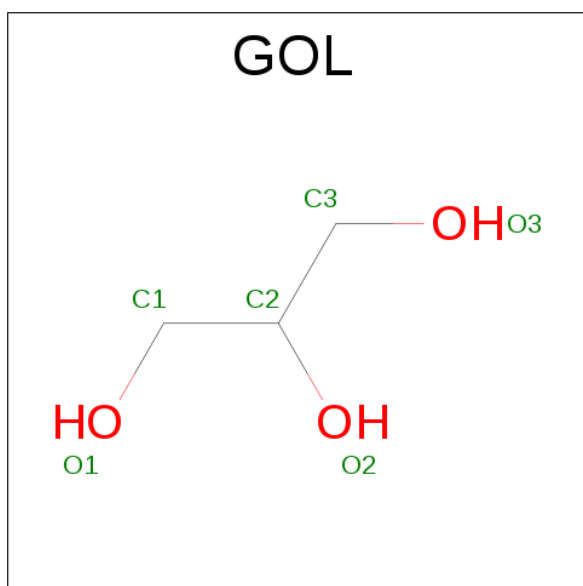


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Na	0	0
			2	2		
4	A	3	Total	Na	0	0
			3	3		
4	C	2	Total	Na	0	0
			2	2		

- 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	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

*Continued from previous page...*

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

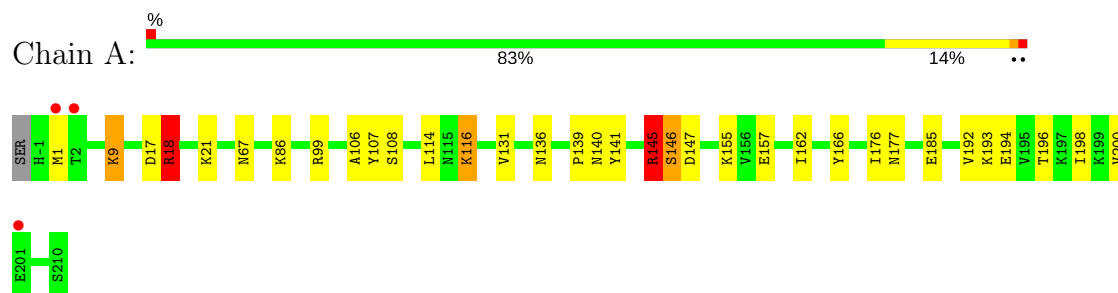
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	199	Total	O	0	0
			199	199		
6	B	145	Total	O	0	0
			145	145		
6	C	145	Total	O	0	0
			145	145		

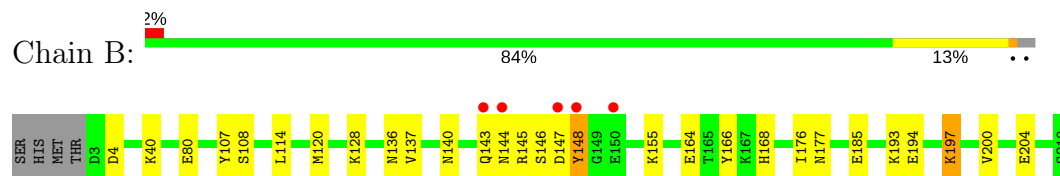
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

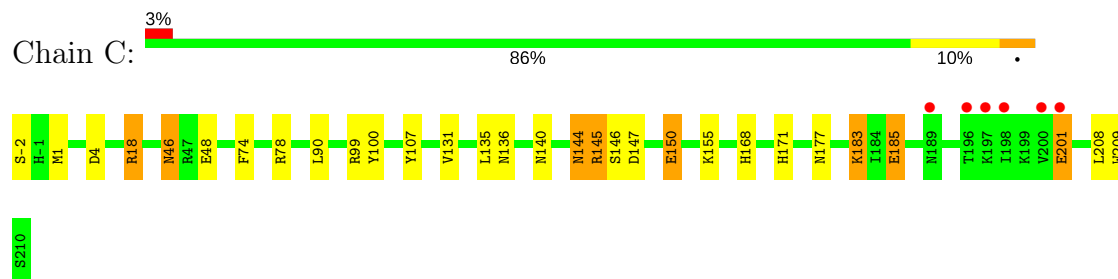
#### • Molecule 1: THYMIDILATE KINASE, PUTATIVE



#### • Molecule 1: THYMIDILATE KINASE, PUTATIVE



#### • Molecule 1: THYMIDILATE KINASE, PUTATIVE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.13Å 110.13Å 120.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.35 – 1.89 37.34 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.3 (95.35-1.89) 84.5 (37.34-1.89)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.160 , 0.203 0.160 , 0.201	Depositor DCC
$R_{free}$ test set	2902 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TMP, GOL, ADP, NA

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	1.26	7/1812 (0.4%)	1.06	8/2446 (0.3%)
1	B	1.18	5/1804 (0.3%)	0.89	1/2435 (0.0%)
1	C	1.19	8/1816 (0.4%)	1.13	9/2448 (0.4%)
All	All	1.21	20/5432 (0.4%)	1.03	18/7329 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	GLU	CB-CG	-9.20	1.34	1.52
1	C	168	HIS	CB-CG	-7.91	1.35	1.50
1	B	197	LYS	CD-CE	-7.85	1.31	1.51
1	A	193	LYS	CB-CG	-7.74	1.31	1.52
1	A	146	SER	CB-OG	7.34	1.51	1.42
1	B	128	LYS	CE-NZ	7.15	1.67	1.49
1	C	171	HIS	CA-CB	-7.04	1.38	1.53
1	C	150	GLU	CG-CD	6.91	1.62	1.51
1	A	185	GLU	CG-CD	6.45	1.61	1.51
1	A	185	GLU	CD-OE2	5.86	1.32	1.25
1	C	131	VAL	CB-CG1	-5.60	1.41	1.52
1	B	193	LYS	CB-CG	-5.60	1.37	1.52
1	C	201	GLU	CB-CG	-5.59	1.41	1.52
1	C	155	LYS	CG-CD	-5.57	1.33	1.52
1	A	106	ALA	CA-CB	5.53	1.64	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	LYS	CG-CD	-5.36	1.34	1.52
1	A	141	TYR	CD1-CE1	5.27	1.47	1.39
1	C	74	PHE	CE2-CZ	5.17	1.47	1.37
1	C	100	TYR	CD1-CE1	5.01	1.46	1.39
1	B	80	GLU	CD-OE1	5.01	1.31	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	ARG	NE-CZ-NH1	17.26	128.93	120.30
1	A	145	ARG	NE-CZ-NH2	15.26	127.93	120.30
1	C	18	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	A	145	ARG	NE-CZ-NH1	-13.24	113.68	120.30
1	C	145	ARG	NE-CZ-NH2	11.62	126.11	120.30
1	C	145	ARG	NE-CZ-NH1	-11.37	114.61	120.30
1	A	18	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	18	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	C	171	HIS	N-CA-CB	7.82	124.67	110.60
1	A	99	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	145	ARG	CD-NE-CZ	6.67	132.93	123.60
1	C	18	ARG	CD-NE-CZ	6.50	132.70	123.60
1	C	78	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	C	183	LYS	CB-CG-CD	-5.70	96.79	111.60
1	A	21	LYS	CD-CE-NZ	5.41	124.14	111.70
1	C	99	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	146	SER	CA-CB-OG	-5.22	97.11	111.20
1	B	155	LYS	CB-CG-CD	-5.03	98.53	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	171	HIS	CA

There are no planarity outliers.

## 5.2 Too-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 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	1769	0	1729	19	0
1	B	1750	0	1717	19	0
1	C	1774	0	1736	13	0
2	A	21	0	13	0	0
2	B	21	0	13	1	0
2	C	21	0	13	1	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	18	0	24	0	0
5	B	24	0	32	0	0
5	C	12	0	16	0	0
6	A	199	0	0	4	0
6	B	145	0	0	5	0
6	C	145	0	0	2	0
All	All	5987	0	5329	51	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 5.

All (51) 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:176:ILE:HD13	1:A:194:GLU:HG2	1.53	0.91
1:A:116:LYS:NZ	6:A:2095:HOH:O	2.08	0.86
1:A:136:ASN:HD22	1:A:177:ASN:HD21	1.23	0.83
1:B:136:ASN:HD22	1:B:177:ASN:HD21	1.26	0.82
1:C:185:GLU:CD	1:C:185:GLU:H	1.88	0.77
1:C:136:ASN:HD22	1:C:177:ASN:HD21	1.33	0.75
1:B:164:GLU:OE2	6:B:2099:HOH:O	2.12	0.67
1:C:147:ASP:O	1:C:150:GLU:HG2	1.94	0.66
1:C:144:ASN:H	1:C:144:ASN:HD22	1.44	0.64
1:B:176:ILE:CD1	1:B:194[A]:GLU:HG2	2.28	0.64
1:B:200:VAL:O	1:B:200:VAL:HG12	1.98	0.63
1:A:176:ILE:HD13	1:A:194:GLU:CG	2.28	0.60
1:B:147:ASP:O	1:B:148:TYR:C	2.41	0.59
1:C:1:MET:HB2	6:C:2003:HOH:O	2.02	0.59
1:A:192:VAL:O	1:A:196:THR:HG23	2.04	0.58
1:A:176:ILE:CD1	1:A:194:GLU:HG2	2.32	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ASP:O	1:B:148:TYR:O	2.23	0.57
1:C:140:ASN:ND2	6:C:2086:HOH:O	2.39	0.54
1:B:40:LYS:HE3	6:B:2060:HOH:O	2.07	0.53
1:B:137:VAL:O	1:B:137:VAL:HG23	2.09	0.53
1:A:157:GLU:CD	1:A:157:GLU:H	2.12	0.52
1:C:46:ASN:HD22	1:C:46:ASN:C	2.13	0.52
1:B:176:ILE:HD12	1:B:194[A]:GLU:HG2	1.92	0.50
1:B:143:GLN:HG3	1:B:144:ASN:OD1	2.12	0.50
1:C:4:ASP:HA	1:C:90:LEU:HD21	1.94	0.50
1:C:46:ASN:ND2	1:C:48:GLU:H	2.10	0.49
1:A:9:LYS:HE2	1:A:198:ILE:CG2	2.43	0.49
1:B:147:ASP:C	6:B:2089:HOH:O	2.51	0.48
1:A:131:VAL:HG21	1:A:176:ILE:HD12	1.96	0.48
1:B:194[A]:GLU:OE1	1:B:197:LYS:HE3	2.12	0.48
1:A:145:ARG:HD3	6:B:2104:HOH:O	2.14	0.48
1:A:9:LYS:HD2	1:A:9:LYS:HA	1.69	0.48
1:A:86:LYS:NZ	6:A:2078:HOH:O	2.41	0.47
1:B:4:ASP:N	1:B:4:ASP:OD1	2.48	0.46
1:A:140:ASN:ND2	6:A:2111:HOH:O	2.46	0.46
1:B:108:SER:HB3	1:B:114:LEU:HD12	1.98	0.45
1:A:67:ASN:ND2	6:A:2054:HOH:O	2.50	0.44
1:B:107:TYR:CE1	2:B:211:TMP:H2'1	2.52	0.43
1:C:107:TYR:CE1	2:C:211:TMP:H2'1	2.53	0.43
1:C:183:LYS:HB3	1:C:185:GLU:OE1	2.18	0.43
1:A:131:VAL:CG2	1:A:176:ILE:HD12	2.49	0.43
1:B:140:ASN:O	1:B:143:GLN:HG2	2.18	0.42
1:C:208:LEU:HA	1:C:209:TRP:HA	1.83	0.42
1:A:108:SER:HB3	1:A:114:LEU:HD12	2.01	0.42
1:B:120:MET:SD	1:B:168:HIS:HE1	2.43	0.41
1:A:18:ARG:NH2	1:A:147:ASP:HB2	2.36	0.41
1:B:200:VAL:HG11	6:B:2067:HOH:O	2.20	0.41
1:B:137:VAL:CG2	1:B:137:VAL:O	2.69	0.41
1:C:136:ASN:HD22	1:C:177:ASN:ND2	2.10	0.41
1:A:107:TYR:CE1	1:A:162:ILE:HD13	2.56	0.40
1:A:17:ASP:O	1:A:18:ARG:HB2	2.21	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	211/212 (100%)	206 (98%)	4 (2%)	1 (0%)	32	20
1	B	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	32	20
1	C	211/212 (100%)	206 (98%)	4 (2%)	1 (0%)	32	20
All	All	632/636 (99%)	616 (98%)	13 (2%)	3 (0%)	32	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	SER
1	B	148	TYR
1	C	146	SER

### 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	196/195 (100%)	188 (96%)	8 (4%)	35	24
1	B	195/195 (100%)	191 (98%)	4 (2%)	59	53
1	C	197/195 (101%)	189 (96%)	8 (4%)	35	24
All	All	588/585 (100%)	568 (97%)	20 (3%)	42	32

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	LYS
1	A	18	ARG
1	A	116	LYS
1	A	139	PRO
1	A	145	ARG
1	A	166	TYR
1	A	200	VAL
1	B	145	ARG
1	B	146	SER
1	B	166	TYR
1	B	204	GLU
1	C	-2	SER
1	C	18	ARG
1	C	46	ASN
1	C	135	LEU
1	C	144	ASN
1	C	145	ARG
1	C	185	GLU
1	C	201	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	34	ASN
1	A	53	GLN
1	A	67	ASN
1	A	177	ASN
1	B	34	ASN
1	B	35	ASN
1	B	67	ASN
1	B	168	HIS
1	B	177	ASN
1	C	34	ASN
1	C	46	ASN
1	C	140	ASN
1	C	144	ASN
1	C	177	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 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	TMP	A	211	4	17,22,22	2.54	8 (47%)	24,33,33	2.70	8 (33%)
3	ADP	A	212	4	25,29,29	1.44	4 (16%)	24,45,45	1.90	4 (16%)
5	GOL	A	215	-	5,5,5	0.56	0	5,5,5	1.64	2 (40%)
5	GOL	A	216	-	5,5,5	0.72	0	5,5,5	0.77	0
5	GOL	A	217	-	5,5,5	0.57	0	5,5,5	1.17	0
2	TMP	B	211	4	17,22,22	1.72	5 (29%)	24,33,33	1.96	4 (16%)
3	ADP	B	212	4	25,29,29	1.16	2 (8%)	24,45,45	2.04	3 (12%)
5	GOL	B	215	-	5,5,5	0.43	0	5,5,5	0.88	0
5	GOL	B	216	-	5,5,5	0.35	0	5,5,5	1.01	1 (20%)
5	GOL	B	217	-	5,5,5	0.56	0	5,5,5	0.32	0
5	GOL	B	218	-	5,5,5	0.48	0	5,5,5	1.07	1 (20%)
2	TMP	C	211	-	17,22,22	1.88	5 (29%)	24,33,33	2.12	8 (33%)
3	ADP	C	212	4	25,29,29	1.43	6 (24%)	24,45,45	1.59	3 (12%)
5	GOL	C	215	-	5,5,5	1.07	0	5,5,5	0.78	0
5	GOL	C	216	-	5,5,5	0.37	0	5,5,5	0.42	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	TMP	A	211	4	-	0/6/22/22	0/2/2/2
3	ADP	A	212	4	-	0/12/32/32	0/3/3/3
5	GOL	A	215	-	-	0/4/4/4	0/0/0/0
5	GOL	A	216	-	-	0/4/4/4	0/0/0/0
5	GOL	A	217	-	-	0/4/4/4	0/0/0/0
2	TMP	B	211	4	-	0/6/22/22	0/2/2/2
3	ADP	B	212	4	-	0/12/32/32	0/3/3/3
5	GOL	B	215	-	-	0/4/4/4	0/0/0/0
5	GOL	B	216	-	-	0/4/4/4	0/0/0/0
5	GOL	B	217	-	-	0/4/4/4	0/0/0/0
5	GOL	B	218	-	-	0/4/4/4	0/0/0/0
2	TMP	C	211	-	-	0/6/22/22	0/2/2/2
3	ADP	C	212	4	-	0/12/32/32	0/3/3/3
5	GOL	C	215	-	-	0/4/4/4	0/0/0/0
5	GOL	C	216	-	-	0/4/4/4	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	211	TMP	P-O3P	-4.07	1.38	1.54
2	A	211	TMP	P-O1P	-3.46	1.39	1.50
3	B	212	ADP	C2'-C1'	-2.94	1.49	1.53
3	C	212	ADP	C2'-C1'	-2.47	1.49	1.53
2	A	211	TMP	P-O2P	-2.34	1.45	1.54
3	A	212	ADP	C2'-C1'	-2.15	1.50	1.53
2	A	211	TMP	O5'-C5'	-2.07	1.36	1.44
2	B	211	TMP	C5'-C4'	2.07	1.58	1.51
2	A	211	TMP	C2-N3	2.08	1.42	1.38
2	C	211	TMP	O3'-C3'	2.09	1.47	1.43
2	C	211	TMP	C2'-C1'	2.12	1.58	1.52
3	C	212	ADP	PB-O3A	2.15	1.63	1.60
3	C	212	ADP	C4-N3	2.21	1.38	1.35
2	B	211	TMP	C4-N3	2.28	1.37	1.33
3	A	212	ADP	O4'-C1'	2.46	1.44	1.41
3	C	212	ADP	C5-C4	2.63	1.46	1.40
2	C	211	TMP	P-O3P	2.64	1.65	1.54
3	A	212	ADP	C5-C4	2.80	1.46	1.40
2	B	211	TMP	C2'-C1'	2.83	1.60	1.52
2	C	211	TMP	C5M-C5	2.86	1.56	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	TMP	O4'-C4'	2.86	1.51	1.45
3	C	212	ADP	C2-N3	3.00	1.37	1.32
3	C	212	ADP	O4'-C1'	3.09	1.45	1.41
3	B	212	ADP	C5-C4	3.36	1.48	1.40
2	A	211	TMP	P-O5'	3.38	1.71	1.60
3	A	212	ADP	PB-O3A	3.79	1.66	1.60
2	B	211	TMP	C5M-C5	4.08	1.58	1.51
2	A	211	TMP	C4-N3	4.17	1.40	1.33
2	C	211	TMP	C4-N3	4.52	1.41	1.33
2	A	211	TMP	C5M-C5	5.36	1.61	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	211	TMP	O2P-P-O5'	-7.94	85.59	106.73
3	B	212	ADP	N3-C2-N1	-7.42	122.39	128.86
3	A	212	ADP	N3-C2-N1	-7.12	122.65	128.86
3	C	212	ADP	N3-C2-N1	-5.69	123.90	128.86
2	C	211	TMP	C5-C6-N1	-4.58	117.19	122.15
2	B	211	TMP	C5-C4-N3	-4.49	120.29	125.24
2	B	211	TMP	C5-C6-N1	-3.80	118.04	122.15
2	A	211	TMP	C5-C4-N3	-3.72	121.13	125.24
2	C	211	TMP	O3P-P-O2P	-3.47	93.61	107.61
2	C	211	TMP	O4'-C1'-N1	-3.25	102.30	107.78
2	C	211	TMP	O3P-P-O5'	-3.07	98.57	106.73
2	C	211	TMP	O3P-P-O1P	-2.99	98.80	110.50
2	A	211	TMP	O4'-C1'-N1	-2.62	103.36	107.78
3	C	212	ADP	C4-C5-N7	-2.60	106.89	109.41
2	A	211	TMP	O4'-C4'-C5'	-2.39	101.32	109.40
3	A	212	ADP	C1'-N9-C4	-2.32	122.63	126.64
5	B	216	GOL	C3-C2-C1	-2.19	102.81	111.52
5	B	218	GOL	C3-C2-C1	-2.08	103.26	111.52
2	A	211	TMP	C5-C6-N1	-2.07	119.91	122.15
3	A	212	ADP	C2-N1-C6	2.08	122.42	118.77
5	A	215	GOL	O2-C2-C3	2.09	118.71	108.84
3	C	212	ADP	O3B-PB-O1B	2.14	118.86	110.50
2	A	211	TMP	O5'-P-O1P	2.53	113.58	106.47
5	A	215	GOL	O2-C2-C1	2.66	121.39	108.84
2	B	211	TMP	O2P-P-O1P	2.80	121.46	110.50
2	C	211	TMP	O2P-P-O5'	2.93	114.53	106.73
3	A	212	ADP	N6-C6-N1	3.20	125.10	118.77
3	B	212	ADP	C4'-O4'-C1'	3.21	113.19	109.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	211	TMP	O5'-P-O1P	3.55	116.43	106.47
2	C	211	TMP	O2P-P-O1P	3.62	124.67	110.50
3	B	212	ADP	C2-N1-C6	3.85	125.50	118.77
2	A	211	TMP	C4-N3-C2	3.97	118.64	115.16
2	B	211	TMP	C4-N3-C2	5.76	120.20	115.16
2	A	211	TMP	O3P-P-O1P	6.39	135.49	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	211	TMP	1	0
2	C	211	TMP	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 ⓘ

### 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	211/212 (99%)	-0.51	3 (1%) 75 78	8, 15, 32, 45	4 (1%)
1	B	208/212 (98%)	-0.33	5 (2%) 59 63	11, 18, 37, 47	10 (4%)
1	C	212/212 (100%)	-0.46	6 (2%) 53 57	11, 19, 35, 40	10 (4%)
All	All	631/636 (99%)	-0.43	14 (2%) 62 66	8, 18, 35, 47	24 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	ASP	4.7
1	B	144	ASN	4.7
1	C	198	ILE	3.0
1	C	196	THR	2.8
1	C	197	LYS	2.8
1	B	148	TYR	2.7
1	C	200	VAL	2.6
1	A	201	GLU	2.5
1	A	1	MET	2.5
1	B	143	GLN	2.5
1	B	150	GLU	2.3
1	C	201	GLU	2.1
1	A	2	THR	2.0
1	C	189	ASN	2.0

### 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 [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	216	6/6	0.93	0.16	5.50	37,44,44,49	0
4	NA	A	218	1/1	0.98	0.21	5.40	35,35,35,35	0
5	GOL	A	217	6/6	0.90	0.14	4.01	34,39,43,43	0
5	GOL	A	215	6/6	0.95	0.09	1.04	16,24,28,36	0
5	GOL	B	216	6/6	0.96	0.11	0.95	15,24,29,34	0
5	GOL	B	215	6/6	0.97	0.11	0.88	15,22,28,32	0
5	GOL	B	218	6/6	0.92	0.09	-0.13	31,34,36,36	0
2	TMP	A	211	21/21	0.99	0.07	-0.21	5,10,21,27	0
3	ADP	A	212	27/27	0.99	0.05	-0.66	10,16,19,20	0
3	ADP	B	212	27/27	0.99	0.06	-0.68	15,25,29,30	0
3	ADP	C	212	27/27	0.99	0.07	-0.70	12,23,25,27	0
2	TMP	B	211	21/21	0.99	0.07	-0.70	10,13,24,27	0
2	TMP	C	211	21/21	0.98	0.06	-0.78	9,12,21,31	0
5	GOL	C	215	6/6	0.97	0.06	-0.80	18,20,21,25	0
5	GOL	B	217	6/6	0.98	0.05	-1.24	15,17,19,19	0
5	GOL	A	216	6/6	0.98	0.06	-1.46	14,17,19,21	0
4	NA	B	213	1/1	0.97	0.08	-	37,37,37,37	0
4	NA	C	213	1/1	0.99	0.06	-	18,18,18,18	0
4	NA	C	214	1/1	0.99	0.03	-	15,15,15,15	0
4	NA	A	213	1/1	0.98	0.05	-	25,25,25,25	0
4	NA	A	214	1/1	1.00	0.04	-	22,22,22,22	0
4	NA	B	214	1/1	0.99	0.06	-	22,22,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.