



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:32 AM GMT

PDB ID : 2DFT  
Title : Structure of shikimate kinase from Mycobacterium tuberculosis complexed with ADP and Mg at 2.8 angstroms of resolution  
Authors : Dias, M.V.; Faim, L.M.; Vasconcelos, I.B.; de Oliveira, J.S.; Basso, L.A.; Santos, D.S.; de Azevedo, W.F.  
Deposited on : 2006-03-03  
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary 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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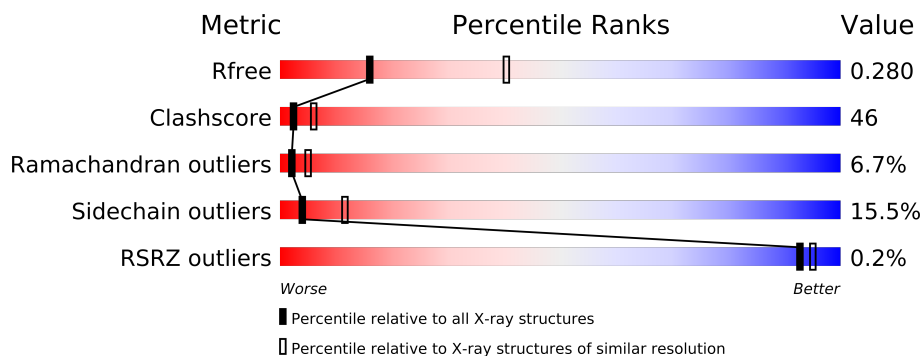
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	176	
1	B	176	
1	C	176	
1	D	176	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	190	-	X
2	MG	B	196	-	X
2	MG	C	202	-	X
2	MG	D	208	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5152 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 Shikimate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1165	717	232	214	2			
1	B	165	Total	C	N	O	S	0	0	0
			1229	759	244	224	2			
1	C	155	Total	C	N	O	S	0	0	0
			1157	713	230	212	2			
1	D	165	Total	C	N	O	S	0	0	0
			1226	757	244	223	2			

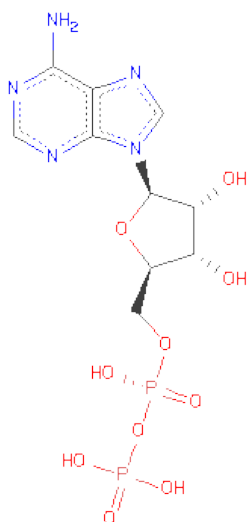
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 5 is water.

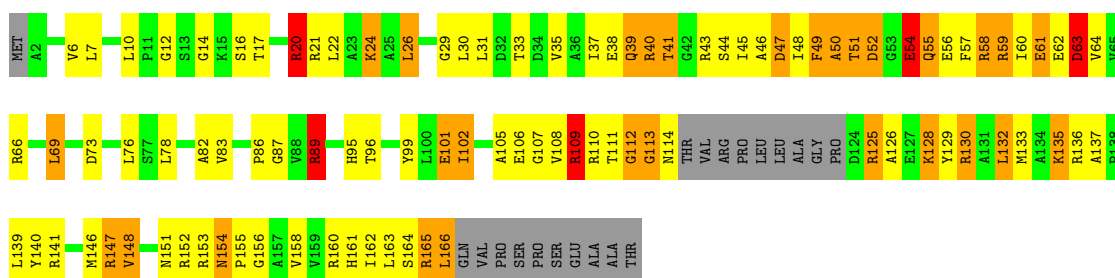
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	B	85	Total	O	0	0
			85	85		
5	C	51	Total	O	0	0
			51	51		
5	D	64	Total	O	0	0
			64	64		

### 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.

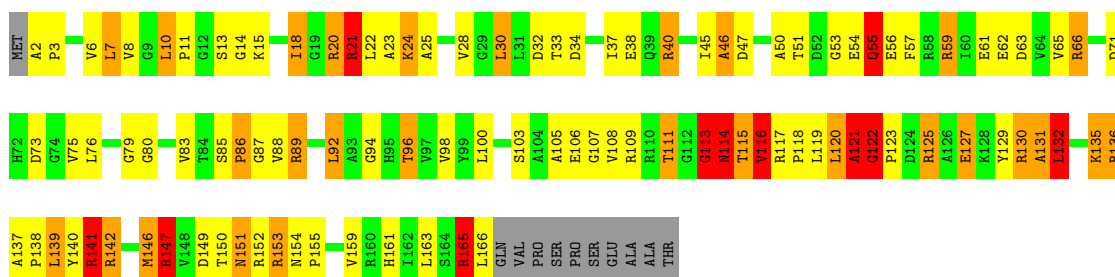
#### • Molecule 1: Shikimate kinase

Chain A:



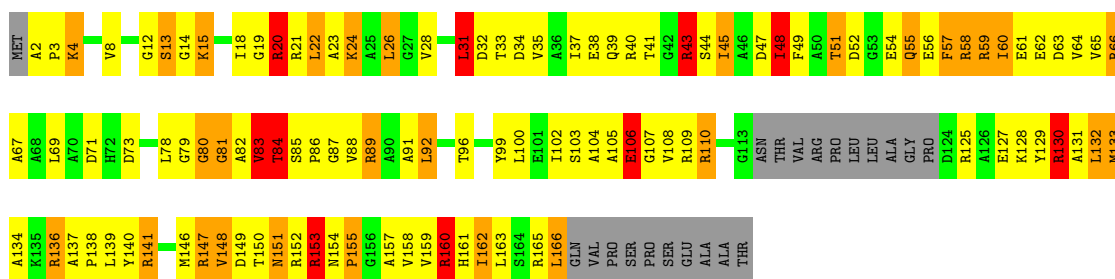
#### • Molecule 1: Shikimate kinase

Chain B:



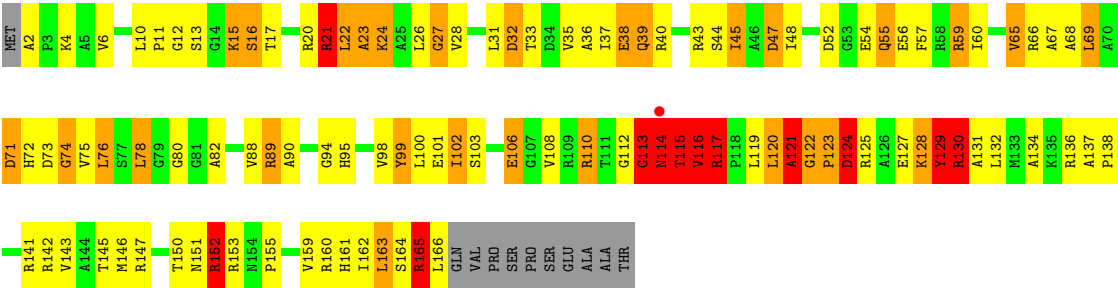
#### • Molecule 1: Shikimate kinase

Chain C:



#### • Molecule 1: Shikimate kinase

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.62Å 62.20Å 170.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.17 – 2.80 57.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (57.17-2.80) 99.7 (57.12-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.183 , 0.282 0.184 , 0.280	Depositor DCC
$R_{free}$ test set	832 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 18.3	EDS
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 16502 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MG, ADP, CL

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	1.37	2/1176 (0.2%)	2.04	38/1584 (2.4%)
1	B	1.33	5/1243 (0.4%)	1.92	33/1679 (2.0%)
1	C	1.44	7/1168 (0.6%)	2.03	35/1573 (2.2%)
1	D	1.39	6/1240 (0.5%)	2.01	43/1674 (2.6%)
All	All	1.38	20/4827 (0.4%)	2.00	149/6510 (2.3%)

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	A	0	3
1	B	0	4
1	C	0	4
1	D	0	6
All	All	0	17

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2	ALA	CA-CB	7.69	1.68	1.52
1	B	83	VAL	CB-CG1	-6.63	1.39	1.52
1	B	127	GLU	CG-CD	6.31	1.61	1.51
1	D	116	VAL	CB-CG2	6.00	1.65	1.52
1	D	129	TYR	CB-CG	-5.91	1.42	1.51

The worst 5 of 149 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	NE-CZ-NH1	-15.45	112.58	120.30
1	C	20	ARG	NE-CZ-NH2	-13.97	113.31	120.30
1	A	20	ARG	NE-CZ-NH2	-13.57	113.52	120.30
1	D	21	ARG	NE-CZ-NH2	-12.74	113.93	120.30
1	D	130	ARG	NE-CZ-NH1	12.73	126.66	120.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Mainchain
1	A	111	THR	Peptide
1	A	113	GLY	Peptide
1	B	113	GLY	Peptide
1	B	114	ASN	Peptide

## 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	1165	0	1208	110	0
1	B	1229	0	1282	114	1
1	C	1157	0	1202	123	1
1	D	1226	0	1275	110	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	27	0	12	6	0
4	B	27	0	12	2	0
4	C	27	0	12	8	0
4	D	27	0	12	6	0
5	A	60	0	0	31	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	85	0	0	47	1
5	C	51	0	0	38	1
5	D	64	0	0	33	1
All	All	5152	0	5015	457	4

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 46.

The worst 5 of 457 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:165:ARG:HH11	1:B:165:ARG:CG	1.34	1.37
1:A:59:ARG:HB2	5:A:278:HOH:O	1.15	1.31
1:C:157:ALA:HB3	5:C:411:HOH:O	1.25	1.29
1:A:125:ARG:HA	5:A:387:HOH:O	1.21	1.28
1:B:116:VAL:CG1	5:B:373:HOH:O	1.66	1.25

All (4) 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)
5:A:436:HOH:O	5:B:441:HOH:O[4.456]	1.71	0.49
1:B:135:LYS:CD	5:A:436:HOH:O[4.556]	1.93	0.27
1:C:96:THR:OG1	1:D:130:ARG:NH2[3.655]	2.04	0.16
5:C:287:HOH:O	5:D:286:HOH:O[3.555]	2.07	0.13

## 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	152/176 (86%)	132 (87%)	14 (9%)	6 (4%)	5	15
1	B	163/176 (93%)	133 (82%)	17 (10%)	13 (8%)	1	3
1	C	151/176 (86%)	129 (85%)	14 (9%)	8 (5%)	3	9
1	D	163/176 (93%)	136 (83%)	12 (7%)	15 (9%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	629/704 (89%)	530 (84%)	57 (9%)	42 (7%)	<b>2</b> <b>5</b>

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	B	46	ALA
1	B	115	THR
1	B	121	ALA
1	B	132	LEU

### 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	116/132 (88%)	97 (84%)	19 (16%)	<b>3</b> <b>10</b>
1	B	123/132 (93%)	108 (88%)	15 (12%)	<b>7</b> <b>20</b>
1	C	115/132 (87%)	93 (81%)	22 (19%)	<b>2</b> <b>6</b>
1	D	122/132 (92%)	104 (85%)	18 (15%)	<b>4</b> <b>13</b>
All	All	476/528 (90%)	402 (84%)	74 (16%)	<b>4</b> <b>11</b>

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	165	ARG
1	C	43	ARG
1	D	127	GLU
1	C	4	LYS
1	C	26	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	151	ASN
1	D	55	GLN

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Mol	Chain	Res	Type
1	C	161	HIS
1	B	39	GLN
1	D	39	GLN

### 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 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	ADP	A	180	2	29,29,29	1.25	4 (13%)	45,45,45	3.00	21 (46%)
4	ADP	B	181	2	29,29,29	1.23	3 (10%)	45,45,45	2.75	20 (44%)
4	ADP	C	182	2	29,29,29	1.11	2 (6%)	45,45,45	2.87	16 (35%)
4	ADP	D	183	2	29,29,29	0.85	0	45,45,45	2.82	14 (31%)

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	ADP	A	180	2	-	0/16/32/32	0/1/3/3
4	ADP	B	181	2	-	0/16/32/32	0/1/3/3
4	ADP	C	182	2	-	0/16/32/32	0/1/3/3
4	ADP	D	183	2	-	0/16/32/32	0/1/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	180	ADP	C8-N9	-3.19	1.31	1.36
4	B	181	ADP	C8-N9	-3.08	1.32	1.36
4	A	180	ADP	C2'-C1'	-3.03	1.49	1.53
4	B	181	ADP	C4-N9	-2.91	1.33	1.37
4	C	182	ADP	C4-N9	-2.69	1.33	1.37

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	183	ADP	N3-C2-N1	-13.29	117.60	128.71
4	C	182	ADP	N3-C2-N1	-11.01	119.51	128.71
4	B	181	ADP	C4-C5-N7	-10.18	100.81	109.52
4	A	180	ADP	N3-C2-N1	-7.15	122.73	128.71
4	C	182	ADP	C8-N9-C4	7.07	112.30	106.90

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	156/176 (88%)	-0.47	0 100 100	12, 32, 53, 68	0
1	B	165/176 (93%)	-0.54	0 100 100	9, 28, 46, 62	0
1	C	155/176 (88%)	-0.44	0 100 100	18, 34, 61, 83	0
1	D	165/176 (93%)	-0.25	1 (0%) 86 88	20, 36, 54, 68	0
All	All	641/704 (91%)	-0.42	1 (0%) 93 95	9, 33, 53, 83	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	ASN	2.3

### 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( $\text{\AA}^2$ )	Q<0.9
2	MG	A	190	1/1	0.23	14.17	22,22,22,22	0
2	MG	B	196	1/1	0.23	4.77	15,15,15,15	0
2	MG	C	202	1/1	0.21	4.17	29,29,29,29	0
2	MG	D	208	1/1	0.20	2.54	41,41,41,41	0
4	ADP	B	181	27/27	0.12	-0.68	10,23,32,36	0
4	ADP	A	180	27/27	0.11	-0.70	10,16,25,32	0
4	ADP	D	183	27/27	0.12	-0.85	17,33,49,52	0
4	ADP	C	182	27/27	0.12	-0.87	7,29,43,54	0
3	CL	B	199	1/1	0.10	-2.03	26,26,26,26	0
3	CL	A	193	1/1	0.07	-2.06	46,46,46,46	0
3	CL	D	211	1/1	0.08	-2.31	34,34,34,34	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.