



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 08:12 PM GMT

PDB ID : 3PP7  
Title : Crystal structure of Leishmania mexicana pyruvate kinase in complex with the drug suramin, an inhibitor of glycolysis.  
Authors : Morgan, H.P.; Auld, D.S.; McNae, I.W.; Nowicki, M.W.; Michels, P.A.M.; Fothergill-Gilmore, L.A.; Walkinshaw, M.D.  
Deposited on : 2010-11-24  
Resolution : 2.35 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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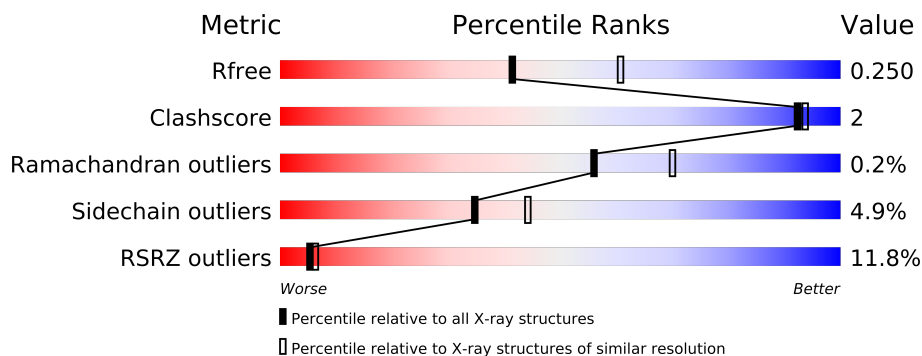
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.35 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	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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	498	
1	B	498	

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	GOL	A	500	-	X

## 2 Entry composition i

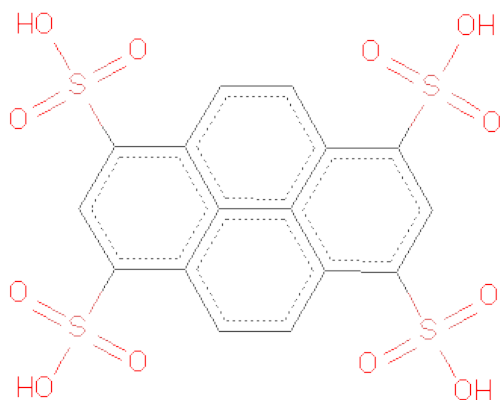
There are 6 unique types of molecules in this entry. The entry contains 8054 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	1	0
			3763	2345	663	729	26			
1	B	494	Total	C	N	O	S	0	0	0
			3766	2347	663	730	26			

- Molecule 2 is PYRENE-1,3,6,8-TETRASULFONICACID (three-letter code: PTK) (formula:  $C_{16}H_{10}O_{12}S_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			32	16	12	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

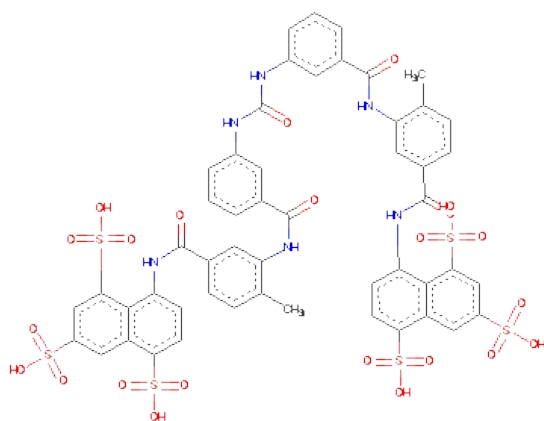


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	K	0	0
			2	2		
4	A	2	Total	K	0	0
			2	2		

- Molecule 5 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFONIC ACID (three-letter code: SVR) (formula: C<sub>51</sub>H<sub>40</sub>N<sub>6</sub>O<sub>23</sub>S<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			41	25	2	11	3		

- Molecule 6 is water.

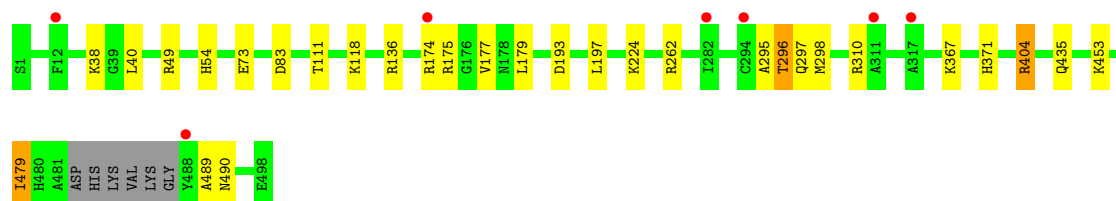
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	236	Total	O	0	0
			236	236		
6	B	200	Total	O	0	0
			200	200		

### 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.

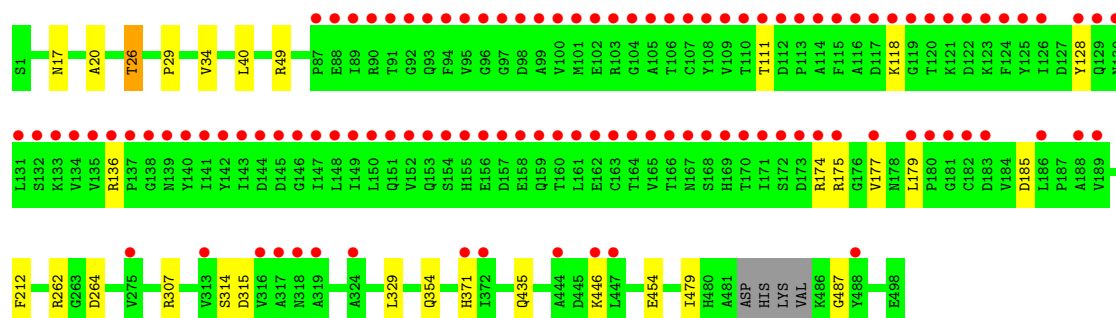
- Molecule 1: Pyruvate kinase

Chain A: 



- Molecule 1: Pyruvate kinase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.77Å 129.48Å 165.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.73 – 2.35 44.73 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (44.73-2.35) 98.0 (44.73-2.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.02	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.55 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.191 , 0.231 0.210 , 0.250	Depositor DCC
$R_{free}$ test set	2761 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.1	EDS
Estimated twinning fraction	0.010 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54537 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: SVR, GOL, K, PTK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	0/3819	0.55	0/5169
1	B	0.42	0/3821	0.56	0/5170
All	All	0.42	0/7640	0.55	0/10339

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	3763	0	0	8	0
1	B	3766	0	0	6	0
2	A	32	0	8	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	B	41	0	18	2	0
6	A	236	0	0	0	0
6	B	200	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8054	0	42	14	0

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 2.

All (14) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:THR:CG2	1:B:329:LEU:O	2.53	0.56
5:B:499:SVR:N63	5:B:499:SVR:S73	2.73	0.55
1:A:54[B]:HIS:C	1:A:54[B]:HIS:CD2	2.84	0.51
1:B:29:PRO:CG	5:B:499:SVR:H56	2.42	0.50
1:A:295:ALA:O	1:A:296:THR:CB	2.64	0.45
1:A:404:ARG:NH2	1:A:404:ARG:CG	2.79	0.44
1:B:20:ALA:N	1:B:354:GLN:OE1	2.49	0.44
1:A:49:ARG:NE	1:A:83:ASP:OD2	2.50	0.44
1:A:193:ASP:O	1:A:197:LEU:N	2.52	0.43
1:B:26:THR:CG2	1:B:49:ARG:NH1	2.83	0.41
1:B:128:TYR:OH	1:B:185:ASP:OD2	2.38	0.41
1:A:38:LYS:CE	1:A:73:GLU:OE1	2.69	0.41
1:A:310:ARG:NH2	1:B:315:ASP:OD1	2.55	0.40
1:A:479:ILE:CD1	1:A:489:ALA:CB	2.99	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	489/498 (98%)	479 (98%)	9 (2%)	1 (0%)	56	70
1	B	490/498 (98%)	477 (97%)	12 (2%)	1 (0%)	56	70
All	All	979/996 (98%)	956 (98%)	21 (2%)	2 (0%)	56	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	487	GLY
1	A	296	THR

### 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	412/416 (99%)	393 (95%)	19 (5%)	37	47
1	B	412/416 (99%)	391 (95%)	21 (5%)	33	41
All	All	824/832 (99%)	784 (95%)	40 (5%)	35	44

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	111	THR
1	A	118	LYS
1	A	136	ARG
1	A	174	ARG
1	A	175	ARG
1	A	177	VAL
1	A	179	LEU
1	A	224	LYS
1	A	262	ARG
1	A	297	GLN
1	A	298	MET
1	A	367	LYS
1	A	371	HIS
1	A	404	ARG
1	A	435	GLN
1	A	453	LYS
1	A	479	ILE
1	A	490	ASN
1	B	17	ASN
1	B	26	THR
1	B	34	VAL
1	B	40	LEU
1	B	111	THR

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Mol	Chain	Res	Type
1	B	118	LYS
1	B	136	ARG
1	B	174	ARG
1	B	175	ARG
1	B	177	VAL
1	B	179	LEU
1	B	212	PHE
1	B	262	ARG
1	B	264	ASP
1	B	307	ARG
1	B	314	SER
1	B	371	HIS
1	B	435	GLN
1	B	446	LYS
1	B	454	GLU
1	B	479	ILE

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 8 ligands modelled in this entry, 4 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	$\# Z  > 2$
2	PTK	A	499	-	35,35,35	1.49	4 (11%)	60,60,60	1.79	21 (35%)
3	GOL	A	500	-	5,5,5	0.20	0	5,5,5	0.67	0
5	SVR	B	499	-	44,44,93	1.24	5 (11%)	67,68,145	1.66	15 (22%)
3	GOL	B	502	-	5,5,5	0.25	0	5,5,5	0.46	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	PTK	A	499	-	-	0/24/24/24	0/0/4/4
3	GOL	A	500	-	-	0/4/4/4	0/0/0/0
5	SVR	B	499	-	-	0/34/34/76	0/2/4/8
3	GOL	B	502	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	499	SVR	C58-C61	3.13	1.56	1.50
5	B	499	SVR	C55-N53	-2.92	1.36	1.41
2	A	499	PTK	CAV-CAZ	-2.87	1.39	1.43
2	A	499	PTK	CAT-CAX	-2.83	1.39	1.43
5	B	499	SVR	C49-C51	2.78	1.55	1.50
2	A	499	PTK	CAS-CAW	-2.43	1.39	1.43
2	A	499	PTK	CAU-CAY	-2.36	1.39	1.43
5	B	499	SVR	C70-C71	2.11	1.40	1.37
5	B	499	SVR	C71-C68	-2.05	1.40	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	499	SVR	O80-S75-C71	4.47	111.27	106.20
5	B	499	SVR	C72-C68-C71	-4.38	118.03	123.20
5	B	499	SVR	C71-C68-C66	3.97	121.41	118.03
5	B	499	SVR	O81-S75-C71	3.74	110.44	106.20
5	B	499	SVR	O78-S73-C69	3.58	110.25	106.20
5	B	499	SVR	O79-S73-C69	3.48	110.32	106.09
2	A	499	PTK	CAQ-CAX-CAT	-3.38	119.22	123.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	499	PTK	OAF-SBE-CAU	3.17	109.79	106.20
2	A	499	PTK	CAM-CAT-SBD	3.15	121.08	117.67
5	B	499	SVR	C66-C69-S73	3.07	124.66	121.05
2	A	499	PTK	CAR-CAZ-CAV	-3.06	119.65	123.81
2	A	499	PTK	OAC-SBD-CAT	3.03	109.77	106.09
2	A	499	PTK	OAE-SBE-CAU	2.98	109.58	106.20
2	A	499	PTK	OAJ-SBD-CAT	2.88	109.47	106.20
2	A	499	PTK	OAA-SBC-CAS	2.86	109.44	106.20
2	A	499	PTK	OAI-SBC-CAS	2.85	109.43	106.20
2	A	499	PTK	OAB-SBC-CAS	2.82	109.53	106.09
2	A	499	PTK	OAL-SBF-CAV	2.82	109.53	106.09
2	A	499	PTK	OAG-SBF-CAV	2.82	109.39	106.20
2	A	499	PTK	OAK-SBE-CAU	2.81	109.51	106.09
5	B	499	SVR	C60-C57-C55	2.81	119.76	117.42
2	A	499	PTK	OAD-SBD-CAT	2.80	109.37	106.20
2	A	499	PTK	CAT-CAX-CBA	2.77	120.39	118.03
2	A	499	PTK	OAH-SBF-CAV	2.72	109.28	106.20
5	B	499	SVR	C70-C71-C68	-2.70	118.52	121.00
5	B	499	SVR	C70-C71-S75	2.68	121.26	117.34
5	B	499	SVR	O82-S75-C71	2.58	109.23	106.09
2	A	499	PTK	CAO-CAW-CAS	-2.53	120.37	123.81
5	B	499	SVR	C74-C69-S73	-2.53	114.92	117.67
5	B	499	SVR	O77-S73-C69	2.43	108.95	106.20
2	A	499	PTK	CAP-CAY-CAU	-2.38	120.58	123.81
5	B	499	SVR	C57-C55-N53	2.32	122.46	118.63
2	A	499	PTK	CAS-CAW-CBA	2.14	119.85	118.03
5	B	499	SVR	C65-C66-C69	-2.11	122.70	126.66
2	A	499	PTK	CAU-CAY-CBB	2.08	119.80	118.03
2	A	499	PTK	CAV-CAZ-CBB	2.05	119.78	118.03

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	492/498 (98%)	0.28	7 (1%) 72 76	38, 55, 94, 109	0
1	B	494/498 (99%)	1.62	110 (22%) 1 1	37, 56, 215, 243	0
All	All	986/996 (98%)	0.95	117 (11%) 5 6	37, 55, 196, 243	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	VAL	23.0
1	B	171	ILE	21.5
1	B	124	PHE	16.9
1	B	172	SER	16.4
1	B	126	ILE	15.6
1	B	92	GLY	14.7
1	B	94	PHE	14.6
1	B	106	THR	14.6
1	B	170	THR	14.2
1	B	104	GLY	12.9
1	B	169	HIS	12.2
1	B	89	ILE	11.6
1	B	138	GLY	10.6
1	B	108	TYR	10.6
1	B	95	VAL	10.2
1	B	137	PRO	10.2
1	B	133	LYS	9.3
1	B	93	GLN	9.2
1	B	142	TYR	9.1
1	B	91	THR	8.8
1	B	103	ARG	8.7
1	B	163	CYS	8.7
1	B	143	ILE	8.7
1	B	119	GLY	8.6

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Mol	Chain	Res	Type	RSRZ
1	B	107	CYS	8.6
1	B	105	ALA	8.6
1	B	175	ARG	8.6
1	B	149	ILE	8.4
1	B	150	LEU	8.4
1	B	161	LEU	8.3
1	B	164	THR	8.3
1	B	90	ARG	8.1
1	B	101	MET	8.0
1	B	165	VAL	7.8
1	B	125	TYR	7.8
1	B	156	GLU	7.8
1	B	167	ASN	7.8
1	B	140	TYR	7.7
1	B	99	ALA	7.7
1	B	134	VAL	7.7
1	B	160	THR	7.5
1	B	155	HIS	7.5
1	B	122	ASP	7.4
1	B	131	LEU	7.2
1	B	152	VAL	7.1
1	B	181	GLY	7.0
1	B	154	SER	6.9
1	B	96	GLY	6.9
1	B	141	ILE	6.8
1	B	139	ASN	6.8
1	B	168	SER	6.5
1	B	166	THR	6.5
1	B	102	GLU	6.5
1	B	157	ASP	6.3
1	B	173	ASP	6.3
1	B	151	GLN	6.2
1	B	121	LYS	6.2
1	B	110	THR	6.1
1	B	153	GLN	6.0
1	B	136	ARG	6.0
1	B	146	GLY	6.0
1	B	148	LEU	5.9
1	B	132	SER	5.8
1	B	162	GLU	5.8
1	B	115	PHE	5.6
1	B	135	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	100	VAL	5.3
1	B	117	ASP	5.1
1	B	177	VAL	4.8
1	B	174	ARG	4.7
1	B	97	GLY	4.7
1	B	158	GLU	4.6
1	B	114	ALA	4.6
1	B	159	GLN	4.5
1	B	180	PRO	4.5
1	B	98	ASP	4.4
1	B	182	CYS	4.2
1	B	179	LEU	4.1
1	B	113	PRO	4.1
1	B	147	ILE	3.9
1	B	188	ALA	3.9
1	B	189	VAL	3.5
1	B	144	ASP	3.4
1	B	116	ALA	3.4
1	B	120	THR	3.3
1	B	88	GLU	3.1
1	B	488	TYR	3.1
1	B	129	GLN	2.9
1	B	183	ASP	2.9
1	B	319	ALA	2.9
1	B	112	ASP	2.8
1	B	123	LYS	2.8
1	B	130	ASN	2.7
1	B	372	ILE	2.7
1	B	444	ALA	2.6
1	A	174	ARG	2.5
1	B	316	VAL	2.5
1	B	446	LYS	2.5
1	B	87	PRO	2.5
1	B	447	LEU	2.5
1	A	317	ALA	2.4
1	A	311	ALA	2.4
1	B	128	TYR	2.3
1	B	145	ASP	2.3
1	B	186	LEU	2.3
1	B	317	ALA	2.3
1	B	118	LYS	2.3
1	A	488	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	111	THR	2.3
1	B	313	VAL	2.2
1	B	318	ASN	2.2
1	A	12	PHE	2.2
1	A	282	ILE	2.2
1	B	371	HIS	2.1
1	B	275	VAL	2.1
1	A	294	CYS	2.1
1	B	324	ALA	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 ⓘ

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	GOL	A	500	6/6	0.24	3.51	61,62,62,62	0
5	SVR	B	499	41/86	0.22	1.97	104,106,108,108	0
3	GOL	B	502	6/6	0.25	1.92	80,81,82,82	0
2	PTK	A	499	32/32	0.20	1.87	118,118,119,119	32
4	K	A	502	1/1	0.10	-0.63	81,81,81,81	0
4	K	B	500	1/1	0.09	-2.05	66,66,66,66	0
4	K	A	501	1/1	0.06	-3.02	55,55,55,55	0
4	K	B	501	1/1	0.04	-4.74	58,58,58,58	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.