



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:55 PM GMT

PDB ID : 3IS4
Title : Crystal structure of Leishmania mexicana pyruvate kinase (LmPYK) in complex with 1,3,6,8-pyrenetetrasulfonic acid
Authors : Walkinshaw, M.D.; Morgan, H.P.
Deposited on : 2009-08-25
Resolution : 2.10 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

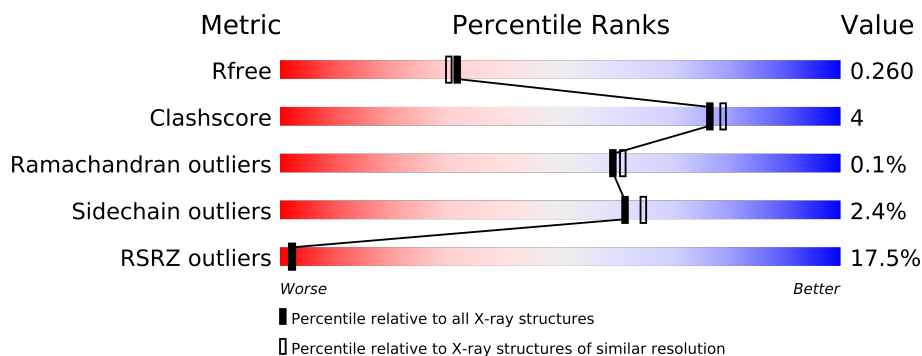
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 ≥ 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	499	
1	B	499	

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	GOL	A	502	-	X
3	PTK	A	501	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8211 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	0	0
			3753	2339	660	728	26			
1	B	492	Total	C	N	O	S	0	0	0
			3753	2339	660	728	26			

There are 8 discrepancies between the modelled and reference sequences:

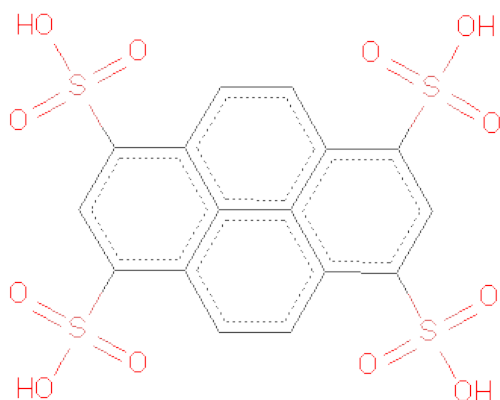
Chain	Residue	Modelled	Actual	Comment	Reference
A	382	SER	GLY	SEE REMARK 999	UNP Q27686
A	389	TYR	SER	SEE REMARK 999	UNP Q27686
A	404	ARG	ALA	SEE REMARK 999	UNP Q27686
A	405	SER	GLY	SEE REMARK 999	UNP Q27686
B	382	SER	GLY	SEE REMARK 999	UNP Q27686
B	389	TYR	SER	SEE REMARK 999	UNP Q27686
B	404	ARG	ALA	SEE REMARK 999	UNP Q27686
B	405	SER	GLY	SEE REMARK 999	UNP Q27686

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 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
3	A	1	Total	C	O	S	0	0
			32	16	12	4		

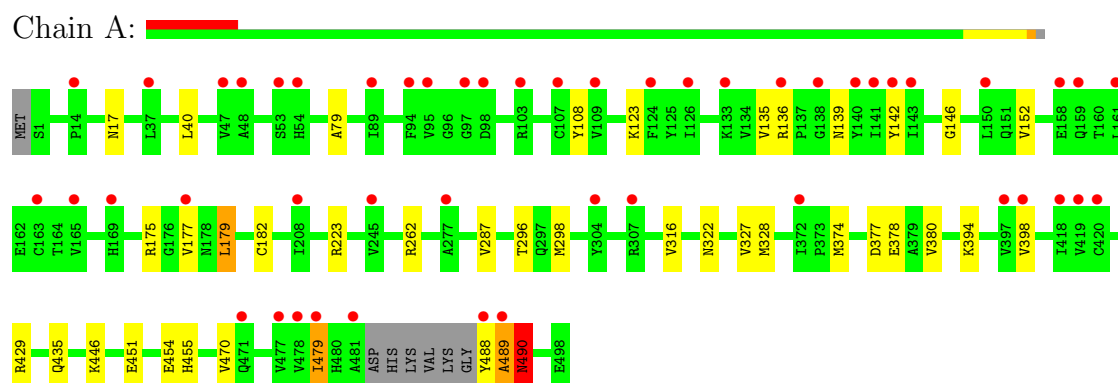
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	350	Total	O	0	0
			350	350		
4	B	293	Total	O	0	0
			293	293		

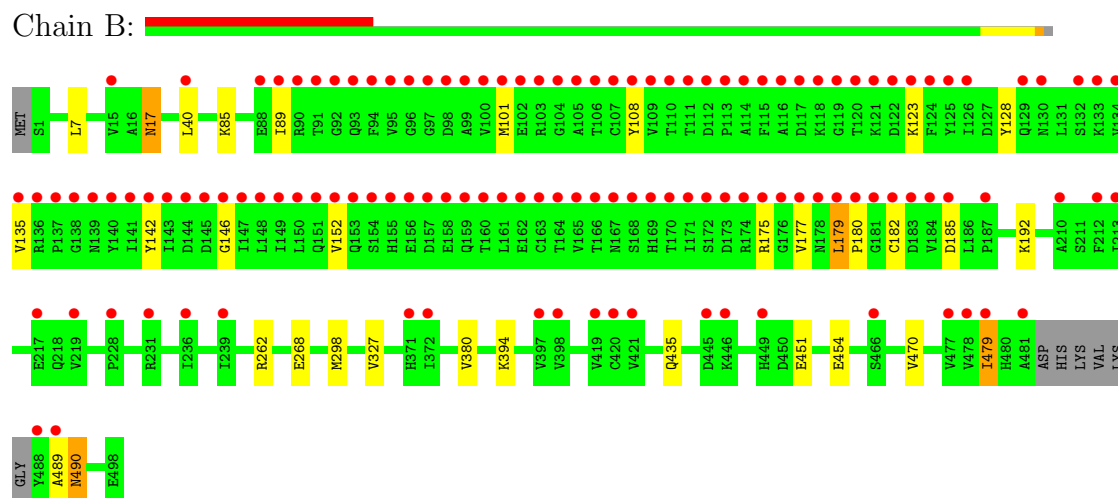
3 Residue-property plots

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



• Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.86Å 129.86Å 165.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.69 – 2.10 20.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.69-2.10) 100.0 (20.69-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.231 , 0.263 0.230 , 0.260	Depositor DCC
R_{free} test set	3865 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 76957 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8211	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: GOL, 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	0.39	0/3808	0.53	2/5154 (0.0%)
1	B	0.39	0/3808	0.50	0/5154
All	All	0.39	0/7616	0.51	2/10308 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ASN	N-CA-CB	5.70	120.85	110.60
1	A	489	ALA	CB-CA-C	5.50	118.35	110.10

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	3753	0	3752	27	0
1	B	3753	0	3752	21	0
2	A	24	0	32	3	0
2	B	6	0	8	0	0
3	A	32	0	10	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	350	0	0	4	0
4	B	293	0	0	2	0
All	All	8211	0	7554	57	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 4.

All (57) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:501:PTK:HAP	3:A:501:PTK:OAK	1.58	0.99
3:A:501:PTK:HAQ	3:A:501:PTK:OAJ	1.62	0.98
3:A:501:PTK:HAR	3:A:501:PTK:OAG	1.57	0.98
3:A:501:PTK:OAB	3:A:501:PTK:HAO	1.82	0.80
1:A:479:ILE:HD11	1:A:489:ALA:HB1	1.66	0.77
1:B:135:VAL:HG11	1:B:152:VAL:HG21	1.75	0.69
1:A:135:VAL:HG11	1:A:152:VAL:HG21	1.76	0.67
1:A:298:MET:HE3	1:A:316:VAL:HG22	1.80	0.63
1:A:298:MET:HE2	1:A:327:VAL:HB	1.80	0.63
1:A:398:VAL:HG13	1:A:479:ILE:HD13	1.84	0.59
1:B:479:ILE:HD11	1:B:489:ALA:CB	2.33	0.59
1:B:179:LEU:HB3	1:B:182:CYS:HB2	1.85	0.58
1:B:394:LYS:HB2	1:B:470:VAL:HG12	1.86	0.57
3:A:501:PTK:CAQ	3:A:501:PTK:OAJ	2.45	0.57
3:A:501:PTK:CAR	3:A:501:PTK:OAG	2.42	0.56
1:B:298:MET:HE2	1:B:327:VAL:HB	1.89	0.54
1:A:179:LEU:HB3	1:A:182:CYS:HB2	1.89	0.54
1:A:223:ARG:HD2	4:A:553:HOH:O	2.06	0.54
1:B:479:ILE:HD11	1:B:489:ALA:HB1	1.89	0.54
3:A:501:PTK:CAP	3:A:501:PTK:OAK	2.42	0.54
1:A:455:HIS:HD2	4:A:559:HOH:O	1.91	0.53
1:B:17:ASN:H	1:B:17:ASN:HD22	1.56	0.53
1:A:377:ASP:HB3	1:A:488:TYR:CD2	2.44	0.53
1:B:298:MET:CE	1:B:327:VAL:HB	2.39	0.53
1:A:380:VAL:HG21	1:A:490:ASN:HA	1.92	0.52
1:A:298:MET:CE	1:A:316:VAL:HG22	2.40	0.50
1:B:380:VAL:HG21	1:B:490:ASN:HA	1.94	0.49
3:A:501:PTK:HOAK	3:A:501:PTK:HAP	1.72	0.49
1:A:451:GLU:CD	1:A:451:GLU:H	2.17	0.48
1:B:180:PRO:HB3	1:B:268:GLU:HB2	1.97	0.47
1:A:298:MET:HB3	1:A:298:MET:HE3	1.74	0.47
1:B:128:TYR:OH	1:B:185:ASP:OD2	2.27	0.47
1:A:479:ILE:HD11	1:A:489:ALA:CB	2.41	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:322:ASN:HA	2:A:502:GOL:H11	1.97	0.46
3:A:501:PTK:CAO	3:A:501:PTK:OAB	2.59	0.45
1:A:322:ASN:HA	2:A:502:GOL:C1	2.46	0.45
1:B:101:MET:HE1	4:B:600:HOH:O	2.16	0.45
1:B:101:MET:CE	4:B:600:HOH:O	2.64	0.45
1:A:287:VAL:HG21	1:B:7:LEU:HD11	1.99	0.45
1:B:85:LYS:HD3	1:B:192:LYS:HD3	1.98	0.44
1:B:108:TYR:O	1:B:123:LYS:HA	2.17	0.44
1:B:89:ILE:HG23	1:B:128:TYR:HB2	2.00	0.44
1:A:108:TYR:O	1:A:123:LYS:HA	2.18	0.44
1:B:17:ASN:N	1:B:17:ASN:HD22	2.13	0.43
1:A:394:LYS:HB2	1:A:470:VAL:HG12	1.99	0.43
1:A:488:TYR:CD2	1:A:489:ALA:O	2.71	0.43
1:B:490:ASN:HD22	1:B:490:ASN:H	1.66	0.43
1:B:142:TYR:HB3	1:B:146:GLY:HA2	2.00	0.43
1:A:298:MET:HG3	1:A:328:MET:O	2.19	0.42
1:A:374:MET:CE	1:A:378:GLU:HG3	2.50	0.41
1:A:136:ARG:H	1:A:139:ASN:ND2	2.19	0.41
1:A:142:TYR:HB3	1:A:146:GLY:HA2	2.02	0.41
1:A:398:VAL:HG22	1:A:479:ILE:HG23	2.03	0.41
1:A:446:LYS:HD3	4:A:815:HOH:O	2.19	0.41
2:A:502:GOL:H12	4:A:547:HOH:O	2.21	0.41
1:A:79:ALA:HB2	1:A:429:ARG:O	2.20	0.41
1:B:451:GLU:CD	1:B:451:GLU:H	2.25	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	488/499 (98%)	476 (98%)	11 (2%)	1 (0%)	56	57
1	B	488/499 (98%)	479 (98%)	9 (2%)	0	100	100
All	All	976/998 (98%)	955 (98%)	20 (2%)	1 (0%)	59	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	411/417 (99%)	401 (98%)	10 (2%)	61	65
1	B	411/417 (99%)	401 (98%)	10 (2%)	61	65
All	All	822/834 (99%)	802 (98%)	20 (2%)	61	65

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

Mol	Chain	Res	Type
1	A	17	ASN
1	A	40	LEU
1	A	175	ARG
1	A	177	VAL
1	A	179	LEU
1	A	262	ARG
1	A	435	GLN
1	A	454	GLU
1	A	479	ILE
1	A	490	ASN
1	B	17	ASN
1	B	40	LEU
1	B	175	ARG
1	B	177	VAL
1	B	179	LEU
1	B	262	ARG
1	B	435	GLN
1	B	454	GLU
1	B	479	ILE
1	B	490	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	139	ASN
1	A	153	GLN
1	A	178	ASN
1	A	471	GLN
1	B	17	ASN
1	B	69	GLN
1	B	139	ASN
1	B	153	GLN
1	B	242	HIS
1	B	490	ASN

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 ⓘ

6 ligands are modelled in this entry.

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	GOL	A	499	-	5,5,5	0.41	0	5,5,5	0.35	0
2	GOL	A	500	-	5,5,5	0.41	0	5,5,5	0.21	0
3	PTK	A	501	-	35,35,35	1.60	4 (11%)	60,60,60	1.84	24 (40%)
2	GOL	A	502	-	5,5,5	0.42	0	5,5,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	503	-	5,5,5	0.32	0	5,5,5	0.30	0
2	GOL	B	499	-	5,5,5	0.33	0	5,5,5	0.36	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	GOL	A	499	-	-	0/4/4/4	0/0/0/0
2	GOL	A	500	-	-	0/4/4/4	0/0/0/0
3	PTK	A	501	-	-	0/24/24/24	0/0/4/4
2	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	GOL	B	499	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PTK	CAV-CAZ	-2.83	1.39	1.43
3	A	501	PTK	CAS-CAW	-2.76	1.39	1.43
3	A	501	PTK	CAT-CAX	-2.76	1.39	1.43
3	A	501	PTK	CAU-CAY	-2.76	1.39	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	PTK	OAD-SBD-CAT	3.13	109.74	106.20
3	A	501	PTK	OAA-SBC-CAS	3.06	109.67	106.20
3	A	501	PTK	OAH-SBF-CAV	3.00	109.61	106.20
3	A	501	PTK	CAR-CAZ-CAV	-2.99	119.74	123.81
3	A	501	PTK	OAE-SBE-CAU	2.98	109.58	106.20
3	A	501	PTK	CAQ-CAX-CAT	-2.91	119.86	123.81
3	A	501	PTK	CAP-CAY-CAU	-2.88	119.89	123.81
3	A	501	PTK	CAO-CAW-CAS	-2.86	119.93	123.81
3	A	501	PTK	CAM-CAT-SBD	2.82	120.73	117.67
3	A	501	PTK	OAF-SBE-CAU	2.80	109.38	106.20
3	A	501	PTK	OAJ-SBD-CAT	2.78	109.35	106.20
3	A	501	PTK	OAI-SBC-CAS	2.78	109.35	106.20
3	A	501	PTK	CAN-CAV-SBF	2.76	120.67	117.67
3	A	501	PTK	OAB-SBC-CAS	2.70	109.38	106.09
3	A	501	PTK	OAL-SBF-CAV	2.70	109.38	106.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	PTK	CAN-CAU-SBE	2.68	120.58	117.67
3	A	501	PTK	OAG-SBF-CAV	2.61	109.16	106.20
3	A	501	PTK	CAM-CAS-SBC	2.60	120.49	117.67
3	A	501	PTK	OAC-SBD-CAT	2.56	109.20	106.09
3	A	501	PTK	OAK-SBE-CAU	2.53	109.17	106.09
3	A	501	PTK	CAS-CAW-CBA	2.30	119.99	118.03
3	A	501	PTK	CAV-CAZ-CBB	2.28	119.97	118.03
3	A	501	PTK	CAT-CAX-CBA	2.20	119.90	118.03
3	A	501	PTK	CAU-CAY-CBB	2.18	119.89	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, 95th 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 ²)	Q<0.9
1	A	492/499 (98%)	0.56	49 (9%) 8 8	20, 33, 55, 60	0
1	B	492/499 (98%)	1.87	124 (25%) 1 1	21, 34, 55, 60	0
All	All	984/998 (98%)	1.22	173 (17%) 2 2	20, 34, 55, 60	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	PHE	17.2
1	B	171	ILE	17.1
1	B	95	VAL	16.9
1	B	172	SER	15.2
1	B	166	THR	14.5
1	B	116	ALA	13.4
1	B	104	GLY	13.1
1	B	115	PHE	13.1
1	B	105	ALA	12.2
1	B	96	GLY	11.7
1	B	142	TYR	11.4
1	B	170	THR	11.3
1	B	167	ASN	11.2
1	B	106	THR	11.1
1	B	103	ARG	10.9
1	B	149	ILE	10.6
1	B	145	ASP	10.6
1	B	155	HIS	10.5
1	B	108	TYR	10.3
1	B	147	ILE	10.2
1	B	169	HIS	10.1
1	B	119	GLY	9.8
1	B	140	TYR	9.6
1	B	136	ARG	9.5

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Mol	Chain	Res	Type	RSRZ
1	B	97	GLY	9.5
1	B	101	MET	9.5
1	B	138	GLY	9.2
1	B	113	PRO	9.2
1	B	109	VAL	9.1
1	B	146	GLY	8.8
1	B	122	ASP	8.8
1	B	159	GLN	8.7
1	B	125	TYR	8.6
1	B	137	PRO	8.6
1	B	168	SER	8.4
1	B	99	ALA	8.4
1	B	154	SER	8.2
1	B	165	VAL	8.2
1	B	124	PHE	8.2
1	B	164	THR	8.2
1	B	152	VAL	7.9
1	B	139	ASN	7.9
1	A	488	TYR	7.8
1	B	153	GLN	7.8
1	B	93	GLN	7.7
1	B	150	LEU	7.5
1	B	98	ASP	7.4
1	B	488	TYR	7.3
1	B	114	ALA	7.2
1	B	156	GLU	7.1
1	B	117	ASP	7.1
1	B	158	GLU	7.1
1	B	179	LEU	6.8
1	B	151	GLN	6.7
1	B	175	ARG	6.7
1	B	182	CYS	6.7
1	B	102	GLU	6.6
1	B	163	CYS	6.5
1	B	92	GLY	6.5
1	B	481	ALA	6.4
1	B	121	LYS	6.3
1	B	157	ASP	6.3
1	B	118	LYS	6.2
1	B	173	ASP	6.2
1	B	112	ASP	6.1
1	B	181	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	126	ILE	6.1
1	B	489	ALA	6.0
1	B	120	THR	5.9
1	B	162	GLU	5.9
1	B	134	VAL	5.9
1	B	133	LYS	5.8
1	A	109	VAL	5.7
1	B	176	GLY	5.5
1	B	100	VAL	5.4
1	B	129	GLN	5.3
1	B	107	CYS	5.3
1	B	123	LYS	5.2
1	B	90	ARG	5.2
1	B	183	ASP	5.1
1	B	111	THR	5.1
1	A	141	ILE	5.0
1	B	174	ARG	4.9
1	B	144	ASP	4.8
1	B	148	LEU	4.7
1	B	110	THR	4.6
1	A	177	VAL	4.3
1	B	160	THR	4.3
1	B	180	PRO	4.2
1	A	481	ALA	3.8
1	B	449	HIS	3.8
1	B	397	VAL	3.8
1	A	158	GLU	3.7
1	A	489	ALA	3.7
1	A	150	LEU	3.6
1	B	91	THR	3.6
1	B	371	HIS	3.6
1	B	213	ILE	3.6
1	B	143	ILE	3.5
1	B	372	ILE	3.5
1	B	161	LEU	3.5
1	B	141	ILE	3.4
1	A	397	VAL	3.2
1	B	88	GLU	3.2
1	A	477	VAL	3.1
1	A	97	GLY	3.1
1	B	478	VAL	3.1
1	A	478	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	89	ILE	3.1
1	B	178	ASN	3.1
1	B	177	VAL	3.0
1	A	143	ILE	2.9
1	A	103	ARG	2.9
1	B	421	VAL	2.9
1	A	126	ILE	2.9
1	B	228	PRO	2.9
1	A	398	VAL	2.8
1	B	479	ILE	2.8
1	B	217	GLU	2.8
1	B	135	VAL	2.8
1	A	163	CYS	2.8
1	A	54	HIS	2.8
1	A	418	ILE	2.7
1	A	124	PHE	2.7
1	A	479	ILE	2.7
1	A	304	TYR	2.7
1	A	161	LEU	2.6
1	B	446	LYS	2.6
1	B	187	PRO	2.6
1	B	15	VAL	2.6
1	B	132	SER	2.6
1	B	231	ARG	2.5
1	B	210	ALA	2.4
1	A	372	ILE	2.4
1	B	445	ASP	2.4
1	B	466	SER	2.4
1	A	89	ILE	2.4
1	B	130	ASN	2.4
1	B	185	ASP	2.4
1	A	107	CYS	2.3
1	A	419	VAL	2.3
1	B	419	VAL	2.3
1	A	208	ILE	2.3
1	A	142	TYR	2.3
1	A	159	GLN	2.3
1	B	239	ILE	2.3
1	A	98	ASP	2.3
1	A	48	ALA	2.3
1	A	471	GLN	2.2
1	B	212	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	95	VAL	2.2
1	A	136	ARG	2.2
1	B	398	VAL	2.2
1	B	477	VAL	2.2
1	A	53	SER	2.2
1	B	420	CYS	2.1
1	A	138	GLY	2.1
1	A	94	PHE	2.1
1	B	219	VAL	2.1
1	A	37	LEU	2.1
1	A	277	ALA	2.1
1	A	245	VAL	2.1
1	A	140	TYR	2.1
1	A	169	HIS	2.1
1	A	420	CYS	2.0
1	B	184	VAL	2.0
1	A	133	LYS	2.0
1	B	236	ILE	2.0
1	A	47	VAL	2.0
1	A	165	VAL	2.0
1	A	307	ARG	2.0
1	B	40	LEU	2.0
1	A	14	PRO	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, 95th 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(\AA^2)	Q<0.9
3	PTK	A	501	32/32	0.27	4.88	100,100,101,101	32
2	GOL	A	502	6/6	0.23	2.97	36,41,42,43	0
2	GOL	A	500	6/6	0.25	1.91	63,63,63,63	0
2	GOL	B	499	6/6	0.21	1.33	67,68,68,68	0
2	GOL	A	503	6/6	0.21	1.13	59,61,62,62	0
2	GOL	A	499	6/6	0.32	0.89	41,44,45,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.