



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:39 AM GMT

PDB ID : 3KTX
Title : Crystal structure of Leishmania mexicana pyruvate kinase (LmPYK) in complex with 1,3,6,8-pyrenetetrasulfonic acid
Authors : Morgan, H.P.; Walkinshaw, M.D.
Deposited on : 2009-11-26
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>

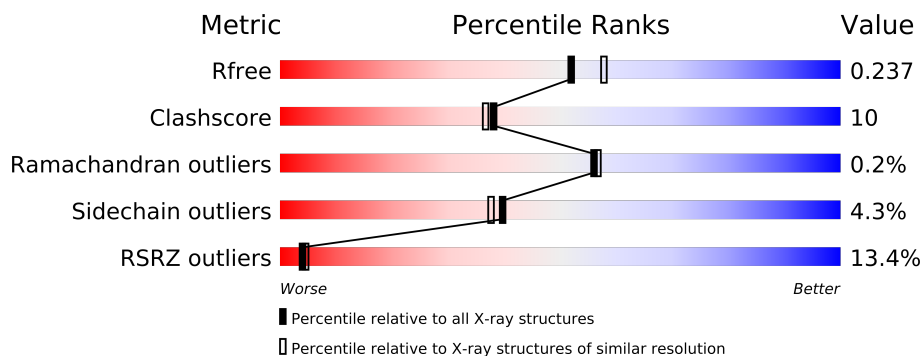
The following versions of software and data (see [references](#)) were used in the production of this report:

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	500	-	X
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 8214 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:

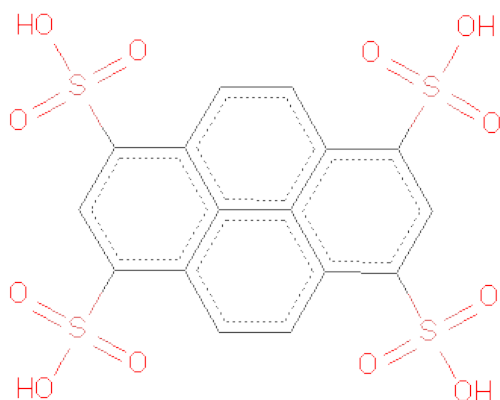
Chain	Residue	Modelled	Actual	Comment	Reference
A	382	SER	GLY	CONFLICT	UNP Q27686
A	389	TYR	SER	CONFLICT	UNP Q27686
A	404	ARG	ALA	CONFLICT	UNP Q27686
A	405	SER	GLY	CONFLICT	UNP Q27686
B	382	SER	GLY	CONFLICT	UNP Q27686
B	389	TYR	SER	CONFLICT	UNP Q27686
B	404	ARG	ALA	CONFLICT	UNP Q27686
B	405	SER	GLY	CONFLICT	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	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.

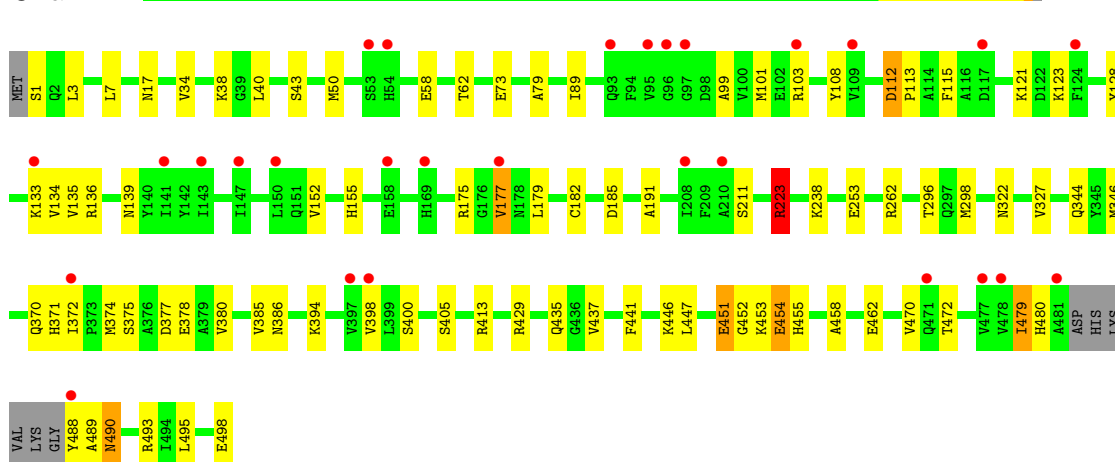
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	344	Total	O	0	0
			344	344		
4	B	296	Total	O	0	0
			296	296		

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.

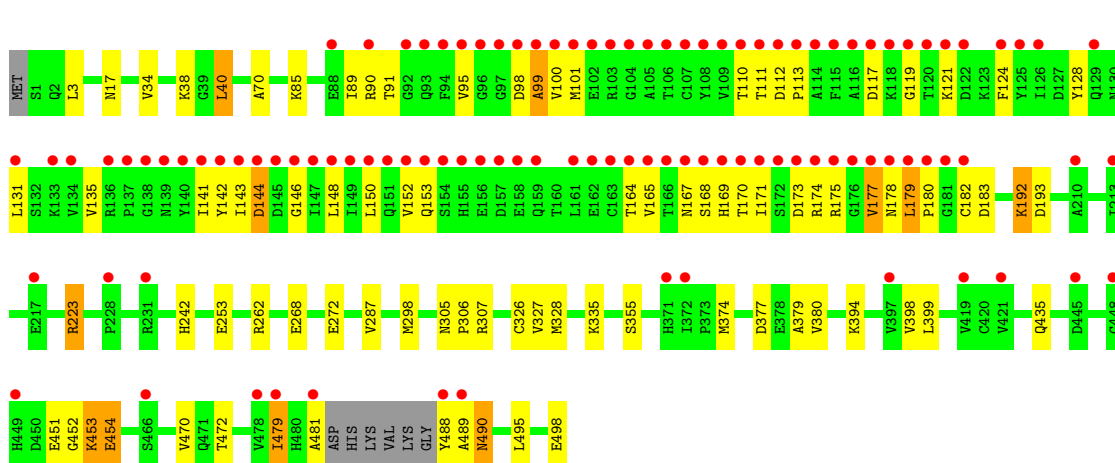
• Molecule 1: Pyruvate kinase

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, 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)	100.0 (20.69-2.10) 100.0 (20.69-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.186 , 0.239 0.186 , 0.237	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 , 53.1	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	0.95	EDS
Total number of atoms	8214	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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	1.13	7/3808 (0.2%)	0.92	5/5154 (0.1%)
1	B	1.05	4/3808 (0.1%)	0.93	5/5154 (0.1%)
All	All	1.09	11/7616 (0.1%)	0.93	10/10308 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	GLU	CG-CD	6.53	1.61	1.51
1	A	458	ALA	CA-CB	6.21	1.65	1.52
1	A	191	ALA	CA-CB	6.09	1.65	1.52
1	A	437	VAL	CB-CG2	5.83	1.65	1.52
1	A	441	PHE	CE2-CZ	5.68	1.48	1.37
1	B	326	CYS	CB-SG	-5.66	1.72	1.81
1	B	192	LYS	CE-NZ	5.64	1.63	1.49
1	A	58	GLU	CG-CD	5.61	1.60	1.51
1	B	355	SER	CB-OG	5.59	1.49	1.42
1	A	385	VAL	CB-CG2	5.21	1.63	1.52
1	B	272	GLU	CG-CD	5.06	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ALA	CB-CA-C	21.84	142.85	110.10
1	B	99	ALA	N-CA-C	-7.84	89.83	111.00
1	A	223	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	112	ASP	CB-CG-OD1	6.26	123.94	118.30
1	B	495	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	193	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	50	MET	CG-SD-CE	5.28	108.64	100.20
1	A	413	ARG	NE-CZ-NH2	-5.12	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	40	LEU	CB-CG-CD1	5.01	119.51	111.00

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	67	0
1	B	3753	0	3752	72	0
2	A	30	0	40	2	0
2	B	6	0	8	3	0
3	A	32	0	10	10	0
4	A	344	0	0	12	0
4	B	296	0	0	6	0
All	All	8214	0	7562	150	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 10.

All (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:501:PTK:OAB	3:A:501:PTK:HAO	1.39	1.19
3:A:501:PTK:OAJ	3:A:501:PTK:HAQ	1.44	1.15
3:A:501:PTK:HAP	3:A:501:PTK:OAK	1.43	1.09
3:A:501:PTK:HAR	3:A:501:PTK:OAG	1.43	1.06
1:A:223:ARG:HD2	4:A:553:HOH:O	1.58	1.01
1:B:142:TYR:CE1	1:B:180:PRO:HG2	2.01	0.95
1:A:99:ALA:HB1	1:A:101:MET:CE	1.96	0.94
1:B:253:GLU:HG3	4:B:591:HOH:O	1.68	0.92
1:A:377:ASP:HB3	1:A:488:TYR:CD2	2.07	0.90
1:A:298:MET:CE	1:A:327:VAL:HB	2.07	0.84
1:A:455:HIS:HD2	4:A:559:HOH:O	1.61	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:ALA:HB1	1:A:101:MET:HE2	1.60	0.82
1:B:143:ILE:O	1:B:144:ASP:HB2	1.80	0.82
3:A:501:PTK:CAP	3:A:501:PTK:OAK	2.29	0.80
1:A:375:SER:OG	1:A:377:ASP:OD2	2.01	0.79
1:A:135:VAL:HG11	1:A:152:VAL:HG21	1.64	0.77
1:B:143:ILE:O	1:B:144:ASP:CB	2.32	0.77
1:A:298:MET:HE1	1:A:327:VAL:HB	1.68	0.76
3:A:501:PTK:CAO	3:A:501:PTK:OAB	2.26	0.76
1:A:99:ALA:CB	1:A:101:MET:CE	2.63	0.75
1:B:298:MET:HE3	1:B:327:VAL:HB	1.69	0.74
1:B:169:HIS:HD2	1:B:171:ILE:HG23	1.51	0.74
1:A:446:LYS:HE2	4:A:713:HOH:O	1.86	0.74
1:A:446:LYS:HE3	4:A:813:HOH:O	1.88	0.74
2:B:499:GOL:O3	4:B:743:HOH:O	1.78	0.74
1:A:398:VAL:HG13	1:A:479:ILE:HD13	1.68	0.74
1:A:472:THR:HG23	1:A:498:GLU:OXT	1.89	0.73
1:B:169:HIS:CD2	1:B:171:ILE:HG23	2.23	0.73
3:A:501:PTK:CAQ	3:A:501:PTK:OAJ	2.30	0.73
1:A:136:ARG:H	1:A:139:ASN:ND2	1.87	0.72
1:A:374:MET:HE1	1:A:378:GLU:HG3	1.73	0.71
1:B:121:LYS:HE3	4:B:715:HOH:O	1.92	0.70
1:B:135:VAL:HG11	1:B:152:VAL:HG21	1.74	0.70
2:B:499:GOL:C3	4:B:743:HOH:O	2.36	0.70
1:A:253:GLU:HG3	4:A:761:HOH:O	1.91	0.70
1:B:100:VAL:HG22	1:B:170:THR:HG23	1.74	0.70
1:A:298:MET:HE2	1:A:327:VAL:HB	1.74	0.69
1:B:142:TYR:CD1	1:B:180:PRO:HG2	2.27	0.69
1:A:377:ASP:HB3	1:A:488:TYR:CE2	2.29	0.68
1:B:479:ILE:HD11	1:B:489:ALA:HB1	1.76	0.66
1:A:155:HIS:HD2	4:A:811:HOH:O	1.78	0.65
1:A:490:ASN:H	1:A:490:ASN:HD22	1.43	0.65
1:B:394:LYS:HB2	1:B:470:VAL:HG12	1.79	0.65
1:A:1:SER:N	4:A:695:HOH:O	2.30	0.64
1:B:99:ALA:HB1	1:B:121:LYS:HB3	1.79	0.64
1:A:380:VAL:HG21	1:A:490:ASN:HA	1.80	0.63
1:A:101:MET:CE	1:A:121:LYS:HA	2.28	0.63
1:B:142:TYR:HB3	1:B:146:GLY:HA2	1.79	0.63
3:A:501:PTK:HOAK	3:A:501:PTK:HAP	1.61	0.62
1:B:90:ARG:HE	1:B:174:ARG:HB3	1.64	0.62
1:B:298:MET:HE3	1:B:327:VAL:CB	2.30	0.61
1:B:85:LYS:HD3	1:B:192:LYS:HD3	1.83	0.60
3:A:501:PTK:CAR	3:A:501:PTK:OAG	2.30	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:298:MET:HE1	1:A:327:VAL:CG1	2.32	0.59
1:B:298:MET:CE	1:B:327:VAL:HB	2.30	0.59
1:B:89:ILE:HB	1:B:177:VAL:HG22	1.84	0.59
1:A:298:MET:HE1	1:A:327:VAL:CB	2.33	0.58
1:B:178:ASN:O	1:B:180:PRO:HD3	2.03	0.58
1:A:479:ILE:HG12	1:A:480:HIS:N	2.18	0.58
1:B:153:GLN:NE2	1:B:164:THR:OG1	2.37	0.57
1:B:95:VAL:HG23	1:B:119:GLY:O	2.04	0.57
1:B:141:ILE:CG2	1:B:143:ILE:HD11	2.35	0.57
1:B:148:LEU:HB2	1:B:169:HIS:CD2	2.39	0.57
1:A:462:GLU:OE1	4:A:576:HOH:O	2.18	0.57
1:B:142:TYR:HB2	1:B:178:ASN:HB2	1.87	0.56
1:A:298:MET:HE3	1:A:346:MET:HE2	1.86	0.56
1:A:298:MET:HE3	1:A:346:MET:CE	2.36	0.56
1:B:380:VAL:HG21	1:B:490:ASN:HA	1.88	0.56
1:B:180:PRO:HB3	1:B:268:GLU:HB2	1.88	0.56
1:B:298:MET:HE3	1:B:327:VAL:CG1	2.37	0.55
1:B:479:ILE:HD11	1:B:489:ALA:CB	2.35	0.55
1:A:134:VAL:HG13	1:A:182:CYS:HB3	1.88	0.55
1:A:101:MET:HE1	1:A:121:LYS:HA	1.88	0.55
1:A:322:ASN:HA	2:A:502:GOL:H11	1.88	0.54
1:A:99:ALA:CB	1:A:101:MET:HE3	2.37	0.54
1:B:298:MET:CE	1:B:327:VAL:HG12	2.38	0.54
1:B:298:MET:CE	1:B:327:VAL:CB	2.85	0.54
1:B:180:PRO:HB3	1:B:268:GLU:CB	2.37	0.54
3:A:501:PTK:HOAB	3:A:501:PTK:HAO	1.64	0.53
1:B:131:LEU:HD11	1:B:141:ILE:HD11	1.89	0.53
1:B:223:ARG:HD2	4:B:637:HOH:O	2.10	0.53
1:A:136:ARG:H	1:A:139:ASN:HD22	1.57	0.52
1:A:135:VAL:HG13	1:A:139:ASN:HB2	1.91	0.51
1:B:89:ILE:HG23	1:B:128:TYR:HB2	1.93	0.51
1:A:3:LEU:HD23	1:A:3:LEU:C	2.31	0.51
1:A:103:ARG:HB2	1:A:103:ARG:HH21	1.75	0.51
1:B:298:MET:HE1	1:B:327:VAL:HG12	1.93	0.51
1:A:89:ILE:CG2	1:A:177:VAL:HG22	2.41	0.50
1:B:307:ARG:HG2	4:B:783:HOH:O	2.12	0.50
1:B:141:ILE:HG21	1:B:143:ILE:HD11	1.93	0.50
1:A:455:HIS:CD2	4:A:559:HOH:O	2.48	0.50
1:B:490:ASN:H	1:B:490:ASN:HD22	1.60	0.49
1:B:179:LEU:HB3	1:B:182:CYS:HB2	1.93	0.49
1:B:110:THR:HG22	1:B:124:PHE:O	2.12	0.49
1:B:472:THR:HG23	1:B:498:GLU:OXT	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:488:TYR:HA	2:A:499:GOL:H31	1.94	0.49
1:A:43:SER:HB3	1:A:344:GLN:HG3	1.94	0.49
1:A:374:MET:CE	1:A:378:GLU:HG3	2.42	0.48
1:B:3:LEU:HD23	1:B:3:LEU:C	2.33	0.48
1:B:452:GLY:HA3	1:B:454:GLU:OE2	2.14	0.48
1:A:115:PHE:CZ	1:A:123:LYS:HE2	2.48	0.47
1:B:335:LYS:HE3	2:B:499:GOL:H12	1.95	0.47
1:A:451:GLU:H	1:A:451:GLU:CD	2.18	0.47
1:A:211:SER:HA	1:A:238:LYS:HD3	1.95	0.47
1:B:98:ASP:O	1:B:99:ALA:HB2	2.15	0.47
1:B:91:THR:O	1:B:174:ARG:HA	2.15	0.47
1:B:179:LEU:O	1:B:182:CYS:HB2	2.14	0.47
1:A:108:TYR:O	1:A:123:LYS:HA	2.14	0.47
1:A:452:GLY:HA3	1:A:454:GLU:OE2	2.15	0.47
1:A:99:ALA:HB3	1:A:101:MET:HE3	1.96	0.46
1:A:446:LYS:HG2	1:A:447:LEU:HD23	1.98	0.46
1:A:490:ASN:N	1:A:490:ASN:HD22	2.10	0.46
1:A:38:LYS:NZ	1:A:73:GLU:OE1	2.36	0.46
1:B:101:MET:HB3	1:B:165:VAL:HG11	1.98	0.46
1:A:493:ARG:NH2	4:A:788:HOH:O	2.48	0.46
1:A:479:ILE:HD11	1:A:489:ALA:HB1	1.98	0.45
1:B:399:LEU:CD2	1:B:453:LYS:HG3	2.45	0.45
1:B:142:TYR:CD1	1:B:180:PRO:CG	2.99	0.45
1:A:128:TYR:OH	1:A:185:ASP:OD2	2.20	0.45
1:A:298:MET:CE	1:A:346:MET:CE	2.95	0.45
1:A:62:THR:HG23	4:A:827:HOH:O	2.17	0.45
1:A:370:GLN:HG3	1:A:374:MET:HE3	1.97	0.44
1:B:452:GLY:O	1:B:453:LYS:HB2	2.18	0.44
1:A:370:GLN:HG3	1:A:374:MET:CE	2.48	0.44
1:B:89:ILE:CG2	1:B:128:TYR:HB2	2.48	0.44
1:B:481:ALA:HB2	1:B:488:TYR:O	2.17	0.43
1:B:298:MET:CE	1:B:327:VAL:CG1	2.95	0.43
1:B:398:VAL:HG13	1:B:479:ILE:HD13	2.00	0.43
1:B:180:PRO:HA	1:B:268:GLU:OE2	2.18	0.43
1:A:298:MET:CE	1:A:346:MET:HE2	2.48	0.43
1:A:400:SER:HB2	1:A:405:SER:OG	2.19	0.43
1:B:183:ASP:OD1	1:B:242:HIS:HE1	2.02	0.42
1:B:135:VAL:CG1	1:B:152:VAL:HG21	2.46	0.42
1:A:79:ALA:HB2	1:A:429:ARG:O	2.19	0.42
1:B:148:LEU:HD13	1:B:169:HIS:HB3	2.02	0.42
1:A:7:LEU:HD11	1:B:287:VAL:HG21	2.00	0.42
1:B:451:GLU:H	1:B:451:GLU:CD	2.22	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:298:MET:HE2	1:B:328:MET:H	1.84	0.42
1:B:150:LEU:HD22	1:B:165:VAL:HG22	2.02	0.41
1:B:34:VAL:O	1:B:38:LYS:HG3	2.20	0.41
1:B:100:VAL:HG22	1:B:170:THR:CG2	2.46	0.41
1:A:452:GLY:C	1:A:454:GLU:OE2	2.58	0.41
1:B:490:ASN:N	1:B:490:ASN:HD22	2.19	0.41
1:B:38:LYS:HG2	1:B:70:ALA:HB1	2.01	0.41
1:B:305:ASN:HB3	1:B:306:PRO:HD2	2.02	0.41
1:A:386:ASN:HB3	4:A:596:HOH:O	2.19	0.41
1:A:394:LYS:HB2	1:A:470:VAL:HG12	2.01	0.41
1:B:374:MET:HE2	1:B:379:ALA:N	2.36	0.41
1:A:112:ASP:HA	1:A:113:PRO:HD3	1.71	0.40
1:B:377:ASP:HB3	1:B:488:TYR:CD2	2.56	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%)	477 (98%)	10 (2%)	1 (0%)	56	57
1	B	488/499 (98%)	462 (95%)	25 (5%)	1 (0%)	56	57
All	All	976/998 (98%)	939 (96%)	35 (4%)	2 (0%)	56	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	ASP
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%)	395 (96%)	16 (4%)	43	43
1	B	411/417 (99%)	392 (95%)	19 (5%)	37	34
All	All	822/834 (99%)	787 (96%)	35 (4%)	40	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	34	VAL
1	A	40	LEU
1	A	133	LYS
1	A	175	ARG
1	A	177	VAL
1	A	179	LEU
1	A	223	ARG
1	A	262	ARG
1	A	371	HIS
1	A	372	ILE
1	A	435	GLN
1	A	453	LYS
1	A	454	GLU
1	A	479	ILE
1	A	490	ASN
1	B	17	ASN
1	B	40	LEU
1	B	111	THR
1	B	112	ASP
1	B	113	PRO
1	B	117	ASP
1	B	167	ASN
1	B	168	SER
1	B	173	ASP
1	B	175	ARG
1	B	177	VAL
1	B	179	LEU
1	B	223	ARG
1	B	262	ARG
1	B	435	GLN
1	B	453	LYS
1	B	454	GLU

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Mol	Chain	Res	Type
1	B	479	ILE
1	B	490	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	435	GLN
1	A	471	GLN
1	A	490	ASN
1	B	17	ASN
1	B	69	GLN
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 ⓘ

7 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	0.77	0	5,5,5	1.39	1 (20%)
2	GOL	A	500	-	5,5,5	0.65	0	5,5,5	1.05	0
3	PTK	A	501	-	35,35,35	1.78	6 (17%)	60,60,60	2.54	27 (45%)
2	GOL	A	502	-	5,5,5	0.72	0	5,5,5	1.62	2 (40%)
2	GOL	A	503	-	5,5,5	0.40	0	5,5,5	0.75	0
2	GOL	A	504	-	5,5,5	0.30	0	5,5,5	0.43	0
2	GOL	B	499	-	5,5,5	0.57	0	5,5,5	0.77	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	A	504	-	-	0/4/4/4	0/0/0/0
2	GOL	B	499	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PTK	CAV-CAZ	-3.40	1.38	1.43
3	A	501	PTK	CAU-CAY	-3.33	1.38	1.43
3	A	501	PTK	CAS-CAW	-3.12	1.38	1.43
3	A	501	PTK	CAT-CAX	-3.01	1.38	1.43
3	A	501	PTK	CAM-CAT	2.30	1.40	1.37
3	A	501	PTK	CAM-CAS	2.27	1.40	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	PTK	CAM-CAS-SBC	6.47	124.69	117.67
3	A	501	PTK	CAM-CAT-SBD	5.76	123.93	117.67
3	A	501	PTK	CAN-CAU-SBE	5.05	123.16	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	PTK	CAN-CAV-SBF	4.80	122.89	117.67
3	A	501	PTK	CAW-CAS-SBC	-4.74	115.47	121.05
3	A	501	PTK	OAA-SBC-CAS	4.47	111.27	106.20
3	A	501	PTK	CAX-CAT-SBD	-4.17	116.14	121.05
3	A	501	PTK	OAD-SBD-CAT	4.13	110.88	106.20
3	A	501	PTK	CAZ-CAV-SBF	-3.69	116.70	121.05
3	A	501	PTK	CAO-CAW-CAS	-3.67	118.82	123.81
3	A	501	PTK	CAY-CAU-SBE	-3.65	116.74	121.05
3	A	501	PTK	CAP-CAY-CAU	-3.53	119.02	123.81
3	A	501	PTK	CAR-CAZ-CAV	-3.34	119.28	123.81
3	A	501	PTK	CAQ-CAX-CAT	-3.28	119.36	123.81
3	A	501	PTK	OAE-SBE-CAU	3.16	109.78	106.20
3	A	501	PTK	OAH-SBF-CAV	2.99	109.59	106.20
3	A	501	PTK	OAC-SBD-CAT	2.81	109.51	106.09
2	A	499	GOL	O2-C2-C1	2.78	120.90	108.22
3	A	501	PTK	CAS-CAW-CBA	2.61	120.25	118.03
3	A	501	PTK	OAF-SBE-CAU	2.58	109.12	106.20
3	A	501	PTK	OAI-SBC-CAS	2.57	109.11	106.20
3	A	501	PTK	OAG-SBF-CAV	2.38	108.89	106.20
3	A	501	PTK	CAT-CAX-CBA	2.37	120.05	118.03
3	A	501	PTK	CAU-CAY-CBB	2.35	120.03	118.03
2	A	502	GOL	O2-C2-C3	-2.27	97.86	108.22
2	A	502	GOL	O1-C1-C2	2.24	120.65	109.71
3	A	501	PTK	OAJ-SBD-CAT	2.13	108.62	106.20
3	A	501	PTK	OAL-SBF-CAV	2.13	108.68	106.09
3	A	501	PTK	CAV-CAZ-CBB	2.07	119.79	118.03
3	A	501	PTK	OAK-SBE-CAU	2.06	108.60	106.09

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%)	0.14	28 (5%)	23 25	20, 34, 55, 70	0
1	B	492/499 (98%)	1.26	105 (21%)	1 1	22, 36, 124, 135	0
All	All	984/998 (98%)	0.70	133 (13%)	4 4	20, 35, 121, 135	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	SER	20.0
1	B	171	ILE	18.7
1	B	104	GLY	16.0
1	B	166	THR	15.0
1	B	95	VAL	13.5
1	B	94	PHE	13.1
1	B	108	TYR	12.6
1	B	103	ARG	12.0
1	B	140	TYR	11.1
1	B	165	VAL	11.1
1	B	115	PHE	10.8
1	B	170	THR	10.8
1	B	149	ILE	9.6
1	B	105	ALA	9.6
1	B	145	ASP	9.4
1	B	142	TYR	9.3
1	B	155	HIS	9.0
1	B	106	THR	9.0
1	B	116	ALA	8.9
1	B	167	ASN	8.8
1	B	113	PRO	8.7
1	B	147	ILE	8.6
1	B	146	GLY	8.5
1	B	150	LEU	8.4

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Mol	Chain	Res	Type	RSRZ
1	B	154	SER	8.4
1	B	169	HIS	7.9
1	B	136	ARG	7.7
1	B	159	GLN	7.6
1	B	99	ALA	7.6
1	B	109	VAL	7.3
1	B	96	GLY	7.2
1	B	168	SER	7.0
1	B	93	GLN	6.8
1	B	117	ASP	6.8
1	B	138	GLY	6.7
1	A	488	TYR	6.7
1	B	122	ASP	6.6
1	B	137	PRO	6.6
1	B	101	MET	6.5
1	B	139	ASN	6.5
1	B	97	GLY	6.4
1	B	156	GLU	6.3
1	B	153	GLN	6.3
1	B	181	GLY	6.2
1	B	114	ALA	6.2
1	B	161	LEU	6.0
1	B	488	TYR	6.0
1	B	143	ILE	6.0
1	B	125	TYR	5.9
1	B	118	LYS	5.8
1	B	148	LEU	5.8
1	B	158	GLU	5.7
1	B	141	ILE	5.7
1	B	98	ASP	5.6
1	B	112	ASP	5.6
1	B	164	THR	5.4
1	B	126	ILE	5.2
1	B	107	CYS	5.1
1	B	489	ALA	5.1
1	B	157	ASP	5.1
1	B	100	VAL	5.1
1	B	124	PHE	4.8
1	B	152	VAL	4.8
1	B	481	ALA	4.7
1	B	129	GLN	4.6
1	A	109	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	175	ARG	4.4
1	B	133	LYS	4.4
1	B	182	CYS	4.3
1	B	92	GLY	4.3
1	B	102	GLU	4.2
1	B	121	LYS	4.2
1	B	162	GLU	4.2
1	B	173	ASP	4.0
1	B	163	CYS	4.0
1	B	151	GLN	3.9
1	B	119	GLY	3.8
1	B	110	THR	3.7
1	B	180	PRO	3.7
1	B	179	LEU	3.6
1	B	397	VAL	3.5
1	B	176	GLY	3.5
1	A	141	ILE	3.3
1	B	131	LEU	3.3
1	B	371	HIS	3.2
1	B	449	HIS	3.2
1	B	144	ASP	3.1
1	A	397	VAL	3.1
1	A	103	ARG	3.1
1	B	228	PRO	3.0
1	B	90	ARG	3.0
1	A	150	LEU	2.9
1	B	120	THR	2.8
1	A	481	ALA	2.8
1	B	213	ILE	2.8
1	B	111	THR	2.7
1	B	134	VAL	2.7
1	B	448	GLY	2.6
1	B	372	ILE	2.6
1	A	54	HIS	2.6
1	B	421	VAL	2.5
1	A	133	LYS	2.5
1	A	93	GLN	2.5
1	A	477	VAL	2.5
1	B	88	GLU	2.5
1	A	158	GLU	2.4
1	B	466	SER	2.4
1	A	124	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	96	GLY	2.4
1	A	177	VAL	2.4
1	B	210	ALA	2.4
1	A	97	GLY	2.4
1	B	177	VAL	2.3
1	B	445	ASP	2.3
1	A	95	VAL	2.3
1	A	478	VAL	2.2
1	B	231	ARG	2.2
1	A	208	ILE	2.2
1	B	178	ASN	2.2
1	A	398	VAL	2.2
1	B	478	VAL	2.2
1	B	217	GLU	2.2
1	A	147	ILE	2.2
1	A	143	ILE	2.1
1	B	174	ARG	2.1
1	A	471	GLN	2.1
1	A	53	SER	2.1
1	A	372	ILE	2.1
1	A	210	ALA	2.1
1	B	419	VAL	2.1
1	A	117	ASP	2.1
1	A	169	HIS	2.0
1	B	479	ILE	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	0.25	3.45	96,98,100,100	32
2	GOL	A	500	6/6	0.25	2.80	53,61,62,62	0
2	GOL	A	502	6/6	0.19	2.59	28,46,48,51	0
2	GOL	A	504	6/6	0.23	1.26	67,69,71,71	0
2	GOL	B	499	6/6	0.18	1.19	48,59,63,65	0
2	GOL	A	503	6/6	0.17	0.69	51,63,65,66	0
2	GOL	A	499	6/6	0.22	0.36	33,48,49,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.