



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:11 AM GMT

PDB ID : 3HQN
Title : Apo crystal structure of Leishmania mexicana(LmPYK)pyruvatekinase
Authors : Morgan, H.P.; Walkinshaw, M.D.
Deposited on : 2009-06-08
Resolution : 2.00 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>

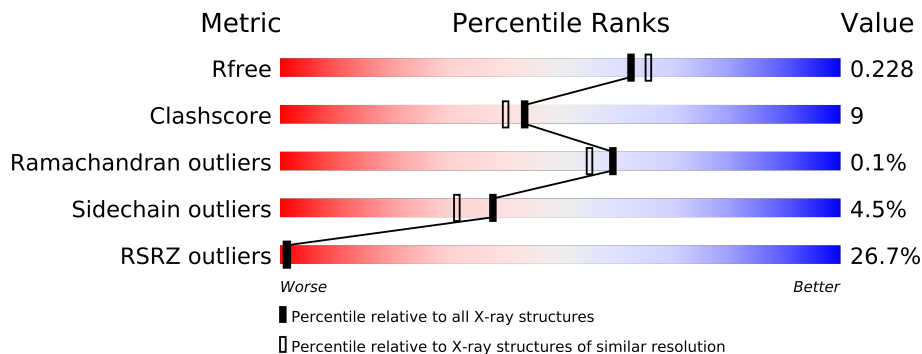
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	D	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	499	-	X
2	GOL	D	499	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8323 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	D	493	Total	C	N	O	S	0	1	0
			3767	2345	666	730	26			
1	A	492	Total	C	N	O	S	154	5	0
			3790	2362	669	733	26			

There are 8 discrepancies between the modelled and reference sequences:

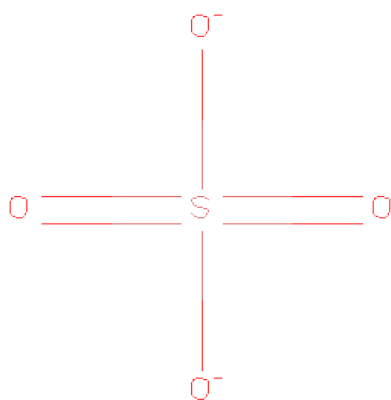
Chain	Residue	Modelled	Actual	Comment	Reference
D	382	SER	GLY	SEE REMARK 999	UNP Q27686
D	389	TYR	SER	SEE REMARK 999	UNP Q27686
D	404	ARG	ALA	SEE REMARK 999	UNP Q27686
D	405	SER	GLY	SEE REMARK 999	UNP Q27686
A	382	SER	GLY	SEE REMARK 999	UNP Q27686
A	389	TYR	SER	SEE REMARK 999	UNP Q27686
A	404	ARG	ALA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

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



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

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

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

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

- Molecule 5 is water.

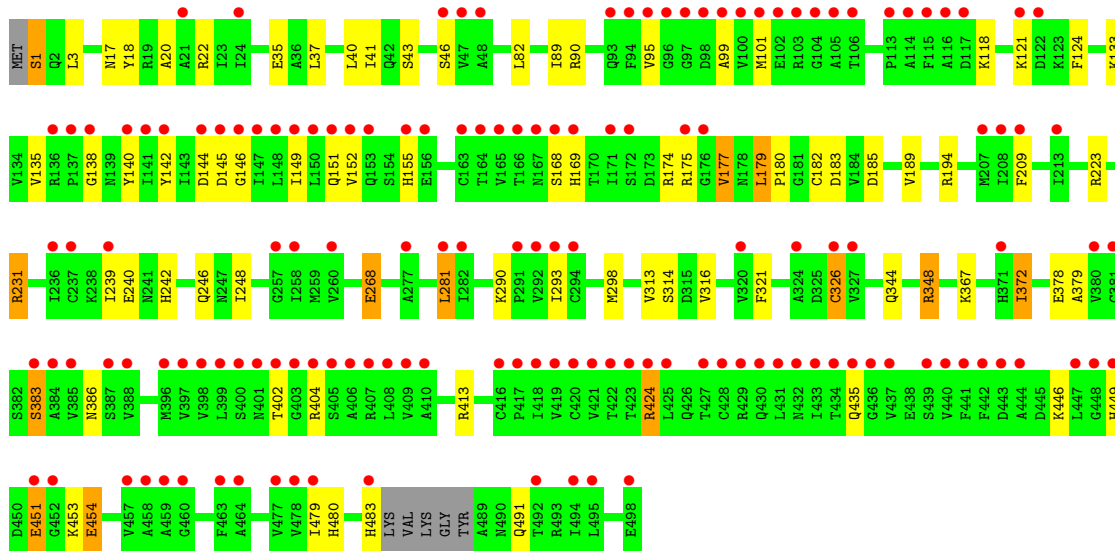
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	394	Total	O	0	0
			394	394		
5	A	340	Total	O	0	0
			340	340		

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.

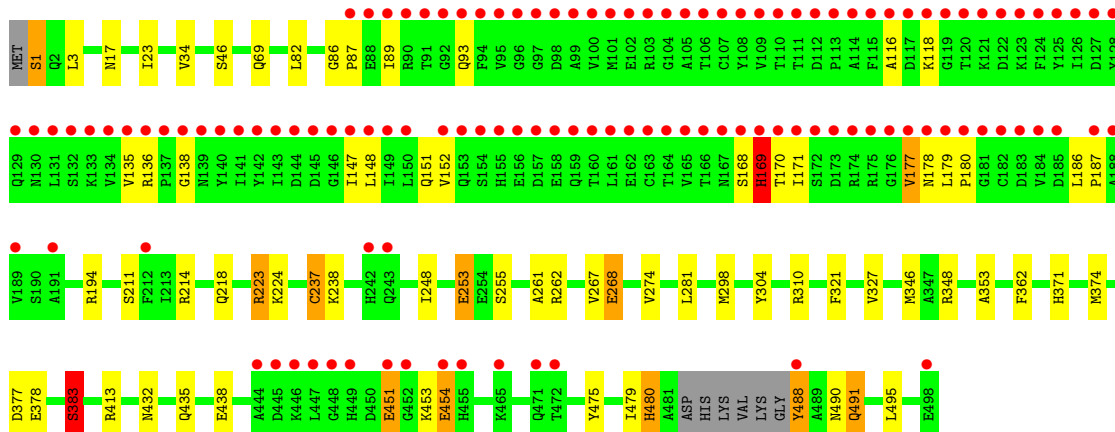
• Molecule 1: Pyruvate kinase

Chain D: 



• Molecule 1: Pyruvate kinase

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.58Å 167.33Å 132.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.32 – 2.00 39.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.32-2.00) 99.7 (39.32-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.169 , 0.209 0.185 , 0.228	Depositor DCC
R_{free} test set	4504 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 89897 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8323	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, K, SO4

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	1.23	10/3856 (0.3%)	0.99	8/5218 (0.2%)
1	D	1.30	14/3825 (0.4%)	1.03	11/5176 (0.2%)
All	All	1.26	24/7681 (0.3%)	1.01	19/10394 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	SER	N-CA	8.73	1.63	1.46
1	A	86	GLY	C-N	7.73	1.49	1.34
1	A	1	SER	N-CA	7.69	1.61	1.46
1	D	378	GLU	CB-CG	-6.70	1.39	1.52
1	D	18	TYR	CE1-CZ	6.25	1.46	1.38
1	A	383	SER	CB-OG	-6.04	1.34	1.42
1	A	304	TYR	CG-CD1	5.95	1.46	1.39
1	D	321	PHE	CD1-CE1	5.93	1.51	1.39
1	A	475	TYR	CD1-CE1	5.67	1.47	1.39
1	D	46	SER	CA-CB	5.64	1.61	1.52
1	D	20	ALA	CA-CB	5.64	1.64	1.52
1	D	35	GLU	CG-CD	5.55	1.60	1.51
1	D	326	CYS	CB-SG	-5.55	1.72	1.81
1	D	209	PHE	CE2-CZ	5.54	1.47	1.37
1	D	290	LYS	CB-CG	5.51	1.67	1.52
1	A	274	VAL	CB-CG1	5.42	1.64	1.52
1	A	321	PHE	CD1-CE1	5.40	1.50	1.39
1	A	261	ALA	CA-CB	5.35	1.63	1.52
1	D	268	GLU	CG-CD	5.33	1.59	1.51
1	A	353	ALA	CA-CB	5.28	1.63	1.52
1	A	362	PHE	CE2-CZ	5.16	1.47	1.37
1	D	451	GLU	CB-CG	5.14	1.61	1.52
1	D	313	VAL	CB-CG2	5.07	1.63	1.52
1	D	451	GLU	CG-CD	5.06	1.59	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	348	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	D	223[A]	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	D	223[B]	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	D	281	LEU	CB-CG-CD2	7.79	124.23	111.00
1	A	169	HIS	CB-CA-C	7.58	125.57	110.40
1	D	413	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	348	ARG	NE-CZ-NH2	6.95	123.77	120.30
1	A	34	VAL	CG1-CB-CG2	6.78	121.74	110.90
1	D	185	ASP	CB-CG-OD2	6.26	123.93	118.30
1	D	194	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	372	ILE	CG1-CB-CG2	-5.80	98.64	111.40
1	D	223[A]	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	D	223[B]	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	495	LEU	CA-CB-CG	5.55	128.08	115.30
1	A	237	CYS	CA-CB-SG	-5.46	104.17	114.00
1	D	367	LYS	CD-CE-NZ	5.21	123.69	111.70
1	A	310	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	413	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	194	ARG	NE-CZ-NH2	5.03	122.81	120.30

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	3790	0	3787	72	1
1	D	3767	0	3766	55	3
2	A	6	0	8	1	0
2	D	12	0	16	2	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
5	A	340	0	0	12	2
5	D	394	0	0	20	0
All	All	8323	0	7577	128	3

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 9.

All (128) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:149:ILE:HG23	5:D:784:HOH:O	1.33	1.22
1:A:383:SER:HB3	5:A:811:HOH:O	0.98	1.14
1:D:424:ARG:HH11	1:D:424:ARG:HB3	1.08	1.11
1:A:116:ALA:O	5:A:693:HOH:O	1.78	1.02
1:D:298:MET:HE3	1:D:316:VAL:HG22	1.48	0.94
1:D:140:TYR:HB3	5:D:784:HOH:O	1.67	0.93
1:D:298:MET:CE	1:D:316:VAL:HG22	2.00	0.92
1:D:424:ARG:HH11	1:D:424:ARG:CB	1.83	0.91
1:A:186:LEU:HB3	1:A:187:PRO:HD2	1.58	0.85
1:D:180:PRO:HD3	5:D:762:HOH:O	1.79	0.81
1:A:488:TYR:CD2	1:A:488:TYR:O	2.32	0.81
1:A:1:SER:HA	5:A:600:HOH:O	1.79	0.80
1:D:424:ARG:HB3	1:D:424:ARG:NH1	1.92	0.79
1:D:142:TYR:HB3	1:D:146:GLY:HA2	1.65	0.79
1:A:180:PRO:HB3	1:A:268:GLU:HB2	1.64	0.78
1:A:138:GLY:HA2	1:A:151:GLN:NE2	1.98	0.77
1:A:298:MET:HE2	1:A:327:VAL:HB	1.69	0.75
1:A:180:PRO:HB3	1:A:268:GLU:CB	2.18	0.73
1:D:179:LEU:HB3	1:D:182:CYS:HB2	1.70	0.73
1:A:377:ASP:HA	1:A:488:TYR:OH	1.89	0.73
1:A:116:ALA:HB1	5:A:693:HOH:O	1.90	0.71
1:D:1:SER:HA	5:D:580:HOH:O	1.89	0.71
1:D:231:ARG:HG2	1:D:231:ARG:HH11	1.57	0.70
1:A:136:ARG:HB3	1:A:136:ARG:HH11	1.54	0.70
1:D:135:VAL:HG11	1:D:152:VAL:HG21	1.74	0.69
1:D:348:ARG:NH2	5:D:868:HOH:O	2.22	0.69
1:A:138:GLY:HA2	1:A:151:GLN:HE21	1.59	0.67
1:A:374:MET:CE	1:A:378:GLU:HG3	2.24	0.67
1:D:246:GLN:HG2	5:A:745:HOH:O	1.95	0.67
1:A:23:ILE:HG23	1:A:346:MET:CE	2.25	0.67
1:D:99:ALA:HB1	5:D:808:HOH:O	1.94	0.67
1:A:136:ARG:NH1	1:A:136:ARG:CB	2.58	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:169:HIS:ND1	1:A:170:THR:O	2.30	0.65
1:D:155:HIS:HD2	5:D:772:HOH:O	1.80	0.65
1:A:180:PRO:HA	1:A:268:GLU:OE1	1.96	0.65
1:A:248:ILE:HG12	1:A:281:LEU:HD22	1.77	0.65
1:A:168:SER:O	1:A:169:HIS:HB2	1.96	0.65
1:A:147:ILE:CG2	1:A:169:HIS:CD2	2.81	0.64
1:A:136:ARG:NH1	1:A:136:ARG:HB2	2.14	0.63
1:D:231:ARG:HG2	1:D:231:ARG:NH1	2.13	0.63
1:A:136:ARG:HH11	1:A:136:ARG:CB	2.10	0.63
1:D:3:LEU:HD23	1:D:3:LEU:C	2.18	0.63
1:A:490:ASN:O	1:A:491:GLN:HB2	2.00	0.61
1:D:451:GLU:H	1:D:451:GLU:CD	2.04	0.60
1:A:186:LEU:HB3	1:A:187:PRO:CD	2.31	0.60
2:D:499:GOL:H31	5:D:873:HOH:O	2.01	0.60
1:D:99:ALA:CB	5:D:808:HOH:O	2.49	0.60
1:A:186:LEU:CB	1:A:187:PRO:HD2	2.32	0.59
1:D:449:HIS:HB3	5:D:688:HOH:O	2.02	0.59
1:A:147:ILE:HG22	1:A:169:HIS:HD2	1.68	0.59
1:A:374:MET:HE2	1:A:378:GLU:HB3	1.84	0.58
1:D:231:ARG:HD3	5:D:741:HOH:O	2.04	0.58
1:A:253:GLU:HB2	5:A:783:HOH:O	2.04	0.57
1:A:147:ILE:HG22	1:A:169:HIS:CD2	2.40	0.57
1:D:483:HIS:HB3	5:D:724:HOH:O	2.05	0.56
1:D:133:LYS:HD2	5:D:754:HOH:O	2.07	0.55
1:A:147:ILE:CG2	1:A:169:HIS:HD2	2.19	0.54
1:A:480[A]:HIS:O	1:A:490:ASN:HA	2.08	0.54
1:D:43:SER:HB3	1:D:344:GLN:HG3	1.90	0.53
1:A:298:MET:CE	1:A:327:VAL:HB	2.37	0.53
1:D:180:PRO:HB3	1:D:268:GLU:HB3	1.89	0.53
1:D:454:GLU:HG3	5:D:848:HOH:O	2.07	0.53
1:A:135:VAL:HG11	1:A:152:VAL:HG21	1.91	0.52
1:A:377:ASP:CA	1:A:488:TYR:OH	2.56	0.52
1:D:89:ILE:CG2	1:D:177:VAL:HG22	2.39	0.51
1:A:374:MET:CE	1:A:378:GLU:CG	2.88	0.50
1:D:189:VAL:O	1:D:189:VAL:HG23	2.10	0.50
1:A:223:ARG:HD2	5:A:809:HOH:O	2.10	0.50
1:A:168:SER:O	1:A:169:HIS:CB	2.59	0.50
1:A:253:GLU:CB	5:A:783:HOH:O	2.60	0.50
1:A:46:SER:HB3	1:A:432:ASN:HB3	1.94	0.49
1:D:424:ARG:HH11	1:D:424:ARG:CG	2.26	0.49
1:A:147:ILE:HG21	1:A:169:HIS:CD2	2.48	0.49
1:D:90:ARG:HD3	1:D:174:ARG:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:402:THR:HG21	1:D:483:HIS:HE1	1.79	0.48
1:A:377:ASP:HB3	1:A:488:TYR:CZ	2.49	0.48
1:D:89:ILE:HG21	1:D:177:VAL:HG22	1.96	0.48
1:A:23:ILE:HG12	1:A:346:MET:HE3	1.96	0.48
1:D:144:ASP:O	1:D:145:ASP:HB2	2.13	0.47
1:D:1:SER:CA	5:D:580:HOH:O	2.55	0.46
1:A:136:ARG:NH1	1:A:136:ARG:HB3	2.24	0.46
1:A:169:HIS:ND1	1:A:170:THR:N	2.64	0.46
1:A:454:GLU:HG3	1:A:454:GLU:H	1.50	0.46
1:A:3:LEU:HD23	1:A:3:LEU:C	2.36	0.46
1:D:168:SER:O	1:D:169:HIS:HB2	2.16	0.46
1:A:377:ASP:HB3	1:A:488:TYR:OH	2.16	0.45
1:A:138:GLY:CA	1:A:151:GLN:HE21	2.27	0.45
1:A:214:ARG:CZ	1:A:218:GLN:HE22	2.30	0.45
1:A:451:GLU:H	1:A:451:GLU:CD	2.20	0.45
1:A:488:TYR:CG	1:A:488:TYR:O	2.69	0.45
1:A:82:LEU:C	1:A:82:LEU:HD23	2.38	0.45
1:A:237:CYS:SG	1:A:255:SER:HB3	2.57	0.44
1:A:211:SER:HA	1:A:238:LYS:HD3	1.98	0.44
1:A:374:MET:HE2	1:A:378:GLU:CB	2.45	0.44
1:A:253:GLU:CG	5:A:783:HOH:O	2.66	0.44
1:A:480[A]:HIS:C	1:A:480[A]:HIS:CD2	2.90	0.44
1:D:121:LYS:HG2	5:D:795:HOH:O	2.18	0.44
1:A:89:ILE:CG2	1:A:177:VAL:HG22	2.48	0.43
1:A:135:VAL:HG12	1:A:136:ARG:N	2.34	0.43
1:A:87:PRO:HG3	1:A:187:PRO:O	2.18	0.43
1:D:386:ASN:ND2	5:D:588:HOH:O	2.52	0.43
1:A:298:MET:O	5:A:800:HOH:O	2.21	0.43
1:A:186:LEU:CD2	1:A:187:PRO:HD2	2.49	0.42
1:A:490:ASN:O	1:A:491:GLN:CB	2.61	0.42
1:D:82:LEU:C	1:D:82:LEU:HD23	2.40	0.42
1:A:180:PRO:CB	1:A:268:GLU:HB2	2.40	0.42
1:A:491:GLN:HE21	1:A:491:GLN:HB2	1.61	0.42
1:A:178:ASN:ND2	1:A:267:VAL:HG11	2.35	0.42
1:D:37:LEU:O	1:D:41:ILE:HG13	2.19	0.42
1:A:438:GLU:HB3	2:A:499:GOL:H2	2.02	0.41
1:D:298:MET:HE3	1:D:316:VAL:CG2	2.34	0.41
1:A:377:ASP:CB	1:A:488:TYR:OH	2.68	0.41
1:D:183:ASP:OD1	1:D:242:HIS:HE1	2.03	0.41
1:A:1:SER:CA	5:A:600:HOH:O	2.55	0.41
1:A:148:LEU:CD2	1:A:171:ILE:HD13	2.50	0.41
1:D:424:ARG:CG	1:D:424:ARG:NH1	2.83	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:116:ALA:CB	5:A:693:HOH:O	2.51	0.41
1:D:379:ALA:O	1:D:383:SER:HB3	2.21	0.41
1:D:293:ILE:HG12	1:D:326:CYS:HB2	2.02	0.41
1:D:101:MET:CE	1:D:124:PHE:CE1	3.04	0.41
1:D:138:GLY:HA2	1:D:151:GLN:HE21	1.85	0.41
1:D:404:ARG:NH1	5:D:780:HOH:O	2.53	0.40
1:D:449:HIS:CE1	5:D:529:HOH:O	2.74	0.40
1:D:248:ILE:HG12	1:D:281:LEU:HD22	2.03	0.40
1:D:240:GLU:OE2	2:D:499:GOL:H12	2.21	0.40
1:D:239:ILE:HG21	1:D:281:LEU:HD11	2.04	0.40
1:D:22:ARG:HH11	1:D:22:ARG:HD3	1.73	0.40
1:D:95:VAL:HA	5:D:709:HOH:O	2.21	0.40

All (3) 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)
1:D:446:LYS:NZ	1:A:69:GLN:OE1[7_545]	1.83	0.37
1:D:446:LYS:CE	5:A:825:HOH:O[7_545]	2.03	0.17
1:D:446:LYS:NZ	5:A:825:HOH:O[7_545]	2.15	0.05

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	493/499 (99%)	477 (97%)	15 (3%)	1 (0%)	56	51
1	D	490/499 (98%)	476 (97%)	14 (3%)	0	100	100
All	All	983/998 (98%)	953 (97%)	29 (3%)	1 (0%)	59	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	GLN

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	416/417 (100%)	394 (95%)	22 (5%)	32	24
1	D	413/417 (99%)	396 (96%)	17 (4%)	41	35
All	All	829/834 (99%)	790 (95%)	39 (5%)	38	29

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	17	ASN
1	D	40	LEU
1	D	118	LYS
1	D	175	ARG
1	D	177	VAL
1	D	179	LEU
1	D	231	ARG
1	D	314	SER
1	D	372	ILE
1	D	383	SER
1	D	424	ARG
1	D	435	GLN
1	D	453	LYS
1	D	454	GLU
1	D	479	ILE
1	D	480	HIS
1	D	491	GLN
1	A	17	ASN
1	A	93	GLN
1	A	118	LYS
1	A	169	HIS
1	A	177	VAL
1	A	179	LEU
1	A	223	ARG
1	A	224	LYS
1	A	253	GLU
1	A	262	ARG
1	A	268	GLU
1	A	371[A]	HIS

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Mol	Chain	Res	Type
1	A	371[B]	HIS
1	A	383	SER
1	A	435	GLN
1	A	451	GLU
1	A	453	LYS
1	A	454	GLU
1	A	479	ILE
1	A	480[A]	HIS
1	A	480[B]	HIS
1	A	488	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	17	ASN
1	D	139	ASN
1	D	151	GLN
1	D	155	HIS
1	D	178	ASN
1	D	242	HIS
1	D	386	ASN
1	D	435	GLN
1	D	449	HIS
1	D	455	HIS
1	A	17	ASN
1	A	151	GLN
1	A	178	ASN
1	A	305	ASN
1	A	435	GLN
1	A	491	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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	GOL	A	499	-	5,5,5	0.24	0	5,5,5	0.79	0
3	SO4	A	500	-	4,4,4	0.71	0	6,6,6	0.83	0
2	GOL	D	499	4	5,5,5	0.46	0	5,5,5	0.75	0
2	GOL	D	500	-	5,5,5	0.58	0	5,5,5	0.68	0
3	SO4	D	501	-	4,4,4	0.65	0	6,6,6	0.66	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
3	SO4	A	500	-	-	0/0/0/0	0/0/0/0
2	GOL	D	499	4	-	0/4/4/4	0/0/0/0
2	GOL	D	500	-	-	0/4/4/4	0/0/0/0
3	SO4	D	501	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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%)	1.69	120 (24%) ⓘ ⓘ	14, 25, 64, 76	101 (20%)
1	D	493/499 (98%)	1.47	145 (29%) ⓘ ⓘ	13, 23, 36, 46	0
All	All	985/998 (98%)	1.58	265 (26%) ⓘ ⓘ	13, 23, 57, 76	101 (10%)

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	ILE	23.7
1	A	166	THR	20.8
1	A	170	THR	19.7
1	A	134	VAL	19.4
1	A	181	GLY	18.5
1	A	100	VAL	16.9
1	A	135	VAL	16.4
1	A	147	ILE	16.2
1	A	140	TYR	15.8
1	A	149	ILE	15.3
1	A	136	ARG	13.8
1	A	95	VAL	12.4
1	A	152	VAL	11.9
1	A	109	VAL	11.5
1	A	104	GLY	11.4
1	A	124	PHE	11.4
1	A	89	ILE	11.4
1	A	138	GLY	10.9
1	A	165	VAL	10.7
1	A	103	ARG	10.2
1	A	178	ASN	10.2
1	A	133	LYS	10.2
1	A	105	ALA	10.1
1	A	164	THR	9.9

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Mol	Chain	Res	Type	RSRZ
1	A	169	HIS	9.6
1	A	101	MET	9.5
1	A	160	THR	9.5
1	A	142	TYR	8.9
1	A	130	ASN	8.8
1	A	125	TYR	8.7
1	A	102	GLU	8.6
1	A	139	ASN	8.3
1	A	107	CYS	8.1
1	D	147	ILE	8.0
1	A	113	PRO	7.8
1	D	149	ILE	7.8
1	A	126	ILE	7.7
1	A	179	LEU	7.4
1	A	99	ALA	7.4
1	A	168	SER	7.3
1	A	141	ILE	7.2
1	A	122	ASP	7.2
1	A	172	SER	7.0
1	A	177	VAL	6.8
1	A	173	ASP	6.8
1	A	143	ILE	6.6
1	A	182	CYS	6.6
1	A	162	GLU	6.5
1	A	91	THR	6.5
1	A	93	GLN	6.5
1	A	175	ARG	6.4
1	A	108	TYR	6.3
1	A	128	TYR	6.3
1	A	121	LYS	6.3
1	A	185	ASP	6.2
1	A	158	GLU	6.1
1	A	112	ASP	6.0
1	D	166	THR	6.0
1	A	144	ASP	5.9
1	A	92	GLY	5.8
1	D	148	LEU	5.8
1	D	406	ALA	5.7
1	A	161	LEU	5.7
1	D	431	LEU	5.7
1	A	137	PRO	5.7
1	A	163	CYS	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	167	ASN	5.5
1	A	98	ASP	5.5
1	D	437	VAL	5.5
1	D	433	ILE	5.5
1	A	94	PHE	5.4
1	D	169	HIS	5.4
1	D	168	SER	5.4
1	A	176	GLY	5.2
1	D	428	CYS	5.2
1	A	150	LEU	5.2
1	D	95	VAL	5.0
1	A	146	GLY	5.0
1	A	96	GLY	5.0
1	D	103	ARG	5.0
1	D	403	GLY	4.9
1	A	159	GLN	4.9
1	A	90	ARG	4.9
1	D	96	GLY	4.8
1	A	180	PRO	4.7
1	A	183	ASP	4.7
1	D	432	ASN	4.6
1	A	106	THR	4.6
1	A	127	ASP	4.6
1	A	153	GLN	4.5
1	D	418	ILE	4.5
1	A	132	SER	4.4
1	D	410	ALA	4.4
1	D	419	VAL	4.4
1	D	425	LEU	4.4
1	A	131	LEU	4.4
1	D	399	LEU	4.3
1	D	421	VAL	4.3
1	D	427	THR	4.3
1	A	110	THR	4.3
1	A	114	ALA	4.3
1	A	97	GLY	4.3
1	A	119	GLY	4.3
1	A	116	ALA	4.2
1	D	97	GLY	4.2
1	A	184	VAL	4.2
1	D	98	ASP	4.2
1	D	434	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	154	SER	4.1
1	D	114	ALA	4.1
1	D	420	CYS	4.1
1	A	174	ARG	4.0
1	D	171	ILE	4.0
1	D	441	PHE	4.0
1	D	101	MET	3.9
1	D	146	GLY	3.9
1	D	429	ARG	3.9
1	A	117	ASP	3.9
1	D	409	VAL	3.8
1	D	398	VAL	3.8
1	D	167	ASN	3.8
1	D	402	THR	3.7
1	D	423	THR	3.7
1	A	88	GLU	3.7
1	A	145	ASP	3.7
1	D	430	GLN	3.6
1	D	94	PHE	3.6
1	D	397	VAL	3.6
1	D	104	GLY	3.5
1	D	408	LEU	3.5
1	A	189	VAL	3.5
1	D	407	ARG	3.5
1	D	151	GLN	3.5
1	D	422	THR	3.4
1	D	163	CYS	3.4
1	D	444	ALA	3.4
1	D	164	THR	3.4
1	D	385	VAL	3.4
1	D	439	SER	3.4
1	D	291	PRO	3.4
1	A	120	THR	3.4
1	D	293	ILE	3.3
1	D	258	ILE	3.3
1	D	442	PHE	3.3
1	D	459	ALA	3.2
1	D	327	VAL	3.2
1	D	326	CYS	3.1
1	D	405	SER	3.1
1	D	292	VAL	3.1
1	D	153	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	436	GLY	3.1
1	D	117	ASP	3.1
1	A	115	PHE	3.1
1	D	142	TYR	3.1
1	D	150	LEU	3.1
1	D	381	CYS	3.0
1	D	380	VAL	3.0
1	D	260	VAL	3.0
1	D	440	VAL	2.9
1	A	123	LYS	2.9
1	D	451	GLU	2.9
1	A	129	GLN	2.9
1	D	371	HIS	2.9
1	D	416	CYS	2.9
1	D	483	HIS	2.9
1	D	140	TYR	2.9
1	D	435	GLN	2.8
1	A	449	HIS	2.8
1	D	152	VAL	2.8
1	D	105	ALA	2.8
1	D	113	PRO	2.8
1	D	478	VAL	2.8
1	D	106	THR	2.8
1	A	242	HIS	2.8
1	D	172	SER	2.7
1	D	175	ARG	2.7
1	A	448	GLY	2.7
1	D	137	PRO	2.7
1	D	237	CYS	2.7
1	D	494	ILE	2.7
1	D	384	ALA	2.7
1	D	396	MET	2.7
1	D	138	GLY	2.7
1	D	449	HIS	2.7
1	D	492	THR	2.7
1	D	498	GLU	2.7
1	D	477	VAL	2.7
1	D	165	VAL	2.6
1	D	457	VAL	2.6
1	D	122	ASP	2.6
1	D	121	LYS	2.6
1	D	320	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	495	LEU	2.6
1	A	148	LEU	2.6
1	A	451	GLU	2.6
1	A	498	GLU	2.6
1	A	111	THR	2.6
1	D	282	ILE	2.6
1	A	471	GLN	2.6
1	D	460	GLY	2.6
1	D	424	ARG	2.6
1	D	115	PHE	2.6
1	A	455	HIS	2.6
1	D	448	GLY	2.5
1	D	145	ASP	2.5
1	D	463	PHE	2.5
1	D	99	ALA	2.5
1	D	281	LEU	2.5
1	D	176	GLY	2.5
1	D	400	SER	2.5
1	A	445	ASP	2.5
1	D	116	ALA	2.5
1	D	479	ILE	2.5
1	A	472	THR	2.5
1	A	446	LYS	2.4
1	D	404	ARG	2.4
1	D	102	GLU	2.4
1	D	447	LEU	2.4
1	D	100	VAL	2.4
1	D	156	GLU	2.4
1	D	401	ASN	2.4
1	A	191	ALA	2.4
1	D	464	ALA	2.4
1	D	209	PHE	2.4
1	A	444	ALA	2.4
1	D	383	SER	2.4
1	A	188	ALA	2.4
1	D	136	ARG	2.3
1	D	141	ILE	2.3
1	A	155	HIS	2.3
1	A	156	GLU	2.3
1	D	144	ASP	2.3
1	D	324	ALA	2.3
1	A	212	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	47	VAL	2.2
1	A	187	PRO	2.2
1	D	417	PRO	2.2
1	D	24	ILE	2.2
1	D	236	ILE	2.2
1	A	447	LEU	2.2
1	A	87	PRO	2.2
1	D	458	ALA	2.2
1	A	118	LYS	2.2
1	D	294	CYS	2.2
1	D	46	SER	2.2
1	D	387	SER	2.2
1	A	454	GLU	2.2
1	D	207	MET	2.1
1	D	48	ALA	2.1
1	D	155	HIS	2.1
1	D	257	GLY	2.1
1	D	208	ILE	2.1
1	D	21	ALA	2.1
1	D	452	GLY	2.1
1	D	239	ILE	2.1
1	A	452	GLY	2.1
1	D	277	ALA	2.1
1	A	157	ASP	2.1
1	A	243	GLN	2.0
1	A	465	LYS	2.0
1	D	388	VAL	2.0
1	A	488	TYR	2.0
1	D	443	ASP	2.0
1	D	93	GLN	2.0
1	D	213	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(Å ²)	Q<0.9
2	GOL	D	499	6/6	0.22	2.61	47,52,55,61	0
2	GOL	A	499	6/6	0.18	2.03	36,56,60,60	0
3	SO4	A	500	5/5	0.15	0.93	42,45,47,48	4
4	K	A	502	1/1	0.10	-0.17	44,44,44,44	0
3	SO4	D	501	5/5	0.17	-1.66	33,39,40,41	3
4	K	D	503	1/1	0.08	-1.97	50,50,50,50	0
4	K	D	502	1/1	0.10	-2.20	43,43,43,43	1
2	GOL	D	500	6/6	0.15	-2.22	47,53,55,61	0
4	K	A	501	1/1	0.08	-2.49	40,40,40,40	1

6.5 Other polymers ⓘ

There are no such residues in this entry.