



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:30 AM UTC

PDB ID : 3HQN / pdb_00003hqn
Title : Apo crystal structure of Leishmania mexicana(LmPYK)pyruvate kinase
Authors : Morgan, H.P.; Walkinshaw, M.D.
Deposited on : 2009-06-08
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

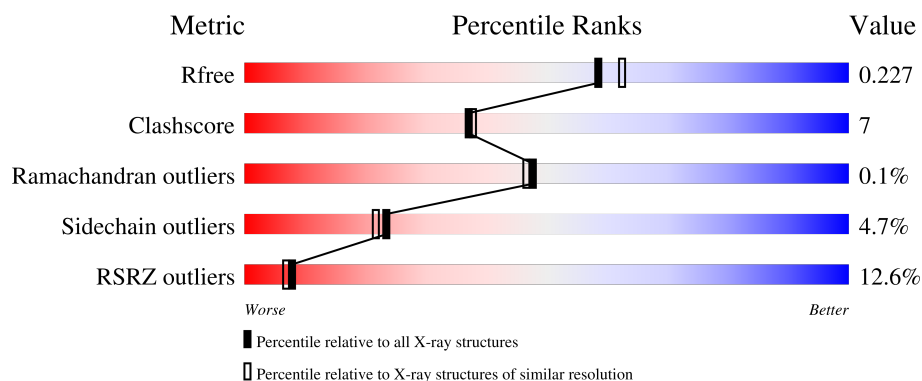
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	499	22% 85% 11% ..
1	D	499	2% 80% 16% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8323 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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 (CCD ID: 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 (CCD ID: K) (formula: K).

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

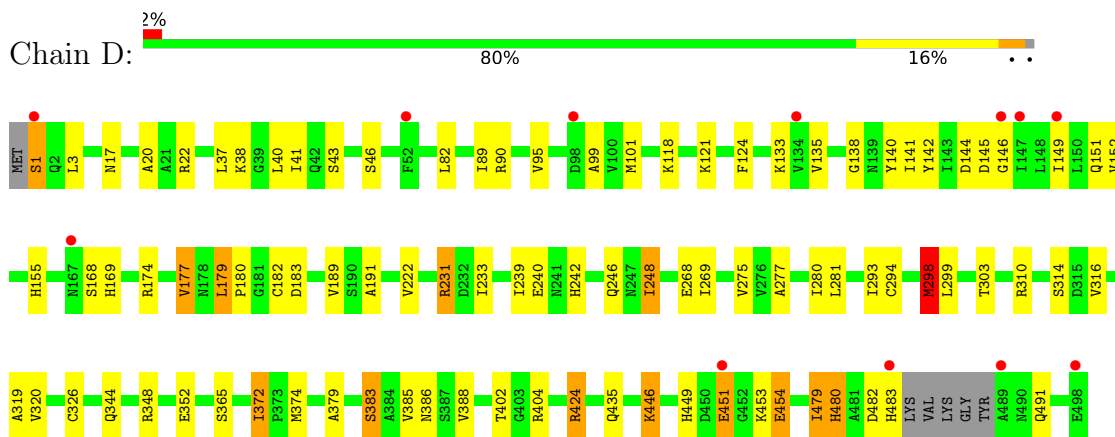
- Molecule 5 is water.

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

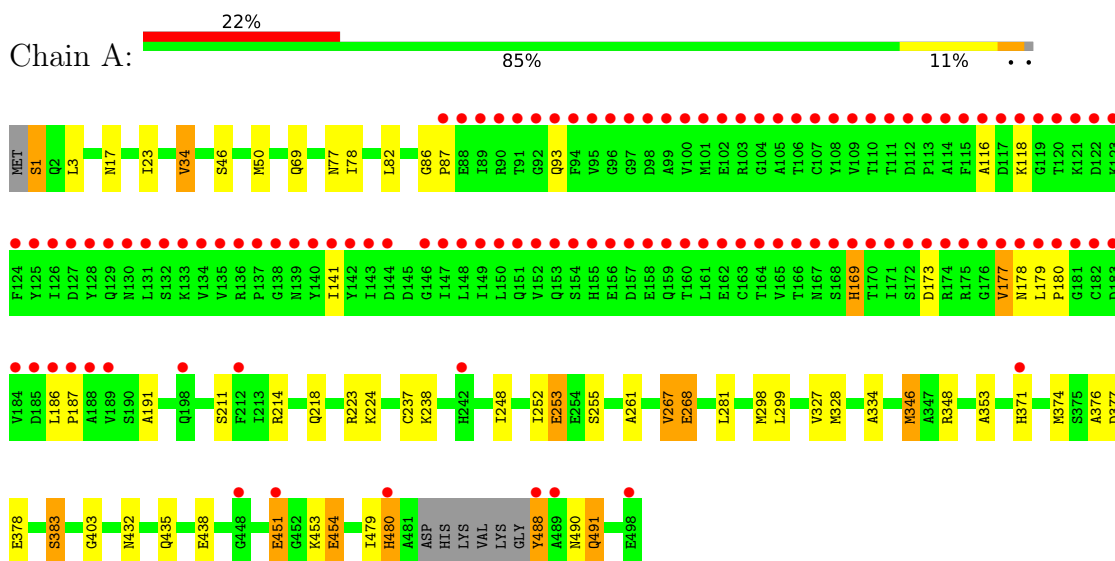
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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	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 0.184 , 0.227	Depositor DCC
R_{free} test set	4504 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, K

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	1.49	17/3856 (0.4%)	1.23	7/5218 (0.1%)
1	D	1.56	26/3825 (0.7%)	1.22	4/5176 (0.1%)
All	All	1.53	43/7681 (0.6%)	1.22	11/10394 (0.1%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	GLY	C-N	11.61	1.49	1.33
1	D	1	SER	N-CA	9.24	1.63	1.46
1	A	1	SER	N-CA	8.15	1.61	1.46
1	D	365	SER	N-CA	7.31	1.55	1.46
1	D	479	ILE	CA-CB	7.08	1.65	1.54
1	A	77	ASN	C-O	6.81	1.32	1.24
1	D	20	ALA	CA-CB	6.77	1.64	1.53
1	D	352	GLU	CA-C	6.66	1.61	1.52
1	D	374	MET	SD-CE	-6.65	1.62	1.79
1	D	372	ILE	CA-C	6.58	1.58	1.52
1	A	353	ALA	CA-CB	6.57	1.63	1.53
1	D	248	ILE	CA-CB	6.31	1.62	1.54
1	D	303	THR	CA-C	6.20	1.60	1.52
1	D	275	VAL	N-CA	6.20	1.53	1.46
1	A	261	ALA	CA-CB	6.03	1.63	1.53
1	D	320	VAL	CA-CB	5.95	1.61	1.54
1	A	177	VAL	CA-CB	5.89	1.64	1.54
1	D	388	VAL	CA-CB	5.79	1.61	1.54
1	A	78	ILE	C-O	-5.70	1.18	1.24
1	A	376	ALA	CA-CB	5.70	1.62	1.53
1	D	385	VAL	CA-CB	5.68	1.61	1.54
1	D	191	ALA	CA-CB	5.66	1.62	1.53
1	D	277	ALA	N-CA	5.58	1.53	1.46
1	D	294	CYS	CA-C	5.54	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	GLY	N-CA	5.54	1.53	1.45
1	D	480	HIS	CA-C	5.53	1.59	1.52
1	D	319	ALA	CA-CB	5.52	1.61	1.53
1	A	346	MET	C-O	-5.44	1.17	1.24
1	A	252	ILE	CA-CB	5.43	1.60	1.54
1	D	141	ILE	CA-C	-5.33	1.46	1.52
1	D	280	ILE	C-O	-5.33	1.18	1.24
1	D	310	ARG	CA-C	5.32	1.59	1.52
1	A	267	VAL	N-CA	5.31	1.52	1.46
1	D	298	MET	C-O	5.23	1.29	1.24
1	A	34	VAL	CA-CB	5.22	1.60	1.54
1	D	46	SER	CA-CB	5.20	1.61	1.54
1	D	222	VAL	N-CA	5.15	1.52	1.46
1	A	50	MET	N-CA	5.08	1.52	1.46
1	A	191	ALA	CA-CB	5.07	1.61	1.53
1	A	328	MET	N-CA	5.04	1.52	1.46
1	A	334	ALA	CA-CB	5.03	1.61	1.53
1	D	482	ASP	N-CA	5.01	1.52	1.46
1	D	233	ILE	CA-CB	5.01	1.60	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	HIS	CB-CA-C	9.04	125.57	110.03
1	A	34	VAL	N-CA-CB	6.96	120.01	110.54
1	D	299	LEU	N-CA-C	-6.50	102.64	110.44
1	A	173	ASP	N-CA-C	6.31	119.14	110.24
1	A	299	LEU	N-CA-C	-6.21	102.98	110.44
1	A	141	ILE	N-CA-C	-6.10	98.74	107.77
1	A	86	GLY	O-C-N	5.64	127.41	121.77
1	A	348	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	D	446	LYS	CB-CA-C	-5.06	101.44	110.70
1	D	269	ILE	CA-C-N	5.04	125.04	119.90
1	D	269	ILE	C-N-CA	5.04	125.04	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3790	0	3787	47	1
1	D	3767	0	3766	57	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
4	D	2	0	0	0	0
5	A	340	0	0	12	2
5	D	394	0	0	21	0
All	All	8323	0	7577	105	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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	1.49	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:D:180:PRO:HD3	5:D:762:HOH:O	1.79	0.81
1:A:488:TYR:O	1:A:488:TYR:CD2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:3:LEU:C	1:D:3:LEU:HD23	2.18	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: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:D:451:GLU:H	1:D:451:GLU:CD	2.04	0.65
1:A:374:MET:HE2	1:A:378:GLU:HB3	1.79	0.65
1:D:231:ARG:HG2	1:D:231:ARG:NH1	2.13	0.63
1:A:327:VAL:HG23	1:A:346:MET:HE3	1.81	0.62
1:A:490:ASN:O	1:A:491:GLN:HB2	2.00	0.61
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:D:449:HIS:HB3	5:D:688:HOH:O	2.02	0.59
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: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: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: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:D:189:VAL:HG23	1:D:189:VAL:O	2.10	0.50
1:A:374:MET:CE	1:A:378:GLU:CG	2.88	0.50
1:A:223:ARG:HD2	5:A:809:HOH:O	2.10	0.50
1:A:3:LEU:C	1:A:3:LEU:HD23	2.36	0.50
1:A:253:GLU:CB	5:A:783:HOH:O	2.60	0.50
1:A:451:GLU:H	1:A:451:GLU:CD	2.20	0.50
1:A:46:SER:HB3	1:A:432:ASN:HB3	1.94	0.49
1:A:82:LEU:C	1:A:82:LEU:HD23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:ARG:HH11	1:D:424:ARG:CG	2.26	0.49
1:A:480[A]:HIS:C	1:A:480[A]:HIS:CD2	2.90	0.48
1:D:90:ARG:HD3	1:D:174:ARG:O	2.13	0.48
1:D:101:MET:HE2	5:D:808:HOH:O	2.13	0.48
1:A:374:MET:HE2	1:A:378:GLU:CB	2.43	0.48
1:D:402:THR:HG21	1:D:483:HIS:HE1	1.79	0.48
1:D:89:ILE:HG21	1:D:177:VAL:HG22	1.96	0.48
1:A:377:ASP:HB3	1:A:488:TYR:CZ	2.49	0.48
1:D:144:ASP:O	1:D:145:ASP:HB2	2.13	0.47
1:D:82:LEU:C	1:D:82:LEU:HD23	2.40	0.47
1:D:1:SER:CA	5:D:580:HOH:O	2.55	0.46
1:A:454:GLU:H	1:A:454:GLU:HG3	1.50	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:214:ARG:CZ	1:A:218:GLN:HE22	2.30	0.45
1:A:488:TYR:O	1:A:488:TYR:CG	2.69	0.45
1:D:101:MET:HE1	1:D:124:PHE:CE1	2.52	0.45
1:A:211:SER:HA	1:A:238:LYS:HD3	1.98	0.44
1:A:237:CYS:SG	1:A:255:SER:HB3	2.57	0.44
1:A:253:GLU:CG	5:A:783:HOH:O	2.66	0.44
1:D:121:LYS:HG2	5:D:795:HOH:O	2.18	0.44
1:A:374:MET:HE2	1:A:378:GLU:CG	2.48	0.43
1:D:386:ASN:ND2	5:D:588:HOH:O	2.52	0.43
1:A:87:PRO:HG3	1:A:187:PRO:O	2.18	0.43
1:A:298:MET:O	5:A:800:HOH:O	2.21	0.43
1:D:37:LEU:O	1:D:41:ILE:HG13	2.19	0.42
1:A:178:ASN:ND2	1:A:267:VAL:HG11	2.35	0.42
1:A:180:PRO:CB	1:A:268:GLU:HB2	2.40	0.42
1:A:491:GLN:HB2	1:A:491:GLN:HE21	1.61	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: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:293:ILE:HG12	1:D:326:CYS:HB2	2.02	0.41
1:D:379:ALA:O	1:D:383:SER:HB3	2.21	0.41
1:D:424:ARG:NH1	1:D:424:ARG:CG	2.83	0.41
1:A:116:ALA:CB	5:A:693:HOH:O	2.51	0.41
1:D:404:ARG:NH1	5:D:780:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ILE:HG12	1:D:281:LEU:HD22	2.03	0.40
1:D:449:HIS:CE1	5:D:529:HOH:O	2.74	0.40
1:D:22:ARG:HH11	1:D:22:ARG:HD3	1.73	0.40
1:D:239:ILE:HG21	1:D:281:LEU:HD11	2.04	0.40
1:D:240:GLU:OE2	2:D:499:GOL:H12	2.21	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	Interatomic distance (Å)	Clash overlap (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%)	43	42
1	D	490/499 (98%)	476 (97%)	14 (3%)	0	100	100
All	All	983/998 (98%)	953 (97%)	29 (3%)	1 (0%)	48	46

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%)	20	18
1	D	413/417 (99%)	394 (95%)	19 (5%)	24	22
All	All	829/834 (99%)	788 (95%)	41 (5%)	23	20

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	17	ASN
1	D	38	LYS
1	D	40	LEU
1	D	118	LYS
1	D	177	VAL
1	D	179	LEU
1	D	231	ARG
1	D	298	MET
1	D	314	SER
1	D	372	ILE
1	D	383	SER
1	D	424	ARG
1	D	435	GLN
1	D	451	GLU
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	34	VAL
1	A	93	GLN
1	A	118	LYS
1	A	169	HIS
1	A	177	VAL
1	A	179	LEU
1	A	186	LEU

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Mol	Chain	Res	Type
1	A	224	LYS
1	A	253	GLU
1	A	268	GLU
1	A	371[A]	HIS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	17	ASN
1	D	77	ASN
1	D	93	GLN
1	D	139	ASN
1	D	151	GLN
1	D	155	HIS
1	D	159	GLN
1	D	178	ASN
1	D	305	ASN
1	D	344	GLN
1	D	371	HIS
1	D	386	ASN
1	D	449	HIS
1	D	455	HIS
1	D	471	GLN
1	A	17	ASN
1	A	151	GLN
1	A	178	ASN
1	A	241	ASN
1	A	305	ASN
1	A	491	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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	$\# Z > 2$
3	SO4	A	500	-	4,4,4	0.25	0	6,6,6	1.01	0
2	GOL	A	499	-	5,5,5	0.30	0	5,5,5	0.79	0
2	GOL	D	499	4	5,5,5	0.50	0	5,5,5	0.80	0
3	SO4	D	501	-	4,4,4	0.49	0	6,6,6	0.89	0
2	GOL	D	500	-	5,5,5	0.62	0	5,5,5	0.79	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	D	499	4	-	3/4/4/4	-
2	GOL	A	499	-	-	2/4/4/4	-
2	GOL	D	500	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	499	GOL	O1-C1-C2-C3
2	A	499	GOL	O1-C1-C2-C3
2	D	499	GOL	O1-C1-C2-O2
2	D	499	GOL	C1-C2-C3-O3
2	D	500	GOL	O1-C1-C2-C3
2	A	499	GOL	O1-C1-C2-O2
2	D	500	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	499	GOL	1	0
2	D	499	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.98	112 (22%) 2 2	3, 21, 37, 58	106 (21%)
1	D	493/499 (98%)	0.06	12 (2%) 59 59	13, 23, 36, 46	1 (0%)
All	All	985/998 (98%)	0.52	124 (12%) 8 7	3, 22, 37, 58	107 (10%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	ASN	11.7
1	A	122	ASP	10.2
1	A	89	ILE	9.8
1	A	138	GLY	9.8
1	A	114	ALA	9.7
1	A	113	PRO	9.5
1	A	147	ILE	8.3
1	A	100	VAL	8.2
1	A	112	ASP	8.1
1	A	153	GLN	7.7
1	A	160	THR	7.4
1	A	187	PRO	7.3
1	A	140	TYR	7.1
1	A	109	VAL	7.0
1	A	115	PHE	6.7
1	A	142	TYR	6.7
1	A	171	ILE	6.6
1	A	95	VAL	6.6
1	A	128	TYR	6.5
1	A	144	ASP	6.4
1	A	108	TYR	6.4
1	A	127	ASP	6.4
1	A	116	ALA	6.3
1	A	120	THR	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	157	ASP	6.3
1	A	102	GLU	6.3
1	A	92	GLY	6.2
1	A	182	CYS	6.2
1	A	180	PRO	6.1
1	A	124	PHE	6.1
1	A	134	VAL	5.9
1	A	152	VAL	5.9
1	A	94	PHE	5.8
1	A	105	ALA	5.7
1	A	129	GLN	5.6
1	A	181	GLY	5.6
1	A	103	ARG	5.5
1	A	163	CYS	5.5
1	A	159	GLN	5.4
1	A	177	VAL	5.4
1	A	107	CYS	5.4
1	A	149	ILE	5.4
1	A	132	SER	5.4
1	A	173	ASP	5.3
1	A	117	ASP	5.2
1	A	119	GLY	5.2
1	A	183	ASP	5.1
1	A	174	ARG	5.0
1	A	133	LYS	4.9
1	A	99	ALA	4.8
1	A	184	VAL	4.8
1	A	170	THR	4.8
1	A	176	GLY	4.8
1	A	91	THR	4.8
1	A	106	THR	4.8
1	A	164	THR	4.7
1	A	123	LYS	4.7
1	A	137	PRO	4.6
1	A	488	TYR	4.5
1	A	135	VAL	4.5
1	A	96	GLY	4.4
1	A	97	GLY	4.3
1	A	175	ARG	4.3
1	A	126	ILE	4.3
1	A	165	VAL	4.2
1	A	98	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	169	HIS	4.2
1	A	121	LYS	4.2
1	A	155	HIS	4.1
1	A	167	ASN	4.0
1	A	111	THR	3.9
1	A	110	THR	3.9
1	A	87	PRO	3.9
1	D	98	ASP	3.8
1	A	90	ARG	3.8
1	A	185	ASP	3.8
1	A	131	LEU	3.7
1	A	158	GLU	3.7
1	A	151	GLN	3.7
1	A	146	GLY	3.7
1	A	139	ASN	3.7
1	A	93	GLN	3.7
1	A	489	ALA	3.7
1	A	186	LEU	3.6
1	A	161	LEU	3.6
1	A	118	LYS	3.6
1	A	172	SER	3.5
1	A	101	MET	3.4
1	A	480[A]	HIS	3.4
1	A	143	ILE	3.4
1	A	166	THR	3.2
1	A	104	GLY	3.2
1	D	149	ILE	3.2
1	A	148	LEU	3.1
1	D	146	GLY	3.1
1	A	179	LEU	2.9
1	A	130	ASN	2.9
1	A	125	TYR	2.9
1	D	489	ALA	2.9
1	D	483	HIS	2.8
1	A	212	PHE	2.8
1	A	88	GLU	2.7
1	A	448	GLY	2.6
1	D	134	VAL	2.6
1	A	136	ARG	2.6
1	A	242	HIS	2.5
1	D	147	ILE	2.5
1	A	198	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	168	SER	2.4
1	A	371[A]	HIS	2.4
1	A	154	SER	2.3
1	A	162	GLU	2.3
1	A	189	VAL	2.3
1	A	188	ALA	2.3
1	A	156	GLU	2.2
1	D	52	PHE	2.2
1	D	451	GLU	2.1
1	D	498	GLU	2.1
1	D	1	SER	2.1
1	D	167	ASN	2.1
1	A	451	GLU	2.1
1	A	498	GLU	2.1
1	A	150	LEU	2.1
1	A	141	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	499	6/6	0.87	0.14	36,56,60,60	0
2	GOL	D	500	6/6	0.89	0.12	47,53,55,61	0
2	GOL	D	499	6/6	0.89	0.11	47,52,55,61	0
3	SO4	A	500	5/5	0.92	0.10	42,45,47,48	4
4	K	A	501	1/1	0.93	0.19	40,40,40,40	1
4	K	D	503	1/1	0.94	0.19	50,50,50,50	0
4	K	D	502	1/1	0.95	0.11	43,43,43,43	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	A	502	1/1	0.96	0.06	44,44,44,44	0
3	SO4	D	501	5/5	0.97	0.10	33,39,40,41	3

6.5 Other polymers [i](#)

There are no such residues in this entry.