Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:15 AM GMT

PDB ID	:	3HQN
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

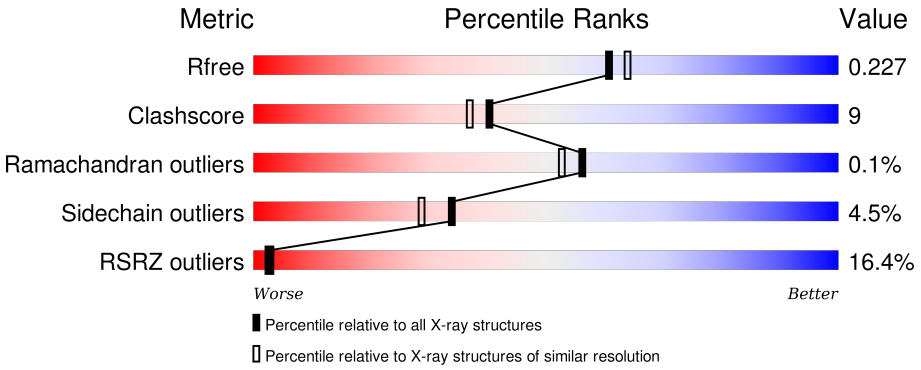
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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 <=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	25% 83% 13%
1	D	499	8% 82% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 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.

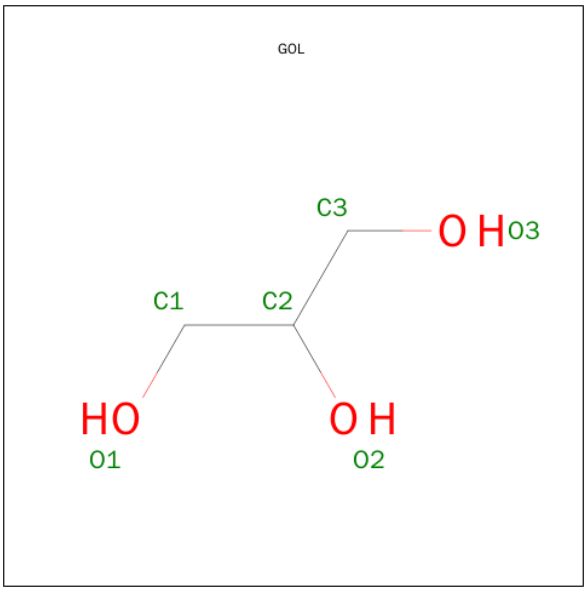
- Molecule 1 is a protein called Pyruvate kinase.

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:

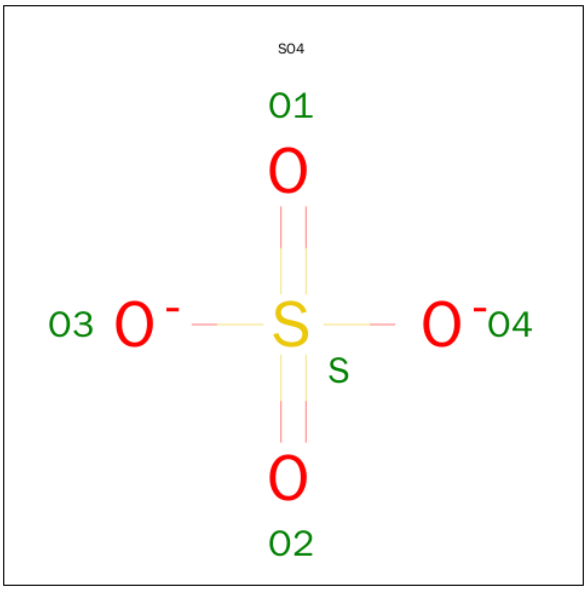
Chain	Residue	Modelled	Actual	Comment	Reference
D	382	SER	GLY	SEE REMARK 999	UNP Q27686
D	389	TYR	SER	SEE REMARK 999	UNP Q27686
D	404	ARG	ALA	SEE REMARK 999	UNP Q27686
D	405	SER	GLY	SEE REMARK 999	UNP Q27686
A	382	SER	GLY	SEE REMARK 999	UNP Q27686
A	389	TYR	SER	SEE REMARK 999	UNP Q27686
A	404	ARG	ALA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

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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: O_4S).



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 5 4 1	0	0

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

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

- Molecule 5 is water.

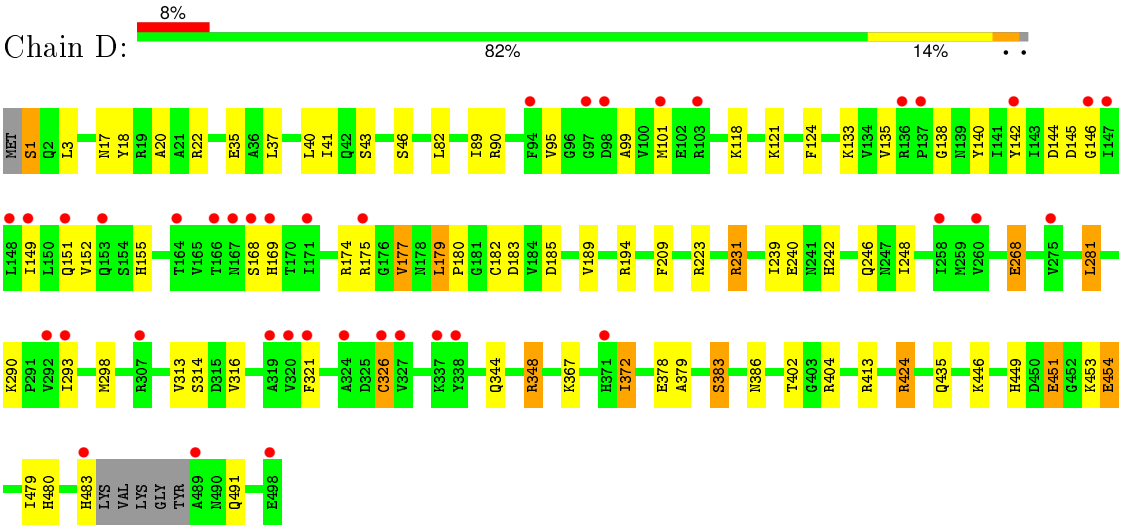
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	394	Total O 394 394	0	0
5	A	340	Total O 340 340	0	0

3 Residue-property plots (i)

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.

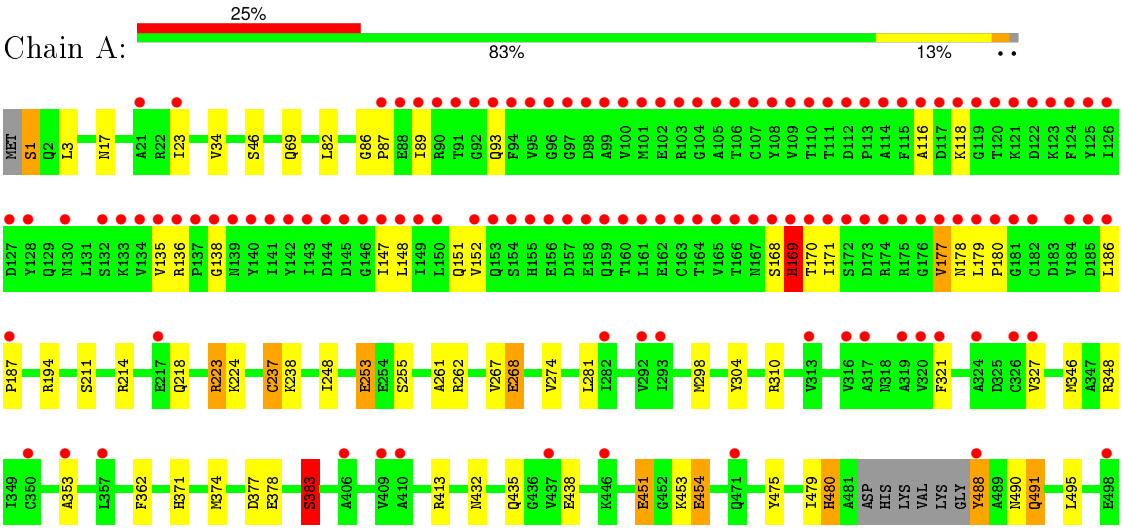
- Molecule 1: Pyruvate kinase

Chain D:



- Molecule 1: Pyruvate kinase

Chain A:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.27%)	DCC
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 89897 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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	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
4	D	2	0	0	0	0
5	A	340	0	0	12	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	394	0	0	20	0
All	All	8323	0	7577	128	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 9.

All (128) 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	1.48	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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ARG:HD3	1:D:174:ARG:O	2.13	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	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 (i)

5.3.1 Protein backbone (i)

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%)	52 48
1	D	490/499 (98%)	476 (97%)	14 (3%)	0	100 100
All	All	983/998 (98%)	953 (97%)	29 (3%)	1 (0%)	56 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	GLN

5.3.2 Protein sidechains (i)

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%)	28	22
1	D	413/417 (99%)	396 (96%)	17 (4%)	37	32
All	All	829/834 (99%)	790 (95%)	39 (5%)	34	27

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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	0.25	0	5,5,5	0.76	0
3	SO4	A	500	-	4,4,4	0.69	0	6,6,6	0.83	0
2	GOL	D	499	4	5,5,5	0.48	0	5,5,5	0.72	0
2	GOL	D	500	-	5,5,5	0.60	0	5,5,5	0.70	0
3	SO4	D	501	-	4,4,4	0.61	0	6,6,6	0.65	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.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	1.79	123 (25%) 1 1	14, 25, 64, 76	101 (20%)
1	D	493/499 (98%)	0.30	39 (7%) 15 16	13, 23, 36, 46	0
All	All	985/998 (98%)	1.04	162 (16%) 2 3	13, 23, 57, 76	101 (10%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	THR	27.5
1	A	166	THR	22.8
1	A	149	ILE	21.2
1	A	171	ILE	19.3
1	A	109	VAL	16.7
1	A	95	VAL	15.5
1	A	100	VAL	14.9
1	A	147	ILE	14.3
1	A	104	GLY	14.3
1	A	122	ASP	14.3
1	A	160	THR	14.3
1	A	164	THR	13.8
1	A	124	PHE	13.5
1	A	125	TYR	13.2
1	A	135	VAL	13.1
1	A	140	TYR	12.5
1	A	134	VAL	11.9
1	A	101	MET	11.8
1	A	89	ILE	11.7
1	A	107	CYS	11.6
1	A	94	PHE	11.1
1	A	96	GLY	10.8
1	A	136	ARG	10.6
1	A	181	GLY	10.5

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Mol	Chain	Res	Type	RSRZ
1	A	165	VAL	10.3
1	A	105	ALA	10.1
1	A	178	ASN	9.8
1	A	106	THR	9.6
1	A	108	TYR	9.5
1	A	168	SER	9.5
1	A	146	GLY	9.4
1	A	152	VAL	9.4
1	A	172	SER	9.0
1	A	169	HIS	8.9
1	A	103	ARG	8.8
1	A	117	ASP	8.7
1	A	167	ASN	8.4
1	A	93	GLN	8.3
1	A	161	LEU	8.3
1	A	139	ASN	7.9
1	A	126	ILE	7.7
1	A	102	GLU	7.5
1	A	133	LYS	7.2
1	A	112	ASP	7.1
1	A	113	PRO	7.0
1	A	99	ALA	7.0
1	A	92	GLY	7.0
1	A	98	ASP	6.8
1	A	115	PHE	6.8
1	A	177	VAL	6.8
1	A	175	ARG	6.8
1	A	162	GLU	6.6
1	A	116	ALA	6.3
1	A	118	LYS	6.2
1	A	97	GLY	6.0
1	A	142	TYR	5.9
1	D	149	ILE	5.9
1	A	153	GLN	5.9
1	A	154	SER	5.9
1	A	123	LYS	5.9
1	A	143	ILE	5.9
1	A	158	GLU	5.7
1	A	159	GLN	5.5
1	A	174	ARG	5.3
1	A	141	ILE	5.1
1	A	182	CYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	150	LEU	5.1
1	A	111	THR	5.0
1	A	173	ASP	5.0
1	D	147	ILE	4.7
1	A	91	THR	4.6
1	A	110	THR	4.5
1	A	138	GLY	4.5
1	A	144	ASP	4.4
1	D	166	THR	4.4
1	A	163	CYS	4.4
1	A	121	LYS	4.4
1	D	98	ASP	4.2
1	A	179	LEU	4.2
1	A	132	SER	4.2
1	A	180	PRO	4.1
1	A	128	TYR	4.0
1	D	148	LEU	4.0
1	A	145	ASP	4.0
1	D	169	HIS	4.0
1	A	114	ALA	3.9
1	A	90	ARG	3.9
1	A	127	ASP	3.8
1	A	137	PRO	3.6
1	A	157	ASP	3.6
1	D	103	ARG	3.6
1	A	88	GLU	3.6
1	A	488	TYR	3.5
1	A	119	GLY	3.4
1	A	120	THR	3.3
1	A	184	VAL	3.3
1	D	146	GLY	3.3
1	A	324	ALA	3.3
1	A	320	VAL	3.2
1	A	319	ALA	3.1
1	A	176	GLY	3.0
1	A	156	GLU	3.0
1	D	94	PHE	3.0
1	D	483	HIS	3.0
1	A	155	HIS	3.0
1	D	168	SER	2.9
1	D	167	ASN	2.8
1	D	164	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	326	CYS	2.8
1	D	320	VAL	2.8
1	A	321	PHE	2.7
1	D	175	ARG	2.7
1	A	148	LEU	2.7
1	A	130	ASN	2.7
1	A	187	PRO	2.7
1	A	293	ILE	2.7
1	D	326	CYS	2.7
1	D	151	GLN	2.6
1	A	185	ASP	2.6
1	A	292	VAL	2.6
1	A	186	LEU	2.6
1	A	21	ALA	2.6
1	A	437	VAL	2.6
1	D	97	GLY	2.6
1	D	136	ARG	2.5
1	D	293	ILE	2.5
1	D	171	ILE	2.5
1	A	498	GLU	2.5
1	D	338	TYR	2.4
1	D	498	GLU	2.4
1	A	327	VAL	2.4
1	D	153	GLN	2.4
1	A	313	VAL	2.4
1	D	337	LYS	2.4
1	D	371	HIS	2.3
1	D	324	ALA	2.3
1	D	489	ALA	2.3
1	D	260	VAL	2.3
1	D	275	VAL	2.3
1	D	319	ALA	2.3
1	A	410	ALA	2.3
1	A	87	PRO	2.2
1	D	327	VAL	2.2
1	A	317	ALA	2.2
1	A	353	ALA	2.2
1	D	101	MET	2.2
1	A	446	LYS	2.2
1	A	350	CYS	2.1
1	A	471	GLN	2.1
1	A	217	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	409	VAL	2.1
1	D	142	TYR	2.1
1	A	282	ILE	2.1
1	A	316	VAL	2.1
1	D	258	ILE	2.1
1	D	137	PRO	2.1
1	D	321	PHE	2.1
1	A	23	ILE	2.0
1	A	357	LEU	2.0
1	A	406	ALA	2.0
1	D	307	ARG	2.0
1	D	292	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	D	499	6/6	0.89	0.21	4.41	47,52,55,61	0
2	GOL	A	499	6/6	0.87	0.19	1.03	36,56,60,60	0
2	GOL	D	500	6/6	0.91	0.14	0.93	47,53,55,61	0
3	SO4	D	501	5/5	0.98	0.13	-0.25	33,39,40,41	3
4	K	A	502	1/1	0.97	0.11	-0.38	44,44,44,44	0
3	SO4	A	500	5/5	0.96	0.11	-0.39	42,45,47,48	4
4	K	D	503	1/1	0.96	0.09	-0.97	50,50,50,50	0
4	K	D	502	1/1	0.95	0.07	-2.06	43,43,43,43	1
4	K	A	501	1/1	0.97	0.08	-3.59	40,40,40,40	1

6.5 Other polymers (i)

There are no such residues in this entry.