Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:31 AM GMT

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

This is a Full wwPDB 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 ⓘ symbol.

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

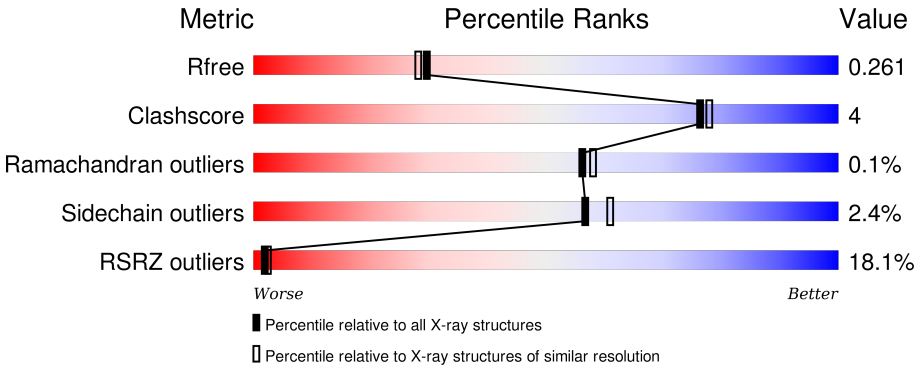
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. 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	10% 90% 7% ••
1	B	499	26% 92% 6% ••

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	A	500	-	-	-	X
2	GOL	A	502	-	-	-	X
3	PTK	A	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8211 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.

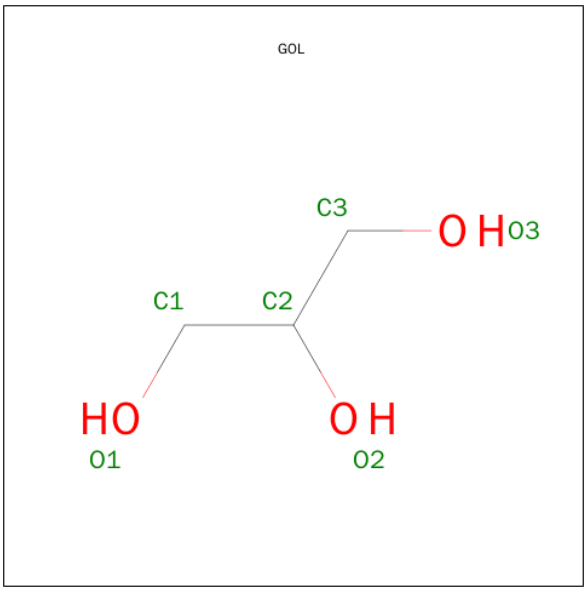
- Molecule 1 is a protein called Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3753	2339	660	728	26			
1	B	492	Total	C	N	O	S	0	0	0
			3753	2339	660	728	26			

There are 8 discrepancies between the modelled and reference sequences:

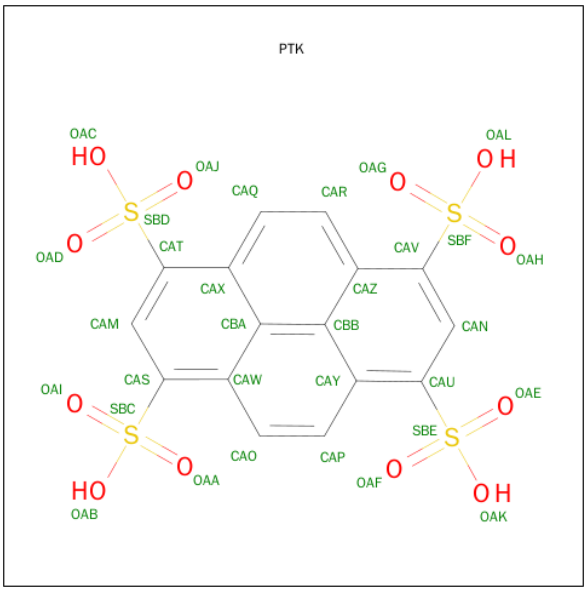
Chain	Residue	Modelled	Actual	Comment	Reference
A	382	SER	GLY	SEE REMARK 999	UNP Q27686
A	389	TYR	SER	SEE REMARK 999	UNP Q27686
A	404	ARG	ALA	SEE REMARK 999	UNP Q27686
A	405	SER	GLY	SEE REMARK 999	UNP Q27686
B	382	SER	GLY	SEE REMARK 999	UNP Q27686
B	389	TYR	SER	SEE REMARK 999	UNP Q27686
B	404	ARG	ALA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

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



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

- Molecule 3 is PYRENE-1,3,6,8-TETRASULFONIC ACID (three-letter code: PTK) (formula: $C_{16}H_{10}O_{12}S_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			32	16	12	4		

- Molecule 4 is water.

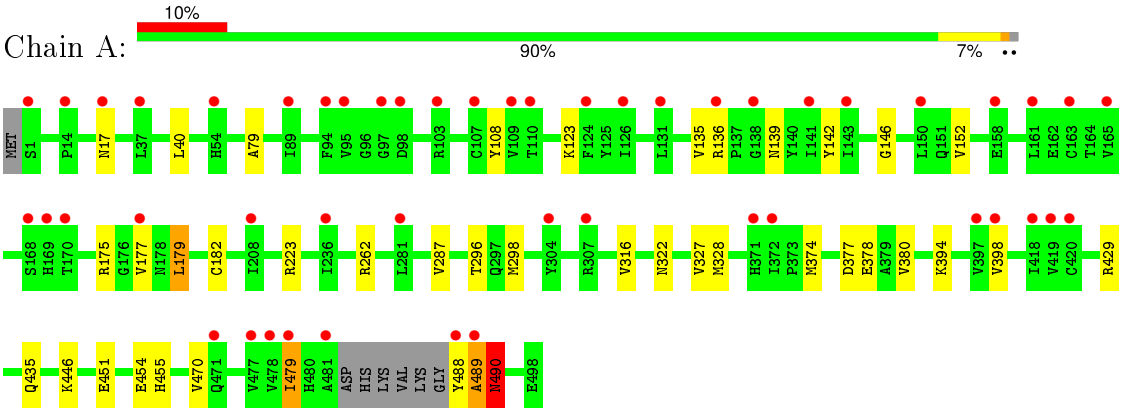
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	350	Total	O	0	0
			350	350		
4	B	293	Total	O	0	0
			293	293		

3 Residue-property plots (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.

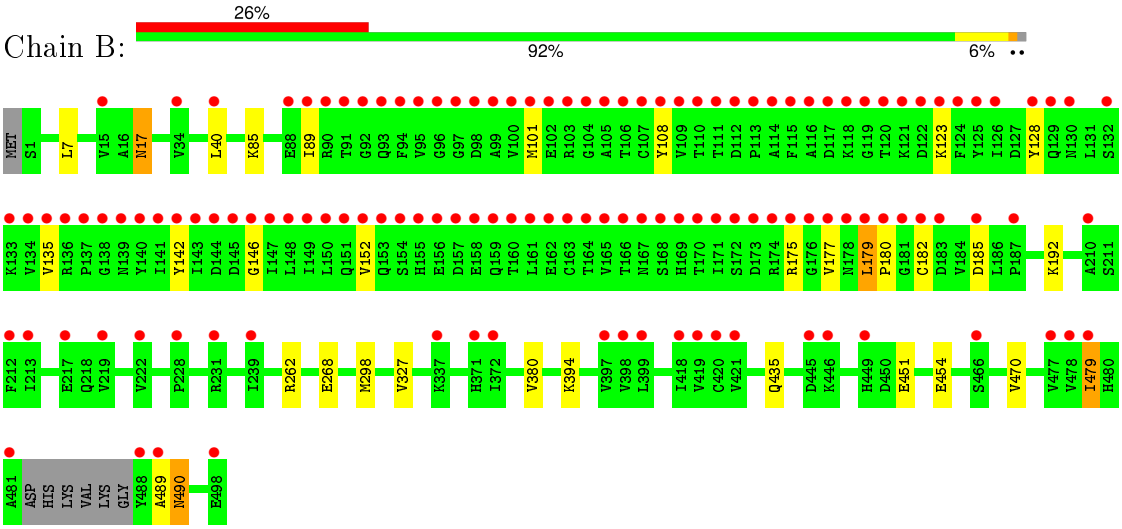
- Molecule 1: Pyruvate kinase

Chain A:



- Molecule 1: Pyruvate kinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	122.86Å 129.86Å 165.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.69 – 2.10 20.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.69-2.10) 100.0 (20.69-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.231 , 0.263 0.230 , 0.261	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)	0.40 , 58.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 76957 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8211	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

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

[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, PTK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/3808	0.53	2/5154 (0.0%)
1	B	0.39	0/3808	0.50	0/5154
All	All	0.39	0/7616	0.51	2/10308 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 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	3753	0	3752	27	0
1	B	3753	0	3752	21	0
2	A	24	0	32	3	0
2	B	6	0	8	0	0
3	A	32	0	10	9	0
4	A	350	0	0	4	0
4	B	293	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8211	0	7554	57	0

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 4.

All (57) 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)
3:A:501:PTK:HAP	3:A:501:PTK:OAK	1.58	0.99
3:A:501:PTK:HAQ	3:A:501:PTK:OAJ	1.62	0.98
3:A:501:PTK:HAR	3:A:501:PTK:OAG	1.57	0.98
3:A:501:PTK:OAB	3:A:501:PTK:HAO	1.82	0.80
1:A:479:ILE:HD11	1:A:489:ALA:HB1	1.66	0.77
1:B:135:VAL:HG11	1:B:152:VAL:HG21	1.75	0.69
1:A:135:VAL:HG11	1:A:152:VAL:HG21	1.76	0.67
1:A:298:MET:HE3	1:A:316:VAL:HG22	1.80	0.63
1:A:298:MET:HE2	1:A:327:VAL:HB	1.80	0.63
1:A:398:VAL:HG13	1:A:479:ILE:HD13	1.84	0.59
1:B:479:ILE:HD11	1:B:489:ALA:CB	2.33	0.59
1:B:179:LEU:HB3	1:B:182:CYS:HB2	1.85	0.58
1:B:394:LYS:HB2	1:B:470:VAL:HG12	1.86	0.57
3:A:501:PTK:CAQ	3:A:501:PTK:OAJ	2.45	0.57
3:A:501:PTK:CAR	3:A:501:PTK:OAG	2.42	0.56
1:B:298:MET:HE2	1:B:327:VAL:HB	1.89	0.54
1:A:179:LEU:HB3	1:A:182:CYS:HB2	1.89	0.54
1:A:223:ARG:HD2	4:A:553:HOH:O	2.06	0.54
1:B:479:ILE:HD11	1:B:489:ALA:HB1	1.89	0.54
3:A:501:PTK:CAP	3:A:501:PTK:OAK	2.42	0.54
1:A:455:HIS:HD2	4:A:559:HOH:O	1.91	0.53
1:B:17:ASN:H	1:B:17:ASN:HD22	1.56	0.53
1:A:377:ASP:HB3	1:A:488:TYR:CD2	2.44	0.53
1:B:298:MET:CE	1:B:327:VAL:HB	2.39	0.53
1:A:380:VAL:HG21	1:A:490:ASN:HA	1.92	0.52
1:A:298:MET:CE	1:A:316:VAL:HG22	2.40	0.50
1:B:380:VAL:HG21	1:B:490:ASN:HA	1.94	0.49
3:A:501:PTK:HOAK	3:A:501:PTK:HAP	1.72	0.49
1:A:451:GLU:CD	1:A:451:GLU:H	2.17	0.48
1:B:180:PRO:HB3	1:B:268:GLU:HB2	1.97	0.47
1:A:298:MET:HB3	1:A:298:MET:HE3	1.74	0.47
1:B:128:TYR:OH	1:B:185:ASP:OD2	2.27	0.47
1:A:479:ILE:HD11	1:A:489:ALA:CB	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:HA	2:A:502:GOL:H11	1.97	0.46
3:A:501:PTK:CAO	3:A:501:PTK:OAB	2.59	0.45
1:A:322:ASN:HA	2:A:502:GOL:C1	2.46	0.45
1:B:101:MET:HE1	4:B:600:HOH:O	2.16	0.45
1:B:101:MET:CE	4:B:600:HOH:O	2.64	0.45
1:A:287:VAL:HG21	1:B:7:LEU:HD11	1.99	0.45
1:B:85:LYS:HD3	1:B:192:LYS:HD3	1.98	0.44
1:B:108:TYR:O	1:B:123:LYS:HA	2.17	0.44
1:B:89:ILE:HG23	1:B:128:TYR:HB2	2.00	0.44
1:A:108:TYR:O	1:A:123:LYS:HA	2.18	0.44
1:B:17:ASN:N	1:B:17:ASN:HD22	2.13	0.43
1:A:394:LYS:HB2	1:A:470:VAL:HG12	1.99	0.43
1:A:488:TYR:CD2	1:A:489:ALA:O	2.71	0.43
1:B:490:ASN:HD22	1:B:490:ASN:H	1.66	0.43
1:B:142:TYR:HB3	1:B:146:GLY:HA2	2.00	0.43
1:A:298:MET:HG3	1:A:328:MET:O	2.19	0.42
1:A:374:MET:CE	1:A:378:GLU:HG3	2.50	0.41
1:A:136:ARG:H	1:A:139:ASN:ND2	2.19	0.41
1:A:142:TYR:HB3	1:A:146:GLY:HA2	2.02	0.41
1:A:398:VAL:HG22	1:A:479:ILE:HG23	2.03	0.41
1:A:446:LYS:HD3	4:A:815:HOH:O	2.19	0.41
2:A:502:GOL:H12	4:A:547:HOH:O	2.21	0.41
1:A:79:ALA:HB2	1:A:429:ARG:O	2.20	0.41
1:B:451:GLU:CD	1:B:451:GLU:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (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	488/499 (98%)	476 (98%)	11 (2%)	1 (0%)	52 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	488/499 (98%)	479 (98%)	9 (2%)	0	100 100
All	All	976/998 (98%)	955 (98%)	20 (2%)	1 (0%)	56 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	THR

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	411/417 (99%)	401 (98%)	10 (2%)	57 61
1	B	411/417 (99%)	401 (98%)	10 (2%)	57 61
All	All	822/834 (99%)	802 (98%)	20 (2%)	57 61

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

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

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Mol	Chain	Res	Type
1	B	262	ARG
1	B	435	GLN
1	B	454	GLU
1	B	479	ILE
1	B	490	ASN

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

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

5.3.3 RNA (i)

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)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	A	499	-	5,5,5	0.42	0	5,5,5	0.30	0
2	GOL	A	500	-	5,5,5	0.43	0	5,5,5	0.21	0
3	PTK	A	501	-	35,35,35	1.69	8 (22%)	50,60,60	1.65	12 (24%)
2	GOL	A	502	-	5,5,5	0.43	0	5,5,5	0.60	0
2	GOL	A	503	-	5,5,5	0.34	0	5,5,5	0.25	0
2	GOL	B	499	-	5,5,5	0.34	0	5,5,5	0.32	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	0/4/4/4
2	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	GOL	B	499	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PTK	CAV-CAZ	-2.80	1.39	1.43
3	A	501	PTK	CAS-CAW	-2.74	1.39	1.43
3	A	501	PTK	CAT-CAX	-2.74	1.39	1.43
3	A	501	PTK	CAU-CAY	-2.74	1.39	1.43
3	A	501	PTK	CAT-SBD	-2.35	1.75	1.78
3	A	501	PTK	CAU-SBE	-2.30	1.75	1.78
3	A	501	PTK	CAV-SBF	-2.30	1.75	1.78
3	A	501	PTK	CAS-SBC	-2.19	1.75	1.78

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	PTK	CAR-CAZ-CAV	-3.08	119.74	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	PTK	CAQ-CAX-CAT	-2.99	119.86	123.83
3	A	501	PTK	CAP-CAY-CAU	-2.96	119.89	123.83
3	A	501	PTK	CAO-CAW-CAS	-2.94	119.93	123.83
3	A	501	PTK	OAG-SBF-CAV	2.61	109.16	106.20
3	A	501	PTK	OAI-SBC-CAS	2.78	109.35	106.20
3	A	501	PTK	OAJ-SBD-CAT	2.78	109.35	106.20
3	A	501	PTK	OAF-SBE-CAU	2.80	109.38	106.20
3	A	501	PTK	OAE-SBE-CAU	2.98	109.58	106.20
3	A	501	PTK	OAH-SBF-CAV	3.00	109.61	106.20
3	A	501	PTK	OAA-SBC-CAS	3.06	109.67	106.20
3	A	501	PTK	OAD-SBD-CAT	3.13	109.74	106.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	PTK	9	0
2	A	502	GOL	3	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%)	0.59	49 (9%) 9 13	20, 33, 55, 60	0
1	B	492/499 (98%)	2.01	129 (26%) 1 1	21, 34, 55, 60	0
All	All	984/998 (98%)	1.30	178 (18%) 2 2	20, 34, 55, 60	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	95	VAL	18.3
1	B	94	PHE	17.6
1	B	171	ILE	16.8
1	B	172	SER	14.5
1	B	104	GLY	14.4
1	B	166	THR	14.2
1	B	115	PHE	13.8
1	B	116	ALA	13.6
1	B	149	ILE	13.4
1	B	170	THR	13.2
1	B	96	GLY	12.7
1	B	142	TYR	12.6
1	B	167	ASN	12.5
1	B	105	ALA	12.4
1	B	147	ILE	11.8
1	B	106	THR	11.3
1	B	109	VAL	11.3
1	B	169	HIS	11.0
1	B	101	MET	10.8
1	B	103	ARG	10.7
1	B	155	HIS	10.7
1	B	145	ASP	10.7
1	B	119	GLY	10.6
1	B	108	TYR	10.5

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Mol	Chain	Res	Type	RSRZ
1	B	140	TYR	10.4
1	B	136	ARG	10.4
1	B	99	ALA	10.1
1	B	113	PRO	10.0
1	B	138	GLY	10.0
1	B	124	PHE	10.0
1	B	122	ASP	9.8
1	B	125	TYR	9.8
1	B	137	PRO	9.8
1	B	146	GLY	9.4
1	A	488	TYR	9.3
1	B	165	VAL	9.3
1	B	150	LEU	9.2
1	B	97	GLY	8.8
1	B	152	VAL	8.8
1	B	154	SER	8.8
1	B	168	SER	8.5
1	B	126	ILE	8.3
1	B	121	LYS	8.3
1	B	114	ALA	8.3
1	B	117	ASP	8.2
1	B	163	CYS	8.1
1	B	139	ASN	8.1
1	B	182	CYS	8.0
1	B	153	GLN	7.9
1	B	488	TYR	7.8
1	B	98	ASP	7.7
1	B	159	GLN	7.6
1	B	93	GLN	7.6
1	B	92	GLY	7.5
1	B	164	THR	7.5
1	B	134	VAL	7.4
1	B	120	THR	7.0
1	B	175	ARG	7.0
1	B	181	GLY	6.9
1	B	156	GLU	6.9
1	B	158	GLU	6.8
1	B	179	LEU	6.8
1	B	157	ASP	6.8
1	B	148	LEU	6.6
1	B	133	LYS	6.6
1	B	151	GLN	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	112	ASP	6.4
1	B	176	GLY	6.4
1	B	123	LYS	6.3
1	B	90	ARG	6.2
1	B	481	ALA	6.2
1	B	173	ASP	6.1
1	A	109	VAL	6.1
1	B	102	GLU	6.0
1	B	107	CYS	5.9
1	B	118	LYS	5.7
1	B	100	VAL	5.7
1	B	183	ASP	5.7
1	B	162	GLU	5.5
1	B	174	ARG	5.3
1	B	489	ALA	5.2
1	B	129	GLN	5.2
1	B	144	ASP	4.9
1	B	111	THR	4.7
1	B	110	THR	4.6
1	A	141	ILE	4.5
1	A	177	VAL	4.5
1	B	372	ILE	4.4
1	B	160	THR	4.3
1	B	141	ILE	4.3
1	B	89	ILE	4.3
1	B	371	HIS	4.3
1	A	489	ALA	3.9
1	A	150	LEU	3.9
1	B	177	VAL	3.9
1	B	397	VAL	3.9
1	B	143	ILE	3.9
1	A	481	ALA	3.8
1	B	213	ILE	3.8
1	B	91	THR	3.8
1	B	180	PRO	3.7
1	B	135	VAL	3.5
1	A	158	GLU	3.4
1	B	449	HIS	3.4
1	B	132	SER	3.4
1	B	178	ASN	3.3
1	A	54	HIS	3.3
1	A	397	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	478	VAL	3.3
1	A	97	GLY	3.3
1	B	446	LYS	3.3
1	A	477	VAL	3.3
1	B	217	GLU	3.2
1	A	143	ILE	3.2
1	A	103	ARG	3.1
1	B	88	GLU	3.1
1	A	479	ILE	3.1
1	A	124	PHE	3.1
1	B	187	PRO	3.1
1	A	126	ILE	3.1
1	B	421	VAL	3.0
1	A	372	ILE	3.0
1	B	161	LEU	3.0
1	B	478	VAL	3.0
1	B	479	ILE	3.0
1	A	304	TYR	2.9
1	A	163	CYS	2.9
1	B	15	VAL	2.9
1	A	398	VAL	2.9
1	B	130	ASN	2.9
1	A	418	ILE	2.8
1	B	231	ARG	2.8
1	B	222	VAL	2.8
1	A	107	CYS	2.7
1	B	185	ASP	2.7
1	A	165	VAL	2.7
1	B	228	PRO	2.6
1	B	445	ASP	2.6
1	A	98	ASP	2.6
1	A	161	LEU	2.6
1	B	419	VAL	2.5
1	A	136	ARG	2.5
1	B	399	LEU	2.5
1	A	95	VAL	2.4
1	B	466	SER	2.4
1	B	219	VAL	2.3
1	A	89	ILE	2.3
1	A	169	HIS	2.3
1	A	307	ARG	2.3
1	B	239	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	208	ILE	2.3
1	A	110	THR	2.3
1	B	40	LEU	2.3
1	A	131	LEU	2.3
1	A	138	GLY	2.2
1	A	471	GLN	2.2
1	B	418	ILE	2.2
1	B	420	CYS	2.2
1	B	210	ALA	2.2
1	A	14	PRO	2.2
1	A	419	VAL	2.2
1	A	420	CYS	2.1
1	A	168	SER	2.1
1	A	94	PHE	2.1
1	B	337	LYS	2.1
1	A	170	THR	2.1
1	A	281	LEU	2.1
1	B	398	VAL	2.1
1	B	212	PHE	2.1
1	A	236	ILE	2.1
1	A	37	LEU	2.1
1	A	371	HIS	2.1
1	B	498	GLU	2.1
1	B	128	TYR	2.1
1	B	34	VAL	2.1
1	A	1	SER	2.0
1	A	17	ASN	2.0
1	B	477	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	A	500	6/6	0.73	0.30	3.10	63,63,63,63	0
2	GOL	A	502	6/6	0.84	0.23	2.96	36,41,42,43	0
2	GOL	A	503	6/6	0.68	0.22	1.15	59,61,62,62	0
2	GOL	B	499	6/6	0.56	0.20	0.94	67,68,68,68	0
2	GOL	A	499	6/6	0.62	0.31	0.77	41,44,45,46	0
3	PTK	A	501	32/32	0.44	0.27	-	100,100,101,101	32

6.5 Other polymers (i)

There are no such residues in this entry.