



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:20 PM GMT

PDB ID : 3QV7
Title : Crystal structure of Leishmania mexicana pyruvate kinase(LmPYK)in complex with ponceau S and acid blue 25.
Authors : Morgan, H.P.; Auld, D.S.; McNae, I.W.; Nowicki, M.W.; Michels, P.A.M.; Fothergill-Gilmore, L.A.; Walkinshaw, M.D.
Deposited on : 2011-02-25
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ](#)) 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

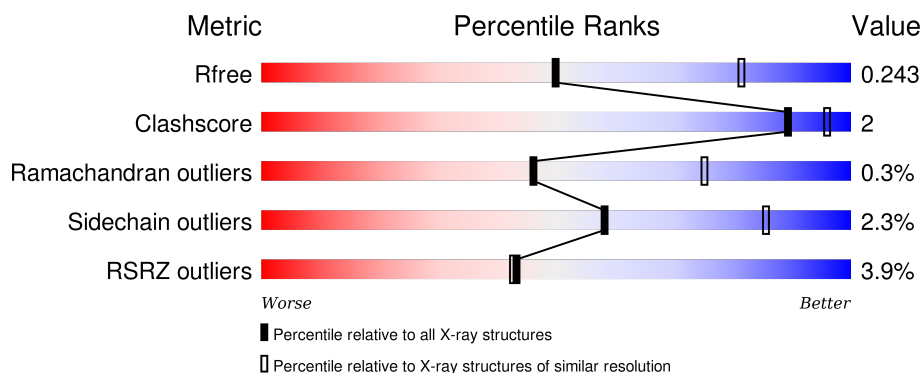
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 $\leq 5\%$. 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	<div> <div>3%</div> <div>91%</div> <div>8% ..</div> </div>
1	B	499	<div> <div>2%</div> <div>75%</div> <div>5%</div> <div>20%</div> </div>
1	C	499	<div> <div>6%</div> <div>74%</div> <div>6%</div> <div>20%</div> </div>
1	D	499	<div> <div>4%</div> <div>93%</div> <div>5% .</div> </div>

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	SO4	D	499	-	-	-	X
3	K	D	501	-	-	-	X
4	QV7	B	501	-	-	-	X
4	QV7	B	504	-	-	-	X
4	QV7	D	503	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14425 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	494	Total	C	N	O	S	0	4	0
			3793	2367	666	734	26			
1	A	493	Total	C	N	O	S	0	3	0
			3774	2355	661	732	26			
1	B	400	Total	C	N	O	S	0	2	0
			3051	1908	540	581	22			
1	C	398	Total	C	N	O	S	0	2	0
			3032	1895	536	579	22			

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

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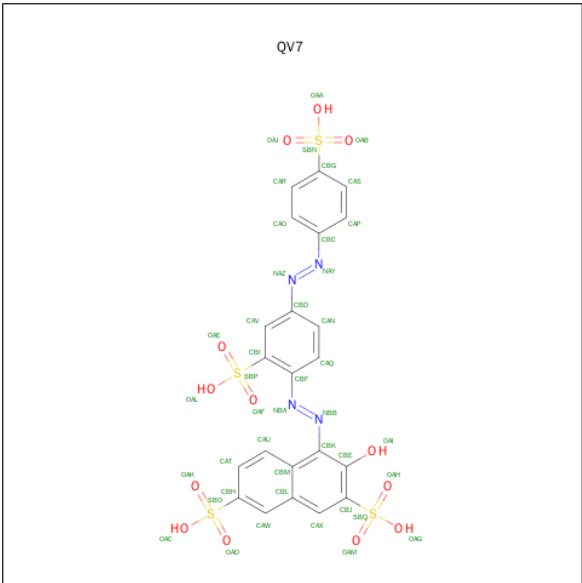
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	K	0	0
			2	2		
3	A	2	Total	K	0	0
			2	2		
3	D	2	Total	K	0	0
			2	2		
3	C	2	Total	K	0	0
			2	2		

- Molecule 4 is 3-HYDROXY-4-[(E)-{2-SULFO-4-[(E)-(4-SULFOPHENYL)DIAZENYL]PHENYL}DIAZENYL]NAPHTHALENE-2,7-DISULFONIC ACID (three-letter code: QV7) (formula: C₂₂H₁₆N₄O₁₃S₄).



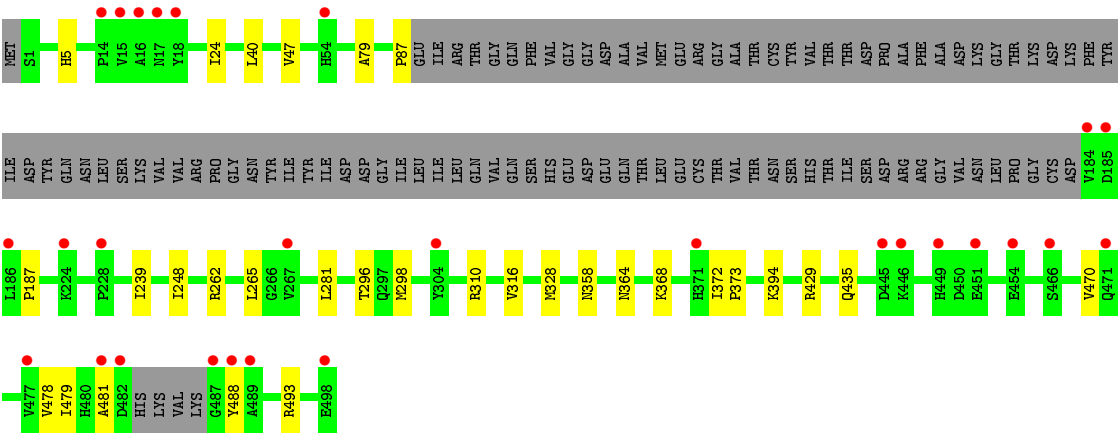
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			43	22	4	13	4		
4	A	1	Total	C	N	O	S	0	0
			43	22	4	13	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 43	C 22	N 4	O 13	S 4	0	0
4	B	1	Total 43	C 22	N 4	O 13	S 4	0	0
4	B	1	Total 43	C 22	N 4	O 13	S 4	0	0

- QV8
-
- The diagram illustrates the chemical structure of QV8, which consists of two fused benzene rings connected by a central carbon atom. The left ring is substituted with eight labels: CAI, CAM, CAJ, CAN, CAW, CAX, CAU, and CAV. The right ring is substituted with seven labels: CAP, CAY, CAS, CAO, CAT, CAZ, and CAG. A central carbon atom is bonded to OAA, OAB, and a nitrogen atom (NH). The nitrogen atom is further bonded to a phenyl ring with four additional substituents: CAR, CAH, CAF, and CAG.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	161	Total O 161 161	0	0
6	A	167	Total O 167 167	0	0
6	B	109	Total O 109 109	0	0
6	C	68	Total O 68 68	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.11Å 164.80Å 123.35Å 90.00° 115.80° 90.00°	Depositor
Resolution (Å)	21.14 – 2.70 21.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (21.14-2.70) 99.8 (21.14-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.215 , 0.244 0.215 , 0.243	Depositor DCC
R_{free} test set	4480 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 89352 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14425	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: K, QV7, QV8, 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	0.31	0/3839	0.46	0/5197
1	B	0.31	0/3101	0.45	0/4193
1	C	0.31	0/3081	0.44	0/4167
1	D	0.32	0/3863	0.45	0/5230
All	All	0.31	0/13884	0.45	0/18787

There are no bond length outliers.

There are no bond angle outliers.

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	3774	0	3775	16	0
1	B	3051	0	3087	11	0
1	C	3032	0	3058	13	0
1	D	3793	0	3788	11	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	43	0	14	0	0
4	B	129	0	42	1	0
4	D	43	0	14	10	0
5	B	27	0	13	5	0
6	A	167	0	0	0	0
6	B	109	0	0	1	0
6	C	68	0	0	0	0
6	D	161	0	0	0	0
All	All	14425	0	13791	67	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 2.

The worst 5 of 67 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)
4:D:503:QV7:CAO	4:D:503:QV7:HAN	1.70	1.20
4:D:503:QV7:NBA	4:D:503:QV7:HAU	1.56	1.19
4:D:503:QV7:CAN	4:D:503:QV7:CAO	2.34	1.04
4:D:503:QV7:HAO	4:D:503:QV7:HAN	1.01	1.00
4:D:503:QV7:CAN	4:D:503:QV7:HAO	1.90	1.00

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	492/499 (99%)	483 (98%)	8 (2%)	1 (0%)	52 80
1	B	398/499 (80%)	389 (98%)	7 (2%)	2 (0%)	34 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	394/499 (79%)	383 (97%)	10 (2%)	1 (0%)	46	75
1	D	494/499 (99%)	480 (97%)	13 (3%)	1 (0%)	52	80
All	All	1778/1996 (89%)	1735 (98%)	38 (2%)	5 (0%)	46	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	296	THR
1	A	296	THR
1	C	296	THR
1	B	188	ALA
1	B	296	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	414/417 (99%)	400 (97%)	14 (3%)	44	75
1	B	333/417 (80%)	326 (98%)	7 (2%)	61	87
1	C	331/417 (79%)	324 (98%)	7 (2%)	61	87
1	D	416/417 (100%)	409 (98%)	7 (2%)	68	90
All	All	1494/1668 (90%)	1459 (98%)	35 (2%)	58	85

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	GLU
1	A	435	GLN
1	C	368	LYS
1	A	262	ARG
1	A	310	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	ASN
1	B	286	ASN
1	C	435	GLN
1	A	471	GLN
1	B	17	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\# Z > 2$
4	QV7	A	499	-	45,46,46	1.31	6 (13%)	66,72,72	1.43	10 (15%)
2	SO4	A	500	-	4,4,4	0.24	0	6,6,6	0.10	0
4	QV7	B	499	-	45,46,46	1.23	4 (8%)	66,72,72	1.51	10 (15%)
5	QV8	B	500	-	30,30,30	1.54	5 (16%)	44,45,45	0.73	0
4	QV7	B	501	-	45,46,46	1.18	4 (8%)	66,72,72	1.85	9 (13%)
4	QV7	B	504	-	45,46,46	1.17	4 (8%)	66,72,72	1.49	10 (15%)
2	SO4	C	499	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	D	499	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	D	500	-	4,4,4	0.22	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	QV7	D	503	-	45,46,46	1.27	4 (8%)	66,72,72	1.36	11 (16%)

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
4	QV7	A	499	-	-	0/34/34/34	0/4/4/4
2	SO4	A	500	-	-	0/0/0/0	0/0/0/0
4	QV7	B	499	-	-	0/34/34/34	0/4/4/4
5	QV8	B	500	-	-	0/10/26/26	0/4/4/4
4	QV7	B	501	-	-	0/34/34/34	0/4/4/4
4	QV7	B	504	-	-	0/34/34/34	0/4/4/4
2	SO4	C	499	-	-	0/0/0/0	0/0/0/0
2	SO4	D	499	-	-	0/0/0/0	0/0/0/0
2	SO4	D	500	-	-	0/0/0/0	0/0/0/0
4	QV7	D	503	-	-	0/34/34/34	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	QV8	CAW-CAU	-4.04	1.39	1.48
4	A	499	QV7	CBF-NBA	-3.95	1.33	1.42
5	B	500	QV8	CAY-CAU	-3.89	1.40	1.48
5	B	500	QV8	CAX-CAV	-3.66	1.40	1.48
4	D	503	QV7	CBF-NBA	-3.58	1.34	1.42

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	QV7	CBE-CBK-NBB	-3.70	120.22	124.16
4	D	503	QV7	CAU-CBM-CBK	-2.93	119.22	123.81
4	A	499	QV7	CAU-CBM-CBK	-2.70	119.59	123.81
4	B	499	QV7	CBE-CBK-NBB	-2.57	121.42	124.16
4	A	499	QV7	CBE-CBK-NBB	-2.54	121.45	124.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	500	QV8	5	0
4	B	501	QV7	1	0
4	D	503	QV7	10	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	493/499 (98%)	-0.08	15 (3%) 54 54	27, 38, 59, 67	0
1	B	400/499 (80%)	-0.14	8 (2%) 68 69	30, 44, 54, 57	0
1	C	398/499 (79%)	0.13	28 (7%) 19 17	37, 51, 64, 71	0
1	D	494/499 (98%)	0.02	18 (3%) 46 46	27, 41, 57, 62	0
All	All	1785/1996 (89%)	-0.02	69 (3%) 43 43	27, 44, 60, 71	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	488	TYR	5.1
1	C	14	PRO	4.4
1	D	449	HIS	4.0
1	A	487	GLY	3.7
1	D	109	VAL	3.6

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	QV7	B	504	43/43	0.81	0.30	3.89	81,87,88,88	0
4	QV7	B	501	43/43	0.72	0.31	3.75	94,101,102,102	0
2	SO4	D	499	5/5	0.81	0.25	3.10	103,103,103,103	0
3	K	D	501	1/1	0.24	0.28	2.07	94,94,94,94	0
5	QV8	B	500	27/27	0.84	0.27	1.55	97,97,98,98	0
4	QV7	D	503	43/43	0.82	0.24	0.80	62,65,66,66	43
4	QV7	A	499	43/43	0.90	0.18	0.49	64,67,70,71	0
2	SO4	A	500	5/5	0.97	0.17	0.05	89,89,89,89	0
3	K	C	500	1/1	0.54	0.18	-0.24	88,88,88,88	0
2	SO4	D	500	5/5	0.97	0.17	-0.50	71,71,71,71	0
4	QV7	B	499	43/43	0.96	0.13	-0.57	41,42,45,45	0
2	SO4	C	499	5/5	0.97	0.11	-1.18	89,89,89,89	0
3	K	D	502	1/1	0.94	0.14	-	65,65,65,65	0
3	K	B	502	1/1	0.92	0.19	-	91,91,91,91	0
3	K	B	503	1/1	0.80	0.11	-	58,58,58,58	0
3	K	C	501	1/1	0.90	0.11	-	61,61,61,61	0
3	K	A	502	1/1	0.78	0.14	-	59,59,59,59	0
3	K	A	501	1/1	0.93	0.07	-	64,64,64,64	0

6.5 Other polymers

There are no such residues in this entry.