Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:20 PM GMT

PDB ID	:	3QV9
Title	:	Crystal structure of Trypanosoma cruzi pyruvate kinase(TcPYK)in complex with ponceau S.
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	:	2.10 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 (i) symbol.

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

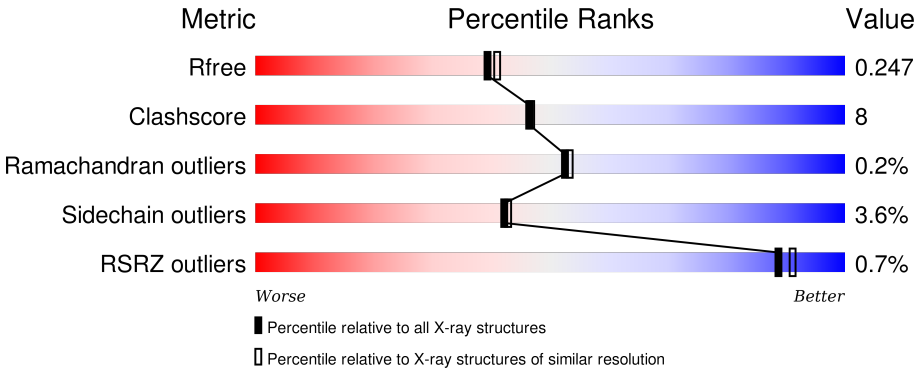
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	% 82% 17%
1	B	499	67% 11% 21%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7464 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.

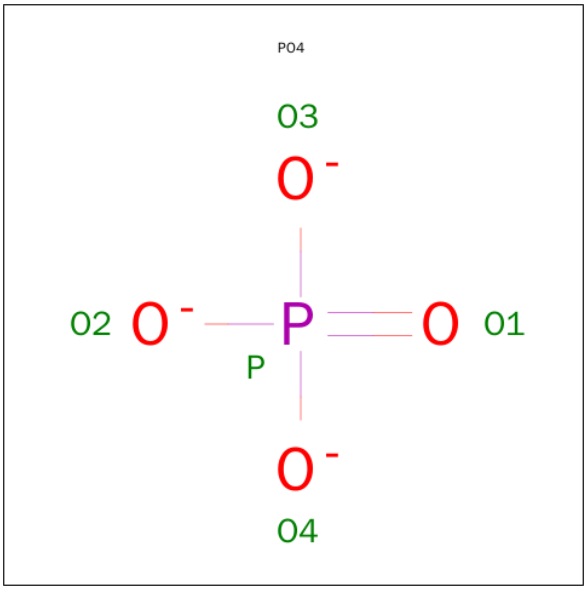
- Molecule 1 is a protein called Pyruvate kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	5	0
			3849	2407	679	734	29			
1	B	394	Total	C	N	O	S	0	3	0
			3014	1871	538	579	26			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

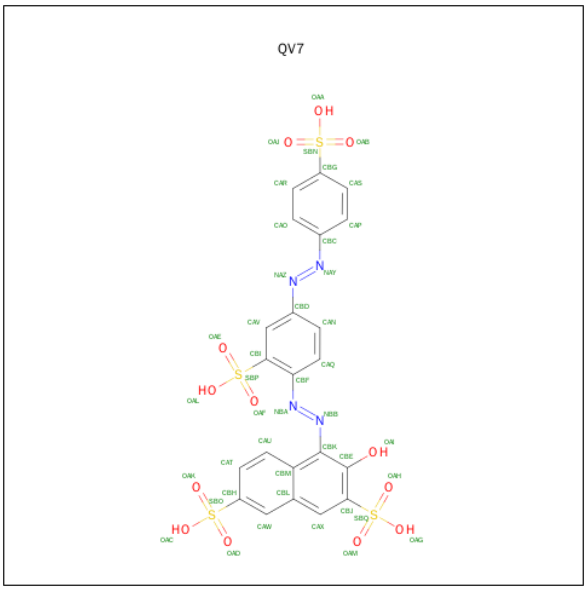
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- 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: $C_{22}H_{16}N_4O_{13}S_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O S 129 66 12 39 12	0	1

- Molecule 5 is water.

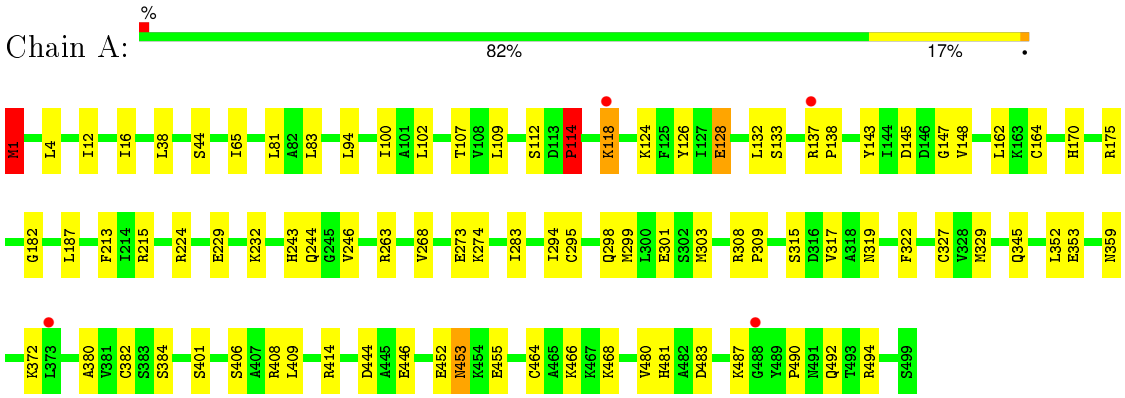
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	257	Total O 257 257	0	0
5	B	208	Total O 208 208	0	0

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.

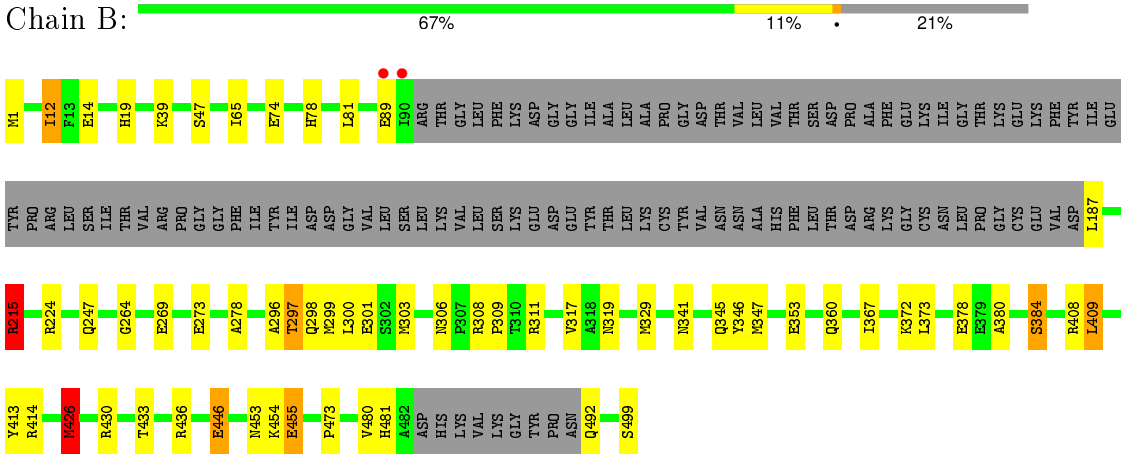
- Molecule 1: Pyruvate kinase 2

Chain A:



- Molecule 1: Pyruvate kinase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.20Å 121.83Å 96.54Å 90.00° 109.81° 90.00°	Depositor
Resolution (Å)	90.82 – 2.10 53.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (90.82-2.10) 98.2 (53.25-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.249 0.198 , 0.247	Depositor DCC
R_{free} test set	3563 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 70415 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7464	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: K, QV7, PO4

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	1.02	3/3923 (0.1%)	0.93	5/5298 (0.1%)
1	B	1.06	1/3060 (0.0%)	1.00	11/4127 (0.3%)
All	All	1.04	4/6983 (0.1%)	0.96	16/9425 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	PHE	CD2-CE2	5.91	1.51	1.39
1	A	452	GLU	CG-CD	5.65	1.60	1.51
1	A	452	GLU	CB-CG	5.39	1.62	1.52
1	B	446	GLU	CB-CG	-5.10	1.42	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	408	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	408	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	B	436	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	414	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	B	409	LEU	CB-CG-CD2	-7.21	98.74	111.00
1	B	224	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	215	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	B	408	ARG	CG-CD-NE	-6.07	99.06	111.80
1	A	224	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	215	ARG	CG-CD-NE	5.70	123.78	111.80
1	B	436	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	480	VAL	CB-CA-C	-5.56	100.84	111.40
1	B	430	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	1	MET	N-CA-C	-5.23	96.87	111.00
1	A	187	LEU	CA-CB-CG	5.19	127.24	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	426	MET	CG-SD-CE	-5.02	92.17	100.20

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	3849	0	3910	64	1
1	B	3014	0	3068	54	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
4	B	129	0	43	1	0
5	A	257	0	0	6	0
5	B	208	0	0	1	0
All	All	7464	0	7021	107	1

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 8.

All (107) 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:B:264:GLY:H	1:B:297:THR:HG21	1.14	1.08
1:B:296:ALA:O	1:B:297:THR:HB	1.52	1.08
1:B:299:MET:HE3	1:B:317:VAL:HG22	1.15	1.08
1:A:299:MET:HE3	1:A:317:VAL:HG22	1.41	1.01
1:A:464:CYS:SG	1:A:468:LYS:NZ	2.34	1.00
1:B:303:MET:HE1	1:B:309:PRO:HG3	1.42	0.98
1:B:299:MET:CE	1:B:317:VAL:HG22	1.95	0.96
1:B:303:MET:CE	1:B:309:PRO:HG3	2.01	0.89
1:B:39:LYS:NZ	1:B:74:GLU:OE2	2.12	0.81
1:B:264:GLY:N	1:B:297:THR:HG21	1.97	0.77
1:B:297:THR:HG23	1:B:298:GLN:HG3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LEU:HD13	1:B:303:MET:HE3	1.69	0.75
1:B:360:GLN:HE22	1:B:414:ARG:HH11	1.36	0.73
1:A:301[B]:GLU:OE1	5:A:855:HOH:O	2.07	0.72
1:A:453:ASN:ND2	5:A:610:HOH:O	2.22	0.72
1:B:299:MET:HE3	1:B:317:VAL:CG2	2.09	0.72
1:B:380:ALA:O	1:B:384:SER:HB3	1.95	0.67
1:B:296:ALA:O	1:B:297:THR:CB	2.33	0.66
1:A:481:HIS:HA	1:A:490:PRO:HB3	1.79	0.65
1:B:360:GLN:NE2	1:B:414:ARG:HH11	1.95	0.64
1:A:481:HIS:CA	1:A:490:PRO:HB3	2.27	0.64
1:B:78:HIS:HE1	1:B:426:MET:CE	2.11	0.63
1:B:473:PRO:HG3	1:B:499:SER:O	1.99	0.62
1:A:319[A]:ASN:OD1	1:B:319:ASN:ND2	2.34	0.60
1:A:446:GLU:HG2	5:A:608:HOH:O	2.01	0.59
1:B:300:LEU:HD13	1:B:303:MET:CE	2.32	0.59
1:B:264:GLY:H	1:B:297:THR:CG2	2.03	0.59
1:A:94:LEU:HB2	1:A:118:LYS:HA	1.83	0.59
1:B:187:LEU:O	1:B:215:ARG:NH2	2.37	0.58
1:A:16:ILE:HG21	1:A:352:LEU:HG	1.86	0.58
1:B:78:HIS:HE1	1:B:426:MET:HE1	1.69	0.57
1:A:44:SER:HB3	1:A:345:GLN:HG3	1.85	0.57
1:A:12:ILE:HD13	1:B:278:ALA:HB2	1.86	0.56
1:A:145:ASP:O	1:A:148:VAL:HG22	2.06	0.55
1:A:444:ASP:OD2	5:A:609:HOH:O	2.18	0.54
1:B:378:GLU:HG2	1:B:409:LEU:HD21	1.89	0.54
1:B:303:MET:HE2	1:B:309:PRO:HG3	1.88	0.53
1:A:118:LYS:O	1:A:118:LYS:HG2	2.07	0.53
1:A:182:GLY:C	1:A:243:HIS:CE1	2.82	0.53
1:B:360:GLN:HE21	1:B:414:ARG:HD2	1.75	0.52
1:A:481:HIS:C	1:A:490:PRO:HB3	2.30	0.52
1:A:137:ARG:O	1:A:138:PRO:C	2.46	0.52
1:A:273:GLU:HG3	1:B:353:GLU:HG3	1.92	0.51
1:A:353:GLU:HG3	1:B:273:GLU:HG3	1.93	0.51
1:A:246:VAL:HG11	1:B:12:ILE:HD11	1.91	0.51
1:B:481:HIS:O	1:B:492:GLN:HB3	2.11	0.51
1:A:147:GLY:HA3	1:A:268:VAL:HG13	1.92	0.50
1:A:4:LEU:HD21	1:B:367:ILE:HD13	1.92	0.50
1:A:112:SER:O	1:A:114:PRO:HD3	2.12	0.50
1:B:14:GLU:HA	1:B:14:GLU:OE1	2.12	0.50
4:B:501[C]:QV7:OAI	4:B:501[C]:QV7:NBA	2.44	0.50
1:A:298:GLN:HB3	1:B:311:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301[B]:GLU:OE2	5:A:759:HOH:O	2.19	0.49
1:A:1:MET:HB3	1:A:359:ASN:HD21	1.77	0.49
1:A:401:SER:HB2	1:A:406:SER:HB3	1.95	0.49
1:A:483:ASP:HB3	1:A:492:GLN:OE1	2.13	0.49
1:A:446:GLU:HA	1:A:446:GLU:OE2	2.14	0.48
1:A:294:ILE:HG12	1:A:327:CYS:HB2	1.95	0.47
1:B:308:ARG:HH21	1:B:308:ARG:HB2	1.79	0.47
1:A:466:LYS:HE2	5:A:820:HOH:O	2.15	0.46
1:A:453:ASN:ND2	1:A:455:GLU:H	2.13	0.46
1:A:273:GLU:CG	1:B:353:GLU:HG3	2.46	0.46
1:A:315:SER:O	1:A:319[B]:ASN:HB2	2.16	0.46
1:A:299:MET:HG3	1:A:329:MET:O	2.16	0.46
1:B:308:ARG:NH2	1:B:308:ARG:HB2	2.31	0.45
1:B:298:GLN:HA	1:B:301[B]:GLU:HG3	1.99	0.45
1:B:341:ASN:O	1:B:345:GLN:HG3	2.17	0.45
1:A:65:ILE:HG12	1:A:81:LEU:HD21	1.98	0.45
1:A:83:LEU:HD23	1:A:83:LEU:C	2.37	0.45
1:B:19:HIS:ND1	5:B:662:HOH:O	2.30	0.44
1:A:148:VAL:HG23	1:A:170:HIS:CE1	2.53	0.44
1:A:380:ALA:O	1:A:384:SER:HB3	2.17	0.44
1:A:481:HIS:NE2	1:A:494:ARG:NE	2.65	0.44
1:B:78:HIS:CE1	1:B:426:MET:CE	2.98	0.44
1:B:47:SER:HB3	1:B:433:THR:HB	1.98	0.44
1:A:453:ASN:HD22	1:A:455:GLU:H	1.65	0.44
1:A:12:ILE:CD1	1:B:278:ALA:HB2	2.48	0.44
1:B:453:ASN:C	1:B:455:GLU:H	2.21	0.44
1:A:100:ILE:HD12	1:A:102:LEU:HD21	1.99	0.44
1:A:126:TYR:CE1	1:A:128:GLU:HA	2.52	0.43
1:A:107:THR:HA	1:A:164:CYS:O	2.18	0.43
1:A:353:GLU:HG3	1:B:273:GLU:CG	2.47	0.43
1:A:143:TYR:HB3	1:A:147:GLY:HA2	2.00	0.43
1:A:283:ILE:HD11	1:A:295[A]:CYS:SG	2.59	0.43
1:A:382:CYS:SG	1:A:409:LEU:HD23	2.59	0.43
1:B:299:MET:HG3	1:B:329:MET:O	2.19	0.43
1:A:229:GLU:O	1:A:232:LYS:HG2	2.19	0.43
1:A:109:LEU:O	1:A:124:LYS:HA	2.19	0.42
1:B:453:ASN:O	1:B:455:GLU:N	2.52	0.42
1:A:481:HIS:O	1:A:492:GLN:HB3	2.19	0.42
1:B:308:ARG:HA	1:B:309:PRO:HD3	1.92	0.42
1:A:213:PHE:O	1:A:215:ARG:HD3	2.20	0.42
1:B:65:ILE:HG12	1:B:81:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:GLN:HA	1:B:301[A]:GLU:HG3	2.01	0.41
1:A:480:VAL:HG12	1:A:490:PRO:HB2	2.01	0.41
1:A:133:SER:HA	1:A:162:LEU:HD21	2.02	0.41
1:B:360:GLN:NE2	1:B:414:ARG:HD2	2.35	0.41
1:A:481:HIS:NE2	1:A:494:ARG:NH2	2.68	0.41
1:A:126:TYR:CZ	1:A:128:GLU:HA	2.55	0.41
1:A:243:HIS:CG	1:A:244:GLN:N	2.88	0.41
1:A:274:LYS:NZ	1:B:353:GLU:OE2	2.53	0.41
1:B:78:HIS:CE1	1:B:426:MET:HE2	2.56	0.40
1:A:126:TYR:CE1	1:A:128:GLU:OE1	2.74	0.40
1:B:413:TYR:O	1:B:414:ARG:HB2	2.21	0.40
1:A:319[A]:ASN:CG	1:B:319:ASN:ND2	2.75	0.40
1:A:308:ARG:HB2	1:A:309:PRO:HD2	2.04	0.40
1:A:38:LEU:HA	1:A:38:LEU:HD23	1.93	0.40

All (1) 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:A:492:GLN:NE2	1:B:492:GLN:OE1[2_656]	1.60	0.60

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	502/499 (101%)	482 (96%)	19 (4%)	1 (0%)	52 53
1	B	391/499 (78%)	381 (97%)	9 (2%)	1 (0%)	46 45
All	All	893/998 (90%)	863 (97%)	28 (3%)	2 (0%)	52 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	454	LYS
1	A	114	PRO

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	425/420 (101%)	414 (97%)	11 (3%)	54 58
1	B	333/420 (79%)	317 (95%)	16 (5%)	31 29
All	All	758/840 (90%)	731 (96%)	27 (4%)	42 43

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	114	PRO
1	A	118	LYS
1	A	128	GLU
1	A	132	LEU
1	A	175	ARG
1	A	263	ARG
1	A	303	MET
1	A	372	LYS
1	A	453	ASN
1	A	487	LYS
1	B	1	MET
1	B	12	ILE
1	B	89	GLU
1	B	215	ARG
1	B	247	GLN
1	B	269	GLU
1	B	297	THR
1	B	306	ASN
1	B	346	TYR
1	B	347	MET
1	B	372	LYS

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Mol	Chain	Res	Type
1	B	373	LEU
1	B	384	SER
1	B	426	MET
1	B	446	GLU
1	B	455	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	179	ASN
1	A	243	HIS
1	A	248	ASN
1	A	341	ASN
1	A	360	GLN
1	A	453	ASN
1	B	62	GLN
1	B	66	ASN
1	B	78	HIS
1	B	204	GLN
1	B	360	GLN
1	B	492	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	PO4	A	501	-	4,4,4	0.49	0	6,6,6	0.30	0
4	QV7	B	501[A]	-	45,46,46	1.31	6 (13%)	66,72,72	1.84	12 (18%)
4	QV7	B	501[B]	-	45,46,46	1.23	5 (11%)	66,72,72	1.70	13 (19%)
4	QV7	B	501[C]	-	45,46,46	1.33	7 (15%)	66,72,72	1.60	10 (15%)

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
3	PO4	A	501	-	-	0/0/0/0	0/0/0/0
4	QV7	B	501[A]	-	-	0/34/34/34	0/4/4/4
4	QV7	B	501[B]	-	-	0/34/34/34	0/4/4/4
4	QV7	B	501[C]	-	-	0/34/34/34	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501[C]	QV7	CBF-NBA	-3.89	1.34	1.42
4	B	501[B]	QV7	CBF-NBA	-3.42	1.35	1.42
4	B	501[A]	QV7	CBJ-SBQ	-2.87	1.74	1.78
4	B	501[B]	QV7	CBD-NAZ	-2.39	1.34	1.44
4	B	501[B]	QV7	CBC-NAY	-2.34	1.34	1.44
4	B	501[C]	QV7	CBC-NAY	-2.26	1.34	1.44
4	B	501[C]	QV7	CBD-NAZ	-2.23	1.35	1.44
4	B	501[A]	QV7	CBI-SBP	-2.11	1.75	1.78
4	B	501[A]	QV7	CBC-NAY	-2.11	1.35	1.44
4	B	501[A]	QV7	CBD-NAZ	-2.06	1.35	1.44
4	B	501[C]	QV7	CBK-CBM	-2.05	1.40	1.43
4	B	501[A]	QV7	CAW-CBH	2.09	1.40	1.36
4	B	501[B]	QV7	CAW-CBH	2.16	1.40	1.36
4	B	501[C]	QV7	CAW-CBH	2.18	1.40	1.36
4	B	501[C]	QV7	CBJ-SBQ	2.61	1.82	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501[A]	QV7	CAX-CBJ	2.62	1.40	1.37
4	B	501[B]	QV7	CAX-CBJ	2.64	1.40	1.37
4	B	501[C]	QV7	CAX-CBJ	2.77	1.40	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501[B]	QV7	CBE-CBK-NBB	-4.99	118.84	124.16
4	B	501[C]	QV7	CBE-CBK-NBB	-3.79	120.13	124.16
4	B	501[C]	QV7	CAX-CBJ-CBE	-3.42	118.16	121.05
4	B	501[A]	QV7	CBE-CBJ-SBQ	-2.89	118.17	121.15
4	B	501[A]	QV7	CAS-CBG-SBN	-2.71	116.58	119.75
4	B	501[A]	QV7	CBE-CBK-NBB	-2.49	121.51	124.16
4	B	501[A]	QV7	CAU-CBM-CBK	-2.27	120.25	123.81
4	B	501[C]	QV7	CAU-CBM-CBK	-2.25	120.28	123.81
4	B	501[B]	QV7	CAX-CBJ-CBE	-2.22	119.18	121.05
4	B	501[B]	QV7	CAU-CBM-CBK	-2.02	120.65	123.81
4	B	501[C]	QV7	CAX-CBJ-SBQ	2.02	121.32	117.82
4	B	501[B]	QV7	OAD-SBO-CBH	2.02	111.59	106.63
4	B	501[C]	QV7	CBC-NAY-NAZ	2.08	123.36	113.28
4	B	501[A]	QV7	OAK-SBO-CBH	2.11	111.81	106.63
4	B	501[B]	QV7	CBM-CBK-NBB	2.19	121.41	115.63
4	B	501[A]	QV7	OAA-SBN-CBG	2.22	113.20	106.94
4	B	501[A]	QV7	OAJ-SBN-CBG	2.33	112.36	106.63
4	B	501[A]	QV7	CAP-CAS-CBG	2.34	122.06	119.48
4	B	501[B]	QV7	CBC-NAY-NAZ	2.42	124.97	113.28
4	B	501[B]	QV7	CBF-NBA-NBB	2.49	120.55	114.55
4	B	501[C]	QV7	CBI-CBF-NBA	2.69	120.64	117.57
4	B	501[B]	QV7	CBI-CBF-NBA	3.15	121.17	117.57
4	B	501[C]	QV7	OAH-SBQ-CBJ	3.26	109.93	106.17
4	B	501[B]	QV7	OAE-SBP-CBI	3.72	110.45	106.17
4	B	501[B]	QV7	CBF-CBI-SBP	4.02	124.43	120.84
4	B	501[B]	QV7	OAF-SBP-CBI	4.09	110.89	106.17
4	B	501[C]	QV7	OAE-SBP-CBI	4.14	110.94	106.17
4	B	501[A]	QV7	CBF-NBA-NBB	4.16	124.58	114.55
4	B	501[A]	QV7	CAR-CBG-SBN	4.40	124.89	119.75
4	B	501[C]	QV7	OAM-SBQ-CBJ	4.45	111.30	106.17
4	B	501[B]	QV7	CBK-NBB-NBA	4.73	123.76	116.10
4	B	501[C]	QV7	CBK-NBB-NBA	5.05	124.28	116.10
4	B	501[B]	QV7	OAM-SBQ-CBJ	5.12	112.07	106.17
4	B	501[A]	QV7	OAH-SBQ-CBJ	6.75	113.95	106.17
4	B	501[A]	QV7	CBK-NBB-NBA	7.48	128.22	116.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501[C]	QV7	1	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	499/499 (100%)	-0.12	4 (0%)	87	90	15, 29, 52, 62	0
1	B	394/499 (78%)	-0.11	2 (0%)	91	93	14, 27, 43, 54	0
All	All	893/998 (89%)	-0.12	6 (0%)	89	91	14, 28, 50, 62	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	ARG	3.1
1	A	373	LEU	2.5
1	B	90	ILE	2.5
1	B	89	GLU	2.4
1	A	488	GLY	2.3
1	A	118	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
4	QV7	B	501[C]	43/43	0.95	0.14	1.77	2,4,6,7	43
4	QV7	B	501[B]	43/43	0.95	0.14	1.23	43,52,64,64	43
4	QV7	B	501[A]	43/43	0.95	0.14	0.82	25,28,40,41	43
3	PO4	A	501	5/5	0.93	0.15	0.55	74,74,76,77	0
2	K	B	502	1/1	0.98	0.12	0.54	48,48,48,48	0
2	K	A	500	1/1	0.98	0.07	-1.68	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.