



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:17 PM GMT

PDB ID : 2X0S
Title : 3.0 A RESOLUTION CRYSTAL STRUCTURE OF GLYCOSOMAL PYRUVATE PHOSPHATE DIKINASE FROM TRYPANOSOMA BRUCEI
Authors : Cosenza, L.W.; Bringaud, F.; Baltz, T.; Vellieux, F.M.D.
Deposited on : 2009-12-17
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

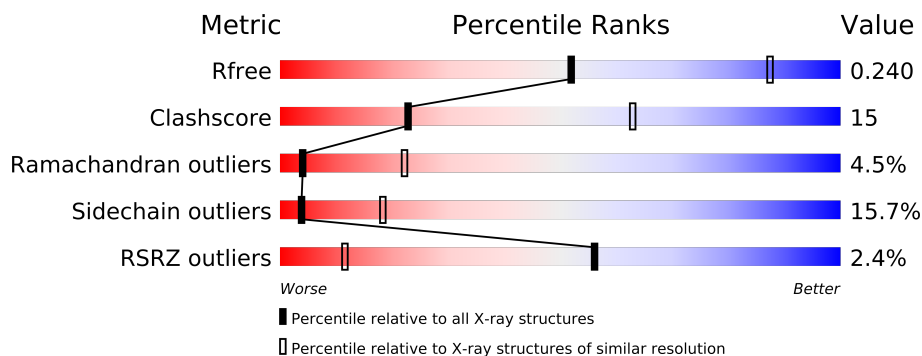
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	913	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6977 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOSPHATE DIKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	899	Total	C	N	O	S	0	2	0
			6941	4357	1255	1280	49			

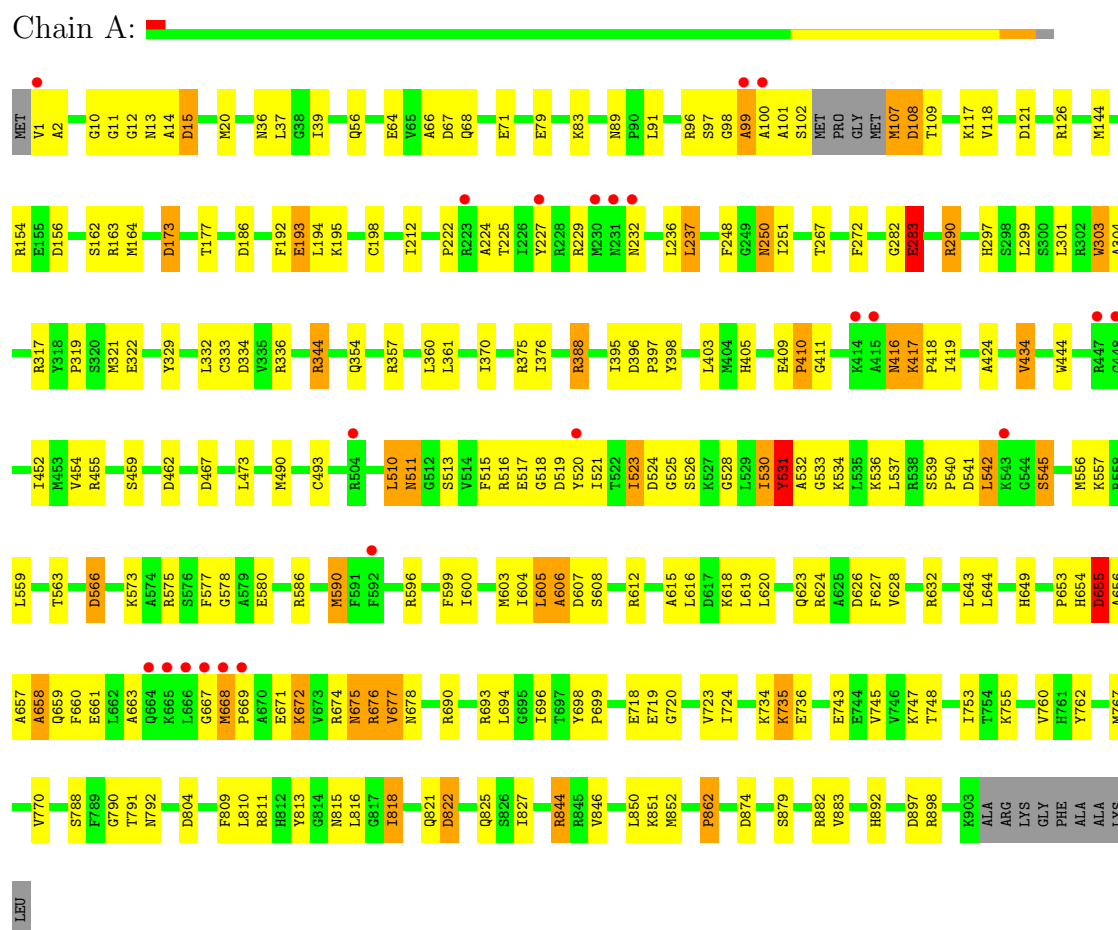
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		

3 Residue-property plots

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 PHOSPHATE DIKINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.17Å 153.50Å 65.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.94 – 3.00 23.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (23.94-3.00) 95.7 (23.94-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.99Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.165 , 0.241 0.166 , 0.240	Depositor DCC
R_{free} test set	1162 reflections (4.82%)	DCC
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 24119 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6977	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.46	0/7070	0.67	0/9531

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6941	0	0	102	0
2	A	36	0	0	4	0
All	All	6977	0	0	102	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (102) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:MET:SD	1:A:107:MET:N	2.48	0.87
1:A:675:ASN:CG	1:A:676:ARG:N	2.41	0.73
1:A:542:LEU:O	1:A:545:SER:N	2.24	0.70
1:A:659:GLN:NE2	1:A:660:PHE:CD2	2.60	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:344:ARG:NH1	1:A:344:ARG:CG	2.56	0.68
1:A:675:ASN:OD1	1:A:676:ARG:N	2.28	0.67
1:A:388:ARG:CG	1:A:388:ARG:NH1	2.59	0.66
1:A:515:PHE:CB	1:A:520:TYR:OH	2.44	0.66
1:A:511:ASN:O	2:A:2018:HOH:O	2.14	0.65
1:A:844:ARG:NH1	1:A:850:LEU:O	2.33	0.62
1:A:528:GLY:CA	2:A:2020:HOH:O	2.48	0.61
1:A:297:HIS:N	1:A:322:GLU:OE1	2.35	0.60
1:A:813:TYR:CD1	1:A:818:ILE:CG1	2.85	0.59
1:A:539:SER:O	1:A:541:ASP:N	2.35	0.59
1:A:248:PHE:N	1:A:354:GLN:NE2	2.50	0.59
1:A:524:ASP:OD1	1:A:525:GLY:N	2.35	0.59
1:A:531:TYR:C	1:A:533:GLY:N	2.54	0.59
1:A:524:ASP:OD1	1:A:524:ASP:C	2.42	0.58
1:A:516:ARG:O	1:A:518:GLY:N	2.38	0.57
1:A:117:LYS:O	1:A:121:ASP:OD1	2.24	0.56
1:A:677:VAL:CG1	1:A:678:ASN:N	2.68	0.56
1:A:409:GLU:O	1:A:411:GLY:N	2.38	0.56
1:A:236:LEU:O	1:A:237:LEU:CB	2.53	0.56
1:A:668:MET:SD	1:A:672:LYS:CB	2.93	0.56
1:A:10:GLY:O	1:A:12:GLY:N	2.39	0.55
1:A:154:ARG:C	1:A:156:ASP:N	2.61	0.55
1:A:557:LYS:NZ	1:A:559:LEU:O	2.41	0.54
1:A:623:GLN:O	1:A:626:ASP:N	2.41	0.54
1:A:612:ARG:NH1	1:A:698:TYR:CE1	2.76	0.53
1:A:519:ASP:CB	1:A:531:TYR:CE1	2.91	0.53
1:A:173:ASP:N	1:A:173:ASP:OD1	2.41	0.52
1:A:575:ARG:O	1:A:578:GLY:N	2.43	0.52
1:A:100:ALA:O	1:A:102:SER:N	2.43	0.52
1:A:724:ILE:CG1	1:A:724:ILE:O	2.59	0.50
1:A:530:ILE:O	1:A:531:TYR:CB	2.59	0.50
1:A:192:PHE:O	1:A:194:LEU:N	2.44	0.50
1:A:616:LEU:O	1:A:619:LEU:N	2.45	0.50
1:A:747:LYS:CG	1:A:748:THR:N	2.74	0.49
1:A:416:ASN:O	1:A:417:LYS:CG	2.61	0.49
1:A:329:TYR:C	1:A:329:TYR:CD2	2.85	0.49
1:A:762:TYR:N	1:A:762:TYR:CD2	2.81	0.49
1:A:417:LYS:N	1:A:418:PRO:CD	2.76	0.48
1:A:718:GLU:O	1:A:720:GLY:N	2.46	0.48
1:A:303:TRP:CD1	1:A:304:ALA:N	2.81	0.48
1:A:528:GLY:N	2:A:2020:HOH:O	2.45	0.48
1:A:539:SER:C	1:A:541:ASP:N	2.66	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:655:ASP:O	1:A:656:ALA:C	2.51	0.48
1:A:809:PHE:CD1	1:A:813:TYR:CE2	3.02	0.47
1:A:282:GLY:O	1:A:283:GLU:CB	2.62	0.47
1:A:821:GLN:O	1:A:822:ASP:C	2.53	0.47
1:A:623:GLN:O	1:A:624:ARG:C	2.50	0.47
1:A:98:GLY:O	1:A:99:ALA:CB	2.63	0.47
1:A:668:MET:CE	1:A:672:LYS:CD	2.93	0.47
1:A:520:TYR:N	1:A:520:TYR:CD1	2.82	0.47
1:A:599:PHE:CD1	1:A:599:PHE:N	2.82	0.47
1:A:250:ASN:C	1:A:250:ASN:ND2	2.69	0.47
1:A:659:GLN:N	1:A:659:GLN:CD	2.69	0.46
1:A:675:ASN:O	1:A:677:VAL:N	2.49	0.46
1:A:193:GLU:CG	1:A:193:GLU:O	2.63	0.46
1:A:66:ALA:O	1:A:67:ASP:C	2.53	0.46
1:A:510:LEU:O	1:A:511:ASN:C	2.54	0.45
1:A:590:MET:O	1:A:623:GLN:NE2	2.50	0.45
1:A:671:GLU:CB	1:A:674:ARG:NH2	2.80	0.45
1:A:154:ARG:O	1:A:156:ASP:N	2.49	0.45
1:A:661:GLU:N	1:A:661:GLU:OE1	2.50	0.45
1:A:334:ASP:C	1:A:334:ASP:OD1	2.55	0.45
1:A:566:ASP:OD1	1:A:566:ASP:N	2.50	0.45
1:A:398:TYR:CE1	1:A:862:PRO:CG	3.00	0.44
1:A:649:HIS:O	1:A:649:HIS:CG	2.70	0.44
1:A:790:GLY:O	1:A:792:ASN:N	2.49	0.44
1:A:693:ARG:O	1:A:696:ILE:CG1	2.65	0.44
1:A:409:GLU:C	1:A:411:GLY:N	2.70	0.44
1:A:370:ILE:CG1	1:A:403:LEU:CD1	2.97	0.43
1:A:693:ARG:NH2	2:A:2023:HOH:O	2.52	0.43
1:A:396:ASP:OD1	1:A:397:PRO:CD	2.67	0.43
1:A:672:LYS:O	1:A:675:ASN:OD1	2.35	0.43
1:A:375:ARG:O	1:A:376:ILE:C	2.57	0.43
1:A:605:LEU:O	1:A:606:ALA:C	2.57	0.43
1:A:734:LYS:O	1:A:736:GLU:N	2.51	0.43
1:A:531:TYR:O	1:A:532:ALA:C	2.57	0.42
1:A:616:LEU:C	1:A:618:LYS:N	2.73	0.42
1:A:882:ARG:O	1:A:883:VAL:C	2.57	0.42
1:A:657:ALA:O	1:A:658:ALA:CB	2.67	0.42
1:A:667:GLY:O	1:A:668:MET:CE	2.68	0.41
1:A:424:ALA:CB	1:A:524:ASP:O	2.68	0.41
1:A:523:ILE:CG1	1:A:524:ASP:N	2.84	0.41
1:A:13:ASN:O	1:A:36:ASN:OD1	2.38	0.41
1:A:192:PHE:C	1:A:194:LEU:N	2.73	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:612:ARG:O	1:A:615:ALA:N	2.54	0.41
1:A:660:PHE:C	1:A:660:PHE:CD1	2.94	0.41
1:A:590:MET:CE	1:A:627:PHE:CE1	3.03	0.41
1:A:605:LEU:O	1:A:607:ASP:N	2.54	0.41
1:A:434:VAL:CG1	1:A:520:TYR:CZ	3.04	0.41
1:A:14:ALA:O	1:A:15:ASP:C	2.59	0.41
1:A:222:PRO:C	1:A:224:ALA:N	2.73	0.41
1:A:409:GLU:CG	1:A:410:PRO:CD	2.99	0.41
1:A:852:MET:N	1:A:874:ASP:OD2	2.54	0.41
1:A:643:LEU:O	1:A:644:LEU:C	2.59	0.40
1:A:539:SER:N	1:A:540:PRO:CD	2.85	0.40
1:A:573:LYS:O	1:A:577:PHE:CD2	2.74	0.40
1:A:521:ILE:CD1	1:A:531:TYR:O	2.69	0.40
1:A:444:TRP:N	1:A:444:TRP:CD1	2.90	0.40

There are no symmetry-related clashes.

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	896/913 (98%)	731 (82%)	125 (14%)	40 (4%)	4 22

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ALA
1	A	101	ALA
1	A	237	LEU
1	A	319	PRO
1	A	417	LYS
1	A	511	ASN
1	A	517	GLU
1	A	531	TYR
1	A	658	ALA

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Mol	Chain	Res	Type
1	A	669	PRO
1	A	675	ASN
1	A	719	GLU
1	A	735	LYS
1	A	2	ALA
1	A	15	ASP
1	A	126	ARG
1	A	193	GLU
1	A	283	GLU
1	A	410	PRO
1	A	416	ASN
1	A	526	SER
1	A	542	LEU
1	A	606	ALA
1	A	608	SER
1	A	653	PRO
1	A	676	ARG
1	A	677	VAL
1	A	791	THR
1	A	11	GLY
1	A	663	ALA
1	A	290	ARG
1	A	654	HIS
1	A	108	ASP
1	A	655	ASP
1	A	822	ASP
1	A	419	ILE
1	A	846	VAL
1	A	818	ILE
1	A	862	PRO
1	A	699	PRO

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	727/735 (99%)	612 (84%)	115 (16%)	4 18

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	20	MET
1	A	37	LEU
1	A	39	ILE
1	A	56	GLN
1	A	64[A]	GLU
1	A	64[B]	GLU
1	A	68	GLN
1	A	71	GLU
1	A	79	GLU
1	A	83	LYS
1	A	89	ASN
1	A	91	LEU
1	A	96	ARG
1	A	97	SER
1	A	107	MET
1	A	108	ASP
1	A	109	THR
1	A	118	VAL
1	A	144	MET
1	A	162	SER
1	A	163[A]	ARG
1	A	164	MET
1	A	173	ASP
1	A	177	THR
1	A	186	ASP
1	A	195	LYS
1	A	198	CYS
1	A	212	ILE
1	A	225	THR
1	A	227	TYR
1	A	229	ARG
1	A	232	ASN
1	A	250	ASN
1	A	251	ILE
1	A	267	THR
1	A	272	PHE
1	A	283	GLU
1	A	290	ARG
1	A	299	LEU
1	A	301	LEU
1	A	303	TRP

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Mol	Chain	Res	Type
1	A	317	ARG
1	A	321	MET
1	A	332	LEU
1	A	333	CYS
1	A	336	ARG
1	A	344	ARG
1	A	357	ARG
1	A	360	LEU
1	A	361	LEU
1	A	388	ARG
1	A	395	ILE
1	A	405	HIS
1	A	434	VAL
1	A	452	ILE
1	A	454	VAL
1	A	455	ARG
1	A	459	SER
1	A	462	ASP
1	A	467	ASP
1	A	473	LEU
1	A	490	MET
1	A	493	CYS
1	A	510	LEU
1	A	513	SER
1	A	523	ILE
1	A	530	ILE
1	A	531	TYR
1	A	534	LYS
1	A	536	LYS
1	A	537	LEU
1	A	545	SER
1	A	556	MET
1	A	563	THR
1	A	566	ASP
1	A	580	GLU
1	A	586	ARG
1	A	590	MET
1	A	596	ARG
1	A	600	ILE
1	A	603	MET
1	A	604	ILE
1	A	605	LEU

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Mol	Chain	Res	Type
1	A	620	LEU
1	A	628	VAL
1	A	632	ARG
1	A	655	ASP
1	A	668	MET
1	A	672	LYS
1	A	690	ARG
1	A	694	LEU
1	A	723	VAL
1	A	735	LYS
1	A	743	GLU
1	A	745	VAL
1	A	753	ILE
1	A	755	LYS
1	A	760	VAL
1	A	767	MET
1	A	770	VAL
1	A	788	SER
1	A	804	ASP
1	A	810	LEU
1	A	811	ARG
1	A	815	ASN
1	A	816	LEU
1	A	825	GLN
1	A	827	ILE
1	A	844	ARG
1	A	851	LYS
1	A	879	SER
1	A	892	HIS
1	A	897	ASP
1	A	898	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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, 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	899/913 (98%)	-0.60	22 (2%) 56 11	23, 69, 163, 358	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	666	LEU	14.2
1	A	664	GLN	10.4
1	A	667	GLY	10.1
1	A	1	VAL	9.1
1	A	665	LYS	7.9
1	A	414	LYS	7.2
1	A	230	MET	4.7
1	A	448	GLY	4.6
1	A	227	TYR	3.6
1	A	447	ARG	3.5
1	A	668	MET	3.4
1	A	504	ARG	3.1
1	A	223	ARG	3.0
1	A	543	LYS	2.6
1	A	100	ALA	2.6
1	A	231	ASN	2.6
1	A	232	ASN	2.4
1	A	669	PRO	2.3
1	A	99	ALA	2.2
1	A	592	PHE	2.1
1	A	520	TYR	2.0
1	A	415	ALA	2.0

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.