



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:11 AM GMT

PDB ID : 3L6V
Title : Crystal Structure of the Xanthomonas campestris Gyrase A C-terminal Domain
Authors : Hsieh, T.J.; Yen, T.J.; Lin, T.S.; Chang, H.T.; Huang, S.Y.; Farh, L.; Chan, N.L.
Deposited on : 2009-12-26
Resolution : 2.19 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 ⓘ](#)) 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

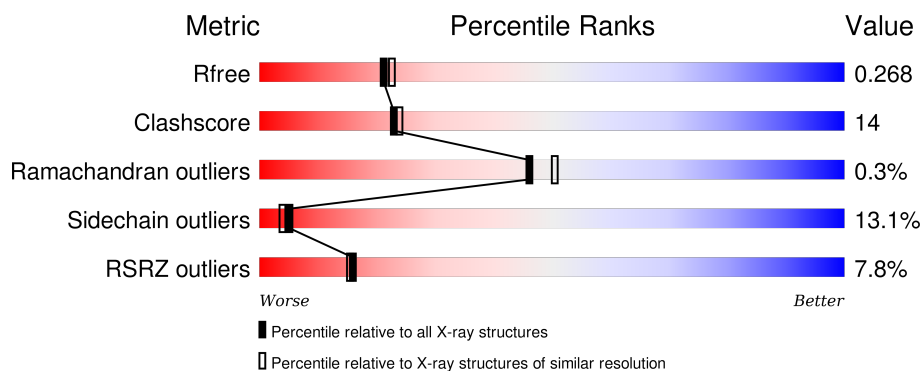
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	370	<div> <div>5%</div> <div>57%</div> <div>21%</div> <div>5%</div> <div>15%</div> </div>
1	B	370	<div> <div>8%</div> <div>65%</div> <div>15%</div> <div>•</div> <div>18%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4921 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2401	1495	450	452	4			
1	B	305	Total	C	N	O	S	0	0	0
			2344	1464	433	443	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	530	MET	LEU	ENGINEERED	UNP Q8PAB1
A	647	MET	PHE	CONFLICT	UNP Q8PAB1
A	830	MET	LEU	CONFLICT	UNP Q8PAB1
B	530	MET	LEU	ENGINEERED	UNP Q8PAB1
B	647	MET	PHE	CONFLICT	UNP Q8PAB1
B	830	MET	LEU	CONFLICT	UNP Q8PAB1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	83	Total	O	0	0
			83	83		
2	B	93	Total	O	0	0
			93	93		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.49 Å 58.97 Å 74.42 Å 79.00° 79.78° 69.62°	Depositor
Resolution (Å)	29.00 – 2.19 25.76 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.00-2.19) 91.9 (25.76-2.19)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.43 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.219 , 0.271 0.218 , 0.268	Depositor DCC
R_{free} test set	2022 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.1	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 40325 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4921	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.19% 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

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	0.88	1/2433 (0.0%)	0.98	9/3285 (0.3%)
1	B	0.82	0/2375	0.92	3/3209 (0.1%)
All	All	0.85	1/4808 (0.0%)	0.95	12/6494 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	538	VAL	CB-CG1	-6.13	1.40	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	739	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	797	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	557	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	830	MET	CG-SD-CE	-5.98	90.64	100.20
1	B	800	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	877	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	838	LEU	CA-CB-CG	5.53	128.02	115.30
1	B	557	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	665	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	557	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	734	LEU	CA-CB-CG	5.12	127.09	115.30
1	A	564	ARG	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	855	GLY	Peptide

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	2401	0	2459	77	0
1	B	2344	0	2398	53	0
2	A	83	0	0	4	0
2	B	93	0	0	5	0
All	All	4921	0	4857	130	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 14.

All (130) 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:A:713:MET:CE	1:A:719:GLY:HA2	1.64	1.27
1:A:713:MET:HE1	1:A:719:GLY:HA2	1.29	1.12
1:A:713:MET:HE3	1:A:719:GLY:HA2	1.39	1.04
1:A:853:THR:HG22	1:A:855:GLY:H	1.31	0.92
1:B:863:LYS:HE3	1:B:864:GLY:H	1.37	0.89
1:B:786:TYR:HB3	1:B:855:GLY:HA3	1.57	0.86
1:A:614:ARG:HH11	1:A:614:ARG:CG	1.93	0.81
1:B:691:ARG:HE	1:B:738:GLU:CD	1.83	0.81
1:A:713:MET:HE2	2:A:69:HOH:O	1.80	0.80
1:A:593:THR:HG23	1:A:595:SER:H	1.46	0.79
1:A:802:THR:HG23	1:A:804:GLY:H	1.46	0.79
1:A:699:ASN:HB2	2:A:92:HOH:O	1.83	0.79
1:B:637:ARG:HG3	1:B:637:ARG:HH11	1.48	0.78
1:A:584:ASN:HD22	1:A:586:HIS:H	1.33	0.77
1:B:682:VAL:HG12	1:B:682:VAL:O	1.85	0.76
1:B:666:LEU:HD23	1:B:670:LYS:HE3	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:THR:HG22	1:A:786:TYR:H	1.55	0.72
1:B:637:ARG:NH1	2:B:168:HOH:O	2.22	0.72
1:A:593:THR:HG22	1:A:597:LYS:H	1.54	0.71
1:A:713:MET:HE1	1:A:719:GLY:CA	2.16	0.70
1:A:782:THR:HG23	1:A:814:ASN:O	1.90	0.70
1:A:713:MET:HE3	1:A:719:GLY:CA	2.19	0.70
1:A:706:GLY:O	1:A:709:THR:HB	1.92	0.69
1:A:649:THR:HG21	1:A:653:THR:HB	1.74	0.69
1:A:614:ARG:HG2	1:A:614:ARG:HH11	1.58	0.68
1:A:567:SER:HB3	1:A:841:THR:HG23	1.74	0.68
1:A:689:GLY:HA2	1:A:707:GLU:OE2	1.94	0.67
1:B:863:LYS:HE3	1:B:864:GLY:N	2.08	0.67
1:B:811:THR:HG23	1:B:814:ASN:H	1.60	0.67
1:B:718:THR:HG23	2:B:79:HOH:O	1.94	0.67
1:B:559:GLN:HG3	1:B:559:GLN:O	1.95	0.66
1:A:853:THR:HG22	1:A:855:GLY:N	2.08	0.66
1:A:548:ALA:HB2	1:A:618:ILE:HG23	1.76	0.65
1:B:713:MET:HE1	1:B:719:GLY:HA2	1.79	0.64
1:A:853:THR:CG2	1:A:854:GLN:N	2.62	0.63
1:A:853:THR:CG2	1:A:855:GLY:H	2.07	0.62
1:A:605:GLN:HE21	1:A:621:TRP:HE1	1.46	0.62
1:B:787:GLY:HA3	1:B:858:LEU:HD11	1.81	0.61
1:A:849:VAL:HG11	1:A:853:THR:HG21	1.81	0.61
1:A:709:THR:HG23	1:A:800:ARG:HE	1.65	0.61
1:A:713:MET:CE	1:A:719:GLY:CA	2.59	0.59
1:B:814:ASN:HD21	1:B:855:GLY:H	1.50	0.59
1:B:718:THR:CG2	2:B:79:HOH:O	2.50	0.59
1:B:551:GLN:HE22	1:B:559:GLN:NE2	2.00	0.59
1:B:637:ARG:CG	1:B:637:ARG:HH11	2.14	0.59
1:A:810:THR:O	1:A:810:THR:HG23	2.02	0.59
1:A:649:THR:HG22	1:A:653:THR:H	1.68	0.59
1:B:649:THR:HG23	1:B:679:ASP:OD2	2.03	0.58
1:A:634:LEU:HD13	1:A:686:LEU:HD13	1.86	0.58
1:A:593:THR:HG21	1:A:628:GLU:OE2	2.04	0.58
1:B:649:THR:CG2	1:B:679:ASP:OD2	2.52	0.58
1:A:655:LYS:HG3	1:A:713:MET:CE	2.34	0.57
1:A:709:THR:HG22	1:A:710:VAL:HG23	1.86	0.57
1:A:584:ASN:ND2	1:A:586:HIS:H	2.02	0.57
1:B:806:ILE:HG21	1:B:852:ASN:ND2	2.20	0.57
1:A:699:ASN:CB	2:A:92:HOH:O	2.46	0.56
1:A:542:LEU:HD13	2:A:133:HOH:O	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:ARG:NH2	2:B:40:HOH:O	2.36	0.56
1:A:593:THR:CG2	1:A:628:GLU:OE2	2.53	0.56
1:A:622:ILE:HG22	1:A:624:LEU:HD13	1.88	0.55
1:B:609:ALA:HB1	1:B:613:ALA:HB3	1.89	0.55
1:A:853:THR:HG22	1:A:854:GLN:N	2.20	0.55
1:B:810:THR:HG23	1:B:810:THR:O	2.07	0.55
1:A:739:ARG:CZ	1:A:797:ARG:HH22	2.20	0.54
1:B:738:GLU:OE2	1:B:738:GLU:HA	2.08	0.54
1:A:649:THR:CG2	1:A:653:THR:HB	2.37	0.54
1:A:614:ARG:NH1	1:A:614:ARG:CG	2.65	0.54
1:B:587:ASP:OD1	1:B:637:ARG:HG2	2.08	0.54
1:B:682:VAL:CG1	1:B:682:VAL:O	2.54	0.54
1:A:649:THR:CG2	1:A:679:ASP:OD2	2.57	0.53
1:A:703:VAL:HG13	1:A:723:ILE:HD12	1.91	0.53
1:B:649:THR:HG23	1:B:679:ASP:OD1	2.08	0.53
1:A:798:LYS:HG3	1:A:802:THR:HG21	1.91	0.53
1:A:655:LYS:HG3	1:A:713:MET:HE3	1.92	0.52
1:A:542:LEU:HD21	1:A:618:ILE:HG12	1.90	0.52
1:B:704:ARG:NH1	1:B:795:TYR:O	2.37	0.52
1:A:614:ARG:HH11	1:A:614:ARG:HG3	1.75	0.51
1:B:831:LEU:HB2	1:B:839:VAL:HG22	1.93	0.50
1:B:649:THR:HG23	1:B:679:ASP:CG	2.32	0.50
1:A:689:GLY:CA	1:A:707:GLU:OE2	2.59	0.50
1:A:802:THR:CG2	1:A:804:GLY:H	2.20	0.49
1:A:639:TYR:HA	1:A:659:LEU:HD13	1.95	0.49
1:A:703:VAL:HG12	1:A:802:THR:HG22	1.94	0.49
1:A:799:GLY:O	1:A:802:THR:HB	2.13	0.49
1:B:555:ALA:O	1:B:559:GLN:HG2	2.13	0.48
1:A:605:GLN:NE2	1:A:621:TRP:HE1	2.11	0.48
1:B:576:PHE:HE1	1:B:830:MET:HE2	1.76	0.48
1:B:587:ASP:CG	1:B:637:ARG:HG2	2.33	0.48
1:A:543:SER:HA	1:A:577:ILE:HA	1.96	0.47
1:A:609:ALA:HB1	1:A:613:ALA:HB3	1.96	0.47
1:A:670:LYS:HB3	1:A:715:ARG:HH21	1.79	0.47
1:A:788:LYS:HE3	1:A:851:ARG:HA	1.96	0.47
1:B:798:LYS:O	1:B:798:LYS:HG3	2.15	0.47
1:B:580:LEU:C	1:B:580:LEU:HD23	2.36	0.46
1:B:576:PHE:CE1	1:B:830:MET:HE2	2.50	0.46
1:B:649:THR:HG21	1:B:653:THR:HB	1.98	0.46
1:A:649:THR:HG21	1:A:679:ASP:OD2	2.15	0.45
1:B:787:GLY:CA	1:B:858:LEU:HD11	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:SER:HB2	1:A:629:ARG:H	1.80	0.45
1:A:655:LYS:HG3	1:A:713:MET:HE2	1.99	0.45
1:A:649:THR:HG23	1:A:651:ASN:H	1.81	0.45
1:B:781:ALA:O	1:B:817:LEU:HD12	2.16	0.45
1:A:798:LYS:HE3	1:A:802:THR:CG2	2.47	0.44
1:B:639:TYR:HA	1:B:659:LEU:HD13	1.99	0.44
1:B:693:VAL:O	1:B:704:ARG:HA	2.17	0.44
1:A:695:LEU:O	1:A:702:THR:HA	2.16	0.44
1:B:695:LEU:O	1:B:702:THR:HA	2.18	0.44
1:A:641:ASP:O	1:A:642:ASN:HB2	2.16	0.44
1:B:787:GLY:HA3	1:B:858:LEU:CD1	2.48	0.44
1:A:614:ARG:HG2	1:A:614:ARG:NH1	2.28	0.44
1:B:581:TRP:CD1	1:B:635:PRO:HG2	2.53	0.44
1:A:599:PHE:CE2	1:A:623:PRO:HD2	2.52	0.44
1:B:778:ILE:HD11	1:B:792:LEU:HD23	2.01	0.43
1:A:699:ASN:HA	1:A:810:THR:HG21	2.01	0.42
1:B:637:ARG:CG	1:B:637:ARG:NH1	2.77	0.42
1:A:649:THR:HG23	1:A:679:ASP:OD2	2.19	0.42
1:A:824:GLY:N	1:A:827:ASP:OD2	2.49	0.42
1:B:705:PHE:CD2	1:B:800:ARG:HG3	2.53	0.42
1:B:806:ILE:HD13	1:B:852:ASN:HD21	1.85	0.42
1:A:564:ARG:HH11	1:A:564:ARG:HB3	1.85	0.42
1:A:781:ALA:O	1:A:817:LEU:HD12	2.20	0.41
1:B:710:VAL:HG22	1:B:800:ARG:HD2	2.01	0.41
1:B:670:LYS:HD3	1:B:715:ARG:NH2	2.35	0.41
1:B:649:THR:HG22	1:B:653:THR:H	1.85	0.41
1:A:593:THR:HG23	1:A:595:SER:N	2.25	0.41
1:A:782:THR:HG21	1:A:786:TYR:HB2	2.03	0.41
1:A:594:SER:CB	1:A:629:ARG:H	2.33	0.41
1:B:860:ARG:HD2	2:B:154:HOH:O	2.21	0.40
1:A:703:VAL:CG1	1:A:802:THR:HG22	2.52	0.40
1:B:649:THR:HG21	1:B:679:ASP:OD2	2.20	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	309/370 (84%)	297 (96%)	10 (3%)	2 (1%)	30	29
1	B	299/370 (81%)	287 (96%)	12 (4%)	0	100	100
All	All	608/740 (82%)	584 (96%)	22 (4%)	2 (0%)	46	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	GLY
1	A	594	SER

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	253/297 (85%)	208 (82%)	45 (18%)	2	1
1	B	249/297 (84%)	228 (92%)	21 (8%)	14	13
All	All	502/594 (84%)	436 (87%)	66 (13%)	5	4

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	531	ASP
1	A	533	ILE
1	A	539	VAL
1	A	542	LEU
1	A	560	ARG
1	A	561	ARG
1	A	564	ARG
1	A	571	THR
1	A	577	ILE
1	A	585	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	593	THR
1	A	594	SER
1	A	614	ARG
1	A	616	ARG
1	A	624	LEU
1	A	638	GLU
1	A	641	ASP
1	A	649	THR
1	A	659	LEU
1	A	668	ARG
1	A	686	LEU
1	A	693	VAL
1	A	707	GLU
1	A	709	THR
1	A	727	LYS
1	A	734	LEU
1	A	739	ARG
1	A	782	THR
1	A	792	LEU
1	A	802	THR
1	A	803	GLN
1	A	810	THR
1	A	830	MET
1	A	839	VAL
1	A	841	THR
1	A	854	GLN
1	A	858	LEU
1	A	859	ILE
1	A	862	SER
1	A	866	LYS
1	A	867	LEU
1	A	868	GLN
1	A	872	ARG
1	A	873	LEU
1	A	877	LEU
1	B	538	VAL
1	B	542	LEU
1	B	624	LEU
1	B	637	ARG
1	B	649	THR
1	B	659	LEU
1	B	671	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	702	THR
1	B	718	THR
1	B	734	LEU
1	B	792	LEU
1	B	810	THR
1	B	822	LEU
1	B	832	ILE
1	B	838	LEU
1	B	841	THR
1	B	842	ARG
1	B	852	ASN
1	B	856	VAL
1	B	863	LYS
1	B	867	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	584	ASN
1	A	605	GLN
1	B	559	GLN
1	B	642	ASN
1	B	852	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](#)

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	313/370 (84%)	0.50	20 (6%)	23 22	14, 28, 44, 56	0
1	B	305/370 (82%)	0.55	28 (9%)	11 10	12, 29, 47, 57	0
All	All	618/740 (83%)	0.53	48 (7%)	16 15	12, 29, 47, 57	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	560	ARG	6.1
1	B	826	THR	6.1
1	A	612	ASN	5.7
1	A	611	SER	5.4
1	B	825	SER	5.2
1	A	562	GLY	4.8
1	B	739	ARG	4.8
1	A	863	LYS	4.2
1	B	855	GLY	3.9
1	A	677	GLU	3.6
1	B	641	ASP	3.6
1	B	690	ASP	3.6
1	A	864	GLY	3.5
1	B	842	ARG	3.5
1	A	561	ARG	3.5
1	B	668	ARG	3.4
1	A	812	GLU	3.3
1	B	775	VAL	3.0
1	B	612	ASN	3.0
1	B	626	SER	2.9
1	A	642	ASN	2.9
1	B	812	GLU	2.9
1	B	738	GLU	2.9
1	B	664	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	531	ASP	2.8
1	A	641	ASP	2.8
1	A	627	GLY	2.7
1	A	826	THR	2.7
1	A	640	ALA	2.7
1	B	875	ALA	2.6
1	B	824	GLY	2.6
1	B	863	LYS	2.6
1	B	638	GLU	2.6
1	B	642	ASN	2.6
1	A	876	SER	2.5
1	A	610	GLY	2.5
1	A	699	ASN	2.5
1	B	627	GLY	2.4
1	B	531	ASP	2.4
1	A	858	LEU	2.3
1	B	568	ALA	2.3
1	A	738	GLU	2.2
1	B	637	ARG	2.2
1	B	864	GLY	2.2
1	B	611	SER	2.1
1	A	638	GLU	2.1
1	B	604	HIS	2.0
1	B	845	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.