Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:35 PM GMT

PDB ID	:	1BJT
Title	:	TOPOISOMERASE II RESIDUES 409-1201
Authors	:	Fass, D.; Bogden, C.E.; Berger, J.M.
Deposited on	:	1998-06-29
Resolution	:	2.50 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:

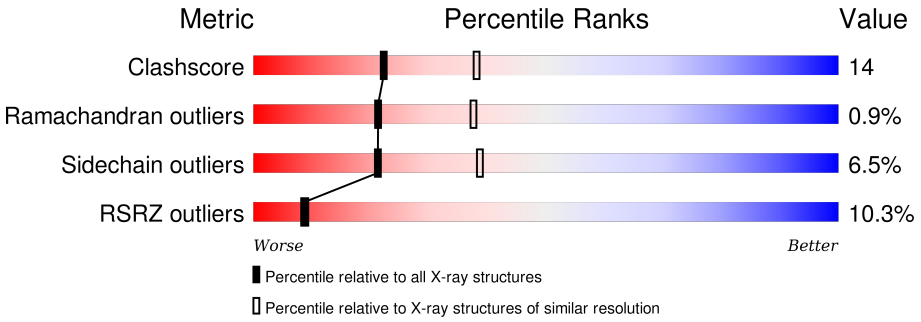
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	793	9% 63% 20% • 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5815 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 TOPOISOMERASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	679	Total	C	N	O	S	0	0	0
			5598	3621	939	1018	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	547	LEU	PRO	CONFLICT	UNP P06786

- Molecule 2 is water.

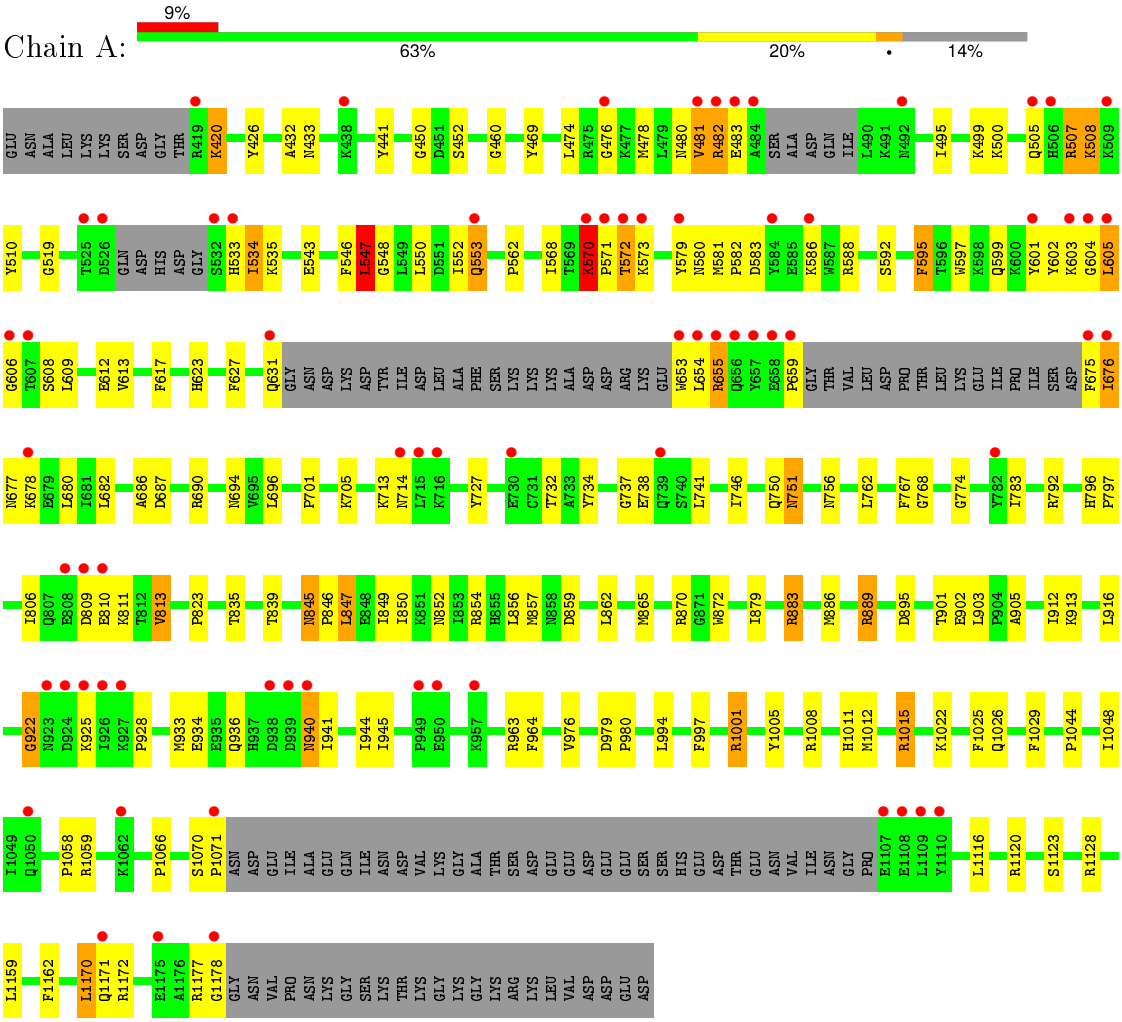
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	217	Total	O	0	0
			217	217		

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: TOPOISOMERASE II

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	103.40Å 145.70Å 161.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.00 – 2.50 13.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (14.00-2.50) 98.0 (13.92-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.58 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.227 , 0.269 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 41302 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5815	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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

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	0.40	0/5727	0.66	2/7718 (0.0%)

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	A	0	1

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	659	PRO	CA-C-O	12.23	149.55	120.20
1	A	1178	GLY	CA-C-O	6.48	132.27	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	676	ILE	Mainchain

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	5598	0	5637	155	0
2	A	217	0	0	3	0
All	All	5815	0	5637	155	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 (155) 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:603:LYS:HB2	1:A:675:PHE:HE1	1.22	1.00
1:A:482:ARG:HD3	1:A:482:ARG:H	1.25	0.98
1:A:627:PHE:HD1	1:A:654:LEU:HD12	1.38	0.88
1:A:623:HIS:CE1	1:A:654:LEU:HD22	2.10	0.87
1:A:903:LEU:HG	1:A:941:ILE:HD13	1.59	0.83
1:A:605:LEU:HG	1:A:606:GLY:N	1.96	0.81
1:A:481:VAL:HG12	1:A:482:ARG:NH1	1.98	0.78
1:A:570:LYS:HB3	1:A:571:PRO:HD3	1.65	0.78
1:A:1120:ARG:HH11	1:A:1120:ARG:HG3	1.49	0.76
1:A:603:LYS:CB	1:A:675:PHE:HE1	1.98	0.75
1:A:568:ILE:O	1:A:573:LYS:HA	1.86	0.75
1:A:603:LYS:HB2	1:A:675:PHE:CE1	2.14	0.73
1:A:655:ARG:H	1:A:655:ARG:HD3	1.53	0.73
1:A:627:PHE:HD1	1:A:654:LEU:CD1	2.02	0.72
1:A:547:LEU:HD22	1:A:547:LEU:H	1.55	0.71
1:A:854:ARG:HA	1:A:857:MET:HE2	1.73	0.71
1:A:655:ARG:CD	1:A:655:ARG:H	2.06	0.67
1:A:481:VAL:HG12	1:A:482:ARG:HH11	1.60	0.66
1:A:852:ASN:HB3	1:A:994:LEU:HD21	1.78	0.65
1:A:588:ARG:HA	1:A:592:SER:OG	1.96	0.65
1:A:856:LEU:HG	1:A:862:LEU:HD21	1.79	0.64
1:A:482:ARG:HD3	1:A:482:ARG:N	2.05	0.63
1:A:562:PRO:HA	1:A:579:TYR:HA	1.79	0.63
1:A:997:PHE:CZ	1:A:1001:ARG:HG3	2.34	0.63
1:A:746:ILE:O	1:A:750:GLN:HG3	1.99	0.63
1:A:768:GLY:HA3	1:A:774:GLY:HA2	1.81	0.62
1:A:481:VAL:HG12	1:A:482:ARG:HD3	1.82	0.61
1:A:627:PHE:HA	1:A:654:LEU:HD11	1.82	0.60
1:A:482:ARG:CD	1:A:482:ARG:H	2.01	0.60
1:A:510:TYR:O	1:A:548:GLY:HA3	2.01	0.60
1:A:1044:PRO:O	1:A:1048:ILE:HG13	2.00	0.60
1:A:849:ILE:N	1:A:865:MET:HE3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:PHE:CD1	1:A:654:LEU:HD12	2.30	0.60
1:A:571:PRO:HG2	1:A:595:PHE:HD1	1.67	0.59
1:A:627:PHE:O	1:A:631:GLN:HG2	2.01	0.59
1:A:570:LYS:HE2	1:A:571:PRO:HG3	1.85	0.59
1:A:568:ILE:HG23	1:A:595:PHE:HB3	1.84	0.58
1:A:507:ARG:HH11	1:A:507:ARG:HG3	1.68	0.58
1:A:823:PRO:HG3	1:A:997:PHE:CD1	2.39	0.58
1:A:474:LEU:HD23	1:A:534:ILE:HD11	1.86	0.58
1:A:553:GLN:HE21	1:A:553:GLN:N	2.01	0.57
1:A:756:ASN:O	1:A:870:ARG:NH1	2.38	0.57
1:A:562:PRO:HG3	1:A:579:TYR:CE2	2.40	0.56
1:A:655:ARG:N	1:A:655:ARG:HD3	2.21	0.56
1:A:922:GLY:H	1:A:928:PRO:HG3	1.71	0.56
1:A:701:PRO:O	1:A:705:LYS:HG3	2.07	0.55
1:A:602:TYR:CZ	1:A:604:GLY:HA3	2.43	0.54
1:A:507:ARG:NH1	1:A:507:ARG:HG3	2.23	0.54
1:A:599:GLN:NE2	1:A:737:GLY:HA2	2.22	0.54
1:A:940:ASN:N	1:A:940:ASN:HD22	2.06	0.53
1:A:623:HIS:HB2	2:A:1363:HOH:O	2.08	0.53
1:A:751:ASN:H	1:A:751:ASN:HD22	1.57	0.53
1:A:687:ASP:OD2	1:A:835:THR:HG23	2.09	0.53
1:A:603:LYS:CB	1:A:675:PHE:CE1	2.83	0.53
1:A:571:PRO:HG2	1:A:595:PHE:CD1	2.43	0.53
1:A:571:PRO:O	1:A:572:THR:HB	2.09	0.53
1:A:627:PHE:CD1	1:A:654:LEU:CD1	2.88	0.52
1:A:903:LEU:CG	1:A:941:ILE:HD13	2.36	0.52
1:A:608:SER:O	1:A:612:GLU:HG2	2.09	0.52
1:A:850:ILE:HD11	1:A:1162:PHE:CD2	2.45	0.51
1:A:806:ILE:O	1:A:813:VAL:HG23	2.09	0.51
1:A:823:PRO:HG2	1:A:994:LEU:HD12	1.92	0.51
1:A:548:GLY:O	1:A:552:ILE:HG13	2.10	0.51
1:A:601:TYR:HE1	1:A:675:PHE:CE1	2.28	0.51
1:A:495:ILE:O	1:A:499:LYS:HG3	2.11	0.51
1:A:1120:ARG:CG	1:A:1120:ARG:HH11	2.23	0.50
1:A:653:TRP:O	1:A:654:LEU:HD23	2.11	0.50
1:A:678:LYS:O	1:A:682:LEU:HB2	2.11	0.49
1:A:592:SER:HB3	1:A:597:TRP:NE1	2.27	0.49
1:A:839:THR:HB	1:A:976:VAL:HB	1.93	0.49
1:A:811:LYS:HB2	1:A:811:LYS:NZ	2.26	0.49
1:A:605:LEU:HG	1:A:606:GLY:H	1.73	0.49
1:A:1022:LYS:O	1:A:1026:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:PRO:HD2	1:A:849:ILE:CG2	2.43	0.48
1:A:979:ASP:HB2	1:A:980:PRO:CD	2.44	0.48
1:A:583:ASP:O	1:A:586:LYS:HG2	2.14	0.48
1:A:879:ILE:HD11	1:A:883:ARG:NH1	2.28	0.48
1:A:925:LYS:HG2	1:A:925:LYS:O	2.14	0.48
1:A:1008:ARG:O	1:A:1012:MET:HG3	2.14	0.48
1:A:746:ILE:HG23	1:A:767:PHE:CD2	2.49	0.47
1:A:751:ASN:O	1:A:870:ARG:NH2	2.47	0.47
1:A:508:LYS:O	1:A:546:PHE:HA	2.13	0.47
1:A:653:TRP:O	1:A:654:LEU:HG	2.14	0.47
1:A:1123:SER:HA	1:A:1128:ARG:HG2	1.97	0.47
1:A:734:TYR:CE1	1:A:741:LEU:HD13	2.49	0.47
1:A:823:PRO:HD2	1:A:849:ILE:HG21	1.97	0.46
1:A:852:ASN:HB3	1:A:994:LEU:CD2	2.43	0.46
1:A:850:ILE:HD11	1:A:1162:PHE:CE2	2.51	0.46
1:A:420:LYS:HE3	1:A:433:ASN:O	2.15	0.46
1:A:562:PRO:O	1:A:602:TYR:HE1	1.99	0.46
1:A:441:TYR:O	1:A:519:GLY:HA3	2.16	0.46
1:A:694:ASN:ND2	1:A:696:LEU:H	2.13	0.46
1:A:543:GLU:HG3	1:A:550:LEU:HD22	1.97	0.46
1:A:592:SER:HB3	1:A:597:TRP:HE1	1.81	0.45
1:A:872:TRP:CH2	1:A:886:MET:HG3	2.52	0.45
1:A:601:TYR:CE2	1:A:680:LEU:HA	2.51	0.45
1:A:588:ARG:O	1:A:592:SER:HB2	2.16	0.45
1:A:845:ASN:ND2	1:A:847:LEU:H	2.14	0.45
1:A:482:ARG:NH1	1:A:482:ARG:O	2.49	0.45
1:A:1029:PHE:CB	1:A:1116:LEU:HD22	2.47	0.45
1:A:879:ILE:HD11	1:A:883:ARG:HH11	1.82	0.45
1:A:432:ALA:HB2	1:A:469:TYR:C	2.38	0.45
1:A:1001:ARG:HD3	1:A:1005:TYR:HE2	1.82	0.44
1:A:768:GLY:CA	1:A:774:GLY:HA2	2.46	0.44
1:A:510:TYR:HD2	1:A:546:PHE:HB3	1.82	0.44
1:A:811:LYS:CB	1:A:811:LYS:NZ	2.80	0.44
1:A:478:MET:HG3	1:A:480:ASN:OD1	2.18	0.44
1:A:450:GLY:HA2	1:A:476:GLY:O	2.17	0.44
1:A:623:HIS:CE1	1:A:655:ARG:O	2.71	0.44
1:A:767:PHE:CE1	1:A:783:ILE:HB	2.53	0.44
1:A:889:ARG:HB3	1:A:902:GLU:HB3	2.00	0.43
1:A:945:ILE:HD13	1:A:964:PHE:CE1	2.53	0.43
1:A:603:LYS:CG	1:A:605:LEU:HB3	2.49	0.43
1:A:654:LEU:HD23	1:A:655:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ILE:HG23	1:A:767:PHE:HD2	1.83	0.43
1:A:811:LYS:HB2	1:A:811:LYS:HZ2	1.84	0.43
1:A:845:ASN:HD22	1:A:845:ASN:C	2.22	0.43
1:A:849:ILE:CA	1:A:865:MET:HE3	2.49	0.43
1:A:1025:PHE:CD1	1:A:1058:PRO:HD2	2.54	0.43
1:A:482:ARG:N	1:A:482:ARG:HH11	2.17	0.42
1:A:570:LYS:CE	1:A:571:PRO:HG3	2.48	0.42
1:A:609:LEU:O	1:A:613:VAL:HG23	2.19	0.42
1:A:653:TRP:O	1:A:655:ARG:NH1	2.51	0.42
1:A:676:ILE:C	1:A:678:LYS:N	2.73	0.42
1:A:845:ASN:ND2	1:A:847:LEU:HB2	2.34	0.42
1:A:796:HIS:HA	1:A:797:PRO:HD2	1.92	0.42
1:A:426:TYR:HE2	1:A:500:LYS:HG2	1.85	0.42
1:A:933:MET:SD	1:A:934:GLU:N	2.92	0.42
1:A:676:ILE:C	1:A:678:LYS:H	2.23	0.42
1:A:581:MET:HB3	1:A:582:PRO:HD3	2.01	0.42
1:A:686:ALA:O	1:A:690:ARG:HG3	2.20	0.42
1:A:653:TRP:O	1:A:654:LEU:CG	2.68	0.42
1:A:535:LYS:HE3	2:A:1219:HOH:O	2.19	0.42
1:A:460:GLY:HA3	1:A:617:PHE:CD2	2.55	0.42
1:A:510:TYR:HE2	1:A:546:PHE:CD1	2.38	0.42
1:A:912:ILE:O	1:A:916:LEU:HG	2.20	0.42
1:A:936:GLN:NE2	1:A:944:ILE:HD12	2.35	0.42
1:A:676:ILE:O	1:A:678:LYS:N	2.53	0.41
1:A:732:THR:HA	1:A:813:VAL:HG12	2.02	0.41
1:A:713:LYS:HB2	1:A:727:TYR:CE2	2.55	0.41
1:A:1070:SER:HA	1:A:1071:PRO:HD3	1.89	0.41
1:A:886:MET:SD	1:A:905:ALA:HB3	2.61	0.41
1:A:809:ASP:O	1:A:810:GLU:HB2	2.20	0.41
1:A:654:LEU:HA	1:A:654:LEU:HD23	1.90	0.41
1:A:732:THR:HA	1:A:813:VAL:CG1	2.51	0.41
1:A:676:ILE:HD13	1:A:676:ILE:HA	2.00	0.41
1:A:676:ILE:HG22	1:A:678:LYS:CG	2.51	0.41
1:A:845:ASN:HD22	1:A:846:PRO:N	2.19	0.41
1:A:845:ASN:HD21	1:A:847:LEU:HB2	1.86	0.41
1:A:1011:HIS:O	1:A:1015:ARG:HD2	2.21	0.41
1:A:1170:LEU:HA	1:A:1170:LEU:HD12	1.85	0.41
1:A:478:MET:HB2	2:A:1376:HOH:O	2.21	0.40
1:A:751:ASN:N	1:A:751:ASN:HD22	2.19	0.40
1:A:845:ASN:HD22	1:A:847:LEU:H	1.70	0.40
1:A:1059:ARG:O	1:A:1066:PRO:HA	2.22	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	667/793 (84%)	626 (94%)	35 (5%)	6 (1%)	21 37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	572	THR
1	A	677	ASN
1	A	420	LYS
1	A	922	GLY
1	A	547	LEU
1	A	570	LYS

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	603/701 (86%)	564 (94%)	39 (6%)	21 39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	452	SER
1	A	481	VAL

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Mol	Chain	Res	Type
1	A	482	ARG
1	A	483	GLU
1	A	505	GLN
1	A	507	ARG
1	A	508	LYS
1	A	533	HIS
1	A	534	ILE
1	A	547	LEU
1	A	553	GLN
1	A	570	LYS
1	A	580	ASN
1	A	595	PHE
1	A	605	LEU
1	A	655	ARG
1	A	714	ASN
1	A	738	GLU
1	A	751	ASN
1	A	762	LEU
1	A	792	ARG
1	A	813	VAL
1	A	845	ASN
1	A	847	LEU
1	A	859	ASP
1	A	883	ARG
1	A	889	ARG
1	A	895	ASP
1	A	901	THR
1	A	913	LYS
1	A	940	ASN
1	A	963	ARG
1	A	1001	ARG
1	A	1015	ARG
1	A	1159	LEU
1	A	1170	LEU
1	A	1171	GLN
1	A	1172	ARG
1	A	1177	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	506	HIS

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Mol	Chain	Res	Type
1	A	540	ASN
1	A	553	GLN
1	A	580	ASN
1	A	623	HIS
1	A	656	GLN
1	A	694	ASN
1	A	714	ASN
1	A	735	HIS
1	A	736	HIS
1	A	751	ASN
1	A	845	ASN
1	A	940	ASN
1	A	974	ASN
1	A	1130	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

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, 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	679/793 (85%)	0.29	70 (10%) 9 9	23, 50, 99, 100	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	PHE	9.6
1	A	657	TYR	9.2
1	A	659	PRO	8.9
1	A	676	ILE	8.1
1	A	573	LYS	7.8
1	A	419	ARG	6.4
1	A	925	LYS	6.0
1	A	1178	GLY	5.9
1	A	653	TRP	5.8
1	A	570	LYS	5.7
1	A	532	SER	5.7
1	A	809	ASP	5.2
1	A	553	GLN	5.2
1	A	810	GLU	5.1
1	A	484	ALA	4.9
1	A	716	LYS	4.8
1	A	678	LYS	4.8
1	A	656	GLN	4.7
1	A	715	LEU	4.6
1	A	605	LEU	4.3
1	A	1110	TYR	3.9
1	A	603	LYS	3.8
1	A	1109	LEU	3.7
1	A	572	THR	3.7
1	A	655	ARG	3.7
1	A	631	GLN	3.6
1	A	586	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	938	ASP	3.6
1	A	601	TYR	3.5
1	A	926	ILE	3.4
1	A	483	GLU	3.4
1	A	482	ARG	3.3
1	A	924	ASP	3.2
1	A	1108	GLU	3.2
1	A	714	ASN	3.1
1	A	730	GLU	3.1
1	A	923	ASN	2.8
1	A	584	TYR	2.8
1	A	438	LYS	2.8
1	A	606	GLY	2.7
1	A	526	ASP	2.6
1	A	604	GLY	2.6
1	A	658	GLU	2.6
1	A	782	TYR	2.5
1	A	949	PRO	2.4
1	A	1071	PRO	2.4
1	A	509	LYS	2.4
1	A	927	LYS	2.4
1	A	939	ASP	2.4
1	A	957	LYS	2.4
1	A	571	PRO	2.4
1	A	525	THR	2.4
1	A	808	GLU	2.4
1	A	505	GLN	2.3
1	A	607	THR	2.3
1	A	506	HIS	2.3
1	A	739	GLN	2.3
1	A	579	TYR	2.3
1	A	1050	GLN	2.3
1	A	1107	GLU	2.3
1	A	1171	GLN	2.3
1	A	476	GLY	2.2
1	A	654	LEU	2.2
1	A	1175	GLU	2.1
1	A	1062	LYS	2.1
1	A	940	ASN	2.1
1	A	481	VAL	2.0
1	A	950	GLU	2.0
1	A	533	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	492	ASN	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.