Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2021 – 01:07 pm GMT

PDB ID	:	6Z03
Title	:	DNA Topoisomerase
Authors	:	Takahashi, T.S.; Gadelle, D.; Forterre, P.; Mayer, C.; Petrella, S.
Deposited on	:	2020-05-07
Resolution	:	2.20 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
https://www.wwpdb.org/validation/2017/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:

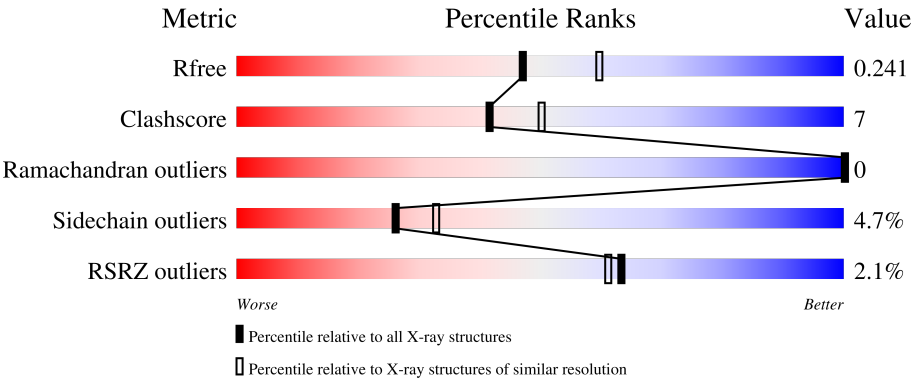
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

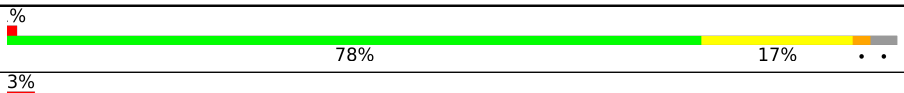
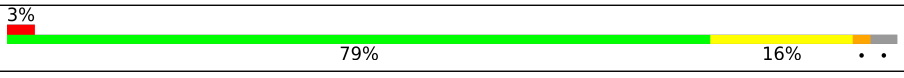
The reported resolution of this entry is 2.20 Å.

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	539	
1	B	539	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9140 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 topoisomerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4357	2786	780	781	10			
1	B	521	Total	C	N	O	S	0	0	0
			4350	2781	779	780	10			

- Molecule 2 is water.

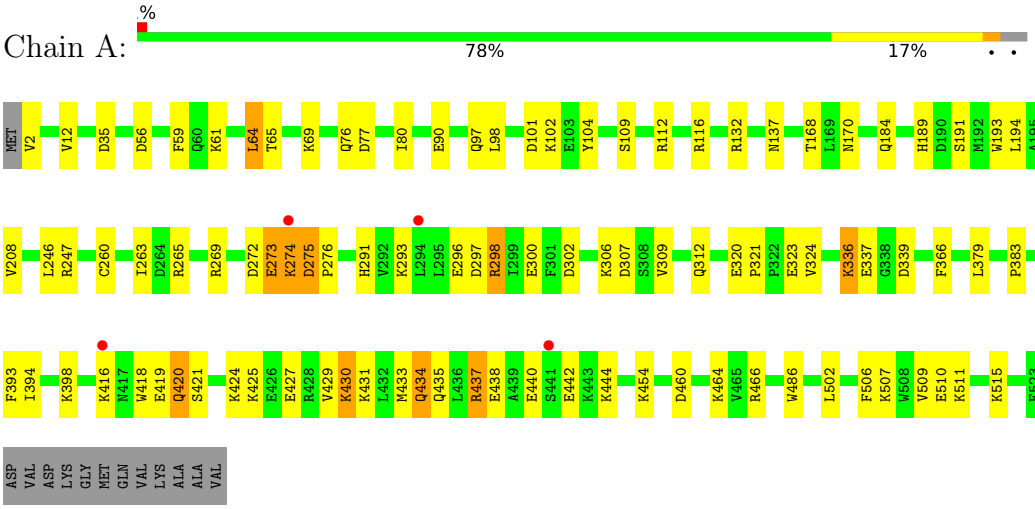
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	209	Total	O	0	0
			209	209		
2	B	224	Total	O	0	0
			224	224		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

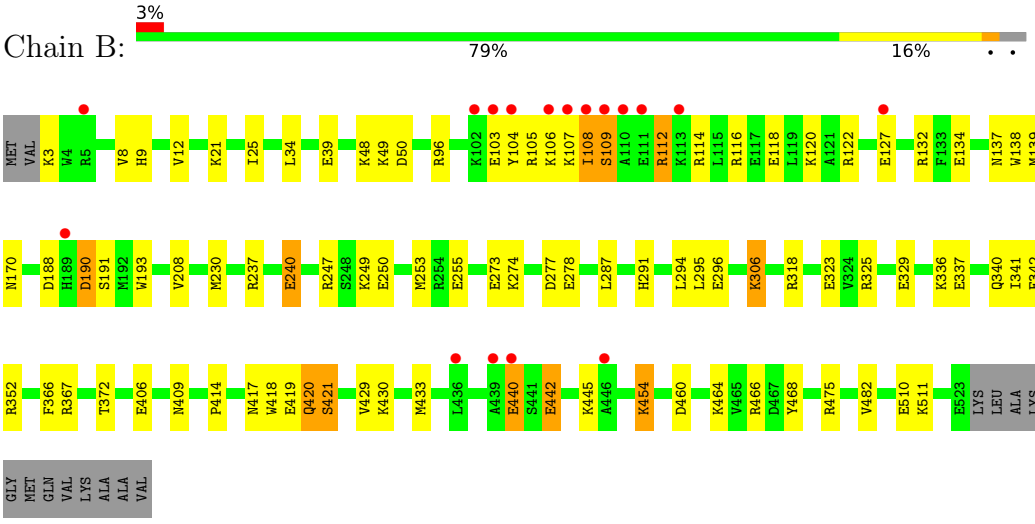
• Molecule 1: DNA topoisomerase I

Chain A:



• Molecule 1: DNA topoisomerase I

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.47Å 94.68Å 92.65Å 90.00° 111.81° 90.00°	Depositor
Resolution (Å)	70.07 – 2.20 70.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.07-2.20) 99.9 (70.07-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.192 , 0.241 0.191 , 0.241	Depositor DCC
R_{free} test set	2972 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9140	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 5.12% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.28	0/4455	0.43	0/5995
1	B	0.28	0/4448	0.43	0/5985
All	All	0.28	0/8903	0.43	0/11980

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

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	4357	0	4415	63	0
1	B	4350	0	4406	61	0
2	A	209	0	0	9	0
2	B	224	0	0	14	0
All	All	9140	0	8821	123	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 7.

All (123) 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:76:GLN:O	2:A:601:HOH:O	1.82	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:NH1	2:A:603:HOH:O	2.02	0.92
1:A:265:ARG:NH2	1:A:320:GLU:OE2	2.02	0.92
1:B:273:GLU:OE2	2:B:601:HOH:O	1.92	0.87
1:A:90:GLU:OE1	2:A:602:HOH:O	1.93	0.85
1:B:247:ARG:HG2	1:B:323:GLU:HG2	1.62	0.81
1:B:296:GLU:OE2	1:B:296:GLU:N	2.13	0.78
1:B:414:PRO:HB3	1:B:466:ARG:HD3	1.64	0.78
1:B:340:GLN:NE2	2:B:603:HOH:O	2.10	0.77
1:A:510:GLU:OE2	2:A:604:HOH:O	2.07	0.72
1:A:507:LYS:O	2:A:605:HOH:O	2.08	0.71
1:A:291:HIS:O	2:A:606:HOH:O	2.11	0.69
1:B:3:LYS:NZ	1:B:190:ASP:O	2.27	0.68
1:B:454:LYS:NZ	2:B:609:HOH:O	2.28	0.66
1:B:240:GLU:O	2:B:604:HOH:O	2.14	0.65
1:A:109:SER:HA	1:A:112:ARG:HG2	1.78	0.65
1:A:383:PRO:HD2	1:A:386:LYS:HD2	1.77	0.65
1:A:273:GLU:OE1	1:A:273:GLU:N	2.22	0.64
1:B:295:LEU:O	1:B:325:ARG:NH2	2.31	0.63
1:A:247:ARG:HG2	1:A:323:GLU:HG2	1.83	0.61
1:A:2:VAL:HG13	1:A:189:HIS:HB3	1.83	0.61
1:A:64:LEU:HD11	1:A:80:ILE:HD13	1.81	0.61
1:B:109:SER:HA	1:B:112:ARG:HG2	1.83	0.61
1:B:336:LYS:HD2	1:B:337:GLU:H	1.66	0.60
1:A:269:ARG:HD2	1:A:273:GLU:OE2	2.01	0.60
1:B:247:ARG:CG	1:B:323:GLU:HG2	2.33	0.59
1:A:515:LYS:NZ	2:A:615:HOH:O	2.36	0.57
1:A:336:LYS:HD3	1:A:337:GLU:H	1.69	0.57
1:B:419:GLU:OE1	2:B:605:HOH:O	2.18	0.56
1:A:296:GLU:H	1:A:296:GLU:CD	2.09	0.56
1:A:306:LYS:O	1:A:309:VAL:HG12	2.06	0.55
1:A:101:ASP:OD1	1:A:104:TYR:N	2.40	0.55
1:A:434:GLN:O	1:A:438:GLU:HG2	2.07	0.55
1:B:237:ARG:NH1	2:B:621:HOH:O	2.40	0.55
1:B:418:TRP:CE2	1:B:466:ARG:HG3	2.42	0.54
1:B:409:ASN:HA	2:B:703:HOH:O	2.06	0.54
1:A:431:LYS:O	1:A:435:GLN:HG3	2.08	0.53
1:B:255:GLU:OE1	1:B:343:GLN:N	2.39	0.53
1:A:170:ASN:HB2	1:A:193:TRP:CZ3	2.45	0.52
1:B:318:ARG:HD2	2:B:608:HOH:O	2.07	0.52
1:B:417:ASN:O	1:B:421:SER:OG	2.26	0.52
1:B:105:ARG:NH2	1:B:352:ARG:HD2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASP:OD1	1:A:312:GLN:HG2	2.09	0.51
1:A:391:GLU:H	1:A:391:GLU:CD	2.13	0.51
1:A:442:GLU:OE2	1:A:442:GLU:HA	2.11	0.51
1:A:321:PRO:O	1:A:324:VAL:HG12	2.10	0.51
1:B:104:TYR:O	1:B:108:ILE:HB	2.10	0.51
1:B:50:ASP:OD2	1:B:96:ARG:NH2	2.42	0.51
1:A:65:THR:O	1:A:69:LYS:HG3	2.11	0.51
1:A:246:LEU:HB3	1:A:323:GLU:HB3	1.93	0.49
1:A:460:ASP:OD2	1:A:464:LYS:NZ	2.43	0.49
1:B:132:ARG:NE	2:B:602:HOH:O	2.00	0.49
1:A:272:ASP:N	1:A:273:GLU:OE1	2.46	0.49
1:A:420:GLN:O	1:A:424:LYS:HG2	2.12	0.49
1:A:97:GLN:NE2	2:A:620:HOH:O	2.46	0.48
1:B:191:SER:HB3	1:B:193:TRP:CD1	2.48	0.48
1:A:511:LYS:HG2	1:B:510:GLU:HB3	1.96	0.47
1:B:460:ASP:O	1:B:464:LYS:HG3	2.14	0.47
1:B:406:GLU:HG2	1:B:468:TYR:CZ	2.50	0.47
1:A:98:LEU:HD13	1:A:104:TYR:CZ	2.49	0.47
1:B:325:ARG:NH1	2:B:616:HOH:O	2.36	0.47
1:B:342:PHE:CD1	1:B:345:ILE:HG13	2.50	0.47
1:B:103:GLU:HA	1:B:106:LYS:HD3	1.96	0.47
1:B:296:GLU:H	1:B:296:GLU:CD	2.05	0.47
1:B:430:LYS:HA	1:B:433:MET:HE2	1.97	0.47
1:B:418:TRP:CD2	1:B:466:ARG:HG3	2.50	0.46
1:B:250:GLU:OE2	1:B:253:MET:N	2.47	0.46
1:A:434:GLN:HA	1:A:437:ARG:HG2	1.98	0.46
1:B:277:ASP:OD2	1:B:278:GLU:N	2.49	0.46
1:B:9:HIS:HE1	1:B:169:LEU:HG	1.82	0.45
1:B:12:VAL:HG11	1:B:208:VAL:HG21	1.97	0.45
1:A:379:LEU:HD22	1:A:486:TRP:CE2	2.51	0.45
1:A:418:TRP:CE2	1:A:466:ARG:HG3	2.51	0.45
1:B:406:GLU:HG2	1:B:468:TYR:CE1	2.51	0.45
1:A:12:VAL:HG11	1:A:208:VAL:HG21	1.98	0.45
1:A:391:GLU:HG3	1:A:454:LYS:HE2	1.98	0.45
1:B:8:VAL:HG12	1:B:127:GLU:HB2	1.98	0.44
1:A:273:GLU:H	1:A:273:GLU:CD	2.08	0.44
1:A:425:LYS:O	1:A:429:VAL:HG12	2.16	0.44
1:A:274:LYS:HD2	1:A:274:LYS:H	1.82	0.44
1:B:287:LEU:HB3	1:B:341:ILE:HD12	1.99	0.44
1:A:196:ARG:HA	1:A:206:LYS:O	2.17	0.44
1:B:442:GLU:OE2	1:B:445:LYS:HE2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:SER:HB3	1:A:193:TRP:CD1	2.52	0.44
1:A:444:LYS:HD2	1:A:444:LYS:H	1.82	0.44
1:A:437:ARG:NH2	2:A:622:HOH:O	2.50	0.44
1:B:429:VAL:O	1:B:433:MET:HG3	2.18	0.44
1:A:298:ARG:HD3	1:A:300:GLU:OE2	2.18	0.43
1:B:48:LYS:NZ	1:B:147:MET:HE1	2.33	0.43
1:B:120:LYS:NZ	1:B:134:GLU:OE2	2.41	0.43
1:B:306:LYS:HB2	1:B:306:LYS:HE2	1.87	0.43
1:B:230:MET:HG3	2:B:648:HOH:O	2.18	0.43
1:B:440:GLU:H	1:B:440:GLU:CD	2.21	0.43
1:A:56:ASP:HB3	1:A:59:PHE:HB2	2.01	0.43
1:B:138:TRP:CZ3	1:B:139:MET:HG2	2.53	0.43
1:A:430:LYS:HA	1:A:430:LYS:HD3	1.82	0.43
1:A:137:ASN:OD1	1:A:137:ASN:N	2.51	0.43
1:A:168:THR:HG23	1:A:184:GLN:HG3	2.01	0.43
1:B:372:THR:HG23	1:B:482:VAL:HG21	2.00	0.42
1:A:433:MET:HE3	1:A:433:MET:HB3	1.76	0.42
1:B:49:LYS:O	2:B:606:HOH:O	2.21	0.42
1:A:424:LYS:O	1:A:427:GLU:HG3	2.18	0.42
1:B:21:LYS:N	1:B:39:GLU:OE1	2.47	0.42
1:B:342:PHE:HB3	1:B:345:ILE:HG13	2.01	0.42
1:B:25:ILE:HG23	1:B:34:LEU:HD11	2.01	0.42
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.87	0.42
1:A:293:LYS:HE2	1:A:300:GLU:HB2	2.02	0.42
1:B:188:ASP:C	1:B:188:ASP:OD1	2.58	0.42
1:A:394:ILE:HG22	1:A:398:LYS:HD2	2.01	0.41
1:A:416:LYS:HA	1:A:416:LYS:HD3	1.74	0.41
1:A:393:PHE:CE1	1:A:486:TRP:CD1	3.07	0.41
1:B:170:ASN:HB2	1:B:193:TRP:CZ3	2.56	0.41
1:A:275:ASP:HA	1:A:276:PRO:HD3	1.86	0.41
1:A:306:LYS:HE2	1:A:307:ASP:OD2	2.21	0.41
1:A:506:PHE:O	1:A:509:VAL:HG12	2.20	0.41
1:B:420:GLN:HG3	1:B:421:SER:N	2.36	0.41
1:B:108:ILE:HD13	1:B:108:ILE:HA	1.86	0.41
1:B:294:LEU:HD21	1:B:329:GLU:HG3	2.02	0.41
1:B:291:HIS:NE2	2:B:613:HOH:O	2.30	0.41
1:B:137:ASN:N	1:B:137:ASN:OD1	2.54	0.41
1:A:260:CYS:HA	1:A:263:ILE:HD12	2.02	0.40
1:B:367:ARG:HD3	2:B:691:HOH:O	2.20	0.40
1:A:336:LYS:O	1:A:339:ASP:HB2	2.21	0.40

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	520/539 (96%)	513 (99%)	7 (1%)	0	100	100
1	B	519/539 (96%)	513 (99%)	6 (1%)	0	100	100
All	All	1039/1078 (96%)	1026 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	460/473 (97%)	438 (95%)	22 (5%)	25	32
1	B	459/473 (97%)	438 (95%)	21 (5%)	27	34
All	All	919/946 (97%)	876 (95%)	43 (5%)	26	33

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	61	LYS
1	A	64	LEU
1	A	77	ASP
1	A	102	LYS
1	A	116	ARG
1	A	194	LEU
1	A	196	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	273	GLU
1	A	274	LYS
1	A	275	ASP
1	A	297	ASP
1	A	298	ARG
1	A	336	LYS
1	A	366	PHE
1	A	419	GLU
1	A	420	GLN
1	A	421	SER
1	A	430	LYS
1	A	434	GLN
1	A	437	ARG
1	A	440	GLU
1	B	107	LYS
1	B	108	ILE
1	B	109	SER
1	B	112	ARG
1	B	114	ARG
1	B	116	ARG
1	B	118	GLU
1	B	122	ARG
1	B	190	ASP
1	B	240	GLU
1	B	249	LYS
1	B	274	LYS
1	B	306	LYS
1	B	366	PHE
1	B	420	GLN
1	B	421	SER
1	B	440	GLU
1	B	442	GLU
1	B	454	LYS
1	B	475	ARG
1	B	511	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	344	ASN
1	A	349	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	417	ASN
1	A	458	ASN
1	B	184	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 monosaccharides 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	522/539 (96%)	-0.03	4 (0%) 86 85	29, 51, 86, 107	0
1	B	521/539 (96%)	0.06	18 (3%) 44 42	27, 49, 99, 137	0
All	All	1043/1078 (96%)	0.01	22 (2%) 63 61	27, 50, 92, 137	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	ALA	5.0
1	B	104	TYR	4.6
1	B	113	LYS	4.5
1	B	106	LYS	4.3
1	B	110	ALA	4.2
1	B	109	SER	3.1
1	B	111	GLU	3.0
1	B	439	ALA	3.0
1	A	274	LYS	2.9
1	B	127	GLU	2.9
1	A	294	LEU	2.7
1	B	5	ARG	2.7
1	B	102	LYS	2.4
1	A	416	LYS	2.4
1	B	107	LYS	2.2
1	B	189	HIS	2.2
1	B	440	GLU	2.2
1	B	108	ILE	2.2
1	B	103	GLU	2.2
1	B	436	LEU	2.2
1	A	441	SER	2.1
1	B	344	ASN	2.1

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 monosaccharides 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.