



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 10:17 AM EDT

PDB ID : 2CSD
Title : Crystal structure of Topoisomerase V (61 kDa fragment)
Authors : Taneja, B.; Patel, A.; Slesarev, A.; Mondragon, A.
Deposited on : unknown
Resolution : 2.90 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

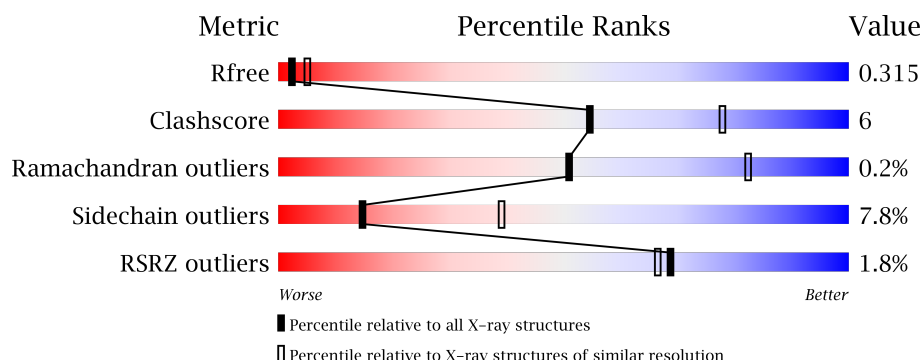
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	519	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>
1	B	519	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>..</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8390 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.

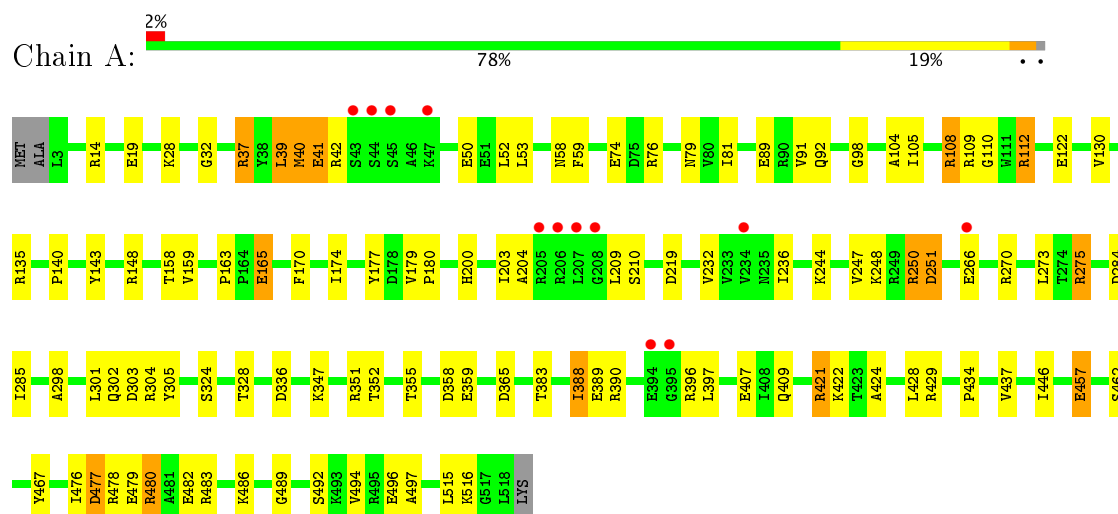
- Molecule 1 is a protein called Topoisomerase V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4195	2625	753	807	10			
1	B	516	Total	C	N	O	S	0	0	0
			4195	2625	753	807	10			

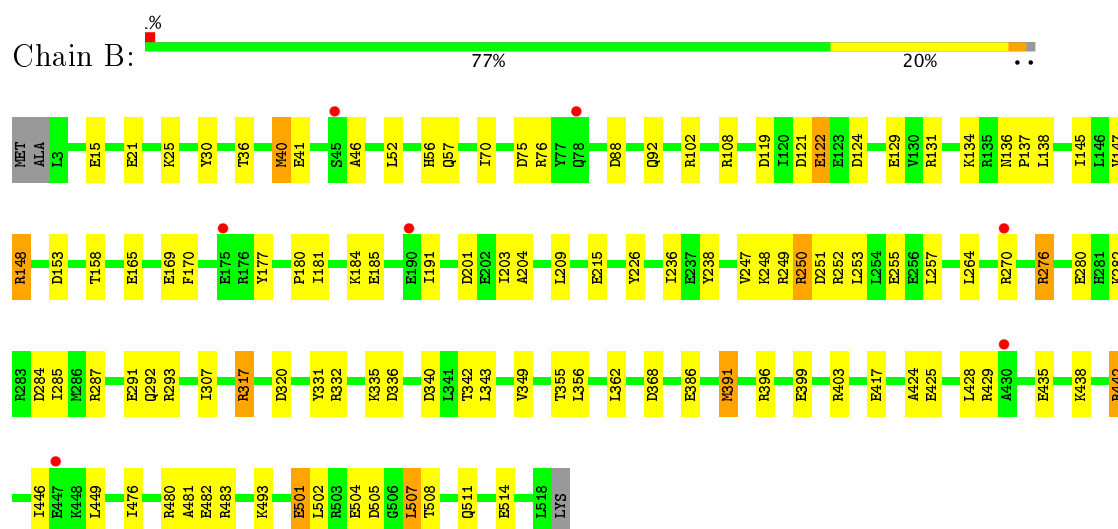
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Topoisomerase V



• Molecule 1: Topoisomerase V



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.50 Å 86.40 Å 175.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.80 – 2.90 28.06 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (28.80-2.90) 99.1 (28.06-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.90 Å)	Xtriage
Refinement program	CNS, REFMAC 5.0	Depositor
R, R_{free}	0.236 , 0.308 0.248 , 0.315	Depositor DCC
R_{free} test set	1319 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8390	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.333 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	0.37	0/4260	0.72	5/5745 (0.1%)
1	B	0.37	0/4260	0.73	13/5745 (0.2%)
All	All	0.37	0/8520	0.72	18/11490 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	336	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	75	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	219	ASP	CB-CG-OD2	5.62	123.35	118.30
1	B	124	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	121	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	340	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	284	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	303	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	505	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	119	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	153	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	320	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	365	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	336	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	477	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	138	LEU	CA-CB-CG	5.04	126.88	115.30
1	B	368	ASP	CB-CG-OD2	5.01	122.81	118.30

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	4195	0	4198	54	0
1	B	4195	0	4198	48	0
All	All	8390	0	8396	100	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 6.

All (100) 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:479:GLU:HG2	1:A:483:ARG:NH1	1.71	1.05
1:A:479:GLU:HG2	1:A:483:ARG:HH12	1.19	1.05
1:B:508:THR:H	1:B:511:GLN:HE21	1.28	0.82
1:A:28:LYS:HG3	1:A:275:ARG:NH2	2.03	0.73
1:A:58:ASN:OD1	1:A:159:VAL:HG23	1.91	0.70
1:B:331:TYR:HE1	1:B:343:LEU:HA	1.57	0.69
1:B:88:ASP:O	1:B:92:GLN:HG2	1.96	0.65
1:B:331:TYR:CE1	1:B:343:LEU:HA	2.32	0.65
1:B:102:ARG:HD2	1:B:147:VAL:O	1.97	0.64
1:A:479:GLU:CG	1:A:483:ARG:HH12	2.04	0.64
1:B:247:VAL:HA	1:B:250:ARG:HD2	1.80	0.64
1:A:163:PRO:HB2	1:A:165:GLU:HG3	1.81	0.62
1:B:501:GLU:O	1:B:504:GLU:HB2	1.99	0.61
1:A:109:ARG:O	1:A:112:ARG:HG2	2.01	0.61
1:B:435:GLU:OE1	1:B:438:LYS:HD2	2.01	0.60
1:B:145:ILE:HD11	1:B:226:TYR:HD2	1.66	0.60
1:A:250:ARG:HG2	1:A:251:ASP:N	2.17	0.59
1:B:424:ALA:O	1:B:428:LEU:HG	2.03	0.58
1:B:502:LEU:O	1:B:507:LEU:HB2	2.04	0.58
1:B:282:LYS:O	1:B:285:ILE:HG22	2.03	0.58
1:A:275:ARG:O	1:A:275:ARG:HD3	2.05	0.56
1:B:36:THR:HG21	1:B:56:HIS:HB2	1.85	0.56
1:B:287:ARG:O	1:B:291:GLU:HB2	2.06	0.55
1:A:200:HIS:HA	1:A:203:ILE:HD12	1.89	0.55
1:A:177:TYR:CZ	1:A:236:ILE:HG13	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:THR:H	1:B:511:GLN:NE2	2.02	0.54
1:B:250:ARG:HG2	1:B:251:ASP:N	2.22	0.54
1:A:298:ALA:O	1:A:302:GLN:HG3	2.07	0.54
1:A:247:VAL:HA	1:A:250:ARG:HD2	1.90	0.54
1:B:36:THR:O	1:B:40:MET:HG2	2.08	0.53
1:B:425:GLU:O	1:B:429:ARG:HG2	2.09	0.52
1:B:276:ARG:O	1:B:280:GLU:HG2	2.10	0.52
1:B:476:ILE:HG22	1:B:481:ALA:HB2	1.91	0.52
1:A:109:ARG:HH11	1:A:112:ARG:HH21	1.57	0.51
1:A:41:GLU:HG2	1:A:41:GLU:O	2.09	0.51
1:A:140:PRO:O	1:A:143:TYR:HB3	2.11	0.50
1:A:383:THR:O	1:A:409:GLN:NE2	2.44	0.50
1:B:46:ALA:O	1:B:52:LEU:HD23	2.12	0.49
1:A:492:SER:O	1:A:496:GLU:HG3	2.14	0.48
1:A:174:ILE:HD13	1:A:232:VAL:HG21	1.95	0.48
1:A:477:ASP:OD1	1:A:480:ARG:HB2	2.14	0.48
1:B:446:ILE:HB	1:B:482:GLU:OE1	2.14	0.47
1:B:15:GLU:HB3	1:B:76:ARG:HD3	1.96	0.47
1:A:482:GLU:HG2	1:A:486:LYS:HD2	1.96	0.47
1:A:424:ALA:O	1:A:428:LEU:HG	2.14	0.47
1:A:446:ILE:HB	1:A:482:GLU:OE1	2.14	0.47
1:B:41:GLU:HG3	1:B:292:GLN:HE22	1.79	0.47
1:B:204:ALA:HB1	1:B:209:LEU:O	2.15	0.47
1:B:317:ARG:HH11	1:B:317:ARG:HB3	1.79	0.47
1:A:89:GLU:HA	1:A:92:GLN:HG2	1.96	0.47
1:B:180:PRO:HB3	1:B:442:ARG:O	2.15	0.46
1:A:457:GLU:OE1	1:A:478:ARG:NH1	2.48	0.46
1:A:79:ASN:O	1:A:81:ILE:HD12	2.16	0.46
1:B:253:LEU:O	1:B:257:LEU:HG	2.16	0.46
1:A:301:LEU:O	1:A:305:TYR:HB2	2.16	0.45
1:B:181:ILE:HG22	1:B:185:GLU:HB2	1.99	0.45
1:B:41:GLU:HG2	1:B:41:GLU:O	2.16	0.45
1:A:497:ALA:O	1:A:516:LYS:NZ	2.50	0.44
1:B:122:GLU:H	1:B:122:GLU:HG2	1.40	0.44
1:A:204:ALA:HB1	1:A:209:LEU:O	2.17	0.44
1:B:145:ILE:HD11	1:B:226:TYR:CD2	2.49	0.44
1:A:40:MET:HE3	1:A:52:LEU:HG	1.98	0.44
1:A:39:LEU:O	1:A:42:ARG:HB2	2.17	0.44
1:A:324:SER:O	1:A:328:THR:HG23	2.17	0.44
1:B:264:LEU:HD23	1:B:264:LEU:C	2.38	0.44
1:A:109:ARG:O	1:A:112:ARG:CG	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:NH1	1:B:238:TYR:HD2	2.16	0.43
1:B:391:MET:HG3	1:B:396:ARG:HH11	1.83	0.43
1:B:57:GLN:HG2	1:B:137:PRO:HD3	2.00	0.43
1:A:32:GLY:HA3	1:A:59:PHE:CD2	2.53	0.43
1:A:210:SER:HB3	1:A:351:ARG:HD3	1.99	0.43
1:A:355:THR:HA	1:A:359:GLU:HG3	2.00	0.43
1:A:494:VAL:HG12	1:A:515:LEU:HD21	1.99	0.43
1:B:21:GLU:O	1:B:25:LYS:HG3	2.18	0.43
1:A:165:GLU:O	1:A:170:PHE:HA	2.18	0.43
1:B:215:GLU:HB3	1:B:226:TYR:CD1	2.53	0.42
1:A:434:PRO:O	1:A:437:VAL:HB	2.19	0.42
1:A:14:ARG:HH11	1:B:238:TYR:HD2	1.68	0.42
1:B:191:ILE:HG21	1:B:203:ILE:HG12	2.02	0.42
1:B:30:TYR:CZ	1:B:129:GLU:HB2	2.55	0.42
1:A:179:VAL:HA	1:A:180:PRO:HD2	1.86	0.42
1:B:165:GLU:HA	1:B:169:GLU:O	2.20	0.42
1:A:19:GLU:HG2	1:A:76:ARG:HH11	1.85	0.42
1:B:165:GLU:O	1:B:170:PHE:HA	2.20	0.42
1:A:347:LYS:NZ	1:A:358:ASP:OD1	2.52	0.41
1:A:244:LYS:O	1:A:248:LYS:HG2	2.20	0.41
1:A:476:ILE:HG23	1:A:480:ARG:HB3	2.02	0.41
1:A:91:VAL:HG11	1:A:98:GLY:O	2.20	0.41
1:B:177:TYR:CZ	1:B:236:ILE:HG13	2.55	0.41
1:B:356:LEU:HD22	1:B:362:LEU:HD12	2.02	0.41
1:A:37:ARG:HA	1:A:37:ARG:HD2	1.77	0.41
1:A:388:ILE:HG22	1:A:389:GLU:N	2.35	0.41
1:A:407:GLU:OE1	1:A:407:GLU:HA	2.20	0.41
1:A:108:ARG:O	1:A:109:ARG:HB2	2.21	0.41
1:A:104:ALA:O	1:A:110:GLY:HA3	2.20	0.41
1:A:421:ARG:HB3	1:A:421:ARG:HE	1.77	0.41
1:B:102:ARG:NH1	1:B:148:ARG:O	2.54	0.41
1:B:399:GLU:O	1:B:403:ARG:HG3	2.21	0.40
1:B:136:ASN:HA	1:B:137:PRO:HD2	1.98	0.40
1:A:467:TYR:OH	1:A:478:ARG:HG2	2.21	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	514/519 (99%)	493 (96%)	20 (4%)	1 (0%)	51	82
1	B	514/519 (99%)	480 (93%)	33 (6%)	1 (0%)	51	82
All	All	1028/1038 (99%)	973 (95%)	53 (5%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	GLY
1	B	355	THR

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	447/449 (100%)	411 (92%)	36 (8%)	14	38
1	B	447/449 (100%)	413 (92%)	34 (8%)	15	41
All	All	894/898 (100%)	824 (92%)	70 (8%)	15	39

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	39	LEU
1	A	40	MET
1	A	41	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	50	GLU
1	A	53	LEU
1	A	74	GLU
1	A	105	ILE
1	A	108	ARG
1	A	112	ARG
1	A	122	GLU
1	A	130	VAL
1	A	135	ARG
1	A	148	ARG
1	A	158	THR
1	A	165	GLU
1	A	250	ARG
1	A	251	ASP
1	A	266	GLU
1	A	270	ARG
1	A	273	LEU
1	A	275	ARG
1	A	284	ASP
1	A	285	ILE
1	A	304	ARG
1	A	352	THR
1	A	388	ILE
1	A	390	ARG
1	A	396	ARG
1	A	397	LEU
1	A	421	ARG
1	A	422	LYS
1	A	429	ARG
1	A	457	GLU
1	A	462	SER
1	A	480	ARG
1	B	40	MET
1	B	70	ILE
1	B	108	ARG
1	B	122	GLU
1	B	131	ARG
1	B	134	LYS
1	B	148	ARG
1	B	158	THR
1	B	184	LYS
1	B	248	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	249	ARG
1	B	250	ARG
1	B	252	ARG
1	B	255	GLU
1	B	270	ARG
1	B	276	ARG
1	B	293	ARG
1	B	307	ILE
1	B	317	ARG
1	B	332	ARG
1	B	335	LYS
1	B	342	THR
1	B	349	VAL
1	B	386	GLU
1	B	391	MET
1	B	417	GLU
1	B	442	ARG
1	B	449	LEU
1	B	480	ARG
1	B	483	ARG
1	B	493	LYS
1	B	501	GLU
1	B	507	LEU
1	B	514	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	246	HIS
1	A	433	ASN
1	B	56	HIS
1	B	292	GLN
1	B	409	GLN
1	B	511	GLN

5.3.3 RNA ⓘ

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	516/519 (99%)	0.00	12 (2%) 61 57	36, 49, 58, 66	1 (0%)
1	B	516/519 (99%)	0.13	7 (1%) 75 74	37, 54, 70, 76	0
All	All	1032/1038 (99%)	0.07	19 (1%) 69 66	36, 52, 68, 76	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	GLU	4.4
1	B	270	ARG	3.8
1	A	395	GLY	3.4
1	A	44	SER	3.2
1	B	45	SER	3.0
1	A	206	ARG	3.0
1	B	190	GLU	2.9
1	B	447	GLU	2.8
1	A	207	LEU	2.8
1	A	45	SER	2.6
1	A	47	LYS	2.6
1	B	78	GLN	2.5
1	A	208	GLY	2.4
1	A	266	GLU	2.4
1	B	430	ALA	2.2
1	A	205	ARG	2.2
1	B	175	GLU	2.2
1	A	43	SER	2.1
1	A	234	VAL	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 [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.