



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:19 AM GMT

PDB ID : 2CSD  
Title : Crystal structure of Topoisomerase V (61 kDa fragment)  
Authors : Taneja, B.; Patel, A.; Slesarev, A.; Mondragon, A.  
Deposited on : 2005-05-21  
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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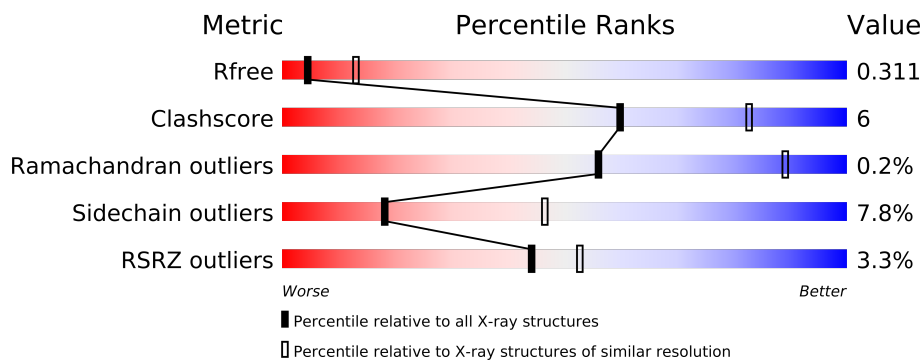
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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  $\geq 3$ , 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	519	
1	B	519	

## 2 Entry composition

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

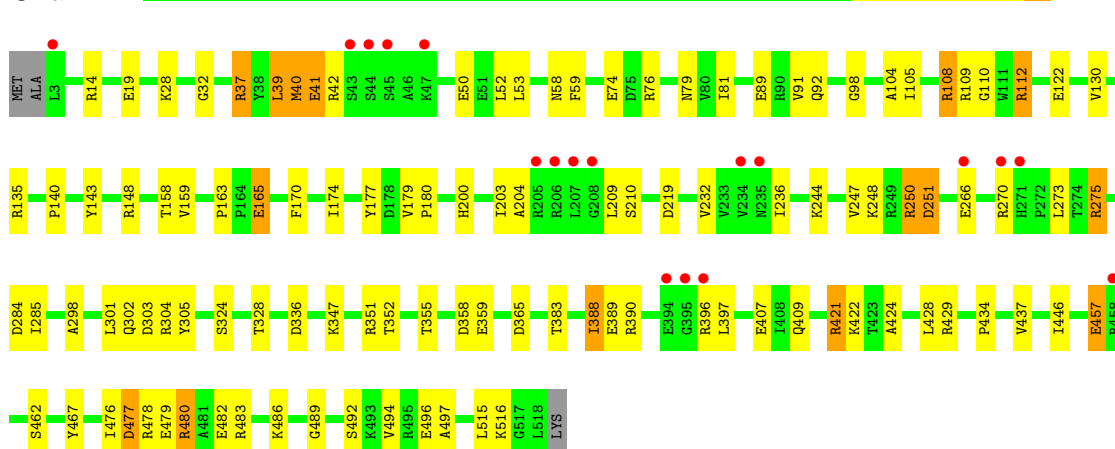
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4195	2625	753	807	10			
1	B	516	Total	C	N	O	S	0	0	0
			4195	2625	753	807	10			

### 3 Residue-property plots

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.

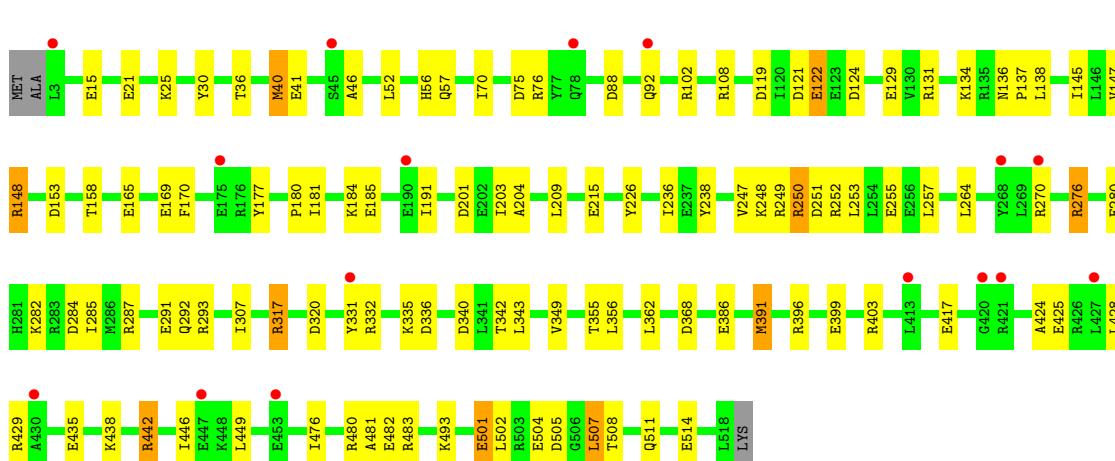
#### • Molecule 1: Topoisomerase V

Chain A:



#### • Molecule 1: Topoisomerase V

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.50Å 86.40Å 175.70Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.236 , 0.308 0.236 , 0.311	Depositor DCC
$R_{free}$ test set	1319 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.4	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 25911 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities 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	0.37	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 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	4195	0	4198	54	0
1	B	4195	0	4198	48	0
All	All	8390	0	8396	100	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 6.

All (100) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:502:LEU:O	1:B:507:LEU:HB2	2.04	0.58
1:B:424:ALA:O	1:B:428:LEU:HG	2.03	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

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Atom-1	Atom-2	Distance(Å)	Clash(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:476:ILE:HG22	1:B:481:ALA:HB2	1.91	0.52
1:B:276:ARG:O	1:B:280:GLU:HG2	2.10	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:317:ARG:HH11	1:B:317:ARG:HB3	1.79	0.47
1:B:204:ALA:HB1	1:B:209:LEU:O	2.15	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:B:253:LEU:O	1:B:257:LEU:HG	2.16	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: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
1:A:14:ARG:NH1	1:B:238:TYR:HD2	2.16	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:21:GLU:O	1:B:25:LYS:HG3	2.18	0.43
1:A:494:VAL:HG12	1:A:515:LEU:HD21	1.99	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:30:TYR:CZ	1:B:129:GLU:HB2	2.55	0.42
1:B:191:ILE:HG21	1:B:203:ILE:HG12	2.02	0.42
1:B:165:GLU:HA	1:B:169:GLU:O	2.20	0.42
1:A:179:VAL:HA	1:A:180:PRO:HD2	1.86	0.42
1:B:165:GLU:O	1:B:170:PHE:HA	2.20	0.42
1:A:19:GLU:HG2	1:A:76:ARG:HH11	1.85	0.42
1:A:347:LYS:NZ	1:A:358:ASP:OD1	2.52	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:A:244:LYS:O	1:A:248:LYS:HG2	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:388:ILE:HG22	1:A:389:GLU:N	2.35	0.41
1:A:37:ARG:HA	1:A:37:ARG:HD2	1.77	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:B:102:ARG:NH1	1:B:148:ARG:O	2.54	0.41
1:A:421:ARG:HB3	1:A:421:ARG:HE	1.77	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%)	56	89
1	B	514/519 (99%)	480 (93%)	33 (6%)	1 (0%)	56	89
All	All	1028/1038 (99%)	973 (95%)	53 (5%)	2 (0%)	56	89

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%)	17	45
1	B	447/449 (100%)	413 (92%)	34 (8%)	19	48
All	All	894/898 (100%)	824 (92%)	70 (8%)	18	46

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	516/519 (99%)	0.06	18 (3%)	42 50	36, 49, 58, 66	1 (0%)
1	B	516/519 (99%)	0.19	16 (3%)	47 55	37, 54, 70, 76	0
All	All	1032/1038 (99%)	0.12	34 (3%)	44 53	36, 52, 68, 76	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	GLU	4.7
1	B	270	ARG	4.4
1	A	395	GLY	3.6
1	B	421	ARG	3.4
1	A	206	ARG	3.4
1	A	44	SER	3.3
1	B	45	SER	3.2
1	A	208	GLY	2.8
1	B	190	GLU	2.8
1	B	447	GLU	2.8
1	B	175	GLU	2.7
1	A	207	LEU	2.6
1	A	234	VAL	2.6
1	B	268	TYR	2.6
1	A	47	LYS	2.6
1	B	453	GLU	2.5
1	B	78	GLN	2.5
1	A	43	SER	2.5
1	A	266	GLU	2.5
1	A	270	ARG	2.4
1	A	45	SER	2.4
1	B	427	LEU	2.4
1	B	430	ALA	2.2
1	A	235	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	92	GLN	2.1
1	B	331	TYR	2.1
1	A	3	LEU	2.1
1	A	205	ARG	2.1
1	A	271	HIS	2.1
1	A	396	ARG	2.1
1	A	458	ARG	2.1
1	B	420	GLY	2.1
1	B	3	LEU	2.0
1	B	413	LEU	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.