



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:47 PM UTC

PDB ID : 8DF7 / pdb_00008df7
Title : Structure of M. kandleri topoisomerase V in complex with DNA. 38 base pair symmetric DNA complex
Authors : Osterman, A.; Mondragon, A.
Deposited on : 2022-06-21
Resolution : 3.52 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

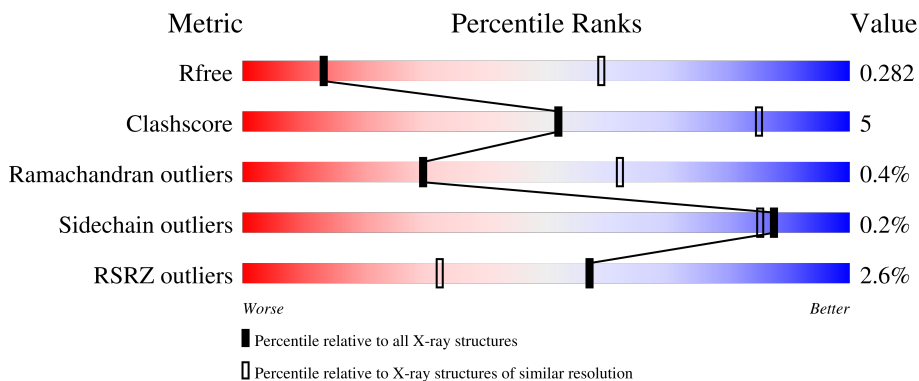
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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 $\leq 5\%$. 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	854	
1	B	854	
2	U	39	
2	V	39	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15168 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
			Total	C	N	O	S			
1	A	850	6802	4255	1222	1315	10	0	0	0
1	B	850	6802	4255	1222	1315	10	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

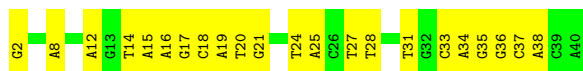
Chain	Residue	Modelled	Actual	Comment	Reference
A	809	ALA	LYS	engineered mutation	UNP Q977W1
A	820	ALA	LYS	engineered mutation	UNP Q977W1
A	831	ALA	LYS	engineered mutation	UNP Q977W1
A	835	ALA	LYS	engineered mutation	UNP Q977W1
A	846	ALA	LYS	engineered mutation	UNP Q977W1
A	851	ALA	LYS	engineered mutation	UNP Q977W1
B	809	ALA	LYS	engineered mutation	UNP Q977W1
B	820	ALA	LYS	engineered mutation	UNP Q977W1
B	831	ALA	LYS	engineered mutation	UNP Q977W1
B	835	ALA	LYS	engineered mutation	UNP Q977W1
B	846	ALA	LYS	engineered mutation	UNP Q977W1
B	851	ALA	LYS	engineered mutation	UNP Q977W1

- Molecule 2 is a DNA chain called DNA (39-MER).

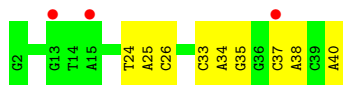
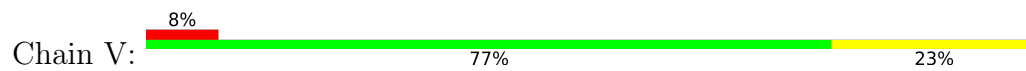
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	U	39	771	364	139	229	39	0	0	0
2	V	39	788	374	144	231	39	0	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	3	Total K 3 3	0	0



- Molecule 2: DNA (39-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.67Å 121.67Å 498.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.10 – 3.52 59.10 – 3.52	Depositor EDS
% Data completeness (in resolution range)	87.4 (59.10-3.52) 87.5 (59.10-3.52)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 3.49Å)	Xtrriage
Refinement program	BUSTER, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.229 , 0.275 0.263 , 0.282	Depositor DCC
R_{free} test set	2130 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	108.2	Xtrriage
Anisotropy	0.035	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 133.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15168	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K

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	0.09	0/6898	0.23	0/9292
1	B	0.09	0/6898	0.23	0/9292
2	U	0.18	0/863	0.37	0/1329
2	V	0.17	0/883	0.34	0/1359
All	All	0.10	0/15542	0.25	0/21272

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 [i](#)

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	6802	0	6862	69	0
1	B	6802	0	6862	71	0
2	U	771	0	421	17	0
2	V	788	0	433	7	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
All	All	15168	0	14578	151	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 5.

All (151) 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)
2:V:37:DC:H2''	2:V:38:DA:H5'	1.66	0.77
1:A:123:GLU:O	1:A:283:ARG:NH2	2.22	0.73
1:A:286:MET:HB3	1:A:292:GLN:HG3	1.72	0.71
1:A:634:LEU:HD21	1:A:664:LEU:HD13	1.73	0.69
1:B:287:ARG:HH22	1:B:296:GLU:HG3	1.58	0.69
2:V:25:DA:H4'	2:V:26:DC:H5'	1.74	0.69
1:B:220:PRO:HB3	1:B:231:ARG:HG3	1.76	0.67
1:A:130:VAL:HG21	1:A:147:VAL:HG11	1.77	0.66
1:A:516:LYS:O	1:A:535:LYS:NZ	2.28	0.66
2:U:14:DT:H2''	2:U:15:DA:C8	2.32	0.65
1:B:518:LEU:HD21	1:B:535:LYS:HD2	1.80	0.63
1:A:220:PRO:HB3	1:A:231:ARG:HG3	1.81	0.63
1:B:54:GLU:HG3	1:B:159:VAL:HG21	1.80	0.62
1:B:289:TYR:O	1:B:291:GLU:N	2.31	0.60
1:B:161:GLU:OE2	1:B:249:ARG:NH1	2.35	0.60
1:A:148:ARG:NH2	1:A:230:SER:OG	2.36	0.57
1:B:804:ARG:NH2	2:V:24:DT:OP1	2.37	0.57
1:A:332:ARG:NH2	1:A:372:GLU:OE2	2.36	0.57
1:B:308:ARG:NH2	1:B:340:ASP:O	2.34	0.57
1:A:834:VAL:HG13	1:A:847:ILE:HG21	1.86	0.56
1:B:130:VAL:HG21	1:B:147:VAL:HG11	1.87	0.56
1:A:461:ARG:NH2	1:B:304:ARG:O	2.39	0.56
1:A:513:ARG:NH1	1:A:522:GLU:OE1	2.39	0.56
1:A:123:GLU:HG3	1:A:299:LEU:HD13	1.87	0.56
1:B:169:GLU:OE1	1:B:172:ARG:NE	2.33	0.55
1:B:834:VAL:HG13	1:B:847:ILE:HG21	1.88	0.55
1:A:513:ARG:HD2	1:A:519:LYS:HG3	1.87	0.55
1:B:79:ASN:N	1:B:88:ASP:OD2	2.38	0.55
1:B:123:GLU:O	1:B:283:ARG:NH2	2.41	0.54
1:A:776:SER:O	1:A:780:GLU:HG2	2.07	0.54
1:B:787:LEU:HD12	1:B:797:ILE:HG23	1.89	0.54
2:U:14:DT:H2''	2:U:15:DA:N7	2.23	0.54
1:A:169:GLU:OE1	1:A:172:ARG:NE	2.34	0.54
1:B:487:LYS:NZ	1:B:505:ASP:OD1	2.42	0.53
1:B:231:ARG:O	1:B:235:ASN:ND2	2.39	0.53
1:B:571:LYS:HD3	1:B:615:GLU:HB3	1.90	0.53
1:A:684:ARG:HB2	1:A:688:ARG:HD3	1.90	0.53
1:B:552:LEU:O	1:B:557:PHE:HB2	2.09	0.52
1:A:811:LEU:HD11	1:A:850:ILE:HD11	1.91	0.52
1:A:71:ASP:O	1:A:102:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ARG:NH1	1:A:515:LEU:O	2.42	0.52
1:A:552:LEU:O	1:A:557:PHE:HB2	2.09	0.52
2:V:34:DA:H2''	2:V:35:DG:C8	2.44	0.52
1:A:112:ARG:HH22	1:A:292:GLN:HG2	1.75	0.52
1:B:677:ARG:HA	1:B:680:VAL:HG22	1.92	0.51
1:A:325:MET:HE1	1:B:704:VAL:HA	1.91	0.51
1:B:634:LEU:HD21	1:B:664:LEU:HD13	1.93	0.51
1:A:240:GLU:HG3	1:A:244:LYS:HE3	1.92	0.51
2:U:18:DC:H2''	2:U:19:DA:C8	2.46	0.51
1:A:677:ARG:HA	1:A:680:VAL:HG22	1.92	0.51
2:V:33:DC:H2''	2:V:34:DA:C8	2.46	0.50
1:A:106:VAL:HG11	1:A:148:ARG:HB2	1.94	0.50
1:B:419:VAL:HG22	1:B:459:VAL:HG13	1.93	0.50
1:B:82:VAL:HB	1:B:87:PHE:CE1	2.47	0.50
1:B:545:ARG:HG2	1:B:565:ILE:HG23	1.95	0.49
1:B:227:SER:OG	1:B:231:ARG:NH2	2.46	0.49
2:U:24:DT:H2''	2:U:25:DA:C8	2.47	0.49
1:A:731:VAL:HG13	1:A:745:VAL:HG11	1.95	0.49
1:A:787:LEU:HD12	1:A:797:ILE:HG23	1.94	0.49
1:B:756:ARG:NH1	1:B:762:PRO:HD3	2.28	0.49
1:B:682:SER:HA	1:B:685:LYS:HE2	1.95	0.48
1:A:830:ARG:NH2	1:A:852:GLY:O	2.46	0.48
1:B:153:ASP:HB3	1:B:243:ALA:HB2	1.95	0.48
1:B:811:LEU:HD11	1:B:850:ILE:HD11	1.95	0.48
1:A:756:ARG:NH1	1:A:762:PRO:HD3	2.28	0.48
1:B:761:THR:HG22	1:B:764:GLU:H	1.78	0.48
1:A:179:VAL:HG21	1:A:232:VAL:HG22	1.96	0.48
1:A:304:ARG:HG2	1:B:472:SER:HB2	1.96	0.48
1:B:123:GLU:HG3	1:B:299:LEU:HD23	1.95	0.48
2:U:20:DT:H2''	2:U:21:DG:C8	2.49	0.48
1:B:356:LEU:HB3	1:B:362:LEU:HD12	1.96	0.47
1:A:20:ARG:NH1	1:A:118:LEU:O	2.47	0.47
2:U:16:DA:H2''	2:U:17:DG:C8	2.49	0.47
1:A:374:PHE:O	1:A:376:SER:N	2.45	0.47
1:B:754:THR:OG1	2:U:12:DA:OP2	2.23	0.47
1:B:187:ARG:O	1:B:190:GLU:HG2	2.14	0.47
1:A:177:TYR:CZ	1:A:236:ILE:HG12	2.50	0.47
1:A:577:ASP:OD1	1:A:580:THR:OG1	2.26	0.47
1:A:51:GLU:O	1:A:54:GLU:HG2	2.16	0.46
1:A:487:LYS:NZ	1:A:505:ASP:OD1	2.46	0.46
1:B:488:TYR:OH	1:B:505:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:O	1:A:190:GLU:HG2	2.16	0.46
1:A:639:LEU:O	1:A:644:TYR:N	2.42	0.46
1:A:822:ARG:HH11	1:A:840:LEU:HD21	1.81	0.46
1:B:242:THR:HG22	1:B:245:ARG:NH2	2.30	0.46
1:B:177:TYR:CZ	1:B:236:ILE:HG12	2.51	0.46
1:A:54:GLU:O	1:A:58:ASN:ND2	2.47	0.46
2:U:37:DC:H2''	2:U:38:DA:H5''	1.96	0.46
1:A:392:TYR:OH	1:A:399:GLU:OE1	2.27	0.46
1:B:332:ARG:NH2	1:B:365:ASP:OD1	2.47	0.46
2:U:27:DT:H2'	2:U:28:DT:H71	1.98	0.46
1:B:513:ARG:NH1	1:B:522:GLU:OE1	2.46	0.45
2:U:33:DC:H2''	2:U:34:DA:C8	2.51	0.45
1:B:591:LEU:N	2:U:8:DA:OP1	2.44	0.45
1:B:761:THR:HG23	1:B:763:ALA:H	1.81	0.45
1:A:102:ARG:O	1:A:105:ILE:HG22	2.16	0.45
1:A:554:GLU:C	1:A:556:GLY:H	2.25	0.45
1:A:624:LEU:O	1:A:630:VAL:HG21	2.16	0.45
1:A:661:VAL:HG11	1:A:664:LEU:HD23	1.99	0.45
1:B:293:ARG:HB2	2:U:31:DT:OP1	2.17	0.45
1:B:289:TYR:C	1:B:291:GLU:H	2.20	0.45
1:B:761:THR:HG22	1:B:764:GLU:HG3	1.98	0.45
1:A:657:LEU:O	1:A:661:VAL:HG12	2.16	0.45
1:A:49:ASP:OD2	1:A:268:TYR:OH	2.27	0.45
1:A:125:VAL:HB	1:A:282:LYS:HD2	1.98	0.45
1:B:69:SER:OG	1:B:250:ARG:NH1	2.36	0.45
1:B:513:ARG:HD3	1:B:522:GLU:OE1	2.17	0.45
1:B:712:LEU:HD21	1:B:740:ILE:HG13	1.99	0.44
1:B:624:LEU:O	1:B:630:VAL:HG21	2.18	0.44
1:A:495:ARG:HA	1:A:515:LEU:HD21	1.99	0.44
1:B:753:LYS:HG2	2:U:12:DA:H3'	2.00	0.44
1:A:480:ARG:HH22	1:A:506:GLY:C	2.26	0.44
1:A:746:ALA:HB1	1:A:753:LYS:HB2	1.99	0.44
1:A:810:ARG:HH12	1:B:501:GLU:CD	2.26	0.44
1:B:545:ARG:NH1	1:B:565:ILE:O	2.50	0.44
1:B:287:ARG:HA	1:B:287:ARG:HD3	1.81	0.44
1:A:301:LEU:HB3	1:A:307:ILE:HD12	1.99	0.44
1:B:158:THR:HG22	1:B:160:ASP:H	1.84	0.43
1:A:433:ASN:OD1	1:A:436:ARG:N	2.45	0.43
1:A:735:LEU:HG	1:A:745:VAL:HG21	2.00	0.43
1:B:335:LYS:HA	1:B:335:LYS:HD2	1.87	0.43
1:B:731:VAL:HG13	1:B:745:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:GLU:C	1:B:556:GLY:H	2.27	0.43
1:A:661:VAL:HG11	1:A:664:LEU:HB3	2.01	0.43
1:B:834:VAL:O	1:B:838:ARG:HG3	2.19	0.43
1:A:102:ARG:O	1:A:106:VAL:HG13	2.18	0.43
1:B:20:ARG:NH1	1:B:118:LEU:O	2.52	0.43
1:B:283:ARG:O	1:B:287:ARG:HG2	2.18	0.43
2:U:16:DA:H2''	2:U:17:DG:H8	1.83	0.43
1:B:495:ARG:NH1	1:B:515:LEU:O	2.52	0.43
1:A:834:VAL:O	1:A:838:ARG:HG3	2.19	0.43
1:A:148:ARG:NE	1:A:218:LYS:HB3	2.35	0.42
1:B:178:ASP:O	1:B:179:VAL:HG22	2.19	0.42
1:A:37:ARG:HD2	2:V:37:DC:H1'	2.02	0.42
1:A:131:ARG:NH2	2:V:40:DA:OP1	2.31	0.42
1:A:634:LEU:HD11	1:A:664:LEU:HB2	2.00	0.42
1:B:746:ALA:HB1	1:B:753:LYS:HB2	2.01	0.42
1:A:23:PHE:HZ	1:A:111:TRP:HB2	1.85	0.42
1:A:545:ARG:HG2	1:A:565:ILE:HG23	2.02	0.41
1:B:16:PHE:CE2	1:B:20:ARG:HD2	2.54	0.41
1:B:138:LEU:HD11	1:B:156:PRO:HD2	2.01	0.41
1:B:374:PHE:O	1:B:376:SER:N	2.48	0.41
1:A:109:ARG:HD3	2:U:2:DG:C6	2.56	0.41
1:A:524:ILE:HD12	1:A:565:ILE:HG12	2.03	0.41
1:B:433:ASN:OD1	1:B:436:ARG:N	2.45	0.41
1:B:82:VAL:HG21	1:B:104:ALA:HB1	2.02	0.41
1:B:624:LEU:HD23	1:B:624:LEU:HA	1.91	0.41
1:A:55:LEU:HD12	1:A:257:LEU:HD22	2.03	0.40
1:B:293:ARG:HE	2:U:31:DT:H5''	1.85	0.40
1:A:774:SER:O	1:A:778:VAL:HG23	2.22	0.40
2:U:35:DG:H2''	2:U:36:DG:H8	1.85	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	848/854 (99%)	816 (96%)	31 (4%)	1 (0%)	48 79
1	B	848/854 (99%)	812 (96%)	30 (4%)	6 (1%)	18 52
All	All	1696/1708 (99%)	1628 (96%)	61 (4%)	7 (0%)	30 62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	290	LEU
1	B	178	ASP
1	B	179	VAL
1	B	375	GLU
1	B	688	ARG
1	B	663	GLY
1	A	781	GLY

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	712/715 (100%)	711 (100%)	1 (0%)	88 87
1	B	712/715 (100%)	710 (100%)	2 (0%)	86 83
All	All	1424/1430 (100%)	1421 (100%)	3 (0%)	87 85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	518	LEU
1	B	179	VAL
1	B	761	THR

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

Mol	Chain	Res	Type
1	A	57	GLN

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Mol	Chain	Res	Type
1	A	78	GLN
1	A	79	ASN
1	A	195	ASN
1	B	57	GLN
1	B	195	ASN
1	B	281	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	850/854 (99%)	0.26	15 (1%) 67 40	53, 120, 190, 235	0
1	B	850/854 (99%)	0.37	28 (3%) 49 27	52, 130, 211, 268	0
2	U	39/39 (100%)	1.03	0 100 100	80, 125, 180, 189	0
2	V	39/39 (100%)	1.21	3 (7%) 19 13	81, 129, 172, 194	0
All	All	1778/1786 (99%)	0.35	46 (2%) 57 32	52, 125, 201, 268	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	ARG	4.5
1	B	166	MET	3.8
1	A	67	ALA	3.8
1	A	147	VAL	3.4
1	B	130	VAL	3.3
1	B	167	ALA	3.2
1	A	3	LEU	3.0
1	B	297	CYS	2.9
1	B	736	GLU	2.9
2	V	13	DG	2.9
1	B	157	VAL	2.9
1	B	58	ASN	2.8
1	B	288	ARG	2.7
1	B	290	LEU	2.7
1	B	147	VAL	2.7
1	B	203	ILE	2.6
1	B	69	SER	2.6
1	A	135	ARG	2.6
1	A	288	ARG	2.5
1	B	174	ILE	2.5
1	A	338	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	104	ALA	2.4
1	B	52	LEU	2.4
1	B	152	VAL	2.3
1	B	156	PRO	2.3
1	A	284	ASP	2.3
1	B	150	GLY	2.3
1	B	3	LEU	2.3
1	A	68	CYS	2.3
1	B	84	GLY	2.3
1	B	338	CYS	2.2
2	V	37	DC	2.2
1	B	229	TRP	2.2
2	V	15	DA	2.2
1	B	30	TYR	2.2
1	A	77	TYR	2.1
1	A	40	MET	2.1
1	A	285	ILE	2.1
1	B	852	GLY	2.0
1	A	141	ALA	2.0
1	A	294	ILE	2.0
1	B	287	ARG	2.0
1	B	155	MET	2.0
1	A	235	ASN	2.0
1	A	290	LEU	2.0
1	B	256	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	K	B	901	1/1	0.81	0.34	22,22,22,22	0
3	K	B	903	1/1	0.84	0.19	48,48,48,48	0
3	K	A	901	1/1	0.88	0.38	10,10,10,10	0
3	K	B	902	1/1	0.90	0.29	38,38,38,38	0
3	K	A	902	1/1	0.92	0.23	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.