



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:09 AM UTC

PDB ID : 8DF9 / pdb_00008df9
Title : Structure of M. kandleri topoisomerase V in complex with DNA. 38 base pair asymmetric DNA complex
Authors : Osterman, A.; Mondragon, A.
Deposited on : 2022-06-21
Resolution : 3.24 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
Xtriage (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

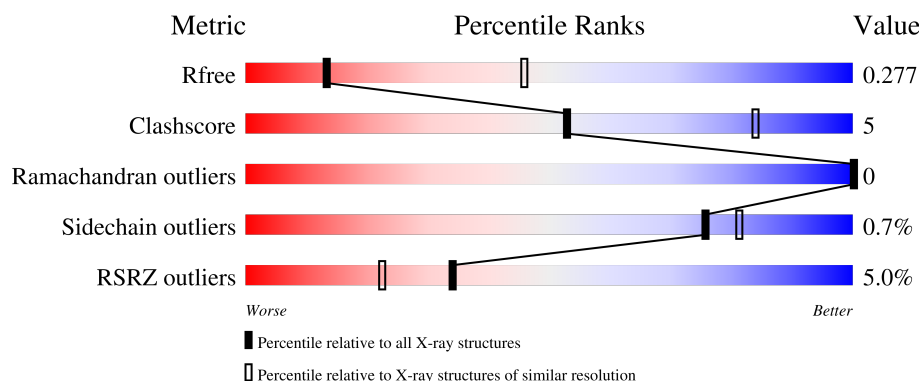
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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.



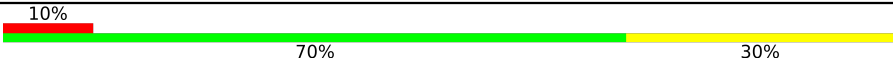
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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 $\leq 5\%$. 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	4% 78% 13% 9%
1	B	854	6% 86% 13% .
2	S	33	3% 70% 30%
3	T	33	73% 27%
4	U	17	6% 59% 41%

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Mol	Chain	Length	Quality of chain
5	V	20	 10% 70% 30%
5	X	20	 5% 60% 40%
6	W	18	 61% 39%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15929 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	781	Total	C	N	O	S	0	0	0
			6249	3911	1122	1206	10			
1	B	845	Total	C	N	O	S	0	0	0
			6765	4231	1214	1310	10			

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 (33-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	33	Total	C	N	O	P	0	0	0
			681	323	130	195	33			

- Molecule 3 is a DNA chain called DNA (33-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	33	Total	C	N	O	P	0	0	0
			669	321	117	199	32			

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*CP*CP*TP*GP*CP*AP*CP*GP*AP*AP*GP*TP*AP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	U	17	Total	C	N	O	P	0	0	0
			350	165	69	99	17			

- Molecule 5 is a DNA chain called DNA (5'-D(P*TP*GP*CP*TP*TP*AP*CP*TP*TP*CP*GP*TP*GP*CP*AP*GP*GP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	V	20	Total	C	N	O	P	0	0	0
			408	195	69	124	20			
5	X	20	Total	C	N	O	P	0	0	0
			392	185	67	120	20			

- Molecule 6 is a DNA chain called DNA (5'-D(P*GP*CP*CP*TP*GP*CP*AP*CP*GP*AP*AP*GP*TP*AP*AP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	W	18	Total	C	N	O	P	0	0	0
			371	175	74	104	18			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	Mg	0	0
			5	5		
7	B	7	Total	Mg	0	0
			7	7		

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	S	1	Total	K	0	0
			1	1		
8	T	1	Total	K	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	11	Total	O	0	0
			11	11		

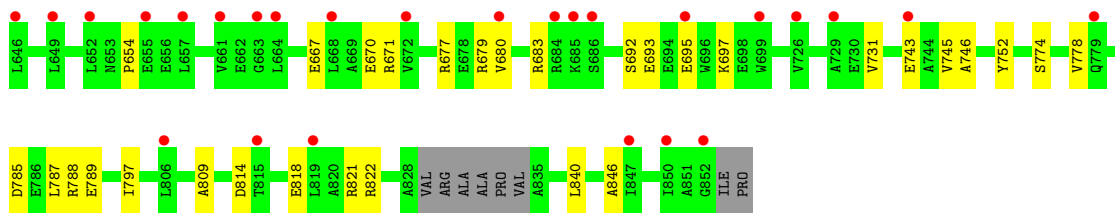
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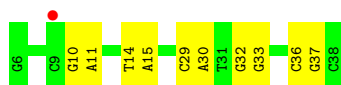
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	19	Total	O	0	0
			19	19		

- Molecule 1: Topoisomerase V





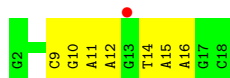
• Molecule 2: DNA (33-MER)



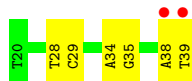
• Molecule 3: DNA (33-MER)



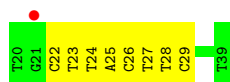
• Molecule 4: DNA (5'-D(P*GP*CP*CP*TP*GP*CP*AP*CP*GP*AP*AP*GP*TP*AP*AP*GP*C)-3')



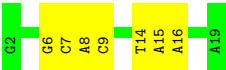
• Molecule 5: DNA (5'-D(P*TP*GP*CP*TP*TP*AP*CP*TP*TP*CP*GP*TP*GP*CP*AP*GP*GP*CP*CP*A)-3')



• Molecule 5: DNA (5'-D(P*TP*GP*CP*TP*TP*AP*CP*TP*TP*CP*GP*TP*GP*CP*AP*GP*GP*CP*CP*A)-3')



• Molecule 6: DNA (5'-D(P*GP*CP*CP*TP*GP*CP*AP*CP*GP*AP*AP*GP*TP*AP*AP*GP*CP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	193.75Å 193.75Å 245.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.28 – 3.24 39.28 – 3.24	Depositor EDS
% Data completeness (in resolution range)	70.3 (39.28-3.24) 70.3 (39.28-3.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.25Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.235 , 0.266 0.245 , 0.277	Depositor DCC
R_{free} test set	2599 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	122.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 108.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15929	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: MG, 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	0.18	0/6338	0.32	0/8540
1	B	0.19	1/6859 (0.0%)	0.32	0/9236
2	S	0.18	0/765	0.33	0/1179
3	T	0.18	0/748	0.35	0/1152
4	U	0.17	0/393	0.29	0/604
5	V	0.21	0/455	0.43	0/700
5	X	0.22	0/437	0.43	0/673
6	W	0.16	0/417	0.34	0/641
All	All	0.19	1/16412 (0.0%)	0.33	0/22725

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	ASP	C-O	-7.12	1.20	1.23

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	6249	0	6307	65	0
1	B	6765	0	6820	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	681	0	371	7	0
3	T	669	0	375	6	0
4	U	350	0	190	4	0
5	V	408	0	228	5	0
5	X	392	0	215	4	0
6	W	371	0	201	5	0
7	A	5	0	0	0	0
7	B	7	0	0	0	0
8	S	1	0	0	0	0
8	T	1	0	0	0	0
9	A	11	0	0	1	0
9	B	19	0	0	0	0
All	All	15929	0	14707	148	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 (148) 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:848:ALA:HA	1:A:852:GLY:HA2	1.69	0.75
1:B:38:TYR:HB2	1:B:285:ILE:HG23	1.72	0.72
4:U:14:DT:H2''	4:U:15:DA:H5''	1.71	0.72
1:B:308:ARG:NH2	1:B:340:ASP:O	2.24	0.70
2:S:10:DG:H2''	2:S:11:DA:H5'	1.74	0.70
1:B:818:GLU:OE1	1:B:821:ARG:NH1	2.25	0.68
1:A:834:VAL:HG13	1:A:847:ILE:HG21	1.77	0.66
3:T:6:DC:H2''	3:T:7:DC:H5''	1.78	0.66
6:W:14:DT:H2''	6:W:15:DA:H5''	1.76	0.66
1:B:21:GLU:HG2	1:B:25:LYS:HE3	1.78	0.65
1:B:524:ILE:HD13	1:B:565:ILE:HG12	1.77	0.64
1:B:809:ALA:HB1	1:B:846:ALA:HB1	1.79	0.64
6:W:6:DG:H2''	6:W:7:DC:H5''	1.79	0.64
1:B:161:GLU:OE2	1:B:246:HIS:NE2	2.32	0.63
1:A:784:PRO:HB2	1:A:788:ARG:HH21	1.64	0.63
1:A:308:ARG:NH2	1:A:340:ASP:O	2.29	0.62
1:B:731:VAL:HG13	1:B:745:VAL:HG11	1.81	0.62
1:A:393:GLU:O	9:A:1001:HOH:O	2.15	0.62
5:V:28:DT:H2''	5:V:29:DC:H5''	1.81	0.62
1:B:342:THR:HG22	1:B:344:GLU:H	1.64	0.62
1:A:731:VAL:HG13	1:A:745:VAL:HG11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:LEU:HD11	1:B:541:ALA:HB2	1.83	0.60
1:A:342:THR:HG22	1:A:344:GLU:H	1.65	0.60
1:B:458:ARG:HH12	1:B:461:ARG:HD3	1.67	0.60
5:X:28:DT:H2''	5:X:29:DC:H5''	1.85	0.58
1:A:830:ARG:HH12	5:V:39:DT:H1'	1.68	0.58
3:T:20:DT:H2''	3:T:21:DG:H5''	1.85	0.58
1:A:38:TYR:HB2	1:A:285:ILE:HG23	1.86	0.56
1:A:21:GLU:HG2	1:A:25:LYS:HE3	1.86	0.56
2:S:36:DC:H2''	2:S:37:DG:H5''	1.86	0.56
1:A:518:LEU:HD21	1:A:535:LYS:HD2	1.87	0.56
1:A:179:VAL:HG13	1:A:231:ARG:HD2	1.88	0.55
1:B:743:GLU:HB2	2:S:15:DA:H3'	1.88	0.55
1:A:491:TYR:OH	1:A:495:ARG:NH1	2.40	0.55
1:A:788:ARG:NH2	1:A:814:ASP:OD1	2.30	0.54
1:B:530:LYS:HD3	1:B:557:PHE:HZ	1.72	0.54
1:B:305:TYR:CD2	1:B:349:VAL:HA	2.43	0.54
1:A:693:GLU:HG3	1:A:718:SER:HB2	1.90	0.54
1:A:180:PRO:O	1:A:231:ARG:NH1	2.41	0.54
1:A:356:LEU:HB3	1:A:362:LEU:HD12	1.89	0.53
1:A:525:VAL:HG11	1:A:530:LYS:HB2	1.91	0.52
1:B:179:VAL:HG13	1:B:231:ARG:HD2	1.90	0.52
1:B:654:PRO:HG2	1:B:670:GLU:HG2	1.90	0.52
1:A:194:GLU:CD	1:B:42:ARG:HH21	2.17	0.52
1:B:518:LEU:HD21	1:B:535:LYS:HD2	1.92	0.52
1:B:619:PRO:HA	1:B:622:LYS:HE2	1.91	0.52
1:B:788:ARG:NH2	1:B:814:ASP:OD1	2.43	0.51
1:B:356:LEU:HB3	1:B:362:LEU:HD12	1.91	0.51
1:A:524:ILE:HD13	1:A:565:ILE:HG12	1.92	0.51
1:B:222:SER:HB3	1:B:227:SER:HB2	1.92	0.51
1:A:521:LEU:HD11	1:A:541:ALA:HB2	1.93	0.50
1:B:142:LEU:HB2	1:B:229:TRP:CE2	2.46	0.50
5:V:38:DA:H2''	5:V:39:DT:H5''	1.93	0.50
1:A:213:GLU:OE2	1:A:845:ARG:NH2	2.45	0.49
1:A:812:ASP:OD1	1:A:815:THR:OG1	2.28	0.49
1:B:125:VAL:O	1:B:282:LYS:NZ	2.31	0.49
1:B:220:PRO:HB3	1:B:231:ARG:HA	1.94	0.49
1:B:532:ASP:O	1:B:536:ARG:HG2	2.12	0.49
1:B:102:ARG:HD2	1:B:147:VAL:O	2.13	0.48
1:B:677:ARG:HA	1:B:680:VAL:HG22	1.95	0.48
2:S:14:DT:H2''	2:S:15:DA:C8	2.48	0.48
1:A:177:TYR:CZ	1:A:236:ILE:HG12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ARG:HH12	1:A:461:ARG:HD3	1.78	0.48
1:B:503:ARG:HH21	1:B:528:LEU:HD13	1.79	0.48
1:B:352:THR:HG23	1:B:377:ILE:HG12	1.95	0.48
1:A:30:TYR:CE1	1:A:129:GLU:HB2	2.49	0.48
1:A:417:GLU:HG2	1:A:458:ARG:HD2	1.95	0.48
4:U:9:DC:H2''	4:U:10:DG:C8	2.50	0.47
1:B:525:VAL:HG11	1:B:530:LYS:HB2	1.96	0.47
1:B:58:ASN:HB3	1:B:257:LEU:HD11	1.95	0.47
6:W:8:DA:H1'	6:W:9:DC:H5'	1.97	0.47
1:B:746:ALA:HA	1:B:752:TYR:HB3	1.96	0.47
4:U:15:DA:H2''	4:U:16:DA:C8	2.50	0.47
1:A:102:ARG:NH1	1:A:148:ARG:O	2.48	0.47
1:A:530:LYS:HD3	1:A:557:PHE:HZ	1.80	0.46
1:A:142:LEU:HB2	1:A:229:TRP:CE2	2.50	0.46
1:A:553:ARG:NH2	1:A:579:GLU:OE2	2.49	0.46
1:B:679:ARG:HD2	1:B:683:ARG:HH12	1.81	0.46
1:A:183:GLU:OE1	1:A:442:ARG:NH2	2.48	0.46
1:B:487:LYS:NZ	1:B:505:ASP:OD1	2.49	0.46
1:B:30:TYR:CE1	1:B:129:GLU:HB2	2.51	0.46
1:B:296:GLU:HG2	1:B:300:LYS:HE3	1.98	0.46
1:A:215:GLU:HB3	1:A:226:TYR:CD2	2.52	0.45
1:B:156:PRO:HG2	1:B:162:VAL:HG22	1.99	0.45
5:V:34:DA:H2''	5:V:35:DG:C8	2.52	0.45
1:A:746:ALA:HA	1:A:752:TYR:HB3	1.98	0.45
1:B:475:GLY:HA3	1:B:511:GLN:HE21	1.82	0.45
2:S:32:DG:H2''	2:S:33:DG:H5''	1.98	0.45
1:A:351:ARG:HH21	1:A:845:ARG:NH1	2.15	0.44
1:A:825:SER:H	1:A:828:ALA:HB3	1.81	0.44
1:B:32:GLY:HA3	1:B:59:PHE:CE1	2.52	0.44
1:A:55:LEU:HD21	1:A:261:LEU:HB2	1.99	0.44
1:A:391:MET:HG2	1:A:396:ARG:HH21	1.81	0.44
3:T:7:DC:H2''	3:T:8:DA:H5'	1.97	0.44
5:X:24:DT:H1'	5:X:25:DA:H5'	1.98	0.44
1:B:37:ARG:O	1:B:41:GLU:HG2	2.18	0.44
1:B:787:LEU:HD12	1:B:797:ILE:HG23	1.99	0.44
2:S:29:DC:H2''	2:S:30:DA:H8	1.83	0.44
1:B:667:GLU:O	1:B:671:ARG:HG2	2.18	0.44
5:X:26:DC:H2''	5:X:27:DT:H5'	1.99	0.44
1:A:341:LEU:HD21	1:A:346:ALA:HB2	2.00	0.44
1:A:446:ILE:HG12	1:A:464:VAL:HG21	1.99	0.44
1:B:470:LEU:HD23	1:B:470:LEU:HA	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ILE:O	1:A:598:LEU:HB2	2.18	0.43
1:A:151:ARG:NH1	1:A:153:ASP:OD1	2.51	0.43
1:B:142:LEU:O	1:B:146:LEU:HG	2.18	0.43
1:B:500:GLU:H	1:B:500:GLU:CD	2.27	0.43
1:B:571:LYS:HD3	1:B:615:GLU:HB3	2.01	0.43
1:A:37:ARG:HH12	1:A:134:LYS:HE3	1.82	0.43
1:A:814:ASP:O	1:A:818:GLU:HG3	2.19	0.43
6:W:15:DA:H2''	6:W:16:DA:C8	2.54	0.43
1:A:473:ILE:HB	1:A:476:ILE:HD12	2.01	0.43
1:A:785:ASP:O	1:A:789:GLU:HG2	2.19	0.43
3:T:29:DC:H2''	3:T:30:DG:H5'	2.00	0.43
1:A:153:ASP:OD1	1:A:153:ASP:N	2.52	0.42
1:A:42:ARG:O	1:B:205:ARG:NH2	2.53	0.42
1:B:774:SER:O	1:B:778:VAL:HG23	2.20	0.42
1:B:785:ASP:O	1:B:789:GLU:HG2	2.19	0.42
5:X:22:DC:H2''	5:X:23:DT:H5''	2.01	0.42
1:A:199:PRO:HG2	1:A:202:GLU:HB2	2.01	0.42
1:A:754:THR:OG1	5:V:35:DG:OP2	2.21	0.42
2:S:14:DT:H2''	2:S:15:DA:H8	1.85	0.42
1:A:707:GLY:O	1:A:710:ARG:HG2	2.20	0.42
3:T:26:DC:H2''	3:T:27:DT:H5'	2.02	0.42
4:U:11:DA:H1'	4:U:12:DA:H5'	2.02	0.42
1:A:28:LYS:HG3	1:A:275:ARG:CZ	2.50	0.42
1:B:822:ARG:HH11	1:B:840:LEU:HD11	1.85	0.42
3:T:27:DT:H6	3:T:27:DT:H2'	1.71	0.42
1:B:692:SER:HB3	1:B:695:GLU:HG3	2.01	0.41
1:A:691:ARG:HB3	1:A:695:GLU:HB3	2.02	0.41
1:A:163:PRO:HA	1:A:164:PRO:HD3	1.99	0.41
1:A:513:ARG:HD2	1:A:519:LYS:HA	2.02	0.41
1:B:55:LEU:HD12	1:B:257:LEU:HD22	2.02	0.41
1:A:311:VAL:HG13	1:A:338:CYS:SG	2.61	0.41
1:A:389:GLU:OE2	1:A:429:ARG:NH2	2.53	0.41
1:B:81:ILE:HD13	1:B:86:ASN:HA	2.03	0.41
1:A:774:SER:O	1:A:778:VAL:HG23	2.21	0.41
1:A:800:ILE:HD12	1:A:800:ILE:HA	1.94	0.41
1:B:171:GLU:CD	1:B:193:ARG:HE	2.29	0.41
1:A:500:GLU:H	1:A:500:GLU:CD	2.29	0.41
1:A:850:ILE:HG22	1:A:851:ALA:N	2.36	0.41
1:B:631:GLY:HA2	1:B:632:PRO:HD3	1.98	0.41
1:B:693:GLU:O	1:B:697:LYS:HG3	2.20	0.41
6:W:7:DC:H2''	6:W:8:DA:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ARG:HH21	1:A:528:LEU:HD13	1.86	0.40
1:A:532:ASP:O	1:A:536:ARG:HG2	2.21	0.40
1:A:81:ILE:HD11	1:A:86:ASN:HD22	1.86	0.40
1:A:20:ARG:HH22	1:A:122:GLU:CD	2.30	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	777/854 (91%)	754 (97%)	23 (3%)	0	100	100
1	B	841/854 (98%)	818 (97%)	23 (3%)	0	100	100
All	All	1618/1708 (95%)	1572 (97%)	46 (3%)	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	655/715 (92%)	649 (99%)	6 (1%)	70	79
1	B	708/715 (99%)	704 (99%)	4 (1%)	78	83
All	All	1363/1430 (95%)	1353 (99%)	10 (1%)	76	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	202	GLU
1	A	393	GLU
1	A	553	ARG
1	A	695	GLU
1	A	850	ILE
1	B	148	ARG
1	B	291	GLU
1	B	303	ASP
1	B	553	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	779	GLN

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 14 ligands modelled in this entry, 14 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	781/854 (91%)	0.31	34 (4%) 39 25	79, 116, 248, 268	0
1	B	845/854 (98%)	0.38	49 (5%) 29 19	78, 121, 244, 251	0
2	S	33/33 (100%)	0.11	1 (3%) 52 34	118, 172, 260, 267	0
3	T	33/33 (100%)	0.04	0 100 100	116, 177, 254, 265	0
4	U	17/17 (100%)	0.54	1 (5%) 28 18	205, 223, 239, 239	0
5	V	20/20 (100%)	0.52	2 (10%) 12 9	198, 231, 283, 296	0
5	X	20/20 (100%)	0.64	1 (5%) 34 22	176, 214, 297, 338	0
6	W	18/18 (100%)	0.47	0 100 100	182, 208, 250, 251	0
All	All	1767/1849 (95%)	0.34	88 (4%) 34 22	78, 123, 246, 338	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	779	GLN	6.4
1	A	743	GLU	6.2
1	B	646	LEU	6.1
1	B	743	GLU	6.0
1	B	686	SER	5.1
1	A	559	ASP	4.4
1	B	663	GLY	4.2
1	A	700	LEU	3.7
1	B	729	ALA	3.4
1	B	630	VAL	3.4
1	B	609	THR	3.3
1	A	606	LEU	3.1
1	B	664	LEU	3.1
1	A	747	ARG	3.1
1	B	806	LEU	3.1
1	A	266	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	520	THR	3.0
1	A	591	LEU	2.9
1	B	627	ILE	2.9
1	B	649	LEU	2.9
1	B	592	LYS	2.8
1	B	612	ALA	2.8
1	B	611	LYS	2.8
1	B	655	GLU	2.8
1	A	572	LEU	2.7
1	A	826	VAL	2.7
1	B	668	LEU	2.7
1	B	567	GLY	2.7
1	B	624	LEU	2.7
1	B	538	TYR	2.7
2	S	9	DC	2.7
1	B	819	LEU	2.6
1	A	545	ARG	2.6
1	A	571	LYS	2.6
1	A	521	LEU	2.6
1	A	853	ILE	2.6
1	A	89	GLU	2.5
1	A	719	ALA	2.5
1	B	638	ILE	2.5
1	B	511	GLN	2.5
1	A	466	GLY	2.4
1	B	565	ILE	2.4
1	A	555	LEU	2.4
1	B	815	THR	2.4
1	A	726	VAL	2.4
1	B	850	ILE	2.4
1	A	616	ILE	2.4
1	A	309	GLU	2.4
1	A	754	THR	2.3
1	A	594	ILE	2.3
1	B	573	ARG	2.3
5	V	39	DT	2.3
1	A	815	THR	2.3
1	B	531	ALA	2.3
5	V	38	DA	2.3
1	B	519	LYS	2.3
1	B	629	GLY	2.3
1	A	520	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	685	LYS	2.3
1	B	779	GLN	2.3
1	B	652	LEU	2.2
1	B	657	LEU	2.2
1	A	311	VAL	2.2
1	B	468	ALA	2.2
1	B	672	VAL	2.2
1	A	696	TRP	2.2
1	A	819	LEU	2.1
1	B	440	LEU	2.1
1	B	680	VAL	2.1
1	B	726	VAL	2.1
1	B	628	GLU	2.1
1	B	852	GLY	2.1
1	B	699	TRP	2.1
1	A	568	ILE	2.1
1	A	830	ARG	2.1
1	B	518	LEU	2.1
1	B	528	LEU	2.1
4	U	13	DG	2.1
5	X	21	DG	2.1
1	B	695	GLU	2.1
1	B	661	VAL	2.0
1	B	847	ILE	2.0
1	A	552	LEU	2.0
1	A	391	MET	2.0
1	B	582	ALA	2.0
1	A	757	ASP	2.0
1	A	474	ARG	2.0
1	B	684	ARG	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(Å ²)	Q<0.9
7	MG	A	901	1/1	0.82	0.19	120,120,120,120	0
7	MG	B	901	1/1	0.82	0.18	154,154,154,154	0
7	MG	B	902	1/1	0.82	0.12	117,117,117,117	0
7	MG	B	903	1/1	0.82	0.12	106,106,106,106	0
7	MG	A	905	1/1	0.83	0.13	141,141,141,141	0
8	K	S	101	1/1	0.84	0.20	132,132,132,132	0
7	MG	A	903	1/1	0.88	0.14	150,150,150,150	0
7	MG	B	907	1/1	0.90	0.13	148,148,148,148	0
7	MG	B	904	1/1	0.93	0.12	160,160,160,160	0
8	K	T	101	1/1	0.95	0.14	118,118,118,118	0
7	MG	B	906	1/1	0.96	0.06	144,144,144,144	0
7	MG	A	902	1/1	0.97	0.07	108,108,108,108	0
7	MG	B	905	1/1	0.98	0.08	107,107,107,107	0
7	MG	A	904	1/1	0.99	0.08	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.