Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2022 – 01:43 PM EDT

PDB ID	:	8DF9
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:

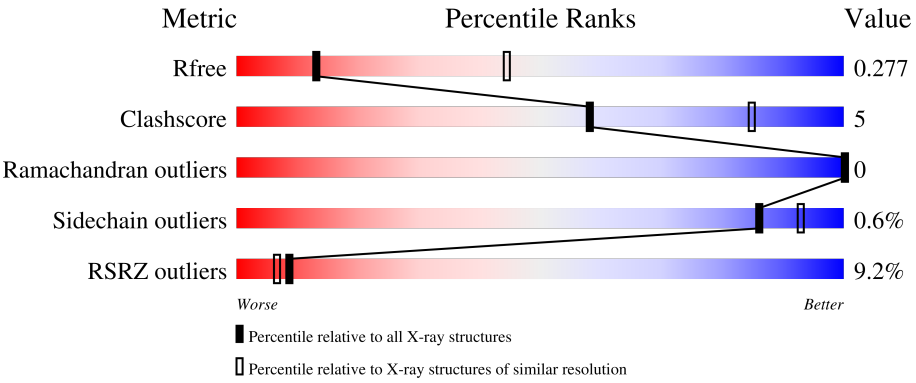
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 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}	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (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 <=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	7% 78% 13% 9%
1	B	854	10% 87% 12% .
2	S	33	18% 70% 30%
3	T	33	12% 73% 27%
4	U	17	6% 59% 41%

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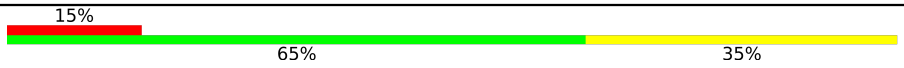
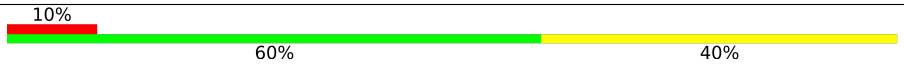
Mol	Chain	Length	Quality of chain
5	V	20	
5	X	20	
6	W	18	

2 Entry composition (i)

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 (three-letter code: 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 (three-letter code: 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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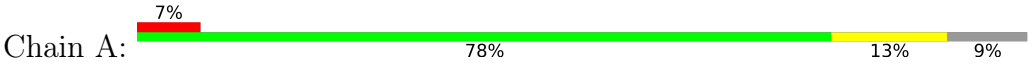
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	19	Total O 19 19	0	0

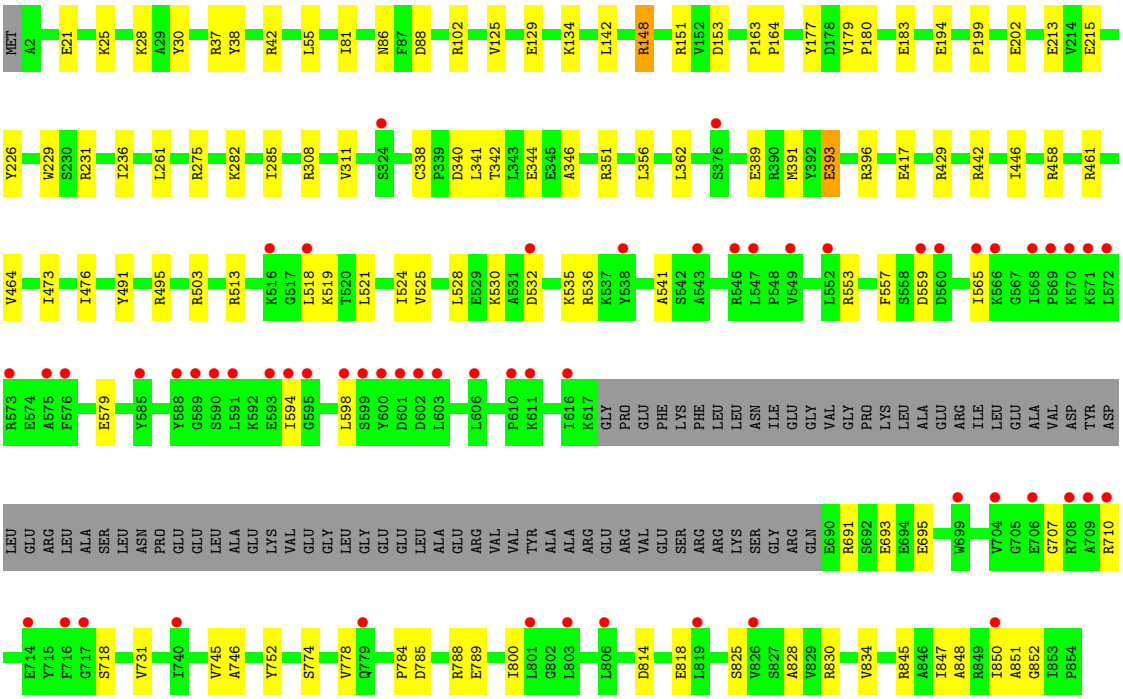
3 Residue-property plots (i)

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: Topoisomerase V

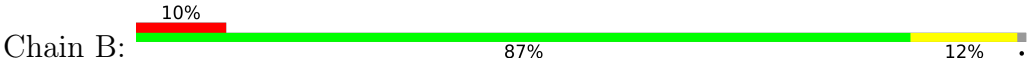
Chain A:

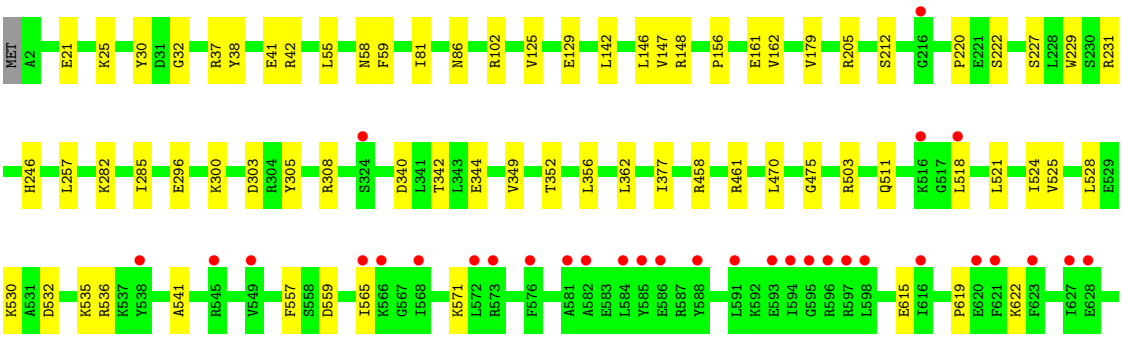


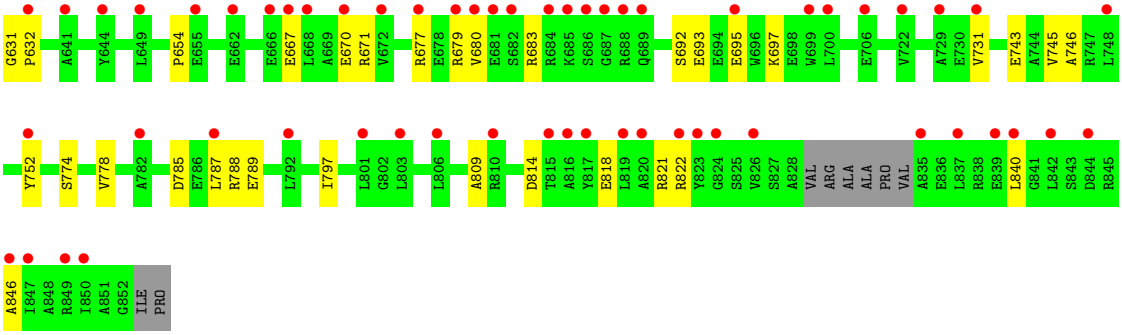


• Molecule 1: Topoisomerase V

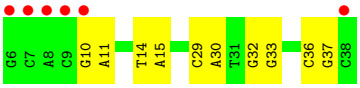
Chain B:



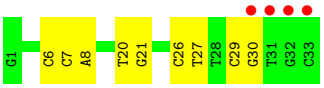




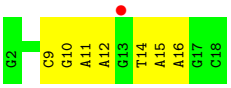
• Molecule 2: DNA (33-MER)



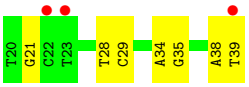
• Molecule 3: DNA (33-MER)



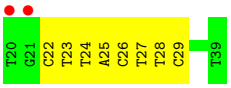
• Molecule 4: DNA (5'-D(P*GP*CP*CP*TP*GP*CP*AP*CP*GP*AP*AP*GP*TP*AP*AP*GP*C)-3')



• 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')

Chain W:

4 Data and refinement statistics (i)

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) 70.4 (39.28-3.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.95%)	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)	0.29 , 88.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

[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

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

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	0.29	0/6338	0.53	0/8540
1	B	0.28	0/6859	0.53	0/9236
2	S	0.51	0/765	0.84	0/1179
3	T	0.51	0/748	0.89	0/1152
4	U	0.49	0/393	0.79	0/604
5	V	0.54	0/455	0.99	1/700 (0.1%)
5	X	0.55	0/437	0.99	0/673
6	W	0.48	0/417	0.85	1/641 (0.2%)
All	All	0.34	0/16412	0.63	2/22725 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	W	2	DG	OP1-P-OP2	-6.74	109.50	119.60
5	V	21	DG	OP1-P-OP2	-6.32	110.13	119.60

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	6249	0	6307	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6765	0	6820	54	0
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	4	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	142	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 (142) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:VAL:HG13	1:A:745:VAL:HG11	1.81	0.61
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:125:VAL:O	1:A:282:LYS:NZ	2.37	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: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: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
1:A:194:GLU:CD	1:B:42:ARG:HH21	2.17	0.47
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: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: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
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: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
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

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%)	651 (99%)	4 (1%)	86	93
1	B	708/715 (99%)	704 (99%)	4 (1%)	86	93
All	All	1363/1430 (95%)	1355 (99%)	8 (1%)	86	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASP
1	A	148	ARG
1	A	393	GLU
1	A	559	ASP
1	B	148	ARG
1	B	212	SER
1	B	303	ASP
1	B	559	ASP

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

Mol	Chain	Res	Type
1	A	78	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

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

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	781/854 (91%)	0.38	58 (7%) 14 10	79, 116, 248, 268	0
1	B	845/854 (98%)	0.56	89 (10%) 6 5	78, 121, 244, 251	0
2	S	33/33 (100%)	0.56	6 (18%) 1 1	118, 172, 260, 267	0
3	T	33/33 (100%)	0.37	4 (12%) 4 3	116, 177, 254, 265	0
4	U	17/17 (100%)	0.24	1 (5%) 22 15	205, 223, 239, 239	0
5	V	20/20 (100%)	0.54	3 (15%) 2 2	198, 231, 283, 296	0
5	X	20/20 (100%)	0.22	2 (10%) 7 5	176, 214, 297, 338	0
6	W	18/18 (100%)	-0.27	0 100 100	182, 208, 250, 251	0
All	All	1767/1849 (95%)	0.46	163 (9%) 9 7	78, 123, 246, 338	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	PRO	7.1
2	S	9	DC	7.0
1	B	686	SER	6.0
1	A	600	TYR	5.7
1	B	596	ARG	5.7
1	A	594	ILE	5.7
1	B	598	LEU	5.7
1	B	662	GLU	5.5
1	B	594	ILE	5.4
1	A	572	LEU	5.4
3	T	33	DC	5.3
3	T	32	DG	5.3
1	A	568	ILE	5.2
1	A	598	LEU	5.2
1	A	559	ASP	5.2
1	B	649	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	681	GLU	5.1
1	B	688	ARG	5.1
1	B	684	ARG	5.1
1	B	685	LYS	5.1
1	B	538	TYR	4.9
1	B	706	GLU	4.9
5	X	20	DT	4.7
1	B	823	TYR	4.5
1	B	806	LEU	4.5
1	B	819	LEU	4.5
1	B	621	PHE	4.3
1	A	590	SER	4.3
1	B	792	LEU	4.2
1	A	606	LEU	4.2
1	B	803	LEU	4.2
1	A	547	LEU	4.1
1	B	722	VAL	4.0
1	B	616	ILE	4.0
1	B	572	LEU	3.9
1	A	706	GLU	3.9
1	B	582	ALA	3.9
1	B	835	ALA	3.9
1	A	588	TYR	3.8
1	B	573	ARG	3.8
1	A	546	ARG	3.7
2	S	10	DG	3.7
1	A	549	VAL	3.6
1	A	566	LYS	3.6
1	B	729	ALA	3.5
2	S	8	DA	3.5
1	B	815	THR	3.5
1	A	801	LEU	3.5
1	A	601	ASP	3.4
1	B	842	LEU	3.3
1	A	569	PRO	3.3
1	B	644	TYR	3.3
1	B	588	TYR	3.3
1	A	602	ASP	3.3
1	B	822	ARG	3.2
1	B	839	GLU	3.2
1	B	568	ILE	3.2
1	B	627	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	573	ARG	3.2
5	V	23	DT	3.2
2	S	7	DC	3.1
1	B	817	TYR	3.1
1	B	655	GLU	3.1
1	B	782	ALA	3.1
1	B	826	VAL	3.1
1	A	716	PHE	3.1
1	B	641	ALA	3.1
2	S	6	DG	3.0
1	B	820	ALA	3.0
1	B	787	LEU	3.0
1	B	623	PHE	3.0
1	A	595	GLY	3.0
2	S	38	DC	3.0
1	A	575	ALA	3.0
1	B	584	LEU	3.0
1	A	717	GLY	2.9
1	A	538	TYR	2.9
1	A	611	LYS	2.9
1	B	518	LEU	2.9
1	B	837	LEU	2.9
1	A	740	ILE	2.8
1	A	803	LEU	2.8
1	A	819	LEU	2.8
1	B	700	LEU	2.8
1	A	708	ARG	2.8
1	B	816	ALA	2.8
1	B	566	LYS	2.8
1	B	585	TYR	2.8
1	B	689	GLN	2.8
1	B	810	ARG	2.8
1	B	847	ILE	2.7
4	U	13	DG	2.7
1	A	560	ASP	2.7
1	A	806	LEU	2.7
1	B	324	SER	2.7
5	X	21	DG	2.7
1	A	709	ALA	2.7
1	B	846	ALA	2.7
1	B	581	ALA	2.6
3	T	30	DG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	576	PHE	2.6
1	B	844	ASP	2.6
1	A	552	LEU	2.6
1	B	840	LEU	2.6
1	B	672	VAL	2.5
1	A	599	SER	2.5
1	A	704	VAL	2.5
1	B	680	VAL	2.5
1	B	824	GLY	2.5
1	B	801	LEU	2.5
1	B	565	ILE	2.5
1	A	591	LEU	2.5
1	A	603	LEU	2.5
1	B	667	GLU	2.5
1	A	616	ILE	2.4
1	B	516	LYS	2.4
1	B	549	VAL	2.4
1	B	687	GLY	2.4
1	B	591	LEU	2.4
3	T	31	DT	2.3
1	B	593	GLU	2.3
1	B	597	ARG	2.3
1	B	677	ARG	2.3
1	A	826	VAL	2.3
5	V	39	DT	2.3
1	B	849	ARG	2.3
1	A	543	ALA	2.3
1	B	670	GLU	2.3
1	A	779	GLN	2.3
1	A	850	ILE	2.3
1	B	695	GLU	2.3
1	B	668	LEU	2.3
1	B	679	ARG	2.3
1	B	586	GLU	2.2
1	A	593	GLU	2.2
1	B	850	ILE	2.2
1	A	699	TRP	2.2
1	A	565	ILE	2.2
1	A	532	ASP	2.2
1	B	620	GLU	2.2
1	B	731	VAL	2.2
1	B	752	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	682	SER	2.2
1	B	632	PRO	2.1
1	A	710	ARG	2.1
1	B	748	LEU	2.1
5	V	22	DC	2.1
1	A	324	SER	2.1
1	A	714	GLU	2.1
1	A	518	LEU	2.1
1	A	516	LYS	2.1
1	B	699	TRP	2.1
1	A	570	LYS	2.1
1	A	576	PHE	2.1
1	A	571	LYS	2.1
1	B	628	GLU	2.1
1	A	376	SER	2.1
1	A	589	GLY	2.1
1	A	585	TYR	2.0
1	B	666	GLU	2.0
1	B	545	ARG	2.0
1	B	216	GLY	2.0
1	B	595	GLY	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 monosaccharides 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, 95^{th} 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	903	1/1	0.79	0.19	150,150,150,150	0
7	MG	B	907	1/1	0.79	0.17	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	A	905	1/1	0.83	0.15	141,141,141,141	0
7	MG	B	906	1/1	0.87	0.08	144,144,144,144	0
7	MG	B	902	1/1	0.91	0.11	117,117,117,117	0
8	K	S	101	1/1	0.91	0.38	132,132,132,132	0
7	MG	B	904	1/1	0.94	0.19	160,160,160,160	0
7	MG	A	901	1/1	0.95	0.34	120,120,120,120	0
7	MG	B	903	1/1	0.95	0.34	106,106,106,106	0
7	MG	A	902	1/1	0.95	0.36	108,108,108,108	0
8	K	T	101	1/1	0.96	0.23	118,118,118,118	0
7	MG	B	901	1/1	0.97	0.41	154,154,154,154	0
7	MG	A	904	1/1	0.98	0.06	105,105,105,105	0
7	MG	B	905	1/1	0.99	0.04	107,107,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.