



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:53 PM GMT

PDB ID : 1R49  
Title : Human topoisomerase I (Topo70) double mutant K532R/Y723F  
Authors : Interthal, H.; Quigley, P.M.; Hol, W.G.; Champoux, J.J.  
Deposited on : 2003-10-03  
Resolution : 3.13 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](mailto: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.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

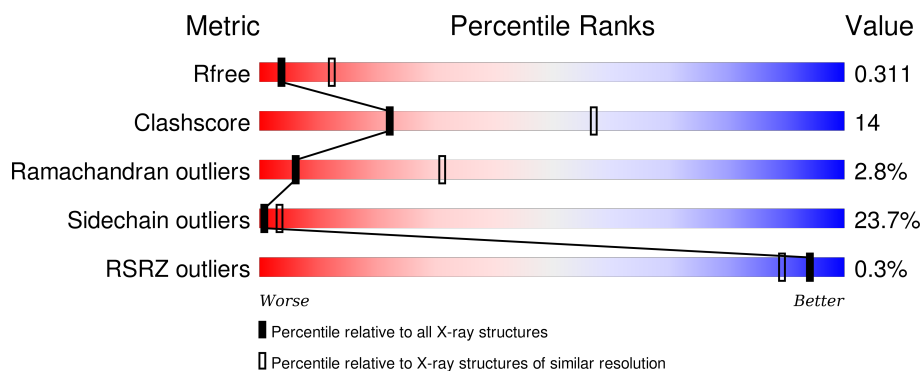
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.13 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))
$R_{free}$	91344	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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. 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	B	22	<div> <div>36%</div> <div>45%</div> <div>18%</div> </div>
2	C	22	<div> <div>23%</div> <div>36%</div> <div>41%</div> </div>
3	A	592	<div> <div>53%</div> <div>31%</div> <div>8%</div> <div>7%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5453 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 DNA chain called 5'-D(\*AP\*AP\*AP\*AP\*AP\*GP\*AP\*CP\*TP\*TP\*AP\*GP\*AP\*AP\*AP\*AP\*AP\*TP\*TP\*TP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	22	Total	C	N	O	P	0	0	0
			451	218	87	125	21			

- Molecule 2 is a DNA chain called 5'-D(P\*AP\*AP\*AP\*AP\*AP\*TP\*TP\*TP\*TP\*TP\*CP\*T\*P\*AP\*AP\*GP\*TP\*CP\*TP\*TP\*TP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			446	217	70	137	22			

- Molecule 3 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	548	Total	C	N	O	S	40	0	0
			4527	2869	801	831	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	532	ARG	LYS	ENGINEERED	UNP P11387
A	723	PHE	TYR	ENGINEERED	UNP P11387

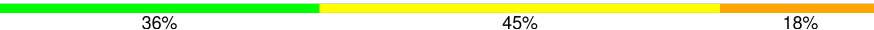
- Molecule 4 is water.

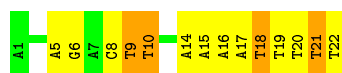
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	1	Total	O	0	0
			1	1		
4	C	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

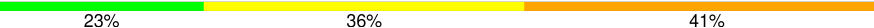
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 5'-D(\*AP\*AP\*AP\*AP\*AP\*GP\*AP\*CP\*TP\*TP\*AP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*TP\*TP\*T)-3'

Chain B: 



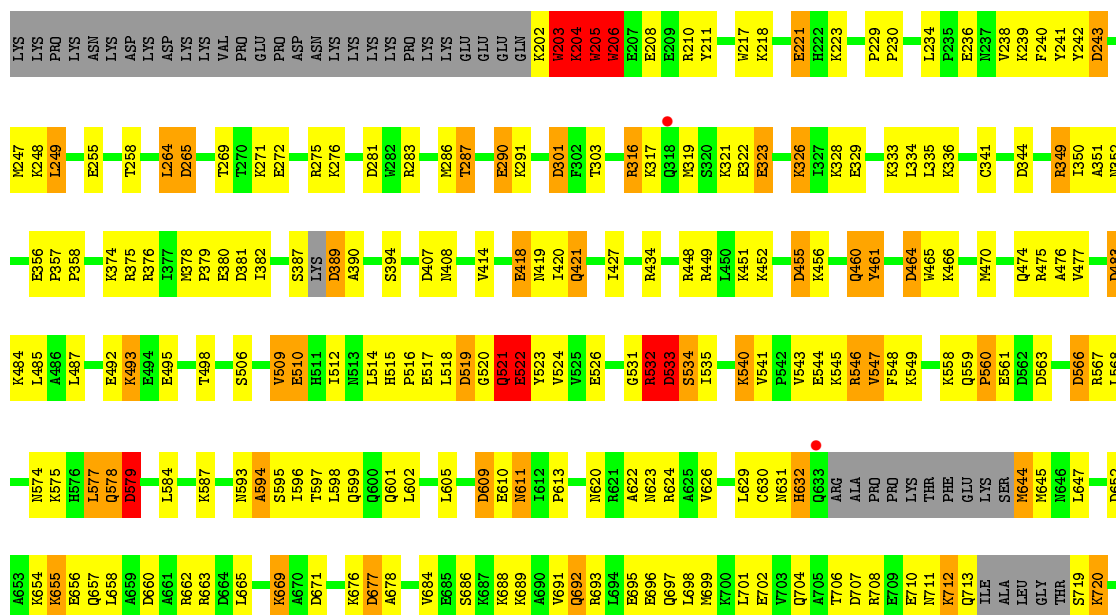
- Molecule 2: 5'-D(P\*AP\*AP\*AP\*AP\*AP\*TP\*TP\*TP\*TP\*TP\*CP\*TP\*AP\*AP\*GP\*TP\*CP\*TP\*TP\*TP\*TP\*T)-3'

Chain C: 



- Molecule 3: DNA topoisomerase I

Chain A: 



L724	D725	P739	L740	E741	K742	K746	T747	Q748	R749	E750	W754	D757	W758	A759	D760	E761	D762	F765
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.94Å 118.64Å 71.65Å 90.00° 98.33° 90.00°	Depositor
Resolution (Å)	47.67 – 3.13 47.60 – 3.13	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-3.13) 93.0 (47.60-3.13)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	61.79 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.277 , 0.339 0.248 , 0.311	Depositor DCC
$R_{free}$ test set	821 reflections (5.59%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.9	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 15497 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	B	1.83	6/508 (1.2%)	1.54	12/782 (1.5%)
2	C	2.47	11/497 (2.2%)	1.93	23/764 (3.0%)
3	A	0.65	8/4621 (0.2%)	0.89	49/6206 (0.8%)
All	All	1.09	25/5626 (0.4%)	1.11	84/7752 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	2	6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	203	TRP	CA-C	25.38	2.19	1.52
1	B	18	DT	C5-C7	-16.21	1.40	1.50
1	B	21	DT	C5-C7	-16.16	1.40	1.50
2	C	120	DT	C5-C7	-16.16	1.40	1.50
2	C	108	DT	C5-C7	-16.15	1.40	1.50
2	C	110	DT	C5-C7	-16.15	1.40	1.50
2	C	122	DT	C5-C7	-16.14	1.40	1.50
1	B	19	DT	C5-C7	-16.13	1.40	1.50
2	C	107	DT	C5-C7	-16.12	1.40	1.50
2	C	109	DT	C5-C7	-16.11	1.40	1.50
2	C	118	DT	C5-C7	-16.09	1.40	1.50
2	C	119	DT	C5-C7	-16.09	1.40	1.50
1	B	9	DT	C5-C7	-16.08	1.40	1.50
1	B	22	DT	C5-C7	-16.08	1.40	1.50
2	C	121	DT	C5-C7	-16.08	1.40	1.50
2	C	106	DT	C5-C7	-16.08	1.40	1.50
1	B	10	DT	C5-C7	-16.07	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	116	DT	C5-C7	-16.05	1.40	1.50
3	A	203	TRP	C-O	14.29	1.50	1.23
3	A	204	LYS	CA-CB	-12.38	1.26	1.53
3	A	203	TRP	C-N	12.01	1.61	1.34
3	A	203	TRP	N-CA	10.68	1.67	1.46
3	A	205	TRP	CZ2-CH2	10.37	1.57	1.37
3	A	208	GLU	CA-CB	-8.52	1.35	1.53
3	A	206	TRP	N-CA	5.71	1.57	1.46

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	203	TRP	CB-CA-C	-17.84	74.71	110.40
3	A	203	TRP	N-CA-CB	-15.42	82.84	110.60
3	A	205	TRP	CZ3-CH2-CZ2	-15.30	103.24	121.60
3	A	204	LYS	CB-CA-C	14.32	139.04	110.40
3	A	203	TRP	N-CA-C	-13.69	74.04	111.00
3	A	205	TRP	N-CA-CB	13.26	134.47	110.60
3	A	205	TRP	CD2-CE2-CZ2	-12.61	107.17	122.30
3	A	204	LYS	CA-CB-CG	11.95	139.69	113.40
3	A	202	LYS	C-N-CA	-9.97	96.79	121.70
2	C	118	DT	C6-C5-C7	-9.64	117.12	122.90
2	C	122	DT	C6-C5-C7	-9.63	117.12	122.90
1	B	19	DT	C6-C5-C7	-9.53	117.18	122.90
2	C	120	DT	C6-C5-C7	-9.35	117.29	122.90
2	C	119	DT	C6-C5-C7	-9.28	117.33	122.90
1	B	21	DT	C6-C5-C7	-9.26	117.34	122.90
2	C	107	DT	C6-C5-C7	-9.25	117.35	122.90
2	C	108	DT	C6-C5-C7	-9.22	117.37	122.90
2	C	110	DT	C6-C5-C7	-9.19	117.38	122.90
1	B	18	DT	C6-C5-C7	-9.19	117.38	122.90
2	C	109	DT	C6-C5-C7	-9.17	117.40	122.90
2	C	121	DT	C6-C5-C7	-9.14	117.41	122.90
1	B	10	DT	C6-C5-C7	-9.11	117.44	122.90
1	B	9	DT	C6-C5-C7	-9.09	117.44	122.90
1	B	22	DT	C6-C5-C7	-9.04	117.47	122.90
2	C	106	DT	C6-C5-C7	-8.79	117.63	122.90
2	C	116	DT	C6-C5-C7	-8.45	117.83	122.90
3	A	206	TRP	N-CA-C	8.35	133.55	111.00
3	A	203	TRP	C-N-CA	8.30	142.44	121.70
3	A	205	TRP	CH2-CZ2-CE2	-8.29	109.11	117.40
3	A	208	GLU	CB-CA-C	8.27	126.93	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	LYS	CB-CA-C	8.14	126.69	110.40
3	A	206	TRP	CB-CA-C	-7.96	94.49	110.40
3	A	208	GLU	CA-CB-CG	7.92	130.82	113.40
2	C	106	DT	C4-C5-C7	7.68	123.61	119.00
2	C	121	DT	C4-C5-C7	7.60	123.56	119.00
1	B	22	DT	C4-C5-C7	7.59	123.55	119.00
2	C	107	DT	C4-C5-C7	7.57	123.54	119.00
2	C	110	DT	C4-C5-C7	7.52	123.51	119.00
2	C	109	DT	C4-C5-C7	7.48	123.49	119.00
2	C	116	DT	C4-C5-C7	7.43	123.46	119.00
1	B	21	DT	C4-C5-C7	7.41	123.45	119.00
1	B	9	DT	C4-C5-C7	7.40	123.44	119.00
1	B	18	DT	C4-C5-C7	7.39	123.43	119.00
2	C	108	DT	C4-C5-C7	7.39	123.43	119.00
1	B	19	DT	C4-C5-C7	7.37	123.42	119.00
2	C	120	DT	C4-C5-C7	7.33	123.40	119.00
1	B	10	DT	C4-C5-C7	7.31	123.39	119.00
2	C	118	DT	C4-C5-C7	7.22	123.33	119.00
2	C	122	DT	C4-C5-C7	7.20	123.32	119.00
2	C	119	DT	C4-C5-C7	7.16	123.30	119.00
3	A	208	GLU	N-CA-CB	6.73	122.71	110.60
3	A	205	TRP	CG-CD2-CE3	-6.41	128.13	133.90
3	A	203	TRP	CA-C-N	6.32	131.11	117.20
3	A	203	TRP	O-C-N	-6.14	112.88	122.70
3	A	243	ASP	CB-CG-OD2	5.78	123.50	118.30
3	A	563	ASP	CB-CG-OD2	5.72	123.45	118.30
3	A	389	ASP	CB-CG-OD2	5.51	123.25	118.30
3	A	281	ASP	CB-CG-OD2	5.45	123.20	118.30
3	A	757	ASP	CB-CG-OD2	5.39	123.16	118.30
3	A	660	ASP	CB-CG-OD2	5.37	123.13	118.30
3	A	609	ASP	CB-CG-OD2	5.36	123.12	118.30
3	A	707	ASP	CB-CG-OD2	5.35	123.11	118.30
3	A	407	ASP	CB-CG-OD2	5.33	123.09	118.30
3	A	206	TRP	CA-C-N	-5.31	105.51	117.20
3	A	483	ASP	CB-CG-OD2	5.31	123.08	118.30
3	A	519	ASP	CB-CG-OD2	5.31	123.08	118.30
3	A	381	ASP	CB-CG-OD2	5.29	123.06	118.30
3	A	301	ASP	CB-CG-OD2	5.25	123.02	118.30
3	A	762	ASP	CB-CG-OD2	5.24	123.02	118.30
3	A	344	ASP	CB-CG-OD2	5.24	123.01	118.30
3	A	455	ASP	CB-CG-OD2	5.23	123.00	118.30
3	A	632	HIS	N-CA-C	5.20	125.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	265	ASP	CB-CG-OD2	5.19	122.97	118.30
3	A	533	ASP	CB-CG-OD2	5.18	122.96	118.30
2	C	119	DT	N3-C4-O4	5.12	122.97	119.90
3	A	677	ASP	CB-CG-OD2	5.12	122.91	118.30
3	A	566	ASP	CB-CG-OD2	5.10	122.89	118.30
3	A	760	ASP	CB-CG-OD2	5.09	122.88	118.30
3	A	725	ASP	CB-CG-OD2	5.08	122.87	118.30
3	A	579	ASP	CB-CG-OD2	5.04	122.84	118.30
3	A	205	TRP	CB-CG-CD1	5.02	133.53	127.00
3	A	652	ASP	CB-CG-OD2	5.02	122.82	118.30
3	A	671	ASP	CB-CG-OD2	5.02	122.81	118.30
3	A	464	ASP	CB-CG-OD2	5.00	122.81	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	204	LYS	CA
3	A	208	GLU	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	203	TRP	Mainchain
3	A	205	TRP	Peptide
3	A	206	TRP	Mainchain,Peptide
3	A	522	GLU	Peptide
3	A	594	ALA	Peptide

## 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	B	451	0	248	16	0
2	C	446	0	252	19	0
3	A	4527	0	4447	108	3
4	A	25	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	3	0	0	0	0
All	All	5453	0	4947	141	3

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 14.

All (141) 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:C:121:DT:H2''	2:C:122:DT:H71	1.18	1.14
3:A:521:GLN:HA	3:A:522:GLU:HB2	1.20	1.14
3:A:521:GLN:HA	3:A:522:GLU:CB	1.82	1.08
3:A:531:GLY:O	3:A:532:ARG:O	1.83	0.96
3:A:523:TYR:HB3	3:A:548:PHE:CD1	2.03	0.93
3:A:644:MET:HB2	3:A:645:MET:HA	1.48	0.92
3:A:644:MET:CB	3:A:645:MET:HA	2.03	0.88
3:A:532:ARG:O	3:A:534:SER:N	2.07	0.87
1:B:20:DT:H2''	1:B:21:DT:C7	2.07	0.84
3:A:466:LYS:HE3	3:A:546:ARG:HD3	1.57	0.84
1:B:20:DT:H2''	1:B:21:DT:H72	1.57	0.84
3:A:523:TYR:HB3	3:A:548:PHE:CE1	2.13	0.83
2:C:104:DA:H2''	2:C:105:DA:OP2	1.80	0.82
2:C:121:DT:H2''	2:C:122:DT:C7	2.05	0.82
3:A:521:GLN:CA	3:A:522:GLU:CB	2.58	0.82
3:A:523:TYR:CB	3:A:548:PHE:CD1	2.62	0.81
3:A:509:VAL:HG22	3:A:560:PRO:HA	1.66	0.78
1:B:20:DT:C2'	1:B:21:DT:H72	2.13	0.78
3:A:255:GLU:O	3:A:258:THR:OG1	2.04	0.75
2:C:107:DT:H4'	2:C:108:DT:OP1	1.84	0.75
2:C:101:DA:H4'	2:C:102:DA:O5'	1.87	0.73
2:C:121:DT:C2'	2:C:122:DT:H71	2.10	0.73
2:C:115:DG:H2'	2:C:116:DT:H72	1.72	0.72
2:C:115:DG:H2'	2:C:116:DT:C7	2.20	0.70
3:A:510:GLU:HG2	3:A:560:PRO:O	1.91	0.69
2:C:118:DT:C2'	2:C:119:DT:H72	2.23	0.68
2:C:118:DT:H2''	2:C:119:DT:C7	2.23	0.68
3:A:622:ALA:O	3:A:626:VAL:HG23	1.94	0.67
3:A:644:MET:HB2	3:A:645:MET:CA	2.24	0.67
3:A:221:GLU:HB2	3:A:390:ALA:HB1	1.77	0.66
2:C:107:DT:H2''	2:C:108:DT:H71	1.76	0.65
2:C:114:DA:N3	3:A:532:ARG:NH1	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:510:GLU:HB3	3:A:560:PRO:HB3	1.79	0.64
1:B:17:DA:C8	1:B:18:DT:H72	2.34	0.61
3:A:594:ALA:HB2	3:A:629:LEU:HD11	1.81	0.61
1:B:8:DC:H2''	1:B:9:DT:H72	1.83	0.61
3:A:240:PHE:CD2	3:A:249:LEU:HD11	2.36	0.60
3:A:518:LEU:HB3	3:A:524:VAL:HG21	1.83	0.60
3:A:514:LEU:HB3	3:A:548:PHE:CZ	2.36	0.60
3:A:523:TYR:HB2	3:A:548:PHE:CD1	2.36	0.60
3:A:574:ASN:O	3:A:578:GLN:HG2	2.02	0.60
3:A:532:ARG:O	3:A:533:ASP:C	2.40	0.59
2:C:108:DT:H1'	2:C:109:DT:H5'	1.83	0.59
1:B:8:DC:C2'	1:B:9:DT:H72	2.34	0.57
3:A:358:PRO:HG3	3:A:376:ARG:HE	1.68	0.57
2:C:118:DT:H2''	2:C:119:DT:H72	1.86	0.57
1:B:8:DC:H2''	1:B:9:DT:C7	2.34	0.56
3:A:594:ALA:O	3:A:724:LEU:HD23	2.05	0.56
3:A:483:ASP:O	3:A:593:ASN:ND2	2.37	0.56
3:A:382:ILE:HG23	3:A:414:VAL:HG13	1.88	0.56
3:A:620:ASN:O	3:A:624:ARG:HG3	2.05	0.55
3:A:611:ASN:OD1	3:A:613:PRO:HD2	2.06	0.55
3:A:521:GLN:CA	3:A:522:GLU:HB3	2.36	0.54
3:A:629:LEU:HD12	3:A:630:CYS:SG	2.48	0.54
3:A:523:TYR:CE2	3:A:545:LYS:HG2	2.43	0.54
3:A:754:TRP:O	3:A:758:MET:HG3	2.07	0.53
3:A:269:THR:O	3:A:275:ARG:HD2	2.08	0.53
1:B:14:DA:H2''	1:B:15:DA:C8	2.44	0.53
3:A:720:LYS:HA	3:A:724:LEU:HD12	1.90	0.52
1:B:16:DA:C8	1:B:16:DA:H5'	2.45	0.52
3:A:746:LYS:O	3:A:750:GLU:HB2	2.10	0.52
3:A:485:LEU:HD11	3:A:541:VAL:HG21	1.91	0.52
1:B:20:DT:H2''	1:B:21:DT:H73	1.89	0.51
3:A:509:VAL:CG2	3:A:560:PRO:HA	2.40	0.51
2:C:106:DT:H2'	2:C:107:DT:H72	1.92	0.51
3:A:326:LYS:HA	3:A:329:GLU:HB2	1.92	0.51
3:A:240:PHE:CE2	3:A:249:LEU:HD21	2.46	0.51
3:A:598:LEU:HD13	3:A:724:LEU:HD22	1.93	0.50
2:C:107:DT:C2'	2:C:108:DT:H71	2.40	0.50
3:A:316:ARG:HA	3:A:319:MET:CG	2.42	0.50
3:A:375:ARG:H	3:A:419:ASN:HD21	1.58	0.50
3:A:465:TRP:CD1	3:A:476:ALA:HB1	2.48	0.49
3:A:230:PRO:HA	3:A:376:ARG:HH12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:DT:H1'	1:B:10:DT:H5'	1.95	0.49
3:A:544:GLU:O	3:A:547:VAL:HG23	2.13	0.49
3:A:387:SER:O	3:A:389:ASP:N	2.45	0.49
3:A:477:VAL:HG13	3:A:547:VAL:HG12	1.95	0.48
3:A:456:LYS:O	3:A:460:GLN:HB2	2.13	0.48
3:A:601:GLN:O	3:A:605:LEU:HB2	2.13	0.48
3:A:493:LYS:HD3	3:A:493:LYS:HA	1.47	0.48
3:A:597:THR:O	3:A:601:GLN:HG2	2.14	0.48
3:A:461:TYR:C	3:A:461:TYR:CD2	2.88	0.48
3:A:485:LEU:HD11	3:A:541:VAL:HG11	1.96	0.48
3:A:520:GLY:C	3:A:521:GLN:HG3	2.33	0.47
3:A:349:ARG:HD2	3:A:350:ILE:O	2.14	0.47
3:A:420:ILE:HG22	3:A:421:GLN:HG2	1.97	0.46
3:A:242:TYR:O	3:A:243:ASP:CB	2.64	0.46
3:A:466:LYS:HE3	3:A:546:ARG:CD	2.39	0.46
3:A:712:LYS:NZ	3:A:713:GLN:H	2.13	0.46
2:C:118:DT:H2'	2:C:119:DT:H72	1.96	0.46
1:B:5:DA:C2	1:B:6:DG:C4	3.04	0.46
3:A:654:LYS:HA	3:A:657:GLN:HB3	1.98	0.45
3:A:380:GLU:OE2	3:A:380:GLU:N	2.50	0.45
3:A:474:GLN:OE1	3:A:566:ASP:O	2.35	0.45
3:A:599:GLN:HE22	3:A:765:PHE:H	1.63	0.45
3:A:518:LEU:C	3:A:520:GLY:N	2.70	0.45
3:A:669:LYS:HB3	3:A:669:LYS:HE2	1.58	0.45
1:B:14:DA:H2''	1:B:15:DA:H8	1.80	0.45
3:A:283:ARG:NH2	3:A:291:LYS:O	2.49	0.45
3:A:475:ARG:HG2	3:A:476:ALA:N	2.32	0.45
3:A:577:LEU:HB3	3:A:584:LEU:HG	2.00	0.44
3:A:739:PRO:HG2	3:A:742:LYS:HG3	1.99	0.44
3:A:578:GLN:H	3:A:578:GLN:HG2	1.51	0.44
3:A:319:MET:HB2	3:A:323:GLU:OE2	2.16	0.44
3:A:577:LEU:C	3:A:579:ASP:H	2.21	0.44
3:A:378:MET:HB3	3:A:379:PRO:CD	2.47	0.44
3:A:419:ASN:N	3:A:419:ASN:OD1	2.44	0.44
3:A:234:LEU:HD22	3:A:238:VAL:HG11	1.99	0.44
2:C:105:DA:H2''	2:C:106:DT:H71	2.00	0.44
3:A:515:HIS:O	3:A:516:PRO:C	2.56	0.43
3:A:301:ASP:OD1	3:A:303:THR:OG1	2.22	0.43
3:A:418:GLU:HG2	3:A:420:ILE:H	1.83	0.43
3:A:464:ASP:HB3	3:A:476:ALA:HB2	2.00	0.43
3:A:512:ILE:HA	3:A:526:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:DT:H3	2:C:102:DA:H61	1.66	0.43
3:A:470:MET:CE	3:A:470:MET:HA	2.49	0.42
3:A:533:ASP:O	3:A:535:ILE:N	2.52	0.42
3:A:712:LYS:HB2	3:A:712:LYS:HE2	1.58	0.42
3:A:356:GLU:HA	3:A:357:PRO:HD3	1.90	0.42
3:A:692:GLN:HA	3:A:695:GLU:HB2	2.00	0.42
3:A:594:ALA:O	3:A:724:LEU:CD2	2.67	0.42
1:B:17:DA:N9	1:B:18:DT:H72	2.34	0.42
3:A:702:GLU:O	3:A:706:THR:HG22	2.18	0.42
3:A:378:MET:HB3	3:A:379:PRO:HD2	2.01	0.42
3:A:217:TRP:CZ2	3:A:408:ASN:HA	2.54	0.42
3:A:546:ARG:HE	3:A:546:ARG:HA	1.85	0.41
3:A:521:GLN:NE2	3:A:521:GLN:O	2.53	0.41
3:A:559:GLN:O	3:A:561:GLU:N	2.53	0.41
3:A:540:LYS:HB2	3:A:540:LYS:HE2	1.34	0.41
1:B:9:DT:C2'	1:B:10:DT:H72	2.50	0.41
3:A:523:TYR:HE2	3:A:545:LYS:HG2	1.85	0.41
3:A:611:ASN:H	3:A:611:ASN:HD22	1.68	0.41
3:A:696:GLU:O	3:A:697:GLN:C	2.59	0.41
3:A:287:THR:HG23	3:A:290:GLU:OE2	2.21	0.41
3:A:352:ASN:HD21	3:A:427:ILE:HA	1.85	0.41
3:A:655:LYS:HG2	3:A:698:LEU:HD11	2.02	0.41
3:A:541:VAL:O	3:A:543:VAL:HG13	2.21	0.41
3:A:264:LEU:HD23	3:A:264:LEU:HA	1.78	0.41
3:A:229:PRO:HA	3:A:230:PRO:HD3	1.98	0.40
3:A:290:GLU:O	3:A:291:LYS:C	2.60	0.40
3:A:283:ARG:HA	3:A:286:MET:HE2	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:204:LYS:NZ	3:A:272:GLU:OE2[1_455]	0.42	1.78
3:A:204:LYS:NZ	3:A:272:GLU:CD[1_455]	1.23	0.97
3:A:204:LYS:CE	3:A:272:GLU:OE2[1_455]	1.54	0.66

## 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	
3	A	540/592 (91%)	494 (92%)	31 (6%)	15 (3%)	6	31

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	204	LYS
3	A	205	TRP
3	A	522	GLU
3	A	532	ARG
3	A	533	ASP
3	A	534	SER
3	A	631	ASN
3	A	210	ARG
3	A	203	TRP
3	A	519	ASP
3	A	677	ASP
3	A	351	ALA
3	A	521	GLN
3	A	678	ALA
3	A	560	PRO

### 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	
3	A	465/536 (87%)	355 (76%)	110 (24%)	1	3

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	204	LYS
3	A	206	TRP
3	A	211	TYR
3	A	218	LYS
3	A	221	GLU
3	A	223	LYS
3	A	236	GLU
3	A	239	LYS
3	A	241	TYR
3	A	247	MET
3	A	248	LYS
3	A	249	LEU
3	A	264	LEU
3	A	265	ASP
3	A	271	LYS
3	A	276	LYS
3	A	287	THR
3	A	290	GLU
3	A	316	ARG
3	A	317	LYS
3	A	321	LYS
3	A	322	GLU
3	A	323	GLU
3	A	326	LYS
3	A	328	LYS
3	A	333	LYS
3	A	334	LEU
3	A	335	LEU
3	A	336	LYS
3	A	341	CYS
3	A	349	ARG
3	A	374	LYS
3	A	394	SER
3	A	418	GLU
3	A	421	GLN
3	A	434	ARG
3	A	448	ARG
3	A	449	ARG
3	A	451	LYS
3	A	452	LYS
3	A	455	ASP
3	A	460	GLN

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Mol	Chain	Res	Type
3	A	461	TYR
3	A	484	LYS
3	A	487	LEU
3	A	492	GLU
3	A	493	LYS
3	A	495	GLU
3	A	498	THR
3	A	506	SER
3	A	509	VAL
3	A	510	GLU
3	A	517	GLU
3	A	521	GLN
3	A	532	ARG
3	A	533	ASP
3	A	540	LYS
3	A	546	ARG
3	A	547	VAL
3	A	549	LYS
3	A	558	LYS
3	A	567	ARG
3	A	568	LEU
3	A	575	LYS
3	A	577	LEU
3	A	578	GLN
3	A	579	ASP
3	A	587	LYS
3	A	595	SER
3	A	596	ILE
3	A	602	LEU
3	A	609	ASP
3	A	610	GLU
3	A	611	ASN
3	A	623	ASN
3	A	632	HIS
3	A	644	MET
3	A	647	LEU
3	A	655	LYS
3	A	656	GLU
3	A	658	LEU
3	A	662	ARG
3	A	663	ARG
3	A	665	LEU

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Mol	Chain	Res	Type
3	A	669	LYS
3	A	676	LYS
3	A	684	VAL
3	A	686	SER
3	A	688	LYS
3	A	689	LYS
3	A	691	VAL
3	A	692	GLN
3	A	693	ARG
3	A	699	MET
3	A	701	LEU
3	A	704	GLN
3	A	708	ARG
3	A	710	GLU
3	A	711	ASN
3	A	712	LYS
3	A	719	SER
3	A	720	LYS
3	A	741	GLU
3	A	742	LYS
3	A	746	LYS
3	A	747	THR
3	A	748	GLN
3	A	749	ARG
3	A	758	MET
3	A	761	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	307	GLN
3	A	318	GLN
3	A	367	HIS
3	A	399	HIS
3	A	421	GLN
3	A	430	ASN
3	A	515	HIS
3	A	521	GLN
3	A	578	GLN
3	A	599	GLN
3	A	657	GLN
3	A	704	GLN

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Mol	Chain	Res	Type
3	A	722	ASN
3	A	748	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 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	B	22/22 (100%)	-0.57	0	100 100	23, 57, 93, 104	0
2	C	22/22 (100%)	-0.39	0	100 100	20, 57, 91, 106	0
3	A	548/592 (92%)	-0.22	2 (0%)	93 86	23, 64, 106, 135	7 (1%)
All	All	592/636 (93%)	-0.24	2 (0%)	94 89	20, 63, 106, 135	7 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	633	GLN	2.5
3	A	318	GLN	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 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.