



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:40 AM UTC

PDB ID : 1A36 / pdb_00001a36
Title : TOPOISOMERASE I/DNA COMPLEX
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Deposited on : 1998-01-29
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

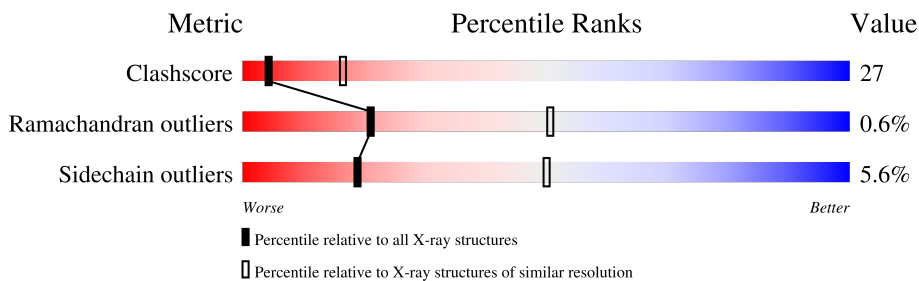
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	22	
2	C	22	
3	A	591	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5285 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 DNA (5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*TP*TP*AP*GP*AP*AP*AP*AP*A P*TP*TP*TP*TP*T)- 3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	22	Total	C	N	O	P	0	0	0
			452	219	87	125	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			444	218	70	135	21			

- Molecule 3 is a protein called TOPOISOMERASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	544	Total	C	N	O	S	0	0	0
			4332	2764	761	784	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	723	PHE	TYR	engineered mutation	UNP P11387

- Molecule 4 is water.

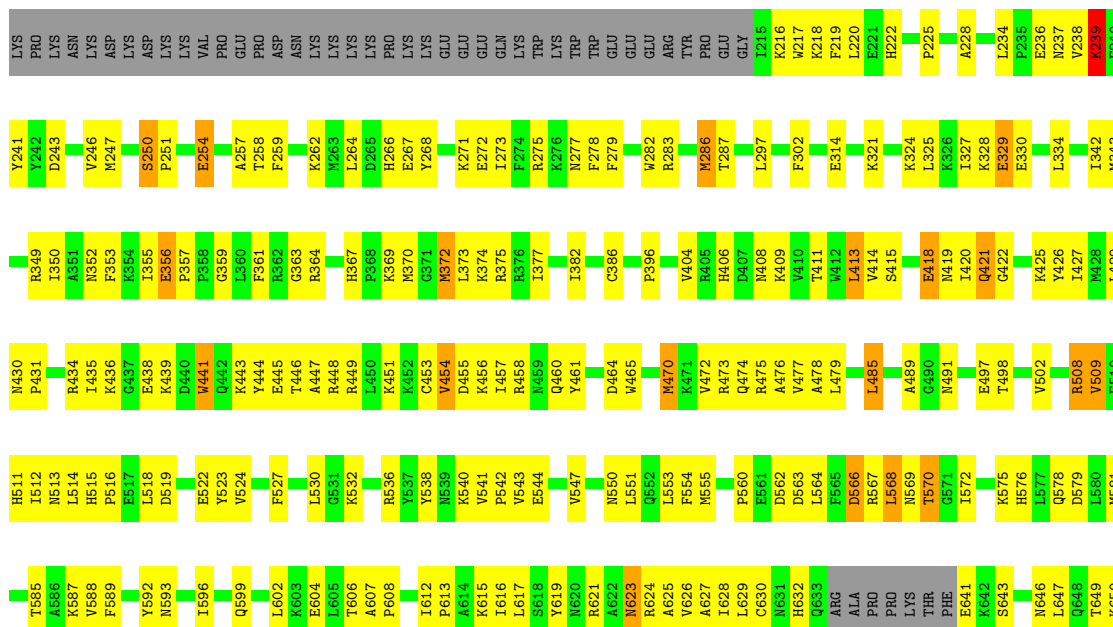
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	O	0	0
			5	5		
4	C	3	Total	O	0	0
			3	3		
4	A	49	Total	O	0	0
			49	49		

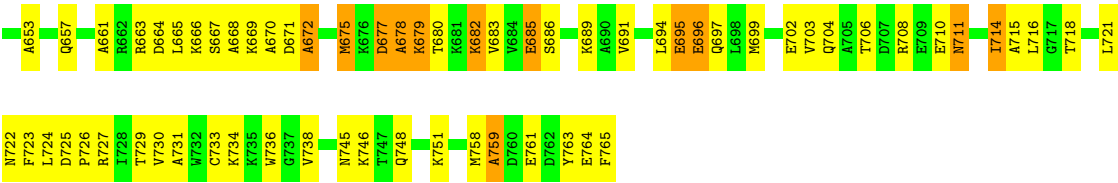
Note EDS was not executed.

- Chain B: 14% 86%



- Molecule 3: TOPOISOMERASE I





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.50Å 118.40Å 71.50Å 90.00° 101.20° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	94.7 (8.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.224 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5285	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

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	0.50	0/509	0.87	0/784
2	C	0.55	0/495	1.00	1/762 (0.1%)
3	A	0.83	2/4422 (0.0%)	1.15	32/5960 (0.5%)
All	All	0.78	2/5426 (0.0%)	1.11	33/7506 (0.4%)

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
2	C	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	286	MET	SD-CE	-5.61	1.65	1.79
3	A	396	PRO	CA-C	5.49	1.54	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	566	ASP	N-CA-C	-9.47	98.31	110.53
3	A	228	ALA	CA-C-N	8.28	125.71	119.66
3	A	228	ALA	C-N-CA	8.28	125.71	119.66
3	A	321	LYS	N-CA-C	-8.18	102.31	111.71
3	A	329	GLU	N-CA-C	-7.20	103.37	111.14
3	A	542	PRO	N-CA-C	-6.95	100.31	110.80
3	A	761	GLU	N-CA-C	-6.62	104.10	111.71
3	A	485	LEU	N-CA-C	6.45	120.89	112.89
3	A	679	LYS	N-CA-C	-6.19	103.84	111.33
3	A	508	ARG	N-CA-C	-6.17	101.36	110.48
3	A	353	PHE	N-CA-C	6.14	120.51	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	672	ALA	N-CA-C	5.99	117.81	111.28
3	A	314	GLU	N-CA-C	-5.95	104.71	111.07
3	A	356	GLU	CA-C-N	5.76	123.86	119.66
3	A	356	GLU	C-N-CA	5.76	123.86	119.66
3	A	250	SER	CA-C-N	5.73	127.00	119.84
3	A	250	SER	C-N-CA	5.73	127.00	119.84
3	A	218	LYS	N-CA-C	-5.61	106.48	113.55
3	A	382	ILE	N-CA-C	5.57	116.60	108.58
3	A	478	ALA	N-CA-C	-5.54	105.14	111.07
3	A	759	ALA	N-CA-C	5.48	117.46	108.52
3	A	441	TRP	N-CA-C	-5.48	105.39	111.36
3	A	239	LYS	N-CA-C	5.46	118.61	110.52
3	A	671	ASP	N-CA-C	-5.29	105.59	111.36
3	A	374	LYS	N-CA-C	-5.28	100.12	108.73
3	A	649	THR	N-CA-C	-5.27	105.45	111.14
3	A	695	GLU	N-CA-C	-5.27	104.95	111.33
2	C	103	DA	C2'-C3'-O3'	-5.21	103.69	111.50
3	A	254	GLU	N-CA-C	-5.20	105.52	111.14
3	A	714	ILE	N-CA-C	5.18	115.73	108.89
3	A	250	SER	N-CA-C	-5.08	103.07	110.08
3	A	287	THR	N-CA-C	-5.03	104.04	110.53
3	A	324	LYS	N-CA-C	5.01	117.13	111.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	108	DT	Sidechain
2	C	115	DG	Sidechain
2	C	121	DT	Sidechain

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	B	452	0	251	35	0
2	C	444	0	256	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4332	0	4261	217	0
4	A	49	0	0	2	0
4	B	5	0	0	0	0
4	C	3	0	0	0	0
All	All	5285	0	4768	268	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 27.

All (268) 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)
3:A:283:ARG:HA	3:A:286:MET:HE3	1.38	1.04
2:C:121:DT:H2''	2:C:122:DT:C5	1.96	0.99
2:C:121:DT:H2''	2:C:122:DT:C7	1.93	0.99
1:B:13:DA:H5'	3:A:364:ARG:NH1	1.82	0.92
2:C:121:DT:H2''	2:C:122:DT:H71	1.53	0.88
3:A:626:VAL:HG11	3:A:724:LEU:HD21	1.55	0.88
1:B:1:DA:H1'	1:B:2:DA:O5'	1.74	0.87
3:A:745:ASN:OD1	3:A:748:GLN:HG3	1.76	0.84
2:C:108:DT:C6	2:C:109:DT:H72	2.14	0.82
3:A:625:ALA:O	3:A:628:ILE:HG22	1.80	0.81
1:B:12:DG:H1'	3:A:364:ARG:HH12	1.43	0.81
3:A:234:LEU:HD22	3:A:238:VAL:HG11	1.63	0.81
1:B:11:DA:C2'	3:A:718:THR:HG21	2.11	0.81
1:B:1:DA:O4'	1:B:2:DA:H5'	1.80	0.80
3:A:446:THR:HG23	3:A:449:ARG:NH2	1.98	0.78
3:A:569:ASN:OD1	3:A:572:ILE:HG13	1.83	0.78
2:C:115:DG:H2'	2:C:116:DT:H72	1.66	0.77
1:B:11:DA:H2''	3:A:718:THR:HG21	1.64	0.77
1:B:13:DA:H5'	3:A:364:ARG:HH11	1.45	0.77
2:C:121:DT:H2''	2:C:122:DT:C6	2.20	0.76
3:A:456:LYS:HE2	3:A:460:GLN:HE21	1.51	0.74
1:B:9:DT:OP1	3:A:439:LYS:HD3	1.89	0.73
3:A:369:LYS:O	3:A:372:MET:HG3	1.89	0.71
3:A:273:ILE:H	3:A:273:ILE:HD12	1.55	0.70
3:A:375:ARG:H	3:A:419:ASN:HD21	1.38	0.70
2:C:106:DT:H2'	2:C:107:DT:H71	1.72	0.70
3:A:641:GLU:C	3:A:643:SER:H	2.01	0.68
2:C:117:DC:H2''	2:C:118:DT:H71	1.76	0.68
1:B:21:DT:H2'	1:B:22:DT:H72	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:259:PHE:HE2	3:A:373:LEU:HD11	1.59	0.68
3:A:225:PRO:HB2	3:A:355:ILE:HG12	1.76	0.67
3:A:236:GLU:O	3:A:239:LYS:HE2	1.95	0.66
1:B:1:DA:C1'	1:B:2:DA:H5'	2.26	0.66
3:A:421:GLN:HE22	3:A:497:GLU:HB3	1.61	0.66
1:B:1:DA:H1'	1:B:2:DA:C5'	2.27	0.65
3:A:421:GLN:NE2	3:A:497:GLU:HB3	2.11	0.65
1:B:17:DA:H2''	1:B:18:DT:H5'	1.77	0.65
1:B:22:DT:H3	2:C:101:DA:H61	1.43	0.65
2:C:121:DT:C2'	2:C:122:DT:C5	2.79	0.64
3:A:663:ARG:O	3:A:666:LYS:HB3	1.98	0.64
1:B:11:DA:H2'	3:A:718:THR:HG21	1.80	0.64
3:A:502:VAL:HG11	3:A:511:HIS:CE1	2.32	0.63
3:A:665:LEU:HG	3:A:669:LYS:HE3	1.80	0.63
3:A:518:LEU:HD21	3:A:540:LYS:HD2	1.80	0.63
3:A:530:LEU:HD23	3:A:536:ARG:HA	1.81	0.63
3:A:502:VAL:HG11	3:A:511:HIS:HE1	1.64	0.62
3:A:527:PHE:O	3:A:538:TYR:HA	1.98	0.62
3:A:736:TRP:HA	3:A:736:TRP:CE3	2.33	0.62
1:B:1:DA:C1'	1:B:2:DA:O5'	2.45	0.61
2:C:117:DC:C2'	2:C:118:DT:H71	2.29	0.61
3:A:283:ARG:CA	3:A:286:MET:HE3	2.22	0.61
1:B:1:DA:C1'	1:B:2:DA:C5'	2.78	0.60
3:A:278:PHE:HE2	3:A:297:LEU:HD13	1.67	0.59
3:A:411:THR:HG22	3:A:435:ILE:HD11	1.85	0.59
3:A:745:ASN:H	3:A:748:GLN:HE21	1.50	0.59
3:A:430:ASN:ND2	3:A:431:PRO:HD2	2.17	0.59
3:A:441:TRP:O	3:A:445:GLU:HG2	2.03	0.59
3:A:470:MET:CE	3:A:553:LEU:HG	2.33	0.58
3:A:568:LEU:HD22	3:A:569:ASN:N	2.17	0.58
3:A:473:ARG:O	3:A:477:VAL:HG23	2.03	0.58
3:A:625:ALA:C	3:A:628:ILE:HG22	2.28	0.58
3:A:220:LEU:HD11	3:A:413:LEU:HD22	1.86	0.58
2:C:109:DT:OP1	3:A:746:LYS:HD2	2.03	0.57
3:A:375:ARG:HH11	3:A:419:ASN:CG	2.12	0.57
3:A:266:HIS:CE1	3:A:268:TYR:CD2	2.92	0.57
3:A:541:VAL:O	3:A:543:VAL:HG13	2.05	0.57
3:A:617:LEU:O	3:A:621:ARG:HG3	2.05	0.57
3:A:259:PHE:CE2	3:A:373:LEU:HD11	2.40	0.57
3:A:576:HIS:O	3:A:579:ASP:HB2	2.04	0.56
3:A:665:LEU:CG	3:A:669:LYS:HE3	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:DA:H8	3:A:426:TYR:OH	1.88	0.56
2:C:115:DG:H2'	2:C:116:DT:C7	2.33	0.56
3:A:513:ASN:ND2	3:A:515:HIS:CE1	2.73	0.56
3:A:241:TYR:CE2	3:A:246:VAL:HG22	2.41	0.56
3:A:516:PRO:O	3:A:522:GLU:HG3	2.06	0.56
3:A:599:GLN:OE1	3:A:765:PHE:HB3	2.06	0.55
3:A:733:CYS:HB3	3:A:738:VAL:O	2.05	0.55
3:A:624:ARG:HG2	3:A:714:ILE:HG21	1.89	0.55
3:A:646:ASN:O	3:A:650:LYS:HG3	2.06	0.55
3:A:627:ALA:CB	3:A:716:LEU:HD23	2.37	0.55
1:B:1:DA:H2''	1:B:2:DA:OP2	2.07	0.54
3:A:599:GLN:HE22	3:A:764:GLU:HA	1.72	0.54
3:A:602:LEU:HD21	3:A:619:TYR:HA	1.89	0.54
3:A:679:LYS:O	3:A:683:VAL:HG23	2.08	0.54
1:B:21:DT:C2'	1:B:22:DT:H72	2.36	0.54
3:A:283:ARG:O	3:A:286:MET:HB2	2.08	0.54
3:A:254:GLU:O	3:A:258:THR:HG23	2.08	0.54
3:A:456:LYS:HE2	3:A:460:GLN:NE2	2.20	0.54
3:A:612:ILE:HB	3:A:613:PRO:HD3	1.90	0.54
3:A:473:ARG:HD3	3:A:550:ASN:OD1	2.07	0.54
3:A:691:VAL:O	3:A:695:GLU:HG3	2.08	0.54
3:A:257:ALA:HB1	3:A:302:PHE:HE1	1.73	0.53
2:C:108:DT:H3'	3:A:745:ASN:HB2	1.90	0.53
3:A:361:PHE:HD1	3:A:370:MET:HA	1.74	0.53
2:C:108:DT:H1'	2:C:109:DT:H5'	1.89	0.53
1:B:6:DG:N2	2:C:118:DT:C2	2.77	0.53
3:A:592:TYR:O	3:A:596:ILE:HG22	2.09	0.53
3:A:624:ARG:HA	3:A:716:LEU:HD21	1.91	0.53
3:A:217:TRP:CZ2	3:A:408:ASN:HA	2.43	0.53
3:A:349:ARG:NH1	3:A:350:ILE:O	2.42	0.53
3:A:523:TYR:O	3:A:543:VAL:HG22	2.09	0.53
3:A:686:SER:HA	3:A:689:LYS:HE3	1.91	0.53
3:A:509:VAL:HG13	3:A:562:ASP:O	2.07	0.52
3:A:632:HIS:HB3	3:A:715:ALA:HB3	1.91	0.52
3:A:258:THR:O	3:A:262:LYS:HG3	2.09	0.52
3:A:518:LEU:HD23	3:A:524:VAL:HG11	1.91	0.52
3:A:453:CYS:SG	3:A:581:MET:SD	3.07	0.52
3:A:325:LEU:O	3:A:329:GLU:HG3	2.09	0.52
3:A:696:GLU:O	3:A:697:GLN:C	2.53	0.52
2:C:106:DT:H6	2:C:106:DT:H5'	1.74	0.51
3:A:619:TYR:CE1	3:A:729:THR:HG23	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:DT:C2'	2:C:122:DT:C7	2.80	0.51
3:A:518:LEU:CD2	3:A:540:LYS:HD2	2.39	0.51
3:A:730:VAL:HG11	3:A:759:ALA:HB3	1.92	0.51
1:B:7:DA:C2	1:B:8:DC:C2	2.99	0.51
3:A:677:ASP:CG	3:A:678:ALA:H	2.18	0.51
3:A:216:LYS:HE3	3:A:409:LYS:O	2.10	0.51
3:A:627:ALA:HB2	3:A:716:LEU:HD23	1.93	0.51
1:B:21:DT:H2''	1:B:22:DT:C6	2.46	0.51
2:C:105:DA:H2''	2:C:106:DT:OP2	2.11	0.51
2:C:121:DT:C2'	2:C:122:DT:H71	2.36	0.51
3:A:414:VAL:HB	3:A:427:ILE:HB	1.92	0.51
3:A:612:ILE:O	3:A:616:ILE:HG13	2.11	0.51
3:A:665:LEU:O	3:A:669:LYS:HG3	2.10	0.51
3:A:518:LEU:HB3	3:A:524:VAL:HG21	1.93	0.50
3:A:699:MET:O	3:A:703:VAL:HG23	2.11	0.50
3:A:434:ARG:HD3	3:A:435:ILE:N	2.26	0.50
3:A:361:PHE:HB2	3:A:420:ILE:HD13	1.93	0.50
3:A:607:ALA:O	3:A:615:LYS:HE2	2.11	0.50
3:A:706:THR:O	3:A:710:GLU:HG3	2.12	0.50
3:A:704:GLN:O	3:A:708:ARG:HG3	2.11	0.50
3:A:443:LYS:NZ	3:A:722:ASN:O	2.42	0.50
3:A:731:ALA:HB2	3:A:763:TYR:HB3	1.93	0.50
3:A:568:LEU:HD22	3:A:569:ASN:H	1.75	0.49
3:A:359:GLY:O	3:A:373:LEU:HD12	2.12	0.49
1:B:10:DT:H3'	3:A:723:PHE:CZ	2.48	0.49
3:A:647:LEU:HD11	3:A:708:ARG:HD2	1.95	0.49
3:A:472:VAL:O	3:A:475:ARG:HB3	2.13	0.49
3:A:367:HIS:CE1	3:A:498:THR:HG22	2.48	0.49
3:A:694:LEU:HD23	3:A:697:GLN:OE1	2.13	0.49
3:A:271:LYS:O	3:A:275:ARG:HG3	2.13	0.48
1:B:9:DT:P	3:A:439:LYS:HZ3	2.36	0.48
1:B:10:DT:H3'	3:A:723:PHE:CE2	2.49	0.48
3:A:477:VAL:HG13	3:A:547:VAL:HG13	1.95	0.48
3:A:461:TYR:O	3:A:476:ALA:HB1	2.13	0.48
2:C:117:DC:H2''	2:C:118:DT:OP2	2.13	0.48
3:A:217:TRP:CD1	3:A:343:MET:HE2	2.49	0.48
3:A:518:LEU:HD12	3:A:519:ASP:H	1.77	0.48
2:C:115:DG:OP1	3:A:532:LYS:HA	2.13	0.48
2:C:121:DT:C2'	2:C:122:DT:C6	2.95	0.48
3:A:470:MET:HE2	3:A:553:LEU:HG	1.96	0.47
2:C:115:DG:C2'	2:C:116:DT:H72	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:283:ARG:HG2	3:A:286:MET:HE3	1.96	0.47
1:B:21:DT:C6	1:B:22:DT:H72	2.50	0.47
3:A:386:CYS:O	3:A:406:HIS:HA	2.15	0.47
3:A:602:LEU:CD2	3:A:619:TYR:HA	2.45	0.47
3:A:602:LEU:C	3:A:604:GLU:N	2.72	0.47
3:A:641:GLU:C	3:A:643:SER:N	2.70	0.47
3:A:509:VAL:CG2	3:A:560:PRO:HA	2.44	0.47
3:A:489:ALA:HB1	3:A:570:THR:HG22	1.96	0.47
3:A:566:ASP:O	3:A:567:ARG:HB2	2.15	0.47
3:A:734:LYS:NZ	3:A:759:ALA:O	2.43	0.47
1:B:4:DA:H2''	1:B:5:DA:OP2	2.15	0.46
3:A:624:ARG:C	3:A:626:VAL:N	2.71	0.46
3:A:279:PHE:CD1	3:A:297:LEU:HB2	2.51	0.46
3:A:352:ASN:OD1	3:A:352:ASN:N	2.47	0.46
3:A:608:PRO:HA	3:A:736:TRP:CH2	2.50	0.46
1:B:17:DA:H2''	1:B:18:DT:C5'	2.44	0.46
3:A:277:ASN:HB3	3:A:372:MET:HG2	1.97	0.46
3:A:434:ARG:HD3	3:A:434:ARG:C	2.40	0.46
3:A:458:ARG:HA	3:A:461:TYR:CE2	2.51	0.46
3:A:454:VAL:O	3:A:458:ARG:HG3	2.16	0.46
3:A:220:LEU:O	3:A:386:CYS:HB2	2.15	0.46
3:A:474:GLN:OE1	3:A:566:ASP:O	2.33	0.45
3:A:721:LEU:O	3:A:751:LYS:NZ	2.49	0.45
3:A:629:LEU:HD12	3:A:630:CYS:N	2.31	0.45
1:B:14:DA:C2	1:B:15:DA:C4	3.04	0.45
3:A:508:ARG:N	3:A:511:HIS:ND1	2.62	0.45
2:C:101:DA:H2''	2:C:102:DA:C8	2.51	0.45
3:A:361:PHE:HB2	3:A:420:ILE:CD1	2.47	0.45
3:A:632:HIS:CD2	3:A:718:THR:OG1	2.70	0.45
2:C:115:DG:H2''	2:C:116:DT:C6	2.52	0.45
1:B:9:DT:O3'	3:A:587:LYS:NZ	2.50	0.45
3:A:217:TRP:CE2	3:A:408:ASN:HA	2.52	0.45
3:A:682:LYS:O	3:A:685:GLU:HB3	2.17	0.45
3:A:514:LEU:HD21	3:A:551:LEU:HD13	1.98	0.45
1:B:11:DA:H2''	1:B:12:DG:OP2	2.17	0.44
2:C:106:DT:OP1	3:A:708:ARG:NH1	2.50	0.44
3:A:569:ASN:OD1	3:A:572:ILE:CG1	2.61	0.44
3:A:653:ALA:O	3:A:657:GLN:HG3	2.16	0.44
3:A:435:ILE:HG23	3:A:436:LYS:N	2.32	0.44
3:A:219:PHE:HE2	3:A:342:ILE:CG2	2.30	0.44
1:B:21:DT:C2'	1:B:22:DT:C7	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:273:ILE:HG22	3:A:277:ASN:ND2	2.33	0.44
3:A:667:SER:HA	3:A:670:ALA:HB3	1.99	0.44
3:A:725:ASP:HA	3:A:726:PRO:HD2	1.85	0.44
3:A:415:SER:HA	3:A:425:LYS:O	2.17	0.44
3:A:334:LEU:HD12	3:A:334:LEU:HA	1.77	0.44
3:A:370:MET:O	3:A:370:MET:HG3	2.17	0.44
3:A:665:LEU:CD2	3:A:669:LYS:HE3	2.48	0.44
3:A:267:GLU:O	3:A:268:TYR:C	2.61	0.43
3:A:272:GLU:O	3:A:273:ILE:C	2.60	0.43
3:A:356:GLU:HA	3:A:357:PRO:HD3	1.82	0.43
3:A:418:GLU:O	3:A:422:GLY:HA2	2.18	0.43
3:A:222:HIS:CD2	3:A:413:LEU:HB3	2.53	0.43
3:A:352:ASN:ND2	3:A:427:ILE:HA	2.34	0.43
3:A:572:ILE:O	3:A:575:LYS:HB3	2.18	0.43
2:C:112:DT:C2'	3:A:356:GLU:OE2	2.66	0.43
3:A:444:TYR:O	3:A:447:ALA:HB3	2.18	0.43
2:C:112:DT:OP2	3:A:356:GLU:HG2	2.19	0.43
3:A:355:ILE:HG21	3:A:377:ILE:HB	1.99	0.43
3:A:509:VAL:HG22	3:A:560:PRO:HA	2.00	0.43
3:A:585:THR:H	3:A:588:VAL:CG2	2.31	0.43
3:A:464:ASP:OD2	3:A:475:ARG:NH2	2.51	0.43
3:A:647:LEU:O	3:A:650:LYS:N	2.51	0.43
3:A:461:TYR:HB2	3:A:476:ALA:HB1	2.01	0.43
3:A:672:ALA:HA	3:A:680:THR:HG21	2.01	0.43
2:C:104:DA:H2''	2:C:105:DA:OP2	2.19	0.43
3:A:219:PHE:CE2	3:A:342:ILE:CG2	3.02	0.43
3:A:540:LYS:HZ3	3:A:540:LYS:HB2	1.83	0.43
1:B:13:DA:H1'	1:B:14:DA:H5'	2.01	0.42
3:A:250:SER:HB2	3:A:251:PRO:HD2	2.02	0.42
3:A:745:ASN:O	3:A:746:LYS:C	2.62	0.42
3:A:369:LYS:HB3	3:A:369:LYS:HE2	1.79	0.42
3:A:606:THR:HG21	3:A:736:TRP:CD1	2.54	0.42
3:A:623:ASN:HD22	3:A:623:ASN:HA	1.61	0.42
2:C:108:DT:H2''	2:C:109:DT:OP2	2.19	0.42
3:A:454:VAL:O	3:A:455:ASP:C	2.62	0.42
3:A:675:MET:C	3:A:677:ASP:H	2.28	0.42
3:A:711:ASN:ND2	3:A:714:ILE:HB	2.34	0.42
2:C:106:DT:H5'	2:C:106:DT:C6	2.54	0.42
3:A:678:ALA:O	3:A:679:LYS:C	2.62	0.42
3:A:727:ARG:HB2	3:A:763:TYR:CE2	2.54	0.42
3:A:429:LEU:HD12	3:A:435:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:435:ILE:CG2	3:A:436:LYS:N	2.83	0.42
3:A:454:VAL:CG1	3:A:455:ASP:N	2.83	0.42
3:A:628:ILE:HG23	3:A:629:LEU:N	2.35	0.42
1:B:22:DT:O2	2:C:101:DA:N1	2.53	0.42
3:A:363:GLY:HA3	3:A:367:HIS:ND1	2.34	0.42
3:A:470:MET:HE2	3:A:554:PHE:HD1	1.83	0.42
3:A:551:LEU:O	3:A:555:MET:HG3	2.20	0.42
3:A:602:LEU:C	3:A:604:GLU:H	2.28	0.42
2:C:115:DG:C2'	2:C:116:DT:C7	2.97	0.41
3:A:661:ALA:O	3:A:664:ASP:HB2	2.20	0.41
3:A:665:LEU:HD21	3:A:669:LYS:HE3	2.02	0.41
2:C:108:DT:O2	2:C:109:DT:O4'	2.38	0.41
3:A:457:ILE:O	3:A:460:GLN:HB2	2.20	0.41
1:B:2:DA:C6	1:B:3:DA:N6	2.89	0.41
3:A:665:LEU:HA	3:A:668:ALA:HB3	2.01	0.41
3:A:246:VAL:HG23	4:A:1052:HOH:O	2.20	0.41
3:A:599:GLN:HE22	3:A:765:PHE:H	1.69	0.41
2:C:106:DT:C2'	2:C:107:DT:H71	2.47	0.41
3:A:225:PRO:HB3	3:A:427:ILE:HD12	2.03	0.41
3:A:327:ILE:HG13	3:A:328:LYS:N	2.34	0.41
3:A:465:TRP:CH2	3:A:544:GLU:HG3	2.56	0.41
3:A:479:LEU:HD11	3:A:589:PHE:CZ	2.56	0.41
3:A:763:TYR:HA	4:A:1040:HOH:O	2.21	0.41
3:A:257:ALA:HB2	3:A:282:TRP:CZ2	2.56	0.41
3:A:485:LEU:HD23	3:A:485:LEU:HA	1.84	0.41
3:A:512:ILE:HD13	3:A:564:LEU:CD2	2.51	0.40
3:A:730:VAL:CG1	3:A:734:LYS:HE3	2.50	0.40
2:C:116:DT:H2'	3:A:491:ASN:HD21	1.87	0.40
3:A:578:GLN:HA	3:A:581:MET:O	2.21	0.40
3:A:746:LYS:H	3:A:746:LYS:HG3	1.63	0.40
3:A:448:ARG:O	3:A:451:LYS:HB3	2.22	0.40
3:A:508:ARG:HA	3:A:563:ASP:HA	2.03	0.40
3:A:513:ASN:ND2	3:A:515:HIS:NE2	2.70	0.40
2:C:111:DC:H2''	2:C:112:DT:C6	2.57	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	
3	A	540/591 (91%)	491 (91%)	46 (8%)	3 (1%)	21	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	677	ASP
3	A	678	ALA
3	A	696	GLU

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	
3	A	446/535 (83%)	421 (94%)	25 (6%)	19	50

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	237	ASN
3	A	239	LYS
3	A	243	ASP
3	A	247	MET
3	A	264	LEU
3	A	330	GLU
3	A	372	MET
3	A	404	VAL

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Mol	Chain	Res	Type
3	A	413	LEU
3	A	418	GLU
3	A	421	GLN
3	A	438	GLU
3	A	454	VAL
3	A	470	MET
3	A	509	VAL
3	A	568	LEU
3	A	570	THR
3	A	593	ASN
3	A	623	ASN
3	A	675	MET
3	A	682	LYS
3	A	685	GLU
3	A	702	GLU
3	A	711	ASN
3	A	758	MET

Sometimes 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	312	GLN
3	A	366	ASN
3	A	399	HIS
3	A	421	GLN
3	A	430	ASN
3	A	460	GLN
3	A	513	ASN
3	A	578	GLN
3	A	599	GLN
3	A	601	GLN
3	A	623	ASN
3	A	631	ASN
3	A	632	HIS

5.3.3 RNA ⓘ

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](#)

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.