Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 11:52 AM EDT

PDB ID	:	1A36
Title	:	TOPOISOMERASE I/DNA COMPLEX
Authors	:	Stewart, L.; Redinbo, M.R.; Qiu, X.; Champoux, J.J.; Hol, W.G.J.
Deposited on	:	1998-01-29
Resolution	:	2.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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.
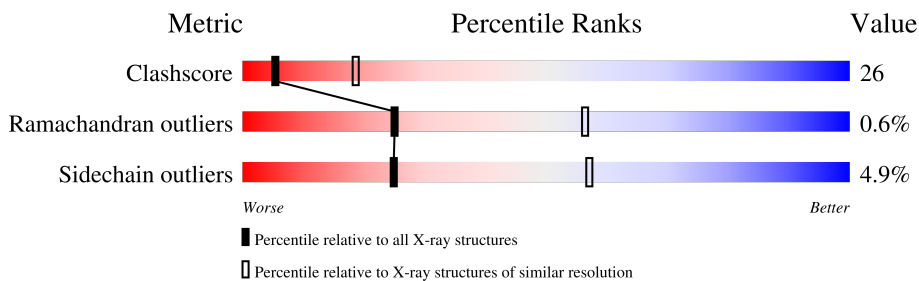
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	22	14% 86%
2	C	22	23% 64% 14%
3	A	591	50% 40% • 8%

2 Entry composition ⓘ

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 452	C 219	N 87	O 125	P 21	0	0	0

- 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 444	C 218	N 70	O 135	P 21	0	0	0

- Molecule 3 is a protein called TOPOISOMERASE I.

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

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 5	O 5	0	0
4	C	3	Total 3	O 3	0	0
4	A	49	Total 49	O 49	0	0

3 Residue-property plots ⓘ

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. 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. 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.

Note EDS was not executed.

• Molecule 1: 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')

Chain B:
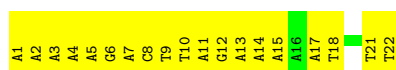
• Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*TP*AP*AP*GP*TP *C P*TP*TP*TP*TP*T)- 3')

Chain C:

• Molecule 3: TOPOISOMERASE I

Chain A:

K676 D677 A678 K679 T680 K681 K682 V683 V684 E685 S686 K689 A690 V691 L694 E695 E696 Q697 L698 M699 E702 V703 Q704 A705 T706 D707 R708 E709 E710 N711 I714 A715 L716 G717 T718 L721 N722 F723 L724 D725 P726 R727 I728 T729 V730 A731 W732 C733 K734 K735 W736 G737 V738 N745

K746 T747 Q748 K751 A759 Y763 E764 F765
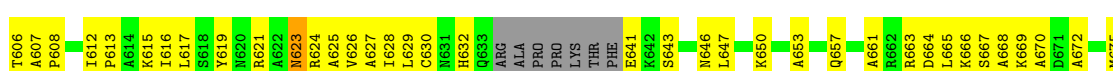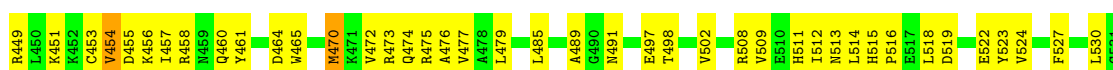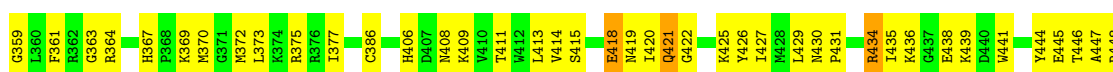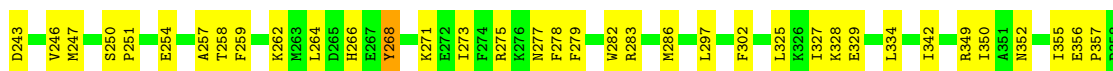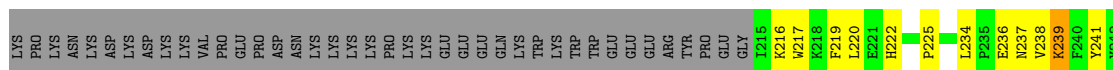
4 Data and refinement statistics (i)

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	0.80	0/509	0.86	0/784
2	C	0.86	0/495	0.97	1/762 (0.1%)
3	A	0.65	0/4422	0.78	0/5960
All	All	0.69	0/5426	0.81	1/7506 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	103	DA	C1'-O4'-C4'	-5.14	104.96	110.10

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	37	0
2	C	444	0	256	40	0
3	A	4332	0	4261	207	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	260	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 26.

All (260) 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: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
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:7:DA:H8	3:A:426:TYR:HH	1.34	0.73
1:B:9:DT:OP1	3:A:439:LYS:HD3	1.89	0.73
3:A:283:ARG:HA	3:A:286:MET:HE2	1.72	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:DT:H2'	2:C:107:DT:H71	1.72	0.70
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
3:A:259:PHE:HE2	3:A:373:LEU:HD11	1.59	0.68
3:A:283:ARG:HG2	3:A:286:MET:HE3	1.75	0.67
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
3:A:641:GLU:C	3:A:643:SER:H	2.01	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:470:MET:HE2	3:A:553:LEU:HG	1.80	0.62
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:HA	3:A:286:MET:CE	2.29	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:A:625:ALA:C	3:A:628:ILE:HG22	2.28	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:375:ARG:HH11	3:A:419:ASN:CG	2.12	0.52
3:A:258:THR:O	3:A:262:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:108:DT:C2'	2:C:109:DT:H71	2.39	0.52
3:A:325:LEU:O	3:A:329:GLU:HG3	2.09	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
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: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: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: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:518:LEU:HD12	3:A:519:ASP:H	1.77	0.48
1:B:9:DT:P	3:A:439:LYS:HZ3	2.37	0.48
2:C:115:DG:OP1	3:A:532:LYS:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:DT:C2'	2:C:122:DT:C6	2.95	0.48
2:C:115:DG:C2'	2:C:116:DT:H72	2.41	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:509:VAL:CG2	3:A:560:PRO:HA	2.44	0.47
3:A:696:GLU:O	3:A:697:GLN:C	2.53	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:677:ASP:CG	3:A:678:ALA:H	2.18	0.47
1:B:4:DA:H2"	1:B:5:DA:OP2	2.15	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: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
2:C:108:DT:C6	2:C:109:DT:H73	2.52	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
3:A:273:ILE:HG22	3:A:277:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:108:DT:C6	2:C:109:DT:C7	3.00	0.44
3:A:415:SER:HA	3:A:425:LYS:O	2.17	0.44
1:B:10:DT:P	3:A:587:LYS:HZ1	2.40	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: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:641:GLU:C	3:A:643:SER:N	2.70	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
1:B:13:DA:H1'	1:B:14:DA:H5'	2.01	0.42
3:A:602:LEU:C	3:A:604:GLU:N	2.72	0.42
3:A:250:SER:HB2	3:A:251:PRO:HD2	2.02	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:363:GLY:HA3	3:A:367:HIS:ND1	2.34	0.42
3:A:551:LEU:O	3:A:555:MET:HG3	2.20	0.42
3:A:624:ARG:C	3:A:626:VAL:N	2.71	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:434:ARG:HD3	3:A:434:ARG:C	2.40	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 ⓘ

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	540/591 (91%)	491 (91%)	46 (8%)	3 (1%)	25	56

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 ⓘ

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%)	424 (95%)	22 (5%)	25	57

All (22) 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	268	TYR
3	A	418	GLU
3	A	421	GLN
3	A	434	ARG
3	A	438	GLU
3	A	454	VAL
3	A	470	MET
3	A	568	LEU
3	A	570	THR
3	A	593	ASN
3	A	623	ASN

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Mol	Chain	Res	Type
3	A	675	MET
3	A	682	LYS
3	A	685	GLU
3	A	699	MET
3	A	702	GLU
3	A	711	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	623	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 ⓘ

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 ⓘ

There are no ligands in this entry.

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 ⓘ

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.