



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:38 PM UTC

PDB ID : 1EJ9 / pdb_00001ej9
Title : CRYSTAL STRUCTURE OF HUMAN TOPOISOMERASE I DNA COMPLEX
Authors : Redinbo, M.R.; Champoux, J.J.; Hol, W.G.
Deposited on : 2000-03-01
Resolution : 2.60 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

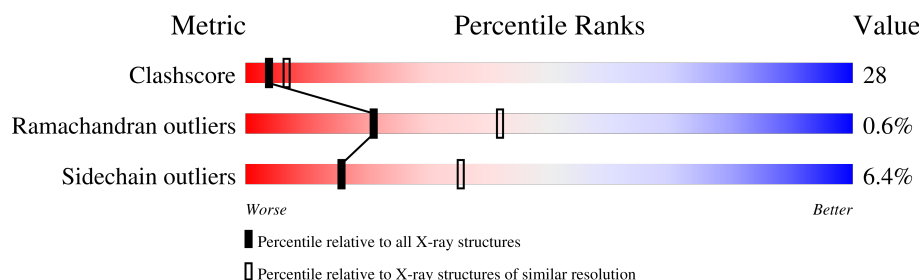
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	C	23	
2	D	23	
3	A	563	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5215 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(*C*AP*AP*AP*AP*AP*GP*AP*CP*TP*C P*AP*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	22	Total	C	N	O	P	0	0	0
			451	218	88	124	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	22	Total	C	N	O	P	0	0	0
			445	218	70	136	21			

- Molecule 3 is a protein called DNA TOPOISOMERASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	483	Total	C	N	O	S	0	0	0
			3966	2547	689	708	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	634	ILE	ARG	engineered mutation	UNP P11387
A	723	PHE	TYR	engineered mutation	UNP P11387

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	33	Total	O	0	0
			33	33		
4	D	50	Total	O	0	0
			50	50		
4	A	270	Total	O	0	0
			270	270		

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(*C*AP*AP*AP*AP*AP*GP*AP*CP*TP*CP*AP*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3')

Chain C: 



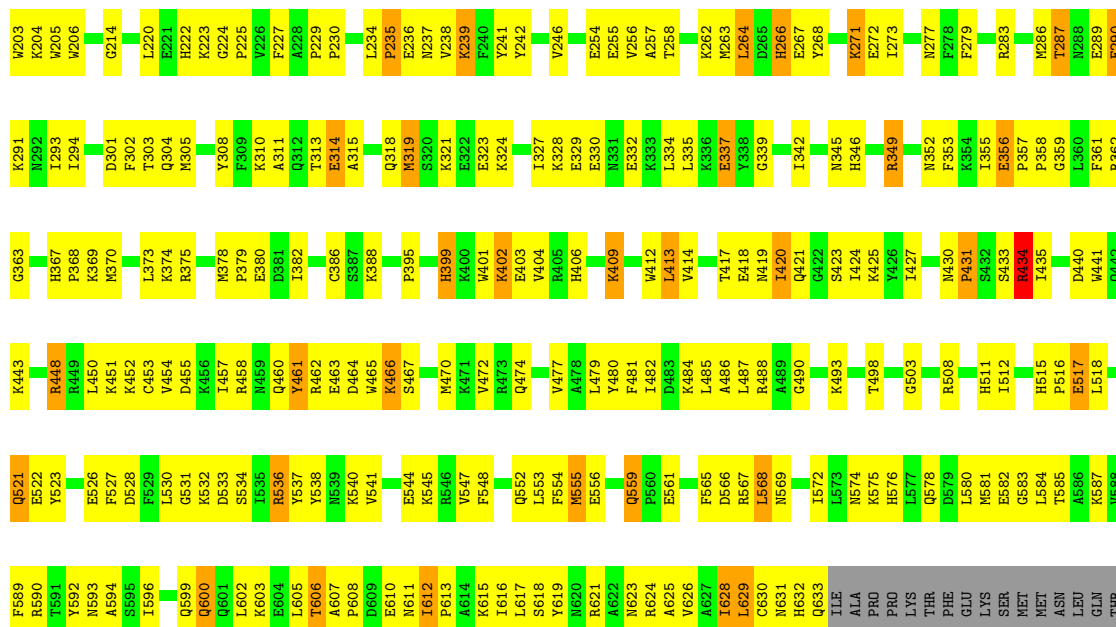
- Molecule 2: DNA (5'-D(*C*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*TP*GP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3')

Chain D: 



- Molecule 3: DNA TOPOISOMERASE I

Chain A: 



GLU	ASN	LYS	GLN	L714	L715	L716	S719	F723	L724	D725	F726	V730	F731	V732	K733	K735	G737	F738	I740	E741	K742	I743	L744	M745	K746	T747	Q748	R749	F752	A753	F754	I755	I756	D757	M758	E761	F762	F763	F764	F765	LYS	ILE	ASP	LYS	LYS	GLU	GLN	LEU	LEU	ALA	ALA	ASP	ALA	ARG	ARG	ASP	LYS	LEU	LEU	LYS	SER	LYS	ALA	ALA	ASP	ASP	LYS	VAL	VAL	LYS	LYS	LYS	LYS	LYS	ALA	VAL	VAL	GLU	SER	SER	LYS	LYS	LYS	LYS	ALA	VAL	GLN	VAL	LEU	LEU	GLU	GLN	THR	ASP	ARG	GLU
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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	56.98Å 124.92Å 72.29Å 90.00° 93.84° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.7 (15.00-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5215	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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	C	0.59	0/508	1.08	3/782 (0.4%)
2	D	0.61	0/496	1.06	2/764 (0.3%)
3	A	0.92	1/4064 (0.0%)	1.22	39/5476 (0.7%)
All	All	0.87	1/5068 (0.0%)	1.19	44/7022 (0.6%)

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
1	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	256	VAL	CA-CB	-5.53	1.47	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	761	GLU	N-CA-C	-9.37	101.06	111.28
3	A	419	ASN	N-CA-C	8.68	121.83	111.33
1	C	10	DC	C2'-C3'-O3'	-8.45	98.83	111.50
3	A	239	LYS	N-CA-C	8.34	123.20	109.95
3	A	420	ILE	N-CA-C	8.12	118.92	110.72
3	A	559	GLN	CA-C-N	7.27	128.93	119.84
3	A	559	GLN	C-N-CA	7.27	128.93	119.84
3	A	484	LYS	N-CA-C	7.15	120.49	111.69
3	A	434	ARG	N-CA-C	-7.12	102.72	111.40
3	A	293	ILE	N-CA-C	7.05	118.01	111.45
3	A	399	HIS	N-CA-C	6.82	118.86	109.18
3	A	541	VAL	N-CA-C	6.70	118.29	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	LYS	N-CA-C	-6.37	104.42	111.36
3	A	409	LYS	N-CA-C	-6.22	105.85	113.50
3	A	271	LYS	N-CA-C	6.19	118.77	110.35
3	A	272	GLU	N-CA-C	6.15	117.65	111.07
3	A	224	GLY	CA-C-N	6.08	126.59	120.14
3	A	224	GLY	C-N-CA	6.08	126.59	120.14
3	A	267	GLU	N-CA-C	-6.06	105.85	113.18
3	A	754	TRP	N-CA-C	-5.94	104.50	110.97
3	A	329	GLU	N-CA-C	-5.87	104.88	111.28
3	A	356	GLU	CA-C-N	5.78	126.34	120.38
3	A	356	GLU	C-N-CA	5.78	126.34	120.38
3	A	606	THR	N-CA-C	5.74	118.02	109.59
2	D	121	DT	C2'-C3'-O3'	-5.56	103.17	111.50
3	A	345	ASN	N-CA-C	5.54	119.74	112.92
2	D	112	DT	C2'-C3'-O3'	-5.49	103.27	111.50
3	A	303	THR	N-CA-C	5.44	116.90	110.97
3	A	287	THR	N-CA-C	-5.41	103.39	110.53
3	A	738	VAL	CB-CA-C	-5.40	104.64	110.85
3	A	378	MET	CA-C-N	5.30	125.11	119.28
3	A	378	MET	C-N-CA	5.30	125.11	119.28
3	A	235	PRO	N-CA-C	-5.28	102.81	111.21
3	A	555	MET	N-CA-C	5.25	119.67	113.16
3	A	374	LYS	N-CA-C	-5.25	100.75	109.46
3	A	448	ARG	N-CA-C	-5.24	105.62	112.23
3	A	536	ARG	N-CA-C	5.23	117.80	109.96
3	A	337	GLU	N-CA-C	5.18	118.06	111.69
1	C	10	DC	N1-C1'-C2'	5.16	121.24	113.50
3	A	612	ILE	CB-CA-C	-5.15	108.81	113.70
1	C	1	DA	O5'-C5'-C4'	-5.13	103.11	110.80
3	A	290	GLU	N-CA-C	-5.09	105.81	111.36
3	A	725	ASP	CA-C-N	5.07	124.73	119.56
3	A	725	ASP	C-N-CA	5.07	124.73	119.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	17	DA	Sidechain
1	C	8	DC	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	C	451	0	250	22	0
2	D	445	0	256	22	0
3	A	3966	0	3923	225	0
4	A	270	0	0	23	0
4	C	33	0	0	2	0
4	D	50	0	0	13	0
All	All	5215	0	4429	261	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 28.

All (261) 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:517:GLU:HG3	3:A:522:GLU:HG3	1.30	1.10
1:C:21:DT:H2'	1:C:22:DT:H72	1.38	1.02
3:A:599:GLN:HE22	3:A:765:PHE:H	1.01	0.97
3:A:367:HIS:HD2	3:A:369:LYS:H	1.12	0.97
2:D:101:DA:H1'	4:D:1064:HOH:O	1.74	0.88
3:A:599:GLN:HE22	3:A:765:PHE:N	1.73	0.87
1:C:18:DT:H73	4:C:1351:HOH:O	1.74	0.87
2:D:106:DT:H71	4:D:1162:HOH:O	1.73	0.86
3:A:745:ASN:H	3:A:748:GLN:NE2	1.72	0.86
3:A:608:PRO:HA	3:A:736:TRP:HZ3	1.42	0.83
2:D:101:DA:H2''	2:D:102:DA:C8	2.15	0.81
2:D:115:DG:H2'	2:D:116:DT:H72	1.63	0.81
3:A:599:GLN:NE2	3:A:765:PHE:H	1.81	0.78
1:C:17:DA:H2''	1:C:18:DT:H5'	1.65	0.77
3:A:315:ALA:HA	3:A:318:GLN:HE21	1.50	0.77
2:D:106:DT:H5''	4:D:1222:HOH:O	1.85	0.77
3:A:349:ARG:HG3	3:A:349:ARG:HH11	1.51	0.76
3:A:367:HIS:CD2	3:A:369:LYS:H	2.01	0.76
3:A:623:ASN:HB3	3:A:716:LEU:HD13	1.67	0.75
3:A:578:GLN:HE21	3:A:583:GLY:H	1.35	0.73
3:A:286:MET:O	3:A:291:LYS:HE3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:318:GLN:HB3	4:A:1163:HOH:O	1.90	0.71
2:D:121:DT:H2'	4:D:1323:HOH:O	1.90	0.71
3:A:328:LYS:O	3:A:332:GLU:HG3	1.92	0.70
3:A:361:PHE:HB2	3:A:420:ILE:HD13	1.74	0.70
3:A:321:LYS:HA	3:A:324:LYS:HE3	1.75	0.69
3:A:544:GLU:HB2	3:A:547:VAL:HG23	1.72	0.69
3:A:254:GLU:O	3:A:258:THR:HG23	1.92	0.69
3:A:417:THR:HG23	4:A:1352:HOH:O	1.93	0.69
3:A:581:MET:HB3	3:A:584:LEU:HD22	1.76	0.68
1:C:21:DT:H2'	1:C:22:DT:C7	2.19	0.68
3:A:453:CYS:O	3:A:457:ILE:HG13	1.93	0.68
3:A:474:GLN:OE1	3:A:567:ARG:HB2	1.94	0.68
2:D:116:DT:H1'	4:D:1309:HOH:O	1.94	0.67
3:A:266:HIS:HB3	3:A:268:TYR:HB2	1.75	0.67
3:A:225:PRO:HB2	3:A:355:ILE:HG12	1.76	0.67
3:A:315:ALA:O	3:A:318:GLN:HG2	1.95	0.66
2:D:117:DC:H5'	4:D:1309:HOH:O	1.95	0.66
3:A:434:ARG:HD3	4:A:1357:HOH:O	1.95	0.65
3:A:608:PRO:HA	3:A:736:TRP:CZ3	2.28	0.65
3:A:515:HIS:CD2	3:A:518:LEU:HD22	2.31	0.65
3:A:283:ARG:O	3:A:291:LYS:HE2	1.97	0.65
3:A:745:ASN:H	3:A:748:GLN:HE21	1.44	0.65
3:A:745:ASN:OD1	3:A:748:GLN:HG3	1.97	0.65
3:A:346:HIS:HD2	4:A:1182:HOH:O	1.79	0.65
3:A:517:GLU:HG2	3:A:521:GLN:O	1.97	0.64
3:A:516:PRO:O	3:A:522:GLU:HG2	1.98	0.64
3:A:273:ILE:HD12	4:A:1108:HOH:O	1.98	0.63
3:A:413:LEU:N	3:A:413:LEU:HD23	2.13	0.62
2:D:101:DA:C1'	4:D:1064:HOH:O	2.40	0.62
2:D:115:DG:H2'	2:D:116:DT:C7	2.27	0.62
3:A:608:PRO:HG3	3:A:736:TRP:HH2	1.64	0.62
3:A:626:VAL:HG11	3:A:724:LEU:HD21	1.81	0.62
3:A:223:LYS:HD3	3:A:337:GLU:O	1.99	0.62
3:A:271:LYS:HB3	4:A:1108:HOH:O	1.99	0.62
3:A:279:PHE:O	3:A:283:ARG:HG3	2.00	0.62
3:A:462:ARG:HG2	3:A:465:TRP:CH2	2.35	0.62
1:C:11:DA:H5''	3:A:532:LYS:HE2	1.81	0.61
3:A:289:GLU:HA	3:A:289:GLU:OE1	2.00	0.61
1:C:8:DC:H5''	4:A:1054:HOH:O	2.00	0.61
3:A:308:TYR:O	3:A:311:ALA:HB3	2.01	0.61
3:A:403:GLU:HG2	3:A:404:VAL:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:615:LYS:HZ3	3:A:736:TRP:HE3	1.49	0.60
3:A:315:ALA:HA	3:A:318:GLN:NE2	2.17	0.59
3:A:470:MET:HE2	3:A:554:PHE:CD2	2.37	0.59
3:A:521:GLN:HG2	4:A:1267:HOH:O	2.01	0.59
1:C:21:DT:H2''	1:C:22:DT:O5'	2.01	0.59
2:D:101:DA:H2''	4:D:1064:HOH:O	2.02	0.59
3:A:610:GLU:O	3:A:615:LYS:HE3	2.03	0.59
3:A:621:ARG:HG2	3:A:624:ARG:NH1	2.18	0.58
3:A:359:GLY:O	3:A:373:LEU:HD12	2.03	0.58
3:A:526:GLU:HG3	3:A:540:LYS:HG2	1.84	0.58
3:A:235:PRO:HD2	3:A:238:VAL:HG21	1.86	0.58
3:A:512:ILE:HD11	3:A:555:MET:SD	2.43	0.58
3:A:612:ILE:HB	3:A:613:PRO:HD3	1.85	0.58
3:A:625:ALA:O	3:A:628:ILE:HG22	2.03	0.58
3:A:358:PRO:HD3	4:A:1046:HOH:O	2.04	0.57
1:C:21:DT:C2'	1:C:22:DT:H72	2.26	0.57
3:A:490:GLY:CA	3:A:503:GLY:HA3	2.35	0.57
3:A:335:LEU:HD12	3:A:339:GLY:HA3	1.87	0.57
3:A:608:PRO:HG3	3:A:736:TRP:CH2	2.39	0.56
3:A:375:ARG:HG2	3:A:375:ARG:HH11	1.71	0.56
3:A:745:ASN:CG	3:A:748:GLN:HG3	2.31	0.56
3:A:590:ARG:HD3	4:A:1048:HOH:O	2.06	0.56
3:A:745:ASN:O	3:A:749:ARG:HG3	2.06	0.55
3:A:754:TRP:CG	3:A:755:ALA:H	2.24	0.55
2:D:114:DA:H4'	3:A:533:ASP:OD1	2.05	0.55
3:A:575:LYS:HD2	4:A:1313:HOH:O	2.06	0.55
3:A:578:GLN:NE2	3:A:583:GLY:H	2.02	0.55
1:C:11:DA:H5''	3:A:532:LYS:CE	2.37	0.55
3:A:508:ARG:HD2	3:A:561:GLU:O	2.07	0.55
3:A:566:ASP:OD2	3:A:567:ARG:HG2	2.06	0.55
3:A:287:THR:OG1	3:A:290:GLU:HG3	2.07	0.54
3:A:735:LYS:HA	3:A:761:GLU:HG3	1.90	0.54
2:D:101:DA:C2'	2:D:102:DA:C8	2.87	0.54
3:A:412:TRP:CD1	3:A:412:TRP:H	2.24	0.54
3:A:412:TRP:C	3:A:413:LEU:HD23	2.33	0.54
3:A:214:GLY:O	3:A:409:LYS:HA	2.08	0.54
3:A:239:LYS:HB2	3:A:304:GLN:OE1	2.07	0.53
1:C:1:DA:O5'	1:C:1:DA:C2'	2.55	0.53
3:A:745:ASN:CG	3:A:748:GLN:HE21	2.17	0.53
1:C:1:DA:O5'	1:C:1:DA:H2'	2.08	0.53
3:A:578:GLN:NE2	3:A:582:GLU:HA	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:257:ALA:HB1	3:A:302:PHE:HE1	1.74	0.52
3:A:434:ARG:CD	4:A:1357:HOH:O	2.57	0.52
3:A:530:LEU:HD23	3:A:536:ARG:HA	1.92	0.52
3:A:479:LEU:HD11	3:A:589:PHE:CZ	2.44	0.52
3:A:624:ARG:O	3:A:628:ILE:HB	2.10	0.52
3:A:477:VAL:O	3:A:480:TYR:HB3	2.10	0.52
3:A:490:GLY:HA2	3:A:503:GLY:HA3	1.92	0.51
3:A:565:PHE:C	3:A:566:ASP:O	2.50	0.51
3:A:629:LEU:C	3:A:629:LEU:HD12	2.35	0.51
1:C:11:DA:P	3:A:488:ARG:HH21	2.33	0.51
3:A:242:TYR:CE1	3:A:294:ILE:HG23	2.45	0.51
3:A:418:GLU:HB2	3:A:425:LYS:HE3	1.93	0.51
3:A:602:LEU:CD2	3:A:619:TYR:HA	2.40	0.51
3:A:754:TRP:CG	3:A:755:ALA:N	2.78	0.51
3:A:242:TYR:CZ	3:A:294:ILE:HA	2.46	0.51
3:A:745:ASN:CB	3:A:748:GLN:HE21	2.23	0.51
3:A:222:HIS:CD2	3:A:413:LEU:HB3	2.46	0.51
3:A:380:GLU:OE2	3:A:399:HIS:HD2	1.94	0.51
3:A:578:GLN:HE21	3:A:583:GLY:N	2.07	0.51
3:A:732:TRP:HZ3	3:A:743:ILE:HD11	1.77	0.50
4:D:1077:HOH:O	3:A:357:PRO:HD2	2.10	0.50
3:A:454:VAL:HG13	3:A:455:ASP:N	2.26	0.50
3:A:616:ILE:O	3:A:619:TYR:HB3	2.11	0.50
3:A:719:SER:HA	3:A:723:PHE:HD1	1.76	0.50
3:A:606:THR:O	3:A:608:PRO:HD3	2.12	0.50
3:A:236:GLU:O	3:A:239:LYS:NZ	2.45	0.50
3:A:569:ASN:OD1	3:A:572:ILE:HG13	2.12	0.50
3:A:517:GLU:HG3	3:A:522:GLU:CG	2.21	0.50
3:A:268:TYR:HE1	3:A:362:ARG:HE	1.58	0.50
3:A:235:PRO:HD2	3:A:238:VAL:CG2	2.43	0.49
3:A:271:LYS:HD2	4:A:1135:HOH:O	2.13	0.49
2:D:101:DA:C2'	4:D:1064:HOH:O	2.57	0.49
3:A:630:CYS:HB3	3:A:632:HIS:CE1	2.48	0.48
3:A:327:ILE:HD13	4:A:1243:HOH:O	2.12	0.48
3:A:517:GLU:HA	3:A:522:GLU:HA	1.95	0.48
2:D:115:DG:H3'	4:D:1052:HOH:O	2.13	0.48
1:C:21:DT:H2''	1:C:22:DT:C6	2.49	0.48
3:A:485:LEU:O	3:A:486:ALA:HB3	2.14	0.48
3:A:553:LEU:O	3:A:556:GLU:HG2	2.14	0.48
3:A:273:ILE:HG22	3:A:277:ASN:ND2	2.29	0.48
3:A:241:TYR:HB2	3:A:301:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:286:MET:HB3	3:A:290:GLU:HB2	1.96	0.47
3:A:457:ILE:HG23	3:A:580:LEU:CD1	2.44	0.47
3:A:470:MET:HE2	3:A:554:PHE:HD2	1.79	0.47
3:A:612:ILE:N	3:A:613:PRO:CD	2.77	0.47
3:A:592:TYR:HE2	4:A:1132:HOH:O	1.97	0.47
3:A:382:ILE:HG23	3:A:414:VAL:CG1	2.45	0.47
3:A:470:MET:HE2	3:A:554:PHE:CE2	2.50	0.47
3:A:599:GLN:O	3:A:603:LYS:HG3	2.15	0.47
1:C:6:DG:H2'	3:A:424:ILE:HD12	1.97	0.47
3:A:448:ARG:O	3:A:451:LYS:HB3	2.15	0.47
3:A:628:ILE:CG2	3:A:629:LEU:N	2.78	0.47
3:A:726:PRO:HG3	3:A:752:PHE:CD2	2.50	0.47
3:A:386:CYS:O	3:A:406:HIS:HA	2.15	0.47
3:A:631:ASN:HD21	3:A:633:GLN:HE21	1.63	0.47
1:C:21:DT:H1'	1:C:22:DT:H5'	1.97	0.46
3:A:361:PHE:CE2	3:A:363:GLY:N	2.83	0.46
3:A:528:ASP:HA	3:A:537:TYR:O	2.15	0.46
3:A:255:GLU:O	3:A:258:THR:OG1	2.27	0.46
3:A:349:ARG:HG3	3:A:349:ARG:NH1	2.25	0.46
3:A:227:PHE:CZ	3:A:379:PRO:HG3	2.50	0.46
3:A:430:ASN:ND2	3:A:431:PRO:HD2	2.31	0.46
3:A:600:GLN:O	3:A:603:LYS:HB2	2.15	0.46
3:A:746:LYS:H	3:A:746:LYS:HG3	1.37	0.46
2:D:117:DC:OP1	3:A:585:THR:HB	2.16	0.46
2:D:115:DG:OP2	3:A:493:LYS:HE2	2.15	0.46
3:A:302:PHE:O	3:A:305:MET:HB2	2.16	0.46
3:A:617:LEU:CD1	3:A:624:ARG:HH22	2.29	0.46
3:A:719:SER:HA	3:A:723:PHE:CD1	2.51	0.46
1:C:8:DC:H2''	1:C:9:DT:H72	1.98	0.45
3:A:402:LYS:HE2	4:A:1320:HOH:O	2.16	0.45
3:A:441:TRP:CZ2	3:A:758:MET:HE1	2.52	0.45
3:A:481:PHE:HB3	3:A:487:LEU:HD12	1.98	0.45
3:A:258:THR:HA	3:A:305:MET:HE2	1.97	0.45
3:A:452:LYS:NZ	4:A:1200:HOH:O	2.49	0.45
3:A:523:TYR:CZ	3:A:545:LYS:HG3	2.51	0.45
2:D:116:DT:C2'	4:D:1016:HOH:O	2.64	0.45
3:A:310:LYS:O	3:A:313:THR:HB	2.17	0.45
3:A:367:HIS:O	3:A:370:MET:HE3	2.17	0.45
3:A:433:SER:HB3	3:A:435:ILE:HG22	1.98	0.45
3:A:596:ILE:HD12	3:A:596:ILE:HA	1.84	0.45
3:A:608:PRO:C	3:A:610:GLU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:574:ASN:OD1	3:A:585:THR:HA	2.17	0.45
3:A:512:ILE:HA	3:A:526:GLU:O	2.17	0.44
3:A:628:ILE:HG22	3:A:629:LEU:N	2.32	0.44
1:C:8:DC:H2''	1:C:9:DT:C7	2.47	0.44
3:A:578:GLN:HG2	3:A:583:GLY:H	1.80	0.44
3:A:388:LYS:HG2	3:A:406:HIS:CG	2.52	0.44
1:C:19:DT:H73	4:C:1254:HOH:O	2.18	0.44
3:A:631:ASN:HD21	3:A:633:GLN:NE2	2.16	0.44
2:D:106:DT:C5'	4:D:1222:HOH:O	2.57	0.44
3:A:463:GLU:O	3:A:466:LYS:HB2	2.18	0.44
3:A:508:ARG:HD3	4:A:1118:HOH:O	2.18	0.44
3:A:733:CYS:HB3	3:A:738:VAL:O	2.16	0.44
3:A:273:ILE:HD12	3:A:273:ILE:H	1.83	0.44
3:A:527:PHE:O	3:A:538:TYR:HA	2.17	0.44
3:A:220:LEU:HA	3:A:342:ILE:O	2.18	0.43
3:A:458:ARG:HB3	3:A:462:ARG:NH1	2.32	0.43
3:A:508:ARG:H	3:A:511:HIS:CE1	2.36	0.43
1:C:1:DA:O5'	1:C:1:DA:C8	2.68	0.43
3:A:739:PRO:O	3:A:742:LYS:HB2	2.17	0.43
3:A:534:SER:N	4:A:1015:HOH:O	2.51	0.43
2:D:101:DA:H2''	2:D:102:DA:H8	1.75	0.43
2:D:107:DT:H2''	2:D:108:DT:OP2	2.19	0.43
3:A:334:LEU:HD23	4:A:1127:HOH:O	2.17	0.43
3:A:754:TRP:H	3:A:754:TRP:CD1	2.36	0.43
3:A:587:LYS:HG3	4:A:1039:HOH:O	2.19	0.43
3:A:599:GLN:HG2	3:A:603:LYS:HE3	2.00	0.43
3:A:605:LEU:HD23	3:A:605:LEU:HA	1.76	0.43
3:A:607:ALA:HB3	3:A:610:GLU:CB	2.49	0.43
3:A:355:ILE:HG21	4:A:1031:HOH:O	2.17	0.43
3:A:466:LYS:HD2	3:A:466:LYS:HA	1.79	0.43
3:A:576:HIS:HE1	4:A:1036:HOH:O	2.02	0.43
3:A:741:GLU:H	3:A:741:GLU:HG3	1.43	0.43
3:A:418:GLU:HG3	3:A:425:LYS:HE3	2.02	0.42
1:C:17:DA:H2''	1:C:18:DT:C5'	2.44	0.42
3:A:352:ASN:O	3:A:427:ILE:HG23	2.20	0.42
3:A:367:HIS:HA	3:A:368:PRO:HD2	1.95	0.42
3:A:450:LEU:O	3:A:451:LYS:C	2.61	0.42
3:A:548:PHE:O	3:A:552:GLN:HG3	2.19	0.42
3:A:263:MET:HE3	3:A:362:ARG:NH2	2.34	0.42
3:A:283:ARG:NH2	3:A:291:LYS:O	2.52	0.42
3:A:356:GLU:HA	3:A:357:PRO:HD3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:203:TRP:O	3:A:205:TRP:N	2.51	0.42
3:A:234:LEU:HD23	3:A:234:LEU:HA	1.88	0.42
3:A:735:LYS:CA	3:A:761:GLU:HG3	2.49	0.42
3:A:283:ARG:HA	3:A:286:MET:HG3	2.02	0.42
3:A:482:ILE:HG12	3:A:487:LEU:O	2.20	0.42
1:C:21:DT:C2'	1:C:22:DT:C7	2.92	0.41
3:A:464:ASP:HB3	3:A:472:VAL:HG12	2.02	0.41
3:A:730:VAL:HG21	3:A:756:ILE:HA	2.00	0.41
3:A:349:ARG:NH1	3:A:349:ARG:CG	2.80	0.41
3:A:375:ARG:HG2	3:A:375:ARG:NH1	2.33	0.41
3:A:395:PRO:HD3	3:A:401:TRP:NE1	2.34	0.41
3:A:458:ARG:HA	3:A:461:TYR:CE1	2.56	0.41
3:A:531:GLY:O	3:A:534:SER:N	2.53	0.41
3:A:611:ASN:CB	3:A:613:PRO:HD2	2.50	0.41
3:A:229:PRO:HA	3:A:230:PRO:HD3	1.82	0.41
3:A:559:GLN:HB3	3:A:561:GLU:OE1	2.21	0.41
3:A:568:LEU:HD23	3:A:569:ASN:H	1.86	0.41
1:C:18:DT:H2'	1:C:19:DT:H71	2.02	0.41
3:A:319:MET:HB2	3:A:323:GLU:OE1	2.20	0.41
3:A:382:ILE:CG2	3:A:414:VAL:HG13	2.50	0.41
3:A:594:ALA:HA	3:A:626:VAL:HG13	2.03	0.41
3:A:335:LEU:HD11	3:A:349:ARG:CZ	2.51	0.41
3:A:464:ASP:C	3:A:466:LYS:N	2.78	0.41
3:A:523:TYR:CE1	3:A:545:LYS:HE2	2.56	0.41
3:A:578:GLN:HA	3:A:581:MET:O	2.21	0.41
3:A:602:LEU:HD21	3:A:619:TYR:HA	2.02	0.41
3:A:617:LEU:O	3:A:618:SER:C	2.62	0.41
3:A:382:ILE:HG23	3:A:414:VAL:HG13	2.03	0.41
3:A:440:ASP:O	3:A:443:LYS:HB3	2.21	0.41
3:A:258:THR:O	3:A:262:LYS:HG3	2.21	0.40
3:A:731:ALA:HB2	3:A:763:TYR:HB3	2.02	0.40
3:A:204:LYS:HG2	3:A:206:TRP:CZ2	2.56	0.40
3:A:339:GLY:HA2	3:A:353:PHE:CD1	2.56	0.40
2:D:115:DG:OP2	3:A:493:LYS:CE	2.69	0.40
3:A:314:GLU:O	3:A:315:ALA:C	2.65	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	479/563 (85%)	448 (94%)	28 (6%)	3 (1%)	21	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	319	MET
3	A	264	LEU
3	A	467	SER

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	419/507 (83%)	392 (94%)	27 (6%)	16	35

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	237	ASN
3	A	246	VAL
3	A	264	LEU
3	A	266	HIS
3	A	314	GLU
3	A	330	GLU
3	A	349	ARG
3	A	413	LEU

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Mol	Chain	Res	Type
3	A	421	GLN
3	A	423	SER
3	A	431	PRO
3	A	434	ARG
3	A	460	GLN
3	A	461	TYR
3	A	466	LYS
3	A	498	THR
3	A	517	GLU
3	A	521	GLN
3	A	568	LEU
3	A	593	ASN
3	A	600	GLN
3	A	628	ILE
3	A	629	LEU
3	A	741	GLU
3	A	743	ILE
3	A	746	LYS
3	A	758	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	266	HIS
3	A	307	GLN
3	A	318	GLN
3	A	367	HIS
3	A	399	HIS
3	A	430	ASN
3	A	460	GLN
3	A	515	HIS
3	A	539	ASN
3	A	559	GLN
3	A	578	GLN
3	A	599	GLN
3	A	623	ASN
3	A	631	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 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.