



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:09 PM GMT

PDB ID : 1A35
Title : HUMAN TOPOISOMERASE I/DNA COMPLEX
Authors : Redinbo, M.R.; Stewart, L.; Kuhn, P.; Champoux, J.J.; Hol, W.G.
Deposited on : 1998-01-29
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

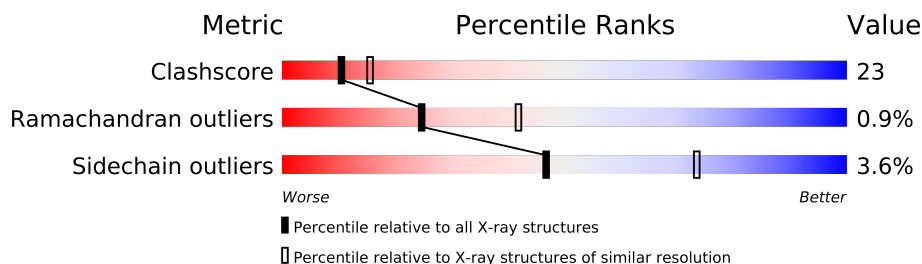
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4947 atoms, of which 0 are hydrogen and 0 are deuterium.

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*AP*(BRU)P*(BRU)P*TP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	22	Total	Br	C	N	O	P	0	0	0
			452	2	217	87	125	21			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	22	Total	Br	C	N	O	P	0	0	0
			444	6	212	70	135	21			

- Molecule 3 is a protein called PROTEIN (DNA TOPOISOMERASE I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	474	Total	C	N	O	S	0	0	0
			3778	2431	662	663	22			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	C	23	Total	O	0	0
			23	23		
4	D	44	Total	O	0	0
			44	44		

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.

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*AP*(BRU)P*(BRU)P*TP*TP*T)-3')

Chain C: 



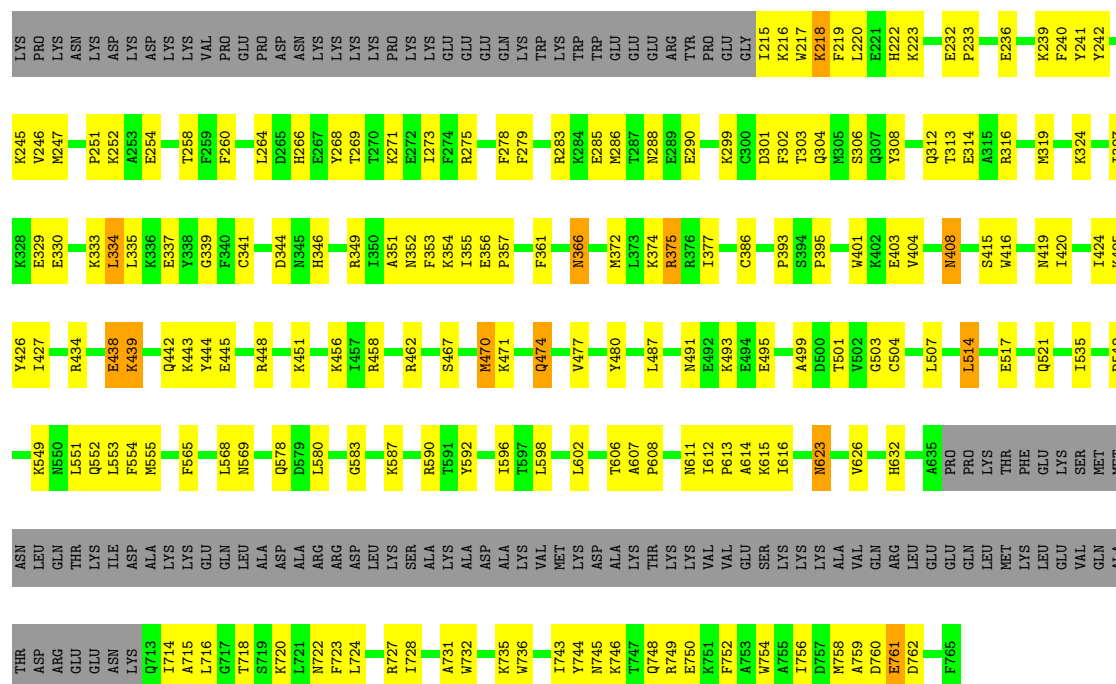
- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*TP*+UP*+UP*+UP*+UP*CP*+UP*AP*AP*GP*TP*CP*TP*TP*TP*+UP*T)-3')

Chain D: 



- Molecule 3: PROTEIN (DNA TOPOISOMERASE I)

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.80Å 66.30Å 71.80Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	87.0 (20.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.209 , 0.308	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4947	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.69	0/464	0.89	1/712 (0.1%)
2	D	0.89	0/360	0.96	0/546
3	A	0.57	0/3868	0.72	0/5222
All	All	0.61	0/4692	0.76	1/6480 (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
1	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	DC	C1'-O4'-C4'	-5.94	104.16	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	8	DC	Sidechain

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	452	0	245	27	0
2	D	444	0	238	34	0
3	A	3778	0	3713	156	0
4	A	206	0	0	36	0
4	C	23	0	0	3	0
4	D	44	0	0	12	0
All	All	4947	0	4196	203	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (203) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:105:DA:H2''	2:D:106:DT:C5'	1.85	1.06
2:D:105:DA:H2''	2:D:106:DT:H5'	1.38	1.03
1:C:8:DC:H2''	1:C:9:DT:C7	1.88	1.03
1:C:8:DC:C2'	1:C:9:DT:H71	1.87	1.02
3:A:623:ASN:HD21	3:A:716:LEU:HB3	1.28	0.97
1:C:8:DC:H2''	1:C:9:DT:H71	0.95	0.94
2:D:118:DT:H5'	4:D:1071:HOH:O	1.68	0.93
2:D:116:DT:H73	4:A:1076:HOH:O	1.70	0.91
2:D:122:DT:H71	4:D:1124:HOH:O	1.71	0.91
3:A:408:ASN:H	3:A:408:ASN:HD22	1.15	0.90
1:C:21:DT:H5''	4:C:1257:HOH:O	1.72	0.88
3:A:720:LYS:HE2	3:A:748:GLN:HE22	1.41	0.83
3:A:470:MET:HB3	4:A:1234:HOH:O	1.77	0.83
1:C:12:DG:H5''	3:A:535:ILE:HD11	1.59	0.82
3:A:487:LEU:HD12	4:A:1200:HOH:O	1.78	0.81
2:D:105:DA:H2''	2:D:106:DT:H5''	1.63	0.79
2:D:110:BRU:H2''	2:D:111:DC:H5'	1.66	0.77
3:A:366:ASN:C	3:A:366:ASN:HD22	1.89	0.75
3:A:504:CYS:SG	4:A:1200:HOH:O	2.46	0.73
2:D:105:DA:C2'	2:D:106:DT:H5''	2.18	0.72
1:C:19:BRU:H1'	1:C:20:DT:H5'	1.70	0.72
3:A:245:LYS:HE3	4:A:1241:HOH:O	1.87	0.72
3:A:732:TRP:HZ3	3:A:743:ILE:HD11	1.55	0.71
2:D:115:DG:H1'	4:D:1037:HOH:O	1.90	0.71
3:A:607:ALA:O	3:A:615:LYS:HE2	1.89	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:354:LYS:HG3	4:A:1046:HOH:O	1.90	0.71
2:D:104:DA:H2"	2:D:105:DA:H5"	1.73	0.70
3:A:286:MET:HB3	3:A:290:GLU:HB2	1.72	0.70
2:D:105:DA:C2'	2:D:106:DT:C5'	2.67	0.70
3:A:372:MET:SD	4:A:1221:HOH:O	2.50	0.70
3:A:612:ILE:HB	3:A:613:PRO:HD3	1.73	0.69
2:D:112:BRU:BR	4:D:1115:HOH:O	2.67	0.68
3:A:587:LYS:HB2	4:A:1141:HOH:O	1.93	0.68
3:A:551:LEU:O	3:A:555:MET:HG3	1.92	0.67
1:C:11:DA:OP2	3:A:723:PHE:HE1	1.77	0.67
3:A:735:LYS:HE2	3:A:761:GLU:O	1.93	0.67
3:A:568:LEU:HD22	3:A:569:ASN:N	2.09	0.67
3:A:720:LYS:HG3	4:A:1176:HOH:O	1.94	0.67
3:A:254:GLU:O	3:A:258:THR:HG23	1.95	0.66
1:C:12:DG:C5'	3:A:535:ILE:HD11	2.25	0.66
3:A:330:GLU:O	3:A:333:LYS:HG2	1.95	0.65
3:A:470:MET:CE	3:A:553:LEU:HG	2.26	0.65
3:A:720:LYS:HE3	4:A:1176:HOH:O	1.96	0.64
3:A:239:LYS:HD3	3:A:246:VAL:HG11	1.80	0.64
2:D:116:DT:C7	4:A:1076:HOH:O	2.38	0.64
2:D:112:BRU:H6	4:D:1107:HOH:O	1.97	0.64
2:D:110:BRU:H2"	2:D:111:DC:C5'	2.28	0.63
3:A:375:ARG:HG2	3:A:419:ASN:ND2	2.13	0.63
3:A:279:PHE:O	3:A:283:ARG:HG3	1.99	0.63
3:A:355:ILE:HG21	3:A:377:ILE:HB	1.81	0.62
3:A:744:TYR:HD1	3:A:748:GLN:HE21	1.48	0.62
1:C:17:DA:C2	2:D:106:DT:N3	2.62	0.62
3:A:732:TRP:CZ3	3:A:743:ILE:HD11	2.34	0.61
3:A:470:MET:HG2	3:A:554:PHE:HE1	1.65	0.61
3:A:218:LYS:HA	3:A:218:LYS:CE	2.30	0.61
3:A:720:LYS:HA	4:A:1275:HOH:O	1.99	0.61
3:A:744:TYR:HD1	3:A:748:GLN:NE2	1.98	0.61
3:A:542:PRO:HD2	4:A:1230:HOH:O	1.99	0.61
1:C:19:BRU:H2"	1:C:20:DT:H71	1.83	0.60
3:A:727:ARG:HG2	3:A:759:ALA:HB2	1.84	0.60
1:C:16:DA:H8	4:C:1060:HOH:O	1.84	0.60
3:A:746:LYS:O	3:A:750:GLU:HG2	2.02	0.60
1:C:11:DA:H2'	1:C:12:DG:C8	2.36	0.60
3:A:218:LYS:HA	3:A:218:LYS:HE3	1.83	0.60
3:A:623:ASN:ND2	3:A:716:LEU:HB3	2.10	0.59
3:A:568:LEU:HD22	3:A:569:ASN:H	1.65	0.59
3:A:503:GLY:O	3:A:507:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:113:DA:C2'	4:D:1001:HOH:O	2.51	0.58
3:A:271:LYS:NZ	4:A:1191:HOH:O	2.36	0.58
1:C:11:DA:OP2	3:A:723:PHE:CE1	2.55	0.58
3:A:443:LYS:HD3	4:A:1089:HOH:O	2.03	0.58
3:A:416:TRP:HH2	4:A:1068:HOH:O	1.87	0.57
1:C:9:DT:H5'	3:A:439:LYS:NZ	2.19	0.57
1:C:19:BRU:C2'	1:C:20:DT:H71	2.35	0.57
3:A:590:ARG:NH1	4:A:1088:HOH:O	2.38	0.57
3:A:756:ILE:HG22	3:A:756:ILE:O	2.05	0.56
3:A:611:ASN:OD1	3:A:614:ALA:HB3	2.05	0.56
3:A:745:ASN:O	3:A:749:ARG:HG3	2.05	0.56
1:C:2:DA:H2''	1:C:3:DA:OP2	2.06	0.56
3:A:408:ASN:N	3:A:408:ASN:HD22	1.89	0.55
1:C:17:DA:H2''	1:C:18:BRU:O5'	2.05	0.55
3:A:366:ASN:ND2	3:A:499:ALA:HA	2.21	0.55
3:A:606:THR:HG21	3:A:736:TRP:NE1	2.21	0.55
3:A:470:MET:HE2	3:A:553:LEU:HG	1.86	0.55
3:A:216:LYS:NZ	4:A:1256:HOH:O	2.39	0.55
3:A:218:LYS:HZ2	3:A:218:LYS:HA	1.70	0.55
3:A:271:LYS:O	3:A:275:ARG:HG3	2.06	0.55
3:A:715:ALA:HB1	4:A:1173:HOH:O	2.07	0.55
3:A:395:PRO:HD3	3:A:401:TRP:NE1	2.22	0.54
3:A:477:VAL:O	3:A:480:TYR:HB3	2.08	0.53
3:A:241:TYR:HB2	3:A:301:ASP:HB3	1.91	0.53
3:A:623:ASN:ND2	3:A:716:LEU:HD13	2.23	0.53
3:A:375:ARG:HH11	3:A:419:ASN:HB3	1.74	0.53
3:A:451:LYS:HG3	3:A:592:TYR:HE1	1.72	0.52
3:A:242:TYR:CE1	3:A:299:LYS:HB2	2.45	0.52
2:D:104:DA:C2'	2:D:105:DA:H5''	2.38	0.51
3:A:744:TYR:HA	3:A:748:GLN:NE2	2.25	0.51
3:A:444:TYR:O	3:A:448:ARG:HG3	2.11	0.51
3:A:346:HIS:CD2	4:A:1188:HOH:O	2.62	0.51
3:A:458:ARG:O	3:A:462:ARG:HB2	2.11	0.51
2:D:115:DG:H3'	4:A:1076:HOH:O	2.11	0.51
1:C:17:DA:H2	2:D:106:DT:H3	1.51	0.51
3:A:240:PHE:HD2	3:A:247:MET:HB3	1.76	0.51
3:A:273:ILE:HG12	4:A:1109:HOH:O	2.10	0.51
3:A:366:ASN:C	3:A:366:ASN:ND2	2.62	0.50
3:A:366:ASN:O	3:A:366:ASN:ND2	2.43	0.50
3:A:215:ILE:HG21	3:A:218:LYS:HZ3	1.76	0.50
1:C:12:DG:H5''	3:A:535:ILE:CD1	2.37	0.50
3:A:493:LYS:HE2	4:A:1258:HOH:O	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:6:DG:H2'	3:A:424:ILE:HD12	1.93	0.49
3:A:415:SER:HA	3:A:425:LYS:O	2.13	0.49
3:A:251:PRO:HG2	4:A:1039:HOH:O	2.12	0.49
3:A:266:HIS:CE1	3:A:268:TYR:CD2	2.99	0.49
1:C:1:DA:H2''	1:C:2:DA:O5'	2.12	0.49
2:D:117:DC:C1'	4:D:1193:HOH:O	2.61	0.49
3:A:728:ILE:HB	4:A:1055:HOH:O	2.12	0.49
3:A:735:LYS:HE2	3:A:761:GLU:C	2.33	0.49
3:A:456:LYS:NZ	3:A:580:LEU:HB3	2.28	0.48
3:A:252:LYS:HE2	3:A:285:GLU:OE1	2.14	0.48
3:A:754:TRP:O	3:A:758:MET:HG2	2.13	0.48
3:A:313:THR:HA	3:A:316:ARG:NH2	2.29	0.48
3:A:352:ASN:O	3:A:427:ILE:HG23	2.14	0.48
3:A:346:HIS:HD2	4:A:1188:HOH:O	1.96	0.48
3:A:471:LYS:HG3	4:A:1142:HOH:O	2.14	0.48
1:C:9:DT:C5'	3:A:439:LYS:NZ	2.75	0.48
3:A:264:LEU:HD23	3:A:269:THR:HG21	1.96	0.48
2:D:117:DC:OP1	3:A:587:LYS:HG2	2.14	0.47
3:A:218:LYS:NZ	3:A:218:LYS:HA	2.29	0.47
3:A:324:LYS:O	3:A:327:ILE:HG13	2.14	0.47
3:A:334:LEU:HD23	3:A:353:PHE:HE1	1.79	0.47
2:D:120:DT:H2'	2:D:121:BRU:BR	2.69	0.47
3:A:403:GLU:HG2	3:A:404:VAL:N	2.29	0.47
2:D:113:DA:H2''	4:D:1001:HOH:O	2.12	0.47
3:A:514:LEU:HD23	3:A:552:GLN:HG2	1.97	0.47
3:A:264:LEU:HD11	3:A:302:PHE:HB2	1.97	0.47
3:A:438:GLU:HB2	4:A:1245:HOH:O	2.14	0.47
3:A:308:TYR:O	3:A:312:GLN:HG2	2.14	0.46
3:A:247:MET:HE3	3:A:247:MET:HB2	1.87	0.46
1:C:17:DA:N1	2:D:106:DT:C4	2.83	0.46
3:A:408:ASN:ND2	3:A:408:ASN:N	2.61	0.46
2:D:104:DA:H2''	2:D:105:DA:C5'	2.44	0.46
3:A:612:ILE:O	3:A:616:ILE:HG13	2.15	0.46
2:D:118:DT:C5'	4:D:1071:HOH:O	2.45	0.46
3:A:222:HIS:HB3	3:A:341:CYS:HB2	1.98	0.46
3:A:632:HIS:CD2	4:A:1148:HOH:O	2.69	0.45
3:A:623:ASN:HD22	3:A:623:ASN:C	2.19	0.45
3:A:602:LEU:HD23	3:A:602:LEU:HA	1.77	0.45
1:C:17:DA:H2''	1:C:18:BRU:H6	1.98	0.45
3:A:236:GLU:HB2	4:A:1127:HOH:O	2.17	0.45
3:A:314:GLU:C	3:A:316:ARG:H	2.17	0.45
3:A:718:THR:O	3:A:722:ASN:N	2.45	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:720:LYS:HE2	3:A:748:GLN:NE2	2.19	0.44
3:A:304:GLN:HE21	3:A:304:GLN:HB3	1.60	0.44
3:A:393:PRO:O	3:A:401:TRP:NE1	2.44	0.44
3:A:260:PHE:HB2	3:A:278:PHE:CE1	2.52	0.44
3:A:607:ALA:HB3	4:A:1053:HOH:O	2.16	0.44
3:A:219:PHE:HB3	3:A:344:ASP:HA	2.00	0.44
4:D:1094:HOH:O	3:A:374:LYS:NZ	2.50	0.44
2:D:105:DA:C1'	2:D:106:DT:H5''	2.48	0.44
3:A:329:GLU:HG2	4:A:1220:HOH:O	2.17	0.44
3:A:220:LEU:HD23	3:A:386:CYS:HA	2.00	0.44
3:A:366:ASN:HD21	3:A:499:ALA:HA	1.82	0.44
3:A:517:GLU:HA	3:A:521:GLN:O	2.18	0.44
3:A:470:MET:HG2	3:A:554:PHE:CE1	2.48	0.43
3:A:470:MET:HE3	3:A:553:LEU:HG	1.98	0.43
2:D:105:DA:H1'	2:D:106:DT:H5''	2.00	0.43
3:A:223:LYS:HG3	3:A:337:GLU:O	2.18	0.43
3:A:266:HIS:CE1	3:A:268:TYR:HD2	2.37	0.43
3:A:752:PHE:HD1	4:A:1120:HOH:O	2.01	0.43
2:D:110:BRU:H1'	2:D:111:DC:H5''	2.00	0.43
2:D:101:DA:H2	4:D:1011:HOH:O	2.00	0.43
3:A:493:LYS:HD3	3:A:493:LYS:HA	1.77	0.43
3:A:316:ARG:HA	3:A:319:MET:HG3	2.01	0.42
3:A:404:VAL:N	4:A:1134:HOH:O	2.52	0.42
3:A:361:PHE:HB2	3:A:420:ILE:HD13	2.01	0.42
3:A:607:ALA:HA	3:A:608:PRO:HD3	1.91	0.42
3:A:760:ASP:C	3:A:762:ASP:H	2.22	0.42
3:A:596:ILE:HA	3:A:596:ILE:HD12	1.81	0.42
3:A:501:THR:HB	4:A:1098:HOH:O	2.18	0.42
3:A:241:TYR:HA	3:A:245:LYS:O	2.19	0.42
3:A:626:VAL:HG11	3:A:724:LEU:HD21	2.00	0.42
1:C:11:DA:C2	2:D:113:DA:C2	3.08	0.42
2:D:117:DC:H1'	4:D:1193:HOH:O	2.19	0.42
3:A:623:ASN:ND2	3:A:623:ASN:C	2.73	0.42
3:A:288:ASN:HD22	3:A:288:ASN:HA	1.67	0.41
1:C:12:DG:H2'	4:C:1123:HOH:O	2.20	0.41
3:A:598:LEU:HB2	3:A:724:LEU:HD22	2.02	0.41
2:D:106:DT:H2''	2:D:107:BRU:O5'	2.21	0.41
3:A:451:LYS:HA	3:A:592:TYR:CE1	2.56	0.41
3:A:303:THR:HA	3:A:306:SER:HB3	2.03	0.41
3:A:578:GLN:HE22	3:A:583:GLY:HA2	1.85	0.41
3:A:239:LYS:H	3:A:304:GLN:NE2	2.18	0.41
3:A:491:ASN:HB2	4:A:1258:HOH:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:549:LYS:HD3	3:A:552:GLN:OE1	2.21	0.41
3:A:474:GLN:NE2	3:A:565:PHE:HA	2.36	0.41
3:A:232:GLU:HA	3:A:233:PRO:HD3	1.86	0.41
3:A:217:TRP:CZ2	3:A:408:ASN:HA	2.56	0.41
3:A:732:TRP:HZ3	3:A:743:ILE:CD1	2.30	0.40
3:A:335:LEU:O	3:A:339:GLY:HA3	2.21	0.40
1:C:6:DG:H2"	3:A:426:TYR:OH	2.21	0.40
3:A:442:GLN:O	3:A:445:GLU:HB2	2.22	0.40
3:A:356:GLU:HA	3:A:357:PRO:HD3	1.76	0.40
3:A:731:ALA:HB1	3:A:735:LYS:HE3	2.04	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	470/591 (80%)	445 (95%)	21 (4%)	4 (1%)	25	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	761	GLU
3	A	495	GLU
3	A	351	ALA
3	A	714	ILE

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	388/535 (72%)	374 (96%)	14 (4%)	47 73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	218	LYS
3	A	334	LEU
3	A	349	ARG
3	A	366	ASN
3	A	375	ARG
3	A	408	ASN
3	A	434	ARG
3	A	438	GLU
3	A	439	LYS
3	A	467	SER
3	A	470	MET
3	A	474	GLN
3	A	514	LEU
3	A	623	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	288	ASN
3	A	304	GLN
3	A	366	ASN
3	A	408	ASN
3	A	421	GLN
3	A	474	GLN
3	A	623	ASN
3	A	748	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	BRU	C	18	1,2	19,21,22	2.20	3 (15%)	22,30,33	1.58	3 (13%)
1	BRU	C	19	1,2	19,21,22	2.14	3 (15%)	22,30,33	1.65	4 (18%)
2	BRU	D	107	1,2	19,21,22	1.98	3 (15%)	22,30,33	2.01	4 (18%)
2	BRU	D	108	1,2	19,21,22	1.99	2 (10%)	22,30,33	1.94	4 (18%)
2	BRU	D	109	1,2	19,21,22	2.09	2 (10%)	22,30,33	2.04	3 (13%)
2	BRU	D	110	1,2	19,21,22	2.17	3 (15%)	22,30,33	1.83	3 (13%)
2	BRU	D	112	1,2	19,21,22	2.00	2 (10%)	22,30,33	1.81	3 (13%)
2	BRU	D	121	1,2	19,21,22	2.25	3 (15%)	22,30,33	1.56	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	BRU	C	18	1,2	-	0/5/21/22	0/2/2/2
1	BRU	C	19	1,2	-	0/5/21/22	0/2/2/2
2	BRU	D	107	1,2	-	0/5/21/22	0/2/2/2
2	BRU	D	108	1,2	-	0/5/21/22	0/2/2/2
2	BRU	D	109	1,2	-	0/5/21/22	0/2/2/2
2	BRU	D	110	1,2	-	0/5/21/22	0/2/2/2
2	BRU	D	112	1,2	-	0/5/21/22	0/2/2/2
2	BRU	D	121	1,2	-	0/5/21/22	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	19	BRU	BR-C5	8.17	2.10	1.90
2	D	121	BRU	BR-C5	8.08	2.10	1.90
1	C	18	BRU	BR-C5	7.93	2.10	1.90
2	D	110	BRU	BR-C5	7.91	2.10	1.90
2	D	109	BRU	BR-C5	7.82	2.09	1.90
2	D	112	BRU	BR-C5	7.71	2.09	1.90
2	D	108	BRU	BR-C5	7.66	2.09	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	107	BRU	BR-C5	7.61	2.09	1.90
2	D	121	BRU	C4-C5	3.89	1.46	1.39
1	C	18	BRU	C4-C5	3.72	1.46	1.39
2	D	109	BRU	C4-C5	3.50	1.45	1.39
2	D	121	BRU	P-OP1	3.15	1.50	1.46
2	D	110	BRU	C4-C5	3.11	1.45	1.39
1	C	18	BRU	P-OP1	2.97	1.50	1.46
2	D	110	BRU	P-OP1	2.93	1.50	1.46
1	C	19	BRU	C4-C5	2.93	1.44	1.39
2	D	108	BRU	C4-C5	2.83	1.44	1.39
2	D	107	BRU	P-OP1	2.40	1.49	1.46
2	D	107	BRU	C4-C5	2.39	1.43	1.39
2	D	112	BRU	P-OP1	2.15	1.49	1.46
1	C	19	BRU	P-OP1	2.14	1.49	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	109	BRU	C6-N1-C2	-6.26	120.63	122.41
2	D	109	BRU	C5-C6-N1	6.11	123.69	119.67
1	C	19	BRU	C5-C6-N1	5.74	123.45	119.67
2	D	107	BRU	C6-N1-C2	-5.71	120.78	122.41
2	D	110	BRU	C5-C6-N1	5.70	123.42	119.67
2	D	121	BRU	C5-C6-N1	5.67	123.40	119.67
2	D	107	BRU	C5-C6-N1	5.60	123.36	119.67
1	C	18	BRU	C5-C6-N1	5.57	123.34	119.67
2	D	108	BRU	C6-N1-C2	-5.52	120.84	122.41
2	D	108	BRU	C5-C6-N1	5.50	123.29	119.67
2	D	110	BRU	C6-N1-C2	-5.48	120.85	122.41
2	D	112	BRU	C5-C6-N1	5.46	123.27	119.67
2	D	112	BRU	C6-N1-C2	-4.31	121.18	122.41
1	C	19	BRU	C6-N1-C2	-3.13	121.52	122.41
1	C	18	BRU	C6-N1-C2	-3.03	121.54	122.41
2	D	121	BRU	C6-N1-C2	-3.03	121.55	122.41
2	D	107	BRU	BR-C5-C6	2.85	123.63	117.98
2	D	108	BRU	BR-C5-C6	2.85	123.63	117.98
1	C	18	BRU	BR-C5-C6	2.58	123.10	117.98
1	C	19	BRU	BR-C5-C6	2.55	123.03	117.98
2	D	109	BRU	BR-C5-C6	2.46	122.86	117.98
2	D	112	BRU	BR-C5-C6	2.42	122.77	117.98
2	D	121	BRU	BR-C5-C6	2.40	122.74	117.98
2	D	110	BRU	BR-C5-C6	2.39	122.72	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	108	BRU	C2'-C1'-N1	2.23	119.89	114.08
1	C	19	BRU	N3-C2-N1	-2.16	114.17	115.97
2	D	107	BRU	C2'-C1'-N1	2.12	119.61	114.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.