Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 03:34 PM EDT

PDB ID	:	1A31
Title	:	HUMAN RECONSTITUTED DNA TOPOISOMERASE I IN COVALENT COMPLEX WITH A 22 BASE PAIR DNA DUPLEX
Authors	:	Redinbo, M.R.; Stewart, L.; Kuhn, P.; Champoux, J.J.; Hol, W.G.J.
Deposited on	:	1998-01-27
Resolution	:	2.10 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:

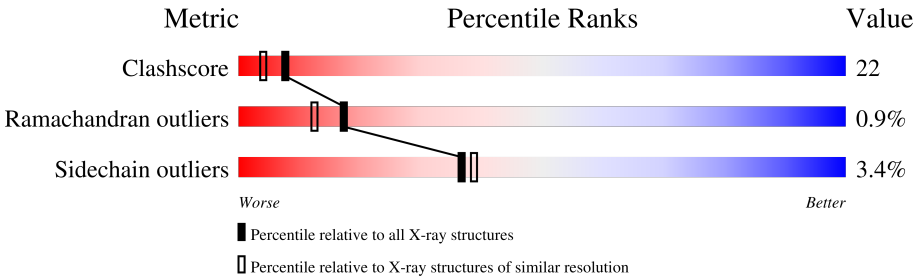
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	C	22	32% 41% 27%
2	D	22	45% 32% 23%
3	A	591	47% 28% . 23%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4991 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*5IUP*5IU*TP*GP*AP*AP*AP*AP*AP*5IUP*5IUP*5IUP*5IUP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	I	N	O	P			
1	C	22	447	213	6	84	124	20	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	I	N	O	P			
2	D	22	445	214	4	73	133	21	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
3	A	458	3690	2365	640	664	1	20	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	723	PTR	TYR	MODIFIED RESIDUE	UNP P11387

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	47	47	47	0	0
4	D	66	66	66	0	0
4	A	296	296	296	0	0

3 Residue-property plots (i)

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.

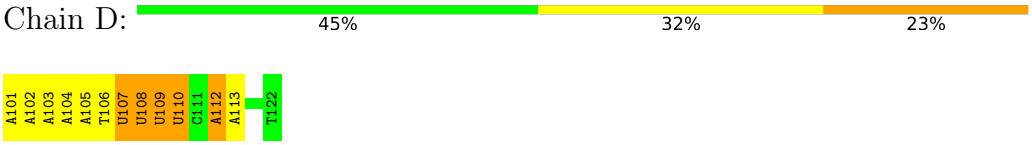
Note EDS was not executed.

• Molecule 1: DNA (5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*5IUP*5IU*TP*GP*AP*AP*AP*AP*AP*5IUP*5IUP*5IUP*5IUP*T)-3')

Chain C:

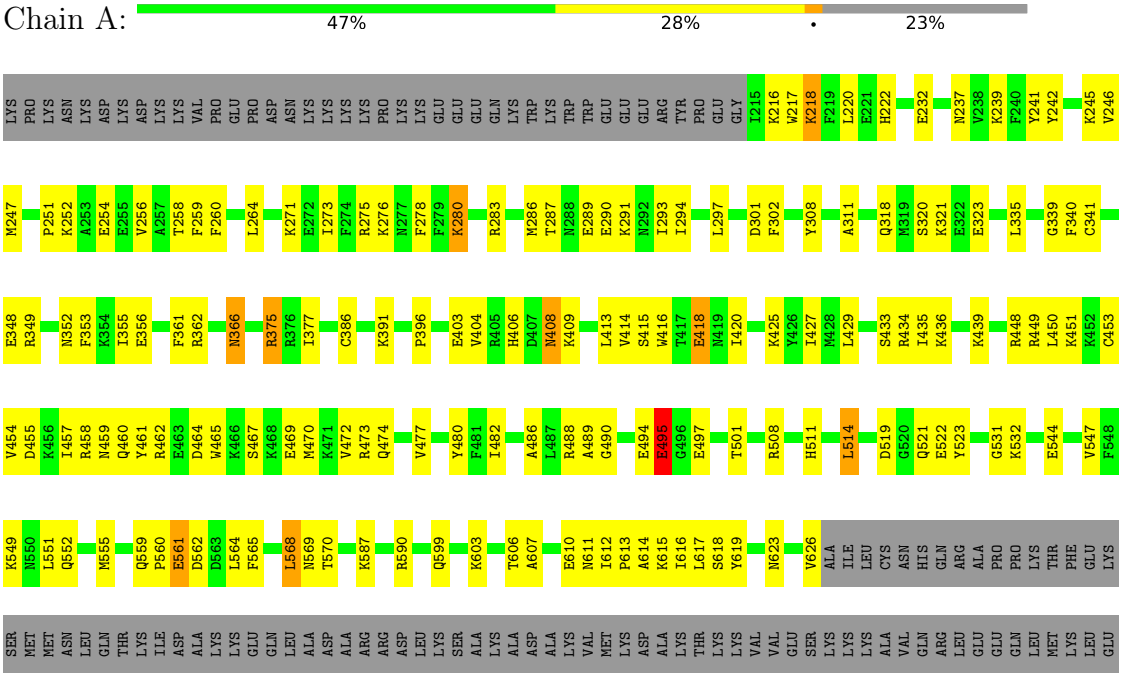
• Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*TP*5IUP*5IUP*5IUP*5IUP*CP*AP*AP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3')

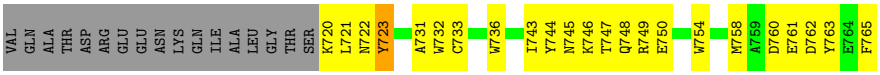
Chain D:



• Molecule 3: PROTEIN (TOPOISOMERASE I)

Chain A:




VAL
GLN
ALA
THR
ASP
ARG
GLU
GLU
ASN
LYS
GLN
ILE
ALA
LEU
GLY
THR
SER
K720
L721
N722
Y723
A731
W732
C733
W736
I743
Y744
N745
K746
T747
Q748
R749
E750
W754
M758
A759
D760
E761
D762
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	72.00Å 66.60Å 71.80Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	97.2 (20.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.247 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4991	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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: 5IU, PTR

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	0.96	0/370	0.91	0/565
2	D	0.92	0/408	0.92	0/625
3	A	0.64	0/3761	0.77	0/5077
All	All	0.70	0/4539	0.80	0/6267

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
2	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	13	DA	Sidechain
1	C	8	DC	Sidechain
2	D	112	DA	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	447	0	234	17	0
2	D	445	0	243	23	0
3	A	3690	0	3588	151	0
4	A	296	0	0	30	0
4	C	47	0	0	2	0
4	D	66	0	0	7	0
All	All	4991	0	4065	187	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 22.

All (187) 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)
1:C:1:DA:H2”	1:C:2:DA:H5’	1.13	1.12
2:D:101:DA:H2”	2:D:102:DA:H5’	1.15	1.10
1:C:1:DA:H2”	1:C:2:DA:C5’	1.87	1.05
2:D:107:5IU:H5”	4:D:1230:HOH:O	1.59	1.02
1:C:8:DC:H2’	1:C:9:5IU:I5	2.30	1.01
2:D:101:DA:H2”	2:D:102:DA:C5’	1.92	1.00
2:D:105:DA:H2”	2:D:106:DT:C5’	1.93	0.99
2:D:105:DA:H2”	2:D:106:DT:H5”	1.48	0.94
3:A:320:SER:HA	4:A:1374:HOH:O	1.71	0.91
2:D:103:DA:H2’	4:D:1120:HOH:O	1.73	0.88
3:A:494:GLU:HG2	3:A:497:GLU:HG3	1.60	0.83
3:A:375:ARG:HG2	3:A:375:ARG:HH11	1.45	0.80
3:A:460:GLN:HB2	4:A:1387:HOH:O	1.81	0.80
3:A:731:ALA:HB2	3:A:763:TYR:HB3	1.63	0.80
2:D:105:DA:C2’	2:D:106:DT:H5”	2.12	0.80
3:A:733:CYS:SG	3:A:743:ILE:HD12	2.21	0.79
3:A:450:LEU:O	3:A:454:VAL:HG23	1.83	0.79
3:A:610:GLU:CB	3:A:615:LYS:HG3	2.13	0.79
1:C:14:DA:H2”	1:C:15:DA:OP2	1.83	0.77
2:D:105:DA:H2”	2:D:106:DT:H5’	1.68	0.75
3:A:237:ASN:HA	4:A:1210:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:362:ARG:HD2	4:A:1233:HOH:O	1.87	0.74
3:A:408:ASN:HD21	3:A:409:LYS:HE3	1.52	0.74
1:C:9:5IU:OP1	3:A:439:LYS:HD2	1.86	0.74
3:A:614:ALA:O	3:A:617:LEU:HB2	1.87	0.74
1:C:19:5IU:H1'	1:C:20:5IU:H5"	1.70	0.73
3:A:403:GLU:HG2	3:A:404:VAL:N	2.02	0.73
3:A:568:LEU:HD22	3:A:569:ASN:N	2.05	0.72
2:D:101:DA:C2'	2:D:102:DA:H5'	2.07	0.72
3:A:488:ARG:NH1	3:A:590:ARG:HH12	1.89	0.71
3:A:568:LEU:HD22	3:A:569:ASN:H	1.55	0.71
3:A:264:LEU:HD11	3:A:302:PHE:HB2	1.74	0.70
2:D:106:DT:H2"	2:D:107:5IU:O5'	1.90	0.70
3:A:477:VAL:O	3:A:480:TYR:HB3	1.91	0.70
3:A:218:LYS:HE3	3:A:218:LYS:HA	1.74	0.70
3:A:289:GLU:HA	4:A:1332:HOH:O	1.92	0.69
2:D:101:DA:C2'	2:D:102:DA:C5'	2.70	0.68
3:A:320:SER:HB2	4:A:1289:HOH:O	1.93	0.67
2:D:104:DA:H1'	2:D:105:DA:H5"	1.77	0.66
3:A:271:LYS:O	3:A:275:ARG:HG3	1.95	0.66
3:A:453:CYS:O	3:A:457:ILE:HG13	1.97	0.65
2:D:101:DA:HO5'	2:D:101:DA:H8	1.45	0.65
3:A:746:LYS:O	3:A:750:GLU:HG2	1.96	0.65
3:A:587:LYS:HE3	4:A:1007:HOH:O	1.97	0.65
3:A:599:GLN:HE22	3:A:765:PHE:H	1.44	0.64
3:A:464:ASP:HB3	3:A:472:VAL:HG12	1.79	0.63
3:A:273:ILE:HG12	4:A:1239:HOH:O	1.99	0.63
1:C:1:DA:C2'	1:C:2:DA:C5'	2.73	0.62
3:A:745:ASN:O	3:A:749:ARG:HG3	2.00	0.62
3:A:427:ILE:HG12	4:A:1284:HOH:O	2.00	0.62
3:A:449:ARG:NH1	4:A:1162:HOH:O	2.31	0.62
3:A:408:ASN:ND2	3:A:409:LYS:HE3	2.15	0.61
3:A:514:LEU:HD23	3:A:552:GLN:HG2	1.83	0.61
3:A:429:LEU:HB3	3:A:433:SER:OG	2.01	0.61
3:A:619:TYR:O	3:A:623:ASN:HB2	2.01	0.61
3:A:467:SER:N	3:A:473:ARG:HE	1.98	0.61
3:A:732:TRP:HZ3	3:A:743:ILE:HD11	1.66	0.61
3:A:335:LEU:HD23	3:A:353:PHE:HE2	1.64	0.60
3:A:747:THR:O	3:A:750:GLU:HB2	2.02	0.60
3:A:239:LYS:HE2	4:A:1210:HOH:O	2.01	0.60
3:A:366:ASN:O	3:A:366:ASN:ND2	2.34	0.60
3:A:355:ILE:HG21	3:A:377:ILE:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:470:MET:O	3:A:474:GLN:N	2.34	0.60
3:A:551:LEU:O	3:A:555:MET:HG3	2.02	0.59
3:A:216:LYS:HB3	3:A:435:ILE:HD11	1.83	0.59
3:A:458:ARG:O	3:A:462:ARG:HB2	2.02	0.59
3:A:436:LYS:HD3	3:A:439:LYS:NZ	2.18	0.58
3:A:335:LEU:HD22	3:A:339:GLY:HA3	1.85	0.58
3:A:251:PRO:HG2	4:A:1047:HOH:O	2.03	0.57
3:A:320:SER:N	3:A:323:GLU:OE1	2.34	0.57
3:A:490:GLY:HA2	4:A:1218:HOH:O	2.04	0.57
3:A:283:ARG:HD3	4:A:1089:HOH:O	2.04	0.57
3:A:361:PHE:HB2	3:A:420:ILE:HD13	1.87	0.57
3:A:241:TYR:CE2	3:A:246:VAL:HG22	2.40	0.56
3:A:320:SER:OG	3:A:323:GLU:HG3	2.04	0.56
3:A:286:MET:HB3	3:A:290:GLU:HB2	1.87	0.56
3:A:391:LYS:HB2	3:A:391:LYS:HZ3	1.71	0.56
3:A:564:LEU:HD23	3:A:565:PHE:CE2	2.40	0.56
4:C:1385:HOH:O	3:A:723:PTR:HE2	2.05	0.56
3:A:611:ASN:OD1	3:A:614:ALA:HB3	2.06	0.55
1:C:8:DC:C2'	1:C:9:5IU:I5	3.18	0.55
3:A:607:ALA:HB3	4:A:1231:HOH:O	2.05	0.55
3:A:754:TRP:O	3:A:758:MET:HG2	2.06	0.55
1:C:19:5IU:H2"	1:C:20:5IU:O5'	2.08	0.54
3:A:287:THR:O	3:A:291:LYS:HG3	2.08	0.54
3:A:489:ALA:HB1	3:A:570:THR:HG22	1.89	0.54
3:A:469:GLU:HG2	4:A:1223:HOH:O	2.08	0.54
1:C:2:DA:H2"	1:C:3:DA:OP2	2.08	0.54
3:A:615:LYS:O	3:A:618:SER:HB2	2.08	0.53
3:A:340:PHE:HA	3:A:348:GLU:O	2.08	0.53
3:A:610:GLU:CB	3:A:615:LYS:HE3	2.39	0.52
3:A:760:ASP:C	3:A:762:ASP:H	2.14	0.52
2:D:112:DA:OP2	3:A:356:GLU:HG2	2.09	0.51
3:A:560:PRO:C	3:A:562:ASP:H	2.13	0.51
3:A:508:ARG:HB2	3:A:511:HIS:CE1	2.45	0.51
3:A:218:LYS:HA	3:A:218:LYS:CE	2.41	0.50
3:A:318:GLN:HG3	4:A:1238:HOH:O	2.11	0.50
3:A:462:ARG:NH2	3:A:544:GLU:OE2	2.44	0.50
3:A:462:ARG:HG2	3:A:465:TRP:CZ3	2.47	0.50
3:A:494:GLU:CG	3:A:497:GLU:HG3	2.36	0.50
3:A:501:THR:HB	3:A:531:GLY:O	2.11	0.50
3:A:522:GLU:O	3:A:523:TYR:HB2	2.12	0.50
1:C:15:DA:C2	2:D:109:5IU:N3	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1071:HOH:O	3:A:532:LYS:HE2	2.10	0.49
3:A:276:LYS:HG3	4:A:1205:HOH:O	2.12	0.49
3:A:242:TYR:CZ	3:A:294:ILE:HA	2.46	0.49
3:A:436:LYS:HD3	3:A:439:LYS:HZ2	1.77	0.49
1:C:21:5IU:C2'	1:C:22:DT:H72	2.42	0.49
3:A:260:PHE:HB2	3:A:278:PHE:CE1	2.48	0.49
3:A:375:ARG:HG2	3:A:375:ARG:NH1	2.15	0.49
3:A:220:LEU:O	3:A:386:CYS:HB2	2.13	0.49
3:A:418:GLU:HG3	4:A:1131:HOH:O	2.13	0.49
1:C:4:DA:N7	4:C:1353:HOH:O	2.35	0.49
1:C:9:5IU:OP2	3:A:436:LYS:HE3	2.13	0.48
3:A:335:LEU:HD23	3:A:353:PHE:CE2	2.48	0.48
3:A:427:ILE:CG1	4:A:1284:HOH:O	2.59	0.48
3:A:482:ILE:O	3:A:486:ALA:HA	2.13	0.48
3:A:720:LYS:C	3:A:722:ASN:H	2.17	0.48
2:D:101:DA:H8	2:D:101:DA:O5'	1.96	0.48
3:A:454:VAL:HG11	3:A:458:ARG:CZ	2.44	0.48
4:D:1344:HOH:O	3:A:362:ARG:HD3	2.13	0.48
3:A:519:ASP:C	3:A:521:GLN:H	2.17	0.47
2:D:104:DA:H2"	2:D:105:DA:OP2	2.14	0.47
3:A:415:SER:HA	3:A:425:LYS:O	2.14	0.47
3:A:448:ARG:O	3:A:451:LYS:HB3	2.15	0.47
2:D:106:DT:H5'	2:D:106:DT:H6	1.80	0.47
3:A:232:GLU:HB2	4:A:1132:HOH:O	2.15	0.47
3:A:494:GLU:HG2	3:A:497:GLU:CG	2.39	0.47
3:A:544:GLU:O	3:A:547:VAL:HB	2.15	0.47
3:A:606:THR:HG21	3:A:736:TRP:NE1	2.29	0.47
3:A:612:ILE:O	3:A:616:ILE:HG13	2.15	0.47
3:A:450:LEU:CD1	3:A:454:VAL:HG22	2.45	0.47
3:A:613:PRO:O	3:A:616:ILE:HB	2.15	0.47
3:A:386:CYS:O	3:A:406:HIS:HA	2.15	0.47
3:A:416:TRP:HZ3	4:A:1284:HOH:O	1.94	0.46
3:A:408:ASN:N	3:A:408:ASN:HD22	2.13	0.46
1:C:13:DA:H4'	1:C:14:DA:OP1	2.14	0.46
3:A:495:GLU:HG2	4:A:1084:HOH:O	2.15	0.46
3:A:275:ARG:HB3	3:A:297:LEU:CD2	2.45	0.46
3:A:352:ASN:O	3:A:427:ILE:HG23	2.16	0.46
3:A:222:HIS:HB3	3:A:341:CYS:HB2	1.96	0.46
3:A:246:VAL:HG12	3:A:247:MET:N	2.30	0.45
3:A:252:LYS:HE3	4:A:1119:HOH:O	2.16	0.45
3:A:760:ASP:C	3:A:762:ASP:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:403:GLU:HG2	3:A:404:VAL:H	1.79	0.45
3:A:414:VAL:HB	3:A:427:ILE:HB	1.99	0.44
2:D:113:DA:H2'	4:D:1008:HOH:O	2.17	0.44
3:A:320:SER:OG	3:A:323:GLU:CG	2.66	0.44
3:A:349:ARG:HB3	4:A:1228:HOH:O	2.16	0.44
2:D:107:5IU:C6	2:D:108:5IU:I5	3.36	0.44
3:A:559:GLN:O	3:A:562:ASP:HB2	2.17	0.44
3:A:732:TRP:CZ3	3:A:743:ILE:HD11	2.49	0.44
3:A:416:TRP:CZ3	4:A:1284:HOH:O	2.57	0.43
3:A:467:SER:H	3:A:473:ARG:HE	1.64	0.43
3:A:744:TYR:HD1	3:A:748:GLN:NE2	2.16	0.43
3:A:461:TYR:HE1	3:A:465:TRP:CZ2	2.35	0.43
3:A:760:ASP:O	3:A:762:ASP:N	2.52	0.43
2:D:101:DA:H1'	2:D:102:DA:H5"	1.99	0.43
3:A:217:TRP:CZ2	3:A:408:ASN:HA	2.54	0.43
3:A:321:LYS:N	4:A:1374:HOH:O	2.48	0.43
1:C:19:5IU:H1'	1:C:20:5IU:C5'	2.46	0.43
3:A:470:MET:O	3:A:474:GLN:HG3	2.18	0.43
3:A:568:LEU:CD2	3:A:569:ASN:H	2.28	0.43
3:A:320:SER:O	3:A:323:GLU:HB2	2.19	0.42
3:A:256:VAL:HA	3:A:259:PHE:CD2	2.54	0.42
3:A:454:VAL:O	3:A:458:ARG:HG3	2.19	0.42
2:D:110:5IU:H3'	4:D:1321:HOH:O	2.19	0.42
3:A:435:ILE:O	3:A:439:LYS:HE3	2.20	0.42
3:A:216:LYS:NZ	4:A:1222:HOH:O	2.47	0.41
3:A:220:LEU:HD11	3:A:413:LEU:HD22	2.02	0.41
3:A:549:LYS:O	3:A:552:GLN:N	2.52	0.41
3:A:733:CYS:SG	3:A:743:ILE:CD1	3.01	0.41
1:C:21:5IU:H2'	1:C:22:DT:H72	2.01	0.41
3:A:283:ARG:O	3:A:291:LYS:HE2	2.20	0.41
3:A:747:THR:HA	3:A:750:GLU:CG	2.50	0.41
3:A:511:HIS:HA	4:A:1094:HOH:O	2.19	0.41
2:D:106:DT:C1'	4:D:1230:HOH:O	2.68	0.41
3:A:247:MET:HE1	3:A:293:ILE:HG21	2.02	0.41
3:A:280:LYS:HB3	3:A:280:LYS:NZ	2.36	0.41
3:A:396:PRO:HD3	4:A:1032:HOH:O	2.19	0.41
3:A:744:TYR:CD1	3:A:748:GLN:NE2	2.89	0.41
3:A:254:GLU:O	3:A:258:THR:HG23	2.21	0.41
3:A:241:TYR:HB2	3:A:301:ASP:HB3	2.04	0.40
3:A:455:ASP:O	3:A:459:ASN:ND2	2.55	0.40
3:A:308:TYR:O	3:A:311:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:599:GLN:NE2	3:A:765:PHE:H	2.12	0.40
3:A:241:TYR:HA	3:A:245:LYS:O	2.22	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	453/591 (77%)	426 (94%)	23 (5%)	4 (1%)	17 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	561	GLU
3	A	721	LEU
3	A	495	GLU
3	A	761	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	381/534 (71%)	368 (97%)	13 (3%)	37 39

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	218	LYS
3	A	280	LYS
3	A	366	ASN
3	A	375	ARG
3	A	408	ASN
3	A	418	GLU
3	A	434	ARG
3	A	495	GLU
3	A	514	LEU
3	A	561	GLU
3	A	568	LEU
3	A	603	LYS
3	A	626	VAL

Sometimes 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	408	ASN
3	A	430	ASN
3	A	459	ASN
3	A	576	HIS
3	A	599	GLN
3	A	722	ASN
3	A	748	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

11 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	$\#\|Z\|>2$
2	5IU	D	107	2,1	18,21,22	1.21	1 (5%)	26,30,33	0.58	0
2	5IU	D	108	2,1	18,21,22	1.30	1 (5%)	26,30,33	0.58	0
1	5IU	C	21	2,1	18,21,22	0.98	1 (5%)	26,30,33	0.59	0
2	5IU	D	109	2,1	18,21,22	1.50	2 (11%)	26,30,33	0.70	0
1	5IU	C	20	2,1	18,21,22	1.05	1 (5%)	26,30,33	0.56	0
1	5IU	C	10	3,2,1	17,20,22	1.32	1 (5%)	22,28,33	1.02	1 (4%)
3	PTR	A	723	3,1	15,16,17	1.87	1 (6%)	19,22,24	1.17	2 (10%)
1	5IU	C	19	2,1	18,21,22	1.01	1 (5%)	26,30,33	0.58	0
2	5IU	D	110	2,1	18,21,22	1.31	1 (5%)	26,30,33	0.54	0
1	5IU	C	18	2,1	18,21,22	1.11	1 (5%)	26,30,33	0.58	0
1	5IU	C	9	2,1	18,21,22	1.37	1 (5%)	26,30,33	0.57	0

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
2	5IU	D	107	2,1	-	0/7/21/22	0/2/2/2
2	5IU	D	108	2,1	-	0/7/21/22	0/2/2/2
1	5IU	C	21	2,1	-	0/7/21/22	0/2/2/2
2	5IU	D	109	2,1	-	3/7/21/22	0/2/2/2
1	5IU	C	20	2,1	-	4/7/21/22	0/2/2/2
1	5IU	C	10	3,2,1	-	0/7/18/22	0/2/2/2
3	PTR	A	723	3,1	-	1/10/11/13	0/1/1/1
1	5IU	C	19	2,1	-	0/7/21/22	0/2/2/2
2	5IU	D	110	2,1	-	0/7/21/22	0/2/2/2
1	5IU	C	18	2,1	-	0/7/21/22	0/2/2/2
1	5IU	C	9	2,1	-	0/7/21/22	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	723	PTR	P-OH	-6.61	1.48	1.59
2	D	109	5IU	C5-I5	-5.40	1.92	2.08
1	C	9	5IU	C5-I5	-5.03	1.93	2.08
2	D	110	5IU	C5-I5	-4.84	1.93	2.08
2	D	108	5IU	C5-I5	-4.73	1.94	2.08
2	D	107	5IU	C5-I5	-4.46	1.94	2.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	10	5IU	C5-I5	-4.40	1.95	2.08
1	C	20	5IU	C5-I5	-4.24	1.95	2.08
1	C	18	5IU	C5-I5	-4.11	1.96	2.08
1	C	21	5IU	C5-I5	-3.82	1.96	2.08
1	C	19	5IU	C5-I5	-3.76	1.97	2.08
2	D	109	5IU	C4-C5	-2.05	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	723	PTR	OH-P-O1P	-2.53	99.77	109.31
3	A	723	PTR	O3P-P-O2P	2.36	116.65	107.64
1	C	10	5IU	O4'-C4'-C5'	-2.15	105.97	109.52

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	723	PTR	O-C-CA-CB
1	C	20	5IU	C2'-C1'-N1-C6
1	C	20	5IU	O4'-C1'-N1-C6
1	C	20	5IU	C2'-C1'-N1-C2
2	D	109	5IU	C2'-C1'-N1-C6
1	C	20	5IU	O4'-C1'-N1-C2
2	D	109	5IU	O4'-C1'-N1-C6
2	D	109	5IU	C2'-C1'-N1-C2

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	107	5IU	3	0
2	D	108	5IU	1	0
1	C	21	5IU	2	0
2	D	109	5IU	1	0
1	C	20	5IU	3	0
3	A	723	PTR	1	0
1	C	19	5IU	3	0
2	D	110	5IU	1	0
1	C	9	5IU	4	0

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.