



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:32 PM UTC

PDB ID : 1A31 / pdb_00001a31
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

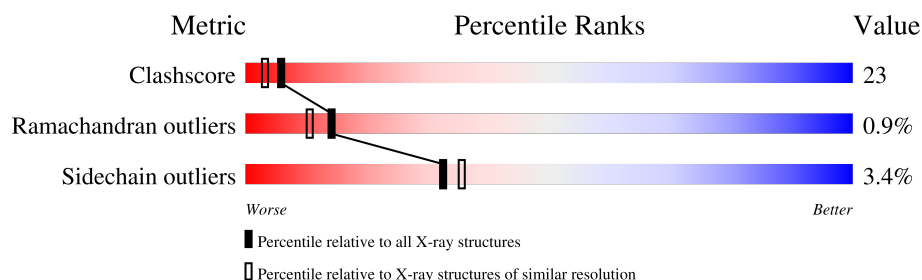
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 $\leq 5\%$

Note EDS was not executed.

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

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*AP*5IUP*5IUP*5IUP*5IUP*T)-3').

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

- 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*T)-3').

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

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

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

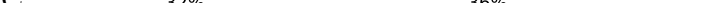
There is a discrepancy between the modelled and reference sequences:

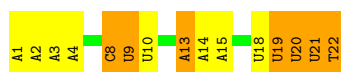
Chain	Residue	Modelled	Actual	Comment	Reference
A	723	PTR	TYR	modified residue	UNP P11387

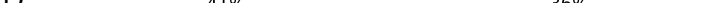
- Molecule 4 is water.

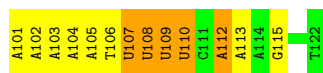
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	47	Total	O	0	0
			47	47		
4	D	66	Total	O	0	0
			66	66		
4	A	296	Total	O	0	0
			296	296		

Note EDS was not executed.

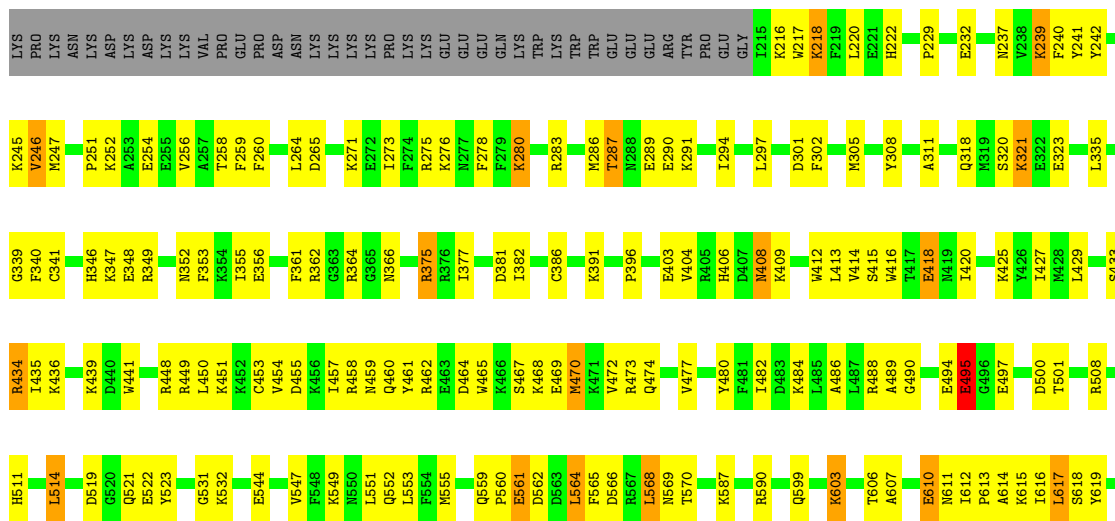
- Chain C:  32% 36% 32%



- Chain D:  41% 36% 23%



- Chain A: 45% 29% . 23%



A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000
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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	72.00 Å 66.60 Å 71.80 Å 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	0.52	0/370	0.93	1/565 (0.2%)
2	D	0.56	0/408	0.98	1/625 (0.2%)
3	A	0.80	2/3761 (0.1%)	1.10	19/5077 (0.4%)
All	All	0.77	2/4539 (0.0%)	1.08	21/6267 (0.3%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	229	PRO	C-O	-5.35	1.20	1.25
3	A	470	MET	SD-CE	5.09	1.92	1.79

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	468	LYS	N-CA-C	-8.24	104.23	112.97
3	A	382	ILE	N-CA-C	6.37	117.76	108.58
3	A	564	LEU	N-CA-C	-6.34	104.29	111.14
3	A	610	GLU	N-CA-C	6.30	119.79	110.46
3	A	246	VAL	N-CA-C	-6.27	103.21	110.05
3	A	434	ARG	N-CA-C	-6.05	104.76	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	115	DG	N9-C1'-C2'	-5.95	104.58	113.50
3	A	347	LYS	N-CA-C	-5.82	101.87	110.48
3	A	346	HIS	N-CA-C	5.79	119.11	110.14
3	A	622	ALA	N-CA-C	-5.77	105.07	111.36
3	A	617	LEU	N-CA-C	-5.75	104.93	111.14
1	C	22	DT	C2'-C3'-O3'	-5.37	103.44	111.50
3	A	500	ASP	N-CA-C	5.35	117.18	108.63
3	A	239	LYS	N-CA-C	5.31	118.24	109.85
3	A	287	THR	N-CA-C	-5.30	103.69	110.53
3	A	412	TRP	N-CA-C	5.21	118.60	110.32
3	A	484	LYS	N-CA-C	5.16	116.72	111.14
3	A	321	LYS	N-CA-C	-5.15	105.79	111.71
3	A	603	LYS	N-CA-C	-5.13	105.60	111.14
3	A	566	ASP	N-CA-C	5.12	117.53	111.33
3	A	265	ASP	N-CA-C	-5.10	106.84	113.16

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

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	161	0
4	A	296	0	0	31	0
4	C	47	0	0	2	0
4	D	66	0	0	7	0
All	All	4991	0	4065	197	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 23.

All (197) 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
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
2:D:101:DA:HO5'	2:D:101:DA:H8	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:A:470:MET:O	3:A:474:GLN:N	2.34	0.60
3:A:441:TRP:CZ2	3:A:758:MET:HE1	2.37	0.59
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:470:MET:HE2	3:A:553:LEU:HG	1.86	0.57
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:436:LYS:HD3	3:A:439:LYS:HZ2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:391:LYS:HB2	3:A:391:LYS:HZ3	1.71	0.56
3:A:560:PRO:C	3:A:562:ASP:H	2.13	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
3:A:760:ASP:C	3:A:762:ASP:H	2.14	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:720:LYS:C	3:A:722:ASN:H	2.17	0.53
3:A:519:ASP:C	3:A:521:GLN:H	2.17	0.52
3:A:610:GLU:CB	3:A:615:LYS:HE3	2.39	0.52
2:D:112:DA:OP2	3:A:356:GLU:HG2	2.09	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
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
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
3:A:760:ASP:C	3:A:762:ASP:N	2.69	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:240:PHE:HB2	3:A:305:MET:HE2	1.96	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:216:LYS:NZ	4:A:1222:HOH:O	2.47	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:247:MET:HE3	3:A:247:MET:HB2	1.77	0.45
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:450:LEU:C	3:A:454:VAL:HG23	2.42	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:560:PRO:C	3:A:562:ASP:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:375:ARG:HH21	3:A:381:ASP:CG	2.27	0.42
3:A:720:LYS:C	3:A:722:ASN:N	2.77	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
3:A:490:GLY:C	4:A:1218:HOH:O	2.61	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:611:ASN:O	3:A:612:ILE:C	2.63	0.42
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:280:LYS:HB3	3:A:280:LYS:NZ	2.36	0.41
3:A:467:SER:C	3:A:469:GLU:H	2.28	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
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

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	453/591 (77%)	426 (94%)	23 (5%)	4 (1%)	14	10

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

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%)	32	35

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	364	ARG
3	A	375	ARG
3	A	408	ASN
3	A	418	GLU
3	A	434	ARG

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Mol	Chain	Res	Type
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	459	ASN
3	A	576	HIS
3	A	599	GLN
3	A	601	GLN
3	A	722	ASN
3	A	748	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
3	PTR	A	723	1,3	15,16,17	1.70	1 (6%)	17,22,24	1.26	2 (11%)
1	5IU	C	18	1,2	18,21,22	1.14	1 (5%)	25,30,33	0.59	0
2	5IU	D	108	1,2	18,21,22	1.36	1 (5%)	25,30,33	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5IU	C	21	1,2	18,21,22	1.03	1 (5%)	25,30,33	0.60	0
1	5IU	C	9	1,2	18,21,22	1.43	1 (5%)	25,30,33	0.59	0
2	5IU	D	107	1,2	18,21,22	1.26	1 (5%)	25,30,33	0.59	0
1	5IU	C	10	1,2,3	17,20,22	1.38	1 (5%)	22,28,33	1.00	0
2	5IU	D	110	1,2	18,21,22	1.37	1 (5%)	25,30,33	0.56	0
2	5IU	D	109	1,2	18,21,22	1.56	2 (11%)	25,30,33	0.72	0
1	5IU	C	20	1,2	18,21,22	1.10	1 (5%)	25,30,33	0.57	0
1	5IU	C	19	1,2	18,21,22	1.04	1 (5%)	25,30,33	0.59	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
3	PTR	A	723	1,3	-	1/10/11/13	0/1/1/1
1	5IU	C	18	1,2	-	0/7/21/22	0/2/2/2
2	5IU	D	108	1,2	-	0/7/21/22	0/2/2/2
1	5IU	C	21	1,2	-	0/7/21/22	0/2/2/2
1	5IU	C	9	1,2	-	0/7/21/22	0/2/2/2
2	5IU	D	107	1,2	-	0/7/21/22	0/2/2/2
1	5IU	C	10	1,2,3	-	0/7/18/22	0/2/2/2
2	5IU	D	110	1,2	-	0/7/21/22	0/2/2/2
2	5IU	D	109	1,2	-	3/7/21/22	0/2/2/2
1	5IU	C	20	1,2	-	4/7/21/22	0/2/2/2
1	5IU	C	19	1,2	-	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	-5.81	1.48	1.59
2	D	109	5IU	C5-I5	-5.72	1.92	2.08
1	C	9	5IU	C5-I5	-5.33	1.93	2.08
2	D	110	5IU	C5-I5	-5.13	1.93	2.08
2	D	108	5IU	C5-I5	-5.01	1.94	2.08
2	D	107	5IU	C5-I5	-4.73	1.94	2.08
1	C	10	5IU	C5-I5	-4.67	1.95	2.08
1	C	20	5IU	C5-I5	-4.49	1.95	2.08
1	C	18	5IU	C5-I5	-4.36	1.96	2.08
1	C	21	5IU	C5-I5	-4.05	1.96	2.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	19	5IU	C5-I5	-3.99	1.97	2.08
2	D	109	5IU	C4-C5	-2.07	1.41	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	723	PTR	OH-P-O1P	-2.91	99.77	109.48
3	A	723	PTR	O3P-P-O2P	2.36	116.65	107.80

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	C2'-C1'-N1-C2
2	D	109	5IU	O4'-C1'-N1-C6

There are no ring outliers.

9 monomers are involved in 15 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides 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.