



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:29 PM UTC

PDB ID : 3PX7 / pdb_00003px7
Title : Crystal Structure of covalent complex of topoisomerase 1A with substrate
Authors : Zhang, Z.; Tse-dinh, Y.C.; Cheng, B.
Deposited on : 2010-12-09
Resolution : 2.30 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

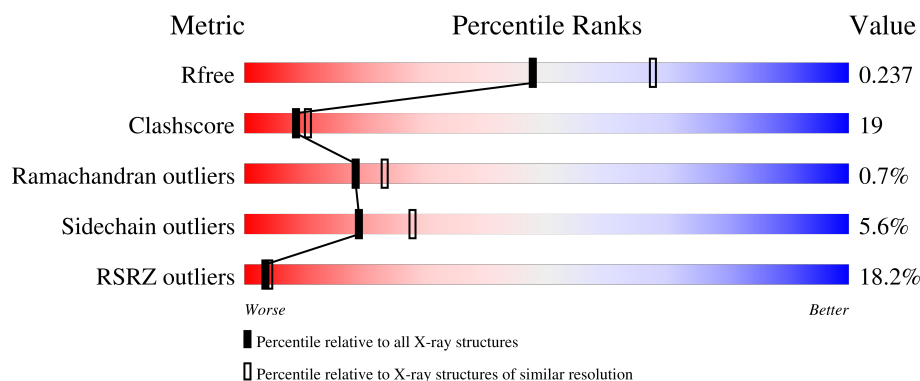
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	17% 62% 27% • 7%
2	B	5	40% 20% 20% 60%
3	C	8	12% 62% 25% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PTR	A	319	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4726 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 protein called DNA topoisomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	P	S	0	0	0
			4407	2772	786	831	1	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ASN	ASP	engineered mutation	UNP C9QXS7

- Molecule 2 is a DNA chain called DNA 5'-D(*TP*TP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	P	0	0	0
			36	20	4	11	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	P	0	0	0
			140	68	25	41	6			

- Molecule 4 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Hg	0	0
			1	1		
4	B	1	Total	Hg	0	0
			1	1		
4	C	1	Total	Hg	0	0
			1	1		

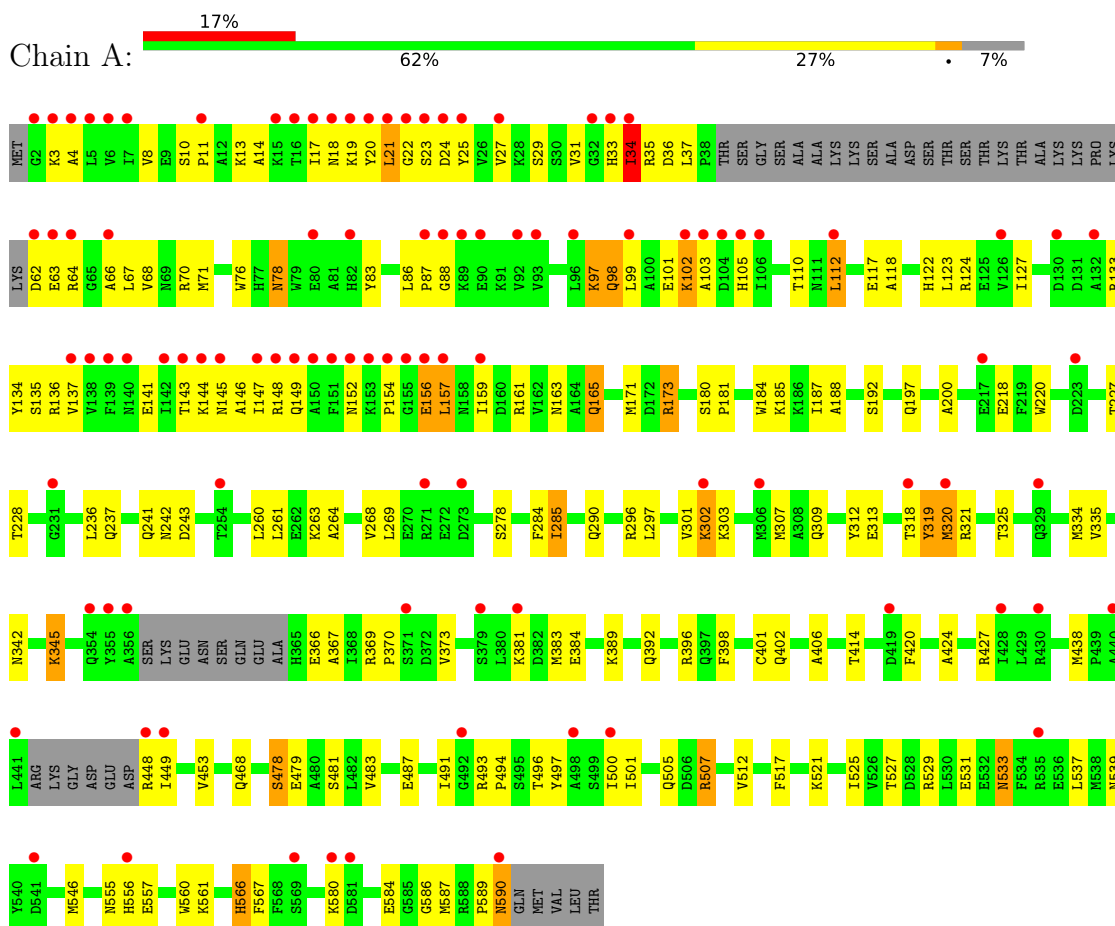
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	133	Total 133	O 133	0	0
5	C	7	Total 7	O 7	0	0

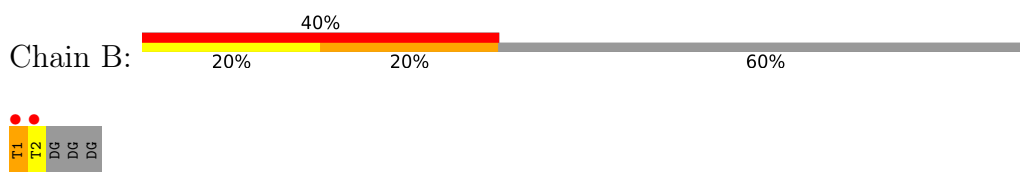
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

• Molecule 1: DNA topoisomerase

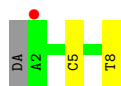


• Molecule 2: DNA 5'-D(*TP*TP*GP*GP*G)-3'



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.60Å 91.76Å 141.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.30 77.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (500.00-2.30) 99.0 (77.06-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.269 0.237 , 0.237	Depositor DCC
R_{free} test set	1811 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG, 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	A	0.43	0/4475	0.86	10/6043 (0.2%)
2	B	0.14	0/39	1.02	1/59 (1.7%)
3	C	0.24	0/156	0.75	0/239
All	All	0.42	0/4670	0.86	11/6341 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	PHE	N-CA-C	6.53	119.15	110.53
2	B	1	DT	P-O3'-C3'	6.44	129.86	120.20
1	A	560	TRP	N-CA-C	6.33	117.84	111.07
1	A	187	ILE	N-CA-C	6.30	117.41	111.48
1	A	478	SER	N-CA-C	-6.05	100.55	109.81
1	A	285	ILE	N-CA-C	-5.97	100.08	108.80
1	A	533	ASN	N-CA-C	5.46	120.10	113.38
1	A	342	ASN	N-CA-C	5.22	119.80	113.38
1	A	200	ALA	N-CA-C	-5.17	105.54	111.07
1	A	589	PRO	N-CA-C	-5.15	103.75	111.57
1	A	491	ILE	N-CA-C	5.13	115.80	110.82

There are no chirality outliers.

There are no planarity outliers.

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	A	4407	0	4378	170	0
2	B	36	0	23	5	0
3	C	140	0	80	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	133	0	0	2	0
5	C	7	0	0	0	0
All	All	4726	0	4481	171	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 19.

All (171) 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:A:320:MET:HE3	1:A:320:MET:H	1.16	1.10
1:A:118:ALA:HB2	1:A:165:GLN:HG2	1.44	1.00
1:A:320:MET:HE3	1:A:320:MET:N	1.79	0.96
1:A:21:LEU:HD21	1:A:25:TYR:HB2	1.53	0.91
1:A:320:MET:H	1:A:320:MET:CE	1.84	0.90
1:A:263:LYS:HD2	1:A:263:LYS:C	1.97	0.90
1:A:302:LYS:H	1:A:302:LYS:HE2	1.35	0.89
1:A:521:LYS:HE3	1:A:525:ILE:HD11	1.57	0.86
1:A:260:LEU:O	1:A:263:LYS:HE3	1.78	0.83
1:A:33:HIS:O	1:A:34:ILE:HG12	1.79	0.82
1:A:112:LEU:H	1:A:112:LEU:HD23	1.43	0.81
1:A:263:LYS:HD2	1:A:264:ALA:N	1.95	0.81
1:A:319:PTR:HA	1:A:320:MET:HE3	1.62	0.80
1:A:478:SER:H	1:A:481:SER:HB3	1.48	0.77
1:A:312:TYR:CG	1:A:320:MET:HE2	2.21	0.76
1:A:309:GLN:HE22	1:A:321:ARG:NH2	1.85	0.74
1:A:302:LYS:H	1:A:302:LYS:CE	2.01	0.74
1:A:171:MET:HE2	1:A:546:MET:HE2	1.69	0.74
1:A:449:ILE:HG13	1:A:449:ILE:O	1.86	0.74
1:A:319:PTR:O1P	1:A:321:ARG:HD2	1.90	0.70
1:A:319:PTR:P	2:B:1:DT:C5'	2.79	0.70
1:A:334:MET:SD	1:A:373:VAL:HG23	2.30	0.70
1:A:118:ALA:CB	1:A:165:GLN:HG2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:HB3	1:A:76:TRP:CD2	2.29	0.68
1:A:373:VAL:HG22	1:A:398:PHE:HE2	1.59	0.67
1:A:366:GLU:HG2	1:A:367:ALA:H	1.59	0.67
1:A:147:ILE:HD12	1:A:148:ARG:N	2.10	0.67
1:A:319:PTR:O3P	3:C:8:DT:H2''	1.97	0.65
1:A:67:LEU:HD13	1:A:71:MET:HE2	1.79	0.65
1:A:302:LYS:HE3	1:A:479:GLU:OE1	1.97	0.64
1:A:37:LEU:CD1	1:A:173:ARG:HG3	2.27	0.64
1:A:124:ARG:HE	1:A:157:LEU:HD21	1.63	0.64
1:A:35:ARG:NH1	1:A:83:TYR:HB2	2.14	0.63
1:A:309:GLN:HE22	1:A:321:ARG:HH22	1.46	0.63
1:A:319:PTR:HA	1:A:320:MET:CE	2.29	0.63
1:A:236:LEU:HD23	1:A:424:ALA:HB2	1.81	0.62
1:A:19:LYS:C	1:A:21:LEU:H	2.07	0.62
1:A:319:PTR:CA	1:A:320:MET:HE3	2.27	0.62
1:A:66:ALA:O	1:A:70:ARG:HG2	2.01	0.61
1:A:345:LYS:HZ2	1:A:345:LYS:HB3	1.65	0.61
1:A:483:VAL:HG23	1:A:501:ILE:HD11	1.82	0.60
1:A:97:LYS:NZ	1:A:127:ILE:HA	2.16	0.60
1:A:319:PTR:C	1:A:320:MET:HE3	2.30	0.60
1:A:278:SER:HB3	1:A:406:ALA:HB3	1.82	0.60
1:A:21:LEU:HD23	1:A:22:GLY:O	2.04	0.58
1:A:112:LEU:H	1:A:112:LEU:CD2	2.14	0.58
1:A:269:LEU:HD12	1:A:414:THR:HG22	1.85	0.58
1:A:156:GLU:N	1:A:156:GLU:OE1	2.36	0.57
1:A:144:LYS:HA	1:A:147:ILE:HG13	1.86	0.57
1:A:496:THR:HG22	1:A:500:ILE:HG12	1.87	0.57
1:A:23:SER:O	1:A:24:ASP:HB3	2.03	0.57
1:A:67:LEU:CD1	1:A:71:MET:HE2	2.34	0.57
1:A:11:PRO:HD2	2:B:2:DT:OP1	2.05	0.57
1:A:313:GLU:OE1	2:B:2:DT:H5'	2.05	0.56
1:A:147:ILE:HD12	1:A:148:ARG:HG3	1.89	0.55
1:A:18:ASN:HA	1:A:21:LEU:HD22	1.89	0.55
1:A:263:LYS:C	1:A:263:LYS:CD	2.76	0.55
1:A:161:ARG:HG3	1:A:161:ARG:HH11	1.72	0.55
1:A:143:THR:HG22	1:A:145:ASN:H	1.72	0.54
1:A:102:LYS:HG2	1:A:102:LYS:O	2.08	0.54
1:A:533:ASN:HD21	1:A:587:MET:HA	1.73	0.54
1:A:285:ILE:HG23	1:A:325:THR:HG22	1.90	0.54
1:A:34:ILE:HD13	1:A:123:LEU:HD23	1.90	0.53
1:A:555:ASN:O	1:A:557:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:O	1:A:263:LYS:CE	2.54	0.53
1:A:36:ASP:CG	1:A:37:LEU:H	2.16	0.53
1:A:290:GLN:CD	1:A:301:VAL:HG13	2.33	0.53
1:A:527:THR:O	1:A:531:GLU:HG3	2.09	0.53
1:A:124:ARG:HG2	1:A:124:ARG:HH11	1.74	0.52
1:A:144:LYS:HA	1:A:147:ILE:CG1	2.40	0.52
1:A:37:LEU:HD12	1:A:173:ARG:HG3	1.92	0.52
1:A:149:GLN:HA	1:A:152:ASN:OD1	2.09	0.52
1:A:3:LYS:HD3	1:A:102:LYS:HE2	1.90	0.51
1:A:319:PTR:OH	2:B:1:DT:H3'	2.11	0.51
1:A:171:MET:CE	1:A:546:MET:HE2	2.37	0.51
1:A:302:LYS:H	1:A:302:LYS:CD	2.23	0.51
1:A:35:ARG:HG2	1:A:83:TYR:HB3	1.93	0.51
1:A:366:GLU:HG2	1:A:367:ALA:N	2.26	0.51
1:A:13:LYS:O	1:A:17:ILE:HG12	2.11	0.50
1:A:296:ARG:O	1:A:297:LEU:HD23	2.11	0.50
1:A:171:MET:HE2	1:A:546:MET:CE	2.41	0.50
1:A:260:LEU:C	1:A:263:LYS:HE3	2.37	0.50
1:A:133:ARG:O	1:A:133:ARG:HG2	2.11	0.50
1:A:184:TRP:HA	1:A:188:ALA:O	2.12	0.49
1:A:78:ASN:ND2	1:A:561:LYS:HD3	2.27	0.49
1:A:180:SER:HB2	1:A:181:PRO:HD3	1.95	0.49
1:A:8:VAL:O	1:A:29:SER:HA	2.13	0.48
1:A:97:LYS:NZ	1:A:127:ILE:HG12	2.28	0.48
1:A:112:LEU:HD23	1:A:112:LEU:N	2.22	0.48
1:A:23:SER:C	1:A:25:TYR:H	2.20	0.48
1:A:521:LYS:O	1:A:525:ILE:HD13	2.13	0.48
1:A:101:GLU:C	1:A:103:ALA:H	2.21	0.48
1:A:242:ASN:O	1:A:243:ASP:HB2	2.12	0.48
1:A:86:LEU:C	1:A:88:GLY:H	2.20	0.48
1:A:302:LYS:HD2	1:A:303:LYS:H	1.79	0.48
1:A:335:VAL:HG11	1:A:402:GLN:HG3	1.96	0.48
1:A:392:GLN:CD	1:A:396:ARG:NH1	2.72	0.48
1:A:580:LYS:O	1:A:586:GLY:HA3	2.14	0.48
1:A:590:ASN:O	1:A:590:ASN:ND2	2.47	0.48
1:A:149:GLN:HA	1:A:152:ASN:CG	2.38	0.47
1:A:505:GLN:NE2	1:A:512:VAL:HG23	2.29	0.47
1:A:525:ILE:O	1:A:529:ARG:HG2	2.13	0.47
1:A:105:HIS:NE2	1:A:135:SER:HB2	2.30	0.47
1:A:3:LYS:CD	1:A:102:LYS:HE2	2.44	0.47
1:A:147:ILE:CD1	1:A:148:ARG:HG3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:HD12	1:A:147:ILE:C	2.39	0.47
1:A:302:LYS:CD	1:A:302:LYS:N	2.78	0.47
1:A:507:ARG:NH2	3:C:5:DC:OP1	2.41	0.47
1:A:218:GLU:OE2	1:A:468:GLN:NE2	2.44	0.47
1:A:117:GLU:HG2	1:A:161:ARG:HB2	1.97	0.47
1:A:312:TYR:CD2	1:A:320:MET:HE2	2.50	0.47
1:A:62:ASP:OD1	1:A:63:GLU:N	2.48	0.46
1:A:384:GLU:HG3	5:A:659:HOH:O	2.13	0.46
1:A:507:ARG:HB2	1:A:507:ARG:NH1	2.31	0.46
1:A:192:SER:OG	1:A:197:GLN:NE2	2.49	0.46
1:A:64:ARG:O	1:A:68:VAL:HG23	2.16	0.46
1:A:268:VAL:HG21	1:A:453:VAL:CG1	2.46	0.46
1:A:31:VAL:HG12	1:A:31:VAL:O	2.15	0.46
1:A:105:HIS:CE1	1:A:135:SER:HB2	2.51	0.45
1:A:227:THR:HG22	1:A:228:THR:O	2.16	0.45
1:A:318:THR:O	1:A:319:PTR:C	2.64	0.45
1:A:369:ARG:HB2	1:A:370:PRO:HD2	1.98	0.45
1:A:4:ALA:HB3	1:A:25:TYR:CD2	2.51	0.45
1:A:124:ARG:HG2	1:A:124:ARG:NH1	2.32	0.45
1:A:220:TRP:CH2	1:A:468:GLN:HB2	2.52	0.45
1:A:97:LYS:HZ1	1:A:127:ILE:HG12	1.81	0.45
1:A:14:ALA:HB1	1:A:27:VAL:HG12	1.97	0.45
1:A:19:LYS:C	1:A:21:LEU:N	2.74	0.45
1:A:479:GLU:HB3	1:A:501:ILE:HD13	1.97	0.45
1:A:19:LYS:O	1:A:21:LEU:N	2.48	0.45
2:B:1:DT:C7	2:B:2:DT:H73	2.47	0.44
1:A:18:ASN:O	1:A:22:GLY:N	2.49	0.44
1:A:97:LYS:NZ	1:A:97:LYS:HA	2.33	0.44
1:A:124:ARG:HG3	1:A:134:TYR:CE2	2.53	0.44
1:A:161:ARG:HG3	1:A:161:ARG:NH1	2.32	0.44
1:A:35:ARG:NE	1:A:122:HIS:HD2	2.15	0.43
1:A:496:THR:O	1:A:500:ILE:HG12	2.18	0.43
1:A:159:ILE:HG12	1:A:163:ASN:ND2	2.32	0.43
1:A:302:LYS:HD2	1:A:302:LYS:N	2.33	0.43
1:A:307:MET:HA	1:A:307:MET:HE2	2.00	0.43
1:A:392:GLN:CG	1:A:396:ARG:NH1	2.81	0.43
1:A:261:LEU:HD21	1:A:420:PHE:CG	2.53	0.43
1:A:580:LYS:HE3	1:A:584:GLU:OE1	2.18	0.43
1:A:185:LYS:HE3	1:A:185:LYS:HB2	1.83	0.43
1:A:320:MET:N	1:A:320:MET:CE	2.58	0.43
1:A:427:ARG:O	1:A:448:ARG:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ASN:ND2	1:A:587:MET:HA	2.34	0.43
1:A:11:PRO:HG3	1:A:31:VAL:HG22	2.00	0.42
1:A:479:GLU:HA	1:A:517:PHE:HE1	1.84	0.42
1:A:590:ASN:N	1:A:590:ASN:HD22	2.17	0.42
1:A:10:SER:HA	1:A:11:PRO:HD3	1.94	0.42
1:A:268:VAL:HG21	1:A:453:VAL:HG11	2.01	0.42
1:A:494:PRO:HA	1:A:497:TYR:CE2	2.55	0.42
1:A:117:GLU:OE1	1:A:136:ARG:NH1	2.53	0.42
1:A:396:ARG:HB3	1:A:438:MET:HG3	2.01	0.42
1:A:566:HIS:ND1	1:A:567:PHE:N	2.67	0.42
1:A:241:GLN:HG2	1:A:242:ASN:ND2	2.35	0.42
1:A:110:THR:O	1:A:136:ARG:NH2	2.53	0.41
1:A:145:ASN:O	1:A:145:ASN:ND2	2.53	0.41
1:A:86:LEU:O	1:A:88:GLY:N	2.54	0.41
1:A:312:TYR:CB	1:A:320:MET:HE2	2.50	0.41
1:A:33:HIS:C	1:A:35:ARG:H	2.28	0.41
1:A:137:VAL:HG12	1:A:154:PRO:HB3	2.01	0.41
1:A:319:PTR:O2P	1:A:319:PTR:HE2	2.20	0.41
1:A:98:GLN:HG3	1:A:99:LEU:N	2.35	0.41
1:A:37:LEU:HD13	1:A:173:ARG:HG3	2.03	0.41
1:A:566:HIS:HE1	5:A:666:HOH:O	2.03	0.41
1:A:33:HIS:C	1:A:34:ILE:HG23	2.46	0.40
1:A:141:GLU:H	1:A:146:ALA:HB1	1.86	0.40
1:A:78:ASN:HD22	1:A:78:ASN:HA	1.61	0.40
1:A:521:LYS:HE3	1:A:525:ILE:CD1	2.41	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	
1	A	543/595 (91%)	517 (95%)	22 (4%)	4 (1%)	18	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	TYR
1	A	34	ILE
1	A	87	PRO
1	A	102	LYS

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	
1	A	467/503 (93%)	441 (94%)	26 (6%)	19	28

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	34	ILE
1	A	78	ASN
1	A	97	LYS
1	A	98	GLN
1	A	112	LEU
1	A	156	GLU
1	A	157	LEU
1	A	165	GLN
1	A	173	ARG
1	A	237	GLN
1	A	302	LYS
1	A	320	MET
1	A	345	LYS
1	A	381	LYS
1	A	383	MET
1	A	389	LYS
1	A	401	CYS
1	A	487	GLU
1	A	493	ARG
1	A	507	ARG

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Mol	Chain	Res	Type
1	A	537	LEU
1	A	539	ASN
1	A	556	HIS
1	A	566	HIS
1	A	590	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	78	ASN
1	A	111	ASN
1	A	122	HIS
1	A	140	ASN
1	A	145	ASN
1	A	152	ASN
1	A	163	ASN
1	A	165	GLN
1	A	166	GLN
1	A	197	GLN
1	A	241	GLN
1	A	242	ASN
1	A	253	GLN
1	A	309	GLN
1	A	353	ASN
1	A	469	HIS
1	A	505	GLN
1	A	514	ASN
1	A	533	ASN
1	A	539	ASN
1	A	548	ASN
1	A	590	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PTR	A	319	2,1	15,16,17	2.02	1 (6%)	17,22,24	0.61	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
1	PTR	A	319	2,1	-	2/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	PTR	OH-CZ	-7.63	1.23	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	319	PTR	N-CA-CB-CG
1	A	319	PTR	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	319	PTR	10	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	551/595 (92%)	1.01	99 (17%) 3 4	23, 45, 93, 106	0
2	B	2/5 (40%)	5.27	2 (100%) 0 0	78, 78, 78, 79	0
3	C	7/8 (87%)	0.86	1 (14%) 6 7	37, 40, 79, 100	0
All	All	560/608 (92%)	1.03	102 (18%) 3 4	23, 45, 93, 106	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ILE	6.4
2	B	1	DT	5.8
1	A	21	LEU	5.1
1	A	2	GLY	4.9
2	B	2	DT	4.8
1	A	4	ALA	4.7
1	A	62	ASP	4.7
1	A	441	LEU	4.7
1	A	33	HIS	4.6
1	A	140	ASN	4.3
1	A	63	GLU	4.2
1	A	354	GLN	4.0
1	A	147	ILE	4.0
1	A	356	ALA	4.0
1	A	556	HIS	3.9
3	C	2	DA	3.8
1	A	143	THR	3.8
1	A	440	ALA	3.8
1	A	306	MET	3.8
1	A	145	ASN	3.8
1	A	5	LEU	3.7
1	A	157	LEU	3.7
1	A	154	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	64	ARG	3.6
1	A	23	SER	3.6
1	A	96	LEU	3.5
1	A	152	ASN	3.5
1	A	22	GLY	3.5
1	A	99	LEU	3.5
1	A	32	GLY	3.5
1	A	428	ILE	3.4
1	A	87	PRO	3.3
1	A	15	LYS	3.3
1	A	20	TYR	3.2
1	A	3	LYS	3.1
1	A	449	ILE	3.0
1	A	151	PHE	3.0
1	A	132	ALA	3.0
1	A	150	ALA	3.0
1	A	19	LYS	3.0
1	A	302	LYS	3.0
1	A	80	GLU	3.0
1	A	112	LEU	2.9
1	A	24	ASP	2.9
1	A	66	ALA	2.9
1	A	144	LYS	2.9
1	A	25	TYR	2.9
1	A	27	VAL	2.9
1	A	104	ASP	2.9
1	A	355	TYR	2.8
1	A	137	VAL	2.8
1	A	103	ALA	2.8
1	A	126	VAL	2.8
1	A	159	ILE	2.7
1	A	88	GLY	2.7
1	A	155	GLY	2.7
1	A	82	HIS	2.7
1	A	581	ASP	2.7
1	A	329	GLN	2.6
1	A	7	ILE	2.6
1	A	102	LYS	2.6
1	A	318	THR	2.6
1	A	106	ILE	2.6
1	A	153	LYS	2.6
1	A	541	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	34	ILE	2.6
1	A	139	PHE	2.5
1	A	92	VAL	2.5
1	A	148	ARG	2.5
1	A	6	VAL	2.5
1	A	217	GLU	2.5
1	A	535	ARG	2.5
1	A	492	GLY	2.4
1	A	381	LYS	2.4
1	A	569	SER	2.4
1	A	590	ASN	2.3
1	A	231	GLY	2.3
1	A	105	HIS	2.3
1	A	90	GLU	2.3
1	A	254	THR	2.3
1	A	17	ILE	2.3
1	A	580	LYS	2.3
1	A	130	ASP	2.3
1	A	273	ASP	2.3
1	A	16	THR	2.3
1	A	93	VAL	2.2
1	A	138	VAL	2.2
1	A	18	ASN	2.2
1	A	500	ILE	2.2
1	A	419	ASP	2.2
1	A	149	GLN	2.2
1	A	271	ARG	2.2
1	A	448	ARG	2.2
1	A	223	ASP	2.2
1	A	379	SER	2.1
1	A	371	SER	2.1
1	A	89	LYS	2.1
1	A	430	ARG	2.1
1	A	320	MET	2.0
1	A	156	GLU	2.0
1	A	498	ALA	2.0
1	A	11	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PTR	A	319	16/17	0.79	0.19	42,49,52,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HG	B	6	1/1	0.94	0.13	52,52,52,52	1
4	HG	A	596	1/1	0.98	0.11	34,34,34,34	1
4	HG	C	9	1/1	0.98	0.23	51,51,51,51	1

6.5 Other polymers [i](#)

There are no such residues in this entry.