



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:30 PM UTC

PDB ID : 1X9S / pdb_00001x9s
Title : T7 DNA polymerase in complex with a primer/template DNA containing a disordered N-2 aminofluorene on the template, crystallized with dideoxy-CTP as the incoming nucleotide.
Authors : Dutta, S.; Li, Y.; Johnson, D.; Dzantiev, L.; Richardson, C.C.; Romano, L.J.; Ellenberger, T.
Deposited on : 2004-08-24
Resolution : 2.70 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

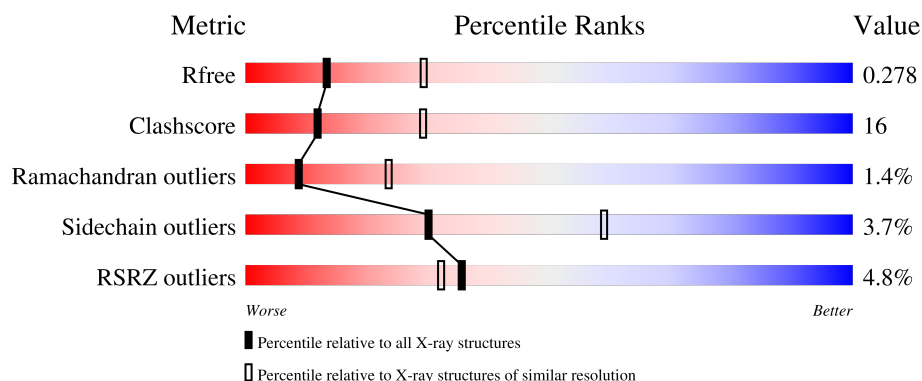
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	P	22	9% 14% 27% 5% 5% 50%
2	T	26	4% 23% 15% 58%
3	A	698	5% 65% 29% • •
4	B	108	2% 63% 31% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6462 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 5'-D(*GP*GP*AP*GP*AP*GP*TP*GP*AP*TP*T*GP*GP*TP*AP*GP*TP*GP*TP*GP*AP*(2DT))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	11	Total	C	N	O	P	0	0	0
			228	110	43	65	10			

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*(AFG)P*AP*TP*CP*AP*CP*AP*C*P*TP*AP*CP*CP*AP*AP*TP*CP*AP*CP*TP*CP*TP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	11	Total	C	N	O	P	0	0	0
			219	105	39	64	11			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	673	Total	C	N	O	S	0	0	0
			5189	3313	887	965	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P00581
A	?	-	ARG	deletion	UNP P00581
A	?	-	PHE	deletion	UNP P00581
A	?	-	GLY	deletion	UNP P00581
A	?	-	SER	deletion	UNP P00581
A	?	-	HIS	deletion	UNP P00581

- Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	105	Total	C	N	O	S	0	0	0
			774	500	121	150	3			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0

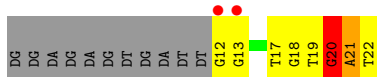
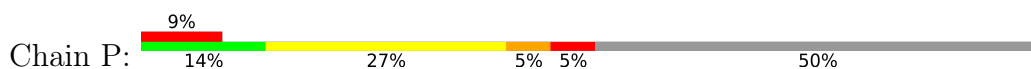
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	6	Total 6	O 6	0	0
6	A	43	Total 43	O 43	0	0
6	B	2	Total 2	O 2	0	0

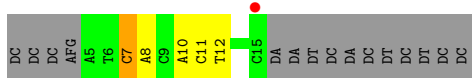
3 Residue-property plots

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.

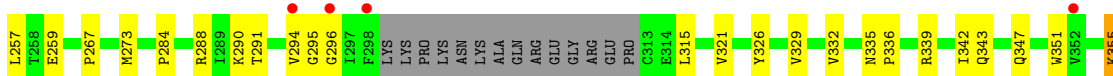
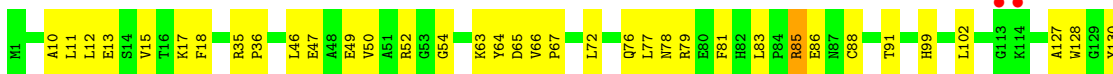
- Molecule 1: 5'-D(*GP*GP*AP*GP*AP*GP*TP*GP*AP*TP*T*GP*GP*TP*AP*GP*TP*GP*TP*GP*AP*(2DT))-3'

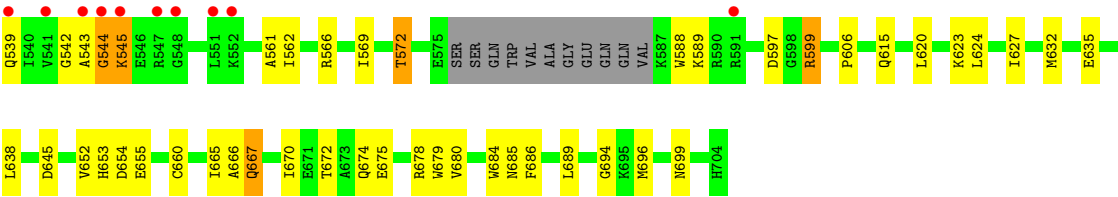


- Molecule 2: 5'-D(*CP*CP*CP*(AFG)P*AP*TP*CP*AP*CP*AP*CP*TP*AP*CP*CP*AP*A
P*TP*CP*AP*CP*TP*CP*TP*CP*C)-3'

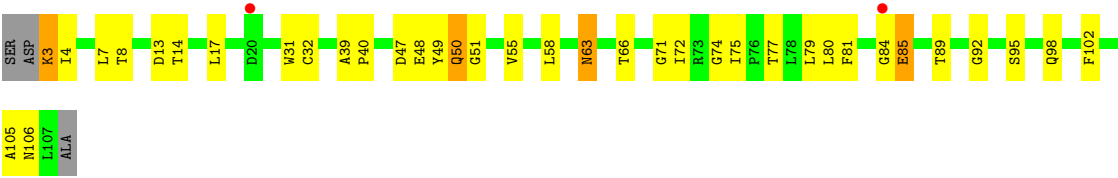


- Molecule 3: DNA polymerase





● Molecule 4: Thioredoxin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.58Å 211.10Å 51.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.64 – 2.70 46.64 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.1 (46.64-2.70) 95.0 (46.64-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.40 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.279 0.225 , 0.278	Depositor DCC
R_{free} test set	1775 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6462	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: MG, 2DT

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	P	0.29	0/235	0.93	1/363 (0.3%)
2	T	0.37	0/244	0.80	0/372
3	A	0.45	0/5318	0.93	15/7226 (0.2%)
4	B	0.44	0/789	0.94	4/1078 (0.4%)
All	All	0.44	0/6586	0.93	20/9039 (0.2%)

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	P	0	2
2	T	0	1
All	All	0	3

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	589	LYS	N-CA-C	-7.51	103.07	112.90
3	A	520	ASN	N-CA-C	-6.83	104.42	112.89
1	P	20	DG	N9-C1'-C2'	-6.65	103.53	113.50
3	A	513	ALA	N-CA-C	-6.62	101.62	110.55
4	B	63	ASN	CA-C-N	6.59	126.72	119.87
4	B	63	ASN	C-N-CA	6.59	126.72	119.87
3	A	196	ILE	N-CA-C	6.46	118.33	108.71
3	A	65	ASP	N-CA-C	6.40	118.79	111.11
3	A	519	ASP	N-CA-C	-6.17	105.45	114.39
3	A	225	ALA	N-CA-C	-5.73	105.12	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	699	ASN	N-CA-C	5.70	116.61	108.74
4	B	66	THR	N-CA-C	5.66	118.30	111.40
3	A	347	GLN	N-CA-C	-5.52	105.35	111.36
3	A	88	CYS	N-CA-C	5.51	118.46	109.59
3	A	127	ALA	N-CA-C	5.50	117.71	111.11
3	A	400	ALA	N-CA-C	5.38	120.33	113.18
4	B	7	LEU	N-CA-C	5.32	117.39	110.53
3	A	199	THR	N-CA-C	-5.29	106.42	112.92
3	A	523	THR	N-CA-C	-5.28	105.42	111.07
3	A	431	THR	N-CA-C	-5.02	101.57	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	20	DG	Sidechain
1	P	21	DA	Sidechain
2	T	7	DC	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	228	0	127	11	0
2	T	219	0	124	6	0
3	A	5189	0	4909	166	0
4	B	774	0	750	20	0
5	A	1	0	0	0	0
6	A	43	0	0	1	0
6	B	2	0	0	0	0
6	T	6	0	0	1	0
All	All	6462	0	5910	194	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 16.

All (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:624:LEU:HD12	3:A:680:VAL:HG22	1.49	0.92
3:A:666:ALA:HB3	3:A:696:MET:HE2	1.53	0.90
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.52	0.90
3:A:624:LEU:HD11	3:A:679:TRP:HZ3	1.39	0.87
3:A:674:GLN:NE2	3:A:678:ARG:HH11	1.77	0.81
3:A:355:LYS:HD2	3:A:355:LYS:H	1.47	0.79
3:A:391:MET:C	3:A:391:MET:HE2	2.09	0.76
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.66	0.75
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.70	0.74
3:A:496:TYR:CZ	3:A:505:ILE:HD11	2.22	0.74
2:T:7:DC:H4'	3:A:431:THR:HG22	1.70	0.73
3:A:35:ARG:HH11	3:A:35:ARG:HG3	1.53	0.73
3:A:294:VAL:HG12	3:A:295:GLY:H	1.54	0.71
4:B:3:LYS:HE2	4:B:50:GLN:OE1	1.90	0.71
3:A:535:GLU:HA	3:A:545:LYS:HA	1.74	0.70
4:B:95:SER:OG	4:B:98:GLN:HG3	1.91	0.69
3:A:252:GLU:OE2	3:A:256:LYS:HE3	1.92	0.69
3:A:13:GLU:H	3:A:13:GLU:CD	2.00	0.68
1:P:21:DA:H2'	1:P:22:2DT:H72	1.76	0.68
3:A:624:LEU:CD1	3:A:680:VAL:HG22	2.24	0.68
3:A:496:TYR:CE1	3:A:505:ILE:HD11	2.28	0.68
3:A:678:ARG:NH2	3:A:689:LEU:HD21	2.09	0.67
3:A:674:GLN:HE21	3:A:678:ARG:HH11	1.42	0.67
3:A:366:ASP:OD1	3:A:387:LYS:HD2	1.93	0.67
3:A:535:GLU:HA	3:A:545:LYS:CA	2.25	0.66
3:A:481:LEU:HD21	3:A:525:ILE:HG12	1.78	0.66
3:A:315:LEU:HD21	4:B:105:ALA:HB1	1.76	0.65
3:A:538:GLY:HA3	3:A:544:GLY:O	1.96	0.65
3:A:597:ASP:OD1	3:A:599:ARG:HD2	1.97	0.65
3:A:91:THR:HB	3:A:181:LEU:CD1	2.27	0.65
3:A:391:MET:HE3	3:A:395:ARG:HG3	1.78	0.64
3:A:284:PRO:HA	3:A:288:ARG:HH21	1.62	0.64
3:A:525:ILE:HG23	3:A:526:TYR:N	2.12	0.63
3:A:391:MET:HE2	3:A:392:ILE:HA	1.80	0.63
3:A:666:ALA:CB	3:A:696:MET:HE2	2.28	0.63
3:A:376:ASP:HB3	3:A:379:LYS:HG3	1.79	0.63
3:A:624:LEU:O	3:A:624:LEU:HD13	1.99	0.63
3:A:391:MET:HE2	3:A:392:ILE:N	2.14	0.63
3:A:235:ASP:OD2	3:A:238:ALA:HB2	2.00	0.62
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.00	0.61
3:A:233:PRO:HB2	3:A:456:GLY:O	2.00	0.61
3:A:448:GLY:O	3:A:452:ARG:HB2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:632:MET:HA	3:A:635:GLU:HG2	1.82	0.61
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.31	0.61
3:A:517:THR:C	3:A:519:ASP:H	2.08	0.61
3:A:15:VAL:HG22	3:A:72:LEU:HD21	1.82	0.61
1:P:12:DG:H2''	1:P:13:DG:OP2	2.02	0.60
3:A:404:LYS:HA	3:A:409:TYR:HE2	1.66	0.59
3:A:678:ARG:HH21	3:A:689:LEU:HD21	1.66	0.59
3:A:86:GLU:HG3	3:A:203:TYR:CE1	2.38	0.58
3:A:391:MET:HE3	3:A:395:ARG:CG	2.34	0.57
3:A:355:LYS:H	3:A:355:LYS:CD	2.17	0.57
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.87	0.57
3:A:35:ARG:HG3	3:A:35:ARG:NH1	2.19	0.57
3:A:376:ASP:HB3	3:A:379:LYS:CG	2.34	0.56
3:A:501:LEU:CD2	3:A:689:LEU:HB3	2.35	0.56
3:A:488:MET:HE2	3:A:496:TYR:HB2	1.88	0.56
1:P:17:DT:H2''	1:P:18:DG:H5'	1.87	0.56
3:A:391:MET:HE2	3:A:392:ILE:CA	2.35	0.56
3:A:624:LEU:HD11	3:A:679:TRP:CZ3	2.30	0.56
3:A:488:MET:HE3	3:A:561:ALA:HB3	1.87	0.56
3:A:666:ALA:O	3:A:670:ILE:HG13	2.06	0.55
2:T:12:DT:H5''	3:A:335:ASN:HD21	1.72	0.55
3:A:235:ASP:CG	3:A:238:ALA:HB2	2.32	0.55
3:A:357:THR:C	3:A:359:LYS:H	2.15	0.55
3:A:474:ILE:HD12	3:A:474:ILE:N	2.22	0.54
3:A:539:GLN:HA	3:A:542:GLY:O	2.07	0.54
3:A:128:TRP:CE3	3:A:177:VAL:HG13	2.42	0.54
3:A:480:GLU:HA	3:A:480:GLU:OE2	2.08	0.54
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.42	0.54
3:A:63:LYS:HE2	3:A:228:GLU:OE2	2.08	0.54
4:B:3:LYS:HB2	4:B:3:LYS:NZ	2.23	0.53
4:B:17:LEU:HA	4:B:84:GLY:HA2	1.90	0.53
3:A:326:TYR:HB3	4:B:92:GLY:HA2	1.89	0.53
3:A:525:ILE:HG23	3:A:526:TYR:H	1.73	0.52
1:P:17:DT:H2''	1:P:18:DG:C5'	2.39	0.52
3:A:46:LEU:O	3:A:50:VAL:HG23	2.10	0.52
3:A:517:THR:O	3:A:519:ASP:N	2.41	0.52
4:B:4:ILE:HG23	4:B:55:VAL:O	2.10	0.52
4:B:13:ASP:HA	4:B:17:LEU:HD12	1.92	0.52
3:A:204:THR:O	3:A:208:SER:HB2	2.10	0.52
3:A:130:TYR:CZ	3:A:134:GLU:HG3	2.45	0.51
2:T:8:DA:H4'	3:A:432:HIS:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:10:DA:H2"	2:T:11:DC:C6	2.44	0.51
3:A:501:LEU:HD21	3:A:689:LEU:HB3	1.92	0.51
3:A:674:GLN:NE2	3:A:678:ARG:NH1	2.52	0.51
3:A:535:GLU:HA	3:A:545:LYS:C	2.36	0.51
3:A:351:TRP:NE1	3:A:372:VAL:HG22	2.26	0.51
3:A:99:HIS:HB3	3:A:102:LEU:HD12	1.93	0.50
3:A:172:VAL:O	3:A:176:VAL:HG23	2.11	0.50
3:A:473:GLY:O	3:A:694:GLY:HA2	2.11	0.50
3:A:543:ALA:O	3:A:544:GLY:C	2.54	0.50
3:A:155:VAL:O	3:A:156:ASP:C	2.54	0.50
3:A:569:ILE:O	3:A:572:THR:HB	2.12	0.50
1:P:17:DT:H1'	1:P:18:DG:H5"	1.94	0.50
3:A:543:ALA:O	3:A:545:LYS:N	2.45	0.50
3:A:49:GLU:HA	3:A:52:ARG:NH1	2.26	0.50
3:A:91:THR:HB	3:A:181:LEU:HD12	1.93	0.50
3:A:363:VAL:O	3:A:368:VAL:HG21	2.11	0.50
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.12	0.49
3:A:432:HIS:ND1	3:A:432:HIS:N	2.60	0.49
3:A:632:MET:HE1	3:A:675:GLU:HB2	1.93	0.49
3:A:351:TRP:CD1	3:A:372:VAL:HG22	2.48	0.49
3:A:484:LEU:O	3:A:488:MET:HG2	2.12	0.49
3:A:510:GLN:O	3:A:513:ALA:O	2.31	0.49
4:B:47:ASP:O	4:B:50:GLN:HB2	2.12	0.49
3:A:223:LEU:O	3:A:226:LYS:HB3	2.13	0.49
3:A:632:MET:HE1	3:A:675:GLU:CB	2.43	0.49
3:A:131:ARG:O	3:A:135:MET:HG2	2.12	0.48
3:A:632:MET:HE2	3:A:672:THR:HG23	1.95	0.48
3:A:142:ASP:HB3	3:A:146:MET:HE3	1.96	0.48
4:B:81:PHE:HA	4:B:85:GLU:O	2.13	0.48
3:A:145:ARG:O	3:A:149:GLU:HG3	2.12	0.48
3:A:147:LEU:HD11	3:A:158:MET:HE2	1.96	0.48
3:A:79:ARG:HD3	6:A:4012:HOH:O	2.13	0.48
3:A:420:VAL:O	3:A:422:PRO:HD3	2.13	0.47
3:A:562:ILE:O	3:A:566:ARG:HG3	2.13	0.47
3:A:13:GLU:CD	3:A:13:GLU:N	2.69	0.47
3:A:436:ASN:O	3:A:439:GLN:HG2	2.15	0.47
4:B:102:PHE:O	4:B:106:ASN:ND2	2.40	0.47
3:A:339:ARG:HA	3:A:342:ILE:HD12	1.95	0.47
3:A:290:LYS:HD3	3:A:291:THR:N	2.29	0.47
3:A:525:ILE:CG2	3:A:526:TYR:N	2.77	0.47
3:A:645:ASP:HB3	3:A:665:ILE:CD1	2.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:48:GLU:C	4:B:50:GLN:H	2.22	0.47
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.49	0.47
3:A:18:PHE:HB2	3:A:72:LEU:HD13	1.98	0.46
1:P:21:DA:H5''	3:A:440:ILE:O	2.15	0.46
3:A:517:THR:C	3:A:519:ASP:N	2.74	0.46
3:A:404:LYS:HA	3:A:409:TYR:CE2	2.49	0.46
3:A:249:ARG:O	3:A:253:LEU:HG	2.16	0.46
3:A:294:VAL:HG12	3:A:295:GLY:N	2.25	0.45
3:A:367:GLU:O	3:A:370:GLU:HB3	2.15	0.45
3:A:443:VAL:HB	3:A:449:GLU:OE1	2.16	0.45
3:A:388:GLU:O	3:A:392:ILE:HG12	2.16	0.45
4:B:71:GLY:O	4:B:72:ILE:C	2.58	0.45
2:T:12:DT:H5''	3:A:335:ASN:ND2	2.30	0.45
3:A:623:LYS:O	3:A:627:ILE:HG13	2.16	0.45
3:A:429:ARG:HD2	3:A:615:GLN:OE1	2.17	0.45
3:A:10:ALA:HB3	3:A:15:VAL:HA	1.99	0.45
3:A:273:MET:CE	3:A:284:PRO:HG3	2.47	0.44
3:A:273:MET:HE1	3:A:284:PRO:HG3	1.98	0.44
3:A:588:TRP:CH2	3:A:606:PRO:HG3	2.51	0.44
3:A:660:CYS:SG	3:A:666:ALA:HA	2.58	0.44
3:A:213:ALA:HB2	3:A:597:ASP:OD1	2.17	0.44
3:A:391:MET:CE	3:A:395:ARG:HG3	2.46	0.44
3:A:470:VAL:HG12	3:A:471:GLN:N	2.32	0.44
3:A:667:GLN:NE2	3:A:696:MET:HE1	2.33	0.44
3:A:674:GLN:HE21	3:A:678:ARG:NH1	2.11	0.44
4:B:77:THR:HG22	4:B:79:LEU:HD13	2.00	0.44
3:A:442:GLY:O	3:A:448:GLY:HA3	2.17	0.43
3:A:66:VAL:HB	3:A:67:PRO:HD3	2.00	0.43
3:A:514:GLU:O	3:A:515:LEU:C	2.61	0.43
3:A:83:LEU:HD23	3:A:83:LEU:HA	1.83	0.43
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.18	0.43
3:A:49:GLU:OE1	3:A:52:ARG:NH1	2.51	0.43
1:P:22:2DT:H4'	3:A:652:VAL:HG12	2.01	0.43
3:A:446:PRO:O	3:A:447:TYR:HB2	2.19	0.43
4:B:74:GLY:O	4:B:77:THR:OG1	2.35	0.43
3:A:267:PRO:HA	3:A:329:VAL:HG12	2.01	0.42
1:P:22:2DT:H3'2	3:A:654:ASP:OD1	2.19	0.42
3:A:597:ASP:OD2	3:A:620:LEU:HD13	2.18	0.42
3:A:481:LEU:HD21	3:A:525:ILE:CG1	2.48	0.42
3:A:47:GLU:HG3	3:A:81:PHE:HE1	1.85	0.42
3:A:684:TRP:O	3:A:685:ASN:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:157:GLY:HA2	3:A:159:GLU:OE1	2.19	0.42
3:A:402:GLY:O	3:A:408:ARG:NE	2.52	0.42
3:A:678:ARG:HE	3:A:689:LEU:HD11	1.85	0.42
3:A:368:VAL:HG23	3:A:369:LEU:N	2.35	0.42
3:A:525:ILE:CG2	3:A:526:TYR:H	2.32	0.42
3:A:35:ARG:NH1	3:A:35:ARG:CG	2.83	0.42
3:A:64:TYR:O	3:A:67:PRO:HD2	2.20	0.41
3:A:257:LEU:C	3:A:259:GLU:H	2.28	0.41
3:A:516:PRO:O	3:A:517:THR:CB	2.68	0.41
3:A:391:MET:HE2	3:A:391:MET:O	2.17	0.41
3:A:624:LEU:HD13	3:A:624:LEU:C	2.45	0.41
3:A:296:GLY:H	3:A:321:VAL:HA	1.86	0.41
3:A:501:LEU:HD22	3:A:689:LEU:HB3	2.01	0.41
3:A:171:ASN:C	3:A:171:ASN:HD22	2.28	0.41
3:A:339:ARG:NH1	3:A:390:LEU:HD13	2.35	0.41
4:B:49:TYR:C	4:B:51:GLY:H	2.29	0.41
1:P:21:DA:H2''	1:P:22:2DT:H6	2.02	0.41
3:A:77:LEU:O	3:A:78:ASN:C	2.62	0.41
3:A:158:MET:HA	3:A:161:TRP:CD2	2.56	0.41
1:P:19:DT:C2	1:P:20:DG:N7	2.89	0.41
3:A:11:LEU:O	3:A:12:LEU:C	2.64	0.41
3:A:17:LYS:HA	3:A:76:GLN:OE1	2.21	0.40
4:B:31:TRP:CD1	4:B:31:TRP:H	2.36	0.40
3:A:467:LYS:HA	3:A:468:PRO:HD3	1.94	0.40
4:B:8:THR:HA	4:B:63:ASN:OD1	2.20	0.40
1:P:21:DA:H2''	1:P:22:2DT:C6	2.52	0.40
2:T:11:DC:H2'	6:T:4030:HOH:O	2.20	0.40
3:A:383:ILE:O	3:A:387:LYS:HG3	2.20	0.40
4:B:32:CYS:HB2	4:B:75:ILE:HD11	2.03	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	667/698 (96%)	620 (93%)	37 (6%)	10 (2%)	8	22
4	B	103/108 (95%)	94 (91%)	8 (8%)	1 (1%)	12	32
All	All	770/806 (96%)	714 (93%)	45 (6%)	11 (1%)	9	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	544	GLY
3	A	545	LYS
3	A	518	ARG
3	A	515	LEU
4	B	50	GLN
3	A	478	GLY
3	A	653	HIS
3	A	358	ASP
3	A	360	GLY
3	A	517	THR

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	511/579 (88%)	495 (97%)	16 (3%)	35	65
4	B	78/87 (90%)	72 (92%)	6 (8%)	12	30
All	All	589/666 (88%)	567 (96%)	22 (4%)	30	59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	85	ARG
3	A	181	LEU
3	A	204	THR
3	A	332	VAL
3	A	343	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	355	LYS
3	A	391	MET
3	A	410	VAL
3	A	426	VAL
3	A	432	HIS
3	A	572	THR
3	A	599	ARG
3	A	638	LEU
3	A	655	GLU
3	A	667	GLN
3	A	686	PHE
4	B	3	LYS
4	B	14	THR
4	B	58	LEU
4	B	80	LEU
4	B	85	GLU
4	B	89	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	60	ASN
3	A	173	GLN
3	A	227	GLN
3	A	266	GLN
3	A	335	ASN
3	A	347	GLN
3	A	502	ASN
3	A	558	ASN
3	A	602	HIS
4	B	62	GLN

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	2DT	P	22	1,2	17,20,21	0.31	0	22,28,31	0.34	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	2DT	P	22	1,2	-	0/7/18/19	0/2/2/2

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.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	22	2DT	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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	P	10/22 (45%)	1.17	2 (20%) 3 2	29, 41, 91, 98	0
2	T	11/26 (42%)	0.29	1 (9%) 15 12	18, 32, 57, 73	0
3	A	673/698 (96%)	0.10	33 (4%) 35 31	9, 27, 66, 83	0
4	B	105/108 (97%)	0.36	2 (1%) 66 63	20, 35, 53, 64	0
All	All	799/854 (93%)	0.15	38 (4%) 35 32	9, 29, 65, 98	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	543	ALA	5.1
1	P	12	DG	5.1
3	A	517	THR	3.8
3	A	518	ARG	3.5
3	A	296	GLY	3.5
3	A	544	GLY	3.3
3	A	536	LYS	3.3
2	T	15	DC	3.2
3	A	530	TYR	3.2
3	A	298	PHE	3.1
3	A	547	ARG	3.1
3	A	537	ILE	3.0
3	A	114	LYS	3.0
3	A	539	GLN	2.9
3	A	515	LEU	2.9
3	A	529	LEU	2.9
1	P	13	DG	2.8
3	A	526	TYR	2.8
3	A	551	LEU	2.8
3	A	528	PHE	2.8
3	A	156	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	538	GLY	2.6
3	A	516	PRO	2.6
3	A	360	GLY	2.5
3	A	591	ARG	2.5
3	A	548	GLY	2.4
3	A	294	VAL	2.4
3	A	520	ASN	2.3
3	A	113	GLY	2.2
3	A	506	HIS	2.2
3	A	552	LYS	2.2
4	B	84	GLY	2.1
3	A	352	VAL	2.1
4	B	20	ASP	2.1
3	A	532	ALA	2.1
3	A	545	LYS	2.1
3	A	541	VAL	2.1
3	A	358	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
1	2DT	P	22	19/20	0.96	0.08	22,26,27,29	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($\text{\AA}^2$)	Q<0.9
5	MG	A	3001	1/1	0.91	0.28	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.