



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:45 PM UTC

PDB ID : 1SL1 / pdb_00001sl1
Title : Binary 5' complex of T7 DNA polymerase with a DNA primer/template containing a cis-syn thymine dimer on the template
Authors : Li, Y.; Dutta, S.; Doublié, S.; Bdour, H.M.; Taylor, J.S.; Ellenberger, T.
Deposited on : 2004-03-05
Resolution : 2.20 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

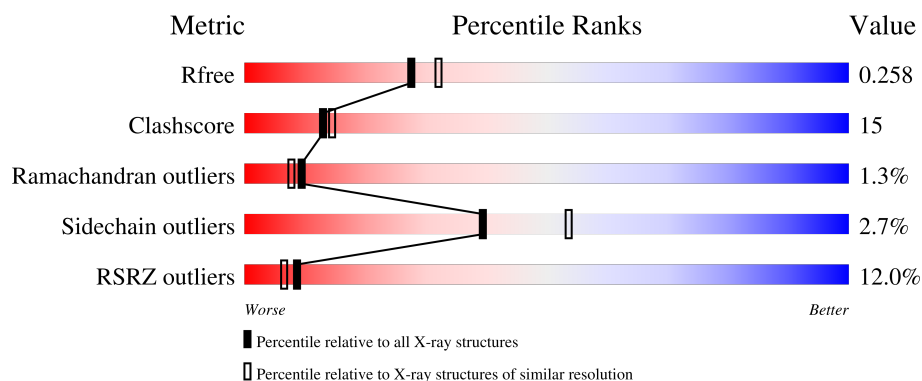
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	5% 14% 23% 5% 59%
2	T	25	8% 16% 20% . 60%
3	A	698	11% 70% 25% . .
4	B	108	12% 67% 29% . .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6654 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(*CP*GP*AP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*TP*(2DA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	9	Total	C	N	O	P	0	0	0
			172	82	28	53	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	10	Total	C	N	O	P	0	0	0
			223	107	42	64	10			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	678	Total	C	N	O	S	0	0	0
			5243	3340	907	972	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.

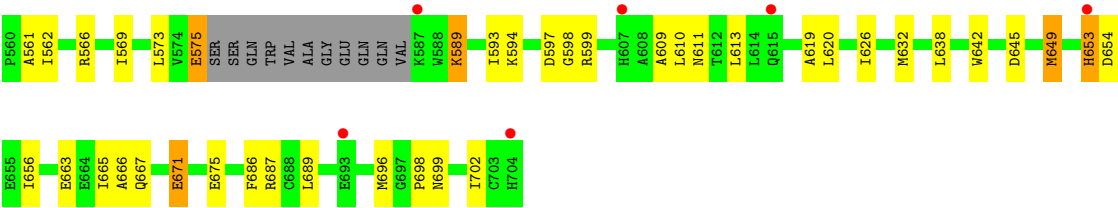
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	105	Total	C	N	O	S	0	0	0
			776	503	122	148	3			

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

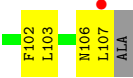
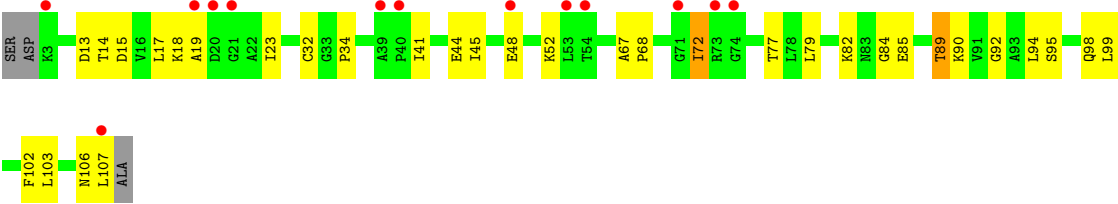
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	6	Total 6	O 6	0	0
6	A	213	Total 213	O 213	0	0
6	B	20	Total 20	O 20	0	0



● 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	104.38Å 214.78Å 52.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.20) 98.5 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.03 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.262 0.240 , 0.258	Depositor DCC
R_{free} test set	2814 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6654	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: TTD, MG, 2DA

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	0.37	0/180	0.68	0/275
2	T	0.27	0/211	0.71	0/324
3	A	0.40	1/5374 (0.0%)	0.88	9/7301 (0.1%)
4	B	0.36	0/791	0.84	0/1079
All	All	0.39	1/6556 (0.0%)	0.87	9/8979 (0.1%)

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	1
2	T	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	649	MET	SD-CE	-5.88	1.64	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	280	GLY	N-CA-C	-6.95	105.16	114.95
3	A	589	LYS	N-CA-C	-6.50	105.50	113.50
3	A	127	ALA	N-CA-C	6.07	118.43	111.02
3	A	225	ALA	N-CA-C	-5.60	105.17	111.28
3	A	9	ASN	N-CA-C	5.37	119.70	113.20
3	A	65	ASP	N-CA-C	5.37	117.55	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	521	ALA	N-CA-C	-5.19	105.53	111.14
3	A	13	GLU	N-CA-C	5.12	117.53	111.33
3	A	699	ASN	N-CA-C	5.03	115.68	108.74

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	19	DC	Sidechain
2	T	8	DG	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	172	0	97	12	0
2	T	223	0	122	10	0
3	A	5243	0	4982	152	0
4	B	776	0	761	22	0
5	A	1	0	0	0	0
6	A	213	0	0	4	0
6	B	20	0	0	0	0
6	T	6	0	0	0	0
All	All	6654	0	5962	185	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 15.

All (185) 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:131:ARG:HB3	3:A:131:ARG:HH11	1.20	1.07
4:B:19:ALA:HB3	4:B:23:ILE:HD11	1.43	0.99
3:A:667:GLN:HG3	3:A:696:MET:HE1	1.55	0.89
3:A:18:PHE:H	3:A:76:GLN:HE22	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:LEU:HD21	3:A:689:LEU:HB3	1.67	0.77
3:A:490:ARG:HH11	3:A:490:ARG:HB2	1.50	0.76
3:A:490:ARG:HH11	3:A:490:ARG:CB	2.02	0.73
3:A:173:GLN:O	3:A:176:VAL:HG22	1.90	0.72
3:A:663:GLU:HG2	3:A:696:MET:SD	2.30	0.72
3:A:131:ARG:HH11	3:A:131:ARG:CB	2.02	0.71
3:A:131:ARG:HB3	3:A:131:ARG:NH1	2.02	0.71
3:A:667:GLN:O	3:A:671:GLU:HG2	1.91	0.71
1:P:18:DG:HI'	3:A:394:LYS:HZ1	1.55	0.71
3:A:364:VAL:HA	3:A:368:VAL:HG21	1.73	0.71
3:A:233:PRO:CD	3:A:649:MET:HE2	2.21	0.70
4:B:95:SER:OG	4:B:98:GLN:HG3	1.94	0.68
3:A:457:ALA:HA	3:A:649:MET:HE1	1.74	0.68
3:A:593:ILE:HD12	3:A:594:LYS:H	1.57	0.68
3:A:513:ALA:HB2	3:A:555:PHE:HB2	1.75	0.68
3:A:321:VAL:HG13	3:A:324:ALA:HB3	1.76	0.67
3:A:429:ARG:HD2	3:A:619:ALA:HB2	1.77	0.67
3:A:164:ASN:HD22	3:A:166:GLU:H	1.44	0.66
3:A:667:GLN:CG	3:A:696:MET:HE1	2.25	0.66
3:A:321:VAL:HG11	4:B:94:LEU:HG	1.79	0.65
3:A:467:LYS:HA	3:A:467:LYS:HE2	1.76	0.65
1:P:18:DG:HI'	3:A:394:LYS:NZ	2.11	0.65
4:B:67:ALA:HB1	4:B:72:ILE:HD12	1.79	0.65
2:T:5:TTD:H2'	2:T:5:TTD:H5R2	1.77	0.65
3:A:79:ARG:HD3	6:A:5050:HOH:O	1.97	0.65
3:A:552:LYS:O	3:A:556:LEU:HD13	1.97	0.64
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.28	0.64
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.32	0.64
3:A:291:THR:HG22	3:A:325:PRO:HB3	1.80	0.64
3:A:145:ARG:O	3:A:149:GLU:HG3	1.97	0.64
3:A:642:TRP:HH2	3:A:649:MET:CE	2.11	0.63
3:A:597:ASP:OD1	3:A:599:ARG:CD	2.47	0.62
3:A:597:ASP:OD1	3:A:599:ARG:HD2	1.99	0.61
3:A:501:LEU:HD21	3:A:689:LEU:CB	2.30	0.61
3:A:164:ASN:ND2	3:A:167:MET:H	1.98	0.61
3:A:18:PHE:H	3:A:76:GLN:NE2	1.95	0.60
3:A:496:TYR:CZ	3:A:505:ILE:HD11	2.36	0.60
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.83	0.60
2:T:5:TTD:H2''	2:T:6:DA:N6	2.18	0.59
3:A:642:TRP:HH2	3:A:649:MET:HE2	1.69	0.58
3:A:632:MET:HE1	3:A:675:GLU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:480:GLU:HB3	3:A:529:LEU:HD13	1.86	0.57
3:A:339:ARG:HB3	3:A:364:VAL:HG21	1.86	0.57
3:A:339:ARG:HB3	3:A:364:VAL:CG2	2.34	0.56
3:A:573:LEU:O	3:A:589:LYS:HG2	2.04	0.56
3:A:321:VAL:HG13	3:A:324:ALA:CB	2.36	0.56
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.87	0.56
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.45	0.56
2:T:5:TTD:H2'	2:T:5:TTD:C5R	2.36	0.56
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.41	0.56
3:A:270:GLY:HA3	3:A:288:ARG:HB3	1.86	0.55
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.88	0.55
3:A:441:PRO:O	3:A:452:ARG:HD3	2.07	0.55
3:A:575:GLU:HB2	3:A:589:LYS:HB3	1.89	0.55
1:P:16:DG:H1'	1:P:17:DT:H5''	1.89	0.55
4:B:95:SER:H	4:B:98:GLN:NE2	2.04	0.55
3:A:138:GLU:HG2	3:A:170:TYR:OH	2.08	0.54
3:A:499:GLU:HG2	3:A:508:LYS:HD2	1.90	0.54
3:A:569:ILE:CG2	3:A:609:ALA:HB1	2.38	0.54
3:A:164:ASN:HD22	3:A:166:GLU:N	2.05	0.53
3:A:516:PRO:HG2	3:A:517:THR:H	1.73	0.53
3:A:111:ARG:HG3	3:A:111:ARG:HH11	1.72	0.53
3:A:442:GLY:O	3:A:448:GLY:HA3	2.09	0.53
4:B:82:LYS:O	4:B:85:GLU:HG2	2.08	0.53
3:A:296:GLY:O	3:A:316:ASP:HB3	2.10	0.52
3:A:53:GLY:HA2	6:A:5155:HOH:O	2.10	0.51
1:P:16:DG:H2''	1:P:17:DT:C5'	2.41	0.51
3:A:507:THR:HG23	3:A:518:ARG:HH21	1.75	0.51
3:A:339:ARG:HD2	3:A:364:VAL:HG23	1.92	0.51
3:A:158:MET:HA	3:A:161:TRP:CE2	2.45	0.51
4:B:44:GLU:O	4:B:48:GLU:HG3	2.10	0.51
2:T:5:TTD:H2'	2:T:5:TTD:O4R	2.10	0.51
3:A:233:PRO:HD2	3:A:649:MET:HE2	1.92	0.51
4:B:103:LEU:O	4:B:107:LEU:HD13	2.10	0.51
3:A:347:GLN:NE2	3:A:353:PRO:HG2	2.26	0.51
3:A:358:ASP:C	3:A:360:GLY:H	2.18	0.50
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.47	0.50
3:A:490:ARG:HB2	3:A:490:ARG:NH1	2.23	0.50
3:A:326:TYR:HB3	4:B:92:GLY:HA2	1.93	0.50
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.11	0.50
3:A:530:TYR:O	3:A:531:GLY:C	2.54	0.50
3:A:569:ILE:HD11	3:A:613:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:698:PRO:CG	3:A:702:ILE:HD12	2.43	0.49
3:A:368:VAL:O	3:A:372:VAL:HG23	2.13	0.49
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.93	0.49
2:T:5:TTD:HT	3:A:527:GLY:HA2	1.78	0.48
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.13	0.48
3:A:512:ALA:O	3:A:513:ALA:HB3	2.13	0.48
3:A:525:ILE:HG23	3:A:526:TYR:N	2.28	0.48
1:P:16:DG:H2''	1:P:17:DT:H5'	1.94	0.48
2:T:10:DA:H3'	3:A:404:LYS:HG3	1.95	0.48
3:A:28:THR:O	3:A:30:GLU:HG3	2.14	0.48
3:A:204:THR:HG22	6:A:5140:HOH:O	2.14	0.48
3:A:698:PRO:HG2	3:A:702:ILE:HD12	1.96	0.48
4:B:77:THR:HG22	4:B:79:LEU:HD13	1.95	0.47
3:A:336:PRO:HB2	3:A:389:TYR:CE1	2.48	0.47
3:A:274:PHE:HD1	3:A:289:ILE:HD13	1.79	0.47
2:T:6:DA:H2'	2:T:7:DG:O4'	2.15	0.47
4:B:67:ALA:HB3	4:B:68:PRO:HD3	1.96	0.47
3:A:566:ARG:HG2	3:A:610:LEU:HD22	1.96	0.47
3:A:364:VAL:HA	3:A:368:VAL:CG2	2.45	0.47
3:A:504:ASP:OD1	3:A:507:THR:HG23	2.13	0.47
4:B:67:ALA:CB	4:B:72:ILE:HD12	2.44	0.47
3:A:509:ASN:O	3:A:512:ALA:O	2.33	0.46
3:A:130:TYR:CZ	3:A:134:GLU:HG3	2.50	0.46
4:B:14:THR:HG23	4:B:15:ASP:N	2.31	0.46
3:A:18:PHE:N	3:A:76:GLN:HE22	2.03	0.46
3:A:436:ASN:O	3:A:439:GLN:HG2	2.15	0.46
3:A:488:MET:HE3	3:A:561:ALA:HB3	1.96	0.46
1:P:19:DC:H2''	1:P:20:DC:C6	2.51	0.46
3:A:211:LEU:HD21	3:A:598:GLY:C	2.41	0.46
1:P:15:DA:H4'	3:A:359:LYS:HD2	1.98	0.46
3:A:535:GLU:HA	3:A:545:LYS:CA	2.46	0.46
3:A:626:ILE:HG22	3:A:656:ILE:HG21	1.98	0.46
3:A:91:THR:HB	3:A:181:LEU:HD13	1.98	0.45
3:A:504:ASP:OD2	3:A:518:ARG:NH2	2.50	0.45
3:A:513:ALA:HB2	3:A:555:PHE:CB	2.46	0.45
3:A:344:LYS:O	3:A:348:GLU:HG3	2.16	0.45
4:B:19:ALA:CB	4:B:23:ILE:HD11	2.31	0.45
3:A:365:ASP:O	3:A:368:VAL:HG22	2.16	0.45
1:P:18:DG:C4	1:P:19:DC:C5	3.05	0.45
3:A:496:TYR:CE1	3:A:505:ILE:HD11	2.52	0.45
3:A:666:ALA:HB3	3:A:696:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:102:PHE:O	4:B:106:ASN:ND2	2.47	0.45
3:A:158:MET:HA	3:A:161:TRP:CD2	2.52	0.45
3:A:642:TRP:HH2	3:A:649:MET:HE3	1.80	0.45
3:A:233:PRO:HB2	3:A:456:GLY:O	2.17	0.45
3:A:270:GLY:C	3:A:288:ARG:HB3	2.42	0.44
4:B:89:THR:O	4:B:90:LYS:HD2	2.18	0.44
3:A:359:LYS:O	3:A:359:LYS:HG2	2.18	0.44
4:B:95:SER:CB	4:B:98:GLN:HE21	2.30	0.44
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.83	0.44
3:A:530:TYR:HA	3:A:611:ASN:ND2	2.33	0.43
3:A:544:GLY:C	3:A:546:GLU:H	2.25	0.43
1:P:17:DT:H2"	1:P:18:DG:C8	2.54	0.43
3:A:79:ARG:HG2	3:A:80:GLU:N	2.34	0.43
3:A:446:PRO:O	3:A:447:TYR:HB2	2.19	0.43
3:A:155:VAL:O	3:A:156:ASP:C	2.62	0.43
3:A:270:GLY:CA	3:A:288:ARG:HB3	2.48	0.43
3:A:368:VAL:HG23	3:A:369:LEU:N	2.33	0.43
3:A:510:GLN:HE22	3:A:518:ARG:HB3	1.84	0.43
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.18	0.43
3:A:429:ARG:NH2	3:A:654:ASP:OD1	2.51	0.43
3:A:569:ILE:HD11	3:A:613:LEU:CD2	2.49	0.43
3:A:535:GLU:HA	3:A:545:LYS:N	2.32	0.42
3:A:638:LEU:CD1	3:A:638:LEU:N	2.83	0.42
4:B:41:ILE:O	4:B:45:ILE:HD13	2.19	0.42
3:A:347:GLN:C	3:A:349:ALA:H	2.26	0.42
3:A:535:GLU:HA	3:A:545:LYS:H	1.84	0.42
3:A:534:ASP:O	3:A:548:GLY:HA3	2.19	0.42
4:B:17:LEU:HA	4:B:84:GLY:HA2	2.01	0.42
3:A:512:ALA:C	3:A:514:GLU:H	2.28	0.42
3:A:474:ILE:HD12	3:A:474:ILE:N	2.35	0.42
3:A:176:VAL:HG23	3:A:177:VAL:N	2.35	0.42
3:A:273:MET:CE	3:A:284:PRO:HG3	2.49	0.42
3:A:422:PRO:HB2	6:A:5038:HOH:O	2.20	0.42
1:P:20:DC:N4	2:T:6:DA:H61	2.17	0.42
1:P:20:DC:H42	2:T:6:DA:H61	1.67	0.42
3:A:593:ILE:CD1	3:A:594:LYS:H	2.30	0.41
3:A:457:ALA:CA	3:A:649:MET:HE1	2.46	0.41
3:A:525:ILE:CG2	3:A:526:TYR:N	2.83	0.41
4:B:13:ASP:OD1	4:B:18:LYS:HE3	2.20	0.41
3:A:235:ASP:HB2	3:A:459:HIS:CE1	2.55	0.41
3:A:276:HIS:CD2	3:A:278:ARG:H	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:111:ARG:HG3	3:A:111:ARG:NH1	2.35	0.41
2:T:9:DC:H4'	3:A:432:HIS:O	2.20	0.41
3:A:131:ARG:CB	3:A:131:ARG:NH1	2.73	0.41
3:A:273:MET:SD	3:A:284:PRO:HA	2.60	0.41
3:A:489:ALA:HA	3:A:492:ASP:OD1	2.21	0.41
4:B:94:LEU:N	4:B:94:LEU:HD12	2.35	0.41
3:A:57:VAL:HG22	3:A:89:ILE:HB	2.02	0.41
3:A:205:THR:HG23	3:A:209:GLU:HG3	2.03	0.41
3:A:490:ARG:O	3:A:490:ARG:HG2	2.21	0.41
3:A:360:GLY:O	3:A:361:ALA:HB2	2.21	0.40
1:P:18:DG:C1'	3:A:394:LYS:HZ1	2.30	0.40
3:A:638:LEU:N	3:A:638:LEU:HD12	2.37	0.40
3:A:343:GLN:CD	3:A:343:GLN:C	2.89	0.40
3:A:353:PRO:HB2	3:A:356:TYR:CZ	2.56	0.40
3:A:559:THR:HG22	3:A:562:ILE:HG13	2.03	0.40
3:A:355:LYS:HG3	3:A:363:VAL:HB	2.04	0.40
3:A:530:TYR:O	3:A:532:ALA:N	2.54	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	672/698 (96%)	641 (95%)	22 (3%)	9 (1%)	9	8
4	B	103/108 (95%)	99 (96%)	3 (3%)	1 (1%)	12	11
All	All	775/806 (96%)	740 (96%)	25 (3%)	10 (1%)	9	8

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP

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Mol	Chain	Res	Type
3	A	531	GLY
3	A	360	GLY
3	A	514	GLU
3	A	544	GLY
4	B	72	ILE
3	A	313	CYS
3	A	545	LYS
3	A	653	HIS
3	A	516	PRO

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	520/579 (90%)	507 (98%)	13 (2%)	42	56
4	B	78/87 (90%)	75 (96%)	3 (4%)	29	40
All	All	598/666 (90%)	582 (97%)	16 (3%)	39	53

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	131	ARG
3	A	164	ASN
3	A	181	LEU
3	A	410	VAL
3	A	429	ARG
3	A	481	LEU
3	A	490	ARG
3	A	518	ARG
3	A	575	GLU
3	A	653	HIS
3	A	671	GLU
3	A	686	PHE
3	A	687	ARG
4	B	52	LYS

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Mol	Chain	Res	Type
4	B	89	THR
4	B	99	LEU

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	76	GLN
3	A	164	ASN
3	A	276	HIS
3	A	343	GLN
3	A	347	GLN
3	A	510	GLN
3	A	704	HIS
4	B	50	GLN
4	B	98	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	2DA	P	22	1	7,10,23	0.45	0	6,12,34	0.43	0
2	TTD	T	5	2	40,40,46	4.12	10 (25%)	58,67,77	3.98	25 (43%)

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	2DA	P	22	1	-	0/3/12/19	0/1/1/3
2	TTD	T	5	2	-	7/19/101/110	0/5/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	5	TTD	C5T-C6T	-20.58	1.32	1.55
2	T	5	TTD	C5-C6	-10.81	1.43	1.55
2	T	5	TTD	C1R-N1T	5.46	1.52	1.45
2	T	5	TTD	C1'-N1	4.44	1.51	1.45
2	T	5	TTD	C2-N3	-3.90	1.31	1.38
2	T	5	TTD	C5A-C5	3.89	1.61	1.53
2	T	5	TTD	C2-N1	3.54	1.43	1.36
2	T	5	TTD	C6T-C6	2.92	1.64	1.56
2	T	5	TTD	C5M-C5T	2.90	1.59	1.53
2	T	5	TTD	O4R-C1R	-2.15	1.37	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	5	TTD	C5-C5T-C6T	10.45	100.58	88.36
2	T	5	TTD	O4'-C1'-N1	-9.65	97.22	108.65
2	T	5	TTD	O4R-C1R-N1T	9.10	119.44	108.65
2	T	5	TTD	O4T-C4T-C5T	8.05	130.20	122.71
2	T	5	TTD	C2'-C1'-N1	8.01	126.41	115.59
2	T	5	TTD	O4'-C1'-C2'	-7.80	97.12	107.09
2	T	5	TTD	C5T-C5-C4	7.31	136.57	112.84
2	T	5	TTD	O5R-PB-O5P	-7.21	80.36	108.94
2	T	5	TTD	C5A-C5-C4	-6.56	97.41	108.19
2	T	5	TTD	C5T-C6T-N1T	5.41	122.83	115.65
2	T	5	TTD	O4P-PB-O5R	-5.31	83.51	107.57
2	T	5	TTD	C5T-C5-C6	-5.16	82.33	88.36
2	T	5	TTD	O3R-PB-O5P	4.90	125.45	109.81
2	T	5	TTD	C5T-C6T-C6	-4.54	82.28	89.26
2	T	5	TTD	C4'-O4R-C1R	-4.54	98.73	109.51
2	T	5	TTD	C2R-C1R-N1T	-4.23	109.87	115.59
2	T	5	TTD	O4T-C4T-N3T	-4.16	113.85	120.59
2	T	5	TTD	O4P-PB-O5P	3.72	129.74	112.44
2	T	5	TTD	C5-C5T-C4T	-3.66	100.96	112.84
2	T	5	TTD	O4'-C4R-C3R	3.50	108.33	104.17
2	T	5	TTD	C2'-C3R-C4R	-3.32	98.30	102.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	5	TTD	O4-C4-C5	2.71	125.23	122.71
2	T	5	TTD	C5A-C5-C5T	-2.25	109.97	116.61
2	T	5	TTD	O4-C4-N3	-2.19	117.05	120.59
2	T	5	TTD	C3'-C2R-C1R	-2.18	97.26	102.60

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	5	TTD	C2'-C1'-N1-C6
2	T	5	TTD	C2'-C1'-N1-C2
2	T	5	TTD	C4R-C3R-O3R-PB
2	T	5	TTD	O4'-C1'-N1-C6
2	T	5	TTD	O4'-C1'-N1-C2
2	T	5	TTD	C3R-O3R-PB-O5P
2	T	5	TTD	C3R-O3R-PB-O4P

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	5	TTD	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	8/22 (36%)	1.00	1 (12%) 8 6	42, 49, 60, 68	0
2	T	9/25 (36%)	0.89	2 (22%) 2 1	35, 49, 64, 68	0
3	A	678/698 (97%)	0.67	80 (11%) 9 7	19, 35, 64, 71	0
4	B	105/108 (97%)	1.03	13 (12%) 8 6	30, 45, 58, 60	0
All	All	800/853 (93%)	0.73	96 (12%) 9 6	19, 37, 63, 71	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	548	GLY	6.5
3	A	539	GLN	5.8
3	A	298	PHE	5.5
3	A	544	GLY	5.4
3	A	547	ARG	5.4
3	A	531	GLY	5.3
3	A	513	ALA	4.8
3	A	294	VAL	4.5
3	A	541	VAL	4.5
3	A	530	TYR	4.4
3	A	587	LYS	4.3
3	A	151	GLY	4.2
3	A	540	ILE	4.1
3	A	299	LYS	4.0
3	A	704	HIS	3.9
3	A	354	THR	3.8
3	A	546	GLU	3.8
3	A	537	ILE	3.8
3	A	311	GLU	3.8
3	A	538	GLY	3.8
4	B	20	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
3	A	321	VAL	3.7
3	A	322	ALA	3.7
3	A	283	LEU	3.5
4	B	73	ARG	3.5
3	A	315	LEU	3.4
3	A	693	GLU	3.3
3	A	358	ASP	3.3
3	A	300	LYS	3.2
3	A	291	THR	3.2
3	A	314	GLU	3.2
4	B	71	GLY	3.2
3	A	313	CYS	3.1
3	A	312	PRO	3.1
3	A	534	ASP	3.1
3	A	545	LYS	3.0
3	A	514	GLU	3.0
4	B	3	LYS	2.9
3	A	295	GLY	2.9
3	A	542	GLY	2.9
2	T	7	DG	2.9
3	A	536	LYS	2.8
3	A	543	ALA	2.8
3	A	297	ILE	2.8
3	A	653	HIS	2.8
3	A	278	ARG	2.8
3	A	364	VAL	2.8
3	A	115	LEU	2.7
3	A	556	LEU	2.7
3	A	532	ALA	2.6
3	A	533	GLY	2.6
4	B	107	LEU	2.6
3	A	145	ARG	2.6
3	A	529	LEU	2.6
3	A	551	LEU	2.6
4	B	48	GLU	2.6
4	B	21	GLY	2.5
3	A	511	ILE	2.5
1	P	19	DC	2.5
4	B	40	PRO	2.5
3	A	526	TYR	2.5
4	B	19	ALA	2.5
4	B	39	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	376	ASP	2.4
3	A	550	GLU	2.4
3	A	111	ARG	2.4
3	A	615	GLN	2.4
3	A	535	GLU	2.4
3	A	137	GLY	2.3
3	A	143	PHE	2.3
3	A	607	HIS	2.3
3	A	549	LYS	2.3
3	A	520	ASN	2.3
3	A	317	THR	2.3
3	A	370	GLU	2.3
3	A	519	ASP	2.2
3	A	403	ASP	2.2
3	A	146	MET	2.2
2	T	8	DG	2.2
3	A	515	LEU	2.1
3	A	293	LYS	2.1
3	A	361	ALA	2.1
4	B	53	LEU	2.1
4	B	74	GLY	2.1
3	A	204	THR	2.1
3	A	169	ASP	2.1
3	A	301	PRO	2.1
3	A	353	PRO	2.1
3	A	552	LYS	2.0
3	A	517	THR	2.0
4	B	54	THR	2.0
3	A	275	CYS	2.0
3	A	141	ASP	2.0
3	A	142	ASP	2.0
3	A	156	ASP	2.0
3	A	318	ARG	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($\text{\AA}^2$)	Q<0.9
2	TTD	T	5	35/41	0.56	0.23	71,73,79,80	0
1	2DA	P	22	10/21	0.80	0.19	59,62,64,64	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	4003	1/1	0.80	0.26	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.