



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:08 am BST

PDB ID : 1SL1
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

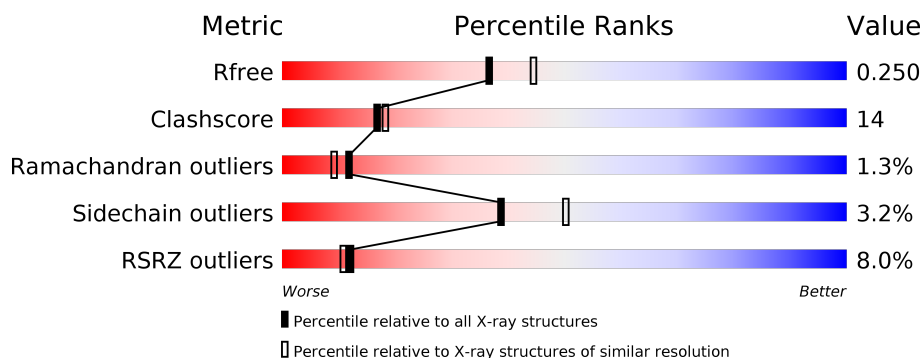
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	
2	T	25	
3	A	698	
4	B	108	

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			

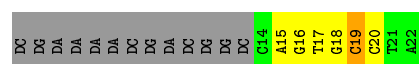
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

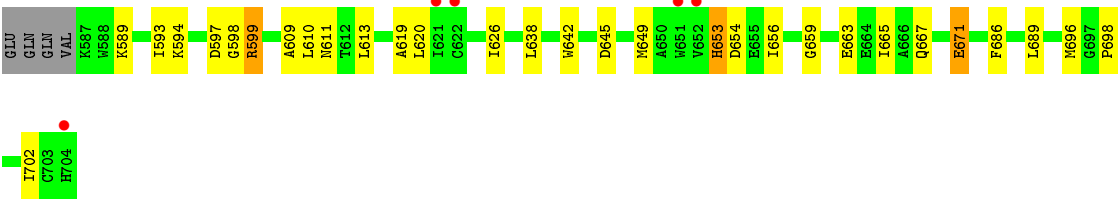
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	6	Total 6	O 6	0	0
6	A	213	Total 213	O 213	0	0
6	B	20	Total 20	O 20	0	0

● Molecule 1: 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'



DC	DC	DC	T5	A6	G7	G8	C9	A10	G14	DC	DC	DG	DT	DC	DG	DT	DT	DT	DT	DC	DG
----	----	----	----	----	----	----	----	-----	-----	----	----	----	----	----	----	----	----	----	----	----	----

A513	A514	L515	P516	T517	R518	A521	L525	Y526	G527	F528	L529	Y530	G531	A532	G533	D534	E535	K536	F537	G538	Q539	I540	A543	G544	K545	E546	A547	G548	K549	E550	L551	K552	F555	L556	E557	A558	R559	F560	A561	I562	R566	I569	L573	V574	E575	SER	SER	GLN	TRP	VAL	ALA	TYR
V420	N421	P422	A425	R429	A430	T431	H432	A433	N436	Q439	I440	P441	G442	P446	Y447	G448	R452	G456	A457	E458	H459	K467	Q471	I474	E480	L481	M488	A489	R490	F491	D492	Y496	E499	I500	L501	D504	I505	H566	T507	K508	N509	Q510	T511	A512								
P301	ASN	LVS	ALA	GLN	ARG	GLY	ARG	F311	P312	C313	D316	V321	A322	G323	P325	Y326	P336	R339	K344	Q347	E348	P353	T354	K355	T357	D358	K359	G360	A361	P362	V363	V364	D365	V368	L369	E370	G371	V372	Y389	K394	K404	Q510	V410									
M167	Y170	N171	V172	Q173	V176	V177	L181	L185	P193	P194	T204	T205	E209	S210	L211	A220	A221	W222	L223	L224	F232	L233	P233	F234	D235	T239	G270	M273	F274	C275	H276	P277	R278	P284	R288	L289	K290	T291	V294	G295	G296	L297	F298	K299	P165	E166						
F18	T28	A29	E30	R35	P36	E49	G53	G54	V57	H62	Q76	R79	E80	R85	I89	T91	V93	L94	R111	Y130	R131	E134	E138	D141	R145	E149	Q150	G151	D156	G157	M158	W161	M164	F165	E166																	



● 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	104.38 Å 214.78 Å 52.18 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 36.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.20) 98.6 (36.90-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.03 (at 2.20 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.262 0.233 , 0.250	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 , 45.4	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: MG, 2DA, TTD

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	0.50	0/180	0.79	0/275
2	T	0.38	0/211	0.76	0/324
3	A	0.34	0/5374	0.57	0/7301
4	B	0.30	0/791	0.55	0/1079
All	All	0.34	0/6556	0.58	0/8979

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

There are no bond length outliers.

There are no bond angle outliers.

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	11	0
2	T	223	0	122	10	0
3	A	5243	0	4982	141	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	174	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 14.

All (174) 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:HH11	3:A:131:ARG:HB3	1.20	1.07
4:B:19:ALA:HB3	4:B:23:ILE:HD11	1.43	0.99
3:A:642:TRP:HH2	3:A:649:MET:HE2	1.29	0.95
3:A:18:PHE:H	3:A:76:GLN:HE22	1.23	0.86
3:A:501:LEU:HD21	3:A:689:LEU:HB3	1.67	0.77
3:A:490:ARG:HB2	3:A:490:ARG:HH11	1.50	0.76
3:A:490:ARG:CB	3:A:490:ARG:HH11	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:667:GLN:HG3	3:A:696:MET:HE1	1.72	0.71
3:A:131:ARG:HH11	3:A:131:ARG:CB	2.02	0.71
3:A:131:ARG:NH1	3:A:131:ARG:HB3	2.02	0.71
3:A:667:GLN:O	3:A:671:GLU:HG2	1.91	0.71
3:A:364:VAL:HA	3:A:368:VAL:HG21	1.73	0.71
4:B:95:SER:OG	4:B:98:GLN:HG3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:164:ASN:HD22	3:A:166:GLU:H	1.44	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
4:B:67:ALA:HB1	4:B:72:ILE:HD12	1.79	0.65
1:P:18:DG:H1'	3:A:394:LYS:NZ	2.11	0.65
3:A:79:ARG:HD3	6:A:5050:HOH:O	1.97	0.65
2:T:5:TTD:H5R2	2:T:5:TTD:H2'	1.77	0.65
1:P:18:DG:H1'	3:A:394:LYS:HZ1	1.62	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: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:642:TRP:CH2	3:A:649:MET:HE2	2.22	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: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:C5R	2:T:5:TTD:H2'	2.36	0.56
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.41	0.56
3:A:488:MET:HE3	3:A:561:ALA:HB3	1.87	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
3:A:642:TRP:HH2	3:A:649:MET:CE	2.11	0.55
4:B:95:SER:H	4:B:98:GLN:NE2	2.04	0.55
1:P:16:DG:H1'	1:P:17:DT:H5''	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:507:THR:HG23	3:A:518:ARG:HH21	1.75	0.51
1:P:16:DG:H2''	1:P:17:DT:C5'	2.41	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
4:B:103:LEU:O	4:B:107:LEU:HD13	2.10	0.51
2:T:5:TTD:O4R	2:T:5:TTD:H2'	2.10	0.51
3:A:347:GLN:NE2	3:A:353:PRO:HG2	2.26	0.51
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.47	0.50
3:A:490:ARG:NH1	3:A:490:ARG:HB2	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:457:ALA:HA	3:A:649:MET:HE1	1.93	0.50
3:A:569:ILE:HD11	3:A:613:LEU:HD22	1.93	0.50
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
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
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
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:358:ASP:C	3:A:360:GLY:H	2.18	0.47
3:A:274:PHE:HD1	3:A:289:ILE:HD13	1.79	0.47
4:B:67:ALA:HB3	4:B:68:PRO:HD3	1.96	0.47
2:T:6:DA:H2'	2:T:7:DG:O4'	2.15	0.47
3:A:566:ARG:HG2	3:A:610:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:436:ASN:O	3:A:439:GLN:HG2	2.15	0.46
3:A:18:PHE:N	3:A:76:GLN:HE22	2.03	0.46
1:P:19:DC:H2"	1:P:20:DC:C6	2.51	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
1:P:15:DA:H4'	3:A:359:LYS:HD2	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
3:A:530:TYR:O	3:A:531:GLY:C	2.54	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
3:A:496:TYR:CE1	3:A:505:ILE:HD11	2.52	0.45
1:P:18:DG:C4	1:P:19:DC:C5	3.05	0.45
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:233:PRO:HB2	3:A:456:GLY:O	2.17	0.45
4:B:89:THR:O	4:B:90:LYS:HD2	2.18	0.44
3:A:359:LYS:HG2	3:A:359:LYS:O	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:446:PRO:O	3:A:447:TYR:HB2	2.19	0.43
3:A:79:ARG:HG2	3:A:80:GLU:N	2.34	0.43
1:P:17:DT:H2"	1:P:18:DG:C8	2.54	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:569:ILE:HD11	3:A:613:LEU:CD2	2.49	0.43
3:A:429:ARG:NH2	3:A:654:ASP:OD1	2.51	0.43
3:A:535:GLU:HA	3:A:545:LYS:N	2.32	0.42
3:A:638:LEU:N	3:A:638:LEU:CD1	2.83	0.42
4:B:41:ILE:O	4:B:45:ILE:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:535:GLU:HA	3:A:545:LYS:H	1.84	0.42
3:A:649:MET:HE3	3:A:659:GLY:HA3	2.00	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:474:ILE:N	3:A:474:ILE:HD12	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: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:211:LEU:HD21	3:A:598:GLY:C	2.41	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
3:A:111:ARG:HG3	3:A:111:ARG:NH1	2.35	0.41
3:A:273:MET:SD	3:A:284:PRO:HA	2.60	0.41
2:T:9:DC:H4'	3:A:432:HIS:O	2.20	0.41
4:B:94:LEU:HD12	4:B:94:LEU:N	2.35	0.41
3:A:131:ARG:NH1	3:A:131:ARG:CB	2.73	0.41
3:A:489:ALA:HA	3:A:492:ASP:OD1	2.21	0.41
3:A:667:GLN:HG3	3:A:696:MET:CE	2.45	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:57:VAL:HG22	3:A:89:ILE:HB	2.02	0.41
3:A:360:GLY:O	3:A:361:ALA:HB2	2.21	0.40
3:A:638:LEU:N	3:A:638:LEU:HD12	2.37	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%)	12	9
4	B	103/108 (95%)	99 (96%)	3 (3%)	1 (1%)	15	14
All	All	775/806 (96%)	740 (96%)	25 (3%)	10 (1%)	12	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
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%)	504 (97%)	16 (3%)	40	51
4	B	78/87 (90%)	75 (96%)	3 (4%)	33	42
All	All	598/666 (90%)	579 (97%)	19 (3%)	39	50

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	62	HIS
3	A	131	ARG

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Mol	Chain	Res	Type
3	A	164	ASN
3	A	171	ASN
3	A	181	LEU
3	A	232	PHE
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	599	ARG
3	A	653	HIS
3	A	671	GLU
3	A	686	PHE
4	B	10	ASP
4	B	89	THR
4	B	99	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	76	GLN
3	A	164	ASN
3	A	276	HIS
3	A	343	GLN
3	A	347	GLN
3	A	510	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	0.50	0	6,12,34	0.44	0
2	TTD	T	5	2	40,40,46	3.94	10 (25%)	58,67,77	3.92	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	-	5/19/101/110	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	-19.52	1.32	1.55
2	T	5	TTD	C5-C6	-10.25	1.43	1.55
2	T	5	TTD	C1R-N1T	5.53	1.52	1.45
2	T	5	TTD	C1'-N1	4.49	1.51	1.45
2	T	5	TTD	C5A-C5	3.92	1.61	1.53
2	T	5	TTD	C2-N3	-3.81	1.31	1.38
2	T	5	TTD	C2-N1	3.31	1.43	1.36
2	T	5	TTD	C5M-C5T	2.93	1.59	1.53
2	T	5	TTD	C6T-C6	2.73	1.64	1.56
2	T	5	TTD	O4R-C1R	-2.12	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	9.81	100.58	88.38
2	T	5	TTD	O4'-C1'-N1	-9.65	97.22	108.65
2	T	5	TTD	O4T-C4T-C5T	9.18	130.20	122.88
2	T	5	TTD	O4R-C1R-N1T	9.10	119.44	108.65
2	T	5	TTD	C2'-C1'-N1	8.01	126.41	115.59
2	T	5	TTD	O5R-PB-O5P	-7.35	80.36	109.07
2	T	5	TTD	O4'-C1'-C2'	-7.30	97.12	107.10
2	T	5	TTD	C5T-C5-C4	7.08	136.57	113.21
2	T	5	TTD	C5A-C5-C4	-6.27	97.41	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	5	TTD	O4P-PB-O5R	-5.22	83.51	107.75
2	T	5	TTD	C5T-C6T-N1T	5.15	122.83	115.61
2	T	5	TTD	C5T-C5-C6	-4.86	82.33	88.38
2	T	5	TTD	C4'-O4R-C1R	-4.43	98.73	109.45
2	T	5	TTD	C5T-C6T-C6	-4.27	82.28	89.28
2	T	5	TTD	O3R-PB-O5P	4.26	125.45	109.47
2	T	5	TTD	C2R-C1R-N1T	-4.23	109.87	115.59
2	T	5	TTD	O4T-C4T-N3T	-4.18	113.85	120.50
2	T	5	TTD	C5-C5T-C4T	-3.71	100.96	113.21
2	T	5	TTD	O4P-PB-O5P	3.54	129.74	112.24
2	T	5	TTD	O4'-C4R-C3R	3.30	108.33	104.09
2	T	5	TTD	C2'-C3R-C4R	-3.15	98.30	102.72
2	T	5	TTD	O4-C4-C5	2.95	125.23	122.88
2	T	5	TTD	C5A-C5-C5T	-2.22	109.97	116.39
2	T	5	TTD	O4-C4-N3	-2.17	117.05	120.50
2	T	5	TTD	C3'-C2R-C1R	-2.11	97.26	102.54

There are no chirality outliers.

All (5) 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

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	8/22 (36%)	-0.16	0 100 100	42, 49, 60, 68	0
2	T	9/25 (36%)	0.36	0 100 100	35, 49, 64, 68	0
3	A	678/698 (97%)	0.33	61 (8%) 9 8	19, 35, 64, 71	0
4	B	105/108 (97%)	0.13	3 (2%) 51 49	31, 45, 58, 60	0
All	All	800/853 (93%)	0.30	64 (8%) 12 11	19, 37, 63, 71	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	544	GLY	7.5
3	A	548	GLY	6.2
3	A	513	ALA	6.0
3	A	298	PHE	5.0
3	A	313	CYS	4.9
3	A	294	VAL	4.5
3	A	545	LYS	4.5
3	A	354	THR	4.3
3	A	546	GLU	4.0
3	A	151	GLY	4.0
3	A	539	GLN	4.0
3	A	540	ILE	3.8
3	A	516	PRO	3.8
3	A	551	LEU	3.4
3	A	297	ILE	3.4
3	A	361	ALA	3.4
3	A	515	LEU	3.4
3	A	358	ASP	3.2
3	A	156	ASP	3.2
3	A	322	ALA	3.1
3	A	321	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	A	295	GLY	2.9
3	A	312	PRO	2.9
3	A	543	ALA	2.9
3	A	534	ASP	2.8
3	A	514	GLU	2.7
3	A	141	ASP	2.7
3	A	111	ARG	2.7
3	A	652	VAL	2.7
3	A	533	GLY	2.7
3	A	549	LYS	2.7
3	A	371	GLY	2.7
4	B	21	GLY	2.6
3	A	300	LYS	2.6
3	A	532	ALA	2.6
3	A	537	ILE	2.6
3	A	420	VAL	2.6
3	A	621	ILE	2.6
3	A	93	VAL	2.6
3	A	360	GLY	2.6
3	A	538	GLY	2.5
3	A	521	ALA	2.5
3	A	145	ARG	2.5
3	A	430	ALA	2.5
3	A	220	ALA	2.5
3	A	530	TYR	2.5
3	A	535	GLU	2.5
3	A	425	ALA	2.5
3	A	422	PRO	2.5
3	A	299	LYS	2.5
3	A	531	GLY	2.4
3	A	221	ALA	2.4
3	A	547	ARG	2.4
3	A	622	CYS	2.4
3	A	556	LEU	2.4
3	A	224	LEU	2.4
4	B	48	GLU	2.3
3	A	433	ALA	2.3
3	A	704	HIS	2.3
3	A	651	TRP	2.2
3	A	558	ASN	2.2
3	A	353	PRO	2.2
4	B	107	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	517	THR	2.1

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(\AA^2)	Q<0.9
2	TTD	T	5	35/41	0.67	0.31	71,73,79,80	0
1	2DA	P	22	10/21	0.88	0.14	59,62,64,64	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
5	MG	A	4003	1/1	0.55	0.34	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.