Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:12 PM GMT

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.; Doublie, 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

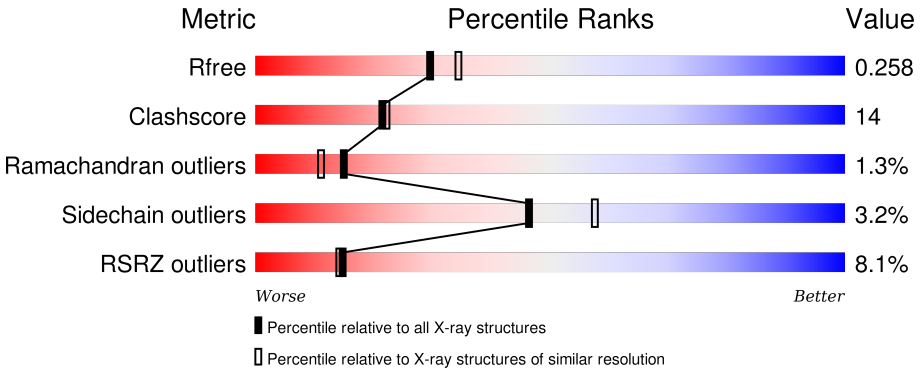
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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. 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 <=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	14% 23% 5% 59%
2	T	25	16% 24% 60%
3	A	698	9% 71% 24%
4	B	108	3% 67% 29%

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
5	MG	A	4003	-	-	-	X

2 Entry composition

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 Mg 1 1	0	0

- Molecule 6 is water.

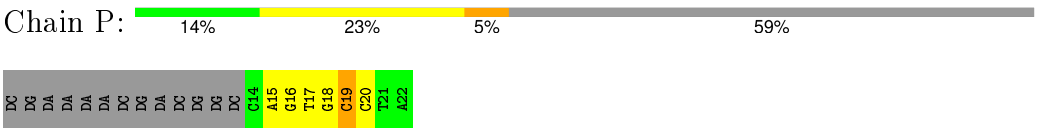
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	213	Total O 213 213	0	0
6	B	20	Total O 20 20	0	0
6	T	6	Total O 6 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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(*CP*GP*AP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*TP*(2DA))-3'

Chain P:

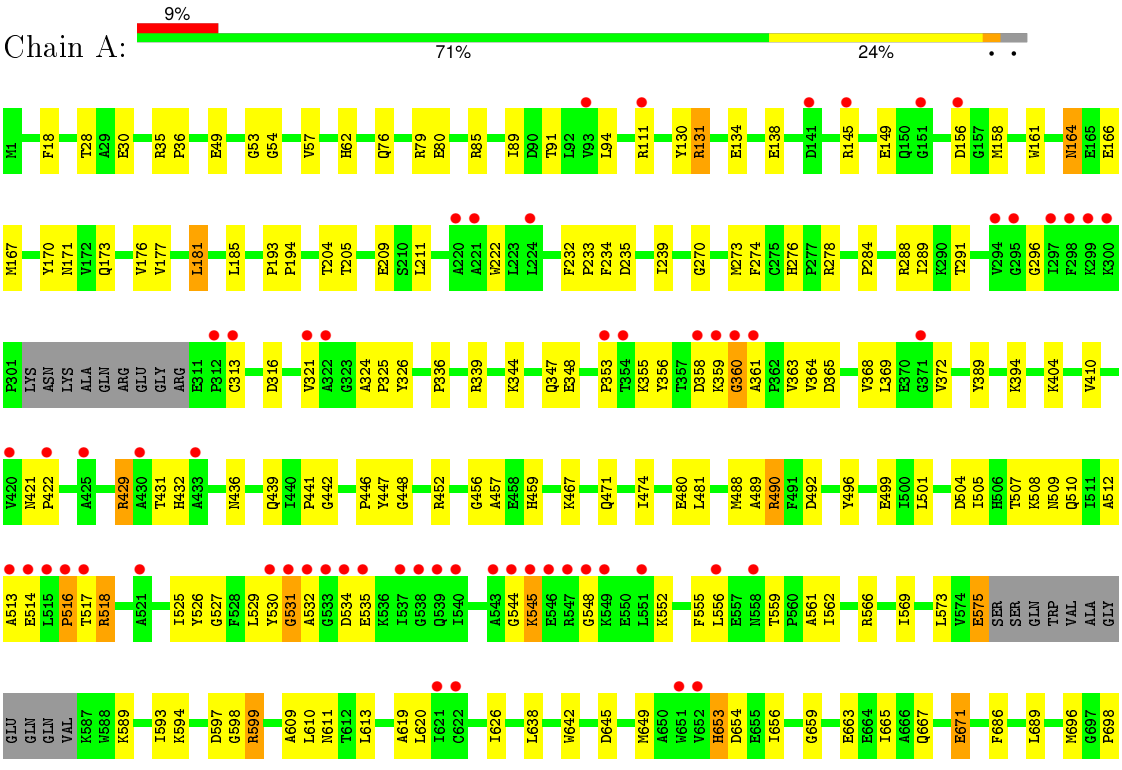


• Molecule 2: 5'-D(*CP*CP*C*(TTD)P*AP*GP*GP*CP*AP*CP*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*TP*CP*G)-3'

Chain T:

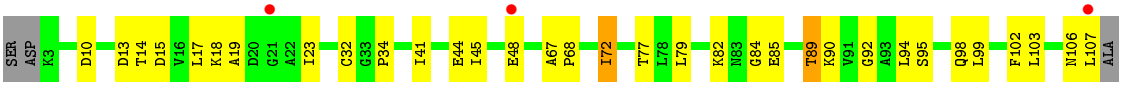
• Molecule 3: DNA polymerase

Chain A:



• Molecule 4: Thioredoxin 1

Chain B:



4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [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%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 59617 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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 (i)

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:HB3	3:A:131:ARG:NH1	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:HE2	3:A:467:LYS:HA	1.76	0.65
1:P:18:DG:H1'	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
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:642:TRP:CH2	3:A:649:MET:HE2	2.22	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: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:642:TRP:HH2	3:A:649:MET:CE	2.11	0.55
3:A:575:GLU:HB2	3:A:589:LYS:HB3	1.89	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
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
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: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: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
2:T:5:TTD:HT	3:A:527:GLY:HA2	1.78	0.48
3:A:525:ILE:HG23	3:A:526:TYR:N	2.28	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
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

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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: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
1:P:19:DC:H2"	1:P:20:DC:C6	2.51	0.46
3:A:626:ILE:HG22	3:A:656:ILE:HG21	1.98	0.46
3:A:535:GLU:HA	3:A:545:LYS:CA	2.46	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
4:B:19:ALA:CB	4:B:23:ILE:HD11	2.31	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
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
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
4:B:95:SER:CB	4:B:98:GLN:HE21	2.30	0.44
3:A:359:LYS:HG2	3:A:359:LYS:O	2.18	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
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:368:VAL:HG23	3:A:369:LEU:N	2.33	0.43
3:A:270:GLY:CA	3:A:288:ARG:HB3	2.48	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
4:B:41:ILE:O	4:B:45:ILE:HD13	2.19	0.42
3:A:638:LEU:N	3:A:638:LEU:CD1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:649:MET:HE3	3:A:659:GLY:HA3	2.00	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: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:H42	2:T:6:DA:H61	1.67	0.42
1:P:20:DC:N4	2:T:6:DA:H61	2.17	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: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:211:LEU:HD21	3:A:598:GLY:C	2.41	0.41
3:A:111:ARG:HG3	3:A:111:ARG:NH1	2.35	0.41
3:A:131:ARG:CB	3:A:131:ARG:NH1	2.73	0.41
3:A:667:GLN:HG3	3:A:696:MET:CE	2.45	0.41
4:B:94:LEU:HD12	4:B:94:LEU:N	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
3:A:489:ALA:HA	3:A:492:ASP:OD1	2.21	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:205:THR:HG23	3:A:209:GLU:HG3	2.03	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:530:TYR:O	3:A:532:ALA:N	2.54	0.40
3:A:355:LYS:HG3	3:A:363:VAL:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	15	11
4	B	103/108 (95%)	99 (96%)	3 (3%)	1 (1%)	19	16
All	All	775/806 (96%)	740 (96%)	25 (3%)	10 (1%)	15	11

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 (i)

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%)	47	59
4	B	78/87 (90%)	75 (96%)	3 (4%)	40	49
All	All	598/666 (90%)	579 (97%)	19 (3%)	46	57

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	6,10,23	0.45	0	7,12,34	0.40	0
2	TTD	T	5	2	39,40,46	3.88	9 (23%)	54,67,77	3.66	23 (42%)

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	-	0/19/101/110	0/3/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	5	TTD	C5T-C6T	-19.19	1.32	1.55
2	T	5	TTD	C5-C6	-10.10	1.43	1.55
2	T	5	TTD	C2-N3	-3.77	1.31	1.38
2	T	5	TTD	O4R-C1R	-2.07	1.37	1.42
2	T	5	TTD	C5M-C5T	2.80	1.59	1.53
2	T	5	TTD	C2-N1	3.21	1.43	1.36
2	T	5	TTD	C5A-C5	3.73	1.61	1.53
2	T	5	TTD	C1'-N1	4.30	1.51	1.45
2	T	5	TTD	C1R-N1T	5.30	1.52	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	5	TTD	C5A-C5-C4	-7.70	97.41	108.41
2	T	5	TTD	O5R-PB-O5P	-7.54	80.36	109.62
2	T	5	TTD	O4'-C1'-C2'	-6.60	97.12	106.86
2	T	5	TTD	O4P-PB-O5R	-4.95	83.51	108.46
2	T	5	TTD	C5T-C5-C6	-4.77	82.33	88.37
2	T	5	TTD	C4'-O4R-C1R	-4.24	98.73	109.46
2	T	5	TTD	C2R-C1R-N1T	-4.22	109.87	115.64
2	T	5	TTD	C5T-C6T-C6	-4.14	82.28	89.27
2	T	5	TTD	C2'-C3R-C4R	-3.96	98.30	103.25
2	T	5	TTD	O4T-C4T-N3T	-3.94	113.85	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	5	TTD	C5-C5T-C4T	-3.56	100.96	113.09
2	T	5	TTD	C3'-C2R-C1R	-2.14	97.26	102.40
2	T	5	TTD	C5A-C5-C5T	-2.05	109.97	116.37
2	T	5	TTD	O4-C4-N3	-2.04	117.05	120.50
2	T	5	TTD	O4-C4-C5	2.84	125.23	122.92
2	T	5	TTD	O4P-PB-O5P	3.18	129.74	112.53
2	T	5	TTD	O3R-PB-O5P	4.07	125.45	109.46
2	T	5	TTD	C5T-C6T-N1T	5.03	122.83	115.70
2	T	5	TTD	PB-O3R-C3R	5.44	139.35	119.41
2	T	5	TTD	C5T-C5-C4	6.89	136.57	113.09
2	T	5	TTD	C2'-C1'-N1	7.86	126.41	115.64
2	T	5	TTD	O4T-C4T-C5T	8.94	130.20	122.92
2	T	5	TTD	C5-C5T-C6T	9.65	100.58	88.37

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
2	T	5	TTD	5	0

5.5 Carbohydrates (i)

There are no carbohydrates 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, 95^{th} 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%)	-0.10	0 100 100	42, 49, 60, 68	0
2	T	9/25 (36%)	0.42	0 100 100	35, 49, 64, 68	0
3	A	678/698 (97%)	0.39	62 (9%) 11 11	19, 35, 64, 71	0
4	B	105/108 (97%)	0.19	3 (2%) 55 54	31, 45, 58, 60	0
All	All	800/853 (93%)	0.36	65 (8%) 15 14	19, 37, 63, 71	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	544	GLY	7.8
3	A	548	GLY	6.4
3	A	513	ALA	6.2
3	A	298	PHE	5.2
3	A	313	CYS	5.2
3	A	294	VAL	4.7
3	A	545	LYS	4.6
3	A	354	THR	4.5
3	A	546	GLU	4.2
3	A	151	GLY	4.2
3	A	539	GLN	4.1
3	A	540	ILE	4.0
3	A	516	PRO	3.9
3	A	297	ILE	3.6
3	A	551	LEU	3.6
3	A	361	ALA	3.5
3	A	515	LEU	3.5
3	A	358	ASP	3.4
3	A	156	ASP	3.3
3	A	322	ALA	3.2
3	A	321	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	295	GLY	3.0
3	A	312	PRO	3.0
3	A	543	ALA	3.0
3	A	534	ASP	2.9
3	A	652	VAL	2.8
3	A	533	GLY	2.8
3	A	141	ASP	2.8
3	A	514	GLU	2.8
3	A	371	GLY	2.8
3	A	111	ARG	2.8
4	B	21	GLY	2.8
3	A	420	VAL	2.7
3	A	537	ILE	2.7
3	A	532	ALA	2.7
3	A	549	LYS	2.7
3	A	93	VAL	2.7
3	A	621	ILE	2.7
3	A	300	LYS	2.7
3	A	360	GLY	2.7
3	A	521	ALA	2.7
3	A	538	GLY	2.7
3	A	220	ALA	2.6
3	A	430	ALA	2.6
3	A	145	ARG	2.6
3	A	530	TYR	2.6
3	A	422	PRO	2.6
3	A	425	ALA	2.6
3	A	531	GLY	2.6
3	A	535	GLU	2.6
3	A	221	ALA	2.6
3	A	622	CYS	2.6
3	A	299	LYS	2.5
3	A	556	LEU	2.5
3	A	547	ARG	2.5
3	A	224	LEU	2.5
3	A	433	ALA	2.4
4	B	48	GLU	2.4
3	A	704	HIS	2.4
3	A	651	TRP	2.4
3	A	558	ASN	2.3
4	B	107	LEU	2.3
3	A	353	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	517	THR	2.2
3	A	359	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	2DA	P	22	10/21	0.88	0.14	-	59,62,64,64	0
2	TTD	T	5	35/41	0.67	0.31	-	71,73,79,80	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	MG	A	4003	1/1	0.55	0.34	8.97	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.