Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:40 PM GMT

PDB ID	:	1L9Z
Title	:	Thermus aquaticus RNA Polymerase Holoenzyme/Fork-Junction Promoter DNA Complex at 6.5 A Resolution
Authors	:	Murakami, K.S.; Masuda, S.; Campbell, E.A.; Muzzin, O.; Darst, S.A.
Deposited on	:	2002-03-27
Resolution	:	6.50 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 (i) symbol.

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

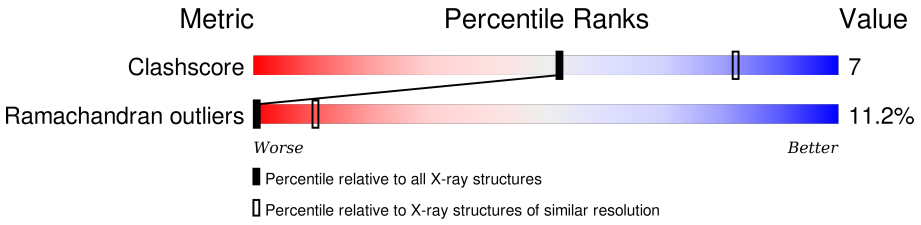
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 6.50 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))
Clashscore	102246	1060 (9.00-3.70)
Ramachandran outliers	100387	1033 (9.00-3.66)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	U	35	26% 54% 20%
2	T	30	60% 13% 27%
3	A	314	62% 9% 29%
3	B	314	61% 9% 30%
4	C	1118	86% 11% .
5	D	1524	66% 11% 22%
6	E	99	88% 5% 7%
7	H	438	63% 10% 27%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10078 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 nontemplate DNA strand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	U	35	Total	C	O	P	0	0	0
			382	175	173	34			

- Molecule 2 is a DNA chain called template DNA strand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	T	30	Total	C	O	P	0	0	0
			327	150	148	29			

- Molecule 3 is a protein called RNA POLYMERASE, ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	A	224	Total	C	N	0	0	0
			672	448	224			
3	B	220	Total	C	N	0	0	0
			660	440	220			

- Molecule 4 is a protein called RNA POLYMERASE, BETA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	C	1084	Total	C	N	0	0	0
			3252	2168	1084			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	DELETION	UNP Q9KWU7

- Molecule 5 is a protein called RNA POLYMERASE, BETA-PRIME SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	D	1183	Total 3549	C 2366	N 1183	0	0	0

- Molecule 6 is a protein called RNA POLYMERASE, OMEGA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	E	92	Total 276	C 184	N 92	0	0	0

- Molecule 7 is a protein called SIGMA FACTOR SIGA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
7	H	319	Total 957	C 638	N 319	0	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total 1	Mg 1	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total 2	Zn 2	0	0

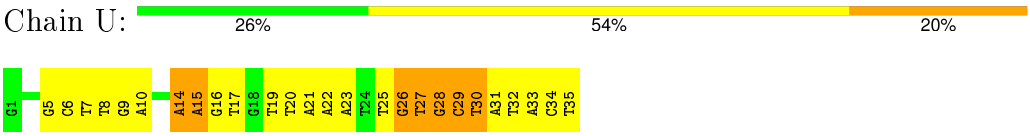
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: nontemplate DNA strand

Chain U:

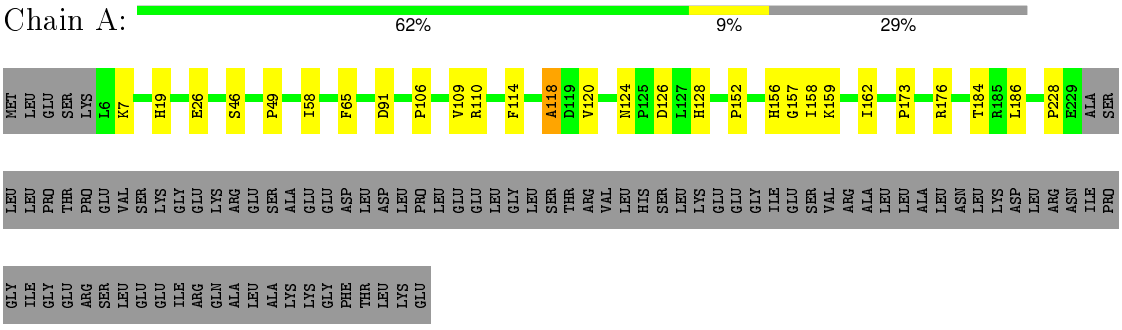


- Molecule 2: template DNA strand

Chain T:

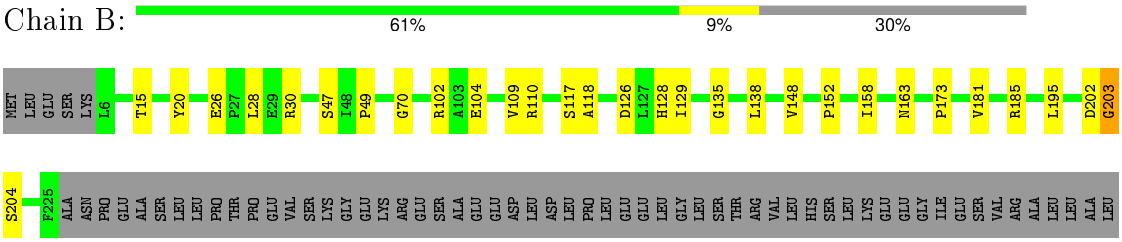
- Molecule 3: RNA POLYMERASE, ALPHA SUBUNIT

Chain A:



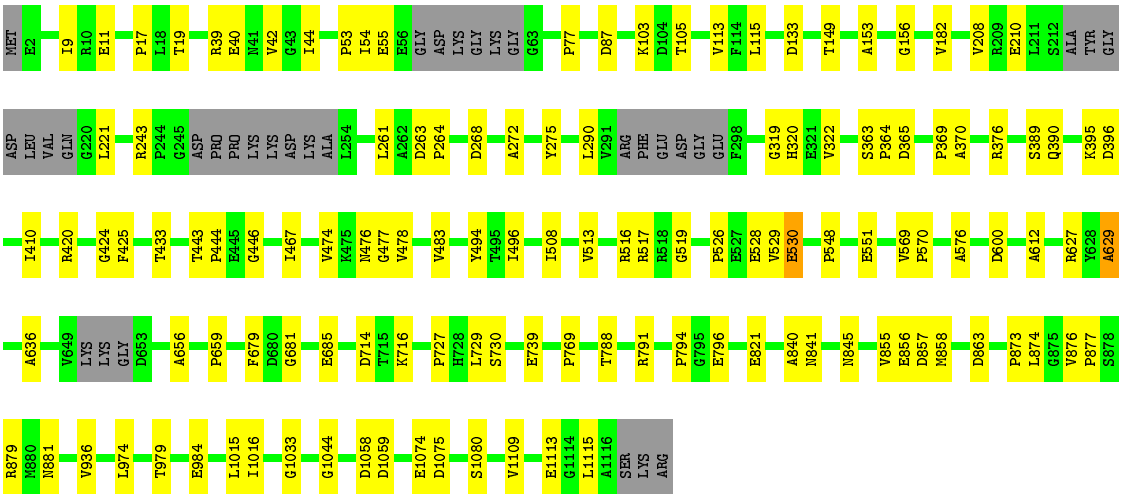
- Molecule 3: RNA POLYMERASE, ALPHA SUBUNIT

Chain B:



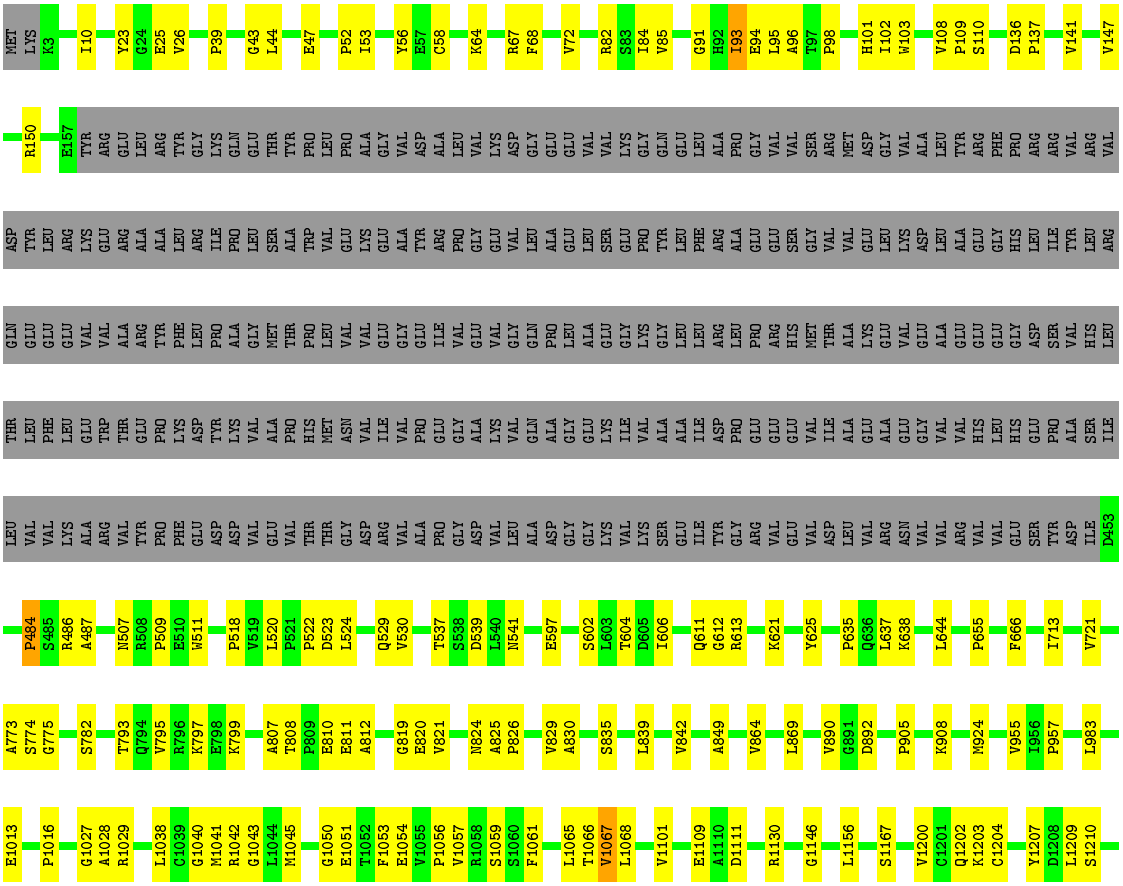
- Molecule 4: RNA POLYMERASE, BETA SUBUNIT

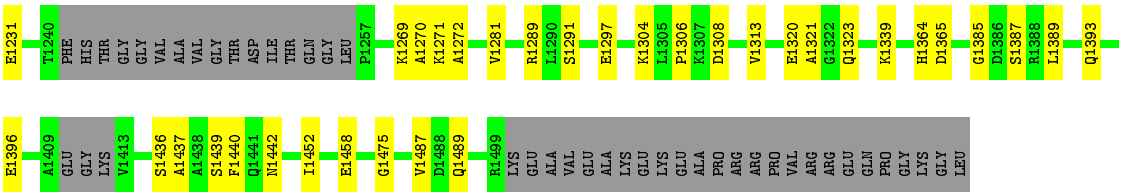
Chain C:



- Molecule 5: RNA POLYMERASE, BETA-PRIME SUBUNIT

Chain D:



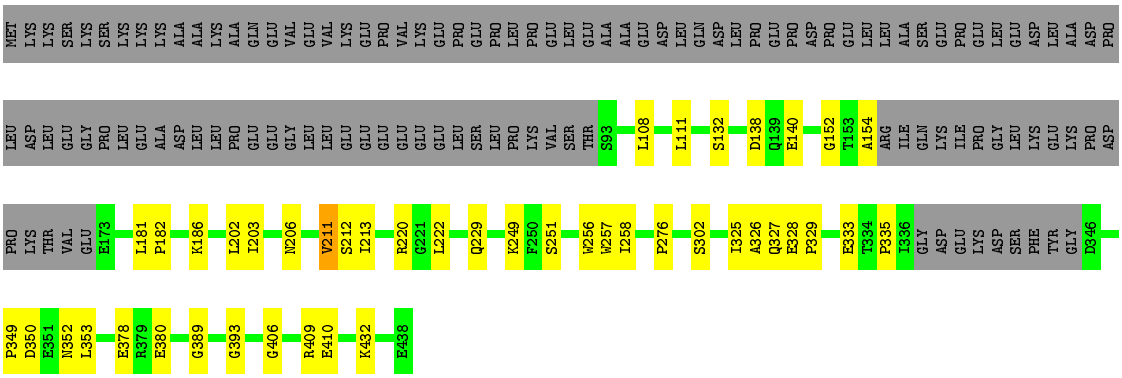


• Molecule 6: RNA POLYMERASE, OMEGA SUBUNIT

Chain E:

• Molecule 7: SIGMA FACTOR SIGA

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	180.95Å 180.95Å 523.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 6.50	Depositor
% Data completeness (in resolution range)	(Not available) (80.00-6.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	?	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10078	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	U	1.48	2/416 (0.5%)	3.85	36/622 (5.8%)
2	T	4.58	8/356 (2.2%)	3.82	23/532 (4.3%)
3	A	0.20	0/671	0.47	0/670
3	B	0.20	0/659	0.53	0/658
4	C	0.19	0/3246	0.41	0/3240
5	D	0.19	0/3545	0.41	0/3541
6	E	0.20	0/275	0.35	0/274
7	H	0.20	0/954	0.49	0/951
All	All	0.93	10/10122 (0.1%)	1.34	59/10488 (0.6%)

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	U	1	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	174	DA	O3'-P	-48.81	1.02	1.61
2	T	185	DC	O3'-P	-48.24	1.03	1.61
2	T	172	DG	O3'-P	-39.32	1.14	1.61
2	T	175	DC	O3'-P	-23.63	1.32	1.61
1	U	26	DG	O3'-P	-23.04	1.33	1.61
2	T	171	DA	O3'-P	17.05	1.81	1.61
1	U	25	DT	O3'-P	-11.97	1.46	1.61
2	T	173	DC	O3'-P	-10.20	1.49	1.61
2	T	186	DT	O3'-P	-9.31	1.50	1.61
2	T	184	DA	O3'-P	6.24	1.68	1.61

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	28	DG	P-O3'-C3'	-45.80	64.74	119.70
1	U	30	DT	P-O3'-C3'	-41.74	69.61	119.70
2	T	171	DA	P-O3'-C3'	-36.19	76.27	119.70
2	T	173	DC	P-O3'-C3'	36.09	163.01	119.70
1	U	28	DG	OP2-P-O3'	30.75	172.85	105.20
2	T	171	DA	OP2-P-O3'	22.82	155.40	105.20
2	T	174	DA	P-O3'-C3'	21.76	145.82	119.70
1	U	28	DG	OP1-P-O3'	-20.74	59.57	105.20
2	T	172	DG	OP1-P-O3'	20.07	149.35	105.20
2	T	185	DC	P-O3'-C3'	19.13	142.65	119.70
2	T	173	DC	OP1-P-O3'	18.91	146.81	105.20
1	U	15	DA	OP2-P-O3'	17.38	143.44	105.20
1	U	30	DT	O3'-P-O5'	17.20	136.69	104.00
2	T	172	DG	OP2-P-O3'	-16.35	69.23	105.20
1	U	30	DT	OP1-P-O3'	-14.79	72.66	105.20
1	U	14	DA	P-O3'-C3'	-14.46	102.34	119.70
2	T	173	DC	OP2-P-O3'	-14.07	74.25	105.20
2	T	171	DA	OP1-P-O3'	-13.82	74.80	105.20
1	U	28	DG	O3'-P-O5'	-13.73	77.92	104.00
2	T	174	DA	OP1-P-O3'	11.48	130.47	105.20
1	U	14	DA	OP1-P-O3'	-11.13	80.72	105.20
1	U	26	DG	P-O3'-C3'	10.46	132.25	119.70
1	U	14	DA	O3'-P-O5'	9.72	122.47	104.00
2	T	171	DA	O3'-P-O5'	-9.68	85.60	104.00
1	U	15	DA	O3'-P-O5'	-9.33	86.27	104.00
2	T	175	DC	P-O3'-C3'	8.87	130.35	119.70
2	T	185	DC	OP2-P-O3'	-8.44	86.62	105.20
1	U	28	DG	C5'-C4'-C3'	-8.22	99.31	114.10
1	U	15	DA	OP1-P-O3'	-7.83	87.97	105.20
1	U	15	DA	P-O3'-C3'	-7.61	110.57	119.70
2	T	174	DA	OP2-P-O3'	-6.98	89.85	105.20
2	T	185	DC	OP1-P-O3'	6.80	120.16	105.20
1	U	29	DC	C4'-C3'-C2'	6.74	109.17	103.10
1	U	14	DA	O4'-C1'-C2'	6.20	110.86	105.90
1	U	27	DT	C5'-C4'-C3'	-6.10	103.13	114.10
1	U	22	DA	O4'-C1'-C2'	6.04	110.74	105.90
1	U	23	DA	O4'-C1'-C2'	5.99	110.69	105.90
1	U	28	DG	C4'-C3'-O3'	5.88	124.41	109.70
1	U	21	DA	O4'-C1'-C2'	5.88	110.60	105.90
1	U	26	DG	OP1-P-O3'	5.79	117.94	105.20
2	T	186	DT	P-O3'-C3'	5.47	126.26	119.70
2	T	176	DA	C4'-C3'-C2'	5.42	107.98	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	20	DT	O4'-C1'-C2'	5.37	110.20	105.90
1	U	30	DT	C5'-C4'-C3'	-5.37	104.43	114.10
2	T	175	DC	O4'-C1'-C2'	5.34	110.17	105.90
1	U	17	DT	O4'-C1'-C2'	5.28	110.13	105.90
2	T	175	DC	OP1-P-O3'	5.26	116.78	105.20
2	T	176	DA	C5'-C4'-C3'	-5.24	104.67	114.10
1	U	7	DT	O4'-C1'-C2'	5.21	110.07	105.90
1	U	19	DT	O4'-C1'-C2'	5.17	110.04	105.90
1	U	29	DC	O5'-P-OP1	5.13	116.86	110.70
1	U	10	DA	O4'-C1'-C2'	5.12	110.00	105.90
2	T	185	DC	O4'-C1'-C2'	5.12	110.00	105.90
2	T	179	DT	O4'-C1'-C2'	5.10	109.98	105.90
1	U	5	DG	O4'-C1'-C2'	5.08	109.96	105.90
1	U	8	DT	O4'-C1'-C2'	5.06	109.95	105.90
1	U	9	DG	O4'-C1'-C2'	5.05	109.94	105.90
1	U	16	DG	O4'-C1'-C2'	5.05	109.94	105.90
1	U	6	DC	O4'-C1'-C2'	5.03	109.92	105.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	U	28	DG	C3'

There are no planarity outliers.

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	U	382	0	212	23	0
2	T	327	0	184	28	0
3	A	672	0	241	2	0
3	B	660	0	238	2	0
4	C	3252	0	1199	10	0
5	D	3549	0	1291	23	0
6	E	276	0	96	0	0
7	H	957	0	339	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	1	0	0	0	0
9	D	2	0	0	0	0
All	All	10078	0	3800	93	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 7.

All (93) 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)
2:T:174:DA:O3'	2:T:175:DC:P	1.02	1.41
2:T:185:DC:O3'	2:T:186:DT:P	1.03	1.40
1:U:29:DC:C1'	1:U:30:DT:H5'	1.49	1.40
1:U:28:DG:C1'	1:U:29:DC:H5'	1.24	1.38
2:T:174:DA:C3'	2:T:175:DC:P	2.34	1.15
1:U:28:DG:C1'	1:U:29:DC:C5'	2.21	1.14
2:T:185:DC:C3'	2:T:186:DT:P	2.34	1.13
2:T:185:DC:HO3'	2:T:186:DT:P	0.98	1.11
2:T:174:DA:HO3'	2:T:175:DC:P	1.12	1.03
2:T:185:DC:O3'	2:T:186:DT:OP2	1.75	1.03
2:T:174:DA:O3'	2:T:175:DC:OP2	1.80	0.98
1:U:29:DC:C1'	1:U:30:DT:C5'	2.45	0.92
5:D:1043:GLY:HA3	5:D:1057:VAL:H	1.41	0.85
1:U:14:DA:H2"	1:U:15:DA:OP2	1.75	0.83
2:T:185:DC:C3'	2:T:186:DT:OP2	2.26	0.83
2:T:176:DA:C3'	2:T:177:DA:H5'	2.12	0.78
2:T:172:DG:C4'	2:T:173:DC:P	2.63	0.77
2:T:172:DG:H4'	2:T:173:DC:P	2.26	0.76
2:T:185:DC:H3'	2:T:186:DT:OP2	1.87	0.73
1:U:27:DT:C1'	1:U:28:DG:H5'	2.18	0.73
2:T:176:DA:C2'	2:T:177:DA:H5'	2.18	0.72
1:U:14:DA:C2'	1:U:15:DA:OP2	2.35	0.71
1:U:29:DC:C2'	1:U:30:DT:H5'	2.22	0.69
2:T:174:DA:C3'	2:T:175:DC:OP2	2.37	0.68
2:T:175:DC:C3'	2:T:176:DA:H5'	2.24	0.68
2:T:171:DA:C1'	2:T:172:DG:H5'	2.25	0.66
1:U:29:DC:O4'	1:U:30:DT:H5'	1.96	0.65
2:T:175:DC:C1'	2:T:176:DA:H5'	2.29	0.62
2:T:172:DG:H4'	2:T:173:DC:OP1	1.99	0.62
3:A:118:ALA:C	3:A:120:VAL:H	2.05	0.58
1:U:33:DA:H2"	1:U:34:DC:OP2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:34:DC:H2"	1:U:35:DT:OP2	2.05	0.56
1:U:32:DT:H2"	1:U:33:DA:OP2	2.05	0.56
1:U:31:DA:H2"	1:U:32:DT:OP2	2.05	0.56
2:T:177:DA:C3'	2:T:178:DT:H5'	2.36	0.55
5:D:1043:GLY:HA3	5:D:1057:VAL:N	2.19	0.53
4:C:1044:GLY:HA2	5:D:1475:GLY:HA2	1.91	0.52
1:U:29:DC:C3'	1:U:30:DT:C5'	2.89	0.51
4:C:474:VAL:C	4:C:476:ASN:H	2.13	0.51
5:D:539:ASP:C	5:D:541:ASN:H	2.14	0.50
1:U:28:DG:O5'	1:U:28:DG:C2'	2.59	0.50
7:H:256:TRP:C	7:H:258:ILE:H	2.13	0.50
4:C:627:ARG:C	4:C:629:ALA:H	2.14	0.50
4:C:208:VAL:C	4:C:210:GLU:H	2.15	0.50
2:T:175:DC:C4'	2:T:176:DA:H5'	2.42	0.50
2:T:176:DA:H2"	2:T:177:DA:H5'	1.94	0.49
5:D:1385:GLY:C	5:D:1387:SER:H	2.16	0.49
5:D:810:GLU:C	5:D:812:ALA:H	2.15	0.49
1:U:27:DT:C2'	1:U:28:DG:O5'	2.60	0.49
2:T:171:DA:C1'	2:T:172:DG:C5'	2.90	0.49
5:D:1066:THR:C	5:D:1068:LEU:H	2.16	0.49
4:C:727:PRO:C	4:C:729:LEU:H	2.17	0.48
5:D:484:PRO:C	5:D:486:ARG:H	2.15	0.48
1:U:27:DT:H2"	1:U:28:DG:O5'	2.13	0.48
2:T:176:DA:C3'	2:T:177:DA:C5'	2.90	0.48
3:B:70:GLY:HA3	3:B:135:GLY:HA3	1.95	0.47
3:B:173:PRO:CA	3:B:203:GLY:HA3	2.44	0.47
7:H:152:GLY:C	7:H:154:ALA:H	2.18	0.47
2:T:175:DC:C3'	2:T:176:DA:C5'	2.93	0.47
7:H:211:VAL:C	7:H:213:ILE:H	2.18	0.47
4:C:679:PHE:C	4:C:681:GLY:H	2.17	0.46
1:U:28:DG:H2"	1:U:29:DC:C3'	2.44	0.46
4:C:528:GLU:C	4:C:530:GLU:H	2.19	0.46
5:D:1202:GLN:C	5:D:1204:CYS:H	2.18	0.46
2:T:176:DA:C1'	2:T:177:DA:H5'	2.45	0.45
5:D:1270:ALA:C	5:D:1272:ALA:H	2.19	0.45
1:U:27:DT:C1'	1:U:28:DG:C5'	2.91	0.45
5:D:604:THR:C	5:D:606:ILE:H	2.19	0.45
5:D:91:GLY:C	5:D:93:ILE:H	2.20	0.44
4:C:320:HIS:C	4:C:322:VAL:H	2.20	0.44
1:U:29:DC:C2'	1:U:30:DT:C5'	2.91	0.44
5:D:1289:ARG:C	5:D:1291:SER:H	2.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:101:HIS:C	5:D:103:TRP:H	2.22	0.44
1:U:29:DC:C3'	1:U:30:DT:H5'	2.47	0.43
4:C:17:PRO:C	4:C:19:THR:H	2.21	0.43
7:H:256:TRP:C	7:H:258:ILE:N	2.72	0.43
5:D:602:SER:C	5:D:604:THR:H	2.23	0.43
7:H:378:GLU:C	7:H:380:GLU:H	2.22	0.43
2:T:175:DC:C2'	2:T:176:DA:H5'	2.49	0.42
5:D:108:VAL:C	5:D:110:SER:H	2.23	0.42
5:D:1043:GLY:C	5:D:1045:MET:H	2.21	0.42
5:D:82:ARG:C	5:D:84:ILE:H	2.23	0.42
5:D:1269:LYS:C	5:D:1271:LYS:H	2.22	0.41
1:U:28:DG:O5'	1:U:28:DG:H2'	2.20	0.41
5:D:91:GLY:C	5:D:93:ILE:N	2.74	0.41
5:D:1065:LEU:C	5:D:1067:VAL:H	2.24	0.41
2:T:177:DA:C2'	2:T:178:DT:H5'	2.50	0.41
5:D:56:TYR:C	5:D:58:CYS:H	2.24	0.41
5:D:509:PRO:C	5:D:511:TRP:H	2.23	0.41
1:U:26:DG:C1'	1:U:27:DT:H5'	2.51	0.41
7:H:138:ASP:C	7:H:140:GLU:H	2.23	0.41
4:C:714:ASP:C	4:C:716:LYS:H	2.23	0.41
3:A:118:ALA:C	3:A:120:VAL:N	2.71	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	222/314 (71%)	149 (67%)	46 (21%)	27 (12%)	0 8
3	B	218/314 (69%)	144 (66%)	47 (22%)	27 (12%)	0 8
4	C	1072/1118 (96%)	710 (66%)	251 (23%)	111 (10%)	1 12
5	D	1175/1524 (77%)	742 (63%)	294 (25%)	139 (12%)	0 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	E	90/99 (91%)	74 (82%)	11 (12%)	5 (6%)	2 28
7	H	313/438 (72%)	227 (72%)	50 (16%)	36 (12%)	0 9
All	All	3090/3807 (81%)	2046 (66%)	699 (23%)	345 (11%)	0 10

All (345) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	58	ILE
3	A	156	HIS
3	A	158	ILE
3	A	186	LEU
3	B	20	TYR
3	B	104	GLU
3	B	117	SER
3	B	128	HIS
3	B	158	ILE
3	B	195	LEU
3	B	204	SER
4	C	11	GLU
4	C	42	VAL
4	C	103	LYS
4	C	263	ASP
4	C	290	LEU
4	C	370	ALA
4	C	410	ILE
4	C	467	ILE
4	C	483	VAL
4	C	517	ARG
4	C	530	GLU
4	C	548	PRO
4	C	551	GLU
4	C	600	ASP
4	C	659	PRO
4	C	739	GLU
4	C	841	ASN
4	C	855	VAL
4	C	856	GLU
4	C	863	ASP
4	C	879	ARG
4	C	1058	ASP
4	C	1074	GLU

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Mol	Chain	Res	Type
5	D	26	VAL
5	D	39	PRO
5	D	44	LEU
5	D	52	PRO
5	D	64	LYS
5	D	98	PRO
5	D	109	PRO
5	D	141	VAL
5	D	484	PRO
5	D	522	PRO
5	D	524	LEU
5	D	529	GLN
5	D	530	VAL
5	D	637	LEU
5	D	666	PHE
5	D	773	ALA
5	D	793	THR
5	D	795	VAL
5	D	808	THR
5	D	829	VAL
5	D	830	ALA
5	D	869	LEU
5	D	892	ASP
5	D	905	PRO
5	D	1013	GLU
5	D	1059	SER
5	D	1067	VAL
5	D	1101	VAL
5	D	1200	VAL
5	D	1203	LYS
5	D	1281	VAL
5	D	1306	PRO
5	D	1313	VAL
5	D	1323	GLN
5	D	1364	HIS
5	D	1365	ASP
5	D	1440	PHE
5	D	1458	GLU
5	D	1487	VAL
6	E	42	PRO
7	H	211	VAL
7	H	328	GLU

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Mol	Chain	Res	Type
7	H	329	PRO
7	H	335	PRO
7	H	349	PRO
7	H	350	ASP
7	H	409	ARG
7	H	410	GLU
3	A	26	GLU
3	A	118	ALA
3	A	128	HIS
3	A	152	PRO
3	B	26	GLU
3	B	47	SER
3	B	109	VAL
3	B	110	ARG
3	B	163	ASN
3	B	185	ARG
3	B	202	ASP
3	B	203	GLY
4	C	87	ASP
4	C	113	VAL
4	C	153	ALA
4	C	268	ASP
4	C	365	ASP
4	C	389	SER
4	C	424	GLY
4	C	444	PRO
4	C	477	GLY
4	C	478	VAL
4	C	529	VAL
4	C	612	ALA
4	C	769	PRO
4	C	788	THR
4	C	840	ALA
4	C	857	ASP
4	C	873	PRO
4	C	936	VAL
4	C	979	THR
4	C	1016	ILE
4	C	1059	ASP
4	C	1113	GLU
4	C	1115	LEU
5	D	10	ILE

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Mol	Chain	Res	Type
5	D	47	GLU
5	D	67	ARG
5	D	72	VAL
5	D	85	VAL
5	D	93	ILE
5	D	95	LEU
5	D	96	ALA
5	D	523	ASP
5	D	782	SER
5	D	821	VAL
5	D	824	ASN
5	D	839	LEU
5	D	908	LYS
5	D	1016	PRO
5	D	1038	LEU
5	D	1041	MET
5	D	1109	GLU
5	D	1156	LEU
5	D	1207	TYR
5	D	1209	LEU
5	D	1210	SER
5	D	1231	GLU
5	D	1297	GLU
5	D	1396	GLU
5	D	1436	SER
5	D	1439	SER
5	D	1442	ASN
5	D	1452	ILE
7	H	108	LEU
7	H	111	LEU
7	H	186	LYS
7	H	203	ILE
7	H	249	LYS
7	H	251	SER
7	H	302	SER
7	H	325	ILE
7	H	327	GLN
7	H	389	GLY
7	H	406	GLY
3	A	19	HIS
3	A	46	SER
3	A	157	GLY

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Mol	Chain	Res	Type
3	A	176	ARG
3	A	184	THR
3	B	15	THR
3	B	28	LEU
4	C	9	ILE
4	C	39	ARG
4	C	40	GLU
4	C	77	PRO
4	C	105	THR
4	C	221	LEU
4	C	272	ALA
4	C	363	SER
4	C	420	ARG
4	C	425	PHE
4	C	446	GLY
4	C	494	TYR
4	C	519	GLY
4	C	526	PRO
4	C	636	ALA
4	C	656	ALA
4	C	685	GLU
4	C	730	SER
4	C	821	GLU
4	C	845	ASN
4	C	874	LEU
4	C	984	GLU
4	C	1080	SER
5	D	23	TYR
5	D	53	ILE
5	D	68	PHE
5	D	94	GLU
5	D	137	PRO
5	D	147	VAL
5	D	507	ASN
5	D	611	GLN
5	D	635	PRO
5	D	644	LEU
5	D	655	PRO
5	D	774	SER
5	D	775	GLY
5	D	807	ALA
5	D	811	GLU

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Mol	Chain	Res	Type
5	D	825	ALA
5	D	924	MET
5	D	983	LEU
5	D	1042	ARG
5	D	1053	PHE
5	D	1056	PRO
5	D	1111	ASP
5	D	1146	GLY
5	D	1308	ASP
5	D	1320	GLU
5	D	1321	ALA
5	D	1389	LEU
5	D	1393	GLN
5	D	1437	ALA
6	E	52	GLU
7	H	212	SER
7	H	220	ARG
7	H	222	LEU
7	H	229	GLN
7	H	257	TRP
7	H	352	ASN
7	H	353	LEU
7	H	393	GLY
7	H	432	LYS
3	A	7	LYS
3	A	49	PRO
3	A	65	PHE
3	A	106	PRO
3	A	110	ARG
3	A	114	PHE
3	A	162	ILE
3	B	30	ARG
3	B	118	ALA
3	B	126	ASP
3	B	138	LEU
4	C	53	PRO
4	C	55	GLU
4	C	115	LEU
4	C	133	ASP
4	C	149	THR
4	C	261	LEU
4	C	319	GLY

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Mol	Chain	Res	Type
4	C	390	GLN
4	C	395	LYS
4	C	396	ASP
4	C	513	VAL
4	C	576	ALA
4	C	629	ALA
4	C	791	ARG
4	C	796	GLU
5	D	25	GLU
5	D	150	ARG
5	D	487	ALA
5	D	612	GLY
5	D	613	ARG
5	D	625	TYR
5	D	638	LYS
5	D	721	VAL
5	D	797	LYS
5	D	799	LYS
5	D	835	SER
5	D	849	ALA
5	D	1028	ALA
5	D	1029	ARG
5	D	1061	PHE
5	D	1489	GLN
7	H	132	SER
7	H	182	PRO
7	H	206	ASN
7	H	276	PRO
7	H	326	ALA
7	H	333	GLU
3	A	109	VAL
3	A	126	ASP
3	A	159	LYS
3	A	228	PRO
3	B	49	PRO
3	B	102	ARG
3	B	148	VAL
4	C	264	PRO
4	C	275	TYR
4	C	376	ARG
4	C	433	THR
4	C	496	ILE

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Mol	Chain	Res	Type
4	C	508	ILE
4	C	569	VAL
4	C	794	PRO
4	C	876	VAL
4	C	1015	LEU
4	C	1075	ASP
5	D	136	ASP
5	D	518	PRO
5	D	537	THR
5	D	621	LYS
5	D	826	PRO
5	D	864	VAL
5	D	1051	GLU
5	D	1304	LYS
6	E	4	PRO
6	E	79	LEU
7	H	202	LEU
3	A	124	ASN
4	C	44	ILE
4	C	516	ARG
4	C	858	MET
4	C	881	ASN
4	C	974	LEU
4	C	1033	GLY
5	D	43	GLY
5	D	597	GLU
5	D	820	GLU
5	D	1050	GLY
5	D	1054	GLU
5	D	1130	ARG
5	D	1167	SER
5	D	1339	LYS
7	H	181	LEU
3	B	129	ILE
3	B	152	PRO
5	D	102	ILE
5	D	955	VAL
5	D	1040	GLY
6	E	41	GLU
3	A	91	ASP
4	C	54	ILE
4	C	364	PRO

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Mol	Chain	Res	Type
4	C	443	THR
5	D	520	LEU
5	D	957	PRO
3	B	181	VAL
4	C	182	VAL
4	C	243	ARG
4	C	877	PRO
5	D	713	ILE
5	D	1027	GLY
3	A	173	PRO
4	C	570	PRO
5	D	819	GLY
5	D	842	VAL
5	D	890	VAL
4	C	156	GLY
4	C	369	PRO
4	C	1109	VAL

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.