



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:17 PM UTC

PDB ID : 6WOY / pdb_00006woy
Title : Thermus thermophilus RNA polymerase initially transcribing complex with 3'dCTP
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2020-04-26
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

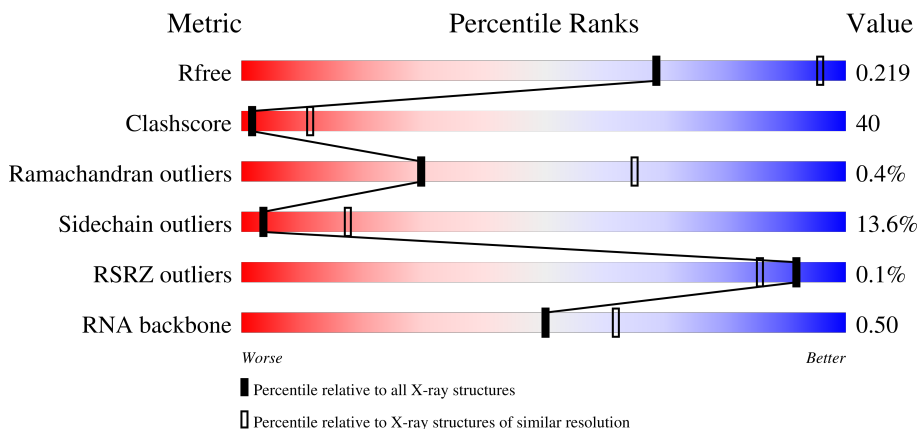
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	A	315	
1	B	315	
2	C	1119	
3	D	1505	

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Mol	Chain	Length	Quality of chain
4	E	99	41%47%6%5%
5	F	423	30%43%8%18%
6	G	22	23%55%23%
7	H	27	30%63%7%
8	I	3	33%67%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28581 atoms, of which 12 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 protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1485	Total	C	N	O	S	0	0	0
			11721	7431	2063	2192	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	86	LYS	ARG	conflict	UNP Q8RQE8

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	P	0	0	0
			351	166	65	103	17			

- Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

- Molecule 8 is a RNA chain called RNA (5'-R(*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	3	Total	C	N	O	P	0	0	0
			62	29	13	18	2			

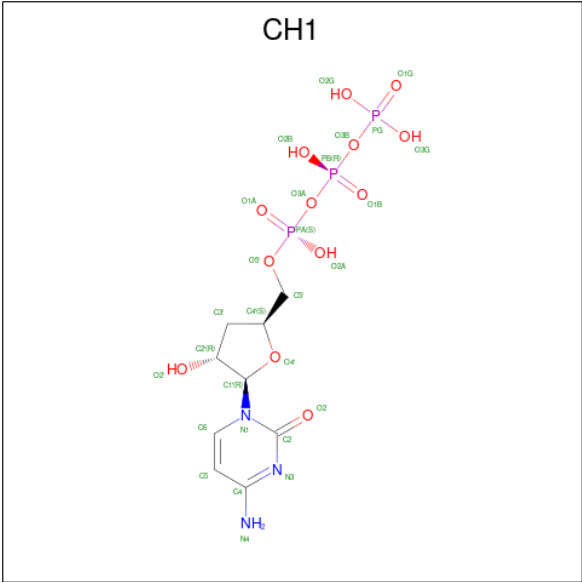
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 11 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CH1) (formula: C₉H₁₆N₃O₁₃P₃).

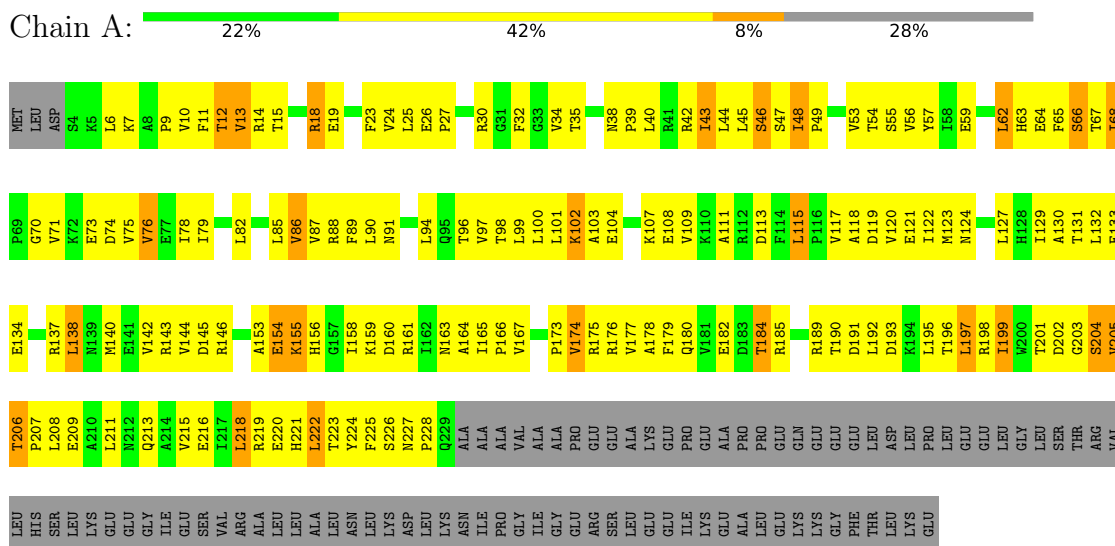


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
11	I	1	40	9	12	3	13	3	0	0

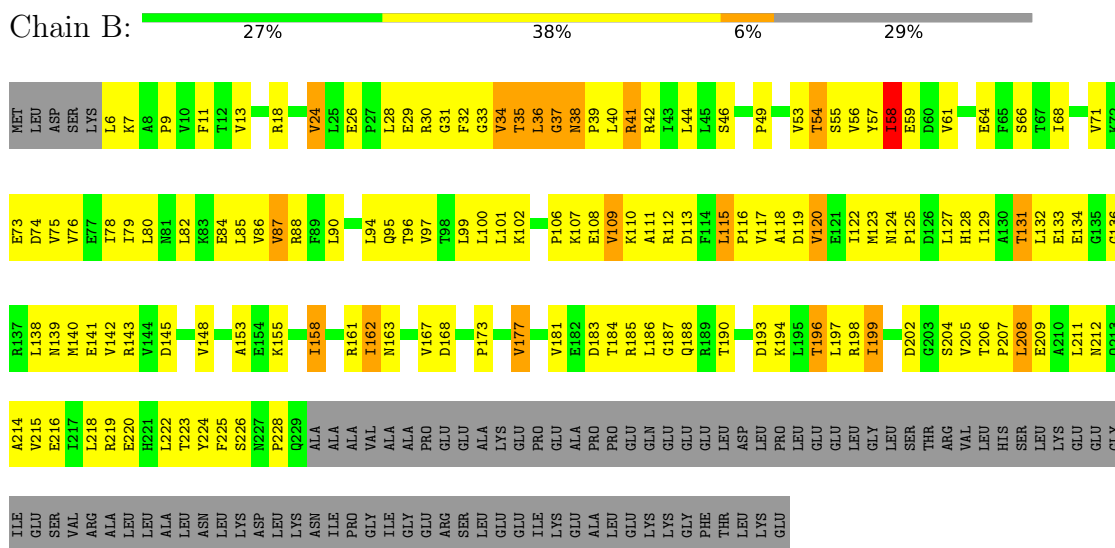
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

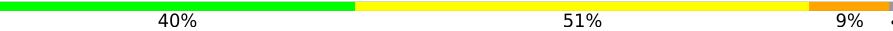
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

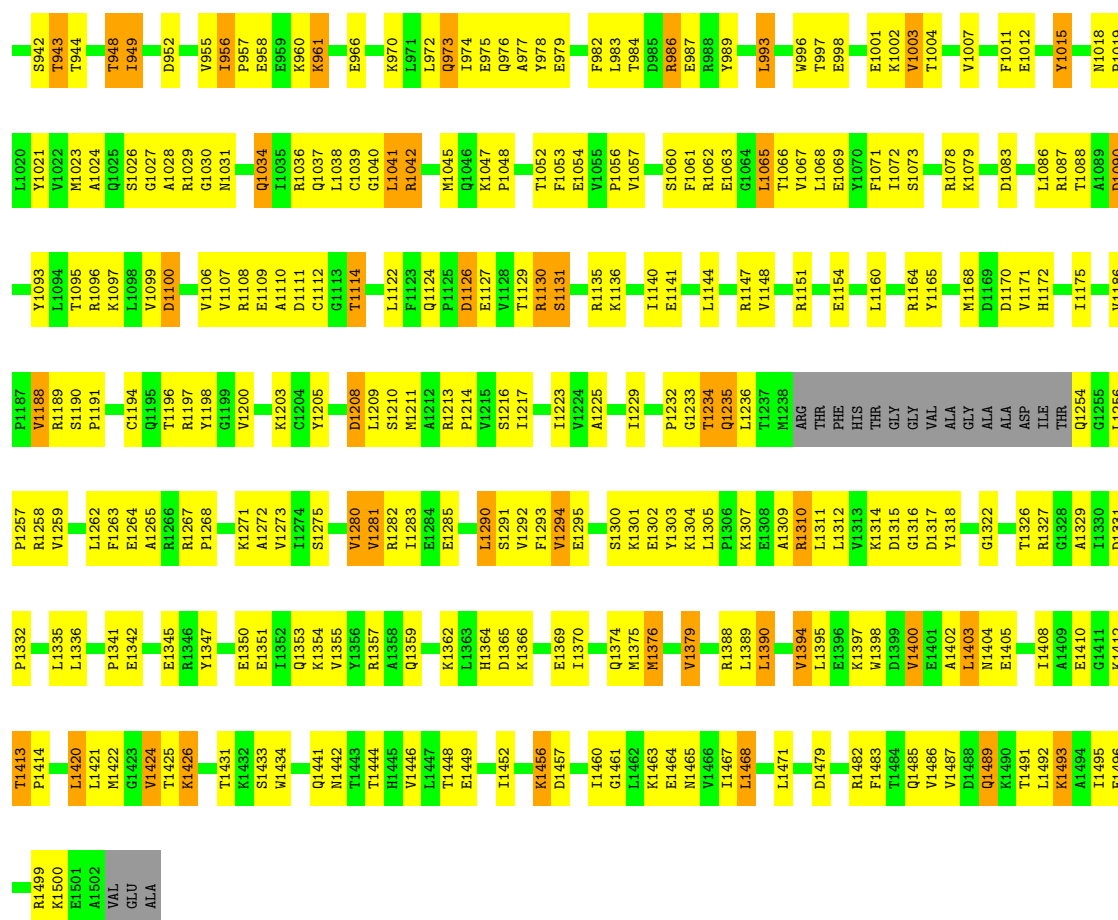


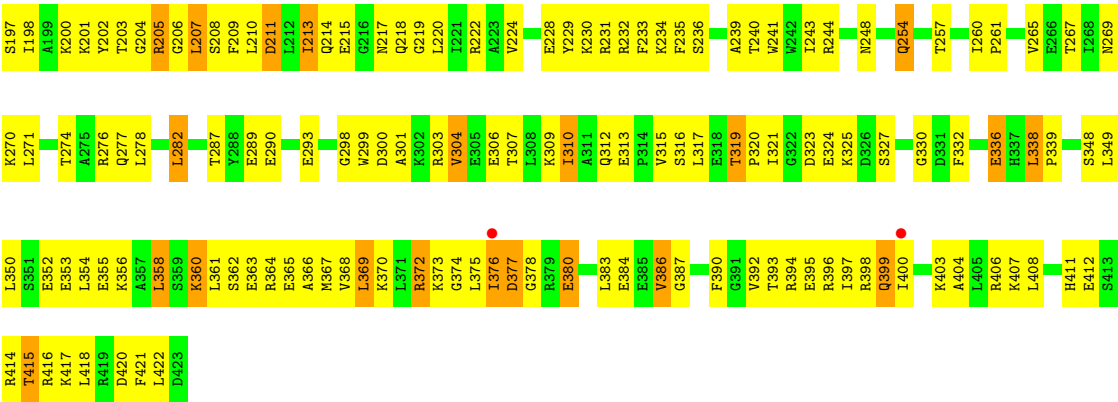
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:  40% 51% 9%

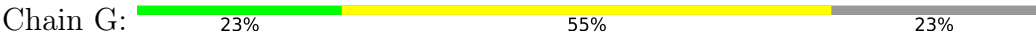
H1	E2	I3	F6	G7	R8	I9	R10	E11	V12	L15	P16	P17	L18	T19	E20	I21	Q22	V23	E24	S25	R28	A29	L30	Q31	A32	D33	V34	P35	P36	E37	K38	R39	E40	M41	T44	Q45	A46	R49	E50	T51	F52	P53	M54	E55	E56	GLU	ASP	LYS	GLY	LYS	GLY	L64	V65			
L66	D67	F68	L69	E70	Y71	E72	L73	G74	E75	P76	F79	Q80	R84	E85	K86	D87	L88	Q91	A92	P93	R97	L98	Q99	L100	A101	E102	I103	P104	T105	G106	L107	S108	K109	E110	D111	E112	L115	G116	H117	I118	P119	L120	M121	T122	E123	D124	F127	I128	L129	M130	G131	A132	D133	V134		
I136	V137	H140	I141	Y142	S143	P144	G145	V146	T149	P150	R154	I162	I163	P164	L165	P166	K167	R168	I172	D173	L174	E175	V176	E177	P178	H179	D180	G181	V182	S183	M184	K185	V186	R189	K190	F191	P192	L193	V194	L195	L196	L197	R198	E199	D200	Q201	E202	T203	L204	V205						
R209	E210	L211	G212	A213	Y214	G215	E216	L217	Q219	G220	L221	H222	D223	E224	S225	V226	F227	A228	R229	R230	E233	A234	L235	L236	R237	L238	F239	L240	L241	P244	G245	D246	P247	P248	R249	R250	A253	V254	L260	I261	A262	D263	P264	R265	R266	Y267	D268	L269	G270	E271	K276	A277	E278			
E279	K280	L281	G282	R283	L285	L290	A291	R292	Q291	F293	E297	F298	K299	D300	E301	V302	F303	L304	P305	T306	L307	R308	Y309	L310	F311	A312	G316	V317	P318	G319	S387	E321	V322	D323	D326	H327	R331	R332	L333	R334	T335	V336	G337	E338	L339	K340	T341	D342	Q343	F344	R345	L348				
L351	A352	R353	G354	V355	R356	P357	R358	K359	L360	K361	G362	S363	E364	P365	S366	L367	T368	P369	A370	K371	L372	R376	P377	L378	E379	A380	A381	L382	R383	E384	F385	F386	S387	R388	S389	Q390	L391	S392	Q393	F394	K395	D396	E397	S402	R403	D481	G482	R405	H406	K407	R408	R409	A412	L413	G414	L418
T419	R420	E421	R422	V423	A424	F425	D426	Y427	R428	H431	R432	T433	G436	R437	L438	E442	T443	P444	E445	G446	A447	N448	T449	G450	L451	L452	T453	S454	R455	L456	R460	V461	D462	T467	R468	Y471	R472	R473	V474	T480	D481	R482	Y485	M486	A488	T489	E490	E491	D492	R493	Y494					
T495	Q498	A499	N500	T501	P502	L503	R507	L508	V513	V514	A515	R516	E517	K518	G519	E520	T521	E522	V524	E528	V529	V534	S535	P536	E537	Q538	F540	S541	V542	N543	T544	N545	L546	L547	E551	H552	D553	D554	R557	A558	L559	M560	M564	Q565	T566	R567	P568	P569	P570	L571						
L572	P577	V578	M580	L583	E584	E585	R586	V587	V588	R589	D590	L591	L592	A593	E594	L595	G596	E597	E598	E599	E602	V603	K605	V606	D607	G608	N609	V613	R614	N615	E616	D617	G618	R619	V623	R626	F628	R629	H630	S631	N632	Q633	Q639	R640	P641	R642	V643	V645								
G646	Q647	R648	V649	K651	L654	L655	A656	G664	F665	L666	A667	G669	Q670	N671	V672	L673	A674	G675	L676	L677	N678	F679	D680	G681	E682	N683	F684	E685	V689	I690	E693	K696	R697	D698	F699	Y700	T701	S702	I703	H704	I705	E706	R707	Y708	E709	I710	E711	R712	R713	D714	K716					
L717	G718	P719	D787	E788	I789	T723	R724	D725	E726	P727	H728	R729	S730	D736	L737	Q738	F739	E740	V742	V743	R744	L745	G746	A747	E748	V749	K750	L751	G752	L753	I754	R755	V756	T759	S760	F761	K762	S765	Q829	V830	R831	L833	Q834	K838	N841	G844	N845	K846	T852	L853	R854					
D784	V785	K786	D787	M788	L789	T789	R791	V792	P793	E796	G797	G798	V799	V800	R801	E802	T803	V804	R805	R807	R808	G809	D810	P811	G812	V813	E814	L815	K816	V819	R820	E821	V822	R823	R824	V825	A828	R829	R830	R831	L833	Q834	K838	N841	G844	N845	K846	T852	L853	R854						
V855	E856	M858	L861	P862	D863	G864	P865	G866	V867	G868	V869	L870	R871	N872	Q873	L874	G875	V876	S877	S878	R879	M880	N881	L882	G883	Q884	E885	L886	E887	T888	H889	L890	G891	L892	Q893	L897	G898	Q899	R900	Y901	I902	P904	I905	F906	D907	G908	K910	I914	N915	E916	L917	Y918	E919			
Q920	A921	F926	K928	R929	K930	G931	E932	G933	H934	G935	V936	D937	K938	R939	E940	V941	E942	V943	R944	R945	R946	A947	E948	R949	L950	G951	L952	V953	T954	K957	T958	P959	E960	E961	Q962	L963	K964	L968	Q969	G970	K971	T1054	L1055	I983	E984	G985	P986	V987	R988	R1063	A1064	A1065	Q990	Y991	M992	E1068
L994	L997	Y998	H999	M1000	V1001	E1002	G1003	K1004	M1005	H1006	A1007	R1008	S1009	P1012	Y1013	S1014	L1015	L1016	Q1019	P1020	L1021	K1024	G1028	G1029	L952	V953	T954	K957	T958	P959	E960	E961	Q962	L963	K964	L968	Q969	G970	K971	T1054	L1055	I983	E984	G985	P986	V987	R988	R1063	A1064	A1065	Q990	Y991	M992	E1068		







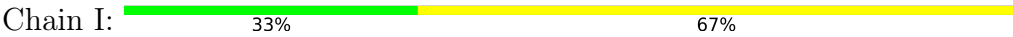
● Molecule 6: DNA (5'-D(P*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*A P*G)-3')



● Molecule 7: DNA (25-MER)



● Molecule 8: RNA (5'-R(*GP*CP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.98Å 102.47Å 296.04Å 90.00° 98.86° 90.00°	Depositor
Resolution (Å)	29.98 – 3.00 29.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.98-3.00) 96.5 (29.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.206 , 0.219 0.206 , 0.219	Depositor DCC
R_{free} test set	2006 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28581	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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, ZN, CH1

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	A	0.41	0/1814	0.64	0/2466
1	B	0.41	0/1799	0.65	0/2447
2	C	0.42	0/8937	0.62	0/12087
3	D	0.44	0/11927	0.67	2/16127 (0.0%)
4	E	0.39	0/775	0.57	0/1045
5	F	0.40	0/2852	0.63	0/3837
6	G	0.51	0/393	0.63	0/605
7	H	0.43	0/580	0.58	0/895
8	I	0.41	0/69	0.50	0/106
All	All	0.43	0/29146	0.64	2/39615 (0.0%)

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	A	0	1
1	B	0	2
2	C	0	2
3	D	0	6
All	All	0	11

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1234	THR	CA-C-N	5.92	132.35	121.70
3	D	1234	THR	C-N-CA	5.92	132.35	121.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	SER	Peptide
1	B	46	SER	Peptide
1	B	58	ILE	Peptide
2	C	268	ASP	Peptide
2	C	766	GLU	Peptide

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	A	1782	0	1834	180	0
1	B	1767	0	1816	194	0
2	C	8770	0	8874	768	1
3	D	11721	0	11941	992	2
4	E	761	0	778	62	0
5	F	2807	0	2882	273	1
6	G	351	0	192	19	0
7	H	516	0	283	29	0
8	I	62	0	34	3	0
9	D	2	0	0	0	0
10	D	2	0	0	0	0
11	I	28	12	11	2	0
All	All	28569	12	28645	2305	2

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 40.

The worst 5 of 2305 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)
7:H:15:DT:H2''	7:H:16:DC:H5'	1.22	1.16
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.24	1.14
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.21	1.13
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.24	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:203:ALA:HB1	3:D:393:ILE:HD11	1.31	1.10

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:GLU:OE2	3:D:1151:ARG:NH1[3_545]	2.04	0.16
3:D:296:GLU:OE2	5:F:222:ARG:NH1[4_1149]	2.12	0.08

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	
1	A	224/315 (71%)	183 (82%)	40 (18%)	1 (0%)	30	65
1	B	222/315 (70%)	187 (84%)	33 (15%)	2 (1%)	14	48
2	C	1107/1119 (99%)	971 (88%)	133 (12%)	3 (0%)	36	70
3	D	1481/1505 (98%)	1302 (88%)	172 (12%)	7 (0%)	24	60
4	E	92/99 (93%)	81 (88%)	11 (12%)	0	100	100
5	F	344/423 (81%)	293 (85%)	51 (15%)	0	100	100
All	All	3470/3776 (92%)	3017 (87%)	440 (13%)	13 (0%)	30	65

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	GLY
3	D	276	ASP
1	A	154	GLU
1	B	36	LEU
3	D	275	GLU

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	
1	A	199/273 (73%)	159 (80%)	40 (20%)	1	7
1	B	197/273 (72%)	175 (89%)	22 (11%)	6	24
2	C	936/941 (100%)	809 (86%)	127 (14%)	3	17
3	D	1249/1265 (99%)	1091 (87%)	158 (13%)	4	20
4	E	83/88 (94%)	75 (90%)	8 (10%)	8	31
5	F	301/371 (81%)	254 (84%)	47 (16%)	2	13
All	All	2965/3211 (92%)	2563 (86%)	402 (14%)	3	17

5 of 402 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	380	GLU
3	D	836	VAL
5	F	400	ILE
3	D	434	ARG
3	D	578	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	737	ASN
3	D	1075	HIS
3	D	767	HIS
3	D	909	ASN
3	D	1235	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	2/3 (66%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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
11	CH1	I	101	9	27,29,29	2.98	9 (33%)	37,45,45	1.36	5 (13%)

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
11	CH1	I	101	9	-	4/22/34/34	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	101	CH1	C3'-C2'	-11.10	1.24	1.52
11	I	101	CH1	O4'-C1'	-6.06	1.28	1.42
11	I	101	CH1	O2-C2	-3.57	1.17	1.23
11	I	101	CH1	C2-N1	-3.49	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	101	CH1	C4-N4	3.16	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	101	CH1	O4'-C4'-C3'	-3.94	100.08	105.07
11	I	101	CH1	O4'-C1'-N1	3.54	116.38	108.36
11	I	101	CH1	C2'-C3'-C4'	2.13	106.82	102.97
11	I	101	CH1	O2A-PA-O5'	2.07	116.96	107.57
11	I	101	CH1	O4'-C1'-C2'	-2.00	104.63	106.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

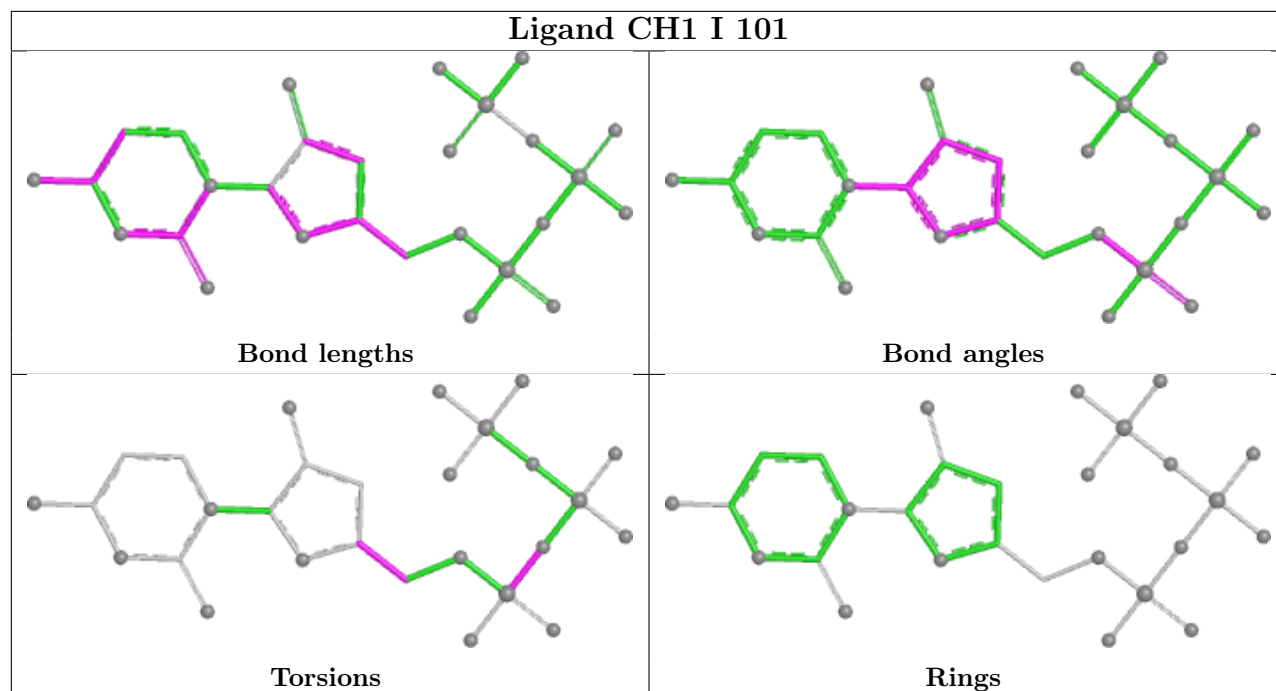
Mol	Chain	Res	Type	Atoms
11	I	101	CH1	C3'-C4'-C5'-O5'
11	I	101	CH1	O4'-C4'-C5'-O5'
11	I	101	CH1	PB-O3A-PA-O1A
11	I	101	CH1	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	I	101	CH1	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	226/315 (71%)	-0.52	0 100 100	58, 79, 98, 110	0
1	B	224/315 (71%)	-0.44	0 100 100	59, 85, 110, 122	0
2	C	1111/1119 (99%)	-0.49	0 100 100	47, 81, 125, 144	0
3	D	1485/1505 (98%)	-0.50	1 (0%) 92 86	40, 75, 122, 141	0
4	E	94/99 (94%)	-0.29	0 100 100	57, 90, 116, 121	0
5	F	346/423 (81%)	-0.34	2 (0%) 85 69	57, 88, 138, 150	0
6	G	17/22 (77%)	-0.43	0 100 100	64, 92, 152, 155	0
7	H	25/27 (92%)	-0.31	0 100 100	77, 106, 149, 157	0
8	I	3/3 (100%)	-1.01	0 100 100	72, 72, 73, 75	0
All	All	3531/3828 (92%)	-0.47	3 (0%) 92 86	40, 81, 126, 157	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	376	ILE	3.3
5	F	400	ILE	2.8
3	D	409	VAL	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

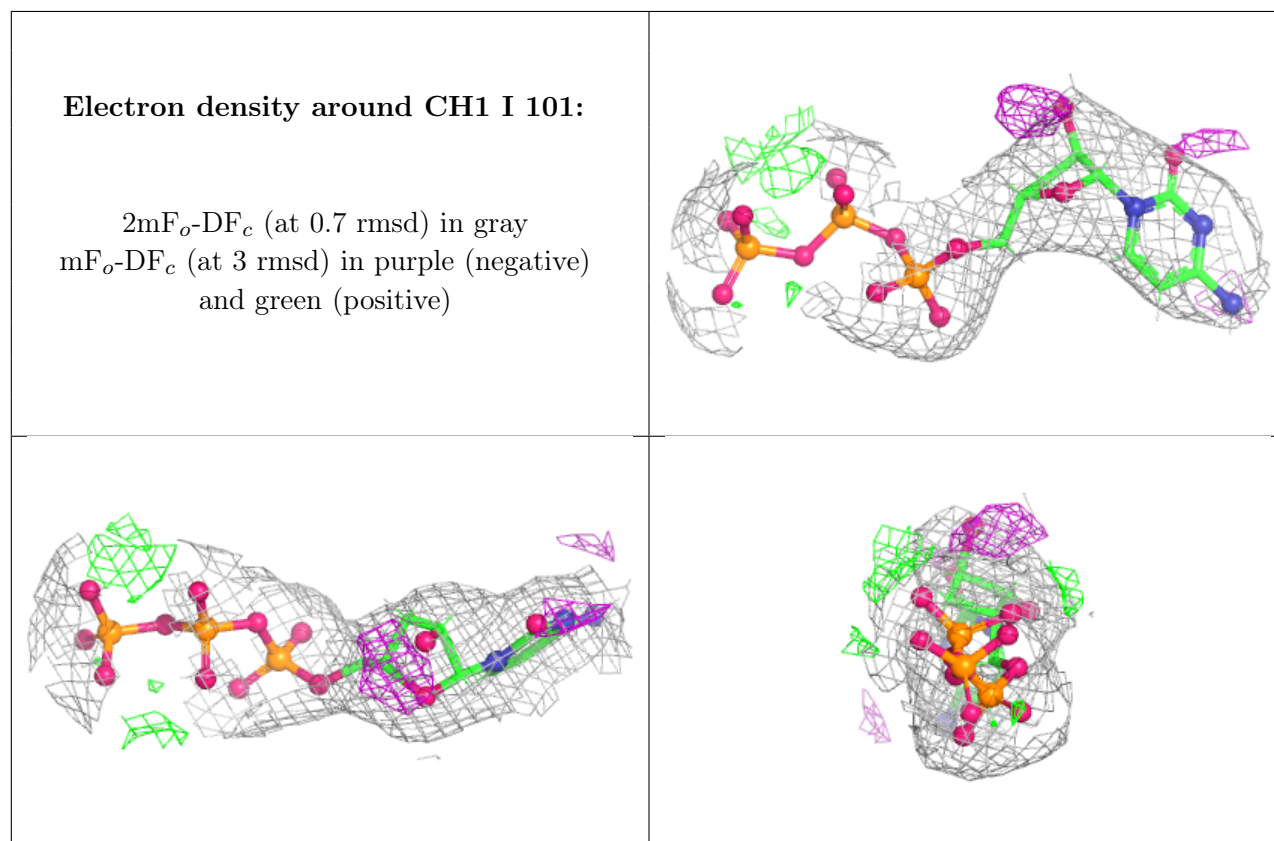
There are no oligosaccharides in this entry.

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
9	MG	D	2002	1/1	0.91	0.10	64,64,64,64	0
11	CH1	I	101	28/28	0.92	0.07	59,77,94,100	0
9	MG	D	2001	1/1	0.97	0.07	47,47,47,47	0
10	ZN	D	2004	1/1	0.99	0.06	76,76,76,76	0
10	ZN	D	2003	1/1	0.99	0.04	96,96,96,96	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.