



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:47 PM GMT

PDB ID : 1H38
Title : STRUCTURE OF A T7 RNA POLYMERASE ELONGATION COMPLEX
AT 2.9Å RESOLUTION
Authors : Tahirov, T.H.; Temyakov, D.; Anikin, M.; Patlan, V.; Mcallister, W.T.; Vasylyev, D.G.; Yokoyama, S.
Deposited on : 2002-08-24
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

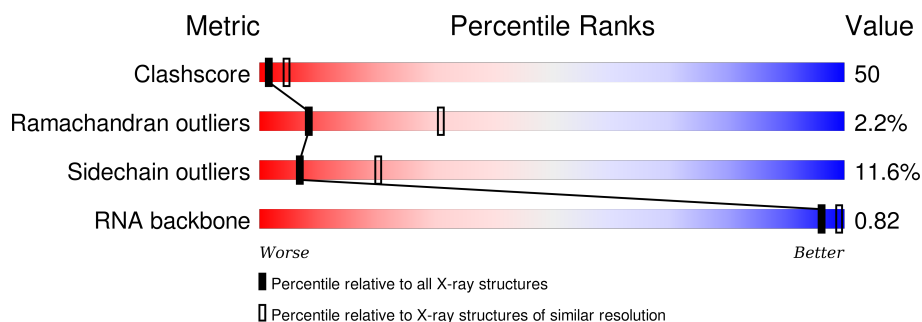
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)


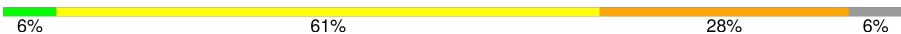

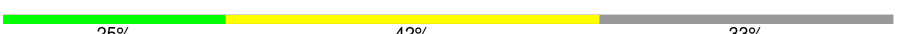



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	883	
1	B	883	
1	C	883	
1	D	883	
2	E	18	
2	H	18	

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Mol	Chain	Length	Quality of chain
2	K	18	
2	N	18	
3	F	12	
3	I	12	
3	L	12	
3	O	12	
4	G	10	
4	J	10	
4	M	10	
4	P	10	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30948 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 protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
1	B	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
1	C	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
1	D	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	P	0	0	0
			345	164	67	98	16			
2	H	18	Total	C	N	O	P	0	0	0
			367	174	72	104	17			
2	K	17	Total	C	N	O	P	0	0	0
			345	164	67	98	16			
2	N	17	Total	C	N	O	P	0	0	0
			345	164	67	98	16			

- Molecule 3 is a RNA chain called 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
3	I	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
3	L	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			

- Molecule 4 is a DNA chain called 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
4	J	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
4	M	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
4	P	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	310	Total	O	0	0
			310	310		
5	B	352	Total	O	0	0
			352	352		
5	C	185	Total	O	0	0
			185	185		
5	D	177	Total	O	0	0
			177	177		
5	E	13	Total	O	0	0
			13	13		
5	F	16	Total	O	0	0
			16	16		
5	G	12	Total	O	0	0
			12	12		
5	H	20	Total	O	0	0
			20	20		
5	I	11	Total	O	0	0
			11	11		
5	J	9	Total	O	0	0
			9	9		
5	K	17	Total	O	0	0
			17	17		
5	L	5	Total	O	0	0
			5	5		

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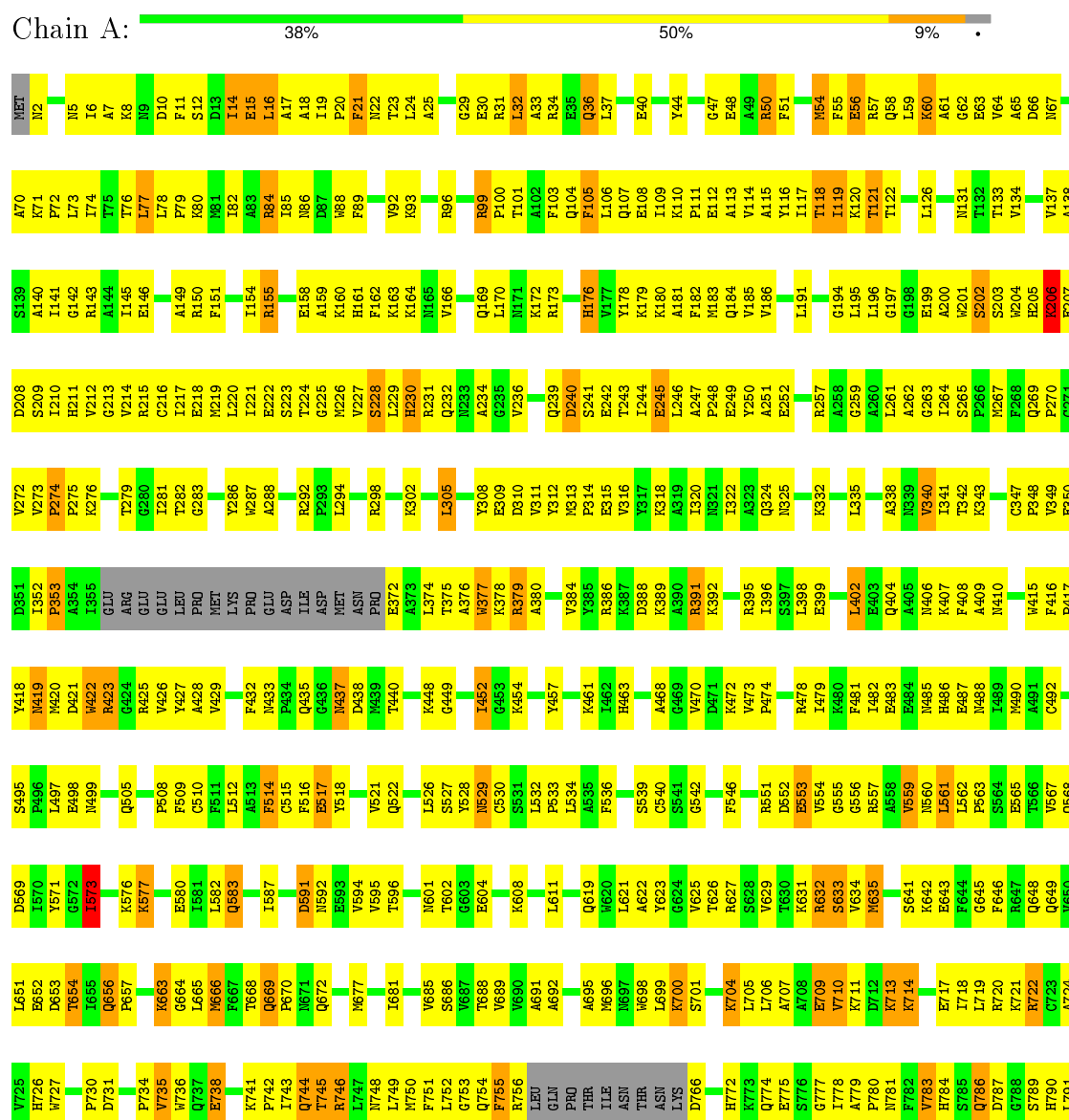
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	8	Total 8	O 8	0	0
5	N	12	Total 12	O 12	0	0
5	O	6	Total 6	O 6	0	0
5	P	9	Total 9	O 9	0	0

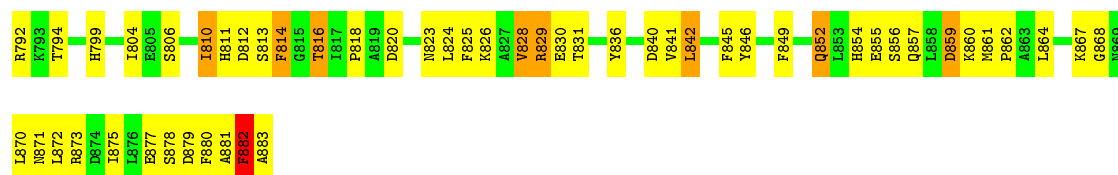
3 Residue-property plots

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.

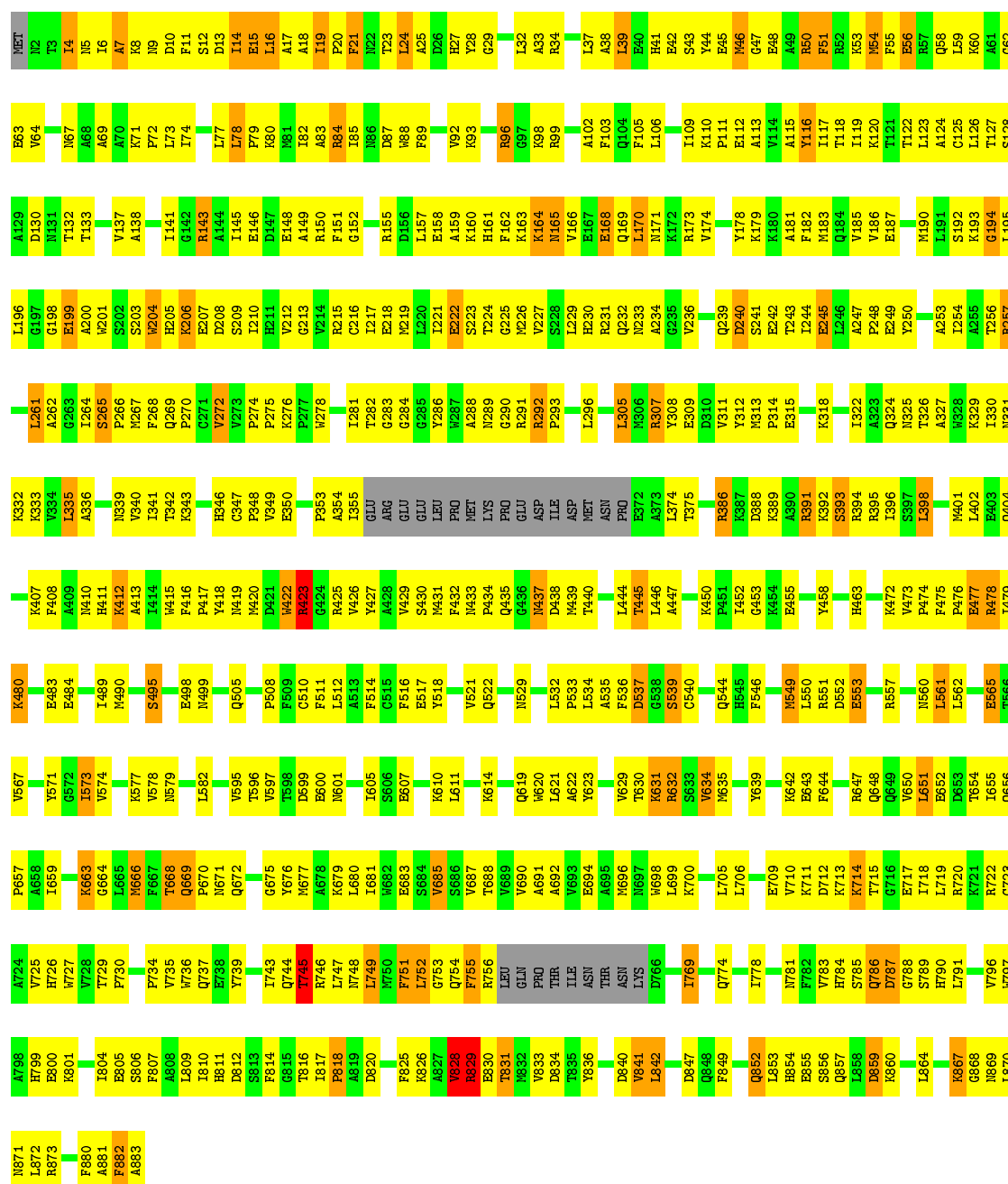
• Molecule 1: DNA-DIRECTED RNA POLYMERASE





• Molecule 1: DNA-DIRECTED RNA POLYMERASE

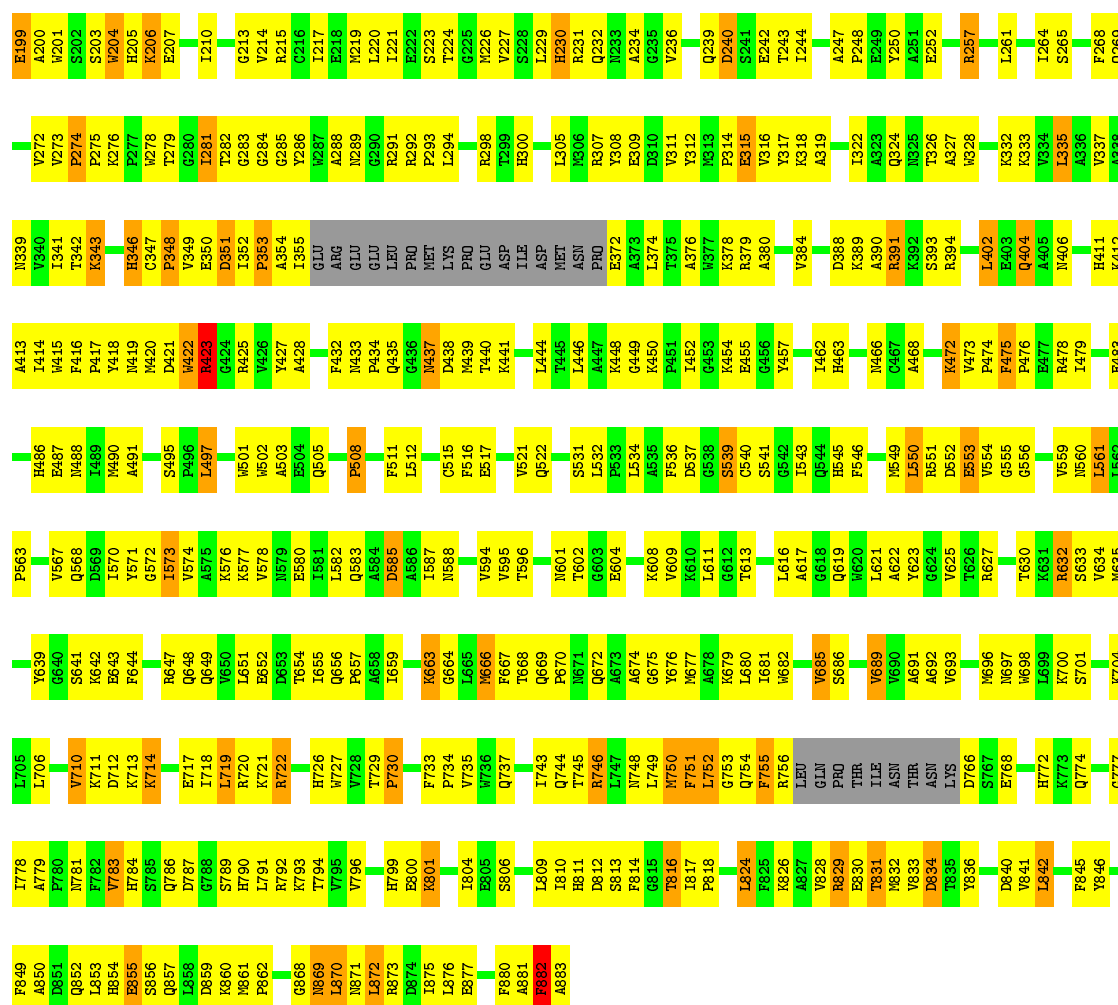
Chain B: 38% 49% 9%



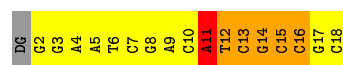
• Molecule 1: DNA-DIRECTED RNA POLYMERASE

Chain C: 39% 49% 8%

Y28	Y29	Y30	Y31	Y32	Y33	Y34	Y35	Y36	Y37	Y38	Y39	Y40	Y41	Y42	Y43	Y44	Y45	Y46	Y47	Y48	Y49	Y50	Y51	Y52	Y53	Y54	Y55	Y56	Y57	Y58	Y59	Y60	Y61	Y62	Y63	Y64	Y65	Y66	Y67	Y68	Y69	Y70	Y71	Y72	Y73	Y74	Y75	Y76	Y77	Y78	Y79	Y80	Y81	Y82	Y83	Y84	Y85	Y86	Y87	Y88	Y89	Y90	Y91	Y92	Y93	Y94	Y95	Y96	Y97	Y98	Y99	Y100	Y101	Y102	Y103	Y104	Y105	Y106	Y107	Y108	Y109	Y110	Y111	Y112	Y113	Y114	Y115	Y116	Y117	Y118	Y119	Y120	Y121	Y122	Y123	Y124	Y125	Y126	Y127	Y128	Y129	Y130	Y131	Y132	Y133	Y134	Y135	Y136	Y137	Y138	Y139	Y140	Y141	Y142	Y143	Y144	Y145	Y146	Y147	Y148	Y149	Y150	Y151	Y152	Y153	Y154	Y155	Y156	Y157	Y158	Y159	Y160	Y161	Y162	Y163	Y164	Y165	Y166	Y167	Y168	Y169	Y170	Y171	Y172	Y173	Y174	Y175	Y176	Y177	Y178	Y179	Y180	Y181	Y182	Y183	Y184	Y185	Y186	Y187	Y188	Y189	Y190	Y191	Y192	Y193	Y194	Y195	Y196	Y197	Y198	Y199	Y200	Y201	Y202	Y203	Y204	Y205	Y206	Y207	Y208	Y209	Y210	Y211	Y212	Y213	Y214	Y215	Y216	Y217	Y218	Y219	Y220	Y221	Y222	Y223	Y224	Y225	Y226	Y227	Y228	Y229	Y230	Y231	Y232	Y233	Y234	Y235	Y236	Y237	Y238	Y239	Y240	Y241	Y242	Y243	Y244	Y245	Y246	Y247	Y248	Y249	Y250	Y251	Y252	Y253	Y254	Y255	Y256	Y257	Y258	Y259	Y260	Y261	Y262	Y263	Y264	Y265	Y266	Y267	Y268	Y269	Y270	Y271	Y272	Y273	Y274	Y275	Y276	Y277	Y278	Y279	Y280	Y281	Y282	Y283	Y284	Y285	Y286	Y287	Y288	Y289	Y290	Y291	Y292	Y293	Y294	Y295	Y296	Y297	Y298	Y299	Y300	Y301	Y302	Y303	Y304	Y305	Y306	Y307	Y308	Y309	Y310	Y311	Y312	Y313	Y314	Y315	Y316	Y317	Y318	Y319	Y320	Y321	Y322	Y323	Y324	Y325	Y326	Y327	Y328	Y329	Y330	Y331	Y332	Y333	Y334	Y335	Y336	Y337	Y338	Y339	Y340	Y341	Y342	Y343	Y344	Y345	Y346	Y347	Y348	Y349	Y350	Y351	Y352	Y353	Y354	Y355	Y356	Y357	Y358	Y359	Y360	Y361	Y362	Y363	Y364	Y365	Y366	Y367	Y368	Y369	Y370	Y371	Y372	Y373	Y374	Y375	Y376	Y377	Y378	Y379	Y380	Y381	Y382	Y383	Y384	Y385	Y386	Y387	Y388	Y389	Y390	Y391	Y392	Y393	Y394	Y395	Y396	Y397	Y398	Y399	Y400	Y401	Y402	Y403	Y404	Y405	Y406	Y407	Y408	Y409	Y410	Y411	Y412	Y413	Y414	Y415	Y416	Y417	Y418	Y419	Y420	Y421	Y422	Y423	Y424	Y425	Y426	Y427	Y428	Y429	Y430	Y431	Y432	Y433	Y434	Y435	Y436	Y437	Y438	Y439	Y440	Y441	Y442	Y443	Y444	Y445	Y446	Y447	Y448	Y449	Y450	Y451	Y452	Y453	Y454	Y455	Y456	Y457	Y458	Y459	Y460	Y461	Y462	Y463	Y464	Y465	Y466	Y467	Y468	Y469	Y470	Y471	Y472	Y473	Y474	Y475	Y476	Y477	Y478	Y479	Y480	Y481	Y482	Y483	Y484	Y485	Y486	Y487	Y488	Y489	Y490	Y491	Y492	Y493	Y494	Y495	Y496	Y497	Y498	Y499	Y500	Y501	Y502	Y503	Y504	Y505	Y506	Y507	Y508	Y509	Y510	Y511	Y512	Y513	Y514	Y515	Y516	Y517	Y518	Y519	Y520	Y521	Y522	Y523	Y524	Y525	Y526	Y527	Y528	Y529	Y530	Y531	Y532	Y533	Y534	Y535	Y536	Y537	Y538	Y539	Y540	Y541	Y542	Y543	Y544	Y545	Y546	Y547	Y548	Y549	Y550	Y551	Y552	Y553	Y554	Y555	Y556	Y557	Y558	Y559	Y560	Y561	Y562	Y563	Y564	Y565	Y566	Y567	Y568	Y569	Y570	Y571	Y572	Y573	Y574	Y575	Y576	Y577	Y578	Y579	Y580	Y581	Y582	Y583	Y584	Y585	Y586	Y587	Y588	Y589	Y590	Y591	Y592	Y593	Y594	Y595	Y596	Y597	Y598	Y599	Y600	Y601	Y602	Y603	Y604	Y605	Y606	Y607	Y608	Y609	Y610	Y611	Y612	Y613	Y614	Y615	Y616	Y617	Y618	Y619	Y620	Y621	Y622	Y623	Y624	Y625	Y626	Y627	Y628	Y629	Y630	Y631	Y632	Y633	Y634	Y635	Y636	Y637	Y638	Y639	Y640	Y641	Y642	Y643	Y644	Y645	Y646	Y647	Y648	Y649	Y650	Y651	Y652	Y653	Y654	Y655	Y656	Y657	Y658	Y659	Y660	Y661	Y662	Y663	Y664	Y665	Y666	Y667	Y668	Y669	Y670	Y671	Y672	Y673	Y674	Y675	Y676	Y677	Y678	Y679	Y680	Y681	Y682	Y683	Y684	Y685	Y686	Y687	Y688	Y689	Y690	Y691	Y692	Y693	Y694	Y695	Y696	Y697	Y698	Y699	Y700	Y701	Y702	Y703	Y704	Y705	Y706	Y707	Y708	Y709	Y710	Y711	Y712	Y713	Y714	Y715	Y716	Y717	Y718	Y719	Y720	Y721	Y722	Y723	Y724	Y725	Y726	Y727	Y728	Y729	Y730	Y731	Y732	Y733	Y734	Y735	Y736	Y737	Y738	Y739	Y740	Y741	Y742	Y743	Y744	Y745	Y746	Y747	Y748	Y749	Y750	Y751	Y752	Y753	Y754	Y755	Y756	Y757	Y758	Y759	Y760	Y761	Y762	Y763	Y764	Y765	Y766	Y767	Y768	Y769	Y770	Y771	Y772	Y773	Y774	Y775	Y776	Y777	Y778	Y779	Y780	Y781	Y782	Y783	Y784	Y785	Y786	Y787	Y788	Y789	Y790	Y791	Y792	Y793	Y794	Y795	Y796	Y797	Y798	Y799	Y800	Y801	Y802	Y803	Y804	Y805	Y806	Y807	Y808	Y809	Y810	Y811	Y812	Y813	Y814	Y815	Y816	Y817	Y818	Y819	Y820	Y821	Y822	Y823	Y824	Y825	Y826	Y827	Y828	Y829	Y830	Y831	Y832	Y833	Y834	Y835	Y836	Y837	Y838	Y839	Y840	Y841	Y842	Y843	Y844	Y845	Y846	Y847	Y848	Y849	Y850	Y851	Y852	Y853	Y854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y862	Y863	Y864	Y865	Y866	Y867	Y868	Y869	Y870	Y871	Y872	Y873	Y874	Y875	Y876	Y877	Y878	Y879	Y880	Y881	Y882	Y883	Y884	Y885	Y886	Y887	Y888	Y889	Y890	Y891	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y902	Y903	Y904	Y905	Y906	Y907	Y908	Y909	Y910	Y911	Y912	Y913	Y914	Y915	Y916	Y917	Y918	Y919	Y920	Y921	Y922	Y923	Y924	Y925	Y926	Y927	Y928	Y929	Y930	Y931	Y932	Y933	Y934	Y935	Y936	Y937	Y938	Y939	Y940	Y941	Y942	Y943	Y944	Y945	Y946	Y947	Y948	Y949	Y950	Y951	Y952	Y953	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y967	Y968	Y969	Y970	Y971	Y972	Y973	Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000	Y1001	Y1002	Y1003	Y1004	Y1005	Y1006	Y1007	Y1008	Y1009	Y1010	Y1011	Y1012	Y1013	Y1014	Y1015	Y1016	Y1017	Y1018	Y1019	Y1020	Y1021	Y1022	Y1023	Y1024	Y1025	Y1026	Y1027	Y1028	Y1029	Y1030	Y1031	Y1032	Y1033	Y1034	Y1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Chain E: 61% 28% 6% 6%



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

Chain H: 17% 39% 39% 6%

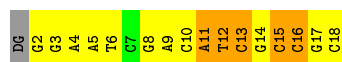


• Molecule 2: 5'-D(*GP*GP*GP*AP*AP*TP*CP*GP*AP*CP *AP*TP*CP*GP*CP*CP*GP*C)-3'

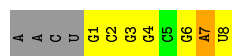
Chain K: 56% 39% 6%



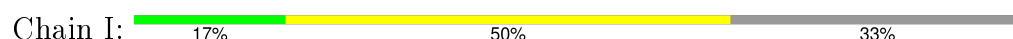
- Molecule 2: 5'-D(*GP*GP*GP*AP*AP*TP*CP*GP*AP*CP *AP*TP*CP*GP*CP*CP*GP*C)-3'



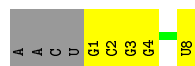
- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'



- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'



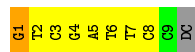
- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'



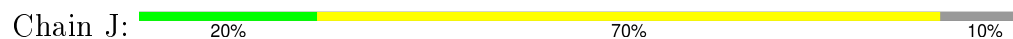
- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'




- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'

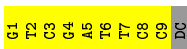


- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'




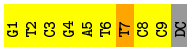
- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'

Chain M:  90% 10%

 G1 T2 C3 G4 A5 T6 T7 C8 C9 DC

- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'

Chain P:  80% 10% 10%

 G1 T2 C3 G4 A5 T6 T7 C8 C9 DC

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.91Å 84.97Å 202.00Å 90.36° 92.97° 109.94°	Depositor
Resolution (Å)	39.93 – 2.90	Depositor
% Data completeness (in resolution range)	98.0 (39.93-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	30948	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.89	9/6897 (0.1%)	0.85	5/9329 (0.1%)
1	B	0.93	2/6897 (0.0%)	0.87	9/9329 (0.1%)
1	C	0.64	0/6897	0.73	0/9329
1	D	0.58	0/6897	0.70	2/9329 (0.0%)
2	E	0.89	0/387	1.06	1/595 (0.2%)
2	H	0.94	0/412	1.03	1/634 (0.2%)
2	K	0.90	0/387	0.97	0/595
2	N	0.80	0/387	0.95	0/595
3	F	1.09	1/191 (0.5%)	0.85	0/297
3	I	0.94	0/191	0.81	0/297
3	L	0.81	0/191	0.79	0/297
3	O	0.61	0/191	0.74	0/297
4	G	0.88	0/199	0.84	0/305
4	J	0.77	0/199	0.93	0/305
4	M	0.68	0/199	0.85	0/305
4	P	0.74	0/199	1.05	0/305
All	All	0.78	12/30721 (0.0%)	0.81	18/42143 (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
2	E	0	6
2	H	0	8
2	K	0	7
2	N	0	6
4	G	0	1
4	J	0	1
4	P	0	1
All	All	0	30

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	CYS	CB-SG	-8.42	1.68	1.82
1	A	573	ILE	CA-CB	7.10	1.71	1.54
1	A	654	THR	CA-CB	5.53	1.67	1.53
1	A	783	VAL	CA-CB	-5.40	1.43	1.54
3	F	7	A	C5-C6	-5.31	1.36	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	ASP	CB-CG-OD1	-8.22	110.90	118.30
1	A	557	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	829	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	B	549	MET	CB-CG-SD	-6.86	91.82	112.40
1	A	787	ASP	CB-CG-OD2	-6.55	112.41	118.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	11	DA	Sidechain
2	E	12	DT	Sidechain
2	E	13	DC	Sidechain
2	E	14	DG	Sidechain
2	E	15	DC	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	A	6746	0	6708	722	0
1	B	6746	0	6708	733	0
1	C	6746	0	6708	680	0
1	D	6746	0	6708	653	0
2	E	345	0	191	30	0
2	H	367	0	202	28	0
2	K	345	0	191	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	345	0	191	21	0
3	F	171	0	89	7	0
3	I	171	0	89	11	0
3	L	171	0	89	9	0
3	O	171	0	89	5	0
4	G	179	0	104	14	0
4	J	179	0	104	8	0
4	M	179	0	104	18	0
4	P	179	0	104	11	0
5	A	310	0	0	102	0
5	B	352	0	0	133	0
5	C	185	0	0	79	0
5	D	177	0	0	105	0
5	E	13	0	0	2	0
5	F	16	0	0	2	0
5	G	12	0	0	5	0
5	H	20	0	0	6	0
5	I	11	0	0	4	0
5	J	9	0	0	4	0
5	K	17	0	0	7	0
5	L	5	0	0	2	0
5	M	8	0	0	1	0
5	N	12	0	0	4	0
5	O	6	0	0	0	0
5	P	9	0	0	3	0
All	All	30948	0	28379	2933	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 50.

The worst 5 of 2933 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)
1:A:668:THR:HG22	1:A:669:GLN:NE2	1.51	1.24
1:C:428:ALA:H	1:C:435:GLN:NE2	1.44	1.15
1:B:50:ARG:HG2	1:B:50:ARG:HH11	1.01	1.14
1:C:133:THR:HA	1:C:243:THR:HG22	1.28	1.10
1:A:120:LYS:HE3	1:A:752:LEU:HD21	1.31	1.10

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	
1	A	851/883 (96%)	740 (87%)	94 (11%)	17 (2%)	9	33
1	B	851/883 (96%)	736 (86%)	98 (12%)	17 (2%)	9	33
1	C	851/883 (96%)	737 (87%)	93 (11%)	21 (2%)	7	27
1	D	851/883 (96%)	735 (86%)	96 (11%)	20 (2%)	7	29
All	All	3404/3532 (96%)	2948 (87%)	381 (11%)	75 (2%)	8	31

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLY
1	A	199	GLU
1	A	539	SER
1	A	663	LYS
1	A	755	PHE

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	703/729 (96%)	615 (88%)	88 (12%)	6	17
1	B	703/729 (96%)	619 (88%)	84 (12%)	6	19
1	C	703/729 (96%)	623 (89%)	80 (11%)	7	21
1	D	703/729 (96%)	628 (89%)	75 (11%)	8	24
All	All	2812/2916 (96%)	2485 (88%)	327 (12%)	7	20

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	668	THR
1	C	120	LYS
1	D	689	VAL
1	B	725	VAL
1	B	829	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	786	GLN
1	C	289	ASN
1	D	744	GLN
1	B	823	ASN
1	C	171	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	F	7/12 (58%)	0	0
3	I	7/12 (58%)	0	0
3	L	7/12 (58%)	0	0
3	O	7/12 (58%)	0	0
All	All	28/48 (58%)	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 ⓘ

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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.