



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:33 PM UTC

PDB ID : 2O5I / pdb_00002o5i
Title : Crystal structure of the T. thermophilus RNA polymerase elongation complex
Authors : Vassilyev, D.G.; Tahirov, T.H.; Vassilyeva, M.N.
Deposited on : 2006-12-06
Resolution : 2.50 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
Xtriage (Phenix) : 2.0
EDS : 3.0
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

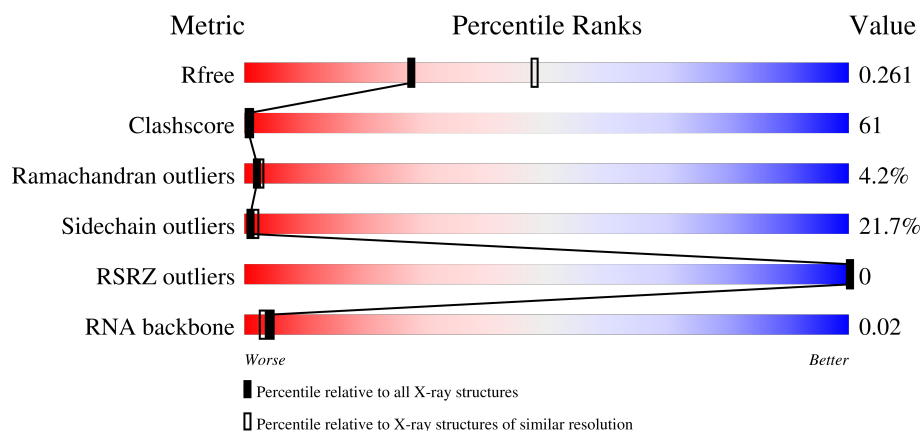
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



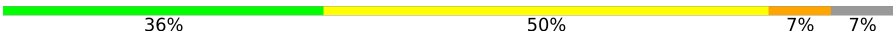
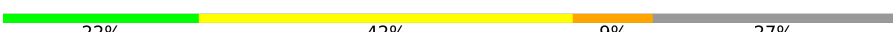
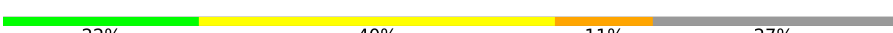
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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	G	23	
1	X	23	
2	H	16	
2	Y	16	

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Mol	Chain	Length	Quality of chain
3	I	14	
3	Z	14	
4	A	315	
4	B	315	
4	K	315	
4	L	315	
5	C	1119	
5	M	1119	
6	D	1524	
6	N	1524	
7	E	99	
7	O	99	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 52719 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(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			
1	X	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			

- Molecule 2 is a RNA chain called 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			
2	Y	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			
3	Z	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
4	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
4	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 5 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
5	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

- Molecule 6 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	1303	Total	C	N	O	S	0	0	0
			10280	6508	1821	1919	32			
6	N	1303	Total	C	N	O	S	0	0	0
			10280	6508	1821	1919	32			

- Molecule 7 is a protein called DNA-directed RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			
7	O	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	N	2	Total	Zn	0	0
			2	2		

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	N	1	Total 1	Mg 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	G	22	Total 22	O 22	0	0
10	H	18	Total 18	O 18	0	0
10	I	36	Total 36	O 36	0	0
10	X	25	Total 25	O 25	0	0
10	Y	16	Total 16	O 16	0	0
10	Z	16	Total 16	O 16	0	0
10	A	144	Total 144	O 144	0	0
10	B	159	Total 159	O 159	0	0
10	C	658	Total 658	O 658	0	0
10	D	760	Total 760	O 760	0	0
10	E	70	Total 70	O 70	0	0
10	K	132	Total 132	O 132	0	0
10	L	121	Total 121	O 121	0	0
10	M	575	Total 575	O 575	0	0
10	N	750	Total 750	O 750	0	0
10	O	61	Total 61	O 61	0	0

3 Residue-property plots

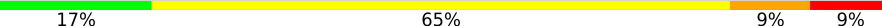
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3'

Chain G: 



- Molecule 1: 5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3'

Chain X: 



- Molecule 2: 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3',

Chain H: 



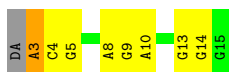
- Molecule 2: 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3',

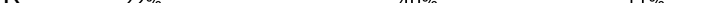
Chain Y: 

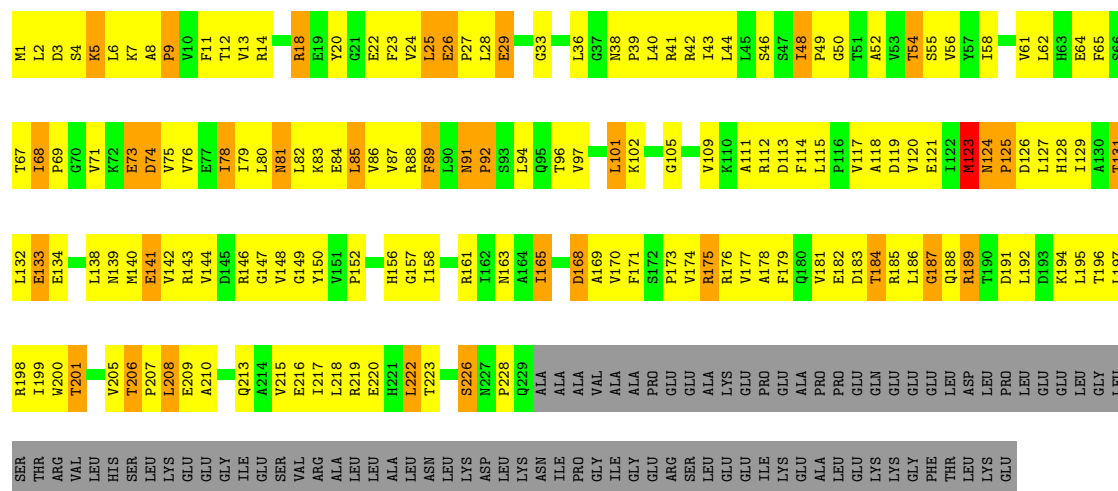


- Molecule 3: 5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3'

Chain I: 

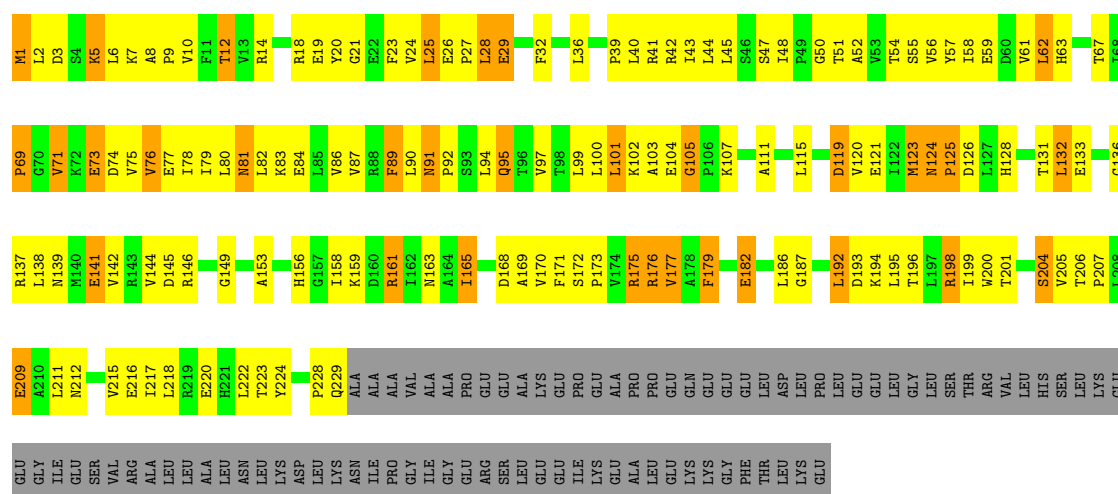


- Chain K:  22% 40% 11% 27%



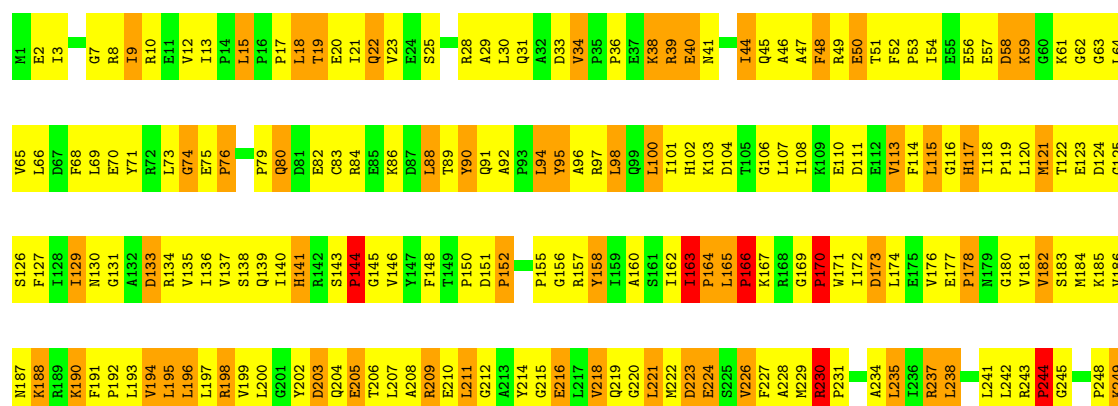
• Molecule 4: DNA-directed RNA polymerase alpha chain

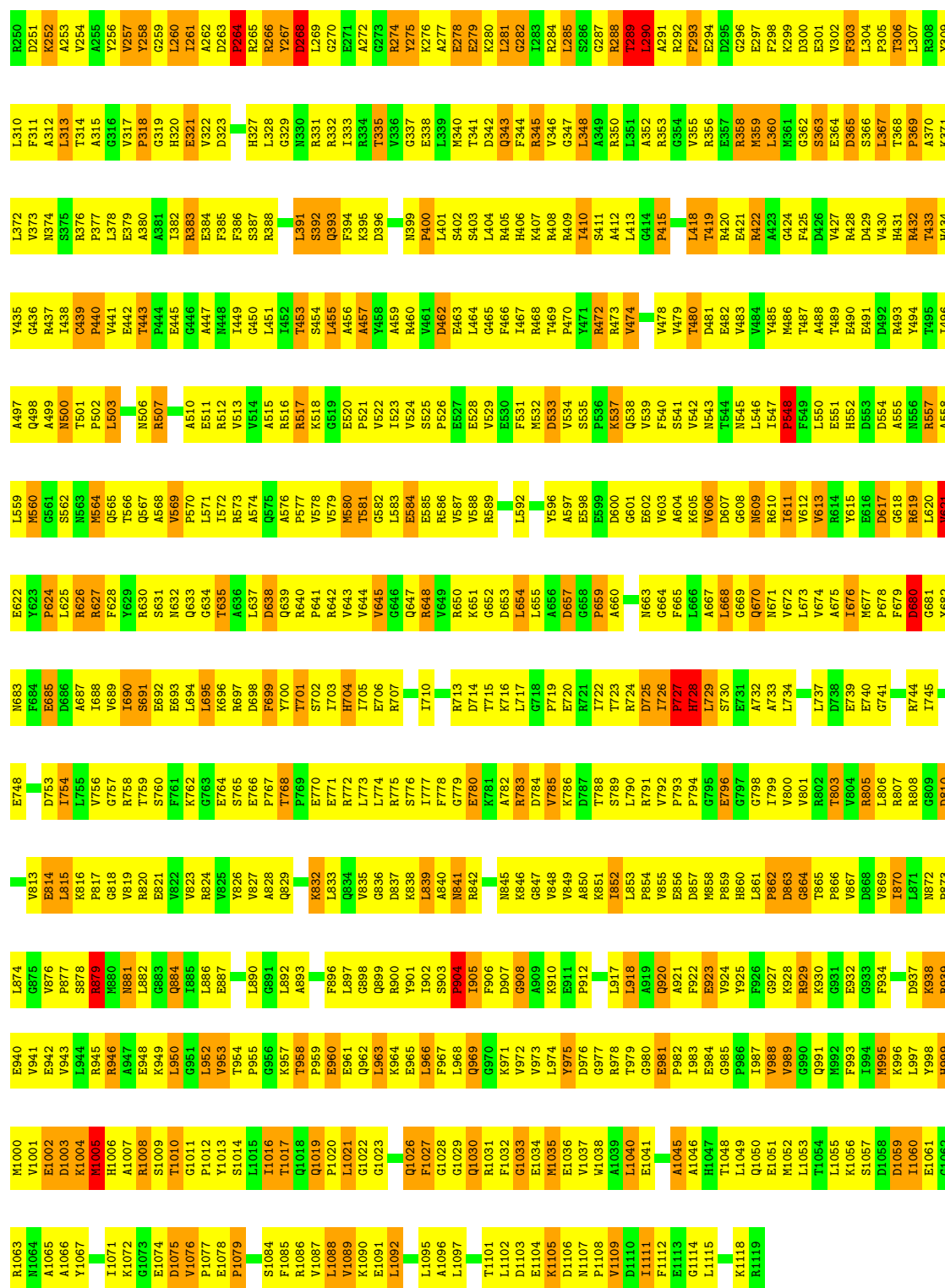
Chain L: 26% 36% 11% 27%



• Molecule 5: DNA-directed RNA polymerase beta chain

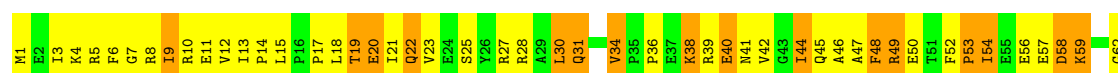
Chain C: 21% 57% 20%





• Molecule 5: DNA-directed RNA polymerase beta chain

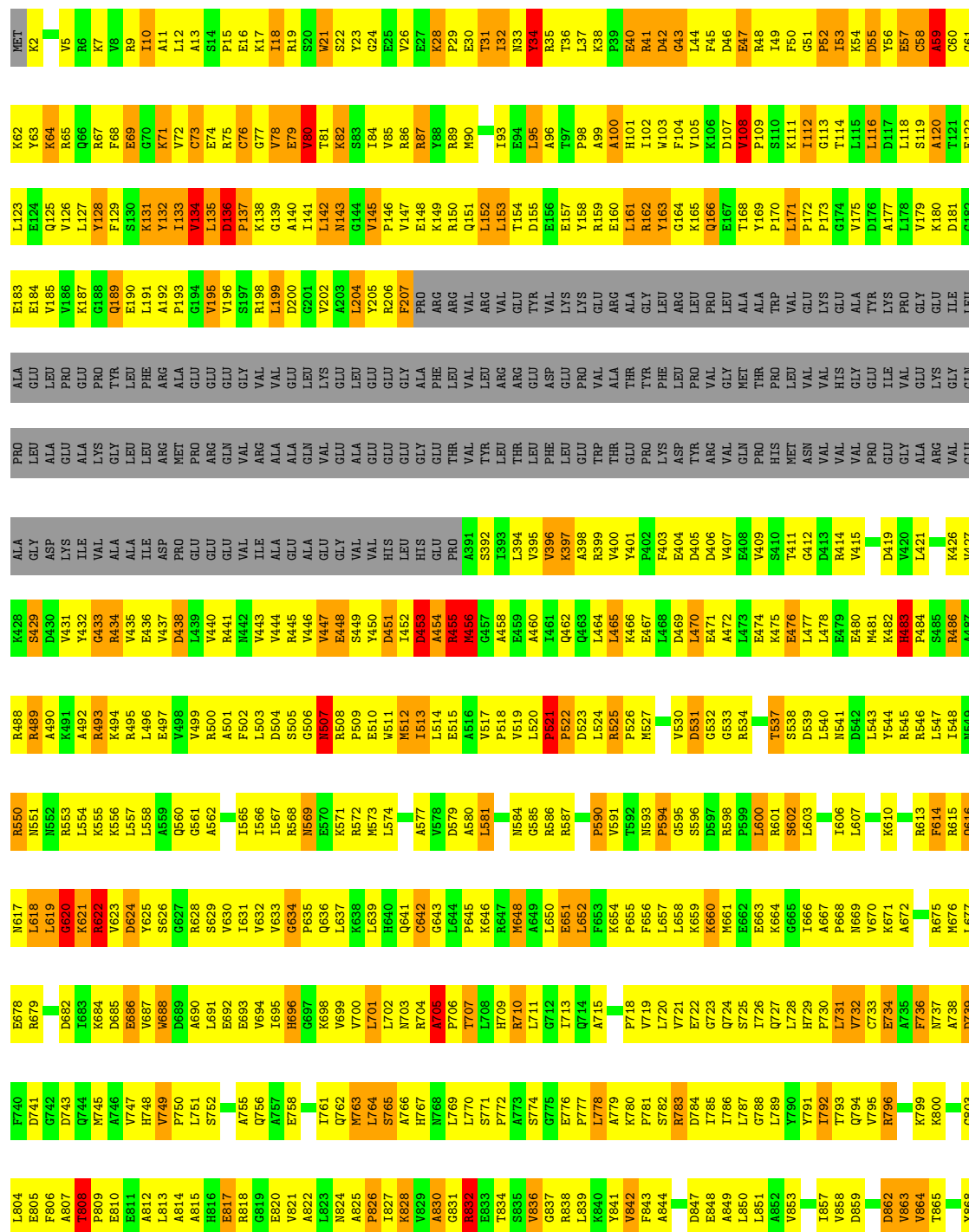
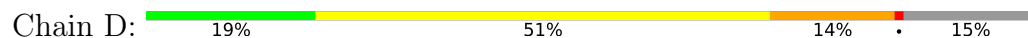
Chain M: 23% 57% 18%





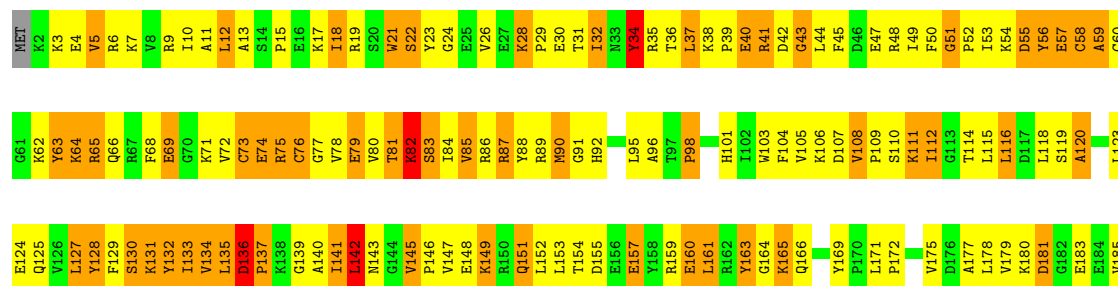


● Molecule 6: DNA-directed RNA polymerase beta' chain

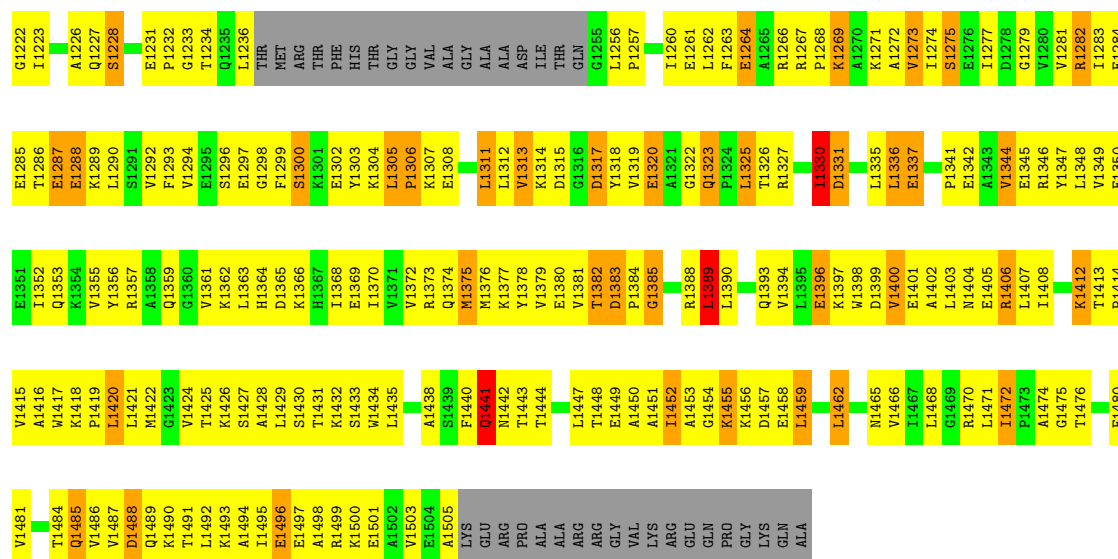




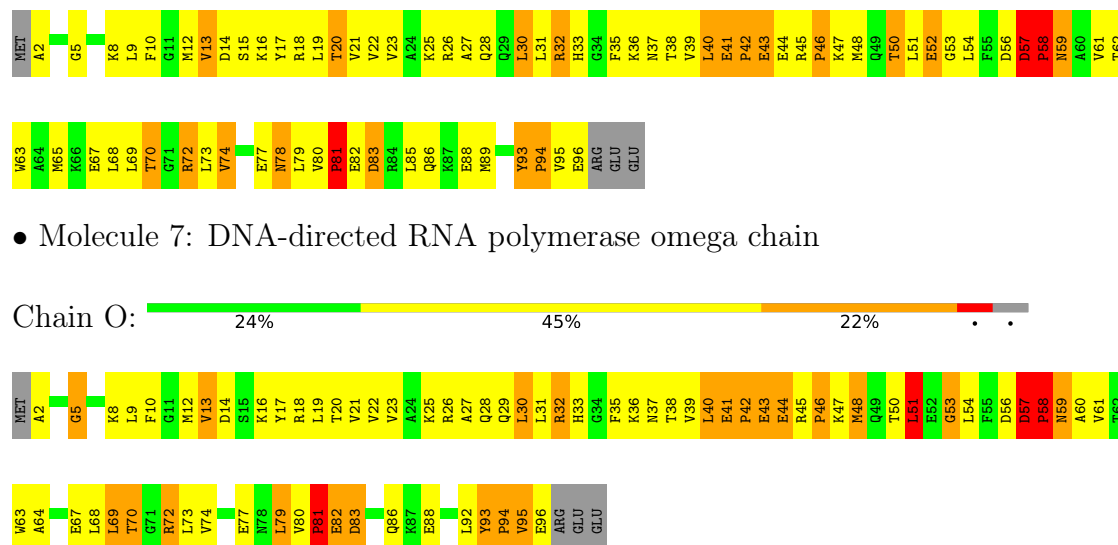
Chain N:



L1144	S1073	S942	P877	L813	H748	K684	L619	R493	P430	I1E	ALA	GLU	W186
Y1145	S1074	T943	G878	A814	W749	D685	G620	K494	V431	VAL	LYS	PRO	K157
R1146	H1075	T944	R879	E817	P750	E686	R621	R495	Y432	ALA	GLY	TYR	Q188
L1147		S945	T880	E818	L751	G687	R622	R496	G433	ALA	LEU	LEU	Q189
R1151	K1078	G946	L881	G819		W688	V623	E497	R434	ILE	LEU	PHE	E190
	K1079	I947	R882	G819	F754	D689	D624	V498	V435	ASP	ARG	ARG	L191
V1155	D1083	T948	A883	E820	A755	A690	W625	Y499	E436	PRO	MET	ALA	A192
L1156	T1084	I949	R884	E820	Q756	L691	S626	R500	D437	GLU	PRO	GLU	P193
	A1085	G950	L885	A822	A757	E692	E564	A501	D438	GLU	ARG	GLU	G194
R1159	L1086	D951	W886	L823	E758	E693	G627	F502	L439	GLU	GLN	GLU	V195
L1160	A1086	D952	A887	L824	A759	V694		L503	V440	VAL	VAL	GLY	V196
L1161	R1087	D953	E888	A825		T695	W631	D504	R441	ILE	ARG	VAL	S197
E1162	A1089	E954	E889	P826	Q762	H696	V632	S505	N442	ALA	ALA	VAL	R198
G1163		V955	W890	L827	W763	G697	V633	G506	V443	GLU	ALA	GLU	L199
R1164	Y1093	I956	E891	R828	L764	K698	G634	N507	V444	ALA	GLN	LEU	D200
Y1165	L1094	P957	D892	W829	S765	V699	P635	R508	R445	VAL	VAL	LYS	
L1166	T1095	E958	E893	A830	A766	W700	Q636	P509	V446	GLY	GLU	GLU	
S1167	R1096	E959	K894	G831	H767	L701	L637	H573	V447	VAL	VAL	VAL	
H1168	K1097	D968	W895	R832		L702	K638	W511	E448	VAL	GLU	GLU	
	L1098	I969	A896	E833	L770	W703	L639	M512	S449	HIS	GLU	GLU	
K1176	Y1099	K970	W897	T834	S771	R704	H640	M512		LEU	GLU	GLY	
A1177	D1100	L964	E898	W835	P772	A705	Q641	D451	D451	HIS	GLY	ALA	
A1178	V1101	E965	L899	W836	A773	P706	C642	E515	I452	GLU	GLU	PHE	
E1179	T1102	E966	I900	C837	S774	T707	C643	A516	D453	PRO	THR	LEU	
		A967	Q901	R838	G775	L708	L644	W517	A454	VAL	VAL	VAL	
L1182	V1106	D968	L902	L839	E776	H709	P645	P518	S392		TYR	LEU	
V1107	V1107	K970	W904	R840	P777	R710	K646	W519	I393	LEU	ARG	ARG	
R1108	L1108	L971	P905	L841	L778		R647	L520	L394	THR	THR	ARG	
E1109	R1109	L972	Q906	W842	A779	W713	M648	D583	G457	LEU	GLU	GLU	
A1110	A1110	L973	E907	F843	K780	Q714	A649	P522	V395	PHE	ASP	VAL	
D1111	D1111	I974	K908	A844	P781	A715	L650	P522	E459	LEU	GLU	GLU	
C1112	C1112	E975	N909	R845	S782	F716	E651	D523	A460	LEU	LEU	PRO	
T1114	T1114	Q976	L911	E848	K783	Q717	L652	R526	I461	TRP	TRP	VAL	
		Y978	L914	L850	D784	P718	F653	P526	Q463	THR	ALA	VAL	
Y1117	Y1117	E979		L851	L785	W719	K654	M527	L464	ALA	GLU	THR	
L1118	L1118	W980	L914	L852	L787		P655		L465	PRO	PRO	TYR	
S1119	S1119	Q917	Q917	W853	G788	Q724	L657	V530	K466	LYS	LYS	PHE	
V1120	V1120	A918	A918	W853	L789	S725	L658	D531	E467	ASP	ASP	LEU	
L1121	L1121	F919	F919	H855		L726	K659	G532	D405	TYR	TYR	LEU	
L1122	L1122	D985	L920	H855	L792	G732	L666	G533	D406	ARG	ARG	VAL	
F1123	F1123	R986	R921	G856	T793	C733	A667	D597	L470	VAL	VAL	GLY	
Q1124	Q1124	E987	L922	W858	Q794	E734	P668	R598	E471	GLN	GLN	MET	
P1125	P1125	R988	G923	W858	W795	H729	W670	P599	A472	PRO	PRO	THR	
		I989	I922	D859	R796	P730	K664	S538		HIS	HIS	TRP	
V1128	V1128	D990	W924	L860	K797	L731	G665	D539	K475	MET	MET	LEU	
T1129	T1129	Q991	E925	L861	L798	W732	L666	L540	E476	ASN	ASN	VAL	
R1130	R1130	F1060	K926	D862	G798	C733	A667	N541	L477	VAL	VAL	VAL	
S1131	S1131	R1062	X926	W863	K799	E734	P668	T604	L478	VAL	VAL	HIS	
L1132	L1132	L983	T927	W864	K800	A735	N669	D605	A416	VAL	VAL	GLY	
R1133	R1133	Q994	R929	T865	G803	F736	K671	L606	P417	PRO	PRO	GLU	
L1134	L1134	L995	L930	W866	L804	W737	A672	L607	C418	GLY	GLY	ILE	
R1135	R1135	W996	E930	R867	A738	A673	K672	S608	D419	VAL	VAL	VAL	
K1136	K1136	L934		W868	F806	F740	R674	G609	H483	ALA	ALA	GLU	
V1137	V1137	T999	Y937	W869	A807	R740	R675		P484	ARG	ARG	LYS	
L1068	L1068	T1000	Y937	R872	R808	D743	R676	R613	L421	VAL	VAL	GLY	
E1069	E1069	E1001	G938		R809	Q744	L677	R550	A422	ALA	ALA	GLY	
T1070	T1070	K1002	P939		E810	W745	E678	N551	K426	PRO	PRO	LEU	
E1141	E1141	V1003	T940		E811	A746	R679	N552	V427	GLY	GLY	LEU	
		T1004	F941		A812	V747		R553	K428	ASP	ASP	ALA	
								L554	S429	LYS	LYS	GLU	



• Molecule 7: DNA-directed RNA polymerase omega chain



• Molecule 7: DNA-directed RNA polymerase omega chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	156.21Å 156.21Å 499.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.2 (20.00-2.50) 83.7 (20.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.267 0.238 , 0.261	Depositor DCC
R_{free} test set	19570 reflections (5.74%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 142.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.149 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52719	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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

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	G	0.62	0/520	1.14	4/798 (0.5%)
1	X	0.57	0/520	1.12	3/798 (0.4%)
2	H	1.43	1/387 (0.3%)	1.99	17/601 (2.8%)
2	Y	1.00	1/387 (0.3%)	2.14	20/601 (3.3%)
3	I	0.54	0/304	0.79	0/467
3	Z	0.48	0/304	0.81	0/467
4	A	0.83	0/1838	1.13	9/2498 (0.4%)
4	B	0.87	1/1838 (0.1%)	1.07	5/2498 (0.2%)
4	K	0.80	2/1838 (0.1%)	1.11	9/2498 (0.4%)
4	L	0.83	1/1838 (0.1%)	1.08	6/2498 (0.2%)
5	C	0.88	2/8997 (0.0%)	1.30	67/12164 (0.6%)
5	M	0.90	4/8997 (0.0%)	1.29	78/12164 (0.6%)
6	D	1.01	29/10452 (0.3%)	1.26	78/14116 (0.6%)
6	N	0.97	22/10452 (0.2%)	1.25	75/14116 (0.5%)
7	E	1.02	2/784 (0.3%)	1.68	20/1057 (1.9%)
7	O	1.02	2/784 (0.3%)	1.63	19/1057 (1.8%)
All	All	0.93	67/50240 (0.1%)	1.27	410/68398 (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	G	0	5
1	X	0	3
2	H	0	2
2	Y	0	3
3	I	0	1
3	Z	0	1
All	All	0	15

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	G	OP3-P	21.78	1.92	1.48
6	D	132	TYR	CA-C	20.07	1.74	1.52
6	D	133	ILE	N-CA	16.41	1.64	1.46
6	D	455	ARG	CA-C	12.58	1.69	1.52
6	N	132	TYR	CA-C	12.20	1.66	1.52

The worst 5 of 410 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	94	PRO	CA-N-CD	-17.09	88.07	112.00
5	C	177	GLU	CA-C-N	15.95	139.78	119.84
5	C	177	GLU	C-N-CA	15.95	139.78	119.84
7	O	94	PRO	N-CA-C	15.93	135.16	113.65
5	M	177	GLU	CA-C-N	14.95	138.52	119.84

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1	DC	Sidechain
1	G	13	DT	Sidechain
1	G	16	DG	Sidechain
1	G	17	DC	Sidechain
1	G	18	DG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	467	0	259	45	0
1	X	467	0	259	34	0
2	H	347	0	174	68	0
2	Y	347	0	175	76	0
3	I	270	0	144	13	0
3	Z	270	0	144	15	0
4	A	1806	0	1861	233	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1806	0	1861	180	0
4	K	1806	0	1861	198	0
4	L	1806	0	1861	176	0
5	C	8829	0	8933	1236	0
5	M	8829	0	8933	1155	0
6	D	10280	0	10510	1464	0
6	N	10280	0	10510	1366	0
7	E	770	0	784	107	0
7	O	770	0	784	108	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	D	1	0	0	0	0
9	N	1	0	0	0	0
10	A	144	0	0	52	0
10	B	159	0	0	38	0
10	C	658	0	0	189	0
10	D	760	0	0	214	0
10	E	70	0	0	17	0
10	G	22	0	0	4	0
10	H	18	0	0	1	0
10	I	36	0	0	4	0
10	K	132	0	0	40	0
10	L	121	0	0	23	0
10	M	575	0	0	169	0
10	N	750	0	0	229	0
10	O	61	0	0	24	0
10	X	25	0	0	5	0
10	Y	16	0	0	2	0
10	Z	16	0	0	2	0
All	All	52719	0	49053	6007	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 61.

The worst 5 of 6007 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)
6:D:132:TYR:C	6:D:132:TYR:CA	1.74	1.54
7:O:95:VAL:CG1	10:O:2132:HOH:O	1.89	1.21
2:H:2:A:OP2	6:D:671:LYS:HD2	1.47	1.14
6:D:165:LYS:HB2	6:D:397:LYS:HB2	1.31	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:619:LEU:HD12	6:N:621:LYS:HZ3	1.08	1.12

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	
4	A	227/315 (72%)	206 (91%)	16 (7%)	5 (2%)	5	9
4	B	227/315 (72%)	205 (90%)	18 (8%)	4 (2%)	6	12
4	K	227/315 (72%)	205 (90%)	17 (8%)	5 (2%)	5	9
4	L	227/315 (72%)	205 (90%)	18 (8%)	4 (2%)	6	12
5	C	1117/1119 (100%)	916 (82%)	142 (13%)	59 (5%)	1	1
5	M	1117/1119 (100%)	918 (82%)	145 (13%)	54 (5%)	2	2
6	D	1297/1524 (85%)	1081 (83%)	165 (13%)	51 (4%)	2	3
6	N	1297/1524 (85%)	1100 (85%)	147 (11%)	50 (4%)	2	3
7	E	93/99 (94%)	76 (82%)	8 (9%)	9 (10%)	0	0
7	O	93/99 (94%)	75 (81%)	9 (10%)	9 (10%)	0	0
All	All	5922/6744 (88%)	4987 (84%)	685 (12%)	250 (4%)	2	2

5 of 250 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	29	GLU
4	A	187	GLY
4	B	29	GLU
4	B	187	GLY
5	C	40	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	202/273 (74%)	163 (81%)	39 (19%)	1	2
4	B	202/273 (74%)	168 (83%)	34 (17%)	2	4
4	K	202/273 (74%)	168 (83%)	34 (17%)	2	4
4	L	202/273 (74%)	165 (82%)	37 (18%)	2	3
5	C	941/941 (100%)	707 (75%)	234 (25%)	0	1
5	M	941/941 (100%)	721 (77%)	220 (23%)	1	1
6	D	1100/1279 (86%)	872 (79%)	228 (21%)	1	2
6	N	1100/1279 (86%)	872 (79%)	228 (21%)	1	2
7	E	84/88 (96%)	60 (71%)	24 (29%)	0	0
7	O	84/88 (96%)	62 (74%)	22 (26%)	0	1
All	All	5058/5708 (89%)	3958 (78%)	1100 (22%)	1	2

5 of 1100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	N	590	PRO
6	N	732	VAL
6	N	581	LEU
6	N	1282	ARG
6	D	618	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
5	M	543	ASN
6	N	724	GLN
5	M	671	ASN
6	N	125	GLN
6	N	1010	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	H	16/16 (100%)	13 (81%)	8 (50%)
2	Y	15/16 (93%)	12 (80%)	7 (46%)
All	All	31/32 (96%)	25 (80%)	15 (48%)

5 of 25 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	2	A
2	H	3	G
2	H	6	U
2	H	7	G
2	H	8	C

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	15	C
2	Y	13	C
2	Y	6	U
2	Y	15	C
2	Y	9	G

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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 ⓘ

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	G	23/23 (100%)	-1.98	0 100 100	16, 38, 58, 69	0
1	X	23/23 (100%)	-1.97	0 100 100	18, 41, 74, 89	0
2	H	16/16 (100%)	-2.07	0 100 100	35, 64, 80, 84	0
2	Y	16/16 (100%)	-2.10	0 100 100	31, 54, 90, 95	0
3	I	13/14 (92%)	-1.92	0 100 100	32, 42, 61, 78	0
3	Z	13/14 (92%)	-1.90	0 100 100	37, 49, 76, 84	0
4	A	229/315 (72%)	-1.42	0 100 100	45, 74, 94, 101	0
4	B	229/315 (72%)	-1.42	0 100 100	57, 79, 94, 104	0
4	K	229/315 (72%)	-1.44	0 100 100	56, 76, 91, 97	0
4	L	229/315 (72%)	-1.41	0 100 100	48, 82, 94, 101	0
5	C	1119/1119 (100%)	-1.45	0 100 100	19, 68, 98, 119	0
5	M	1119/1119 (100%)	-1.46	0 100 100	32, 68, 96, 108	0
6	D	1303/1524 (85%)	-1.45	0 100 100	34, 68, 94, 110	0
6	N	1303/1524 (85%)	-1.44	0 100 100	35, 69, 95, 108	0
7	E	95/99 (95%)	-1.47	0 100 100	50, 70, 90, 96	0
7	O	95/99 (95%)	-1.36	0 100 100	41, 72, 98, 102	0
All	All	6054/6850 (88%)	-1.45	0 100 100	16, 70, 95, 119	0

There are no RSRZ outliers to report.

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

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
8	ZN	D	4058	1/1	1.00	0.03	82,82,82,82	0
8	ZN	D	6112	1/1	1.00	0.01	65,65,65,65	0
8	ZN	N	5058	1/1	1.00	0.01	71,71,71,71	0
8	ZN	N	7112	1/1	1.00	0.02	73,73,73,73	0
9	MG	D	8001	1/1	1.00	0.01	27,27,27,27	0
9	MG	N	8002	1/1	1.00	0.04	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.