



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 09:57 AM EDT

PDB ID : 4WQS
Title : Thermus thermophilus RNA polymerase backtracked complex
Authors : Murayama, Y.; Sekine, S.; Yokoyama, S.
Deposited on : 2014-10-22
Resolution : 4.31 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

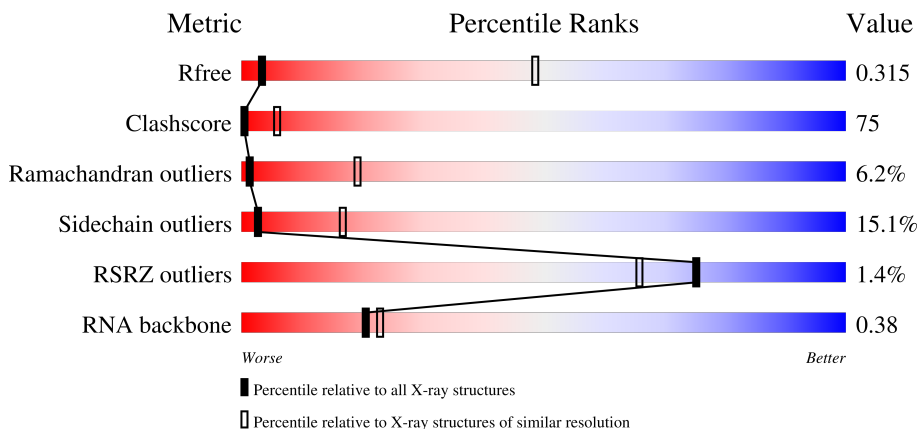
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.31 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}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)
RNA backbone	3102	1058 (5.60-3.00)

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	 21% 45% 7% 27%
1	B	315	 3% 27% 40% . 27%
1	K	315	 27% 41% 5% 27%
1	L	315	 24% 43% 5% 27%

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	G	28	
5	X	28	
6	H	16	
6	Y	16	
7	I	21	
7	Z	21	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 48166 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 subunit alpha.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1151	Total	C	N	O	S	0	0	0
			9097	5753	1629	1682	33			
3	N	1288	Total	C	N	O	S	0	0	0
			10175	6441	1804	1899	31			

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

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

- Molecule 5 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	27	Total	C	N	O	P	0	0	0
			548	259	104	158	27			
5	X	27	Total	C	N	O	P	0	0	0
			548	259	104	158	27			

- Molecule 6 is a RNA chain called RNA (5'-R(P*CP*CP*AP*GP*CP*CP*GP*GP*CP*GP*CP*UP*CP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	16	Total	C	N	O	P	0	0	0
			340	151	61	112	16			
6	Y	15	Total	C	N	O	P	0	0	0
			318	141	56	106	15			

- Molecule 7 is a DNA chain called DNA (5'-D(P*GP*TP*AP*GP*CP*TP*TP*GP*TP*GP*GP*TP*AP*GP*TP*GP*AP*CP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	17	Total	C	N	O	P	0	0	0
			357	169	65	106	17			
7	Z	17	Total	C	N	O	P	0	0	0
			357	169	65	106	17			

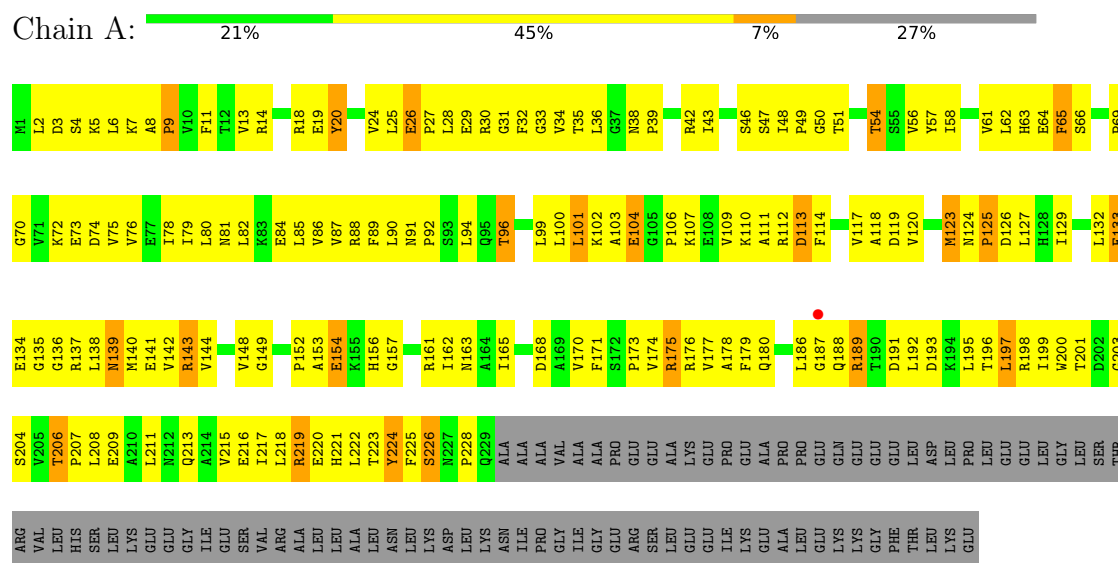
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

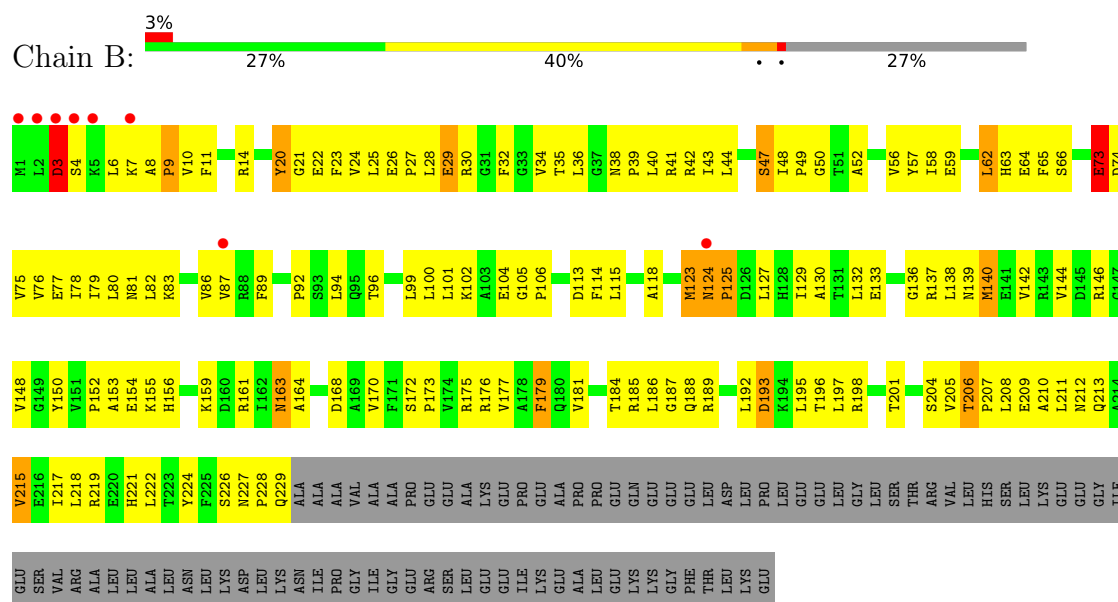
3 Residue-property plots

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.

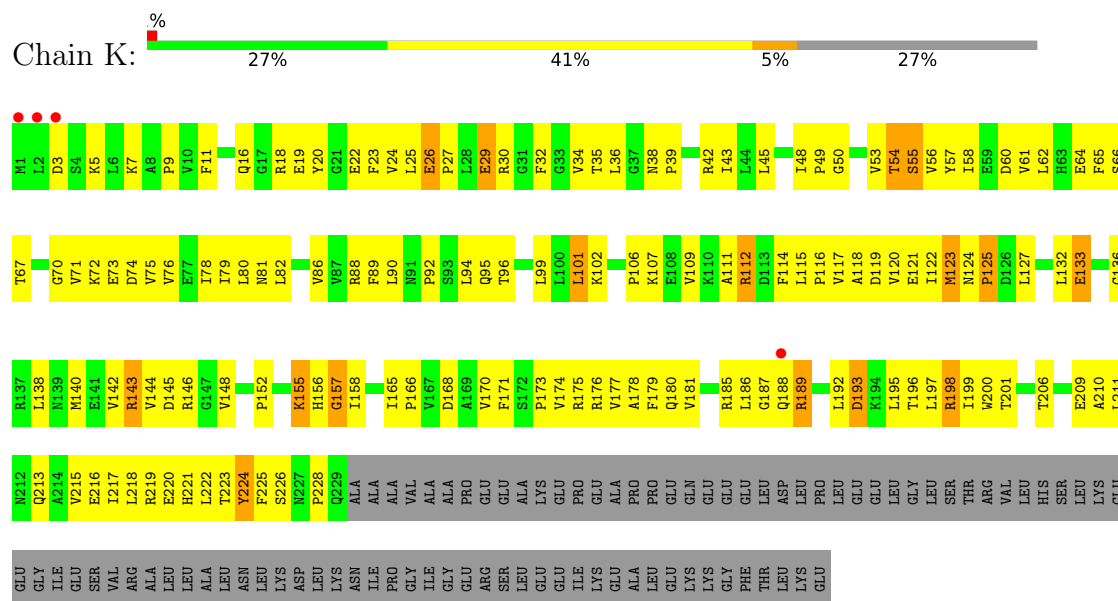
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

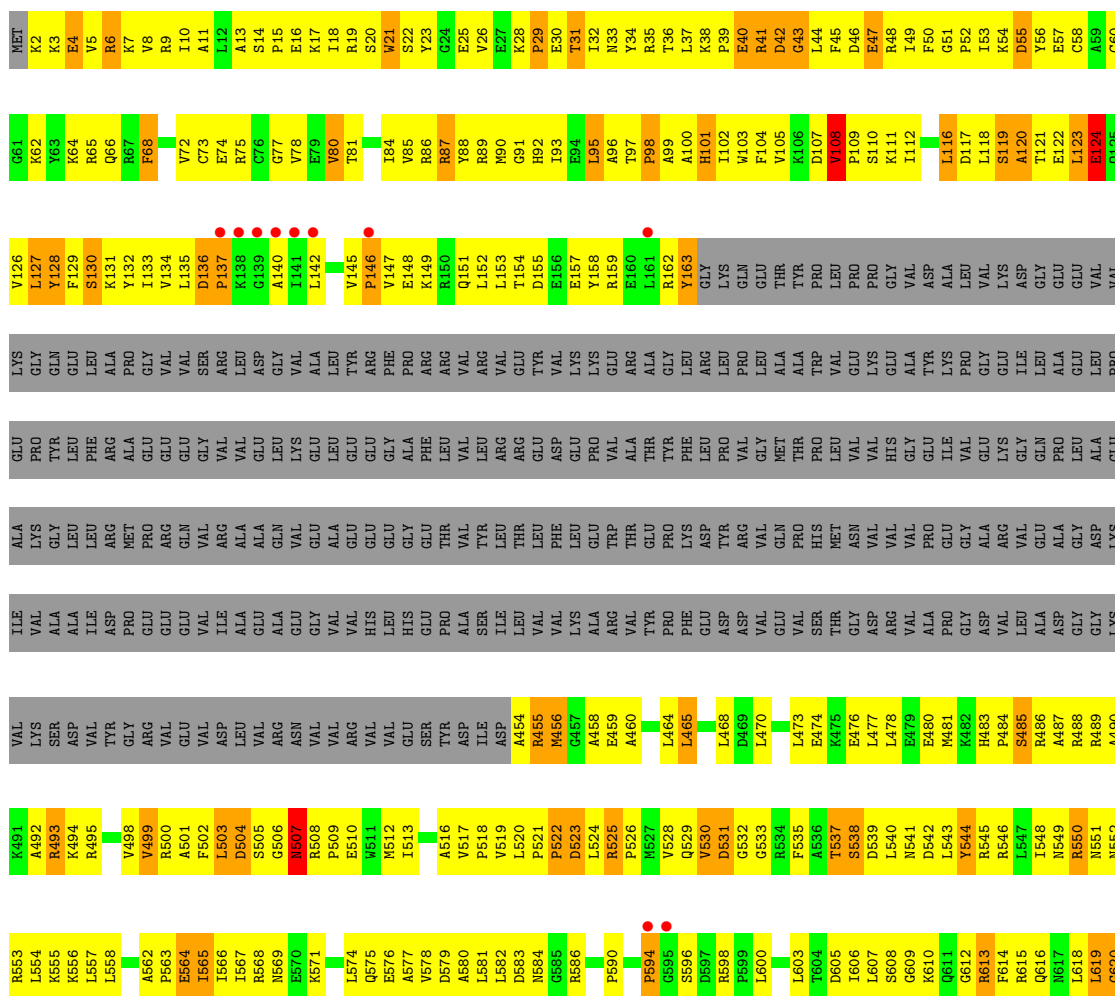


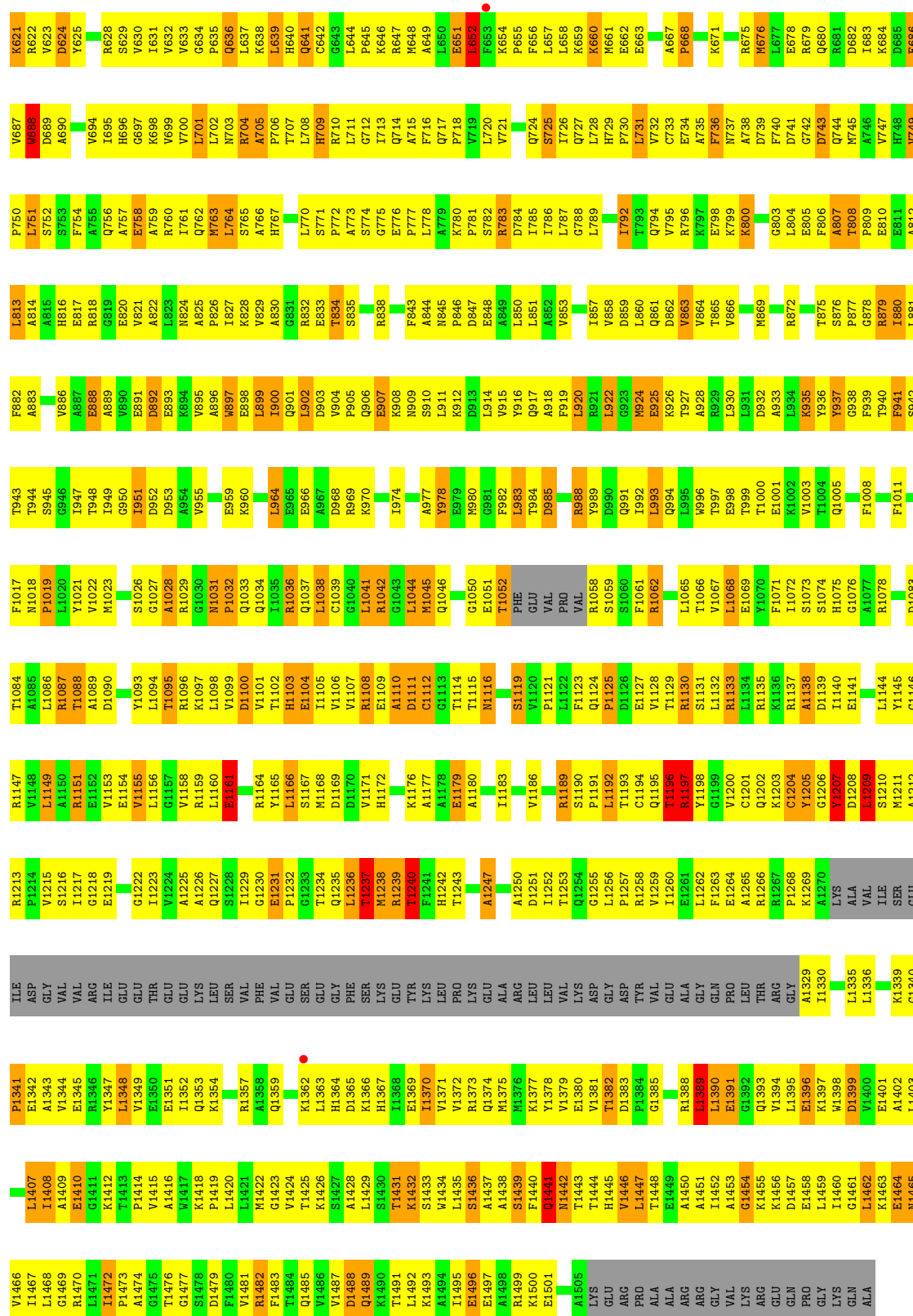
• Molecule 1: DNA-directed RNA polymerase subunit alpha



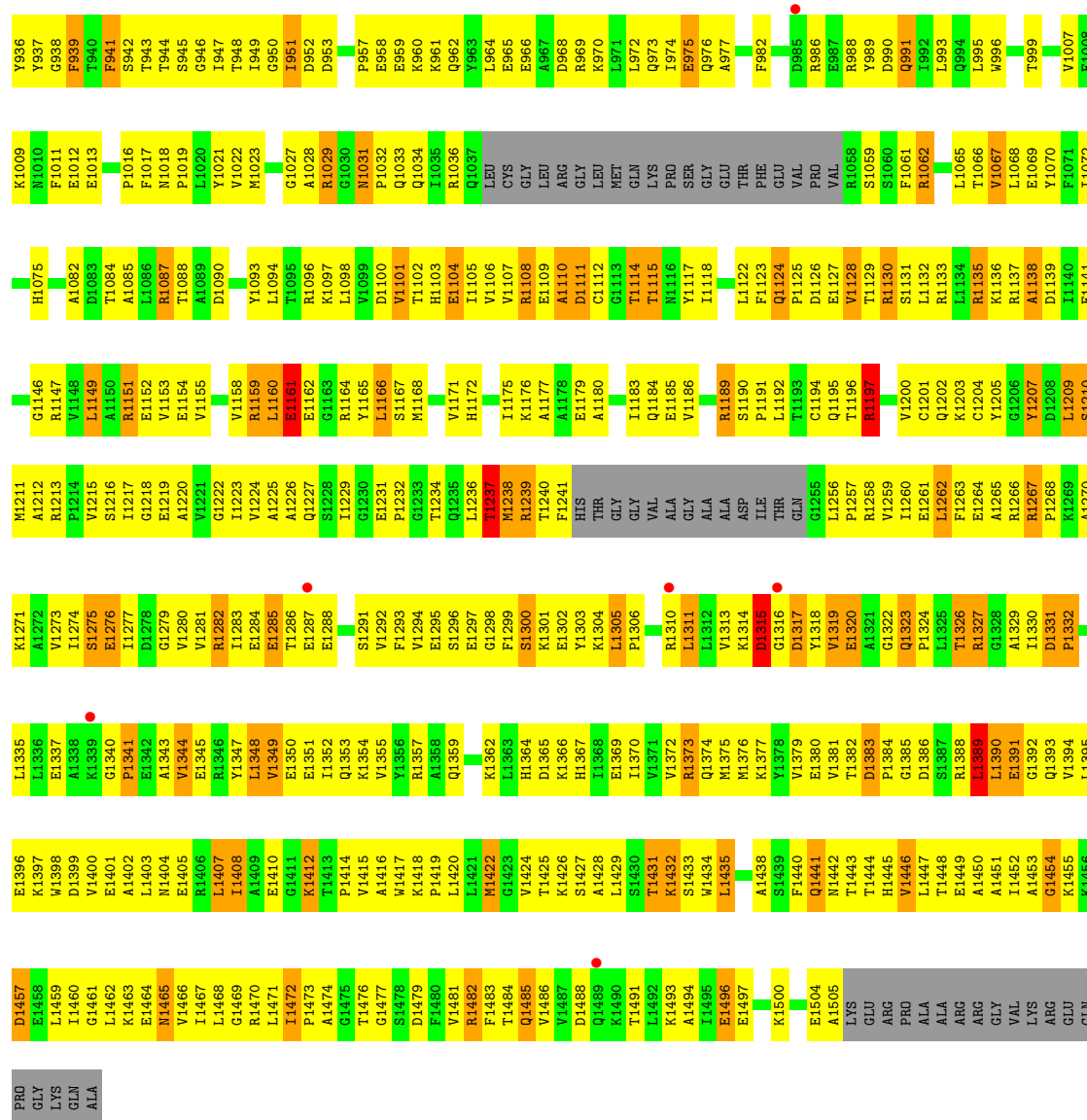
M1036	Y975	F906	H843	E771	E706	V644	E584	B517	T453	F386	H330	Y258	F191	F127
E1036	D976	D907	K846	R772	R707	V645	E585	K518	S454	S387	E321	G259	P192	I128
M1037	G977	G908	G847	S776	E709	G646	E586	G519	A456	R388	V322	L260	L193	I129
M1038	R978				I710	Q647	E587	E520	A457	S389	D323	T281	V194	N130
A1039	T979					R648	E588	P521	Y458	Q390	D324	A282	G131	A132
L1040	G980	P912	A850	E780		V649	E589	V522	A459	L391	I325	L263	L196	A133
E1041	E981		K851	R783	R713	R650	D590	I523	R460	S392	D326	P264	L197	D133
A1042	P982	L918	I852	R784	D714	K651	S591	V524	R461	Q393	H327	R265	R198	R134
Y1043	F983	A919	L853	D784		G652	E592	V525	Y461	F394	L328	R266	V199	V135
G1044	E984	Q920	P854	R785	P719	D653	E593	P526	D462	K395	G329	Z287		I136
A1045	G985	A921	V855	R786	E720	L654	A594		E463	K396	N330	D288	V137	V137
A1046	P986	F922	E856	D787	R721	L655	L595	F531	L464	E397	R331	L269	S138	S138
H1047	R987	E923	D857	T788	I722	L656	E596	M532	G465	T398	R332	G270	Q204	Q139
T1048	V988	V924	H858	S789	I723	D657	E597	D533	F466	N399	I333	E271	E205	I140
L1049	V989	Y925	P859	L790		G659	E598	V534	L467	P400	A272	T206	T206	H141
Q1050	G990	F926	H860	R791	D725		E599		R468	R394	L328	G273	L207	R142
					I726				T469	S402	V366	R274	A208	S143
L1053	Q991	G927	L861	P792	H726				P470	S403	G337	Y275	R209	P144
T1054	N992	P862	D863	P793	E728				Y471	R405	E338	K276	E210	G145
T1055	F993	R929	G863	T794	L729				R472	R406	L339	A277	L211	V146
L1056	T994	K930	G864	G795					R473	R407	F340	E278	G212	V147
K1056	M995	G931	T865	E796					V474	R408	D342	E279	A213	F148
S1057	K996	P866	V867	G797						R409	Q343	K280	Y214	
D1058	L997	V867		G798						R409	F344	L281	D151	
L1059	Y998	D937	D868	I799	A733				V478	T410	E216	E215	P152	
T1060	H999	K938	V669	V800	R735				Y479	T410	E217	E216		
E1061	M1000	R939	I870	V801	D736				T480	S411	L217	L217		
G1062	V1001	E940	L871	E802	L737				D481	L413	L218	V218	G156	
T1063	E1002	S878	N872	T803	D738				E482	L413	G219	Q219	R157	
M1064	D1003	E942	P873	H804	E739				V483	G414	L348	G287	Y158	
A1065	K1004	L874	A675	A675	L550				V484	P415	A349	R288	L221	I159
M1066	M1005	L944	G875	G741					V485	G416	R350	W292	A160	A160
Y1067	H1006	R945	R876	G812	G742				H486	G417	L351	D295	S161	S161
	A1007	R946	P877	V813	V743				T487	L418	A352	D223	E224	I162
I1071	R1008	A947	S878	E814	R744				A488	R353	R292	E225	P163	I163
K1072	S1009	E948	R879	L815	I745				T489	G354	F293	S226	L165	P164
G1073	T1010	K949	H880	P817	G746				R422	V355	E294	F227	P166	
E1074	G1011	L950	N881	K816					A423	R356	D295	G296		
D1075	P1012		L882	G818	E748				C424	E357	G296		P231	
	Y1013		G883	V819	V749				F425	R358	E297			
P1079	S1014	T954	Q884	R820	K750				D426	M359	F298	L236	G169	
G1080	L1015	P955	I885		P751						K299	T236	P170	
V1081	I1016	G956	T888	R824	G752				D429	D365	D300	R237	I172	
P1082	T1017	K957	H889	E825	D753				V430	S366	E301	L238	D173	
E1083	Q1018	T958	V826	V826	I754				H431	L367	V302	F239	L174	
S1084	Q1019	P959	L890	V827	L755				R432	T368	F303	T240	E175	
F1085	P1020	E960	G891	A828	V756				T433	P369	L304	L241	V176	
M1086	L1021	E961	L892	Q829	G757				H434	P305	P305	L242	E177	
V1087	G1022	Q962	A893	K830	R758				Y435	K371	T306	R243	P178	
L1088	G1023	L963	G894	R831	T759				C436	L307	L307	P244	R179	
V1089	K1024	K964	V895	K832	S760				R437	R308	G245	G245	G180	
K1090	A1025	E965	F896	L833	F761				R506	R374	Y309	D246	V181	
E1091	Q1026	L966	L897	Q834	K762				R507	L438	L310	P247	V182	
L1092	F1027	F967	G898	V835	G763				I598	G375	F311		S183	
Q1093	G1028	L968	Q899	G836	E764				A509	P440	R376	R250	M184	
A1094	Q1029	Q969	R900	D837	S765				V441	P377	A312	K251	K185	
L1095	G1030	G370	Y901	K838	E766				E442	L378	L313	K252	V186	
A1096	R1031	K371	I902	L839	P767				T443	E443	T314	A253	M187	
L1097	F1032	V972	S903	A840	T768				V513	P444	I382		K188	
D1098	G1033	V973	P904	R841	P769				L451		R383	P318	R189	
V1099	E1034	L974	I905	R842	E770				R516	L452	F385	G319	K190	







E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935																																																																																																																																																																																											
V749	P750	L751	D689	S752	S753	F754	A755	F756	A757	F758	A759	R760	L761	Q762	M763	L764	S765	A766	R767	P768	L769	S770	S771	S772	G773	F774	G775	F776	P777	L778	A779	K780	L781	S782	R783	D784	I785	L786	L787	G788	L789	L790	Y791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935																																																																																																																												
E686	V687	D688	S689	F690	A691	F692	A693	F694	A695	F696	A697	R698	L699	Q700	M701	L702	S703	A704	P705	L706	S707	S708	S709	S710	S711	S712	S713	S714	S715	S716	S717	S718	S719	S720	S721	S722	S723	S724	S725	S726	S727	S728	S729	S730	S731	S732	S733	S734	S735	S736	S737	S738	S739	S740	S741	S742	S743	S744	S745	S746	S747	S748	S749	S750	S751	S752	S753	S754	S755	S756	S757	S758	S759	S760	S761	S762	S763	S764	S765	S766	S767	S768	S769	S770	S771	S772	S773	S774	S775	S776	S777	S778	S779	S780	S781	S782	S783	S784	S785	S786	S787	S788	S789	S790	S791	S792	S793	S794	S795	S796	S797	S798	S799	S800	S801	S802	S803	S804	S805	S806	S807	S808	S809	S810	S811	S812	S813	S814	S815	S816	S817	S818	S819	S820	S821	S822	S823	S824	S825	S826	S827	S828	S829	S830	S831	S832	S833	S834	S835	S836	S837	S838	S839	S840	S841	S842	S843	S844	S845	S846	S847	S848	S849	S850	S851	S852	S853	S854	S855	S856	S857	S858	S859	S860	S861	S862	S863	S864	S865	S866	S867	S868	S869	S870	S871	S872	S873	S874	S875	S876	S877	S878	S879	S880	S881	S882	S883	S884	S885	S886	S887	S888	S889	S890	S891	S892	S893	S894	S895	S896	S897	S898	S899	S900	S901	S902	S903	S904	S905	S906	S907	S908	S909	S910	S911	S912	S913	S914	S915	S916	S917	S918	S919	S920	S921	S922	S923	S924	S925	S926	S927	S928	S929	S930	S931	S932	S933	S934	S935																																																														
K621	R622	V623	D624	Y625	G626	F627	R628	S629	V630	L631	V632	V633	G634	L637	K638	L639	H640	Q641	G642	L643	L644	P645	K646	A649	L650	D653	N654	L655	G658	R656	R657	P655	F656	L657	L658	K659	K660	M661	E662	E663	K664	L665	A667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	E678	R679	Q680	R681	D682	L683	K684	D685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935
K621	R622	V623	D624	Y625	G626	F627	R628	S629	V630	L631	V632	V633	G634	L637	K638	L639	H640	Q641	G642	L643	L644	P645	K646	A649	L650	D653	N654	L655	G658	R656	R657	P655	F656	L657	L658	K659	K660	M661	E662	E663	K664	L665	A667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	E678	R679	Q680	R681	D682	L683	K684	D685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935
E686	V687	D688	S689	F690	A691	F692	A693	F694	A695	F696	A697	R698	L699	Q700	M701	L702	S703	A704	P705	L706	S707	S708	S709	S710	S711	S712	S713	S714	S715	S716	S717	S718	S719	S720	S721	S722	S723	S724	S725	S726	S727	S728	S729	S730	S731	S732	S733	S734	S735	S736	S737	S738	S739	S740	S741	S742	S743	S744	S745	S746	S747	S748	S749	S750	S751	S752	S753	S754	S755	S756	S757	S758	S759	S760	S761	S762	S763	S764	S765	S766	S767	S768	S769	S770	S771	S772	S773	S774	S775	S776	S777	S778	S779	S780	S781	S782	S783	S784	S785	S786	S787	S788	S789	S790	S791	S792	S793	S794	S795	S796	S797	S798	S799	S800	S801	S802	S803	S804	S805	S806	S807	S808	S809	S810	S811	S812	S813	S814	S815	S816	S817	S818	S819	S820	S821	S822	S823	S824	S825	S826	S827	S828	S829	S830	S831	S832	S833	S834	S835	S836	S837	S838	S839	S840	S841	S842	S843	S844	S845	S846	S847	S848	S849	S850	S851	S852	S853	S854	S855	S856	S857	S858	S859	S860	S861	S862	S863	S864	S865	S866	S867	S868	S869	S870	S871	S872	S873	S874	S875	S876	S877	S878	S879	S880	S881	S882	S883	S884	S885	S886	S887	S888	S889	S890	S891	S892	S893	S894	S895	S896	S897	S898	S899	S900	S901	S902	S903	S904	S905	S906	S907	S908	S909	S910	S911	S912	S913	S914	S915	S916	S917	S918	S919	S920	S921	S922	S923	S924	S925	S926	S927	S928	S929	S930	S931	S932	S933	S934	S935																																																														
K64	R65	Q66	F67	S68	K69	L70	V71	L72	S73	F74	A75	P76	L77	Q78	M79	L80	S81	A82	P83	L84	S85	S86	S87	S88	S89	S90	S91	S92	S93	S94	S95	S96	S97	S98	S99	S00	S01	S02	S03	S04	S05	S06	S07	S08	S09	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26	S27	S28	S29	S30	S31	S32	S33	S34	S35	S36	S37	S38	S39	S40	S41	S42	S43	S44	S45	S46	S47	S48	S49	S50	S51	S52	S53	S54	S55	S56	S57	S58	S59	S60	S61	S62	S63	S64	S65	S66																																																																																																																																																																																																																	

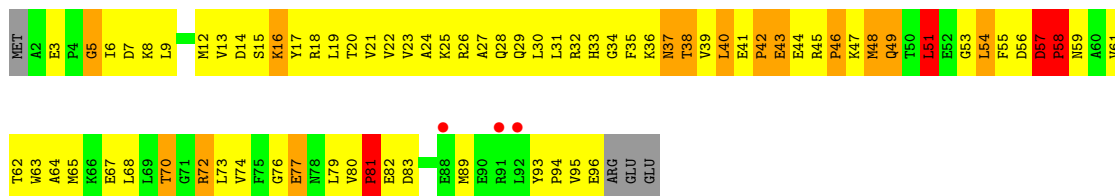


• Molecule 4: DNA-directed RNA polymerase subunit omega

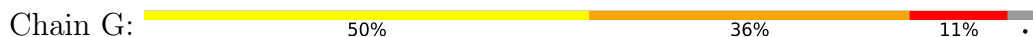


• Molecule 4: DNA-directed RNA polymerase subunit omega





• Molecule 5: DNA (28-MER)



• Molecule 5: DNA (28-MER)



• Molecule 6: RNA (5'-R(P*CP*CP*AP*GP*CP*CP*GP*GP*CP*GP*CP*UP*CP*GP*CP*A)-3')



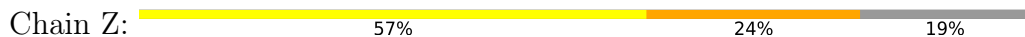
• Molecule 6: RNA (5'-R(P*CP*CP*AP*GP*CP*CP*GP*GP*CP*GP*CP*UP*CP*GP*CP*A)-3')



• Molecule 7: DNA (5'-D(P*GP*TP*AP*GP*CP*TP*TP*GP*TP*GP*GP*TP*AP*GP*TP*GP*AP*CP*GP*AP*G)-3')



• Molecule 7: DNA (5'-D(P*GP*TP*AP*GP*CP*TP*TP*GP*TP*GP*GP*TP*AP*GP*TP*GP*AP*CP*GP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	155.98Å 155.98Å 495.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.15 – 4.31 44.15 – 4.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.15-4.31) 99.4 (44.15-4.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 4.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.281 , 0.311 0.285 , 0.315	Depositor DCC
R_{free} test set	3821 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.499 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	48166	wwPDB-VP
Average B, all atoms (Å ²)	250.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% 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: 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	A	0.38	0/1838	0.69	0/2498
1	B	0.43	0/1838	0.68	0/2498
1	K	0.45	0/1838	0.70	0/2498
1	L	0.42	0/1838	0.67	0/2498
2	C	0.49	0/8997	0.79	3/12164 (0.0%)
2	M	0.48	0/8997	0.78	4/12164 (0.0%)
3	D	0.51	1/9249 (0.0%)	0.83	10/12482 (0.1%)
3	N	0.51	0/10344	0.81	8/13968 (0.1%)
4	E	0.50	0/784	0.87	2/1057 (0.2%)
4	O	0.46	0/784	0.84	2/1057 (0.2%)
5	G	0.99	1/614 (0.2%)	1.41	9/943 (1.0%)
5	X	0.93	0/614	1.43	11/943 (1.2%)
6	H	1.14	3/378 (0.8%)	1.56	6/585 (1.0%)
6	Y	1.15	3/353 (0.8%)	1.45	5/546 (0.9%)
7	I	0.94	1/400 (0.2%)	1.46	7/616 (1.1%)
7	Z	0.90	1/400 (0.2%)	1.28	3/616 (0.5%)
All	All	0.53	10/49266 (0.0%)	0.84	70/67133 (0.1%)

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
5	G	0	10
5	X	0	11
6	H	0	4
6	Y	0	5
7	I	0	6
7	Z	0	4
All	All	0	40

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	1	DG	OP3-P	-7.99	1.51	1.61
7	I	1	DG	OP3-P	-7.84	1.51	1.61
6	Y	11	C	N1-C2	-7.40	1.32	1.40
6	H	11	C	N1-C2	-7.38	1.32	1.40
6	H	1	C	OP3-P	-7.06	1.52	1.61

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	1	DG	O5'-P-OP1	-18.71	88.24	110.70
7	Z	1	DG	O5'-P-OP1	-16.85	90.48	110.70
6	H	5	C	N1-C1'-C2'	-15.07	94.41	114.00
6	Y	5	C	N1-C1'-C2'	-9.98	101.02	112.00
7	I	1	DG	O5'-P-OP2	9.33	121.90	110.70

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	10	DA	Sidechain
5	G	2	DT	Sidechain
5	G	3	DC	Sidechain
5	G	4	DA	Sidechain
5	G	9	DC	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	257	0
1	B	1806	0	1861	180	0
1	K	1806	0	1861	189	0
1	L	1806	0	1861	203	0
2	C	8829	0	8933	1430	0
2	M	8829	0	8933	1425	0
3	D	9097	0	9316	1626	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	10175	0	10401	1763	0
4	E	770	0	784	124	0
4	O	770	0	784	151	0
5	G	548	0	301	113	0
5	X	548	0	301	93	0
6	H	340	0	176	76	0
6	Y	318	0	165	56	0
7	I	357	0	194	68	0
7	Z	357	0	194	71	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
All	All	48166	0	47926	7162	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 75.

The worst 5 of 7162 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:C:52:PHE:CZ	2:C:68:PHE:HB2	1.22	1.67
3:D:897:TRP:HA	3:D:900:ILE:CG1	1.33	1.56
3:D:1041:LEU:HD11	3:D:1045:MET:SD	1.55	1.44
3:D:705:ALA:HB1	6:H:14:G:N2	1.24	1.40
3:D:705:ALA:CB	6:H:14:G:H21	1.40	1.32

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	227/315 (72%)	194 (86%)	24 (11%)	9 (4%)	3 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	227/315 (72%)	195 (86%)	23 (10%)	9 (4%)	3	26
1	K	227/315 (72%)	193 (85%)	26 (12%)	8 (4%)	3	29
1	L	227/315 (72%)	201 (88%)	17 (8%)	9 (4%)	3	26
2	C	1117/1119 (100%)	893 (80%)	151 (14%)	73 (6%)	1	18
2	M	1117/1119 (100%)	889 (80%)	153 (14%)	75 (7%)	1	18
3	D	1143/1524 (75%)	903 (79%)	167 (15%)	73 (6%)	1	19
3	N	1280/1524 (84%)	1011 (79%)	190 (15%)	79 (6%)	1	19
4	E	93/99 (94%)	67 (72%)	15 (16%)	11 (12%)	0	6
4	O	93/99 (94%)	69 (74%)	13 (14%)	11 (12%)	0	6
All	All	5751/6744 (85%)	4615 (80%)	779 (14%)	357 (6%)	1	19

5 of 357 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	29	GLU
1	A	118	ALA
1	A	133	GLU
1	A	187	GLY

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	
1	A	202/273 (74%)	178 (88%)	24 (12%)	5	23
1	B	202/273 (74%)	182 (90%)	20 (10%)	8	29
1	K	202/273 (74%)	182 (90%)	20 (10%)	8	29
1	L	202/273 (74%)	182 (90%)	20 (10%)	8	29
2	C	941/941 (100%)	790 (84%)	151 (16%)	2	15
2	M	941/941 (100%)	794 (84%)	147 (16%)	2	16
3	D	968/1279 (76%)	806 (83%)	162 (17%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	1088/1279 (85%)	919 (84%)	169 (16%)	2	16
4	E	84/88 (96%)	70 (83%)	14 (17%)	2	14
4	O	84/88 (96%)	70 (83%)	14 (17%)	2	14
All	All	4914/5708 (86%)	4173 (85%)	741 (15%)	3	17

5 of 741 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	310	LEU
3	N	85	VAL
2	M	433	THR
2	M	309	TYR
2	M	824	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	841	ASN
2	M	889	HIS
4	O	37	ASN
3	N	1031	ASN
3	N	1034	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	H	15/16 (93%)	5 (33%)	1 (6%)
6	Y	14/16 (87%)	3 (21%)	1 (7%)
All	All	29/32 (90%)	8 (27%)	2 (6%)

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	H	4	G
6	H	5	C
6	H	6	C
6	H	15	C
6	H	16	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	H	5	C
6	Y	5	C

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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 ⓘ

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	229/315 (72%)	-0.77	1 (0%) 92 87	154, 243, 347, 432	0
1	B	229/315 (72%)	-0.48	8 (3%) 44 35	202, 343, 460, 525	0
1	K	229/315 (72%)	-0.59	4 (1%) 70 61	157, 255, 375, 500	0
1	L	229/315 (72%)	-0.49	4 (1%) 70 61	193, 363, 452, 538	0
2	C	1119/1119 (100%)	-0.75	6 (0%) 91 86	12, 213, 336, 454	0
2	M	1119/1119 (100%)	-0.72	8 (0%) 87 82	60, 238, 426, 549	0
3	D	1151/1524 (75%)	-0.73	12 (1%) 82 74	8, 205, 382, 548	0
3	N	1288/1524 (84%)	-0.59	33 (2%) 56 46	81, 249, 452, 545	0
4	E	95/99 (95%)	-0.53	3 (3%) 47 37	156, 217, 337, 395	0
4	O	95/99 (95%)	-0.62	3 (3%) 47 37	205, 297, 426, 451	0
5	G	27/28 (96%)	-0.76	0 100 100	152, 210, 372, 381	0
5	X	27/28 (96%)	-0.67	0 100 100	238, 279, 353, 374	0
6	H	16/16 (100%)	0.21	1 (6%) 20 16	97, 189, 363, 385	0
6	Y	15/16 (93%)	-0.24	0 100 100	208, 249, 351, 378	0
7	I	17/21 (80%)	-0.65	0 100 100	215, 276, 418, 428	0
7	Z	17/21 (80%)	-0.72	0 100 100	264, 305, 348, 352	0
All	All	5902/6874 (85%)	-0.67	83 (1%) 75 66	8, 240, 416, 549	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	140	ALA	12.4
3	N	175	VAL	12.4
3	D	141	ILE	9.5
1	B	3	ASP	8.7
1	L	68	ILE	7.5

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 monosaccharides 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(\AA^2)	Q<0.9
8	ZN	N	1601	1/1	0.97	0.13	72,72,72,72	0
8	ZN	D	1601	1/1	0.98	0.05	72,72,72,72	0
8	ZN	N	1602	1/1	0.98	0.11	72,72,72,72	0
8	ZN	D	1602	1/1	0.99	0.14	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.