



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:02 PM GMT

PDB ID : 2A69  
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic rifapentin  
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-07-02  
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

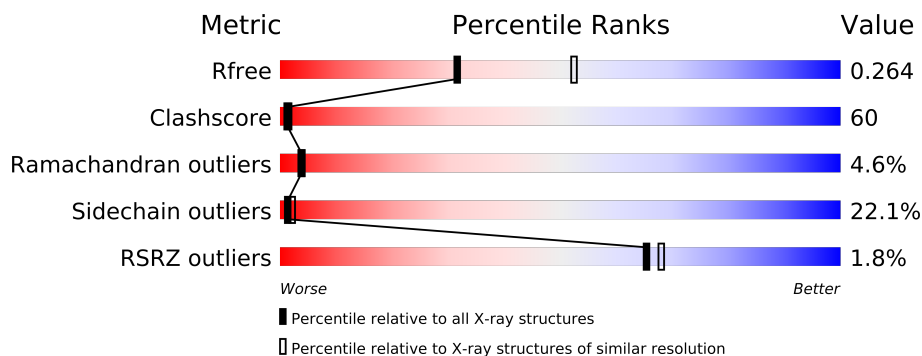
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	MG	A	9043	-	X
6	MG	A	9384	-	X
6	MG	B	9040	-	X
6	MG	B	9056	-	X
6	MG	C	9025	-	X
6	MG	C	9067	-	X
6	MG	D	9064	-	X
6	MG	D	9373	-	X
6	MG	F	9159	-	X
6	MG	F	9376	-	X
6	MG	L	9306	-	X
6	MG	M	9190	-	X
6	MG	M	9416	-	X
6	MG	N	9192	-	X
6	MG	N	9193	-	X
6	MG	N	9217	-	X
6	MG	N	9253	-	X
6	MG	N	9267	-	X
6	MG	N	9444	-	X
6	MG	O	9198	-	X
7	RPT	C	8001	-	X
7	RPT	M	8002	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60572 atoms, of which 0 are hydrogen and 0 are deuterium.

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 alpha chain.

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 beta chain.

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 beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

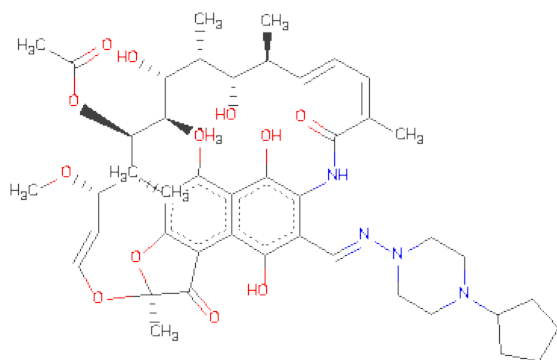
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	20	Total	Mg	0	0
			20	20		
6	D	106	Total	Mg	0	0
			106	106		
6	K	19	Total	Mg	0	0
			19	19		
6	E	5	Total	Mg	0	0
			5	5		
6	B	21	Total	Mg	0	0
			21	21		
6	C	73	Total	Mg	0	0
			73	73		
6	A	33	Total	Mg	0	0
			33	33		
6	N	92	Total	Mg	0	0
			92	92		
6	O	8	Total	Mg	0	0
			8	8		
6	L	17	Total	Mg	0	0
			17	17		
6	F	28	Total	Mg	0	0
			28	28		
6	M	65	Total	Mg	0	0
			65	65		

- Molecule 7 is RIFAPENTINE (three-letter code: RPT) (formula: C<sub>47</sub>H<sub>64</sub>N<sub>4</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			63	47	4	12		
7	M	1	Total	C	N	O	0	0
			63	47	4	12		

- 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		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	239	Total	O	0	0
			239	239		
9	B	258	Total	O	0	0
			258	258		
9	C	979	Total	O	0	0
			979	979		
9	D	1252	Total	O	0	0
			1252	1252		
9	E	117	Total	O	0	0
			117	117		

*Continued on next page...*

*Continued from previous page...*

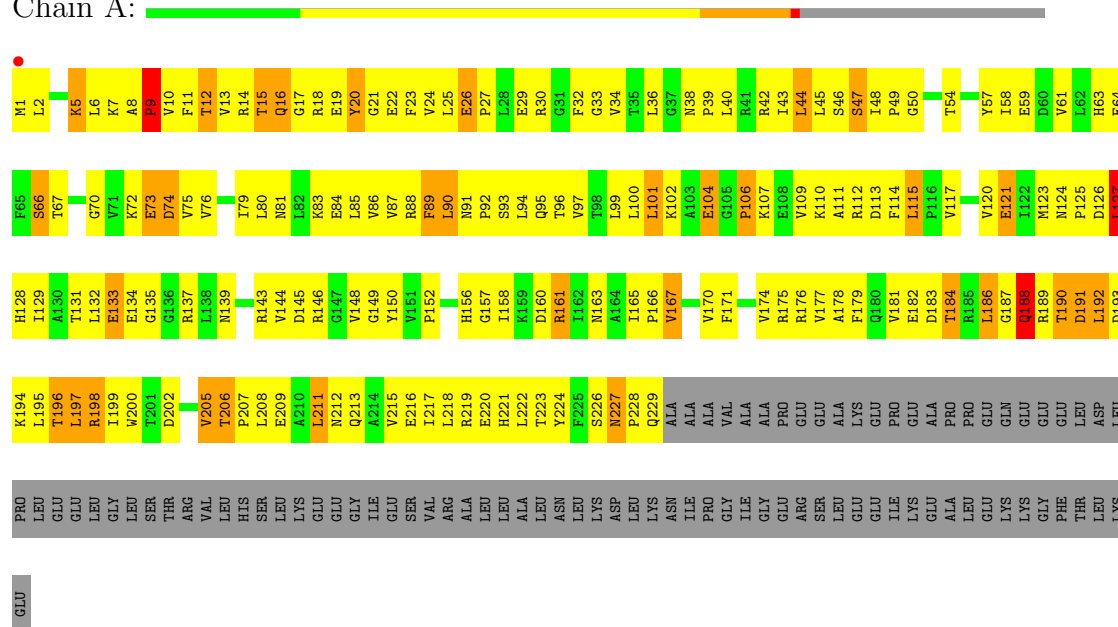
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	420	Total 420	O 420	0	0
9	K	183	Total 183	O 183	0	0
9	L	219	Total 219	O 219	0	0
9	M	998	Total 998	O 998	0	0
9	N	1265	Total 1265	O 1265	0	0
9	O	108	Total 108	O 108	0	0
9	P	361	Total 361	O 361	0	0

### 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.

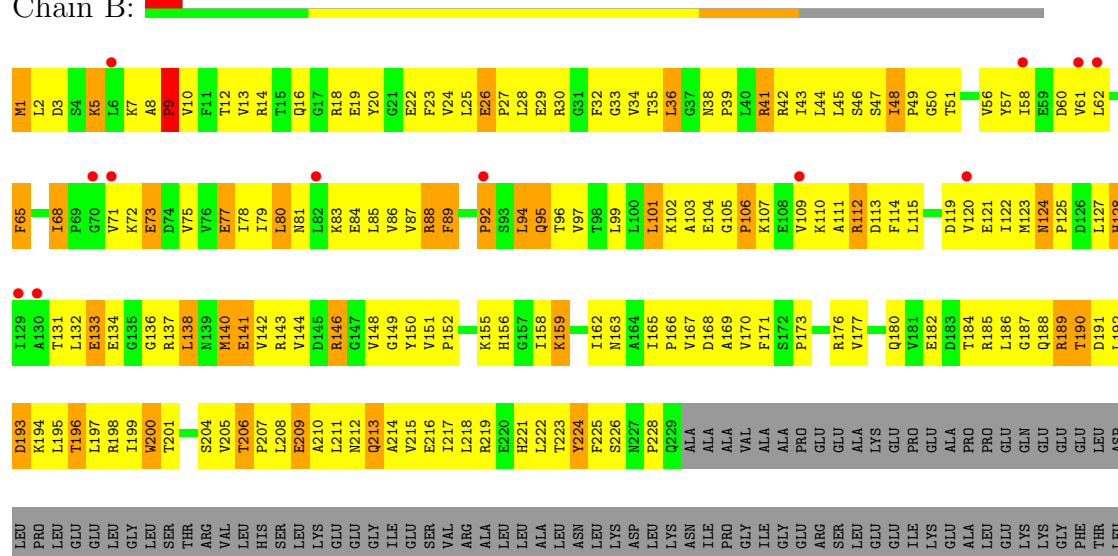
- Molecule 1: DNA-directed RNA polymerase alpha chain

Chain A:



- Molecule 1: DNA-directed RNA polymerase alpha chain

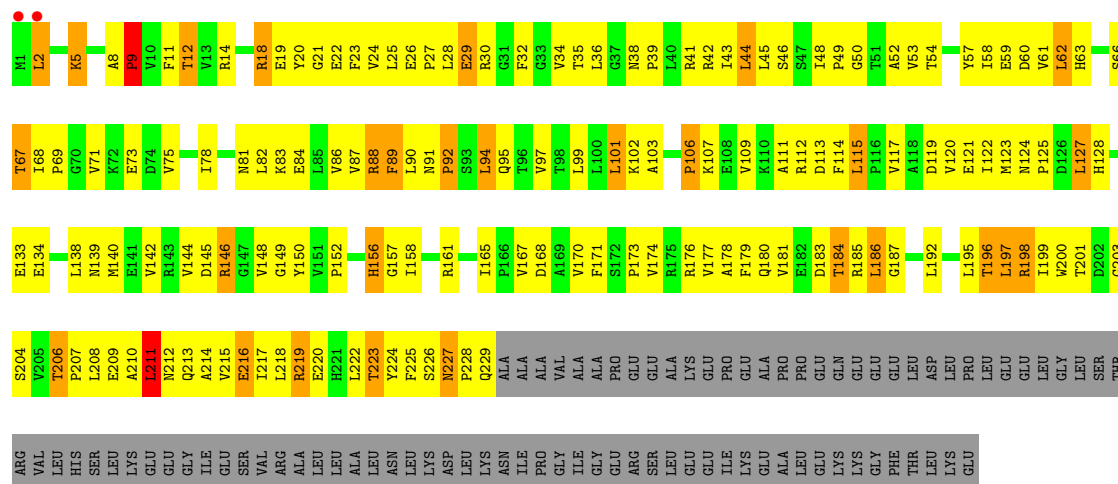
Chain B:



LYS  
GLU

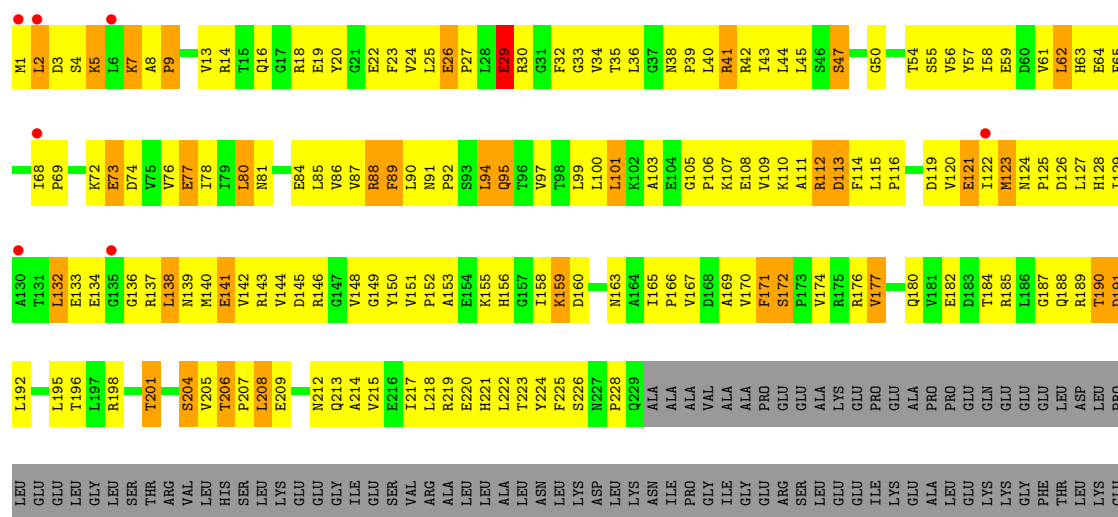
- Molecule 1: DNA-directed RNA polymerase alpha chain

Chain K:



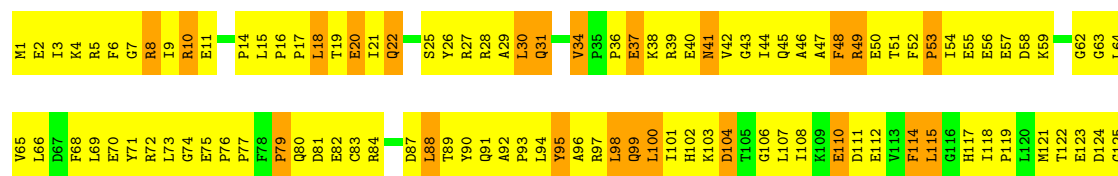
- Molecule 1: DNA-directed RNA polymerase alpha chain

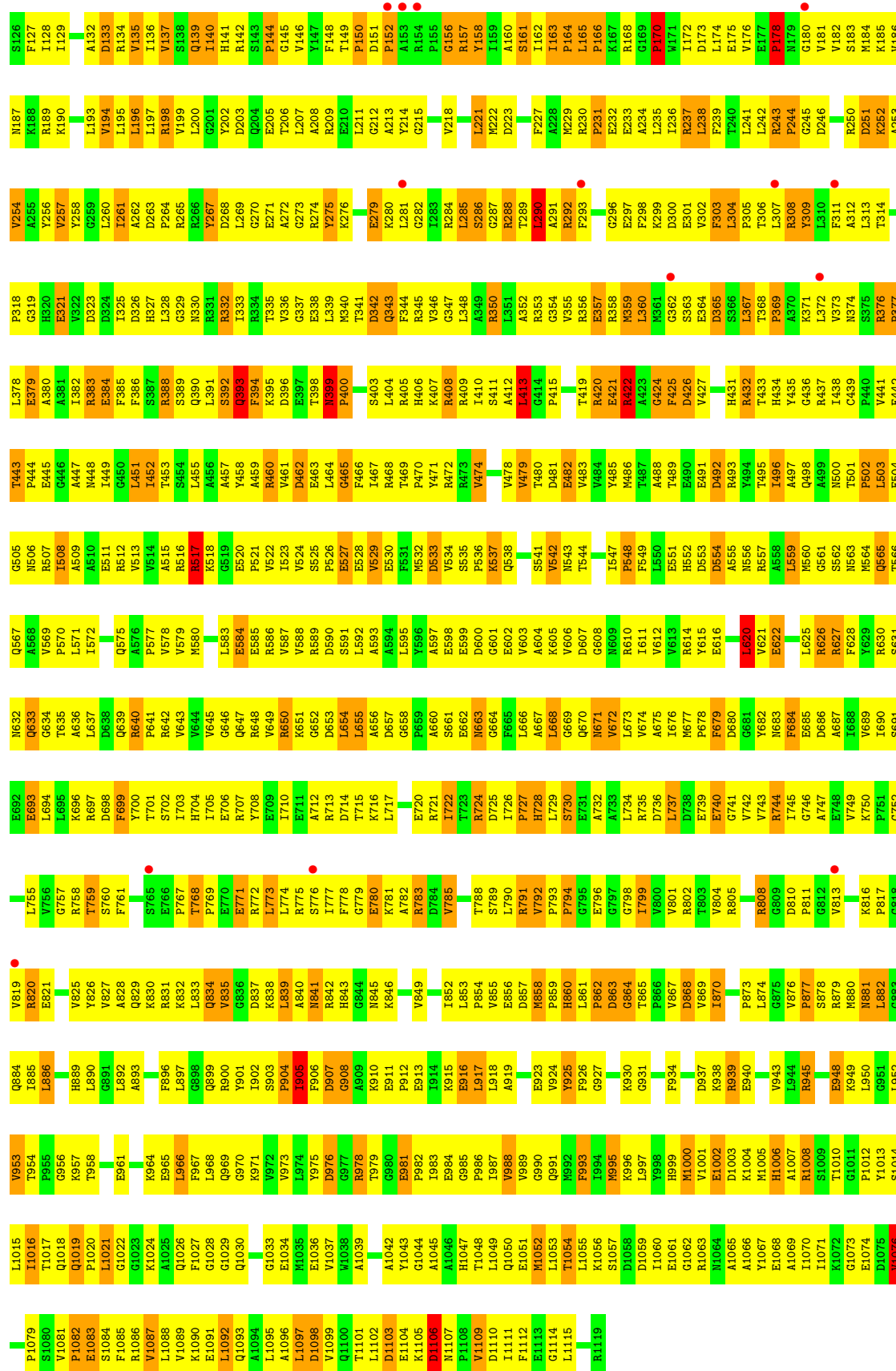
Chain L:



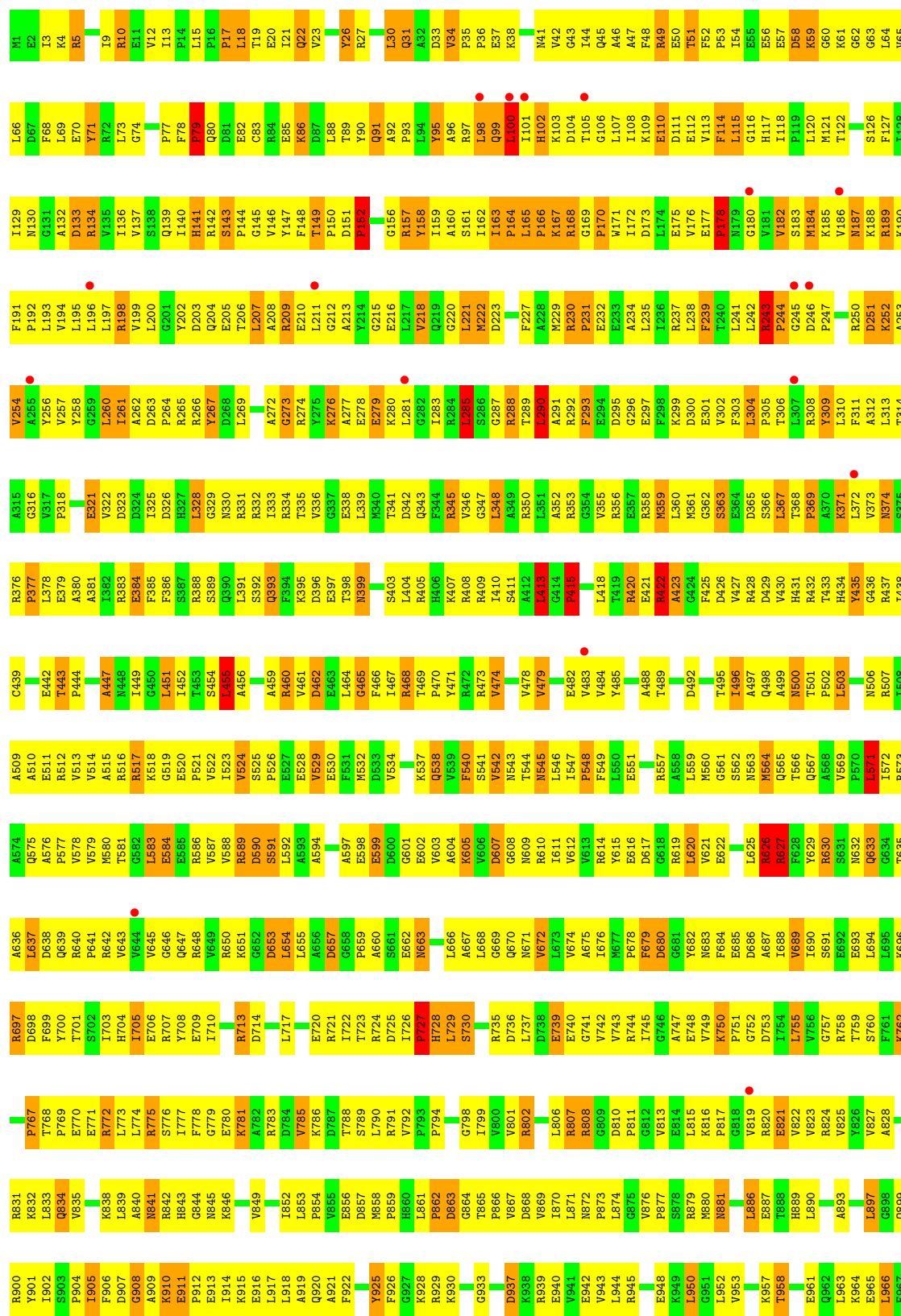
- Molecule 2: DNA-directed RNA polymerase beta chain

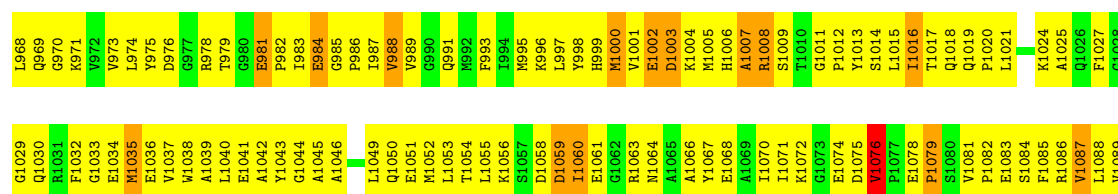
Chain C:





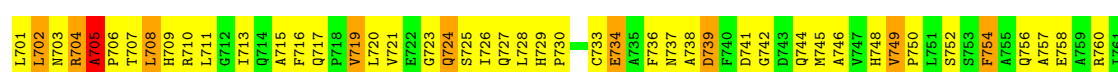
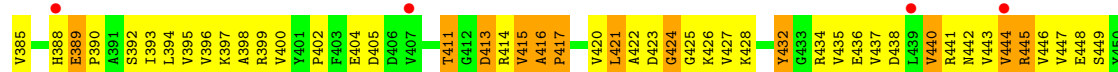
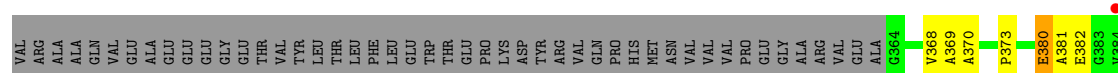
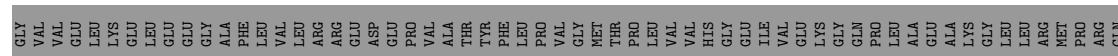
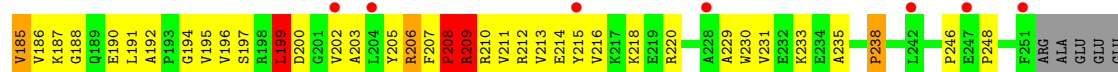
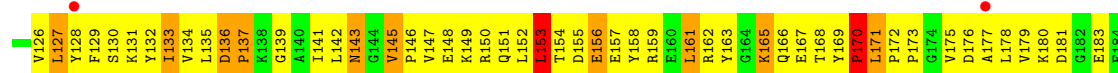
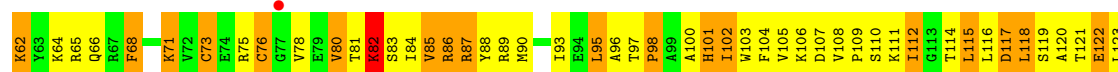
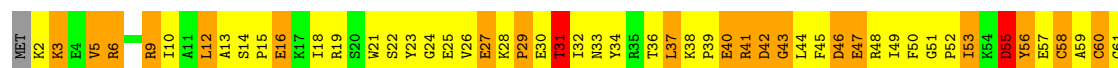
Chain M:





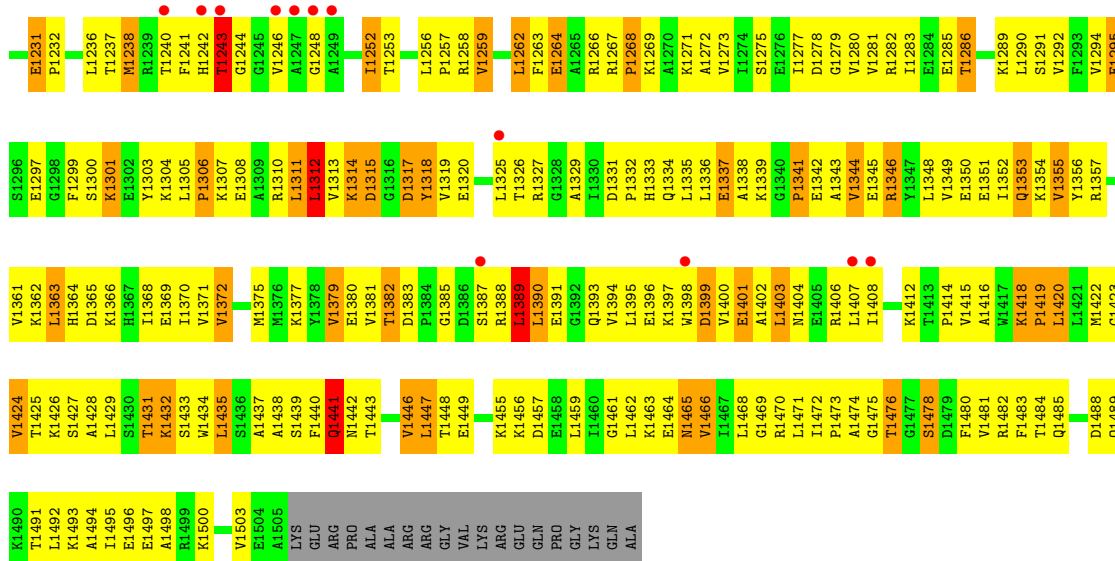
### • Molecule 3: DNA-directed RNA polymerase beta' chain

Chain D:



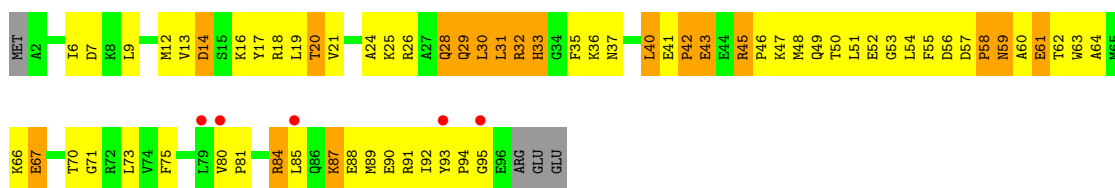


E1161	L1098	P1032	A967	E998	E833	S771	R704	G643	A577	L514	T452	P390	GLU	E190
R1164	V1099	Q1033	D968	L899	T834	P772	A705	L644	V578	E515	D453	A391	LEU	L191
Y1165	D1100	Q1034	R969	I900	S835	A773	P706	P645	D579	A516	A454	S392	GLU	A192
L1166	V1101	I1035	K970	Q901	V836	S774	T707	R646	A580	V517	R455	I393	GLU	P193
S1167	T1102	R1036	L972	L902	G837	G775	L708	R647	L581	P518	M456	L394	GLY	V195
H1103	H1037	Q1037	L971	D903	R838	E776	H709	M648	L582	V519		V395	GLY	V196
M1168	E1104	L1038	Q973	V904	F843	P777	R710		D583	L520	E459	V396	PHE	V197
D1169	T1105	C1039	I974	P905	A844	L778	L711	E551	N884	P521	A460	K397	LEU	S197
P1170	V1106	G1040	E975	Q906	E906			L652	G585	P522	I461	K397	VAL	R198
V1171	L1107	L1041	Q976	E907	D847	P781	Q714	F653	R586	D523	Q462	R399	TYR	L199
H1172	R1108	L1042	A977	S910	E848	S782	A715	K654	R587	L524	Q463	V400	ARG	D200
L1173	E1109	G1043	Y978	I911	A849	R783	F716	P655	G588	R525	L464	Y401	ARG	G201
L1174	A1110	L1044	E979	K912	L850	R784	Q717	F656	A589	P526	L465	Y402	LEU	V202
I1175	D1111	H1045	H980	K912	L851	L785	F718	L657	P590	M527	K466	F403	ASP	A203
K1176	C1112	Q1046	G981	D913	A852	V719	V719	L658	V591	V528	E467	E404	GLU	L204
A1177	G1113	L1047	F982	L914	V853	L787	L720	K659	T592	Q529	L468		PRO	Y205
L1178	P1048	P1048	L983	V915	V853	L788	V721	G660	N593	V530	D469		VAL	R206
E1179	T1115	S1049	T984	Y916	A854	L789	E722	M661	P594	G533	L470	E407	THR	F207
	N1116	G1050	D985		H855	V790	G723	E662		R534	E471		GLU	P208
E1182	Y1117	E1051	R986	F919	G856	V791	I726	E663	R598	R534	E474	T411	PRO	R209
I1183	T1118	L920	E987	L920	L857	L792	I726	K664		F535		G412	LYS	R210
Q1184	S1119	F1053	R988	R921	V858	T793	Q727	G665	R601	A536	E475	D413	PHE	V211
E1185			Y989	L922	D859	Q794	L728	T666	S602	T537	E476	R414	TYR	R212
P1187	L1122	V1057	R990	G923	L860	V795	H729	A667	L603	S538	L477	V415	VAL	V213
V1188	Q1124	R1058	Q991	K924	Q861	R796	P730	P668	T604	D539	L478	A416	GLY	E214
R1189	P1125	S1059	T992		D862	K797	L731	M669	D605	L540	E479	P417	MET	Y215
S1190	F1126	F1061	A928	T927	V863	V799	V732	V670	L606	M541	E480	G418	PRO	Y216
P1191	D1126	R1062	L995	L931	V864	K799	C733	K671	L607	D542	M481	D419	PRO	R207
L1192	E1127	E1063	Y996	L931	T865	R800	E734	A672	S608	L543		V420	MET	F207
T1193	V1128	G1064	T997	D939	V866	G801	A735	A673	G609	R546	H483	L421	ASN	R220
C1194	R1130	L1065	E998	A933	R867	R802	F736	R674	K610	L547	P484	A422	VAL	L223
Q1195	T1066	T1066	T999		V868	G803	N737	R675	Q611	I548	S485	D423	HIS	R224
R1197	R1133	V1087	T1000	Y937	G870	E805	A738	L677	Q616	M549	R486	G424	VAL	L225
Y1198	L1134	L1088	E1001	F941	K871	F806		L677	N617	R550	A487	K426	GLU	A235
	K1135	E1069	K1002	S942	R872	A807	D743	R679	L618	R489	R488	V427	GLY	Y236
	K1136	Y1070	V1003	T943	L873	T808	Q744	Q680	L619	N551	R489	K428	VAL	K237
	R1137		T1004	T943	E874	P809	M745	R681	G620	L554	K491	S429	ALA	A239
	A1138	S1073	Q1005	T944	T875	E810		D682	K621	K555	A492	D430	LYS	V231
	D1139	S1074	A1006	S945	S876	E811	H748	T683	R622	R556	R493	V431	GLY	A235
	I1140	H1075	F1007	G946	P877	A812	V749	K684	V623	L557	K494	V437	PRO	Y236
	E1141	G1076	F1008	I947	G878	L813	P750	D685	D624	L558	R495	G433	LEU	K237
	A1142	A1077	K1009	T948	R879	A814	L751	E686	G625	A559	L496	R434	ALA	P238
	G1143	R1077	M1010	T949	I880		S752	V687	S626	Q560	E497	V435	GLU	
	L1144	K1079	F1011	G950	L881	E817	S753	M688	G627	G561	V498	E436	ALA	P246
	Y1145	D1083	E1012	T951	P882	R818	F754	D689	R628	A562	V499	V437	LYS	E247
	G1146	S1210	N1018	D952	A883	G819	A755	A690	S629	P563	R500	D438	GLY	P248
	R1147	F1007	A1007	D953	R884	E820	Q756	L691	V630	E564	F501	L439	LEU	
	V1148	A1085	M1019	I957	T885	V821	A757	E692	I631	I565	F502	V440	LEU	F251
	L1149	L1086	L1020	T956	V886	A822	E758	E693	V632	I566	L503	R441	ARG	ARG
	A1150	R1087	Y1021	P957	A837	L823	A759	V694	V633	I567	D504	N442	MET	ALA
	R1151		V1022	E958	E888	N824	R760	P695	G634	R568	S505	V442	PRO	GLU
	E1152	D1090	M1023	D952	A889	A825		H696	P635	N569	G506	V444	ARG	GLU
	V1153	G1092	E959	K960	R890	P826	Q756	G697	Q636	E570	N507	R445	GLN	GLU
	E1154	Y1093	K961	T962	E891	I827	S765	V698	K637	K571	R508	V446	VAL	GLY
	V1155	G1027	Q962	Q962	D892	K828	A766	V699	K638	R572	P509	V447	ARG	VAL
	L1156	L1094	Y963	Y963	D892	V829	H767	V700	L639	M573	E510	E448	ALA	VAL
		T1095	L964	L964	V895	A830	H769	L701	H640	L574	M511	S449	ALA	GLU
	R1159	R1096	G1030	E965	V895	L769	L770	L702	Q641	Q575	M512	Y450	GLN	GLU
		K1097	M1031	E966	W897	R832		N703	C642	E576	I513	D451	VAL	LVS



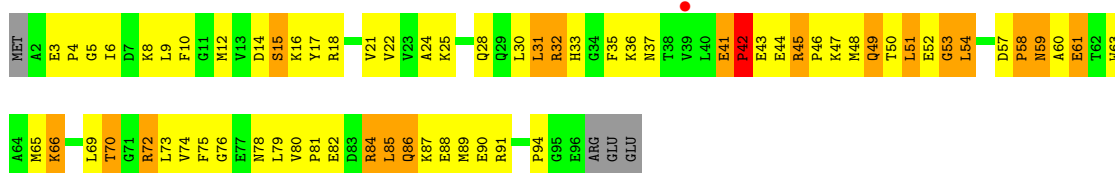
• Molecule 4: RNA polymerase omega chain

Chain E:



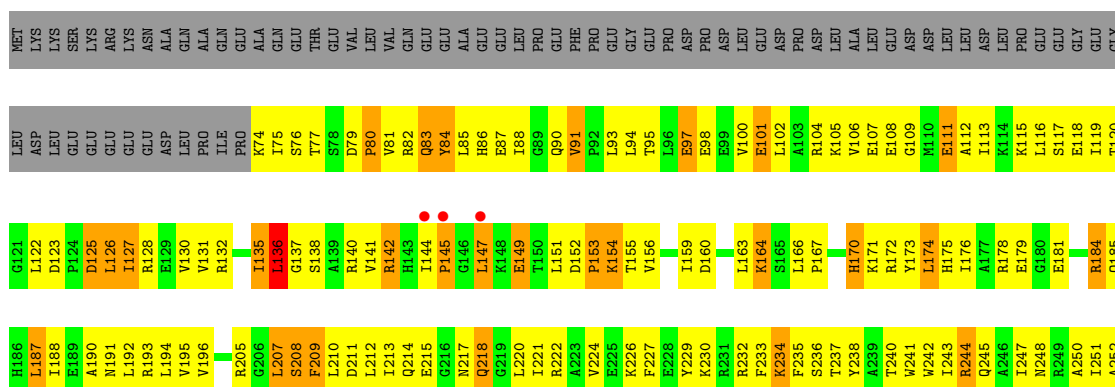
• Molecule 4: RNA polymerase omega chain

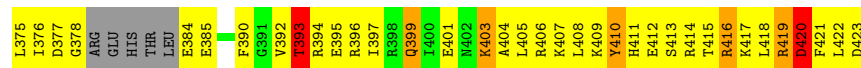
Chain O:



• Molecule 5: RNA polymerase sigma factor rpoD

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 92.6 (24.85-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.267 0.228 , 0.264	Depositor DCC
$R_{free}$ test set	29710 reflections (6.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 81.1	EDS
Estimated twinning fraction	0.499 for -h,-k,l 0.076 for h,-h-k,-l 0.076 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 517107 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	60572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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, RPT

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	0.81	1/1838 (0.1%)	0.88	4/2498 (0.2%)
1	B	0.74	0/1838	0.81	2/2498 (0.1%)
1	K	0.75	0/1838	0.86	3/2498 (0.1%)
1	L	0.73	1/1838 (0.1%)	0.80	2/2498 (0.1%)
2	C	0.83	2/8997 (0.0%)	0.89	7/12164 (0.1%)
2	M	0.81	0/8997	0.88	8/12164 (0.1%)
3	D	0.84	0/10975	0.94	20/14836 (0.1%)
3	N	0.82	0/10975	0.92	17/14836 (0.1%)
4	E	0.84	0/783	0.94	0/1054
4	O	0.82	0/783	0.96	2/1054 (0.2%)
5	F	0.74	0/2812	0.82	4/3781 (0.1%)
5	P	0.71	0/2812	0.80	1/3781 (0.0%)
All	All	0.81	4/54486 (0.0%)	0.89	70/73662 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	6.06	1.45	1.34
1	L	172	SER	N-CA	-5.43	1.35	1.46
2	C	792	VAL	CB-CG1	-5.28	1.41	1.52
2	C	393	GLN	CD-OE1	5.25	1.35	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1389	LEU	CA-CB-CG	8.13	133.99	115.30
1	K	211	LEU	CA-CB-CG	8.11	133.95	115.30
1	B	138	LEU	CA-CB-CG	7.70	133.00	115.30
1	A	192	LEU	CA-CB-CG	7.60	132.79	115.30
3	D	199	LEU	CA-CB-CG	-7.59	97.84	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	232	0
1	B	1806	0	1861	216	0
1	K	1806	0	1861	173	0
1	L	1806	0	1861	186	0
2	C	8829	0	8933	1215	0
2	M	8829	0	8933	1174	0
3	D	10797	0	10873	1490	0
3	N	10797	0	10873	1288	0
4	E	769	0	775	89	0
4	O	769	0	775	95	0
5	F	2771	0	2844	346	0
5	P	2771	0	2844	352	0
6	A	33	0	0	0	0
6	B	21	0	0	0	0
6	C	73	0	0	0	0
6	D	106	0	0	0	0
6	E	5	0	0	0	0
6	F	28	0	0	0	0
6	K	19	0	0	0	0
6	L	17	0	0	0	0
6	M	65	0	0	0	0
6	N	92	0	0	0	0
6	O	8	0	0	0	0
6	P	20	0	0	0	0
7	C	63	0	62	6	0
7	M	63	0	62	7	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	A	239	0	0	50	0
9	B	258	0	0	46	0
9	C	979	0	0	224	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	1252	0	0	277	0
9	E	117	0	0	28	0
9	F	420	0	0	94	0
9	K	183	0	0	39	0
9	L	219	0	0	46	0
9	M	998	0	0	249	0
9	N	1265	0	0	250	0
9	O	108	0	0	26	0
9	P	361	0	0	78	0
All	All	60572	0	54418	6470	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 60.

The worst 5 of 6470 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.07	1.11
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.13	1.11
3:D:1087:ARG:HG2	3:D:1234:THR:HA	1.27	1.07
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.36	1.05
2:M:605:LYS:HB2	2:M:610:ARG:HH12	1.16	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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%)	201 (88%)	21 (9%)	5 (2%)	10 15
1	B	227/315 (72%)	198 (87%)	23 (10%)	6 (3%)	8 11
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	13 20
1	L	227/315 (72%)	203 (89%)	20 (9%)	4 (2%)	13 20
2	C	1117/1119 (100%)	907 (81%)	157 (14%)	53 (5%)	4 3

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	1117/1119 (100%)	906 (81%)	158 (14%)	53 (5%)	4	3
3	D	1388/1524 (91%)	1108 (80%)	207 (15%)	73 (5%)	3	2
3	N	1388/1524 (91%)	1105 (80%)	208 (15%)	75 (5%)	3	2
4	E	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	6	8
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	6	8
5	F	341/423 (81%)	285 (84%)	38 (11%)	18 (5%)	3	2
5	P	341/423 (81%)	287 (84%)	38 (11%)	16 (5%)	4	3
All	All	6786/7590 (89%)	5550 (82%)	923 (14%)	313 (5%)	4	4

5 of 313 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	PRO

### 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%)	159 (79%)	43 (21%)	1	2
1	B	202/273 (74%)	161 (80%)	41 (20%)	2	3
1	K	202/273 (74%)	158 (78%)	44 (22%)	1	2
1	L	202/273 (74%)	160 (79%)	42 (21%)	2	3
2	C	941/941 (100%)	714 (76%)	227 (24%)	1	1
2	M	941/941 (100%)	738 (78%)	203 (22%)	1	2
3	D	1123/1279 (88%)	868 (77%)	255 (23%)	1	2
3	N	1123/1279 (88%)	871 (78%)	252 (22%)	1	2
4	E	83/87 (95%)	62 (75%)	21 (25%)	1	1
4	O	83/87 (95%)	65 (78%)	18 (22%)	1	2

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	295/370 (80%)	233 (79%)	62 (21%)	1	2
5	P	295/370 (80%)	246 (83%)	49 (17%)	3	6
All	All	5692/6446 (88%)	4435 (78%)	1257 (22%)	1	2

5 of 1257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	28	GLN
1	L	55	SER
3	N	1363	LEU
4	E	84	ARG
5	F	365	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	218	GLN
2	M	117	HIS
4	O	86	GLN
5	F	337	HIS
1	K	229	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 493 ligands modelled in this entry, 491 are monoatomic - leaving 2 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	$\# Z  > 2$
7	RPT	C	8001	-	68,68,68	2.84	24 (35%)	101,101,101	1.34	13 (12%)
7	RPT	M	8002	-	68,68,68	2.90	24 (35%)	101,101,101	1.33	10 (9%)

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
7	RPT	C	8001	-	-	0/64/96/96	0/2/6/6
7	RPT	M	8002	-	-	0/64/96/96	0/2/6/6

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RPT	C2-C1	9.66	1.52	1.38
7	C	8001	RPT	C2-C1	8.35	1.50	1.38
7	C	8001	RPT	O5-C29	8.18	1.55	1.39
7	M	8002	RPT	O5-C29	8.00	1.54	1.39
7	C	8001	RPT	O6-C27	7.13	1.58	1.43

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	8001	RPT	C2-N1-C15	4.96	134.26	123.69
7	M	8002	RPT	C2-N1-C15	4.40	133.05	123.69
7	M	8002	RPT	C20-C21-C22	4.22	121.58	114.50
7	M	8002	RPT	C24-C23-C22	4.16	121.68	115.35
7	C	8001	RPT	C20-C21-C22	3.97	121.16	114.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	229/315 (72%)	-0.16	1 (0%) 90 92	27, 63, 91, 115	0
1	B	229/315 (72%)	0.03	12 (5%) 26 27	48, 93, 115, 119	0
1	K	229/315 (72%)	-0.14	2 (0%) 81 82	34, 65, 94, 134	0
1	L	229/315 (72%)	-0.07	7 (3%) 47 48	52, 92, 110, 131	0
2	C	1119/1119 (100%)	-0.20	14 (1%) 74 76	21, 75, 106, 118	0
2	M	1119/1119 (100%)	-0.16	17 (1%) 70 72	25, 79, 109, 122	0
3	D	1392/1524 (91%)	-0.13	26 (1%) 64 66	24, 65, 112, 132	0
3	N	1392/1524 (91%)	-0.11	33 (2%) 56 58	25, 69, 117, 138	0
4	E	95/99 (95%)	-0.13	5 (5%) 25 26	42, 83, 108, 126	0
4	O	95/99 (95%)	-0.24	1 (1%) 77 79	46, 80, 107, 114	0
5	F	345/423 (81%)	-0.22	6 (1%) 67 69	49, 84, 110, 127	0
5	P	345/423 (81%)	-0.14	8 (2%) 57 60	63, 89, 114, 124	0
All	All	6818/7590 (89%)	-0.14	132 (1%) 65 66	21, 75, 112, 138	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	802	ALA	7.3
3	D	1240	THR	6.4
3	N	1249	ALA	5.3
2	C	180	GLY	5.2
3	N	1243	THR	5.1

### 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

There are no carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	C	9067	1/1	0.17	39.00	57,57,57,57	0
6	MG	N	9217	1/1	0.16	32.33	48,48,48,48	0
6	MG	B	9056	1/1	0.14	23.40	43,43,43,43	0
6	MG	D	9373	1/1	0.14	10.00	51,51,51,51	0
6	MG	C	9025	1/1	0.14	8.49	39,39,39,39	0
6	MG	A	9384	1/1	0.16	5.74	39,39,39,39	0
6	MG	M	9190	1/1	0.16	5.50	29,29,29,29	0
6	MG	L	9306	1/1	0.12	5.29	57,57,57,57	0
6	MG	A	9043	1/1	0.17	4.22	37,37,37,37	0
6	MG	N	9192	1/1	0.12	3.88	62,62,62,62	0
6	MG	N	9253	1/1	0.12	3.54	42,42,42,42	0
7	RPT	C	8001	63/63	0.23	3.53	26,40,66,82	0
6	MG	M	9416	1/1	0.12	3.43	45,45,45,45	0
6	MG	N	9193	1/1	0.15	3.43	34,34,34,34	0
6	MG	N	9444	1/1	0.15	3.20	49,49,49,49	0
6	MG	D	9064	1/1	0.15	3.00	44,44,44,44	0
6	MG	F	9376	1/1	0.20	2.77	62,62,62,62	0
6	MG	B	9040	1/1	0.17	2.59	36,36,36,36	0
6	MG	O	9198	1/1	0.12	2.50	36,36,36,36	0
6	MG	N	9267	1/1	0.12	2.29	42,42,42,42	0
7	RPT	M	8002	63/63	0.22	2.26	33,45,55,57	0
6	MG	F	9159	1/1	0.15	2.23	57,57,57,57	0
6	MG	D	9006	1/1	0.12	2.00	40,40,40,40	0
8	ZN	N	7059	1/1	0.13	1.89	93,93,93,93	0
6	MG	D	9023	1/1	0.14	1.80	34,34,34,34	0
8	ZN	N	7113	1/1	0.13	1.62	84,84,84,84	0
6	MG	P	9209	1/1	0.15	1.51	46,46,46,46	0
6	MG	A	9016	1/1	0.16	1.46	36,36,36,36	0
6	MG	L	9289	1/1	0.15	1.46	62,62,62,62	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	M	9256	1/1	0.18	1.32	56,56,56,56	0
6	MG	C	9086	1/1	0.14	1.31	39,39,39,39	0
6	MG	B	9136	1/1	0.12	1.22	47,47,47,47	0
6	MG	P	9235	1/1	0.16	1.12	40,40,40,40	0
6	MG	D	9140	1/1	0.14	1.00	40,40,40,40	0
6	MG	N	9259	1/1	0.15	0.95	34,34,34,34	0
6	MG	C	9360	1/1	0.13	0.94	53,53,53,53	0
6	MG	A	9368	1/1	0.15	0.88	43,43,43,43	0
6	MG	D	9041	1/1	0.14	0.86	47,47,47,47	0
6	MG	B	9093	1/1	0.15	0.81	40,40,40,40	0
6	MG	D	9084	1/1	0.11	0.71	37,37,37,37	0
6	MG	N	9199	1/1	0.11	0.70	35,35,35,35	0
6	MG	L	9309	1/1	0.15	0.67	49,49,49,49	0
6	MG	M	9260	1/1	0.13	0.64	36,36,36,36	0
6	MG	M	9321	1/1	0.13	0.58	41,41,41,41	0
6	MG	M	9241	1/1	0.12	0.53	36,36,36,36	0
6	MG	P	9258	1/1	0.14	0.53	51,51,51,51	0
6	MG	D	9095	1/1	0.15	0.52	30,30,30,30	0
6	MG	C	9169	1/1	0.15	0.48	42,42,42,42	0
6	MG	M	9312	1/1	0.13	0.45	37,37,37,37	0
6	MG	C	9071	1/1	0.12	0.44	42,42,42,42	0
6	MG	P	9202	1/1	0.11	0.41	49,49,49,49	0
6	MG	M	9210	1/1	0.13	0.40	41,41,41,41	0
6	MG	N	9181	1/1	0.16	0.38	47,47,47,47	0
6	MG	K	9191	1/1	0.16	0.36	32,32,32,32	0
6	MG	M	9400	1/1	0.14	0.36	40,40,40,40	0
6	MG	A	9002	1/1	0.17	0.34	31,31,31,31	0
6	MG	D	9011	1/1	0.13	0.33	33,33,33,33	0
6	MG	C	9022	1/1	0.13	0.31	37,37,37,37	0
6	MG	N	9473	1/1	0.14	0.26	51,51,51,51	0
6	MG	L	9183	1/1	0.14	0.26	37,37,37,37	0
6	MG	N	9221	1/1	0.13	0.26	44,44,44,44	0
6	MG	C	9049	1/1	0.12	0.25	46,46,46,46	0
6	MG	D	9453	1/1	0.12	0.21	38,38,38,38	0
6	MG	C	9112	1/1	0.12	0.18	39,39,39,39	0
6	MG	C	9003	1/1	0.14	0.15	38,38,38,38	0
6	MG	D	9024	1/1	0.14	0.14	36,36,36,36	0
6	MG	N	9207	1/1	0.14	0.13	41,41,41,41	0
6	MG	D	9146	1/1	0.11	0.12	31,31,31,31	0
6	MG	M	9220	1/1	0.12	0.11	51,51,51,51	0
6	MG	K	9410	1/1	0.16	0.09	36,36,36,36	0
6	MG	N	9206	1/1	0.16	0.07	31,31,31,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	M	9407	1/1	0.15	0.06	35,35,35,35	0
6	MG	B	9033	1/1	0.14	0.05	33,33,33,33	0
6	MG	F	9375	1/1	0.14	0.02	36,36,36,36	0
6	MG	D	9038	1/1	0.14	0.02	39,39,39,39	0
6	MG	N	9215	1/1	0.13	0.01	32,32,32,32	0
6	MG	N	9398	1/1	0.15	-0.02	48,48,48,48	0
6	MG	N	9233	1/1	0.15	-0.04	62,62,62,62	0
6	MG	N	9293	1/1	0.17	-0.05	42,42,42,42	0
6	MG	D	9349	1/1	0.14	-0.08	33,33,33,33	0
6	MG	B	9103	1/1	0.13	-0.14	43,43,43,43	0
6	MG	C	9455	1/1	0.12	-0.14	40,40,40,40	0
6	MG	A	9075	1/1	0.12	-0.15	36,36,36,36	0
6	MG	C	9050	1/1	0.16	-0.19	37,37,37,37	0
6	MG	D	9330	1/1	0.14	-0.20	39,39,39,39	0
6	MG	A	9013	1/1	0.12	-0.21	44,44,44,44	0
6	MG	N	9288	1/1	0.10	-0.24	49,49,49,49	0
6	MG	C	9076	1/1	0.13	-0.24	33,33,33,33	0
6	MG	K	9301	1/1	0.14	-0.24	43,43,43,43	0
6	MG	F	9356	1/1	0.15	-0.31	37,37,37,37	0
6	MG	D	9029	1/1	0.12	-0.32	33,33,33,33	0
6	MG	C	9051	1/1	0.13	-0.32	37,37,37,37	0
6	MG	N	9322	1/1	0.11	-0.33	54,54,54,54	0
6	MG	N	9418	1/1	0.11	-0.34	49,49,49,49	0
6	MG	B	9104	1/1	0.11	-0.35	45,45,45,45	0
8	ZN	D	7112	1/1	0.11	-0.35	80,80,80,80	0
6	MG	D	9328	1/1	0.12	-0.35	30,30,30,30	0
6	MG	D	9158	1/1	0.13	-0.36	60,60,60,60	0
6	MG	A	9068	1/1	0.13	-0.38	39,39,39,39	0
6	MG	N	9185	1/1	0.17	-0.38	56,56,56,56	0
6	MG	F	9105	1/1	0.14	-0.39	36,36,36,36	0
6	MG	A	9010	1/1	0.13	-0.39	30,30,30,30	0
6	MG	D	9072	1/1	0.14	-0.40	32,32,32,32	0
6	MG	F	9148	1/1	0.09	-0.41	54,54,54,54	0
6	MG	N	9231	1/1	0.11	-0.42	52,52,52,52	0
6	MG	N	9179	1/1	0.13	-0.43	33,33,33,33	0
6	MG	M	9452	1/1	0.13	-0.43	42,42,42,42	0
6	MG	E	9007	1/1	0.11	-0.45	40,40,40,40	0
6	MG	C	9026	1/1	0.14	-0.46	42,42,42,42	0
6	MG	M	9242	1/1	0.12	-0.46	35,35,35,35	0
6	MG	C	9019	1/1	0.14	-0.48	57,57,57,57	0
6	MG	M	9320	1/1	0.11	-0.49	34,34,34,34	0
6	MG	E	9045	1/1	0.13	-0.53	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9143	1/1	0.11	-0.53	35,35,35,35	0
6	MG	D	9133	1/1	0.13	-0.53	42,42,42,42	0
6	MG	N	9240	1/1	0.14	-0.57	46,46,46,46	0
6	MG	P	9189	1/1	0.12	-0.58	49,49,49,49	0
6	MG	M	9208	1/1	0.10	-0.58	39,39,39,39	0
6	MG	F	9123	1/1	0.10	-0.60	37,37,37,37	0
6	MG	K	9432	1/1	0.15	-0.66	49,49,49,49	0
6	MG	A	9106	1/1	0.13	-0.67	38,38,38,38	0
6	MG	N	9302	1/1	0.10	-0.68	31,31,31,31	0
6	MG	M	9275	1/1	0.14	-0.68	55,55,55,55	0
6	MG	D	9127	1/1	0.14	-0.69	48,48,48,48	0
6	MG	M	9205	1/1	0.12	-0.70	38,38,38,38	0
6	MG	M	9247	1/1	0.08	-0.70	51,51,51,51	0
6	MG	M	9295	1/1	0.08	-0.70	42,42,42,42	0
6	MG	C	9065	1/1	0.10	-0.71	37,37,37,37	0
6	MG	D	9018	1/1	0.11	-0.73	39,39,39,39	0
6	MG	C	9145	1/1	0.13	-0.74	66,66,66,66	0
6	MG	N	9445	1/1	0.10	-0.74	51,51,51,51	0
6	MG	M	9224	1/1	0.13	-0.77	40,40,40,40	0
6	MG	M	9219	1/1	0.10	-0.78	47,47,47,47	0
6	MG	D	9329	1/1	0.12	-0.79	33,33,33,33	0
6	MG	D	9174	1/1	0.12	-0.79	47,47,47,47	0
6	MG	P	9277	1/1	0.11	-0.80	41,41,41,41	0
6	MG	D	9005	1/1	0.12	-0.82	40,40,40,40	0
6	MG	P	9280	1/1	0.10	-0.82	51,51,51,51	0
6	MG	M	9319	1/1	0.12	-0.82	41,41,41,41	0
6	MG	D	9121	1/1	0.10	-0.83	35,35,35,35	0
6	MG	F	9035	1/1	0.11	-0.83	40,40,40,40	0
6	MG	M	9434	1/1	0.11	-0.84	34,34,34,34	0
6	MG	A	9380	1/1	0.11	-0.85	44,44,44,44	0
6	MG	F	9393	1/1	0.12	-0.86	38,38,38,38	0
6	MG	C	9031	1/1	0.11	-0.87	40,40,40,40	0
6	MG	D	9014	1/1	0.10	-0.87	41,41,41,41	0
6	MG	L	9252	1/1	0.09	-0.88	45,45,45,45	0
6	MG	D	9113	1/1	0.11	-0.88	34,34,34,34	0
6	MG	M	9261	1/1	0.12	-0.88	47,47,47,47	0
6	MG	N	9431	1/1	0.12	-0.89	39,39,39,39	0
6	MG	P	9399	1/1	0.12	-0.90	34,34,34,34	0
6	MG	C	9053	1/1	0.13	-0.90	30,30,30,30	0
6	MG	D	9073	1/1	0.12	-0.90	34,34,34,34	0
6	MG	N	9236	1/1	0.10	-0.90	39,39,39,39	0
6	MG	M	9203	1/1	0.11	-0.91	32,32,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9184	1/1	0.10	-0.94	29,29,29,29	0
6	MG	N	9200	1/1	0.10	-0.97	38,38,38,38	0
6	MG	C	9107	1/1	0.09	-0.98	42,42,42,42	0
6	MG	D	9028	1/1	0.13	-0.99	34,34,34,34	0
6	MG	A	9012	1/1	0.11	-0.99	47,47,47,47	0
6	MG	L	9218	1/1	0.10	-1.00	33,33,33,33	0
6	MG	C	9394	1/1	0.10	-1.08	33,33,33,33	0
6	MG	M	9196	1/1	0.09	-1.10	42,42,42,42	0
6	MG	A	9111	1/1	0.11	-1.10	35,35,35,35	0
6	MG	E	9074	1/1	0.09	-1.13	59,59,59,59	0
6	MG	D	9347	1/1	0.10	-1.14	49,49,49,49	0
6	MG	N	9402	1/1	0.08	-1.16	45,45,45,45	0
6	MG	M	9440	1/1	0.11	-1.16	50,50,50,50	0
6	MG	C	9046	1/1	0.12	-1.17	38,38,38,38	0
6	MG	C	9176	1/1	0.09	-1.17	28,28,28,28	0
6	MG	M	9486	1/1	0.09	-1.18	48,48,48,48	0
6	MG	D	9077	1/1	0.11	-1.21	35,35,35,35	0
6	MG	N	9232	1/1	0.09	-1.22	47,47,47,47	0
6	MG	C	9377	1/1	0.10	-1.22	44,44,44,44	0
6	MG	D	9118	1/1	0.12	-1.23	44,44,44,44	0
6	MG	M	9310	1/1	0.07	-1.24	46,46,46,46	0
6	MG	M	9201	1/1	0.10	-1.24	45,45,45,45	0
6	MG	F	9370	1/1	0.09	-1.25	46,46,46,46	0
6	MG	K	9251	1/1	0.12	-1.25	43,43,43,43	0
6	MG	N	9417	1/1	0.10	-1.26	39,39,39,39	0
6	MG	D	9341	1/1	0.10	-1.29	41,41,41,41	0
6	MG	N	9318	1/1	0.12	-1.33	34,34,34,34	0
6	MG	D	9339	1/1	0.14	-1.34	37,37,37,37	0
6	MG	M	9442	1/1	0.08	-1.34	59,59,59,59	0
6	MG	F	9060	1/1	0.12	-1.34	41,41,41,41	0
6	MG	K	9213	1/1	0.11	-1.34	43,43,43,43	0
6	MG	B	9359	1/1	0.12	-1.37	52,52,52,52	0
6	MG	D	9062	1/1	0.07	-1.37	47,47,47,47	0
6	MG	D	9036	1/1	0.09	-1.39	44,44,44,44	0
6	MG	F	9008	1/1	0.09	-1.40	40,40,40,40	0
6	MG	N	9484	1/1	0.08	-1.42	37,37,37,37	0
6	MG	N	9249	1/1	0.10	-1.42	45,45,45,45	0
6	MG	F	9390	1/1	0.07	-1.43	46,46,46,46	0
6	MG	N	9317	1/1	0.10	-1.43	43,43,43,43	0
6	MG	D	9089	1/1	0.09	-1.44	36,36,36,36	0
6	MG	N	9426	1/1	0.10	-1.44	41,41,41,41	0
6	MG	F	9098	1/1	0.11	-1.44	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	F	9048	1/1	0.10	-1.44	41,41,41,41	0
6	MG	P	9228	1/1	0.09	-1.44	43,43,43,43	0
6	MG	N	9303	1/1	0.08	-1.45	54,54,54,54	0
6	MG	K	9180	1/1	0.11	-1.45	42,42,42,42	0
6	MG	D	9161	1/1	0.09	-1.46	57,57,57,57	0
6	MG	C	9020	1/1	0.10	-1.46	34,34,34,34	0
6	MG	B	9032	1/1	0.06	-1.46	34,34,34,34	0
6	MG	C	9178	1/1	0.09	-1.50	39,39,39,39	0
6	MG	C	9462	1/1	0.08	-1.53	43,43,43,43	0
6	MG	N	9316	1/1	0.08	-1.55	37,37,37,37	0
6	MG	D	9009	1/1	0.09	-1.56	43,43,43,43	0
6	MG	M	9300	1/1	0.10	-1.57	39,39,39,39	0
6	MG	D	9374	1/1	0.10	-1.60	41,41,41,41	0
6	MG	N	9238	1/1	0.11	-1.61	43,43,43,43	0
6	MG	F	9157	1/1	0.12	-1.63	42,42,42,42	0
6	MG	D	9069	1/1	0.13	-1.63	48,48,48,48	0
6	MG	D	9034	1/1	0.09	-1.65	41,41,41,41	0
8	ZN	D	7058	1/1	0.08	-1.66	106,106,106,106	0
6	MG	B	9358	1/1	0.08	-1.67	39,39,39,39	0
6	MG	B	9059	1/1	0.08	-1.67	48,48,48,48	0
6	MG	M	9411	1/1	0.10	-1.69	47,47,47,47	0
6	MG	D	9058	1/1	0.09	-1.71	38,38,38,38	0
6	MG	P	9255	1/1	0.13	-1.72	34,34,34,34	0
6	MG	C	9015	1/1	0.09	-1.72	38,38,38,38	0
6	MG	D	9351	1/1	0.07	-1.73	43,43,43,43	0
6	MG	A	9342	1/1	0.13	-1.75	39,39,39,39	0
6	MG	D	9147	1/1	0.10	-1.75	41,41,41,41	0
6	MG	N	9327	1/1	0.08	-1.75	40,40,40,40	0
6	MG	D	9001	1/1	0.10	-1.76	36,36,36,36	0
6	MG	N	9269	1/1	0.07	-1.83	42,42,42,42	0
6	MG	M	9409	1/1	0.11	-1.85	36,36,36,36	0
6	MG	D	9087	1/1	0.07	-1.86	43,43,43,43	0
6	MG	K	9188	1/1	0.12	-1.87	40,40,40,40	0
6	MG	F	9109	1/1	0.11	-1.88	60,60,60,60	0
6	MG	D	9137	1/1	0.08	-1.88	47,47,47,47	0
6	MG	M	9212	1/1	0.08	-1.89	32,32,32,32	0
6	MG	C	9115	1/1	0.12	-1.91	36,36,36,36	0
6	MG	M	9234	1/1	0.12	-1.93	53,53,53,53	0
6	MG	C	9042	1/1	0.07	-1.94	47,47,47,47	0
6	MG	M	9299	1/1	0.09	-1.94	43,43,43,43	0
6	MG	C	9092	1/1	0.06	-1.95	44,44,44,44	0
6	MG	D	9386	1/1	0.11	-1.96	40,40,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9102	1/1	0.14	-1.96	44,44,44,44	0
6	MG	D	9130	1/1	0.10	-1.96	51,51,51,51	0
6	MG	D	9120	1/1	0.09	-1.96	31,31,31,31	0
6	MG	M	9263	1/1	0.11	-1.98	56,56,56,56	0
6	MG	A	9354	1/1	0.09	-2.01	37,37,37,37	0
6	MG	D	9017	1/1	0.12	-2.02	42,42,42,42	0
6	MG	N	9323	1/1	0.10	-2.03	38,38,38,38	0
6	MG	N	9243	1/1	0.10	-2.04	35,35,35,35	0
6	MG	N	9292	1/1	0.13	-2.07	56,56,56,56	0
6	MG	K	9223	1/1	0.10	-2.11	32,32,32,32	0
6	MG	B	9131	1/1	0.09	-2.11	33,33,33,33	0
6	MG	D	9333	1/1	0.08	-2.13	33,33,33,33	0
6	MG	M	9268	1/1	0.10	-2.16	32,32,32,32	0
6	MG	C	9119	1/1	0.07	-2.17	43,43,43,43	0
6	MG	N	9186	1/1	0.12	-2.18	49,49,49,49	0
6	MG	D	9052	1/1	0.07	-2.20	65,65,65,65	0
6	MG	N	9467	1/1	0.12	-2.20	35,35,35,35	0
6	MG	M	9195	1/1	0.09	-2.23	34,34,34,34	0
6	MG	C	9061	1/1	0.07	-2.26	34,34,34,34	0
6	MG	C	9170	1/1	0.07	-2.27	41,41,41,41	0
6	MG	A	9125	1/1	0.13	-2.28	36,36,36,36	0
6	MG	D	9365	1/1	0.07	-2.28	41,41,41,41	0
6	MG	P	9226	1/1	0.08	-2.31	43,43,43,43	0
6	MG	A	9124	1/1	0.13	-2.33	39,39,39,39	0
6	MG	C	9138	1/1	0.09	-2.35	43,43,43,43	0
6	MG	A	9027	1/1	0.08	-2.36	37,37,37,37	0
6	MG	D	9054	1/1	0.07	-2.38	44,44,44,44	0
6	MG	N	9429	1/1	0.11	-2.39	45,45,45,45	0
6	MG	N	9415	1/1	0.08	-2.40	42,42,42,42	0
6	MG	A	9081	1/1	0.08	-2.45	40,40,40,40	0
6	MG	A	9332	1/1	0.07	-2.46	35,35,35,35	0
6	MG	N	9214	1/1	0.10	-2.47	33,33,33,33	0
6	MG	C	9154	1/1	0.08	-2.51	43,43,43,43	0
6	MG	M	9248	1/1	0.09	-2.52	48,48,48,48	0
6	MG	N	9229	1/1	0.07	-2.55	41,41,41,41	0
6	MG	M	9471	1/1	0.09	-2.57	47,47,47,47	0
6	MG	D	9166	1/1	0.09	-2.57	40,40,40,40	0
6	MG	F	9057	1/1	0.09	-2.58	30,30,30,30	0
6	MG	N	9287	1/1	0.10	-2.61	53,53,53,53	0
6	MG	K	9244	1/1	0.08	-2.61	44,44,44,44	0
6	MG	M	9250	1/1	0.08	-2.61	38,38,38,38	0
6	MG	N	9211	1/1	0.11	-2.62	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9379	1/1	0.11	-2.62	47,47,47,47	0
6	MG	B	9080	1/1	0.11	-2.63	56,56,56,56	0
6	MG	N	9262	1/1	0.10	-2.64	51,51,51,51	0
6	MG	N	9298	1/1	0.06	-2.74	55,55,55,55	0
6	MG	M	9239	1/1	0.07	-2.75	34,34,34,34	0
6	MG	D	9346	1/1	0.07	-2.75	47,47,47,47	0
6	MG	K	9264	1/1	0.08	-2.76	42,42,42,42	0
6	MG	M	9441	1/1	0.08	-2.78	45,45,45,45	0
6	MG	D	9141	1/1	0.06	-2.78	50,50,50,50	0
6	MG	P	9315	1/1	0.09	-2.80	35,35,35,35	0
6	MG	M	9401	1/1	0.11	-2.84	37,37,37,37	0
6	MG	N	9419	1/1	0.11	-2.87	51,51,51,51	0
6	MG	N	9271	1/1	0.08	-2.90	43,43,43,43	0
6	MG	D	9030	1/1	0.09	-2.96	48,48,48,48	0
6	MG	C	9122	1/1	0.11	-3.00	56,56,56,56	0
6	MG	D	9070	1/1	0.08	-3.03	33,33,33,33	0
6	MG	A	9156	1/1	0.08	-3.05	43,43,43,43	0
6	MG	P	9436	1/1	0.10	-3.09	49,49,49,49	0
6	MG	O	9266	1/1	0.08	-3.16	47,47,47,47	0
6	MG	L	9182	1/1	0.05	-3.24	47,47,47,47	0
6	MG	A	9088	1/1	0.07	-3.40	36,36,36,36	0
6	MG	M	9305	1/1	0.09	-3.45	46,46,46,46	0
6	MG	D	9367	1/1	0.06	-3.57	31,31,31,31	0
6	MG	C	9114	1/1	0.09	-3.60	30,30,30,30	0
6	MG	O	9197	1/1	0.05	-3.81	57,57,57,57	0
6	MG	L	9466	1/1	0.11	-3.83	49,49,49,49	0
6	MG	D	9165	1/1	0.08	-3.85	32,32,32,32	0
6	MG	C	9004	1/1	0.10	-3.86	39,39,39,39	0
6	MG	M	9324	1/1	0.08	-4.23	41,41,41,41	0
6	MG	D	9338	1/1	0.11	-4.44	42,42,42,42	0
6	MG	N	9270	1/1	0.05	-4.46	39,39,39,39	0
6	MG	C	9079	1/1	0.11	-5.00	38,38,38,38	0
6	MG	K	9433	1/1	0.08	-5.86	50,50,50,50	0
6	MG	P	9285	1/1	0.09	-5.89	56,56,56,56	0
6	MG	C	9391	1/1	0.07	-6.27	60,60,60,60	0
6	MG	N	9465	1/1	0.10	-6.67	49,49,49,49	0
6	MG	L	9314	1/1	0.08	-6.76	56,56,56,56	0
6	MG	D	9100	1/1	0.09	-7.47	43,43,43,43	0
6	MG	C	9021	1/1	0.10	-9.67	37,37,37,37	0
6	MG	N	9430	1/1	0.09	-17.91	57,57,57,57	0
6	MG	P	9297	1/1	0.10	-20.75	45,45,45,45	0
6	MG	O	9420	1/1	0.10	-24.60	51,51,51,51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	A	9352	1/1	0.11	-32.00	46,46,46,46	0
6	MG	N	9451	1/1	0.06	-44.50	41,41,41,41	0
6	MG	M	9447	1/1	0.07	-46.67	64,64,64,64	0
6	MG	M	9294	1/1	0.10	-291.00	52,52,52,52	0
6	MG	C	9340	1/1	0.10	-	60,60,60,60	0
6	MG	C	9355	1/1	0.13	-	58,58,58,58	0
6	MG	L	9437	1/1	0.07	-	40,40,40,40	0
6	MG	F	9139	1/1	0.11	-	38,38,38,38	0
6	MG	M	9237	1/1	0.17	-	52,52,52,52	0
6	MG	F	9387	1/1	0.12	-	53,53,53,53	0
6	MG	D	9335	1/1	0.06	-	52,52,52,52	0
6	MG	C	9461	1/1	0.08	-	50,50,50,50	0
6	MG	D	9480	1/1	0.12	-	55,55,55,55	0
6	MG	F	9363	1/1	0.13	-	53,53,53,53	0
6	MG	N	9449	1/1	0.09	-	51,51,51,51	0
6	MG	N	9468	1/1	0.11	-	55,55,55,55	0
6	MG	L	9421	1/1	0.13	-	53,53,53,53	0
6	MG	D	9173	1/1	0.09	-	48,48,48,48	0
6	MG	C	9372	1/1	0.09	-	61,61,61,61	0
6	MG	B	9083	1/1	0.15	-	40,40,40,40	0
6	MG	B	9110	1/1	0.14	-	49,49,49,49	0
6	MG	D	9396	1/1	0.11	-	62,62,62,62	0
6	MG	A	9345	1/1	0.13	-	41,41,41,41	0
6	MG	D	9039	1/1	0.12	-	44,44,44,44	0
6	MG	C	9142	1/1	0.15	-	48,48,48,48	0
6	MG	D	9134	1/1	0.15	-	47,47,47,47	0
6	MG	D	9364	1/1	0.14	-	47,47,47,47	0
6	MG	L	9414	1/1	0.14	-	51,51,51,51	0
6	MG	F	9172	1/1	0.11	-	51,51,51,51	0
6	MG	F	9101	1/1	0.13	-	44,44,44,44	0
6	MG	B	9116	1/1	0.11	-	38,38,38,38	0
6	MG	D	9132	1/1	0.10	-	43,43,43,43	0
6	MG	K	9290	1/1	0.12	-	51,51,51,51	0
6	MG	D	9108	1/1	0.15	-	51,51,51,51	0
6	MG	N	9204	1/1	0.20	-	44,44,44,44	0
6	MG	D	9334	1/1	0.12	-	54,54,54,54	0
6	MG	M	9227	1/1	0.13	-	35,35,35,35	0
6	MG	D	9348	1/1	0.15	-	57,57,57,57	0
6	MG	L	9246	1/1	0.13	-	52,52,52,52	0
6	MG	M	9222	1/1	0.11	-	35,35,35,35	0
6	MG	A	9357	1/1	0.12	-	54,54,54,54	0
6	MG	L	9278	1/1	0.12	-	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	M	9412	1/1	0.14	-	43,43,43,43	0
6	MG	D	9456	1/1	0.12	-	55,55,55,55	0
6	MG	N	9274	1/1	0.19	-	40,40,40,40	0
6	MG	C	9160	1/1	0.10	-	44,44,44,44	0
6	MG	D	9385	1/1	0.14	-	35,35,35,35	0
6	MG	C	9044	1/1	0.16	-	34,34,34,34	0
6	MG	C	9090	1/1	0.11	-	47,47,47,47	0
6	MG	D	9063	1/1	0.09	-	33,33,33,33	0
6	MG	N	9187	1/1	0.18	-	33,33,33,33	0
6	MG	D	9129	1/1	0.15	-	42,42,42,42	0
6	MG	L	9245	1/1	0.10	-	62,62,62,62	0
6	MG	O	9296	1/1	0.13	-	42,42,42,42	0
6	MG	L	9307	1/1	0.11	-	35,35,35,35	0
6	MG	M	9424	1/1	0.14	-	34,34,34,34	0
6	MG	F	9383	1/1	0.11	-	48,48,48,48	0
6	MG	K	9405	1/1	0.13	-	56,56,56,56	0
6	MG	P	9325	1/1	0.13	-	49,49,49,49	0
6	MG	P	9482	1/1	0.12	-	48,48,48,48	0
6	MG	D	9163	1/1	0.15	-	52,52,52,52	0
6	MG	K	9257	1/1	0.11	-	58,58,58,58	0
6	MG	O	9254	1/1	0.09	-	39,39,39,39	0
6	MG	L	9283	1/1	0.13	-	59,59,59,59	0
6	MG	N	9408	1/1	0.14	-	45,45,45,45	0
6	MG	M	9281	1/1	0.12	-	49,49,49,49	0
6	MG	M	9284	1/1	0.16	-	54,54,54,54	0
6	MG	A	9078	1/1	0.13	-	66,66,66,66	0
6	MG	N	9427	1/1	0.15	-	58,58,58,58	0
6	MG	D	9151	1/1	0.16	-	57,57,57,57	0
6	MG	C	9487	1/1	0.12	-	32,32,32,32	0
6	MG	C	9055	1/1	0.11	-	38,38,38,38	0
6	MG	N	9428	1/1	0.11	-	42,42,42,42	0
6	MG	C	9047	1/1	0.12	-	53,53,53,53	0
6	MG	D	9331	1/1	0.19	-	43,43,43,43	0
6	MG	N	9265	1/1	0.15	-	61,61,61,61	0
6	MG	D	9337	1/1	0.16	-	53,53,53,53	0
6	MG	N	9291	1/1	0.13	-	64,64,64,64	0
6	MG	K	9470	1/1	0.14	-	55,55,55,55	0
6	MG	A	9460	1/1	0.08	-	55,55,55,55	0
6	MG	C	9464	1/1	0.08	-	48,48,48,48	0
6	MG	C	9362	1/1	0.16	-	55,55,55,55	0
6	MG	B	9478	1/1	0.13	-	61,61,61,61	0
6	MG	D	9152	1/1	0.12	-	67,67,67,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9085	1/1	0.20	-	49,49,49,49	0
6	MG	D	9459	1/1	0.06	-	54,54,54,54	0
6	MG	D	9117	1/1	0.13	-	48,48,48,48	0
6	MG	O	9483	1/1	0.10	-	63,63,63,63	0
6	MG	C	9037	1/1	0.18	-	51,51,51,51	0
6	MG	K	9438	1/1	0.11	-	52,52,52,52	0
6	MG	N	9311	1/1	0.11	-	39,39,39,39	0
6	MG	K	9413	1/1	0.11	-	54,54,54,54	0
6	MG	A	9477	1/1	0.18	-	52,52,52,52	0
6	MG	N	9435	1/1	0.25	-	53,53,53,53	0
6	MG	M	9273	1/1	0.14	-	44,44,44,44	0
6	MG	N	9472	1/1	0.17	-	56,56,56,56	0
6	MG	M	9474	1/1	0.14	-	49,49,49,49	0
6	MG	D	9388	1/1	0.10	-	37,37,37,37	0
6	MG	D	9096	1/1	0.16	-	60,60,60,60	0
6	MG	N	9404	1/1	0.13	-	55,55,55,55	0
6	MG	F	9389	1/1	0.11	-	53,53,53,53	0
6	MG	A	9153	1/1	0.16	-	66,66,66,66	0
6	MG	E	9155	1/1	0.16	-	44,44,44,44	0
6	MG	P	9216	1/1	0.14	-	48,48,48,48	0
6	MG	N	9313	1/1	0.11	-	43,43,43,43	0
6	MG	N	9448	1/1	0.10	-	51,51,51,51	0
6	MG	M	9272	1/1	0.17	-	45,45,45,45	0
6	MG	K	9469	1/1	0.13	-	50,50,50,50	0
6	MG	D	9344	1/1	0.13	-	55,55,55,55	0
6	MG	D	9336	1/1	0.11	-	53,53,53,53	0
6	MG	A	9171	1/1	0.12	-	58,58,58,58	0
6	MG	C	9463	1/1	0.10	-	55,55,55,55	0
6	MG	D	9135	1/1	0.14	-	50,50,50,50	0
6	MG	N	9308	1/1	0.16	-	55,55,55,55	0
6	MG	C	9149	1/1	0.17	-	48,48,48,48	0
6	MG	D	9091	1/1	0.13	-	27,27,27,27	0
6	MG	C	9361	1/1	0.12	-	41,41,41,41	0
6	MG	O	9439	1/1	0.18	-	56,56,56,56	0
6	MG	M	9406	1/1	0.17	-	67,67,67,67	0
6	MG	C	9162	1/1	0.14	-	50,50,50,50	0
6	MG	N	9423	1/1	0.18	-	58,58,58,58	0
6	MG	N	9476	1/1	0.10	-	54,54,54,54	0
6	MG	M	9485	1/1	0.08	-	54,54,54,54	0
6	MG	C	9381	1/1	0.09	-	53,53,53,53	0
6	MG	D	9150	1/1	0.15	-	31,31,31,31	0
6	MG	D	9343	1/1	0.11	-	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9304	1/1	0.12	-	47,47,47,47	0
6	MG	D	9397	1/1	0.12	-	51,51,51,51	0
6	MG	D	9082	1/1	0.14	-	60,60,60,60	0
6	MG	N	9276	1/1	0.08	-	61,61,61,61	0
6	MG	B	9457	1/1	0.08	-	43,43,43,43	0
6	MG	D	9392	1/1	0.13	-	52,52,52,52	0
6	MG	A	9097	1/1	0.17	-	34,34,34,34	0
6	MG	M	9225	1/1	0.16	-	56,56,56,56	0
6	MG	C	9353	1/1	0.11	-	48,48,48,48	0
6	MG	C	9371	1/1	0.17	-	54,54,54,54	0
6	MG	C	9350	1/1	0.08	-	60,60,60,60	0
6	MG	N	9279	1/1	0.12	-	54,54,54,54	0
6	MG	C	9366	1/1	0.15	-	41,41,41,41	0
6	MG	C	9454	1/1	0.10	-	55,55,55,55	0
6	MG	C	9175	1/1	0.15	-	68,68,68,68	0
6	MG	N	9286	1/1	0.15	-	31,31,31,31	0
6	MG	B	9094	1/1	0.16	-	38,38,38,38	0
6	MG	N	9194	1/1	0.13	-	51,51,51,51	0
6	MG	F	9099	1/1	0.15	-	56,56,56,56	0
6	MG	M	9475	1/1	0.06	-	62,62,62,62	0
6	MG	B	9458	1/1	0.08	-	44,44,44,44	0
6	MG	N	9326	1/1	0.15	-	62,62,62,62	0
6	MG	C	9126	1/1	0.10	-	46,46,46,46	0
6	MG	A	9395	1/1	0.15	-	50,50,50,50	0
6	MG	N	9422	1/1	0.15	-	56,56,56,56	0
6	MG	D	9167	1/1	0.12	-	49,49,49,49	0
6	MG	C	9168	1/1	0.11	-	45,45,45,45	0
6	MG	D	9369	1/1	0.12	-	49,49,49,49	0
6	MG	P	9446	1/1	0.15	-	34,34,34,34	0
6	MG	N	9450	1/1	0.11	-	48,48,48,48	0
6	MG	F	9481	1/1	0.09	-	57,57,57,57	0
6	MG	N	9425	1/1	0.13	-	46,46,46,46	0
6	MG	E	9479	1/1	0.12	-	62,62,62,62	0
6	MG	N	9443	1/1	0.15	-	54,54,54,54	0
6	MG	N	9403	1/1	0.14	-	34,34,34,34	0
6	MG	F	9382	1/1	0.10	-	40,40,40,40	0
6	MG	D	9177	1/1	0.14	-	64,64,64,64	0
6	MG	C	9164	1/1	0.11	-	49,49,49,49	0
6	MG	B	9378	1/1	0.14	-	47,47,47,47	0
6	MG	D	9144	1/1	0.12	-	39,39,39,39	0
6	MG	P	9282	1/1	0.10	-	56,56,56,56	0
6	MG	A	9066	1/1	0.15	-	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9128	1/1	0.13	-	52,52,52,52	0
6	MG	M	9230	1/1	0.12	-	50,50,50,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.