



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 04:23 pm BST

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 X-ray Structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

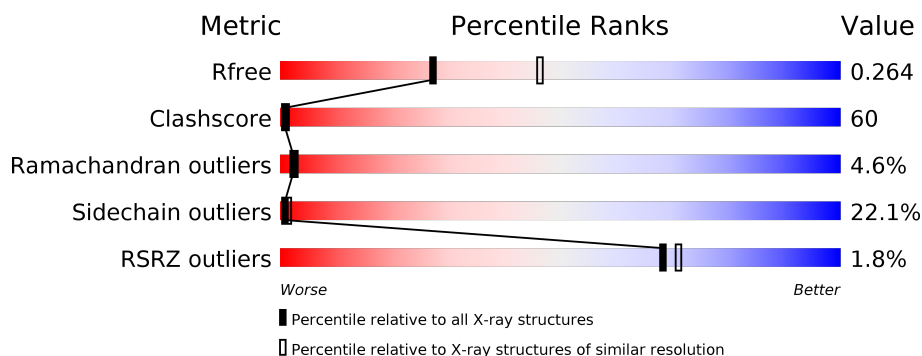
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	<div> <div>17%</div> <div>44%</div> <div>10%</div> <div>27%</div> </div>
1	B	315	<div>4%</div> <div>18%</div> <div>43%</div> <div>11%</div> <div>27%</div>

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Mol	Chain	Length	Quality of chain
3	D	1524	<p>23% 52% 16% 9%</p>
3	N	1524	<p>25% 51% 14% 9%</p>
4	E	99	<p>28% 49% 18% 5%</p>
4	O	99	<p>27% 49% 18% 6%</p>
5	F	423	<p>20% 46% 14% 18%</p>
5	P	423	<p>20% 49% 11% 18%</p>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60572 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 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			

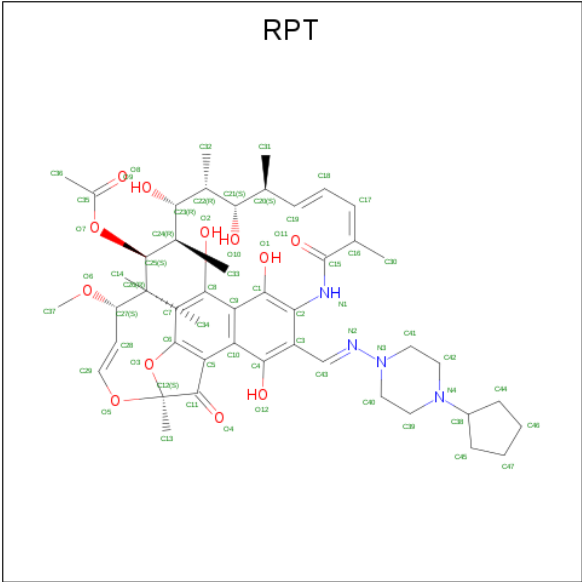
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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		

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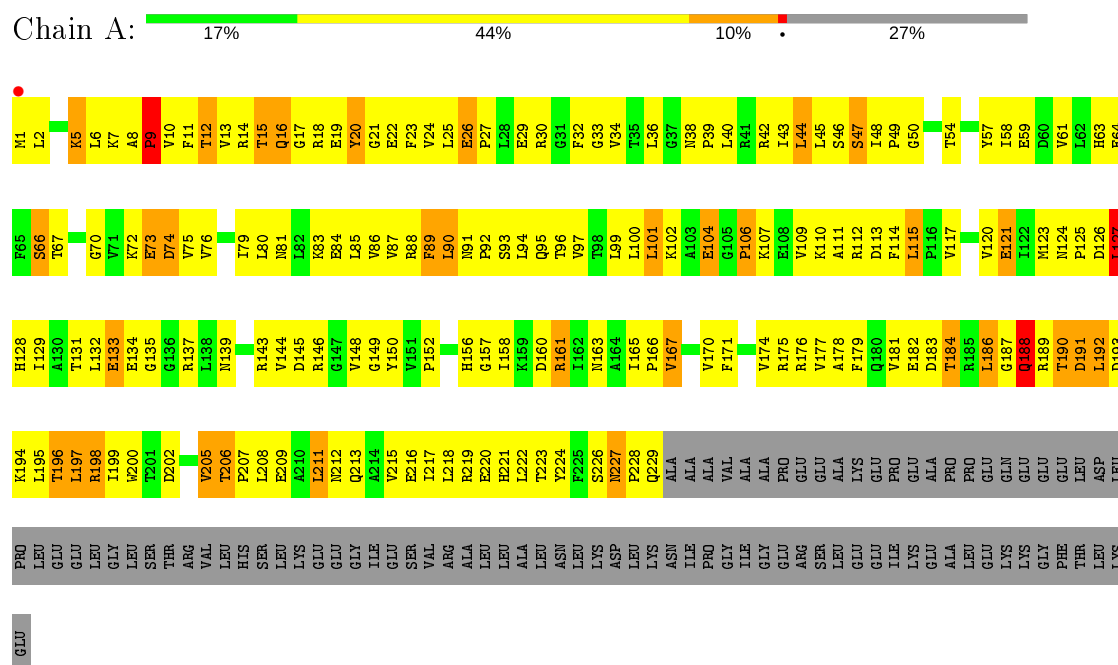
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	420	Total 420	O 420	0	0
9	K	183	Total 183	O 183	0	0
9	L	219	Total 219	O 219	0	0
9	M	998	Total 998	O 998	0	0
9	N	1265	Total 1265	O 1265	0	0
9	O	108	Total 108	O 108	0	0
9	P	361	Total 361	O 361	0	0

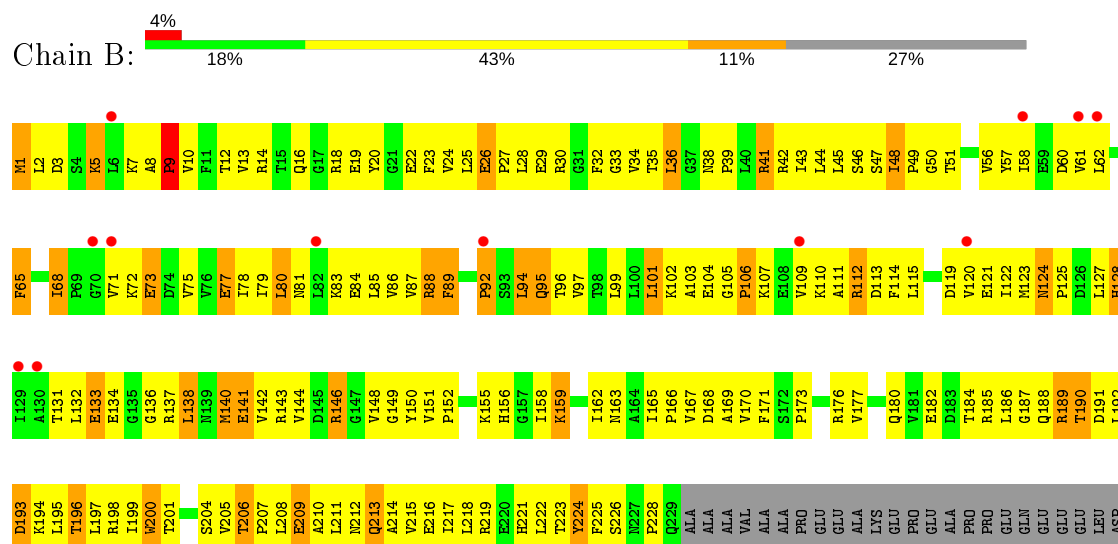
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

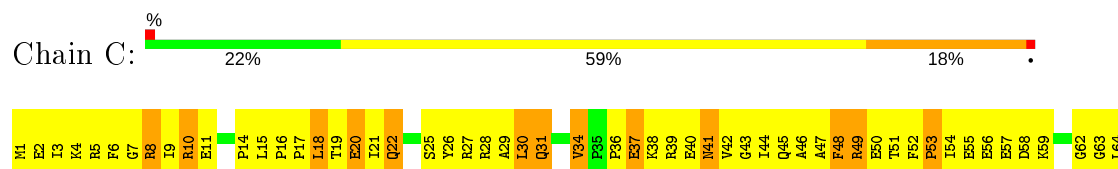
#### • Molecule 1: DNA-directed RNA polymerase alpha chain



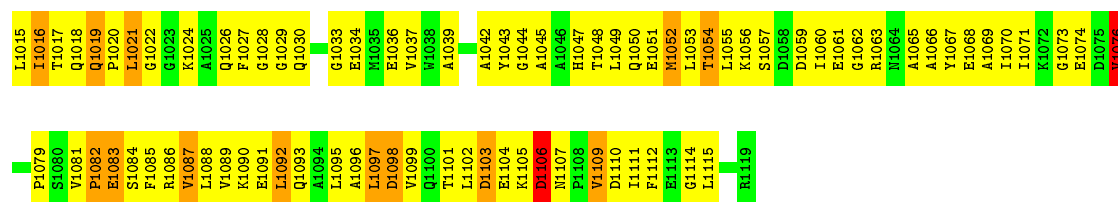
#### • Molecule 1: DNA-directed RNA polymerase alpha chain



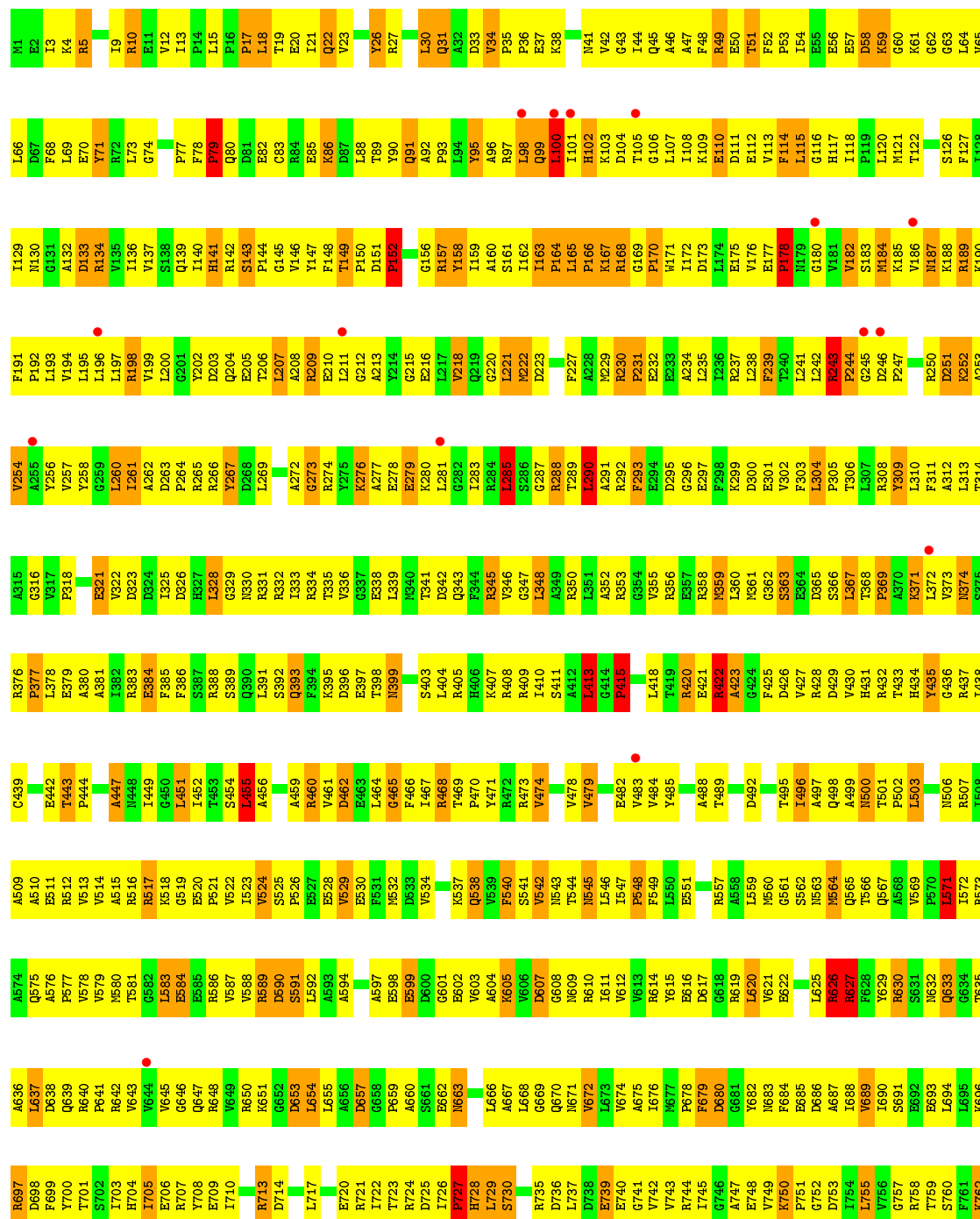


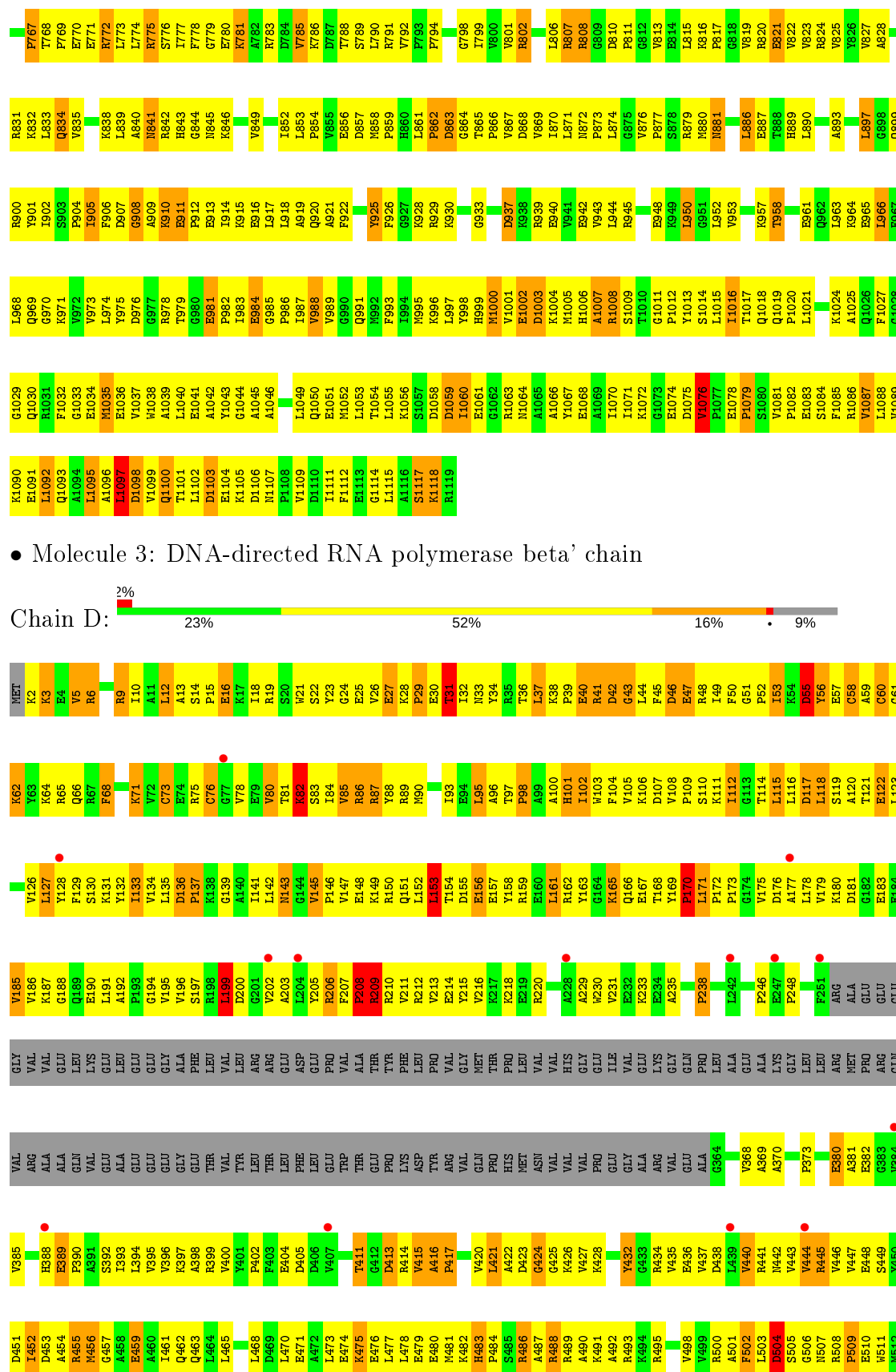






• Molecule 2: DNA-directed RNA polymerase beta chain

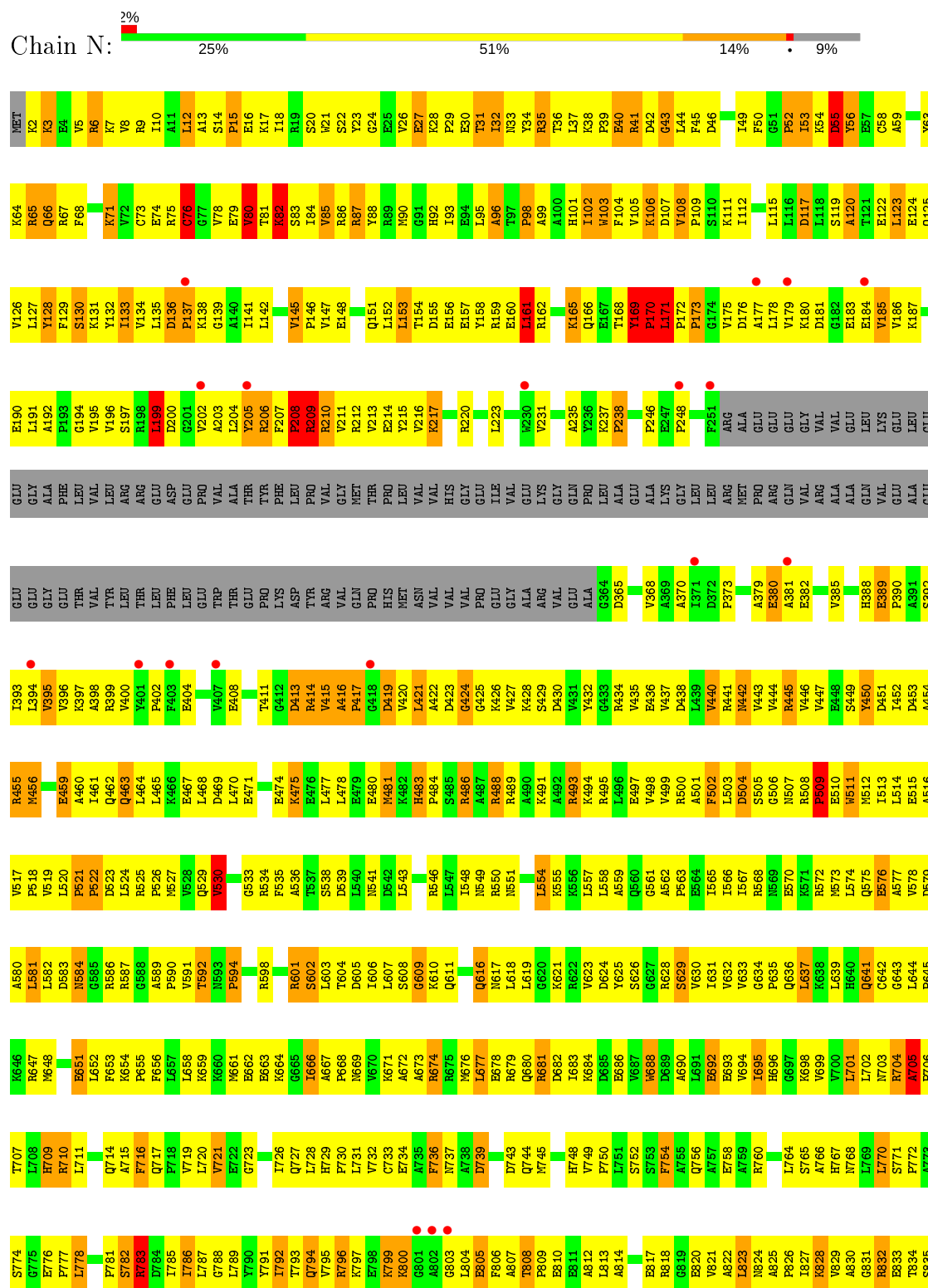


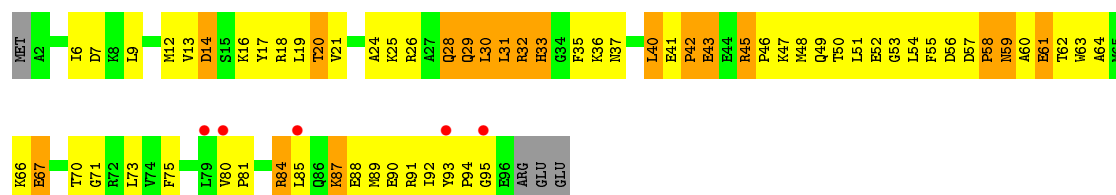


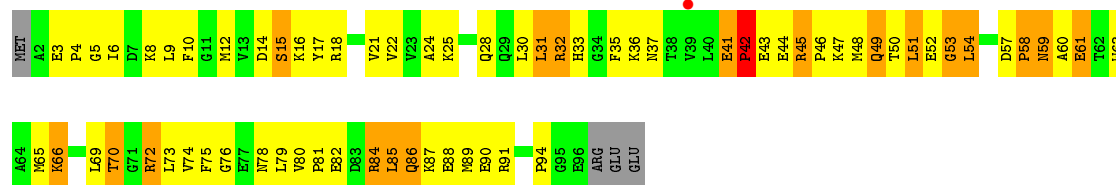
M1404	E1344	V1280	E1219	E1154	R1087	S1026	E959	V890	P826	Q762	L701	L574	E1513
E1405	E1345	V1281	V1221	L1156	D1090	G1027	K960	E891	I827	M763	L702	Q575	E515
R1406	R1346	I1282	I1223	L1157	S1091	A1028	Y963	E893	K828	L764	N703	E876	E516
L1407	I1347	E1283	G1222	E1284	G1092	R1029	L964	K904	V829	S765	R704	A577	A517
A1408	L1348	E1284	I1223	E1285	Y1093	G1030	E965	V895	A830	A766	A705	V578	A518
A1409	V1349	E1285	V1224	E1286	L1160	E1084	E966	E896	E832	P767	P706	D579	P518
E1410	E1350	T1286	A1225	E1161	L1094	M1031	E967	A896	R833	L768	L707	A580	V519
E1411	E1351	E1287	A1226	E1162	T1095	P1032	E968	E897	E833	L769	L708	L581	L520
K1412	Q1288	E1288	Q1227	G1163	R1096	Q1033	D968	E898	7834	L770	H710	L582	P521
K1413	Q1353	K1269	S1228	G1164	K1097	Q1034	R969	L939	S835	K646	R710	D583	P522
K1414	K1354	L1290	H1239	V1165	L1098	L1035	K970	I900	V836	L711	R711	N584	P523
V1415	V1355	S1291	G1230	L1166	V1099	R1036	L971	Q901	E837	G774	G712	G585	D523
A1416	Y1356	V1292	E1231	S1167	D1100	Q1037	L972	I902	R839	G775	E713	E596	L524
V1417	R1357	F1293	P1232	M1168	T1101	L1038	Q973	D903	L839	E776	Q714	R587	P526
K1418	A1358	V1294	G1233	L1169	V1102	C1039	I974	V0904	K840	P777	A715	G588	M527
Q1359	Q1359	P1419	T1234	D1170	H1103	G1040	E975	E906	H841		F716	A589	V528
G1360	G1360	F1299	Q1235	H1171	E1104	L1041	Q976	Q905	H842	K780	Q717	F653	Q529
V1361	V1361	L1236	L1236	H1172	T1105	R1042	A977	E907	F843	E781	F718	K854	V530
K1362	K1362	T1237	T1237	L1173	V1106	G1043	Y978	K908	A844	S782	V719	P855	D531
K1301	K1301	L1310	L1310	L1174	E1107	L1044	E979	N909	R845	R783	L720	F856	G532
V1424	H1364	E1302	R1239	L1175	R1108	M1045	N980	S910	P846	D784	V721	L557	G533
T1425	D1365	Y1303	T1240	K1176	E1109	Q1046	G981	L911	D847	I785	E722	L658	R534
K1426	K1366	K1304	H1241	A1177	K1047	K1047	F982	K912	E848	I786	G723	K659	F535
S1427	H1367	L1305	H1242	A1178	G1112	P1048	L983	E913	L849	L787	Q724	K660	A536
A1428	L1368	P1306	T1243	E1179	G1113	E1051	T984	I914	L850	G788	W725	M861	P598
S1430	E1369	K1307	G1244	L1114	T1115	T1052	D985	Y916	L851	L789	L726	E862	S538
T1431	V1370	E1308	G1245	L1116	T1116	F1053	E987	Q917	A852	Y790	L728	K664	R601
K1432	V1371	A1309	A1246	N1116	Y1117		R988	A918	V853	E791	H729	G665	L540
S1433	R1373	L1310	G1248	V1186	L1118	P1056	Y989	F919	I857	I792	W730	E666	L603
V1434	Q1374	L1312		L1188	S1119	V1057		I920	V859	Q794		L666	
L1435	M1375	V1313	D1251	R1189	V1120	R1058	T992	R921	L859	W795	C733	A667	L606
S1436	M1376	K1314	I1252	S1190	P1121	S1059		L922	P859	R796	L740	P668	L607
A1437	K1377	D1315	T1253	P1191	L1314	S1060	L995	G923	Q861	K797	A735	N669	S608
A1438	Y1378	G1316	Q1254	L1192	Q1124	F1061	W996	N924	D862	E798	F736	V670	R546
S1439	V1379	D1317	G1255	T1193		R1062	T997	E925	V863	K799	N737	K671	G609
F1440	E1380	Y1318	L1256	C1193	E1127	E1063	E998	K926	H864	L799	A672	A672	Q611
N1441	V1381	V1319	P1257	T1196	T1128	G1064	T999	T927	R865	R800	A738	R674	N549
N1442	T1382	E1320	R1258	L1196	L1129	L1065	T000	A928	V866	A802	D739	R675	R550
T1443	D1383	K1197	V1259	R1192	R1130	T1066	E1001	R929	R867	G803	H741	M676	N552
	P1384	A1321	I1260	Y1198	L1430	V1067	K1002	L930	V868	L804	G742	L677	R553
	G1385	P1324	E1261		R1135	L1068	V1003	L931	N869	E805	D743	E678	L554
	D1386	L1325	L1262	C1201	K1136	E1069	T1004		G870	F806	Q744	R679	K555
	L1447	L1325	F1263	Q1202	R1337	T1070	Q1005	T940	K871	Q880	L619	R679	
	R1387	T1326	E1264	K1203	F11071	A1071	A1006	T943	R872	T808	A746	R681	L558
	L1388	R1327	A1265	G1204	D1139	I1072	V1007	T943	L873	P809	D882	K621	A559
	L1389		A1266	E1205	A1138	S1073	T1008	T944	E874	R810	I683	G820	L659
	E1390	D1331	R1267	G1206	E1141	S1074	K1009		T875	E811	H748	R622	Q560
	A1453	E1391	P1268	I1207	A1142	H1075	L1010	E947	S876	A812	V749	V623	G561
	K1455	P1332	K1269	D1208	A1143	G1076	P877	T948	P877	L751	F750	D885	R622
	K1456	Q1393	L1209	D1208	L1444	A1077	E1012	I949	G878	L813	L752	E886	A562
	D1457	V1394	A1270	L1209	L1444							V887	E564
	L1395	K1271	K1271	S1210	Y1145	K1078	Y1015	G950	R879	E817	S753	W688	
	E1396	L1336	A1272	S1211	G1146	R1478		I951	L880	R818	F754		I565
	K1397	E1337	V1273	A1212	R1147	G1080	P1016	D952					I566
	V1398	L1338	I1274	E1213	V1148	G1081		D953				V694	L567
	L1462	K1398	S1275	P1214	L1149	A1082	P1019	A954	R884	E820	A755	L695	R568
	K1463	L1379	E1276	E1214	A1150	D1083	L1020	V956				H696	N569
	E1464	V1400	I1277	S1216	R1151	T1084	Y1021	I955				G697	E570
	N1465	E1401	D1278	G1216	E1452	K1085	L1022	A887				K698	G634
	V1466	A1402	A1270	L1217	V1152	A1086	M1022	P857				V699	P635
		A1403	A1270	L1403	E1452	L1088	M1022	E889				W700	R572
													R572



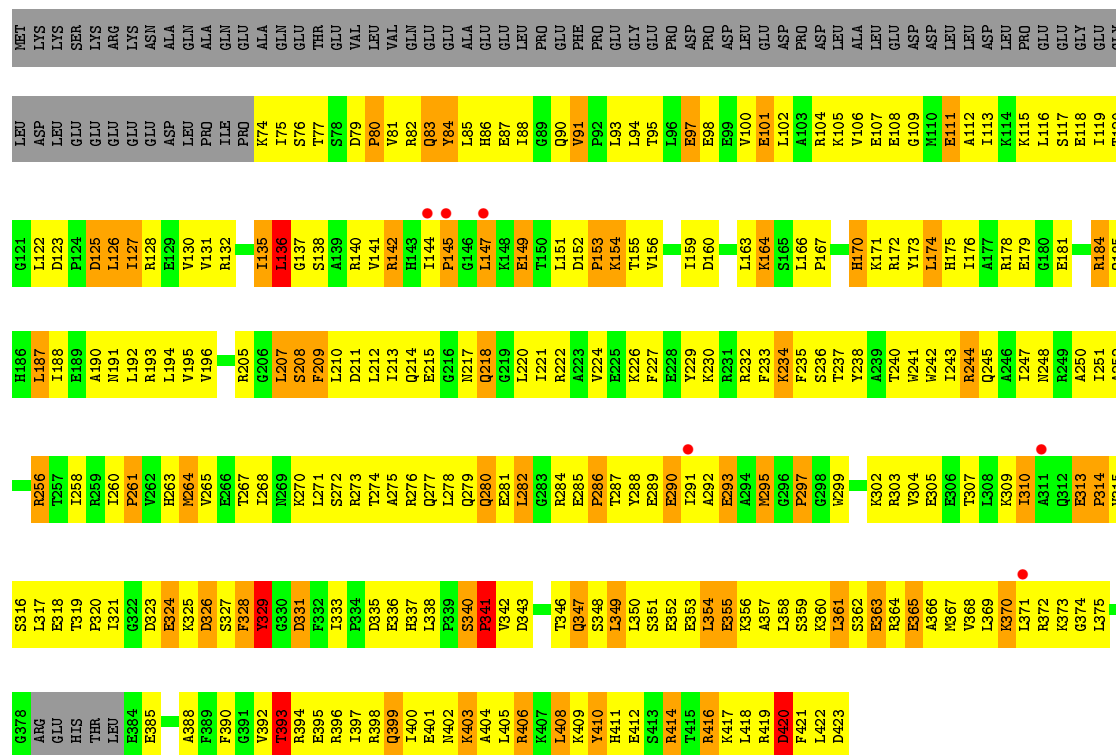
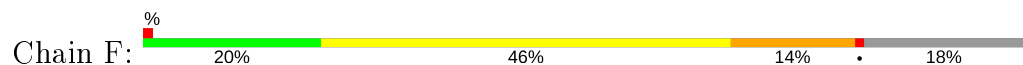
• Molecule 3: DNA-directed RNA polymerase beta' chain



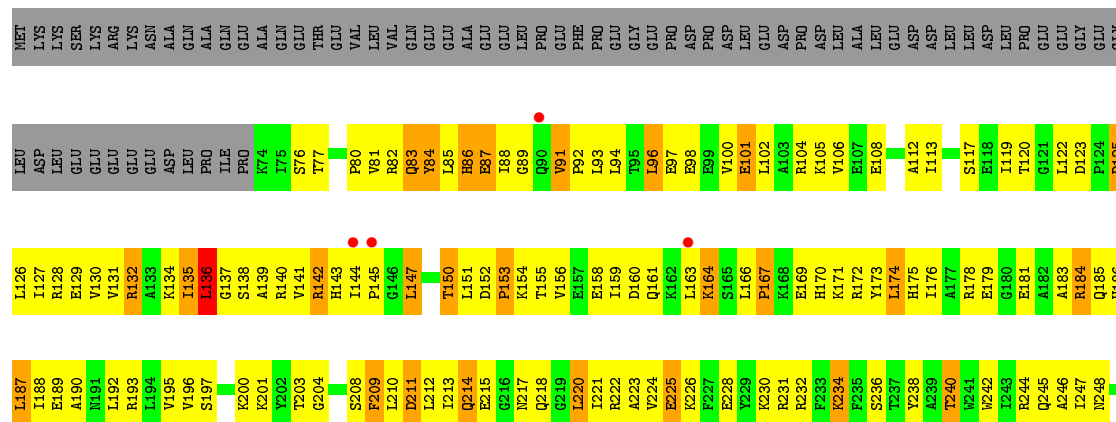
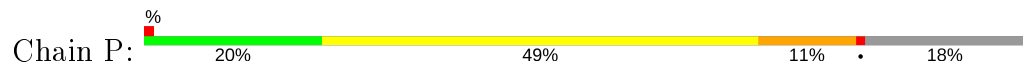




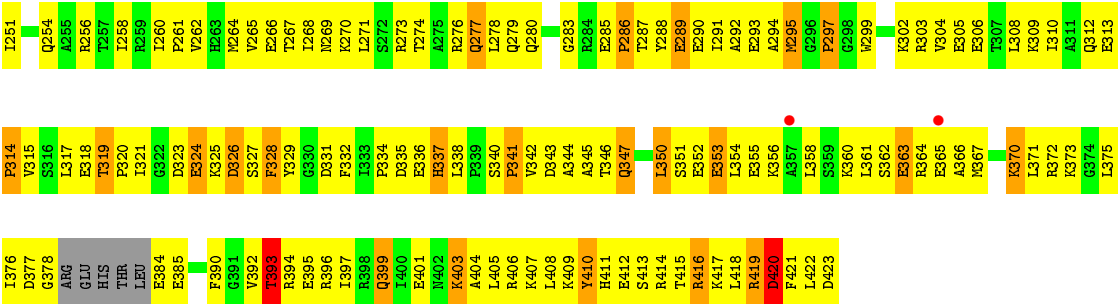
• Molecule 5: RNA polymerase sigma factor rpoD



• Molecule 5: RNA polymerase sigma factor rpoD







## 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) 92.5 (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 (5.75%)	wwPDB-VP
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> )	0.27 , 76.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.076 for h,-h-k,-l 0.076 for -k,-h,-l	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.

<sup>2</sup>Theoretical 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, 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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
9	D	1252	0	0	277	0
9	E	117	0	0	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 60.

The worst 5 of 6470 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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 [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%)	201 (88%)	21 (9%)	5 (2%)	6	10
1	B	227/315 (72%)	198 (87%)	23 (10%)	6 (3%)	5	8
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	8	14
1	L	227/315 (72%)	203 (89%)	20 (9%)	4 (2%)	8	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1117/1119 (100%)	907 (81%)	157 (14%)	53 (5%)	2	2
2	M	1117/1119 (100%)	906 (81%)	158 (14%)	53 (5%)	2	2
3	D	1388/1524 (91%)	1108 (80%)	207 (15%)	73 (5%)	2	2
3	N	1388/1524 (91%)	1105 (80%)	208 (15%)	75 (5%)	2	2
4	E	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	4	5
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	4	5
5	F	341/423 (81%)	285 (84%)	38 (11%)	18 (5%)	2	2
5	P	341/423 (81%)	287 (84%)	38 (11%)	16 (5%)	2	2
All	All	6786/7590 (89%)	5550 (82%)	923 (14%)	313 (5%)	2	2

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%)	1	2
1	K	202/273 (74%)	158 (78%)	44 (22%)	1	1
1	L	202/273 (74%)	160 (79%)	42 (21%)	1	2
2	C	941/941 (100%)	714 (76%)	227 (24%)	0	1
2	M	941/941 (100%)	738 (78%)	203 (22%)	1	1
3	D	1123/1279 (88%)	868 (77%)	255 (23%)	1	1
3	N	1123/1279 (88%)	871 (78%)	252 (22%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	83/87 (95%)	62 (75%)	21 (25%)	0	1
4	O	83/87 (95%)	65 (78%)	18 (22%)	1	1
5	F	295/370 (80%)	233 (79%)	62 (21%)	1	2
5	P	295/370 (80%)	246 (83%)	49 (17%)	2	4
All	All	5692/6446 (88%)	4435 (78%)	1257 (22%)	1	1

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 molecules 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	M	8002	-	68,68,68	2.52	22 (32%)	101,101,101	1.22	9 (8%)
7	RPT	C	8001	-	68,68,68	2.45	22 (32%)	101,101,101	1.23	11 (10%)

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	M	8002	-	-	20/64/96/96	0/6/6/6
7	RPT	C	8001	-	-	12/64/96/96	0/6/6/6

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RPT	C39-N4	6.55	1.59	1.47
7	M	8002	RPT	C42-N4	6.42	1.59	1.47
7	C	8001	RPT	O6-C27	6.22	1.58	1.43
7	C	8001	RPT	O5-C29	6.12	1.55	1.39
7	M	8002	RPT	O5-C29	5.98	1.54	1.39

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RPT	C24-C23-C22	3.73	121.68	115.43
7	C	8001	RPT	C24-C23-C22	3.28	120.92	115.43
7	M	8002	RPT	C20-C21-C22	3.25	121.58	114.96
7	C	8001	RPT	C25-O7-C35	3.23	122.72	117.72
7	C	8001	RPT	C2-N1-C15	3.10	134.26	124.11



There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	8002	RPT	C28-C27-O6-C37
7	M	8002	RPT	C44-C38-N4-C39
7	M	8002	RPT	C45-C38-N4-C39
7	M	8002	RPT	C45-C38-N4-C42
7	C	8001	RPT	C26-C27-C28-C29

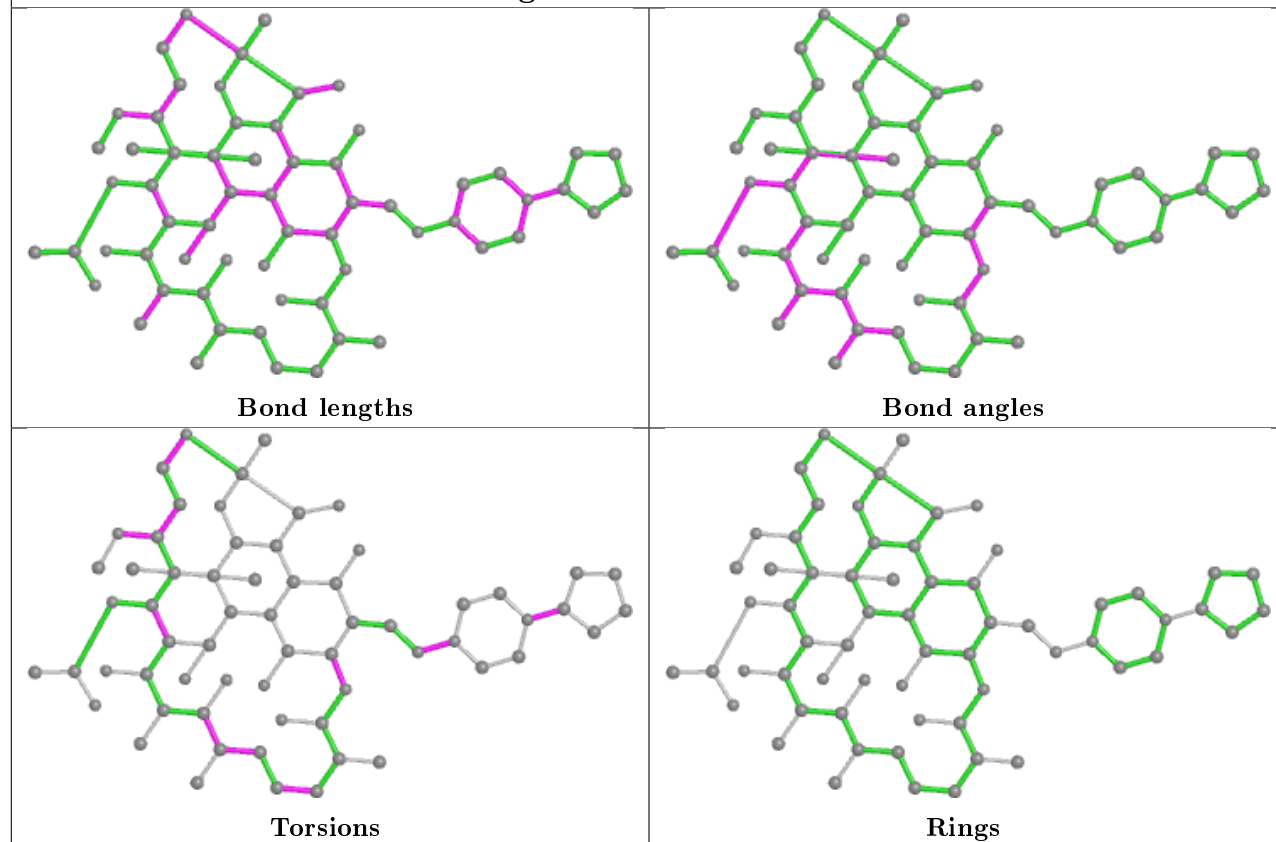
There are no ring outliers.

2 monomers are involved in 13 short contacts:

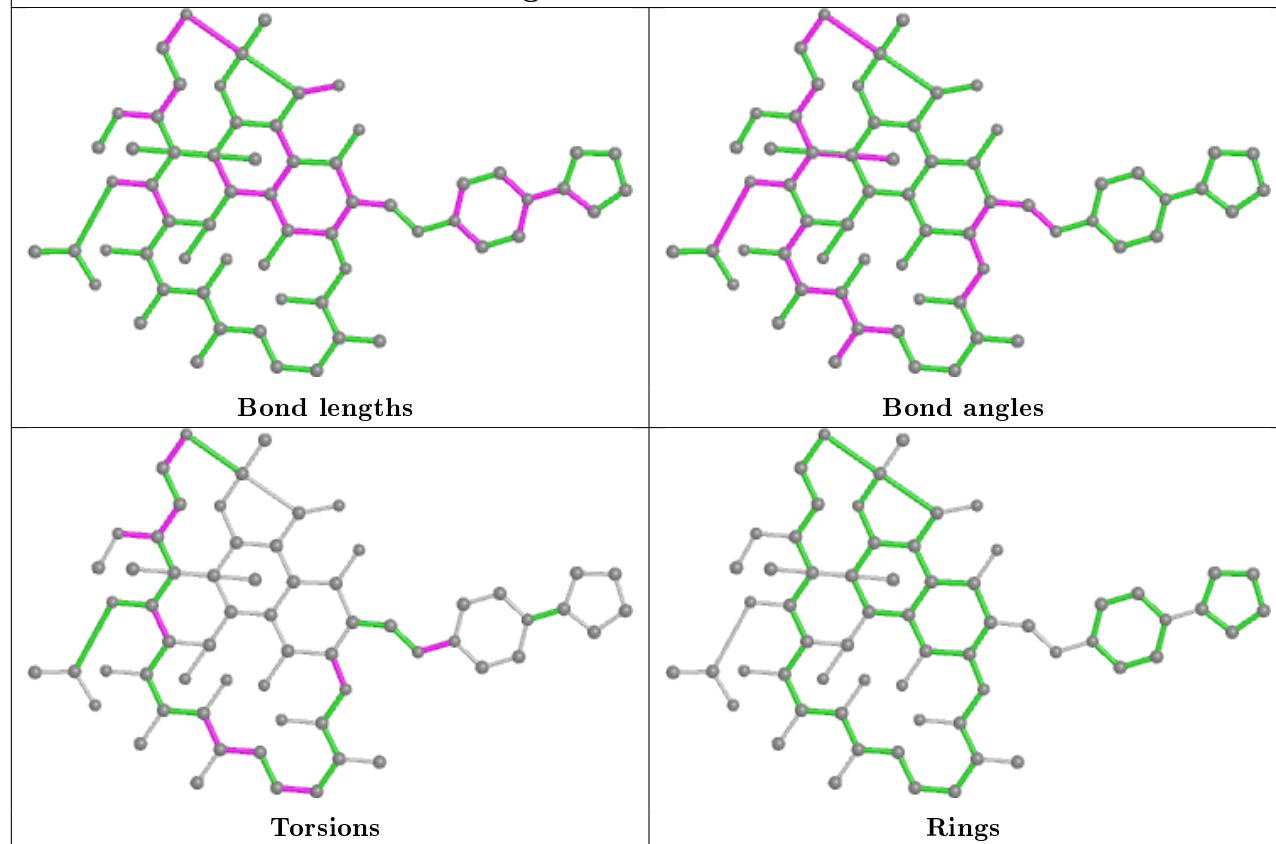
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	8002	RPT	7	0
7	C	8001	RPT	6	0

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

## Ligand RPT M 8002



## Ligand RPT C 8001



## 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, 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%)	-0.31	1 (0%) 92 93	27, 63, 91, 115	0
1	B	229/315 (72%)	-0.11	12 (5%) 27 29	48, 93, 115, 119	0
1	K	229/315 (72%)	-0.30	2 (0%) 84 86	34, 65, 94, 134	0
1	L	229/315 (72%)	-0.21	6 (2%) 56 59	52, 92, 110, 131	0
2	C	1119/1119 (100%)	-0.34	14 (1%) 77 79	21, 75, 106, 118	0
2	M	1119/1119 (100%)	-0.31	15 (1%) 77 79	25, 79, 109, 122	0
3	D	1392/1524 (91%)	-0.27	24 (1%) 70 72	24, 65, 112, 132	0
3	N	1392/1524 (91%)	-0.25	31 (2%) 62 65	25, 69, 117, 138	0
4	E	95/99 (95%)	-0.27	5 (5%) 26 28	42, 83, 108, 126	0
4	O	95/99 (95%)	-0.39	1 (1%) 80 82	46, 80, 107, 114	0
5	F	345/423 (81%)	-0.36	6 (1%) 70 72	49, 84, 110, 127	0
5	P	345/423 (81%)	-0.28	6 (1%) 70 72	63, 89, 114, 124	0
All	All	6818/7590 (89%)	-0.29	123 (1%) 68 71	21, 75, 112, 138	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	802	ALA	7.6
3	D	1240	THR	5.8
3	N	1249	ALA	5.5
2	C	180	GLY	5.3
3	D	1245	GLY	5.3

### 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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ZN	D	7058	1/1	0.87	0.07	106,106,106,106	0
6	MG	M	9256	1/1	0.89	0.17	56,56,56,56	0
6	MG	C	9362	1/1	0.90	0.15	55,55,55,55	0
6	MG	N	9192	1/1	0.91	0.12	62,62,62,62	0
6	MG	D	9161	1/1	0.91	0.09	57,57,57,57	0
6	MG	C	9168	1/1	0.91	0.10	45,45,45,45	0
6	MG	K	9470	1/1	0.91	0.13	55,55,55,55	0
6	MG	N	9221	1/1	0.92	0.13	44,44,44,44	0
6	MG	D	9330	1/1	0.92	0.14	39,39,39,39	0
6	MG	F	9390	1/1	0.93	0.07	46,46,46,46	0
6	MG	C	9350	1/1	0.93	0.07	60,60,60,60	0
6	MG	P	9226	1/1	0.93	0.08	43,43,43,43	0
6	MG	A	9078	1/1	0.93	0.13	66,66,66,66	0
6	MG	D	9001	1/1	0.93	0.10	36,36,36,36	0
6	MG	F	9109	1/1	0.94	0.11	60,60,60,60	0
6	MG	N	9449	1/1	0.94	0.09	51,51,51,51	0
6	MG	M	9263	1/1	0.94	0.10	56,56,56,56	0
6	MG	A	9357	1/1	0.94	0.11	54,54,54,54	0
6	MG	L	9414	1/1	0.94	0.13	51,51,51,51	0
6	MG	C	9067	1/1	0.94	0.17	57,57,57,57	0
6	MG	O	9420	1/1	0.94	0.10	51,51,51,51	0
6	MG	C	9149	1/1	0.94	0.16	48,48,48,48	0
6	MG	P	9202	1/1	0.94	0.10	49,49,49,49	0
6	MG	D	9102	1/1	0.94	0.13	44,44,44,44	0
6	MG	C	9049	1/1	0.94	0.10	46,46,46,46	0
6	MG	M	9411	1/1	0.94	0.09	47,47,47,47	0
6	MG	L	9182	1/1	0.94	0.05	47,47,47,47	0
6	MG	N	9427	1/1	0.94	0.14	58,58,58,58	0
6	MG	N	9313	1/1	0.94	0.10	43,43,43,43	0
6	MG	M	9447	1/1	0.94	0.07	64,64,64,64	0
6	MG	N	9194	1/1	0.94	0.12	51,51,51,51	0
6	MG	M	9324	1/1	0.95	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9217	1/1	0.95	0.15	48,48,48,48	0
6	MG	N	9200	1/1	0.95	0.10	38,38,38,38	0
6	MG	M	9471	1/1	0.95	0.08	47,47,47,47	0
6	MG	D	9036	1/1	0.95	0.09	44,44,44,44	0
6	MG	N	9233	1/1	0.95	0.14	62,62,62,62	0
6	MG	N	9327	1/1	0.95	0.07	40,40,40,40	0
6	MG	F	9148	1/1	0.95	0.08	54,54,54,54	0
6	MG	N	9291	1/1	0.95	0.12	64,64,64,64	0
6	MG	C	9162	1/1	0.95	0.12	50,50,50,50	0
6	MG	D	9082	1/1	0.95	0.14	60,60,60,60	0
6	MG	P	9297	1/1	0.95	0.09	45,45,45,45	0
6	MG	D	9014	1/1	0.95	0.10	41,41,41,41	0
6	MG	M	9294	1/1	0.96	0.09	52,52,52,52	0
6	MG	M	9210	1/1	0.96	0.13	41,41,41,41	0
6	MG	M	9406	1/1	0.96	0.15	67,67,67,67	0
6	MG	M	9261	1/1	0.96	0.11	47,47,47,47	0
6	MG	C	9175	1/1	0.96	0.14	68,68,68,68	0
6	MG	N	9292	1/1	0.96	0.12	56,56,56,56	0
6	MG	N	9326	1/1	0.96	0.14	62,62,62,62	0
6	MG	D	9453	1/1	0.96	0.11	38,38,38,38	0
6	MG	B	9359	1/1	0.96	0.10	52,52,52,52	0
6	MG	M	9234	1/1	0.96	0.12	53,53,53,53	0
6	MG	C	9372	1/1	0.96	0.09	61,61,61,61	0
6	MG	D	9365	1/1	0.96	0.06	41,41,41,41	0
7	RPT	M	8002	63/63	0.96	0.22	33,45,55,57	0
6	MG	L	9278	1/1	0.96	0.11	44,44,44,44	0
6	MG	F	9370	1/1	0.96	0.09	46,46,46,46	0
6	MG	M	9225	1/1	0.96	0.14	56,56,56,56	0
6	MG	D	9062	1/1	0.96	0.08	47,47,47,47	0
6	MG	C	9047	1/1	0.96	0.12	53,53,53,53	0
6	MG	D	9054	1/1	0.96	0.08	44,44,44,44	0
6	MG	C	9355	1/1	0.96	0.12	58,58,58,58	0
6	MG	A	9081	1/1	0.96	0.08	40,40,40,40	0
7	RPT	C	8001	63/63	0.96	0.23	26,40,66,82	0
6	MG	L	9218	1/1	0.96	0.09	33,33,33,33	0
6	MG	O	9198	1/1	0.96	0.12	36,36,36,36	0
6	MG	A	9013	1/1	0.96	0.12	44,44,44,44	0
6	MG	E	9074	1/1	0.96	0.09	59,59,59,59	0
6	MG	N	9426	1/1	0.96	0.09	41,41,41,41	0
6	MG	D	9096	1/1	0.96	0.15	60,60,60,60	0
6	MG	C	9381	1/1	0.96	0.08	53,53,53,53	0
6	MG	C	9391	1/1	0.96	0.06	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	P	9209	1/1	0.96	0.15	46,46,46,46	0
6	MG	C	9019	1/1	0.96	0.13	57,57,57,57	0
6	MG	D	9009	1/1	0.96	0.09	43,43,43,43	0
6	MG	F	9172	1/1	0.96	0.11	51,51,51,51	0
6	MG	B	9059	1/1	0.96	0.07	48,48,48,48	0
6	MG	D	9373	1/1	0.97	0.12	51,51,51,51	0
6	MG	L	9289	1/1	0.97	0.14	62,62,62,62	0
6	MG	D	9073	1/1	0.97	0.12	34,34,34,34	0
6	MG	A	9352	1/1	0.97	0.10	46,46,46,46	0
6	MG	D	9166	1/1	0.97	0.09	40,40,40,40	0
6	MG	C	9107	1/1	0.97	0.09	42,42,42,42	0
6	MG	C	9122	1/1	0.97	0.10	56,56,56,56	0
6	MG	D	9348	1/1	0.97	0.14	57,57,57,57	0
6	MG	M	9412	1/1	0.97	0.14	43,43,43,43	0
6	MG	D	9006	1/1	0.97	0.12	40,40,40,40	0
6	MG	M	9201	1/1	0.97	0.10	45,45,45,45	0
6	MG	N	9232	1/1	0.97	0.08	47,47,47,47	0
6	MG	F	9376	1/1	0.97	0.19	62,62,62,62	0
6	MG	D	9158	1/1	0.97	0.12	60,60,60,60	0
6	MG	P	9216	1/1	0.97	0.13	48,48,48,48	0
6	MG	M	9475	1/1	0.97	0.05	62,62,62,62	0
6	MG	B	9458	1/1	0.97	0.08	44,44,44,44	0
6	MG	C	9022	1/1	0.97	0.12	37,37,37,37	0
6	MG	C	9360	1/1	0.97	0.13	53,53,53,53	0
6	MG	C	9178	1/1	0.97	0.09	39,39,39,39	0
6	MG	C	9119	1/1	0.97	0.07	43,43,43,43	0
6	MG	D	9174	1/1	0.97	0.12	47,47,47,47	0
6	MG	A	9156	1/1	0.97	0.08	43,43,43,43	0
6	MG	M	9275	1/1	0.97	0.12	55,55,55,55	0
6	MG	N	9276	1/1	0.97	0.08	61,61,61,61	0
6	MG	P	9189	1/1	0.97	0.11	49,49,49,49	0
6	MG	D	9041	1/1	0.97	0.13	47,47,47,47	0
6	MG	D	9030	1/1	0.97	0.09	48,48,48,48	0
6	MG	M	9237	1/1	0.97	0.15	52,52,52,52	0
6	MG	C	9160	1/1	0.97	0.09	44,44,44,44	0
6	MG	K	9188	1/1	0.97	0.12	40,40,40,40	0
6	MG	D	9167	1/1	0.97	0.12	49,49,49,49	0
6	MG	B	9104	1/1	0.97	0.10	45,45,45,45	0
6	MG	L	9245	1/1	0.97	0.09	62,62,62,62	0
6	MG	D	9177	1/1	0.97	0.13	64,64,64,64	0
6	MG	F	9123	1/1	0.97	0.09	37,37,37,37	0
6	MG	K	9257	1/1	0.97	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	A	9171	1/1	0.97	0.11	58,58,58,58	0
6	MG	D	9087	1/1	0.97	0.07	43,43,43,43	0
6	MG	L	9252	1/1	0.97	0.09	45,45,45,45	0
6	MG	K	9433	1/1	0.97	0.07	50,50,50,50	0
6	MG	D	9346	1/1	0.97	0.07	47,47,47,47	0
6	MG	K	9410	1/1	0.97	0.15	36,36,36,36	0
6	MG	N	9211	1/1	0.97	0.10	44,44,44,44	0
6	MG	F	9389	1/1	0.97	0.11	53,53,53,53	0
6	MG	M	9196	1/1	0.97	0.09	42,42,42,42	0
6	MG	M	9273	1/1	0.97	0.12	44,44,44,44	0
6	MG	D	9388	1/1	0.97	0.09	37,37,37,37	0
6	MG	N	9473	1/1	0.97	0.12	51,51,51,51	0
6	MG	A	9153	1/1	0.97	0.15	66,66,66,66	0
6	MG	B	9103	1/1	0.97	0.12	43,43,43,43	0
6	MG	F	9060	1/1	0.97	0.10	41,41,41,41	0
6	MG	P	9325	1/1	0.97	0.12	49,49,49,49	0
6	MG	D	9095	1/1	0.97	0.15	30,30,30,30	0
6	MG	D	9165	1/1	0.97	0.07	32,32,32,32	0
6	MG	A	9125	1/1	0.97	0.12	36,36,36,36	0
6	MG	D	9367	1/1	0.97	0.06	31,31,31,31	0
6	MG	F	9099	1/1	0.97	0.13	56,56,56,56	0
6	MG	K	9251	1/1	0.97	0.11	43,43,43,43	0
6	MG	N	9422	1/1	0.97	0.14	56,56,56,56	0
6	MG	D	9017	1/1	0.97	0.10	42,42,42,42	0
6	MG	N	9450	1/1	0.97	0.10	48,48,48,48	0
6	MG	N	9425	1/1	0.97	0.12	46,46,46,46	0
6	MG	M	9219	1/1	0.97	0.09	47,47,47,47	0
6	MG	A	9066	1/1	0.97	0.14	47,47,47,47	0
6	MG	D	9127	1/1	0.97	0.14	48,48,48,48	0
6	MG	N	9465	1/1	0.98	0.08	49,49,49,49	0
6	MG	O	9296	1/1	0.98	0.11	42,42,42,42	0
6	MG	M	9424	1/1	0.98	0.13	34,34,34,34	0
6	MG	P	9280	1/1	0.98	0.10	51,51,51,51	0
6	MG	F	9356	1/1	0.98	0.14	37,37,37,37	0
6	MG	M	9310	1/1	0.98	0.07	46,46,46,46	0
6	MG	D	9121	1/1	0.98	0.09	35,35,35,35	0
6	MG	C	9138	1/1	0.98	0.08	43,43,43,43	0
6	MG	D	9108	1/1	0.98	0.15	51,51,51,51	0
6	MG	L	9246	1/1	0.98	0.12	52,52,52,52	0
6	MG	C	9128	1/1	0.98	0.12	52,52,52,52	0
6	MG	A	9460	1/1	0.98	0.07	55,55,55,55	0
6	MG	K	9405	1/1	0.98	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9184	1/1	0.98	0.10	29,29,29,29	0
6	MG	C	9340	1/1	0.98	0.09	60,60,60,60	0
6	MG	C	9004	1/1	0.98	0.10	39,39,39,39	0
6	MG	E	9045	1/1	0.98	0.12	61,61,61,61	0
6	MG	D	9374	1/1	0.98	0.10	41,41,41,41	0
6	MG	C	9461	1/1	0.98	0.07	50,50,50,50	0
6	MG	N	9428	1/1	0.98	0.10	42,42,42,42	0
6	MG	N	9265	1/1	0.98	0.14	61,61,61,61	0
6	MG	C	9015	1/1	0.98	0.09	38,38,38,38	0
6	MG	M	9434	1/1	0.98	0.11	34,34,34,34	0
6	MG	N	9445	1/1	0.98	0.10	51,51,51,51	0
6	MG	O	9439	1/1	0.98	0.16	56,56,56,56	0
6	MG	D	9118	1/1	0.98	0.11	44,44,44,44	0
6	MG	M	9441	1/1	0.98	0.07	45,45,45,45	0
6	MG	A	9016	1/1	0.98	0.14	36,36,36,36	0
6	MG	D	9397	1/1	0.98	0.12	51,51,51,51	0
6	MG	M	9452	1/1	0.98	0.13	42,42,42,42	0
6	MG	D	9163	1/1	0.98	0.14	52,52,52,52	0
6	MG	D	9379	1/1	0.98	0.11	47,47,47,47	0
6	MG	L	9309	1/1	0.98	0.13	49,49,49,49	0
6	MG	A	9111	1/1	0.98	0.09	35,35,35,35	0
6	MG	N	9214	1/1	0.98	0.10	33,33,33,33	0
6	MG	M	9407	1/1	0.98	0.14	35,35,35,35	0
6	MG	N	9215	1/1	0.98	0.12	32,32,32,32	0
6	MG	N	9415	1/1	0.98	0.07	42,42,42,42	0
6	MG	D	9344	1/1	0.98	0.11	55,55,55,55	0
6	MG	D	9152	1/1	0.98	0.12	67,67,67,67	0
6	MG	N	9419	1/1	0.98	0.11	51,51,51,51	0
6	MG	P	9228	1/1	0.98	0.09	43,43,43,43	0
6	MG	P	9235	1/1	0.98	0.16	40,40,40,40	0
6	MG	D	9137	1/1	0.98	0.08	47,47,47,47	0
6	MG	D	9349	1/1	0.98	0.13	33,33,33,33	0
6	MG	M	9284	1/1	0.98	0.14	54,54,54,54	0
6	MG	D	9338	1/1	0.98	0.10	42,42,42,42	0
6	MG	N	9253	1/1	0.98	0.12	42,42,42,42	0
6	MG	A	9010	1/1	0.98	0.12	30,30,30,30	0
6	MG	C	9154	1/1	0.98	0.07	43,43,43,43	0
6	MG	D	9052	1/1	0.98	0.07	65,65,65,65	0
6	MG	N	9231	1/1	0.98	0.11	52,52,52,52	0
6	MG	D	9069	1/1	0.98	0.12	48,48,48,48	0
6	MG	C	9464	1/1	0.98	0.06	48,48,48,48	0
6	MG	D	9173	1/1	0.98	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9021	1/1	0.98	0.09	37,37,37,37	0
6	MG	A	9027	1/1	0.98	0.08	37,37,37,37	0
6	MG	F	9387	1/1	0.98	0.10	53,53,53,53	0
6	MG	K	9438	1/1	0.98	0.10	52,52,52,52	0
6	MG	C	9142	1/1	0.98	0.15	48,48,48,48	0
6	MG	D	9113	1/1	0.98	0.11	34,34,34,34	0
6	MG	M	9305	1/1	0.98	0.09	46,46,46,46	0
6	MG	N	9204	1/1	0.98	0.19	44,44,44,44	0
6	MG	M	9212	1/1	0.98	0.08	32,32,32,32	0
6	MG	N	9243	1/1	0.98	0.09	35,35,35,35	0
6	MG	N	9185	1/1	0.98	0.14	56,56,56,56	0
6	MG	L	9314	1/1	0.98	0.07	56,56,56,56	0
6	MG	N	9435	1/1	0.98	0.23	53,53,53,53	0
6	MG	B	9080	1/1	0.98	0.10	56,56,56,56	0
6	MG	C	9112	1/1	0.98	0.11	39,39,39,39	0
6	MG	C	9090	1/1	0.98	0.10	47,47,47,47	0
6	MG	N	9404	1/1	0.98	0.12	55,55,55,55	0
6	MG	K	9301	1/1	0.98	0.12	43,43,43,43	0
6	MG	A	9012	1/1	0.98	0.10	47,47,47,47	0
6	MG	F	9383	1/1	0.98	0.11	48,48,48,48	0
6	MG	C	9394	1/1	0.98	0.09	33,33,33,33	0
6	MG	F	9159	1/1	0.98	0.15	57,57,57,57	0
6	MG	N	9270	1/1	0.98	0.05	39,39,39,39	0
6	MG	N	9181	1/1	0.98	0.16	47,47,47,47	0
6	MG	L	9283	1/1	0.98	0.12	59,59,59,59	0
6	MG	M	9241	1/1	0.98	0.11	36,36,36,36	0
6	MG	C	9065	1/1	0.98	0.10	37,37,37,37	0
6	MG	N	9287	1/1	0.98	0.09	53,53,53,53	0
6	MG	L	9421	1/1	0.98	0.12	53,53,53,53	0
6	MG	P	9285	1/1	0.98	0.09	56,56,56,56	0
6	MG	K	9290	1/1	0.98	0.12	51,51,51,51	0
6	MG	M	9205	1/1	0.98	0.11	38,38,38,38	0
6	MG	F	9105	1/1	0.98	0.14	36,36,36,36	0
6	MG	B	9478	1/1	0.98	0.12	61,61,61,61	0
6	MG	D	9459	1/1	0.98	0.05	54,54,54,54	0
6	MG	C	9037	1/1	0.98	0.16	51,51,51,51	0
6	MG	B	9056	1/1	0.98	0.13	43,43,43,43	0
6	MG	F	9098	1/1	0.98	0.11	54,54,54,54	0
6	MG	A	9477	1/1	0.98	0.18	52,52,52,52	0
6	MG	K	9264	1/1	0.98	0.08	42,42,42,42	0
6	MG	C	9025	1/1	0.98	0.14	39,39,39,39	0
6	MG	F	9008	1/1	0.98	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9267	1/1	0.98	0.12	42,42,42,42	0
6	MG	M	9440	1/1	0.98	0.10	50,50,50,50	0
6	MG	D	9064	1/1	0.98	0.14	44,44,44,44	0
6	MG	D	9369	1/1	0.98	0.10	49,49,49,49	0
6	MG	K	9191	1/1	0.98	0.15	32,32,32,32	0
6	MG	F	9375	1/1	0.98	0.13	36,36,36,36	0
6	MG	D	9018	1/1	0.98	0.11	39,39,39,39	0
6	MG	D	9063	1/1	0.98	0.08	33,33,33,33	0
6	MG	O	9197	1/1	0.98	0.04	57,57,57,57	0
6	MG	N	9423	1/1	0.98	0.17	58,58,58,58	0
6	MG	M	9247	1/1	0.98	0.07	51,51,51,51	0
6	MG	N	9293	1/1	0.98	0.15	42,42,42,42	0
6	MG	D	9392	1/1	0.98	0.12	52,52,52,52	0
6	MG	N	9298	1/1	0.98	0.05	55,55,55,55	0
6	MG	N	9259	1/1	0.98	0.15	34,34,34,34	0
6	MG	A	9068	1/1	0.98	0.12	39,39,39,39	0
6	MG	F	9363	1/1	0.98	0.12	53,53,53,53	0
6	MG	M	9250	1/1	0.98	0.07	38,38,38,38	0
6	MG	D	9028	1/1	0.98	0.13	34,34,34,34	0
6	MG	N	9286	1/1	0.98	0.14	31,31,31,31	0
6	MG	N	9322	1/1	0.98	0.10	54,54,54,54	0
6	MG	A	9384	1/1	0.98	0.14	39,39,39,39	0
6	MG	M	9239	1/1	0.98	0.07	34,34,34,34	0
6	MG	C	9092	1/1	0.98	0.06	44,44,44,44	0
6	MG	D	9024	1/1	0.98	0.14	36,36,36,36	0
6	MG	N	9236	1/1	0.98	0.10	39,39,39,39	0
6	MG	D	9135	1/1	0.98	0.14	50,50,50,50	0
6	MG	D	9132	1/1	0.98	0.10	43,43,43,43	0
6	MG	E	9479	1/1	0.98	0.10	62,62,62,62	0
6	MG	K	9213	1/1	0.98	0.11	43,43,43,43	0
6	MG	E	9007	1/1	0.98	0.11	40,40,40,40	0
6	MG	N	9429	1/1	0.98	0.10	45,45,45,45	0
6	MG	P	9282	1/1	0.98	0.09	56,56,56,56	0
6	MG	B	9093	1/1	0.98	0.15	40,40,40,40	0
6	MG	B	9457	1/1	0.98	0.07	43,43,43,43	0
6	MG	N	9431	1/1	0.99	0.12	39,39,39,39	0
6	MG	N	9472	1/1	0.99	0.15	56,56,56,56	0
6	MG	C	9020	1/1	0.99	0.10	34,34,34,34	0
6	MG	D	9343	1/1	0.99	0.10	59,59,59,59	0
6	MG	M	9442	1/1	0.99	0.07	59,59,59,59	0
6	MG	K	9413	1/1	0.99	0.10	54,54,54,54	0
6	MG	D	9329	1/1	0.99	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9038	1/1	0.99	0.14	39,39,39,39	0
6	MG	D	9337	1/1	0.99	0.15	53,53,53,53	0
6	MG	D	9336	1/1	0.99	0.10	53,53,53,53	0
6	MG	A	9097	1/1	0.99	0.16	34,34,34,34	0
6	MG	D	9386	1/1	0.99	0.11	40,40,40,40	0
6	MG	M	9203	1/1	0.99	0.11	32,32,32,32	0
6	MG	C	9371	1/1	0.99	0.15	54,54,54,54	0
6	MG	N	9402	1/1	0.99	0.07	45,45,45,45	0
6	MG	A	9043	1/1	0.99	0.17	37,37,37,37	0
6	MG	M	9195	1/1	0.99	0.08	34,34,34,34	0
6	MG	B	9094	1/1	0.99	0.15	38,38,38,38	0
6	MG	P	9399	1/1	0.99	0.11	34,34,34,34	0
6	MG	C	9042	1/1	0.99	0.07	47,47,47,47	0
6	MG	C	9176	1/1	0.99	0.09	28,28,28,28	0
6	MG	N	9199	1/1	0.99	0.11	35,35,35,35	0
6	MG	A	9332	1/1	0.99	0.06	35,35,35,35	0
6	MG	A	9395	1/1	0.99	0.14	50,50,50,50	0
6	MG	N	9207	1/1	0.99	0.13	41,41,41,41	0
6	MG	D	9130	1/1	0.99	0.09	51,51,51,51	0
6	MG	D	9011	1/1	0.99	0.12	33,33,33,33	0
6	MG	N	9318	1/1	0.99	0.11	34,34,34,34	0
6	MG	N	9443	1/1	0.99	0.13	54,54,54,54	0
6	MG	F	9382	1/1	0.99	0.09	40,40,40,40	0
6	MG	N	9308	1/1	0.99	0.15	55,55,55,55	0
6	MG	N	9179	1/1	0.99	0.12	33,33,33,33	0
6	MG	M	9272	1/1	0.99	0.17	45,45,45,45	0
6	MG	C	9126	1/1	0.99	0.10	46,46,46,46	0
6	MG	C	9366	1/1	0.99	0.14	41,41,41,41	0
6	MG	N	9304	1/1	0.99	0.11	47,47,47,47	0
6	MG	N	9262	1/1	0.99	0.09	51,51,51,51	0
6	MG	L	9437	1/1	0.99	0.06	40,40,40,40	0
6	MG	F	9139	1/1	0.99	0.10	38,38,38,38	0
6	MG	F	9481	1/1	0.99	0.08	57,57,57,57	0
6	MG	D	9146	1/1	0.99	0.10	31,31,31,31	0
6	MG	D	9335	1/1	0.99	0.06	52,52,52,52	0
6	MG	D	9144	1/1	0.99	0.12	39,39,39,39	0
6	MG	M	9242	1/1	0.99	0.11	35,35,35,35	0
6	MG	C	9353	1/1	0.99	0.10	48,48,48,48	0
6	MG	D	9089	1/1	0.99	0.09	36,36,36,36	0
6	MG	F	9048	1/1	0.99	0.10	41,41,41,41	0
6	MG	D	9100	1/1	0.99	0.08	43,43,43,43	0
6	MG	B	9378	1/1	0.99	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	B	9083	1/1	0.99	0.13	40,40,40,40	0
6	MG	D	9133	1/1	0.99	0.13	42,42,42,42	0
6	MG	N	9417	1/1	0.99	0.09	39,39,39,39	0
6	MG	N	9186	1/1	0.99	0.12	49,49,49,49	0
6	MG	D	9029	1/1	0.99	0.12	33,33,33,33	0
6	MG	P	9315	1/1	0.99	0.08	35,35,35,35	0
6	MG	A	9088	1/1	0.99	0.07	36,36,36,36	0
6	MG	P	9436	1/1	0.99	0.11	49,49,49,49	0
6	MG	B	9033	1/1	0.99	0.14	33,33,33,33	0
6	MG	C	9145	1/1	0.99	0.13	66,66,66,66	0
6	MG	A	9002	1/1	0.99	0.17	31,31,31,31	0
6	MG	L	9306	1/1	0.99	0.11	57,57,57,57	0
6	MG	M	9190	1/1	0.99	0.16	29,29,29,29	0
6	MG	C	9115	1/1	0.99	0.11	36,36,36,36	0
6	MG	N	9288	1/1	0.99	0.09	49,49,49,49	0
6	MG	D	9334	1/1	0.99	0.10	54,54,54,54	0
6	MG	P	9277	1/1	0.99	0.09	41,41,41,41	0
6	MG	D	9140	1/1	0.99	0.13	40,40,40,40	0
6	MG	D	9480	1/1	0.99	0.10	55,55,55,55	0
6	MG	A	9106	1/1	0.99	0.12	38,38,38,38	0
6	MG	N	9468	1/1	0.99	0.10	55,55,55,55	0
6	MG	A	9345	1/1	0.99	0.12	41,41,41,41	0
6	MG	C	9026	1/1	0.99	0.13	42,42,42,42	0
6	MG	D	9456	1/1	0.99	0.10	55,55,55,55	0
6	MG	N	9274	1/1	0.99	0.18	40,40,40,40	0
6	MG	D	9339	1/1	0.99	0.14	37,37,37,37	0
6	MG	D	9134	1/1	0.99	0.13	47,47,47,47	0
6	MG	C	9462	1/1	0.99	0.08	43,43,43,43	0
6	MG	D	9396	1/1	0.99	0.10	62,62,62,62	0
6	MG	D	9328	1/1	0.99	0.12	30,30,30,30	0
6	MG	N	9316	1/1	0.99	0.08	37,37,37,37	0
6	MG	N	9430	1/1	0.99	0.08	57,57,57,57	0
6	MG	A	9368	1/1	0.99	0.13	43,43,43,43	0
6	MG	B	9136	1/1	0.99	0.10	47,47,47,47	0
8	ZN	N	7113	1/1	0.99	0.13	84,84,84,84	0
6	MG	P	9255	1/1	0.99	0.12	34,34,34,34	0
6	MG	N	9302	1/1	0.99	0.10	31,31,31,31	0
6	MG	C	9071	1/1	0.99	0.11	42,42,42,42	0
6	MG	B	9116	1/1	0.99	0.09	38,38,38,38	0
6	MG	B	9110	1/1	0.99	0.12	49,49,49,49	0
6	MG	M	9486	1/1	0.99	0.07	48,48,48,48	0
6	MG	O	9254	1/1	0.99	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9323	1/1	0.99	0.09	38,38,38,38	0
6	MG	K	9223	1/1	0.99	0.09	32,32,32,32	0
6	MG	D	9072	1/1	0.99	0.14	32,32,32,32	0
6	MG	M	9222	1/1	0.99	0.10	35,35,35,35	0
6	MG	N	9229	1/1	0.99	0.07	41,41,41,41	0
6	MG	A	9124	1/1	0.99	0.12	39,39,39,39	0
6	MG	A	9380	1/1	0.99	0.11	44,44,44,44	0
6	MG	M	9416	1/1	0.99	0.11	45,45,45,45	0
6	MG	F	9157	1/1	0.99	0.11	42,42,42,42	0
6	MG	B	9032	1/1	0.99	0.06	34,34,34,34	0
6	MG	L	9466	1/1	0.99	0.10	49,49,49,49	0
6	MG	D	9333	1/1	0.99	0.07	33,33,33,33	0
6	MG	D	9385	1/1	0.99	0.13	35,35,35,35	0
6	MG	D	9364	1/1	0.99	0.12	47,47,47,47	0
6	MG	N	9418	1/1	0.99	0.10	49,49,49,49	0
6	MG	A	9354	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9005	1/1	0.99	0.11	40,40,40,40	0
6	MG	N	9187	1/1	0.99	0.18	33,33,33,33	0
6	MG	C	9377	1/1	0.99	0.09	44,44,44,44	0
6	MG	D	9085	1/1	0.99	0.18	49,49,49,49	0
6	MG	C	9053	1/1	0.99	0.12	30,30,30,30	0
6	MG	O	9483	1/1	0.99	0.09	63,63,63,63	0
6	MG	N	9467	1/1	0.99	0.12	35,35,35,35	0
6	MG	L	9307	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9129	1/1	0.99	0.14	42,42,42,42	0
6	MG	D	9347	1/1	0.99	0.09	49,49,49,49	0
6	MG	D	9023	1/1	0.99	0.14	34,34,34,34	0
6	MG	M	9295	1/1	0.99	0.08	42,42,42,42	0
6	MG	N	9444	1/1	0.99	0.15	49,49,49,49	0
6	MG	A	9342	1/1	0.99	0.12	39,39,39,39	0
6	MG	N	9484	1/1	0.99	0.07	37,37,37,37	0
6	MG	C	9044	1/1	0.99	0.14	34,34,34,34	0
6	MG	N	9317	1/1	0.99	0.09	43,43,43,43	0
6	MG	D	9151	1/1	0.99	0.15	57,57,57,57	0
6	MG	N	9206	1/1	0.99	0.16	31,31,31,31	0
6	MG	M	9227	1/1	0.99	0.12	35,35,35,35	0
6	MG	E	9155	1/1	0.99	0.14	44,44,44,44	0
6	MG	N	9451	1/1	0.99	0.06	41,41,41,41	0
6	MG	D	9077	1/1	0.99	0.11	35,35,35,35	0
6	MG	N	9398	1/1	0.99	0.15	48,48,48,48	0
6	MG	M	9260	1/1	0.99	0.12	36,36,36,36	0
6	MG	D	9070	1/1	0.99	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9046	1/1	0.99	0.11	38,38,38,38	0
6	MG	K	9432	1/1	0.99	0.13	49,49,49,49	0
6	MG	N	9238	1/1	0.99	0.11	43,43,43,43	0
6	MG	C	9463	1/1	0.99	0.09	55,55,55,55	0
6	MG	C	9114	1/1	0.99	0.09	30,30,30,30	0
6	MG	F	9035	1/1	0.99	0.10	40,40,40,40	0
6	MG	D	9039	1/1	0.99	0.12	44,44,44,44	0
8	ZN	N	7059	1/1	0.99	0.12	93,93,93,93	0
6	MG	C	9051	1/1	0.99	0.12	37,37,37,37	0
6	MG	C	9143	1/1	0.99	0.10	35,35,35,35	0
6	MG	M	9220	1/1	0.99	0.11	51,51,51,51	0
6	MG	N	9240	1/1	0.99	0.14	46,46,46,46	0
6	MG	M	9299	1/1	0.99	0.09	43,43,43,43	0
6	MG	N	9476	1/1	0.99	0.09	54,54,54,54	0
6	MG	B	9131	1/1	0.99	0.08	33,33,33,33	0
6	MG	C	9055	1/1	0.99	0.11	38,38,38,38	0
6	MG	D	9150	1/1	0.99	0.14	31,31,31,31	0
6	MG	C	9086	1/1	0.99	0.14	39,39,39,39	0
6	MG	M	9224	1/1	0.99	0.13	40,40,40,40	0
6	MG	D	9120	1/1	0.99	0.08	31,31,31,31	0
6	MG	D	9331	1/1	0.99	0.18	43,43,43,43	0
6	MG	M	9400	1/1	0.99	0.12	40,40,40,40	0
6	MG	M	9268	1/1	0.99	0.09	32,32,32,32	0
8	ZN	D	7112	1/1	0.99	0.10	80,80,80,80	0
6	MG	M	9208	1/1	0.99	0.10	39,39,39,39	0
6	MG	M	9300	1/1	0.99	0.09	39,39,39,39	0
6	MG	C	9003	1/1	0.99	0.13	38,38,38,38	0
6	MG	N	9303	1/1	0.99	0.08	54,54,54,54	0
6	MG	N	9279	1/1	0.99	0.11	54,54,54,54	0
6	MG	M	9312	1/1	0.99	0.12	37,37,37,37	0
6	MG	C	9454	1/1	0.99	0.09	55,55,55,55	0
6	MG	D	9147	1/1	0.99	0.10	41,41,41,41	0
6	MG	M	9474	1/1	0.99	0.14	49,49,49,49	0
6	MG	C	9455	1/1	0.99	0.11	40,40,40,40	0
6	MG	C	9061	1/1	0.99	0.07	34,34,34,34	0
6	MG	D	9141	1/1	0.99	0.06	50,50,50,50	0
6	MG	C	9169	1/1	0.99	0.13	42,42,42,42	0
6	MG	D	9351	1/1	0.99	0.06	43,43,43,43	0
6	MG	L	9183	1/1	0.99	0.13	37,37,37,37	0
6	MG	D	9034	1/1	0.99	0.08	41,41,41,41	0
6	MG	N	9448	1/1	0.99	0.09	51,51,51,51	0
6	MG	F	9393	1/1	0.99	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	K	9469	1/1	0.99	0.12	50,50,50,50	0
6	MG	C	9170	1/1	0.99	0.06	41,41,41,41	0
6	MG	P	9446	1/1	0.99	0.13	34,34,34,34	0
6	MG	D	9058	1/1	0.99	0.08	38,38,38,38	0
6	MG	C	9079	1/1	0.99	0.11	38,38,38,38	0
6	MG	B	9358	1/1	0.99	0.07	39,39,39,39	0
6	MG	D	9084	1/1	0.99	0.11	37,37,37,37	0
6	MG	D	9341	1/1	0.99	0.10	41,41,41,41	0
6	MG	N	9403	1/1	0.99	0.12	34,34,34,34	0
6	MG	C	9031	1/1	0.99	0.10	40,40,40,40	0
6	MG	K	9244	1/1	0.99	0.07	44,44,44,44	0
6	MG	C	9164	1/1	0.99	0.10	49,49,49,49	0
6	MG	B	9040	1/1	0.99	0.16	36,36,36,36	0
6	MG	N	9269	1/1	0.99	0.07	42,42,42,42	0
6	MG	C	9050	1/1	0.99	0.15	37,37,37,37	0
6	MG	M	9409	1/1	0.99	0.10	36,36,36,36	0
6	MG	A	9075	1/1	0.99	0.10	36,36,36,36	0
6	MG	M	9281	1/1	0.99	0.11	49,49,49,49	0
6	MG	K	9180	1/1	1.00	0.11	42,42,42,42	0
6	MG	M	9485	1/1	1.00	0.07	54,54,54,54	0
6	MG	N	9408	1/1	1.00	0.14	45,45,45,45	0
6	MG	F	9101	1/1	1.00	0.12	44,44,44,44	0
6	MG	D	9117	1/1	1.00	0.13	48,48,48,48	0
6	MG	C	9361	1/1	1.00	0.10	41,41,41,41	0
6	MG	O	9266	1/1	1.00	0.08	47,47,47,47	0
6	MG	M	9321	1/1	1.00	0.12	41,41,41,41	0
6	MG	N	9193	1/1	1.00	0.15	34,34,34,34	0
6	MG	M	9320	1/1	1.00	0.11	34,34,34,34	0
6	MG	D	9091	1/1	1.00	0.13	27,27,27,27	0
6	MG	P	9258	1/1	1.00	0.14	51,51,51,51	0
6	MG	F	9057	1/1	1.00	0.09	30,30,30,30	0
6	MG	M	9230	1/1	1.00	0.11	50,50,50,50	0
6	MG	N	9249	1/1	1.00	0.10	45,45,45,45	0
6	MG	N	9311	1/1	1.00	0.10	39,39,39,39	0
6	MG	C	9487	1/1	1.00	0.11	32,32,32,32	0
6	MG	N	9271	1/1	1.00	0.07	43,43,43,43	0
6	MG	C	9076	1/1	1.00	0.12	33,33,33,33	0
6	MG	M	9319	1/1	1.00	0.12	41,41,41,41	0
6	MG	P	9482	1/1	1.00	0.11	48,48,48,48	0
6	MG	M	9401	1/1	1.00	0.10	37,37,37,37	0
6	MG	M	9248	1/1	1.00	0.08	48,48,48,48	0

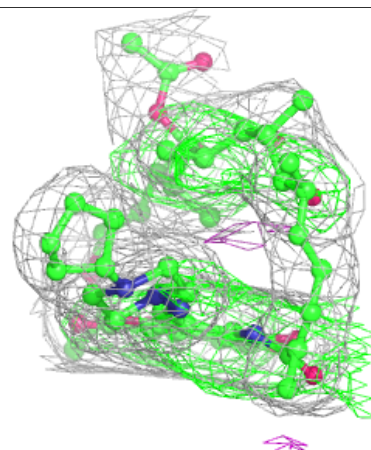
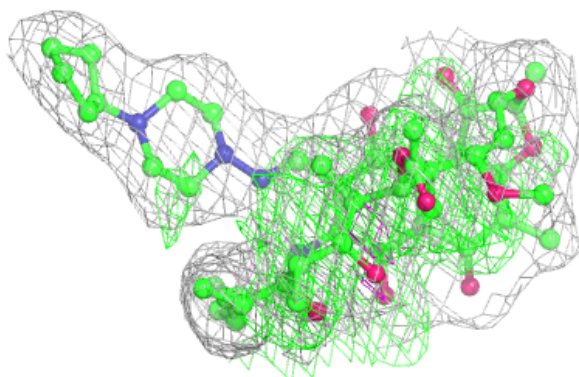
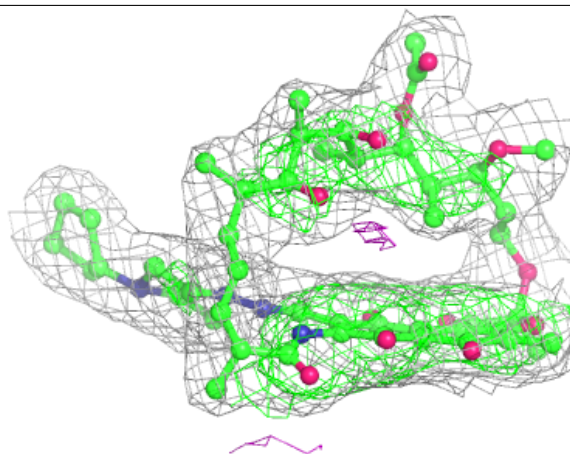
The following is a graphical depiction of the model fit to experimental electron density of all

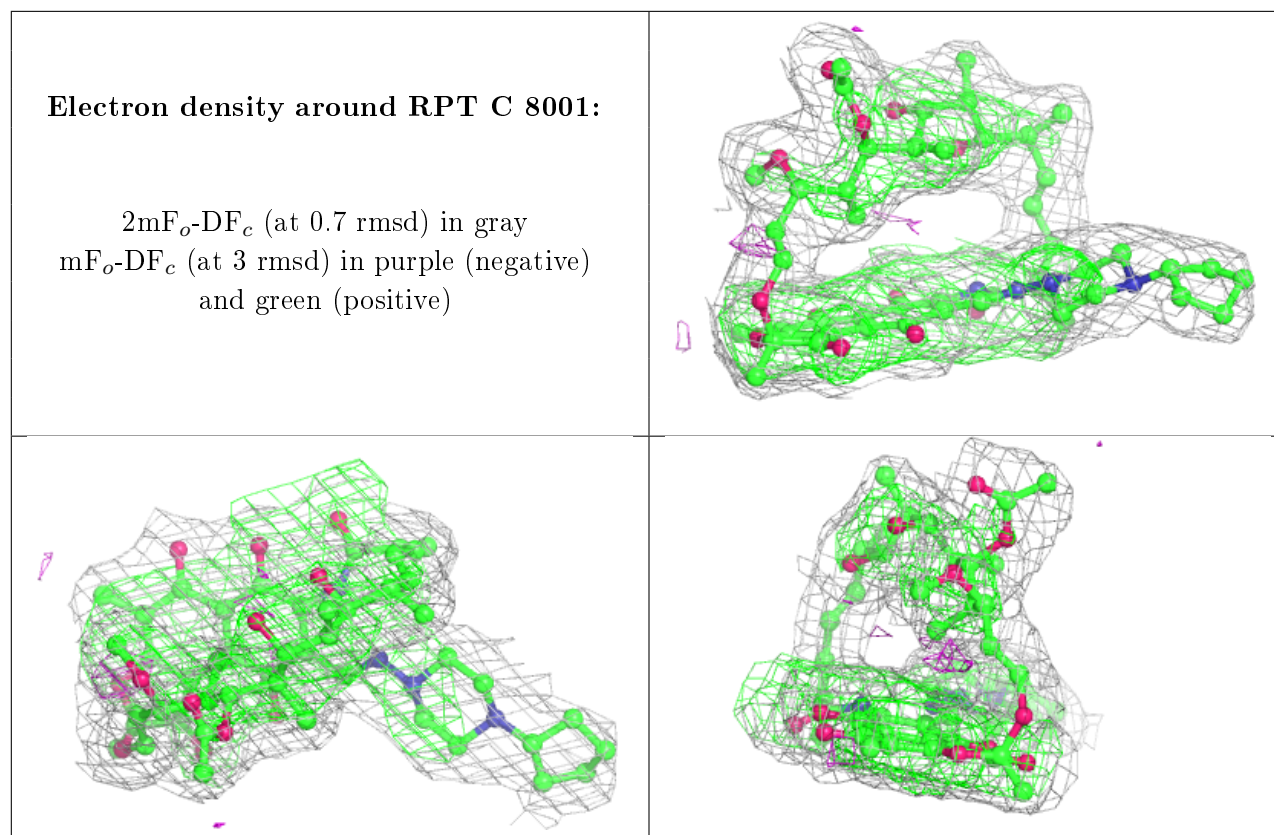


instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around RPT M 8002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.