



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 01:43 pm BST

PDB ID : 2A68
Title : Crystal structure of the T. thermophilus RNA polymerase holoenzyme in complex with antibiotic rifabutin
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 : 2005-07-01
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

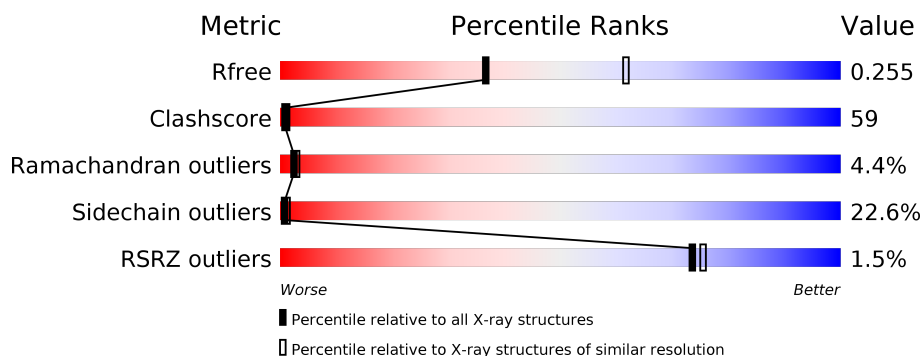
1 Overall quality at a glance ⓘ

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 ≥ 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></div> <div>14% 44% 14% 27%</div> </div>
1	B	315	<div> <div>4%</div> <div>20% 41% 11% 27%</div> </div>
1	K	315	<div> <div>%</div> <div>17% 40% 15% 27%</div> </div>
1	L	315	<div> <div>3%</div> <div>20% 42% 11% 27%</div> </div>
2	C	1119	<div> <div>%</div> <div>23% 59% 17%</div> </div>
2	M	1119	<div> <div>%</div> <div>25% 58% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div><div></div><div></div><div></div><div></div></div><div>%23%51%16%•9%</div></div>
3	N	1524	<div><div><div></div><div></div><div></div><div></div></div><div>2%25%51%15%•9%</div></div>
4	E	99	<div><div><div></div><div></div><div></div><div></div></div><div>2%27%58%11%•</div></div>
4	O	99	<div><div><div></div><div></div><div></div><div></div></div><div>%22%56%17%••</div></div>
5	F	423	<div><div><div></div><div></div><div></div><div></div></div><div>2%21%48%11%•18%</div></div>
5	P	423	<div><div><div></div><div></div><div></div><div></div></div><div>2%24%47%10%18%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 61089 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			

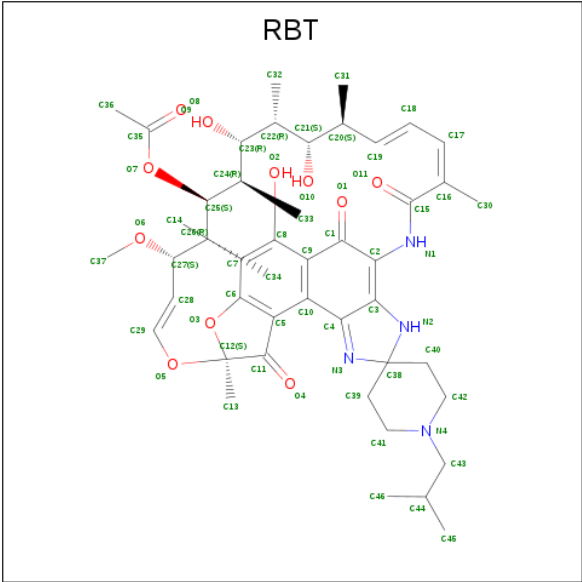
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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	137	Total	Mg	0	0
			137	137		
6	K	21	Total	Mg	0	0
			21	21		
6	E	10	Total	Mg	0	0
			10	10		
6	B	23	Total	Mg	0	0
			23	23		
6	C	81	Total	Mg	0	0
			81	81		
6	A	31	Total	Mg	0	0
			31	31		
6	N	108	Total	Mg	0	0
			108	108		
6	O	6	Total	Mg	0	0
			6	6		
6	L	25	Total	Mg	0	0
			25	25		
6	F	31	Total	Mg	0	0
			31	31		
6	M	69	Total	Mg	0	0
			69	69		

- Molecule 7 is RIFABUTIN (three-letter code: RBT) (formula: C₄₆H₆₂N₄O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			61	46	4	11		
7	M	1	Total	C	N	O	0	0
			61	46	4	11		

- 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	253	Total	O	0	0
			253	253		
9	B	307	Total	O	0	0
			307	307		
9	C	1000	Total	O	0	0
			1000	1000		
9	D	1418	Total	O	0	0
			1418	1418		
9	E	112	Total	O	0	0
			112	112		

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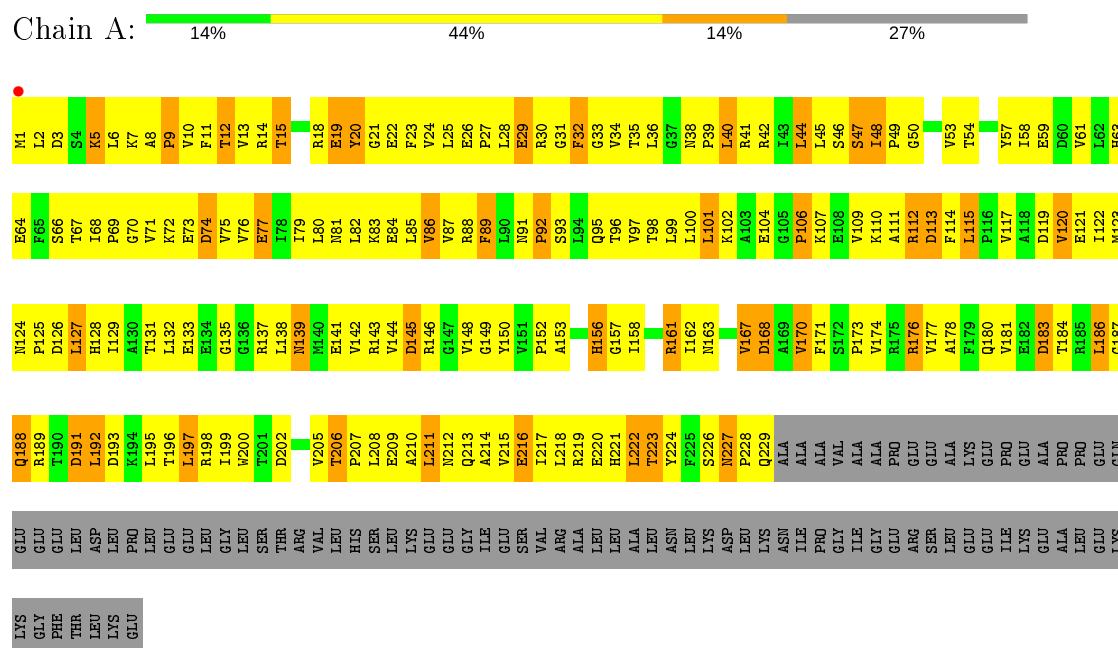
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	456	Total 456	O 456	0	0
9	K	213	Total 213	O 213	0	0
9	L	237	Total 237	O 237	0	0
9	M	998	Total 998	O 998	0	0
9	N	1357	Total 1357	O 1357	0	0
9	O	117	Total 117	O 117	0	0
9	P	377	Total 377	O 377	0	0

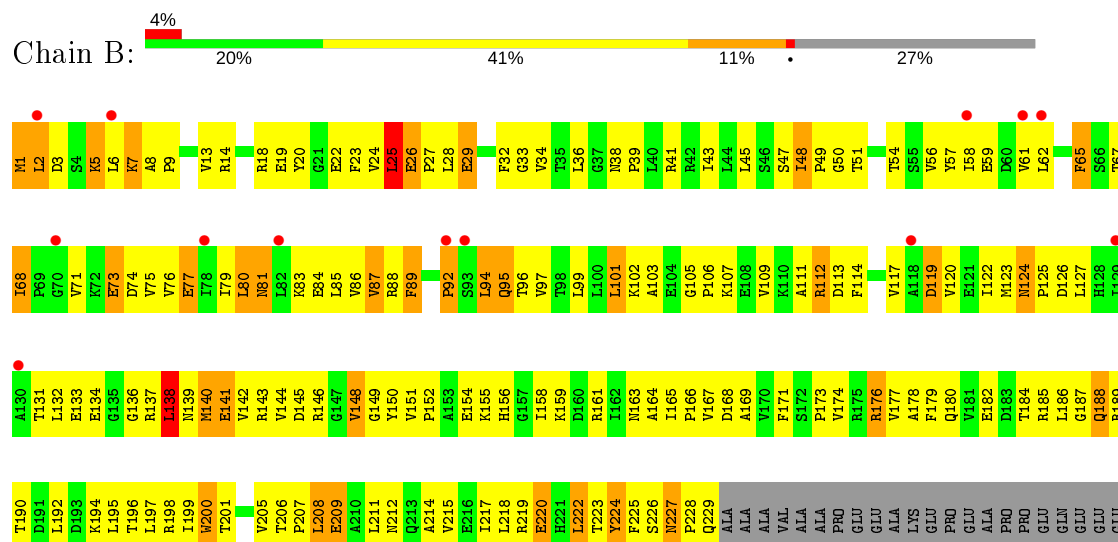
3 Residue-property plots

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

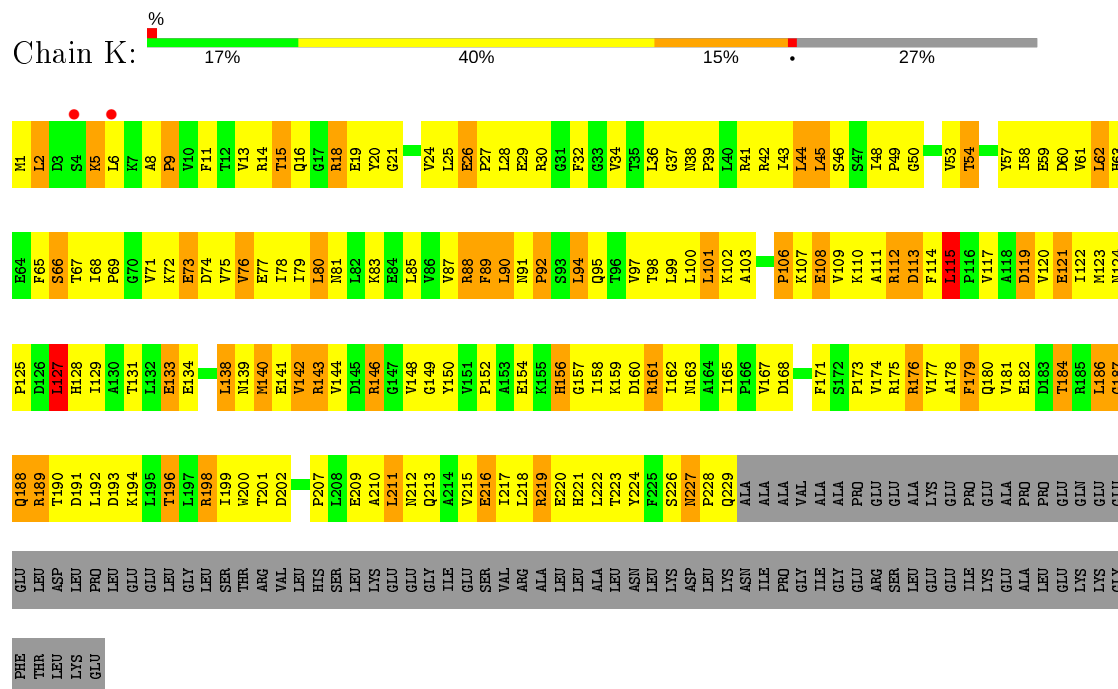


• Molecule 1: DNA-directed RNA polymerase alpha chain

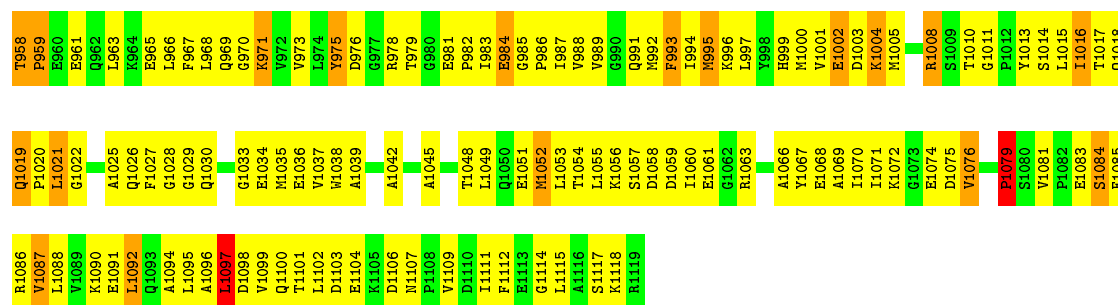


LEU	ASP	LEU	PRO	GLU	GLU	LEU	GLY	SER	THR	ARG	VAL	LEU	HIS	SER	LEU	LYS	GLU	GLY	LEU	LYS	GLY	LYS	PHE
THR	LEU	LYS	GLU																				

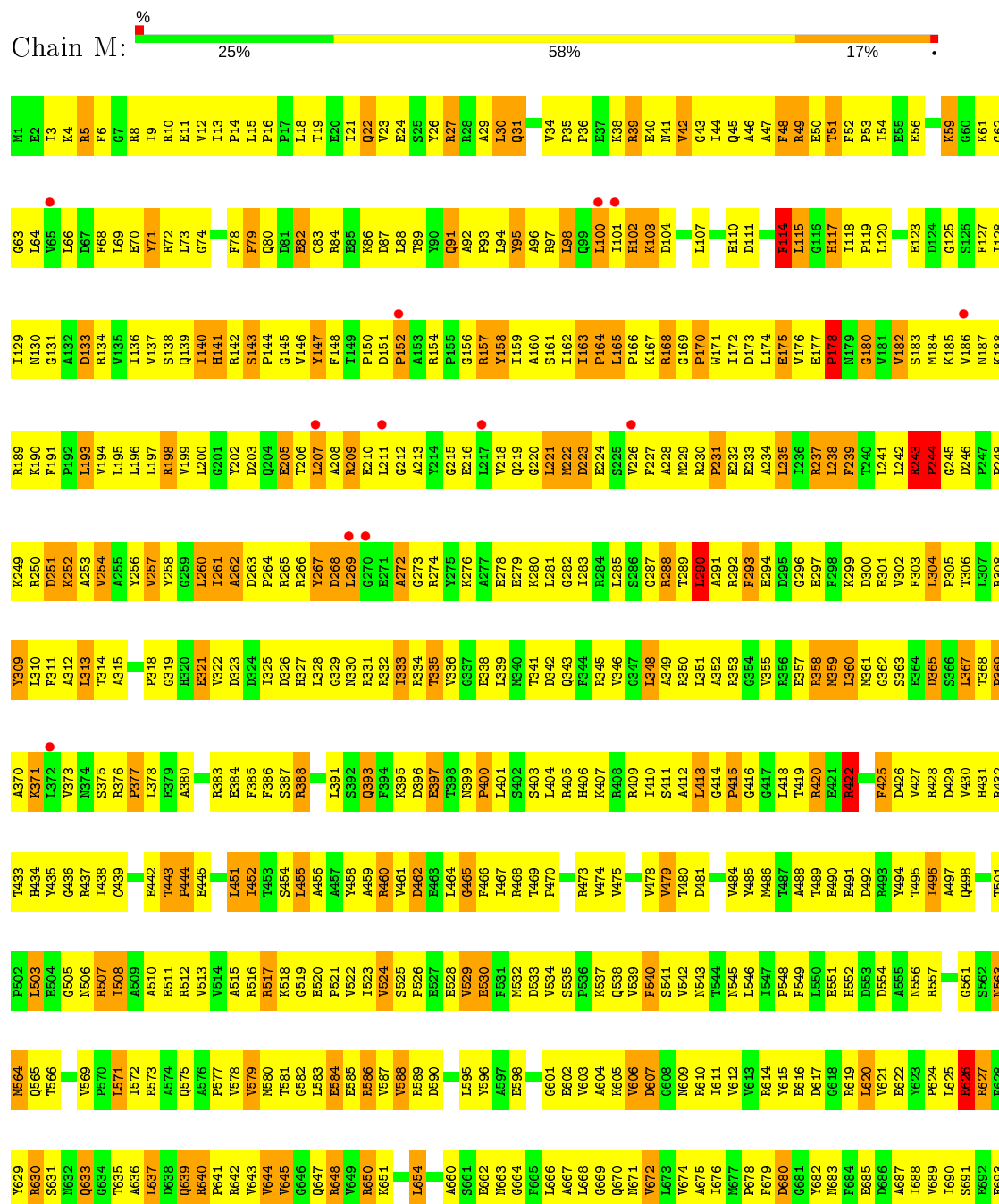
• Molecule 1: DNA-directed RNA polymerase alpha chain



L987	Q829	F761	R697	Q634	V569	I508	T443	A381	V254	K190	I128	V65	M1
Q830	R330		D698	T635	P570	A509	P444	I382	A295	K191	I129	L66	E2
R831	R831	T768	P699	A636	L571	A510		R383	V256	P192		D67	I3
R832	R832		Y700	L637	I572	E511	M448	E384	V257	L193	A132	F68	K4
R833	R833		T701	D638	R573	R513	I449	F385	Y258	V194	D133	L69	R5
R834	R834	E771	R702	Q639	A574	R512	G450	F386	G259	V195	R134	E70	F6
R835	R835	R772	I703	R640	Q575	R514	L451	G387	L260	L196	V135	Y71	G7
R836	R836	L773	H704	P641	A576	A515	L452	R388	I261	L197	L136	R72	R8
R837	R837	L774	T705	R642	P577	R516		S389	A262	K198	V137	L73	I9
R838	R838		R706	V643	V578	K518	L455	Q390	P263	V199	S138	G74	R10
R839	R839	R775	R707	V644	V579	R517	A456	L391	P264	L200	Q139	E75	E11
R840	R840	R776	R708	V645	M580	G519	A457	S392	R265	G201	I140	V12	V12
R841	R841	R777	R709	G646	T581	E520	Y458	Q393	R266	V202	H141	F77	I13
R842	R842	G779	I710	Q647	G582	P521	A459	F394	Y267	G203		F78	P14
R843	R843	E780		R648	L583	V522	R460	K395	D268	Q204	P144	P79	L15
R844	R844	K781	R713	V649	E584	I523	V461	T335	L269	E205	G145	Q80	P16
R845	R845	A782	D714	R650	E585	V524	D462	G337	E271	T206	V146		P17
R846	R846		T715	K651	R586	R525	E463	E338	E272	L207	Y147	R84	L18
			K716	G652	V587	P526	L464	N399	A272	A208	F148	T19	T19
			L717	D653	R588	E527	G465	P400	G273	E209	T149	E20	E20
				L654	R589	E528	F466	L401	R274	E210	P150	L87	L21
				L655	D590	E530	R468	S402	Y275	G212	P152	L88	Q22
				A656		F531	T469	S403	K276				
				D657		M632	P470	F344		A213	R154	T89	S25
					L595	M632	Y471	R405	E279	Y214		Y90	Y26
				A660	A597	D833		H406	K280	G215	P155	Q91	
					E598	V534	R472	R407	L281	E216	G156	A92	A29
				G664	E599	S535	R473	R408	G282	L217	R157	P93	L30
				F665	D600	P336	Y474	R409	L285	V218	Y158	L94	Q31
				R666	G601	K537	V475	I410	L285	E219	I159	Y95	A32
				A667	E602	Q638		S411	S286	G220	A160	D33	D33
				L668	R603	V539	V478	A412	G287	L221	S161	R97	V34
				G669	A604	F540	V479	L413	R288	K222	I162	L98	P35
				K670	K605	S541	T480	G414	T289	D223	I163	Q99	P36
				N671	V606	V542	D481	P415	L290	E224	P164	L100	E37
				V672	D607	N643	E482	G416	A291	S225	L165	I101	K38
				L673	G608			G417	R292	V226	P166	H102	R39
				V674	R609			L418	P293	F227	K187	K103	E40
					R610	I546	Y485	T419	E294	K228	R168	D104	M41
				A675	P548	I547	M486	R420		K229	G169	T105	V42
				L676	V612	P549	T487	E421	E297	R230	P170	G43	G43
				M677	V613	L550	A488	R422	F298	G106	W171	L107	I44
				F679	R614	E551	T489	A423	K299	E232	I172	I108	Q45
				D680	V615	H552	E491	G424	D300	E233	D173	K109	A46
				G681	E616	D553	D492	F425	E501	A234	L174	E10	A47
					L620	E554	R493	D426	F302	I236	V176	D111	F48
				V621	N555	A555	Y494	V427	F303	I236	G106	E112	R49
				E622	R557	N556	T495	R428	L304	R237	V113	F114	E50
				Y623	A558	R557	I496	D429	P305	L238	P178	T51	T51
				F624	L559	A558	A497	V430	T306	F239	N179	F52	F52
				L687	M560	M560	Q498	H431	L307	G180	G116	P53	P53
				L688	L625	R626	A499	R432	R308	V181	H117	I54	I54
				G689	R626	G561	N500	T433	Y309	V182	I118	E55	E55
				I690	R627	S662	T501	H434	L310	G245	P119	E56	E56
				S691	F628	N563	P502	G435	F311	D246	M184	L120	L120
				E692	Y629	M664	L503	Y436	A312		K185	K59	K59
				R693	R630	Q665	E504	R437	L313	R250	V186	G60	G60
				L694	S631	T566	E504		T314	D251	N187	R61	R61
				L695	Q667	Q667	N506	V441	E379	K252	K188		
				S760	A568		R507	E442	P318	A253	R199	L64	L64

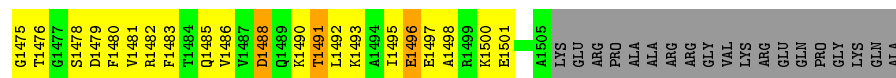


• Molecule 2: DNA-directed RNA polymerase beta chain

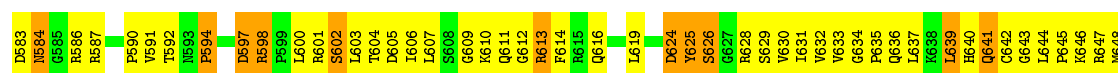
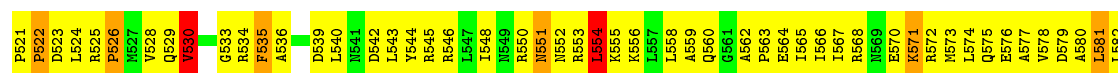
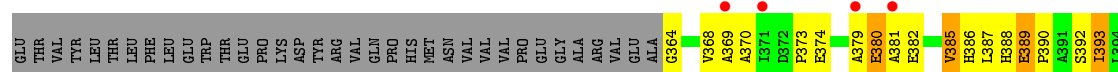
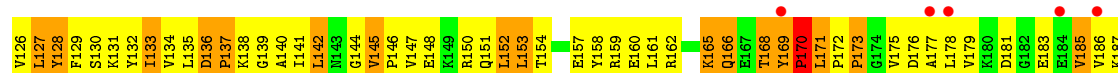
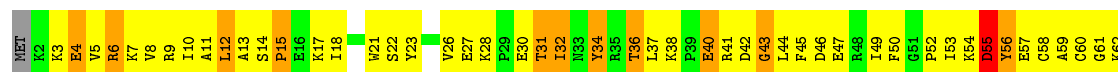


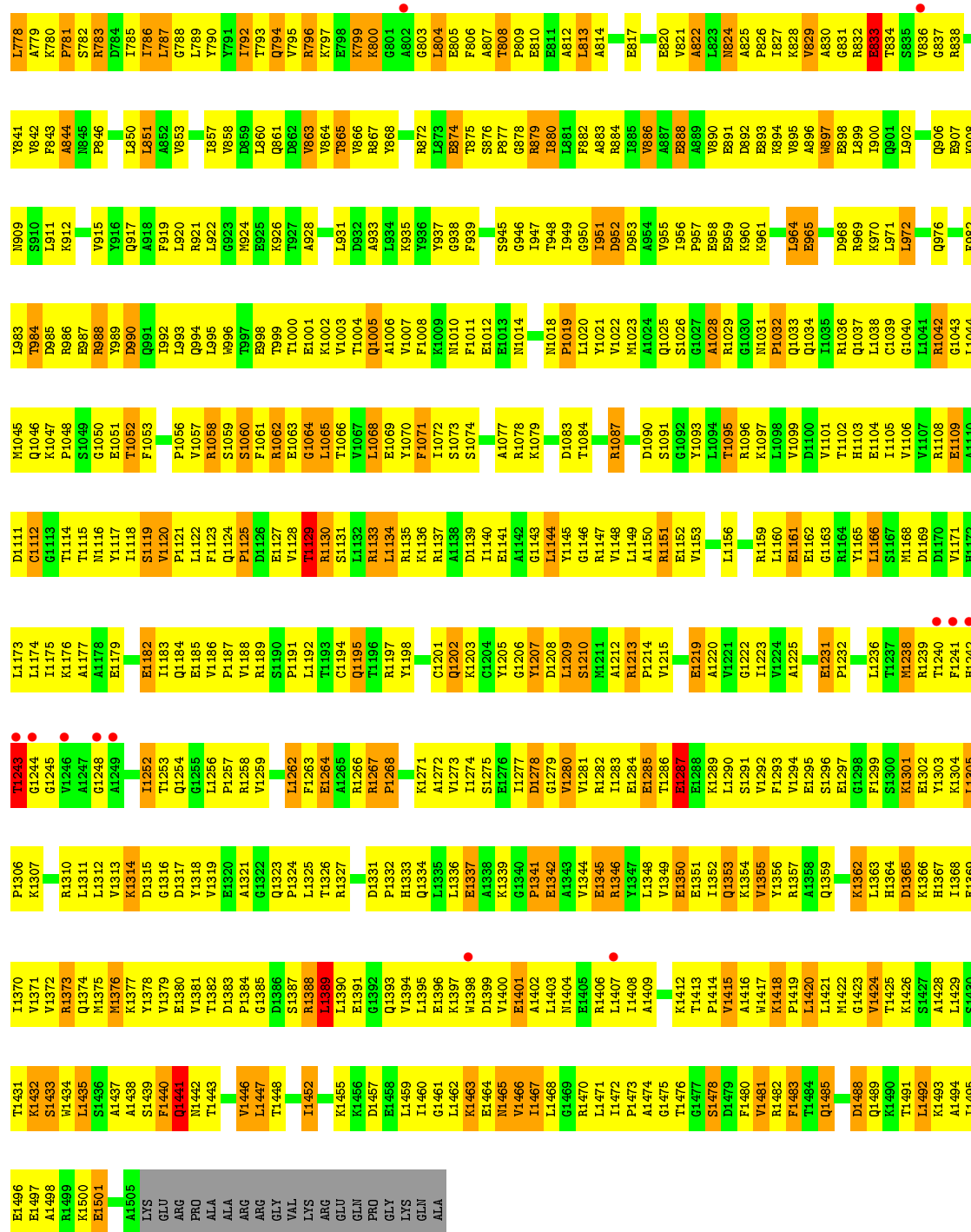


E1350	E1351	E1286	E1285	G1157	L1094	P1032	L964	E998	T834	S774	L708	L644	A580	V517	L452
E1352	E1353	E1287	E1288	R1158	T1095	Q1033	E995	L999	S835	G775	H709	F645	L581	P518	D453
Q1353	Q1354	E1289	E1290	L1160	K1097	L1035	D968	Q901	H836	E776	L711	R646	L582	V519	A454
K1355	K1356	E1161	E1162	L1099	L1160	Q1037	K970	D903	H839	L778	H713	A649	G584	P521	R455
S1291	V1292	G1163	G1164	D1100	V1101	L1038	L971	V904	H840	A779	H714	L650	G585	P522	M456
R1357	E1231	L1165	L1166	T1102	T1101	C1039	L972	P905	H841	F781	A715	E651	R586	D523	A458
A1358	P1232	L1167	L1168	V1103	V1102	G1040	Q973	Q906	H842	S782	F716	L652	A589	L524	A459
Q1359	G1233	L1169	L1170	H1103	H1104	P1041	E974	E907	H843	R783	Q717	F653	P590	R525	E460
E1295	E1296	L1171	L1172	L1105	L1106	L1042	E975	K908	A844	D784	Q718	R654	V591	P526	I461
		T1234	M1168	T1105	T1106	G1043	Q976	N909		H785	W719	P655	V528	M527	Q462
		T1235	D1169	L1106	L1107	L1044	A977	S910	D847	H786	W720	F656	H593	Q529	Q463
		L1236	D1170	V1107	V1108	H1045	Y978	L911	E848	L787	W721	L657	L464	V530	L465
		L1237	H1171	L1108	L1109	Q1046		L912	E849	G788	E722	L658	L466	D531	K466
		T1238	E1172	E1108	E1109	K1047	L983	K912	H850	S789	E723	L659	E467	G532	K467
		L1239	L1173	L1109	L1110	P1048	T984	D913	L851	Y790	Q724	R660	L468	G533	L469
		L1240	L1174	L1111	L1112	S1049	D985	V915	A852	Y791	S725	R661	L469	R534	D469
		F1241	L1175	G1112	G1113	G1050	R986	Y916	H853	H792	W726	E662	L600	P535	
		H1242	K1176	G1114	T1114	E1051	E987	Q917		H793	Q727	E663	R601	A556	
		T1243	A1177	T1115		T1052	R988	Q918	H857	Q794	L728		S602	T537	A472
		G1244	E1178		S1119	F1053		F919	H858	H795		T666	G602	L473	L474
		G1245	E1179	V1120	V1121	E1054	Q991	L920	H859	R796	E722	L668	L603	S538	E474
		V1246	A1180	L1120	L1121	P1056	I992	R921	L860	H797	E733	P668	L604	D539	K475
		G1247	G1181	P1121	L1122	V1057	I993	L922	O861	E798	E734	H669	T605	L540	E476
		A1248	E1182	F1123	F1124	V1058	Q994	G923	H862	K799	A785	H670	L607	D542	L477
		L1249	T1183	F1125	G1126	S1059	H996	H924	H863	R800	F736	R671	S608	L543	E479
		D1251		P1125	P1126	L1067	I997	K926	H864	A801	H737	A672	G609	Y544	
		T1252		P1127	L1127	S1060	T998	T927	H865	A802	A738	R674	R610	R546	K481
		T1253		P1128	L1128	L1062	T999	A928	H866	H804	F740	H675	G612	L547	H483
		L1254		E1189	E1190	E1063	T1000	R929	H867	L804	D741	H676	R613	L548	P484
		T1382		S1190	T1129	G1064	E1001	L930	H869	R806	H742	L677	R614	N549	S485
		P1257		P1191	L1130	L1065	K1002	L931	H870	A807	D743	H678	R615	R550	R486
		R1258		L1192	S1131	T1066	V1003	D932	H871	H808	Q744	R679	Q616	N551	
		V1259		T1193	L1132	V1067	T1004		H872	P809	H745	Q680	N617	N552	R489
		C1194		R1133	R1134	L1068	Q1005	K935	L873	E810	A746	R681	L618	R553	A490
		L1260		L1135	L1136	E1069	A1006		E874	E811	W747	D682	L619	K554	K491
		E1261		R1136	R1137	Y1070	V1007	T940	H875	A812	H748		R622	K555	A492
		L1262		T1196	S876	F1071	F1008	T943	H876	L813	W749		V623	R493	K494
		F1263		Y1198	E1071	S1072	N1009	T944	H877	A814	F750	H688	D624	R495	
		A1265			A1138	S1073	F1011		H879	H816	S752	H689	Y625	V498	
		A1266		G1201	L1139	H1074	F1012	T947	H880	E817	S753	A690	R628	V499	V498
		R1267		Q1202	L1140	H1075	E1011	T948	L881	R818	F754	L691	S629	R500	R500
		P1268		K1203	E1141	G1076	E1013	T949	H882	E820	A755	E692	V630	I566	A501
		K1269		C1204	G1143	H1077	Y1015	G950	A883	E821	Q756	H694	I631	I567	F502
		A1270		G1206	L1144	G1079	P1016	H951	H884	A822	A757		V632	R568	L503
		A1271		Y1207	Y1145			D952	H885	L823		H696	V633	N569	D604
		A1272		D1208	G1146	A1082	P1019	D953		L824	H760		G634	E570	S505
		V1273		L1209	L1147	T1083	L1020	A954	E888	H624	I761		P635	K571	P509
		L1274		S1210	V1148	A1085	T1084	V955	A889	A825	Q762		P636	R572	P509
		T1277		M1211	L1149	L1086	M1023	V956	H890	R826	H763		Q636	R573	E510
		L1278		L1150	L1151	R1087		P957	E891	L827	L764		L637	M573	L574
		G1279		R1152	T1088	H1078	S1026	E958	H892	H828	S765		K638	L574	Q575
		V1280		R1214	E1151	A1089	G1027	E959	E893	H829	A766		L639	Q576	I513
		V1281		V1215	V1153	D1090	A1028	K960	H894	A830	H767		H640	E577	L514
		R1282		V1216	E1154	S1091	L1029	Q961	H895	H831			Q641	A578	E515
		L1283		I1217	E1155	G1092	G1030	K962	A896	R832	L770		P706	V578	L515
		E1284		G1218	L1156	Y1093	M1031	Y963	H897	E833			G643	D579	A516



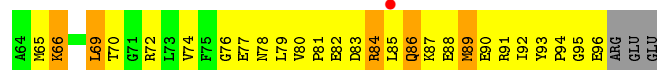
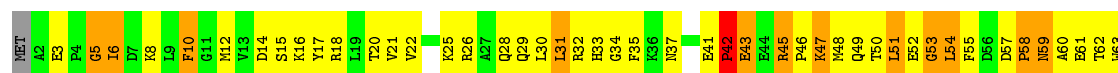
• Molecule 3: DNA-directed RNA polymerase beta' chain



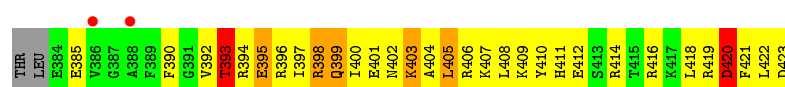
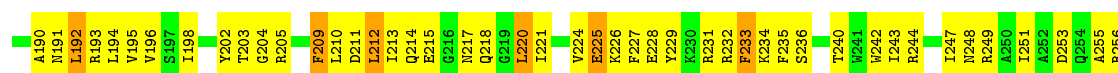




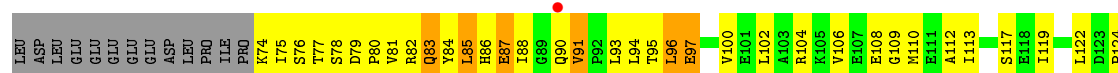
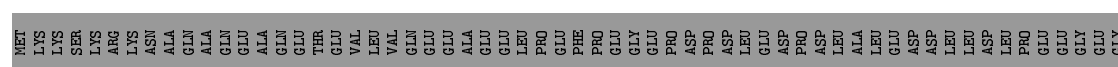
- Molecule 4: RNA polymerase omega chain



- Molecule 5: RNA polymerase sigma factor rpoD



- Molecule 5: RNA polymerase sigma factor rpoD



G391	K325	P261	I188	D125
V392	D326	V262	E189	L126
T393	S327	H263	A190	I127
R394	F328	M264	N191	R128
E395	Y329	V265	L192	E129
R396	G330	E266	R193	V130
I397	D331	T267	L194	V131
R398	F332	I268	V195	A132
Q399	I333	M269	V196	A133
I400	P334	K270	S197	K134
E401	D335	L271	I198	I135
M402	E336	S272	A199	L136
K403	H337	R273	K200	G137
A404	L338	T274	K201	S138
L405		A275	T202	A139
R406	P341	R276	T203	R140
L408	V342	Q277	G204	V141
K409	D343	L278	L207	R142
Y410	A344	Q279	S208	H143
H411	A345	Q280	P209	I144
E412	T346	E281	L210	P145
S413	S348		D211	G146
R414	L349	P286	L212	L147
T415	L350	T287	L213	
R416	S351	Y288	Q214	T150
R417	E352	E289	E215	L151
L418	E353	E290	G216	D152
R419	L354	I291	N217	P153
D420	E355	A292	Q218	K154
F421	K356		G219	T155
L422	A357	K295	L220	V156
D423	L358	G296	I221	
		P297	R232	I159
		G298	Y238	D160
	L361	W299	W242	Q161
	E362	D300	I243	K162
	E363	A301	R244	L163
	R364	K302	Q245	K164
	E365	R303	A246	S165
	A366	V304	I247	L166
	K367	E305	N248	P167
	V368	E306	I251	K168
	L369	T307	A252	E169
	K370	L308	T257	H170
	L371	R309	I260	K171
	R372	I310		R172
	K373	A311		Y173
	G374	Q312		L174
	L375	E313		H175
		P314		I176
	G376	V315		A177
	ARG	S316		R178
	GLU	L317		
	HIS	E318		E181
	THR	T319		A182
	LEU	P320		A183
		I321		R184
	E384	G322		Q185
	E385	D323		H186
		E324		L187
	F390			

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	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) 91.2 (24.85-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.257 0.223 , 0.255	Depositor DCC
R_{free} test set	29386 reflections (5.75%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.085 for h,-h-k,-l 0.085 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	61089	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: ZN, RBT, MG

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	0.79	1/1838 (0.1%)	0.86	2/2498 (0.1%)
1	B	0.73	0/1838	0.82	3/2498 (0.1%)
1	K	0.75	0/1838	0.84	2/2498 (0.1%)
1	L	0.71	1/1838 (0.1%)	0.78	0/2498
2	C	0.81	0/8997	0.88	6/12164 (0.0%)
2	M	0.79	0/8997	0.88	8/12164 (0.1%)
3	D	0.82	0/10975	0.93	22/14836 (0.1%)
3	N	0.80	0/10975	0.91	14/14836 (0.1%)
4	E	0.82	0/783	0.98	1/1054 (0.1%)
4	O	0.84	0/783	0.96	1/1054 (0.1%)
5	F	0.73	0/2812	0.82	2/3781 (0.1%)
5	P	0.71	0/2812	0.80	1/3781 (0.0%)
All	All	0.79	2/54486 (0.0%)	0.88	62/73662 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	5.18	1.44	1.34
1	L	172	SER	N-CA	-5.06	1.36	1.46

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LEU	CA-CB-CG	8.26	134.29	115.30
3	D	199	LEU	CA-CB-CG	-8.08	96.72	115.30
3	N	199	LEU	CA-CB-CG	-7.83	97.28	115.30
3	N	1389	LEU	CA-CB-CG	7.33	132.15	115.30
5	F	361	LEU	CA-CB-CG	7.04	131.49	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	231	0
1	B	1806	0	1861	211	0
1	K	1806	0	1861	199	0
1	L	1806	0	1861	202	0
2	C	8829	0	8933	1201	0
2	M	8829	0	8933	1179	0
3	D	10797	0	10873	1404	0
3	N	10797	0	10873	1285	0
4	E	769	0	775	92	0
4	O	769	0	775	99	0
5	F	2771	0	2844	340	0
5	P	2771	0	2844	315	0
6	A	31	0	0	0	0
6	B	23	0	0	0	0
6	C	81	0	0	0	0
6	D	137	0	0	0	0
6	E	10	0	0	0	0
6	F	31	0	0	0	0
6	K	21	0	0	0	0
6	L	25	0	0	0	0
6	M	69	0	0	0	0
6	N	108	0	0	0	0
6	O	6	0	0	0	0
6	P	20	0	0	0	0
7	C	61	0	61	3	0
7	M	61	0	61	3	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	A	253	0	0	49	0
9	B	307	0	0	49	0
9	C	1000	0	0	202	0
9	D	1418	0	0	282	0
9	E	112	0	0	22	0
9	F	456	0	0	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	213	0	0	34	0
9	L	237	0	0	58	0
9	M	998	0	0	255	0
9	N	1357	0	0	240	0
9	O	117	0	0	26	0
9	P	377	0	0	75	0
All	All	61089	0	54416	6365	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 59.

The worst 5 of 6365 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:42:ARG:HH12	2:C:857:ASP:HB3	1.08	1.12
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.27	1.11
3:N:1045:MET:HG2	3:N:1073:SER:HA	1.35	1.08
2:C:630:ARG:HH21	2:C:705:ILE:HG22	1.18	1.07
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.34	1.06

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%)	204 (90%)	19 (8%)	4 (2%)	8	14
1	B	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	6	10
1	K	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	8	14
1	L	227/315 (72%)	205 (90%)	18 (8%)	4 (2%)	8	14
2	C	1117/1119 (100%)	911 (82%)	153 (14%)	53 (5%)	2	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	1117/1119 (100%)	904 (81%)	168 (15%)	45 (4%)	3	3
3	D	1388/1524 (91%)	1112 (80%)	202 (15%)	74 (5%)	2	2
3	N	1388/1524 (91%)	1118 (80%)	195 (14%)	75 (5%)	2	2
4	E	93/99 (94%)	74 (80%)	15 (16%)	4 (4%)	2	3
4	O	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	2	3
5	F	341/423 (81%)	286 (84%)	40 (12%)	15 (4%)	2	3
5	P	341/423 (81%)	290 (85%)	37 (11%)	14 (4%)	3	3
All	All	6786/7590 (89%)	5585 (82%)	900 (13%)	301 (4%)	2	3

5 of 301 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	156	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	148 (73%)	54 (27%)	0	0
1	B	202/273 (74%)	164 (81%)	38 (19%)	1	2
1	K	202/273 (74%)	144 (71%)	58 (29%)	0	0
1	L	202/273 (74%)	159 (79%)	43 (21%)	1	2
2	C	941/941 (100%)	738 (78%)	203 (22%)	1	1
2	M	941/941 (100%)	737 (78%)	204 (22%)	1	1
3	D	1123/1279 (88%)	841 (75%)	282 (25%)	0	1
3	N	1123/1279 (88%)	865 (77%)	258 (23%)	1	1
4	E	83/87 (95%)	67 (81%)	16 (19%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	83/87 (95%)	61 (74%)	22 (26%)	0	0
5	F	295/370 (80%)	235 (80%)	60 (20%)	1	2
5	P	295/370 (80%)	247 (84%)	48 (16%)	2	4
All	All	5692/6446 (88%)	4406 (77%)	1286 (23%)	1	1

5 of 1286 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	33	HIS
1	L	29	GLU
3	N	1396	GLU
5	F	87	GLU
1	K	2	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 174 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	277	GLN
1	L	212	ASN
3	N	1374	GLN
1	K	63	HIS
1	K	227	ASN

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 568 ligands modelled in this entry, 566 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	RBT	C	8001	6	61,66,66	2.90	22 (36%)	86,101,101	1.87	19 (22%)
7	RBT	M	8002	-	61,66,66	2.86	24 (39%)	86,101,101	1.95	18 (20%)

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	RBT	C	8001	6	-	18/59/116/116	0/5/6/6
7	RBT	M	8002	-	-	16/59/116/116	0/5/6/6

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	8001	RBT	C9-C8	8.84	1.58	1.41
7	M	8002	RBT	C9-C8	8.54	1.57	1.41
7	M	8002	RBT	C8-C7	7.03	1.54	1.40
7	C	8001	RBT	C8-C7	6.71	1.54	1.40
7	C	8001	RBT	C5-C6	6.59	1.48	1.39

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RBT	C42-C40-C38	7.37	122.58	112.64
7	C	8001	RBT	C42-C40-C38	7.35	122.55	112.64
7	M	8002	RBT	C41-C39-C38	7.18	122.32	112.64
7	C	8001	RBT	C41-C39-C38	7.09	122.20	112.64
7	M	8002	RBT	C39-C38-N3	-5.00	106.87	111.42

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

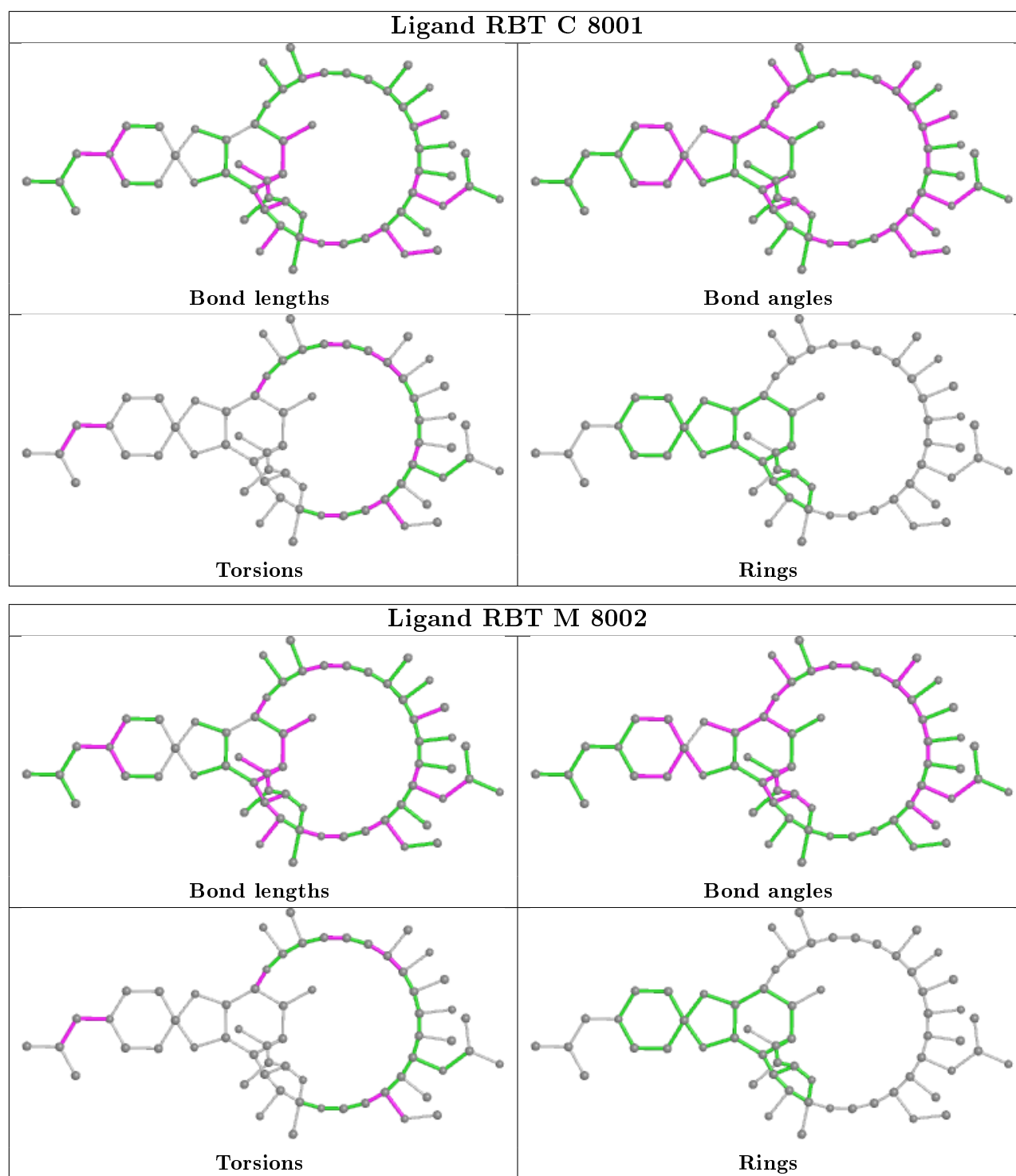
Mol	Chain	Res	Type	Atoms
7	C	8001	RBT	C1-C2-N1-C15
7	C	8001	RBT	C3-C2-N1-C15
7	C	8001	RBT	C16-C17-C18-C19
7	C	8001	RBT	C26-C27-C28-C29
7	C	8001	RBT	C26-C27-O6-C37

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	8001	RBT	3	0
7	M	8002	RBT	3	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/315 (72%)	-0.40	1 (0%) 92 93	29, 60, 84, 110	0
1	B	229/315 (72%)	-0.13	13 (5%) 23 25	44, 89, 114, 118	0
1	K	229/315 (72%)	-0.40	2 (0%) 84 86	33, 58, 89, 120	0
1	L	229/315 (72%)	-0.25	8 (3%) 44 47	49, 89, 109, 119	0
2	C	1119/1119 (100%)	-0.39	10 (0%) 84 86	14, 74, 102, 117	0
2	M	1119/1119 (100%)	-0.39	12 (1%) 80 82	19, 71, 103, 119	0
3	D	1392/1524 (91%)	-0.36	17 (1%) 79 80	19, 62, 107, 125	0
3	N	1392/1524 (91%)	-0.36	24 (1%) 70 72	23, 65, 107, 131	0
4	E	95/99 (95%)	-0.40	2 (2%) 63 66	41, 77, 107, 120	0
4	O	95/99 (95%)	-0.44	1 (1%) 80 82	33, 72, 94, 103	0
5	F	345/423 (81%)	-0.39	7 (2%) 65 68	46, 81, 104, 118	0
5	P	345/423 (81%)	-0.30	8 (2%) 60 63	53, 81, 108, 123	0
All	All	6818/7590 (89%)	-0.36	105 (1%) 73 75	14, 70, 105, 131	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	145	PRO	5.8
3	N	1243	THR	5.8
2	M	269	LEU	5.2
3	D	1244	GLY	4.8
3	D	1240	THR	4.8

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	B	9163	1/1	0.92	0.06	44,44,44,44	0
6	MG	N	9538	1/1	0.92	0.10	42,42,42,42	0
6	MG	L	9258	1/1	0.94	0.10	47,47,47,47	0
6	MG	M	9364	1/1	0.94	0.08	37,37,37,37	0
6	MG	F	9410	1/1	0.94	0.12	47,47,47,47	0
6	MG	N	9354	1/1	0.95	0.07	42,42,42,42	0
6	MG	N	9235	1/1	0.95	0.12	63,63,63,63	0
6	MG	C	9068	1/1	0.95	0.12	37,37,37,37	0
8	ZN	D	7058	1/1	0.95	0.07	100,100,100,100	0
6	MG	B	9199	1/1	0.95	0.10	52,52,52,52	0
6	MG	C	9398	1/1	0.95	0.10	44,44,44,44	0
6	MG	N	9250	1/1	0.95	0.16	61,61,61,61	0
6	MG	N	9503	1/1	0.96	0.12	52,52,52,52	0
6	MG	N	9349	1/1	0.96	0.06	37,37,37,37	0
6	MG	M	9261	1/1	0.96	0.10	45,45,45,45	0
6	MG	O	9359	1/1	0.96	0.08	57,57,57,57	0
6	MG	P	9322	1/1	0.96	0.12	43,43,43,43	0
6	MG	A	9062	1/1	0.96	0.11	45,45,45,45	0
6	MG	D	9084	1/1	0.96	0.10	47,47,47,47	0
6	MG	M	9383	1/1	0.96	0.09	46,46,46,46	0
6	MG	K	9257	1/1	0.96	0.12	57,57,57,57	0
6	MG	D	9147	1/1	0.96	0.09	40,40,40,40	0
6	MG	D	9520	1/1	0.96	0.14	46,46,46,46	0
6	MG	D	9155	1/1	0.96	0.12	56,56,56,56	0
6	MG	C	9190	1/1	0.96	0.07	40,40,40,40	0
6	MG	A	9514	1/1	0.96	0.12	42,42,42,42	0
7	RBT	M	8002	61/61	0.96	0.18	28,39,48,54	0
6	MG	F	9048	1/1	0.96	0.16	50,50,50,50	0
6	MG	D	9111	1/1	0.96	0.09	43,43,43,43	0
6	MG	N	9474	1/1	0.96	0.13	56,56,56,56	0
6	MG	M	9255	1/1	0.96	0.13	58,58,58,58	0
6	MG	C	9177	1/1	0.96	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	N	9253	1/1	0.96	0.08	39,39,39,39	0
6	MG	A	9413	1/1	0.96	0.10	46,46,46,46	0
6	MG	M	9267	1/1	0.96	0.12	41,41,41,41	0
6	MG	M	9220	1/1	0.96	0.13	45,45,45,45	0
6	MG	C	9399	1/1	0.96	0.10	43,43,43,43	0
6	MG	K	9351	1/1	0.97	0.09	37,37,37,37	0
6	MG	M	9334	1/1	0.97	0.09	44,44,44,44	0
6	MG	N	9358	1/1	0.97	0.12	48,48,48,48	0
6	MG	N	9230	1/1	0.97	0.09	40,40,40,40	0
6	MG	E	9467	1/1	0.97	0.12	52,52,52,52	0
6	MG	M	9325	1/1	0.97	0.10	44,44,44,44	0
6	MG	A	9430	1/1	0.97	0.11	35,35,35,35	0
6	MG	N	9539	1/1	0.97	0.10	57,57,57,57	0
6	MG	D	9095	1/1	0.97	0.06	40,40,40,40	0
6	MG	D	9548	1/1	0.97	0.12	51,51,51,51	0
6	MG	D	9543	1/1	0.97	0.12	46,46,46,46	0
6	MG	D	9423	1/1	0.97	0.09	44,44,44,44	0
6	MG	D	9042	1/1	0.97	0.12	47,47,47,47	0
6	MG	P	9304	1/1	0.97	0.10	57,57,57,57	0
6	MG	M	9259	1/1	0.97	0.17	57,57,57,57	0
6	MG	C	9414	1/1	0.97	0.07	41,41,41,41	0
6	MG	N	9486	1/1	0.97	0.09	44,44,44,44	0
6	MG	D	9523	1/1	0.97	0.11	41,41,41,41	0
6	MG	N	9208	1/1	0.97	0.12	35,35,35,35	0
6	MG	C	9455	1/1	0.97	0.12	61,61,61,61	0
6	MG	N	9244	1/1	0.97	0.08	37,37,37,37	0
6	MG	A	9107	1/1	0.97	0.07	40,40,40,40	0
6	MG	A	9145	1/1	0.97	0.11	45,45,45,45	0
6	MG	D	9518	1/1	0.97	0.11	55,55,55,55	0
6	MG	M	9312	1/1	0.97	0.10	37,37,37,37	0
6	MG	K	9363	1/1	0.97	0.09	47,47,47,47	0
6	MG	C	9081	1/1	0.97	0.13	52,52,52,52	0
6	MG	N	9327	1/1	0.97	0.11	54,54,54,54	0
6	MG	L	9249	1/1	0.97	0.07	51,51,51,51	0
7	RBT	C	8001	61/61	0.97	0.19	25,37,42,48	0
6	MG	D	9096	1/1	0.97	0.14	43,43,43,43	0
6	MG	A	9559	1/1	0.97	0.12	45,45,45,45	0
6	MG	O	9209	1/1	0.97	0.11	37,37,37,37	0
6	MG	N	9246	1/1	0.97	0.13	49,49,49,49	0
6	MG	N	9555	1/1	0.97	0.11	56,56,56,56	0
6	MG	N	9247	1/1	0.97	0.08	29,29,29,29	0
6	MG	C	9023	1/1	0.97	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	A	9050	1/1	0.97	0.10	41,41,41,41	0
6	MG	D	9066	1/1	0.97	0.11	49,49,49,49	0
6	MG	N	9508	1/1	0.97	0.11	41,41,41,41	0
6	MG	L	9346	1/1	0.97	0.14	52,52,52,52	0
6	MG	C	9047	1/1	0.97	0.06	47,47,47,47	0
6	MG	L	9483	1/1	0.97	0.15	44,44,44,44	0
6	MG	P	9284	1/1	0.97	0.10	51,51,51,51	0
6	MG	F	9010	1/1	0.97	0.17	57,57,57,57	0
6	MG	C	9156	1/1	0.97	0.12	43,43,43,43	0
6	MG	D	9152	1/1	0.97	0.11	32,32,32,32	0
6	MG	M	9348	1/1	0.97	0.11	63,63,63,63	0
6	MG	M	9473	1/1	0.97	0.11	42,42,42,42	0
6	MG	D	9026	1/1	0.97	0.12	37,37,37,37	0
6	MG	N	9551	1/1	0.97	0.08	40,40,40,40	0
6	MG	E	9184	1/1	0.97	0.16	48,48,48,48	0
6	MG	M	9332	1/1	0.97	0.13	54,54,54,54	0
6	MG	N	9554	1/1	0.97	0.11	45,45,45,45	0
6	MG	C	9192	1/1	0.97	0.10	55,55,55,55	0
6	MG	D	9067	1/1	0.97	0.12	49,49,49,49	0
6	MG	N	9381	1/1	0.97	0.07	35,35,35,35	0
6	MG	F	9461	1/1	0.97	0.12	52,52,52,52	0
6	MG	C	9549	1/1	0.98	0.11	48,48,48,48	0
6	MG	N	9490	1/1	0.98	0.12	41,41,41,41	0
6	MG	N	9498	1/1	0.98	0.09	45,45,45,45	0
6	MG	N	9207	1/1	0.98	0.10	30,30,30,30	0
6	MG	C	9007	1/1	0.98	0.11	34,34,34,34	0
6	MG	D	9172	1/1	0.98	0.10	35,35,35,35	0
6	MG	D	9401	1/1	0.98	0.12	40,40,40,40	0
6	MG	M	9283	1/1	0.98	0.14	35,35,35,35	0
6	MG	D	9202	1/1	0.98	0.18	61,61,61,61	0
6	MG	N	9342	1/1	0.98	0.07	48,48,48,48	0
6	MG	D	9445	1/1	0.98	0.13	48,48,48,48	0
6	MG	P	9558	1/1	0.98	0.09	44,44,44,44	0
6	MG	A	9097	1/1	0.98	0.09	41,41,41,41	0
6	MG	D	9123	1/1	0.98	0.14	37,37,37,37	0
6	MG	M	9347	1/1	0.98	0.11	37,37,37,37	0
6	MG	P	9541	1/1	0.98	0.10	44,44,44,44	0
6	MG	N	9365	1/1	0.98	0.12	43,43,43,43	0
6	MG	D	9466	1/1	0.98	0.10	57,57,57,57	0
6	MG	D	9168	1/1	0.98	0.06	38,38,38,38	0
6	MG	C	9546	1/1	0.98	0.06	49,49,49,49	0
6	MG	N	9314	1/1	0.98	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	C	9124	1/1	0.98	0.08	33,33,33,33	0
6	MG	N	9301	1/1	0.98	0.08	50,50,50,50	0
6	MG	D	9003	1/1	0.98	0.06	43,43,43,43	0
6	MG	M	9377	1/1	0.98	0.12	39,39,39,39	0
6	MG	A	9001	1/1	0.98	0.18	26,26,26,26	0
6	MG	N	9295	1/1	0.98	0.05	48,48,48,48	0
6	MG	N	9504	1/1	0.98	0.10	32,32,32,32	0
6	MG	D	9002	1/1	0.98	0.16	29,29,29,29	0
6	MG	E	9131	1/1	0.98	0.08	47,47,47,47	0
6	MG	N	9297	1/1	0.98	0.13	48,48,48,48	0
6	MG	B	9092	1/1	0.98	0.11	50,50,50,50	0
6	MG	L	9505	1/1	0.98	0.10	58,58,58,58	0
6	MG	A	9078	1/1	0.98	0.13	34,34,34,34	0
6	MG	D	9424	1/1	0.98	0.14	50,50,50,50	0
6	MG	N	9313	1/1	0.98	0.09	39,39,39,39	0
6	MG	M	9478	1/1	0.98	0.06	35,35,35,35	0
6	MG	D	9449	1/1	0.98	0.07	29,29,29,29	0
6	MG	M	9219	1/1	0.98	0.10	39,39,39,39	0
6	MG	B	9101	1/1	0.98	0.08	40,40,40,40	0
6	MG	N	9242	1/1	0.98	0.12	36,36,36,36	0
6	MG	C	9515	1/1	0.98	0.08	41,41,41,41	0
6	MG	D	9397	1/1	0.98	0.12	31,31,31,31	0
6	MG	N	9319	1/1	0.98	0.11	41,41,41,41	0
6	MG	C	9457	1/1	0.98	0.10	40,40,40,40	0
6	MG	M	9233	1/1	0.98	0.15	38,38,38,38	0
6	MG	C	9157	1/1	0.98	0.16	44,44,44,44	0
6	MG	B	9395	1/1	0.98	0.11	56,56,56,56	0
6	MG	C	9063	1/1	0.98	0.10	32,32,32,32	0
6	MG	P	9317	1/1	0.98	0.18	53,53,53,53	0
6	MG	D	9012	1/1	0.98	0.06	39,39,39,39	0
6	MG	B	9389	1/1	0.98	0.10	37,37,37,37	0
6	MG	N	9310	1/1	0.98	0.08	36,36,36,36	0
6	MG	D	9015	1/1	0.98	0.12	37,37,37,37	0
6	MG	K	9553	1/1	0.98	0.09	50,50,50,50	0
6	MG	D	9039	1/1	0.98	0.11	40,40,40,40	0
6	MG	E	9151	1/1	0.98	0.05	48,48,48,48	0
6	MG	C	9396	1/1	0.98	0.14	57,57,57,57	0
6	MG	K	9214	1/1	0.98	0.20	31,31,31,31	0
6	MG	N	9228	1/1	0.98	0.08	49,49,49,49	0
6	MG	D	9447	1/1	0.98	0.10	50,50,50,50	0
6	MG	M	9293	1/1	0.98	0.11	43,43,43,43	0
6	MG	N	9526	1/1	0.98	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9112	1/1	0.98	0.13	39,39,39,39	0
6	MG	F	9153	1/1	0.98	0.07	39,39,39,39	0
6	MG	F	9429	1/1	0.98	0.12	57,57,57,57	0
6	MG	D	9059	1/1	0.98	0.10	40,40,40,40	0
6	MG	D	9099	1/1	0.98	0.07	38,38,38,38	0
6	MG	D	9516	1/1	0.98	0.05	51,51,51,51	0
6	MG	D	9140	1/1	0.98	0.13	43,43,43,43	0
6	MG	C	9014	1/1	0.98	0.14	45,45,45,45	0
6	MG	N	9281	1/1	0.98	0.09	50,50,50,50	0
6	MG	C	9458	1/1	0.98	0.09	38,38,38,38	0
6	MG	A	9102	1/1	0.98	0.09	38,38,38,38	0
6	MG	K	9344	1/1	0.98	0.12	55,55,55,55	0
6	MG	C	9191	1/1	0.98	0.13	44,44,44,44	0
6	MG	N	9534	1/1	0.98	0.09	54,54,54,54	0
6	MG	L	9213	1/1	0.98	0.23	49,49,49,49	0
6	MG	C	9141	1/1	0.98	0.12	45,45,45,45	0
6	MG	N	9499	1/1	0.98	0.08	38,38,38,38	0
6	MG	M	9290	1/1	0.98	0.12	48,48,48,48	0
6	MG	M	9285	1/1	0.98	0.13	43,43,43,43	0
6	MG	N	9262	1/1	0.98	0.14	49,49,49,49	0
6	MG	D	9432	1/1	0.98	0.10	47,47,47,47	0
6	MG	M	9211	1/1	0.98	0.10	28,28,28,28	0
6	MG	D	9019	1/1	0.98	0.15	35,35,35,35	0
6	MG	M	9540	1/1	0.98	0.16	63,63,63,63	0
6	MG	D	9110	1/1	0.98	0.13	38,38,38,38	0
6	MG	N	9315	1/1	0.98	0.11	41,41,41,41	0
6	MG	N	9245	1/1	0.98	0.12	28,28,28,28	0
6	MG	M	9276	1/1	0.98	0.14	54,54,54,54	0
6	MG	L	9311	1/1	0.98	0.07	33,33,33,33	0
6	MG	B	9419	1/1	0.98	0.11	46,46,46,46	0
6	MG	B	9079	1/1	0.98	0.11	28,28,28,28	0
6	MG	M	9485	1/1	0.98	0.06	42,42,42,42	0
6	MG	D	9041	1/1	0.98	0.10	32,32,32,32	0
6	MG	C	9083	1/1	0.98	0.11	48,48,48,48	0
6	MG	L	9378	1/1	0.98	0.14	47,47,47,47	0
6	MG	A	9522	1/1	0.98	0.11	57,57,57,57	0
6	MG	D	9009	1/1	0.98	0.12	53,53,53,53	0
6	MG	D	9057	1/1	0.98	0.11	33,33,33,33	0
6	MG	B	9427	1/1	0.98	0.11	42,42,42,42	0
6	MG	M	9557	1/1	0.98	0.09	54,54,54,54	0
6	MG	D	9036	1/1	0.98	0.13	41,41,41,41	0
6	MG	C	9076	1/1	0.98	0.11	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	N	9266	1/1	0.98	0.08	36,36,36,36	0
6	MG	D	9104	1/1	0.98	0.09	35,35,35,35	0
6	MG	L	9532	1/1	0.98	0.08	51,51,51,51	0
6	MG	D	9451	1/1	0.98	0.09	37,37,37,37	0
6	MG	N	9341	1/1	0.98	0.13	38,38,38,38	0
6	MG	N	9506	1/1	0.98	0.10	56,56,56,56	0
6	MG	D	9034	1/1	0.98	0.16	37,37,37,37	0
6	MG	O	9362	1/1	0.98	0.04	49,49,49,49	0
6	MG	F	9206	1/1	0.98	0.12	33,33,33,33	0
6	MG	B	9148	1/1	0.98	0.15	54,54,54,54	0
6	MG	K	9217	1/1	0.98	0.06	36,36,36,36	0
6	MG	M	9229	1/1	0.98	0.09	35,35,35,35	0
6	MG	N	9338	1/1	0.98	0.12	42,42,42,42	0
6	MG	D	9055	1/1	0.98	0.09	51,51,51,51	0
6	MG	K	9484	1/1	0.98	0.11	30,30,30,30	0
6	MG	C	9183	1/1	0.98	0.16	44,44,44,44	0
6	MG	N	9529	1/1	0.98	0.08	55,55,55,55	0
6	MG	D	9108	1/1	0.98	0.11	51,51,51,51	0
6	MG	F	9167	1/1	0.98	0.12	59,59,59,59	0
6	MG	M	9488	1/1	0.98	0.12	42,42,42,42	0
6	MG	A	9109	1/1	0.98	0.09	33,33,33,33	0
6	MG	M	9350	1/1	0.98	0.09	37,37,37,37	0
6	MG	F	9448	1/1	0.98	0.10	38,38,38,38	0
6	MG	N	9292	1/1	0.98	0.16	52,52,52,52	0
6	MG	F	9437	1/1	0.98	0.09	47,47,47,47	0
6	MG	M	9309	1/1	0.98	0.15	35,35,35,35	0
6	MG	C	9406	1/1	0.98	0.10	47,47,47,47	0
6	MG	M	9227	1/1	0.98	0.10	44,44,44,44	0
6	MG	L	9556	1/1	0.98	0.09	58,58,58,58	0
6	MG	K	9367	1/1	0.98	0.09	38,38,38,38	0
6	MG	D	9441	1/1	0.98	0.10	46,46,46,46	0
6	MG	B	9150	1/1	0.98	0.10	43,43,43,43	0
6	MG	M	9243	1/1	0.98	0.11	45,45,45,45	0
6	MG	M	9298	1/1	0.98	0.12	43,43,43,43	0
6	MG	N	9232	1/1	0.98	0.10	33,33,33,33	0
6	MG	A	9165	1/1	0.98	0.11	65,65,65,65	0
6	MG	N	9288	1/1	0.98	0.10	33,33,33,33	0
6	MG	D	9517	1/1	0.99	0.09	45,45,45,45	0
6	MG	C	9521	1/1	0.99	0.12	45,45,45,45	0
6	MG	F	9072	1/1	0.99	0.07	40,40,40,40	0
6	MG	D	9446	1/1	0.99	0.10	36,36,36,36	0
6	MG	N	9256	1/1	0.99	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	O	9355	1/1	0.99	0.14	36,36,36,36	0
6	MG	B	9137	1/1	0.99	0.09	35,35,35,35	0
6	MG	F	9135	1/1	0.99	0.14	42,42,42,42	0
6	MG	N	9379	1/1	0.99	0.06	56,56,56,56	0
6	MG	N	9475	1/1	0.99	0.07	43,43,43,43	0
6	MG	C	9088	1/1	0.99	0.12	36,36,36,36	0
6	MG	M	9340	1/1	0.99	0.10	43,43,43,43	0
6	MG	N	9280	1/1	0.99	0.09	34,34,34,34	0
6	MG	N	9218	1/1	0.99	0.12	32,32,32,32	0
6	MG	C	9462	1/1	0.99	0.12	50,50,50,50	0
6	MG	D	9454	1/1	0.99	0.08	42,42,42,42	0
6	MG	E	9438	1/1	0.99	0.10	38,38,38,38	0
6	MG	K	9265	1/1	0.99	0.13	37,37,37,37	0
6	MG	F	9054	1/1	0.99	0.07	37,37,37,37	0
6	MG	F	9197	1/1	0.99	0.10	39,39,39,39	0
6	MG	C	9422	1/1	0.99	0.13	41,41,41,41	0
6	MG	B	9180	1/1	0.99	0.09	36,36,36,36	0
6	MG	C	9029	1/1	0.99	0.12	36,36,36,36	0
6	MG	N	9273	1/1	0.99	0.17	30,30,30,30	0
6	MG	P	9274	1/1	0.99	0.11	45,45,45,45	0
6	MG	F	9435	1/1	0.99	0.08	40,40,40,40	0
6	MG	N	9376	1/1	0.99	0.13	31,31,31,31	0
6	MG	N	9226	1/1	0.99	0.07	30,30,30,30	0
6	MG	C	9011	1/1	0.99	0.10	39,39,39,39	0
6	MG	N	9320	1/1	0.99	0.11	41,41,41,41	0
6	MG	N	9248	1/1	0.99	0.06	47,47,47,47	0
6	MG	E	9186	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9154	1/1	0.99	0.12	31,31,31,31	0
6	MG	C	9545	1/1	0.99	0.10	45,45,45,45	0
6	MG	D	9169	1/1	0.99	0.12	45,45,45,45	0
6	MG	L	9471	1/1	0.99	0.10	33,33,33,33	0
6	MG	M	9384	1/1	0.99	0.10	35,35,35,35	0
6	MG	P	9333	1/1	0.99	0.07	28,28,28,28	0
6	MG	D	9189	1/1	0.99	0.10	34,34,34,34	0
6	MG	M	9336	1/1	0.99	0.10	31,31,31,31	0
6	MG	M	9287	1/1	0.99	0.08	36,36,36,36	0
6	MG	D	9463	1/1	0.99	0.11	32,32,32,32	0
6	MG	F	9407	1/1	0.99	0.07	32,32,32,32	0
6	MG	D	9122	1/1	0.99	0.10	31,31,31,31	0
6	MG	D	9119	1/1	0.99	0.09	44,44,44,44	0
6	MG	B	9103	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9077	1/1	0.99	0.10	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	C	9439	1/1	0.99	0.10	35,35,35,35	0
6	MG	N	9356	1/1	0.99	0.14	29,29,29,29	0
6	MG	P	9326	1/1	0.99	0.08	39,39,39,39	0
6	MG	M	9321	1/1	0.99	0.13	40,40,40,40	0
6	MG	P	9502	1/1	0.99	0.07	43,43,43,43	0
6	MG	D	9519	1/1	0.99	0.12	55,55,55,55	0
6	MG	A	9560	1/1	0.99	0.13	49,49,49,49	0
6	MG	C	9044	1/1	0.99	0.08	37,37,37,37	0
6	MG	L	9300	1/1	0.99	0.07	58,58,58,58	0
6	MG	D	9038	1/1	0.99	0.11	35,35,35,35	0
6	MG	C	9196	1/1	0.99	0.13	30,30,30,30	0
6	MG	C	9205	1/1	0.99	0.12	53,53,53,53	0
6	MG	C	9025	1/1	0.99	0.10	39,39,39,39	0
6	MG	D	9393	1/1	0.99	0.13	35,35,35,35	0
6	MG	F	9164	1/1	0.99	0.11	29,29,29,29	0
6	MG	B	9146	1/1	0.99	0.09	44,44,44,44	0
6	MG	N	9335	1/1	0.99	0.10	33,33,33,33	0
6	MG	B	9512	1/1	0.99	0.20	53,53,53,53	0
6	MG	E	9115	1/1	0.99	0.08	39,39,39,39	0
6	MG	C	9121	1/1	0.99	0.15	43,43,43,43	0
6	MG	D	9175	1/1	0.99	0.09	40,40,40,40	0
6	MG	F	9053	1/1	0.99	0.10	34,34,34,34	0
6	MG	D	9159	1/1	0.99	0.11	35,35,35,35	0
6	MG	P	9329	1/1	0.99	0.07	46,46,46,46	0
6	MG	B	9391	1/1	0.99	0.12	27,27,27,27	0
6	MG	D	9100	1/1	0.99	0.07	31,31,31,31	0
6	MG	C	9415	1/1	0.99	0.11	38,38,38,38	0
6	MG	M	9251	1/1	0.99	0.13	33,33,33,33	0
6	MG	D	9021	1/1	0.99	0.12	34,34,34,34	0
6	MG	N	9375	1/1	0.99	0.10	43,43,43,43	0
6	MG	A	9178	1/1	0.99	0.09	28,28,28,28	0
6	MG	N	9307	1/1	0.99	0.09	38,38,38,38	0
6	MG	A	9411	1/1	0.99	0.10	31,31,31,31	0
6	MG	M	9481	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9561	1/1	0.99	0.06	38,38,38,38	0
8	ZN	N	7113	1/1	0.99	0.11	79,79,79,79	0
6	MG	D	9416	1/1	0.99	0.09	48,48,48,48	0
6	MG	D	9136	1/1	0.99	0.10	41,41,41,41	0
6	MG	D	9073	1/1	0.99	0.15	38,38,38,38	0
6	MG	N	9289	1/1	0.99	0.09	35,35,35,35	0
6	MG	C	9144	1/1	0.99	0.09	39,39,39,39	0
6	MG	D	9166	1/1	0.99	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9049	1/1	0.99	0.14	31,31,31,31	0
6	MG	D	9203	1/1	0.99	0.09	46,46,46,46	0
6	MG	N	9368	1/1	0.99	0.09	41,41,41,41	0
6	MG	A	9139	1/1	0.99	0.10	35,35,35,35	0
6	MG	C	9074	1/1	0.99	0.13	30,30,30,30	0
6	MG	N	9509	1/1	0.99	0.11	31,31,31,31	0
6	MG	D	9443	1/1	0.99	0.07	47,47,47,47	0
6	MG	C	9071	1/1	0.99	0.13	39,39,39,39	0
6	MG	C	9456	1/1	0.99	0.07	37,37,37,37	0
6	MG	C	9420	1/1	0.99	0.07	37,37,37,37	0
6	MG	M	9366	1/1	0.99	0.10	41,41,41,41	0
6	MG	C	9020	1/1	0.99	0.14	28,28,28,28	0
6	MG	E	9187	1/1	0.99	0.12	39,39,39,39	0
6	MG	A	9018	1/1	0.99	0.14	31,31,31,31	0
6	MG	D	9065	1/1	0.99	0.14	44,44,44,44	0
6	MG	L	9272	1/1	0.99	0.10	29,29,29,29	0
6	MG	D	9562	1/1	0.99	0.17	49,49,49,49	0
6	MG	M	9252	1/1	0.99	0.12	37,37,37,37	0
6	MG	M	9472	1/1	0.99	0.06	51,51,51,51	0
6	MG	D	9417	1/1	0.99	0.11	35,35,35,35	0
6	MG	P	9296	1/1	0.99	0.07	42,42,42,42	0
6	MG	D	9129	1/1	0.99	0.09	38,38,38,38	0
6	MG	F	9032	1/1	0.99	0.09	32,32,32,32	0
6	MG	C	9428	1/1	0.99	0.12	42,42,42,42	0
6	MG	D	9094	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9090	1/1	0.99	0.11	48,48,48,48	0
6	MG	F	9035	1/1	0.99	0.10	40,40,40,40	0
6	MG	A	9394	1/1	0.99	0.10	46,46,46,46	0
6	MG	D	9544	1/1	0.99	0.11	49,49,49,49	0
6	MG	L	9271	1/1	0.99	0.09	39,39,39,39	0
6	MG	B	9033	1/1	0.99	0.10	44,44,44,44	0
6	MG	K	9496	1/1	0.99	0.09	42,42,42,42	0
6	MG	N	9316	1/1	0.99	0.09	32,32,32,32	0
6	MG	C	9028	1/1	0.99	0.07	41,41,41,41	0
6	MG	N	9476	1/1	0.99	0.06	44,44,44,44	0
6	MG	M	9222	1/1	0.99	0.09	33,33,33,33	0
6	MG	M	9323	1/1	0.99	0.10	37,37,37,37	0
6	MG	L	9236	1/1	0.99	0.08	41,41,41,41	0
6	MG	F	9045	1/1	0.99	0.10	40,40,40,40	0
6	MG	D	9016	1/1	0.99	0.07	38,38,38,38	0
6	MG	P	9536	1/1	0.99	0.07	41,41,41,41	0
6	MG	M	9361	1/1	0.99	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	N	9282	1/1	0.99	0.06	38,38,38,38	0
6	MG	M	9500	1/1	0.99	0.09	46,46,46,46	0
6	MG	M	9268	1/1	0.99	0.11	37,37,37,37	0
6	MG	M	9385	1/1	0.99	0.10	29,29,29,29	0
6	MG	C	9130	1/1	0.99	0.14	42,42,42,42	0
6	MG	L	9345	1/1	0.99	0.12	42,42,42,42	0
6	MG	D	9460	1/1	0.99	0.14	38,38,38,38	0
6	MG	C	9198	1/1	0.99	0.11	36,36,36,36	0
6	MG	F	9513	1/1	0.99	0.14	43,43,43,43	0
6	MG	A	9194	1/1	0.99	0.09	40,40,40,40	0
6	MG	F	9465	1/1	0.99	0.06	36,36,36,36	0
6	MG	N	9291	1/1	0.99	0.15	55,55,55,55	0
6	MG	D	9093	1/1	0.99	0.11	34,34,34,34	0
6	MG	D	9060	1/1	0.99	0.11	35,35,35,35	0
6	MG	P	9353	1/1	0.99	0.11	44,44,44,44	0
6	MG	D	9091	1/1	0.99	0.14	47,47,47,47	0
6	MG	F	9525	1/1	0.99	0.08	54,54,54,54	0
6	MG	N	9277	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9425	1/1	0.99	0.09	44,44,44,44	0
6	MG	N	9215	1/1	0.99	0.10	40,40,40,40	0
6	MG	M	9216	1/1	0.99	0.12	44,44,44,44	0
6	MG	C	9431	1/1	0.99	0.06	42,42,42,42	0
6	MG	N	9270	1/1	0.99	0.13	47,47,47,47	0
6	MG	M	9489	1/1	0.99	0.09	43,43,43,43	0
6	MG	P	9275	1/1	0.99	0.09	32,32,32,32	0
6	MG	A	9126	1/1	0.99	0.10	39,39,39,39	0
6	MG	N	9324	1/1	0.99	0.08	39,39,39,39	0
6	MG	C	9524	1/1	0.99	0.08	45,45,45,45	0
6	MG	D	9125	1/1	0.99	0.10	35,35,35,35	0
6	MG	A	9200	1/1	0.99	0.10	49,49,49,49	0
6	MG	C	9056	1/1	0.99	0.06	34,34,34,34	0
6	MG	D	9405	1/1	0.99	0.10	38,38,38,38	0
6	MG	C	9193	1/1	0.99	0.09	37,37,37,37	0
6	MG	M	9373	1/1	0.99	0.12	38,38,38,38	0
6	MG	L	9479	1/1	0.99	0.10	48,48,48,48	0
6	MG	E	9402	1/1	0.99	0.12	39,39,39,39	0
6	MG	M	9497	1/1	0.99	0.12	43,43,43,43	0
6	MG	N	9221	1/1	0.99	0.10	30,30,30,30	0
6	MG	A	9024	1/1	0.99	0.10	29,29,29,29	0
6	MG	C	9098	1/1	0.99	0.09	52,52,52,52	0
6	MG	L	9530	1/1	0.99	0.10	58,58,58,58	0
6	MG	F	9133	1/1	0.99	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9403	1/1	0.99	0.16	30,30,30,30	0
6	MG	K	9493	1/1	0.99	0.09	38,38,38,38	0
6	MG	P	9240	1/1	0.99	0.11	38,38,38,38	0
6	MG	A	9440	1/1	0.99	0.10	53,53,53,53	0
6	MG	D	9418	1/1	0.99	0.08	47,47,47,47	0
6	MG	M	9224	1/1	0.99	0.06	38,38,38,38	0
6	MG	C	9170	1/1	0.99	0.10	36,36,36,36	0
6	MG	C	9185	1/1	0.99	0.18	60,60,60,60	0
6	MG	D	9452	1/1	0.99	0.10	32,32,32,32	0
6	MG	D	9128	1/1	0.99	0.11	35,35,35,35	0
6	MG	D	9070	1/1	0.99	0.10	46,46,46,46	0
6	MG	D	9052	1/1	0.99	0.09	36,36,36,36	0
6	MG	C	9408	1/1	0.99	0.12	38,38,38,38	0
6	MG	K	9492	1/1	0.99	0.10	40,40,40,40	0
6	MG	A	9173	1/1	0.99	0.10	41,41,41,41	0
6	MG	N	9343	1/1	0.99	0.09	45,45,45,45	0
6	MG	N	9237	1/1	0.99	0.14	40,40,40,40	0
6	MG	N	9305	1/1	0.99	0.09	42,42,42,42	0
6	MG	B	9442	1/1	0.99	0.12	47,47,47,47	0
6	MG	C	9161	1/1	0.99	0.07	40,40,40,40	0
6	MG	N	9386	1/1	0.99	0.08	46,46,46,46	0
6	MG	C	9171	1/1	0.99	0.09	33,33,33,33	0
6	MG	L	9374	1/1	0.99	0.09	47,47,47,47	0
6	MG	D	9459	1/1	0.99	0.10	33,33,33,33	0
6	MG	L	9234	1/1	0.99	0.07	41,41,41,41	0
6	MG	D	9082	1/1	0.99	0.11	30,30,30,30	0
6	MG	N	9550	1/1	0.99	0.09	34,34,34,34	0
6	MG	D	9436	1/1	0.99	0.09	46,46,46,46	0
6	MG	N	9501	1/1	0.99	0.08	47,47,47,47	0
6	MG	D	9120	1/1	0.99	0.07	34,34,34,34	0
6	MG	M	9382	1/1	0.99	0.09	33,33,33,33	0
6	MG	N	9357	1/1	0.99	0.09	41,41,41,41	0
6	MG	D	9158	1/1	0.99	0.08	31,31,31,31	0
6	MG	N	9286	1/1	0.99	0.12	46,46,46,46	0
6	MG	D	9142	1/1	0.99	0.11	40,40,40,40	0
8	ZN	D	7112	1/1	0.99	0.13	72,72,72,72	0
6	MG	D	9174	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9433	1/1	0.99	0.12	46,46,46,46	0
6	MG	D	9051	1/1	0.99	0.07	36,36,36,36	0
6	MG	D	9181	1/1	0.99	0.06	36,36,36,36	0
6	MG	C	9113	1/1	0.99	0.16	47,47,47,47	0
6	MG	A	9116	1/1	0.99	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9132	1/1	0.99	0.10	33,33,33,33	0
6	MG	K	9507	1/1	0.99	0.14	45,45,45,45	0
6	MG	C	9031	1/1	0.99	0.12	43,43,43,43	0
6	MG	N	9263	1/1	0.99	0.08	37,37,37,37	0
6	MG	N	9371	1/1	0.99	0.10	30,30,30,30	0
6	MG	M	9318	1/1	0.99	0.14	51,51,51,51	0
6	MG	M	9328	1/1	0.99	0.09	48,48,48,48	0
6	MG	N	9294	1/1	0.99	0.07	49,49,49,49	0
6	MG	M	9210	1/1	0.99	0.13	35,35,35,35	0
6	MG	M	9369	1/1	0.99	0.09	35,35,35,35	0
6	MG	F	9542	1/1	0.99	0.19	50,50,50,50	0
6	MG	C	9005	1/1	0.99	0.08	31,31,31,31	0
6	MG	C	9204	1/1	0.99	0.12	41,41,41,41	0
6	MG	L	9480	1/1	0.99	0.13	36,36,36,36	0
6	MG	D	9138	1/1	0.99	0.12	38,38,38,38	0
6	MG	B	9434	1/1	0.99	0.11	35,35,35,35	0
6	MG	K	9279	1/1	0.99	0.11	36,36,36,36	0
6	MG	P	9388	1/1	0.99	0.08	45,45,45,45	0
6	MG	M	9223	1/1	0.99	0.10	48,48,48,48	0
6	MG	D	9134	1/1	0.99	0.10	40,40,40,40	0
6	MG	N	9238	1/1	0.99	0.16	29,29,29,29	0
6	MG	L	9260	1/1	0.99	0.09	41,41,41,41	0
6	MG	M	9535	1/1	0.99	0.12	40,40,40,40	0
6	MG	A	9117	1/1	0.99	0.07	32,32,32,32	0
6	MG	M	9537	1/1	0.99	0.13	38,38,38,38	0
6	MG	K	9370	1/1	0.99	0.06	46,46,46,46	0
6	MG	D	9118	1/1	0.99	0.12	34,34,34,34	0
6	MG	D	9085	1/1	0.99	0.10	32,32,32,32	0
6	MG	N	9533	1/1	0.99	0.12	33,33,33,33	0
6	MG	F	9089	1/1	0.99	0.10	48,48,48,48	0
6	MG	C	9004	1/1	0.99	0.09	30,30,30,30	0
6	MG	D	9061	1/1	0.99	0.11	35,35,35,35	0
6	MG	M	9372	1/1	0.99	0.09	47,47,47,47	0
6	MG	D	9017	1/1	0.99	0.07	37,37,37,37	0
6	MG	P	9269	1/1	0.99	0.09	41,41,41,41	0
6	MG	D	9008	1/1	0.99	0.13	37,37,37,37	0
6	MG	D	9058	1/1	0.99	0.11	41,41,41,41	0
6	MG	N	9482	1/1	0.99	0.14	52,52,52,52	0
6	MG	D	9464	1/1	0.99	0.12	38,38,38,38	0
6	MG	C	9426	1/1	0.99	0.06	47,47,47,47	0
6	MG	K	9487	1/1	0.99	0.12	36,36,36,36	0
6	MG	P	9494	1/1	0.99	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	N	9552	1/1	0.99	0.11	46,46,46,46	0
6	MG	N	9303	1/1	0.99	0.12	35,35,35,35	0
6	MG	D	9114	1/1	0.99	0.10	32,32,32,32	0
6	MG	D	9162	1/1	0.99	0.11	44,44,44,44	0
6	MG	L	9330	1/1	0.99	0.09	41,41,41,41	0
6	MG	N	9387	1/1	0.99	0.07	28,28,28,28	0
6	MG	D	9105	1/1	0.99	0.07	48,48,48,48	0
6	MG	M	9254	1/1	0.99	0.08	34,34,34,34	0
6	MG	C	9046	1/1	0.99	0.09	31,31,31,31	0
6	MG	D	9392	1/1	0.99	0.09	46,46,46,46	0
6	MG	C	9444	1/1	0.99	0.09	40,40,40,40	0
6	MG	A	9412	1/1	0.99	0.12	33,33,33,33	0
6	MG	B	9040	1/1	0.99	0.16	29,29,29,29	0
6	MG	B	9450	1/1	0.99	0.08	46,46,46,46	0
6	MG	N	9225	1/1	0.99	0.08	40,40,40,40	0
6	MG	N	9306	1/1	0.99	0.13	30,30,30,30	0
6	MG	N	9339	1/1	0.99	0.11	34,34,34,34	0
6	MG	C	9400	1/1	0.99	0.12	49,49,49,49	0
6	MG	D	9064	1/1	0.99	0.11	41,41,41,41	0
6	MG	D	9188	1/1	0.99	0.09	37,37,37,37	0
6	MG	K	9495	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9075	1/1	0.99	0.11	39,39,39,39	0
6	MG	N	9352	1/1	0.99	0.05	44,44,44,44	0
6	MG	F	9080	1/1	0.99	0.12	30,30,30,30	0
6	MG	C	9086	1/1	0.99	0.10	34,34,34,34	0
6	MG	C	9022	1/1	0.99	0.12	28,28,28,28	0
6	MG	N	9528	1/1	0.99	0.10	40,40,40,40	0
6	MG	C	9409	1/1	0.99	0.12	49,49,49,49	0
6	MG	C	9201	1/1	0.99	0.08	45,45,45,45	0
6	MG	D	9037	1/1	1.00	0.08	31,31,31,31	0
6	MG	C	9390	1/1	1.00	0.12	30,30,30,30	0
6	MG	B	9176	1/1	1.00	0.09	41,41,41,41	0
8	ZN	N	7059	1/1	1.00	0.12	83,83,83,83	0
6	MG	D	9195	1/1	1.00	0.08	32,32,32,32	0
6	MG	E	9511	1/1	1.00	0.12	42,42,42,42	0
6	MG	L	9299	1/1	1.00	0.07	36,36,36,36	0
6	MG	D	9510	1/1	1.00	0.12	51,51,51,51	0
6	MG	D	9043	1/1	1.00	0.11	28,28,28,28	0
6	MG	F	9547	1/1	1.00	0.09	52,52,52,52	0
6	MG	N	9527	1/1	1.00	0.14	42,42,42,42	0
6	MG	N	9531	1/1	1.00	0.10	38,38,38,38	0
6	MG	F	9030	1/1	1.00	0.11	36,36,36,36	0

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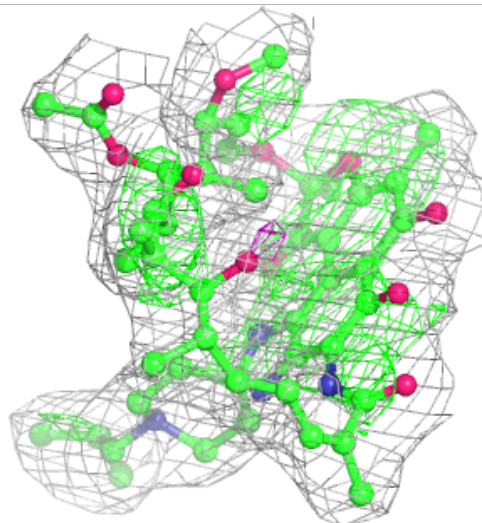
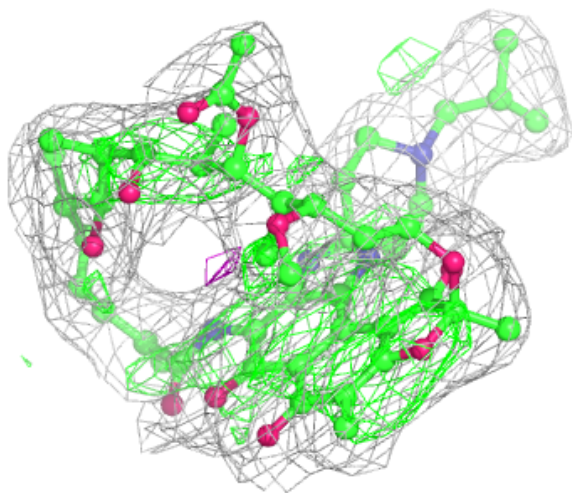
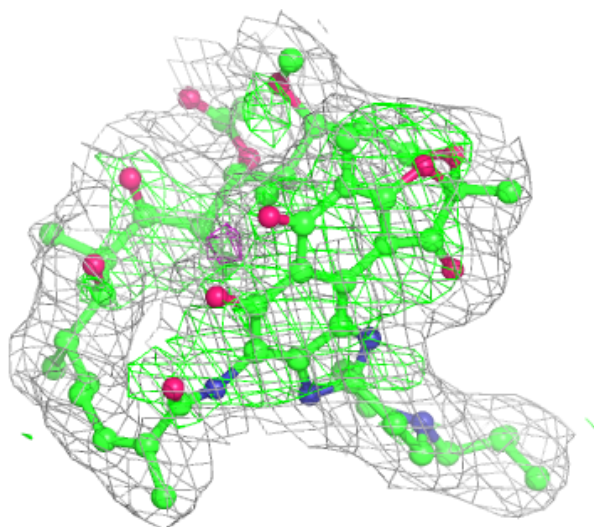
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9006	1/1	1.00	0.14	30,30,30,30	0
6	MG	P	9239	1/1	1.00	0.11	33,33,33,33	0
6	MG	K	9264	1/1	1.00	0.09	36,36,36,36	0
6	MG	N	9308	1/1	1.00	0.12	31,31,31,31	0
6	MG	D	9453	1/1	1.00	0.12	31,31,31,31	0
6	MG	O	9337	1/1	1.00	0.08	34,34,34,34	0
6	MG	D	9182	1/1	1.00	0.07	46,46,46,46	0
6	MG	D	9087	1/1	1.00	0.09	27,27,27,27	0
6	MG	N	9302	1/1	1.00	0.14	48,48,48,48	0
6	MG	N	9468	1/1	1.00	0.11	35,35,35,35	0
6	MG	N	9470	1/1	1.00	0.15	27,27,27,27	0
6	MG	N	9360	1/1	1.00	0.05	39,39,39,39	0
6	MG	C	9160	1/1	1.00	0.12	46,46,46,46	0
6	MG	N	9491	1/1	1.00	0.11	43,43,43,43	0
6	MG	M	9380	1/1	1.00	0.08	32,32,32,32	0
6	MG	M	9241	1/1	1.00	0.09	35,35,35,35	0
6	MG	K	9212	1/1	1.00	0.08	33,33,33,33	0
6	MG	F	9421	1/1	1.00	0.13	30,30,30,30	0
6	MG	L	9278	1/1	1.00	0.08	46,46,46,46	0
6	MG	A	9404	1/1	1.00	0.16	55,55,55,55	0
6	MG	D	9149	1/1	1.00	0.13	42,42,42,42	0
6	MG	C	9027	1/1	1.00	0.12	28,28,28,28	0
6	MG	C	9106	1/1	1.00	0.09	37,37,37,37	0
6	MG	O	9231	1/1	1.00	0.15	41,41,41,41	0
6	MG	D	9179	1/1	1.00	0.09	30,30,30,30	0
6	MG	M	9469	1/1	1.00	0.14	39,39,39,39	0
6	MG	D	9069	1/1	1.00	0.12	32,32,32,32	0
6	MG	K	9477	1/1	1.00	0.11	38,38,38,38	0
6	MG	M	9331	1/1	1.00	0.08	49,49,49,49	0
6	MG	C	9127	1/1	1.00	0.10	41,41,41,41	0
6	MG	D	9143	1/1	1.00	0.14	35,35,35,35	0
6	MG	D	9013	1/1	1.00	0.09	34,34,34,34	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.

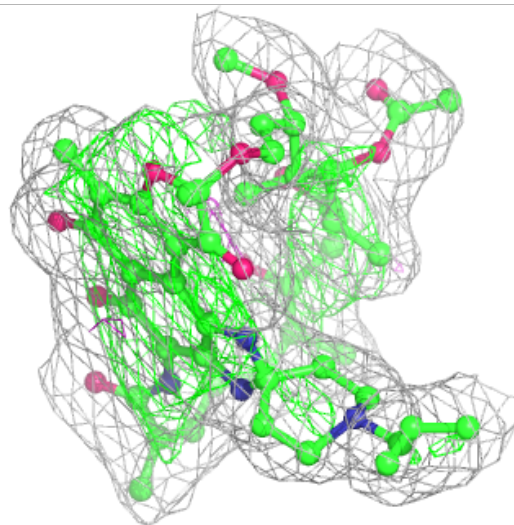
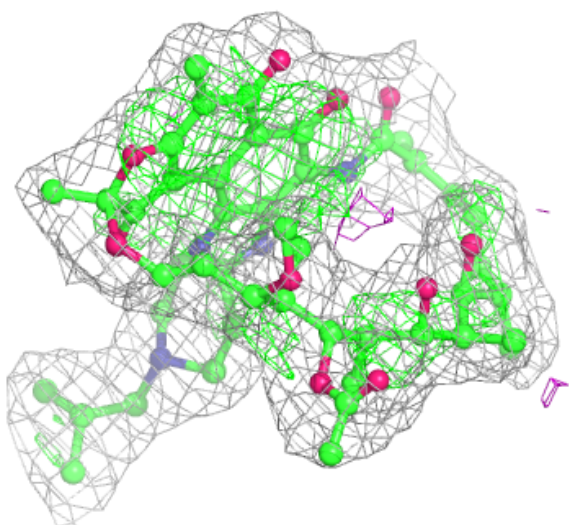
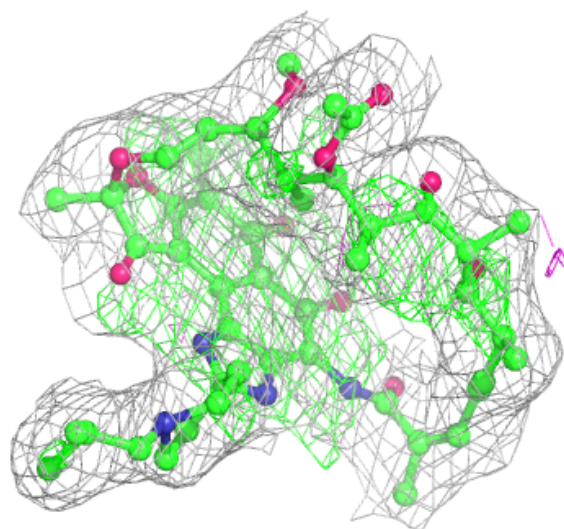
Electron density around RBT M 8002:

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



Electron density around RBT C 8001:

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.