



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 06:15 AM EDT

PDB ID : 6CUX
Title : Escherichia coli RpoB S531L mutant RNA polymerase holoenzyme in complex with Kanglemycin A
Authors : Molodtsov, V.; Murakami, K.S.
Deposited on : 2018-03-26
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

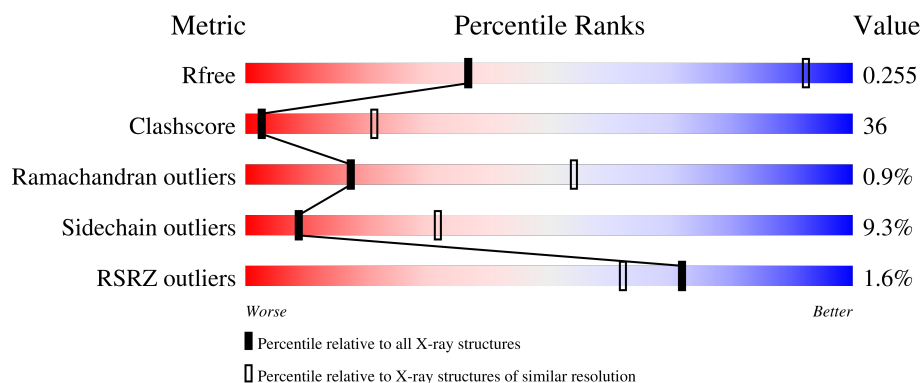
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div>33%</div> <div>29%</div> <div>7%</div> <div>31%</div> </div>
1	B	329	<div> <div>23%</div> <div>39%</div> <div>•</div> <div>35%</div> </div>
1	G	329	<div> <div>29%</div> <div>34%</div> <div>6%</div> <div>32%</div> </div>
1	H	329	<div> <div>28%</div> <div>34%</div> <div>•</div> <div>35%</div> </div>
2	C	1342	<div> <div>44%</div> <div>49%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	J	1502	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55005 atoms, of which 62 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1753	1091	311	345	6			
1	B	214	Total	C	N	O	S	0	0	0
			1649	1029	290	324	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	215	Total	C	N	O	S	0	0	0
			1659	1037	291	325	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1339	Total	C	N	O	S	0	0	0
			10548	6620	1834	2050	44			
2	I	1328	Total	C	N	O	S	0	0	0
			10486	6583	1822	2038	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	531	LEU	SER	conflict	UNP P0A8V2
I	531	LEU	SER	conflict	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9089	5714	1627	1702	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

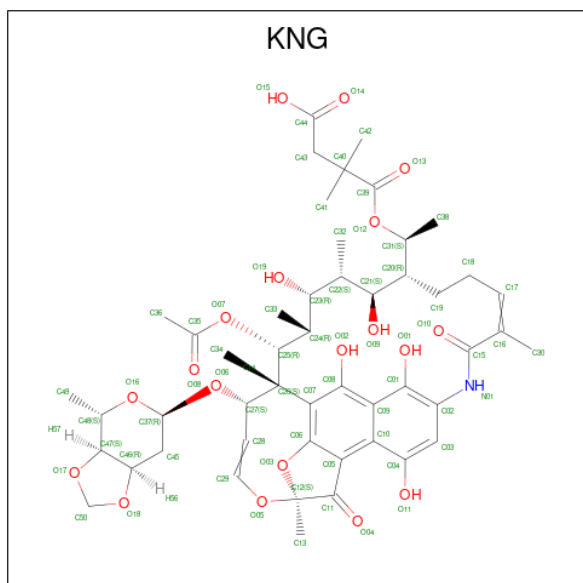
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is Kanglemycin A (three-letter code: KNG) (formula: $C_{50}H_{67}NO_{19}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			132	50	62	1	19		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	J	1	Total	Mg	0	0
			1	1		

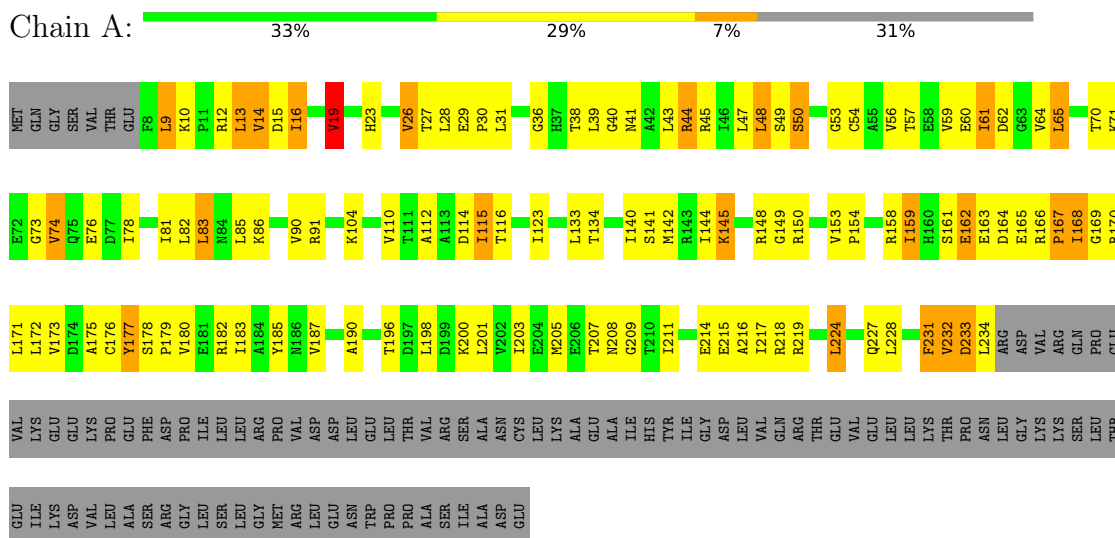
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

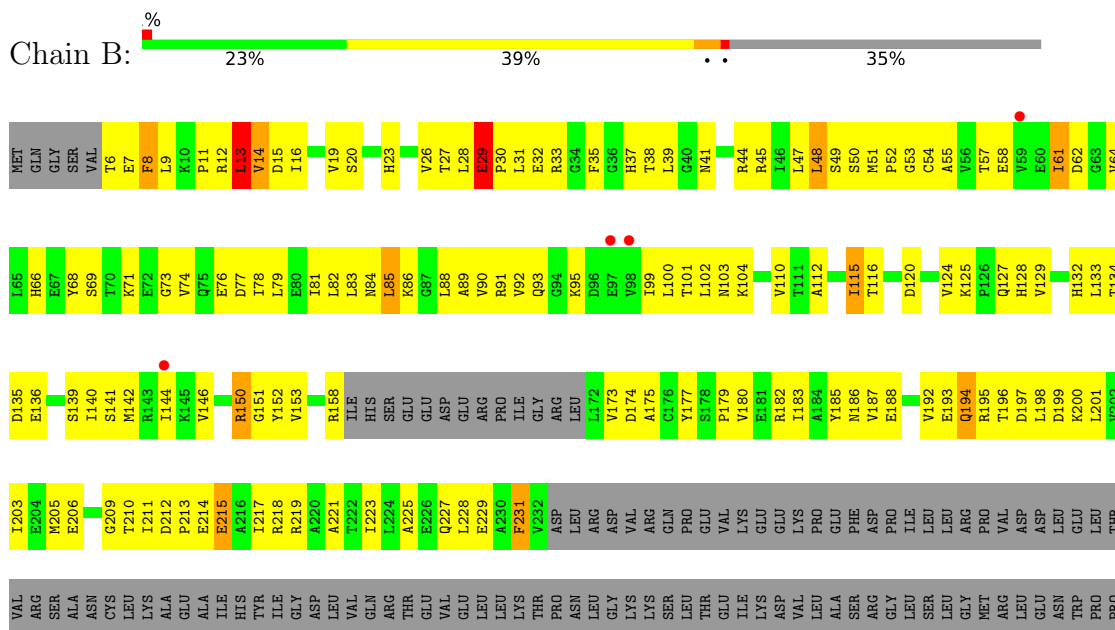
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

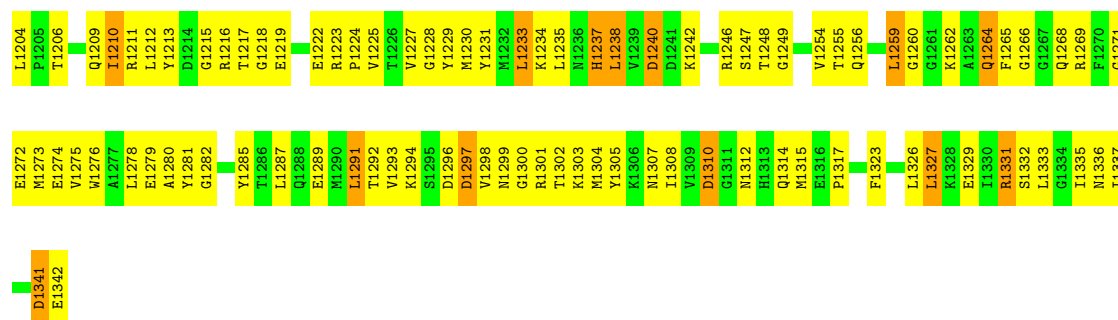
• Molecule 1: DNA-directed RNA polymerase subunit alpha



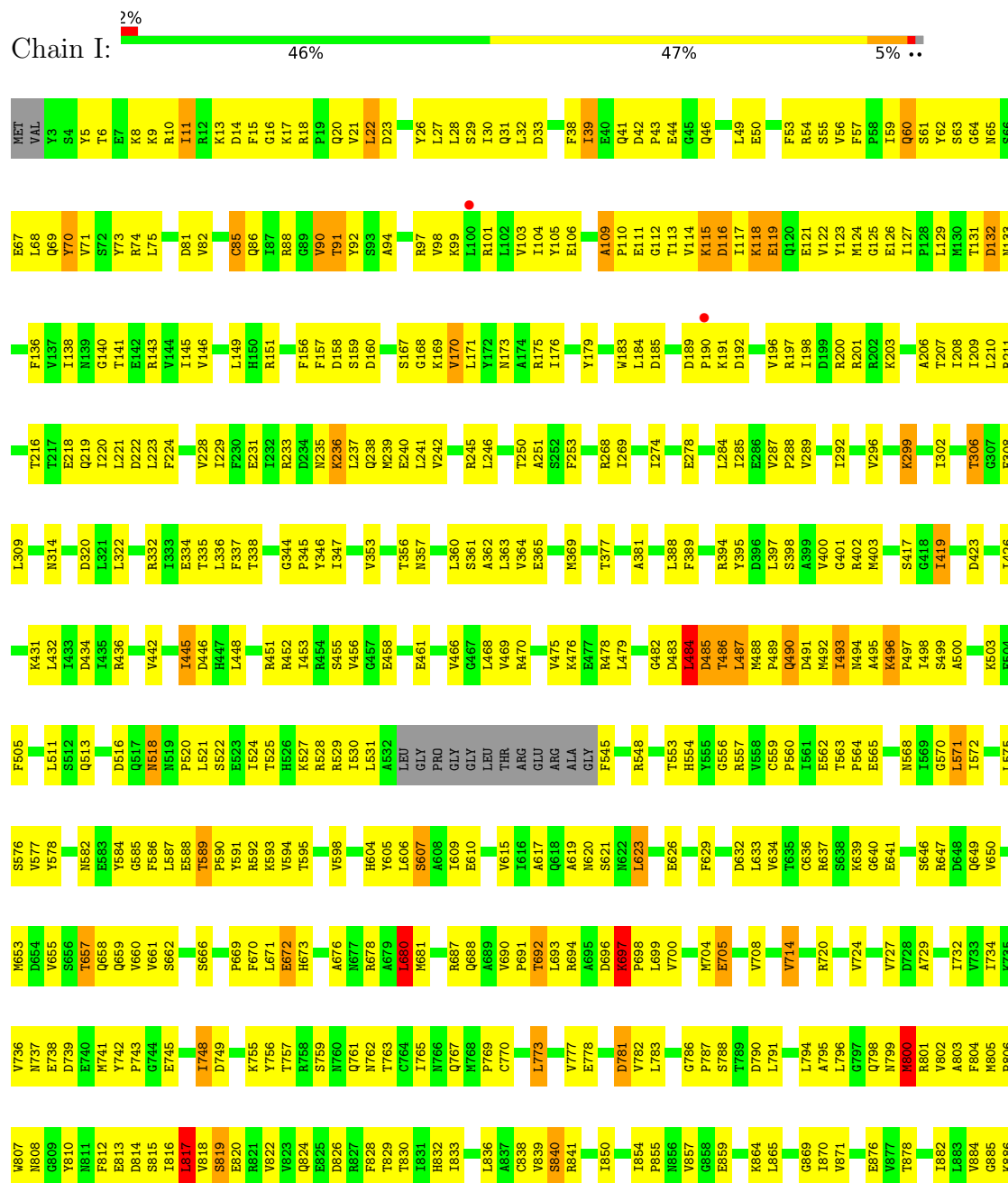
• Molecule 1: DNA-directed RNA polymerase subunit alpha

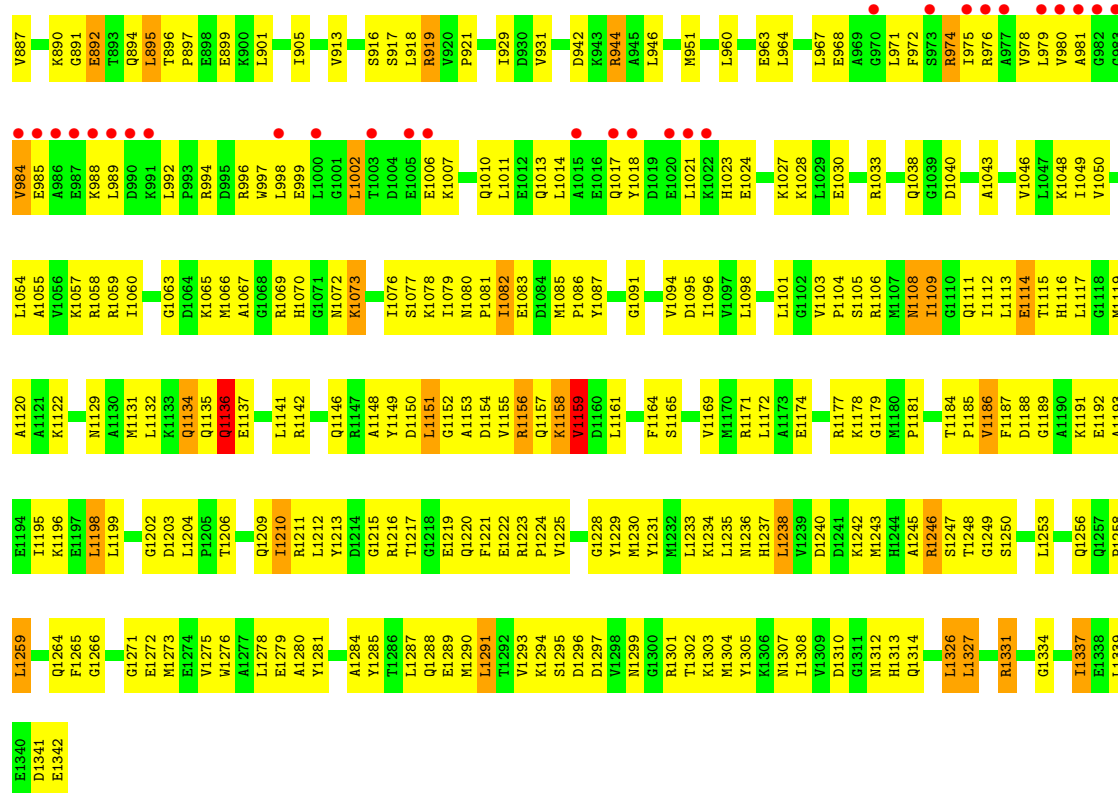


L1141	M1066	V980	P889	L817	D749	E672	T600	L531	R454	L360	V287	Q219	M139	R74
L1142	R1069	G891	K890	V818	Y751	H673	D601	P535	S455	G361	P288	I220	G140	L75
F1144	E1083	L1002	F906	A837	T765	P691	V615	R548	E472	P375	I302	R233	F156	G89
T1145	E1084	L1001	S911	W839	Q767	T693	A617	H550	E477	T377	D303	K236	S159	Y92
Q1146	K1073	E985	Q894	S840	W768	R694	A619	P552	L479	E382	G307	L237	D160	S93
R1147	G1074	A986	T896	R841	L773	A695	N620	T553	S480	F385	E308	Q238	K161	A94
L1148	V1075	K987	E897	D842	E774	D696	E610	H554	L481	G310	C311	M239	G162	Y91
Y1149	I1076	K988	P897	E755	E775	K697	L623	Y555	G482	F390	D483	E240	K163	R97
D1150	S1077	E989	E898	R827	T757	N684	E610	F545	R470	E374	D300	F230	S152	Q86
L1151	K1078	E990	K900	H832	Q761	Q688	Y614	F545	V471	E374	D300	F230	P153	I87
G1152	I1079	L992	L901	H832	T762	A689	Y614	F545	R471	E374	D300	F230	P153	R88
A1153	M1080	L1000	F906	L836	T762	A689	V615	R548	E472	P375	I302	R233	F156	G89
D1154	P1081	G1001	E1016	A837	T765	P691	V615	R548	E472	P375	I302	R233	F157	V90
V1155	L1082	V1155	F906	E837	T765	P691	A617	H550	E477	T377	D303	K236	D168	T91
K1156	E1083	L1002	S911	W839	Q767	T693	A617	H550	E477	T377	D303	K236	S159	Y92
Q1157	E1084	L1001	S911	W839	Q767	T693	A617	H550	E477	T377	D303	K236	S159	Y92
L1158	M1085	E1006	Q912	S840	W768	R694	A619	P552	L479	E382	G307	L237	D160	S93
K1159	P1086	K1007	V913	R841	L773	A695	N620	T553	S480	F385	E308	Q238	K161	A94
V1160	Y1087	Q1008	S916	D842	E774	D696	E610	H554	L481	G310	C311	M239	G162	Y91
L1161	E1088	L1011	S917	T843	E775	K697	L623	Y555	G482	F390	D483	E240	K163	R97
S1162	E1089	L1011	S917	T843	E775	K697	L623	Y555	G482	F390	D483	E240	K163	R97
T1163	L1011	L1011	S917	T843	E775	K697	L623	Y555	G482	F390	D483	E240	K163	R97
F1164	V1094	L1014	R919	P847	E778	G703	E630	R557	L484	D393	A312	V242	S167	K99
S1165	D1095	A1015	V920	E848	R779	G703	E630	R557	L484	D393	A312	V242	S167	K99
L1166	L1095	E1016	P921	E848	R779	G703	E630	R557	L484	D393	A312	V242	S167	K99
V1169	L1101	Q1017	E705	E780	D781	E705	E630	R557	L484	D393	A312	V242	S167	K99
K1170	L1101	Q1017	E705	E780	D781	E705	E630	R557	L484	D393	A312	V242	S167	K99
L1171	S1105	Y1018	V924	T851	W782	L783	E635	T563	Q490	G401	S318	R247	R175	I104
E1174	R1106	L1021	I929	D853	A784	W714	C636	P564	D491	R402	L319	E249	I176	E106
M1175	M107	E1024	D930	I854	T715	R715	R637	E565	M492	N406	L321	T250	I177	E106
L1176	N1108	E1024	D930	I854	T715	R715	R637	E565	M492	N406	L321	T250	I177	E106
R1177	G1110	K1027	V931	V857	T789	A716	K639	G566	I493	R407	A322	D254	R180	A109
K1178	Q1111	L1027	F934	G858	D790	R718	G640	N568	A494	R407	A322	D254	R180	A109
L1179	T1112	K1082	D942	E859	L791	K719	E641	I569	K496	E412	K324	I255	D185	G112
M1180	L1113	L1037	R943	E860	G792	R720	S642	G570	P497	E413	L325	L255	D185	G112
P1181	E1114	T1037	R944	A861	E793	G721	F645	L571	I498	E413	L325	L255	D185	G112
L1182	A945	L1115	A945	R864	A795	G722	F645	L571	I498	E413	L325	L255	D185	G112
T1183	H1116	L1040	L946	L865	G797	W724	R647	S576	K503	K422	G329	E264	D192	I117
L1184	L1117	D1041	L946	L865	G797	W724	R647	S576	K503	K422	G329	E264	D192	I117
P1185	G1118	L1042	K951	D866	Q798	Y726	Q649	V577	Q510	D423	K331	K265	K118	I117
L1186	M1119	A1043	K952	E867	Q798	Y726	Q649	V577	Q510	D423	K331	K265	K118	I117
F1187	A1120	P1044	L953	S868	M800	W727	D651	Y578	L512	I426	R332	R267	E119	E119
L1188	A1121	D1045	R801	G869	R801	D728	D651	Y578	L512	I426	R332	R267	E119	E119
G1189	K1122	V1046	K958	Y872	W802	A729	M653	N582	Q513	K431	T335	T270	E120	Q120
L1190	G1123	L1047	K958	Y872	W802	A729	M653	N582	Q513	K431	T335	T270	E120	Q120
K1191	T1124	K1043	S861	L873	F894	V733	V655	F586	M515	D434	L336	A271	R201	G125
E1192	L1129	I1049	E962	W877	M805	I734	V655	L587	Q517	D435	T339	R272	R201	G125
L1193	M1129	A1055	E963	T878	M805	I734	V655	L587	Q517	D435	T339	R272	R201	G125
E1194	L1130	L964	E963	T878	M805	I734	V655	L587	Q517	D435	T339	R272	R201	G125
L1195	M1131	L964	E963	T878	M805	I734	V655	L587	Q517	D435	T339	R272	R201	G125
K1196	L1132	L966	Q965	G879	W807	K735	T657	T589	N518	R436	T339	R272	R201	G125
L1197	R1058	L1059	Q965	G879	W807	K735	T657	T589	N518	R436	T339	R272	R201	G125
E1197	K1133	R1059	L967	D881	G809	E738	V660	R592	D443	D443	Y346	L277	A206	M130
L1198	Q1134	I1060	L971	L883	M811	E740	S662	V594	H526	L448	S349	E278	I209	D132
L1199	Q1135	P1062	L971	L883	M811	E740	S662	V594	H526	L448	S349	E278	I209	D132
K1200	E1137	G1063	K886	E813	R812	E745	A665	T595	D596	L284	K527	R283	R211	G134
L1201	L1136	P1062	K886	E813	R812	E745	A665	T595	D596	L284	K527	R283	R211	G134
E1202	D1064	R974	S815	S815	E745	E745	A665	T595	D596	L284	K527	R283	R211	G134
L1203	K1065	T075	E745	E745	E745	E745	A665	T595	D596	L284	K527	R283	R211	G134

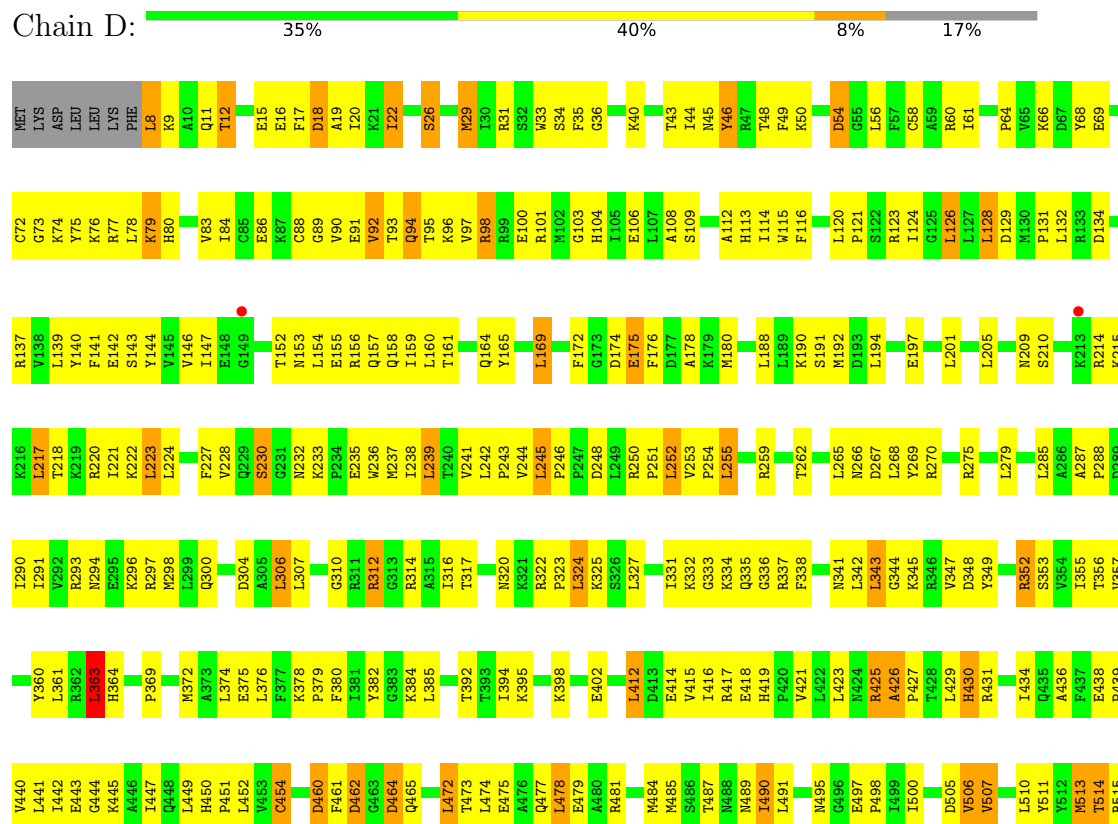


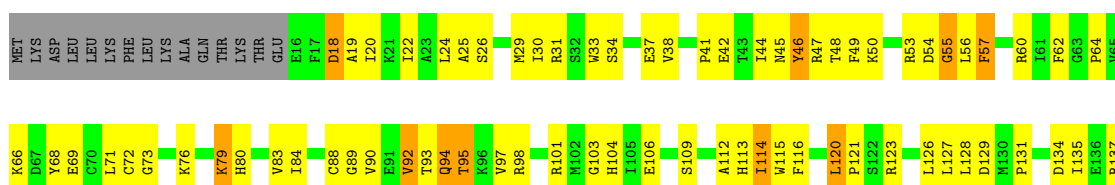
• Molecule 2: DNA-directed RNA polymerase subunit beta





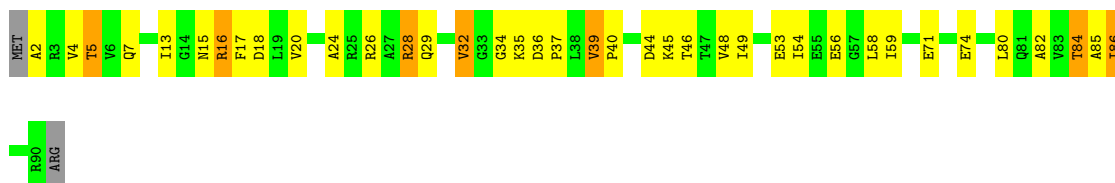
• Molecule 3: DNA-directed RNA polymerase subunit beta'



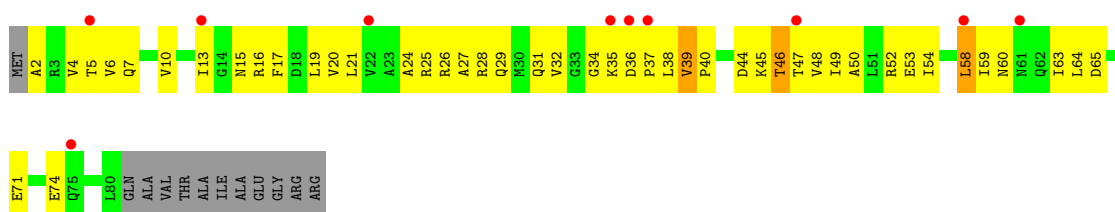


H1218	R1148	VAL	ILE	ASN	A904	D830	I755	A688	V609	V526	D460	P369	E297	T218	V138
D1219	R1149	LEU	THR	SER	R905	V831	E756		R610	L527	F461	P372	M296	K219	L139
I1220	P1150	ILE	GLU	SER	G906	R332	I757	D691	I611	T528	D462	A373	V303	R220	I140
L1221	K1151	PRO	VAL	GLY	H907	E933	P758	R692	L612		G463	L374	D304	I221	F141
R1222	E1152	GLY	SER	LYS	I908	V839	N762	S694	G613	K531	D464	E375	A305	K222	E142
H1227	P1153	THR	GLY	LEU	I909	V839	N763	S695	L614	E532	D465		L306	L223	S143
A1228	A1154	ASP	PHE	VAL			E763	K695	K615	R535	M466	P379	L307	F227	Y144
I1155	I1155	MET	VAL	ILE	E913	V843	R764	A696	P616	L536	A467				V145
L1156	A1157	PRO	ARG	THR	A914	T844	R765	A697	F620	G540	P471	Y382	R312	N232	V146
E1158	E1158	ALA	PHE	ARG	I915	A845	G766	M698		L541	L472	K384	T317	K233	I147
		GLN	THR	ARG	G916	E846	L767	D699		A542	T473	R388		P234	E155
V1163	V1163	TYR	ASP	ASN	V917	D847	N768	N700	Q623	L544	L474		M320	E235	L154
S1164	S1164	LEU	ILE	THR	I918	V848	V769	L701	T627	A546	A475	R321	R321	P236	E156
F1165	F1165	LEU	ASP	GLU	A919	L849	L770	Q702	G628	R547	Q477	K395	R323	Q157	Q158
G1166	G1166	PRO	ASP	LEU	Q920	K850	Y771	T703	F629	H545	L478		R322	I238	I159
K1167	K1167	GLY	GLN	LYS	S922	T853	Y772	E704		A546	L478		R323	L242	L243
E1168	E1168	THR	THR	ILE	I923	A854	I774	V705	A633	R547	E479	H400	K325	V244	L160
T1169	T1169	ALA	ASP	ASP	G924			T707	R634	V548			K325	P243	L161
K1170	K1170	VAL	ILE	ASP	E925			N708		K549	A480	E405		V244	E162
G1171	G1171	GLU	ARG	PHE	P926			R709	S638	V550	R481		D329	L245	E163
		THR	ARG	THR				D710	V639	R551	A482	V408	I331	P246	E163
V1246	R1174	GLU	THR	ARG	L930	N861	R780	G711	G640	L552	L483		K332	P247	Q164
K1247	L1175	THR	ASP	LYS	T931	T862		Q712	I641	K557	M484	E414	G333	D248	Y165
I1248	V1176	GLY	LYS	GLU	MET	L863	L783				M485		K334	L249	
I1177	I1177	VAL	LEU	GLU	ARG	L864			R644		S486	V415	K334	R250	L169
		GLN	THR	THR	THR	L865	L788		V645	T567	T487	I416	K335	R251	
D1181	D1181	ILE	GLY	TYR	PHE	H865			P646	S568	N488	R417	G336	L252	F172
I1182	I1182	SER	LEU	LYS	HIS	E866	N792	S718	P647	L569	N489	E418	R337	P253	
S1183	S1183	SER	SER	VAL	ILE	Q867		F719		K570	N490	H419	F338	P254	E175
V1265	V1184	GLY	SER	PRO	GLY	V868	T797	N720	K650	R571	L491	P420	R339	L255	F176
I1266	P1185	ASP	LEU	TYR	GLY	C869	R798	S721		T572	S492	V421	Q340	D256	D177
T1267	Y1186	VAL	VAL	GLY	ALA	D870	R799	I722	I653	P493	P493	L422	R341	G257	A178
R1268	E1187	LEU	VAL	ALA	SER	L871	L800	Y723	I654	V574	A494	N423	L342	G258	K179
Q1269		ALA	LEU	VAL	ALA	L872	N801	M724		G575		N424	L343		M180
M1260	P1191	ARG	ASP	LEU	ARG	E873	D802	M725	A657	R576	P498	R425	G344	T262	
L1261	K1192	SER	ALA	ALA	ALA	E874	V803	A726	E658	L579	L499	A426	K345	L265	A184
R1262	V1193	LYS	ALA	LYS	ALA	N875	A804	D727	R659		I500	P427	R346	N266	I185
K1263	R1194	GLN	GLU	GLY	ALA	S876	Q805	S728	E660	T582	V501	T428	V347	L267	Q186
A1264	Q1195	ARG	ASP	GLY	GLY	S877	D806		V661	V583		L429	D348	L267	A187
T1265	L1196	THR	THR	GLY	SER	D878	L807	G731	E662		D505	H430	Y349	L268	L188
I1266	N1197	GLY	ALA	GLU	SER	A879	V808	R731	E663	V587		R431	S350	Y269	L189
	V1198	ILE	GLN	GLN	ILE	V880	V809	G732	I664	L587	V506		G351	R270	K190
A1269	F1199	THR	VAL	VAL	GLN	K881	T810	A735		P588	V507	E438	R352		S191
	E1200	LYS	ALA	ALA	VAL	V882	E811		S670	Y589		P439	R352	M192	
D1273	G1201	ASP	ASP	GLY	LYS	R883	C914	Q738	G671	S590	L510	V440	V354	I273	D193
F1274	E1202	ILE	LEU	GLY	ASN	S884	L672	R739		T591	V511	T447	T355	N274	
L1275	R1203	THR	ARG	GLU	LYS	V885	G815	L740	V673	V592	V512	I442	T356	R275	
E1276	V1204	GLY	PRO	THR	GLY		T816	A741	T674	N593	M513	G444	V357	L279	Q196
G1277	E1205	VAL	ALA	VAL	SER	D889	G742			O594	T514	G444	G358		L201
A1278	R1206	LEU	ALA	LEU	ILE	T890	T620	N743	E677	A595	C517	K445	P359	L282	
Q1279	G1207	LYS	ASN	LYS	ILE		M821	R744	R678	L596	V518	A446	Y360	L282	L205
V1280	D1208	ILE	TRP	TRP	LEU	G893	M822	G745	V679	G597	N519	T447	L361	P288	
E1281	V1209	VAL	ASP	SER	SER	V894	T823	L746	N680	K598	N519		L362	D289	S210
I1282	I1210	ASP	PRO	ASN	ASN		P824	M747	K681		A520	H450	R363	I290	
S1283	S1211	VAL	VAL	VAL	VAL	H897	V825	M748	V682	I601	K521	P451	H364	I291	K213
R1284		GLN	THR	HIS	LYS		T826	K749	I683		S522	L452	Q385	V292	R214
V1285	E1215	GLY	MET	THR	SER	R901	E827	P750		M604	S523		G386	R293	K215
K1286	A1216	ASN	PRO	VAL	VAL	D902	G828	I754	I685		E524	C454	G387	K216	
	P1217	VAL	ASP	VAL		L903	G829			C608	M525		L368	K217	L217

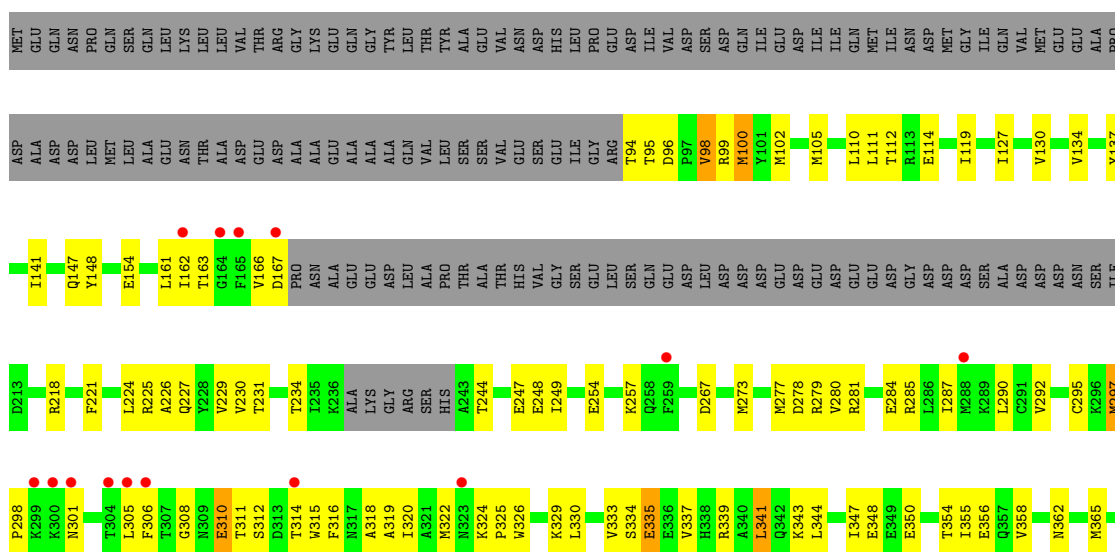
- Molecule 4: DNA-directed RNA polymerase subunit omega

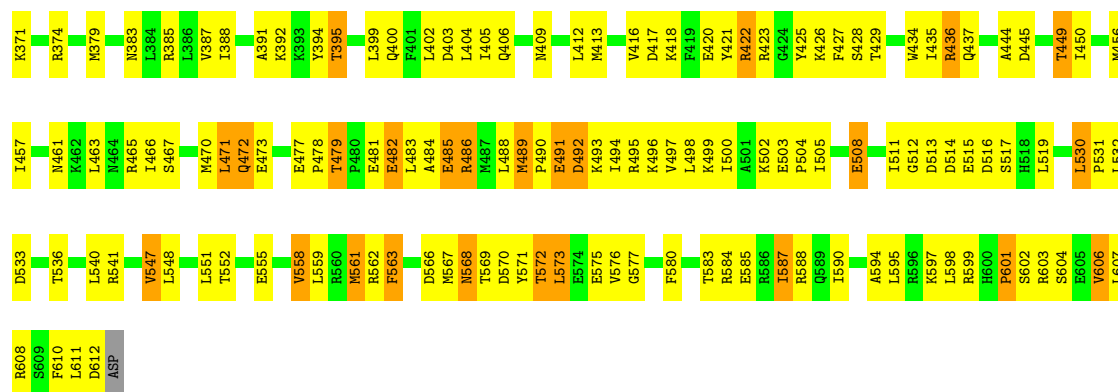


- Molecule 4: DNA-directed RNA polymerase subunit omega

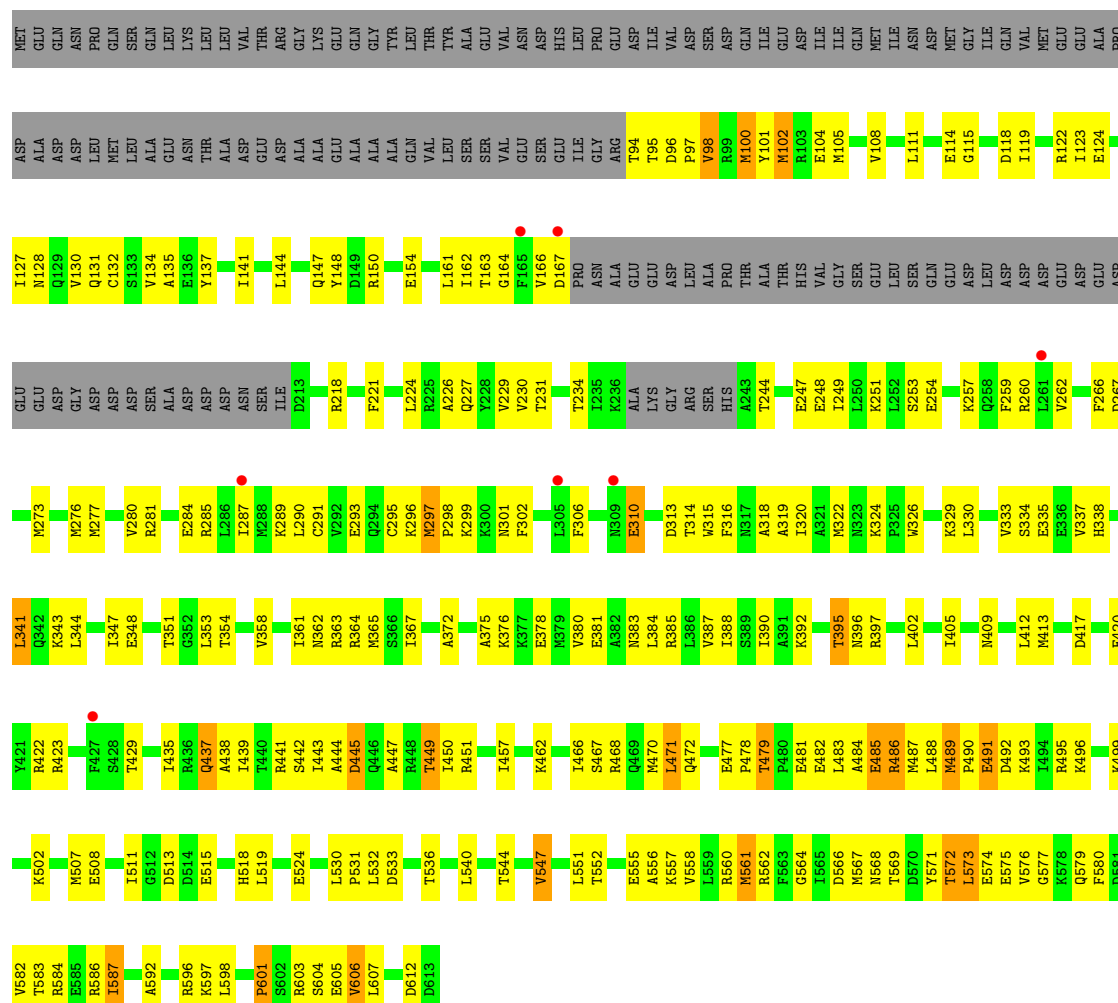


- Molecule 5: RNA polymerase sigma factor RpoD





• Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	188.17Å 204.69Å 311.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.03 – 4.10 45.03 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.03-4.10) 99.0 (45.03-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 4.13Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.210 , 0.255 0.210 , 0.255	Depositor DCC
R_{free} test set	2001 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	190.5	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 182.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55005	wwPDB-VP
Average B, all atoms (Å ²)	241.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KNG, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	1/1774 (0.1%)	1.07	9/2405 (0.4%)
1	B	0.63	0/1668	1.07	7/2260 (0.3%)
1	G	0.50	0/1751	0.82	2/2373 (0.1%)
1	H	0.47	0/1678	0.79	0/2274
2	C	0.67	6/10716 (0.1%)	0.98	24/14458 (0.2%)
2	I	0.56	2/10653 (0.0%)	0.85	14/14373 (0.1%)
3	D	0.71	8/9229 (0.1%)	1.08	42/12459 (0.3%)
3	J	0.60	1/9140 (0.0%)	0.92	16/12341 (0.1%)
4	E	0.62	0/693	0.85	0/935
4	K	0.30	0/629	0.50	0/847
5	F	0.51	0/3864	0.79	2/5194 (0.0%)
5	L	0.48	0/3872	0.76	0/5205
All	All	0.61	18/55667 (0.0%)	0.93	116/75124 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
4	E	0	1
5	F	0	1
5	L	0	1
All	All	0	12

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	517	CYS	CB-SG	-9.59	1.66	1.82
2	C	1274	GLU	CG-CD	7.89	1.63	1.51
3	D	426	ALA	C-N	-6.92	1.21	1.34
3	D	727	ASP	CB-CG	5.86	1.64	1.51
2	C	838	CYS	CB-SG	-5.63	1.72	1.81

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1296	ASP	CB-CG-OD2	-10.40	108.94	118.30
2	C	1233	LEU	CA-CB-CG	9.43	137.00	115.30
2	C	1291	LEU	CA-CB-CG	9.27	136.63	115.30
2	C	1151	LEU	CA-CB-CG	-9.11	94.34	115.30
3	D	605	LEU	CB-CG-CD2	-8.72	96.18	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	GLU	Peptide
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1780	152	0
1	B	1649	0	1674	184	0
1	G	1730	0	1756	191	0
1	H	1659	0	1692	173	0
2	C	10548	0	10553	852	0
2	I	10486	0	10496	746	0
3	D	9089	0	9265	765	0
3	J	9001	0	9169	751	0
4	E	691	0	695	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	59	0
5	F	3813	0	3880	264	0
5	L	3821	0	3884	246	0
6	C	70	62	0	10	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	2	0
All	All	54943	62	55478	4003	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 36.

The worst 5 of 4003 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.21	1.21
5:L:561:MET:HA	5:L:567:MET:HE1	1.27	1.17
2:C:1271:GLY:HA2	3:D:343:LEU:HD11	1.22	1.16
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	1.78	1.16
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.21	1.15

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	225/329 (68%)	198 (88%)	20 (9%)	7 (3%)	4	31
1	B	210/329 (64%)	186 (89%)	19 (9%)	5 (2%)	6	35
1	G	222/329 (68%)	194 (87%)	23 (10%)	5 (2%)	6	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	211/329 (64%)	187 (89%)	17 (8%)	7 (3%)	4	29
2	C	1335/1342 (100%)	1226 (92%)	100 (8%)	9 (1%)	22	60
2	I	1324/1342 (99%)	1220 (92%)	96 (7%)	8 (1%)	25	63
3	D	1162/1407 (83%)	1068 (92%)	86 (7%)	8 (1%)	22	60
3	J	1151/1407 (82%)	1060 (92%)	78 (7%)	13 (1%)	14	50
4	E	87/91 (96%)	82 (94%)	4 (5%)	1 (1%)	14	50
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	426 (92%)	35 (8%)	1 (0%)	47	80
5	L	463/613 (76%)	426 (92%)	36 (8%)	1 (0%)	47	80
All	All	6929/8222 (84%)	6347 (92%)	517 (8%)	65 (1%)	17	54

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	B	13	LEU
1	B	29	GLU
2	C	2	VAL
2	C	3	TYR

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	194/286 (68%)	180 (93%)	14 (7%)	14	42
1	B	182/286 (64%)	172 (94%)	10 (6%)	21	50
1	G	191/286 (67%)	177 (93%)	14 (7%)	14	41
1	H	184/286 (64%)	176 (96%)	8 (4%)	29	56
2	C	1151/1157 (100%)	1045 (91%)	106 (9%)	9	32
2	I	1147/1157 (99%)	1042 (91%)	105 (9%)	9	32
3	D	970/1168 (83%)	868 (90%)	102 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	960/1168 (82%)	863 (90%)	97 (10%)	7	28
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	25
4	K	67/75 (89%)	63 (94%)	4 (6%)	19	47
5	F	417/540 (77%)	375 (90%)	42 (10%)	7	28
5	L	418/540 (77%)	377 (90%)	41 (10%)	8	29
All	All	5953/7024 (85%)	5402 (91%)	551 (9%)	9	32

5 of 551 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	720	ASN
3	J	849	LEU
3	J	717	VAL
5	L	335	GLU
3	D	798	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	1116	HIS
3	J	488	ASN
2	I	1136	GLN
2	I	1314	GLN
3	J	716	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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
6	KNG	C	2001	-	75,75,75	3.77	29 (38%)	104,114,114	2.96	39 (37%)

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
6	KNG	C	2001	-	-	36/76/113/113	0/5/6/6

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2001	KNG	O18-C46	-14.63	1.20	1.44
6	C	2001	KNG	O17-C47	-9.86	1.21	1.43
6	C	2001	KNG	O03-C06	9.82	1.56	1.37
6	C	2001	KNG	C04-C10	8.96	1.59	1.43
6	C	2001	KNG	O16-C37	8.26	1.62	1.42

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2001	KNG	C34-C26-C27	-8.72	93.15	110.93
6	C	2001	KNG	C49-C48-C47	8.51	126.36	113.41
6	C	2001	KNG	C25-C26-C27	7.48	132.41	112.02
6	C	2001	KNG	C24-C23-C22	7.46	127.92	115.43
6	C	2001	KNG	O03-C06-C07	6.85	132.93	121.14

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

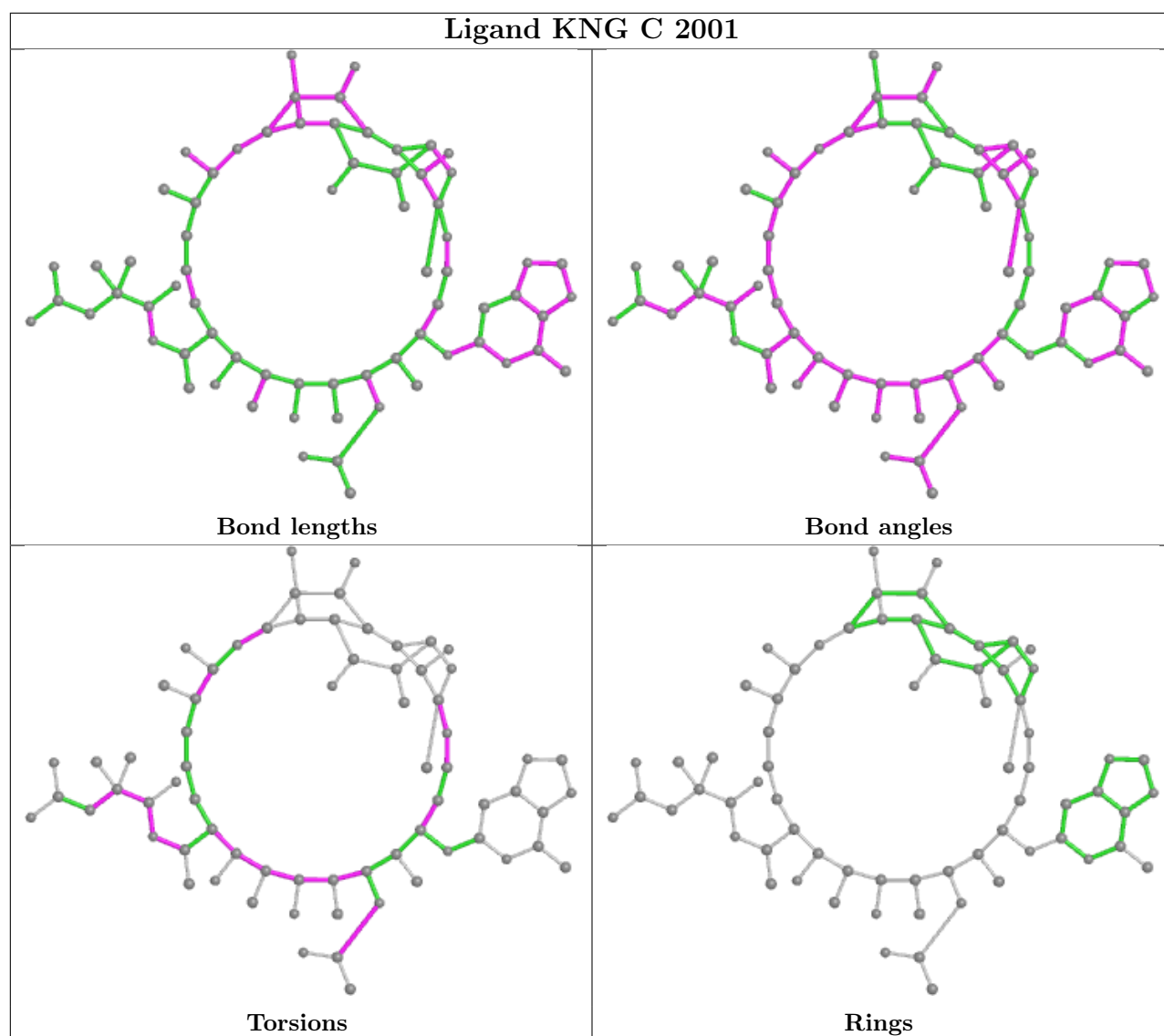
Mol	Chain	Res	Type	Atoms
6	C	2001	KNG	C21-C22-C23-O19
6	C	2001	KNG	O19-C23-C24-C25
6	C	2001	KNG	O19-C23-C24-C33
6	C	2001	KNG	C23-C24-C25-C26
6	C	2001	KNG	C23-C24-C25-O07

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2001	KNG	10	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	227/329 (68%)	-0.31	0 100 100	160, 212, 279, 349	0
1	B	214/329 (65%)	-0.19	4 (1%) 66 58	155, 250, 349, 390	0
1	G	224/329 (68%)	-0.28	2 (0%) 84 77	194, 274, 328, 348	0
1	H	215/329 (65%)	0.09	8 (3%) 41 33	247, 309, 348, 370	0
2	C	1339/1342 (99%)	-0.21	17 (1%) 77 68	124, 208, 314, 382	0
2	I	1328/1342 (98%)	-0.13	31 (2%) 60 51	186, 241, 336, 473	0
3	D	1166/1407 (82%)	-0.29	4 (0%) 94 90	129, 188, 298, 360	0
3	J	1155/1407 (82%)	-0.20	15 (1%) 77 68	164, 229, 312, 374	0
4	E	89/91 (97%)	-0.10	0 100 100	198, 267, 290, 306	0
4	K	79/91 (86%)	0.73	10 (12%) 3 5	329, 403, 484, 493	0
5	F	468/613 (76%)	-0.18	14 (2%) 50 39	156, 283, 413, 445	0
5	L	469/613 (76%)	-0.23	7 (1%) 73 63	193, 275, 393, 414	0
All	All	6973/8222 (84%)	-0.19	112 (1%) 72 62	124, 232, 349, 493	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	9.5
2	I	983	GLY	6.9
2	I	987	GLU	6.3
2	I	980	VAL	5.6
2	I	976	ARG	5.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

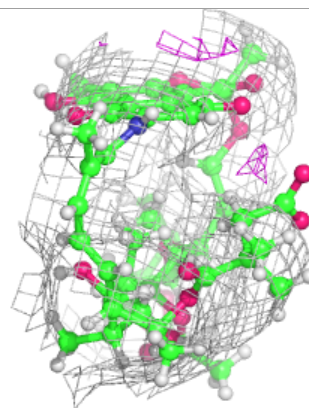
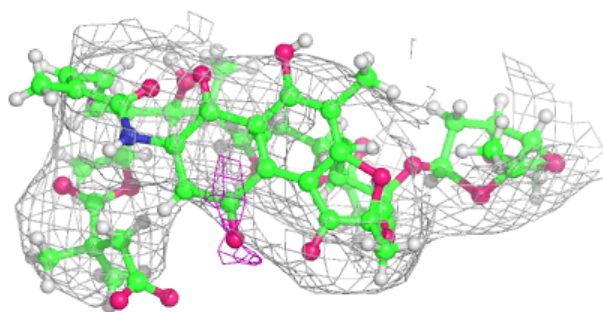
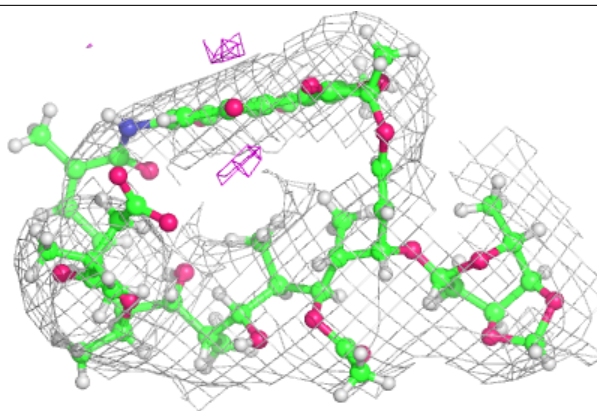
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	KNG	C	2001	70/70	0.93	0.28	155,226,287,292	0
8	ZN	D	1502	1/1	0.95	0.11	192,192,192,192	0
7	MG	J	1501	1/1	0.96	0.34	154,154,154,154	0
8	ZN	J	1502	1/1	0.96	0.06	215,215,215,215	0
7	MG	D	1501	1/1	0.98	0.46	196,196,196,196	0
8	ZN	D	1503	1/1	0.99	0.29	258,258,258,258	0
8	ZN	J	1503	1/1	0.99	0.28	197,197,197,197	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 KNG C 2001:

$2mF_o-DF_c$ (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.