



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:58 PM UTC

PDB ID : 6CUX / pdb\_00006cux  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

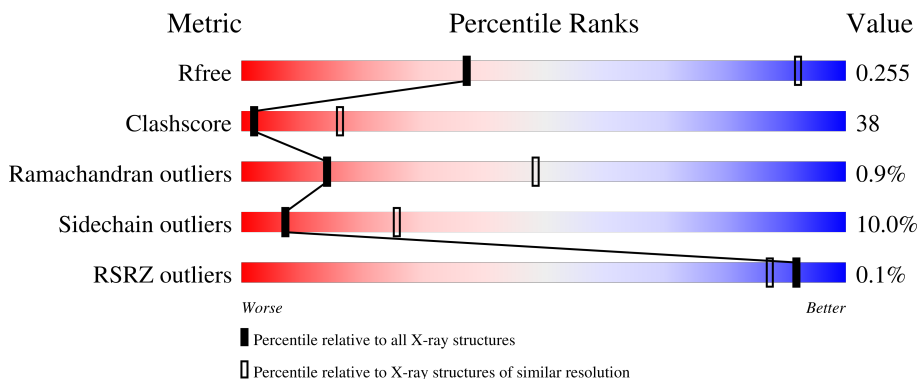
# 1 Overall quality at a glance

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.





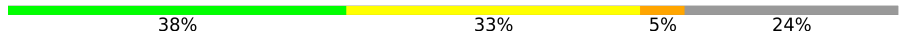
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	 33% 31% 6% 31%
1	B	329	 24% 37% • 35%
1	G	329	 28% 35% 5% 32%
1	H	329	 28% 34% • 35%
2	C	1342	 44% 49% 6%

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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 [i](#)

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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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			

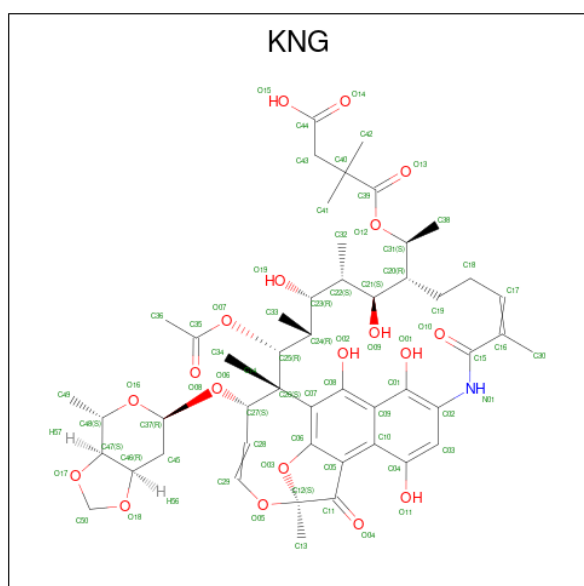
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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 (CCD ID: KNG) (formula: C<sub>50</sub>H<sub>67</sub>NO<sub>19</sub>).



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 (CCD ID: 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		

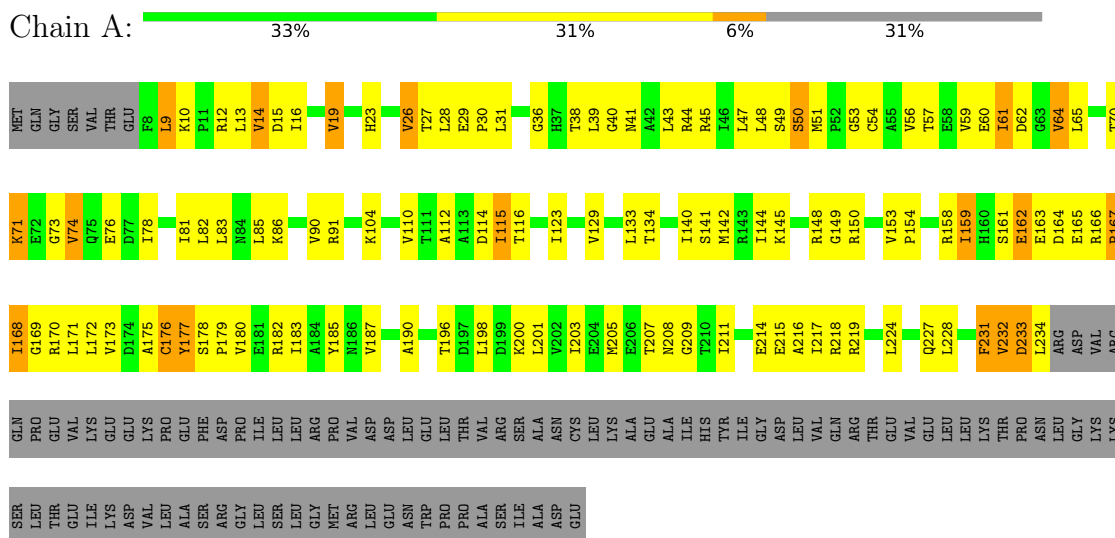
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

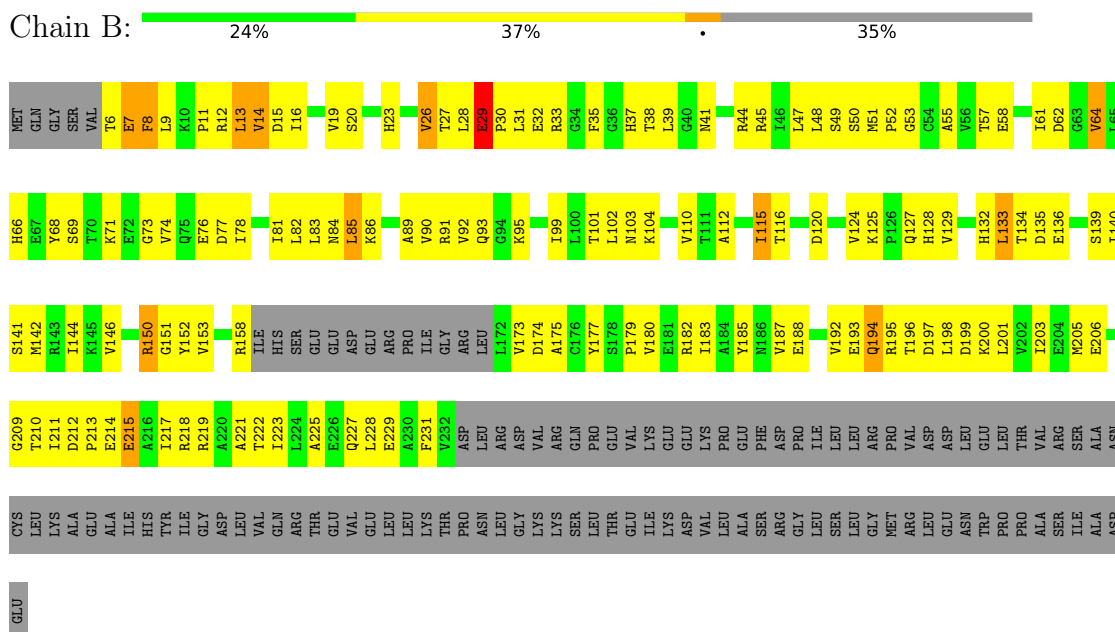
### 3 Residue-property plots [i](#)

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

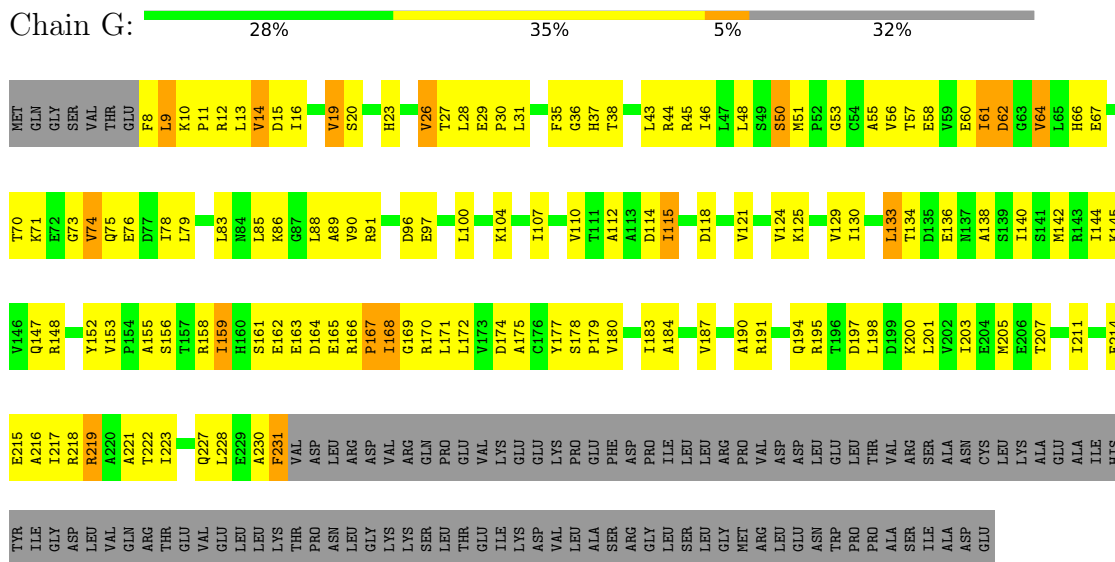
- Molecule 1: DNA-directed RNA polymerase subunit alpha



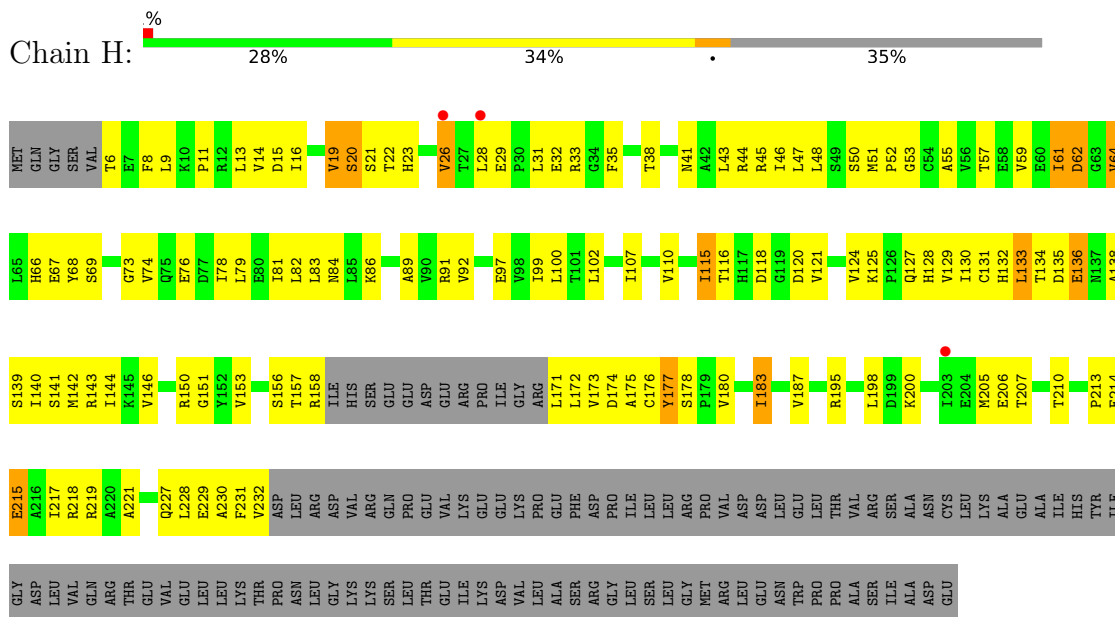
- Molecule 1: DNA-directed RNA polymerase subunit alpha



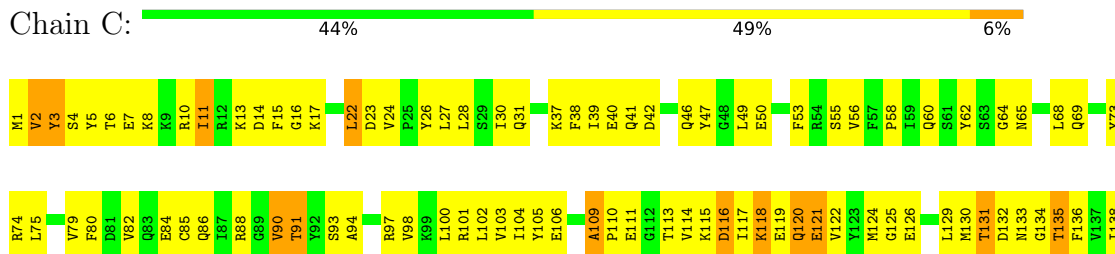
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



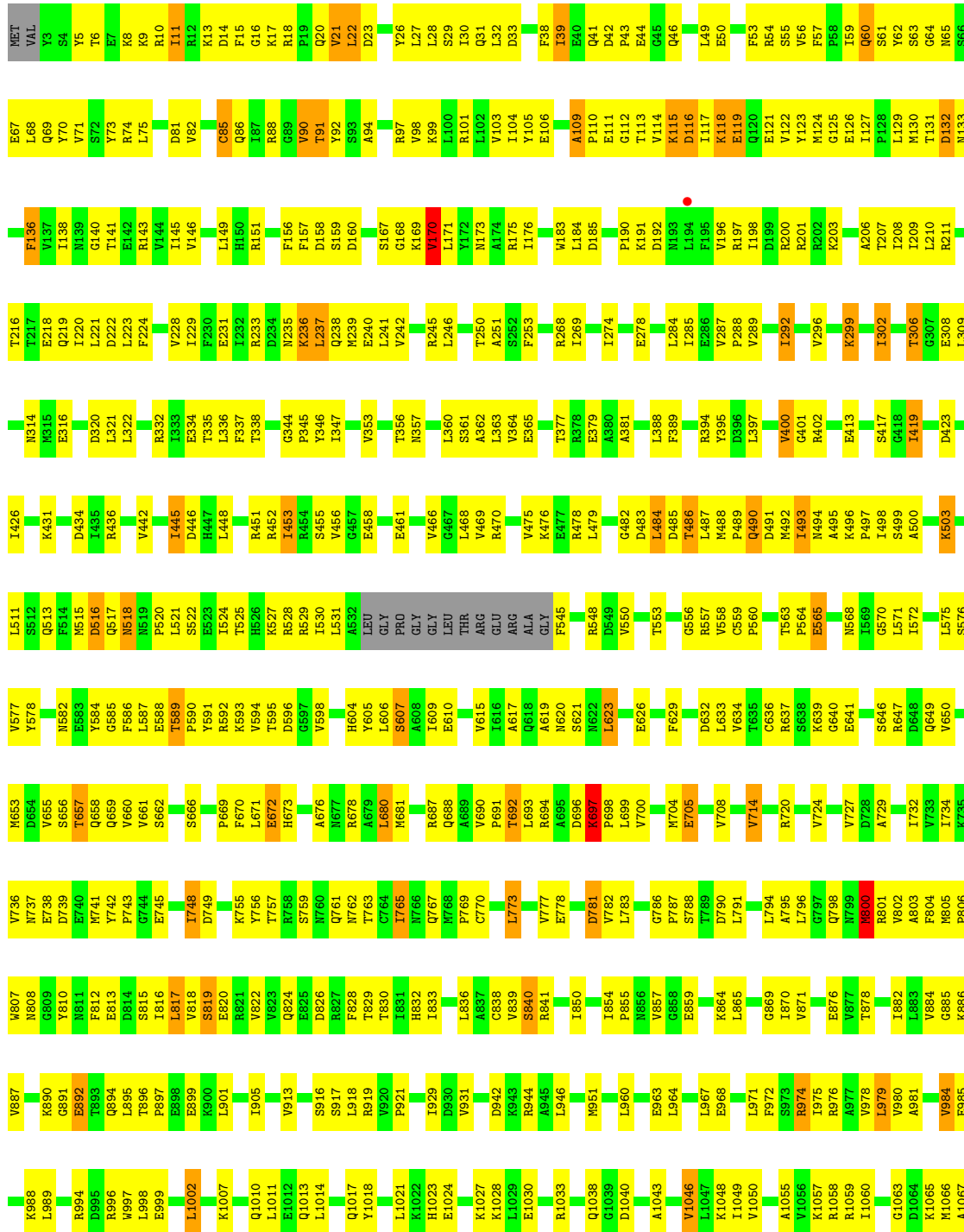
- Molecule 2: DNA-directed RNA polymerase subunit beta



G1218	D1154	I1079	E985	I895	V823	K755	M681	S607	ARG	R465	K369	K299	D222	M139
E1219	V1155	M1060	A986	T896	D826	T756	M684	A608	GLU	V466	M370	D300	L223	G140
E1222	R1156	P1081	E987	F897	R827	T757	M685	F629	ARG	G467	E374	I302	F224	I145
R1223	Q1157	I1082	K988	E988	R828	F758	M686	E610	A643	L468	P375	D303	E226	V146
P1224	E1083	E1083	K991	E989	H832	Q761	Q688	Y614	G544	V469	P376	T306	K227	S147
V1225	V1159	D1084	L992	K900	L836	T762	Q689	V615	F545	R470	T377	G307	V228	Q148
V1227	D1160	M1085	L992	L901	L837	T763	A689	V616	R548	E472	R378	E308	I229	L149
G1228	S1162	P1086	L1002	F906	A837	G764	V690	A617	D549	E308	E379	F230	I229	H150
Y1229	D1088	D1088	K1007	S911	C838	T765	P691	A617	D549	E477	E379	L309	E231	R151
F1229	F1164	M1089	Q1008	S911	W766	T766	T692	Q618	V550	R478	E382	I310	I232	S152
S1165	S1165	Q1008	Q1008	D912	Q767	M768	L693	A619	H551	R478	E382	I310	I232	S152
M1230	S1165	Q1008	Q1008	D912	Q767	M768	L693	A619	H551	R478	E382	I310	I232	S152
M1231	S1165	Q1008	Q1008	D912	Q767	M768	L693	A619	H551	R478	E382	I310	I232	S152
M1232	S1165	Q1008	Q1008	D912	Q767	M768	L693	A619	H551	R478	E382	I310	I232	S152
L1233	V1169	L1011	L1011	Y913	L773	L773	D696	L623	T553	S480	F385	A312	R233	P153
K1234	M1170	L1101	L1014	S916	G774	G774	D696	L623	T553	L481	F390	A315	K236	F156
L1235	R1171	L1014	L1014	S917	E775	E775	D697	F629	G556	D482	F390	A315	L237	F157
M1236	E1015	A1015	E1015	P698	G776	G776	L699	V630	F558	D483	R394	E316	Q238	D158
H1237	E1016	R1016	R1016	R919	E778	E778	L699	E631	C559	L484	R394	E316	M239	S159
L1238	M1175	Q1017	E848	R779	E779	E779	G703	D632	P560	D485	L397	E240	E240	D160
V1239	R1177	Y1018	E849	R779	E780	E780	G704	L633	P561	T486	L397	E240	L241	K161
D1240	K1178	L1021	D851	V924	D781	D781	E705	V634	E562	L487	L320	Y242	L242	G162
K1242	M1180	E1024	R852	V924	L783	L783	E705	V634	E562	M488	L321	Y242	L242	K163
R1246	P1181	K1027	L854	V924	A784	A784	E705	V634	E562	M488	L321	Y242	L242	K163
S1247	I1182	E1027	L854	V924	A784	A784	E705	V634	E562	M488	L321	Y242	L242	K163
T1248	A1183	K1032	L854	V924	A784	A784	E705	V634	E562	M488	L321	Y242	L242	K163
G1249	P1185	E1032	L854	V924	A784	A784	E705	V634	E562	M488	L321	Y242	L242	K163
L1253	M1186	T1037	E860	D942	E792	E792	G713	T635	P564	P489	V400	L322	E244	S167
Y1254	F1187	T1037	E861	D942	E792	E792	G713	T635	P564	P489	V400	L322	E244	S167
T1255	F1188	D1040	R864	A945	L794	L794	G713	T635	P564	P489	V400	L322	E244	S167
Q1256	G1189	D1041	R864	A945	L794	L794	G713	T635	P564	P489	V400	L322	E244	S167
L1259	K1191	E1043	D866	L946	E867	E867	G713	T635	P564	P489	V400	L322	E244	S167
K1262	E1192	P1044	E868	S868	E868	E868	G713	T635	P564	P489	V400	L322	E244	S167
Q1263	E1192	P1044	E868	S868	E868	E868	G713	T635	P564	P489	V400	L322	E244	S167
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Q1267	E1192	P1044	E868	S868	E868	E868	G713	T635	P564	P489	V400	L322	E244	S167
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R1269	E1192	P1044	E868	S868	E868	E868	G713	T635	P564	P489	V400	L322	E244	S167
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G1271	E1192	P1044	E868	S868	E868	E868	G713	T635	P564	P489	V400	L322	E244	S167
E1272	E1192	P1044	E868	S868	E868	E868	G713	T635	P564	P489	V400	L322	E244	S167
M1273	E1192	P1044	E868	S868	E868	E868	G713	T635	P564	P489	V400	L322	E244	S167
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L1327	E1192	P1044	E868	S868	E868	E868	G713	T635	P564	P489	V400	L322	E244	S167
L1328	E1192	P1044	E868	S868	E868	E868	G713	T635	P564	P489	V400	L322	E244	S167
L1329	E1192	P1044	E868	S868	E868	E868	G713	T635	P564	P489	V400	L322	E244	S167
L1330	E1192	P1044</												



• Molecule 2: DNA-directed RNA polymerase subunit beta

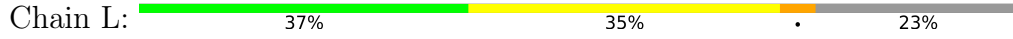




Q736	M821	V885	ALA	LEU	L1138	E1281	M1360	G1376	E16	NET	D67	R137	K296	D329	G333	K341	L342	L343	G344	K345	V346	D348	Y349	S350	G351	K352	S353	V354	I355	T356	V357	G358	Y360	L361	R362	D289	L363	H364	I365	G366	I737	M822	V886	ASN	LYS	L1139	Y1282	V1351	D1368	G17	E16	LYS	D67	V138	R297	D329	G333	K334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	I1210	S1211	P1214	A1215	A1216	P1217	I1220	L1221	R1222	L1223	H1227	T1230	R1231	Y1232	I1233	V1234	N1235	E1236	V1237	Q1238	Y1241	Q1244	G1245	V1246	K1247	I1248	N1249	K1250	K1251	H1252	I1253	E1254	V1255	V1257	M1260	L1261	R1262	K1263	A1264	T1265	I1266	V1267	N1268	D1273	F1274	L1275	E1276	G1277	V1204	E1205	R1206	V1280	V1281	V1282	V1283	V1284	V1285	V1286	V1287	V1288	V1289	V1290	V1291	V1292	V1293	V1294	V1295	V1296	V1297	V1298	V1299	V1300	V1301	V1302	V1303	V1304	V1305	V1306	V1307	V1308	V1309	V1310	V1311	V1312	V1313	V1314	V1315	V1316	V1317	V1318	V1319	V1320	V1321	V1322	V1323	V1324	V1325	V1326	V1327	V1328	V1329	V1330	V1331	V1332	V1333	V1334	V1335	V1336	V1337	V1338	V1339	V1340	V1341	V1342	V1343	V1344	V1345	V1346	V1347	V1348	V1349	V1350	V1351	V1352	V1353	V1354	V1355	V1356	V1357	V1358	V1359	V1360	V1361	V1362	V1363	V1364	V1365	V1366	V1367	V1368	V1369	V1370	V1371	V1372	V1373	V1374	V1375	V1376	V1377	V1378	V1379	V1380	V1381	V1382	V1383	V1384	V1385	V1386	V1387	V1388	V1389	V1390	V1391	V1392	V1393	V1394	V1395	V1396	V1397	V1398	V1399	V1400	V1401	V1402	V1403	V1404	V1405	V1406	V1407	V1408	V1409	V1410	V1411	V1412	V1413	V1414	V1415	V1416	V1417	V1418	V1419	V1420	V1421	V1422	V1423	V1424	V1425	V1426	V1427	V1428	V1429	V1430	V1431	V1432	V1433	V1434	V1435	V1436	V1437	V1438	V1439	V1440	V1441	V1442	V1443	V1444	V1445	V1446	V1447	V1448	V1449	V1450	V1451	V1452	V1453	V1454	V1455	V1456	V1457	V1458	V14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MET	ASP	I127	ASP	M273	K343	R423	M607	E585	E586	E587	A592	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613	
GLU	ALA	M128	GLU	M276	L344	I423	E508	R586	I587	A592	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613		
GLN	ASP	Q129	ASP	M277	I347	T429	I511	R586	I587	A592	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613		
ASN	ASP	V130	ASP	M277	E348	I435	D513	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
PRO	LEU	Q131	MET	V280	T351	I436	D514	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLN	LEU	C132	LEU	R281	G352	R436	E515	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
SER	ALA	S133	ALA	R281	T354	Q437	E515	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLN	GLU	V134	GLU	E284	T354	A438	H518	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
LEU	ASN	E136	ASN	R285	T354	I439	L519	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
LYS	THR	E137	THR	R285	T354	I439	L519	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
LEU	ALA	Y137	ALA	R286	V358	R441	L519	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
VAL	ASP	I141	ASP	I287	R359	S442	L519	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
THR	GLU	T142	GLU	M288	D860	I443	E524	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLY	ASP	Y143	ASP	K289	I361	A444	L530	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLY	ARG	Y143	ARG	L290	N362	D445	P531	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
LYS	ALA	L144	ALA	C291	R363	Q446	L532	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLU	GLU	Q147	GLU	V292	R364	A447	D533	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLN	ALA	D149	ALA	E293	M365	R448	T536	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLY	ALA	R150	ALA	Q294	S866	I449	L540	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
TYR	ALA	E154	ALA	C295	I372	I450	L540	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
LEU	GLN	VAL	GLN	K296	A372	R451	L544	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
THR	LEU	E154	LEU	M297	I457	I457	T544	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
TYR	VAL	L161	VAL	P298	K462	V547	V547	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ALA	SER	I162	SER	K299	I466	I466	L551	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLU	SER	T163	SER	K299	S467	S467	T552	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
VAL	VAL	G164	VAL	N301	R468	R468	T552	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ASN	GLU	F165	GLU	F302	M379	M379	E555	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ASP	SER	F165	SER	F302	M379	M379	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
HIS	GLU	V166	GLU	L305	E381	E381	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
LEU	ILE	D167	ILE	F306	I382	I382	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
PRO	GLY	D167	GLY	F306	I382	I382	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLU	ARG	T94	ARG	E310	N383	N383	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ASP	ALA	T95	ALA	D313	L384	L384	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ILE	GLU	D96	GLU	T314	R385	R385	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
VAL	VAL	P97	VAL	T314	R385	R385	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ASP	ASP	P97	ASP	W315	V387	V387	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
SER	SER	V98	SER	F316	I388	I388	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ASP	ASP	R99	ASP	R317	S389	S389	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ASP	ALA	M100	ALA	A318	I390	I390	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLN	THR	Y101	THR	A318	I390	I390	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ILE	ALA	M102	ALA	I320	K392	K392	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLU	THR	R103	THR	A321	T244	T244	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ILE	THR	E104	THR	M322	E247	E247	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ILE	VAL	M106	VAL	M322	E247	E247	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLN	GLY	V108	GLY	M323	E248	E248	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
MET	SER	V108	SER	K324	L249	L249	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ILE	ILE	L111	ILE	P325	K251	K251	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ASN	LEU	L111	LEU	W326	L252	L252	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ASP	SER	E114	SER	K329	S253	S253	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
MET	GLN	G115	GLN	L330	E254	E254	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLY	GLU	D118	GLU	V333	Q257	Q257	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ILE	ILE	I119	ILE	S334	Q258	Q258	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
VAL	ASP	D118	ASP	S334	Q258	Q258	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
MET	ASP	I119	ASP	V337	F259	F259	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLU	ASP	R122	ASP	H338	R260	R260	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
GLU	GLU	I123	GLU	L341	L261	L261	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
ALA	ASP	E124	ASP	L341	V262	V262	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					
PRO	GLU	I124	GLU	Q342	D267	D267	A556	R596	K597	L598	P601	S602	R603	S604	E605	V606	L607	D612	D613					

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 98.9 (45.03-4.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 4.13Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.210 , 0.255 0.212 , 0.255	Depositor DCC
$R_{free}$ test set	2002 reflections (2.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	190.5	Xtrriage
Anisotropy	0.237	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 206.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	55005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	241.0	wwPDB-VP

Xtrriage'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.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.64	0/1774	1.11	3/2405 (0.1%)
1	B	0.63	0/1668	1.18	2/2260 (0.1%)
1	G	0.44	0/1751	0.85	0/2373
1	H	0.45	0/1678	0.90	0/2274
2	C	0.65	0/10716	1.07	15/14458 (0.1%)
2	I	0.53	0/10653	0.93	6/14373 (0.0%)
3	D	0.70	1/9229 (0.0%)	1.17	11/12459 (0.1%)
3	J	0.58	0/9140	1.03	10/12341 (0.1%)
4	E	0.63	0/693	0.94	0/935
4	K	0.26	0/629	0.54	0/847
5	F	0.49	0/3864	0.89	5/5194 (0.1%)
5	L	0.45	0/3872	0.83	1/5205 (0.0%)
All	All	0.59	1/55667 (0.0%)	1.02	53/75124 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	426	ALA	C-N	-5.45	1.21	1.33

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	42	GLU	CA-CB-CG	7.93	129.96	114.10
5	F	563	PHE	CA-C-N	-7.82	106.09	121.41
5	F	563	PHE	C-N-CA	-7.82	106.09	121.41
1	A	177	TYR	CA-CB-CG	7.31	127.06	113.90
3	D	344	GLY	CA-C-N	6.46	133.88	121.54

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

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	158	0
1	B	1649	0	1674	187	0
1	G	1730	0	1756	196	0
1	H	1659	0	1692	176	0
2	C	10548	0	10553	876	0
2	I	10486	0	10496	764	0
3	D	9089	0	9265	796	0
3	J	9001	0	9169	779	0
4	E	691	0	695	40	0
4	K	627	0	634	62	0
5	F	3813	0	3880	275	0
5	L	3821	0	3884	263	0
6	C	70	62	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4146	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 38.

The worst 5 of 4146 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
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
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.30	1.14

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%)	3	25
1	B	210/329 (64%)	186 (89%)	19 (9%)	5 (2%)	4	30
1	G	222/329 (68%)	194 (87%)	23 (10%)	5 (2%)	5	31
1	H	211/329 (64%)	187 (89%)	17 (8%)	7 (3%)	3	24
2	C	1335/1342 (100%)	1226 (92%)	100 (8%)	9 (1%)	18	55
2	I	1324/1342 (99%)	1220 (92%)	96 (7%)	8 (1%)	21	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1162/1407 (83%)	1068 (92%)	86 (7%)	8 (1%)	18	55
3	J	1151/1407 (82%)	1060 (92%)	78 (7%)	13 (1%)	11	44
4	E	87/91 (96%)	82 (94%)	4 (5%)	1 (1%)	11	44
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	426 (92%)	35 (8%)	1 (0%)	43	76
5	L	463/613 (76%)	426 (92%)	36 (8%)	1 (0%)	43	76
All	All	6929/8222 (84%)	6347 (92%)	517 (8%)	65 (1%)	14	49

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 [i](#)

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%)	179 (92%)	15 (8%)	12	34
1	B	182/286 (64%)	171 (94%)	11 (6%)	17	42
1	G	191/286 (67%)	177 (93%)	14 (7%)	13	36
1	H	184/286 (64%)	175 (95%)	9 (5%)	22	46
2	C	1151/1157 (100%)	1035 (90%)	116 (10%)	7	25
2	I	1147/1157 (99%)	1034 (90%)	113 (10%)	7	26
3	D	970/1168 (83%)	859 (89%)	111 (11%)	5	21
3	J	960/1168 (82%)	852 (89%)	108 (11%)	5	22
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	19
4	K	67/75 (89%)	62 (92%)	5 (8%)	12	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	417/540 (77%)	375 (90%)	42 (10%)	7	25
5	L	418/540 (77%)	376 (90%)	42 (10%)	7	26
All	All	5953/7024 (85%)	5358 (90%)	595 (10%)	7	26

5 of 595 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	374	LEU
5	L	471	LEU
3	J	514	THR
3	J	363	LEU
3	J	881	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	409	ASN
3	J	1366	HIS
2	I	165	HIS
3	J	1279	GLN
5	L	345	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	3.81	30 (40%)	107,114,114	2.95	42 (39%)

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 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2001	KNG	O18-C46	-14.51	1.20	1.44
6	C	2001	KNG	O03-C06	10.20	1.56	1.37
6	C	2001	KNG	O17-C47	-10.11	1.21	1.43
6	C	2001	KNG	C04-C10	9.74	1.59	1.43
6	C	2001	KNG	O16-C37	7.88	1.62	1.42

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2001	KNG	C34-C26-C27	-8.81	93.15	110.95
6	C	2001	KNG	C49-C48-C47	8.72	126.36	113.39
6	C	2001	KNG	C25-C26-C27	7.51	132.41	111.99
6	C	2001	KNG	C24-C23-C22	7.51	127.92	115.41
6	C	2001	KNG	O07-C35-C36	7.06	123.69	111.09

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

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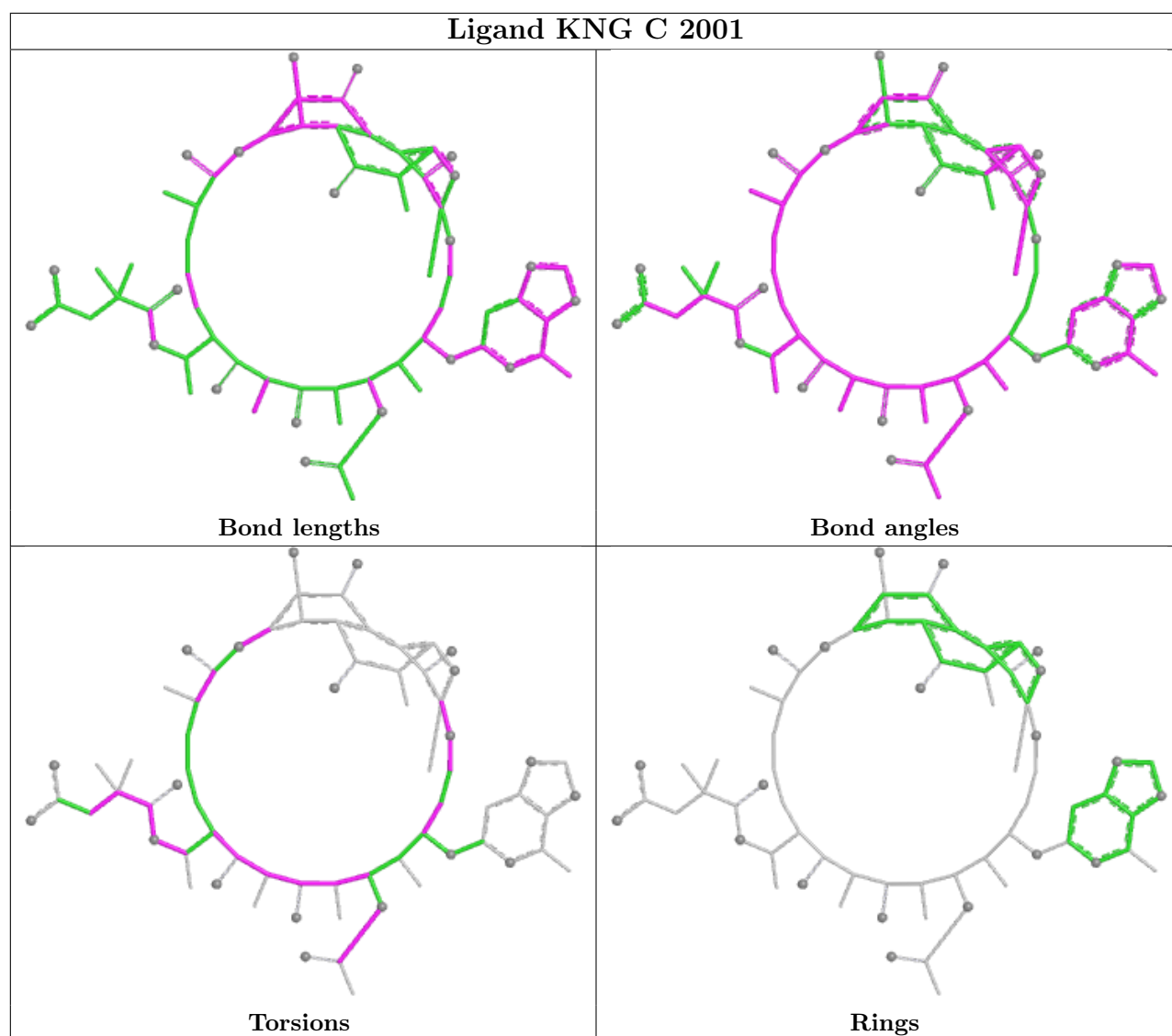
Mol	Chain	Res	Type	Atoms
6	C	2001	KNG	O19-C23-C24-C25
6	C	2001	KNG	O19-C23-C24-C33
6	C	2001	KNG	C23-C24-C25-C26
6	C	2001	KNG	C23-C24-C25-O07

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	227/329 (68%)	-0.66	0 100 100	160, 212, 279, 349	0
1	B	214/329 (65%)	-0.61	0 100 100	155, 250, 349, 390	0
1	G	224/329 (68%)	-0.73	0 100 100	194, 274, 328, 348	0
1	H	215/329 (65%)	-0.56	3 (1%) 73 56	247, 309, 348, 370	0
2	C	1339/1342 (99%)	-0.66	0 100 100	124, 208, 314, 382	0
2	I	1328/1342 (98%)	-0.70	1 (0%) 92 87	186, 241, 336, 473	0
3	D	1166/1407 (82%)	-0.69	0 100 100	129, 188, 298, 360	0
3	J	1155/1407 (82%)	-0.71	0 100 100	164, 229, 312, 374	0
4	E	89/91 (97%)	-0.72	0 100 100	198, 267, 290, 306	0
4	K	79/91 (86%)	-0.78	0 100 100	329, 403, 484, 493	0
5	F	468/613 (76%)	-0.75	0 100 100	156, 283, 413, 445	0
5	L	469/613 (76%)	-0.75	0 100 100	193, 275, 393, 414	0
All	All	6973/8222 (84%)	-0.69	4 (0%) 92 87	124, 232, 349, 493	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	203	ILE	3.5
1	H	28	LEU	2.7
1	H	26	VAL	2.4
2	I	194	LEU	2.0

### 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](#)

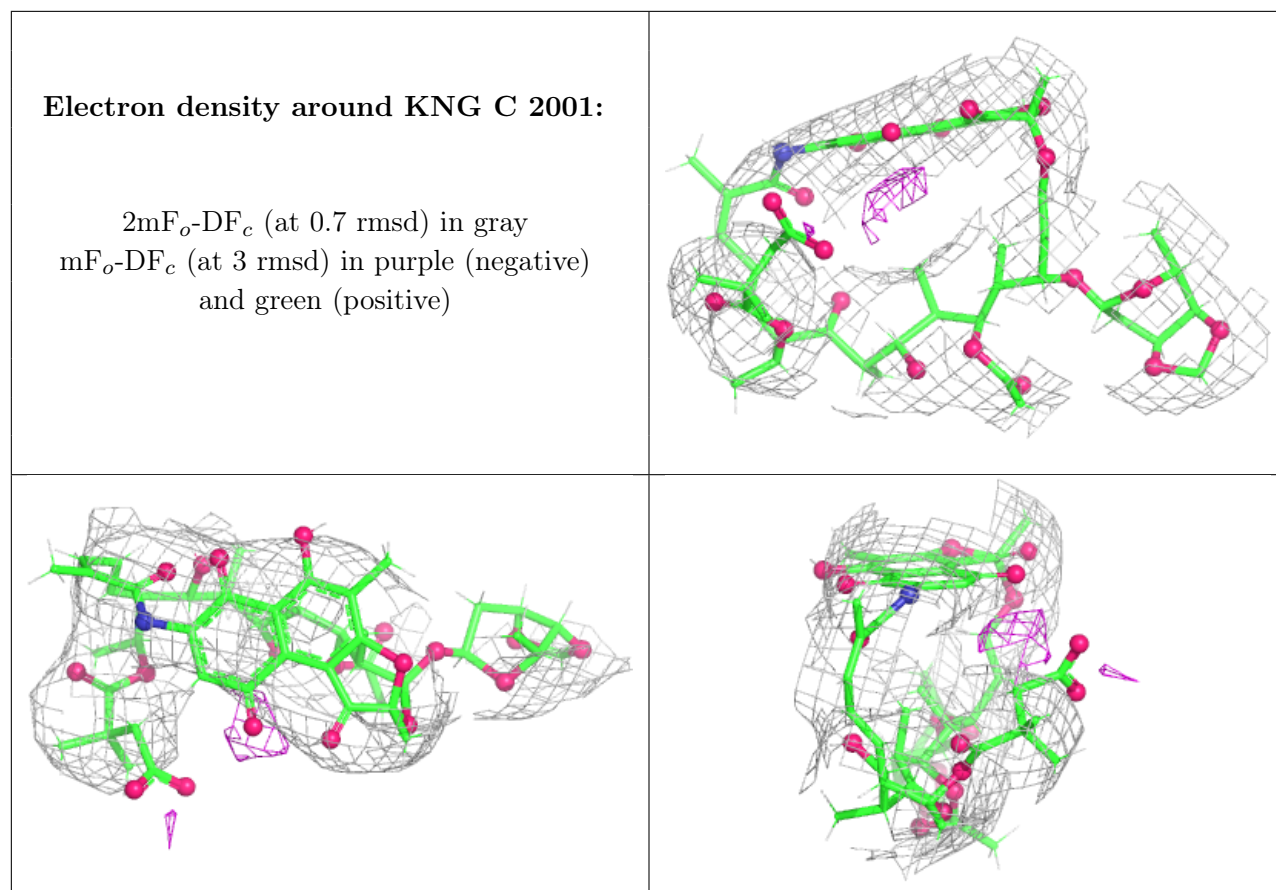
There are no oligosaccharides in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MG	J	1501	1/1	0.87	0.10	154,154,154,154	0
6	KNG	C	2001	70/70	0.88	0.07	155,226,287,292	0
7	MG	D	1501	1/1	0.94	0.08	196,196,196,196	0
8	ZN	J	1502	1/1	0.99	0.02	215,215,215,215	0
8	ZN	D	1503	1/1	1.00	0.04	258,258,258,258	0
8	ZN	D	1502	1/1	1.00	0.03	192,192,192,192	0
8	ZN	J	1503	1/1	1.00	0.03	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.