



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:38 PM GMT

PDB ID : 2PPB
Title : Crystal structure of the T. thermophilus RNAP polymerase elongation complex with the ntp substrate analog and antibiotic streptolydigin
Authors : Vassilyev, D.G.; Vassilyeva, M.N.; Artsimovitch, I.; Landick, R.
Deposited on : 2007-04-28
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

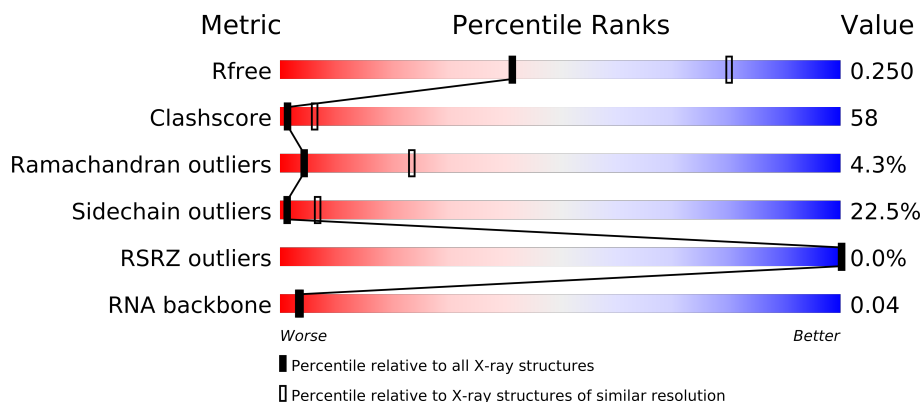
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




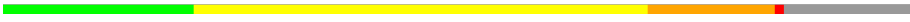
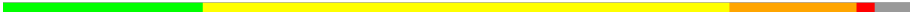

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	G	23	
1	X	23	
2	H	16	
2	Y	16	
3	I	14	
3	Z	14	
4	A	315	
4	B	315	
4	K	315	
4	L	315	
5	C	1119	
5	M	1119	

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Mol	Chain	Length	Quality of chain
6	D	1524	
6	N	1524	
7	E	99	
7	O	99	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 51962 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a DNA chain called DNA (5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			
1	X	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			

- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			
2	Y	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			
3	Z	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
4	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
4	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 5 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
5	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

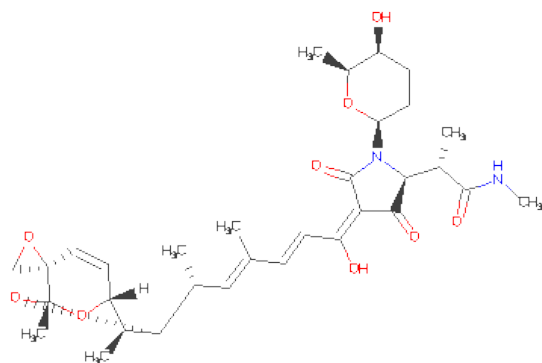
- Molecule 6 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	1314	Total	C	N	O	S	0	0	0
			10373	6565	1838	1937	33			
6	N	1314	Total	C	N	O	S	0	0	0
			10373	6565	1838	1937	33			

- Molecule 7 is a protein called DNA-directed RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			
7	O	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

- Molecule 8 is STREPTOLYDIGIN (three-letter code: STD) (formula: C₃₂H₄₄N₂O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			43	32	2	9		
8	N	1	Total	C	N	O	0	0
			43	32	2	9		

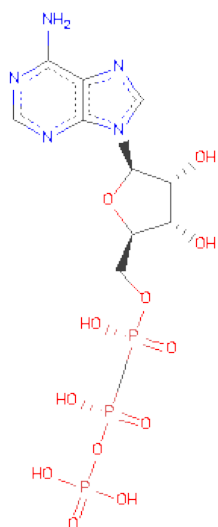
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		
9	N	2	Total	Zn	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Mg	0	0
			2	2		
10	N	2	Total	Mg	0	0
			2	2		

- Molecule 11 is DIPHOSPHOMETHYLPHOSPHONICACID ADENOSYL ESTER (three-letter code: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
11	M	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	78	Total	O	0	0
			78	78		
12	B	117	Total	O	0	0
			117	117		
12	C	408	Total	O	0	0
			408	408		
12	D	531	Total	O	0	0
			531	531		
12	E	34	Total	O	0	0
			34	34		
12	G	39	Total	O	0	0
			39	39		
12	H	22	Total	O	0	0
			22	22		
12	I	31	Total	O	0	0
			31	31		
12	K	81	Total	O	0	0
			81	81		
12	L	95	Total	O	0	0
			95	95		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	396	Total 396	O 396	0	0
12	N	510	Total 510	O 510	0	0
12	O	53	Total 53	O 53	0	0
12	X	31	Total 31	O 31	0	0
12	Y	26	Total 26	O 26	0	0
12	Z	18	Total 18	O 18	0	0

3 Residue-property plots

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

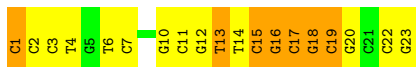
- Molecule 1: DNA (5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3')

Chain G: 



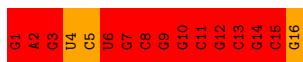
- Molecule 1: DNA (5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3')

Chain X: 



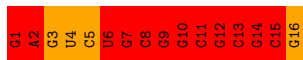
- Molecule 2: RNA (5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3')

Chain H: 



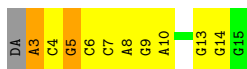
- Molecule 2: RNA (5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3')

Chain Y: 



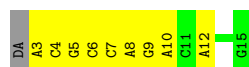
- Molecule 3: DNA (5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3')

Chain I: 



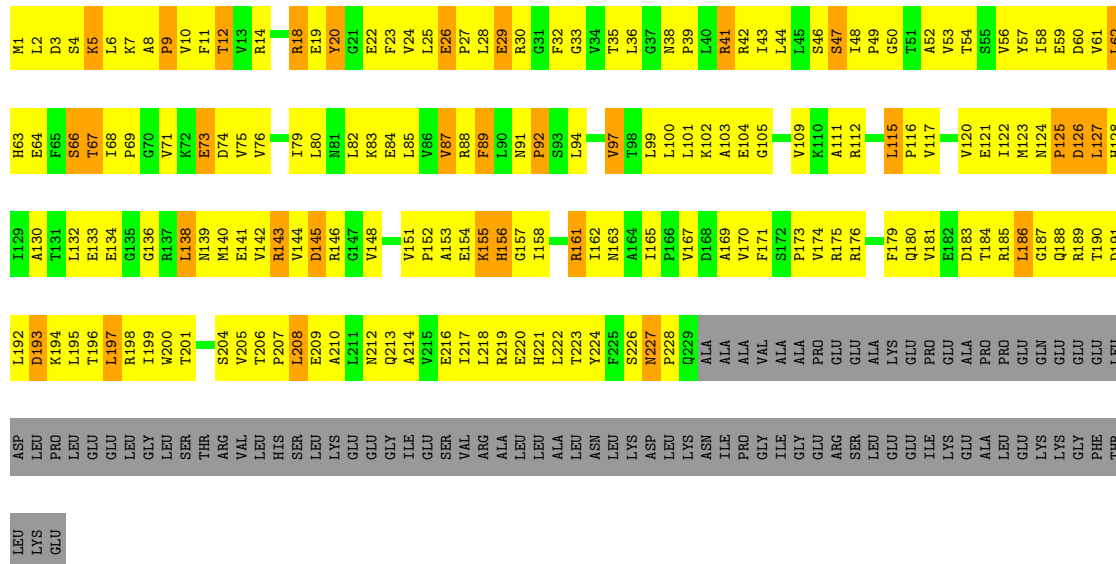
- Molecule 3: DNA (5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3')

Chain Z: 



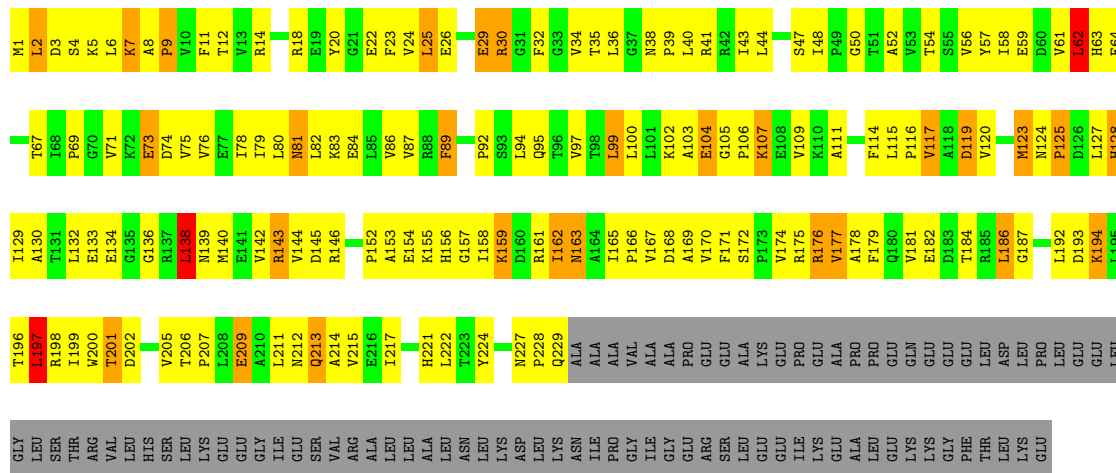
• Molecule 4: DNA-directed RNA polymerase alpha chain

Chain A:



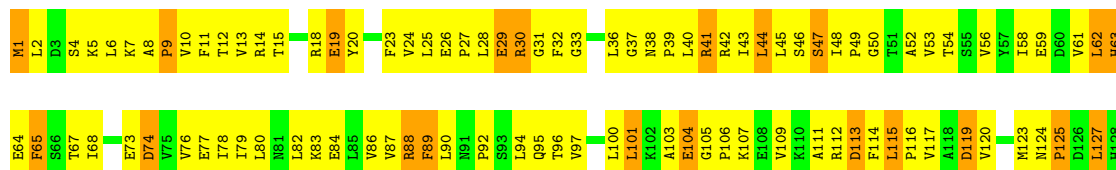
• Molecule 4: DNA-directed RNA polymerase alpha chain

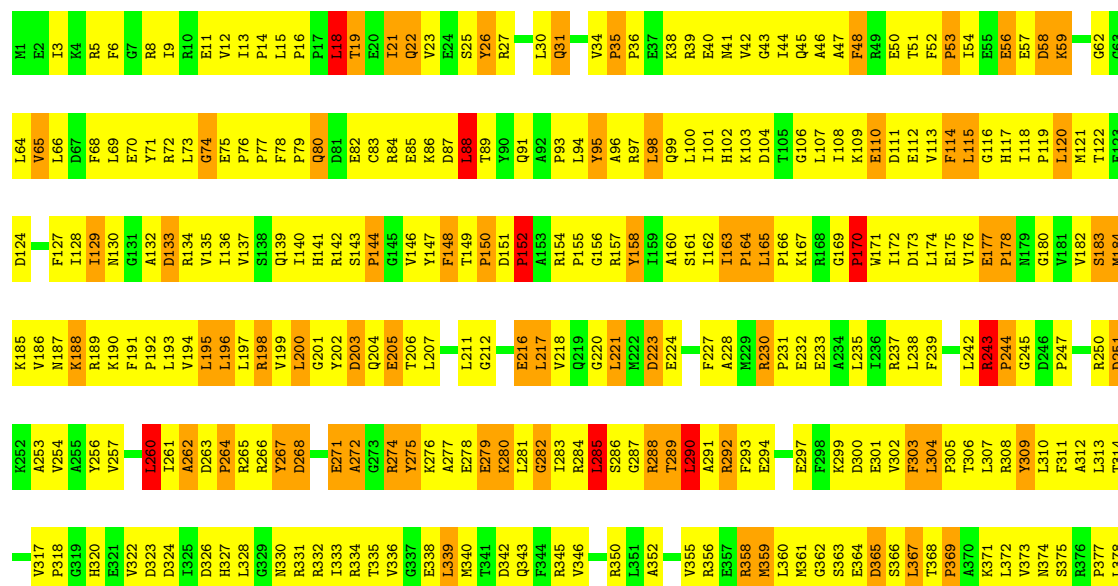
Chain B:

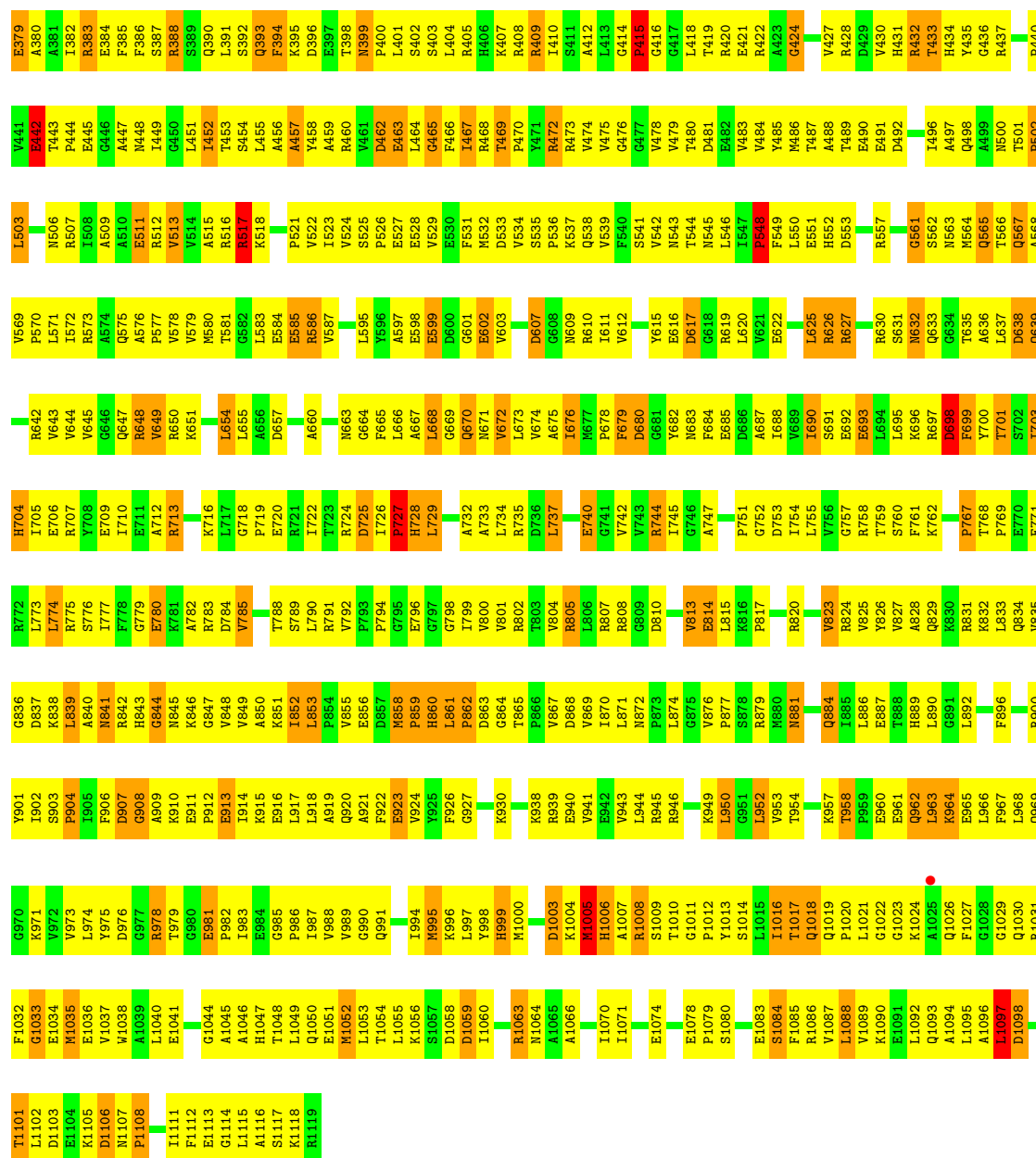


• Molecule 4: DNA-directed RNA polymerase alpha chain

Chain K:









E1152	A1085	P1019	D953	E893	A825	I761	I695	I631	N569	S505	V443	P193	E1127
V1153	L1086	L1020	A954	E894	F826	Q762	V632	V632	E570	G506	V444	GLU	Y128
E1154	L1087	Y1021	V955	K934	I827	M763	K698	Q636	K571	N507	R445	GLU	F129
V1155	T1088	Y1022	V956	K935	K828	L764	V699	Q637	R572	R508	V446	GLU	S130
L1156	A1089	M1023	A957	A896	W829	S765	V700	L637	M573	P509	V447	GLY	K131
	D1090	A1024	E958	V897	A830	A766	L701	K638	L574	E510	E448	VAL	Y132
R1159	Y1093	Q1025	E959	E898	G831	H767	L702	L639	Q575	W511	S449	VAL	I133
L1160	L1094	S1026	K960	L899	R832		M703	H640	E576	M512	Y450	VAL	I134
E1161	L1094	G1027	K961	I900	E833	L770	R704	Q641	A577	I513	D451	GLN	V135
E1162	T1095	A1028	Q962	Q901	T834	S771	A705	C642	V578	L514	I452	VAL	D136
G1163	R1096	G1029	Y963	L902	S835	P772	P706	G643	D579	E515	D453	GLU	A203
R1164	K1097	G1030	L964	D903	V836	A773	T707	L644	A580	A516	A454	ALA	L204
L1165	L1098	G1031	E965	V904	C837	S774	L708	P645	L581	V517	R455	GLU	K138
L1166	V1099	P1032	E966	P905	R838	G775	H709	K646	L582	P518	K486	GLU	G139
S1167	D1100	Q1033	Q906	Q906	K839	E776	R710	R647	D583	V519	G457	GLY	Q205
M1168	V1101	Q1034	E907	E907	R840		L711	M648	M584	L520	A458	GLU	R206
D1169	T1102	Q1037	R969	K970	Y841	A779	R703	A649	R587	P522	A460	THR	P207
L1170	L1105	L1038	K970	K908	Y842	K780	Q714	L650		R521	A461	PHE	L142
V1171	V1106	C1039	L972	S910	F843	S781	A715	E651		D523	I461	VAL	G144
H1172	V1107	G1039	Q973	L911	A844	S782	F716	L652	P580	L524	Q462	VAL	V145
L1173	L1108	G1040	I974	K912	R845	R783	Q717	F653	V591	R525	Q463	ARG	P146
L1174	E1108	L1041	E975	D913	F846	H784	P718	K654	T592	P526	L464	GLU	E148
I1175	E1109	R1042	Q976	L914	D847	I785	V719	P655	M593	M527	L465	GLU	K149
K1176	A1110	Q1046	A977	V915	E848	L786	L720	F656	P594	V528		VAL	R150
A1177	D1111	K1047	Y978	Y916	A849	L787		L657	G595	Q529	L468	LYS	Q151
A1178	C1112	K1047	E979	Q917	L850	G788	G723	L658	S596	V530	D489	LYS	L152
E1179	E1179	P1048		A918	L851	L789	Q724	K659	D597	D531	L470	GLU	L153
A1180	T1114	S1048	L983	F919	A852	Y790	S725	K660	R598	G532	E471	ALA	E157
G1181	T1115	G1050	T984	L920	W853	I791	I726	M661	P599	G533	A472	ALA	Y158
E1182	N1116	E1051	D985	R921	H847	I792	Q727	G662	L600	R534	L473	PRO	E159
I1183	Y1117	T1052	R986	L922	V858	T793	L728	K663	R601	F535	E474	LYS	R169
Q1184	L1118	F1053	E987	G923	P859	Q794	H729	K664	S602	A536	E475	LEU	E160
E1185	S1119	P1056	R988	M924	L860	V795	P730	G665	L603	T537	E476	LEU	L161
P1187	V1188	V1057	E989	K926	D862	R796	L731	I666	T604	S538	L477	PRO	R162
R1189	F1123	S1058	Q991	T927	W863	K799	E734	N669	I606	D605	L478	LEU	Y163
S1190	Q1124	S1060	I992	A928	V864	K800	A735	V670	L607	D542	E479	ALA	G164
P1191	P1125	F1061	L993	R929	T865	G801	F736	K671	S608	L543	E480	ALA	K165
L1192	D1126	R1062	Q994	L930	V866	A902	N737	A672	G609	T544	K481	TRP	Q166
T1193	E1127	E1063	W996	D932	R867	G803	A738	A673	K610	R545	K482	VAL	E167
C1194	V1128	G1064	T997	A933	Y868	L804	F739	R674	Q611	R546	P484	VAL	Y169
Q1195	T1129	L1065	E998	L934	M869	E905	F740	R675	G612	L547	S485	GLY	
T1196	T1066	V1067			B872	F806	D741	M676	R613	I548	A487	ALA	P172
R1197	L1134	L1067	E1001	Y937	L873	T808	D743	E678	R614	N549	D439	TYR	
Y1198	R1135	E1069	K1002	G938	E874	P809	Q744	E679	R615	R550	V420	LYS	V175
G1199	V1200	Y1070	V1003	F939	T875		M745	Q680	Q616	N551	L421	PRO	D176
V1201	A1138	F1071	T1004	F941	S876	A812	A746	R681	L618	N552	A422	GLY	A177
Q1202	D1139	I1072	Q1005	S942	P877	L813	V747	D682	L619	R553	K491	GLU	L178
K1203	I1140	H1075	A1006	T943	C878	A814	H748	I683	G620	K555	R493	ILE	V179
C1204	L1144	R1078	N1010	T944	R879	A815	V749	K684	K621	R556	K494	GLN	K180
Y1205	Y1145	G1206	F1011	S945	L881	H816	P750	E686	R622		R435	ALA	D181
Y1207	G1146	K1079	E1012	I947	F882	E817	L751	G688	V623	A562	V435	GLY	R182
D1208	R1147	G1080	Y1015	T948	T885	G820	F754	W689	G626	P563	E436	LEU	E183
L1209	V1148	G1081	P1016	I949	V886	V821		K689	G627	I565	F502	PRO	E184
S1210	L1149	A1082	F1017	G950	A897	A822	E758	A690	R628	I566	V440	GLU	V185
M1211	A1150	D1083	I951	I951		L823	A759	L691	S629		R441	LYS	Q189
A1212	R1151	T1084	N1018	D952	W890	N824	R760	V694	V630	R568	D504	ARG	E190
													L191
													PHE
													LEU
													ARG

GLY	L1459	L1395	D1331	P1268	D1208	L1144	K1079	M1018	D953	A887	E820	A757	T695
LYS	I1460	E1396	P1332	K1269	L1209	Y1145	A1082	P1019	A954	E891	V621	E758	H696
GLN	G1461	K1397	L1335	A1272	M1211	G1146	T1083	L1020	P955	E891	A822	A759	G697
ALA	L1462	M1398	L1336	V1273	A1212	T1147	T1084	L1021	P956	E892	L1823	A760	K698
	K1463	D1399	E1337	V1274	R1213	V1148	A1085	V1022	P957	E893	K824	I761	V699
	E1464	V1400	E1338	S1275	R1214	V1149	L1086	M1023	P958	E894	A825	I762	V700
	M1465	E1401	A1339	S1276	V1215	A1150	R1087	M1026	P959	E895	P826	I763	L701
	V1466	A1402	K1340	I1277	S1216	R1151	D1090	S1026	K960	E896	I827	L764	L702
	L1467	L1403	G1340	D1278	I1217	E1154	A1093	G1027	P961	E897	K828	S765	N703
	L1468	P1341	E1342	G1279	G1218	V1155	V1093	A1028	P962	E898	V829	A766	R704
	G1469	E1405	R1343	V1280	E1219	V1156	L1094	R1029	P963	E899	A830	H767	A705
	R1470	R1406	A1344	V1281	A1220	L1157	L1095	G1030	P964	E900	G831	N768	P706
	L1471	L1407	V1344	V1282	V1221	G1157	T1096	M1031	P965	E901	R832	N769	T707
	L1472	E1408	E1345	E1283	G1222	V1158	K1097	P1032	P966	E902	E833	L770	L708
	P1473	A1409	R1346	I1284	I1223	R1159	L1098	G1033	P967	E903	T834	S771	H709
	L1474	E1410	G1347	E1285	V1224	V1160	V1099	L1035	P968	E904	V836	A773	R710
	G1475	G1411	V1349	T1286	A1225	E1161	V1105	G1040	P969	E905	G837	A774	L711
	R1476	K1412	E1350	E1287	A1226	F1162	L1041	R1036	P970	E906	R838	S774	G712
	L1477	T1413	E1351	E1288	Q1227	G1163	V1101	Q1037	P971	E907	L839	G775	I713
	G1478	V1414	L1352	E1289	S1228	T1164	T1102	L1038	P972	E908	L911	E776	Q714
	S1479	P1415	K1353	R1289	I1229	Y1165	H1103	C1039	P973	E909	K912	P777	A715
	D1479	A1416	V1354	S1291	G1230	L1166	E1104	G1040	P974	E910	D913	L778	F716
	F1480	A1417	V1355	E1292	E1231	S1167	T1105	L1041	P975	E911	L914	A779	Q717
	V1481	P1419	Y1356	F1293	E1232	M1168	V1106	R1042	P976	E912	V915	K780	P718
	R1482	L1420	R1357	F1294	G1233	D1169	V1107	G1043	P977	E913	K844	P781	V719
	F1483	L1421	A1358	E1295	G1234	V1170	T1108	L1044	P978	E914	R845	S782	L720
	T1484	E1485	Q1359	E1296	Q1235	V1171	E1109	M1045	P979	E915	P946	R783	V721
	Q1486	V1486	G1360	S1296	L1236	L1171	R1110	A1046	P980	E916	D847	R784	E722
	L1487	T1425	V1361	E1297	L1237	L1174	D1111	K1047	P981	E917	E848	I785	G723
	D1488	K1426	K1362	G1298	T1237	L1175	C1112	P1048	P982	E918	L920	I786	Q724
	Q1489	S1427	L1363	F1299	M1238	K1176	G1113	S1049	P983	E919	L850	L787	S725
	K1490	A1428	H1364	S1300	E1239	A1177	T1114	G1050	P984	E920	L851	Q788	L726
	L1491	L1429	K1365	K1301	T1240	A1178	T1115	E1051	P985	E921	V858	L789	Q727
	F1492	S1430	H1366	E1302	H1242	E1179	Y1116	F1052	P986	E922	D859	Y790	L728
	K1493	T1431	H1367	F1303	T1243	E1183	Y1117	F1053	P987	E923	L860	I792	H729
	A1494	K1434	E1368	K1304	GLY	L1183	L1118	E1054	P988	E924	Q861	T793	L731
	I1495	S1433	E1369	L1305	GLY	Q1184	S1119	V1055	D990	E925	L930	Q794	V732
	E1496	W1434	L1370	P1306	VAL	E1185	V1120	P1056	P991	E926	L931	R795	C733
	E1497	T1443	V1371	P1307	ALA	V1186	P1121	V1057	P992	E927	D932	K799	A735
	A1498	S1436	R1372	E1307	GLY	P1187	L1122	R1058	P993	E928	L934	K800	F736
	R1499	A1437	R1373	Q1374	ALA	V1188	F1123	S1059	Q994	E929	V866	E737	N737
	K1500	A1438	Q1375	M1375	ALA	L1189	Q1124	S1060	L995	E930	Y867	A738	A738
	S1439	F1440	E1376	E1379	D1251	S1190	P1125	F1061	P996	E931	Y868	D739	D739
	Q1441	Q1441	Y1378	K1314	L1252	P1191	D1126	R1062	T999	E932	H869	L804	F740
	N1442	N1442	V1379	D1315	T1253	C1194	E1127	E1063	P999	E933	G870	E805	D741
	T1443	E1380	E1380	G1316	Q1254	C1195	V1128	G1064	T1000	E934	K871	F806	G742
	T1444	V1381	D1317	D1317	G1255	T1196	T1129	L1065	T1001	E935	L873	A807	D743
	H1445	T1382	T1382	V1318	L1256	R1197	R1130	T1066	K1002	E936	F941	T808	Q744
	V1446	D1383	V1319	P1257	P1257	V1198	S1131	V1067	V1003	E937	T943	P809	W745
	A1450	P1384	E1320	R1258	R1258	G1199	L1132	L1068	T1004	E938	T875	E810	A746
	A1451	G1385	A1321	V1259	V1259	G1199	R1133	L1069	Q1005	E939	S876	E811	V749
	I1452	D1386	G1322	L1260	E1261	V1200	L1134	Y1070	P977	E940	S945	A812	P750
	A1453	S1387	Q1323	E1261	E1261	C1201	R1135	F1071	V1007	E941	G946	L813	P750
	G1454	R1388	P1324	L1262	F1263	Q1202	K1136	I1072	F1011	E942	T948	A814	L751
	L1455	L1389	L1325	F1263	E1264	K1203	R1137	E1012	E1012	E943	I949	E817	F754
	K1455	L1390	T1326	E1264	E1265	C1204	A1138	H1075	E1013	E944	T948	R818	A755
	R1456	E1391	R1327	E1265	R1266	Y1205	D1139	G1076	N1014	E945	I949	E819	Q756
	L1457	E1391	R1327	R1266	R1266	I1140	I1140	A1077	E1014	E946	I949	E819	Q756
	E1458	V1394	I1330	I1267	I1267	Y1207	E1141	R1078	Y1015	E947	V886	E819	Q756

• Molecule 7: DNA-directed RNA polymerase omega chain

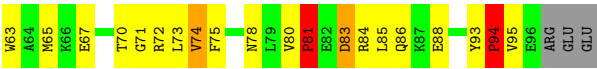
Chain E:

MET	A2	E3	F4	G5	I6	O7	K8	M12	V13	D14	S15	K16	Y17	R18	L19	T20	V21	V22	V23	A24	K25	R26	A27	Q28	Q29	L30	L31	R32	R33	G34	F35	K36	N37	T38	V39	L40	E41	E42	E43	E44	R45	P46	K47	N48	Q49	T50	L51	E52	G53	L54	D57	P58	N59	A60	V61	T62	N63
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● Molecule 7: DNA-directed RNA polymerase omega chain

Chain O:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	155.38Å 155.38Å 496.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 39.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.8 (40.00-3.00) 82.1 (39.78-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.266 0.226 , 0.250	Depositor DCC
R_{free} test set	10938 reflections (6.05%)	DCC
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 122.3	EDS
Estimated twinning fraction	0.147 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 191828 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	51962	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: STD, APC, ZN, 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	G	0.90	1/520 (0.2%)	1.13	2/798 (0.3%)
1	X	0.97	1/520 (0.2%)	1.14	0/798
2	H	1.48	5/387 (1.3%)	2.79	37/601 (6.2%)
2	Y	1.46	2/387 (0.5%)	2.77	38/601 (6.3%)
3	I	0.81	0/304	1.22	3/467 (0.6%)
3	Z	0.76	0/304	1.10	1/467 (0.2%)
4	A	0.73	0/1838	0.79	2/2498 (0.1%)
4	B	0.73	0/1838	0.78	4/2498 (0.2%)
4	K	0.72	0/1838	0.82	3/2498 (0.1%)
4	L	0.76	0/1838	0.79	3/2498 (0.1%)
5	C	0.77	0/8997	0.89	15/12164 (0.1%)
5	M	0.79	2/8997 (0.0%)	0.90	14/12164 (0.1%)
6	D	0.82	12/10547 (0.1%)	0.93	21/14245 (0.1%)
6	N	0.81	7/10547 (0.1%)	0.90	16/14245 (0.1%)
7	E	0.77	1/784 (0.1%)	1.06	3/1057 (0.3%)
7	O	0.81	1/784 (0.1%)	1.07	4/1057 (0.4%)
All	All	0.81	32/50430 (0.1%)	0.97	166/68656 (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	G	0	6
1	X	0	7
2	H	0	2
2	Y	0	1
6	D	0	1
All	All	0	17

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	133	ILE	N-CA	11.89	1.70	1.46
6	D	132	TYR	CA-C	9.71	1.78	1.52
2	Y	1	G	C3'-O3'	8.60	1.54	1.42
2	H	1	G	OP3-P	-7.94	1.51	1.61
6	D	456	MET	N-CA	7.80	1.61	1.46

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	G	N9-C1'-C2'	25.00	146.50	114.00
2	Y	1	G	N9-C1'-C2'	20.87	141.13	114.00
2	Y	1	G	P-O3'-C3'	19.40	142.98	119.70
2	H	1	G	P-O3'-C3'	19.01	142.51	119.70
2	Y	2	A	O4'-C1'-N9	16.04	121.03	108.20

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1	DC	Sidechain
1	G	13	DT	Sidechain
1	G	15	DC	Sidechain
1	G	16	DG	Sidechain
1	G	17	DC	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	467	0	259	46	0
1	X	467	0	259	45	0
2	H	347	0	174	75	0
2	Y	347	0	174	61	0
3	I	270	0	144	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Z	270	0	144	18	0
4	A	1806	0	1861	186	0
4	B	1806	0	1861	178	0
4	K	1806	0	1861	206	0
4	L	1806	0	1861	173	0
5	C	8829	0	8933	1078	0
5	M	8829	0	8933	1061	0
6	D	10373	0	10599	1472	0
6	N	10373	0	10599	1397	0
7	E	770	0	784	124	0
7	O	770	0	784	105	0
8	D	43	0	34	6	0
8	N	43	0	31	6	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	2	0	0	0	0
10	N	2	0	0	0	0
11	D	31	0	14	5	0
11	M	31	0	14	2	0
12	A	78	0	0	13	0
12	B	117	0	0	29	0
12	C	408	0	0	103	0
12	D	531	0	0	107	0
12	E	34	0	0	17	0
12	G	39	0	0	6	0
12	H	22	0	0	6	0
12	I	31	0	0	3	0
12	K	81	0	0	26	0
12	L	95	0	0	12	0
12	M	396	0	0	100	0
12	N	510	0	0	120	0
12	O	53	0	0	16	0
12	X	31	0	0	5	0
12	Y	26	0	0	3	0
12	Z	18	0	0	3	0
All	All	51962	0	49323	5743	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 58.

The worst 5 of 5743 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:133:ILE:N	6:D:133:ILE:CA	1.70	1.55
6:D:132:TYR:C	6:D:132:TYR:CA	1.78	1.49
7:E:92:LEU:HD23	12:E:113:HOH:O	1.25	1.32
2:Y:2:A:OP2	6:N:671:LYS:NZ	1.72	1.21
6:D:87:ARG:HD3	6:D:524:LEU:HD11	1.30	1.12

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	227/315 (72%)	208 (92%)	16 (7%)	3 (1%)	18	62
4	B	227/315 (72%)	208 (92%)	15 (7%)	4 (2%)	13	53
4	K	227/315 (72%)	208 (92%)	16 (7%)	3 (1%)	18	62
4	L	227/315 (72%)	206 (91%)	18 (8%)	3 (1%)	18	62
5	C	1117/1119 (100%)	922 (82%)	136 (12%)	59 (5%)	3	18
5	M	1117/1119 (100%)	919 (82%)	137 (12%)	61 (6%)	3	16
6	D	1308/1524 (86%)	1104 (84%)	145 (11%)	59 (4%)	4	22
6	N	1308/1524 (86%)	1099 (84%)	158 (12%)	51 (4%)	5	26
7	E	93/99 (94%)	73 (78%)	13 (14%)	7 (8%)	2	8
7	O	93/99 (94%)	73 (78%)	12 (13%)	8 (9%)	1	5
All	All	5944/6744 (88%)	5020 (84%)	666 (11%)	258 (4%)	4	23

5 of 258 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	29	GLU
4	B	29	GLU
4	B	187	GLY
5	C	152	PRO
5	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	
4	A	202/273 (74%)	159 (79%)	43 (21%)	1	8
4	B	202/273 (74%)	162 (80%)	40 (20%)	2	11
4	K	202/273 (74%)	155 (77%)	47 (23%)	1	6
4	L	202/273 (74%)	153 (76%)	49 (24%)	1	5
5	C	941/941 (100%)	723 (77%)	218 (23%)	1	6
5	M	941/941 (100%)	714 (76%)	227 (24%)	1	5
6	D	1111/1279 (87%)	875 (79%)	236 (21%)	1	8
6	N	1111/1279 (87%)	863 (78%)	248 (22%)	1	7
7	E	84/88 (96%)	66 (79%)	18 (21%)	1	8
7	O	84/88 (96%)	67 (80%)	17 (20%)	2	10
All	All	5080/5708 (89%)	3937 (78%)	1143 (22%)	1	7

5 of 1143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	1345	GLU
4	L	181	VAL
6	N	1156	LEU
6	D	1465	ASN
4	K	143	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 151 such sidechains are listed below:

Mol	Chain	Res	Type
6	D	1441	GLN
5	M	91	GLN
6	N	1124	GLN
7	E	29	GLN
4	L	16	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	H	16/16 (100%)	11 (68%)	6 (37%)
2	Y	16/16 (100%)	11 (68%)	7 (43%)
All	All	32/32 (100%)	22 (68%)	13 (40%)

5 of 22 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	2	A
2	H	3	G
2	H	6	U
2	H	7	G
2	H	8	C

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	12	G
2	Y	1	G
2	Y	9	G
2	H	9	G
2	Y	8	C

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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
11	APC	D	5999	10	33,33,33	4.64	4 (12%)	52,52,52	1.76	10 (19%)
8	STD	D	7001	-	47,47,47	7.79	28 (59%)	73,73,73	2.72	22 (30%)
11	APC	M	6999	10	33,33,33	4.55	4 (12%)	52,52,52	1.70	11 (21%)
8	STD	N	8001	-	47,47,47	7.62	30 (63%)	73,73,73	2.73	20 (27%)

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
11	APC	D	5999	10	-	0/20/38/38	0/1/3/3
8	STD	D	7001	-	-	0/31/101/101	0/2/5/5
11	APC	M	6999	10	-	0/20/38/38	0/1/3/3
8	STD	N	8001	-	-	0/31/101/101	0/2/5/5

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	7001	STD	O5-C19	-28.47	1.19	1.42
8	N	8001	STD	O5-C19	-27.78	1.19	1.42
8	D	7001	STD	C16-C17	-23.97	1.28	1.53
8	N	8001	STD	C16-C17	-23.14	1.29	1.53
11	D	5999	APC	PB-C3A	-18.71	1.63	1.79

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	8001	STD	C5-C1-C2	9.43	134.35	120.25
8	D	7001	STD	C19-O5-C13	9.21	122.53	112.98
8	D	7001	STD	C5-C1-C2	9.02	133.74	120.25
8	N	8001	STD	C19-O5-C13	8.85	122.15	112.98
8	N	8001	STD	O8-C17-C30	-7.60	105.96	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	G	23/23 (100%)	-0.57	0	100	100	23, 43, 66, 69	0
1	X	23/23 (100%)	-0.57	0	100	100	9, 37, 77, 92	0
2	H	16/16 (100%)	-0.42	0	100	100	24, 52, 92, 93	0
2	Y	16/16 (100%)	-0.40	0	100	100	25, 43, 96, 99	0
3	I	13/14 (92%)	-0.62	0	100	100	39, 55, 76, 77	0
3	Z	13/14 (92%)	-0.71	0	100	100	50, 61, 75, 79	0
4	A	229/315 (72%)	-0.31	0	100	100	31, 58, 73, 77	0
4	B	229/315 (72%)	-0.32	0	100	100	34, 62, 75, 83	0
4	K	229/315 (72%)	-0.32	0	100	100	30, 57, 71, 76	0
4	L	229/315 (72%)	-0.27	0	100	100	37, 62, 76, 87	0
5	C	1119/1119 (100%)	-0.35	1 (0%)	93	63	7, 54, 77, 90	0
5	M	1119/1119 (100%)	-0.34	0	100	100	18, 54, 76, 90	0
6	D	1314/1524 (86%)	-0.32	0	100	100	11, 56, 79, 89	0
6	N	1314/1524 (86%)	-0.32	1 (0%)	93	63	8, 56, 76, 91	0
7	E	95/99 (95%)	-0.41	0	100	100	42, 58, 67, 71	0
7	O	95/99 (95%)	-0.35	0	100	100	33, 59, 75, 80	0
All	All	6076/6850 (88%)	-0.33	2 (0%)	100	100	7, 56, 77, 99	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	N	416	ALA	2.7
5	C	1025	ALA	2.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
10	MG	D	9002	1/1	0.15	0.56	25,25,25,25	0
11	APC	D	5999	31/31	0.16	0.20	30,38,64,65	0
8	STD	D	7001	43/43	0.18	0.08	11,24,27,28	0
8	STD	N	8001	43/43	0.18	-0.15	14,32,53,55	0
11	APC	M	6999	31/31	0.15	-0.26	35,45,57,58	0
9	ZN	D	8112	1/1	0.08	-1.29	58,58,58,58	0
9	ZN	N	8212	1/1	0.11	-1.66	54,54,54,54	0
9	ZN	N	7158	1/1	0.07	-1.82	70,70,70,70	0
9	ZN	D	7058	1/1	0.07	-2.11	87,87,87,87	0
10	MG	D	9001	1/1	0.08	-2.35	22,22,22,22	0
10	MG	N	9003	1/1	0.10	-3.53	21,21,21,21	0
10	MG	N	9004	1/1	0.09	-8.01	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.