



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:50 AM UTC

PDB ID : 1SMY / pdb_00001smy
Title : Structural basis for transcription regulation by alarmone ppGpp
Authors : Artsimovitch, I.; Patlan, V.; Sekine, S.; Vassilyeva, M.N.; Hosaka, T.; Ochi, K.; Yokoyama, S.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-03-10
Resolution : 2.70 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

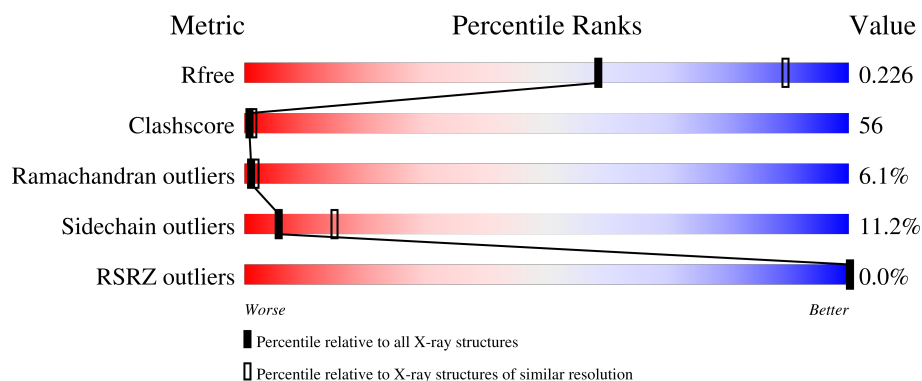
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	315	
1	B	315	
1	K	315	
1	L	315	

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Mol	Chain	Length	Quality of chain
2	C	1119	 27% 59% 13% .
2	M	1119	 26% 62% 10% .
3	D	1524	 26% 53% 10% . 9%
3	N	1524	 28% 53% 10% . 9%
4	E	99	 23% 60% 9% . .
4	O	99	 32% 47% 12% . .
5	F	423	 22% 50% 9% . 18%
5	P	423	 21% 52% 7% . 18%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 63021 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8828	5581	1577	1646	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8828	5581	1577	1646	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA POLYMERASE OMEGA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

- Molecule 5 is a protein called principal sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2770	1744	504	518	4			
5	P	345	Total	C	N	O	S	0	0	0
			2770	1744	504	518	4			

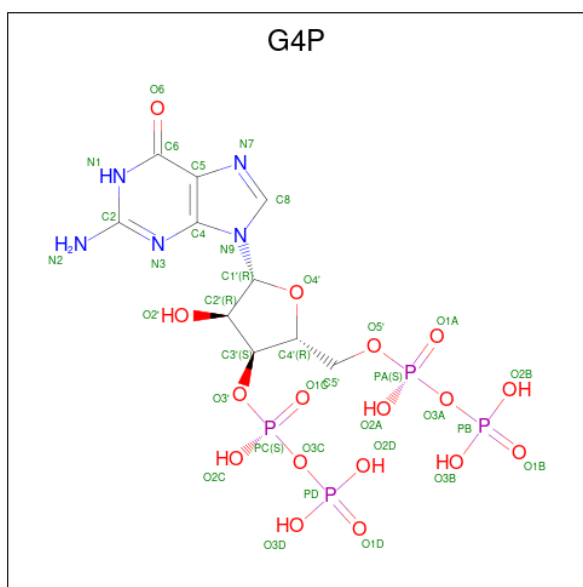
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	Mg	0	0
			29	29		
6	B	22	Total	Mg	0	0
			22	22		
6	C	92	Total	Mg	0	0
			92	92		
6	D	150	Total	Mg	0	0
			150	150		
6	E	17	Total	Mg	0	0
			17	17		
6	F	49	Total	Mg	0	0
			49	49		
6	M	1	Total	Mg	0	0
			1	1		
6	N	2	Total	Mg	0	0
			2	2		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	N	1	Total 36	C 10	N 5	O 17	P 4	0	0
8	N	1	Total 36	C 10	N 5	O 17	P 4	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	296	Total O 296 296	0	0
9	B	307	Total O 307 307	0	0
9	C	1308	Total O 1308 1308	0	0
9	D	1745	Total O 1745 1745	0	0
9	E	160	Total O 160 160	0	0
9	F	619	Total O 619 619	0	0
9	K	316	Total O 316 316	0	0
9	L	341	Total O 341 341	0	0
9	M	1401	Total O 1401 1401	0	0
9	N	1794	Total O 1794 1794	0	0

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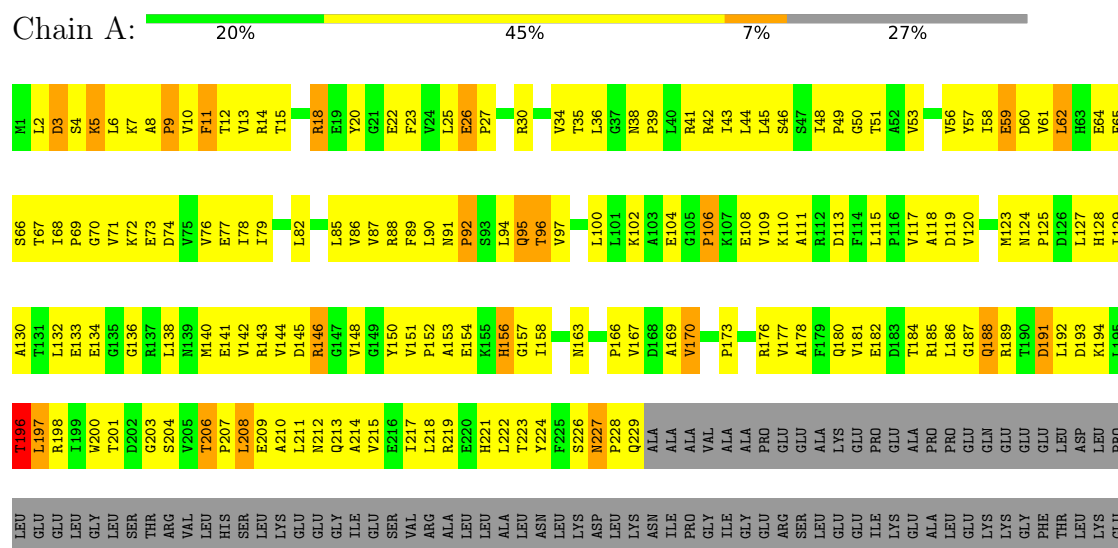
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	O	203	Total 203	O 203	0	0
9	P	541	Total 541	O 541	0	0

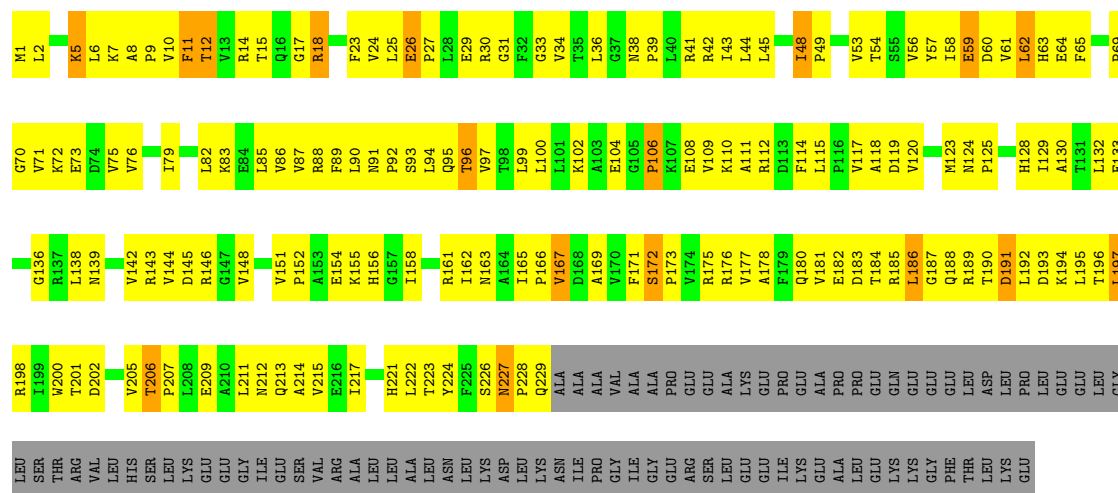
3 Residue-property plots

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.

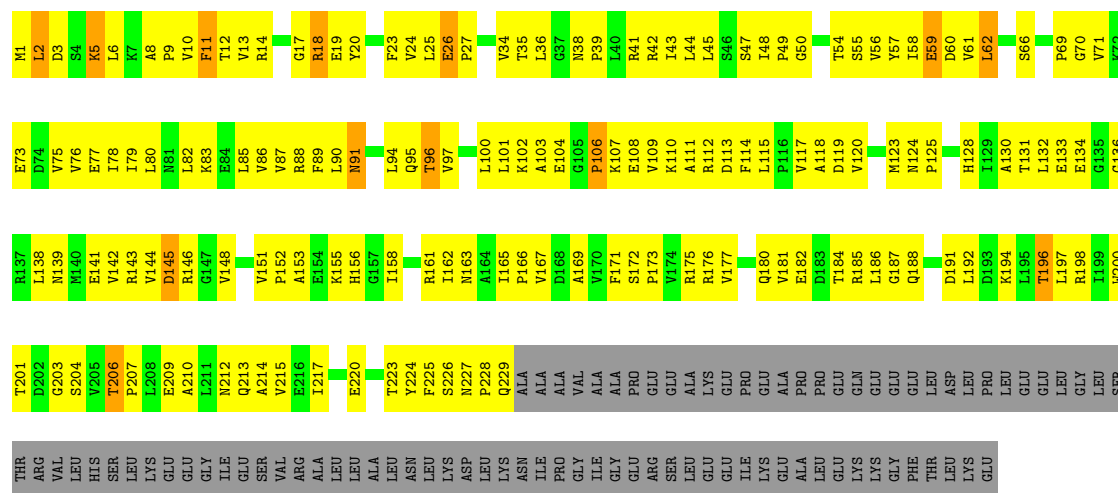
• Molecule 1: DNA-directed RNA polymerase alpha chain



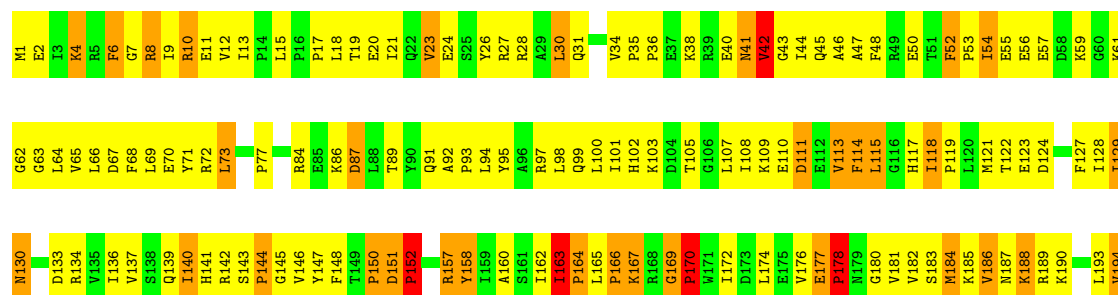
Chain K: 21% 46% 5% 27%



Chain L: 22% 47% . 27%



Chain C: 27% 59% 13%





G977	A909	N845	R172	Y708	R640	P577	A515	F385	E321	G259	L196	D133	H1
R978	K910	K946	L773	E709	P641	V678	R516	F386	V322	L260	L197	R134	E2
T979	E911	G947	L774	I710	R642	V679	S454	S389	D323	T261	R198	V135	I3
G980	P912	V848	R775	E711	V643	N580	K518	Q390	D324	G262	V199	A262	K4
E981	E913	V849	S776	A712	V644	T581	Q519	A456	I325	D263	L200	V137	R5
P982	I914	A850	L777	R713	V645	G582	E520	A457	R326	P264	G201	S138	F6
I983	K915	V853	F778	E714	G646	L583	P521	V458	H327	R265	Y202	Q139	G7
E984	E916	L852	G779	K716	Q647	E584	V522	A459	L328	R266	D203	H140	R8
G985	L917	L853	E780	E715	R648	E585	I523	R460		Y267	Q204	H141	R9
P986	P918	V854	K781	P719	V649	R586	V524	D396	R331	D268	Q205	R142	R10
I987	L919	V855	E782	E720	R650	V587	S525	D462	R332	D269	E206	S143	E11
V988	Q920	E856	R783	R721	G651	V588	P526	T398	I333	A272	L207	P144	V12
V989		D857	D784	I722	G652	R589	E527	L464	R334	G273	A208	P145	I13
G990	Y925	R858	V785	T723	D653	D590	E528	G465	T335		R209	V146	P14
Q991	F926	P859	K786	R724	L654		F531	S402	G336	R274	E210	Y147	P16
N992	G927	H860		D725	L655		M532	R468	G337	Y275	L211	F148	L15
F993	R928		S789	I726	A656		V534	L404	E338	K276	G212	T149	P17
K996	R929	G864	L790	L734	D657	L595	V534	R406	L339	A277	E216	P150	L18
L997	K930	T865	R791	H728	G658	V596		H408	K340	E278		D151	T19
Y998	G931	P866	V792	L729	P659	A597	S535	R407	T341	E279		P152	E20
H999	E932	V867		S730	A660	E598	P536	R408	D342	R280	E217		L21
M1000	D937	D868	G798	L734	S661	E599	K537	V475	Q343	L281	V218	Y158	Q22
V1001	K938	V869	I799	E740	E662	D600	Q538	R409	F344	G282	Q219	T89	V23
E1002	R339	L870	V800	G741	N663	G601	V539	G476	R345	I283	G220	I159	E24
D1003		L871	V801	E742	G664	E602	F540	G477	V346	R284	L221	A160	S25
K1004	V943	R872	R802	L737	A667	V603	S541	V478	G347	L285	K222	S161	Y26
M1005	L944	P873	T803	D738	L668	A604	V542	T480	L348	S286	D223	I162	R27
L1006	R945	L874	D810	E739	G669	K605	N543	D481	A349	E224	L94	I163	R28
A1007	A1007	G875	P811	E740	Q670	V606	T544	G416	R350	S225	P164	A96	A29
R1008	A947	V876	N545	G741	N671	D607	G417	V483	L351	V226	L165	R97	L30
S1009	E948	P877	G812	V742	N672	G608	L546	V484	A352	F227	P166	L98	Q31
		S878	V813	V743	V672	N609	T547	Y485	R353	A291	K167	Q99	
		R879	L673	R744	L673	R610	F548	R420	G354	R292	R168	L100	V34
		N880	V674	I745	A675	T611	F549	G424	V355		R230	I101	P35
		L881	G675	G746	L550	V612	L550	F425	R356		P170	H102	P36
		L882	L676	A747	E551	V613	E551	D426	K359	E297	Y171	K103	E37
		G883	N677	E748	E491	R614	H552	V492	E233	E297	I172	D173	K38
		Q884	P678	V749	D492	V615	D553	V427	L360	F298	D173	L174	R39
		T885	P679	E816	R493	E554	D554	R428		K299	L107	I108	E40
		L886	F679	P751	A555	N556	A555		S363		I108	K109	N41
		T888	N683	G752	F684	L620	R557			E301	E176	E110	V42
		H889	E685	I754	E685	V621				L238	E177	D111	G43
		L892	D686	L755	D686	E622	N560			F303	R178	E112	I44
		A993	A687	V756	A687		G561			L241	R179	V113	Q45
		F996	I690	G757	I690	L625	S562			R243	G180	F114	A46
		L897	S691	T759	S691	R626	N563			P244	V181	L115	A47
		Q898	K830	T759	S691	R627	N564			G116	V182	G116	F48
		Q899	R831	S760	E692	F628	O565			H117	D246	S183	R49
		Q899	K832	F763	E693	V629	T566			P247	M184	E118	E50
		R900	L694	K762	L694	R630	Q567			P248	K185	P119	T51
		Y901	L695	G763	L695	S631	A568			F311	V186	L120	F52
		Y902	K696	E764	K696	N632	V569			R250	K188	M121	P53
		G970	R697	S765	R697	Q633	P570			D251	K189		E55
		S903	L839	E766	G634	L508	O565			T314	K252		E56
		P904	S903	F767	D698	L571	A509			A315	A253	K190	E57
		I905	A840	P767	F699	T635	L572			C316	V254	F191	D58
		P906	N841	T768	Y700	T636	R573			V317	A255	P192	E59
		D907	T701	P769	T701	L637	A574			P318	Y256	L193	D60
		G908	H843	E770	H843	D638	V513			V257	V194	K61	E60
			G844	E771	R707	Q639	A576			H320	Y258		E61

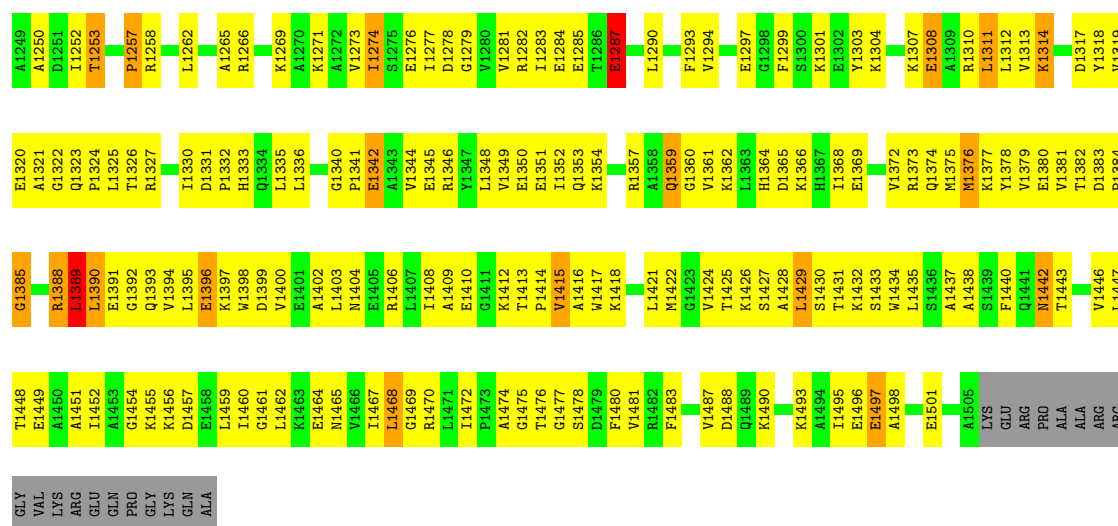
GLY	T1448	G1385	G1322	G1285	G1184	T1115	L1044	Y978	K908	F843
VAL	E1449	G1386	Q1323	L1286	E1185	M1116	M1045		L911	A844
LYS	A1450	R1388	P1324	P1257	F1186	Y1117	K1046	L983	K912	N845
ARG	A1451	L1389	L1325	R1258	P1187	L1118	K1047	T984	L914	N846
GLU	I1452	L1390	T1326	V1259	L1188	S1119		D985	D913	D847
GLN		E1391	R1327	L1260	R1189	V1120	E1051	R986	E848	E849
P80	K1456	G1392	G1328	E1281	L1192	P1121	T1052	F987	L850	L851
GLY	D1457	Q1393	A1329	L1282	T1193	F1122	F1053	Y988	A849	
LYS	E1458	V1394	I1330	F1283	T1193	F1123			L922	A852
GLN	L1459	L1395	D1331	A1264	Q1194	Q1124	P1056	D990	A853	
ALA	L1460	E1396	P1332	A1265	Q1195	P1125	P1057	D991		
	G1461	K1397	H1333	R1266	T1196	D1126	R1058	Q991	E925	V858
	L1462	V1398	Q1334	R1267	R1197	E1127	S1059	Q992	K926	D859
	K1463	D1399	L1335	F1288	Y1198	V1128	S1060	Q994	T927	L860
	E1464	V1400	L1336	K1289	V1199	T1129	P1061	Q995	A928	Q861
	L1465	E1401	E1337	A1270	V1200	R1130	R1062	N996	R929	D862
	V1466	G1402	A1338	K1271	Q1201	S1131	E1063	T997	L930	V863
	I1467	L1468	K1339	A1272	Q1202	L1132	G1064	E998	L931	
	L1468	E1405	G1340	V1273	K1203	R1133	L1065	T999	D864	T865
	G1469	R1406	P1341	I1274	C1204	L1134	T1066	A933	T866	V866
	L1470	L1407	E1342	S1275		R1135	V1067	L934	R867	Y868
	L1471	I1408	A1343	E1276	Y1207	L1144	Y1003	K935	M869	Y870
	L1472	I1409	V1344	I1277	D1208	Y1145	L1068	Y936	K871	R872
	P1473	E1410	E1345	D1278	L1209	A1136	E1069	Y937	E873	T875
	A1474	G1411	R1346	G1279	S1210	A1138	Y1070	Q1005	S876	P877
	G1475	K1412	Y1347	V1280	M1211	D1139	F1071	A1006	G878	G879
		T1413	L1348	E1281	A1212	T1140	I1072	V1007	I880	F882
	V1486	P1414	E1351	I1282	R1213	L1144	S1073	F1008	L881	F883
	D1487	V1415	I1352	I1283	P1214	Y1146	G1076	K1009	A884	L885
	Q1488	A1416	Q1353	E1284	V1215	E1013	H1075	L1012	E888	
	K1490	V1417	K1354	E1285	L1216	A1146	A1077	E1014	P957	A889
		K1418	K1355	F1286	I1217	R1147	R1078	N1014	E890	
		L1419	V1356	E1287	G1218	V1148		Y1015		
		L1420	Y1357	E1288	E1219	A1150	T1084	F1017		
		M1422	A1358	F1293	G1222	R1087	R1088	P1019		
		G1423	Q1359	V1294	I1223	R1151	A1089	L1020		
		V1424	G1360			E1152		Y1021		
		T1425	V1361	S1300	E1231	V1155	G1092	M1022		
		K1426	K1362	K1301	P1232	L1156	Y1093	M1023		
		S1427	L1363	E1302	G1233	R1159	L1094			
		A1428	H1364	Y1303	T1234	L1160	T1095	S1026		
		L1429	D1365	K1304	G1235	G1163	R1096	G1027		
		S1430	K1366	P1306	T1237	R1164	K1097	A1028		
		T1431			L1236	Y1165	L1098	R1029		
		K1432	E1369	E1307	M1238	R1164	V1099	G1030		
		S1433			T1240	Y1165	D1100	M1031		
		W1434	V1372	A1309	T1240	S1167	V1101	Y963		
		L1435	R1373	R1310		M1168	T1102	L964		
		S1436	Q1374	L1311	T1243	D1169	H1103	E965		
		A1437	M1375	L1312	G1244		E1104	E966		
		A1438	M1376	V1313			I1105	A967		
		S1439	K1377	D1314	A1247	L1173	E1109	L899		
		F1440	K1378	D1315	L1174	L1175	Q1037	I900		
		V1379	V1379	G1316	A1249	I1176	L1038	Q901		
		Q1441	G1381	D1317	A1250	K1176	Q1033	L902		
		N1442	V1381	Y1318	D1251	A1177	Q1034	T903		
		T1443	T1382	V1319	I1252		Q1034	L971		
			T1382	V1320	I1252		E1104	L972		
			P1384	A1321	Q1254		I1105	Q976		
								A977		

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

Chain N:  28% 53% 10% 9%

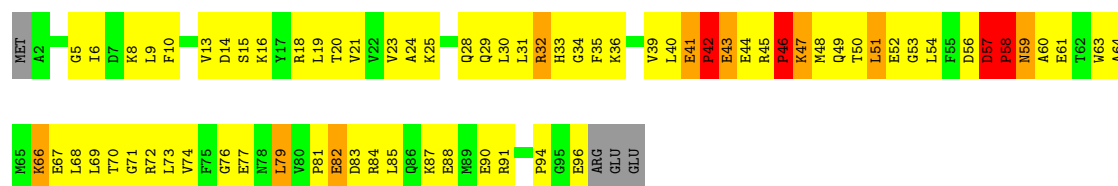
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K2	R65	V126	L161	R66	Q66	L127	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146
K3	R66	L127	L128	L129	E4	F68	F69	F70	F71	F72	F73	F74	F75	F76	F77	F78	F79	F80	F81	F82	F83	F84	F85	F86	
V5	R67	F129	F130	F131	G70	K131	K132	K133	K134	K135	K136	K137	K138	K139	K140	K141	K142	K143	K144	K145	K146	K147	K148	K149	
R6	F68	S120	S121	S122	G70	K131	K132	K133	K134	K135	K136	K137	K138	K139	K140	K141	K142	K143	K144	K145	K146	K147	K148	K149	
K7	G70	K131	K132	K133	K134	K135	K136	K137	K138	K139	K140	K141	K142	K143	K144	K145	K146	K147	K148	K149	K150	K151	K152	K153	
V8	K71	Y132	Y133	Y134	Y135	Y136	Y137	Y138	Y139	Y140	Y141	Y142	Y143	Y144	Y145	Y146	Y147	Y148	Y149	Y150	Y151	Y152	Y153	Y154	
R9	Y72	I133	I134	I135	I136	I137	I138	I139	I140	I141	I142	I143	I144	I145	I146	I147	I148	I149	I150	I151	I152	I153	I154	I155	
I10	Y73	V134	V135	V136	V137	V138	V139	V140	V141	V142	V143	V144	V145	V146	V147	V148	V149	V150	V151	V152	V153	V154	V155	V156	
A11	E74	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	
L12	R75	D136	D137	D138	D139	D140	D141	D142	D143	D144	D145	D146	D147	D148	D149	D150	D151	D152	D153	D154	D155	D156	D157	D158	
A13	G76	P137	P138	P139	P140	P141	P142	P143	P144	P145	P146	P147	P148	P149	P150	P151	P152	P153	P154	P155	P156	P157	P158	P159	
S14	G77	K138	K139	K140	K141	K142	K143	K144	K145	K146	K147	K148	K149	K150	K151	K152	K153	K154	K155	K156	K157	K158	K159	K160	
P15	V78	A139	A140	A141	A142	A143	A144	A145	A146	A147	A148	A149	A150	A151	A152	A153	A154	A155	A156	A157	A158	A159	A160	A161	
E16	E79	G140	G141	G142	G143	G144	G145	G146	G147	G148	G149	G150	G151	G152	G153	G154	G155	G156	G157	G158	G159	G160	G161	G162	
K17	T80	H140	H141	H142	H143	H144	H145	H146	H147	H148	H149	H150	H151	H152	H153	H154	H155	H156	H157	H158	H159	H160	H161	H162	
I18	T81	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	
R19	K82	M143	M144	M145	M146	M147	M148	M149	M150	M151	M152	M153	M154	M155	M156	M157	M158	M159	M160	M161	M162	M163	M164	M165	
S20	S83	G144	G145	G146	G147	G148	G149	G150	G151	G152	G153	G154	G155	G156	G157	G158	G159	G160	G161	G162	G163	G164	G165	G166	
W21	T84	V145	V146	V147	V148	V149	V150	V151	V152	V153	V154	V155	V156	V157	V158	V159	V160	V161	V162	V163	V164	V165	V166	V167	
E22	V85	P146	P147	P148	P149	P150	P151	P152	P153	P154	P155	P156	P157	P158	P159	P160	P161	P162	P163	P164	P165	P166	P167	P168	
Y23	R86	V147	V148	V149	V150	V151	V152	V153	V154	V155	V156	V157	V158	V159	V160	V161	V162	V163	V164	V165	V166	V167	V168	V169	
G24	R87	E148	E149	E150	E151	E152	E153	E154	E155	E156	E157	E158	E159	E160	E161	E162	E163	E164	E165	E166	E167	E168	E169	E170	
E25	R88	K149	K150	K151	K152	K153	K154	K155	K156	K157	K158	K159	K160	K161	K162	K163	K164	K165	K166	K167	K168	K169	K170	K171	
V26	R89	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	
E27	N90	Q151	Q152	Q153	Q154	Q155	Q156	Q157	Q158	Q159	Q160	Q161	Q162	Q163	Q164	Q165	Q166	Q167	Q168	Q169	Q170	Q171	Q172	Q173	
	G91	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	
E30	T30	T154	T155	T156	T157	T158	T159	T160	T161	T162	T163	T164	T165	T166	T167	T168	T169	T170	T171	T172	T173	T174	T175	T176	
T31	T31	T154	T155	T156	T157	T158	T159	T160	T161	T162	T163	T164	T165	T166	T167	T168	T169	T170	T171	T172	T173	T174	T175	T176	
I32	I32	I154	I155	I156	I157	I158	I159	I160	I161	I162	I163	I164	I165	I166	I167	I168	I169	I170	I171	I172	I173	I174	I175	I176	
R33	R33	R154	R155	R156	R157	R158	R159	R160	R161	R162	R163	R164	R165	R166	R167	R168	R169	R170	R171	R172	R173	R174	R175	R176	
Y34	Y34	Y154	Y155	Y156	Y157	Y158	Y159	Y160	Y161	Y162	Y163	Y164	Y165	Y166	Y167	Y168	Y169	Y170	Y171	Y172	Y173	Y174	Y175	Y176	
R35	R35	R154	R155	R156	R157	R158	R159	R160	R161	R162	R163	R164	R165	R166	R167	R168	R169	R170	R171	R172	R173	R174	R175	R176	

P1187	G1112	P1048	R988	L911	D847	I785	A715	L850	D583	L514	I452	A391	LYS	G188
V1188	G1113	S1049	P989	K912	E848	I786	F716	E651	N584	E515	D453	S392	GLU	Q189
R1189	T1114	G1050	P990		A849	L787		L852	G585	A516	A454	T393	LEU	E190
S1190	T1115	E1051	Q991	Q917	L850	G788	V719	F853	R586	P517	R455	L394	GLU	L191
P1191	T1116	T1052	Q992	A918	L851	L789		K654	R587	P518	R456	V395	GLU	A192
L1192	Y1117	F1053	L993	F919	A852		V720	P655	G588	V519	G457	V396	GLY	P193
T1193	L1118	E1054	Q994	L920	V853		V721	F656	A589	L520	A458	K397	ALA	G194
C1194	S1119	V1055	L995	L921	V854	I792	E722	L857	P590	P521	E459		PHE	V195
Q1195	L1120	P1056	W996	L922	A854	T793	G723	L858		P522	A460	A398	LEU	V196
T1196	T1121	T1057	T997		V858	T794	Q724	L859	N593		I461	R399	THR	S197
R1197	F1122	R1058	E998	E925	D859	R796	L728	K660	P594	D523	Q462	Y401	VAL	L198
Y1198	F1123	S1059	T999	K926	L860	G797	H729	M661	G595	L524	Q463	P402	LEU	L199
L1199	F1124	T1060	T1000	T927	Q861	E798		E662	R596	R525	Q464		ARG	L199
V1200	P1125	F1061	A928	A928	D862	K799	V732	E663	S596	P526	L464	F403	THR	D200
C1201	L1126	R1062	R929	R929	V863	G733		K664	D597	M527	L465		GLU	G201
K1202	E1127	E1063	L1002	L930	V864	E734		P599	R598		K466	D406	ASP	A203
K1203	G1064	G1064	T1004	L931	T865	F735		P599	L800	F535	E467	Y407	GLU	A203
C1204	L1128	L1065	Q1005	L931	T866	A736		P599	L800	F535	E467	Y407	GLU	A203
Y1205	R1130	T1066	Q1005	L931	T866	A736		P599	L800	F535	E467	Y407	GLU	A203
G1206		V1067	A1006	K935	R867	F805		K664	R598	F535	E467	Y407	GLU	A203
Y1207	R1133	E1069	F1008	Y936	R868	F806		K664	P599	F535	E467	Y407	GLU	A203
D1208	L1134	E1069	F1008	Y936	R868	F806		K664	P599	F535	E467	Y407	GLU	A203
L1209	R1135	E1069	F1008	Y936	R868	F806		K664	P599	F535	E467	Y407	GLU	A203
M1211	R1137	S1073	F1011	S942	K871	P809		K664	P599	F535	E467	Y407	GLU	A203
S1210	K1136	S1074	E1012	T943	R872	E810		K664	P599	F535	E467	Y407	GLU	A203
A1212	R1137	H1075	E1013	T944	R873	E811		K664	P599	F535	E467	Y407	GLU	A203
R1213	L1144	G1076	N1014	S945	T875	L813		K664	P599	F535	E467	Y407	GLU	A203
P1214	Y1145	A1077	Y1015	G946	S876	A814		K664	P599	F535	E467	Y407	GLU	A203
G1215	G1146	R1078	F1016	G947	P877	A815		K664	P599	F535	E467	Y407	GLU	A203
Y1215	R1147	G1079	F1017	T948	G878	H816		K664	P599	F535	E467	Y407	GLU	A203
T1217	L1148	G1080	N1018	T948	R879	E817		K664	P599	F535	E467	Y407	GLU	A203
G1218	L1149	P1019	F1019	S942	R879	E817		K664	P599	F535	E467	Y407	GLU	A203
E1219	L1155	D1083	L1020	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
G1222	V1155	T1084	L1021	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
L1223	L1156	A1085	Y1021	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
V1224	G1157	L1086	V1022	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
A1225	L1158	R1087	M1023	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
L1226	R1159	T1088	Q1025	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
G1227	L1160	A1089	S1026	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
S1228	E1161	D1090	G1027	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
L1229	E1162	S1091	A1028	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
E1231	R1164	G1092	R1029	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
P1232	Y1165	L1094	N1031	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
G1233	L1166	T1095	F1032	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
T1234	S1167	R1096	Q1033	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
L1235	M1168	K1097	Q1034	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
L1236	D1169	L1098	I1035	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
T1237	L1175	V1099	R1036	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
M1238	K1176	D1100	Q1037	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
R1239	E1179	T1101	L1038	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
F1241	L1180	H1103	C1039	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
H1242	G1181	A1180	G1040	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
T1243	G1182	I1105	L1041	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
G1244	E1182	V1106	G1042	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
G1245	T1183	L1044	R1043	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
V1246	Q1184	M1045	L1044	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
A1247	E1185	E1109	Q1046	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203
G1248	V1186	D1111	K1047	D962	I880	R818		K664	P599	F535	E467	Y407	GLU	A203



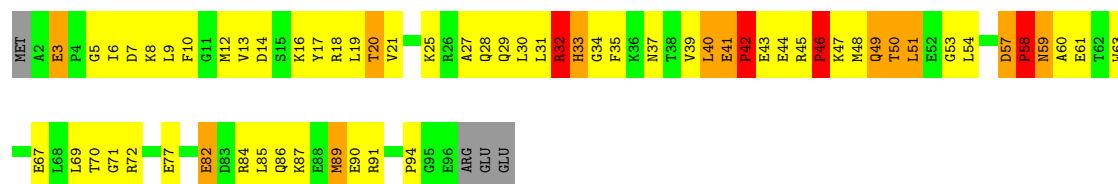
• Molecule 4: RNA POLYMERASE OMEGA SUBUNIT

Chain E: 23% 60% 9%



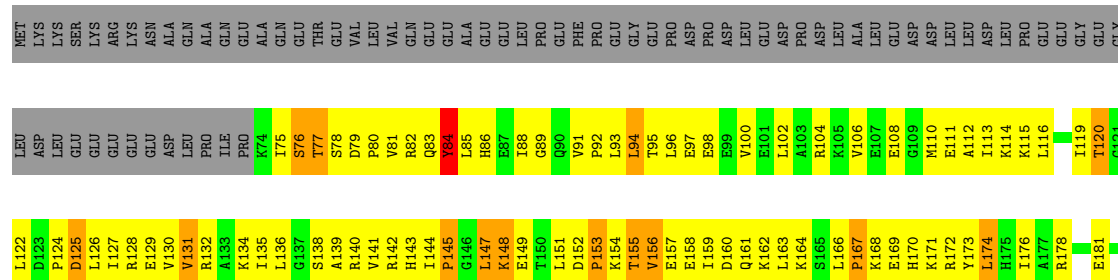
• Molecule 4: RNA POLYMERASE OMEGA SUBUNIT

Chain O: 32% 47% 12%



• Molecule 5: principal sigma factor

Chain F: 22% 50% 9% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.70) 97.1 (40.00-2.71)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.266 (Not available) , 0.226	Depositor DCC
R_{free} test set	14873 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.086 for h,-h-k,-l 0.086 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	63021	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: G4P, 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	A	0.70	1/1838 (0.1%)	0.95	0/2498
1	B	0.67	0/1838	0.92	0/2498
1	K	0.74	2/1838 (0.1%)	0.98	3/2498 (0.1%)
1	L	0.66	0/1838	0.91	2/2498 (0.1%)
2	C	0.75	1/8996 (0.0%)	1.12	37/12164 (0.3%)
2	M	0.74	3/8996 (0.0%)	1.13	35/12164 (0.3%)
3	D	0.75	1/10975 (0.0%)	1.15	60/14836 (0.4%)
3	N	0.75	1/10975 (0.0%)	1.14	58/14836 (0.4%)
4	E	0.76	0/783	1.10	0/1054
4	O	0.75	0/783	1.14	3/1054 (0.3%)
5	F	0.68	0/2811	1.09	11/3781 (0.3%)
5	P	0.66	1/2811 (0.0%)	1.07	9/3781 (0.2%)
All	All	0.74	10/54482 (0.0%)	1.10	218/73662 (0.3%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	474	VAL	CA-CB	7.09	1.61	1.53
1	K	48	ILE	CA-C	6.75	1.59	1.52
3	D	207	PHE	CA-C	6.09	1.58	1.52
1	K	48	ILE	C-N	5.95	1.40	1.33
5	P	144	ILE	CA-CB	5.85	1.57	1.54

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	207	PHE	CA-C-N	14.18	137.57	119.84
3	N	207	PHE	C-N-CA	14.18	137.57	119.84
3	D	207	PHE	CA-C-N	13.81	137.10	119.84
3	D	207	PHE	C-N-CA	13.81	137.10	119.84
2	C	177	GLU	CA-C-N	13.19	136.33	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	216	0
1	B	1806	0	1861	195	0
1	K	1806	0	1861	197	0
1	L	1806	0	1861	187	0
2	C	8828	0	8933	1048	0
2	M	8828	0	8933	1086	0
3	D	10797	0	10873	1289	0
3	N	10797	0	10873	1265	0
4	E	769	0	775	107	0
4	O	769	0	775	104	0
5	F	2770	0	2844	331	0
5	P	2770	0	2844	371	0
6	A	29	0	0	0	0
6	B	22	0	0	0	0
6	C	92	0	0	0	0
6	D	150	0	0	0	0
6	E	17	0	0	0	0
6	F	49	0	0	0	0
6	M	1	0	0	0	0
6	N	2	0	0	0	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	N	72	0	22	9	0
9	A	296	0	0	67	0
9	B	307	0	0	66	0
9	C	1308	0	0	282	0
9	D	1745	0	0	323	0
9	E	160	0	0	38	0
9	F	619	0	0	99	0
9	K	316	0	0	72	0
9	L	341	0	0	65	0
9	M	1401	0	0	327	0
9	N	1794	0	0	333	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	O	203	0	0	34	0
9	P	541	0	0	96	0
All	All	63021	0	54316	6100	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 56.

The worst 5 of 6100 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:34:VAL:HB	2:C:38:LYS:HG3	1.28	1.11
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.33	1.10
2:M:857:ASP:HB2	2:M:978:ARG:HG2	1.34	1.10
8:N:9100:G4P:H5''	8:N:9100:G4P:H8	1.14	1.09
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.35	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	187 (82%)	33 (14%)	7 (3%)	3	8
1	B	227/315 (72%)	183 (81%)	38 (17%)	6 (3%)	4	11
1	K	227/315 (72%)	186 (82%)	32 (14%)	9 (4%)	2	5
1	L	227/315 (72%)	185 (82%)	37 (16%)	5 (2%)	5	14
2	C	1117/1119 (100%)	856 (77%)	194 (17%)	67 (6%)	1	2
2	M	1117/1119 (100%)	863 (77%)	187 (17%)	67 (6%)	1	2
3	D	1388/1524 (91%)	1047 (75%)	248 (18%)	93 (7%)	1	1
3	N	1388/1524 (91%)	1042 (75%)	251 (18%)	95 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	93/99 (94%)	72 (77%)	11 (12%)	10 (11%)	0	0
4	O	93/99 (94%)	70 (75%)	13 (14%)	10 (11%)	0	0
5	F	341/423 (81%)	264 (77%)	53 (16%)	24 (7%)	1	1
5	P	341/423 (81%)	267 (78%)	53 (16%)	21 (6%)	1	2
All	All	6786/7590 (89%)	5222 (77%)	1150 (17%)	414 (6%)	1	2

5 of 414 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	188	GLN
1	B	118	ALA
2	C	10	ARG
2	C	59	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	183 (91%)	19 (9%)	8	21
1	B	202/273 (74%)	186 (92%)	16 (8%)	11	28
1	K	202/273 (74%)	187 (93%)	15 (7%)	13	32
1	L	202/273 (74%)	191 (95%)	11 (5%)	20	45
2	C	941/941 (100%)	817 (87%)	124 (13%)	4	10
2	M	941/941 (100%)	834 (89%)	107 (11%)	5	14
3	D	1123/1279 (88%)	990 (88%)	133 (12%)	5	13
3	N	1123/1279 (88%)	990 (88%)	133 (12%)	5	13
4	E	83/87 (95%)	71 (86%)	12 (14%)	3	8
4	O	83/87 (95%)	71 (86%)	12 (14%)	3	8
5	F	295/370 (80%)	261 (88%)	34 (12%)	5	14
5	P	295/370 (80%)	272 (92%)	23 (8%)	11	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5692/6446 (88%)	5053 (89%)	639 (11%)	6 15

5 of 639 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	1026	GLN
3	N	1124	GLN
3	N	53	ILE
2	M	1015	LEU
3	N	521	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 182 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	567	GLN
3	N	575	GLN
2	M	670	GLN
2	M	1030	GLN
3	N	737	ASN

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 368 ligands modelled in this entry, 366 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	G4P	N	9100	6	36,38,38	1.40	2 (5%)	56,61,61	1.37	10 (17%)
8	G4P	N	9101	6	36,38,38	1.08	3 (8%)	56,61,61	1.18	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	G4P	N	9100	6	-	8/27/43/43	0/3/3/3
8	G4P	N	9101	6	-	10/27/43/43	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	9100	G4P	PC-O3C	6.21	1.66	1.59
8	N	9100	G4P	PD-O3D	2.82	1.65	1.54
8	N	9101	G4P	PD-O3D	2.48	1.64	1.54
8	N	9101	G4P	PA-O3A	2.27	1.61	1.59
8	N	9101	G4P	C6-N1	2.26	1.43	1.38

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	9101	G4P	O3'-C3'-C4'	4.38	125.47	110.03
8	N	9100	G4P	O3A-PA-O1A	-3.31	100.75	110.70
8	N	9100	G4P	C2'-C3'-C4'	3.09	108.65	103.24
8	N	9100	G4P	O3B-PB-O3A	-3.07	94.35	104.64
8	N	9100	G4P	O3'-PC-O1C	-2.88	100.61	109.81

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	9100	G4P	PA-O3A-PB-O2B
8	N	9100	G4P	C5'-O5'-PA-O3A

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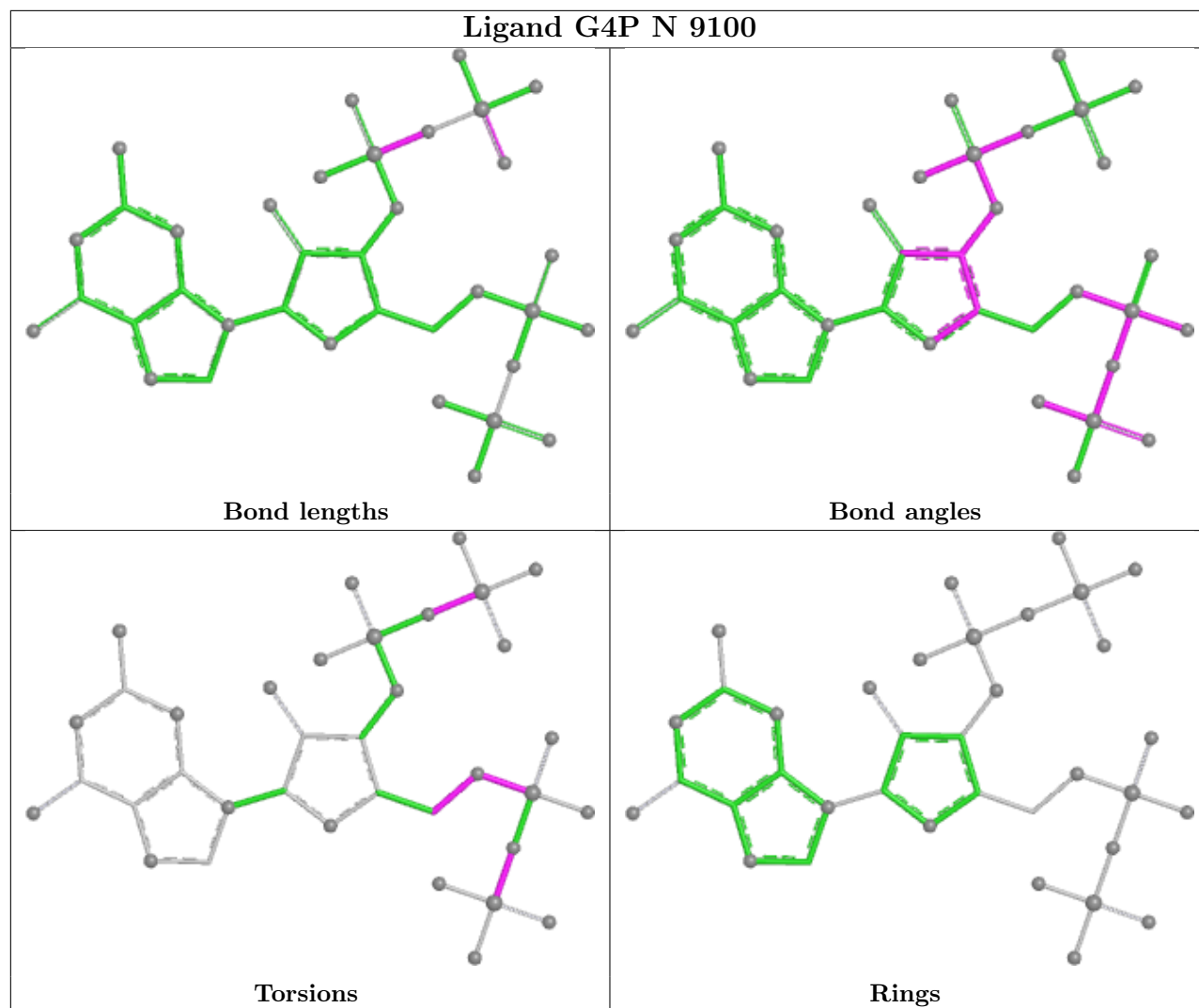
Mol	Chain	Res	Type	Atoms
8	N	9100	G4P	C5'-O5'-PA-O1A
8	N	9100	G4P	C4'-C5'-O5'-PA
8	N	9100	G4P	PC-O3C-PD-O3D

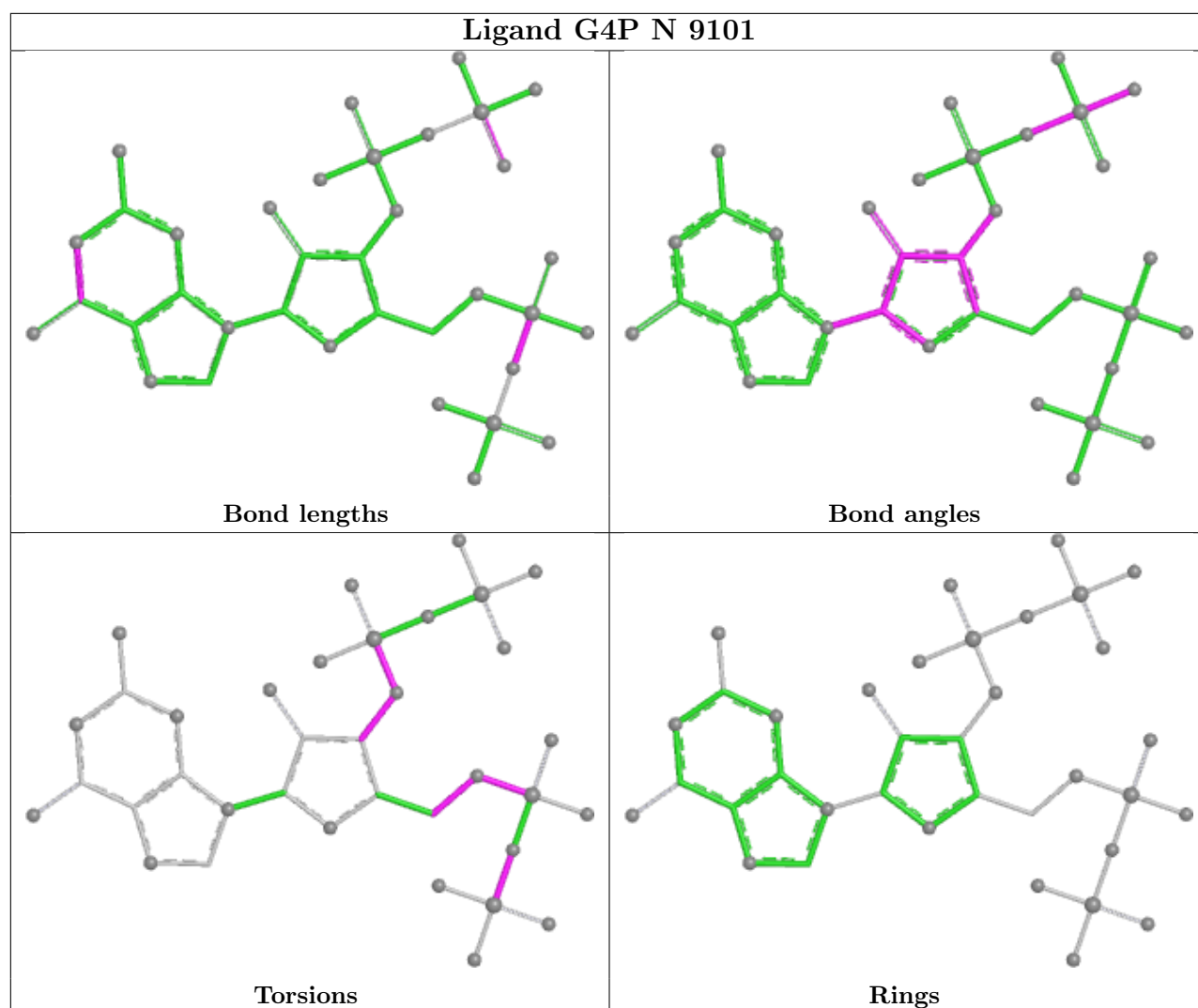
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	9100	G4P	4	0
8	N	9101	G4P	5	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(Å²)	Q<0.9
1	A	229/315 (72%)	-1.76	0	100	100	39, 65, 90, 121	0
1	B	229/315 (72%)	-1.64	0	100	100	58, 82, 103, 129	0
1	K	229/315 (72%)	-1.73	0	100	100	42, 65, 87, 117	0
1	L	229/315 (72%)	-1.64	0	100	100	54, 88, 104, 122	0
2	C	1119/1119 (100%)	-1.66	0	100	100	31, 73, 106, 124	0
2	M	1119/1119 (100%)	-1.62	1 (0%)	92	91	30, 75, 110, 122	0
3	D	1392/1524 (91%)	-1.65	0	100	100	33, 71, 108, 152	0
3	N	1392/1524 (91%)	-1.63	0	100	100	35, 71, 108, 145	0
4	E	95/99 (95%)	-1.78	0	100	100	49, 79, 103, 109	0
4	O	95/99 (95%)	-1.74	0	100	100	42, 81, 111, 119	0
5	F	345/423 (81%)	-1.53	0	100	100	53, 84, 111, 126	0
5	P	345/423 (81%)	-1.53	0	100	100	41, 83, 110, 117	0
All	All	6818/7590 (89%)	-1.64	1 (0%)	100	100	30, 74, 108, 152	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	39	ARG	2.4

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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	9384	1/1	0.99	0.02	20,20,20,20	0
6	MG	A	9212	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9224	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9227	1/1	1.00	0.02	20,20,20,20	0
6	MG	A	9254	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9268	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9273	1/1	1.00	0.02	20,20,20,20	0
6	MG	A	9295	1/1	1.00	0.02	20,20,20,20	0
6	MG	A	9318	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9327	1/1	1.00	0.02	20,20,20,20	0
6	MG	A	9329	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9334	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9365	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9368	1/1	1.00	0.03	20,20,20,20	0
6	MG	A	9394	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9423	1/1	1.00	0.02	20,20,20,20	0
6	MG	A	9437	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9442	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9462	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9464	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9473	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9486	1/1	1.00	0.02	20,20,20,20	0
6	MG	A	9487	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9517	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9520	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9521	1/1	1.00	0.02	20,20,20,20	0
6	MG	A	9543	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9544	1/1	1.00	0.02	20,20,20,20	0
6	MG	A	9555	1/1	1.00	0.03	20,20,20,20	0
6	MG	B	9228	1/1	1.00	0.02	20,20,20,20	0
6	MG	B	9230	1/1	1.00	0.01	20,20,20,20	0
6	MG	B	9235	1/1	1.00	0.02	20,20,20,20	0
6	MG	B	9256	1/1	1.00	0.03	20,20,20,20	0
6	MG	B	9260	1/1	1.00	0.02	20,20,20,20	0
6	MG	B	9280	1/1	1.00	0.02	20,20,20,20	0
6	MG	B	9281	1/1	1.00	0.02	20,20,20,20	0
6	MG	B	9306	1/1	1.00	0.01	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	B	9311	1/1	1.00	0.07	20,20,20,20	0
6	MG	B	9412	1/1	1.00	0.03	20,20,20,20	0
6	MG	B	9413	1/1	1.00	0.04	20,20,20,20	0
6	MG	B	9420	1/1	1.00	0.01	20,20,20,20	0
6	MG	B	9426	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9427	1/1	1.00	0.03	20,20,20,20	0
6	MG	B	9446	1/1	1.00	0.04	20,20,20,20	0
6	MG	B	9458	1/1	1.00	0.03	20,20,20,20	0
6	MG	B	9485	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9488	1/1	1.00	0.01	20,20,20,20	0
6	MG	B	9491	1/1	1.00	0.01	20,20,20,20	0
6	MG	B	9541	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9552	1/1	1.00	0.03	20,20,20,20	0
6	MG	B	9560	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9202	1/1	1.00	0.03	43,43,43,43	0
6	MG	C	9210	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9213	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9217	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9219	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9221	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9222	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9223	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9231	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9238	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9239	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9243	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9255	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9257	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9259	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9263	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9264	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9266	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9267	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9272	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9282	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9284	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9287	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9289	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9292	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9293	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9299	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9300	1/1	1.00	0.03	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	C	9313	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9316	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9320	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9321	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9328	1/1	1.00	0.07	20,20,20,20	0
6	MG	C	9330	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9335	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9338	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9339	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9345	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9346	1/1	1.00	0.07	20,20,20,20	0
6	MG	C	9347	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9348	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9354	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9356	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9358	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9359	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9364	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9367	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9371	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9378	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9381	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9383	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9385	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9387	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9395	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9396	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9397	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9405	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9408	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9411	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9418	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9422	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9429	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9430	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9438	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9441	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9444	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9451	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9454	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9459	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9465	1/1	1.00	0.05	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	C	9466	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9474	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9476	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9489	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9493	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9497	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9501	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9507	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9509	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9511	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9514	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9519	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9522	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9524	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9525	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9534	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9542	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9549	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9550	1/1	1.00	0.01	20,20,20,20	0
6	MG	C	9553	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9554	1/1	1.00	0.02	20,20,20,20	0
6	MG	C	9561	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9201	1/1	1.00	0.01	30,30,30,30	0
6	MG	D	9203	1/1	1.00	0.03	25,25,25,25	0
6	MG	D	9204	1/1	1.00	0.04	38,38,38,38	0
6	MG	D	9208	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9211	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9214	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9215	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9216	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9218	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9220	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9225	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9226	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9232	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9233	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9234	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9236	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9237	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9240	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9241	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9242	1/1	1.00	0.01	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	9246	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9247	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9248	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9252	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9253	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9258	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9261	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9262	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9265	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9269	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9271	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9274	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9276	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9277	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9279	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9283	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9285	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9286	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9291	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9294	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9296	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9301	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9304	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9307	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9308	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9312	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9314	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9315	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9317	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9319	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9322	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9325	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9331	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9332	1/1	1.00	0.00	20,20,20,20	0
6	MG	D	9333	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9336	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9337	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9342	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9343	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9344	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9349	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9350	1/1	1.00	0.02	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	9351	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9353	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9355	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9357	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9360	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9361	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9362	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9363	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9369	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9370	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9372	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9376	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9377	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9379	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9380	1/1	1.00	0.01	20,20,20,20	0
6	MG	A	9209	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9386	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9390	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9391	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9392	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9393	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9399	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9400	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9401	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9402	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9403	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9404	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9406	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9409	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9410	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9416	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9417	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9419	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9421	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9428	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9433	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9434	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9435	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9439	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9440	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9443	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9447	1/1	1.00	0.01	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	9448	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9452	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9455	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9456	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9460	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9461	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9467	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9469	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9470	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9472	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9475	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9477	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9478	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9479	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9480	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9481	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9482	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9490	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9492	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9498	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9499	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9502	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9503	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9505	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9506	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9510	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9512	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9515	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9518	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9523	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9526	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9527	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9528	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9529	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9532	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9533	1/1	1.00	0.02	20,20,20,20	0
6	MG	D	9535	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9536	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9539	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9546	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9547	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9548	1/1	1.00	0.01	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	9556	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9557	1/1	1.00	0.01	20,20,20,20	0
6	MG	D	9559	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9562	1/1	1.00	0.02	20,20,20,20	0
6	MG	E	9249	1/1	1.00	0.01	20,20,20,20	0
6	MG	E	9275	1/1	1.00	0.01	20,20,20,20	0
6	MG	E	9288	1/1	1.00	0.02	20,20,20,20	0
6	MG	E	9341	1/1	1.00	0.03	20,20,20,20	0
6	MG	E	9352	1/1	1.00	0.01	20,20,20,20	0
6	MG	E	9366	1/1	1.00	0.04	20,20,20,20	0
6	MG	E	9373	1/1	1.00	0.02	20,20,20,20	0
6	MG	E	9389	1/1	1.00	0.02	20,20,20,20	0
6	MG	E	9415	1/1	1.00	0.02	20,20,20,20	0
6	MG	E	9431	1/1	1.00	0.04	20,20,20,20	0
6	MG	E	9432	1/1	1.00	0.05	20,20,20,20	0
6	MG	E	9449	1/1	1.00	0.01	20,20,20,20	0
6	MG	E	9457	1/1	1.00	0.04	20,20,20,20	0
6	MG	E	9484	1/1	1.00	0.02	20,20,20,20	0
6	MG	E	9494	1/1	1.00	0.02	20,20,20,20	0
6	MG	E	9538	1/1	1.00	0.01	20,20,20,20	0
6	MG	E	9551	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9229	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9244	1/1	1.00	0.05	20,20,20,20	0
6	MG	F	9245	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9250	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9251	1/1	1.00	0.04	20,20,20,20	0
6	MG	F	9270	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9278	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9290	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9297	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9298	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9302	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9303	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9305	1/1	1.00	0.08	20,20,20,20	0
6	MG	F	9309	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9310	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9323	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9324	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9326	1/1	1.00	0.05	20,20,20,20	0
6	MG	F	9340	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9374	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9375	1/1	1.00	0.01	20,20,20,20	0

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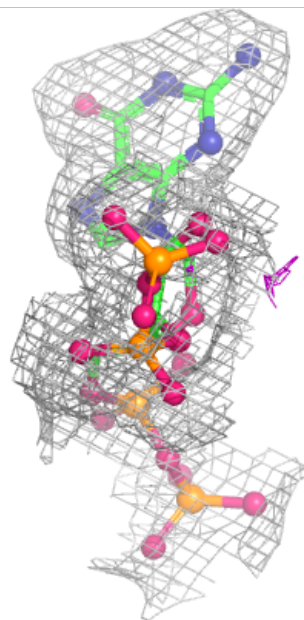
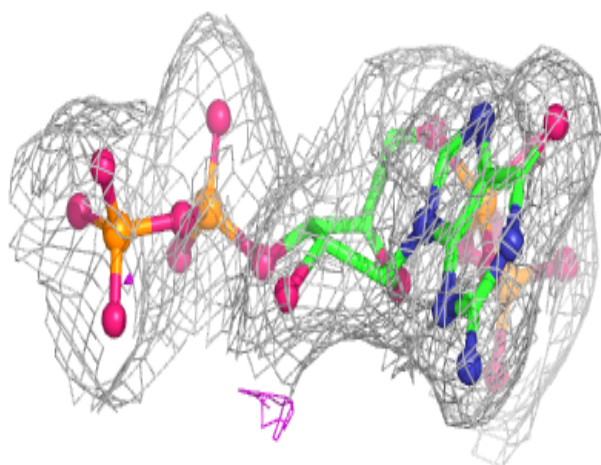
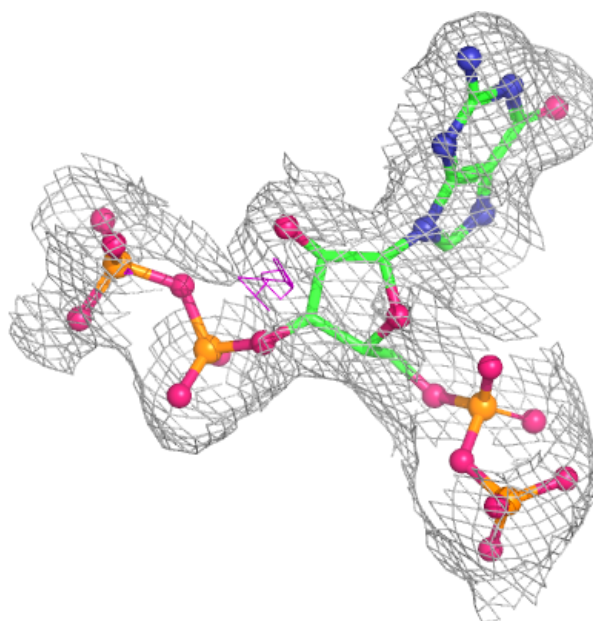
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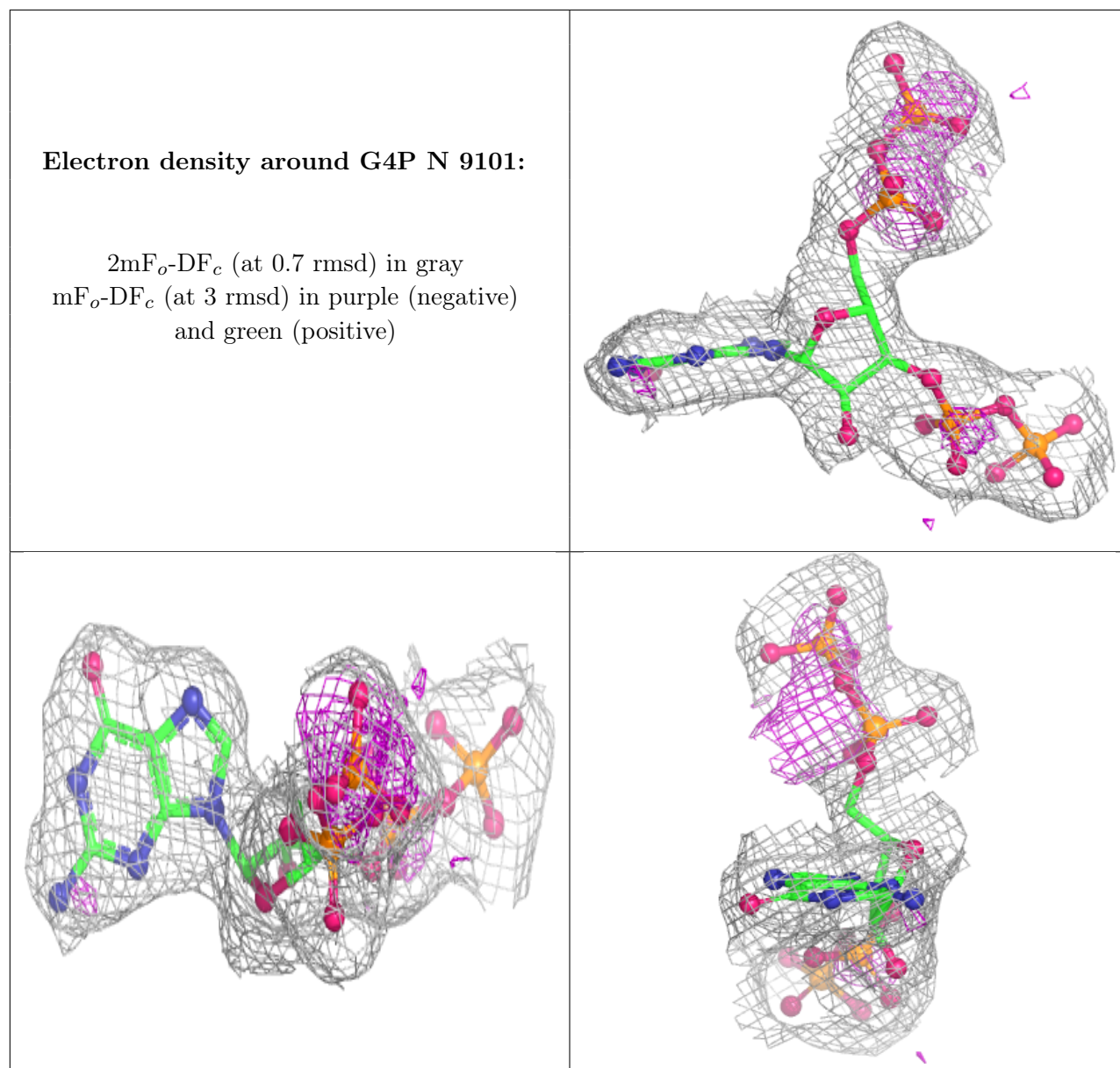
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	F	9382	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9388	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9398	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9407	1/1	1.00	0.04	20,20,20,20	0
6	MG	F	9414	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9424	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9425	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9436	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9445	1/1	1.00	0.04	20,20,20,20	0
6	MG	F	9450	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9453	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9463	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9468	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9471	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9483	1/1	1.00	0.04	20,20,20,20	0
6	MG	F	9495	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9496	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9500	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9504	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9508	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9513	1/1	1.00	0.04	20,20,20,20	0
6	MG	F	9516	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9530	1/1	1.00	0.04	20,20,20,20	0
6	MG	F	9531	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9537	1/1	1.00	0.04	20,20,20,20	0
6	MG	F	9540	1/1	1.00	0.01	20,20,20,20	0
6	MG	F	9545	1/1	1.00	0.02	20,20,20,20	0
6	MG	F	9558	1/1	1.00	0.01	20,20,20,20	0
6	MG	M	9206	1/1	1.00	0.03	38,38,38,38	0
6	MG	N	9205	1/1	1.00	0.01	16,16,16,16	0
6	MG	N	9207	1/1	1.00	0.07	37,37,37,37	0
7	ZN	D	9102	1/1	1.00	0.02	115,115,115,115	0
7	ZN	D	9103	1/1	1.00	0.01	87,87,87,87	0
7	ZN	N	9104	1/1	1.00	0.02	116,116,116,116	0
7	ZN	N	9105	1/1	1.00	0.01	80,80,80,80	0
8	G4P	N	9100	36/36	1.00	0.02	35,45,54,55	0
8	G4P	N	9101	36/36	1.00	0.02	35,45,50,50	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 G4P N 9100:

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 ⓘ

There are no such residues in this entry.