



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 11:58 am BST

PDB ID : 1SMY
Title : Structural basis for transcription regulation by alarmone ppGpp
Authors : Artsimovitch, I.; Patlan, V.; Sekine, S.; Vassylyeva, M.N.; Hosaka, T.; Ochi, K.; Yokoyama, S.; Vassylyev, 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

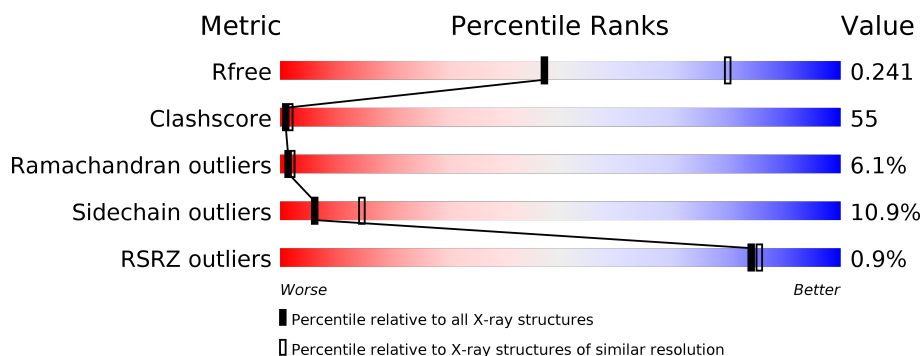
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	<div> <div>21%</div> <div>44%</div> <div>8%</div> <div>27%</div> </div>
1	B	315	<div> <div>21%</div> <div>46%</div> <div>5%</div> <div>27%</div> </div>
1	K	315	<div> <div>21%</div> <div>46%</div> <div>5%</div> <div>27%</div> </div>
1	L	315	<div> <div>23%</div> <div>46%</div> <div>•</div> <div>27%</div> </div>
2	C	1119	<div> <div>28%</div> <div>59%</div> <div>12%</div> <div>•</div> </div>
2	M	1119	<div> <div>27%</div> <div>62%</div> <div>10%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%27%53%10%•9%</div></div>
3	N	1524	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%29%52%9%•9%</div></div>
4	E	99	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>25%58%9%••</div></div>
4	O	99	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>33%51%8%••</div></div>
5	F	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%22%50%8%•18%</div></div>
5	P	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>21%52%7%18%</div></div>

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			

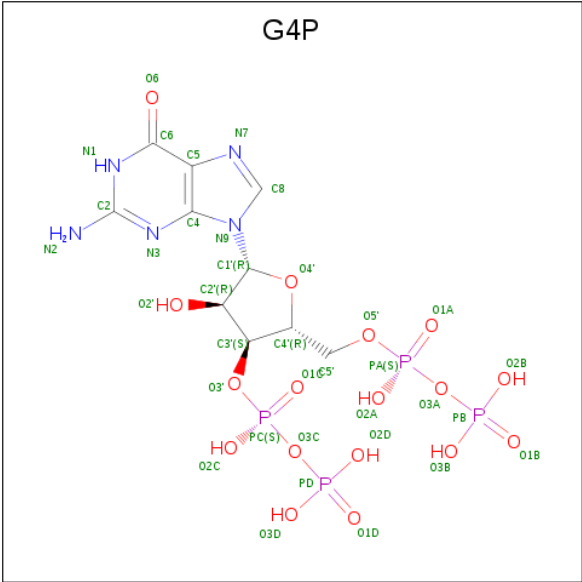
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is ZINC ION (three-letter code: 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 (three-letter code: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).



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

- Molecule 9 is water.

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

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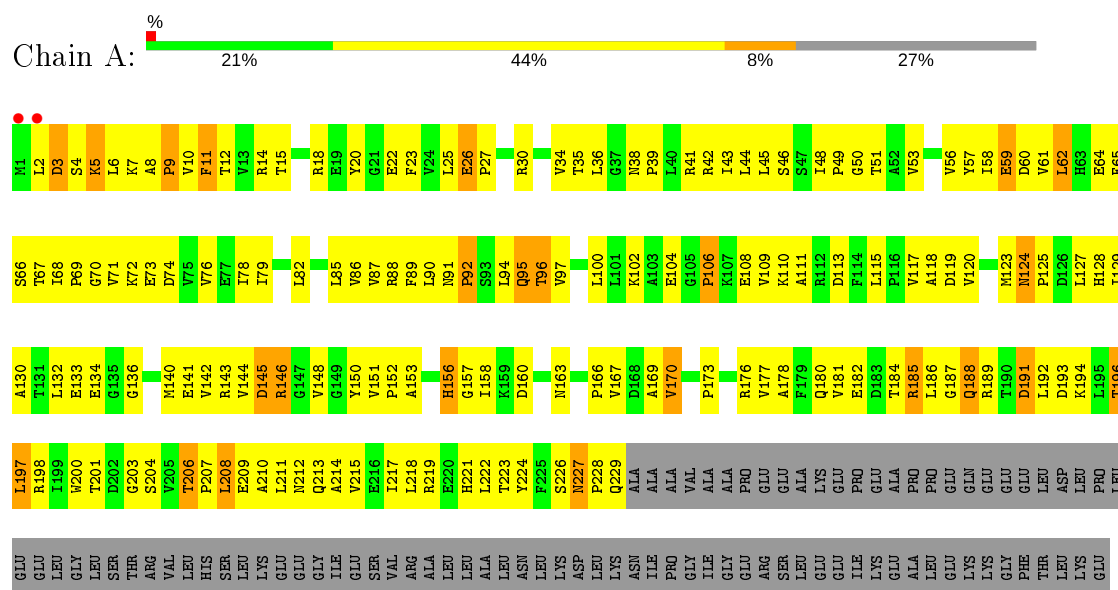
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	O	203	Total 203	O 203	0	0
9	P	541	Total 541	O 541	0	0

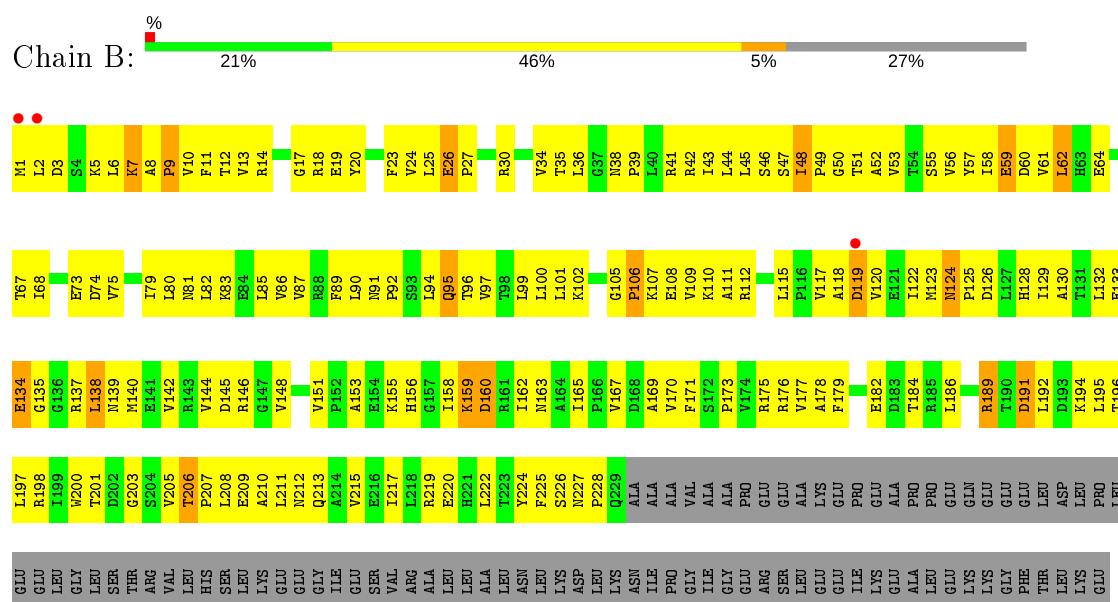
3 Residue-property plots

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

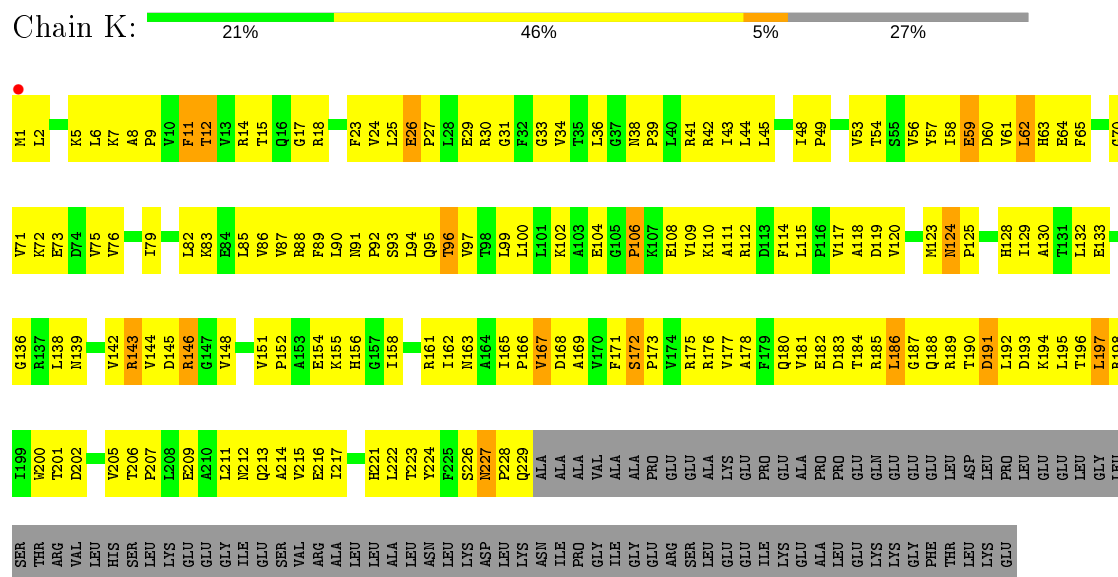
• Molecule 1: DNA-directed RNA polymerase alpha chain



• Molecule 1: DNA-directed RNA polymerase alpha chain

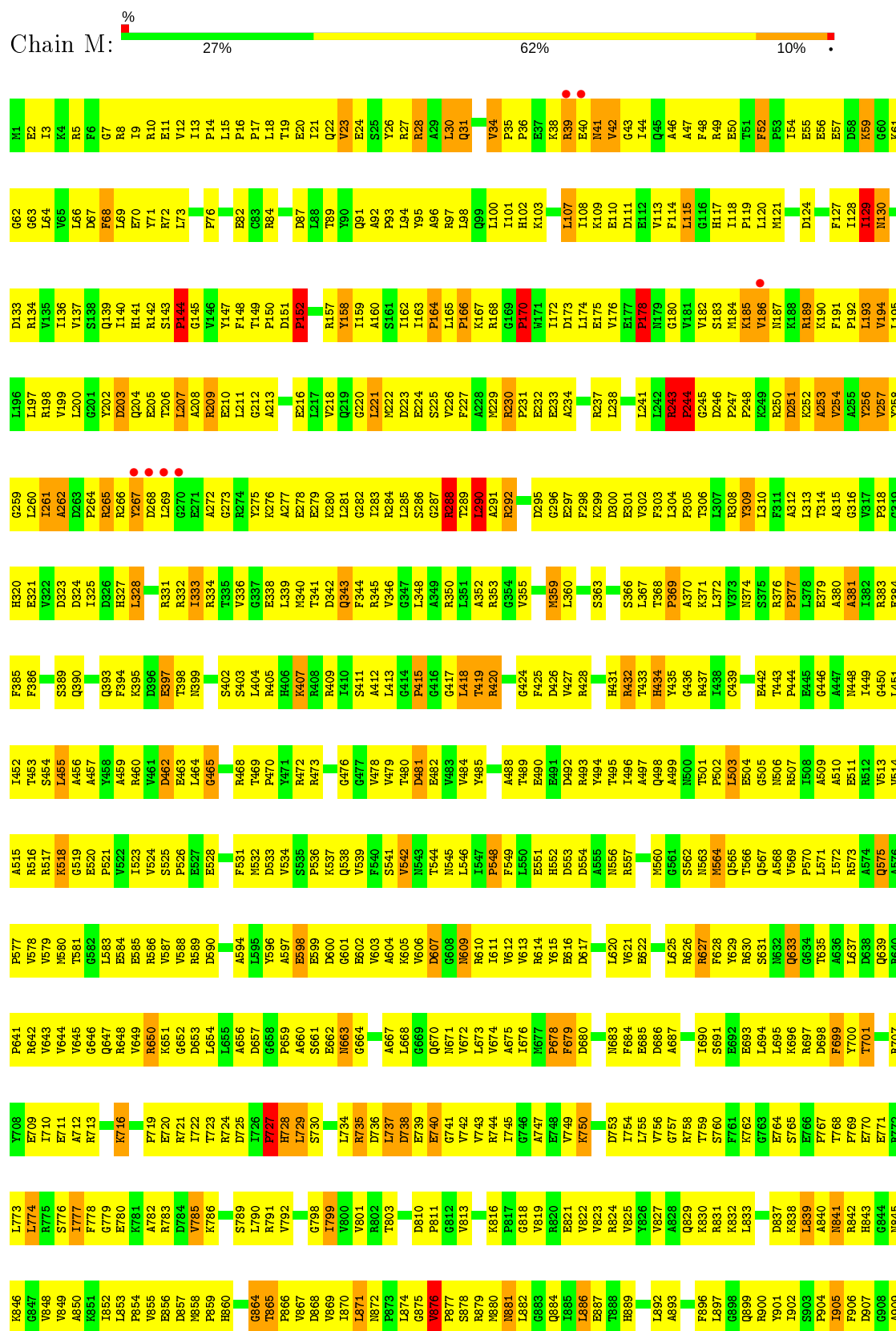


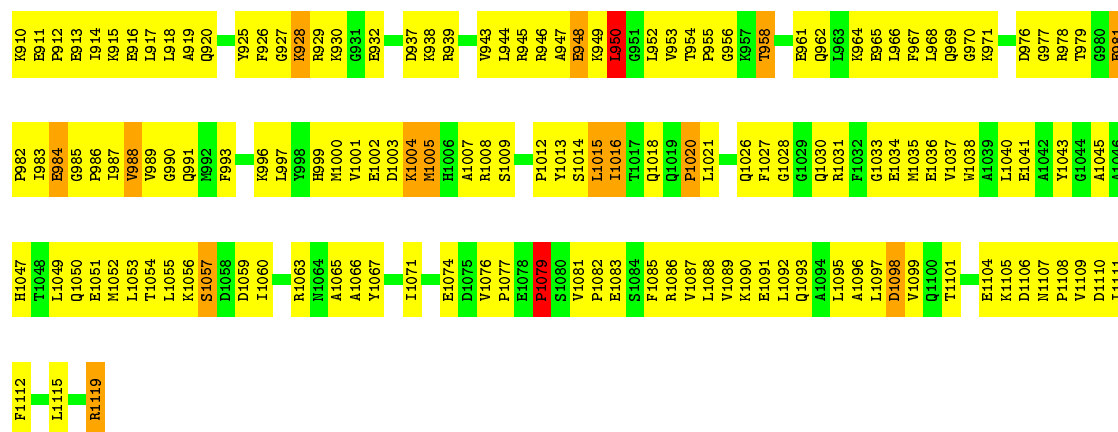
- Molecule 1: DNA-directed RNA polymerase alpha chain



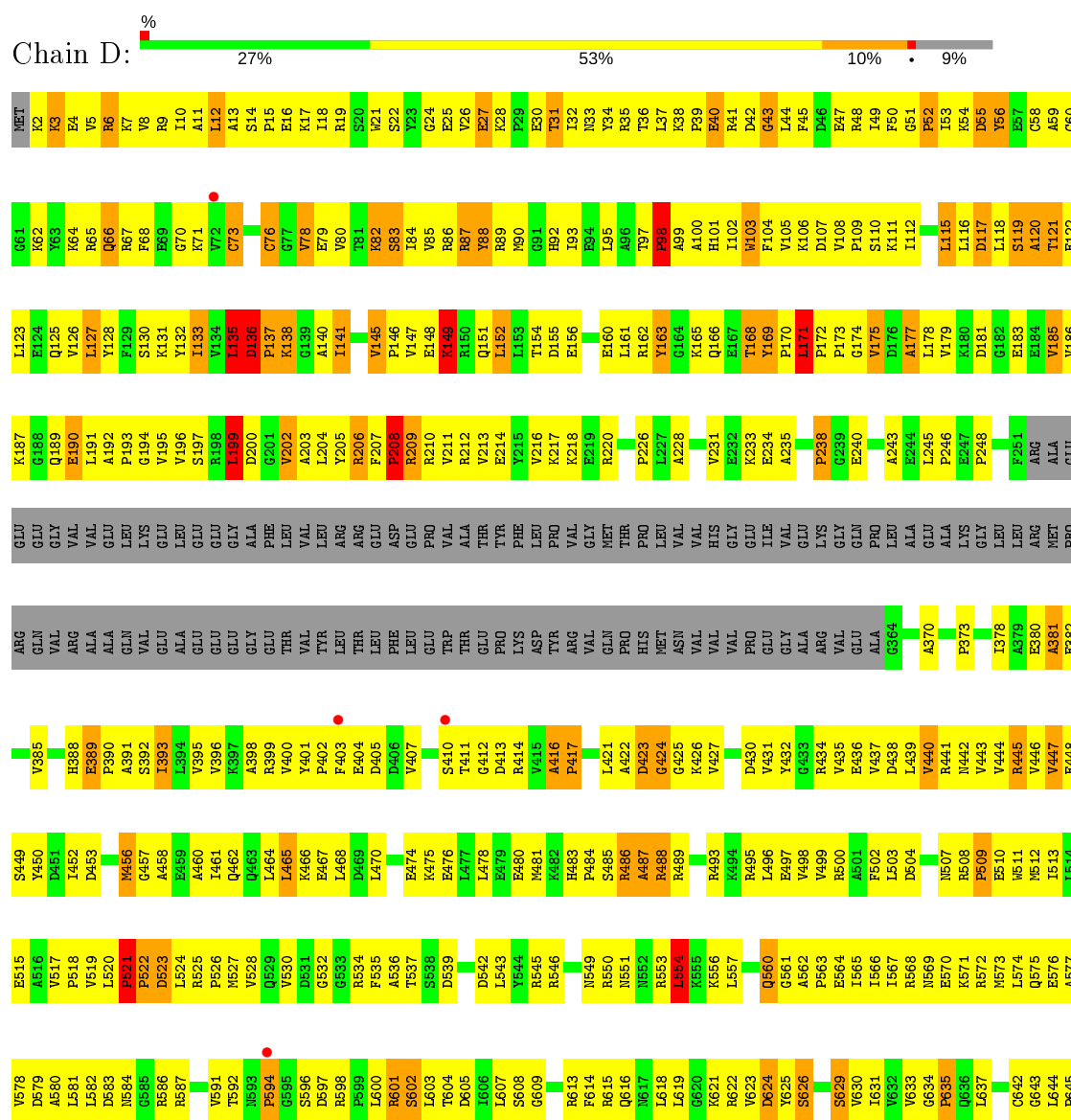


• Molecule 2: DNA-directed RNA polymerase beta chain

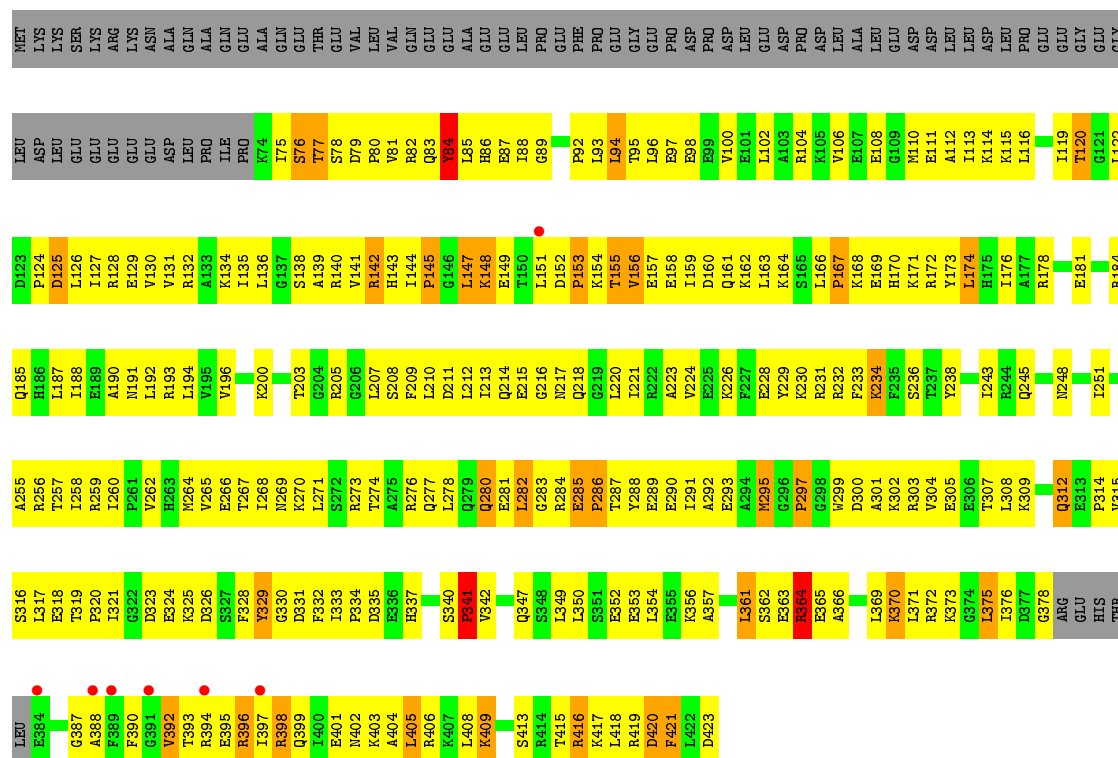




• Molecule 3: DNA-directed RNA polymerase beta' chain



1992	A918	L850	G788	V719	L652	G585	A516	D453	I393	ALA	LEU	G188	Q125	K64	MET
1993	F919	L851	L789	L720	F653	R586	F517	A454	L394	GLU	GLU	Q189	V126	K65	K2
Q994	L920	A952	L792	V721	K654	R587	P518	R455	V395	GLU	GLU	E190	L127	Q66	K3
1995	R921	G851	G792	E722	P655	G588	P519	M456	V396	GLY	GLY	L191	F128	R67	E4
W996	L922	A854	T793	G723	F656	A589	L520	Q457	K397	GLY	ALA	A192	F129	F68	V5
E998	E925	V858	G794	Q724	L657	P590	P921	A458	A398	GLU	PHE	P193	S130	R69	R6
T999	K926	D859	V795	L728	K659	P594	P522	E459	R399	THR	LEU	G194	K131	G70	K7
T1000	T927	L860	K797	H729	K660	G595	D523	A460	V400	VAL	VAL	V195	Y132	K71	V8
E1001	E928	Q861	K798	E729	M661	G596	L524	I461	Y401	TYR	LEU	V196	I133	V72	R9
R929	R929	E798	K799	V732	E662	D597	P526	Q462	P402	THR	ARG	S197	V134	C73	I10
T1003	K863	K800	G800	G733	E663	R598	M527	Q463	F403	THR	ARG	L135	E74	E74	A11
T1004	L831	V864	G801	E734	K664	P599	V528	L464	E404	LEU	GLU	L192	D136	K75	L12
Q1005	G801	T865	G801	A735	E665	L600	G538	L465	D405	PHE	ASP	D200	P137	C76	A13
A1006	V865	V865	L804	F736	M669	R601	F535	K466	D406	LEU	GLU	G201	K138	G77	S14
V1007	R867	R867	E805	M737	V670	S602	A536	E457	V407	GLU	PRO	V202	G139	V78	P15
F1008	F968	R806	F806	A738	K671	L603	T537	D469	V409	THR	VAL	A203	A140	E79	E16
F939	G870	R807	A807	D739	A672	T604	S538	L470	S410	GLU	ALA	L204	I141	V80	K17
T1010	G870	T808	T808	D739	A673	D605	D539	E471	T411	PRO	TYR	R206	I143	K82	R19
F1011	K871	P809	P809	D743	R674	I606	L543	A472	Q412	LYS	PHE	F207	G144	S83	S20
E1012	R872	L807	E811	Q744	R675	L607	L544	L473	D413	LEU	ASP	F208	V145	184	W21
T944	L873	L873	E811	M745	M676	S608	R544	E474	R414	TYR	PRO	R209	P146	V85	S22
S945	E945	E874	A812	A746	K684	G609	R545	K475	V415	ARG	VAL	R210	V147	R86	Y23
T1015	G946	T875	L813	V747	R679	K610	R546	E476	A416	VAL	GLY	V211	E148	R87	G24
P1016	I947	S876	A814	H748	Q680	O611	I547	L477	P417	GLN	MET	R212	K143	V88	E25
F1017	T948	P877	A815	V749	R681	G612	I548	L478	Q418	PRO	THR	V213	R150	R89	V26
P1018	R816	G878	E816	P750	D682	R613	M549	E479	D419	HIS	PRO	E214	Q151	R90	E27
M1019	R879	R879	E817	L751	L683	F614	R550	E480	V420	MET	LEU	Y215	L152	G91	E30
L1020	D952	I880	R818	S752	K684	R614	M551	M481	L421	ASN	VAL	V216	L153	R92	T31
Y1021	D953	G819	G819	S753	D685	L619	M552	D423	A422	VAL	VAL	K217	T154	I93	T32
V1022	A954	E820	E820	F754	E686	G620	R553	P484	D424	VAL	HIS	A221	D155	E94	I32
M1023	R955	V821	V821	A755	R687	K621	L554	S485	Q424	VAL	GLY	K221	E156	L95	R33
A1024	A956	A822	A822	Q756	E688	R622	K555	R486	Q425	PRO	GLY	P226	L161	A99	L37
Q1025	P957	E888	L823	A757	D689	V623	K556	A487	K426	GLU	ILE	R227	R162	P98	T36
E958	E958	A889	N824	E758	A690	D624	L557	R488	V427	GLY	VAL	L227	K161	R97	R35
G1027	E959	V890	A825	A759	L691	V625	L558	R489	K428	ALA	ARG	Y231	K162	A99	L37
A1028	E959	E891	P826	R760	E692	K638	A559	A490	S429	ALA	LYS	K231	R162	A100	K38
R1029	E992	E892	I827	R763	E693	R628	Q580	D430	D430	VAL	GLY	E232	K165	H01	P39
G1030	T963	E893	K828	L764	V694	S629	G561	R493	V431	GLU	GLN	R233	Q166	I102	E40
M1031	L964	K894	V829	V630	K630	S630	G561	K494	Y432	ALA	PRO	E234	E167	M103	R41
E965	E965	V895	A830	S765	K698	I631	I565	R495	Q433	G364	LEU	K238	T168	F104	D42
Q1033	E966	A896	G831	A766	V699	V632	I566	L496	R434	ALA	ALA	G239	Y169	V105	G43
Q1034	A967	V897	R832	H767	V700	V633	I567	E497	V435	GLU	ALA	G239	P170	K106	L44
T1035	D968	E998	E833	N768	L701	G634	R568	V498	E436	ALA	LYS	L245	P172	D107	F45
A1036	R968	L899	T834	L769	L702	P635	R569	R500	V437	ALA	GLY	P246	P173	V108	D46
Q1037	K970	I900	S835	L770	N703	Q636	E570	R500	D438	GLY	LEU	F251	G174	P109	E47
L1038	L902	Q801	V836	S771	R704	L637	K571	A501	L439	ARG	ARG	D251	D175	S110	F50
Q1039	L971	L902	G837	P772	A705	K638	R572	L503	V440	LEU	LEU	K111	V175	K112	I49
G1040	I974	D803	R838	A773	P706	K638	M573	L503	R441	ARG	ARG	D176	D176	G51	P52
L1041	E975	V804	L839	S774	T707	O641	L574	D504	I442	PRO	MET	ALA	A177	P52	
R1042	P905	P905	K840		L703	O642	Q575		V443	ARG	ARG	GLU	L178	L145	D55
L983	Q906	Q906	T841	P777	H709	G643	E576	M507	V444	ARG	ARG	GLU	V179	L146	
T984	E907	R710	V842	L644	R710	L644	A577	R508	R445	GLN	GLN	GLU	K180	D117	
M1045	K908	F843	F843	P781	L711	P645	V578	R508	V446	VAL	VAL	GLY	D181	L118	
Q1046	R986	N909	G712	S782	G712	K646	E510	R509	V446	ARG	ARG	VAL	G182	S119	C58
K1047	E987	K845	N845	R783	L713	R647	A580	M511	E448	ALA	ALA	VAL	E183	A120	A59
F1048	R988	L911	F846	D784	Q714	K648	L581	M512	S449	ALA	ALA	GLU	E184	T121	C60
G1049	R989	R912	E848	I786	A716	K649	L582	I513	V450	GLN	GLN	LEU	V185	E122	G61
E1051	Q991	Q917	A849	L787	F716	L650	M584	E515	I452	VAL	VAL	LYS	K187	L123	K62
						E651								E124	Y63



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 50.12 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.70) 97.1 (50.12-2.71)	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 0.186 , 0.241	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)	0.22 , 59.4	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	0.94	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.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.68	0/1838	0.70	0/2498
1	B	0.68	0/1838	0.68	0/2498
1	K	0.68	0/1838	0.72	1/2498 (0.0%)
1	L	0.68	0/1838	0.67	1/2498 (0.0%)
2	C	0.75	0/8996	0.79	4/12164 (0.0%)
2	M	0.74	0/8996	0.78	4/12164 (0.0%)
3	D	0.74	0/10975	0.81	10/14836 (0.1%)
3	N	0.73	0/10975	0.81	14/14836 (0.1%)
4	E	0.74	0/783	0.81	0/1054
4	O	0.75	0/783	0.81	0/1054
5	F	0.65	0/2811	0.75	1/3781 (0.0%)
5	P	0.64	0/2811	0.74	1/3781 (0.0%)
All	All	0.72	0/54482	0.78	36/73662 (0.0%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	243	ARG	C-N-CD	-9.21	100.34	120.60
3	D	199	LEU	CA-CB-CG	-8.95	94.72	115.30
3	N	199	LEU	CA-CB-CG	-8.85	94.94	115.30
1	K	197	LEU	CA-CB-CG	8.22	134.21	115.30
2	C	243	ARG	C-N-CD	-7.23	104.69	120.60

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	211	0
1	B	1806	0	1861	191	0
1	K	1806	0	1861	196	0
1	L	1806	0	1861	183	0
2	C	8828	0	8933	1013	0
2	M	8828	0	8933	1065	0
3	D	10797	0	10873	1260	0
3	N	10797	0	10873	1227	0
4	E	769	0	775	104	0
4	O	769	0	775	96	0
5	F	2770	0	2844	327	0
5	P	2770	0	2844	363	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	281	0
9	D	1745	0	0	322	0
9	E	160	0	0	37	0
9	F	619	0	0	99	0
9	K	316	0	0	72	0
9	L	341	0	0	64	0
9	M	1401	0	0	325	0
9	N	1794	0	0	330	0
9	O	203	0	0	33	0
9	P	541	0	0	96	0
All	All	63021	0	54316	5952	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 55.

The worst 5 of 5952 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

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	
1	A	227/315 (72%)	187 (82%)	33 (14%)	7 (3%)	4	9
1	B	227/315 (72%)	183 (81%)	38 (17%)	6 (3%)	5	13
1	K	227/315 (72%)	186 (82%)	32 (14%)	9 (4%)	3	6
1	L	227/315 (72%)	185 (82%)	37 (16%)	5 (2%)	6	17
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
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%)	181 (90%)	21 (10%)	7	16
1	B	202/273 (74%)	186 (92%)	16 (8%)	12	28
1	K	202/273 (74%)	187 (93%)	15 (7%)	13	32
1	L	202/273 (74%)	190 (94%)	12 (6%)	19	43
2	C	941/941 (100%)	827 (88%)	114 (12%)	5	11
2	M	941/941 (100%)	838 (89%)	103 (11%)	6	14
3	D	1123/1279 (88%)	992 (88%)	131 (12%)	5	12
3	N	1123/1279 (88%)	987 (88%)	136 (12%)	5	11
4	E	83/87 (95%)	73 (88%)	10 (12%)	5	11
4	O	83/87 (95%)	73 (88%)	10 (12%)	5	11
5	F	295/370 (80%)	263 (89%)	32 (11%)	6	15
5	P	295/370 (80%)	273 (92%)	22 (8%)	13	31
All	All	5692/6446 (88%)	5070 (89%)	622 (11%)	6	14

5 of 622 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1487	VAL
1	L	145	ASP
3	N	1287	GLU
4	E	61	GLU

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Mol	Chain	Res	Type
5	F	362	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	337	HIS
2	M	41	ASN
4	O	33	HIS
1	K	81	ASN
1	L	81	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 carbohydrates 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	30,38,38	1.54	4 (13%)	43,61,61	2.31	13 (30%)
8	G4P	N	9101	6	30,38,38	1.68	6 (20%)	43,61,61	2.25	11 (25%)

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	-	8/23/43/43	0/3/3/3
8	G4P	N	9101	6	-	8/23/43/43	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	9101	G4P	C6-N1	5.77	1.43	1.33
8	N	9100	G4P	C6-N1	4.36	1.40	1.33
8	N	9101	G4P	O4'-C1'	3.85	1.46	1.41
8	N	9100	G4P	O4'-C1'	3.17	1.45	1.41
8	N	9101	G4P	C8-N7	-2.77	1.29	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	9100	G4P	C5-C6-N1	-8.42	111.91	123.43
8	N	9101	G4P	C5-C6-N1	-8.34	112.03	123.43
8	N	9100	G4P	C6-N1-C2	5.66	124.92	115.93
8	N	9101	G4P	C6-N1-C2	5.33	124.39	115.93
8	N	9101	G4P	PC-O3C-PD	-5.30	114.65	132.83

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

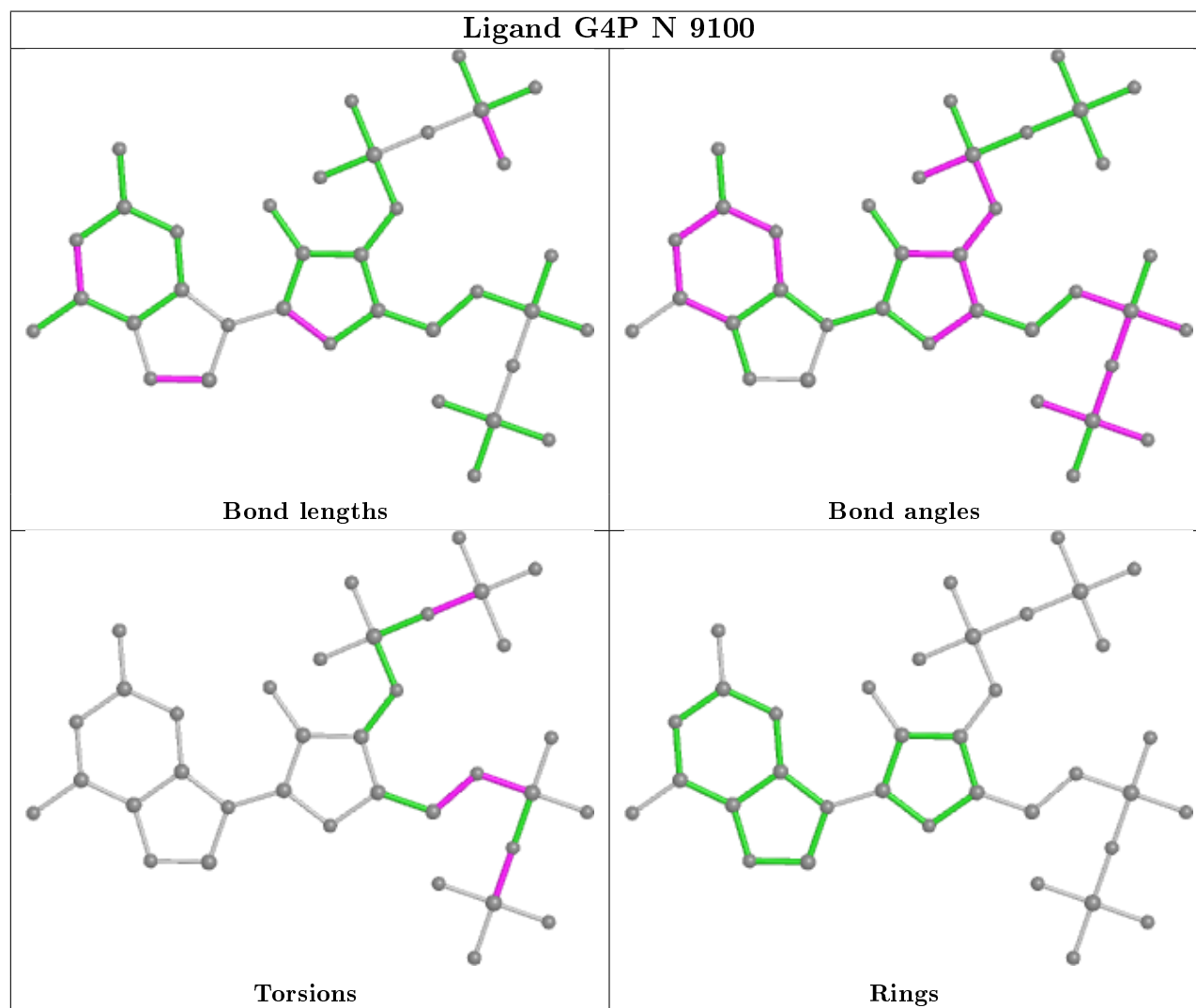
Mol	Chain	Res	Type	Atoms
8	N	9101	G4P	PA-O3A-PB-O3B
8	N	9101	G4P	C5'-O5'-PA-O1A
8	N	9101	G4P	C5'-O5'-PA-O2A
8	N	9101	G4P	C2'-C3'-O3'-PC
8	N	9100	G4P	PA-O3A-PB-O2B

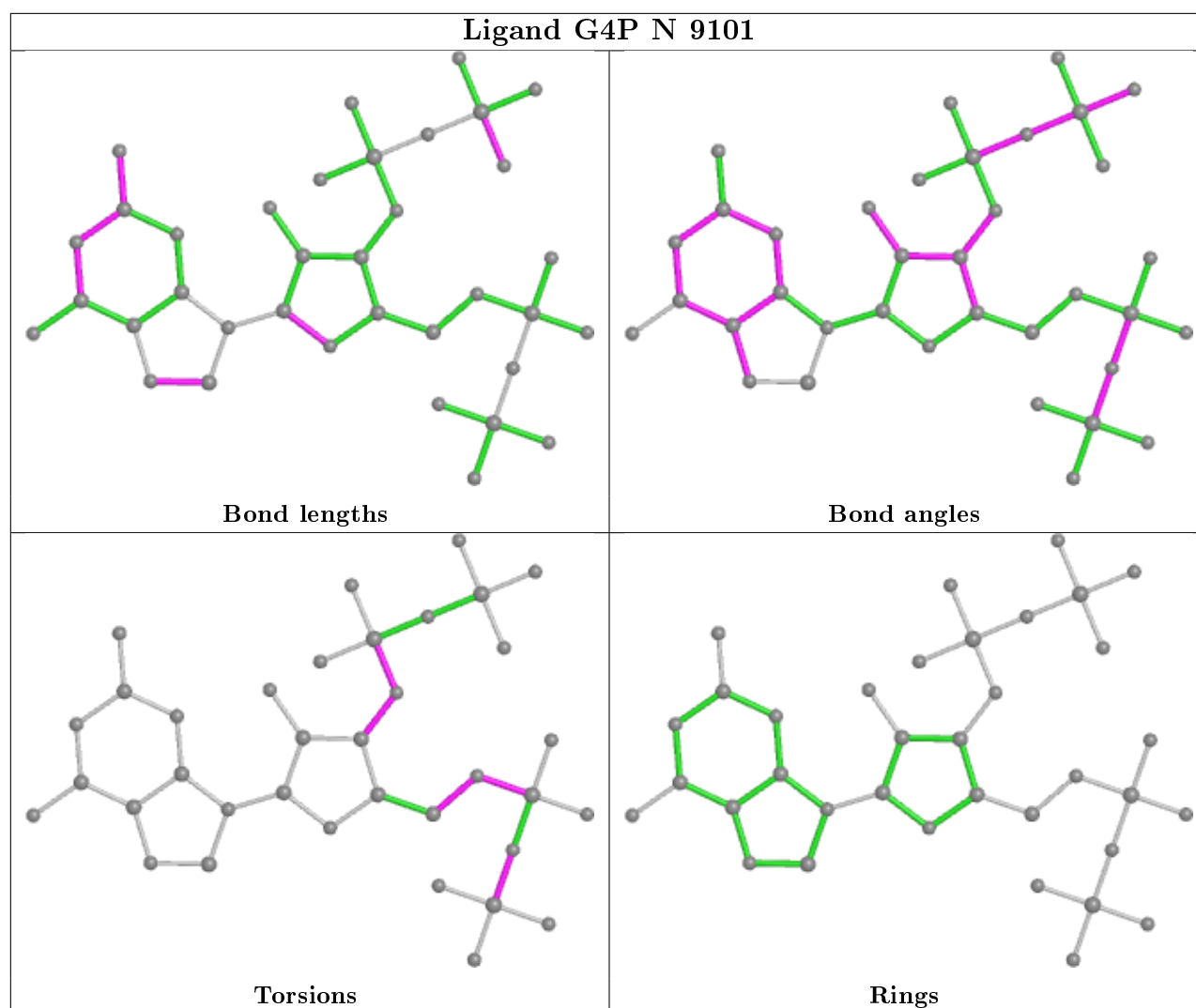
There are no ring outliers.

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(Å ²)	Q<0.9
1	A	229/315 (72%)	-0.74	2 (0%) 84 85	39, 65, 90, 121	0
1	B	229/315 (72%)	-0.70	3 (1%) 77 78	58, 82, 103, 129	0
1	K	229/315 (72%)	-0.72	1 (0%) 92 93	42, 65, 87, 117	0
1	L	229/315 (72%)	-0.71	2 (0%) 84 85	54, 88, 104, 122	0
2	C	1119/1119 (100%)	-0.80	1 (0%) 95 96	31, 73, 106, 124	0
2	M	1119/1119 (100%)	-0.76	7 (0%) 89 91	30, 75, 110, 122	0
3	D	1392/1524 (91%)	-0.70	16 (1%) 80 82	33, 71, 108, 152	0
3	N	1392/1524 (91%)	-0.72	17 (1%) 79 80	35, 71, 108, 145	0
4	E	95/99 (95%)	-0.90	0 100 100	49, 79, 103, 109	0
4	O	95/99 (95%)	-0.77	0 100 100	42, 81, 111, 119	0
5	F	345/423 (81%)	-0.61	7 (2%) 65 67	53, 84, 111, 126	0
5	P	345/423 (81%)	-0.66	2 (0%) 89 91	41, 83, 110, 117	0
All	All	6818/7590 (89%)	-0.73	58 (0%) 84 85	30, 74, 108, 152	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	1246	VAL	7.3
3	D	1245	GLY	7.2
3	D	1246	VAL	6.5
3	N	1247	ALA	6.2
3	D	1243	THR	5.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	ZN	D	9102	1/1	0.96	0.06	115,115,115,115	0
6	MG	D	9416	1/1	0.96	0.08	20,20,20,20	0
6	MG	C	9202	1/1	0.96	0.07	43,43,43,43	0
6	MG	D	9384	1/1	0.96	0.07	20,20,20,20	0
6	MG	D	9240	1/1	0.96	0.08	20,20,20,20	0
6	MG	D	9204	1/1	0.96	0.05	38,38,38,38	0
6	MG	C	9272	1/1	0.97	0.07	20,20,20,20	0
6	MG	D	9201	1/1	0.97	0.11	30,30,30,30	0
6	MG	F	9250	1/1	0.97	0.06	20,20,20,20	0
6	MG	C	9525	1/1	0.97	0.05	20,20,20,20	0
6	MG	C	9257	1/1	0.97	0.06	20,20,20,20	0
6	MG	D	9528	1/1	0.97	0.06	20,20,20,20	0
6	MG	A	9394	1/1	0.97	0.09	20,20,20,20	0
6	MG	M	9206	1/1	0.97	0.10	38,38,38,38	0
6	MG	C	9554	1/1	0.98	0.06	20,20,20,20	0
6	MG	F	9398	1/1	0.98	0.07	20,20,20,20	0
6	MG	C	9356	1/1	0.98	0.07	20,20,20,20	0
6	MG	F	9496	1/1	0.98	0.05	20,20,20,20	0
6	MG	C	9320	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9301	1/1	0.98	0.05	20,20,20,20	0
6	MG	D	9220	1/1	0.98	0.07	20,20,20,20	0
6	MG	B	9235	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9518	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9271	1/1	0.98	0.06	20,20,20,20	0
6	MG	F	9290	1/1	0.98	0.06	20,20,20,20	0
6	MG	E	9431	1/1	0.98	0.07	20,20,20,20	0
6	MG	F	9305	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9390	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9406	1/1	0.98	0.05	20,20,20,20	0
7	ZN	D	9103	1/1	0.98	0.09	87,87,87,87	0
6	MG	C	9238	1/1	0.98	0.07	20,20,20,20	0
7	ZN	N	9105	1/1	0.98	0.10	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9241	1/1	0.98	0.06	20,20,20,20	0
6	MG	C	9299	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9214	1/1	0.98	0.07	20,20,20,20	0
6	MG	C	9210	1/1	0.98	0.05	20,20,20,20	0
6	MG	C	9364	1/1	0.98	0.06	20,20,20,20	0
6	MG	C	9354	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9355	1/1	0.98	0.13	20,20,20,20	0
6	MG	D	9216	1/1	0.98	0.08	20,20,20,20	0
6	MG	D	9460	1/1	0.98	0.04	20,20,20,20	0
6	MG	D	9226	1/1	0.98	0.04	20,20,20,20	0
6	MG	D	9294	1/1	0.98	0.07	20,20,20,20	0
6	MG	C	9441	1/1	0.98	0.05	20,20,20,20	0
6	MG	C	9519	1/1	0.98	0.05	20,20,20,20	0
7	ZN	N	9104	1/1	0.98	0.05	116,116,116,116	0
6	MG	D	9480	1/1	0.98	0.07	20,20,20,20	0
6	MG	B	9485	1/1	0.98	0.05	20,20,20,20	0
6	MG	D	9386	1/1	0.98	0.04	20,20,20,20	0
6	MG	B	9413	1/1	0.98	0.05	20,20,20,20	0
6	MG	D	9532	1/1	0.98	0.04	20,20,20,20	0
6	MG	E	9341	1/1	0.98	0.06	20,20,20,20	0
6	MG	E	9249	1/1	0.98	0.09	20,20,20,20	0
6	MG	F	9545	1/1	0.98	0.08	20,20,20,20	0
6	MG	F	9500	1/1	0.98	0.08	20,20,20,20	0
8	G4P	N	9100	36/36	0.98	0.11	35,45,54,55	0
6	MG	D	9237	1/1	0.98	0.05	20,20,20,20	0
6	MG	A	9318	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9465	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9368	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9353	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9504	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9303	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9265	1/1	0.99	0.09	20,20,20,20	0
6	MG	F	9251	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9342	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9243	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9463	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9533	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9408	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9333	1/1	0.99	0.05	20,20,20,20	0
6	MG	E	9432	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9348	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9393	1/1	0.99	0.08	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	C	9359	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9443	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9325	1/1	0.99	0.10	20,20,20,20	0
6	MG	C	9444	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9273	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9295	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9423	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9302	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9330	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9517	1/1	0.99	0.06	20,20,20,20	0
6	MG	E	9373	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9331	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9328	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9451	1/1	0.99	0.11	20,20,20,20	0
6	MG	D	9546	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9414	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9334	1/1	0.99	0.04	20,20,20,20	0
6	MG	E	9415	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9298	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9440	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9304	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9526	1/1	0.99	0.07	20,20,20,20	0
6	MG	B	9552	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9332	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9400	1/1	0.99	0.08	20,20,20,20	0
6	MG	C	9489	1/1	0.99	0.11	20,20,20,20	0
6	MG	E	9494	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9487	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9222	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9472	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9244	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9217	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9309	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9558	1/1	0.99	0.07	20,20,20,20	0
6	MG	B	9491	1/1	0.99	0.08	20,20,20,20	0
6	MG	C	9430	1/1	0.99	0.06	20,20,20,20	0
6	MG	B	9488	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9512	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9464	1/1	0.99	0.06	20,20,20,20	0
6	MG	E	9484	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9362	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9516	1/1	0.99	0.09	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9439	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9470	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9456	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9548	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9300	1/1	0.99	0.03	20,20,20,20	0
6	MG	D	9559	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9529	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9550	1/1	0.99	0.08	20,20,20,20	0
6	MG	F	9340	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9378	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9523	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9269	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9483	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9358	1/1	0.99	0.07	20,20,20,20	0
6	MG	A	9327	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9454	1/1	0.99	0.07	20,20,20,20	0
6	MG	B	9306	1/1	0.99	0.10	20,20,20,20	0
6	MG	B	9311	1/1	0.99	0.11	20,20,20,20	0
6	MG	D	9258	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9442	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9530	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9506	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9467	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9361	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9323	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9445	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9513	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9477	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9503	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9557	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9536	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9479	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9372	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9497	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9297	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9562	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9261	1/1	0.99	0.10	20,20,20,20	0
6	MG	C	9239	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9326	1/1	0.99	0.04	20,20,20,20	0
6	MG	N	9205	1/1	0.99	0.08	16,16,16,16	0
6	MG	D	9296	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9336	1/1	0.99	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9285	1/1	0.99	0.11	20,20,20,20	0
6	MG	F	9382	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9425	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9229	1/1	0.99	0.11	20,20,20,20	0
6	MG	D	9286	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9403	1/1	0.99	0.04	20,20,20,20	0
6	MG	B	9260	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9283	1/1	0.99	0.10	20,20,20,20	0
6	MG	C	9395	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9490	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9474	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9255	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9317	1/1	0.99	0.12	20,20,20,20	0
6	MG	E	9551	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9363	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9450	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9396	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9371	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9370	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9561	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9291	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9434	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9203	1/1	0.99	0.08	25,25,25,25	0
6	MG	F	9468	1/1	0.99	0.06	20,20,20,20	0
6	MG	E	9538	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9502	1/1	0.99	0.10	20,20,20,20	0
6	MG	C	9267	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9233	1/1	0.99	0.06	20,20,20,20	0
6	MG	B	9280	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9448	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9225	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9410	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9473	1/1	0.99	0.05	20,20,20,20	0
6	MG	B	9458	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9495	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9391	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9405	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9539	1/1	0.99	0.03	20,20,20,20	0
8	G4P	N	9101	36/36	0.99	0.11	35,45,50,50	0
6	MG	D	9344	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9262	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9365	1/1	0.99	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	A	9486	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9369	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9315	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9377	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9252	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9433	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9367	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9407	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9399	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9223	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9287	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9219	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9277	1/1	0.99	0.09	20,20,20,20	0
6	MG	B	9446	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9263	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9452	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9505	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9316	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9375	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9475	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9520	1/1	0.99	0.08	20,20,20,20	0
6	MG	C	9293	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9227	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9211	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9236	1/1	0.99	0.08	20,20,20,20	0
6	MG	F	9424	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9478	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9466	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9212	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9417	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9345	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9308	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9221	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9508	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9515	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9381	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9218	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9498	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9404	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9501	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9524	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9507	1/1	0.99	0.03	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	F	9374	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9339	1/1	0.99	0.11	20,20,20,20	0
6	MG	D	9527	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9357	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9453	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9307	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9310	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9542	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9556	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9511	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9274	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9476	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9409	1/1	0.99	0.11	20,20,20,20	0
6	MG	D	9246	1/1	0.99	0.07	20,20,20,20	0
6	MG	E	9389	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9385	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9282	1/1	0.99	0.05	20,20,20,20	0
6	MG	B	9256	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9514	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9499	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9264	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9422	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9531	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9438	1/1	0.99	0.11	20,20,20,20	0
6	MG	E	9449	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9401	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9289	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9482	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9247	1/1	0.99	0.07	20,20,20,20	0
6	MG	B	9230	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9383	1/1	0.99	0.04	20,20,20,20	0
6	MG	B	9427	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9540	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9419	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9313	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9337	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9469	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9421	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9387	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9481	1/1	0.99	0.08	20,20,20,20	0
6	MG	C	9321	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9543	1/1	0.99	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	F	9245	1/1	0.99	0.09	20,20,20,20	0
6	MG	E	9352	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9253	1/1	0.99	0.08	20,20,20,20	0
6	MG	B	9228	1/1	1.00	0.08	20,20,20,20	0
6	MG	D	9376	1/1	1.00	0.04	20,20,20,20	0
6	MG	B	9426	1/1	1.00	0.06	20,20,20,20	0
6	MG	A	9555	1/1	1.00	0.04	20,20,20,20	0
6	MG	F	9278	1/1	1.00	0.07	20,20,20,20	0
6	MG	C	9411	1/1	1.00	0.11	20,20,20,20	0
6	MG	A	9462	1/1	1.00	0.07	20,20,20,20	0
6	MG	A	9437	1/1	1.00	0.07	20,20,20,20	0
6	MG	B	9560	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9349	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9547	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9429	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9380	1/1	1.00	0.10	20,20,20,20	0
6	MG	F	9436	1/1	1.00	0.11	20,20,20,20	0
6	MG	D	9455	1/1	1.00	0.10	20,20,20,20	0
6	MG	D	9428	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9397	1/1	1.00	0.05	20,20,20,20	0
6	MG	E	9366	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9234	1/1	1.00	0.09	20,20,20,20	0
6	MG	C	9346	1/1	1.00	0.10	20,20,20,20	0
6	MG	F	9324	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9461	1/1	1.00	0.06	20,20,20,20	0
6	MG	A	9224	1/1	1.00	0.07	20,20,20,20	0
6	MG	E	9275	1/1	1.00	0.10	20,20,20,20	0
6	MG	D	9392	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9312	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9492	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9549	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9379	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9232	1/1	1.00	0.10	20,20,20,20	0
6	MG	D	9435	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9213	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9509	1/1	1.00	0.06	20,20,20,20	0
6	MG	B	9420	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9343	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9553	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9284	1/1	1.00	0.07	20,20,20,20	0
6	MG	C	9335	1/1	1.00	0.08	20,20,20,20	0
6	MG	D	9242	1/1	1.00	0.11	20,20,20,20	0

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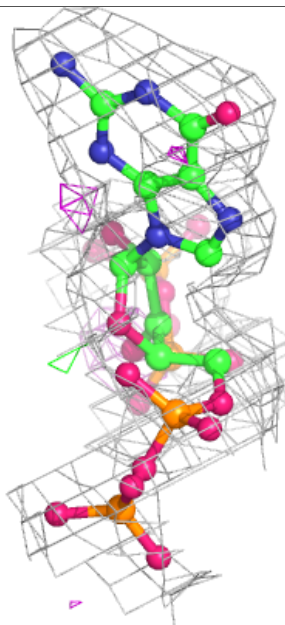
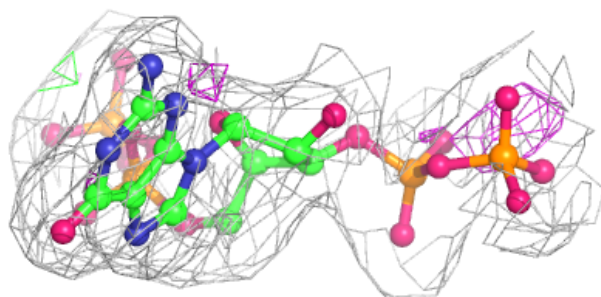
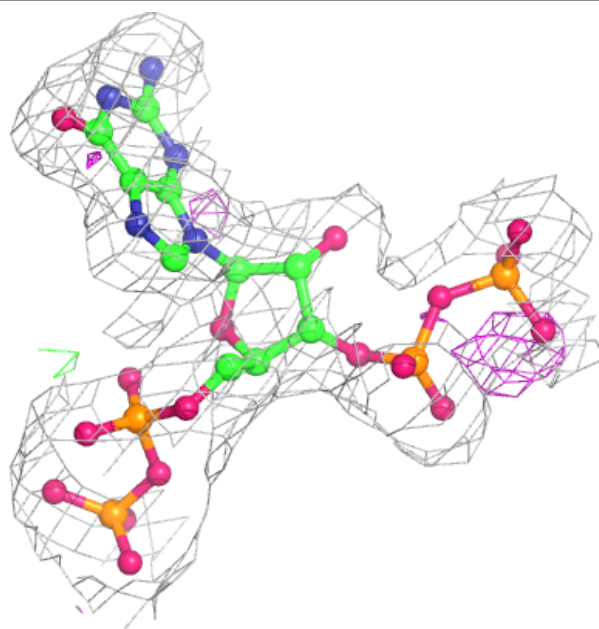
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	9279	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9418	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9314	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9541	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9319	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9254	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9447	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9231	1/1	1.00	0.10	20,20,20,20	0
6	MG	D	9208	1/1	1.00	0.10	20,20,20,20	0
6	MG	C	9338	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9522	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9534	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9266	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9360	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9215	1/1	1.00	0.08	20,20,20,20	0
6	MG	N	9207	1/1	1.00	0.07	37,37,37,37	0
6	MG	D	9510	1/1	1.00	0.08	20,20,20,20	0
6	MG	D	9276	1/1	1.00	0.05	20,20,20,20	0
6	MG	E	9288	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9459	1/1	1.00	0.06	20,20,20,20	0
6	MG	A	9329	1/1	1.00	0.08	20,20,20,20	0
6	MG	D	9322	1/1	1.00	0.09	20,20,20,20	0
6	MG	F	9537	1/1	1.00	0.05	20,20,20,20	0
6	MG	F	9388	1/1	1.00	0.09	20,20,20,20	0
6	MG	B	9281	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9347	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9521	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9259	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9535	1/1	1.00	0.06	20,20,20,20	0
6	MG	F	9471	1/1	1.00	0.08	20,20,20,20	0
6	MG	A	9544	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9350	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9412	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9292	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9248	1/1	1.00	0.06	20,20,20,20	0
6	MG	F	9270	1/1	1.00	0.03	20,20,20,20	0
6	MG	E	9457	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9268	1/1	1.00	0.10	20,20,20,20	0
6	MG	A	9209	1/1	1.00	0.20	20,20,20,20	0
6	MG	D	9402	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9493	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9351	1/1	1.00	0.09	20,20,20,20	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.

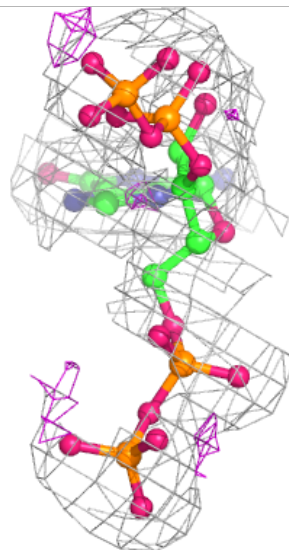
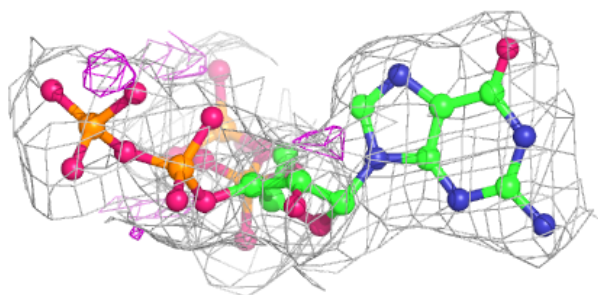
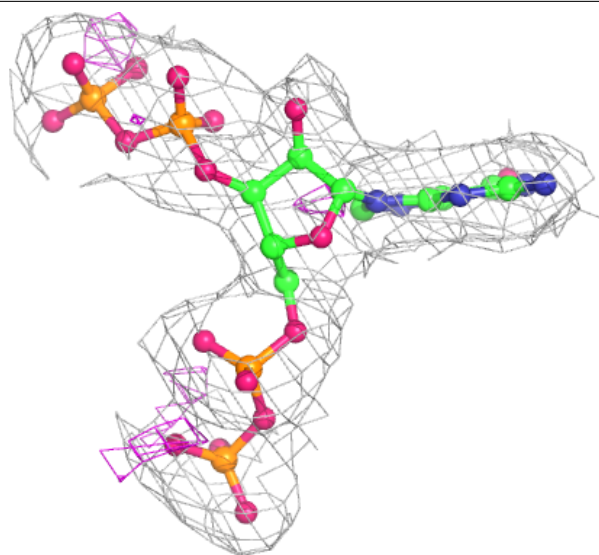
Electron density around G4P N 9100:

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



Electron density around G4P N 9101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.