



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 05:46 am BST

PDB ID : 2BE5
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with inhibitor tagetitoxin
Authors : Vassylyev, D.G.; Svetlov, V.; Vassylyeva, M.N.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Artsimovitch, I.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-10-22
Resolution : 2.40 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

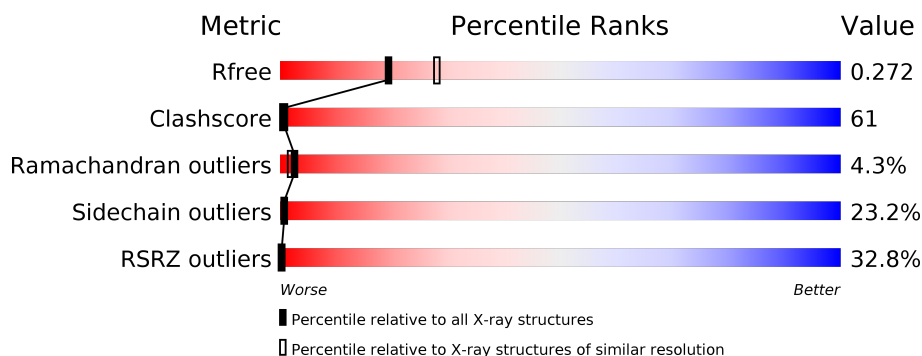
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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>22%</div> <div> <div>14%</div> <div>45%</div> <div>12%</div> <div>27%</div> </div> </div>
1	B	315	<div> <div>25%</div> <div> <div>18%</div> <div>44%</div> <div>10%</div> <div>27%</div> </div> </div>
1	K	315	<div> <div>22%</div> <div> <div>18%</div> <div>43%</div> <div>11%</div> <div>27%</div> </div> </div>
1	L	315	<div> <div>22%</div> <div> <div>15%</div> <div>45%</div> <div>12%</div> <div>27%</div> </div> </div>
2	C	1119	<div> <div>37%</div> <div> <div>23%</div> <div>58%</div> <div>18%</div> </div> </div>
2	M	1119	<div> <div>38%</div> <div> <div>23%</div> <div>60%</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div></div><div>25%</div><div>21%</div><div>54%</div><div>15%</div><div>•</div><div>9%</div></div>
3	N	1524	<div><div></div><div>25%</div><div>22%</div><div>51%</div><div>17%</div><div>•</div><div>9%</div></div>
4	E	99	<div><div></div><div>23%</div><div>24%</div><div>56%</div><div>15%</div><div>•</div><div>•</div></div>
4	O	99	<div><div></div><div>22%</div><div>29%</div><div>44%</div><div>22%</div><div>•</div><div></div></div>
5	F	423	<div><div></div><div>37%</div><div>20%</div><div>49%</div><div>11%</div><div>•</div><div>18%</div></div>
5	P	423	<div><div></div><div>35%</div><div>21%</div><div>48%</div><div>12%</div><div></div><div>18%</div></div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 61800 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
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	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 chain.

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 RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

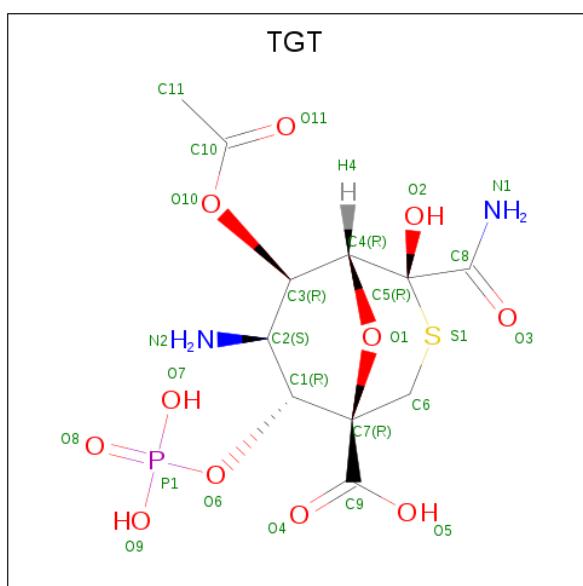
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	N	2	Total	Mg	0	0
			2	2		

- 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 TAGETITOXIN (three-letter code: TGT) (formula: C₁₁H₁₇N₂O₁₁PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	D	1	Total 26	C 11	N 2	O 11	P 1	S 1	0	0
8	N	1	Total 26	C 11	N 2	O 11	P 1	S 1	0	0

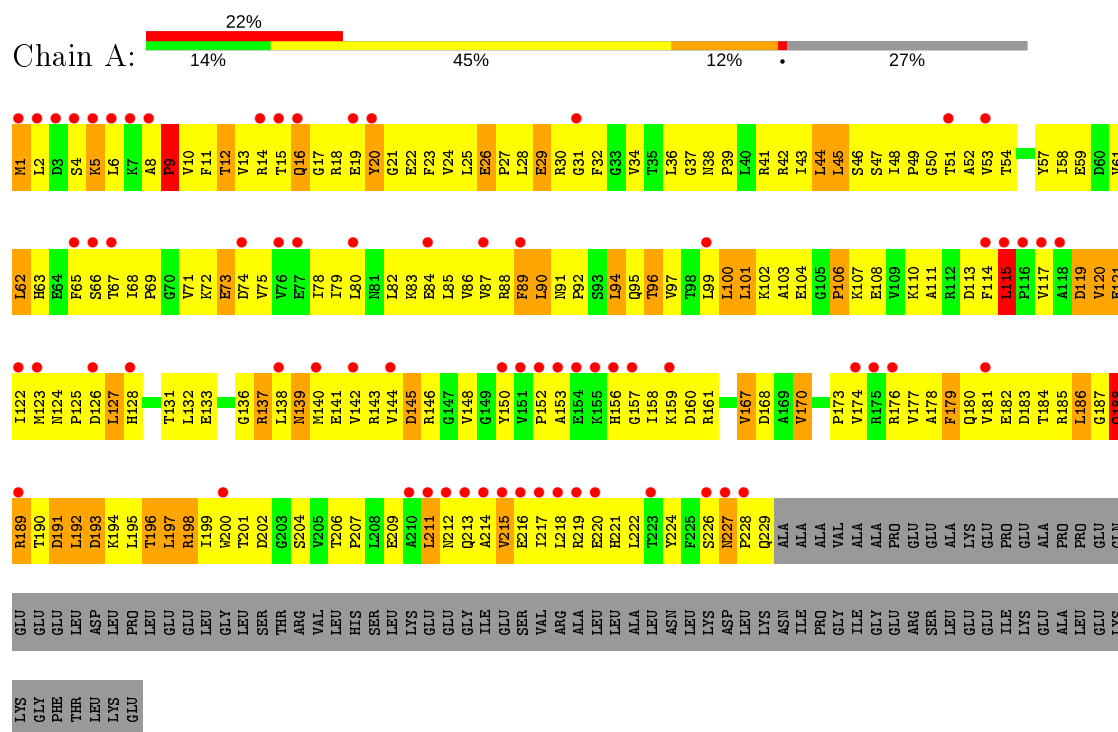
- Molecule 9 is water.

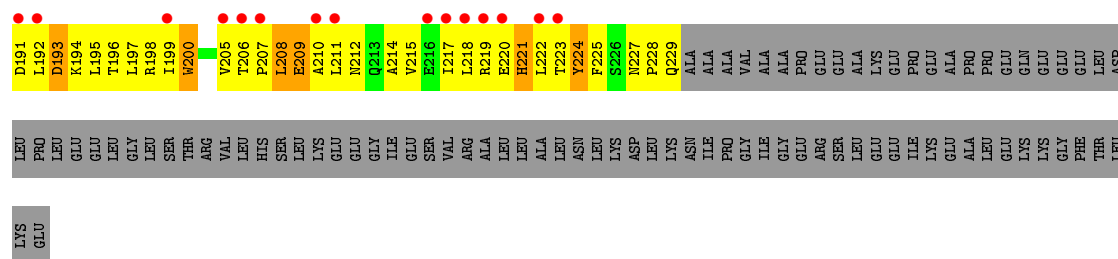
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	250	Total 250	O 250	0	0
9	B	329	Total 329	O 329	0	0
9	C	1321	Total 1321	O 1321	0	0
9	D	1655	Total 1655	O 1655	0	0
9	E	176	Total 176	O 176	0	0
9	F	519	Total 519	O 519	0	0
9	K	278	Total 278	O 278	0	0
9	L	309	Total 309	O 309	0	0
9	M	1236	Total 1236	O 1236	0	0
9	N	1552	Total 1552	O 1552	0	0
9	O	137	Total 137	O 137	0	0
9	P	422	Total 422	O 422	0	0

3 Residue-property plots

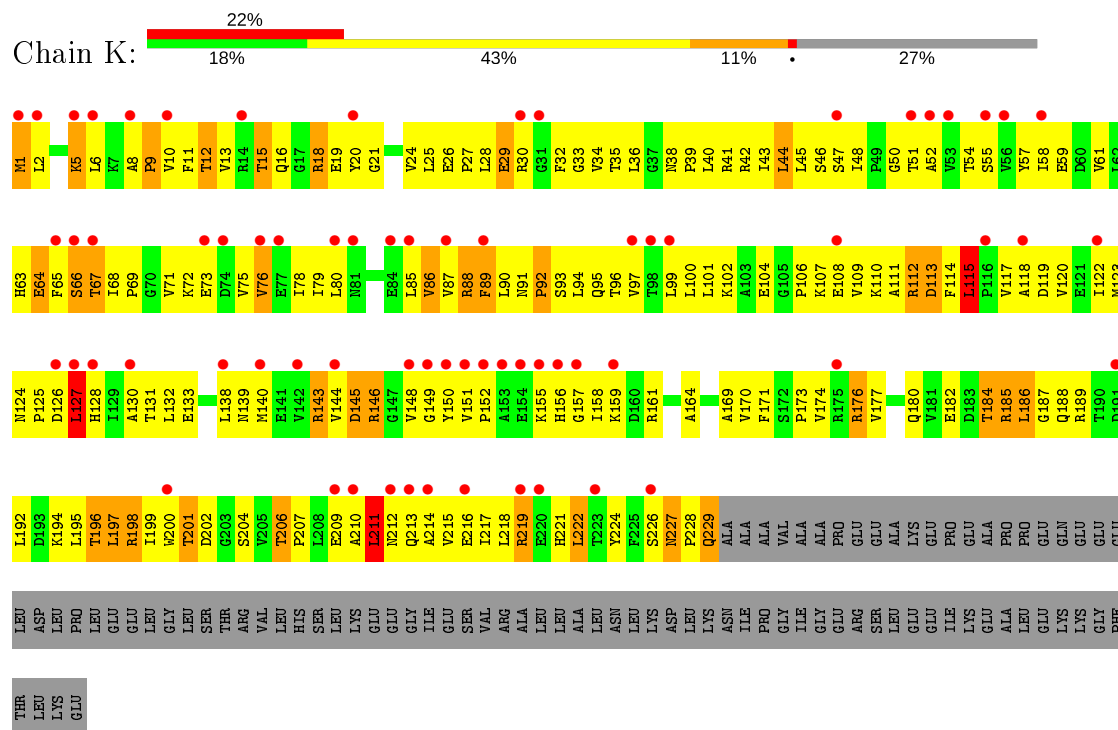
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

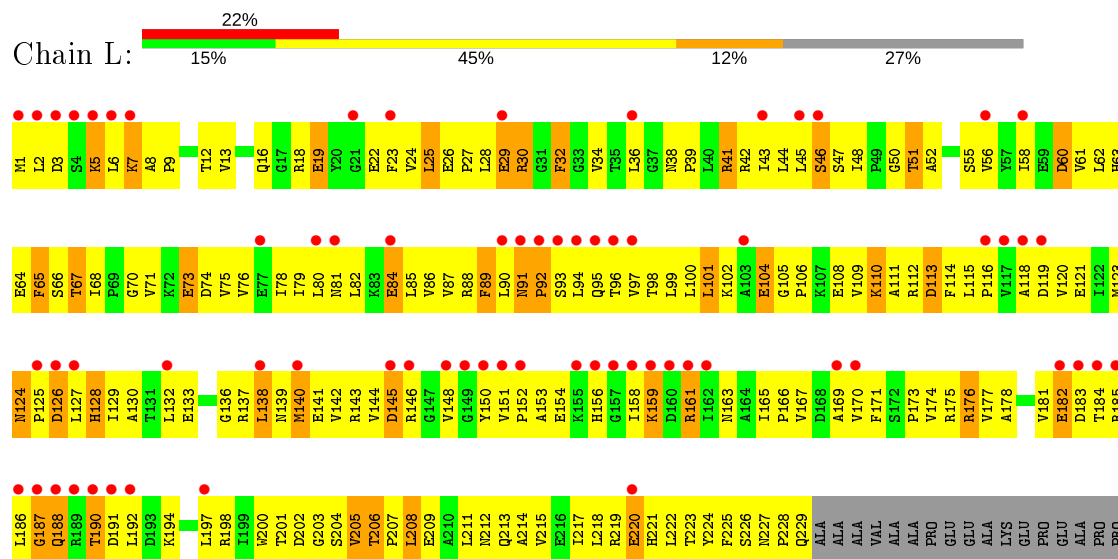


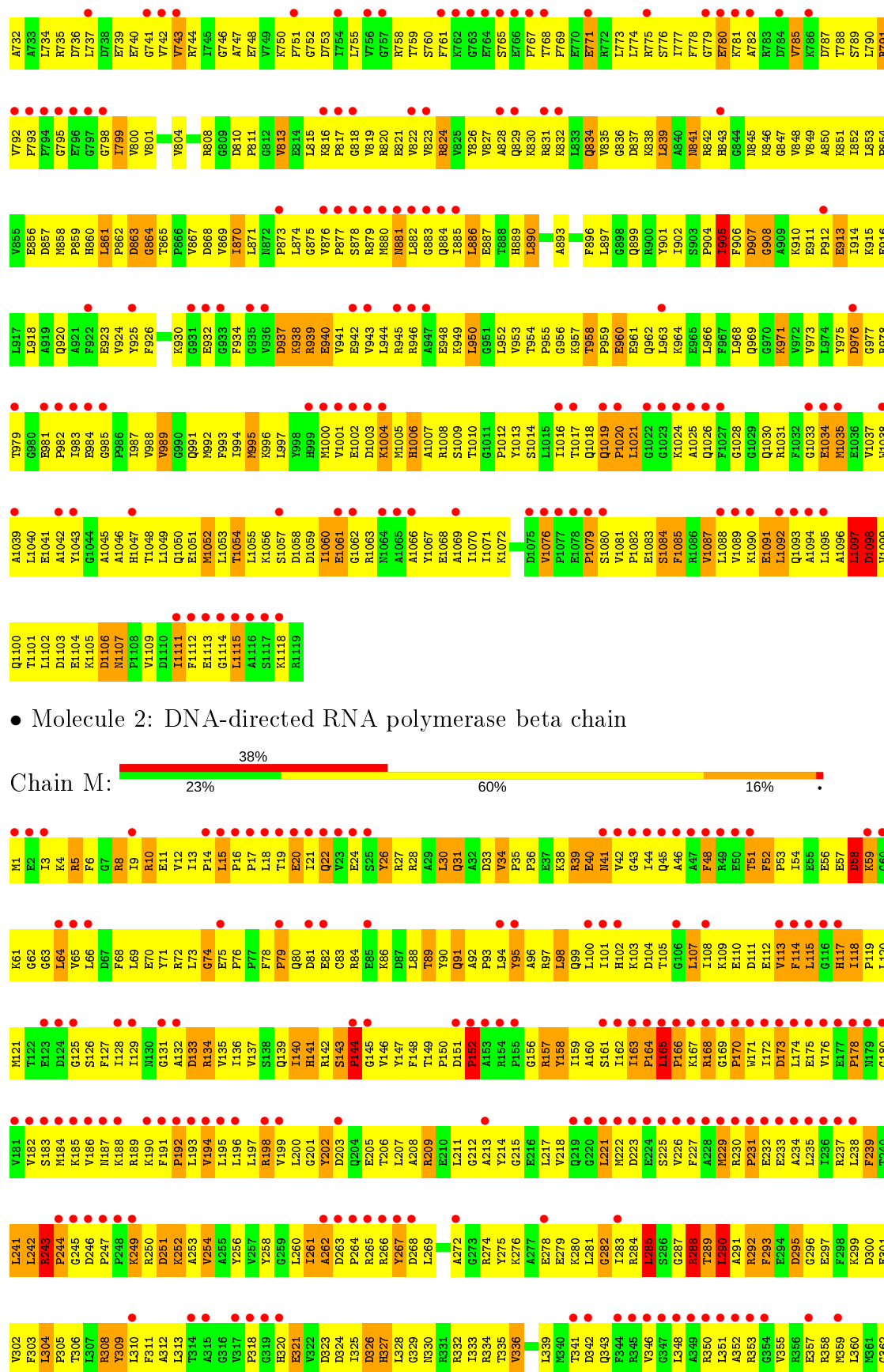


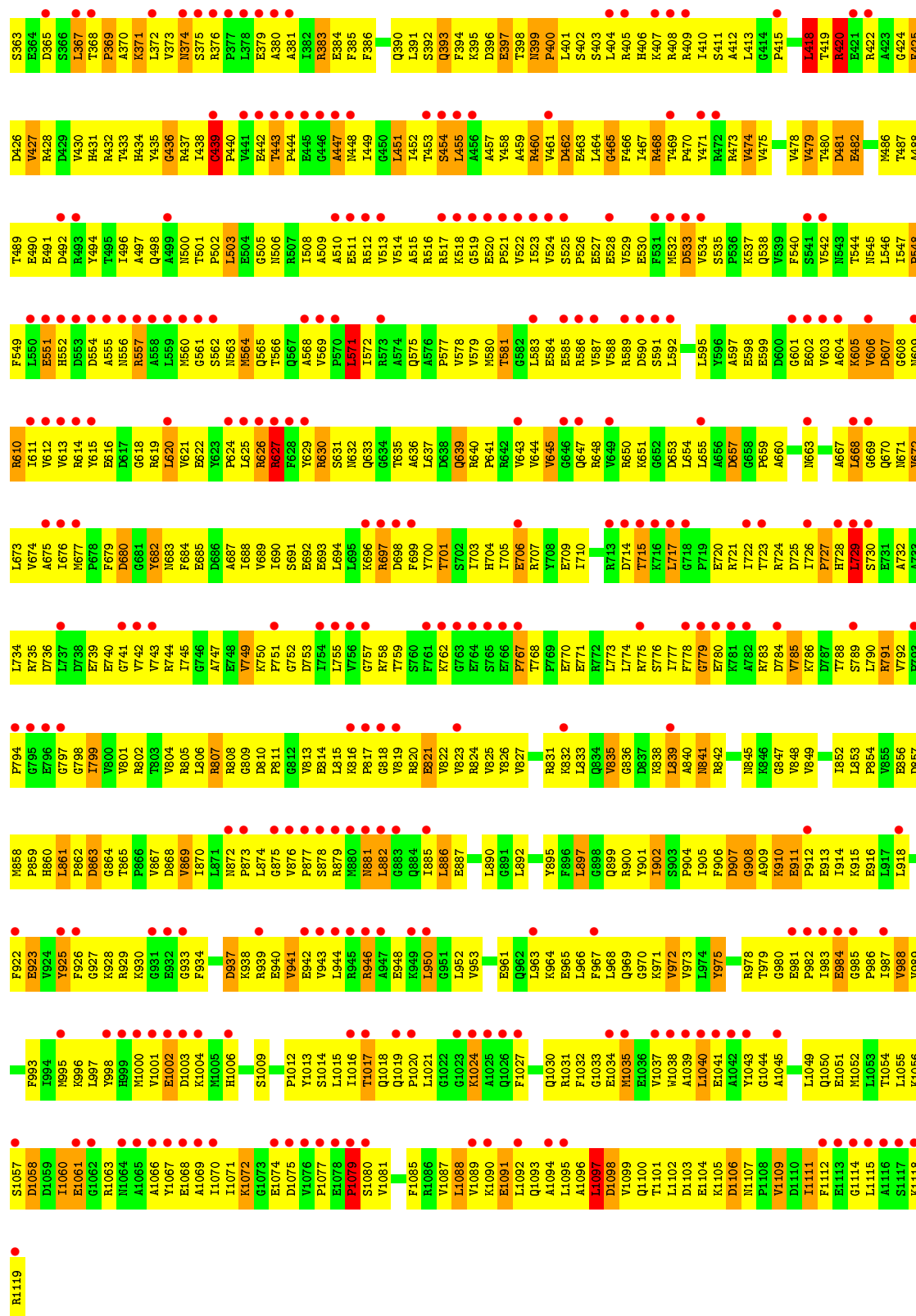
• Molecule 1: DNA-directed RNA polymerase alpha chain



• Molecule 1: DNA-directed RNA polymerase alpha chain







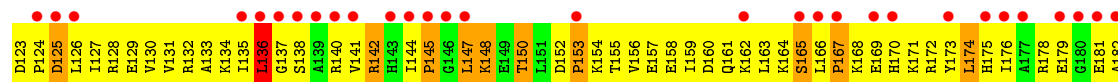
• Molecule 3: DNA-directed RNA polymerase beta' chain

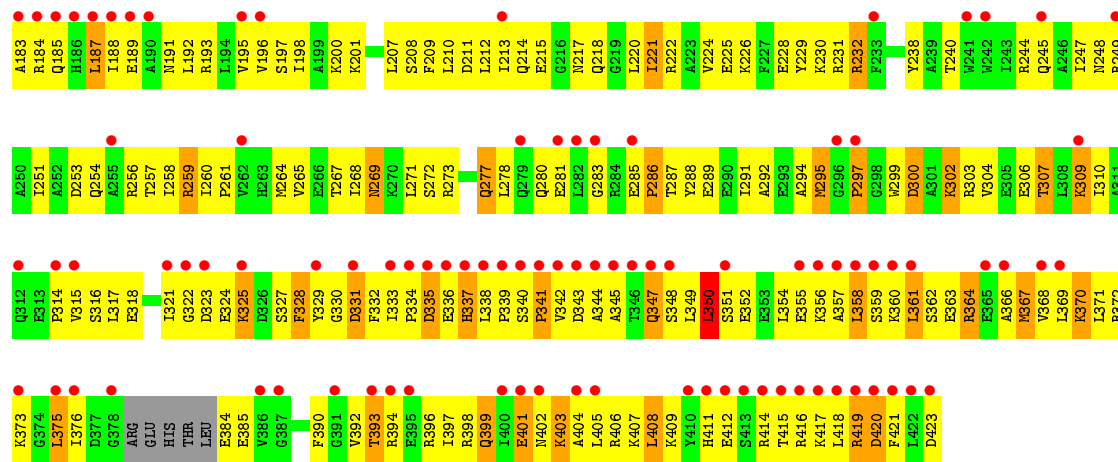


G803	D741	R679	L617	L557	L496	V435	P373	LEU	F251	L123	G81	MET
L804	G742	Q680	L618	L558	E497	E436	P374	ARG	V185	E124	K62	K2
E805	D743	D681	L619	A559	V498	D437	E374	ALA	V186	E125	K63	K3
F806	Q744	D682	Q620	Q560	V499	D438		GLU	K187	Q126	K64	E4
A807	M745	I683	G621	A561	R500	L439	V377	GLU	G188	L127	R65	V5
T808	K746	K684	R622	A562	A501	V440	I378	GLN	G189	L128	Q66	R6
P809	L747	D685	R623	P563	F502	R441	A379	VAL	E190	F129	R67	K7
E810	H748	E686	D624	E564	L503	N442	E380	ARG	L191	S130	F68	V8
E811	V749	D687	D625	S565	D504	N443	E381	VAL	A192	K131	E69	R9
A812	P750	W688	S626	S505	S505	V444	E382	ALA	P193	I132	E70	I10
L813	L751	D689	G627	S506	G506	R445		GLN	G194	I133	V72	A11
A814	S752	A690	R628	R507	R507	V446	V385	VAL	V195	V134	G73	L12
A815	S753	S629	S629	R508	R508	V447	H386	GLU	V196	V135	E74	L13
H816	F754	E691	V630	P509	P509	E448	L387	LEU	S197	D136	R75	S14
E817	A755	E692	L631	E510	R888	S449	H388	GLU	R198	P137	C76	P15
R818	Q756	G693	R632	W511	Q450	Y450	E389	GLU	L199	K138	G77	E16
C819	A757	I695	V633	M512	D451	D451	P390	GLY	D200	G139	V78	K17
E820	E758	G634	V634	L574	A521	A521	A391	GLY	G201	A140	E79	I18
W821	A759	H697	R635	O575	D453	D453	S392	PHE	I202	I141	R80	R19
A822	R760	K698	Q636	E576	A454	A454	I393	LEU	Z203	L142	T81	S20
L823	L761	V699	L637	A577	R455	R455	I394	VAL	L204		R82	W21
N824	Q762	W700	R638	V578	P518	P518	V395	LEU	R205	P146	S83	S22
A825	M763	L701	L639	D579	V519	L639	V396	ARG	R206	V147	I84	Y23
P826	L764	L702	W640	A580	L520	L520	K397	THR	F207	E148	V85	G24
L827	S765	N703	Q641	L581	P521	A459	A398	LEU	P208	K149	R86	E25
K828	A766	R704	C642	L582	P522	I461	R399	PHE	R209		R87	V26
H829	H767	A705	G643	D683	D523	Q462	V400	LEU	R210	R150	Y88	E27
N830	Q768	P706	L644	N584	L524	Q463	Y401	GLU	Q151	L152	R89	K28
G831	L769	T707	P645	Q585	R525	L464	P402	VAL	R212	M90	P29	E30
R832	L770	L708	K646	R586	P526	L465	F403	THR	L153	G91	E90	T31
E833	S771	H709	R647	R587	M527	K466	E404	GLU	E214	T154	H92	
T834	F772	R710	V648	G588	V528	E467	D405	PRO	E215	D155	I93	I32
S835	A773	L711	A649	A589	Q529	L468	D406	PHE	E216	E156	E94	N33
H836	S774	L650	P590	P590	V530	D469	V407	LEU	R217	E157	L95	Y34
R837	Q775	E651	V591	T592	D531	L470	E408	PRO	A221	Y158	A96	R35
R838	E776	L652	T593	G533	G533	E471	V409	ARG	E222	E159	T97	T36
L839	P777	Q717	N593	R534	R534	L473	T411	GLN	L223	E160	P98	L37
K840	L778	P718	P594	F535	F535	E474	G412	THR	A226	L161	A99	K38
Y841		V719	G595	A536	A536	K475	D413	PRO	P226	R162	A100	P39
Y842	S781	L720	S596	D542	D542	K481	L421	LEU		Y163	H101	E40
F843	S782	V721	D597	L543	L543	K482	R414	VAL	A229	G164	I102	R41
A844	R783	E722	R598	S538	S538	L477	V415	ASN		K165	V103	D42
H845	L784	G723	P599	D539	D539	L478	A416	VAL	V231	Q166	F104	G43
P846	I785	Q724	L600	L540	L540	E479	P417	HIS	E232	E167	V105	L44
D847	L786	S725	R601	N541	N541	E480	G418	GLY	E233	T168	K106	F45
E848	L787	I726	S602	D542	D542	M481		VAL	K234	Y169	D107	D46
A849	G788	Q727	L603	L544	L544	K483	A422	ILE	E234	P170	V108	E47
L850	L789	L728	T604	Y544	Y544	H483	D423	GLY	A235	L171	P109	R48
L851	Y790	H729	D605	R546	R546	P484	G424	ALA	P238	P172	S110	I49
A852	Y791	P730	L606	L547	L547	S485	G425	ARG		P173	K111	F50
V853	I792	L731	L607	L548	L548	A487	K426	GLN	G174	V175	I112	G51
A854	T793	N669	S608	L549	L549	R488	F427	PRO	I241	V176	L115	P52
H855	Q794	V670	G609	N549	N549	R489	L242	LEU	A243	D176	L116	I53
G856	K795	E734	R610	R550	R550	K489	K428	ALA		A177	L117	K54
L857	R796	A735	D611	N551	N551	A490	S429	ALA	P246	L178	D117	D55
V858	K797	F736	R612	N552	N552	K491	D430	GLU	E247	V179	L118	Y56
D859	E798	N737	R613	R553	R553	A492	V431	ALA	P248	K180	S119	E57
L860	K799	A738	F614	L554	L554	R493	Y432	LYS	F249	D181	A120	C58
Q861	K800	D739	Q616	K555	K555	K494	G433	LEU	L250	G182	GLY	A59
D862		F740			K556	R495	R434			E183	E122	C60

T927	R866	G803	D743	R679	Q616	K555	K494	G433	V368	LYS	P248	V185	L123
A928	R867	L804	Q744	Q680	M617	K556	R495	R434	A369	GLY	T249	V186	E124
R929	Y868	E805	M745	R881	L618	L557	L496	V435	A370	LEU	L250	K187	Q125
L930	M869	F806	A746	D882	G619	L558	E497	E436	F251	LEU	ARG	G188	V126
L931	G870	A807	V747	I883	G620	I683	R500	V437	P373	ARG	ALA	Q189	L127
D932	K871	R808	H748	K684	K621	G561	R500	D438		MET	VAL	E190	Y128
A933	R872	P809	V749	D885	R622	A562	A501	L439		PRO	GLU	L191	F129
	L873	E810	P750	E886	R623	F563	F502	V440		ARG	GLU	A192	S130
Y936	E874	E811	L751	R887	D624	E564	L503	R441		GLN	GLU	P193	K131
Y937	S875	A812	S752	M688	Y625	I565	D504	N442		VAL	GLY	G194	Y132
	S876	L813	S753	D889		S505	S505	V443		ARG	VAL	V195	I133
T940	R877		F754	A690	R628	I566	G506	V444		ALA	VAL	V196	V134
F941	G878	E817	A755	L691	R629	R568	M507	R445		ALA	GLU	S197	L135
S942	R879	E817	Q756	E892	V630	M569	R508	V446		GLN	LEU	R198	D136
T943	L880	E820	A757	E893	I631	E570	P509	V447		VAL	LYS	L199	P137
T944	L881	R821	E758	V694	V632	K571	P510	V448		GLU	GLU	D200	K138
S945	F882	A822	A759	I895	V633	R572	M511	S449		ALA	LEU	G201	G139
G946	A883	L823	R760	H696	G634	M573	M512	Q450		GLU	GLU	V202	A140
I947	R884	R824	I761	G697	P635	L574	I513	D481		GLU	GLU	A203	I141
T948	V885	A825	Q762	K698	Q636	Q575	L514	L462		GLY	GLY	L204	L142
R949	R886	R826	Q763	K699	L637	E576	E515	D463		GLY	ALA	I393	
G950	A887	R827	L764	V700	K638	A516	A516	A454		THR	PHE	R206	V146
R951	E888	R828	S765	L701	L639	V517	R455	R455		THR	LEU	F207	P146
D952	A889	R829	A766	L702	H640	P518	P518	M456		VAL	VAL	P208	V147
D953	R890	A830	H767	N703	Q641	A580	V519	K397		THR	LEU	R209	E148
A954	E891	E831	N768	R704	C642	L581	L520	A398		LEU	ARG	R210	K149
V955	D892	R832	L769	A705	G643	L582	P521	A460		THR	ARG	R399	R150
I956	E893	E833	L770	F706	L644	D583	P522	I461		LEU	GLU	V211	Q151
P957	K894	T834	S771	T707	P645	M584	D523	Q462		PHE	ASP	V213	L152
E958	V895	S835	P772	L708	K646	G585	L524	Q463		LEU	GLU	E214	L153
E959	A896	V836	A773	H709	R647	R586	R525	L464		THR	PRO	V215	T154
K960	R897	Q837	S774	R710	M643	R587	P526	L465		THR	VAL	V216	D155
K961	E898	R838	G775	L711	A649	G588	M527	K466		ALA	ALA	K217	E156
Q962	L899	L839	E776	G712	L650	A589	V528	E467		GLU	THR	D418	E157
Y963	R900	R840	P777	I713	E651	P590	Q529	L468		PRO	TYR	E219	Y158
L964	Q901	Y841	L778	I714		V530	V530	D469		LYS	PHE	R220	R159
E965	L902	V842	A779	Q715	K654	T592	D531	L470		ASP	LEU	A221	E160
E966	D903	F843	K780	F716	P655	M593	G532	E471		THR	PRO	G222	L161
A967	F904	A844	F781	Q717	F656	P594	G533	A472		ARG	VAL	L223	R162
D968	P905	M845	S782	F718	L657	G595	M541	L473		VAL	GLY	R224	Y163
R969	Q906	R846	R783	V719	L658	S596	F535	E474		GLN	MET	D413	G164
E970	E907	D847	D784	L720	K659	D597	A536	K475		PRO	THR	P226	K165
L971	K908	E848	I785	L720	K660	R598	T537	E476		HIS	PRO	Q166	Q166
L972	R909	R849	L786	S725	M661	P599	S538	L477		MET	LEU	E167	E167
Q973	S910	L850	L787	I726	E662	L600	S539	L478		VAL	VAL	V230	E168
E974	R911	L851	G788	Q727	E663	R601	L540	E479		VAL	VAL	V231	Y169
E975	L912	A852	L789	L728		S602	M541	E480		HIS	HIS	E232	P170
Q976	D913	V853	V790	H729	L603	L603	D542	M481		VAL	GLY	E233	L171
A977	L914	A854	Y791	P730	A667	T604	L543	K482		VAL	GLY	A235	P172
Y978	V915	R855	I792	L731	P668	D605	Y544	H483		PRO	ILE	V236	P173
E979	R916	G856	T793	V732	M669	L606	R545	P484		GLY	VAL	D423	
M980	Q917	R857	Q794	C733	V670	L607	R546	S485		ALA	GLU	P238	D176
			V795	E734	K671	S608	L547	R486		LYS	LYS	G425	A177
F982	L920	D859	R796	A735	A672	G609	I548	A487		VAL	GLY	E240	L178
	R921	R860	K797	F736	A673	K610	M549	R488		VAL	GLN	T241	V179
L922	L922	O861	N737	R674	R674	O611	R550	R489		ALA	PRO	L242	K180
G923	G923	D862	R675	R675	G612	G612	M551	A490			LEU	A243	D161
R986	R924	R863	R676	M676	R613	R613	M552	R491			ALA	D430	G182
E987	E925	V864	L677	L677	F614	F614	R553	A492			ALA	E246	E183
R988											GLU	P247	E184
Y989	Y926	T865	E678	G742	R615	R615	L554	R493			ALA	E247	







4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.40 36.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.40) 95.2 (36.81-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.274 0.235 , 0.272	Depositor DCC
R_{free} test set	34795 reflections (5.75%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.065 for h,-h-k,-l 0.065 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for -h,-k,l	Depositor
Outliers	0 of 604645 reflections	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	61800	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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: ZN, MG, TGT

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	0.77	0/1838	0.86	3/2498 (0.1%)
1	B	0.70	0/1838	0.83	4/2498 (0.2%)
1	K	0.76	0/1838	0.85	4/2498 (0.2%)
1	L	0.73	0/1838	0.76	0/2498
2	C	0.81	0/8997	0.89	8/12164 (0.1%)
2	M	0.80	2/8997 (0.0%)	0.89	12/12164 (0.1%)
3	D	0.82	0/10975	0.92	21/14836 (0.1%)
3	N	0.80	1/10975 (0.0%)	0.92	17/14836 (0.1%)
4	E	0.80	0/783	0.94	0/1054
4	O	0.81	0/783	0.92	0/1054
5	F	0.71	0/2812	0.81	1/3781 (0.0%)
5	P	0.72	0/2812	0.78	2/3781 (0.1%)
All	All	0.79	3/54486 (0.0%)	0.89	72/73662 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	733	CYS	CB-SG	-5.54	1.72	1.81
2	M	202	TYR	CD2-CE2	5.05	1.47	1.39
2	M	682	TYR	CD2-CE2	5.02	1.46	1.39

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LEU	CA-CB-CG	10.11	138.56	115.30
3	N	199	LEU	CA-CB-CG	-8.78	95.11	115.30
2	M	557	ARG	NE-CZ-NH2	7.73	124.17	120.30
3	D	199	LEU	CA-CB-CG	-7.64	97.72	115.30
3	N	1389	LEU	CA-CB-CG	7.54	132.65	115.30

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	232	0
1	B	1806	0	1861	217	0
1	K	1806	0	1861	195	0
1	L	1806	0	1861	216	0
2	C	8829	0	8933	1248	0
2	M	8829	0	8933	1139	0
3	D	10797	0	10873	1481	0
3	N	10797	0	10873	1398	0
4	E	769	0	775	101	0
4	O	769	0	775	98	0
5	F	2771	0	2844	350	0
5	P	2771	0	2844	345	0
6	C	1	0	0	0	0
6	D	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	D	26	0	15	3	0
8	N	26	0	14	1	0
9	A	250	0	0	46	0
9	B	329	0	0	67	0
9	C	1321	0	0	266	0
9	D	1655	0	0	324	0
9	E	176	0	0	32	0
9	F	519	0	0	103	0
9	K	278	0	0	43	0
9	L	309	0	0	68	0
9	M	1236	0	0	259	0
9	N	1552	0	0	306	0
9	O	137	0	0	23	0
9	P	422	0	0	84	0
All	All	61800	0	54323	6611	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 61.

The worst 5 of 6611 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:M:409:ARG:HA	2:M:454:SER:HA	1.20	1.15
3:D:1045:MET:HG2	3:D:1073:SER:HA	1.33	1.10
3:D:119:SER:HB2	3:D:123:LEU:H	1.23	1.04
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.41	1.02
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.43	1.01

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%)	200 (88%)	22 (10%)	5 (2%)	6	7
1	B	227/315 (72%)	200 (88%)	22 (10%)	5 (2%)	6	7
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	8	10
1	L	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	8	10
2	C	1117/1119 (100%)	927 (83%)	138 (12%)	52 (5%)	2	1
2	M	1117/1119 (100%)	926 (83%)	142 (13%)	49 (4%)	2	2
3	D	1388/1524 (91%)	1155 (83%)	168 (12%)	65 (5%)	2	1
3	N	1388/1524 (91%)	1133 (82%)	187 (14%)	68 (5%)	2	1
4	E	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	2	2
4	O	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	2	2
5	F	341/423 (81%)	290 (85%)	35 (10%)	16 (5%)	2	1
5	P	341/423 (81%)	288 (84%)	38 (11%)	15 (4%)	2	2
All	All	6786/7590 (89%)	5671 (84%)	824 (12%)	291 (4%)	2	2

5 of 291 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	231	PRO

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%)	149 (74%)	53 (26%)	0	0
1	B	202/273 (74%)	167 (83%)	35 (17%)	2	2
1	K	202/273 (74%)	154 (76%)	48 (24%)	0	0
1	L	202/273 (74%)	152 (75%)	50 (25%)	0	0
2	C	941/941 (100%)	722 (77%)	219 (23%)	1	1
2	M	941/941 (100%)	731 (78%)	210 (22%)	1	1
3	D	1123/1279 (88%)	861 (77%)	262 (23%)	1	1
3	N	1123/1279 (88%)	832 (74%)	291 (26%)	0	0
4	E	83/87 (95%)	65 (78%)	18 (22%)	1	1
4	O	83/87 (95%)	61 (74%)	22 (26%)	0	0
5	F	295/370 (80%)	234 (79%)	61 (21%)	1	1
5	P	295/370 (80%)	242 (82%)	53 (18%)	1	2
All	All	5692/6446 (88%)	4370 (77%)	1322 (23%)	1	1

5 of 1322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	136	LEU
1	L	197	LEU
3	N	1401	GLU
5	F	249	ARG

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Mol	Chain	Res	Type
1	K	112	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1441	GLN
1	K	229	GLN
3	N	1465	ASN
4	E	28	GLN
5	F	218	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 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	TGT	N	9002	6	18,27,27	4.73	14 (77%)	18,44,44	2.80	6 (33%)
8	TGT	D	9001	6	18,27,27	4.29	14 (77%)	18,44,44	2.74	7 (38%)

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	TGT	N	9002	6	-	4/8/57/57	0/1/2/2
8	TGT	D	9001	6	-	3/8/57/57	0/1/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	9001	TGT	O11-C10	9.53	1.55	1.20
8	N	9002	TGT	O11-C10	8.80	1.53	1.20
8	N	9002	TGT	O3-C8	8.54	1.41	1.23
8	N	9002	TGT	C1-C2	5.90	1.63	1.53
8	D	9001	TGT	C3-C4	5.77	1.64	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	9001	TGT	O10-C10-C11	7.11	124.18	111.09
8	N	9002	TGT	C3-O10-C10	6.95	128.47	117.72
8	N	9002	TGT	O10-C10-C11	6.89	123.76	111.09
8	D	9001	TGT	C3-O10-C10	5.92	126.88	117.72
8	D	9001	TGT	O9-P1-O6	3.42	121.31	105.99

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

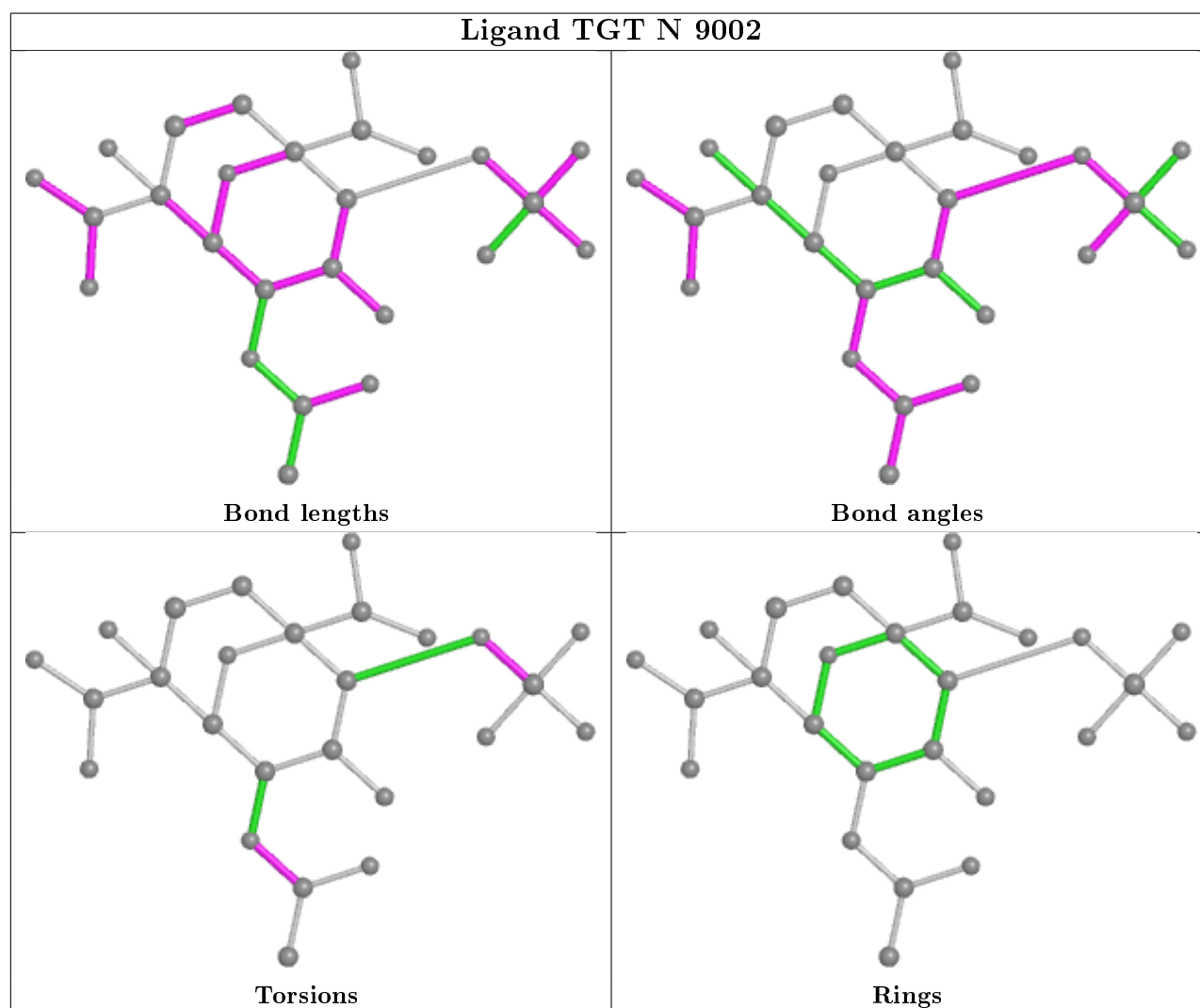
Mol	Chain	Res	Type	Atoms
8	D	9001	TGT	C11-C10-O10-C3
8	D	9001	TGT	O11-C10-O10-C3
8	N	9002	TGT	C11-C10-O10-C3
8	N	9002	TGT	O11-C10-O10-C3
8	N	9002	TGT	C1-O6-P1-O9

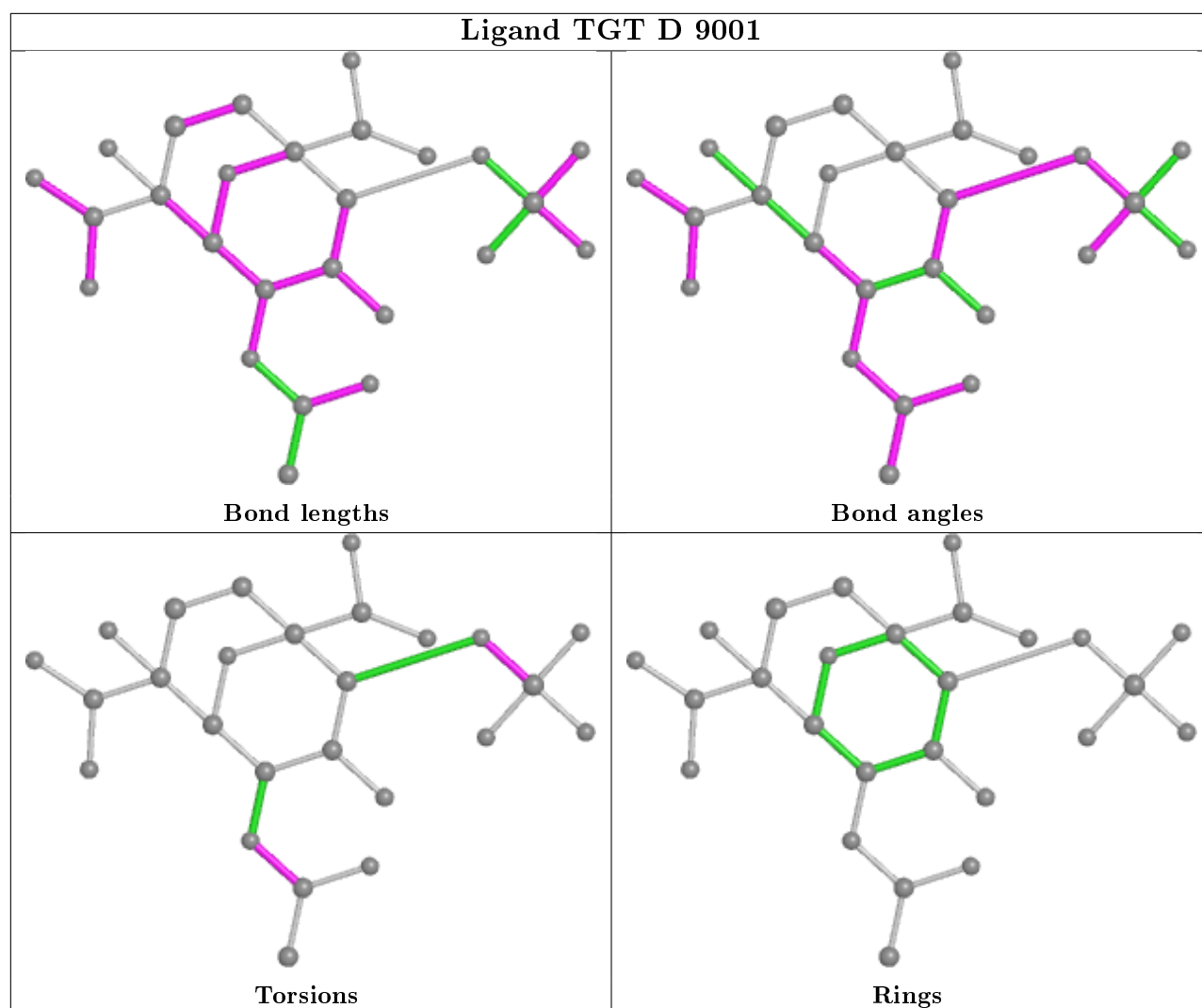
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	9002	TGT	1	0
8	D	9001	TGT	3	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%)	2.02	70 (30%) 0 0	18, 47, 72, 88	0
1	B	229/315 (72%)	2.74	80 (34%) 0 0	34, 66, 82, 88	0
1	K	229/315 (72%)	1.39	69 (30%) 0 0	21, 43, 70, 92	0
1	L	229/315 (72%)	2.07	69 (30%) 0 0	34, 62, 82, 95	0
2	C	1119/1119 (100%)	3.02	409 (36%) 0 0	15, 58, 81, 94	0
2	M	1119/1119 (100%)	3.12	422 (37%) 0 0	15, 55, 81, 97	0
3	D	1392/1524 (91%)	1.93	383 (27%) 0 0	15, 49, 82, 97	0
3	N	1392/1524 (91%)	1.97	384 (27%) 0 0	16, 48, 83, 105	0
4	E	95/99 (95%)	1.35	23 (24%) 0 0	30, 59, 82, 103	0
4	O	95/99 (95%)	1.69	22 (23%) 0 0	22, 59, 77, 87	0
5	F	345/423 (81%)	3.86	158 (45%) 0 0	38, 63, 83, 97	0
5	P	345/423 (81%)	3.90	150 (43%) 0 0	41, 64, 85, 92	0
All	All	6818/7590 (89%)	2.51	2239 (32%) 0 0	15, 54, 82, 105	0

The worst 5 of 2239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	854	ALA	66.8
3	N	1246	VAL	60.6
3	N	532	GLY	59.3
3	N	533	GLY	56.7
3	N	1248	GLY	56.6

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 ⓘ

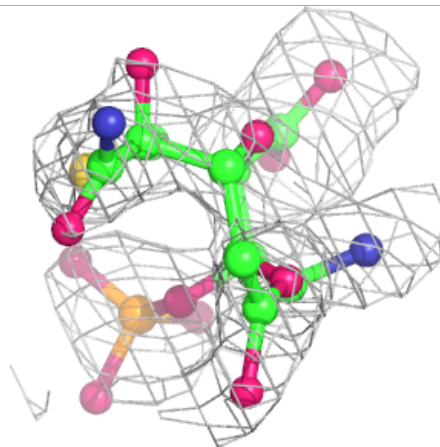
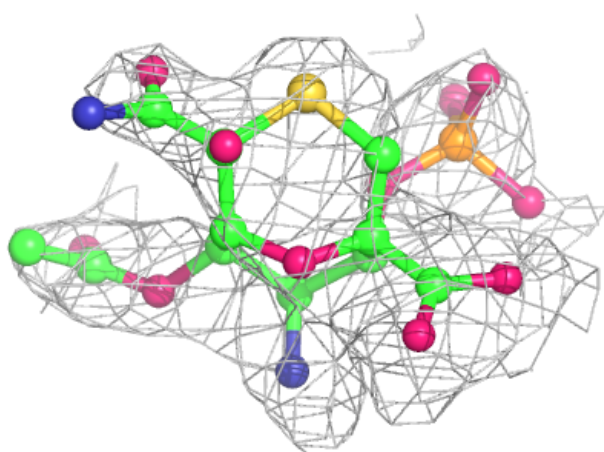
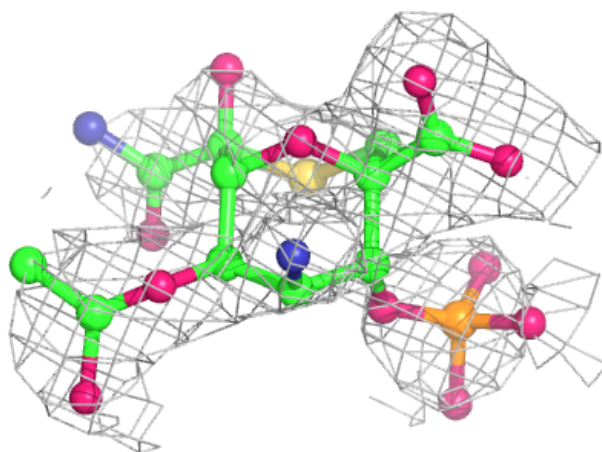
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	TGT	D	9001	26/26	0.81	0.43	44,47,50,52	0
8	TGT	N	9002	26/26	0.81	0.61	41,47,51,52	0
6	MG	C	9004	1/1	0.97	0.06	17,17,17,17	0
6	MG	N	9005	1/1	0.98	0.03	13,13,13,13	0
6	MG	D	9003	1/1	0.98	0.06	17,17,17,17	0
6	MG	N	9006	1/1	0.99	0.04	4,4,4,4	0
7	ZN	D	9112	1/1	0.99	0.05	50,50,50,50	0
7	ZN	N	9059	1/1	0.99	0.06	42,42,42,42	0
7	ZN	N	9113	1/1	0.99	0.10	41,41,41,41	0
7	ZN	D	9058	1/1	1.00	0.17	56,56,56,56	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.

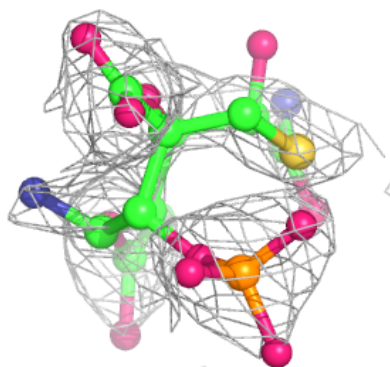
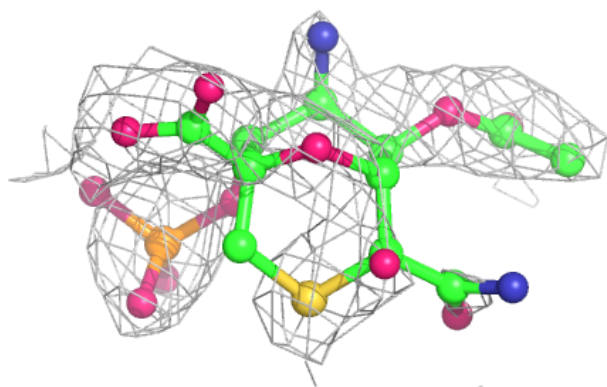
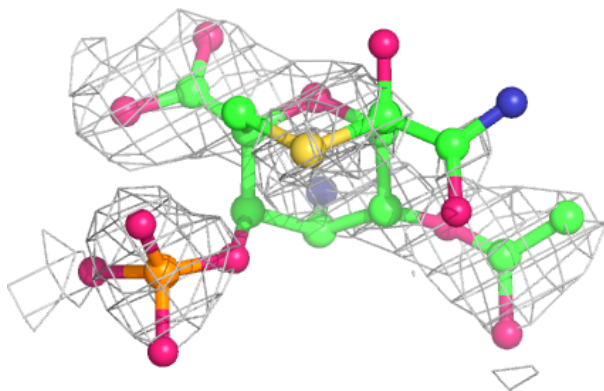
Electron density around TGT D 9001:

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



Electron density around TGT N 9002:

$2mF_o-DF_c$ (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.