



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 6, 2020 – 11:19 pm BST

PDB ID : 2A6H  
Title : Crystal structure of the T. thermophilus RNA polymerase holoenzyme in complex with antibiotic sterptolydigin  
Authors : Temiakov, D.; Zenkin, N.; Vassilyeva, M.N.; Perederina, A.; Tahirov, T.H.; Savkina, M.; Zorov, S.; Nikiforov, V.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Severinov, K.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-07-02  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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



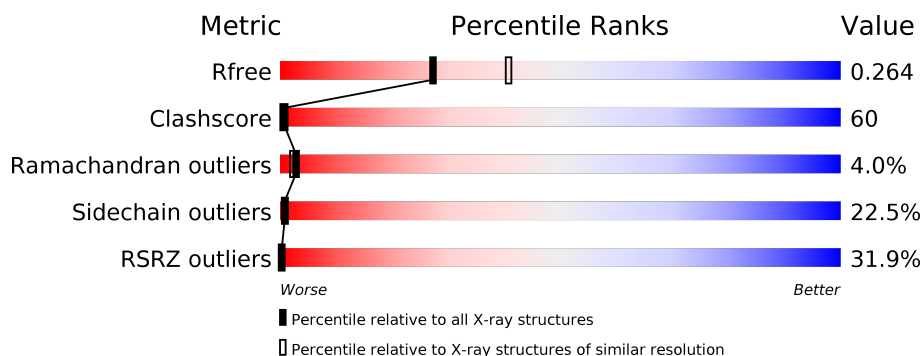
# 1 Overall quality at a glance

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

Mol	Chain	Length	Quality of chain
1	A	315	<div> <div>21%</div> <div>16% 43% 13% 27%</div> </div>
1	B	315	<div> <div>23%</div> <div>16% 43% 13% 27%</div> </div>
1	K	315	<div> <div>19%</div> <div>23% 41% 8% 27%</div> </div>
1	L	315	<div> <div>26%</div> <div>20% 39% 12% 27%</div> </div>
2	C	1119	<div> <div>38%</div> <div>24% 57% 19%</div> </div>
2	M	1119	<div> <div>35%</div> <div>25% 55% 19%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div></div><div>23%</div><div></div><div>22%</div><div>52%</div><div>15%</div><div></div><div>9%</div></div>
3	N	1524	<div><div></div><div>24%</div><div></div><div>25%</div><div>49%</div><div>15%</div><div></div><div>9%</div></div>
4	E	99	<div><div></div><div>28%</div><div></div><div>27%</div><div>53%</div><div>15%</div><div></div><div></div></div>
4	O	99	<div><div></div><div>32%</div><div></div><div>24%</div><div>53%</div><div>18%</div><div></div><div></div></div>
5	F	423	<div><div></div><div>35%</div><div></div><div>20%</div><div>49%</div><div>11%</div><div></div><div>18%</div></div>
5	P	423	<div><div></div><div>30%</div><div></div><div>21%</div><div>49%</div><div>11%</div><div></div><div>18%</div></div>



## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60908 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	1381	Total	C	N	O	S	0	0	0
			10728	6776	1912	2007	33			
3	N	1381	Total	C	N	O	S	0	0	0
			10728	6776	1912	2007	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

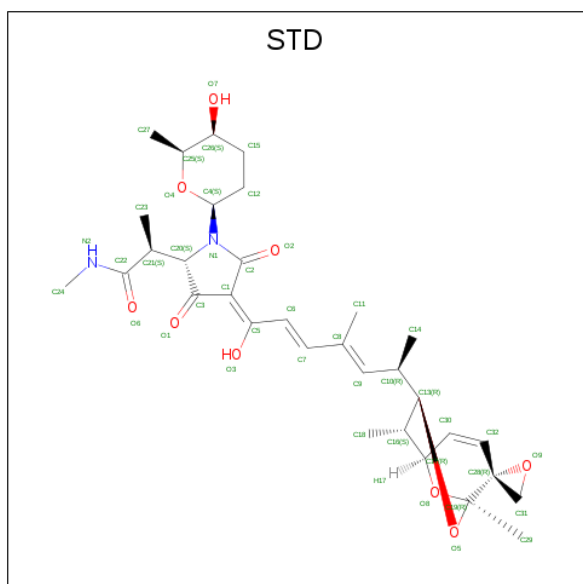
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			



- 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
			2771	1744	504	519	4		
5	P	345	Total	C	N	O	S	0	0
			2771	1744	504	519	4		

- Molecule 6 is STREPTOLYDIGIN (three-letter code: STD) (formula:  $C_{32}H_{44}N_2O_9$ ).



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0

- Molecule 9 is water.

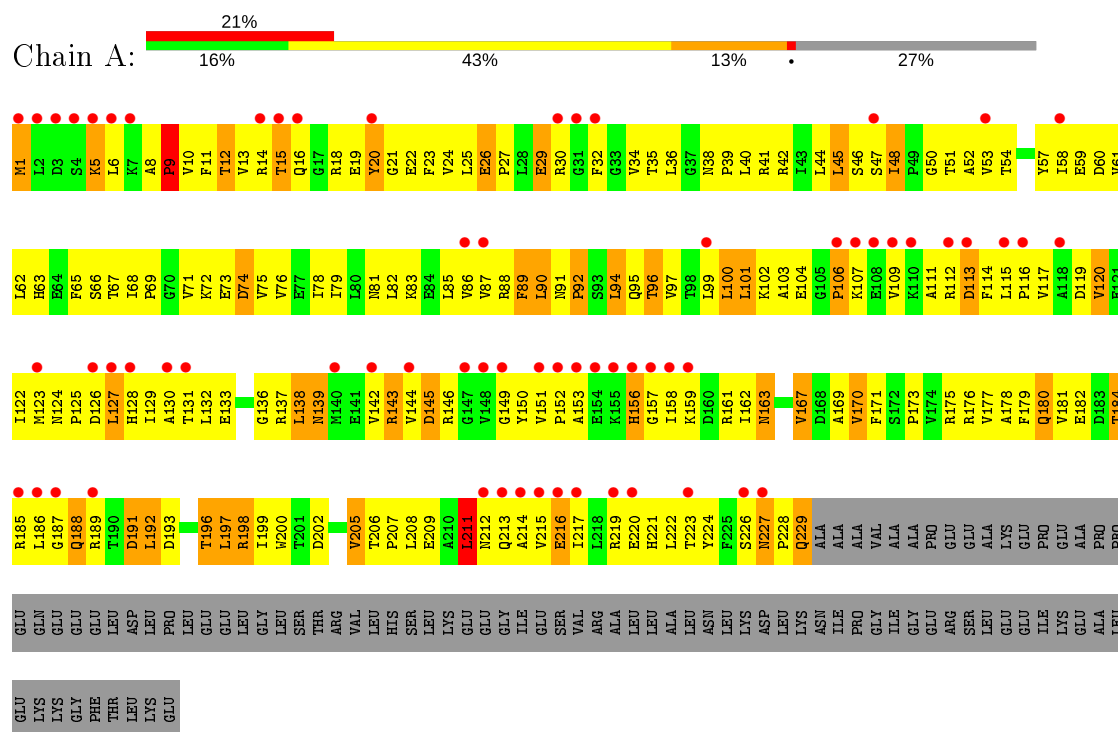
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	232	Total O 232 232	0	0
9	B	304	Total O 304 304	0	0
9	C	1144	Total O 1144 1144	0	0
9	D	1546	Total O 1546 1546	0	0
9	E	130	Total O 130 130	0	0
9	F	491	Total O 491 491	0	0
9	K	229	Total O 229 229	0	0
9	L	274	Total O 274 274	0	0
9	M	1072	Total O 1072 1072	0	0
9	N	1392	Total O 1392 1392	0	0
9	O	137	Total O 137 137	0	0
9	P	447	Total O 447 447	0	0



### 3 Residue-property plots

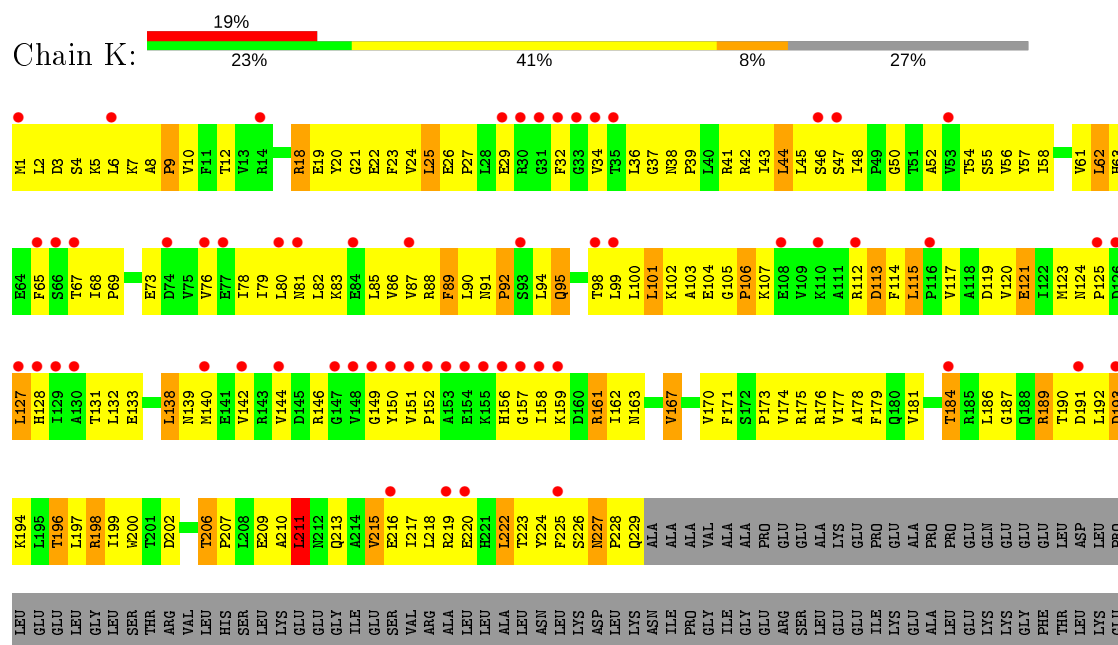
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

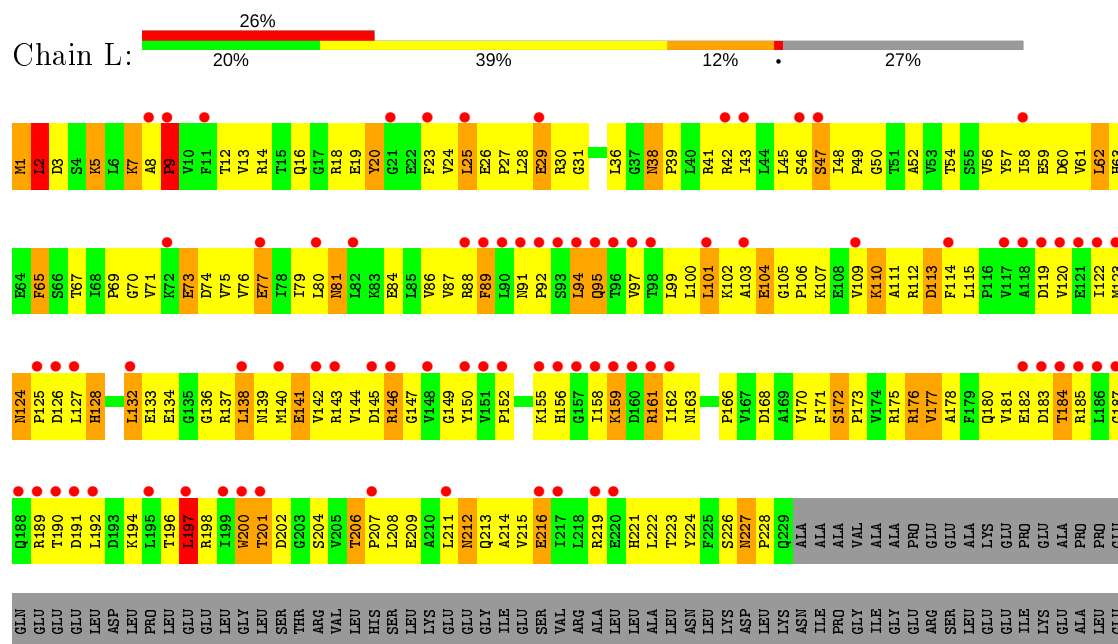




- Molecule 1: DNA-directed RNA polymerase alpha chain



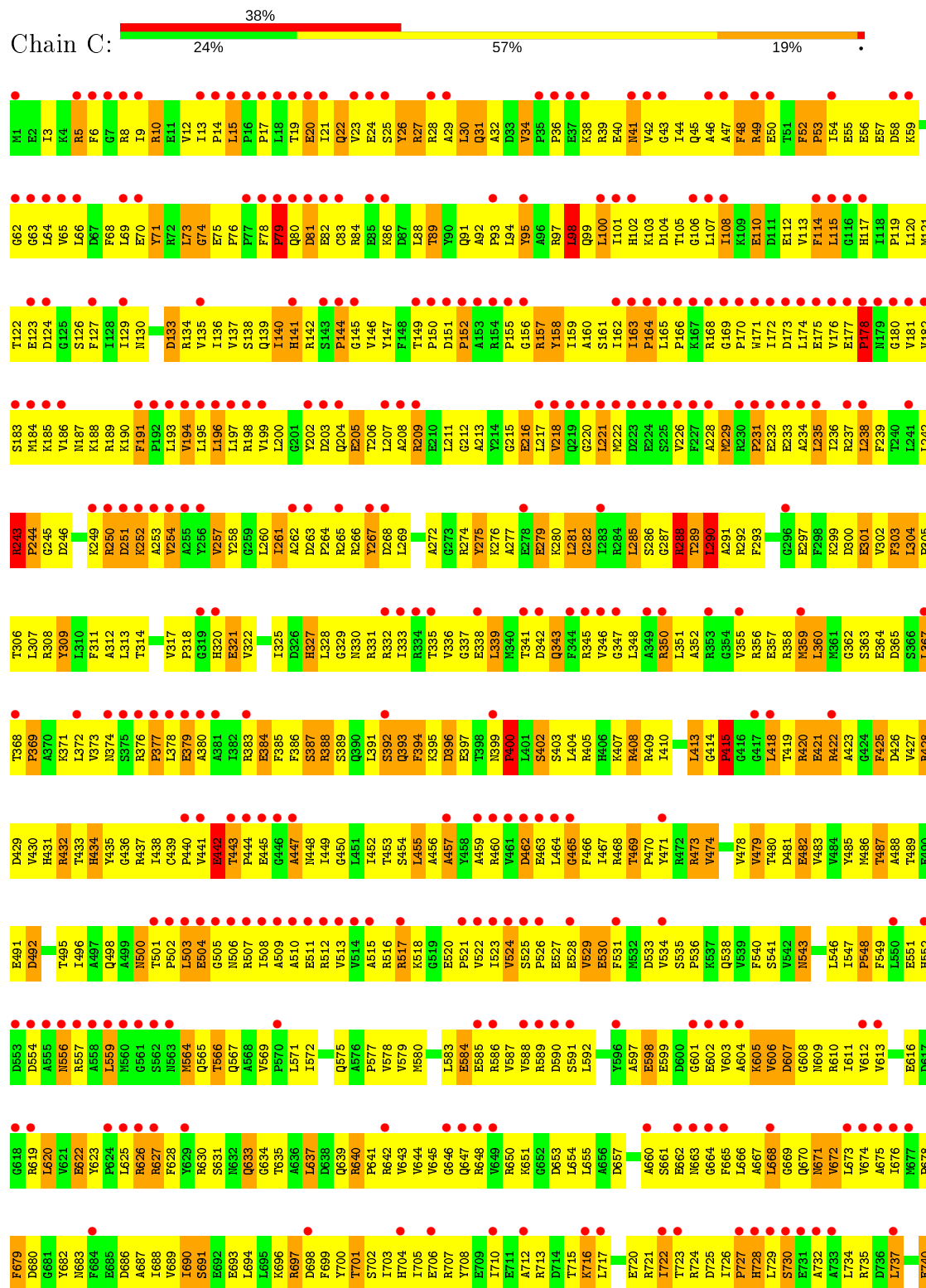
- Molecule 1: DNA-directed RNA polymerase alpha chain



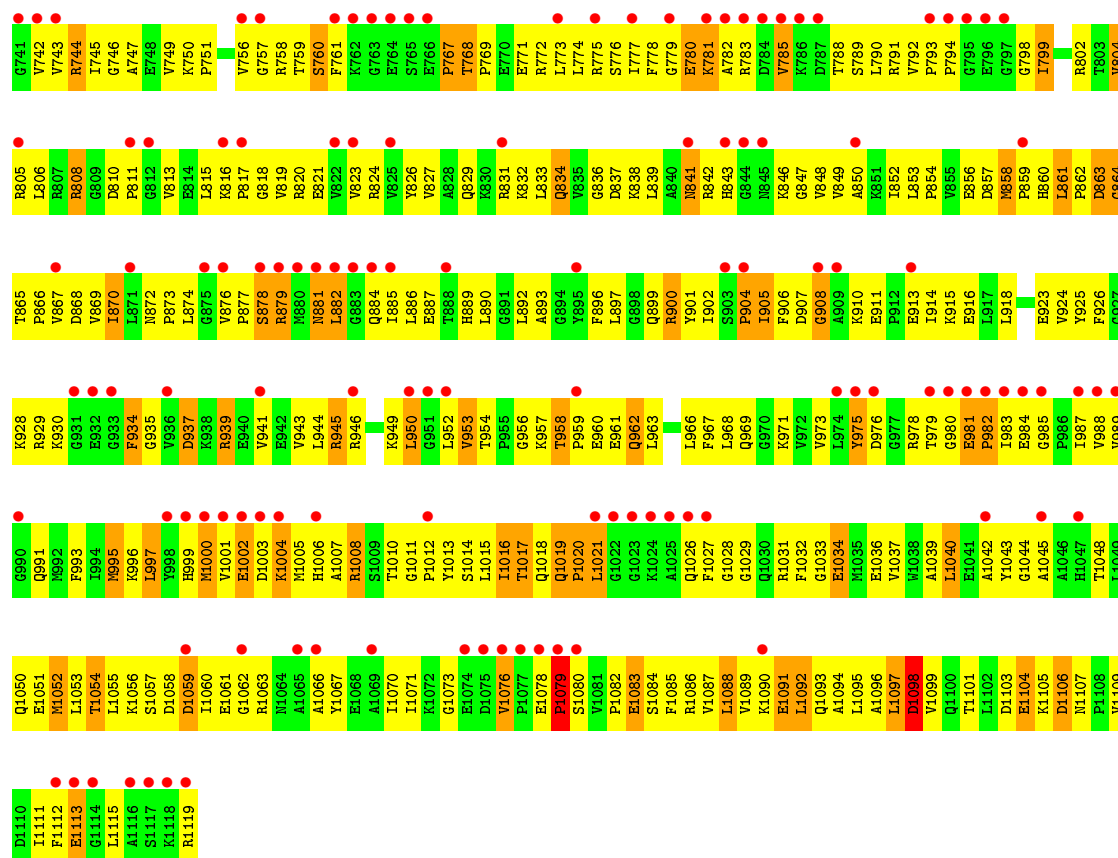


LYS  
LYS  
GLY  
PHE  
THR  
LEU  
LYS  
GLU

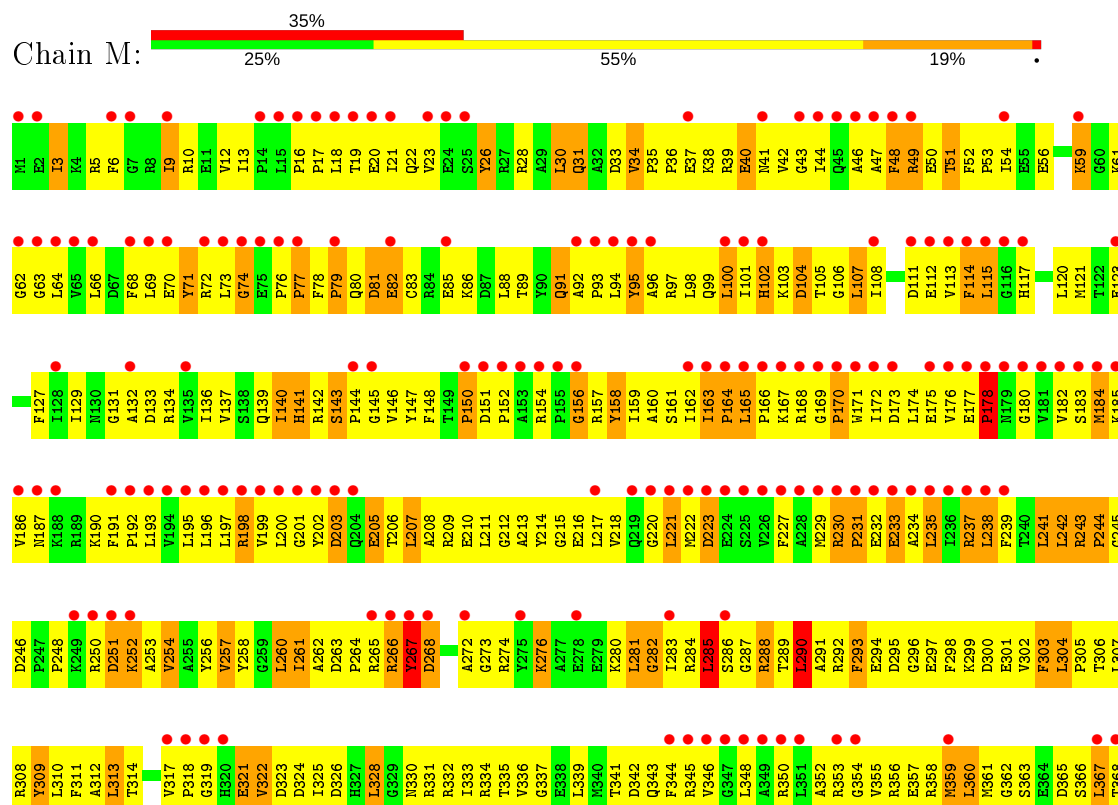
• Molecule 2: DNA-directed RNA polymerase beta chain



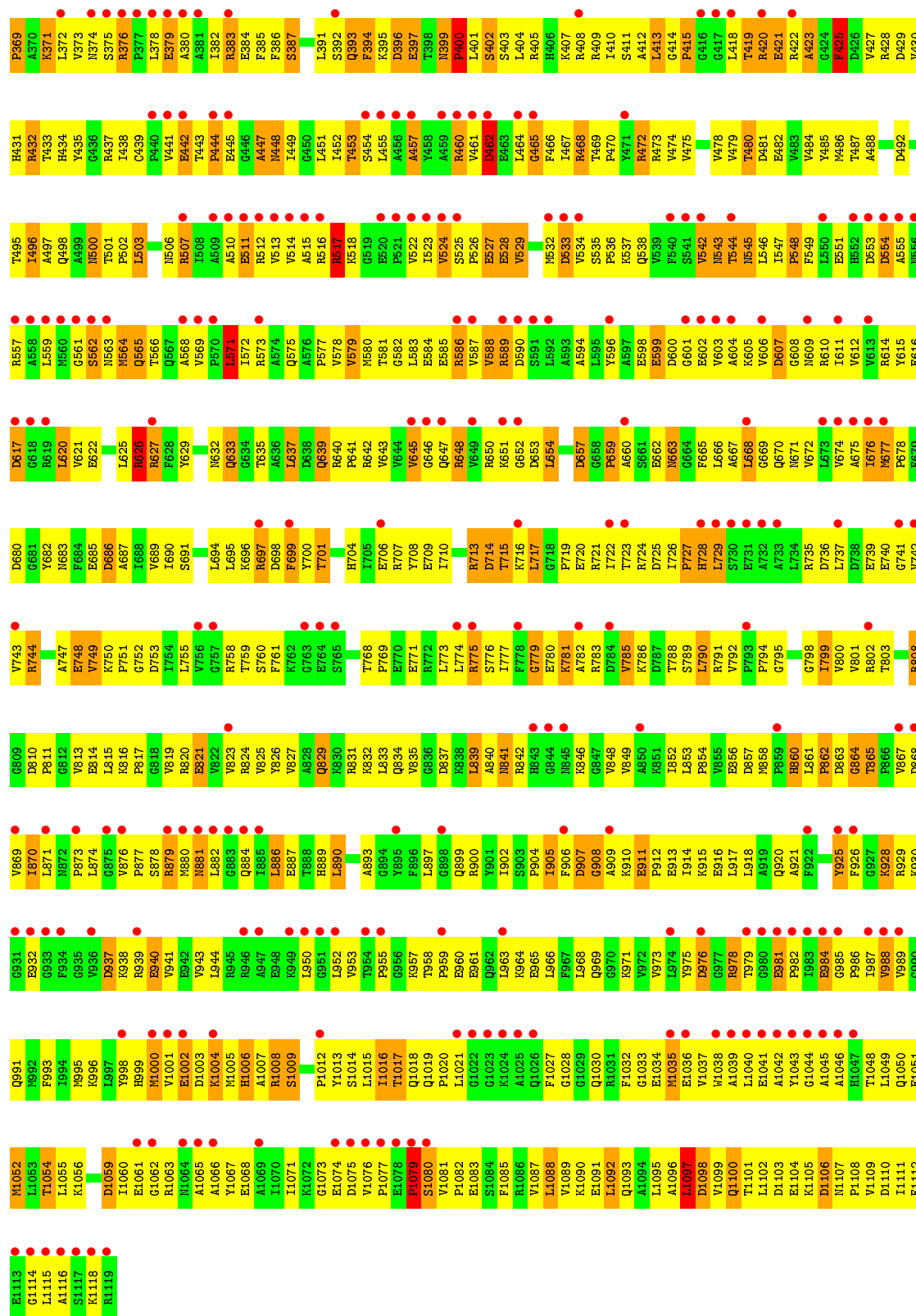




• Molecule 2: DNA-directed RNA polymerase beta chain



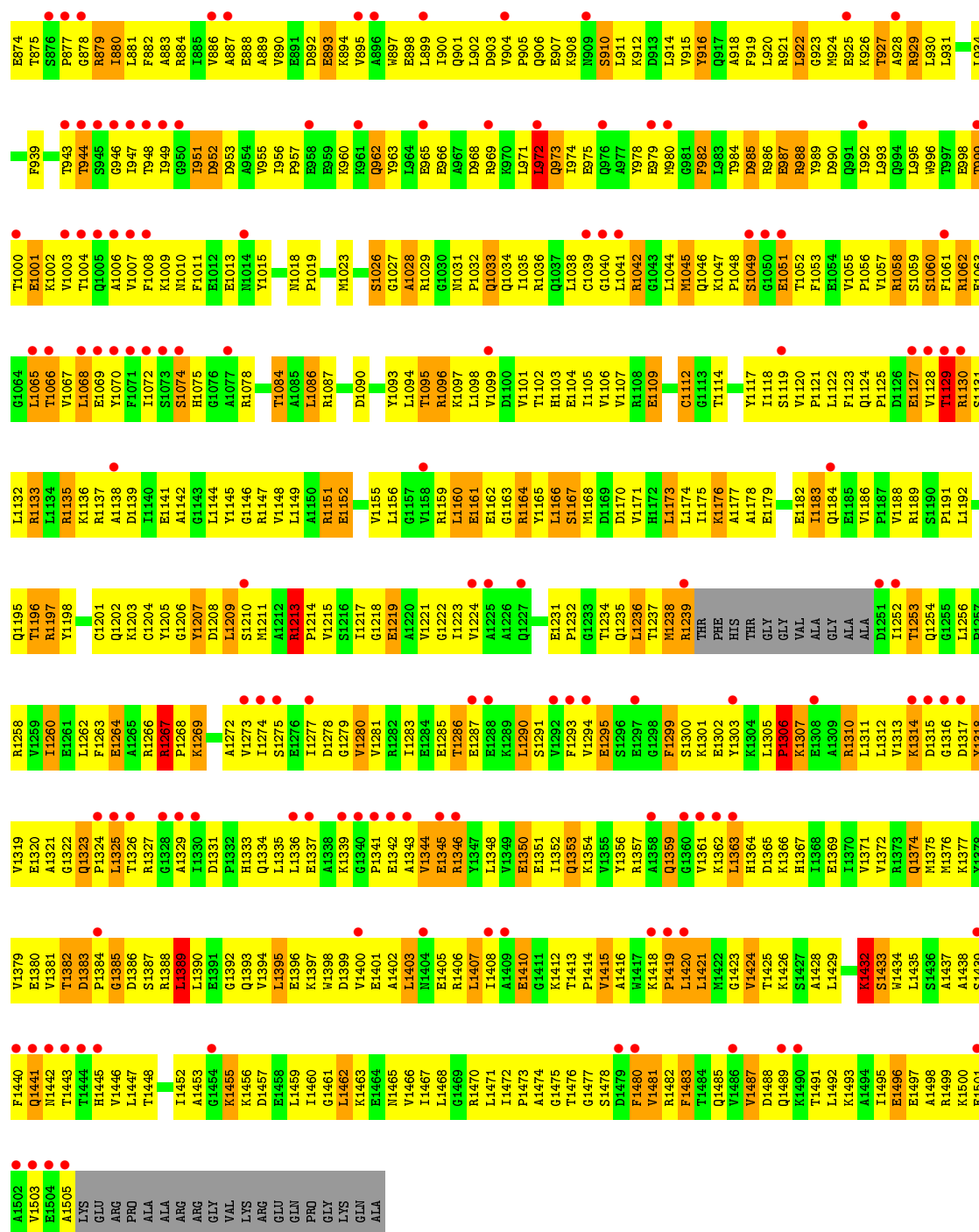








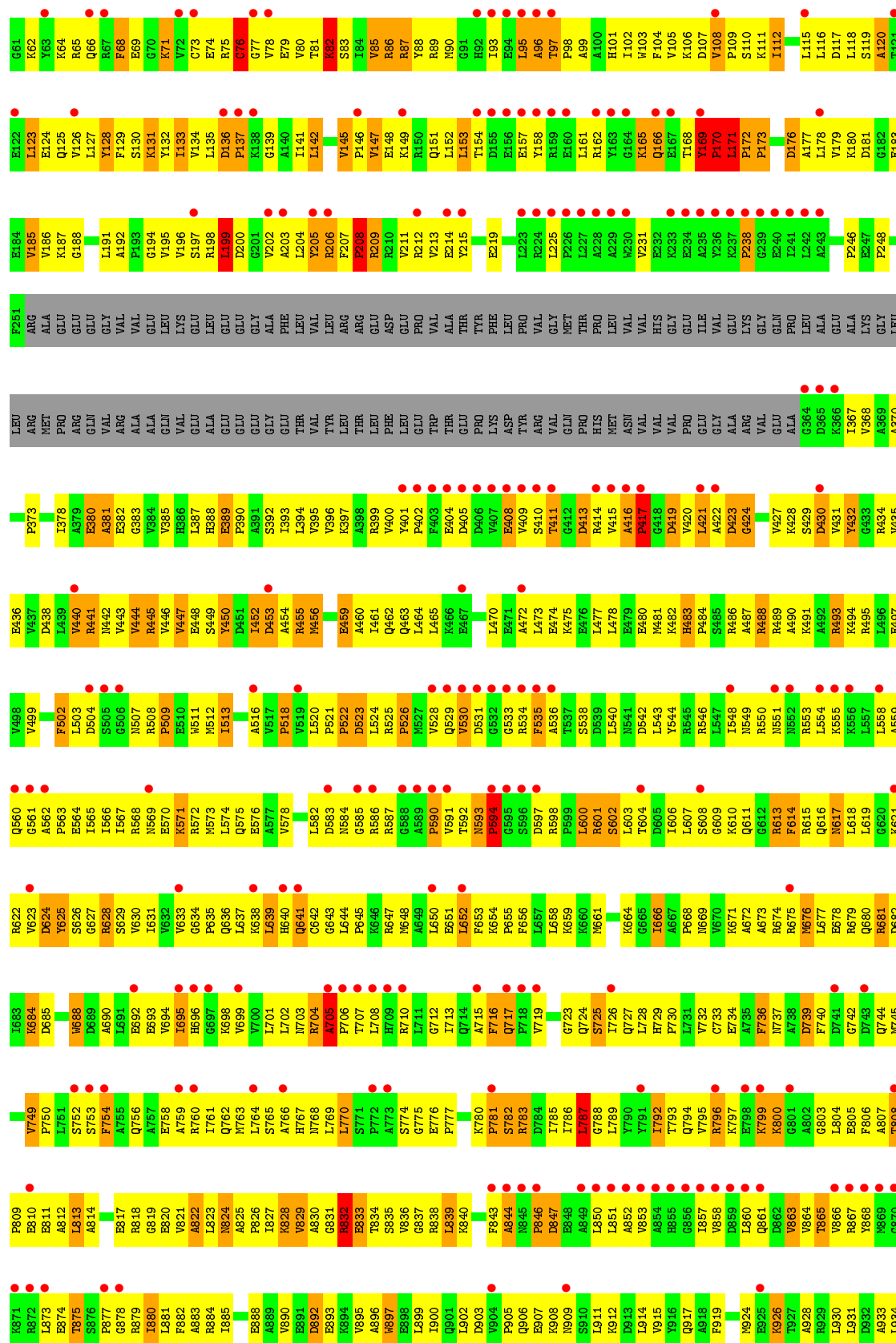




• Molecule 3: DNA-directed RNA polymerase beta' chain







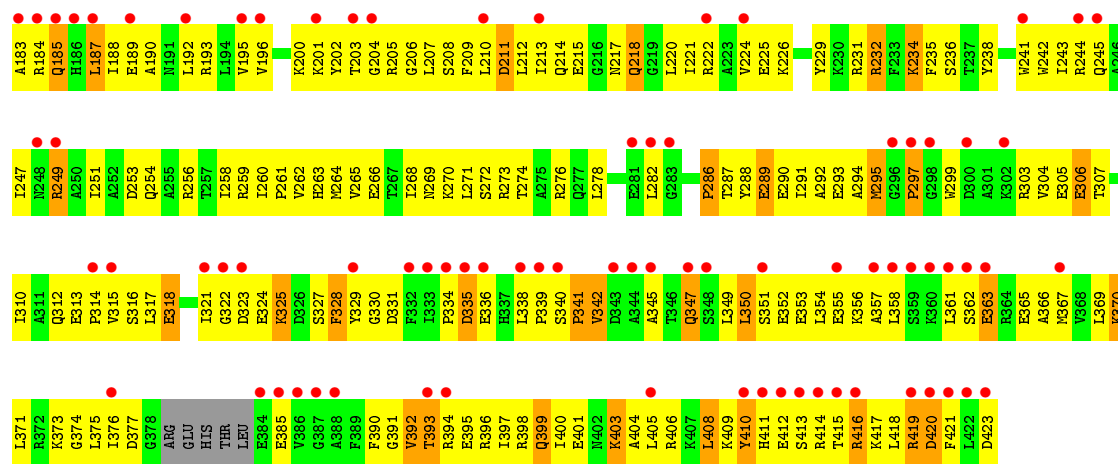














## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.40 34.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.40) 91.0 (34.69-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.268 0.230 , 0.264	Depositor DCC
$R_{free}$ test set	33251 reflections (5.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.079 for h,-h-k,-l 0.079 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.72	EDS
Total number of atoms	60908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: STD, 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	0.80	1/1838 (0.1%)	0.87	3/2498 (0.1%)
1	B	0.75	0/1838	0.84	6/2498 (0.2%)
1	K	0.75	0/1838	0.83	1/2498 (0.0%)
1	L	0.73	1/1838 (0.1%)	0.77	3/2498 (0.1%)
2	C	0.83	1/8997 (0.0%)	0.89	7/12164 (0.1%)
2	M	0.82	0/8997	0.90	10/12164 (0.1%)
3	D	0.82	0/10903	0.93	18/14736 (0.1%)
3	N	0.81	0/10903	0.93	19/14736 (0.1%)
4	E	0.82	0/783	0.96	0/1054
4	O	0.84	1/783 (0.1%)	0.95	1/1054 (0.1%)
5	F	0.72	0/2812	0.83	4/3781 (0.1%)
5	P	0.73	0/2812	0.82	3/3781 (0.1%)
All	All	0.80	4/54342 (0.0%)	0.90	75/73462 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	17	TYR	CD1-CE1	6.19	1.48	1.39
1	A	48	ILE	C-N	5.79	1.45	1.34
1	L	172	SER	N-CA	-5.30	1.35	1.46
2	C	191	PHE	C-N	5.26	1.44	1.34

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1389	LEU	CA-CB-CG	8.52	134.89	115.30
3	D	76	CYS	CA-CB-SG	8.24	128.84	114.00
3	D	199	LEU	CA-CB-CG	-8.01	96.89	115.30
2	M	165	LEU	C-N-CD	-7.94	103.13	120.60
3	N	199	LEU	CA-CB-CG	-7.89	97.16	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	239	0
1	B	1806	0	1861	210	0
1	K	1806	0	1861	178	0
1	L	1806	0	1861	205	0
2	C	8829	0	8933	1211	0
2	M	8829	0	8933	1154	0
3	D	10728	0	10809	1434	0
3	N	10728	0	10809	1309	0
4	E	769	0	775	89	0
4	O	769	0	775	118	0
5	F	2771	0	2844	364	0
5	P	2771	0	2844	336	0
6	D	43	0	31	4	0
6	N	43	0	31	6	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0
9	A	232	0	0	42	0
9	B	304	0	0	53	0
9	C	1144	0	0	274	0
9	D	1546	0	0	310	0
9	E	130	0	0	20	0
9	F	491	0	0	108	0
9	K	229	0	0	33	0
9	L	274	0	0	51	0
9	M	1072	0	0	223	0
9	N	1392	0	0	261	0
9	O	137	0	0	26	0
9	P	447	0	0	72	0
All	All	60908	0	54228	6435	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 60.

The worst 5 of 6435 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)
3:N:131:LYS:HG2	3:N:568:ARG:HG2	1.30	1.08
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.09	1.06
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.36	1.05
1:K:42:ARG:HH12	2:M:857:ASP:HB3	1.22	1.05
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.38	1.03

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%)	201 (88%)	21 (9%)	5 (2%)	6	7
1	B	227/315 (72%)	200 (88%)	21 (9%)	6 (3%)	5	5
1	K	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	12	17
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	8	10
2	C	1117/1119 (100%)	924 (83%)	143 (13%)	50 (4%)	2	2
2	M	1117/1119 (100%)	920 (82%)	149 (13%)	48 (4%)	2	2
3	D	1375/1524 (90%)	1129 (82%)	186 (14%)	60 (4%)	2	2
3	N	1375/1524 (90%)	1129 (82%)	181 (13%)	65 (5%)	2	1
4	E	93/99 (94%)	73 (78%)	16 (17%)	4 (4%)	2	2
4	O	93/99 (94%)	73 (78%)	16 (17%)	4 (4%)	2	2
5	F	341/423 (81%)	288 (84%)	42 (12%)	11 (3%)	4	3
5	P	341/423 (81%)	291 (85%)	37 (11%)	13 (4%)	3	2
All	All	6760/7590 (89%)	5632 (83%)	855 (13%)	273 (4%)	3	2



5 of 273 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	178	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%)	154 (76%)	48 (24%)	0	0
1	B	202/273 (74%)	162 (80%)	40 (20%)	1	1
1	K	202/273 (74%)	165 (82%)	37 (18%)	1	2
1	L	202/273 (74%)	156 (77%)	46 (23%)	1	1
2	C	941/941 (100%)	720 (76%)	221 (24%)	1	1
2	M	941/941 (100%)	722 (77%)	219 (23%)	1	1
3	D	1118/1279 (87%)	848 (76%)	270 (24%)	0	0
3	N	1118/1279 (87%)	860 (77%)	258 (23%)	1	1
4	E	83/87 (95%)	65 (78%)	18 (22%)	1	1
4	O	83/87 (95%)	67 (81%)	16 (19%)	1	1
5	F	295/370 (80%)	237 (80%)	58 (20%)	1	1
5	P	295/370 (80%)	245 (83%)	50 (17%)	2	2
All	All	5682/6446 (88%)	4401 (78%)	1281 (22%)	1	1

5 of 1281 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	7	ASP
1	L	138	LEU
3	N	1372	VAL
4	E	89	MET

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Mol	Chain	Res	Type
5	F	399	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 166 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	337	HIS
1	L	227	ASN
4	O	28	GLN
1	K	38	ASN
1	K	227	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 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
6	STD	N	8002	-	42,47,47	7.09	24 (57%)	47,73,73	2.35	10 (21%)
6	STD	D	8001	-	42,47,47	7.16	24 (57%)	47,73,73	2.24	10 (21%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	STD	N	8002	-	-	15/31/101/101	0/5/5/5
6	STD	D	8001	-	-	13/31/101/101	0/5/5/5

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	8001	STD	O5-C19	-28.16	1.18	1.43
6	N	8002	STD	O5-C19	-27.26	1.18	1.43
6	N	8002	STD	C23-C21	-14.56	1.21	1.53
6	D	8001	STD	C23-C21	-14.50	1.22	1.53
6	D	8001	STD	C18-C16	-13.42	1.25	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	8002	STD	C19-O5-C13	9.36	122.91	112.80
6	D	8001	STD	C19-O5-C13	7.86	121.29	112.80
6	D	8001	STD	O8-C17-C30	-6.73	105.06	111.68
6	N	8002	STD	O8-C17-C30	-6.54	105.26	111.68
6	N	8002	STD	C2-C1-C3	-4.87	102.67	107.80

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	8001	STD	O4-C4-N1-C20
6	D	8001	STD	C1-C5-C6-C7
6	D	8001	STD	O3-C5-C6-C7
6	D	8001	STD	C9-C10-C13-C16
6	D	8001	STD	C9-C10-C13-O5

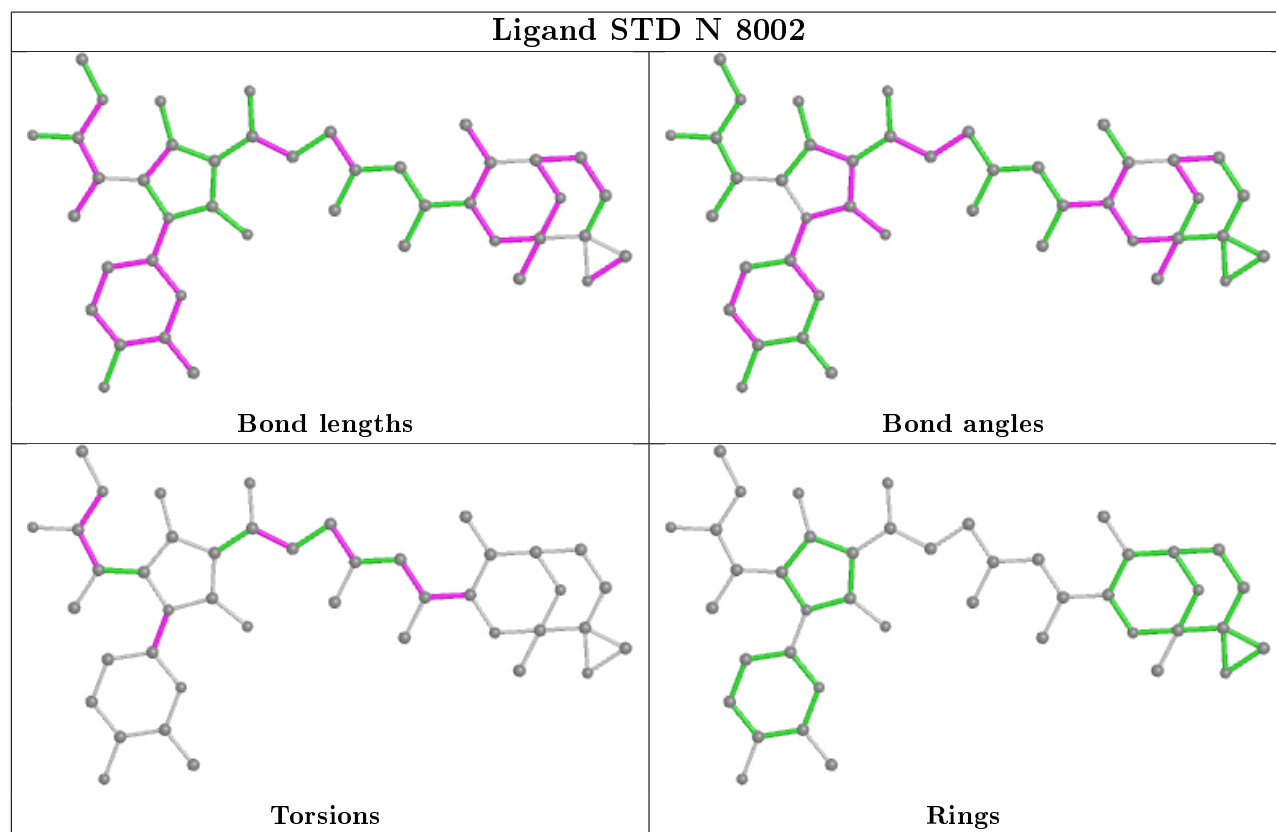
There are no ring outliers.

2 monomers are involved in 10 short contacts:

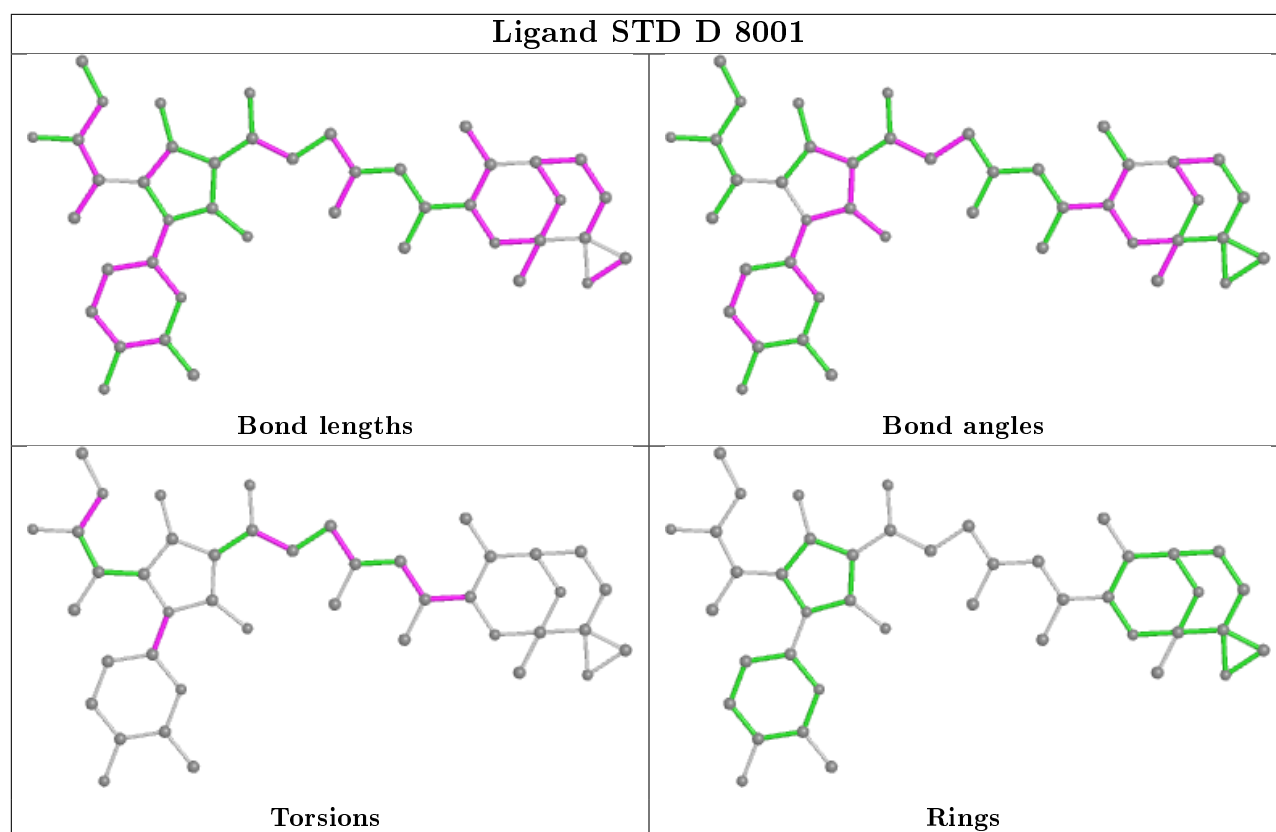
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	8002	STD	6	0
6	D	8001	STD	4	0



The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	229/315 (72%)	2.28	66 (28%) 0 0	31, 63, 90, 117	0
1	B	229/315 (72%)	2.69	74 (32%) 0 0	53, 90, 112, 118	0
1	K	229/315 (72%)	1.53	59 (25%) 0 0	33, 62, 87, 122	0
1	L	229/315 (72%)	3.11	82 (35%) 0 0	50, 87, 110, 125	0
2	C	1119/1119 (100%)	3.16	424 (37%) 0 0	25, 78, 104, 116	0
2	M	1119/1119 (100%)	2.82	396 (35%) 0 0	23, 72, 104, 115	0
3	D	1381/1524 (90%)	1.84	357 (25%) 0 0	27, 67, 107, 119	0
3	N	1381/1524 (90%)	1.85	373 (27%) 0 0	27, 68, 108, 120	0
4	E	95/99 (95%)	1.87	28 (29%) 0 0	44, 81, 108, 128	0
4	O	95/99 (95%)	1.95	32 (33%) 0 0	44, 75, 93, 105	0
5	F	345/423 (81%)	3.54	146 (42%) 0 0	55, 84, 107, 122	0
5	P	345/423 (81%)	3.06	129 (37%) 0 0	62, 84, 108, 116	0
All	All	6796/7590 (89%)	2.45	2166 (31%) 0 0	23, 73, 106, 128	0

The worst 5 of 2166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	405	ASP	71.3
3	N	406	ASP	57.5
1	A	1	MET	54.5
3	D	853	VAL	52.8
3	N	407	VAL	49.0

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

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



### 6.3 Carbohydrates ⓘ

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

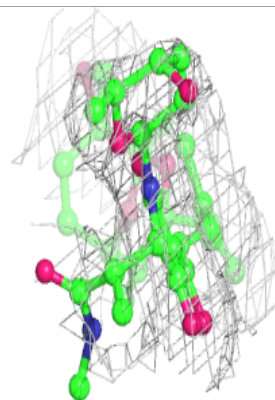
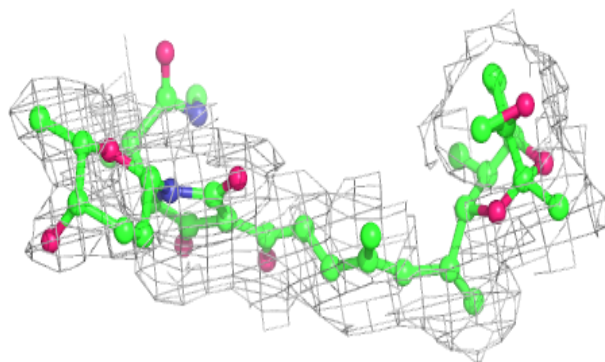
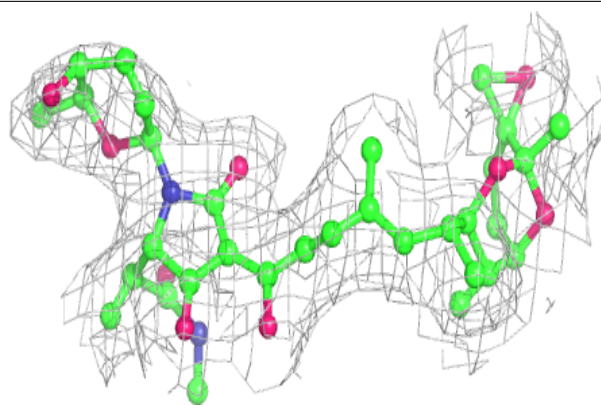
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	STD	N	8002	43/43	0.76	0.15	27,35,41,48	0
6	STD	D	8001	43/43	0.86	0.13	25,35,40,43	0
8	MG	N	9002	1/1	0.88	0.51	53,53,53,53	0
8	MG	D	9001	1/1	0.94	0.19	29,29,29,29	0
7	ZN	N	7459	1/1	0.95	0.10	64,64,64,64	0
7	ZN	N	7413	1/1	0.99	0.11	65,65,65,65	0
7	ZN	D	7458	1/1	0.99	0.09	64,64,64,64	0
7	ZN	D	7412	1/1	0.99	0.06	58,58,58,58	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.

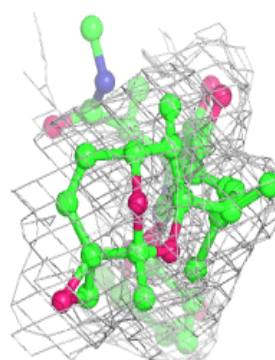
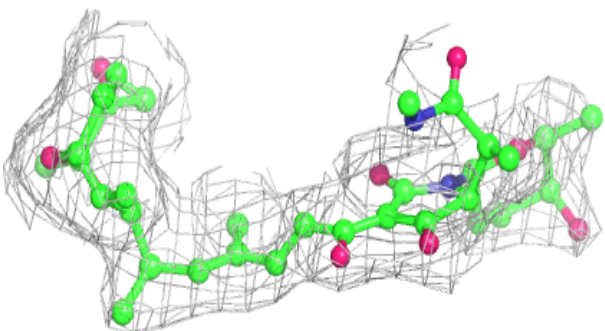
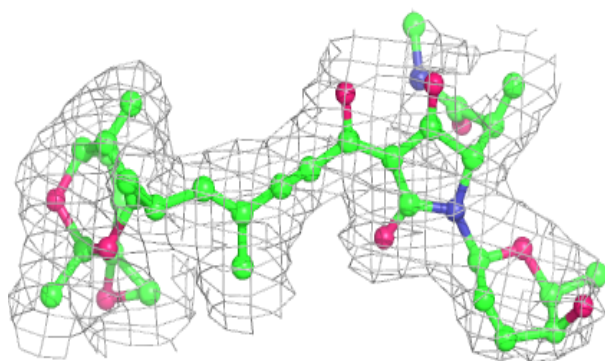


**Electron density around STD N 8002:**

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

**Electron density around STD D 8001:**

$2mF_o-DF_c$  (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.