



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 03:34 AM UTC

PDB ID : 2BE5 / pdb\_00002be5  
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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

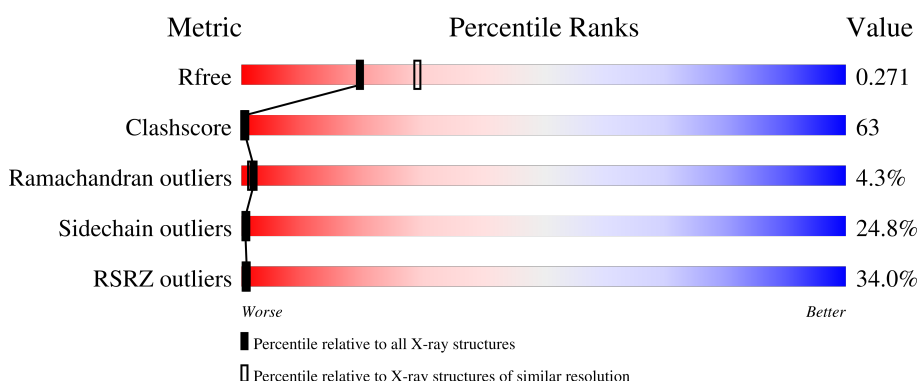
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of 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	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	

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Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

## 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
			Total	C	N	O	S			
1	A	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	B	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	K	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	L	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0

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

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

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

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

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

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

- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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

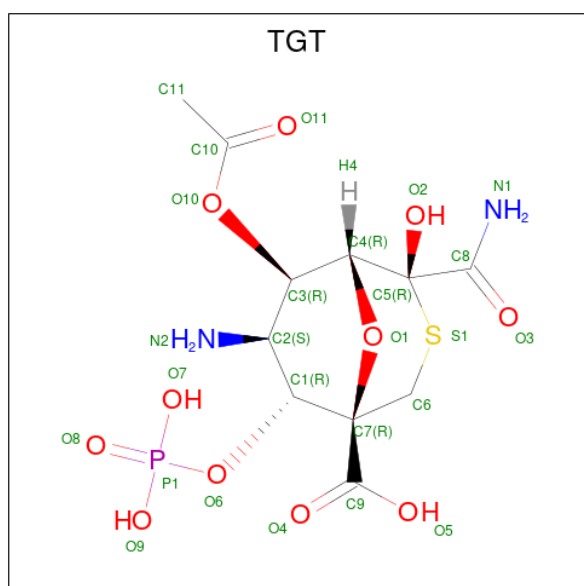
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 8 is TAGETITOXIN (CCD ID: TGT) (formula: C<sub>11</sub>H<sub>17</sub>N<sub>2</sub>O<sub>11</sub>PS).



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

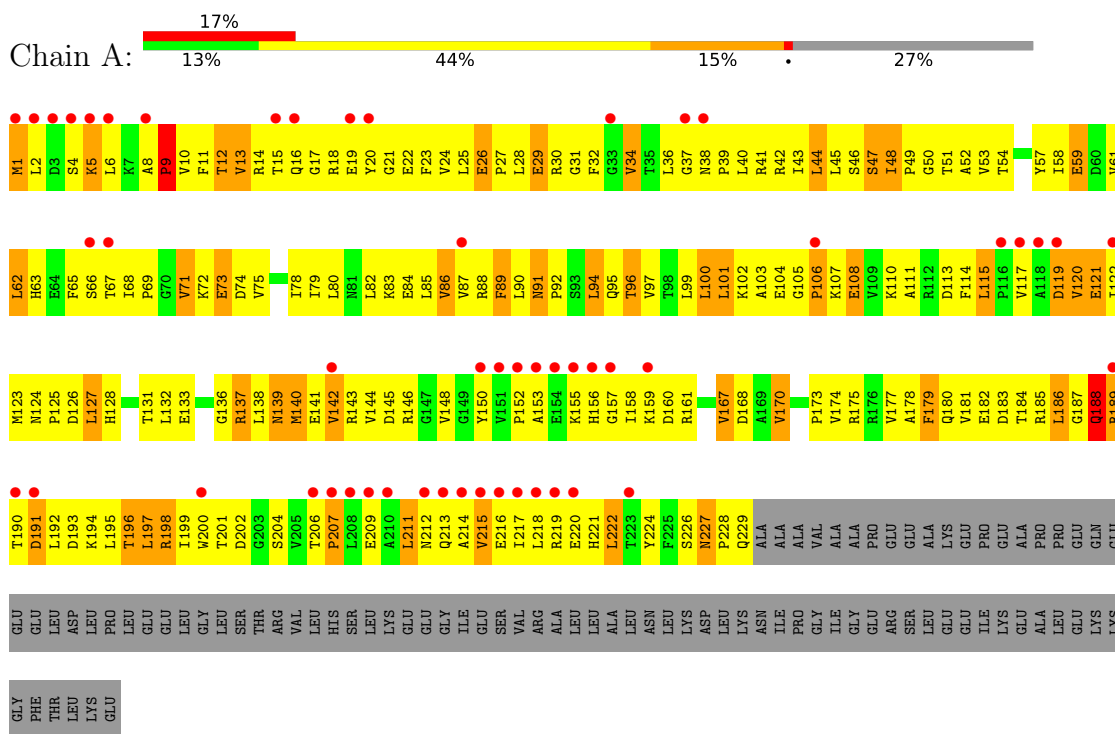
- Molecule 9 is water.

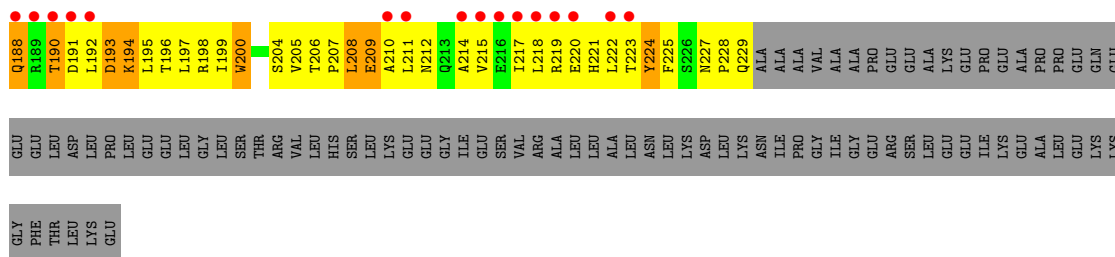
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	250	Total	O	0	0
			250	250		
9	B	329	Total	O	0	0
			329	329		
9	C	1321	Total	O	0	0
			1321	1321		
9	D	1655	Total	O	0	0
			1655	1655		
9	E	176	Total	O	0	0
			176	176		
9	F	519	Total	O	0	0
			519	519		
9	K	278	Total	O	0	0
			278	278		
9	L	309	Total	O	0	0
	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

### 3 Residue-property plots i

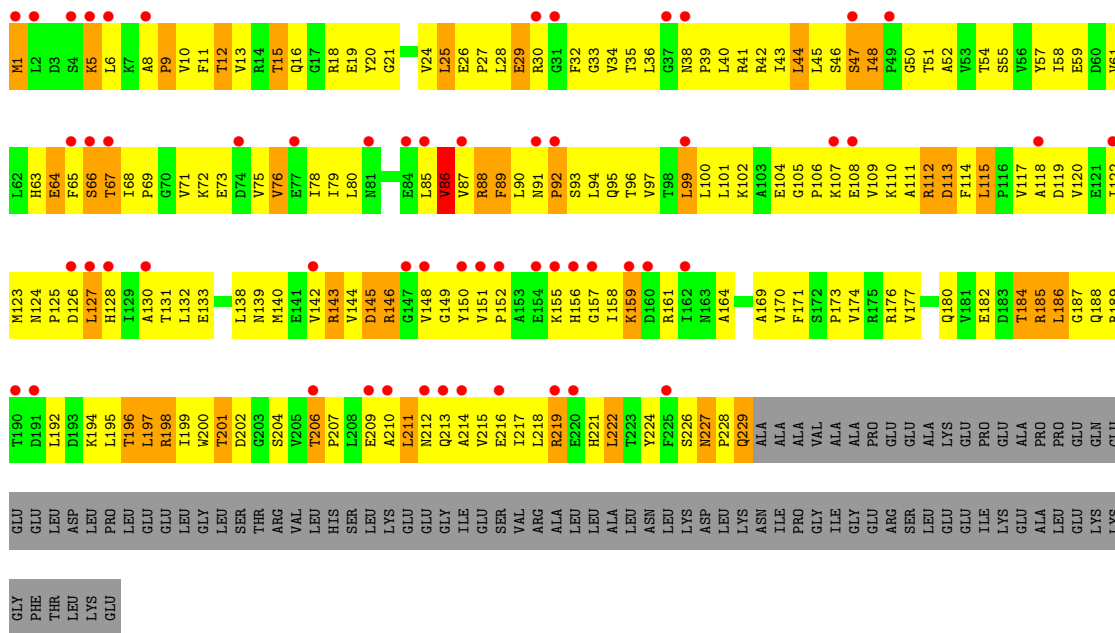
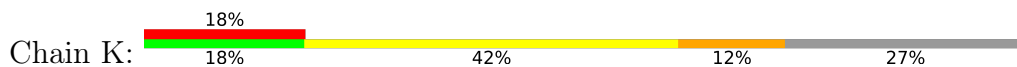
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA-directed RNA polymerase alpha chain

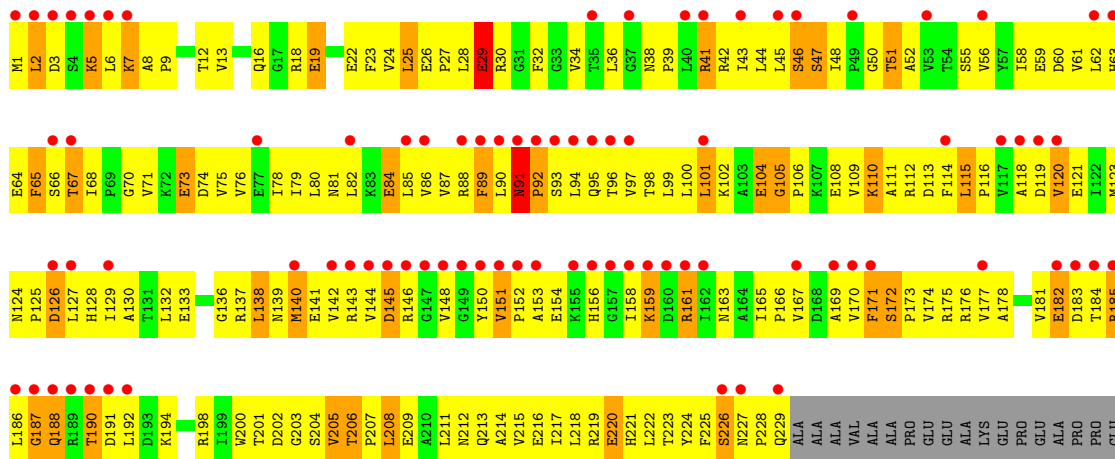
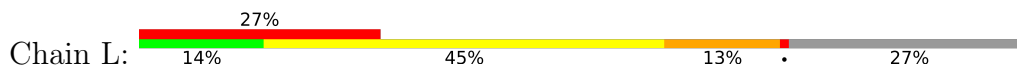




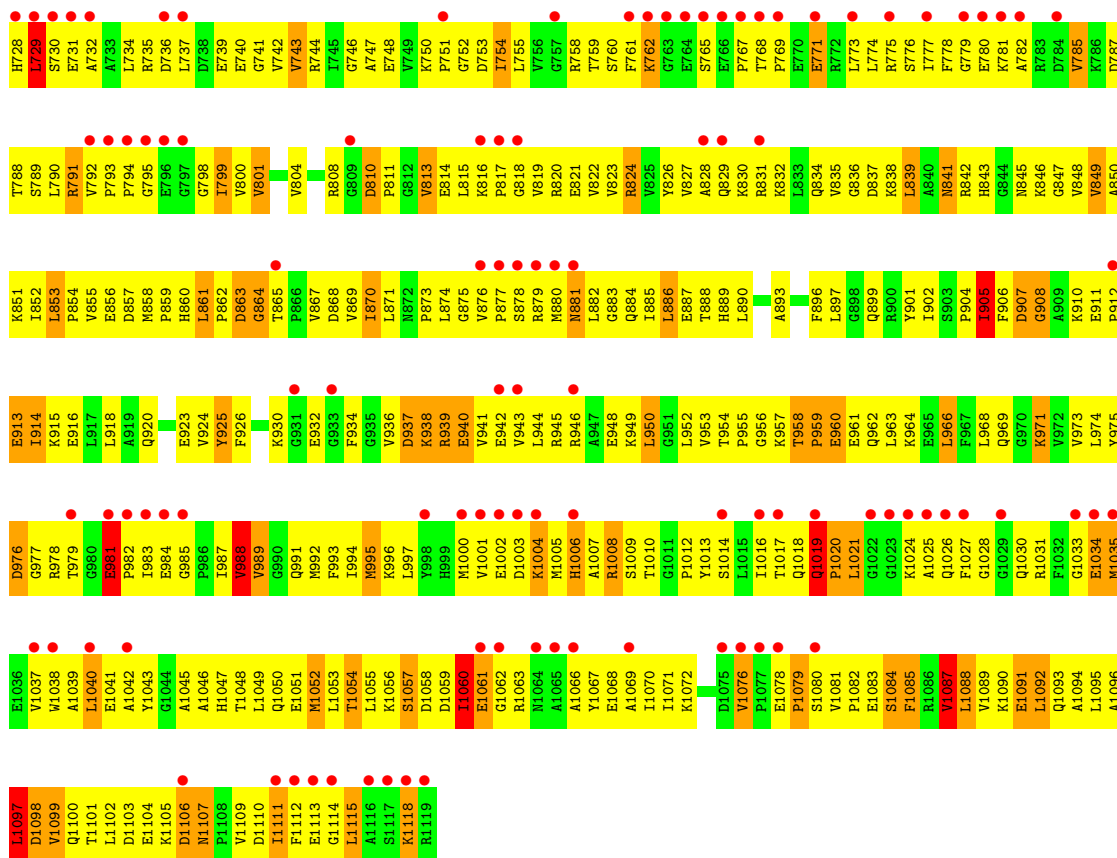
● Molecule 1: DNA-directed RNA polymerase alpha chain



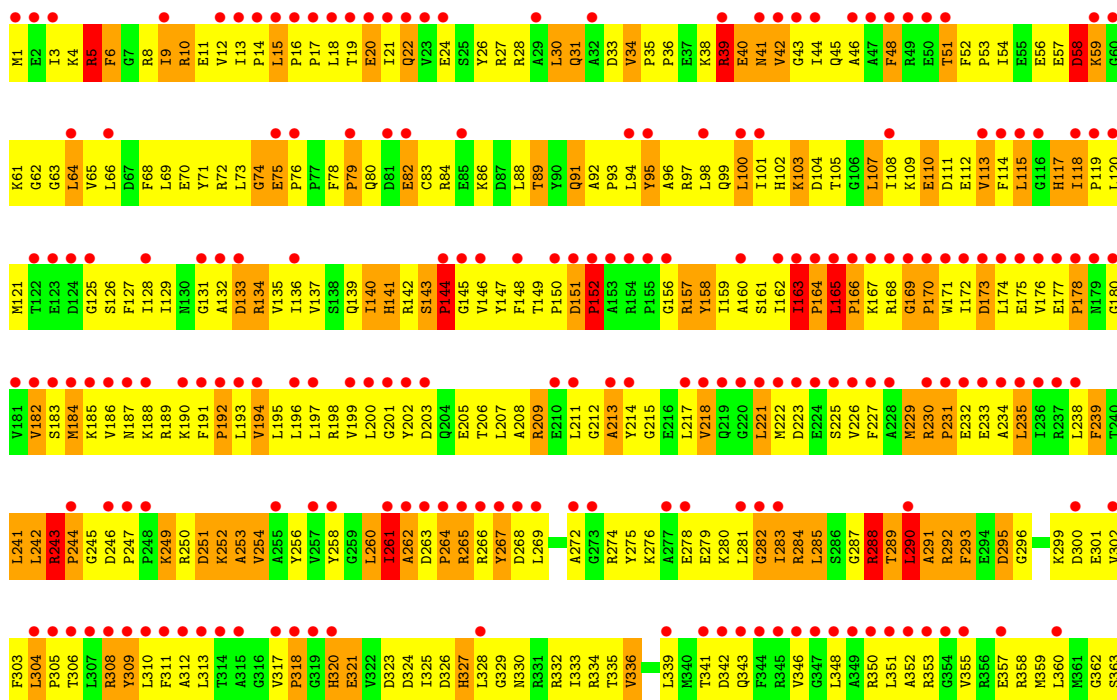
● Molecule 1: DNA-directed RNA polymerase alpha chain

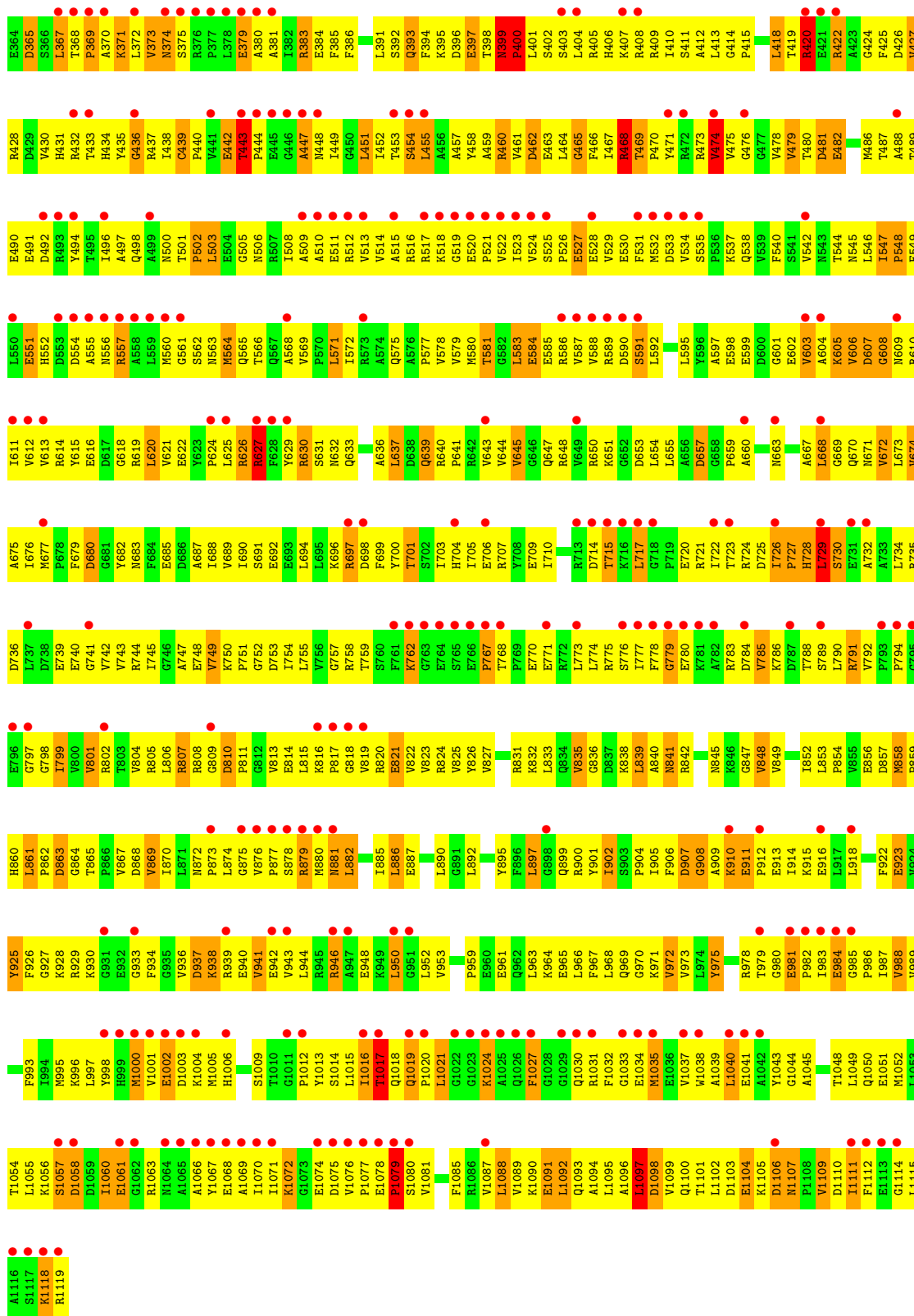




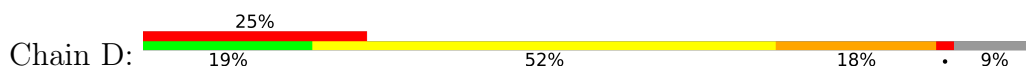


● Molecule 2: DNA-directed RNA polymerase beta chain

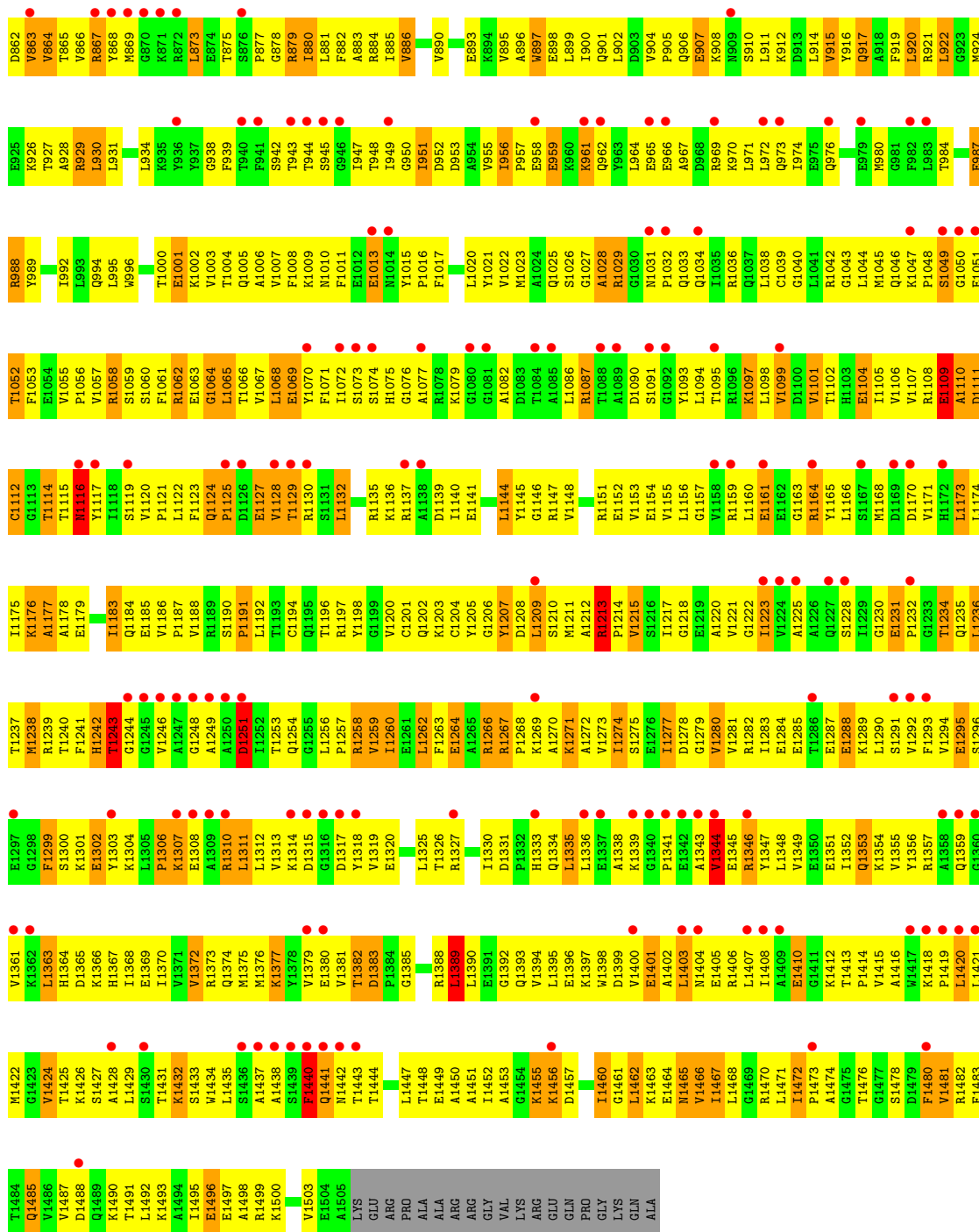




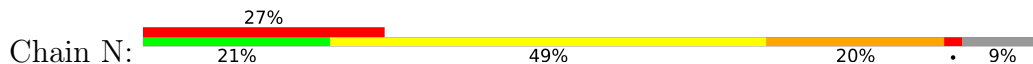
● Molecule 3: DNA-directed RNA polymerase beta' chain







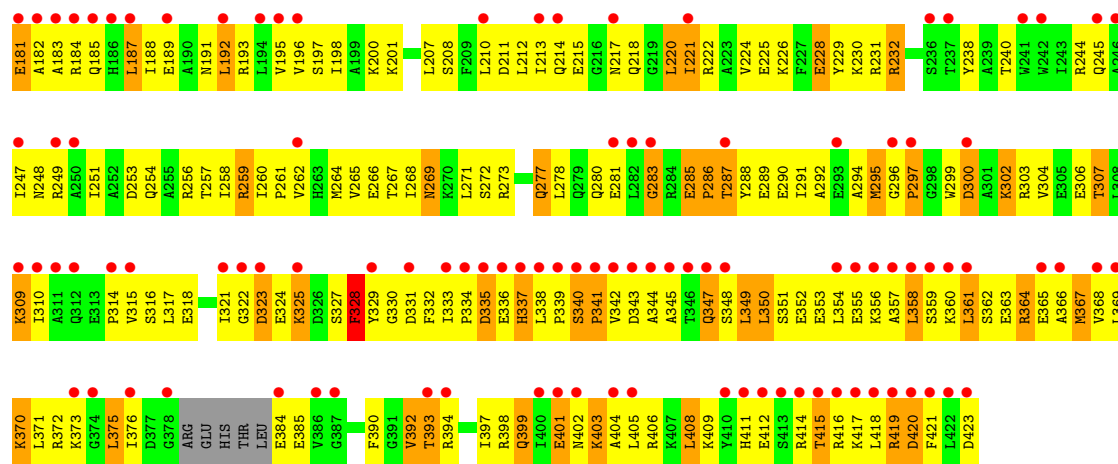
• Molecule 3: DNA-directed RNA polymerase beta' chain











## 4 Data and refinement statistics i

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 25.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.40) 95.2 (25.00-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.65 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.274 0.234 , 0.271	Depositor DCC
$R_{free}$ test set	34795 reflections (5.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtrriage
Anisotropy	0.106	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	-0.43 , 436.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.499 for -h,-k,l 0.065 for h,-h-k,-l 0.065 for -k,-h,-l	Xtrriage
Reported twinning fraction	0.500 for H, K, L 0.500 for -h,-k,l	Depositor
Outliers	0 of 604645 reflections	Xtrriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	61800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage'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.*

<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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TGT, 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%)	1.16	10/2498 (0.4%)
1	B	0.73	0/1838	1.07	9/2498 (0.4%)
1	K	0.78	1/1838 (0.1%)	1.10	5/2498 (0.2%)
1	L	0.76	2/1838 (0.1%)	1.05	8/2498 (0.3%)
2	C	0.87	8/8997 (0.1%)	1.27	84/12164 (0.7%)
2	M	0.85	4/8997 (0.0%)	1.27	86/12164 (0.7%)
3	D	0.88	7/10975 (0.1%)	1.31	101/14836 (0.7%)
3	N	0.88	11/10975 (0.1%)	1.33	99/14836 (0.7%)
4	E	0.90	1/783 (0.1%)	1.32	9/1054 (0.9%)
4	O	0.85	0/783	1.33	9/1054 (0.9%)
5	F	0.77	2/2812 (0.1%)	1.17	13/3781 (0.3%)
5	P	0.77	1/2812 (0.0%)	1.17	15/3781 (0.4%)
All	All	0.85	38/54486 (0.1%)	1.26	448/73662 (0.6%)

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	13	ALA	CA-CB	-8.12	1.42	1.53
3	N	172	PRO	CA-C	7.77	1.56	1.51
2	C	163	ILE	CA-CB	7.67	1.62	1.53
1	L	171	PHE	CA-C	-7.27	1.42	1.52
4	E	65	MET	SD-CE	6.86	1.96	1.79

The worst 5 of 448 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	508	ARG	CA-C-N	18.62	138.06	119.82
3	N	508	ARG	C-N-CA	18.62	138.06	119.82
3	N	1124	GLN	CA-C-N	16.64	140.64	119.84
3	N	1124	GLN	C-N-CA	16.64	140.64	119.84
3	N	207	PHE	CA-C-N	16.44	140.39	119.84

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	233	0
1	B	1806	0	1861	222	0
1	K	1806	0	1861	200	0
1	L	1806	0	1861	220	0
2	C	8829	0	8933	1274	0
2	M	8829	0	8933	1163	0
3	D	10797	0	10873	1517	0
3	N	10797	0	10873	1438	0
4	E	769	0	775	104	0
4	O	769	0	775	102	0
5	F	2771	0	2844	357	0
5	P	2771	0	2844	350	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	268	0
9	D	1655	0	0	329	0
9	E	176	0	0	33	0
9	F	519	0	0	104	0
9	K	278	0	0	42	0
9	L	309	0	0	70	0
9	M	1236	0	0	260	0
9	N	1552	0	0	306	0
9	O	137	0	0	25	0
9	P	422	0	0	85	0
All	All	61800	0	54323	6768	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 63.

The worst 5 of 6768 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:N:567:ILE:HG22	3:N:571:LYS:HZ1	1.11	1.08
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

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%)	5	6
1	B	227/315 (72%)	200 (88%)	22 (10%)	5 (2%)	5	6
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	6	9
1	L	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	6	9
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	1
3	D	1388/1524 (91%)	1155 (83%)	168 (12%)	65 (5%)	2	1
3	N	1388/1524 (91%)	1133 (82%)	187 (14%)	68 (5%)	1	1
4	E	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	2	1
4	O	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	2	1
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	1
All	All	6786/7590 (89%)	5671 (84%)	824 (12%)	291 (4%)	2	1

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 [i](#)

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%)	143 (71%)	59 (29%)	0	0
1	B	202/273 (74%)	169 (84%)	33 (16%)	2	3
1	K	202/273 (74%)	152 (75%)	50 (25%)	1	1
1	L	202/273 (74%)	154 (76%)	48 (24%)	1	1
2	C	941/941 (100%)	715 (76%)	226 (24%)	1	1
2	M	941/941 (100%)	722 (77%)	219 (23%)	1	1
3	D	1123/1279 (88%)	829 (74%)	294 (26%)	0	0
3	N	1123/1279 (88%)	813 (72%)	310 (28%)	0	0
4	E	83/87 (95%)	64 (77%)	19 (23%)	1	1
4	O	83/87 (95%)	61 (74%)	22 (26%)	0	0
5	F	295/370 (80%)	222 (75%)	73 (25%)	1	1
5	P	295/370 (80%)	237 (80%)	58 (20%)	1	2
All	All	5692/6446 (88%)	4281 (75%)	1411 (25%)	1	1

5 of 1411 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	605	LYS
3	N	652	LEU
2	M	727	PRO
2	M	603	VAL

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Mol	Chain	Res	Type
3	N	76	CYS

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

Mol	Chain	Res	Type
2	M	374	ASN
3	N	549	ASN
2	M	543	ASN
2	M	841	ASN
3	N	717	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 oligosaccharides 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	D	9001	6	23,27,27	4.37	19 (82%)	24,44,44	2.56	8 (33%)
8	TGT	N	9002	6	23,27,27	4.75	17 (73%)	24,44,44	2.61	8 (33%)

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	D	9001	6	-	6/14/57/57	0/2/2/2
8	TGT	N	9002	6	-	6/14/57/57	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	9001	TGT	O11-C10	9.66	1.55	1.21
8	N	9002	TGT	O11-C10	8.91	1.53	1.21
8	N	9002	TGT	O3-C8	8.83	1.41	1.23
8	N	9002	TGT	C6-C7	6.86	1.58	1.52
8	D	9001	TGT	C6-C7	6.60	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	9001	TGT	O10-C10-C11	7.34	124.18	111.09
8	N	9002	TGT	O10-C10-C11	7.10	123.76	111.09
8	N	9002	TGT	C3-O10-C10	6.92	128.47	117.72
8	D	9001	TGT	C3-O10-C10	5.89	126.88	117.72
8	D	9001	TGT	O9-P1-O6	3.97	121.31	105.85

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

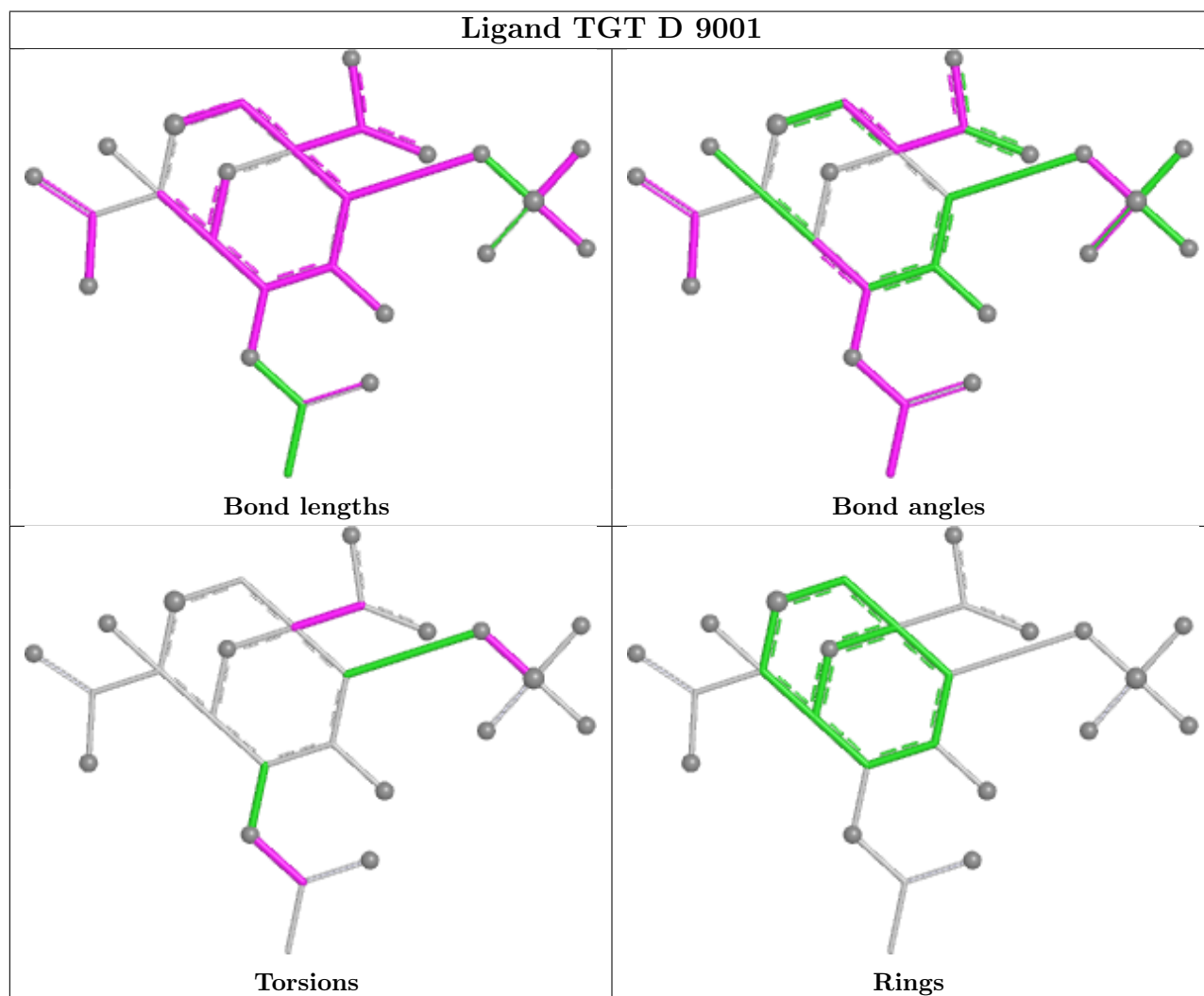
Mol	Chain	Res	Type	Atoms
8	D	9001	TGT	O1-C7-C9-O5
8	D	9001	TGT	C11-C10-O10-C3
8	N	9002	TGT	O1-C7-C9-O5
8	N	9002	TGT	C11-C10-O10-C3
8	D	9001	TGT	O11-C10-O10-C3

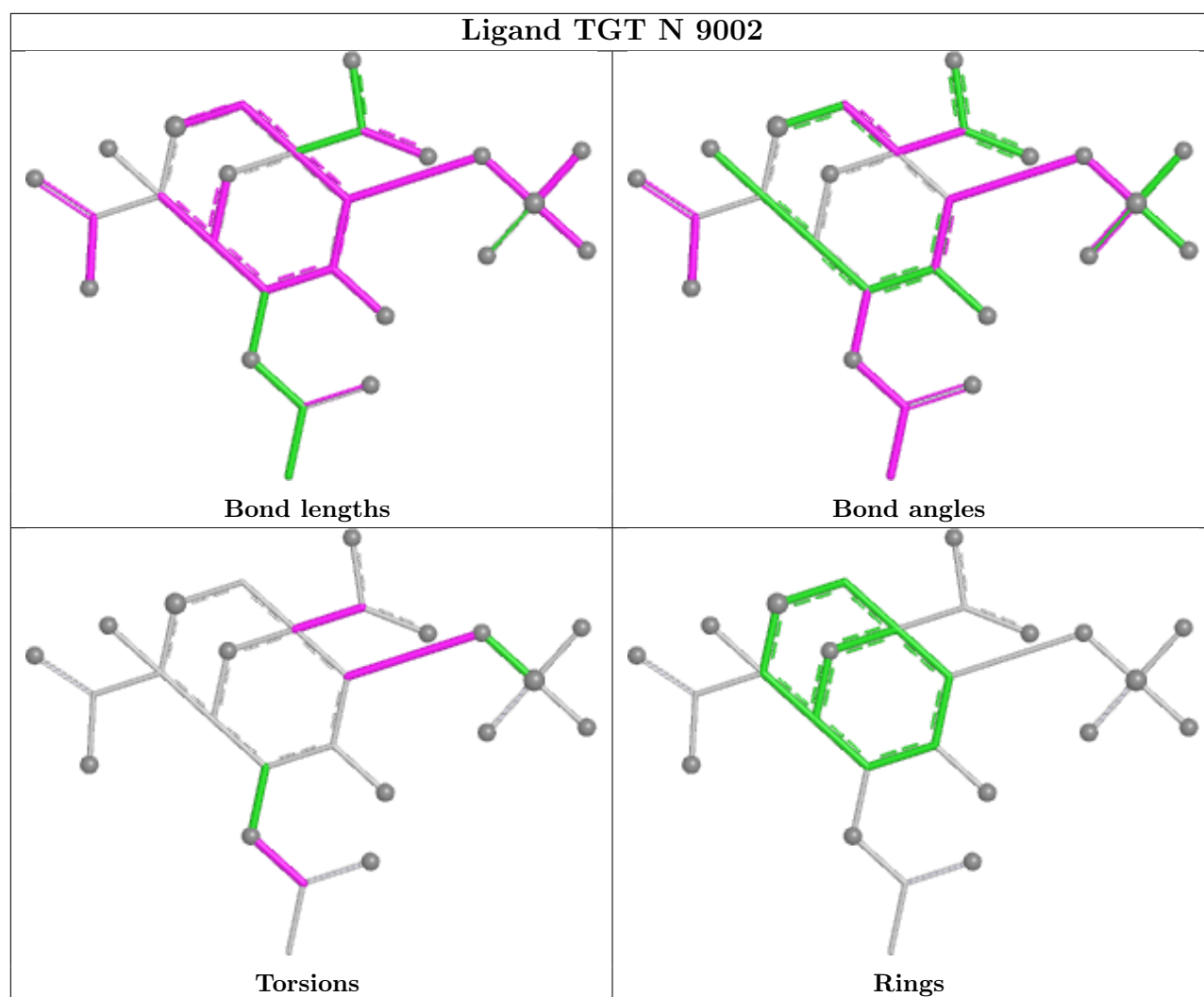
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	9001	TGT	3	0
8	N	9002	TGT	1	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%)	1.75	52 (22%) 2 2	18, 47, 72, 88	0
1	B	229/315 (72%)	2.50	91 (39%) 1 0	34, 66, 82, 88	0
1	K	229/315 (72%)	1.35	57 (24%) 2 1	21, 43, 70, 92	0
1	L	229/315 (72%)	2.58	84 (36%) 1 1	34, 62, 82, 95	0
2	C	1119/1119 (100%)	2.50	428 (38%) 1 0	15, 58, 81, 94	0
2	M	1119/1119 (100%)	2.58	436 (38%) 1 0	15, 55, 81, 97	0
3	D	1392/1524 (91%)	1.87	385 (27%) 1 1	15, 49, 82, 97	0
3	N	1392/1524 (91%)	1.89	412 (29%) 1 1	16, 48, 83, 105	0
4	E	95/99 (95%)	1.70	28 (29%) 1 1	30, 59, 82, 103	0
4	O	95/99 (95%)	1.81	29 (30%) 1 1	22, 59, 77, 87	0
5	F	345/423 (81%)	2.84	154 (44%) 0 0	38, 63, 83, 97	0
5	P	345/423 (81%)	2.93	165 (47%) 0 0	41, 64, 85, 92	0
All	All	6818/7590 (89%)	2.22	2321 (34%) 1 1	15, 54, 82, 105	0

The worst 5 of 2321 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	153	ALA	24.4
2	M	153	ALA	21.6
1	L	90	LEU	21.3
1	L	95	GLN	21.2
5	F	386	VAL	21.1

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

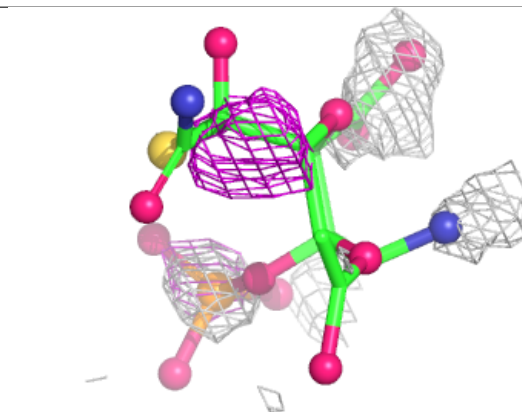
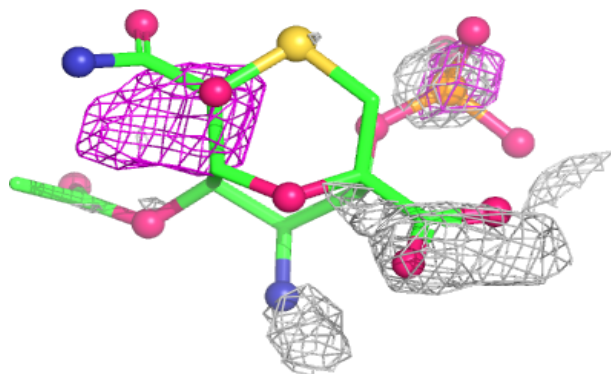
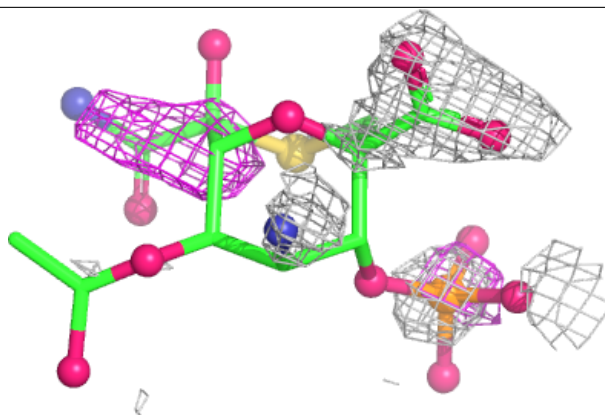
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
8	TGT	D	9001	26/26	0.92	0.21	44,47,50,52	0
8	TGT	N	9002	26/26	0.92	0.22	41,47,51,52	0
6	MG	N	9005	1/1	0.99	0.06	13,13,13,13	0
6	MG	N	9006	1/1	0.99	0.07	4,4,4,4	0
7	ZN	D	9058	1/1	0.99	0.02	56,56,56,56	0
6	MG	C	9004	1/1	0.99	0.03	17,17,17,17	0
6	MG	D	9003	1/1	0.99	0.05	17,17,17,17	0
7	ZN	N	9113	1/1	1.00	0.01	41,41,41,41	0
7	ZN	D	9112	1/1	1.00	0.03	50,50,50,50	0
7	ZN	N	9059	1/1	1.00	0.04	42,42,42,42	0

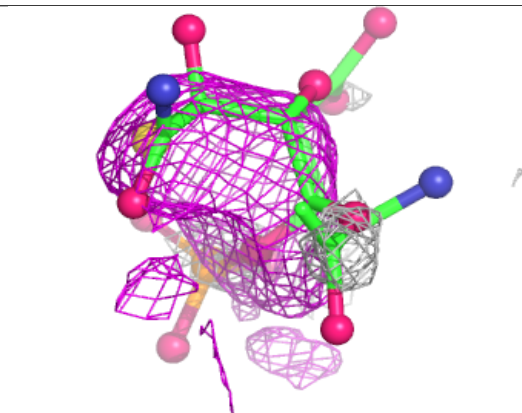
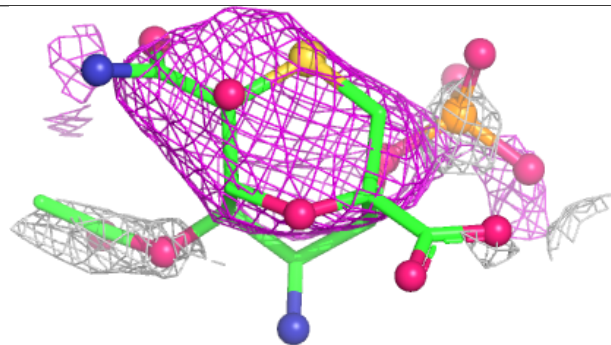
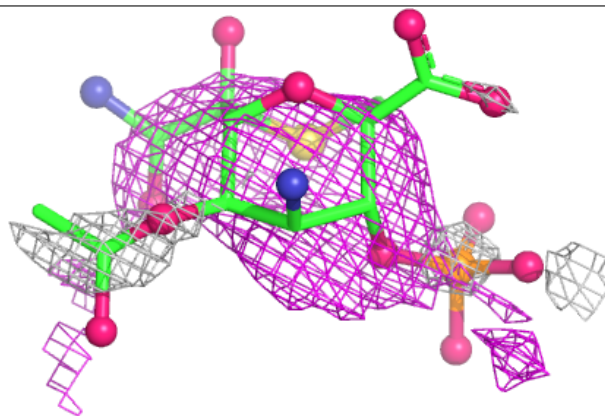
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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

There are no such residues in this entry.