



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 04:12 PM UTC

PDB ID : 2A6H / pdb_00002a6h
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

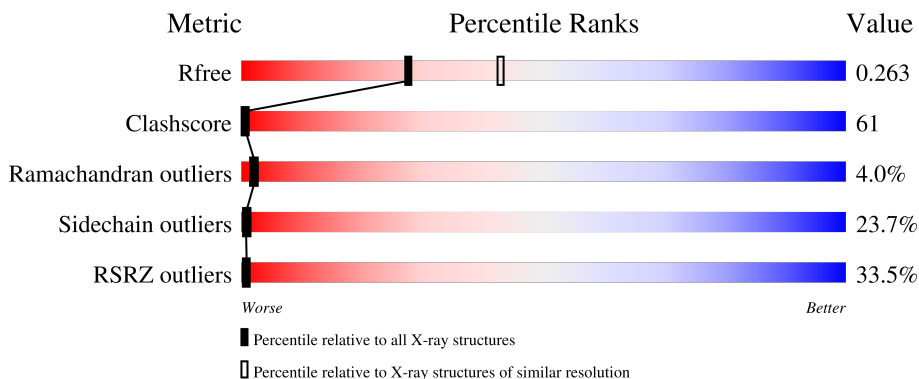
1 Overall quality at a glance

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 ≥ 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	21% 16% 43% 14% 27%
1	B	315	22% 17% 42% 14% 27%
1	K	315	19% 23% 38% 12% 27%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	L	315	
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

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			

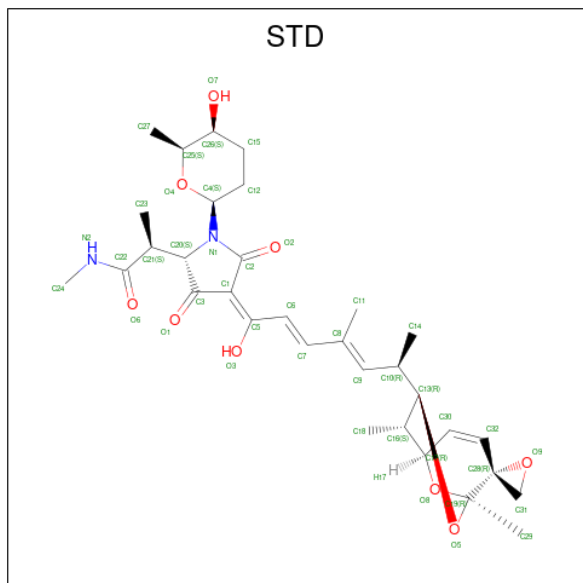
- Molecule 4 is a protein called RNA polymerase omega chain.

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	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 STREPTOLYDIGIN (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

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

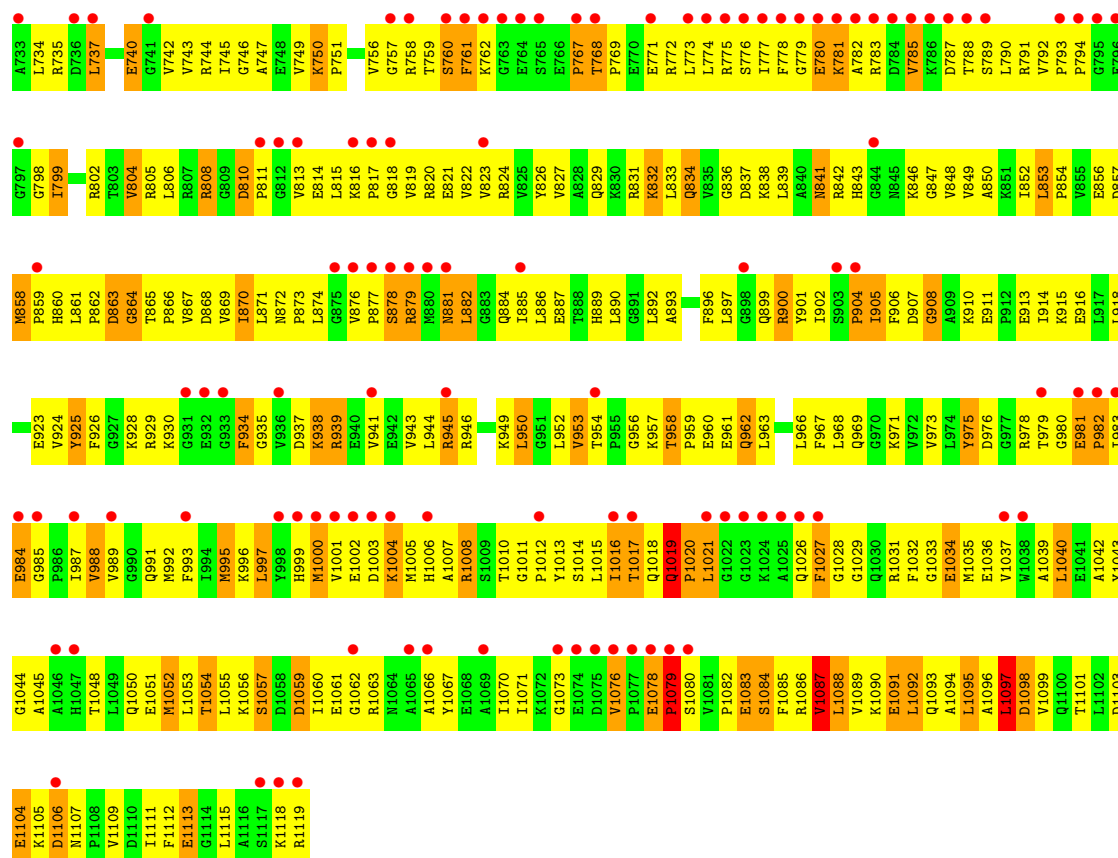
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

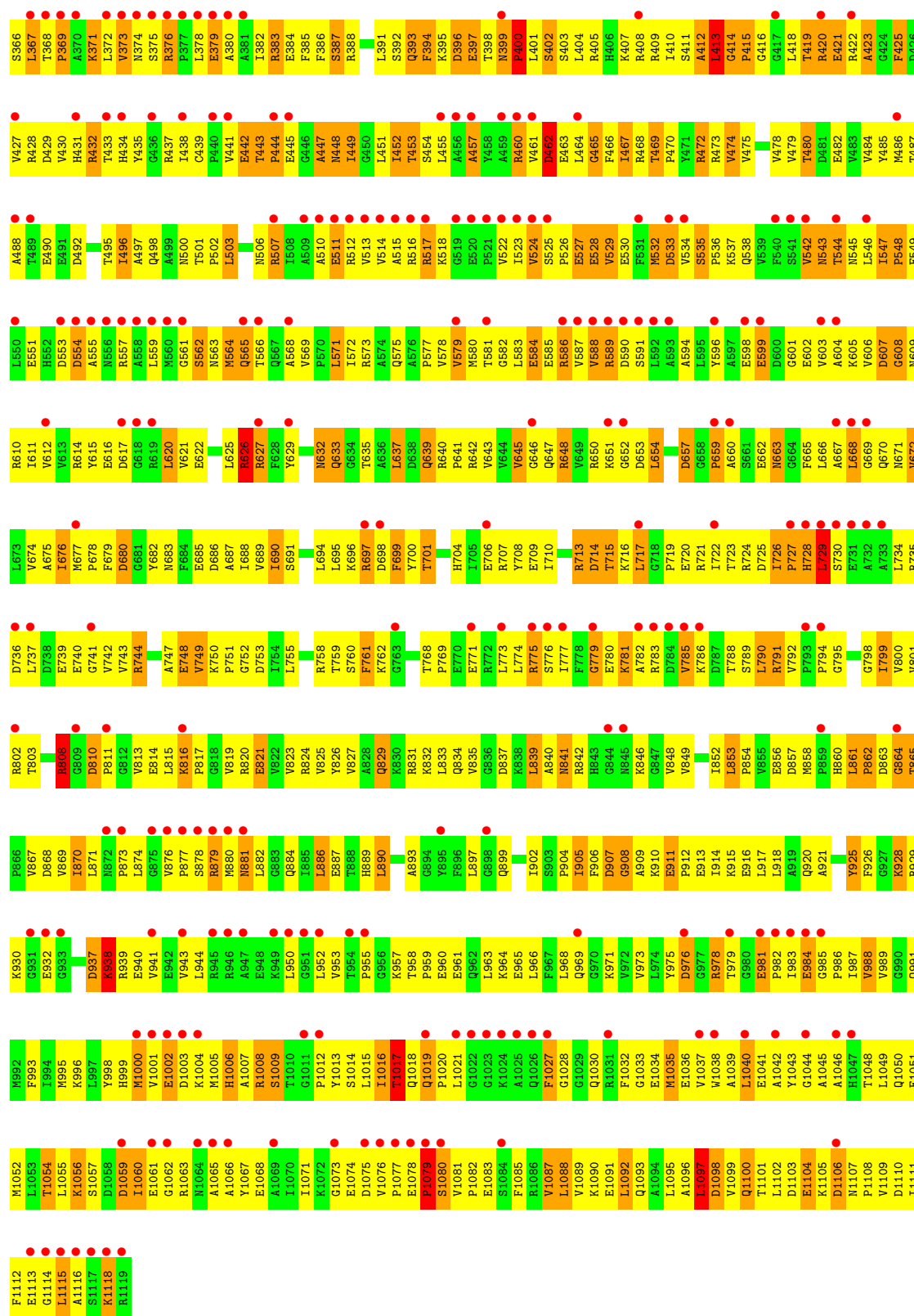
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0

- Molecule 9 is water.

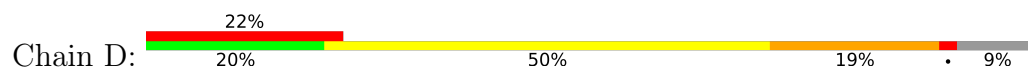
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	232	Total O 232 232	0	0
9	B	304	Total O 304 304	0	0
9	C	1144	Total O 1144 1144	0	0
9	D	1546	Total O 1546 1546	0	0
9	E	130	Total O 130 130	0	0
9	F	491	Total O 491 491	0	0
9	K	229	Total O 229 229	0	0
9	L	274	Total O 274 274	0	0
9	M	1072	Total O 1072 1072	0	0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





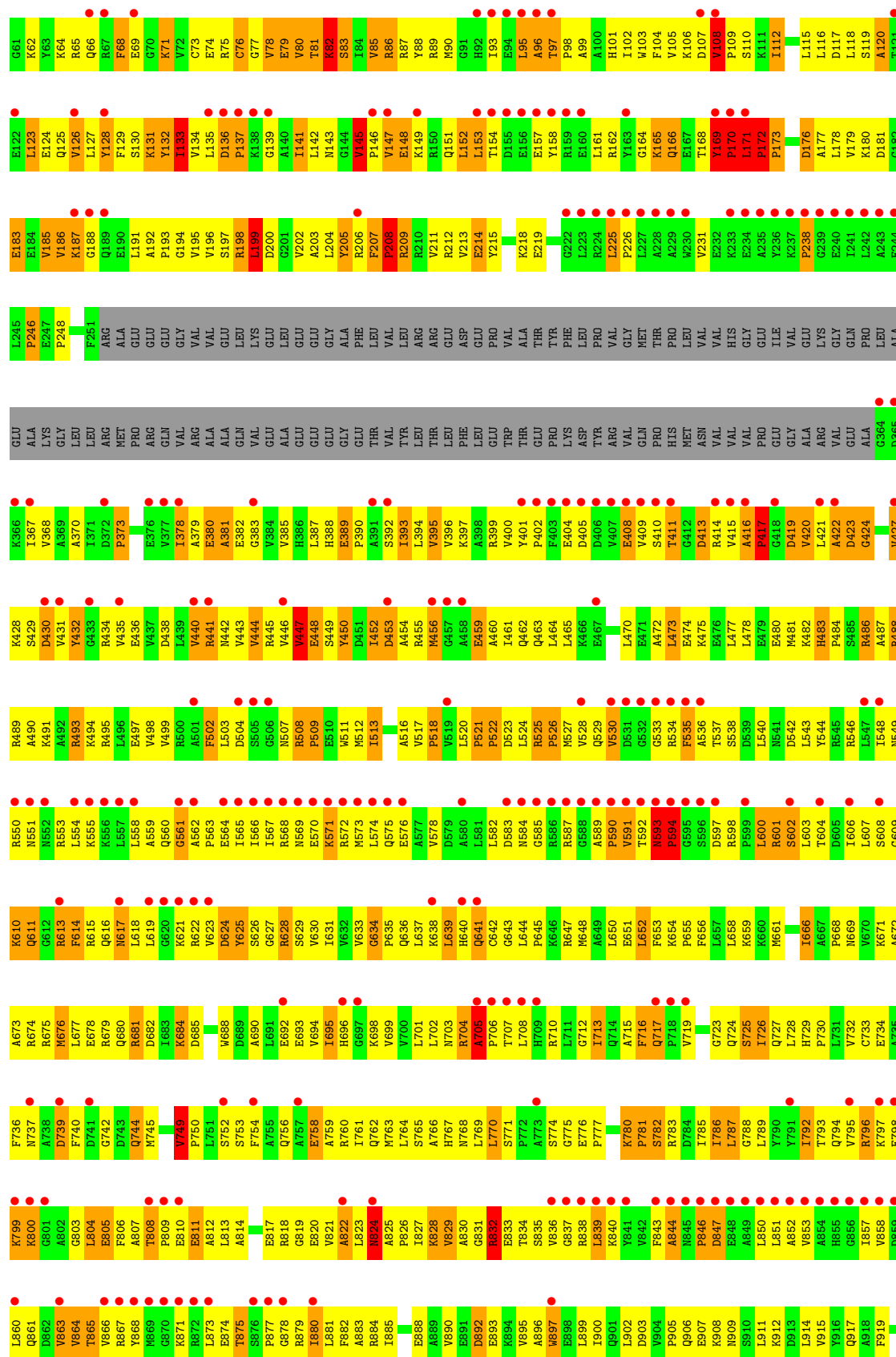


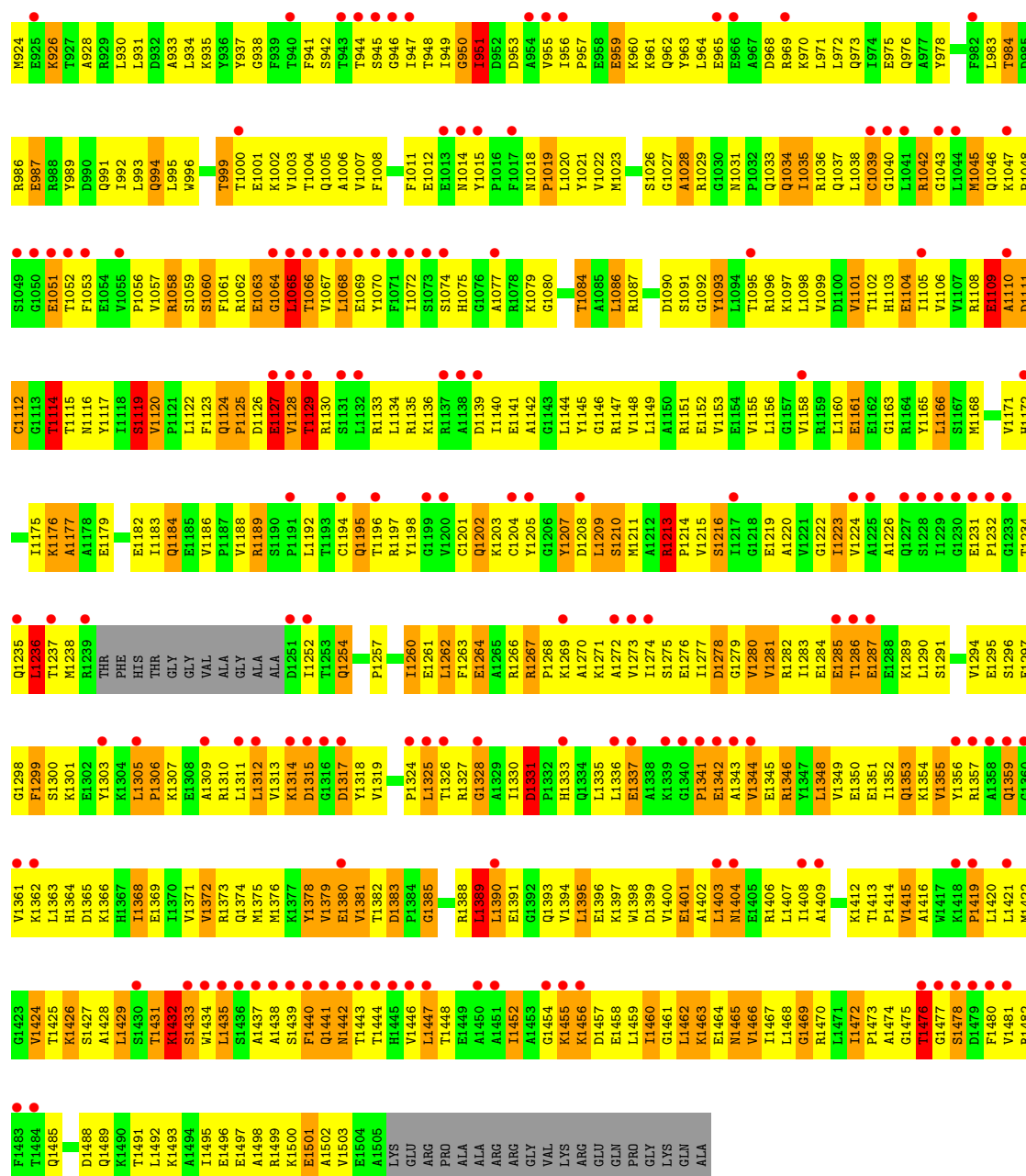
● Molecule 3: DNA-directed RNA polymerase beta' chain







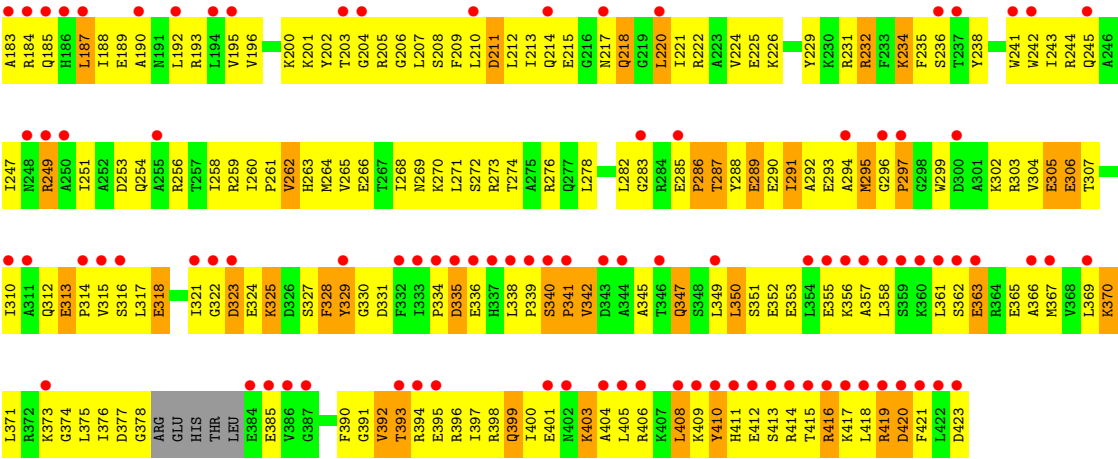




Chain 0:

Chain F:

Chain P:



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 25.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.40) 91.1 (25.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.268 0.229 , 0.263	Depositor DCC
R_{free} test set	33251 reflections (5.76%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-0.65 , 989.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	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	0.81	EDS
Total number of atoms	60908	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, STD, 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	0.89	3/1838 (0.2%)	1.19	11/2498 (0.4%)
1	B	0.79	1/1838 (0.1%)	1.10	9/2498 (0.4%)
1	K	0.79	1/1838 (0.1%)	1.12	10/2498 (0.4%)
1	L	0.76	3/1838 (0.2%)	1.06	9/2498 (0.4%)
2	C	0.90	10/8997 (0.1%)	1.30	86/12164 (0.7%)
2	M	0.89	5/8997 (0.1%)	1.29	85/12164 (0.7%)
3	D	0.91	11/10903 (0.1%)	1.33	108/14736 (0.7%)
3	N	0.91	16/10903 (0.1%)	1.34	116/14736 (0.8%)
4	E	0.87	0/783	1.39	12/1054 (1.1%)
4	O	0.90	1/783 (0.1%)	1.38	12/1054 (1.1%)
5	F	0.77	0/2812	1.20	13/3781 (0.3%)
5	P	0.80	2/2812 (0.1%)	1.20	14/3781 (0.4%)
All	All	0.88	53/54342 (0.1%)	1.28	485/73462 (0.7%)

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	191	PHE	CA-C	9.73	1.61	1.52
1	A	48	ILE	C-N	9.58	1.45	1.33
2	C	163	ILE	CA-CB	8.84	1.63	1.53
2	M	163	ILE	CA-CB	8.55	1.62	1.53
2	C	191	PHE	C-N	8.18	1.44	1.33

The worst 5 of 485 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	207	PHE	CA-C-N	17.11	141.22	119.84
3	D	207	PHE	C-N-CA	17.11	141.22	119.84
3	N	207	PHE	CA-C-N	16.96	141.04	119.84
3	N	207	PHE	C-N-CA	16.96	141.04	119.84
3	N	1124	GLN	CA-C-N	16.75	140.78	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	240	0
1	B	1806	0	1861	214	0
1	K	1806	0	1861	181	0
1	L	1806	0	1861	207	0
2	C	8829	0	8933	1233	0
2	M	8829	0	8933	1179	0
3	D	10728	0	10809	1475	0
3	N	10728	0	10809	1345	0
4	E	769	0	775	89	0
4	O	769	0	775	119	0
5	F	2771	0	2844	373	0
5	P	2771	0	2844	341	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	55	0
9	C	1144	0	0	276	0
9	D	1546	0	0	314	0
9	E	130	0	0	20	0
9	F	491	0	0	108	0
9	K	229	0	0	34	0
9	L	274	0	0	52	0
9	M	1072	0	0	227	0
9	N	1392	0	0	263	0
9	O	137	0	0	27	0
9	P	447	0	0	72	0
All	All	60908	0	54228	6581	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 6581 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%)	5	6
1	B	227/315 (72%)	200 (88%)	21 (9%)	6 (3%)	4	4
1	K	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	9	14
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	6	9
2	C	1117/1119 (100%)	924 (83%)	143 (13%)	50 (4%)	2	1
2	M	1117/1119 (100%)	920 (82%)	149 (13%)	48 (4%)	2	1
3	D	1375/1524 (90%)	1129 (82%)	186 (14%)	60 (4%)	2	1
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	1
4	O	93/99 (94%)	73 (78%)	16 (17%)	4 (4%)	2	1
5	F	341/423 (81%)	288 (84%)	42 (12%)	11 (3%)	3	3
5	P	341/423 (81%)	291 (85%)	37 (11%)	13 (4%)	2	2
All	All	6760/7590 (89%)	5632 (83%)	855 (13%)	273 (4%)	2	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%)	157 (78%)	45 (22%)	1	1
1	B	202/273 (74%)	160 (79%)	42 (21%)	1	1
1	K	202/273 (74%)	158 (78%)	44 (22%)	1	1
1	L	202/273 (74%)	159 (79%)	43 (21%)	1	1
2	C	941/941 (100%)	719 (76%)	222 (24%)	1	1
2	M	941/941 (100%)	711 (76%)	230 (24%)	1	1
3	D	1118/1279 (87%)	828 (74%)	290 (26%)	0	0
3	N	1118/1279 (87%)	842 (75%)	276 (25%)	1	1
4	E	83/87 (95%)	67 (81%)	16 (19%)	1	2
4	O	83/87 (95%)	66 (80%)	17 (20%)	1	1
5	F	295/370 (80%)	227 (77%)	68 (23%)	1	1
5	P	295/370 (80%)	239 (81%)	56 (19%)	1	2
All	All	5682/6446 (88%)	4333 (76%)	1349 (24%)	1	1

5 of 1349 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	668	LEU
3	N	847	ASP
2	M	829	GLN
2	M	663	ASN

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Mol	Chain	Res	Type
3	N	166	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 193 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	99	GLN
2	M	899	GLN
2	M	179	ASN
2	M	552	HIS
3	N	125	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 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	-	41,47,47	7.26	24 (58%)	50,73,73	2.86	12 (24%)
6	STD	D	8001	-	41,47,47	7.28	22 (53%)	50,73,73	2.77	13 (26%)

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	-	-	16/31/101/101	0/6/5/5
6	STD	D	8001	-	-	14/31/101/101	0/6/5/5

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	8001	STD	O5-C19	-28.88	1.18	1.43
6	N	8002	STD	O5-C19	-27.96	1.18	1.43
6	N	8002	STD	C23-C21	-14.85	1.21	1.53
6	D	8001	STD	C23-C21	-14.78	1.22	1.53
6	D	8001	STD	C18-C16	-13.71	1.25	1.53

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	8001	STD	C20-N1-C2	-10.34	103.15	113.06
6	N	8002	STD	C20-N1-C2	-10.16	103.32	113.06
6	N	8002	STD	C19-O5-C13	9.80	122.91	112.81
6	D	8001	STD	C19-O5-C13	8.23	121.29	112.81
6	D	8001	STD	O8-C17-C30	-7.27	105.06	111.68

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

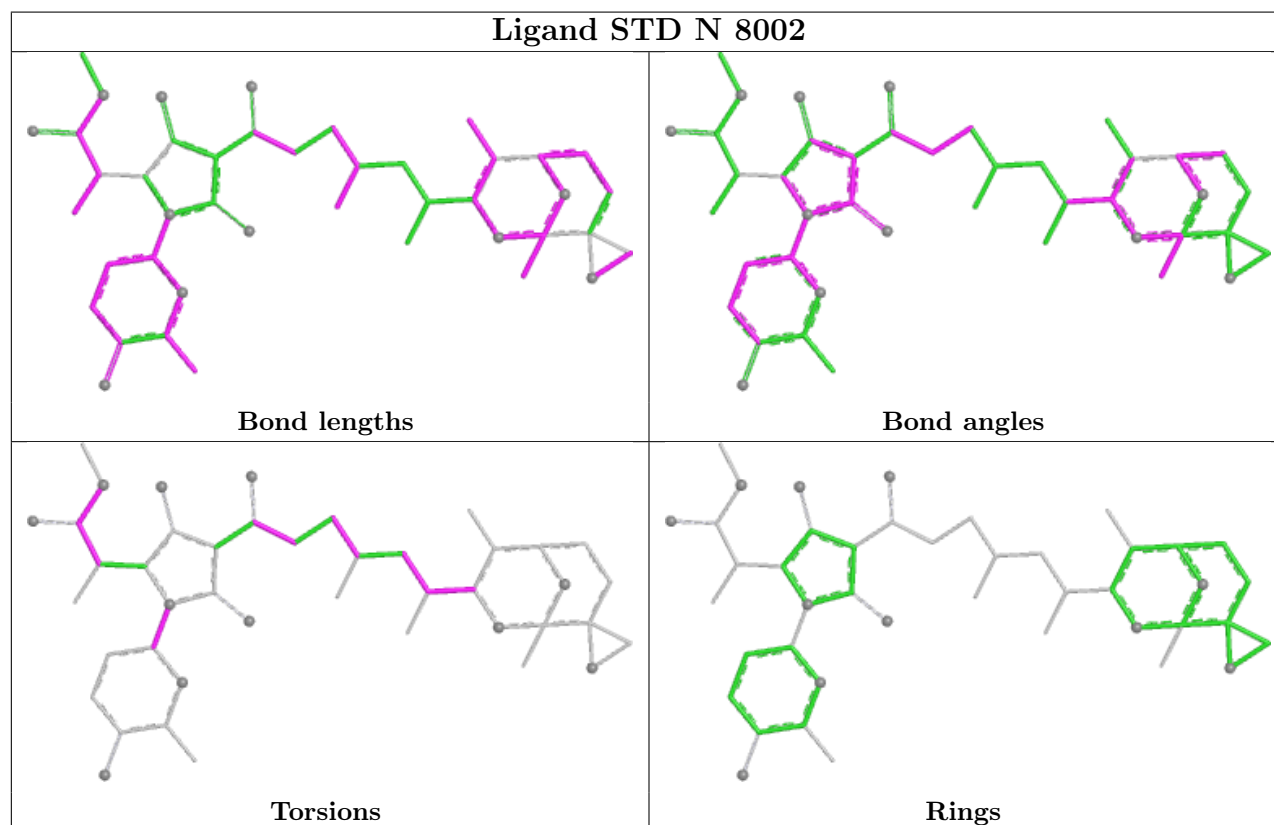
Mol	Chain	Res	Type	Atoms
6	D	8001	STD	O4-C4-N1-C20
6	D	8001	STD	C1-C5-C6-C7
6	D	8001	STD	O3-C5-C6-C7
6	D	8001	STD	C9-C10-C13-C16
6	D	8001	STD	C9-C10-C13-O5

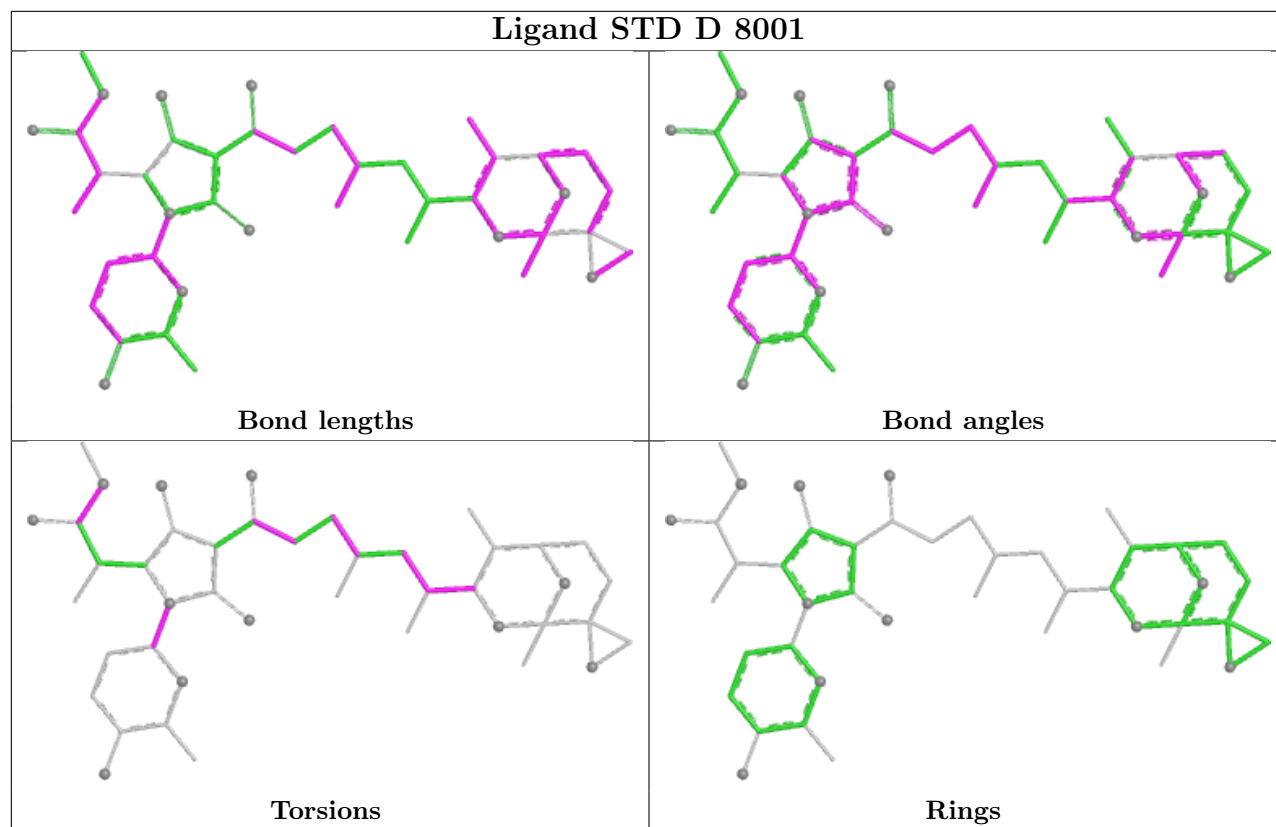
There are no ring outliers.

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, 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%)	1.99	66 (28%) 1 1	31, 63, 90, 117	0
1	B	229/315 (72%)	2.22	69 (30%) 1 1	53, 90, 112, 118	0
1	K	229/315 (72%)	1.49	61 (26%) 1 1	33, 62, 87, 122	0
1	L	229/315 (72%)	2.52	65 (28%) 1 1	50, 87, 110, 125	0
2	C	1119/1119 (100%)	2.64	472 (42%) 0 0	25, 78, 104, 116	0
2	M	1119/1119 (100%)	2.49	430 (38%) 1 0	23, 72, 104, 115	0
3	D	1381/1524 (90%)	1.65	337 (24%) 2 1	27, 67, 107, 119	0
3	N	1381/1524 (90%)	1.86	404 (29%) 1 1	27, 68, 108, 120	0
4	E	95/99 (95%)	1.91	32 (33%) 1 1	44, 81, 108, 128	0
4	O	95/99 (95%)	2.44	39 (41%) 0 0	44, 75, 93, 105	0
5	F	345/423 (81%)	2.59	147 (42%) 0 0	55, 84, 107, 122	0
5	P	345/423 (81%)	2.64	153 (44%) 0 0	62, 84, 108, 116	0
All	All	6796/7590 (89%)	2.16	2275 (33%) 1 1	23, 73, 106, 128	0

The worst 5 of 2275 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	153	ALA	26.9
2	C	153	ALA	25.3
1	L	119	ASP	24.0
1	L	91	ASN	23.2
1	L	90	LEU	22.8

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](#)

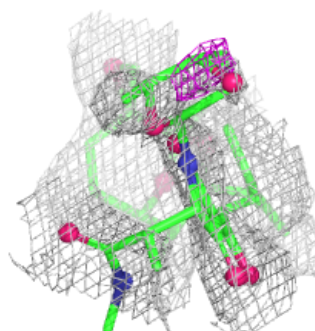
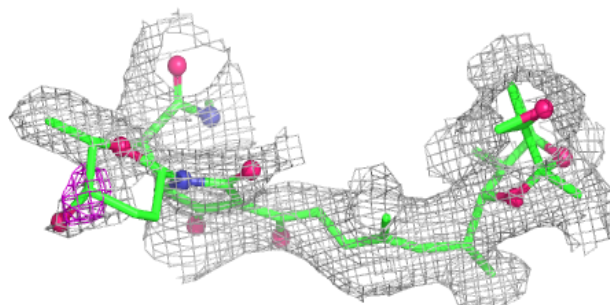
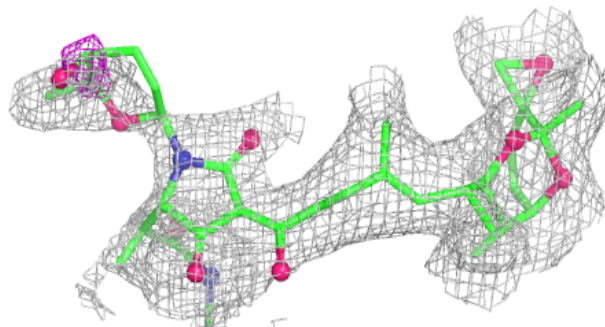
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	STD	N	8002	43/43	0.94	0.08	27,35,41,48	0
6	STD	D	8001	43/43	0.95	0.07	25,35,40,43	0
8	MG	N	9002	1/1	0.95	0.50	53,53,53,53	0
8	MG	D	9001	1/1	0.98	0.16	29,29,29,29	0
7	ZN	N	7459	1/1	0.99	0.04	64,64,64,64	0
7	ZN	N	7413	1/1	1.00	0.02	65,65,65,65	0
7	ZN	D	7412	1/1	1.00	0.03	58,58,58,58	0
7	ZN	D	7458	1/1	1.00	0.07	64,64,64,64	0

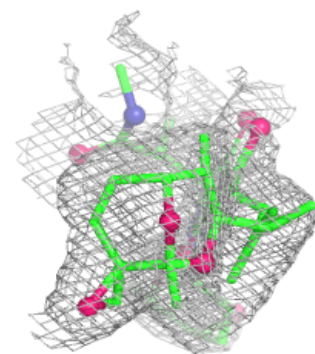
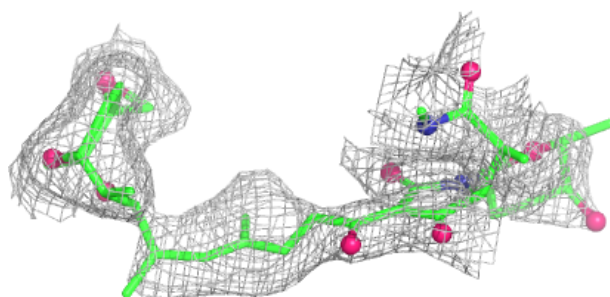
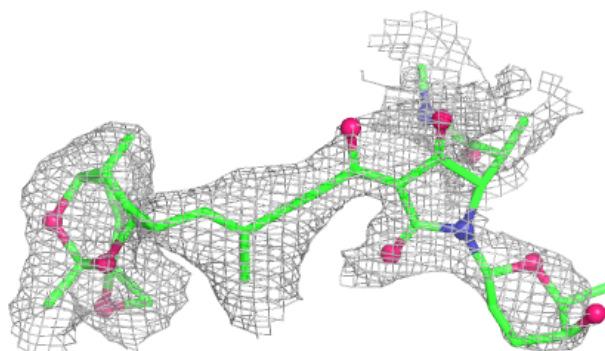
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

There are no such residues in this entry.