wwPDB X-ray Structure Validation Summary Report (i)

May 1, 2025 – 04:10 PM JST

PDB ID	:	9LNV / pdb_00009lnv
Title	:	Crystal structure of T2R-TTL-YQVB6 Complex
Authors	:	Wu, C.Y.; Wang, Y.X.; Chen, Q.F.
Deposited on	:	2025-01-22
Resolution	:	2.67 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 (i) 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 (i)) were used in the production of this report:

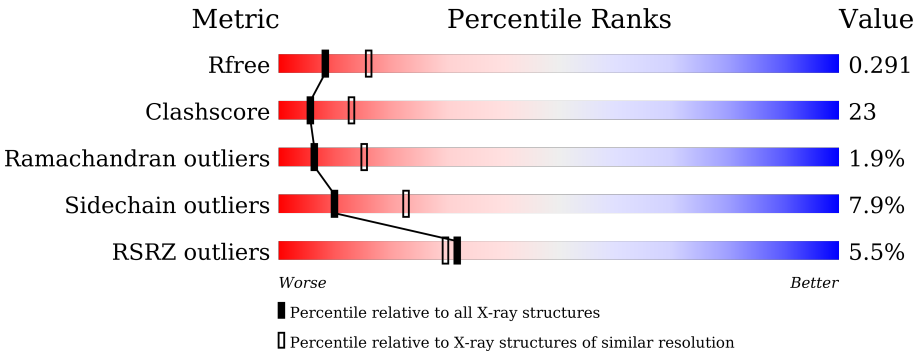
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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}	164625	4708 (2.70-2.66)
Clashscore	180529	5138 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

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 <=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	450	3% 56% 36% 6% •
1	C	450	2% 62% 34% • •
2	B	445	2% 61% 33% • •
2	D	445	9% 43% 45% 7% 5%
3	E	143	6% 48% 30% 5% • 16%
4	F	384	11% 45% 36% 6% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	A1EPR	C	504	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 17621 atoms, of which 58 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	5	9	0
			3465	2200	584	657	24			
1	C	440	Total	C	N	O	S	8	7	0
			3466	2197	584	662	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	424	Total	C	N	O	S	14	4	0
			3343	2102	567	646	28			
2	B	428	Total	C	N	O	S	6	2	0
			3370	2118	576	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			991	612	180	194	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

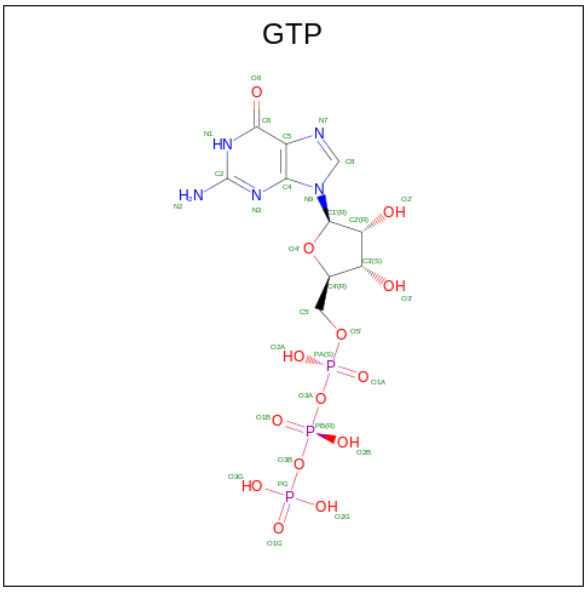
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	9	4	0
			2729	1762	457	496	14			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 32 10 5 14 3	32	0
5	C	1	Total C N O P 32 10 5 14 3	32	0

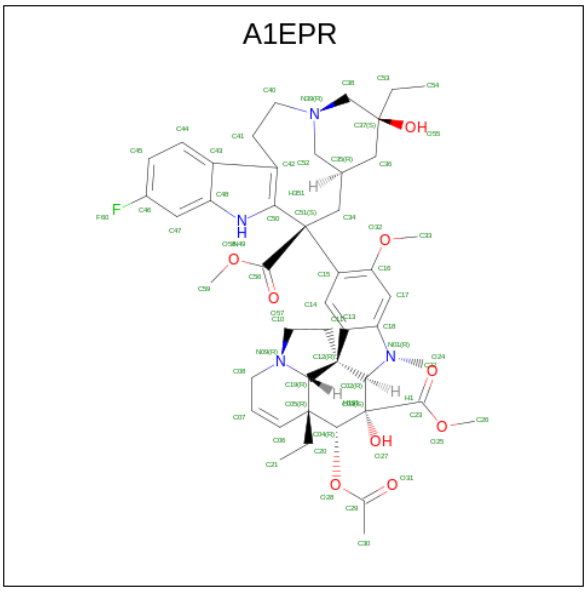
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	1	0
6	C	1	Total Mg 1 1	1	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

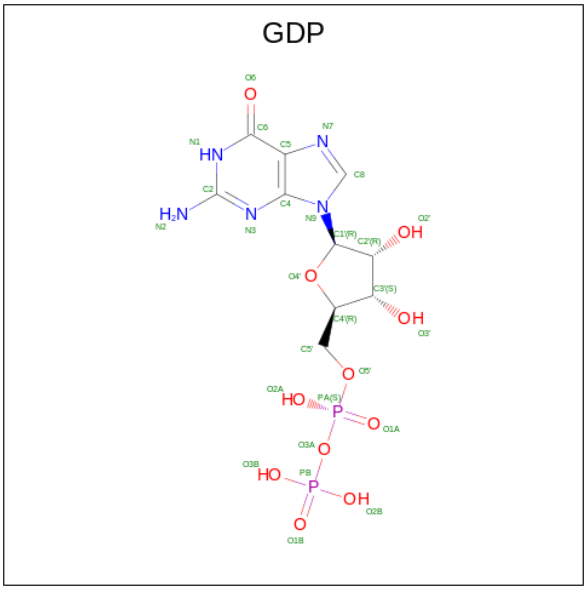
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	1	0
7	C	1	Total Ca 1 1	1	0

- Molecule 8 is 10'-fluorovinblastine (CCD ID: A1EPR) (formula: $C_{46}H_{57}FN_4O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	C	1	Total	C	F	H	N	O	0	0
			118	46	1	58	4	9		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	P	28	0
			28	10	5	11	2		
9	B	1	Total	C	N	O	P	28	0
			28	10	5	11	2		

- Molecule 10 is water.

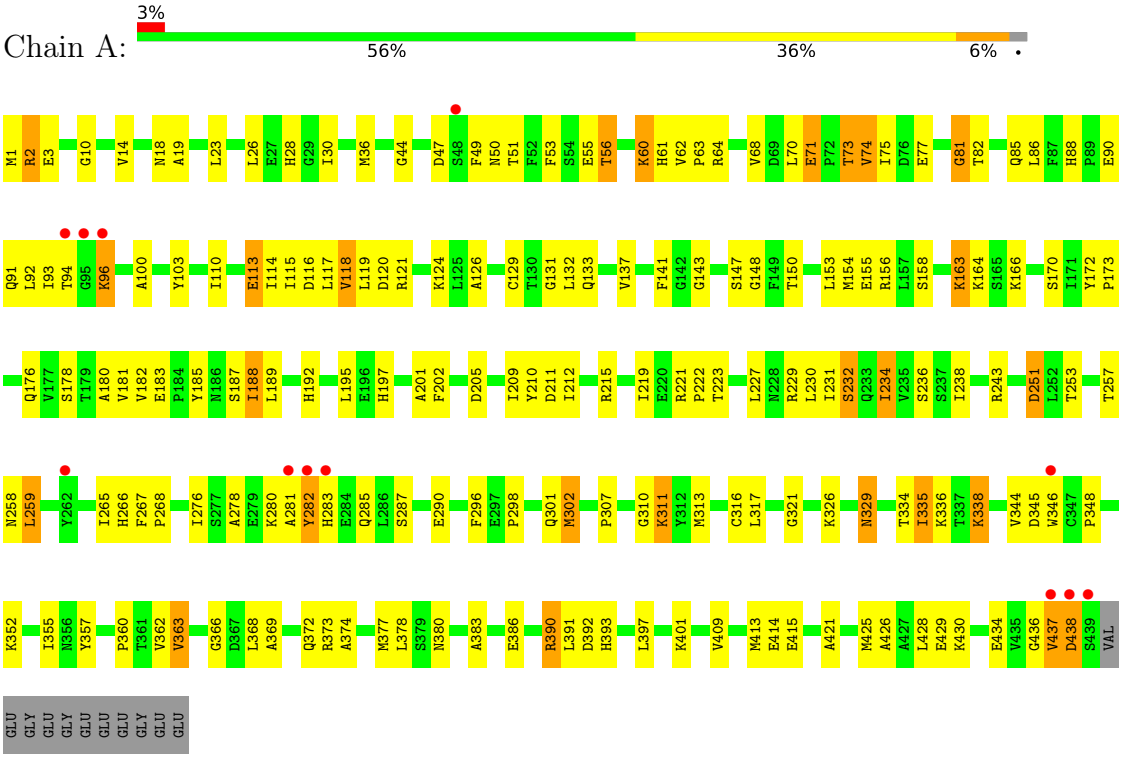
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	6	Total O 6 6	0	0
10	B	9	Total O 9 9	0	0

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.

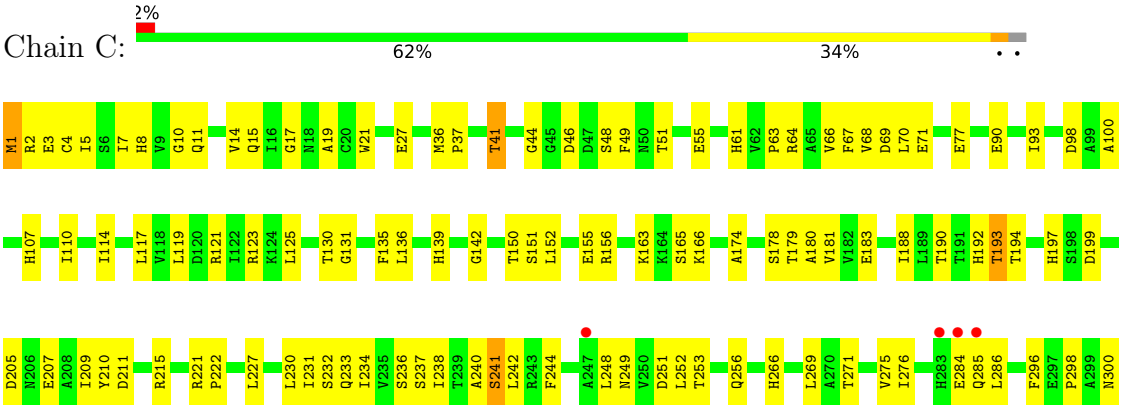
• Molecule 1: Detyrosinated tubulin alpha-1B chain

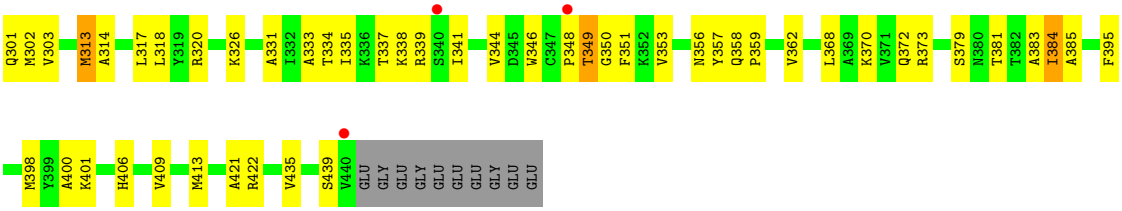
Chain A:



• Molecule 1: Detyrosinated tubulin alpha-1B chain

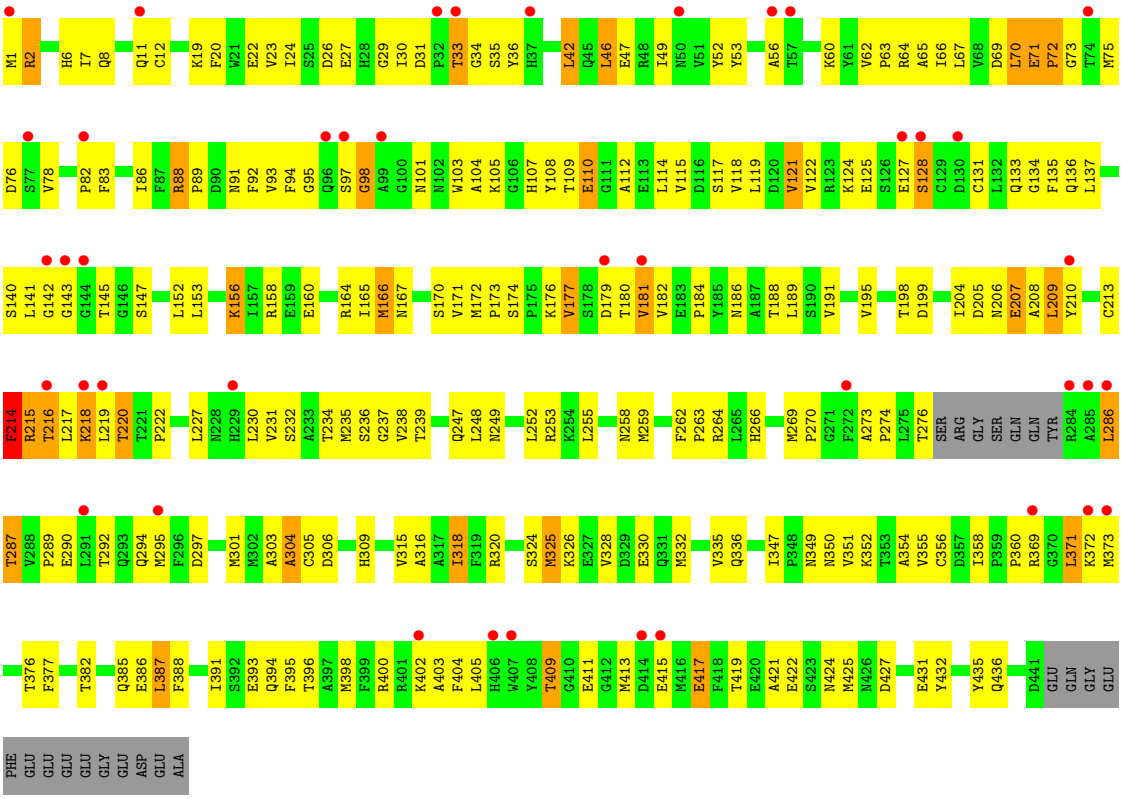
Chain C:





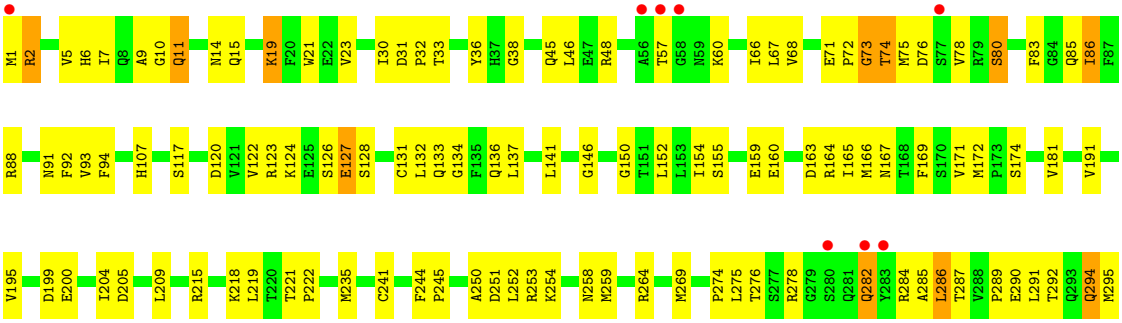
• Molecule 2: Tubulin beta chain

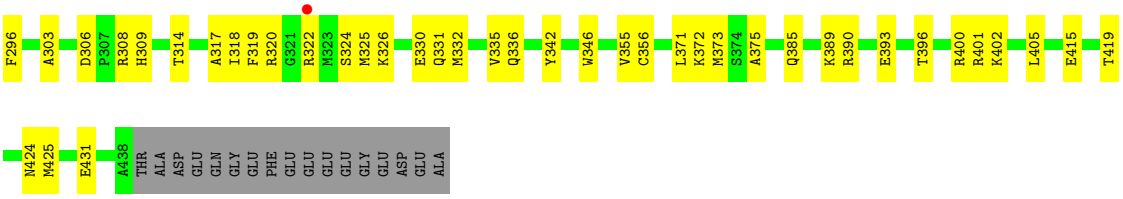
Chain D:



• Molecule 2: Tubulin beta chain

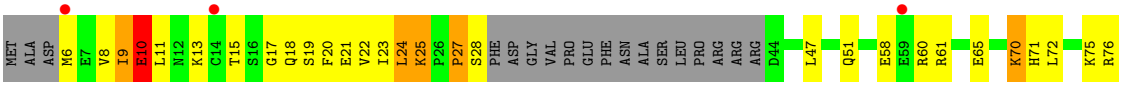
Chain B:

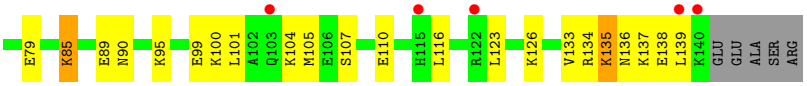




• Molecule 3: Stathmin-4

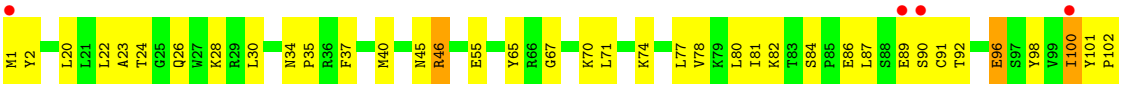
Chain E:

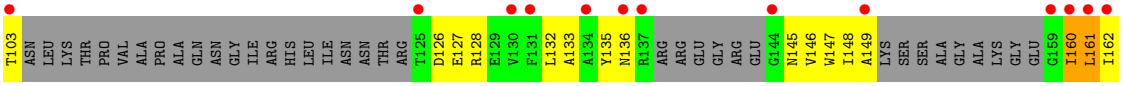


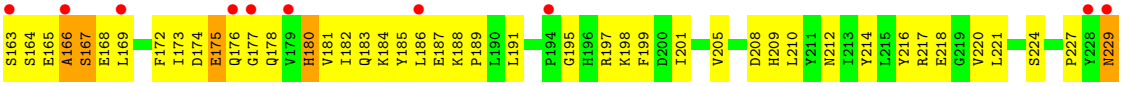


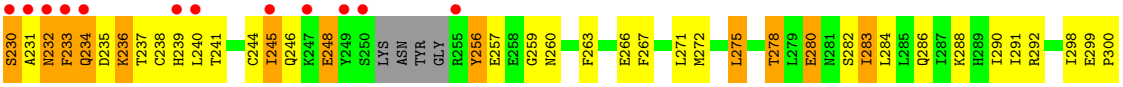
• Molecule 4: Tubulin tyrosine ligase

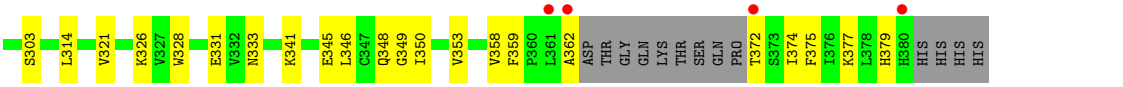
Chain F:











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.21Å 156.47Å 184.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.42 – 2.67 91.42 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (91.42-2.67) 99.7 (91.42-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.65Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.218 , 0.288 0.223 , 0.291	Depositor DCC
R_{free} test set	4488 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17621	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A1EPR, GTP, CA, MG, GDP

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	0.36	0/3571	0.55	0/4849
1	C	0.40	0/3565	0.58	0/4842
2	B	0.40	0/3451	0.58	0/4675
2	D	0.31	0/3428	0.50	0/4645
3	E	0.37	0/999	0.54	0/1325
4	F	0.30	0/2802	0.47	0/3789
All	All	0.36	0/17816	0.54	0/24125

There are no bond length outliers.

There are no bond angle outliers.

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	3465	0	3402	156	0
1	C	3466	0	3393	144	0
2	B	3370	0	3250	126	0
2	D	3343	0	3230	218	0
3	E	991	0	1012	42	0
4	F	2729	0	2715	131	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	C	60	58	0	3	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	9	0	0	2	0
10	C	6	0	0	5	0
All	All	17563	58	17050	788	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 23.

The worst 5 of 788 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:B:154:ILE:HG12	2:B:166:MET:HE2	1.30	1.12
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.12	1.09
2:D:360:PRO:HG2	2:D:371:LEU:HD12	1.35	1.07
2:D:135:PHE:HB2	2:D:166:MET:CE	1.92	0.99
2:D:166:MET:HE3	2:D:166:MET:HA	1.41	0.99

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	446/450 (99%)	403 (90%)	37 (8%)	6 (1%)	10 23
1	C	445/450 (99%)	422 (95%)	20 (4%)	3 (1%)	19 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	428/445 (96%)	401 (94%)	23 (5%)	4 (1%)	14 32
2	D	424/445 (95%)	368 (87%)	44 (10%)	12 (3%)	4 9
3	E	116/143 (81%)	106 (91%)	6 (5%)	4 (3%)	3 6
4	F	323/384 (84%)	284 (88%)	28 (9%)	11 (3%)	3 6
All	All	2182/2317 (94%)	1984 (91%)	158 (7%)	40 (2%)	6 16

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	A	438	ASP
1	C	349	THR
2	D	215	ARG
2	D	216	THR

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	378/378 (100%)	337 (89%)	41 (11%)	5 11
1	C	378/378 (100%)	360 (95%)	18 (5%)	21 44
2	B	369/383 (96%)	351 (95%)	18 (5%)	21 44
2	D	369/383 (96%)	337 (91%)	32 (9%)	8 18
3	E	108/127 (85%)	94 (87%)	14 (13%)	3 7
4	F	303/342 (89%)	276 (91%)	27 (9%)	8 17
All	All	1905/1991 (96%)	1755 (92%)	150 (8%)	10 23

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	180	HIS
2	B	282	GLN

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Mol	Chain	Res	Type
4	F	232	ASN
4	F	345	GLU
1	C	237	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	339	ASN
2	D	349	ASN
2	B	339	ASN
2	B	229	HIS
2	B	247	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
9	GDP	B	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	A1EPR	C	504	-	64,68,68	5.09	30 (46%)	81,110,110	2.59	28 (34%)
9	GDP	D	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.56	7 (21%)
5	GTP	A	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.63	7 (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
9	GDP	B	501	-	-	0/12/32/32	0/3/3/3
8	A1EPR	C	504	-	1/1/17/17	8/38/131/131	0/7/9/9
9	GDP	D	501	-	-	0/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	504	A1EPR	C06-C07	12.68	1.56	1.32
8	C	504	A1EPR	C18-C13	12.20	1.54	1.39
8	C	504	A1EPR	C14-C13	11.44	1.56	1.39
8	C	504	A1EPR	C14-C15	10.54	1.55	1.39
8	C	504	A1EPR	C16-C15	10.06	1.57	1.39

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	504	A1EPR	C11-C12-C13	-10.00	94.12	112.35
8	C	504	A1EPR	C11-C12-C02	7.34	126.17	112.34
8	C	504	A1EPR	O28-C29-C30	6.49	123.03	111.09
8	C	504	A1EPR	C14-C13-C18	-5.67	115.55	120.31
8	C	504	A1EPR	C12-C19-C05	-5.13	114.40	118.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	504	A1EPR	N39

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A

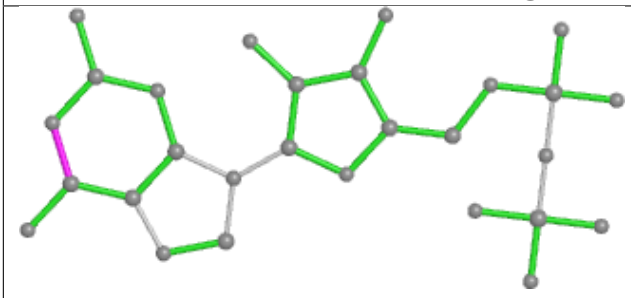
There are no ring outliers.

1 monomer is involved in 3 short contacts:

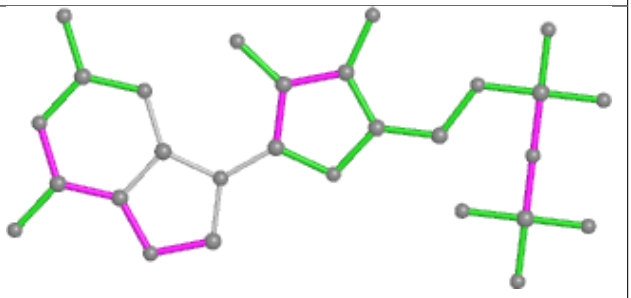
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	504	A1EPR	3	0

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 then 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.

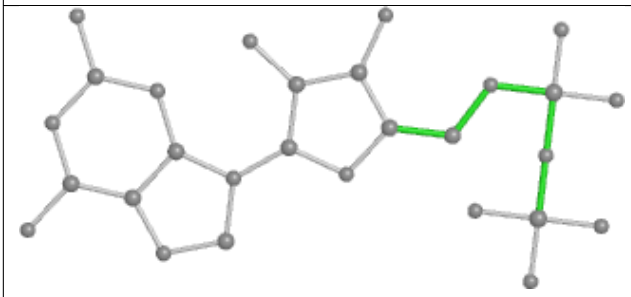
Ligand GDP B 501



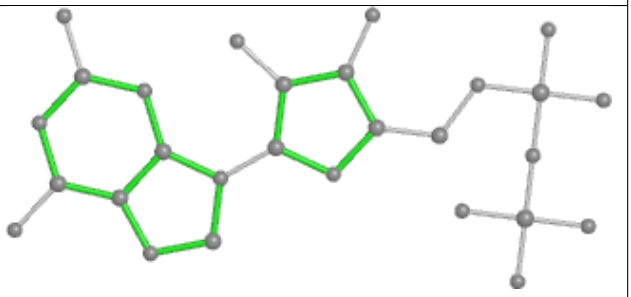
Bond lengths



Bond angles

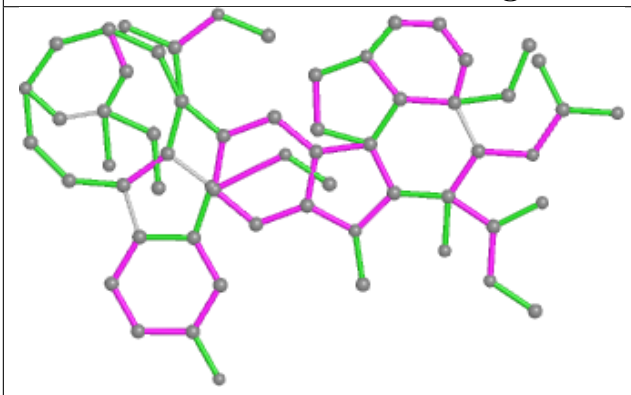


Torsions

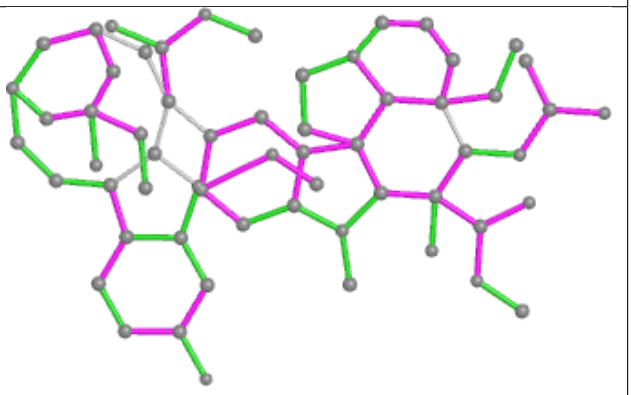


Rings

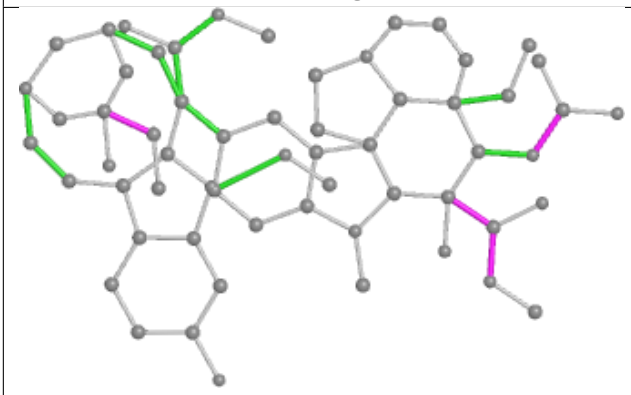
Ligand A1EPR C 504



Bond lengths



Bond angles



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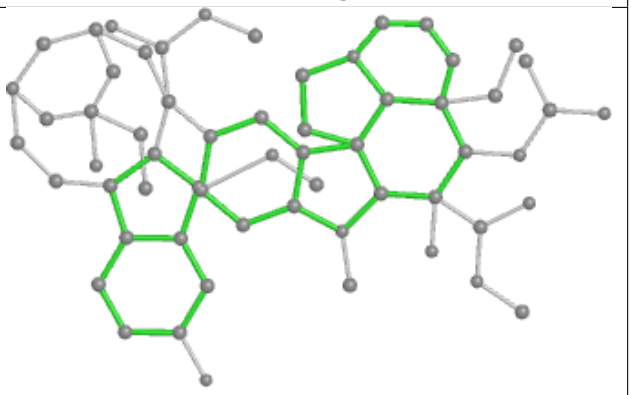
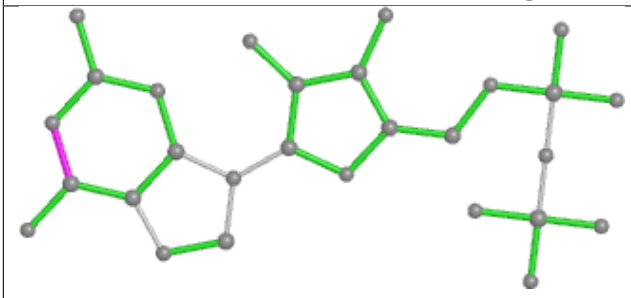
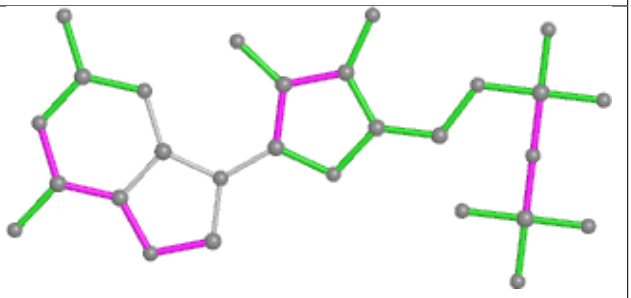


Rings

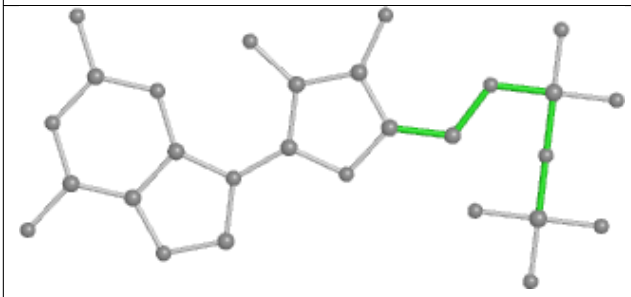
Ligand GDP D 501



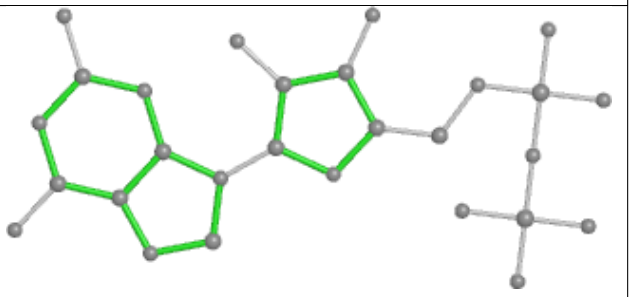
Bond lengths



Bond angles

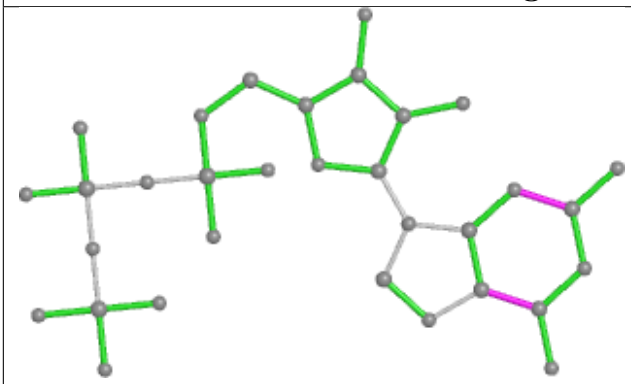


Torsions

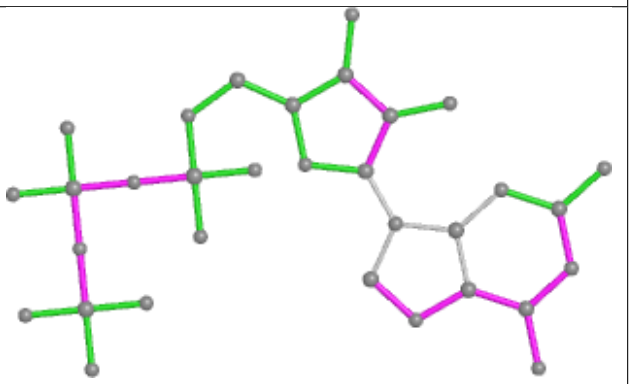


Rings

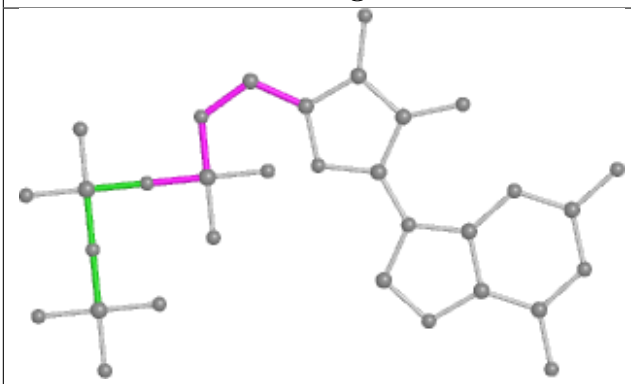
Ligand GTP C 501



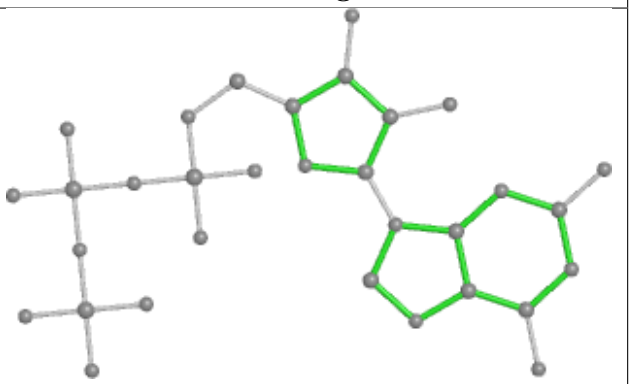
Bond lengths



Bond angles

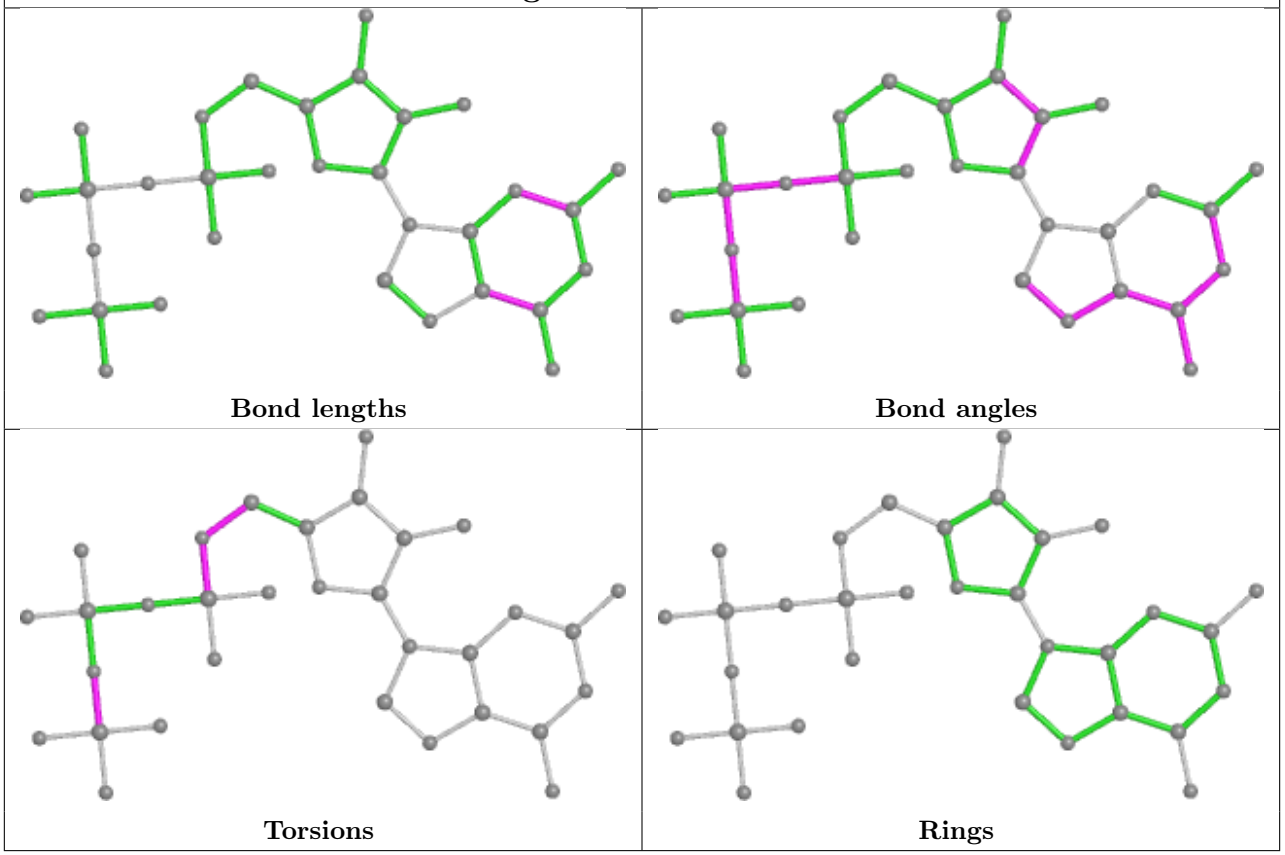


Torsions



Rings

Ligand GTP A 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	439/450 (97%)	-0.07	12 (2%) 56 55	20, 41, 68, 116	9 (2%)
1	C	440/450 (97%)	-0.27	7 (1%) 70 70	16, 35, 56, 72	7 (1%)
2	B	428/445 (96%)	-0.31	9 (2%) 63 62	20, 34, 65, 105	5 (1%)
2	D	424/445 (95%)	0.65	41 (9%) 15 14	28, 58, 90, 124	6 (1%)
3	E	120/143 (83%)	0.54	8 (6%) 25 23	28, 55, 82, 93	0
4	F	331/384 (86%)	0.63	43 (12%) 9 8	29, 59, 110, 128	4 (1%)
All	All	2182/2317 (94%)	0.12	120 (5%) 32 30	16, 45, 87, 128	31 (1%)

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	6.6
2	D	1	MET	5.6
4	F	231	ALA	5.5
2	B	1	MET	5.4
4	F	234	GLN	5.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.