wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2024 – 09:44 PM EST

PDB ID	:	5S63
Title	:	Tubulin-Z2241115980-complex
Authors	:	Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on	:	2020-11-08
Resolution	:	2.60 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:

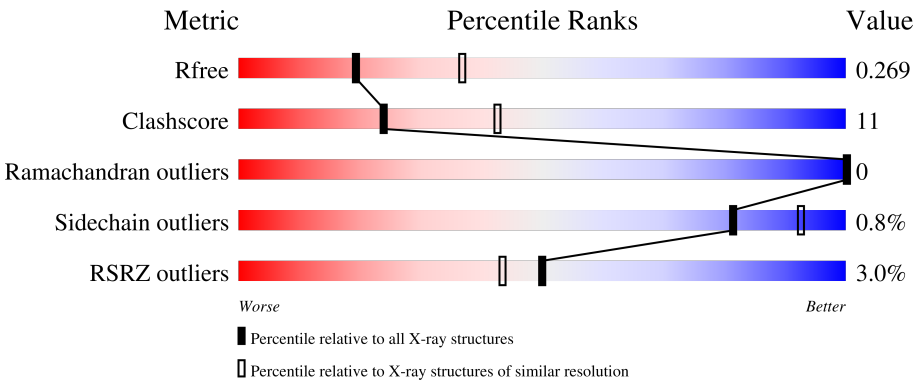
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	451	.% 72% 25% •
1	C	451	2% 79% 18% •
2	B	445	2% 69% 26% •
2	D	445	5% 69% 27% •
3	E	143	8% 72% 14% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	3% 67% 24% 9%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17882 atoms, of which 16 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3424	2167	582	653	22	0	0	0
1	C	440	3443	2178	585	657	23	0	1	0

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	425	3359	2109	577	646	27	13	1	0
2	D	427	3348	2101	571	649	27	5	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	1014	625	183	201	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

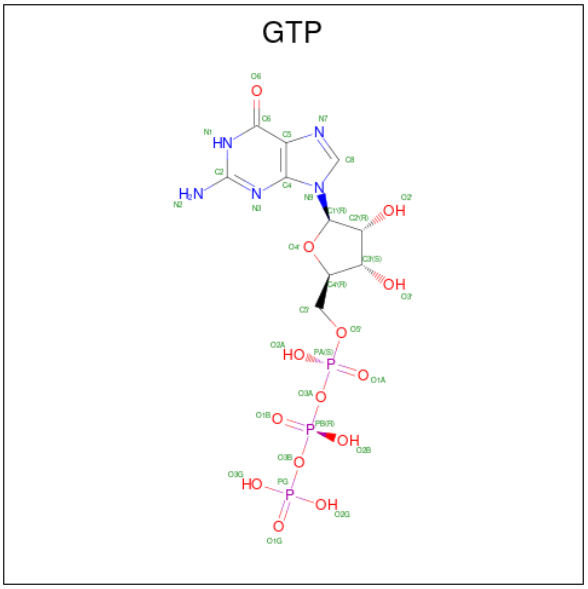
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	349	2863	1835	492	522	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

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

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

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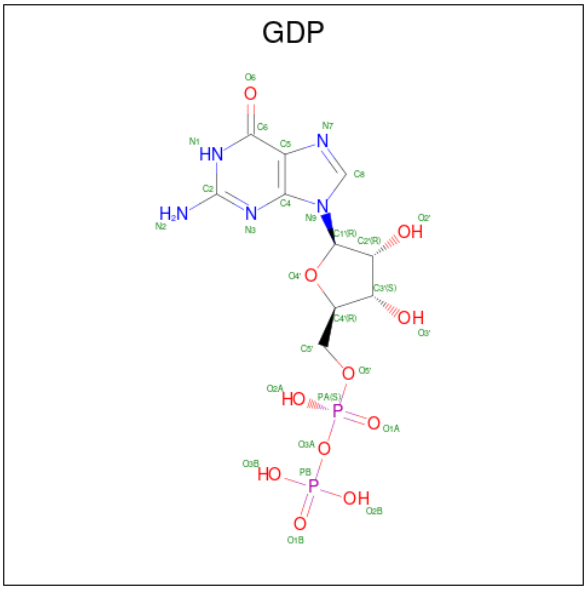
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	F	1	1	1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

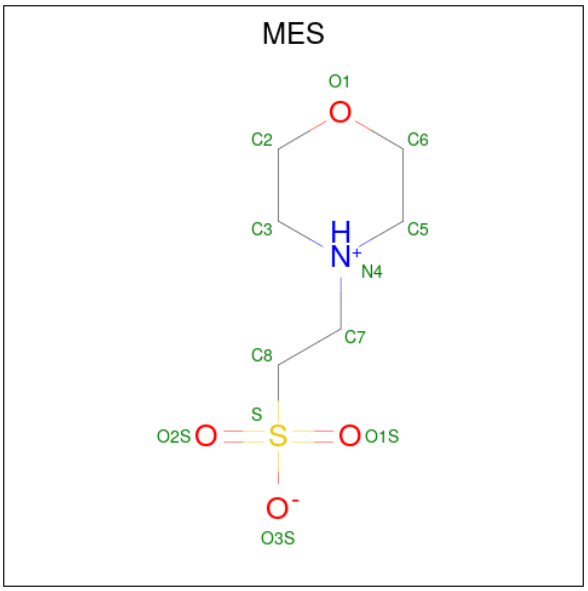
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	B	1	1	1	0	0
			Total	Ca		
7	C	1	1	1	0	0
			Total	Ca		
7	E	1	1	1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



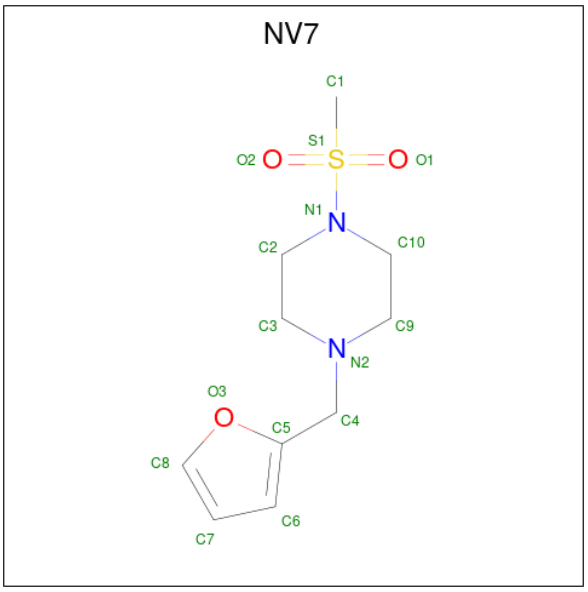
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
8	D	1	28	10	5	11	2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



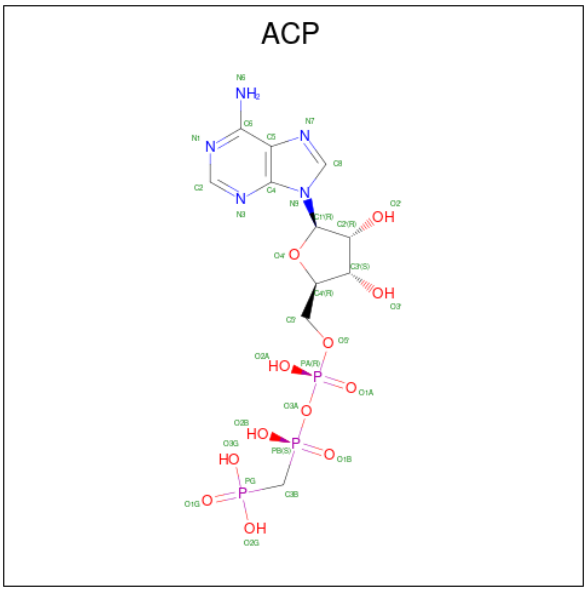
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is 1-[(furan-2-yl)methyl]-4-(methylsulfonyl)piperazine (three-letter code: NV7) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
10	C	1	32	10	16	2	3	1	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	F	1	31	11	5	12	3	0	0

- Molecule 12 is water.

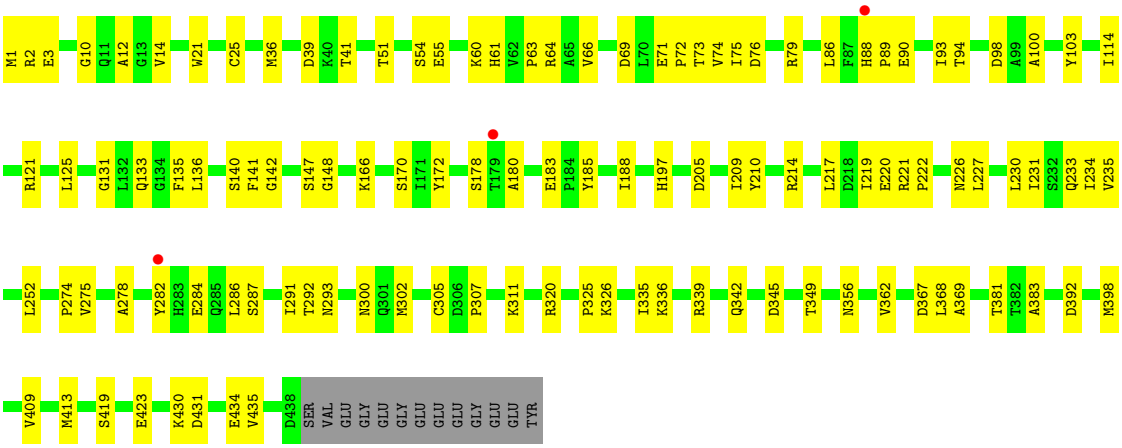
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	35	35	35	0	0
12	B	39	39	39	0	0
12	C	124	124	124	0	0
12	D	17	17	17	0	0
12	E	6	6	6	0	0
12	F	6	6	6	0	0

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.

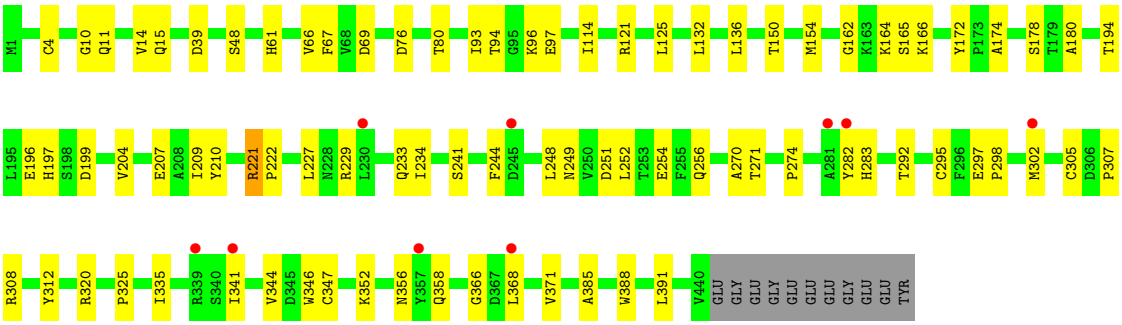
• Molecule 1: Tubulin alpha-1B chain

Chain A:



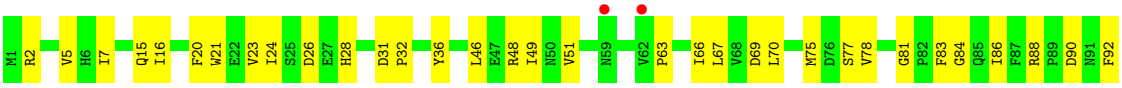
• Molecule 1: Tubulin alpha-1B chain

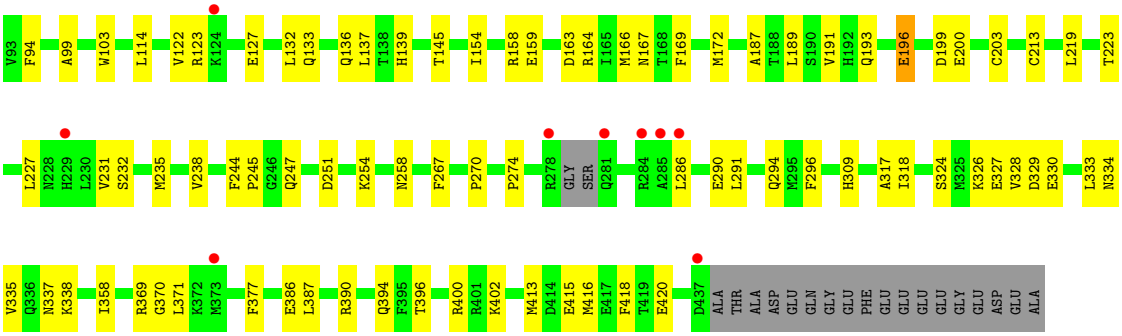
Chain C:



• Molecule 2: Tubulin beta-2B chain

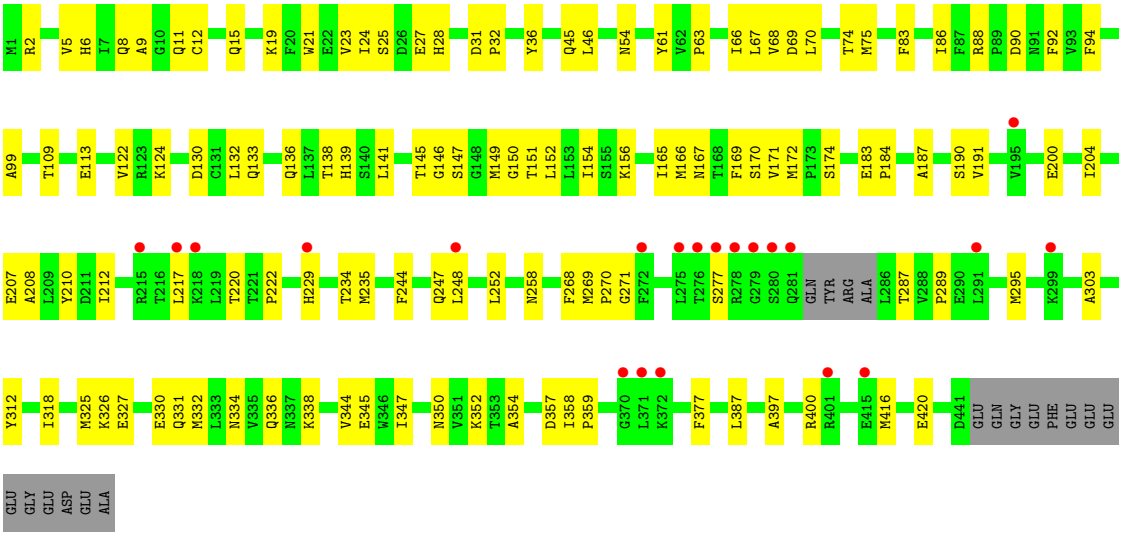
Chain B:





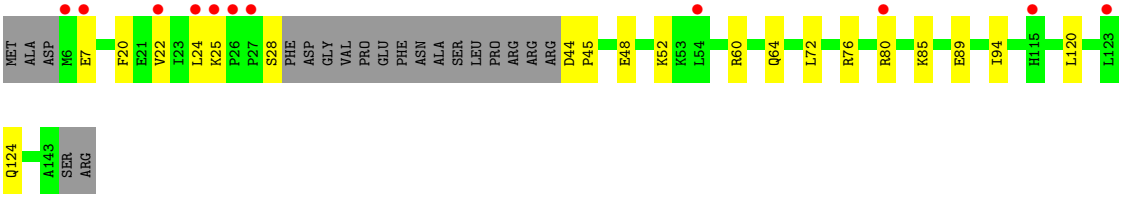
- Molecule 2: Tubulin beta-2B chain

Chain D:



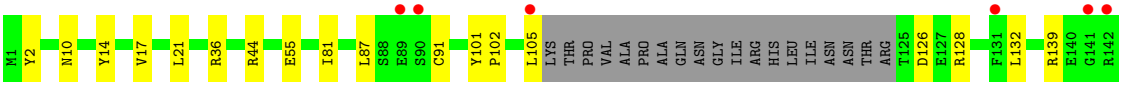
- Molecule 3: Stathmin-4

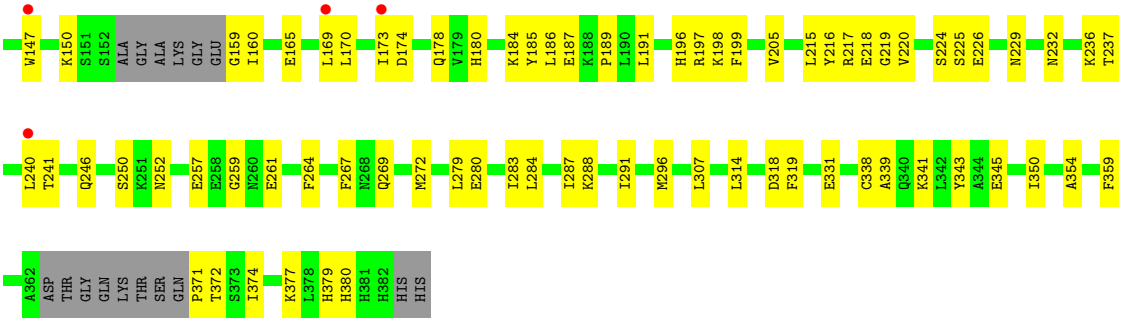
Chain E:



- Molecule 4: Tubulin-Tyrosine Ligase

Chain F:




W147
K150
S151
S152
ALA
GLY
ALA
LYS
GLY
GLU
G159
I160
E165
L169
L170
I173
D174
Q178
V179
H180
K184
Y185
L186
E187
K188
P189
L190
L191
H196
R197
K198
F199
V205
L215
Y216
R217
E218
G219
V220
S224
S225
E226
N229
N232
K236
T237
L240
T241
Q246
S250
K251
N252
E257
E258
G259
N260
E261
F264
F267
N268
Q269
M272
L279
E280
I283
L284
I287
K288
I291
M296
L307
L314
D318
F319
E331
C338
A339
Q340
K341
L342
Y343
A344
E345
I350
A354
F359
A362
ASP
THR
GLY
GLN
LYS
THR
SER
GLN
P371
T372
S373
I374
K377
L378
H379
H380
H381
H382
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.22Å 159.10Å 179.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.78 – 2.60 119.11 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (62.78-2.60) 98.3 (119.11-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.213 , 0.268 0.215 , 0.269	Depositor DCC
R_{free} test set	4496 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	65.5	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17882	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NV7, GTP, MG, MES, CA, ACP, 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	0.26	0/3502	0.41	0/4754
1	C	0.26	0/3521	0.43	0/4780
2	B	0.26	0/3433	0.42	0/4647
2	D	0.25	0/3421	0.41	0/4633
3	E	0.24	0/1022	0.34	0/1356
4	F	0.24	0/2930	0.40	0/3959
All	All	0.25	0/17829	0.41	0/24129

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 (i)

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	3424	0	3335	84	0
1	C	3443	0	3352	63	1
2	B	3359	0	3235	82	0
2	D	3348	0	3224	85	0
3	E	1014	0	1029	17	1
4	F	2863	0	2826	69	0
5	A	32	0	12	1	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	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	4	0
9	B	12	0	12	4	0
10	C	16	16	0	1	0
11	F	31	0	14	4	0
12	A	35	0	0	4	0
12	B	39	0	0	1	0
12	C	124	0	0	4	0
12	D	17	0	0	0	0
12	E	6	0	0	1	0
12	F	6	0	0	1	0
All	All	17866	16	17075	386	1

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 11.

The worst 5 of 386 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:D:217:LEU:HA	2:D:277:SER:HB3	1.43	1.00
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.57	0.86
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.58	0.84
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.60	0.83
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.63	0.81

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:GLY:O	3:E:80:ARG:NH1[4_455]	2.14	0.06

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	436/451 (97%)	419 (96%)	17 (4%)	0	100	100
1	C	439/451 (97%)	429 (98%)	10 (2%)	0	100	100
2	B	422/445 (95%)	409 (97%)	13 (3%)	0	100	100
2	D	423/445 (95%)	408 (96%)	15 (4%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	341/384 (89%)	321 (94%)	20 (6%)	0	100	100
All	All	2180/2319 (94%)	2104 (96%)	76 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	369/379 (97%)	365 (99%)	4 (1%)	73	88
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	88
2	B	368/383 (96%)	364 (99%)	4 (1%)	73	88
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	92
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1902/1993 (95%)	1887 (99%)	15 (1%)	81	92

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	291	LEU
2	D	229	HIS
1	C	48	SER
2	D	247	GLN
1	C	347	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	229	ASN
4	F	333	ASN
2	B	294	GLN
1	C	11	GLN
1	C	85	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
5	GTP	C	602	6	26,34,34	1.11	2 (7%)	32,54,54	1.37	5 (15%)
11	ACP	F	401	6	27,33,33	1.39	5 (18%)	32,52,52	1.50	4 (12%)
8	GDP	B	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.12	3 (10%)
9	MES	B	504	-	12,12,12	2.26	1 (8%)	14,16,16	2.00	6 (42%)
8	GDP	D	501	6	24,30,30	0.95	1 (4%)	30,47,47	1.16	4 (13%)
10	NV7	C	601	-	14,17,17	1.12	2 (14%)	20,24,24	0.74	1 (5%)
5	GTP	A	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.45	5 (15%)

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
5	GTP	C	602	6	-	9/18/38/38	0/3/3/3
11	ACP	F	401	6	-	11/15/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
10	NV7	C	601	-	-	4/9/20/20	0/2/2/2
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.55	1.66	1.77
5	A	501	GTP	C5-C6	-3.81	1.39	1.47
5	C	602	GTP	C5-C6	-3.73	1.39	1.47
10	C	601	NV7	C6-C5	-3.37	1.35	1.39
11	F	401	ACP	PG-O2G	2.95	1.61	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	401	ACP	PB-O3A-PA	-4.38	118.67	132.56
9	B	504	MES	C5-N4-C3	3.74	117.25	108.83
11	F	401	ACP	C3'-C2'-C1'	3.47	106.21	100.98
5	A	501	GTP	PA-O3A-PB	-3.42	121.08	132.83
5	C	602	GTP	PA-O3A-PB	-3.26	121.65	132.83

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	602	GTP	C5'-O5'-PA-O1A
5	C	602	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A

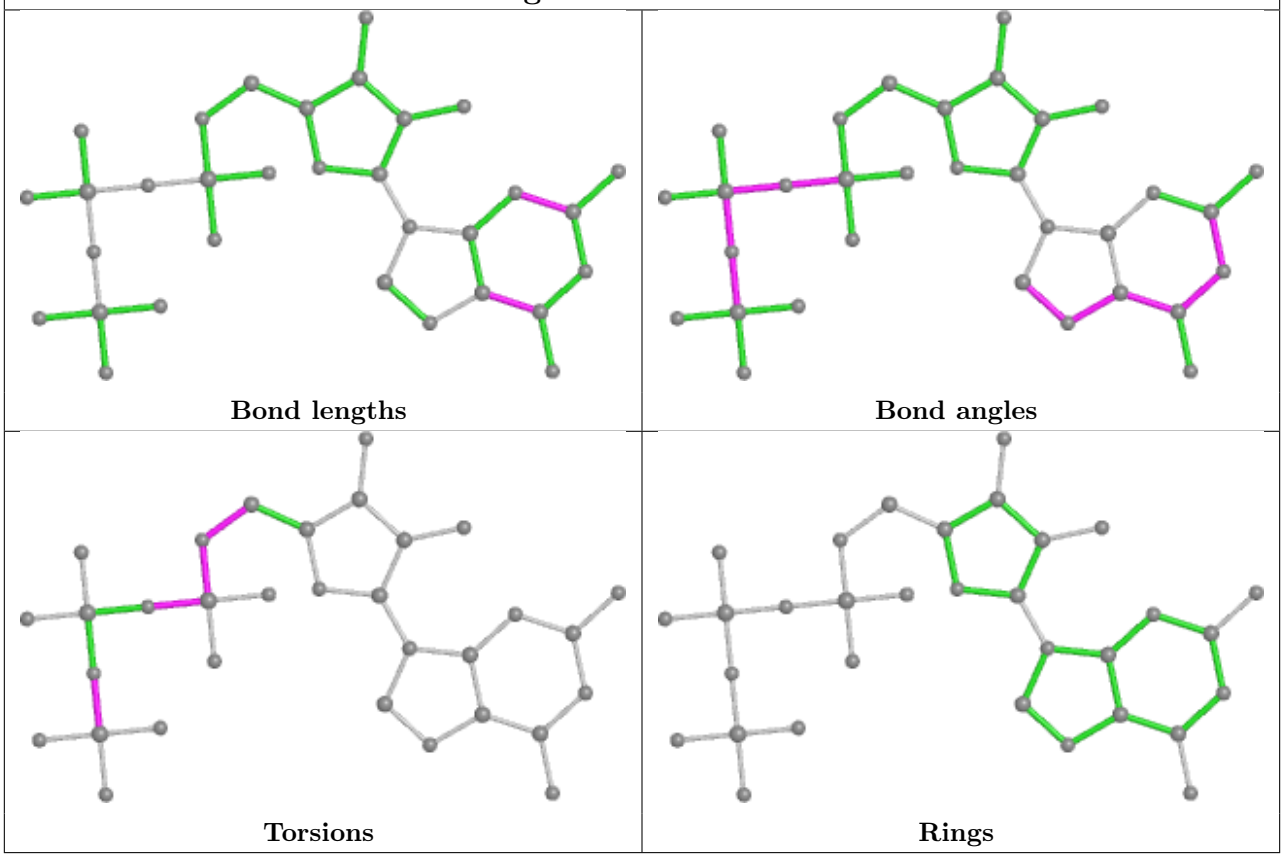
There are no ring outliers.

6 monomers are involved in 15 short contacts:

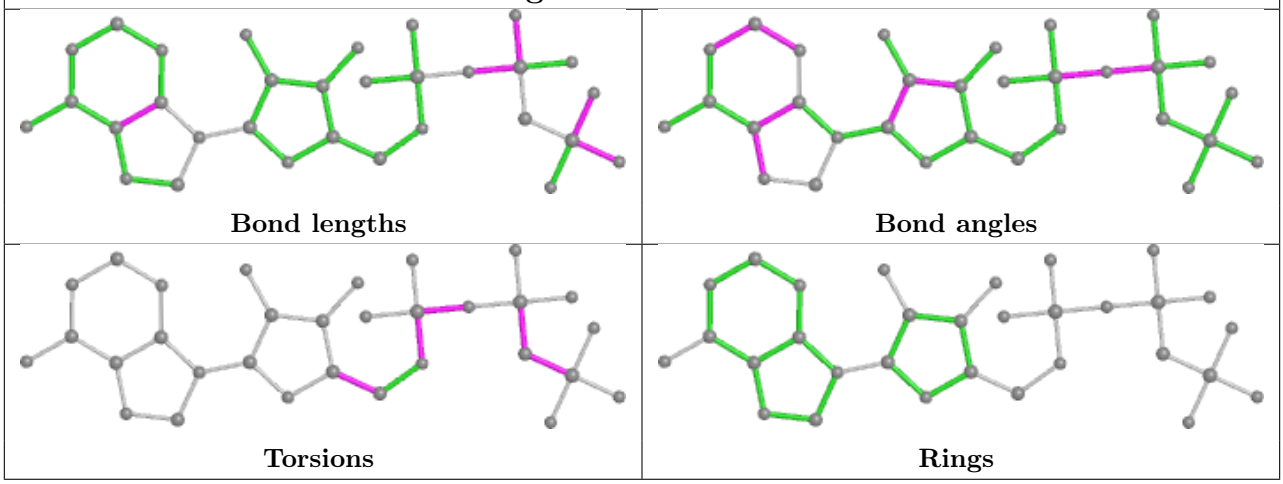
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	4	0
8	B	501	GDP	1	0
9	B	504	MES	4	0
8	D	501	GDP	4	0
10	C	601	NV7	1	0
5	A	501	GTP	1	0

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 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.

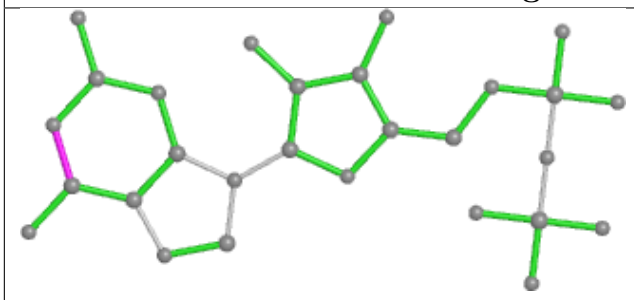
Ligand GTP C 602



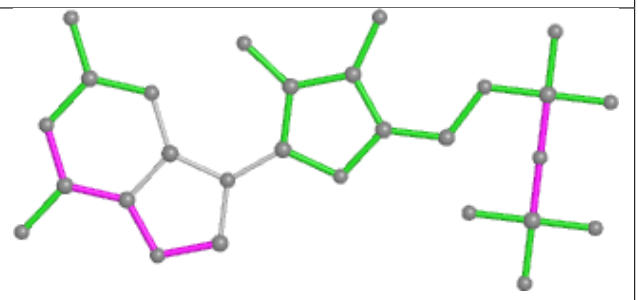
Ligand ACP F 401



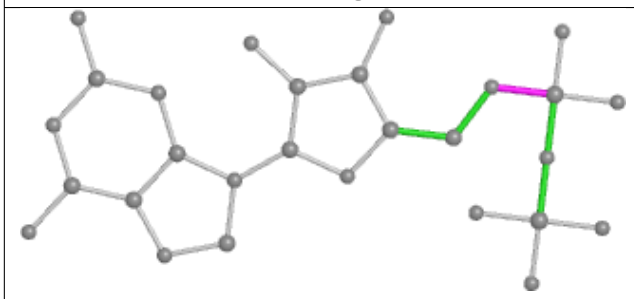
Ligand GDP B 501



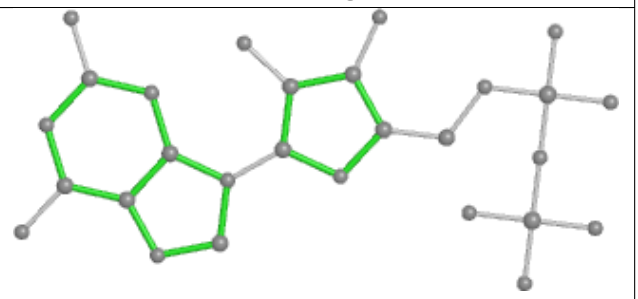
Bond lengths



Bond angles

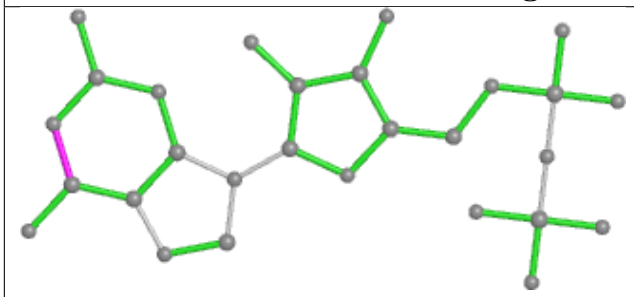


Torsions

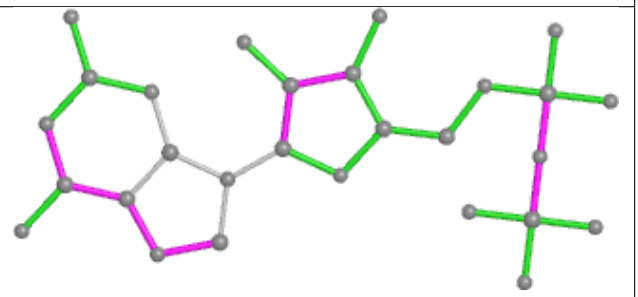


Rings

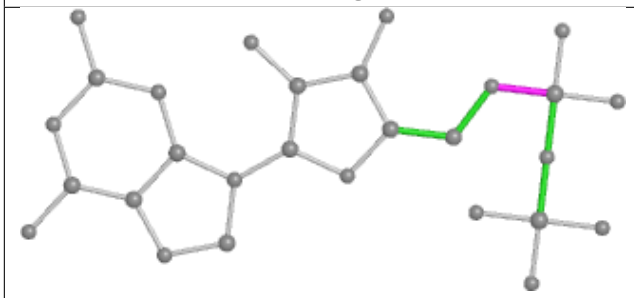
Ligand GDP D 501



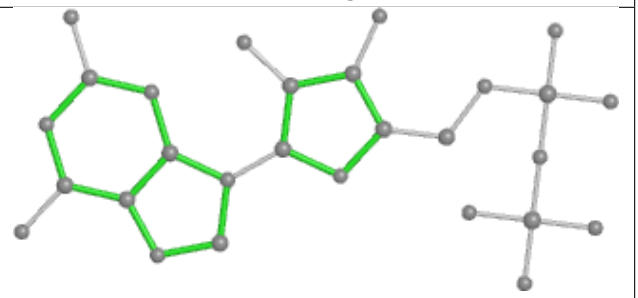
Bond lengths



Bond angles

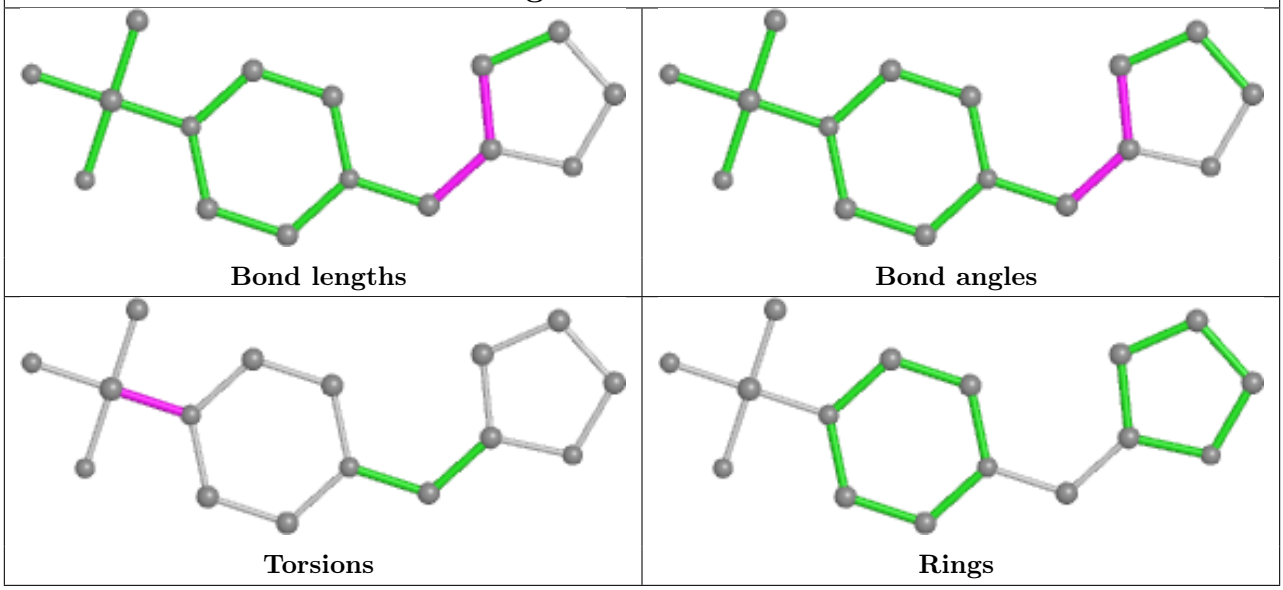


Torsions

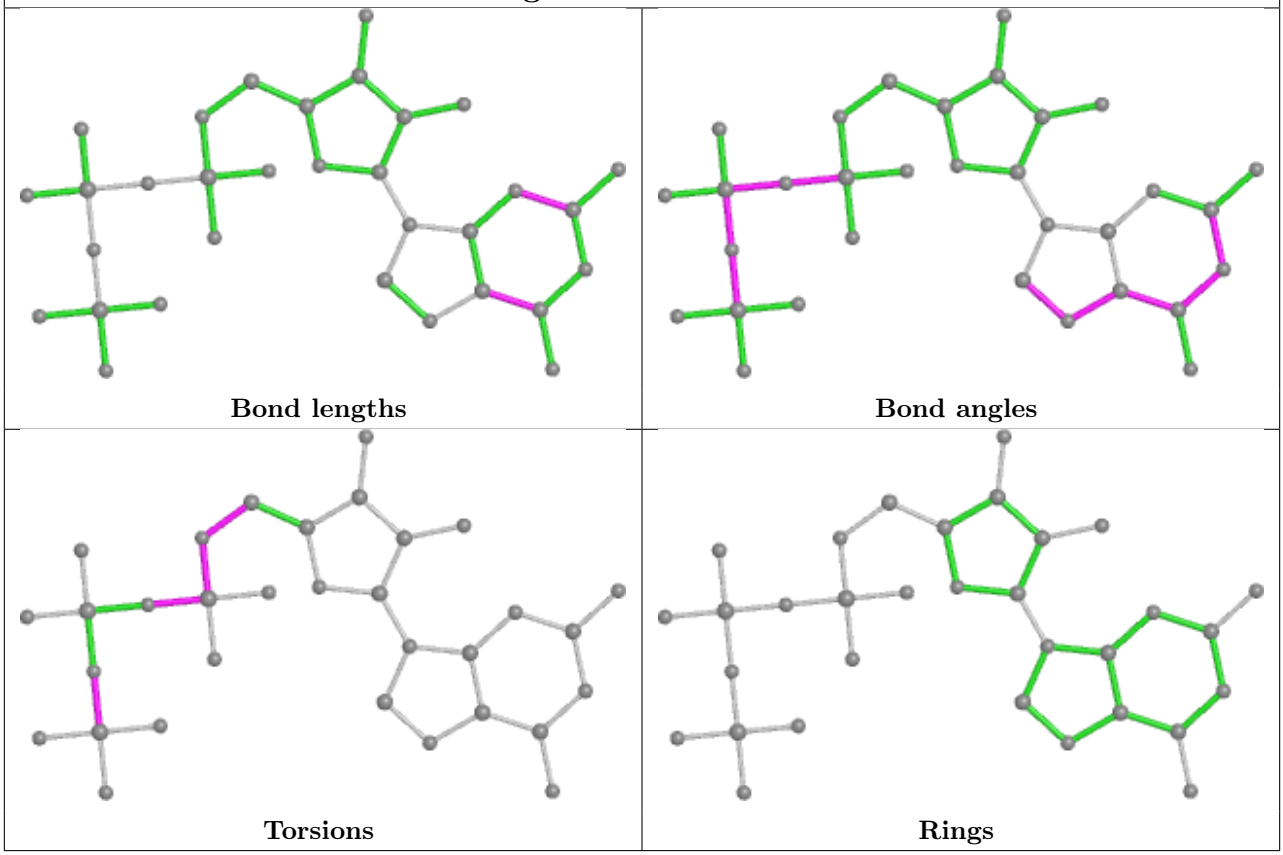


Rings

Ligand NV7 C 601



Ligand GTP A 501



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	438/451 (97%)	0.15	3 (0%)	87	86	55, 70, 106, 190	0
1	C	440/451 (97%)	0.17	9 (2%)	65	60	46, 59, 86, 125	0
2	B	425/445 (95%)	0.26	11 (2%)	56	50	47, 70, 112, 162	3 (0%)
2	D	427/445 (95%)	0.25	21 (4%)	29	23	55, 81, 116, 164	4 (0%)
3	E	123/143 (86%)	0.56	11 (8%)	9	6	64, 88, 132, 177	0
4	F	349/384 (90%)	0.09	10 (2%)	51	45	65, 100, 169, 208	0
All	All	2202/2319 (94%)	0.21	65 (2%)	50	43	46, 74, 132, 208	7 (0%)

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	281	GLN	6.4
2	B	281	GLN	6.1
2	D	277	SER	5.4
2	D	276	THR	5.0
2	D	280	SER	4.9

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 monosaccharides in this entry.

6.4 Ligands (i)

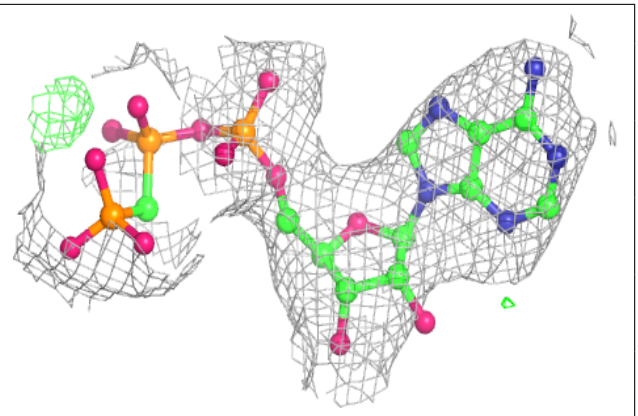
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

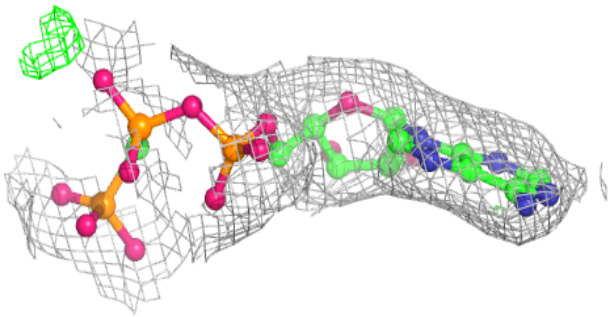
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	E	201	1/1	0.75	0.14	97,97,97,97	0
6	MG	D	502	1/1	0.80	0.19	79,79,79,79	0
9	MES	B	504	12/12	0.85	0.23	114,123,140,141	0
11	ACP	F	401	31/31	0.86	0.14	99,112,124,127	0
7	CA	B	503	1/1	0.88	0.08	105,105,105,105	0
6	MG	B	502	1/1	0.93	0.16	46,46,46,46	0
7	CA	A	503	1/1	0.93	0.13	92,92,92,92	0
8	GDP	D	501	28/28	0.95	0.18	72,76,83,88	0
10	NV7	C	601	16/16	0.97	0.19	66,72,85,87	0
6	MG	F	402	1/1	0.97	0.19	99,99,99,99	0
5	GTP	C	602	32/32	0.98	0.17	42,51,55,58	0
6	MG	A	502	1/1	0.98	0.16	58,58,58,58	0
5	GTP	A	501	32/32	0.98	0.17	51,57,61,63	0
6	MG	C	603	1/1	0.98	0.17	55,55,55,55	0
7	CA	C	604	1/1	0.98	0.10	78,78,78,78	0
8	GDP	B	501	28/28	0.99	0.15	39,50,55,56	0

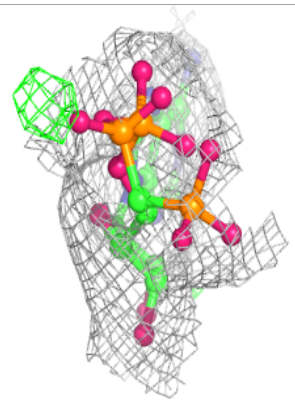
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

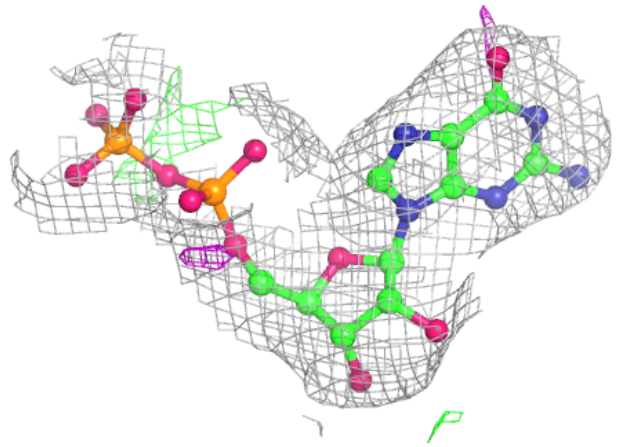


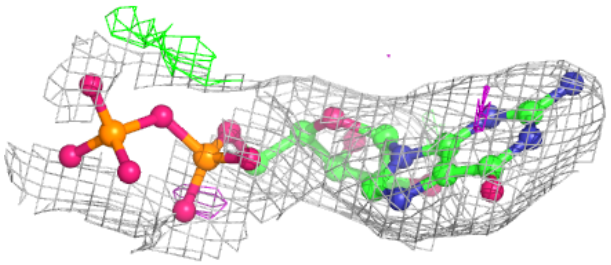


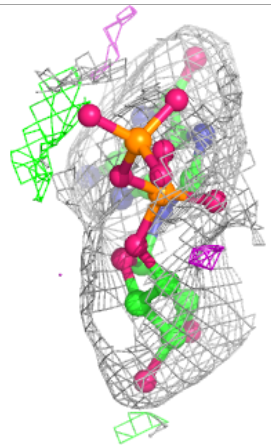


Electron density around GDP D 501:

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

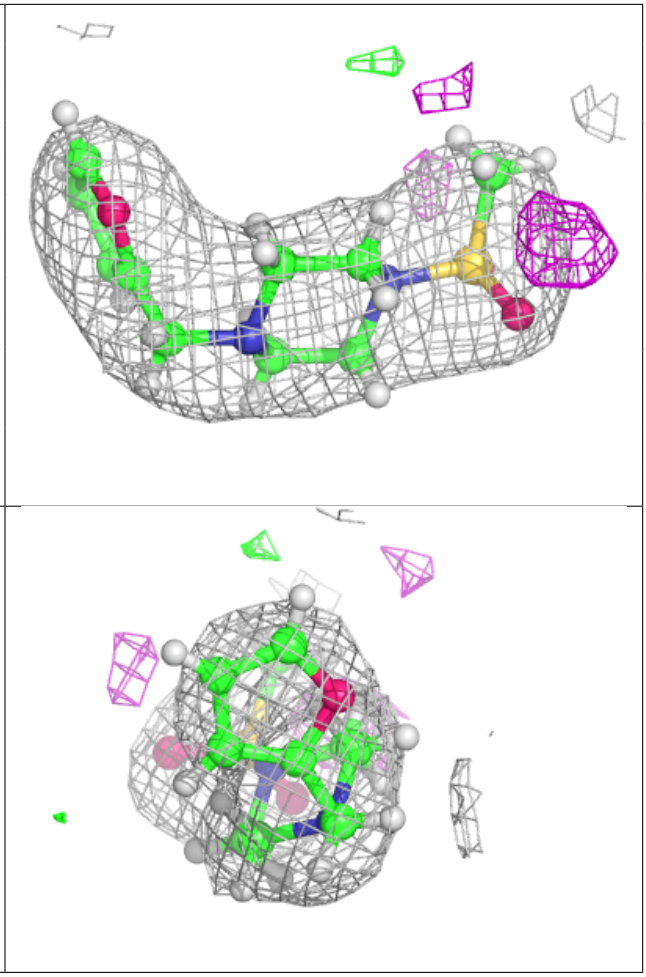






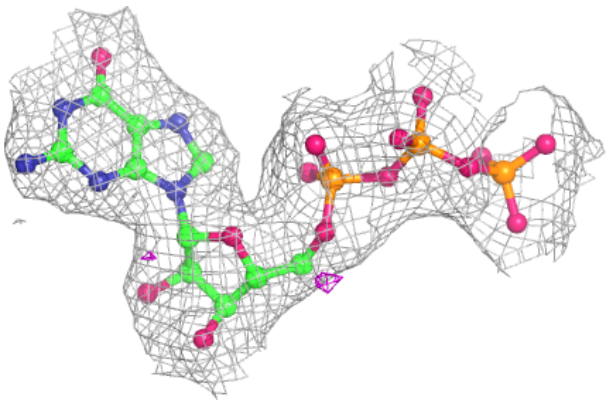
Electron density around NV7 C 601:

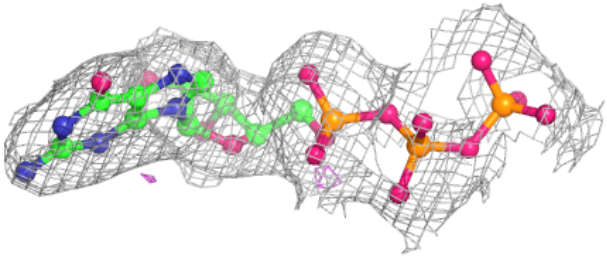
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

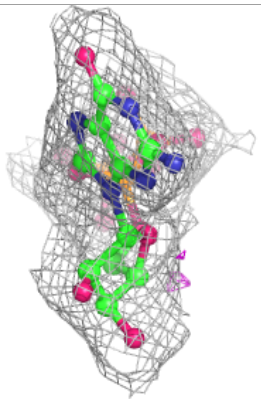


Electron density around GTP C 602:

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

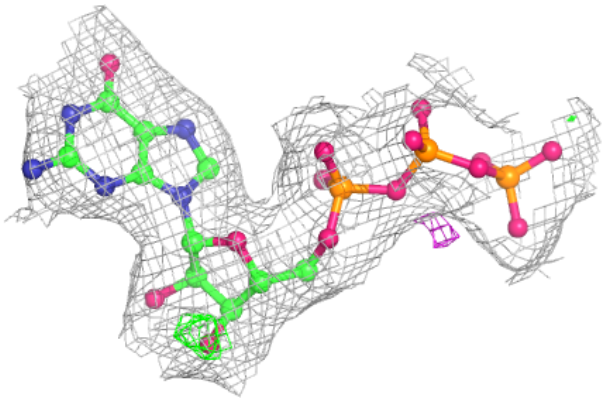


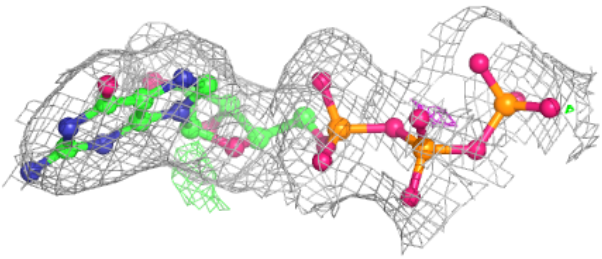


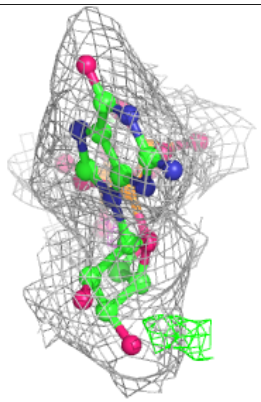


Electron density around GTP A 501:

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

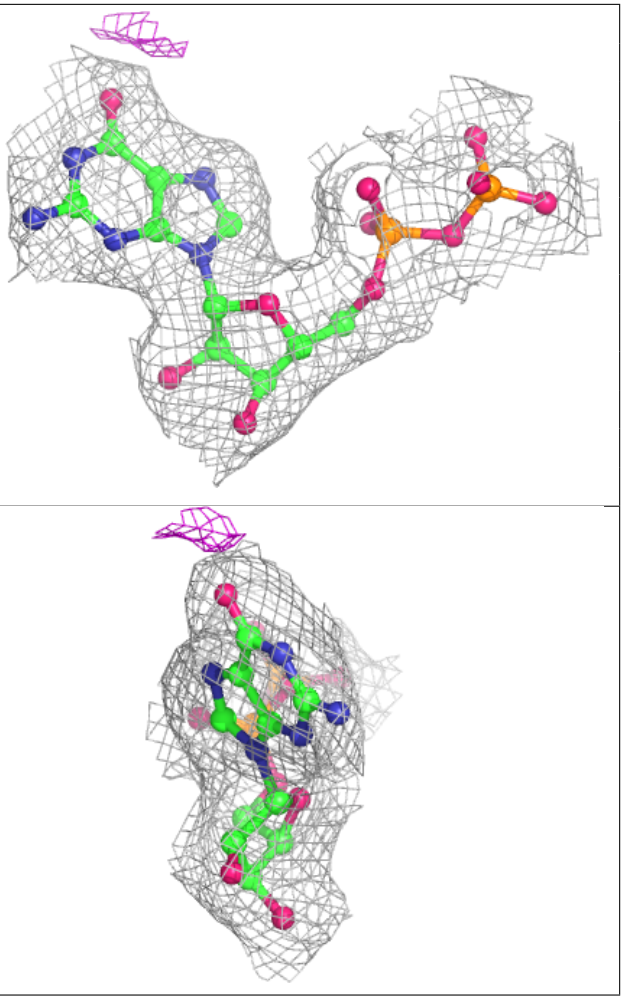






Electron density around GDP B 501:

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.