



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 03:26 AM UTC

PDB ID : 9LNW / pdb_00009lnw
Title : Crystal structure of T2R-TTL-YQVB8 Complex
Authors : Wu, C.Y.; Wang, Y.X.; Chen, Q.F.
Deposited on : 2025-01-22
Resolution : 2.55 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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

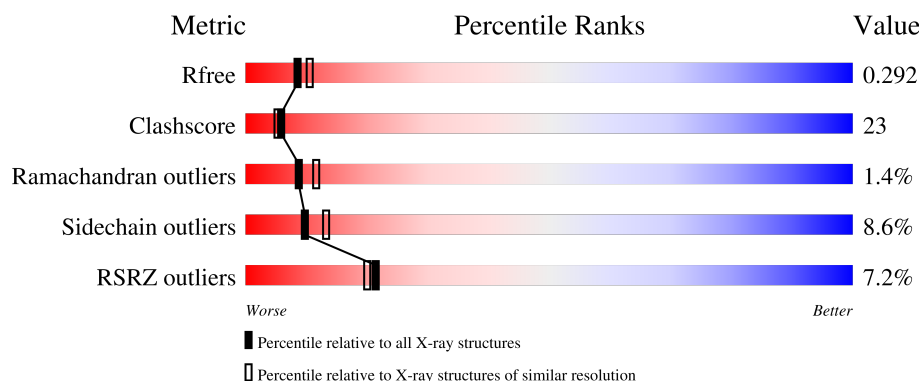
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	450	4% 56% 36% 5%
1	C	450	4% 64% 31% .
2	B	445	2% 64% 29% .
2	D	445	11% 48% 40% 7% 5%
3	E	143	10% 48% 33% . 16%

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Mol	Chain	Length	Quality of chain
4	F	384	14% 47% 34% • • 14%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17615 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	0	9	0
			3465	2200	584	657	24			
1	C	440	Total	C	N	O	S	4	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

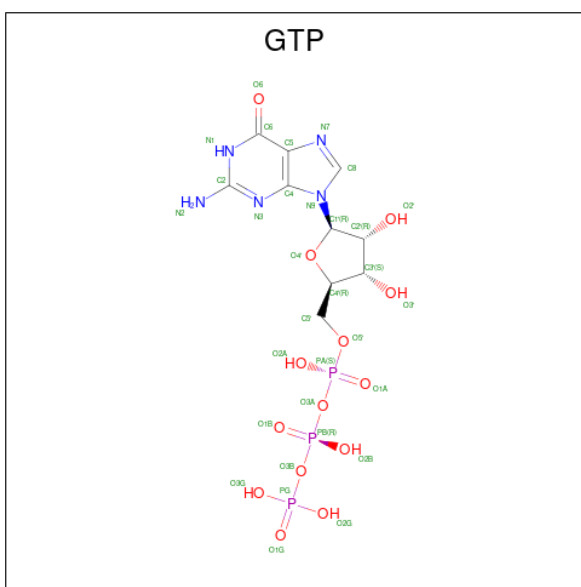
- Molecule 4 is a protein called Tubulin tyrosine ligase.

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	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	32	0
			32	10	5	14	3		

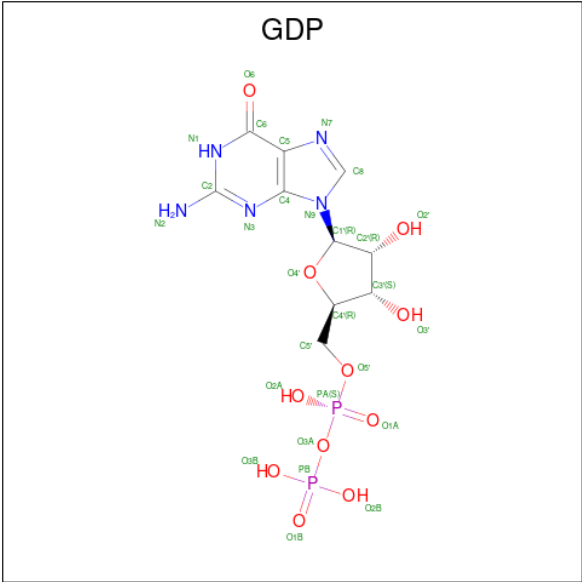
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

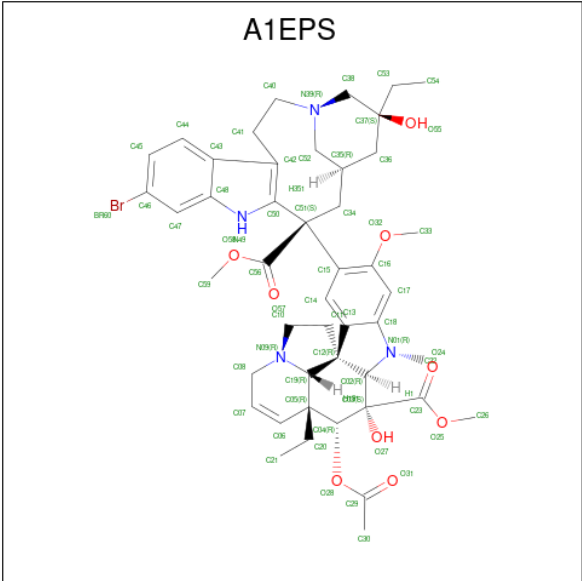
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	1	0
			1	1		
7	C	1	Total	Ca	1	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 9 is 10'-bromovinblastine (CCD ID: A1EPS) (formula: C₄₆H₅₇BrN₄O₉) (labeled as "Ligand of Interest" by depositor).



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

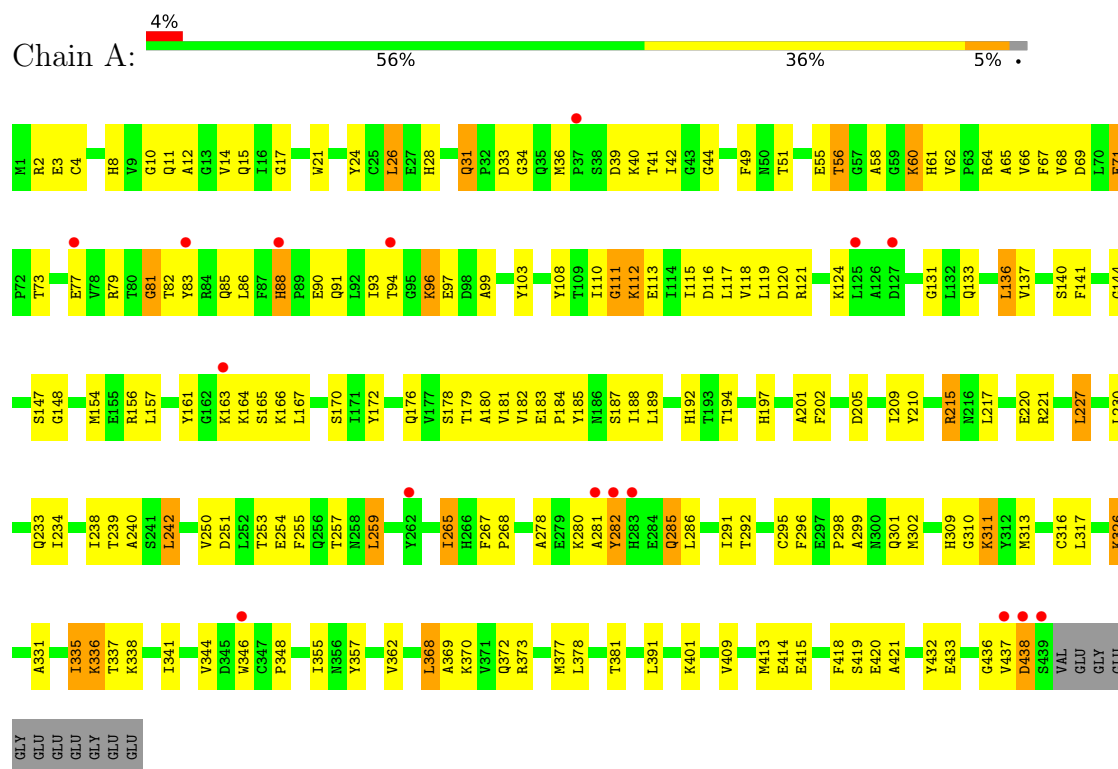
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	4	Total 4	O 4	0	0
10	B	5	Total 5	O 5	0	0

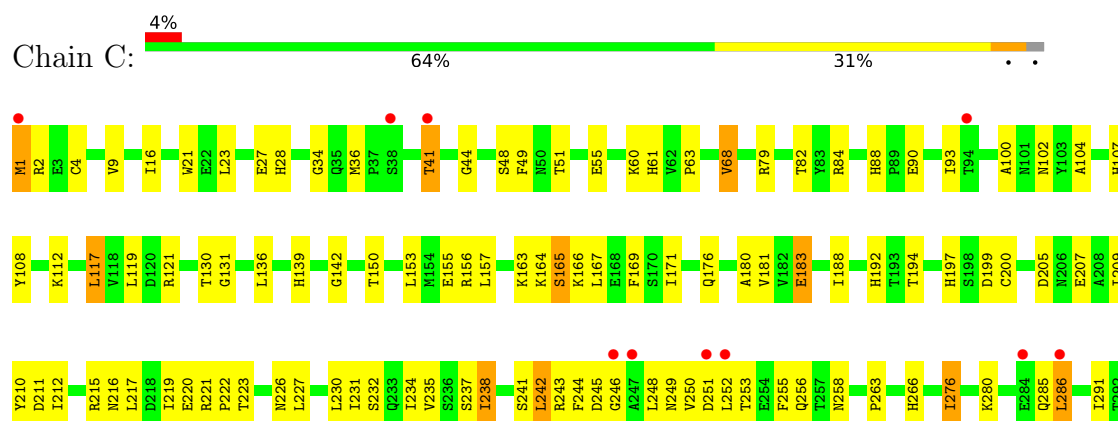
3 Residue-property plots

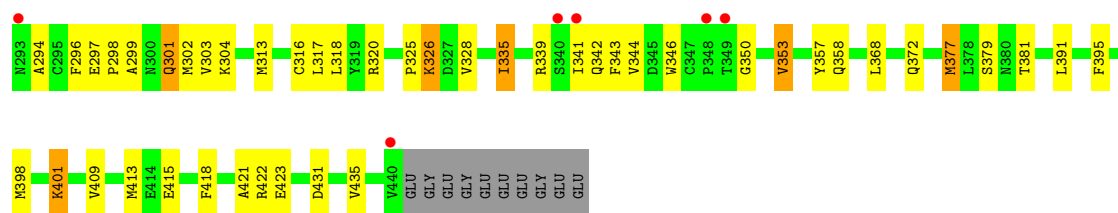
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

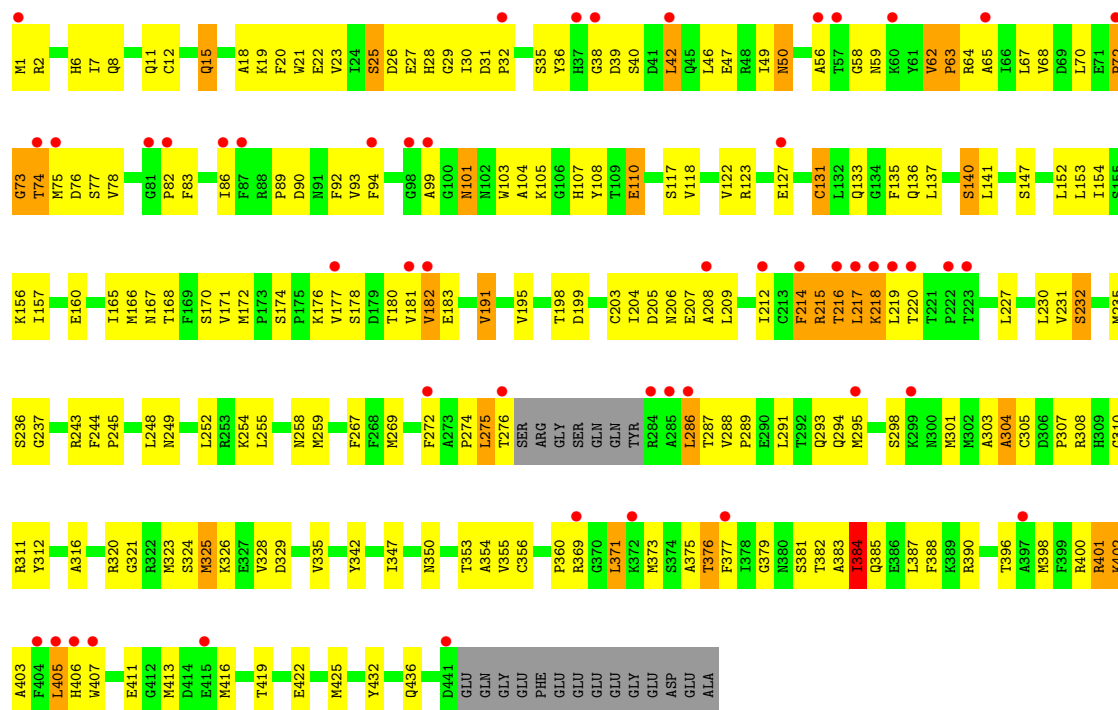


- Molecule 1: Detyrosinated tubulin alpha-1B chain

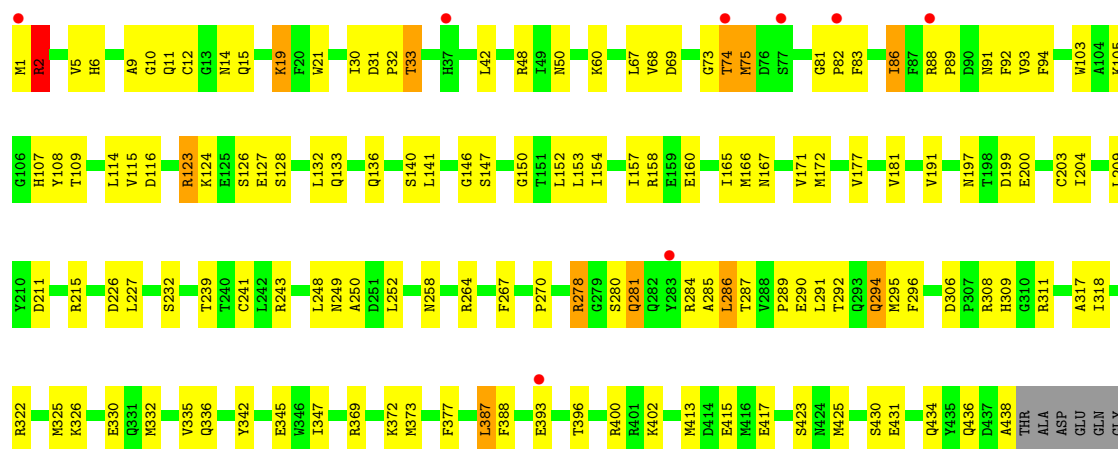




● Molecule 2: Tubulin beta chain



● Molecule 2: Tubulin beta chain



GLU
PHE
GLU
GLU
GLU
GLU
GLY
GLY
ASP
GLU
ALA

● Molecule 3: Stathmin-4



RET
ALA
ASP
N6
E7
V8
T9
E10
C14
T15
S16
G17
Q18
S19
V22
T23
L24
V25
P26
P27
S28
PHE
ASP
GLY
VAL
L123
PRO
GLU
Q124
PHE
ASN
K126
ALA
D127
SER
LEU
A130
PRO
ARG
E132
ARG
D44
P45
S46
L47
I50
Q51
K52
K53
L54
E55
E59
R60
R61
K62
E65
L68
R76

E17
K85
E88
F83
I94
K95
E99
K100
L101
A102
Q103
M105
E106
E110
H115
L116
M119
R122
L123
E125
K126
D127
K128
H129
A130
E131
E132
V133
R134
K135
M136
K137
E138
L139
K140
GLU
ALA
SER
ARG

● Molecule 4: Tubulin tyrosine ligase



M1
Y2
T3
F4
S12
V13
V17
L20
T24
K28
R29
L30
D33
N34
P35
R36
F37
N38
L39
K40
L41
R44
N45
R46
E55
L61
R66
K70
L71
C72
V78
K79
L80
I81
K82
T83
S84
S88
E89
S90
C91
T92
W93
Y98
V99
I100

Y101
P102
T103
ASN
LEU
LYS
THR
PRO
VAL
ALA
PRO
ALA
GLN
ASN
GLY
ILE
ARG
HIS
LEU
ILE
ASN
ASN
THR
ARG
T125
D126
E127
R128
F131
L132
A133
A134
Y135
N136
R137
ARG
ARG
GLY
GLY
ARG
GLU
G144
N145
V146
W147
I148
A149
LYS
SER
SER
ALA
GLY
ALA
LYS
GLY
GLU
G159
I160
L161

I162
S163
S164
E165
A166
S167
E168
L169
D171
F172
I173
D174
E175
V179
H180
Y181
I182
Q183
K184
Y185
L186
E187
L190
P194
R197
K198
F199
V205
L206
D207
D208
H209
Y214
L215
Y216
R217
E218
G219
V220
L221
S224
S225
T228
N229
S230
A231
N232
F233
Q234
D235
K236

T237
C238
H239
L240
T241
N242
H243
C244
I245
Q246
K247
E248
Y249
S250
LYS
ASN
TYR
GLY
R255
E258
G259
N260
M261
M262
F263
E266
L275
N276
T277
T278
S282
L283
L284
L285
T290
I291
R292
L295
M296
C297
I298
I302
K305
H306
Q310
F319
M320
V321
D322

L325
E331
V332
N333
K341
L342
Y343
G349
A354
V358
F359
P360
L361
A362
ASP
THR
GLY
GLN
LYS
THR
SER
GLN
PRO
T372
S373
I374
F375
I376
K377
L378
H379
H380
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.82Å 155.76Å 185.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.21 – 2.55 91.21 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.6 (91.21-2.55) 97.6 (91.21-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.55Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.225 , 0.292 0.228 , 0.292	Depositor DCC
R_{free} test set	4878 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17615	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: GTP, GDP, A1EPS, MG, CA

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	0.37	0/3571	0.54	0/4849
1	C	0.42	0/3565	0.60	0/4842
2	B	0.41	0/3451	0.57	0/4675
2	D	0.31	0/3428	0.49	0/4645
3	E	0.37	0/999	0.51	0/1325
4	F	0.31	0/2802	0.51	0/3789
All	All	0.37	0/17816	0.54	0/24125

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1
4	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	76	ARG	Sidechain
4	F	89	GLU	Peptide

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	3401	176	0
1	C	3466	0	3393	153	0
2	B	3370	0	3249	119	0
2	D	3343	0	3230	201	0
3	E	991	0	1012	51	0
4	F	2729	0	2715	123	0
5	A	32	0	12	0	0
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	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	60	58	0	7	0
10	B	5	0	0	0	0
10	C	4	0	0	0	0
All	All	17557	58	17048	790	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 790 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:135:PHE:HB2	2:D:166:MET:HE1	1.31	1.11
2:B:1:MET:HE2	2:B:1:MET:HA	1.41	1.03
2:D:166:MET:HE3	2:D:166:MET:HA	1.42	0.97
1:C:285:GLN:NE2	1:C:372:GLN:OE1	1.97	0.97
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.46	0.96

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%)	411 (92%)	29 (6%)	6 (1%)	9	12
1	C	445/450 (99%)	422 (95%)	22 (5%)	1 (0%)	43	56
2	B	428/445 (96%)	407 (95%)	18 (4%)	3 (1%)	18	25
2	D	424/445 (95%)	375 (88%)	36 (8%)	13 (3%)	3	2
3	E	116/143 (81%)	109 (94%)	6 (5%)	1 (1%)	14	20
4	F	323/384 (84%)	281 (87%)	35 (11%)	7 (2%)	5	5
All	All	2182/2317 (94%)	2005 (92%)	146 (7%)	31 (1%)	9	11

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	A	438	ASP
2	D	64	ARG
2	D	72	PRO
2	D	73	GLY

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%)	6	7
1	C	378/378 (100%)	353 (93%)	25 (7%)	15	21
2	B	369/383 (96%)	344 (93%)	25 (7%)	14	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	369/383 (96%)	340 (92%)	29 (8%)	11	16
3	E	108/127 (85%)	95 (88%)	13 (12%)	5	5
4	F	303/342 (89%)	267 (88%)	36 (12%)	5	5
All	All	1905/1991 (96%)	1736 (91%)	169 (9%)	10	12

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	90	SER
4	F	378	LEU
4	F	136	ASN
4	F	233	PHE
2	B	75	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
4	F	242	ASN
2	D	294	GLN
4	F	239	HIS
2	D	15	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
8	GDP	B	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
5	GTP	C	501	6	33,34,34	0.97	1 (3%)	50,54,54	1.56	9 (18%)
9	A1EPS	B	502	-	67,68,68	5.16	32 (47%)	84,110,110	3.40	35 (41%)
8	GDP	D	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
5	GTP	A	501	6	33,34,34	0.97	1 (3%)	50,54,54	1.60	9 (18%)

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	GDP	B	501	-	-	1/16/32/32	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
9	A1EPS	B	502	-	-	15/40/131/131	0/7/9/9
8	GDP	D	501	-	-	0/16/32/32	0/3/3/3
5	GTP	A	501	6	-	3/22/38/38	0/3/3/3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	A1EPS	C18-C13	13.80	1.55	1.39
9	B	502	A1EPS	C06-C07	13.00	1.55	1.32
9	B	502	A1EPS	C14-C15	12.61	1.57	1.39
9	B	502	A1EPS	C14-C13	11.51	1.55	1.39
9	B	502	A1EPS	C44-C43	10.87	1.56	1.39

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	502	A1EPS	O55-C37-C53	-17.02	79.99	108.74
9	B	502	A1EPS	C11-C12-C13	-10.46	93.33	112.36
9	B	502	A1EPS	O55-C37-C36	-8.19	88.20	109.33
9	B	502	A1EPS	C11-C12-C02	7.28	126.28	112.17
8	B	501	GDP	C5-C4-N3	-6.18	118.55	128.39

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

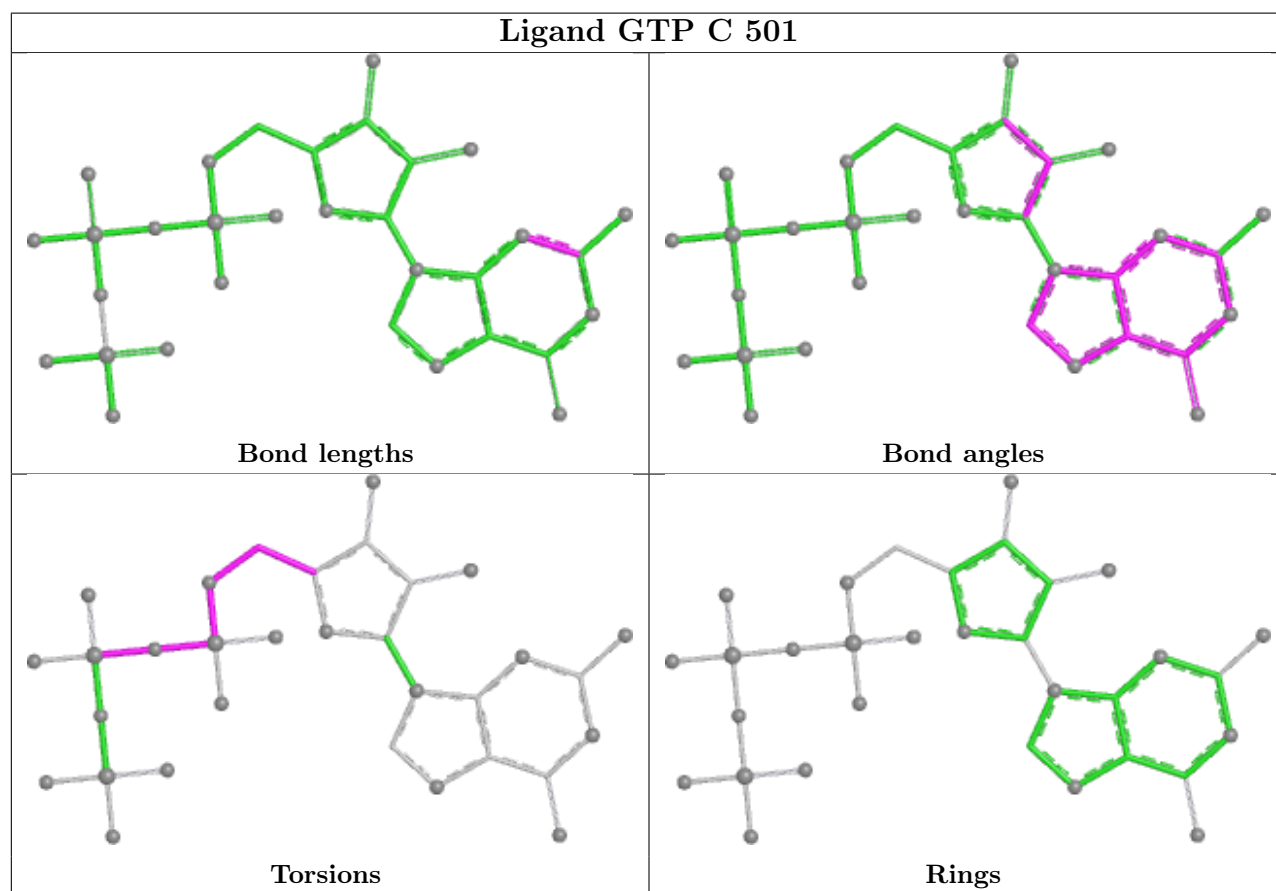
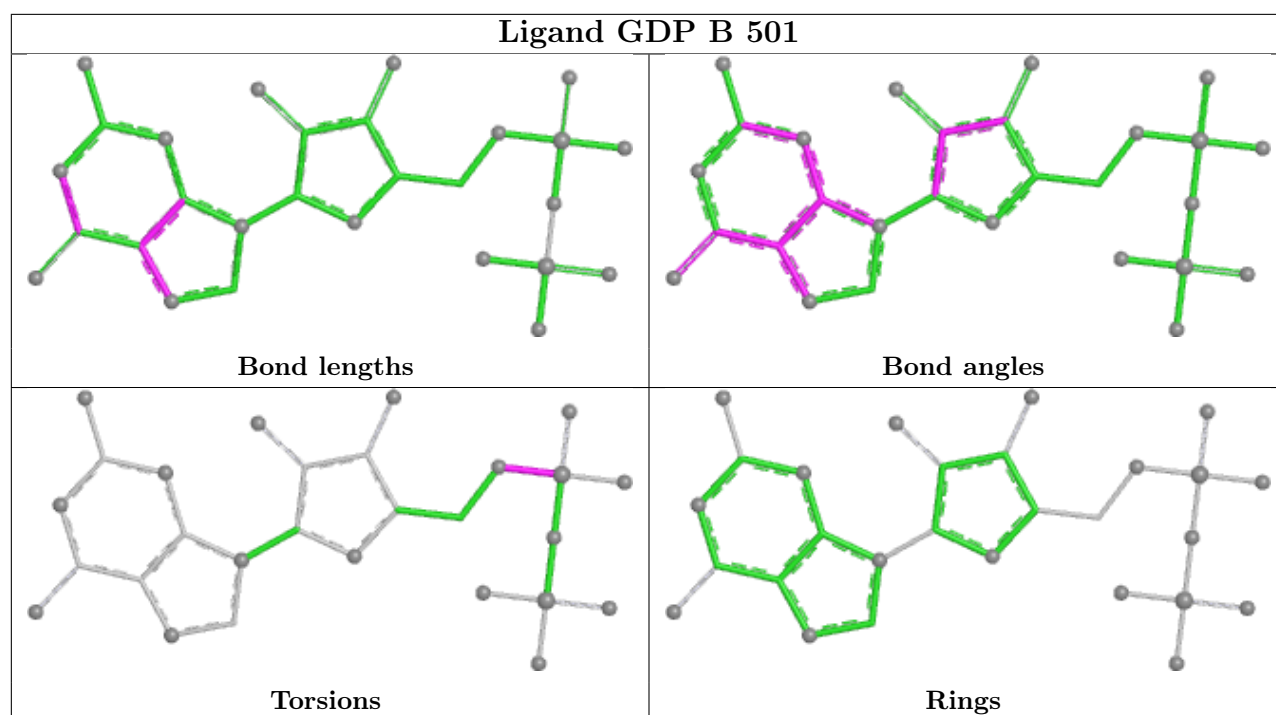
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3A-PA-O5'
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

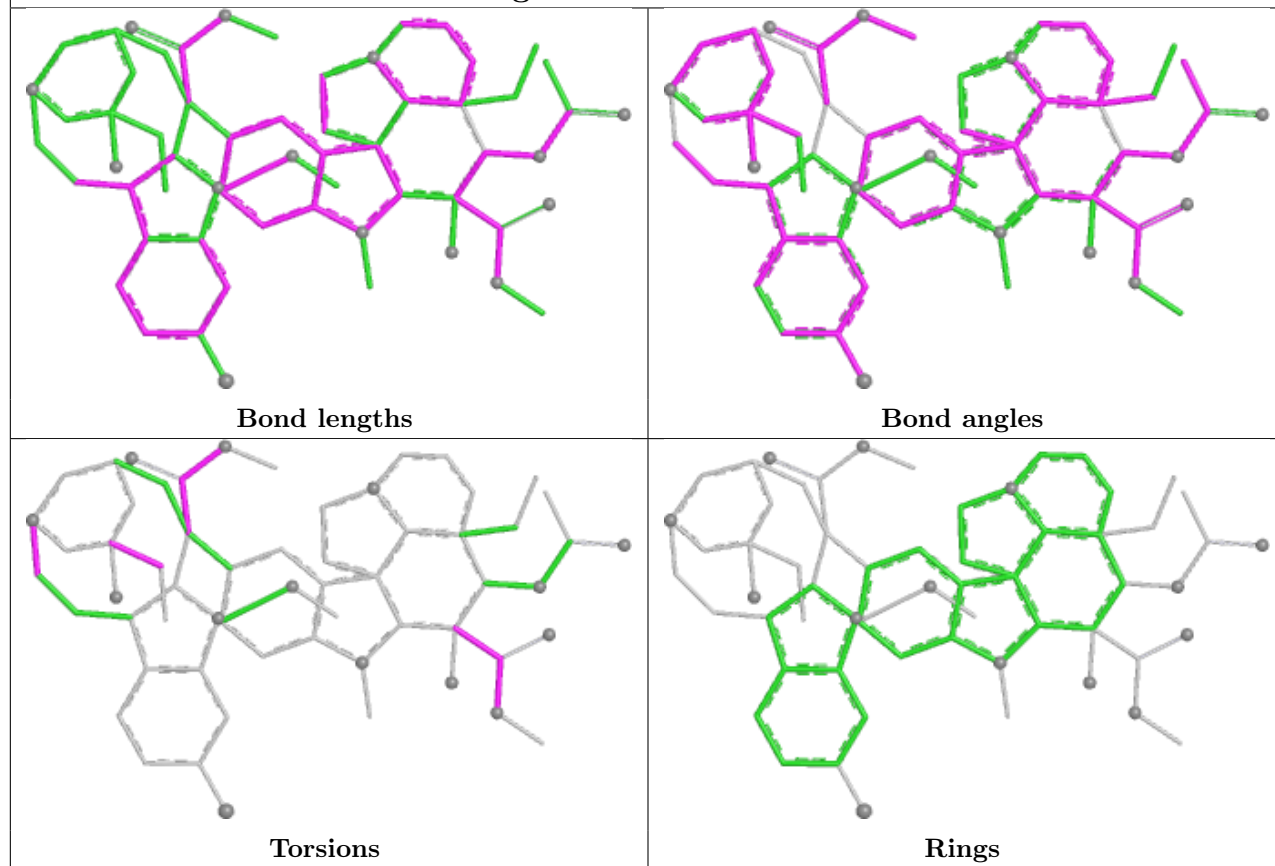
1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	502	A1EPS	7	0

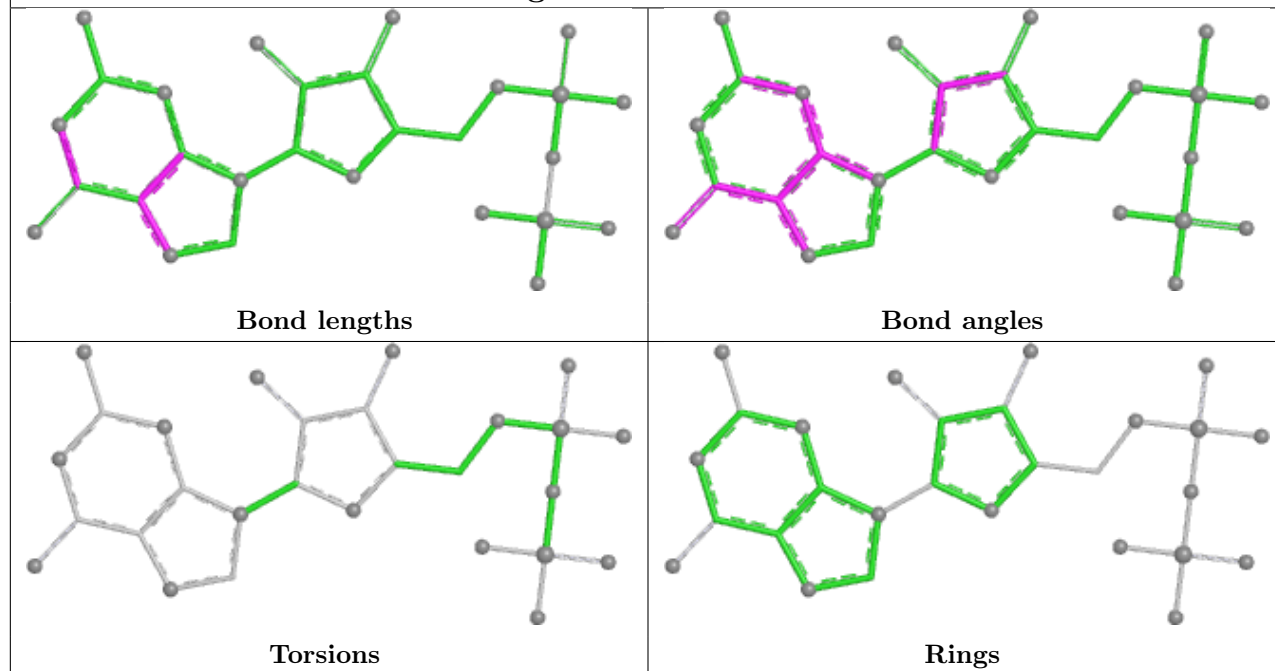
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

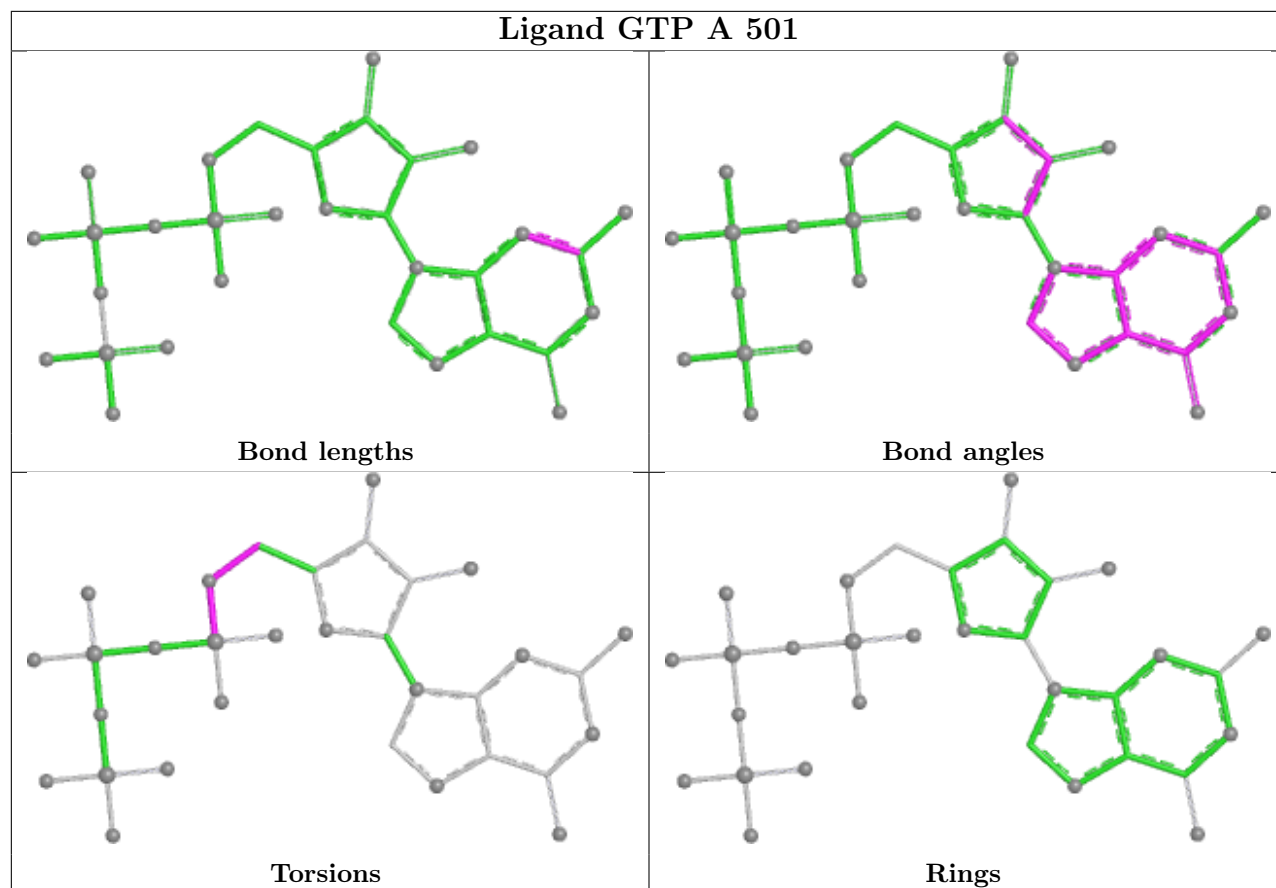


Ligand A1EPS B 502



Ligand GDP D 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	439/450 (97%)	0.34	16 (3%) 46 47	22, 41, 65, 99	9 (2%)
1	C	440/450 (97%)	0.15	16 (3%) 46 47	17, 35, 56, 72	7 (1%)
2	B	428/445 (96%)	0.03	8 (1%) 66 66	16, 34, 62, 84	4 (0%)
2	D	424/445 (95%)	0.99	50 (11%) 9 8	29, 56, 83, 107	7 (1%)
3	E	120/143 (83%)	0.97	14 (11%) 9 8	29, 55, 79, 86	0
4	F	331/384 (86%)	0.99	54 (16%) 4 3	28, 58, 99, 114	4 (1%)
All	All	2182/2317 (94%)	0.50	158 (7%) 21 20	16, 44, 81, 114	31 (1%)

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	5.3
1	A	439	SER	5.1
4	F	233	PHE	4.8
4	F	125	THR	4.7
1	A	282	TYR	4.6

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](#)

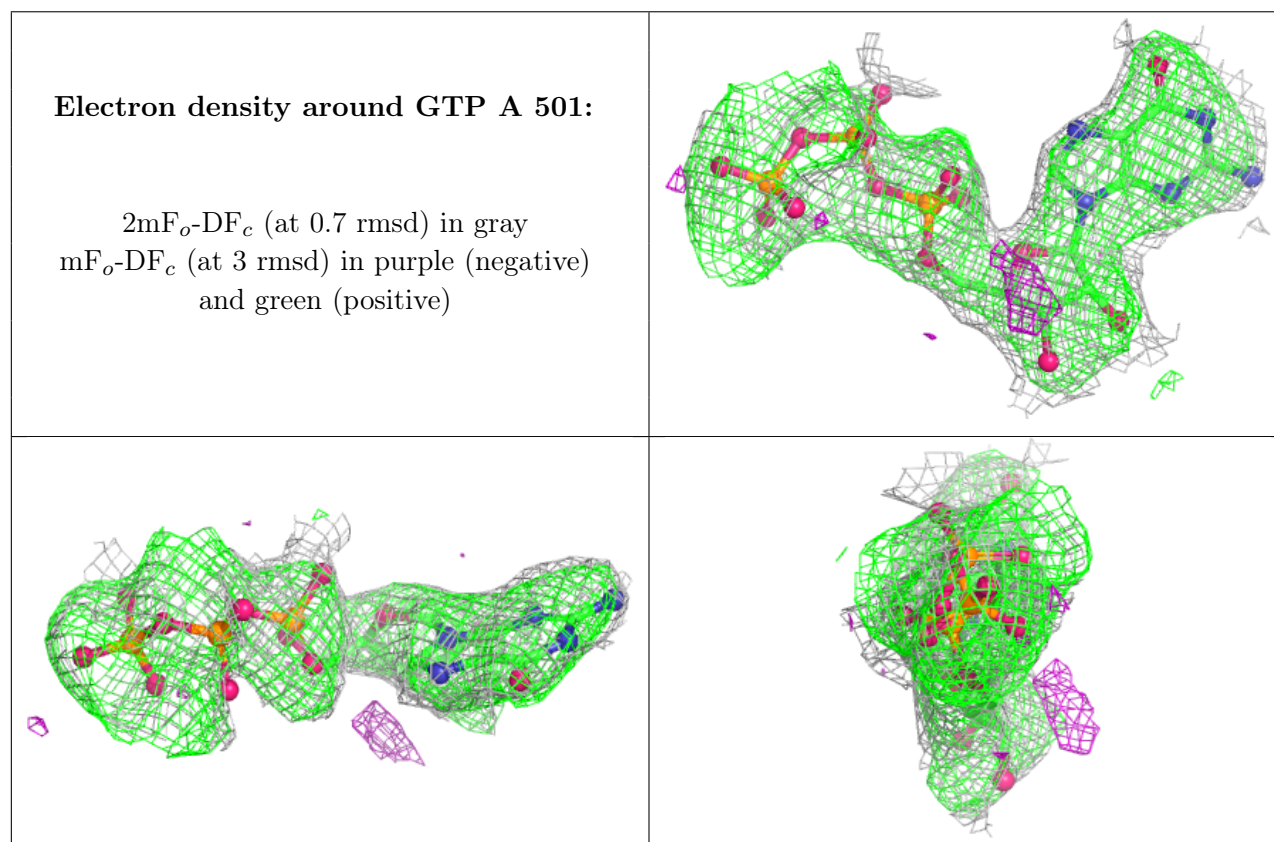
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

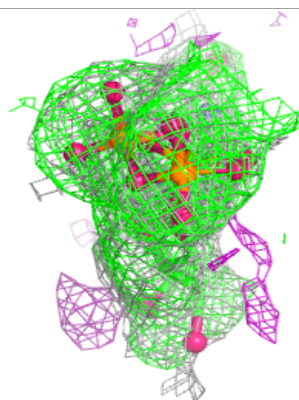
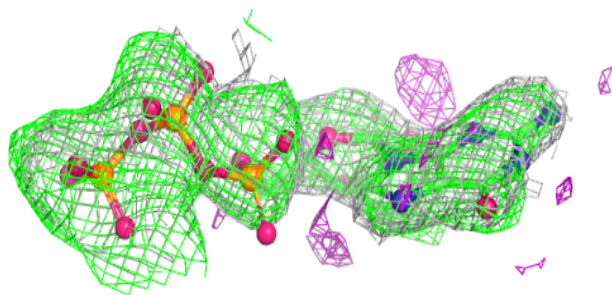
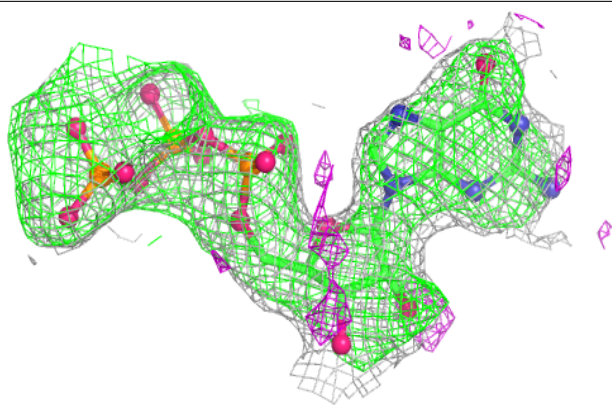
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GTP	A	501	32/32	-	-	27,31,32,37	32
5	GTP	C	501	32/32	-	-	26,27,30,35	32
6	MG	A	502	1/1	-	-	33,33,33,33	1
6	MG	C	502	1/1	-	-	28,28,28,28	1
7	CA	A	503	1/1	-	-	61,61,61,61	1
7	CA	C	503	1/1	-	-	44,44,44,44	1
8	GDP	D	501	28/28	-	-	56,61,64,66	28
8	GDP	B	501	28/28	-	-	21,25,26,27	28
9	A1EPS	B	502	60/60	0.96	0.09	18,32,46,58	0

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

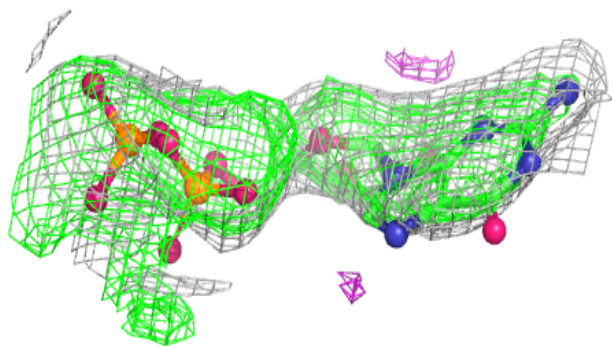
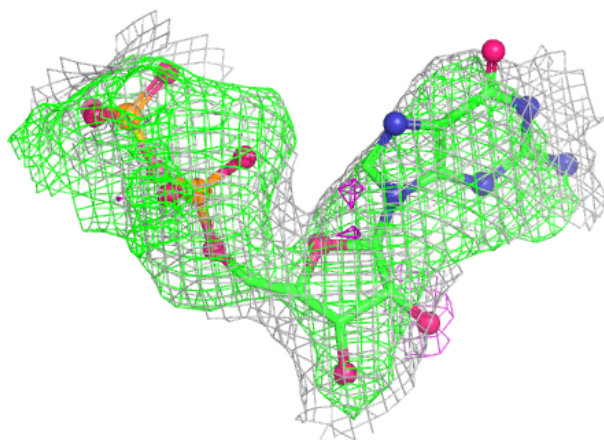


Electron density around GTP C 501:

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

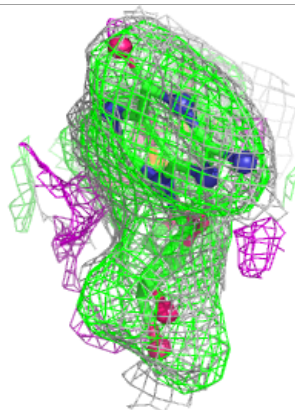
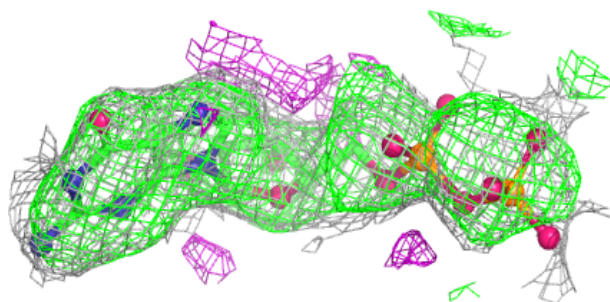
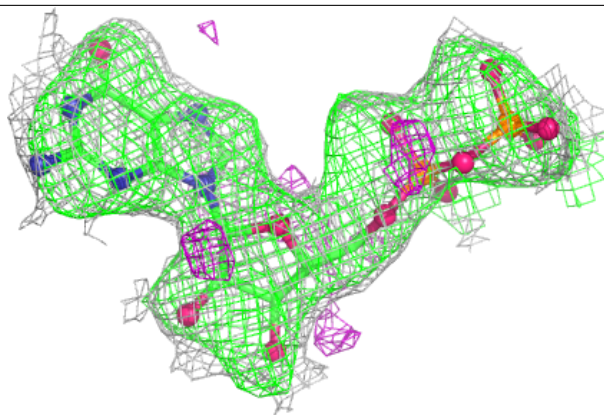
**Electron density around GDP D 501:**

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



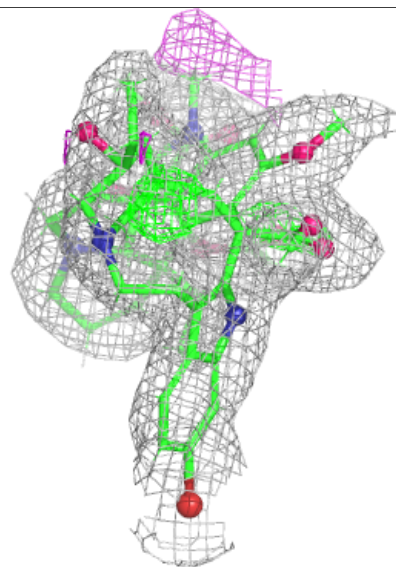
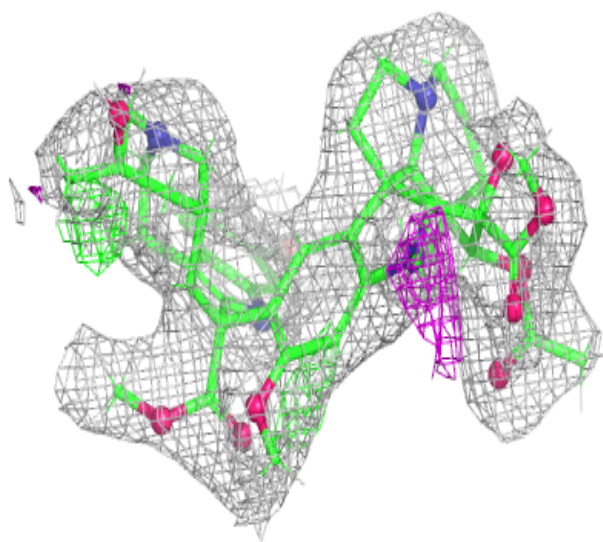
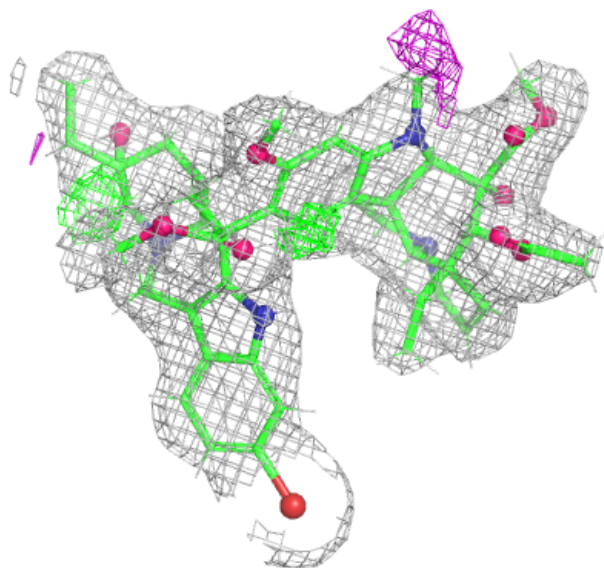
Electron density around GDP B 501:

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



Electron density around A1EPS B 502:

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.