



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 12:07 AM BST

PDB ID : 5XHC
Title : Crystal structure of T2R-TTL-PO10 complex
Authors : Chu, Y.; Wang, Y.; Yang, J.; Li, W.
Deposited on : 2017-04-20
Resolution : 2.75 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

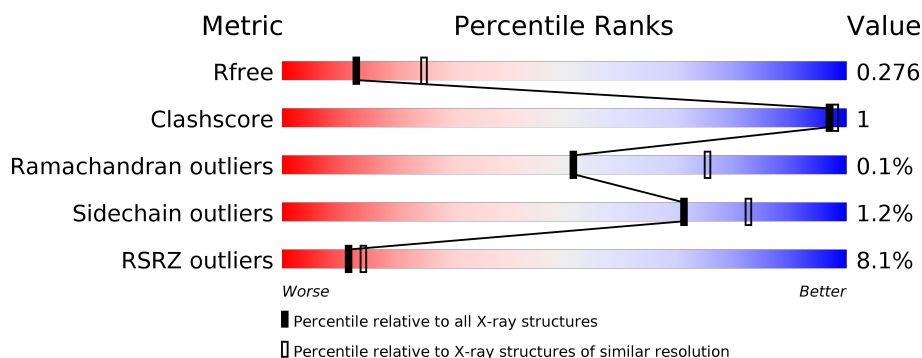
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on 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	<div> <div>4%</div> <div>94%</div> <div>• •</div> </div>
1	C	450	<div> <div>95%</div> <div>• •</div> </div>
2	B	445	<div> <div>3%</div> <div>92%</div> <div>• 5%</div> </div>
2	D	445	<div> <div>13%</div> <div>92%</div> <div>• 5%</div> </div>
3	E	184	<div> <div>6%</div> <div>64%</div> <div>• 35%</div> </div>
4	F	384	<div> <div>18%</div> <div>79%</div> <div>• 20%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17462 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3441	2179	586	652	24			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2200	589	668	25			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	2	0
			3353	2107	574	645	27			
2	D	421	Total	C	N	O	S	0	1	0
			3306	2079	562	638	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	2	0
			1004	621	181	196	6			

- Molecule 4 is a protein called TUBULIN TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	309	Total	C	N	O	S	0	3	0
			2553	1645	438	455	15			

There are 6 discrepancies between the modelled and reference sequences:

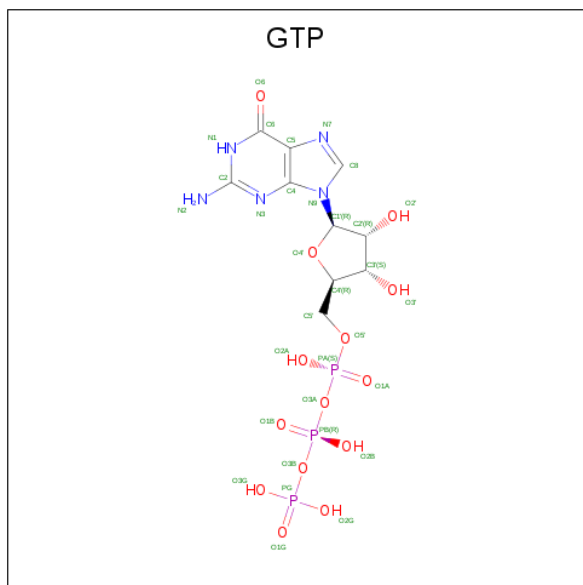
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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Chain	Residue	Modelled	Actual	Comment	Reference
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
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

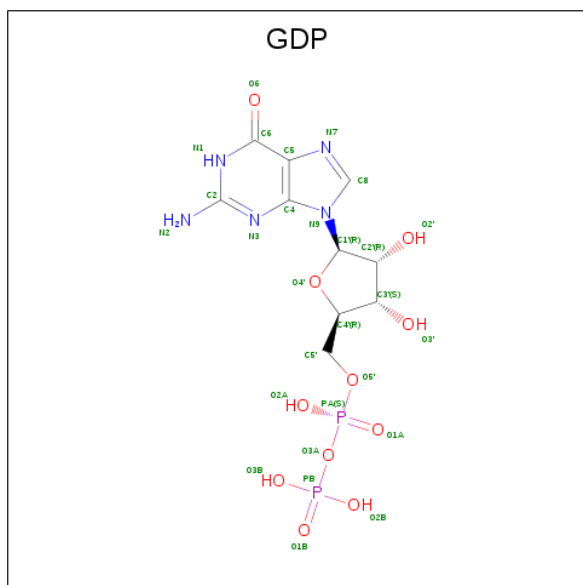
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Mg	0	0
			2	2		
7	D	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

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



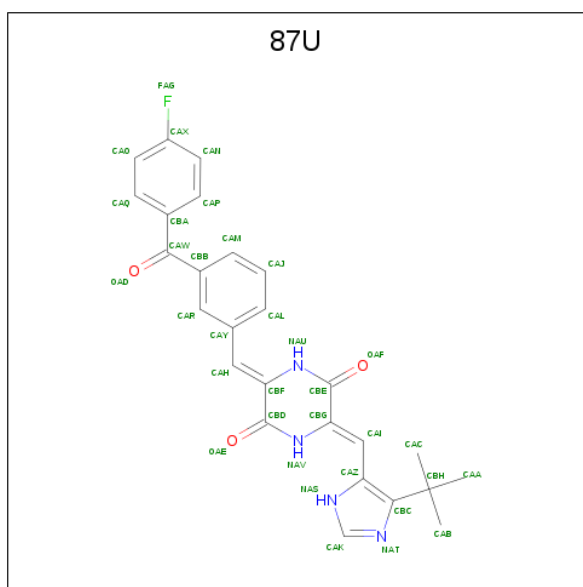
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



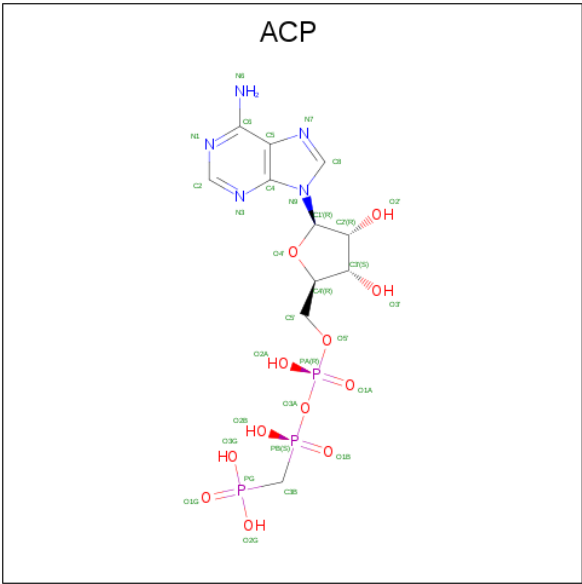
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is (3Z,6Z)-3-[(4-tert-butyl-1H-imidazol-5-yl)methylidene]-6-[[3-(4-fluorophenyl)carbonylphenyl]methylidene]piperazine-2,5-dione (three-letter code: 87U) (formula: C₂₆H₂₃FN₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	F	N	O	0	0
			34	26	1	4	3		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

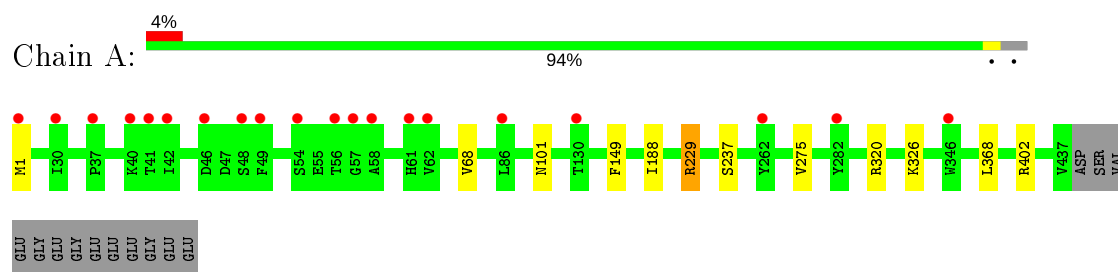
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	20	Total	O	0	0
			20	20		
12	B	22	Total	O	0	0
			22	22		
12	C	55	Total	O	0	0
			55	55		
12	E	2	Total	O	0	0
			2	2		
12	F	4	Total	O	0	0
			4	4		

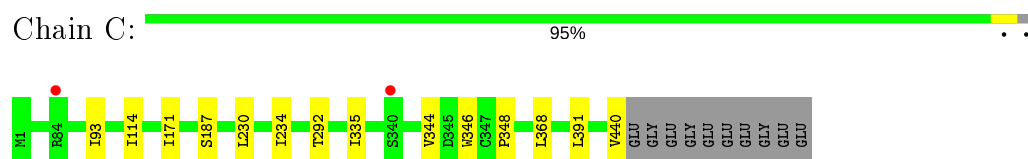
3 Residue-property plots [i](#)

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.

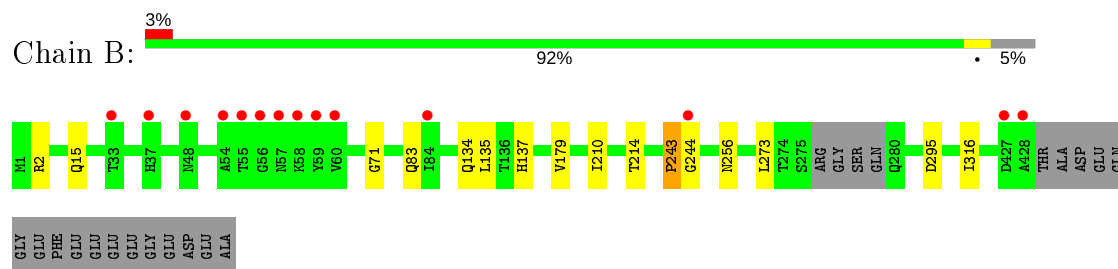
- Molecule 1: Tubulin alpha chain



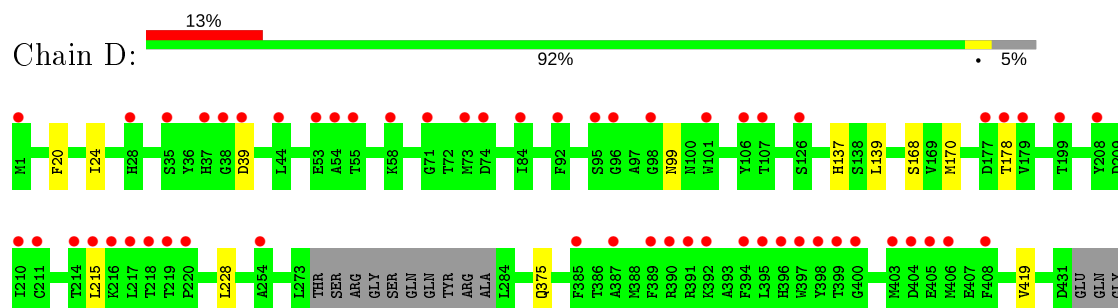
- Molecule 1: Tubulin alpha chain



- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain



GLU
PHE
GLU
GLU
GLU
GLU
GLY
GLU
ASP
GLU
ALA

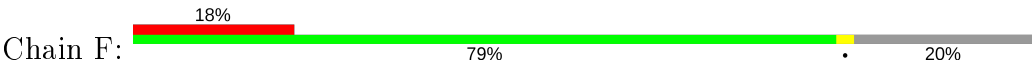
● Molecule 3: Stathmin-4



Tyr
Lys
Glu
Lys
Met
Lys
Glu
Leu
Pro
Val
Ser
Leu
Phe
Cys
Ser
Phe
Leu
Ser
Asp
Pro
Leu
Asn
Lys
Ser
Ser
Tyr
Lys
Tyr
Glu
Ala
Asp
Thr
Val
Asp
Leu
Asn
Trp
Cys
Val
Ile
Ser
Asp
Phe
P26
P27
Ser
Phe
Asp
Gly
Val
Pro
Glu
Phe
Asn
Ala
Ser
Leu

Pro
Arg
Arg
Arg
D44
P45
S46
L47
E48
Q51
E59
K128
E131
E132
V133
N136
K137
E138
L139
K140
E141
Glu
Ala
Ser
Arg

● Molecule 4: TUBULIN TYROSINE LIGASE



M1
V6
E9
N10
Y14
V17
L20
L21
L22
N27
R31
K32
Y98
V99
I100
Y101
P102
Thr
Asn
Leu
Lys
Thr
Pro
Val
Ala
Ala
Pro
Ala
Gln
Asn
Gly
Ile
Arg
His
Leu
Ile
Asn
Asn
Thr
Arg
Thr
Asp
Glu
Arg
Glu
Val
P194
P195
P196
H196
R197
K197
Ala
Ala
Tyr
Asn
Arg

Arg
Arg
Glu
Gly
Arg
Glu
G144
N145
V146
I147
I148
A149
K150
S151
Ser
Ala
Gly
Ala
Lys
Gly
Glu
G159
I160
L161
I162
S163
S164
E165
A166
Ser
Glu
Leu
Leu
Asp
Phe
Ile
Asp
Glu
Gln
Gln
Val
H180
V181
I182
Q183
K184
L191
L192
E193
P194
G195
H196
R197
K197
F199
Y211

T223
S224
E225
E226
Y227
P228
N229
S230
A231
F233
N232
Q234
D235
K236
T237
C238
E239
L240
T241
N242
H243
C244
I245
Q246
K247
Glu
Tyr
Ser
Lys
N252
Y253
Q254
R255
Y256
E257
E258
G259
N260
M320
A335
G349
L361
A362
Asp
Thr
Gly
Gln
Lys
Thr
Ser
Gln
Pro
Thr
S373
I374

H384

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.26Å 157.88Å 182.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.38 – 2.75 49.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (119.38-2.75) 98.5 (49.93-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.227 , 0.277 0.228 , 0.276	Depositor DCC
R_{free} test set	3932 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17462	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CA, 87U, GTP, ACP, MES

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	0/3525	0.59	0/4784
1	C	0.37	0/3572	0.60	0/4850
2	B	0.39	0/3427	0.60	0/4640
2	D	0.38	0/3379	0.55	0/4577
3	E	0.38	0/1018	0.53	0/1350
4	F	0.38	0/2618	0.54	0/3537
All	All	0.38	0/17539	0.57	0/23738

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	3441	0	3363	9	0
1	C	3482	0	3384	7	0
2	B	3353	0	3228	7	0
2	D	3306	0	3181	6	0
3	E	1004	0	1028	0	0
4	F	2553	0	2519	2	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
5	D	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
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	1	0
10	B	34	0	0	2	0
11	F	31	0	14	0	0
12	A	20	0	0	0	0
12	B	22	0	0	0	0
12	C	55	0	0	0	0
12	E	2	0	0	0	0
12	F	4	0	0	0	0
All	All	17462	0	16791	30	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 1.

The worst 5 of 30 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)
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:HH11	1.07	1.20
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:CG	1.75	0.98
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	1.87	0.84
2:B:243:PRO:HB2	2:B:244:GLY:HA2	1.67	0.75
2:B:243:PRO:CB	2:B:244:GLY:HA2	2.22	0.69

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	439/450 (98%)	426 (97%)	13 (3%)	0	100	100
1	C	446/450 (99%)	435 (98%)	11 (2%)	0	100	100
2	B	422/445 (95%)	407 (96%)	13 (3%)	2 (0%)	29	47
2	D	417/445 (94%)	404 (97%)	12 (3%)	1 (0%)	47	69
3	E	118/184 (64%)	116 (98%)	2 (2%)	0	100	100
4	F	300/384 (78%)	286 (95%)	14 (5%)	0	100	100
All	All	2142/2358 (91%)	2074 (97%)	65 (3%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	B	71	GLY
2	D	39	ASP

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	372/378 (98%)	364 (98%)	8 (2%)	52	70
1	C	379/378 (100%)	377 (100%)	2 (0%)	88	92
2	B	367/383 (96%)	360 (98%)	7 (2%)	57	73
2	D	362/383 (94%)	361 (100%)	1 (0%)	92	95
3	E	110/168 (66%)	107 (97%)	3 (3%)	44	65
4	F	281/342 (82%)	278 (99%)	3 (1%)	73	84
All	All	1871/2032 (92%)	1847 (99%)	24 (1%)	71	81

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	83	GLN
2	B	214	THR
4	F	32	LYS
2	B	135	LEU
2	B	137	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
2	B	83	GLN
1	C	249	ASN
3	E	136	ASN
4	F	252	ASN

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 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	MES	B	504	-	12,12,12	2.03	1 (8%)	14,16,16	7.44	10 (71%)
10	87U	B	505	-	29,37,37	2.45	8 (27%)	35,54,54	1.71	9 (25%)
9	MES	B	507	-	12,12,12	2.04	2 (16%)	14,16,16	6.14	6 (42%)
5	GTP	D	501	7	26,34,34	1.25	2 (7%)	33,54,54	1.94	8 (24%)
11	ACP	F	401	-	27,33,33	2.01	8 (29%)	32,52,52	1.34	3 (9%)
8	GDP	B	502	7	24,30,30	1.23	2 (8%)	31,47,47	1.98	6 (19%)
5	GTP	C	501	7	26,34,34	1.14	2 (7%)	33,54,54	1.96	10 (30%)
5	GTP	A	501	7	26,34,34	1.17	2 (7%)	33,54,54	1.93	9 (27%)

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	MES	B	504	-	-	3/6/14/14	0/1/1/1
10	87U	B	505	-	-	2/18/22/22	0/4/4/4
9	MES	B	507	-	-	2/6/14/14	0/1/1/1
5	GTP	D	501	7	-	4/18/38/38	0/3/3/3
11	ACP	F	401	-	-	4/15/38/38	0/3/3/3
8	GDP	B	502	7	-	3/12/32/32	0/3/3/3
5	GTP	C	501	7	-	6/18/38/38	0/3/3/3
5	GTP	A	501	7	-	3/18/38/38	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-6.41	1.68	1.77
9	B	507	MES	C8-S	-6.36	1.68	1.77
10	B	505	87U	CBE-NAU	5.51	1.42	1.33
11	F	401	ACP	PG-O1G	5.46	1.61	1.50
10	B	505	87U	FAG-CAX	-5.44	1.23	1.36

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	MES	O1S-S-C8	-18.77	84.32	106.92
9	B	507	MES	O3S-S-O1S	-13.37	78.60	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	MES	O2S-S-C8	11.41	120.65	106.92
9	B	504	MES	O3S-S-O1S	-10.64	85.27	111.27
9	B	507	MES	O3S-S-C8	10.52	122.79	105.77

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	504	MES	N4-C7-C8-S
9	B	504	MES	C7-C8-S-O2S
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
10	B	505	87U	CBG-CAI-CAZ-NAS

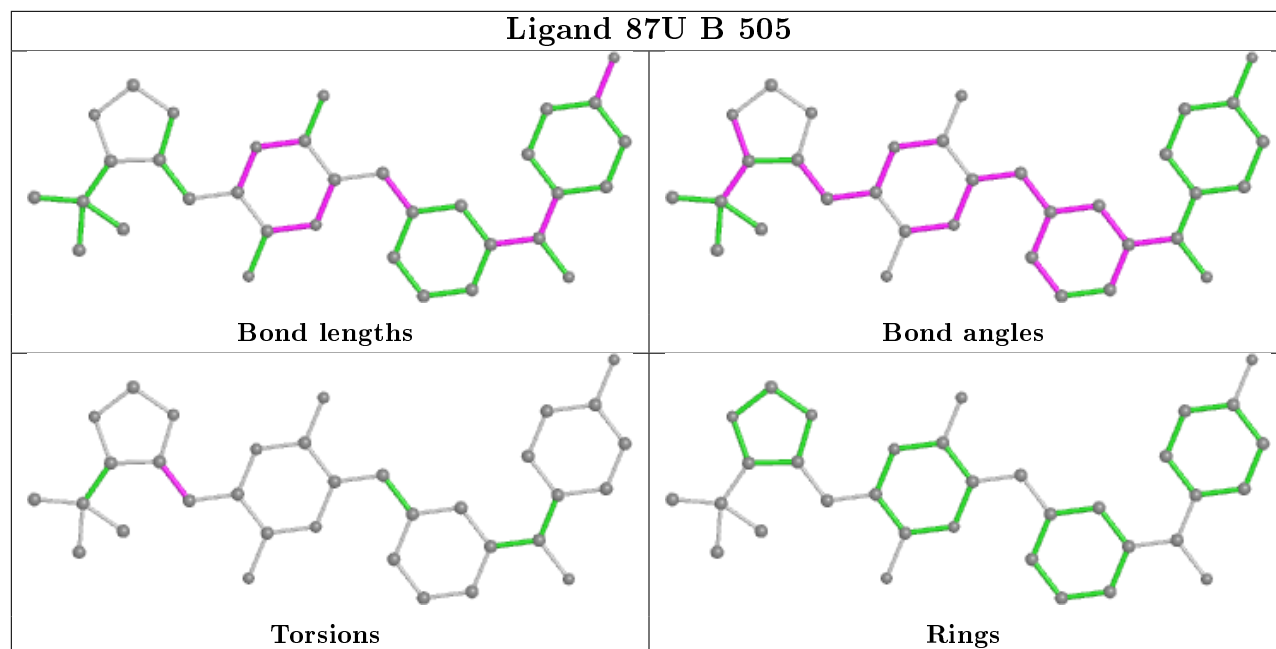
There are no ring outliers.

2 monomers are involved in 3 short contacts:

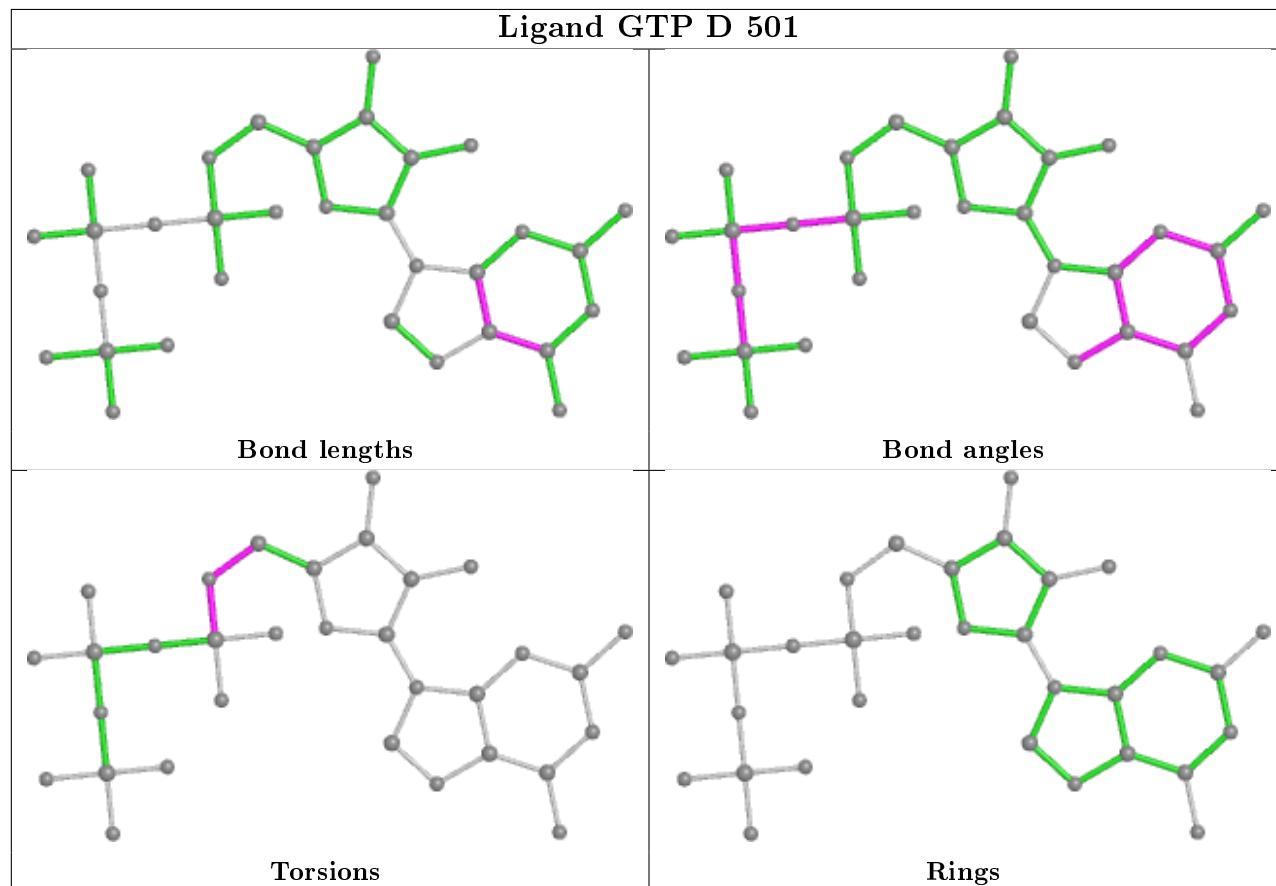
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	87U	2	0
9	B	507	MES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

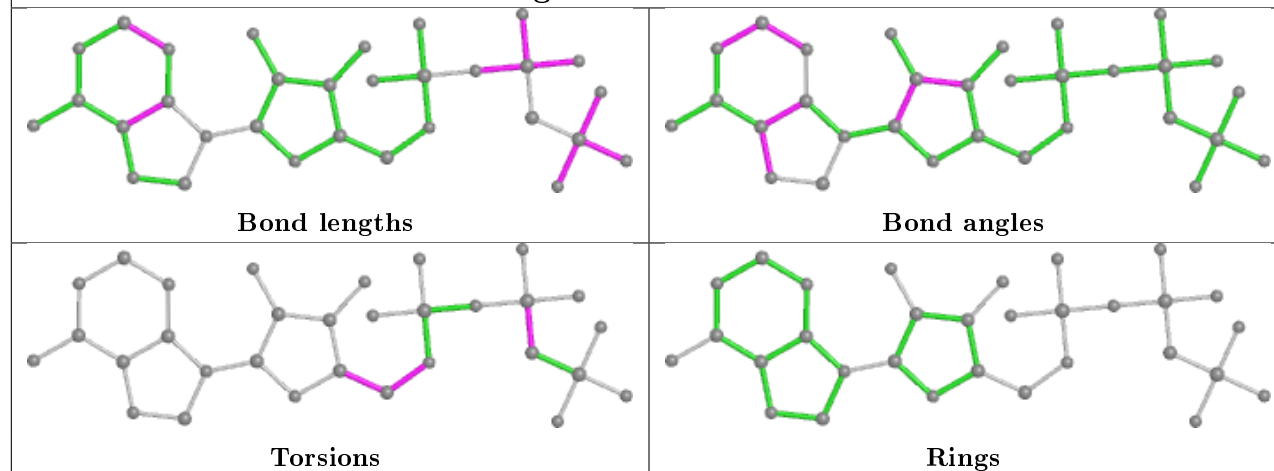
Ligand 87U B 505



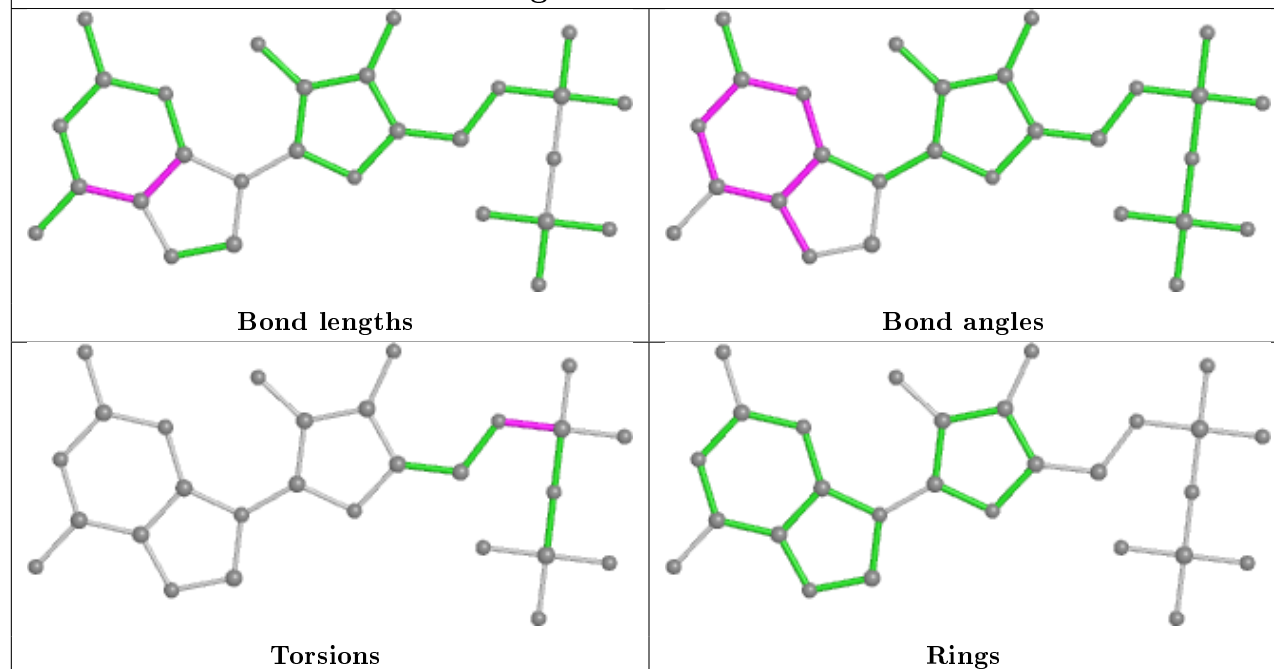
Ligand GTP D 501

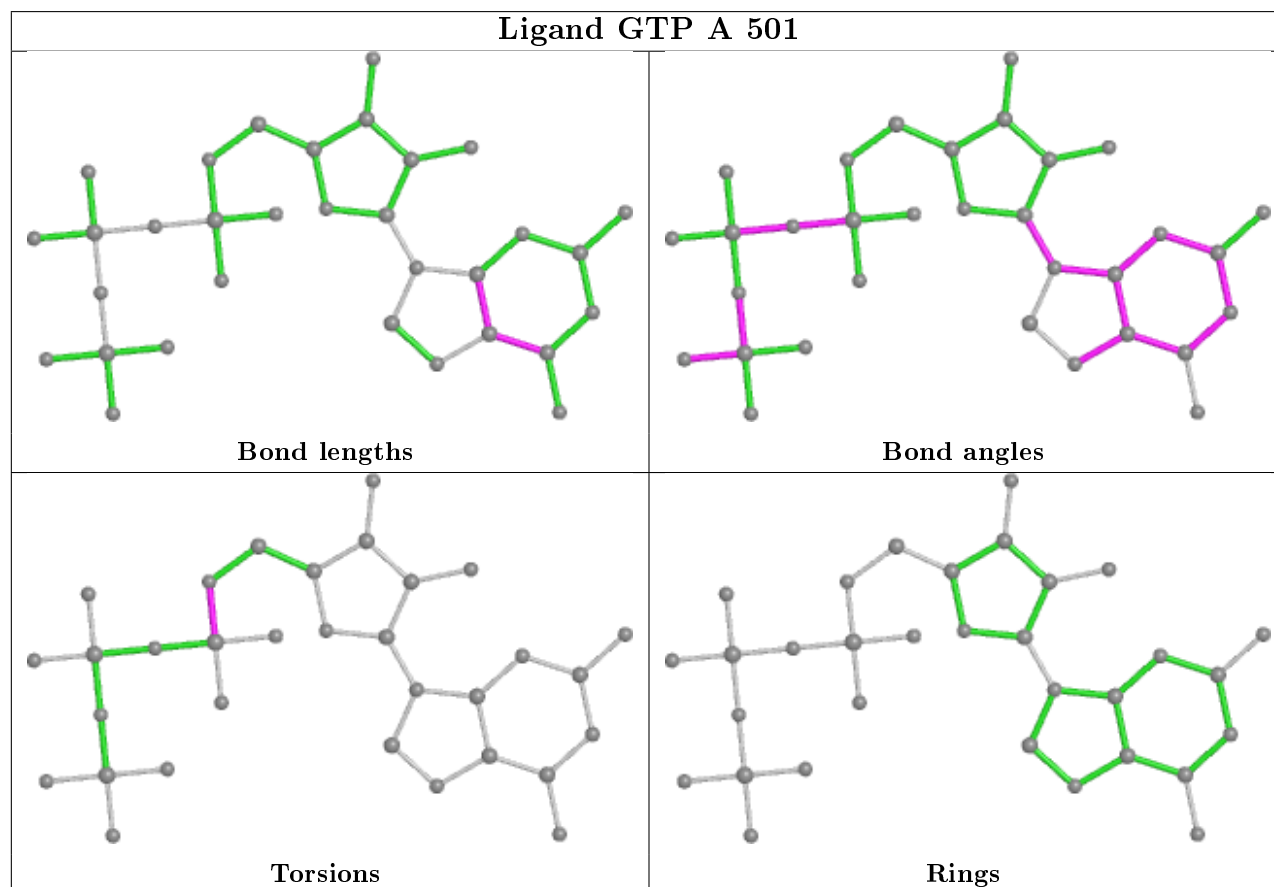
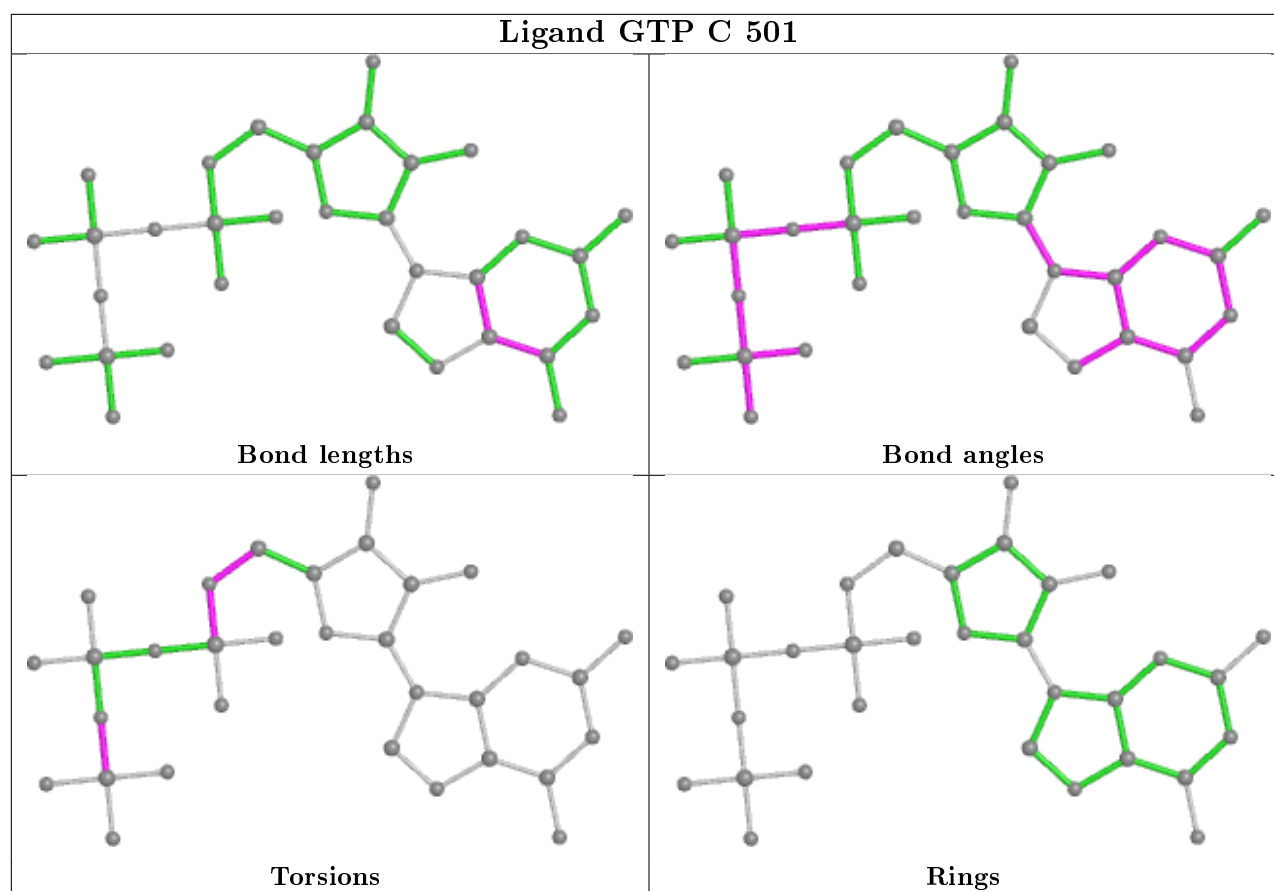


Ligand ACP F 401



Ligand GDP B 502





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	437/450 (97%)	0.20	20 (4%) 32 39	23, 45, 71, 91	0
1	C	440/450 (97%)	-0.08	2 (0%) 91 94	19, 36, 58, 80	1 (0%)
2	B	424/445 (95%)	0.21	14 (3%) 46 54	25, 45, 75, 102	1 (0%)
2	D	421/445 (94%)	0.79	56 (13%) 3 4	35, 64, 96, 126	4 (0%)
3	E	120/184 (65%)	0.64	11 (9%) 9 10	34, 64, 95, 106	0
4	F	309/384 (80%)	1.06	71 (22%) 0 0	35, 68, 107, 122	0
All	All	2151/2358 (91%)	0.41	174 (8%) 12 14	19, 51, 92, 126	6 (0%)

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	182	ILE	9.1
2	D	37	HIS	8.3
4	F	233	PHE	6.4
2	D	395	LEU	5.7
4	F	100	ILE	5.5

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

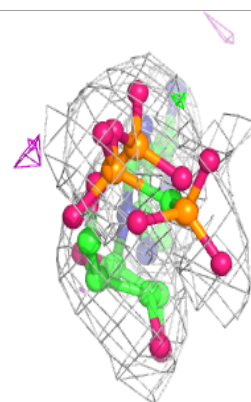
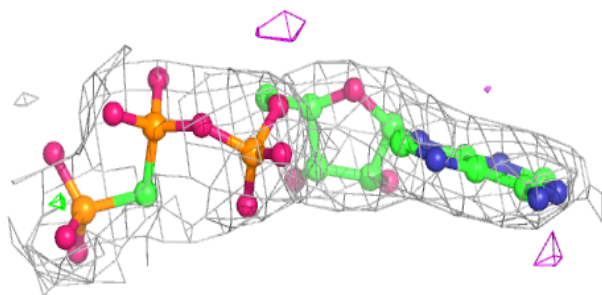
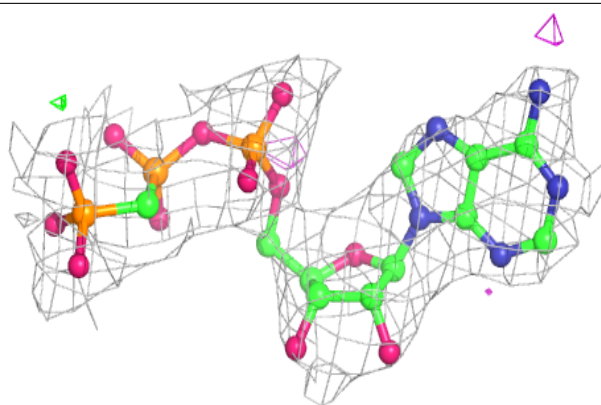
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	D	502	1/1	0.85	0.13	52,52,52,52	0
11	ACP	F	401	31/31	0.85	0.29	79,83,112,115	0
9	MES	B	507	12/12	0.88	0.44	95,97,101,104	0
6	CA	B	506	1/1	0.88	0.15	78,78,78,78	0
6	CA	C	503	1/1	0.89	0.10	56,56,56,56	0
9	MES	B	504	12/12	0.89	0.21	70,74,76,78	0
5	GTP	D	501	32/32	0.93	0.17	45,49,67,70	0
10	87U	B	505	34/34	0.94	0.20	48,54,55,55	0
6	CA	A	502	1/1	0.96	0.13	67,67,67,67	0
7	MG	B	503	1/1	0.97	0.11	24,24,24,24	0
8	GDP	B	502	28/28	0.98	0.15	22,25,26,28	0
7	MG	C	502	1/1	0.98	0.11	24,24,24,24	0
5	GTP	C	501	32/32	0.98	0.14	24,26,28,30	0
7	MG	B	501	1/1	0.98	0.18	22,22,22,22	0
5	GTP	A	501	32/32	0.98	0.15	26,28,30,30	0

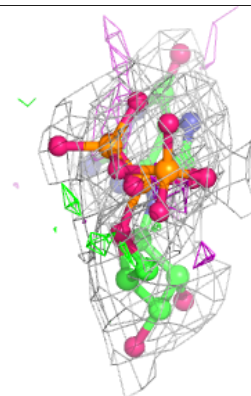
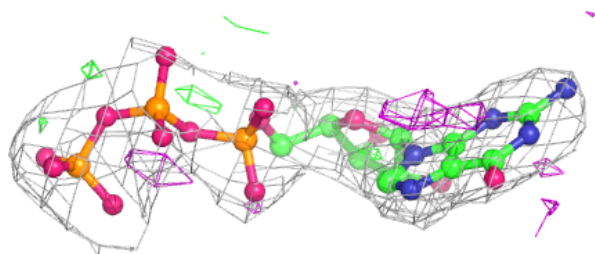
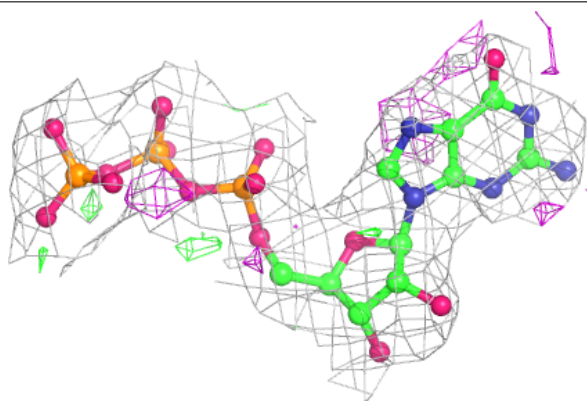
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

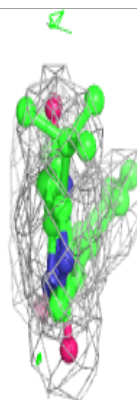
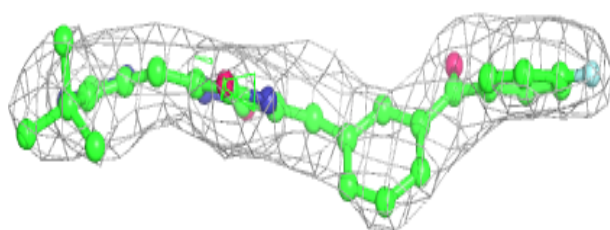
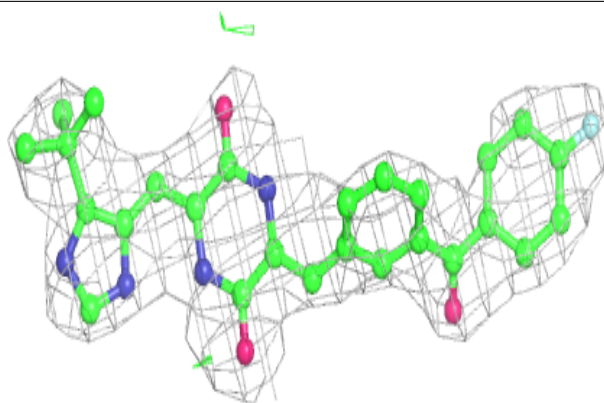
**Electron density around GTP D 501:**

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

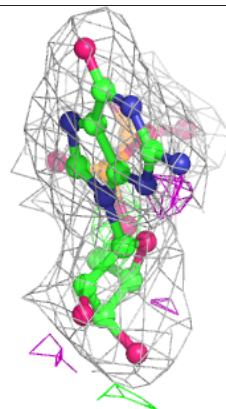
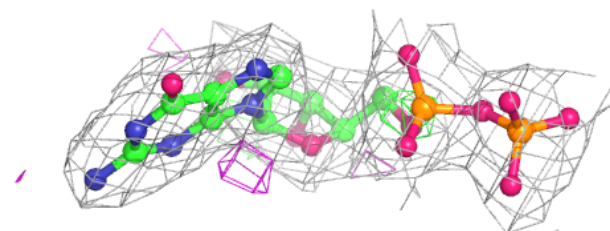
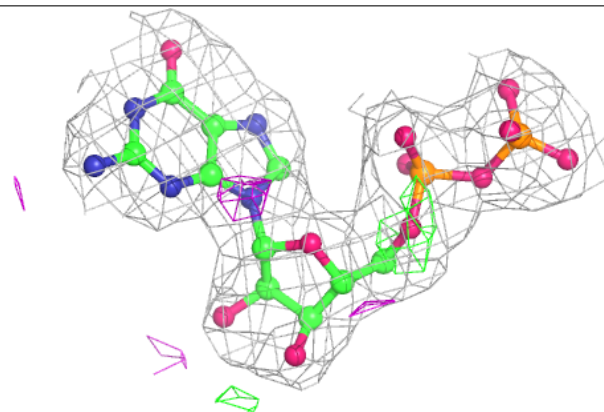


Electron density around 87U B 505:

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

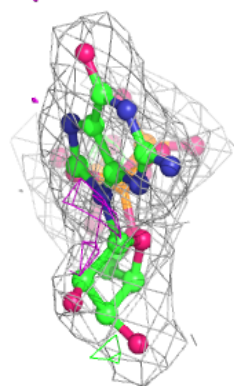
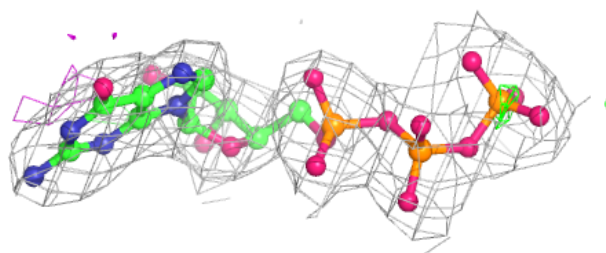
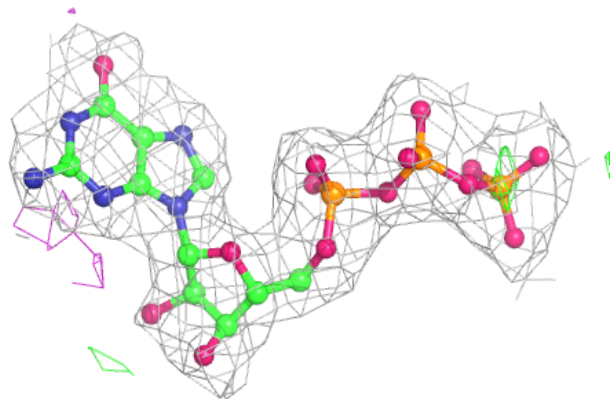
**Electron density around GDP B 502:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

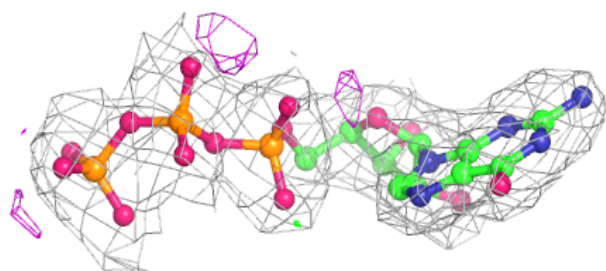
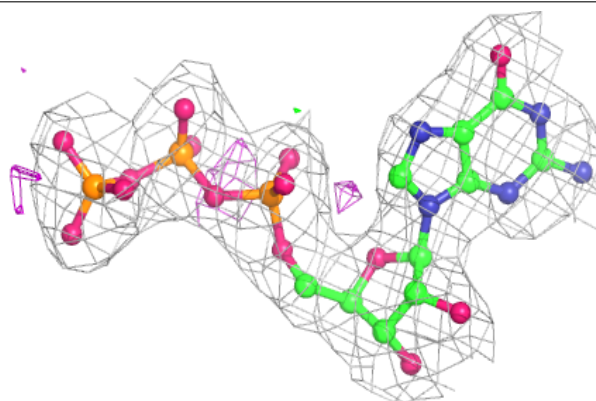


Electron density around GTP C 501:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.