



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:20 pm BST

PDB ID : 5XLZ
Title : The crystal structure of tubulin complexed with a benzylidene derivative of 9(10H)-anthracenone
Authors : Yu, Y.; Chen, Q.
Deposited on : 2017-05-12
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.11
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) : 2.11

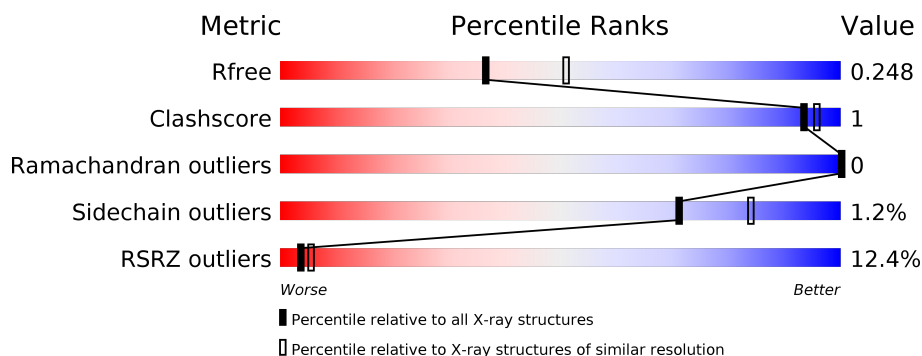
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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>5%</div> <div>95%</div> <div>• •</div> </div>
1	C	450	<div> <div>2%</div> <div>95%</div> <div>• •</div> </div>
2	B	445	<div> <div>7%</div> <div>91%</div> <div>• •</div> </div>
2	D	445	<div> <div>16%</div> <div>90%</div> <div>• 5%</div> </div>
3	E	143	<div> <div>10%</div> <div>83%</div> <div>• 15%</div> </div>
4	F	384	<div> <div>33%</div> <div>82%</div> <div>5% 13%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 35306 atoms, of which 16927 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
1	A	437	Total	C	H	N	O	S	0	7	0
			6791	2179	3345	586	657	24			
1	C	440	Total	C	H	N	O	S	0	4	0
			6806	2184	3351	587	659	25			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	4	0
			6629	2121	3248	581	653	26			
2	D	421	Total	C	H	N	O	S	0	1	0
			6510	2086	3190	566	641	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	2	0
			2031	623	1021	184	198	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	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
4	F	334	Total	C	H	N	O	S	0	2	0
			5460	1766	2707	472	501	14			

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
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

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

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

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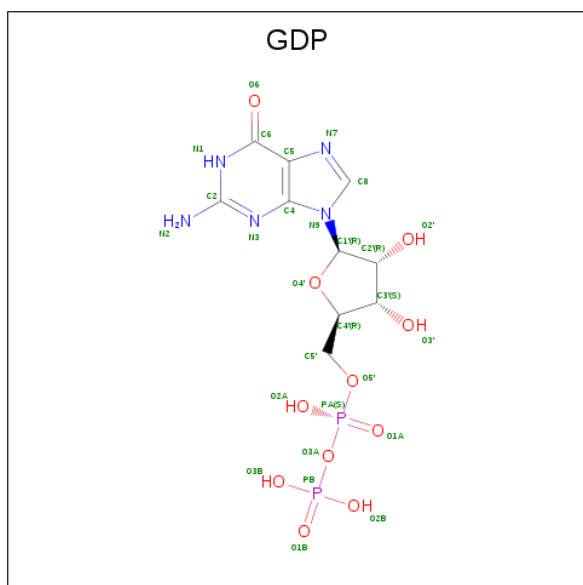
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



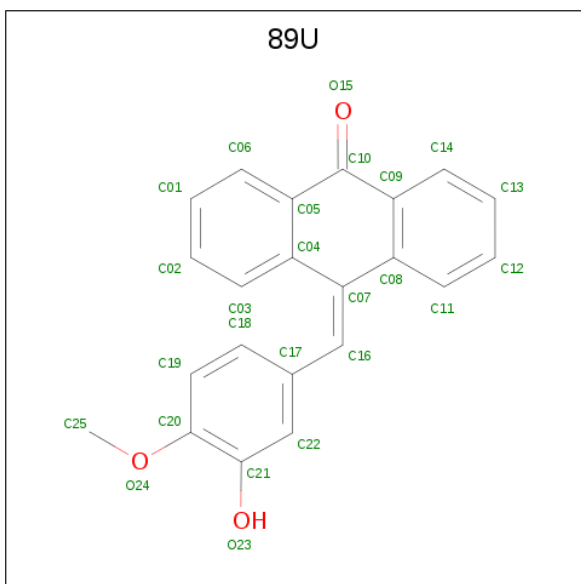
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
8	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		
9	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 10 is 10-[(4-methoxy-3-oxidanyl-phenyl)methylidene]anthracen-9-one (three-letter code: 89U) (formula: C₂₂H₁₆O₃).



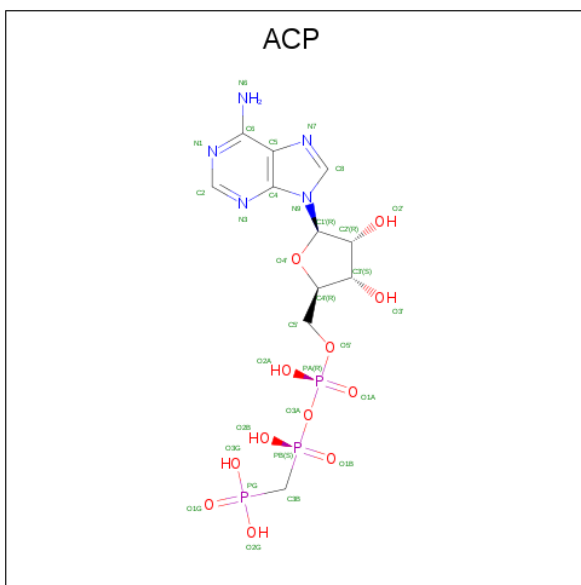
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			25	22	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			25	22	3		

- 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
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

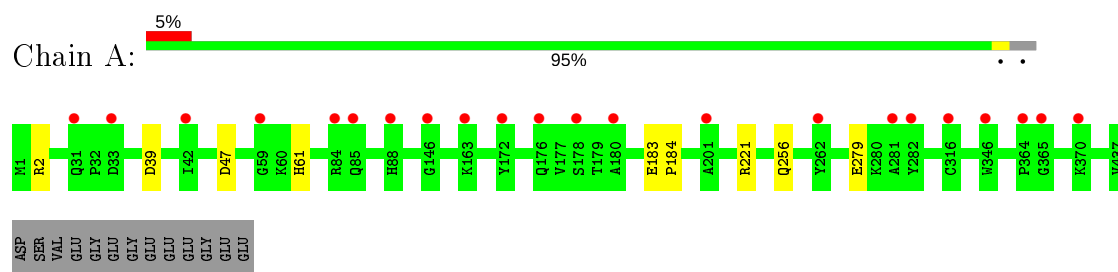
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	150	Total	O	0	0
			150	150		
12	B	153	Total	O	0	0
			153	153		
12	C	286	Total	O	0	0
			286	286		
12	D	85	Total	O	0	0
			85	85		
12	E	36	Total	O	0	0
			36	36		
12	F	69	Total	O	0	0
			69	69		

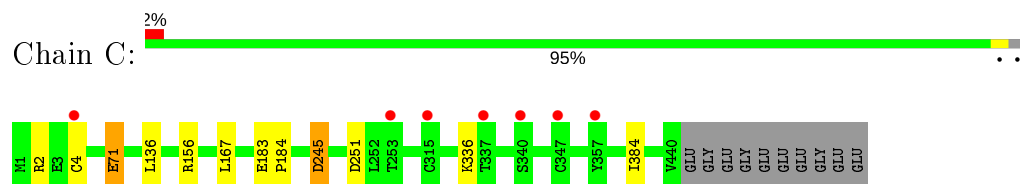
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

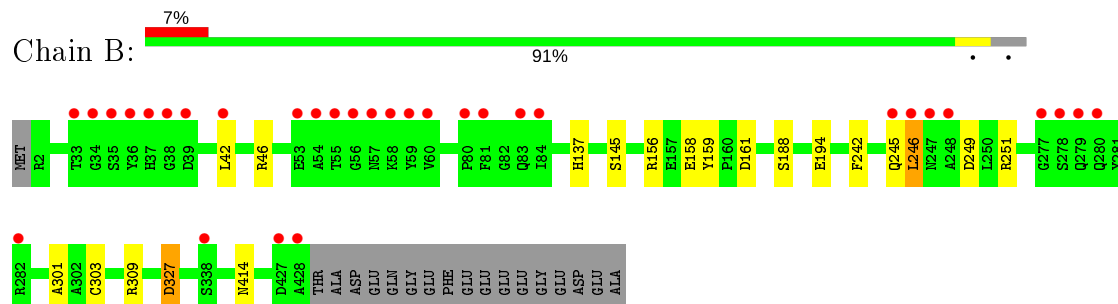
- Molecule 1: Tubulin alpha-1B chain



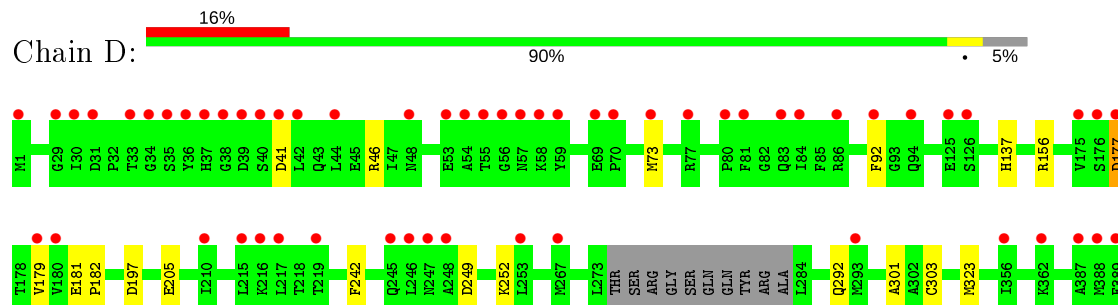
- Molecule 1: Tubulin alpha-1B chain

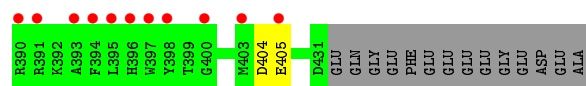


- Molecule 2: Tubulin beta-2B chain

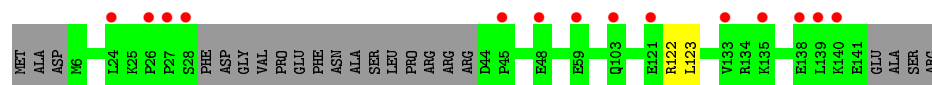
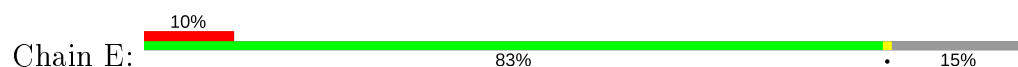


- Molecule 2: Tubulin beta-2B chain

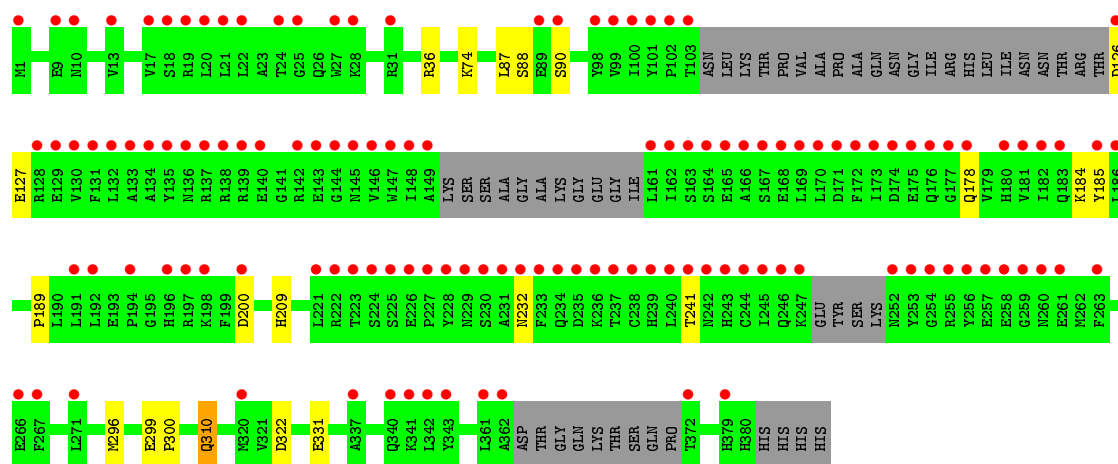
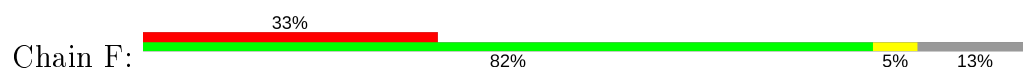




● Molecule 3: Stathmin-4



● Molecule 4: Tubulin Tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.47Å 158.44Å 181.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.67 – 2.30 48.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (42.67-2.30) 98.0 (48.24-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.216 , 0.247 0.221 , 0.248	Depositor DCC
R_{free} test set	1343 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.9	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	0.93	EDS
Total number of atoms	35306	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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, 89U, CA, 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	0.22	0/3548	0.38	0/4815
1	C	0.22	0/3539	0.38	0/4805
2	B	0.22	0/3473	0.40	1/4702 (0.0%)
2	D	0.22	0/3393	0.37	0/4595
3	E	0.21	0/1027	0.32	0/1363
4	F	0.21	0/2821	0.36	0/3811
All	All	0.22	0/17801	0.38	1/24091 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	246	LEU	C-N-CA	7.39	140.18	121.70

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	3446	3345	3322	5	0
1	C	3455	3351	3357	7	0
2	B	3381	3248	3238	12	0
2	D	3320	3190	3201	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1010	1021	1014	2	0
4	F	2753	2707	2712	13	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	10	12	0	0
9	B	24	25	25	0	0
10	B	25	0	0	0	0
10	D	25	0	0	0	0
11	F	31	0	14	1	0
12	A	150	0	0	1	0
12	B	153	0	0	5	0
12	C	286	0	0	3	0
12	D	85	0	0	2	0
12	E	36	0	0	0	0
12	F	69	0	0	3	0
All	All	18379	16927	16931	47	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.

All (47) 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:159:TYR:N	12:B:601:HOH:O	2.07	0.88
2:B:414:ASN:ND2	12:B:602:HOH:O	2.18	0.75
2:B:161:ASP:O	2:B:251[B]:ARG:NH2	2.27	0.67
1:C:156:ARG:NH1	12:C:607:HOH:O	2.28	0.66
1:A:221:ARG:NH2	2:B:327:ASP:OD2	2.30	0.65
2:D:292:GLN:NE2	12:D:604:HOH:O	2.30	0.63
12:D:601:HOH:O	3:E:122:ARG:NH2	2.34	0.61
4:F:126:ASP:N	12:F:505:HOH:O	2.36	0.59
2:B:158:GLU:N	12:B:601:HOH:O	2.35	0.58
2:D:404:ASP:OD1	2:D:405:GLU:N	2.36	0.58
4:F:331:GLU:OE2	11:F:401:ACP:H3B2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:SER:OG	2:B:188:SER:OG	2.21	0.57
1:C:245:ASP:N	1:C:245:ASP:OD1	2.38	0.57
2:B:145:SER:HG	2:B:188:SER:HG	1.54	0.56
4:F:184:LYS:NZ	4:F:185:TYR:O	2.38	0.56
4:F:178:GLN:OE1	4:F:178:GLN:N	2.40	0.55
2:D:46:ARG:NH1	2:D:242:PHE:O	2.41	0.54
1:C:336:LYS:NZ	12:C:621:HOH:O	2.40	0.53
2:D:156:ARG:NH1	2:D:197:ASP:OD2	2.41	0.52
4:F:126:ASP:OD1	4:F:127:GLU:N	2.43	0.52
2:B:309:ARG:NH1	12:B:617:HOH:O	2.42	0.52
1:A:2:ARG:NH2	12:A:619:HOH:O	2.43	0.51
1:C:71:GLU:O	12:C:601:HOH:O	2.20	0.50
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.42	0.49
2:B:156:ARG:NH1	2:B:194[A]:GLU:O	2.46	0.49
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.53	0.48
4:F:232:ASN:O	12:F:501:HOH:O	2.20	0.47
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.34	0.47
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.26	0.44
2:D:177:ASP:N	2:D:177:ASP:OD1	2.51	0.44
2:D:181:GLU:N	2:D:182:PRO:HD2	2.33	0.43
4:F:36:ARG:NH2	12:F:510:HOH:O	2.51	0.43
2:B:156:ARG:C	12:B:601:HOH:O	2.57	0.43
4:F:209:HIS:HB2	4:F:310[A]:GLN:HG2	2.02	0.42
2:D:301:ALA:O	2:D:303:CYS:N	2.53	0.42
1:C:183:GLU:N	1:C:184:PRO:CD	2.83	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.42
2:D:73:MET:HG3	2:D:92:PHE:HB3	2.03	0.41
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.03	0.41
2:D:156:ARG:HG2	3:E:123:LEU:HD11	2.03	0.41
2:B:46:ARG:NH1	2:B:242:PHE:O	2.54	0.40
2:B:301:ALA:O	2:B:303:CYS:N	2.50	0.40
4:F:299:GLU:N	4:F:300:PRO:HD2	2.36	0.40
2:D:249:ASP:OD1	2:D:252:LYS:N	2.46	0.40
4:F:189:PRO:HA	4:F:322:ASP:HA	2.01	0.40
1:A:47:ASP:OD1	1:A:47:ASP:N	2.54	0.40
4:F:87:LEU:O	4:F:88:SER:OG	2.26	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	442/450 (98%)	427 (97%)	15 (3%)	0	100	100
1	C	442/450 (98%)	433 (98%)	9 (2%)	0	100	100
2	B	429/445 (96%)	414 (96%)	15 (4%)	0	100	100
2	D	418/445 (94%)	410 (98%)	8 (2%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	326/384 (85%)	318 (98%)	8 (2%)	0	100	100
All	All	2176/2317 (94%)	2121 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	375/378 (99%)	372 (99%)	3 (1%)	81	91
1	C	375/378 (99%)	370 (99%)	5 (1%)	69	82
2	B	373/383 (97%)	367 (98%)	6 (2%)	62	78
2	D	365/383 (95%)	359 (98%)	6 (2%)	62	78
3	E	111/127 (87%)	111 (100%)	0	100	100
4	F	303/342 (89%)	299 (99%)	4 (1%)	69	82
All	All	1902/1991 (96%)	1878 (99%)	24 (1%)	71	82

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	279[A]	GLU
1	A	279[B]	GLU
2	B	42	LEU
2	B	137	HIS
2	B	245	GLN
2	B	246	LEU
2	B	249	ASP
2	B	327	ASP
1	C	2	ARG
1	C	71	GLU
1	C	245	ASP
1	C	251	ASP
1	C	384	ILE
2	D	41	ASP
2	D	137	HIS
2	D	177	ASP
2	D	179	VAL
2	D	205	GLU
2	D	323	MET
4	F	90	SER
4	F	296	MET
4	F	310[A]	GLN
4	F	310[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	6	24,30,30	1.11	2 (8%)	31,47,47	1.94	8 (25%)
5	GTP	C	501	6	26,34,34	0.95	1 (3%)	33,54,54	1.73	6 (18%)
9	MES	B	505	-	12,12,12	2.27	1 (8%)	14,16,16	1.59	4 (28%)
5	GTP	A	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.74	6 (18%)
9	MES	B	503	-	12,12,12	2.27	1 (8%)	14,16,16	2.58	6 (42%)
5	GTP	D	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.82	7 (21%)
10	89U	D	502	-	28,28,28	1.20	6 (21%)	40,40,40	1.19	6 (15%)
11	ACP	F	401	-	27,33,33	3.07	10 (37%)	32,52,52	4.36	12 (37%)
10	89U	B	504	-	28,28,28	1.28	7 (25%)	40,40,40	1.12	5 (12%)

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	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
9	MES	B	505	-	-	5/6/14/14	0/1/1/1
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
5	GTP	D	501	6	-	6/18/38/38	0/3/3/3
10	89U	D	502	-	-	2/6/22/22	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	-	-	8/15/38/38	0/3/3/3
10	89U	B	504	-	-	2/6/22/22	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	8.06	1.67	1.58
9	B	503	MES	C8-S	-7.62	1.66	1.77
9	B	505	MES	C8-S	-7.59	1.66	1.77
11	F	401	ACP	O4'-C1'	7.12	1.51	1.41
11	F	401	ACP	PB-O1B	6.15	1.66	1.51
11	F	401	ACP	C2-N3	5.00	1.40	1.32
11	F	401	ACP	PG-O3G	4.25	1.64	1.54
8	B	501	GDP	C6-C5	3.89	1.48	1.41
11	F	401	ACP	C2-N1	3.24	1.39	1.33
5	A	501	GTP	C6-N1	3.04	1.38	1.33
5	D	501	GTP	C6-N1	3.01	1.38	1.33
5	C	501	GTP	C6-N1	3.01	1.38	1.33
11	F	401	ACP	C5-C4	-2.88	1.33	1.40
11	F	401	ACP	C6-C5	-2.79	1.32	1.43
11	F	401	ACP	PG-O2G	2.67	1.61	1.54
10	D	502	89U	C08-C07	2.42	1.53	1.47
11	F	401	ACP	C2'-C1'	-2.38	1.50	1.53
10	B	504	89U	C08-C07	2.34	1.53	1.47
10	B	504	89U	O24-C20	2.33	1.40	1.37
10	B	504	89U	C04-C07	2.33	1.53	1.47
10	B	504	89U	C09-C10	2.32	1.53	1.48
8	B	501	GDP	C5-C4	2.32	1.47	1.40
10	D	502	89U	C04-C07	2.31	1.53	1.47
10	D	502	89U	C09-C10	2.26	1.53	1.48
10	D	502	89U	C05-C10	2.21	1.53	1.48
10	B	504	89U	C05-C10	2.21	1.53	1.48
10	B	504	89U	O15-C10	-2.16	1.18	1.22
10	B	504	89U	O23-C21	2.11	1.40	1.36
10	D	502	89U	O15-C10	-2.08	1.19	1.22
10	D	502	89U	O23-C21	2.03	1.40	1.36

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	O4'-C4'-C3'	-14.92	75.60	105.11
11	F	401	ACP	O4'-C1'-C2'	-12.59	88.52	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	N3-C2-N1	-6.70	118.21	128.68
11	F	401	ACP	O5'-C5'-C4'	6.19	130.29	108.99
11	F	401	ACP	C1'-N9-C4	-6.13	115.87	126.64
11	F	401	ACP	C2'-C3'-C4'	-5.51	91.94	102.64
5	D	501	GTP	N3-C2-N1	-5.42	119.99	127.22
5	A	501	GTP	N3-C2-N1	-5.29	120.17	127.22
5	C	501	GTP	N3-C2-N1	-5.20	120.28	127.22
9	B	503	MES	C7-N4-C5	5.01	124.05	111.23
11	F	401	ACP	O2B-PB-C3B	4.59	125.38	106.58
9	B	503	MES	C6-C5-N4	-4.57	103.17	110.10
8	B	501	GDP	C6-C5-C4	-4.43	116.57	120.80
9	B	503	MES	C5-N4-C3	4.42	118.78	108.83
8	B	501	GDP	C6-N1-C2	4.38	122.90	115.93
8	B	501	GDP	C2-N3-C4	4.38	120.36	115.36
5	D	501	GTP	C2-N3-C4	4.15	120.09	115.36
5	A	501	GTP	C2-N3-C4	4.06	120.00	115.36
5	C	501	GTP	C2-N3-C4	4.06	119.99	115.36
8	B	501	GDP	C5-C6-N1	-3.92	118.07	123.43
5	D	501	GTP	PB-O3B-PG	-3.76	119.93	132.83
10	B	504	89U	O24-C20-C21	3.71	119.94	114.57
9	B	505	MES	C5-N4-C3	3.53	116.78	108.83
8	B	501	GDP	N3-C2-N1	-3.47	122.60	127.22
10	D	502	89U	O24-C20-C21	3.19	119.19	114.57
11	F	401	ACP	C5-C6-N6	-3.19	115.50	120.35
5	C	501	GTP	PB-O3B-PG	-3.19	121.88	132.83
5	A	501	GTP	PB-O3B-PG	-3.16	121.98	132.83
5	D	501	GTP	PA-O3A-PB	-3.00	122.54	132.83
5	C	501	GTP	C5-C6-N1	-2.99	119.34	123.43
5	A	501	GTP	C5-C6-N1	-2.98	119.36	123.43
8	B	501	GDP	PA-O3A-PB	-2.97	122.64	132.83
5	D	501	GTP	C5-C6-N1	-2.94	119.41	123.43
5	C	501	GTP	PA-O3A-PB	-2.91	122.85	132.83
5	A	501	GTP	PA-O3A-PB	-2.87	122.97	132.83
9	B	505	MES	O2S-S-C8	2.77	110.25	106.92
10	D	502	89U	C25-O24-C20	-2.76	113.36	117.53
5	D	501	GTP	C6-N1-C2	2.71	120.23	115.93
11	F	401	ACP	O2G-PG-C3B	-2.62	100.05	106.40
5	A	501	GTP	C6-N1-C2	2.62	120.09	115.93
11	F	401	ACP	O1G-PG-C3B	2.62	116.89	111.24
10	D	502	89U	C08-C07-C04	2.61	120.00	114.88
5	C	501	GTP	C6-N1-C2	2.59	120.05	115.93
10	B	504	89U	C08-C07-C04	2.59	119.97	114.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O2S-S-C8	2.52	109.95	106.92
8	B	501	GDP	C4-C5-N7	-2.50	106.80	109.40
10	B	504	89U	C11-C08-C07	-2.48	117.76	122.64
10	D	502	89U	C11-C08-C07	-2.47	117.79	122.64
10	B	504	89U	C03-C04-C07	-2.43	117.86	122.64
10	D	502	89U	C03-C04-C07	-2.42	117.87	122.64
9	B	503	MES	O1S-S-C8	2.35	109.74	106.92
9	B	505	MES	O1S-S-C8	2.34	109.73	106.92
10	D	502	89U	O24-C20-C19	-2.34	120.36	124.37
11	F	401	ACP	O3G-PG-O2G	-2.28	101.43	108.08
10	B	504	89U	O24-C20-C19	-2.10	120.77	124.37
11	F	401	ACP	O2B-PB-O1B	2.10	117.09	110.07
9	B	505	MES	O3S-S-C8	2.09	109.16	105.77
9	B	503	MES	C7-N4-C3	2.09	116.59	111.23
5	D	501	GTP	C3'-C2'-C1'	2.03	104.03	100.98
8	B	501	GDP	O2B-PB-O3A	2.02	111.42	104.64

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	505	MES	C7-C8-S-O1S
9	B	505	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
10	D	502	89U	C04-C07-C16-C17
10	D	502	89U	C08-C07-C16-C17
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	C4'-C5'-O5'-PA
11	F	401	ACP	O4'-C4'-C5'-O5'
10	B	504	89U	C04-C07-C16-C17

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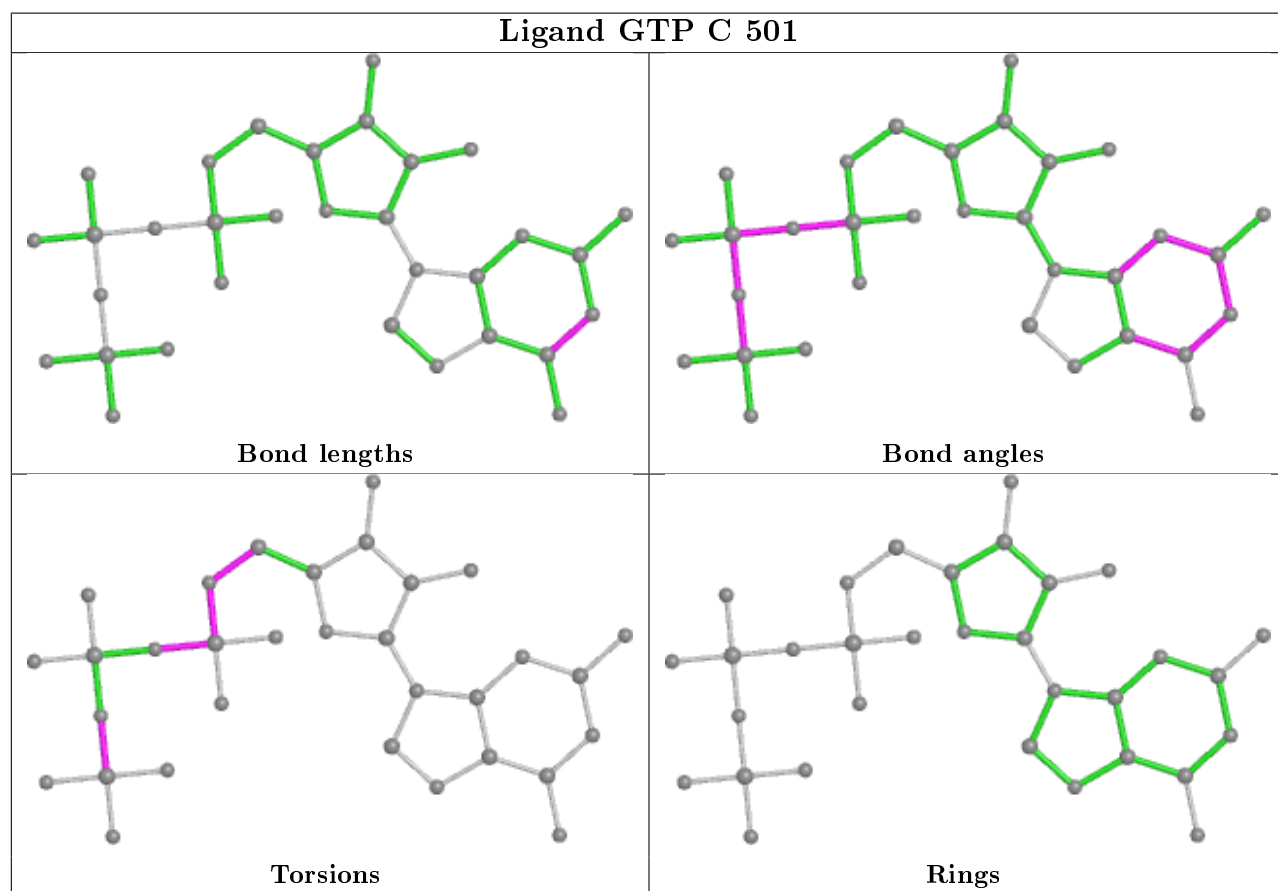
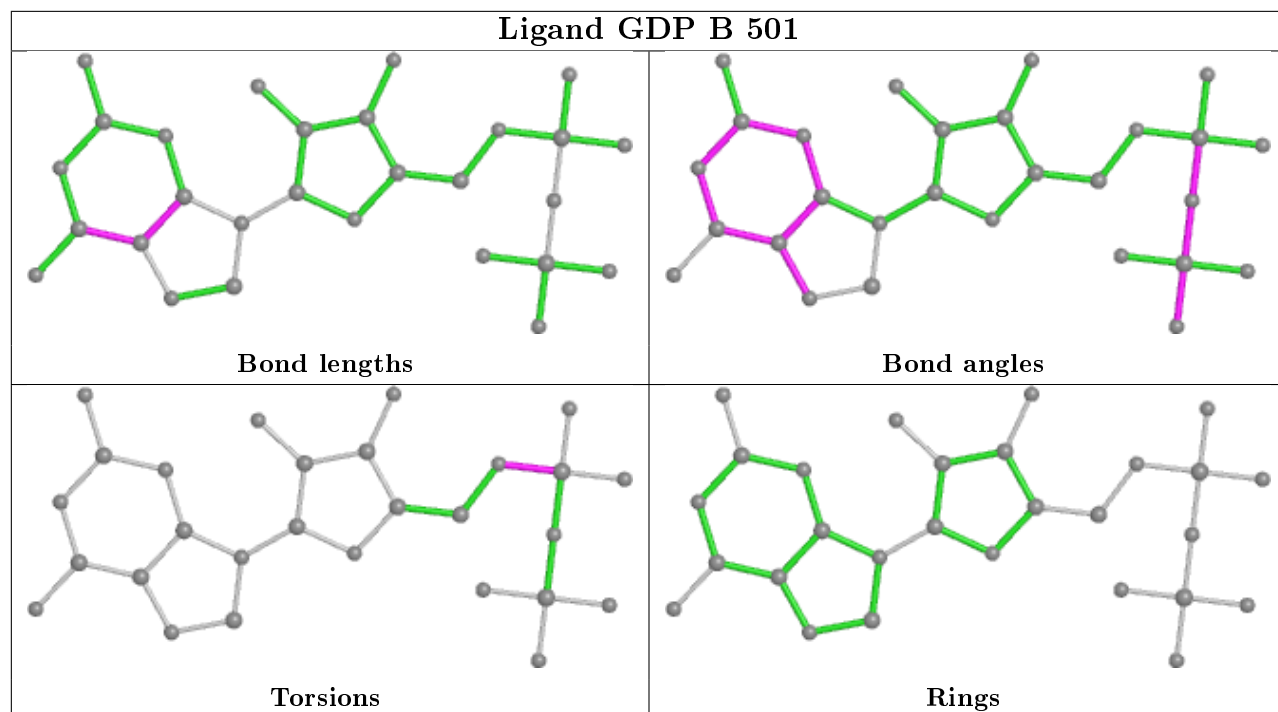
Mol	Chain	Res	Type	Atoms
10	B	504	89U	C08-C07-C16-C17
11	F	401	ACP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3B-PG-O1G
9	B	505	MES	C8-C7-N4-C5
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
9	B	505	MES	C7-C8-S-O2S
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PG-C3B-PB-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	C4'-C5'-O5'-PA
9	B	505	MES	C8-C7-N4-C3
11	F	401	ACP	PB-O3A-PA-O2A
5	D	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O3G
8	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O1G

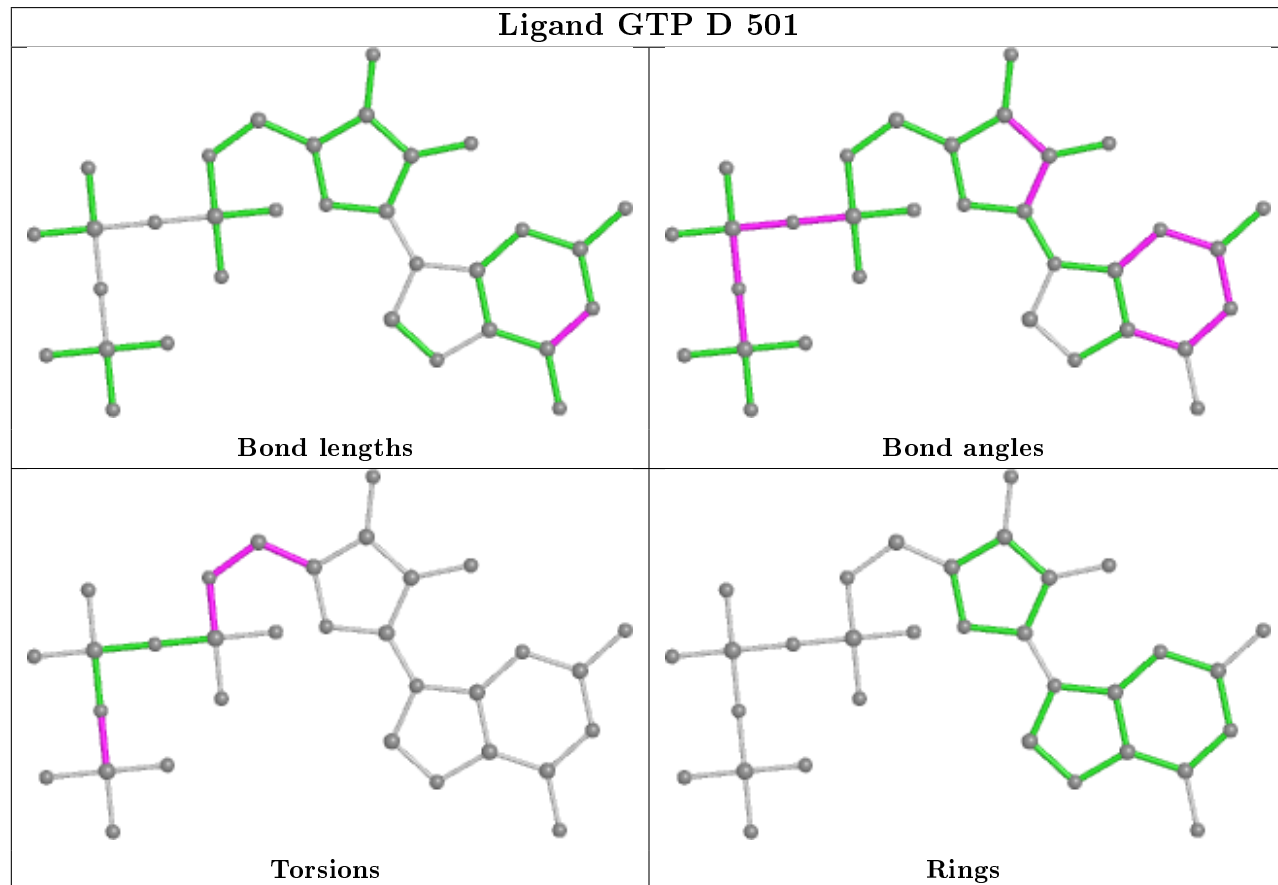
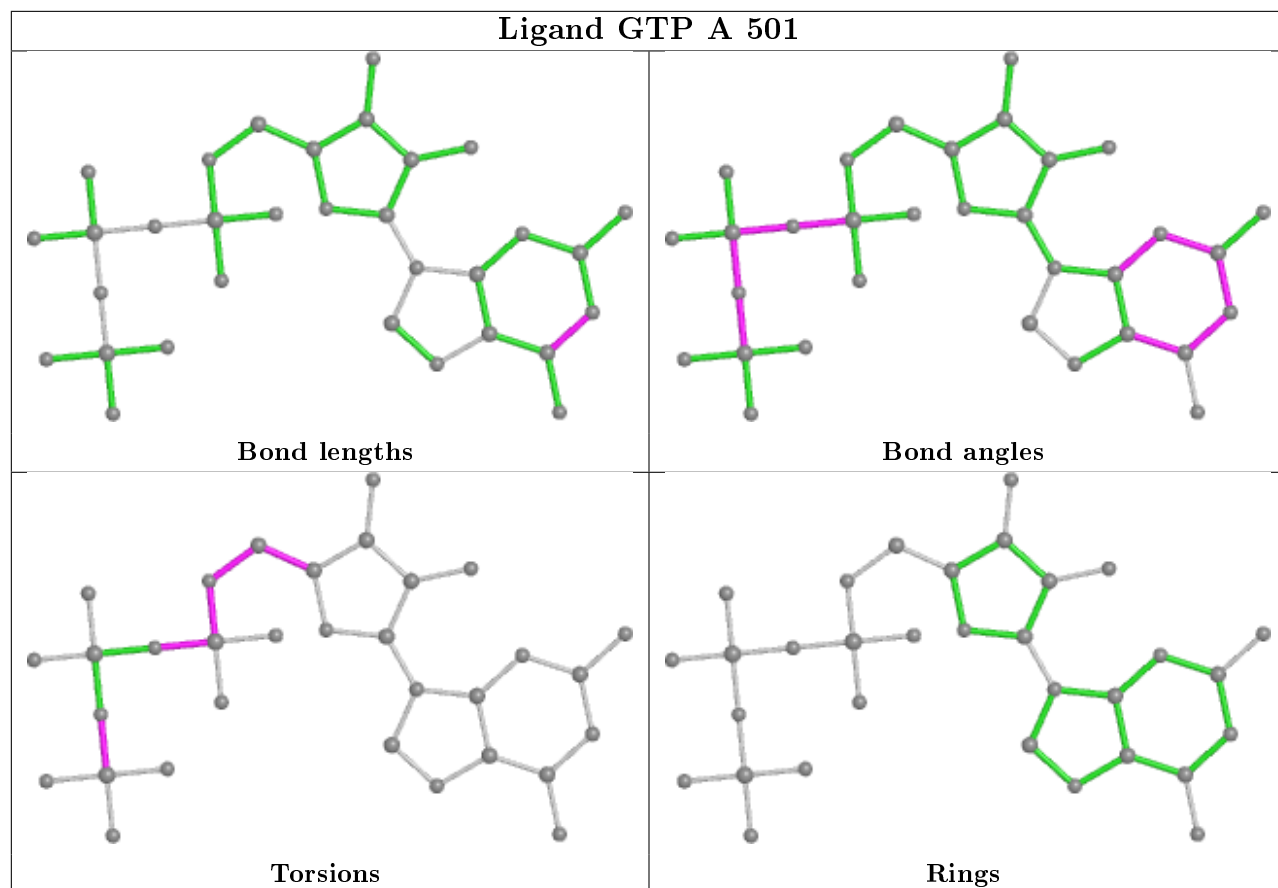
There are no ring outliers.

1 monomer is involved in 1 short contact:

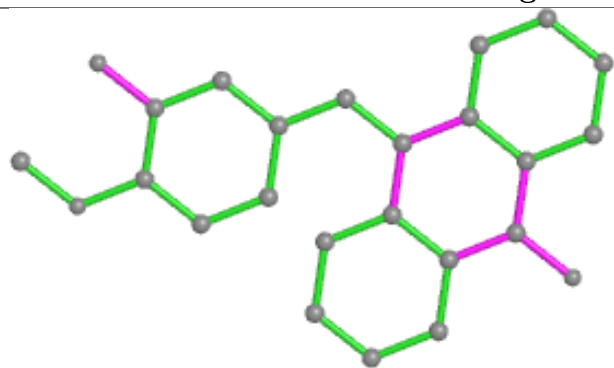
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	1	0

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.

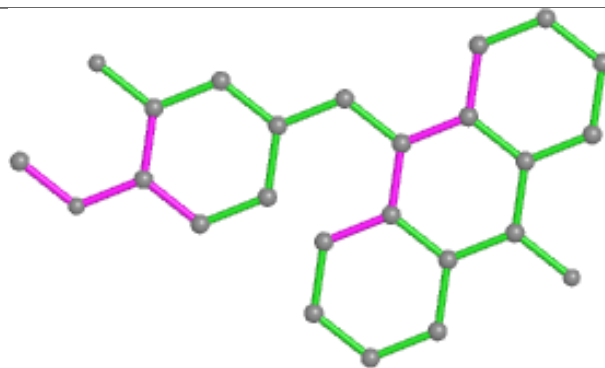




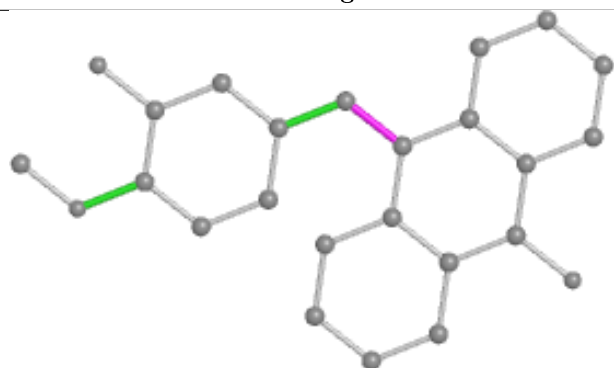
Ligand 89U D 502



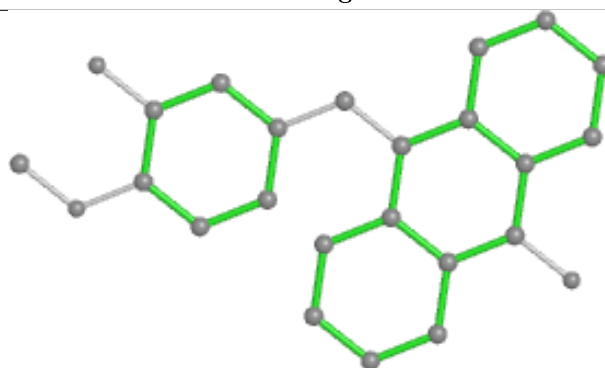
Bond lengths



Bond angles

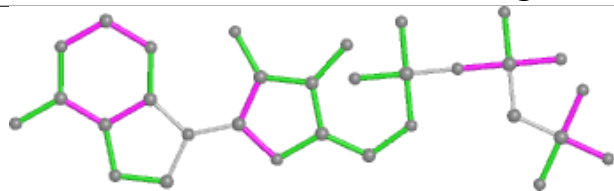


Torsions

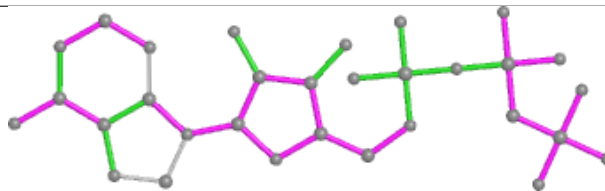


Rings

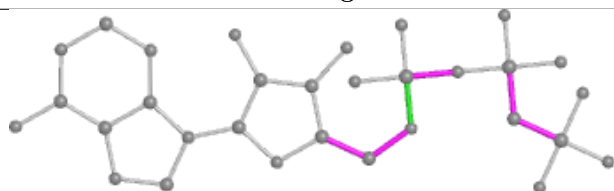
Ligand ACP F 401



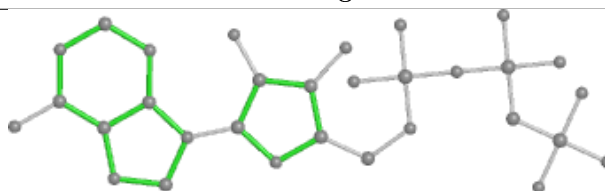
Bond lengths



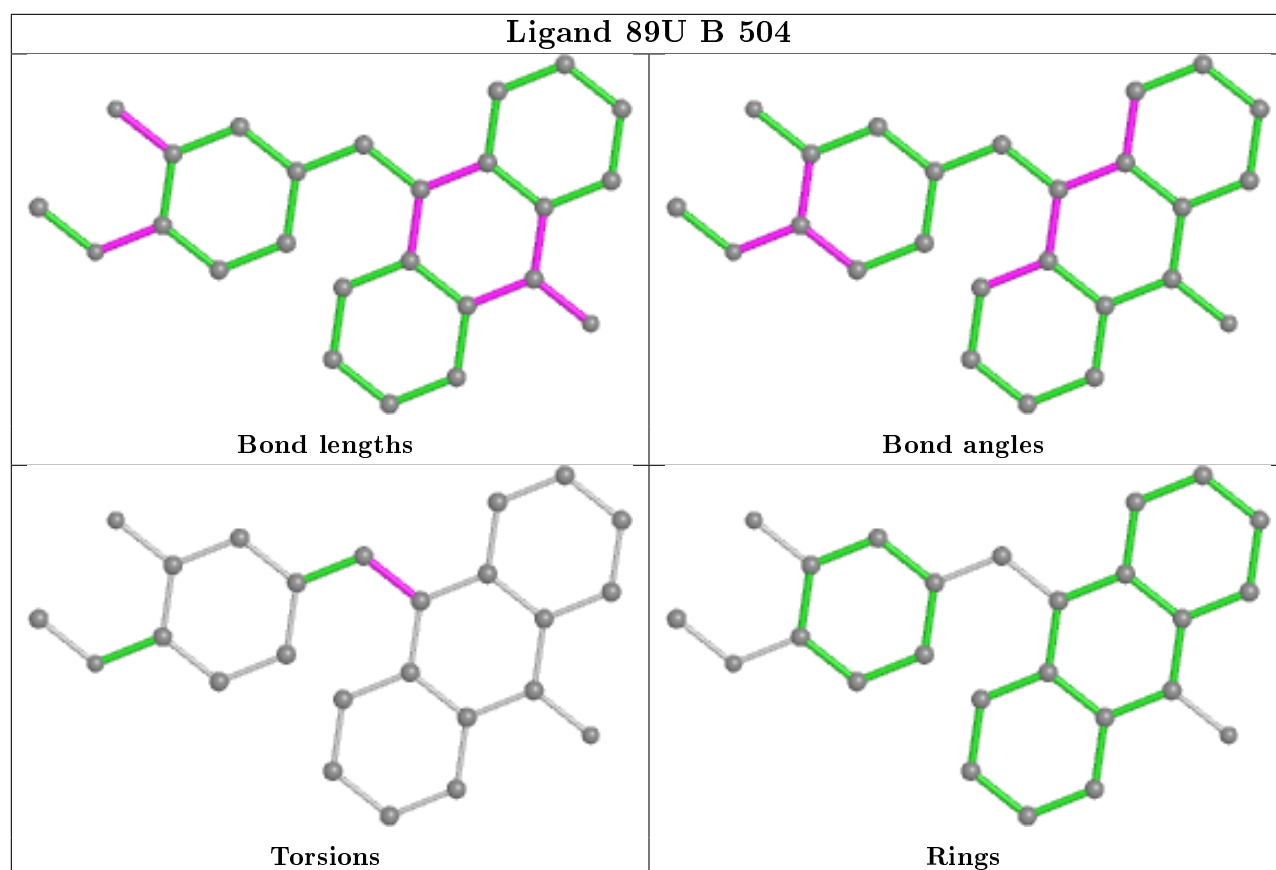
Bond angles



Torsions



Rings



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 ⓘ

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, 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%)	0.46	22 (5%) 28 35	20, 37, 65, 92	0
1	C	440/450 (97%)	0.09	7 (1%) 72 77	13, 26, 52, 71	0
2	B	427/445 (95%)	0.43	32 (7%) 14 19	16, 36, 74, 126	0
2	D	421/445 (94%)	0.95	69 (16%) 1 2	22, 50, 88, 114	0
3	E	121/143 (84%)	0.69	14 (11%) 4 6	23, 51, 84, 99	0
4	F	334/384 (86%)	2.00	127 (38%) 0 0	30, 62, 134, 147	0
All	All	2180/2317 (94%)	0.72	271 (12%) 4 5	13, 41, 95, 147	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	11.4
4	F	244	CYS	10.6
4	F	233	PHE	10.5
4	F	245	ILE	10.0
4	F	253	TYR	10.0
4	F	169	LEU	9.9
4	F	240	LEU	9.9
4	F	231	ALA	9.8
4	F	243	HIS	9.8
4	F	234	GLN	8.9
2	B	57	ASN	8.6
4	F	225	SER	8.5
2	B	56	GLY	8.1
4	F	259	GLY	8.0
4	F	232	ASN	8.0
4	F	130	VAL	7.5
4	F	239	HIS	7.4
2	D	55	THR	7.4
4	F	247	LYS	7.2

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Mol	Chain	Res	Type	RSRZ
4	F	254	GLY	7.2
4	F	256	TYR	7.2
2	D	247	ASN	7.1
4	F	246	GLN	7.0
4	F	236	LYS	7.0
4	F	182	ILE	6.9
4	F	103	THR	6.8
4	F	138	ARG	6.7
4	F	177	GLY	6.5
2	B	55	THR	6.5
4	F	161	LEU	6.4
4	F	22	LEU	6.1
4	F	255	ARG	6.1
4	F	170	LEU	6.1
4	F	237	THR	6.0
4	F	101	TYR	5.9
4	F	166	ALA	5.9
2	D	390	ARG	5.8
2	B	279	GLN	5.7
4	F	139	ARG	5.7
4	F	252	ASN	5.6
4	F	238	CYS	5.6
4	F	136	ASN	5.5
4	F	133	ALA	5.5
4	F	132	LEU	5.4
1	A	282	TYR	5.4
4	F	142	ARG	5.4
2	D	397	TRP	5.3
4	F	226	GLU	5.3
4	F	258	GLU	5.3
2	D	177	ASP	5.2
4	F	235	ASP	5.1
2	D	394	PHE	5.1
4	F	176	GLN	5.1
2	D	245	GLN	5.1
4	F	99	VAL	5.0
2	B	54	ALA	4.9
2	B	58	LYS	4.8
4	F	257	GLU	4.8
4	F	167	SER	4.8
4	F	137	ARG	4.8
4	F	362	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
4	F	131	PHE	4.7
4	F	260	ASN	4.7
4	F	145	ASN	4.7
4	F	242	ASN	4.6
2	D	179	VAL	4.6
4	F	180	HIS	4.6
4	F	100	ILE	4.6
4	F	102	PRO	4.6
4	F	149	ALA	4.6
4	F	172	PHE	4.6
3	E	139	LEU	4.5
4	F	241	THR	4.5
2	D	73	MET	4.5
4	F	175	GLU	4.5
4	F	135	TYR	4.4
4	F	17	VAL	4.4
4	F	194	PRO	4.4
2	D	81	PHE	4.4
4	F	178	GLN	4.2
1	A	262	TYR	4.2
4	F	197	ARG	4.2
2	D	37	HIS	4.1
4	F	223	THR	4.1
1	A	281	ALA	4.1
4	F	379	HIS	4.1
4	F	134	ALA	4.1
2	D	217	LEU	4.0
2	B	247	ASN	4.0
2	D	175	VAL	3.9
2	D	1	MET	3.9
2	B	38	GLY	3.9
4	F	191	LEU	3.9
4	F	228	TYR	3.9
2	D	391	ARG	3.8
4	F	163	SER	3.8
2	D	388	MET	3.7
4	F	227	PRO	3.7
2	D	219	THR	3.7
4	F	230	SER	3.7
4	F	126	ASP	3.6
4	F	361	LEU	3.6
4	F	372	THR	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	174	ASP	3.6
4	F	224	SER	3.6
2	D	405	GLU	3.6
4	F	128	ARG	3.6
4	F	168	GLU	3.5
4	F	162	ILE	3.5
4	F	192	LEU	3.5
4	F	196	HIS	3.5
4	F	24	THR	3.5
4	F	129	GLU	3.5
2	B	33	THR	3.5
4	F	21	LEU	3.4
3	E	28	SER	3.4
4	F	263	PHE	3.4
2	B	84	ILE	3.4
4	F	10	ASN	3.4
4	F	229	ASN	3.4
2	D	84	ILE	3.4
4	F	25	GLY	3.3
2	B	428	ALA	3.3
4	F	320	MET	3.3
2	D	356	ILE	3.3
4	F	143	GLU	3.3
2	B	37	HIS	3.3
4	F	27	TRP	3.2
4	F	90	SER	3.2
3	E	27	PRO	3.2
2	D	58	LYS	3.2
2	B	277	GLY	3.2
2	D	35	SER	3.2
2	B	34	GLY	3.2
4	F	147	TRP	3.2
4	F	20	LEU	3.2
4	F	148	ILE	3.1
4	F	342	LEU	3.1
2	D	44	LEU	3.1
2	D	362	LYS	3.1
2	B	36	TYR	3.1
2	D	54	ALA	3.1
2	B	248	ALA	3.1
4	F	144	GLY	3.1
2	B	35	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	427	ASP	3.0
2	D	180	VAL	3.0
3	E	135	LYS	3.0
3	E	26	PRO	3.0
4	F	271	LEU	3.0
3	E	48	GLU	3.0
4	F	98	TYR	3.0
1	C	340	SER	3.0
4	F	186	LEU	3.0
2	D	57	ASN	3.0
4	F	340	GLN	2.9
4	F	13	VAL	2.9
1	A	346	TRP	2.9
2	D	42	LEU	2.9
4	F	337	ALA	2.9
2	D	53	GLU	2.9
2	D	36	TYR	2.9
1	C	315[A]	CYS	2.8
3	E	140	LYS	2.8
2	D	86	ARG	2.8
1	A	365	GLY	2.8
2	D	39	ASP	2.8
2	D	210	ILE	2.8
4	F	185	TYR	2.8
3	E	45	PRO	2.8
2	D	56	GLY	2.8
2	D	70	PRO	2.7
4	F	18	SER	2.7
2	D	83	GLN	2.7
1	C	4[A]	CYS	2.7
4	F	165	GLU	2.7
2	B	59	TYR	2.7
4	F	181	VAL	2.7
2	D	94	GLN	2.7
2	B	282	ARG	2.7
4	F	171	ASP	2.7
2	D	77	ARG	2.7
1	A	370	LYS	2.7
4	F	140	GLU	2.7
2	D	246	LEU	2.6
1	A	84	ARG	2.6
2	D	400	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	280	GLN	2.6
2	D	126	SER	2.6
2	D	216	LYS	2.6
4	F	222	ARG	2.6
1	A	163	LYS	2.5
2	D	80	PRO	2.5
4	F	19	ARG	2.5
1	C	357	TYR	2.5
1	C	337	THR	2.5
2	D	31	ASP	2.5
1	A	364	PRO	2.5
2	D	29	GLY	2.5
2	D	48	ASN	2.5
2	D	125	GLU	2.5
4	F	1	MET	2.5
2	D	248	ALA	2.5
3	E	59	GLU	2.4
2	B	42	LEU	2.4
2	B	278	SER	2.4
2	D	34	GLY	2.4
4	F	341	LYS	2.4
4	F	31	ARG	2.4
2	D	38	GLY	2.4
3	E	133	VAL	2.4
4	F	266	GLU	2.4
2	D	30	ILE	2.3
1	A	59	GLY	2.3
1	A	178	SER	2.3
2	B	80	PRO	2.3
2	B	245	GLN	2.3
2	D	267	MET	2.3
4	F	183	GLN	2.3
1	A	33	ASP	2.3
1	A	180	ALA	2.3
4	F	9	GLU	2.3
2	D	33	THR	2.3
1	A	88	HIS	2.3
4	F	221	LEU	2.3
4	F	28	LYS	2.3
3	E	24	LEU	2.2
2	B	83	GLN	2.2
4	F	198	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	39	ASP	2.2
1	A	31	GLN	2.2
3	E	138	GLU	2.2
1	C	253	THR	2.2
2	B	81	PHE	2.2
2	D	92	PHE	2.2
2	D	403	MET	2.2
2	D	389	PHE	2.2
2	D	59	TYR	2.2
3	E	121	GLU	2.2
4	F	146	VAL	2.2
2	D	387	ALA	2.2
2	D	253	LEU	2.2
2	B	53	GLU	2.2
4	F	343	TYR	2.1
1	A	201	ALA	2.1
2	D	176	SER	2.1
4	F	267	PHE	2.1
3	E	103	GLN	2.1
1	A	316[A]	CYS	2.1
2	D	396	HIS	2.1
2	D	293	MET	2.1
1	A	176[A]	GLN	2.1
2	D	393	ALA	2.1
2	D	69	GLU	2.1
2	B	338	SER	2.1
1	A	42	ILE	2.1
1	C	347[A]	CYS	2.1
1	A	146	GLY	2.1
2	B	246	LEU	2.1
4	F	89	GLU	2.1
4	F	261	GLU	2.1
4	F	164	SER	2.1
1	A	85	GLN	2.0
2	B	60	VAL	2.0
2	D	41	ASP	2.0
1	A	172	TYR	2.0
2	D	398	TYR	2.0
2	D	395	LEU	2.0
4	F	200	ASP	2.0
2	D	215	LEU	2.0
2	D	40	SER	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

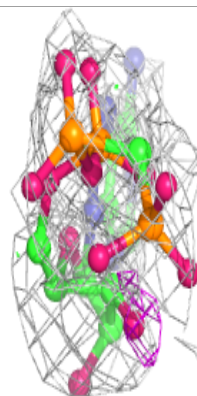
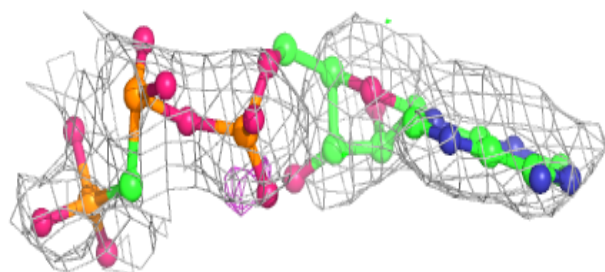
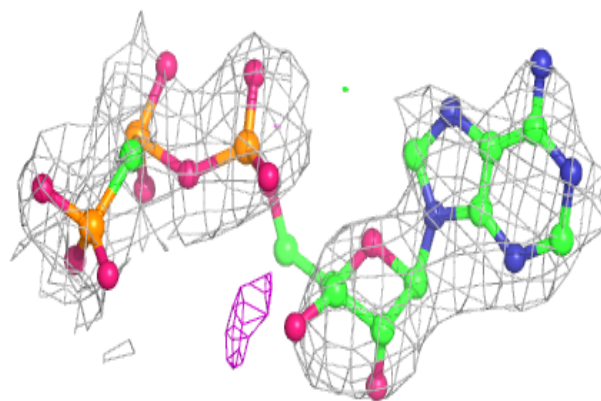
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	503	1/1	0.73	0.25	69,69,69,69	0
11	ACP	F	401	31/31	0.75	0.27	78,90,123,137	0
9	MES	B	505	12/12	0.80	0.30	60,82,95,119	0
7	CA	A	503	1/1	0.80	0.10	62,62,62,62	0
10	89U	D	502	25/25	0.81	0.25	31,46,60,73	0
10	89U	B	504	25/25	0.86	0.24	30,43,52,53	0
5	GTP	D	501	32/32	0.91	0.18	45,56,78,138	0
7	CA	C	503	1/1	0.95	0.06	40,40,40,40	0
5	GTP	A	501	32/32	0.96	0.21	14,24,33,35	0
6	MG	C	502	1/1	0.96	0.21	19,19,19,19	0
9	MES	B	503	12/12	0.96	0.16	31,40,49,51	0
6	MG	A	502	1/1	0.97	0.19	24,24,24,24	0
8	GDP	B	501	28/28	0.97	0.20	13,24,31,34	0
5	GTP	C	501	32/32	0.98	0.17	9,18,24,27	0
6	MG	B	502	1/1	0.98	0.21	16,16,16,16	0

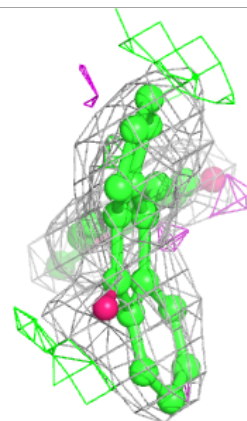
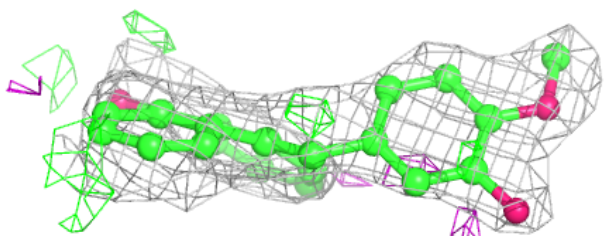
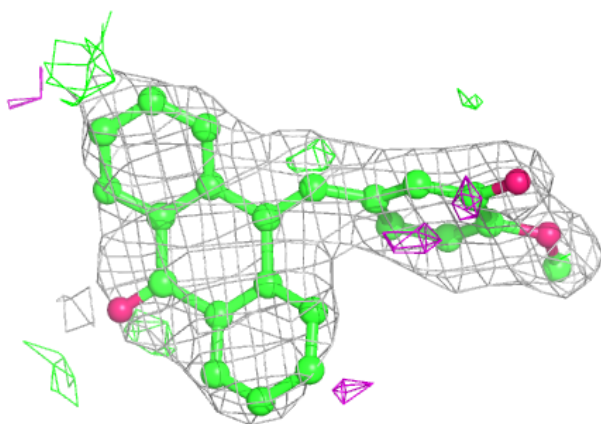
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

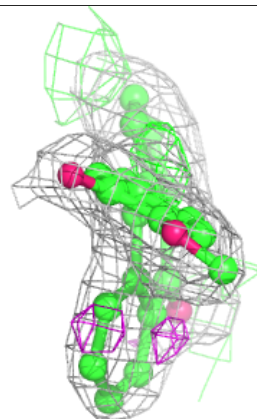
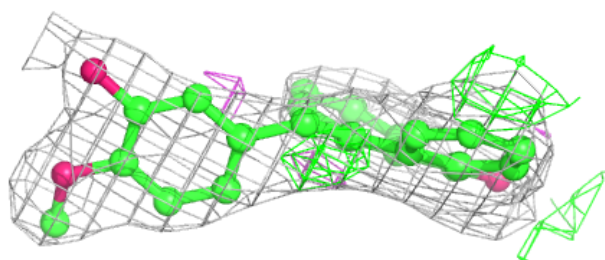
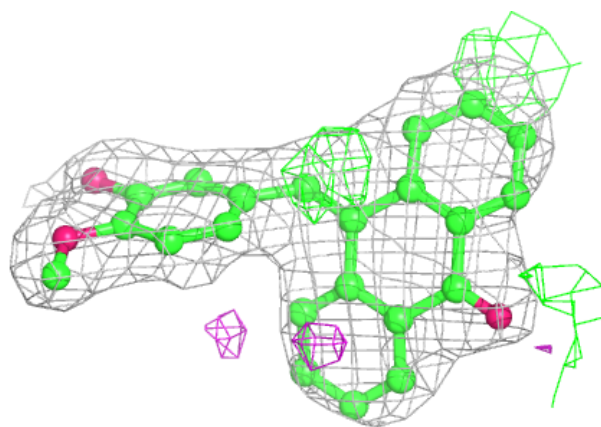
**Electron density around 89U D 502:**

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

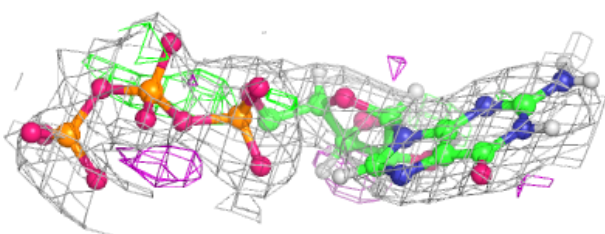
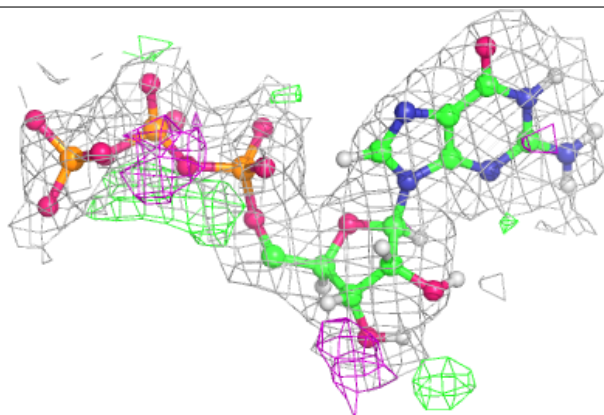


Electron density around 89U B 504:

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

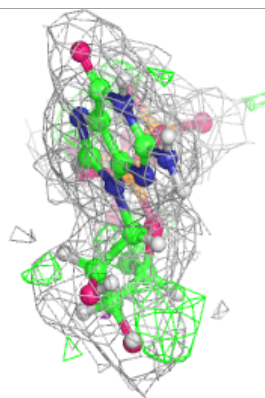
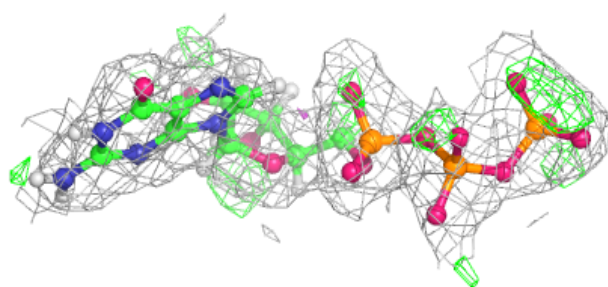
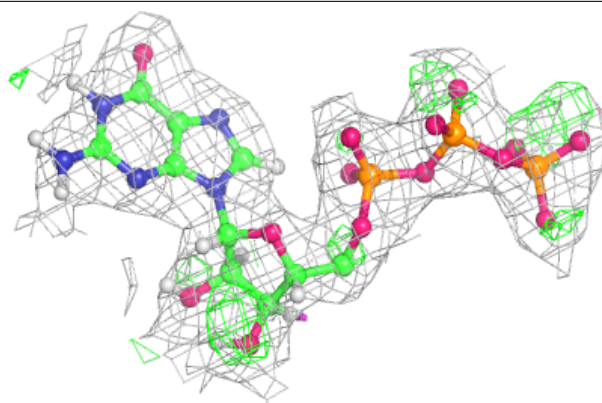
**Electron density around GTP D 501:**

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

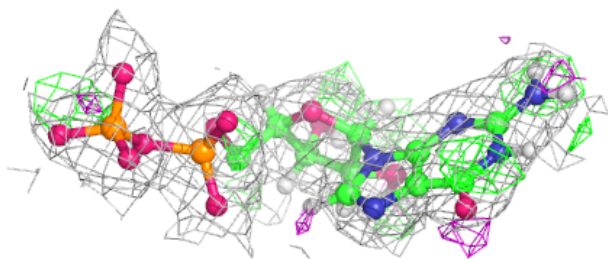
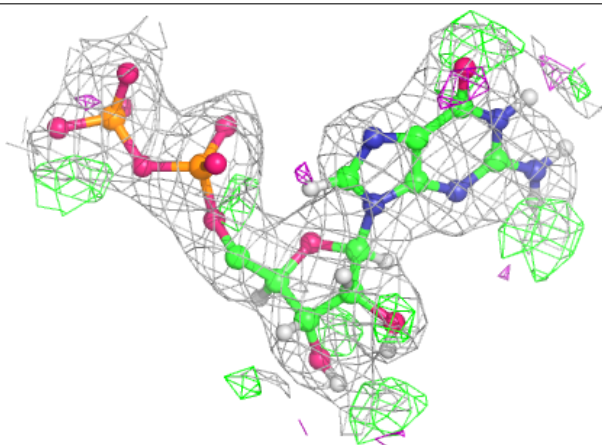


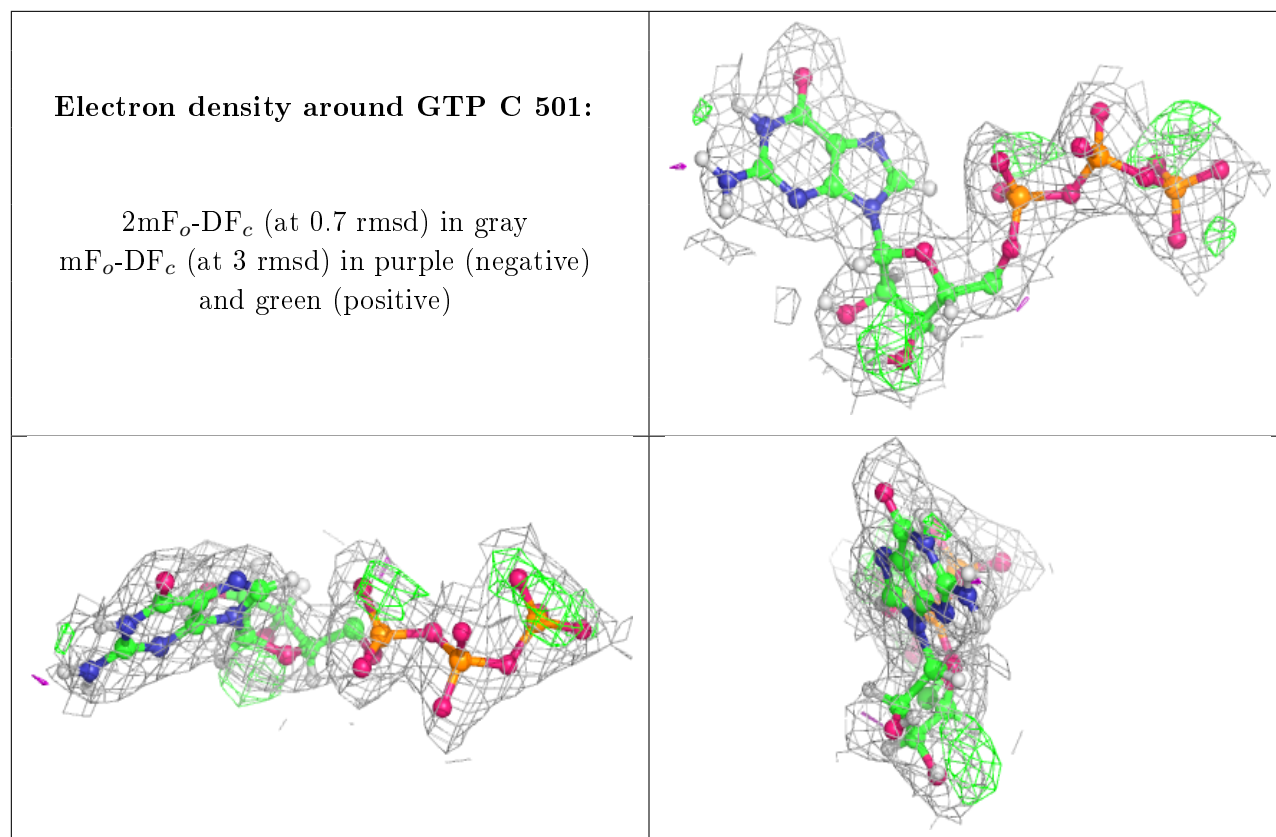
Electron density around GTP A 501:

$2mF_o-DF_c$ (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.