



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 06:11 AM UTC

PDB ID : 5S4N / pdb_00005s4n
Title : Tubulin-Z285782452-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.53 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

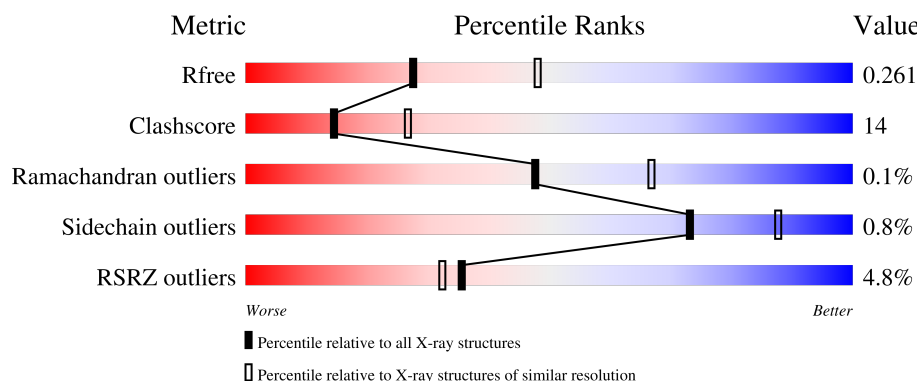
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	451	4% 69% 28% ..
1	C	451	4% 73% 25% .
2	B	445	4% 63% 32% .
2	D	445	4% 67% 29% .
3	E	143	8% 68% 17% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	6% 64% 26% 9%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17930 atoms, of which 44 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	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	1	1	0
			3359	2109	577	646	27			
2	D	431	Total	C	N	O	S	5	0	0
			3368	2113	575	653	27			

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

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

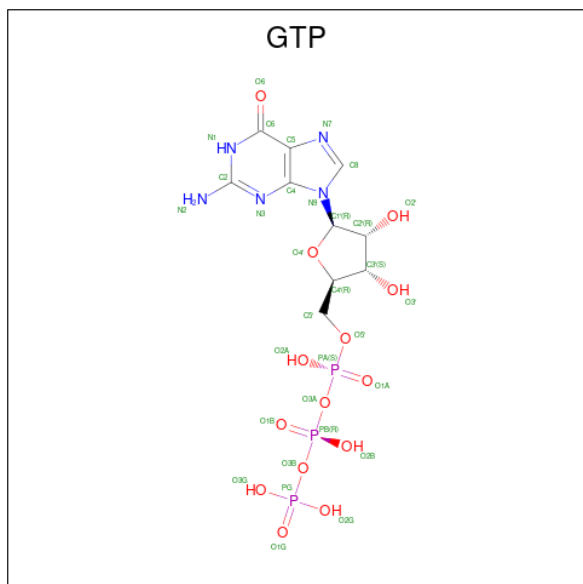
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	349	Total	C	N	O	S	0	0	0
			2853	1830	489	520	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 (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	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	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	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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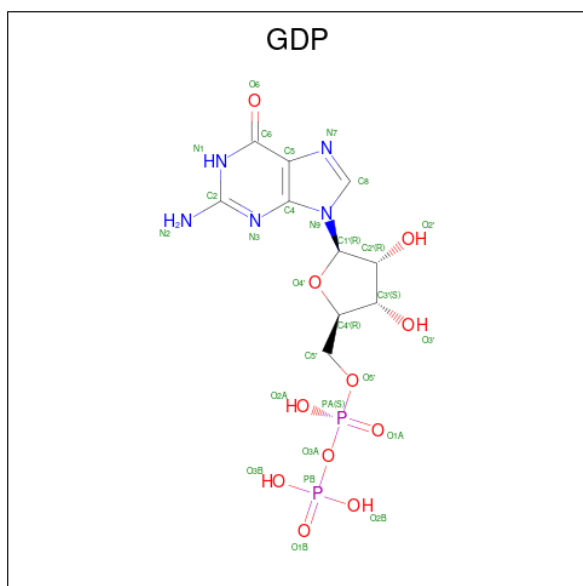
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

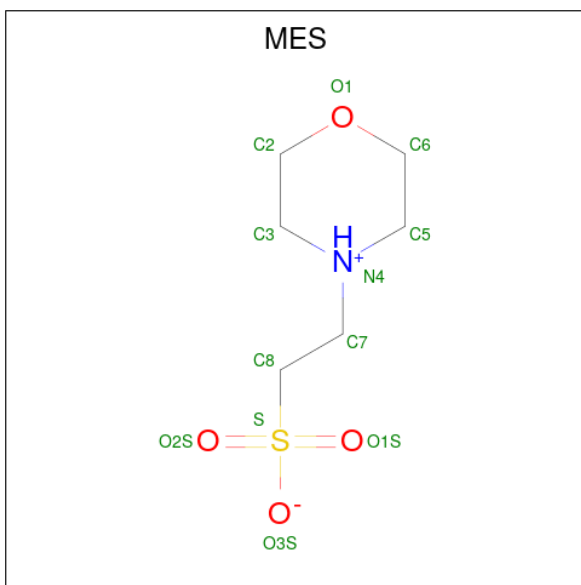
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

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



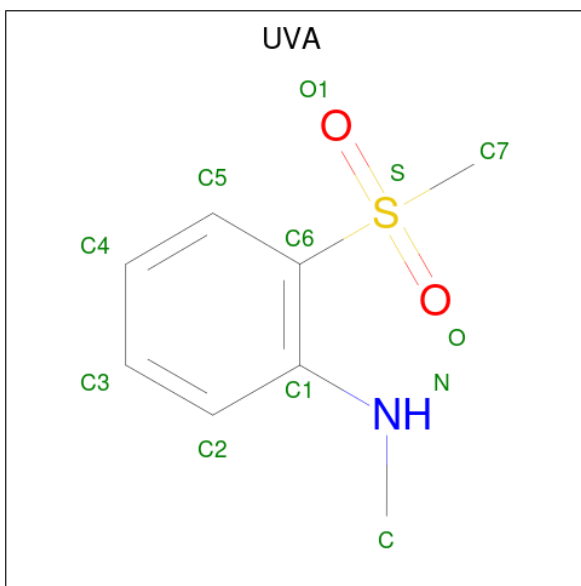
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 10 is N-methyl-2-(methylsulfonyl)aniline (CCD ID: UVA) (formula: $C_8H_{11}NO_2S$) (labeled as "Ligand of Interest" by depositor).



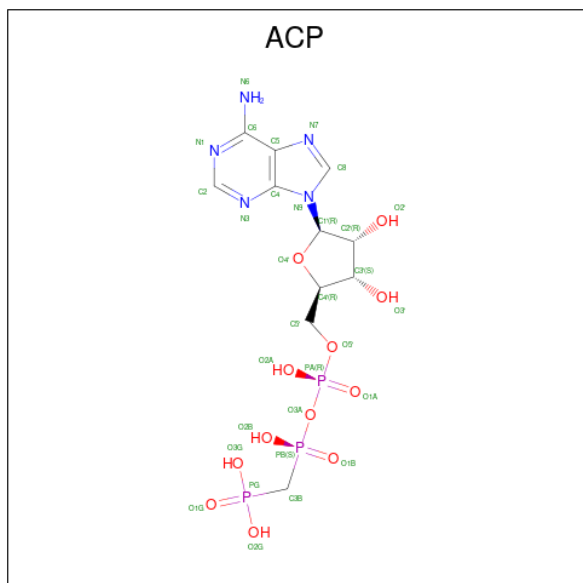
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			23	8	11	1	2	1		
10	B	1	Total	C	H	N	O	S	0	0
			23	8	11	1	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			23	8	11	1	2	1		
10	D	1	Total	C	H	N	O	S	0	0
			23	8	11	1	2	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: 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		

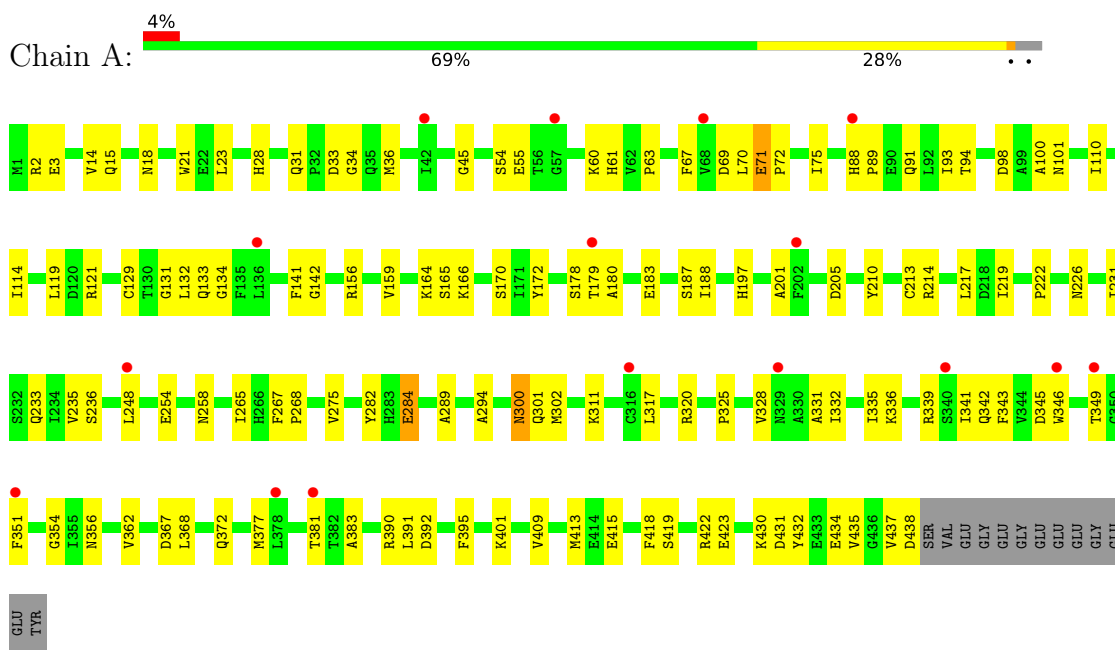
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	31	Total	O	0	0
			31	31		
12	B	44	Total	O	0	0
			44	44		
12	C	108	Total	O	0	0
			108	108		
12	D	12	Total	O	0	0
			12	12		
12	E	9	Total	O	0	0
			9	9		
12	F	1	Total	O	0	0
			1	1		

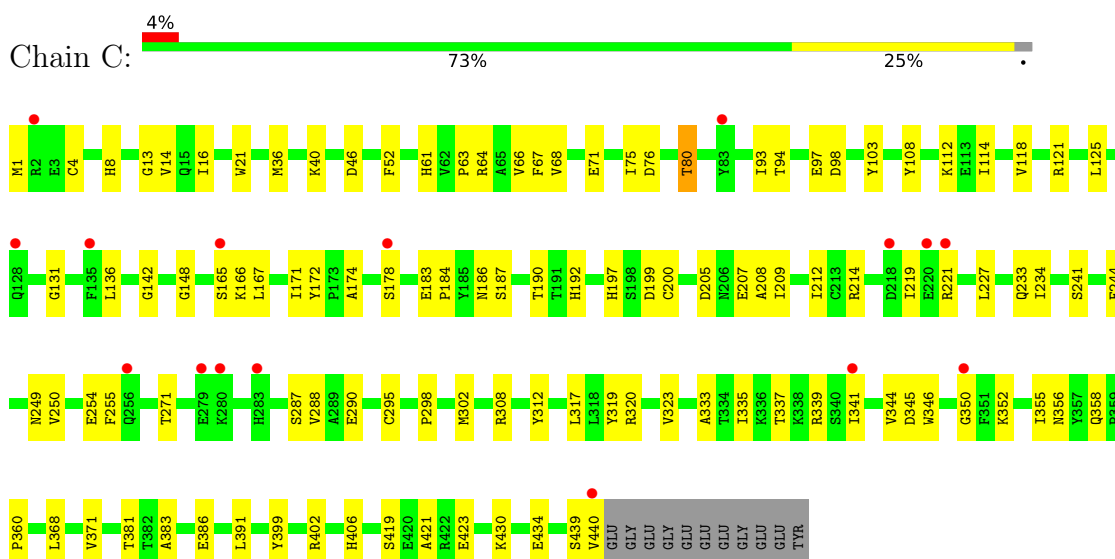
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain



Chain B:

Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.10). The x-axis shows positions 1 to 100. A color scale at the top indicates conservation levels: 4% (red), 63% (green), and 32% (yellow).

Position	Amino Acid	Information Content (bits)
1	M413	0.00
2	M425	0.00
3	Q433	0.00
4	D437	0.00
5	ALA	0.00
6	THR	0.00
7	ALA	0.00
8	ASP	0.00
9	GLU	0.00
10	GLN	0.00
11	GLY	0.00
12	GLU	0.00
13	PHE	0.00
14	GLU	0.00
15	GLU	0.00
16	GLU	0.00
17	GLU	0.00
18	GLY	0.00
19	ASP	0.00
20	ALA	0.00
21	P307	0.00
22	R308	0.00
23	H309	0.00
24	I318	0.00
25	F319	0.00
26	R320	0.00
27	M323	0.00
28	S324	0.00
29	M325	0.00
30	K326	0.00
31	E327	0.00
32	GLN	0.00
33	V328	0.00
34	D329	0.00
35	E330	0.00
36	L333	0.00
37	N334	0.00
38	V335	0.00
39	N337	0.00
40	K338	0.00
41	Y342	0.00
42	E345	0.00
43	W346	0.00
44	I347	0.00
45	F348	0.00
46	N349	0.00
47	N350	0.00
48	V351	0.00
49	K352	0.00
50	C356	0.00
51	D357	0.00
52	I358	0.00
53	P359	0.00
54	P360	0.00
55	R369	0.00
56	M373	0.00
57	S374	0.00
58	A375	0.00
59	T376	0.00
60	F377	0.00
61	Q385	0.00
62	E386	0.00
63	L387	0.00
64	F388	0.00
65	K389	0.00
66	S392	0.00
67	F404	0.00
68	L405	0.00
69	C412	0.00
70	L219	0.00
71	T220	0.00
72	T221	0.00
73	P222	0.00
74	D226	0.00
75	L230	0.00
76	V231	0.00
77	S232	0.00
78	M235	0.00
79	T239	0.00
80	L242	0.00
81	R243	0.00
82	F244	0.00
83	P245	0.00
84	L248	0.00
85	N249	0.00
86	A250	0.00
87	D251	0.00
88	L252	0.00
89	R253	0.00
90	K254	0.00
91	L255	0.00
92	N258	0.00
93	H266	0.00
94	F267	0.00
95	F268	0.00
96	M269	0.00
97	P270	0.00
98	P274	0.00
99	R278	0.00
100	GLY	0.00
101	SER	0.00
102	Q281	0.00
103	Q282	0.00
104	Y283	0.00
105	L286	0.00
106	T292	0.00
107	M295	0.00
108	F296	0.00
109	D297	0.00
110	S298	0.00
111	M302	0.00
112	A303	0.00
113	A304	0.00
114	C305	0.00
115	F306	0.00
116	D120	0.00
117	V121	0.00
118	V122	0.00
119	R123	0.00
120	K124	0.00
121	E127	0.00
122	L132	0.00
123	Q133	0.00
124	Q136	0.00
125	L141	0.00
126	T145	0.00
127	G148	0.00
128	M149	0.00
129	I154	0.00
130	S155	0.00
131	K156	0.00
132	I157	0.00
133	R158	0.00
134	E159	0.00
135	E160	0.00
136	Y161	0.00
137	M165	0.00
138	N167	0.00
139	T168	

Chain D:

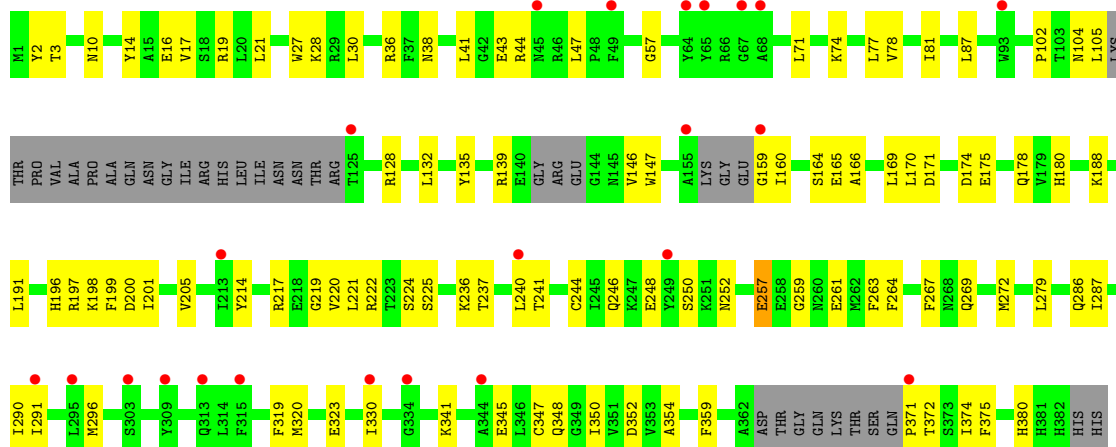
67% 29% 4%

Chain E:

Amino Acid	Category
MET	Grey
ALA	Grey
ASP	Grey
M6	Yellow
E7	Red
F8	Red
I9	Yellow
Q18	Yellow
S19	Yellow
F20	Yellow
E21	Yellow
V22	Red
L23	Yellow
L24	Yellow
K25	Yellow
P26	Red
P27	Red
S28	Yellow
PHE	Grey
ASP	Grey
GLY	Grey
VAL	Grey
PRO	Grey
GLU	Grey
PHE	Grey
ASN	Grey
ALA	Grey
SER	Grey
LEU	Grey
PRO	Grey
ARG	Grey
ARG	Grey
D44	Red
P45	Yellow
S46	Yellow
L47	Yellow
E48	Yellow
E49	Yellow
K52	Yellow
E58	Yellow
R61	Yellow
R76	Red
V82	Yellow
K85	Yellow
E89	Yellow



● 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	105.26Å 158.63Å 179.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.81 – 2.53 90.81 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.5 (90.81-2.53) 99.5 (90.81-2.53)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.216 , 0.258 0.221 , 0.261	Depositor DCC
R_{free} test set	5070 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17930	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: UVA, GDP, GTP, MES, MG, CA, ACP

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	0.11	0/3502	0.28	0/4754
1	C	0.12	0/3521	0.30	0/4780
2	B	0.12	0/3433	0.29	0/4647
2	D	0.12	0/3442	0.29	0/4664
3	E	0.10	0/1022	0.22	0/1356
4	F	0.09	0/2919	0.28	0/3944
All	All	0.12	0/17839	0.28	0/24145

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3334	108	0
1	C	3443	0	3352	83	0
2	B	3359	0	3235	114	0
2	D	3368	0	3236	101	1
3	E	1014	0	1029	23	1
4	F	2853	0	2816	82	0
5	A	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	2	0
9	B	12	0	12	1	0
10	B	36	33	0	0	0
10	D	12	11	0	0	0
11	F	31	0	14	3	0
12	A	31	0	0	6	0
12	B	44	0	0	3	0
12	C	108	0	0	3	0
12	D	12	0	0	1	0
12	E	9	0	0	1	0
12	F	1	0	0	0	0
All	All	17886	44	17076	488	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 488 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:381:THR:HG22	1:A:383:ALA:H	1.28	0.97
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.30	0.96
2:D:323:MET:HE2	2:D:373:MET:HG2	1.51	0.91
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.52	0.89
4:F:269:GLN:HA	4:F:272:MET:HE2	1.55	0.88

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:372:LYS:NZ	3:E:58:GLU:OE2[4_455]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	419 (96%)	17 (4%)	0	100	100
1	C	439/451 (97%)	425 (97%)	14 (3%)	0	100	100
2	B	422/445 (95%)	400 (95%)	21 (5%)	1 (0%)	43	62
2	D	429/445 (96%)	409 (95%)	19 (4%)	1 (0%)	43	62
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	339/384 (88%)	322 (95%)	17 (5%)	0	100	100
All	All	2184/2319 (94%)	2093 (96%)	89 (4%)	2 (0%)	48	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	278	ARG
2	B	251	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	365 (99%)	4 (1%)	65	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	372/379 (98%)	370 (100%)	2 (0%)	81	91
2	B	368/383 (96%)	366 (100%)	2 (0%)	81	91
2	D	368/383 (96%)	364 (99%)	4 (1%)	65	83
3	E	110/127 (87%)	108 (98%)	2 (2%)	51	75
4	F	313/342 (92%)	311 (99%)	2 (1%)	78	90
All	All	1900/1993 (95%)	1884 (99%)	16 (1%)	73	88

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	43	GLU
3	E	128	LYS
2	D	26	ASP
3	E	22	VAL
1	C	381	THR

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

Mol	Chain	Res	Type
4	F	183	GLN
4	F	333	ASN
1	C	133	GLN
1	C	283	HIS
1	C	329	ASN

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 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	D	501	6	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
8	GDP	B	501	6	29,30,30	1.17	3 (10%)	45,47,47	1.70	7 (15%)
10	UVA	B	506	-	12,12,12	0.33	0	17,17,17	0.92	1 (5%)
10	UVA	D	503	-	12,12,12	0.27	0	17,17,17	0.90	1 (5%)
5	GTP	C	501	6	33,34,34	1.00	3 (9%)	50,54,54	1.51	8 (16%)
9	MES	B	504	-	12,12,12	2.34	1 (8%)	15,16,16	1.91	4 (26%)
10	UVA	B	507	-	12,12,12	0.31	0	17,17,17	0.88	1 (5%)
11	ACP	F	401	6	31,33,33	1.66	8 (25%)	47,52,52	1.89	10 (21%)
10	UVA	B	505	-	12,12,12	0.29	0	17,17,17	0.87	1 (5%)
5	GTP	A	501	6	33,34,34	1.00	3 (9%)	50,54,54	1.55	8 (16%)

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	D	501	6	-	2/16/32/32	0/3/3/3
8	GDP	B	501	6	-	2/16/32/32	0/3/3/3
10	UVA	B	506	-	-	0/8/8/8	0/1/1/1
10	UVA	D	503	-	-	0/8/8/8	0/1/1/1
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
10	UVA	B	507	-	-	0/8/8/8	0/1/1/1
11	ACP	F	401	6	-	10/19/38/38	0/3/3/3
10	UVA	B	505	-	-	0/8/8/8	0/1/1/1
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.83	1.66	1.77
11	F	401	ACP	C5-C4	4.72	1.47	1.39
8	B	501	GDP	C5-C4	3.19	1.47	1.38
8	D	501	GDP	C5-C4	3.09	1.47	1.38
11	F	401	ACP	PG-O2G	3.00	1.61	1.55

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-6.14	118.62	128.39
8	B	501	GDP	C5-C4-N3	-5.99	118.86	128.39
11	F	401	ACP	C5-C4-N3	-5.82	118.71	126.72
8	D	501	GDP	C2-N3-C4	4.96	120.85	112.30
8	B	501	GDP	C2-N3-C4	4.95	120.83	112.30

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

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

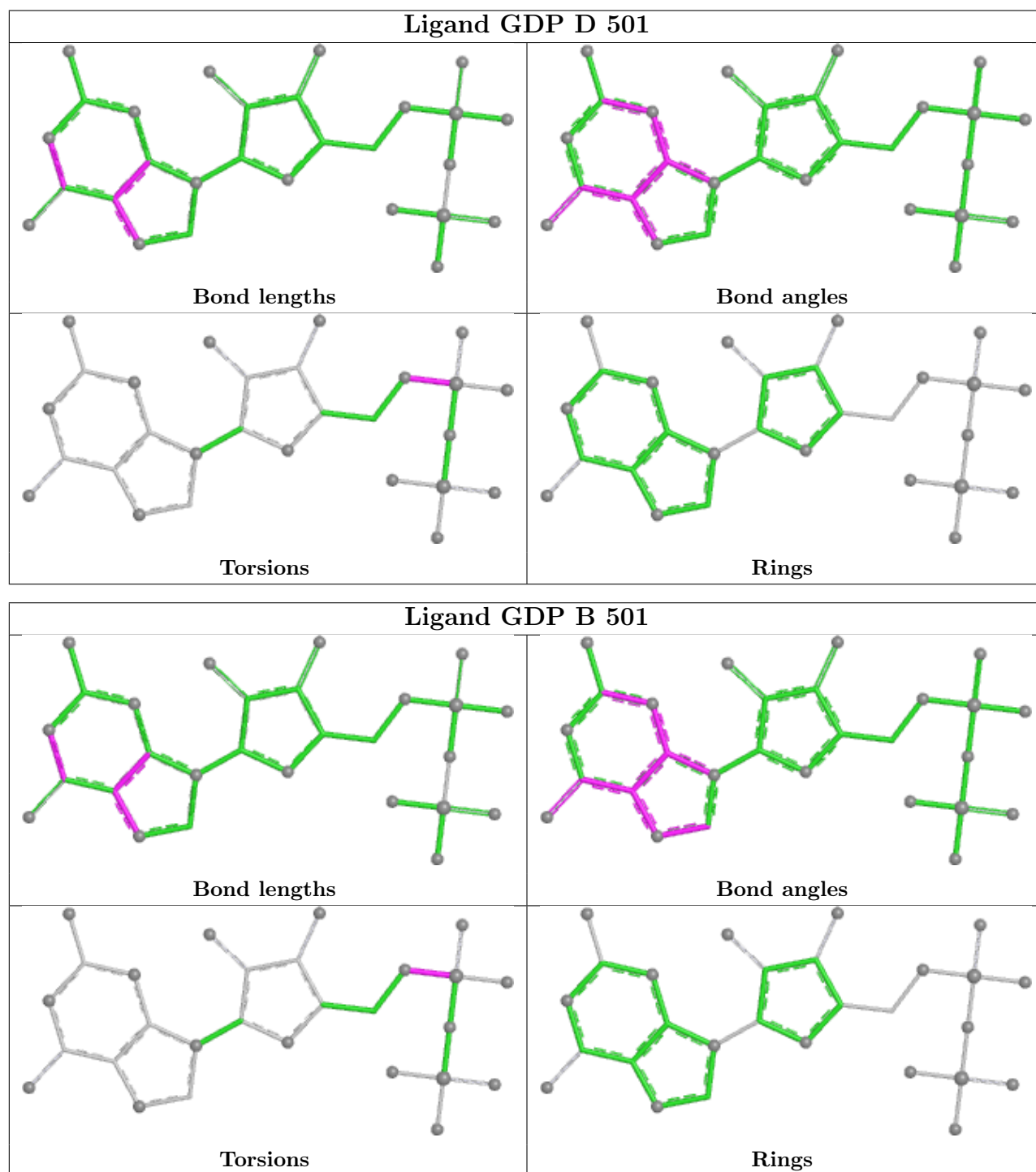
There are no ring outliers.

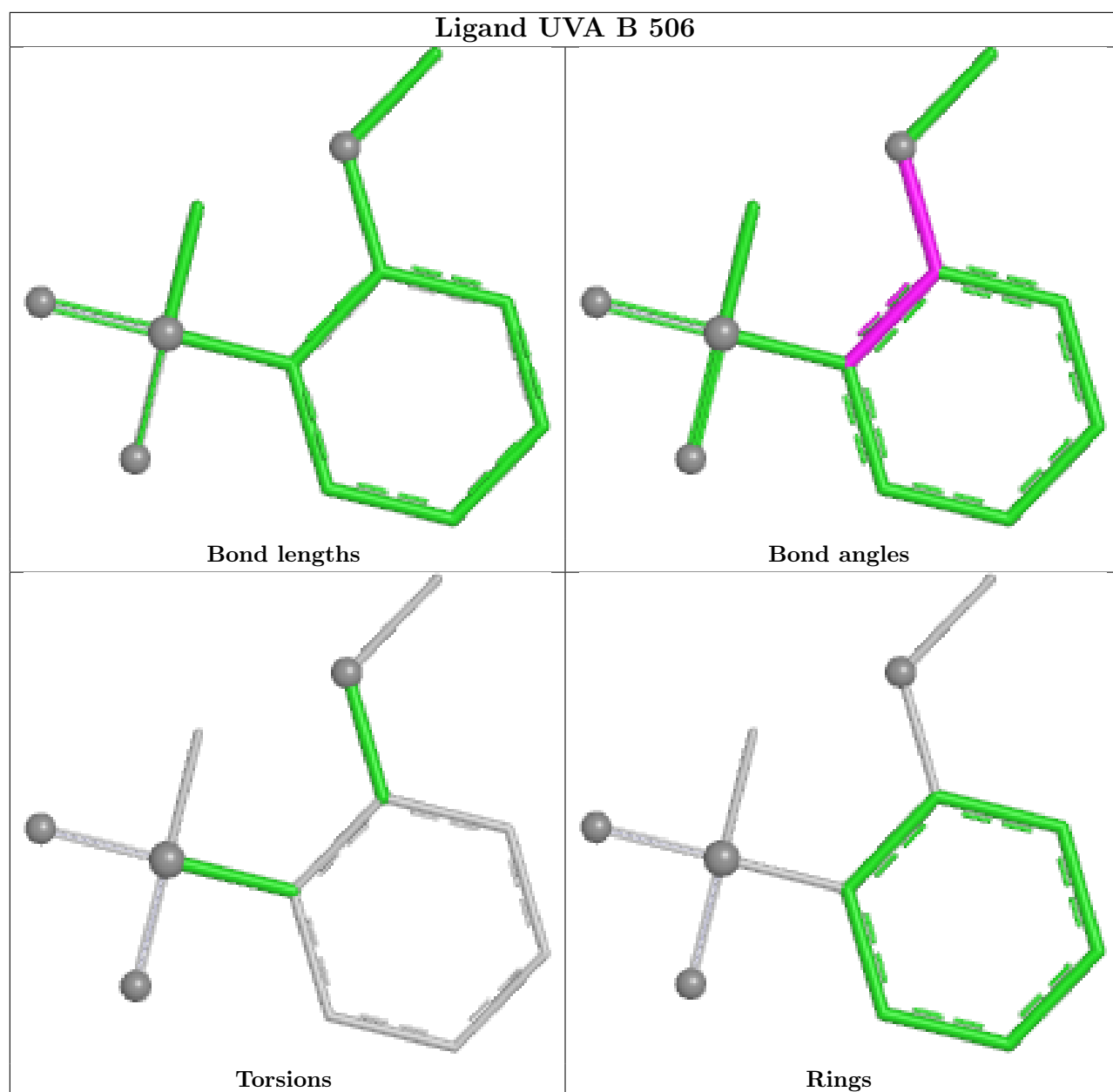
5 monomers are involved in 9 short contacts:

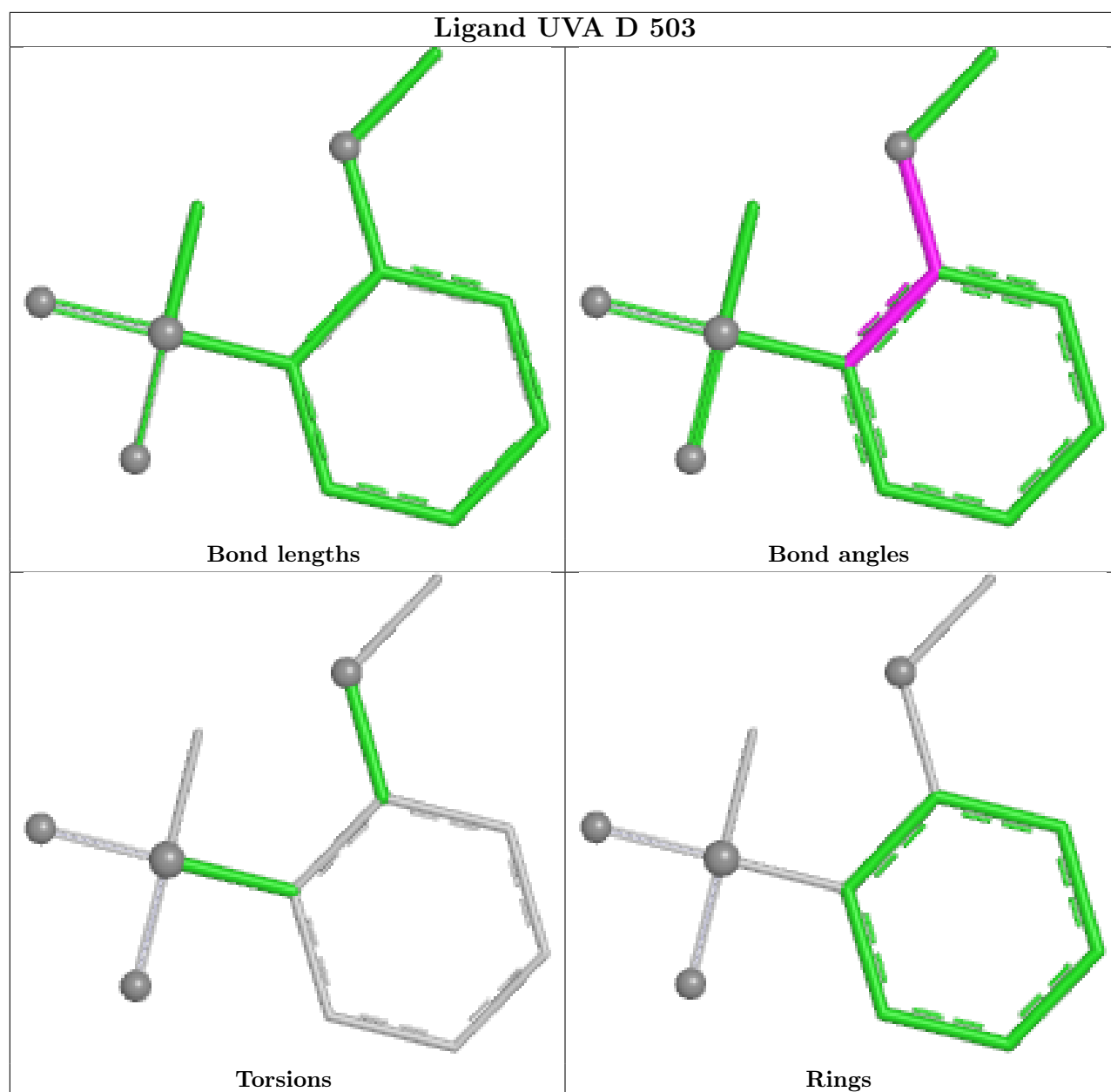
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	2	0
8	B	501	GDP	1	0
9	B	504	MES	1	0
11	F	401	ACP	3	0
5	A	501	GTP	2	0

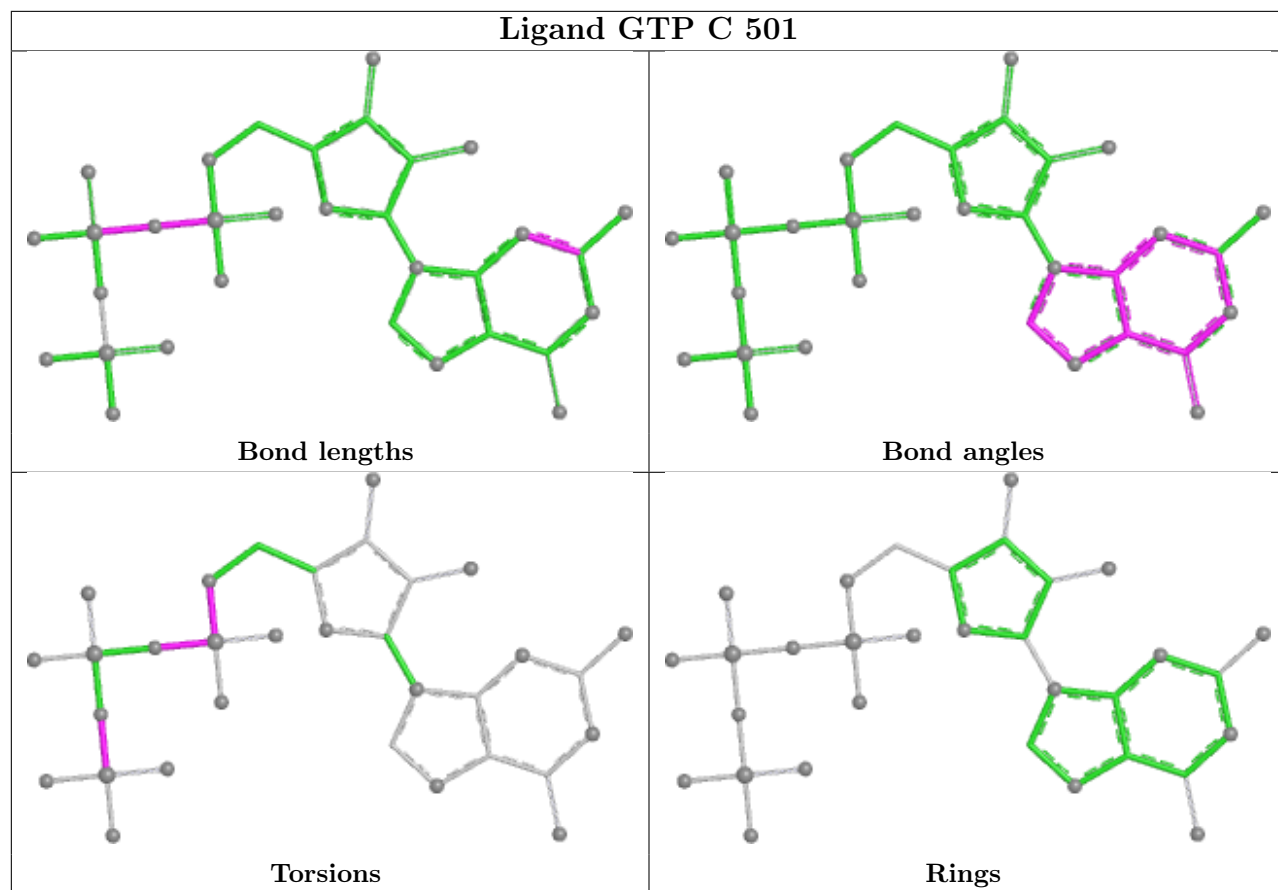
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

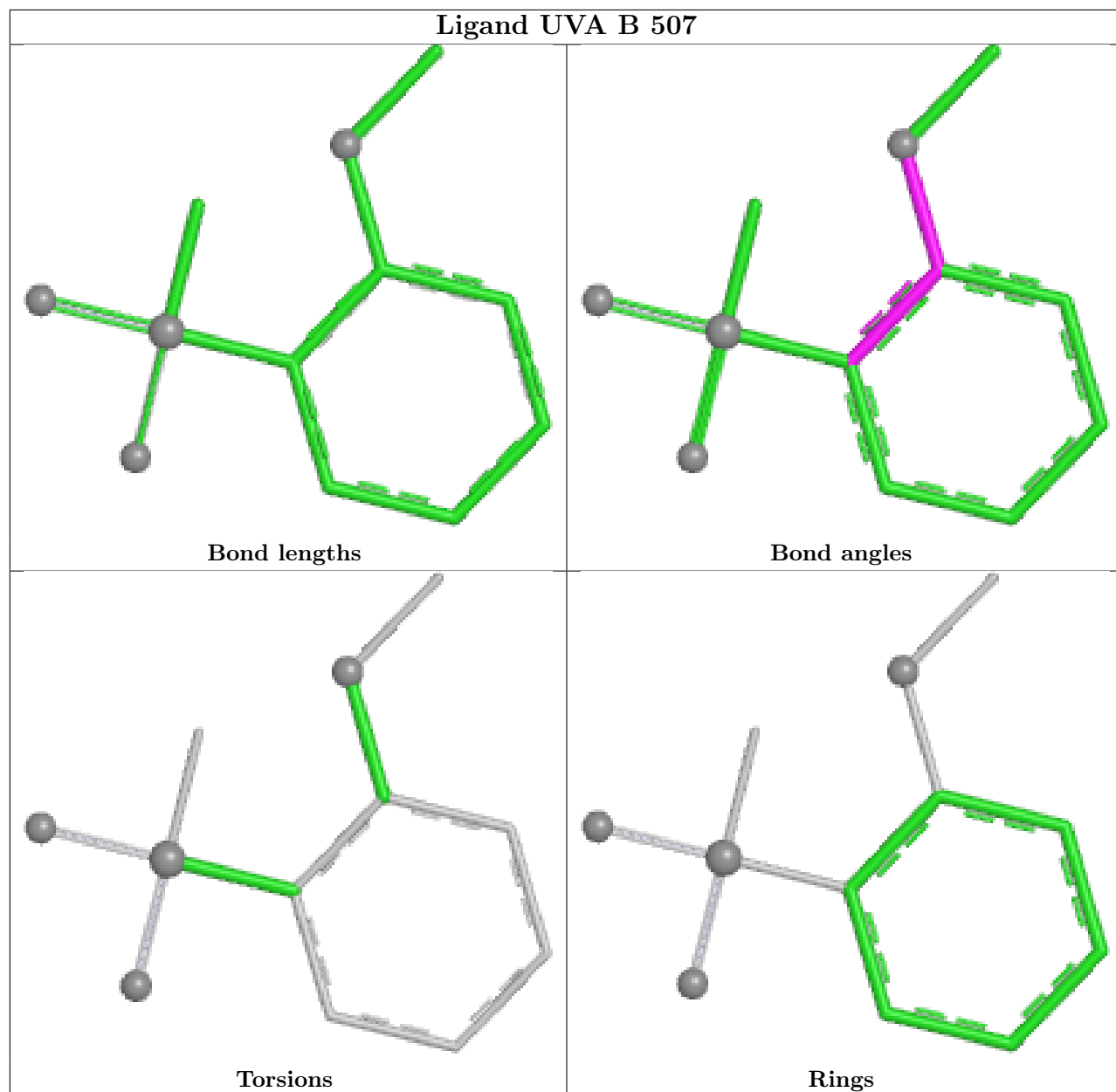




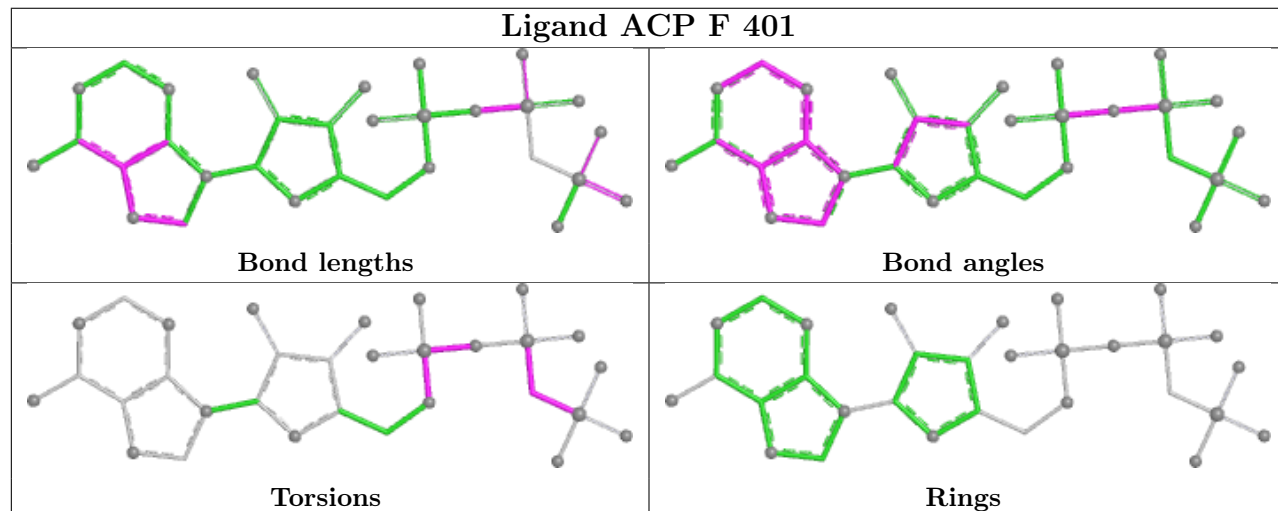


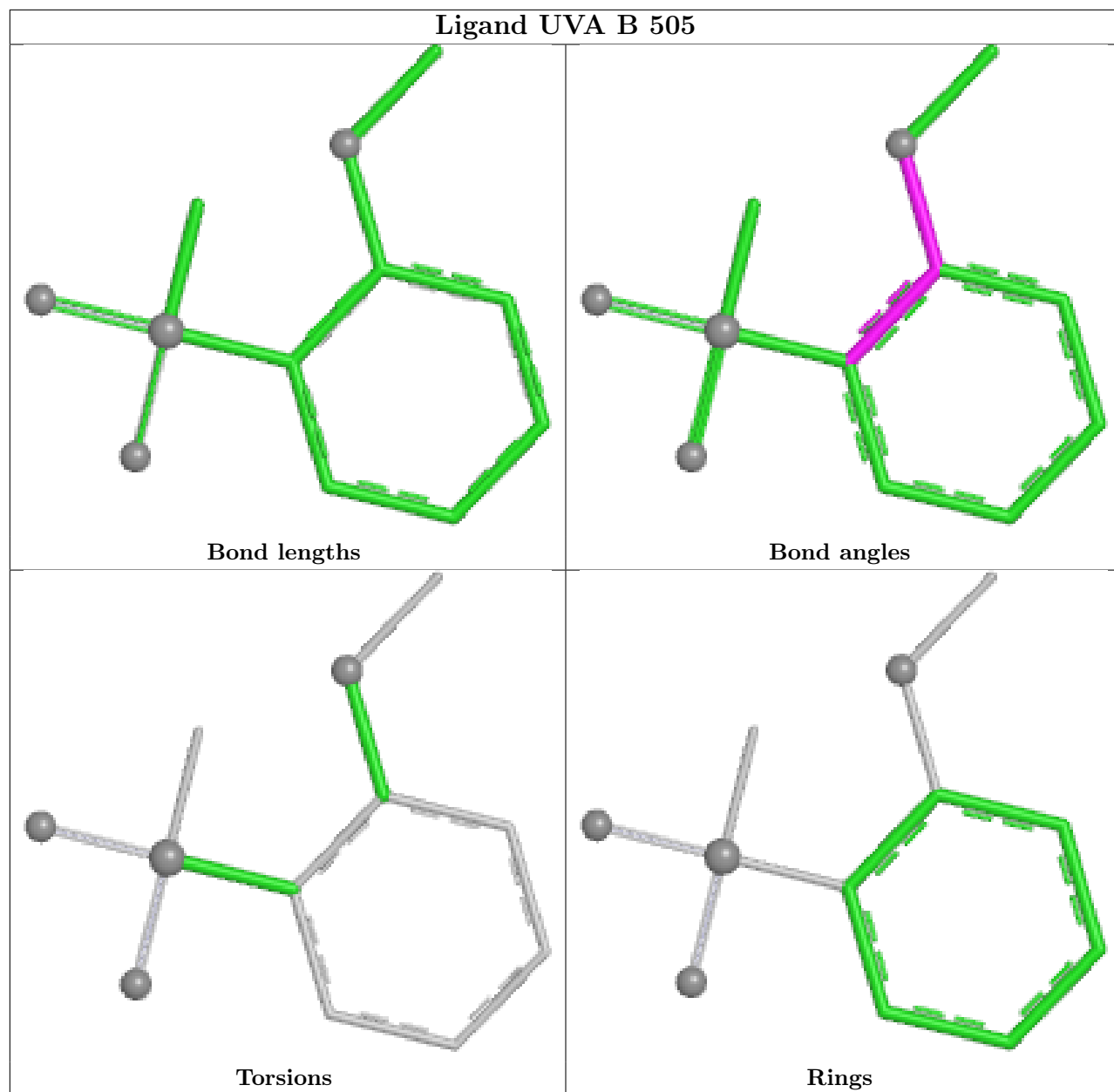


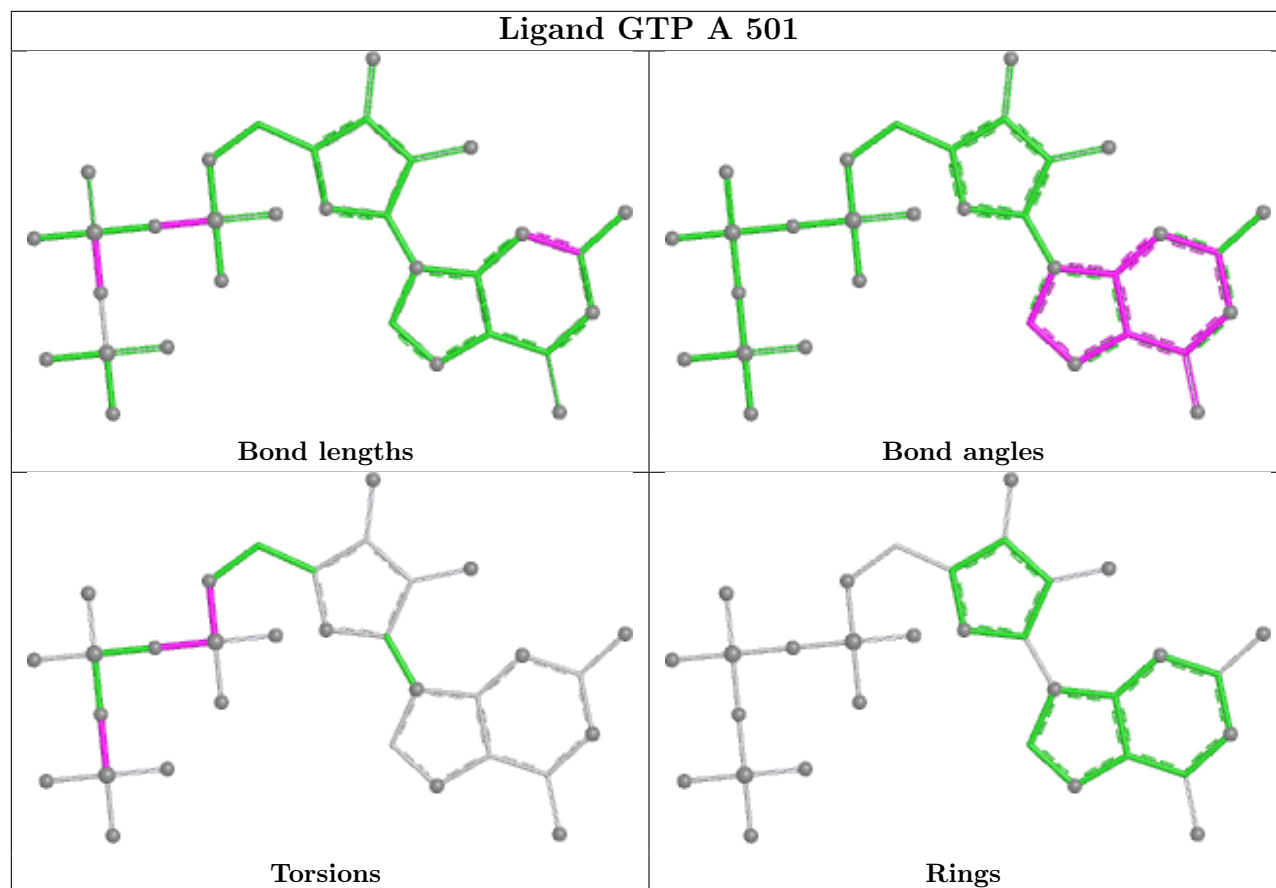
Ligand UVA B 507



Ligand ACP F 401







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	0.47	16 (3%)	45	41	63, 82, 125, 204	0
1	C	440/451 (97%)	0.21	16 (3%)	46	42	37, 69, 100, 153	1 (0%)
2	B	425/445 (95%)	0.39	18 (4%)	40	37	39, 78, 125, 161	3 (0%)
2	D	431/445 (96%)	0.48	20 (4%)	37	34	65, 88, 129, 211	4 (0%)
3	E	123/143 (86%)	0.71	12 (9%)	13	11	71, 94, 144, 182	0
4	F	349/384 (90%)	0.74	23 (6%)	24	22	80, 119, 179, 213	0
All	All	2206/2319 (95%)	0.46	105 (4%)	35	32	37, 85, 147, 213	8 (0%)

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	155	ALA	5.5
2	B	249	ASN	5.4
3	E	24	LEU	5.1
2	B	248	LEU	4.4
2	B	250	ALA	4.2

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 ⓘ

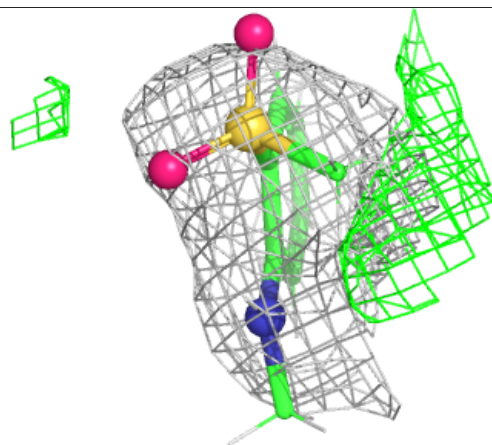
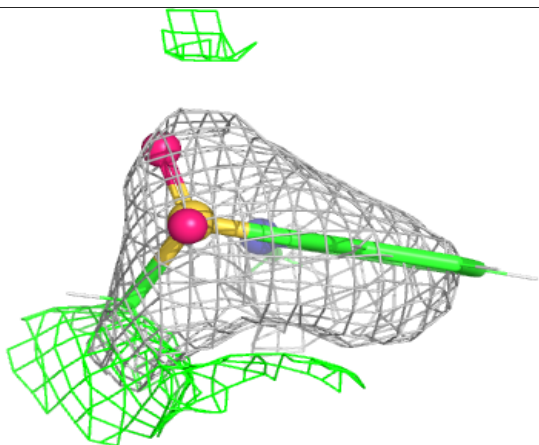
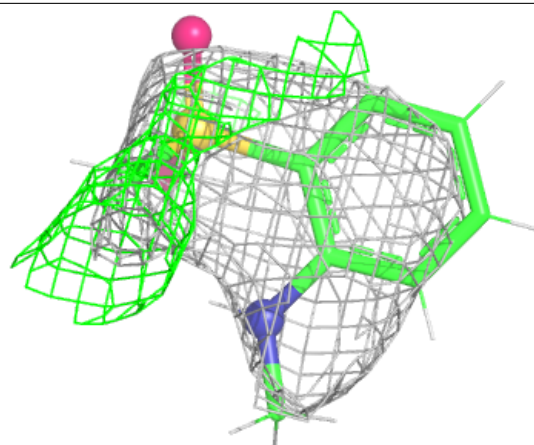
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	503	1/1	0.63	0.16	133,133,133,133	0
6	MG	D	502	1/1	0.73	0.10	92,92,92,92	0
10	UVA	B	507	12/12	0.77	0.24	91,110,122,126	23
9	MES	B	504	12/12	0.85	0.13	88,94,104,110	0
6	MG	A	502	1/1	0.87	0.11	69,69,69,69	0
11	ACP	F	401	31/31	0.88	0.09	115,125,134,138	0
10	UVA	D	503	12/12	0.92	0.10	75,86,103,104	0
10	UVA	B	506	12/12	0.92	0.11	66,80,97,97	0
8	GDP	D	501	28/28	0.93	0.09	77,85,92,97	0
6	MG	F	402	1/1	0.93	0.07	117,117,117,117	0
7	CA	E	201	1/1	0.95	0.07	100,100,100,100	0
5	GTP	A	501	32/32	0.96	0.07	59,65,71,76	0
6	MG	B	502	1/1	0.96	0.12	61,61,61,61	0
8	GDP	B	501	28/28	0.97	0.06	52,59,63,67	0
10	UVA	B	505	12/12	0.97	0.07	70,78,93,94	0
5	GTP	C	501	32/32	0.97	0.07	54,61,66,69	0
7	CA	C	503	1/1	0.99	0.02	92,92,92,92	0
7	CA	A	503	1/1	0.99	0.05	109,109,109,109	0
6	MG	C	502	1/1	1.00	0.04	61,61,61,61	0

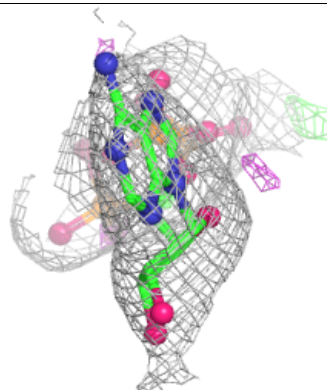
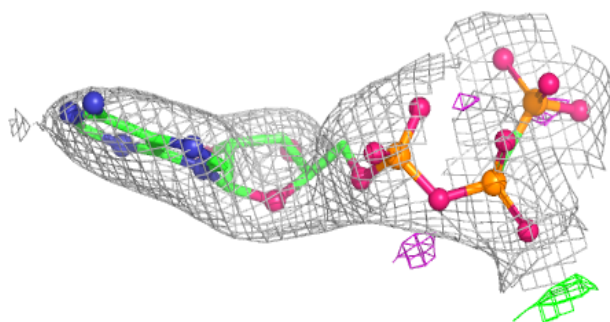
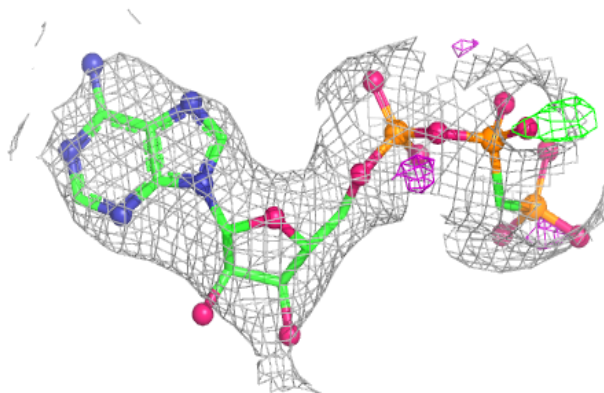
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UVA B 507:

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

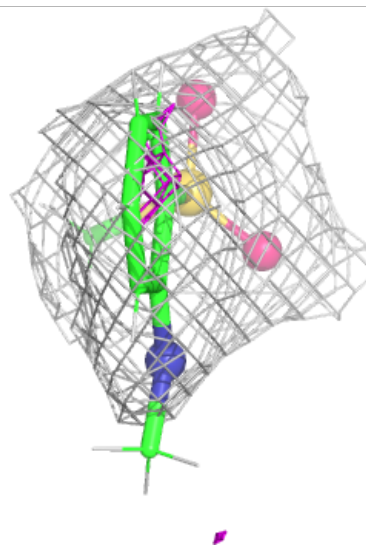
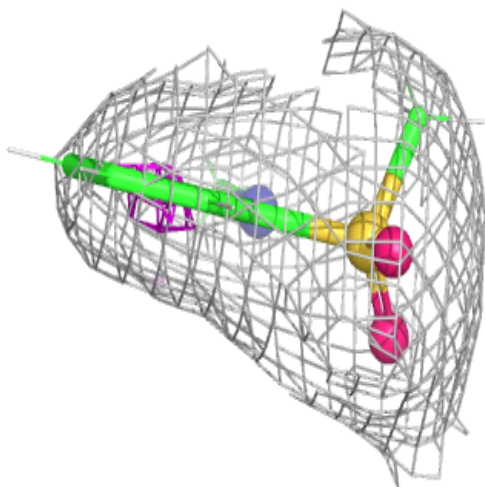
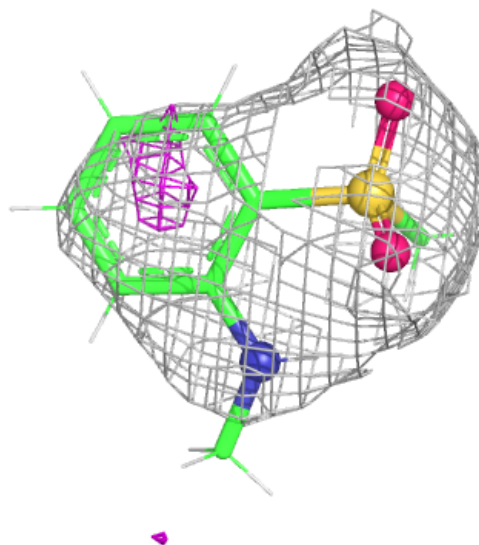
**Electron density around ACP F 401:**

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



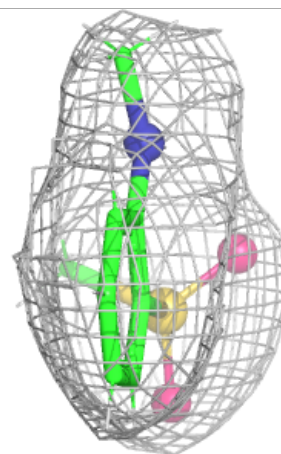
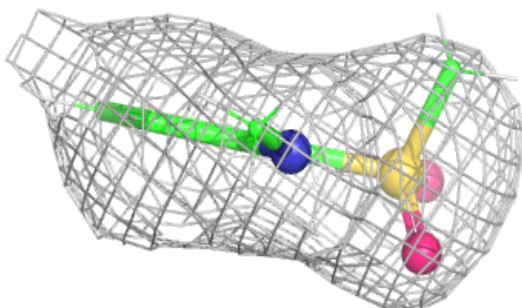
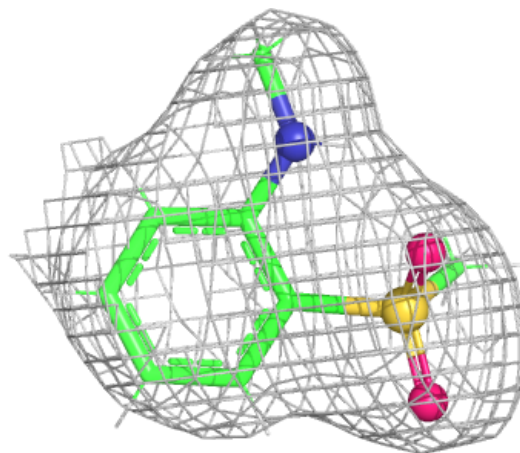
Electron density around UVA D 503:

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



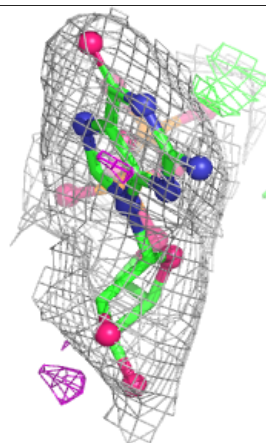
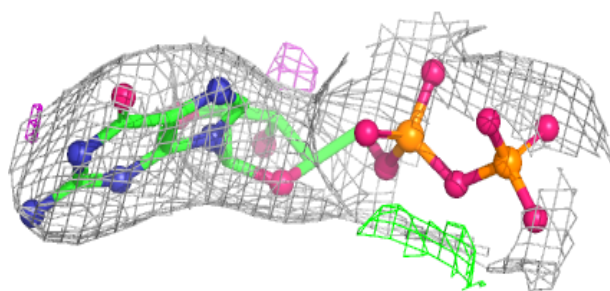
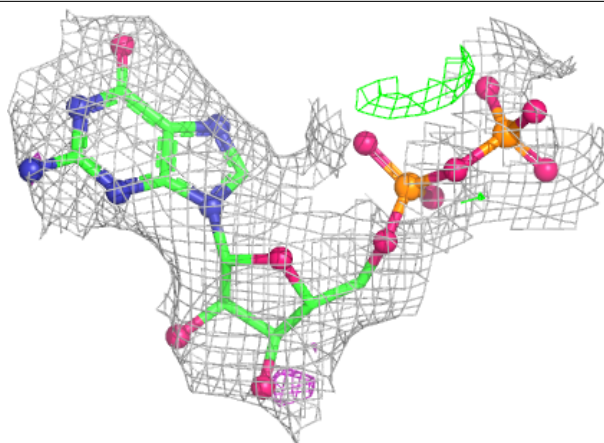
Electron density around UVA B 506:

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

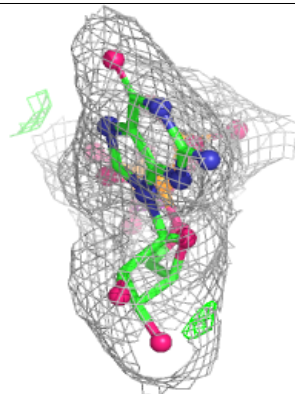
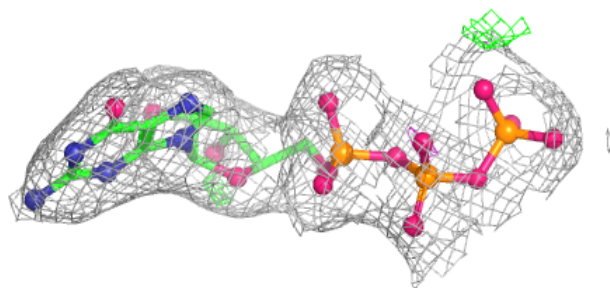
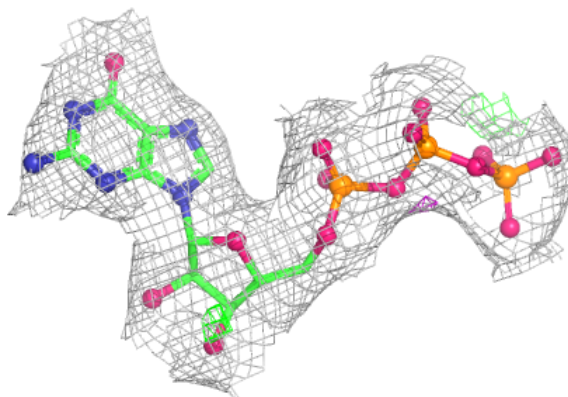


Electron density around GDP D 501:

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and green (positive)

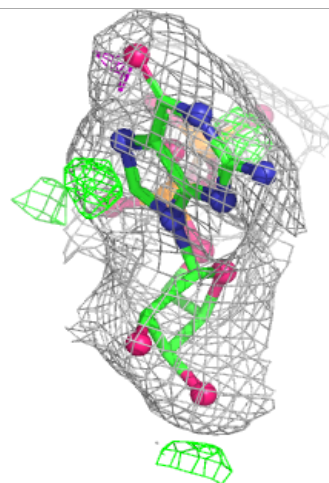
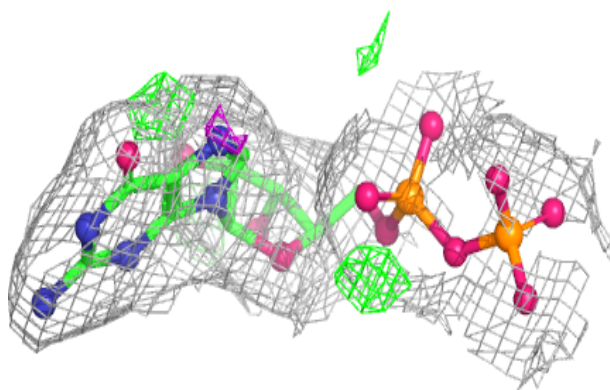
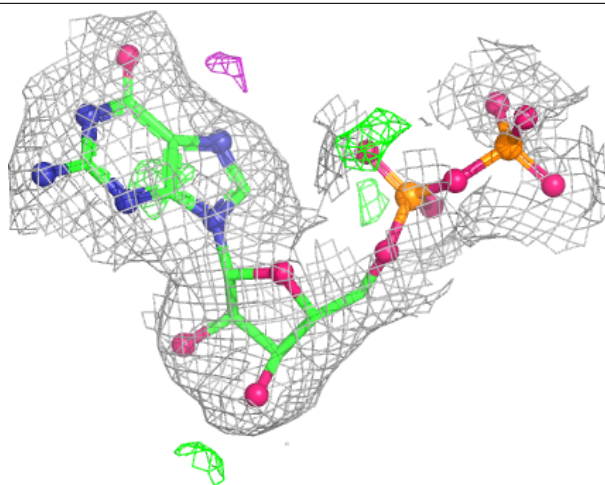
**Electron density around GTP A 501:**

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



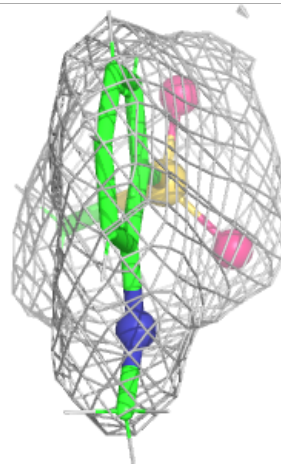
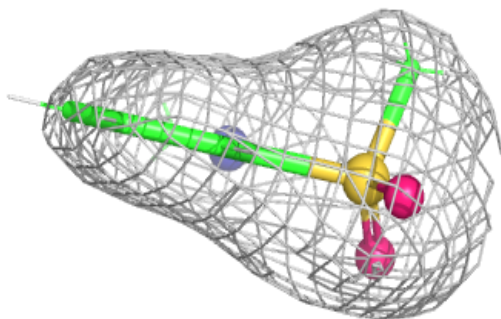
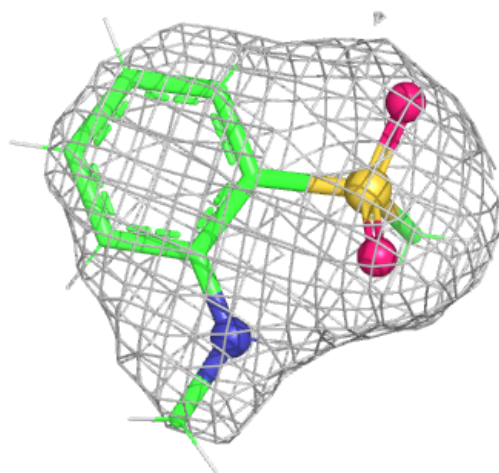
Electron density around GDP B 501:

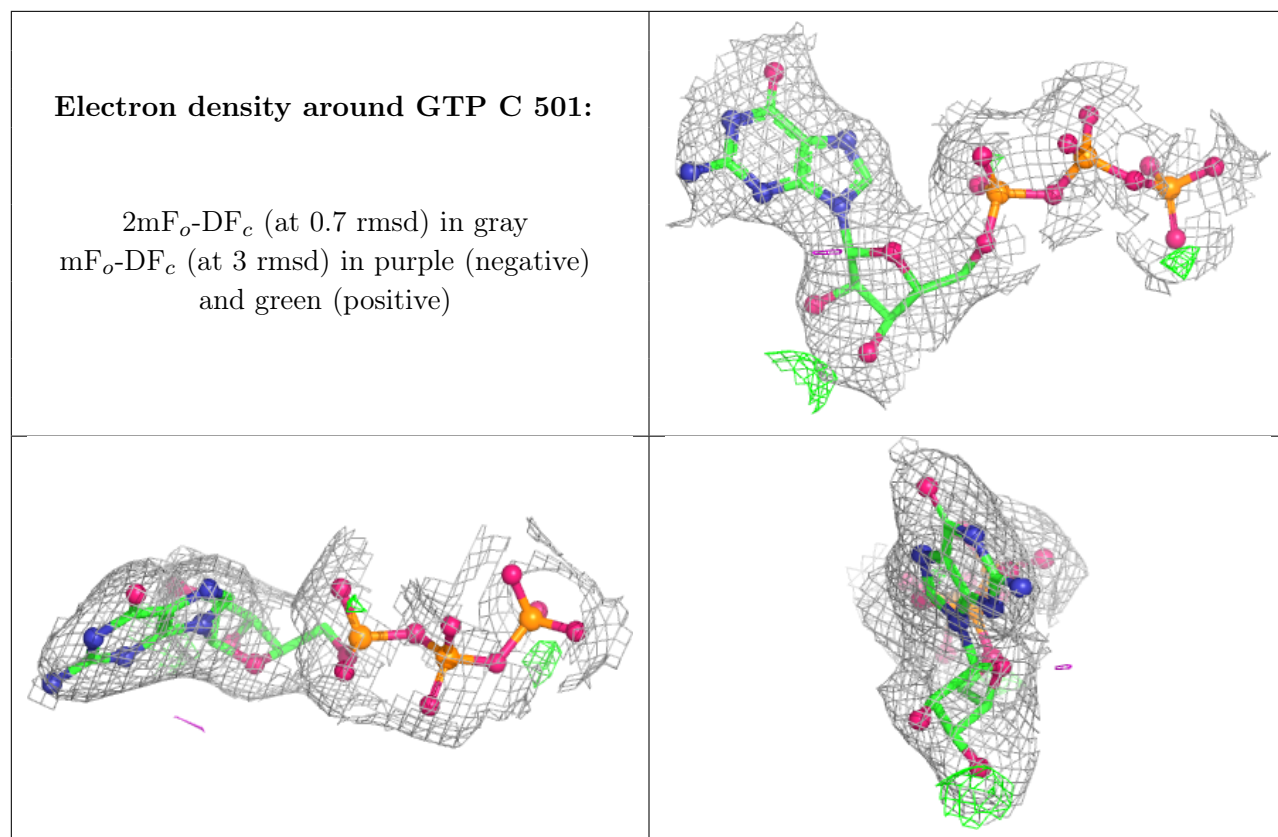
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UVA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.