



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:35 PM UTC

PDB ID : 8YER / pdb_00008yer
Title : Tubulin-RB3_SLD-TTL in complex with compound 4
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2024-02-23
Resolution : 2.71 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

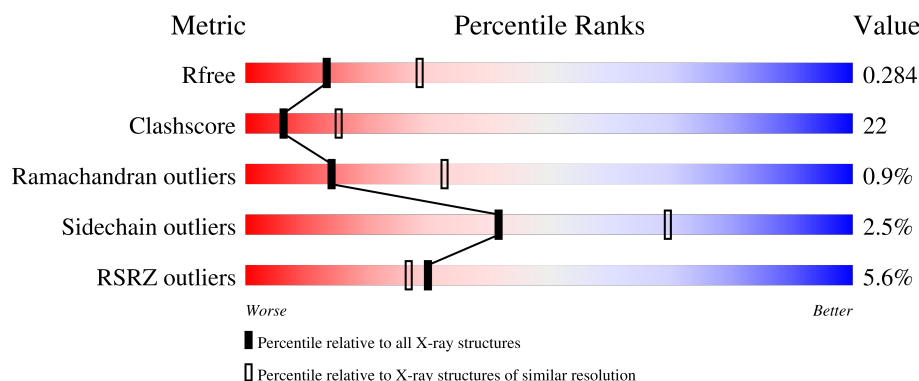
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	440	10% 60% 37% ..
1	C	440	72% 26% .
2	B	431	63% 35% ..
2	D	431	10% 53% 43% ..
3	E	143	4% 50% 32% 15%

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Mol	Chain	Length	Quality of chain
4	F	380	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17484 atoms, of which 52 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3405	2154	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3433	2172	583	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3351	2104	572	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3300	2076	559	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	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

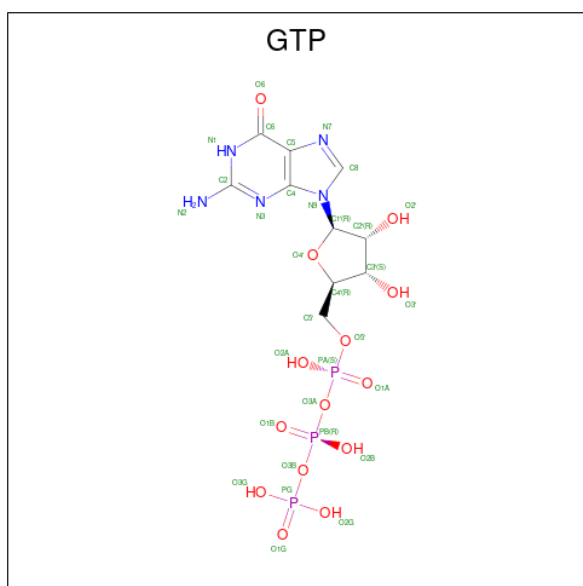
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2713	1740	466	493	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8C9FGJ1
F	380	HIS	-	expression tag	UNP A0A8C9FGJ1

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



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

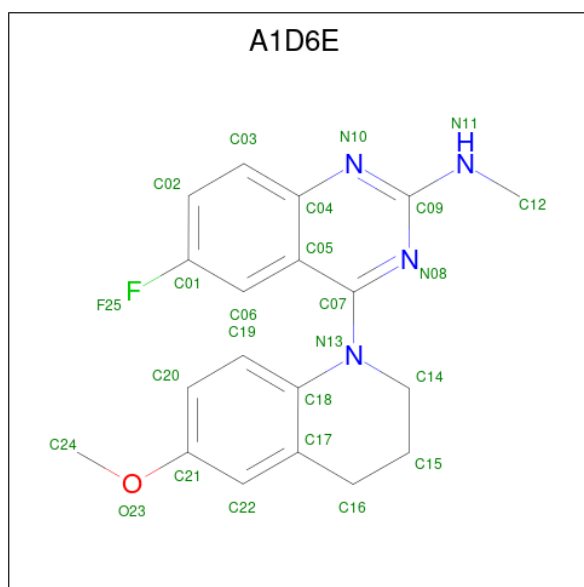
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		

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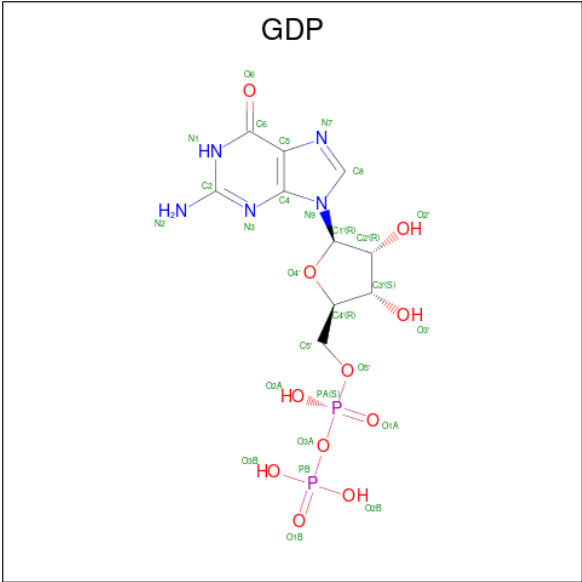
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	1	0
			1	1		

- Molecule 8 is 6-fluoranyl-4-(6-methoxy-3,4-dihydro-2 {H}-quinolin-1-yl)- {N}-methyl-quinazolin-2-amine (CCD ID: A1D6E) (formula: C₁₉H₁₉FN₄O) (labeled as "Ligand of Interest" by depositor).



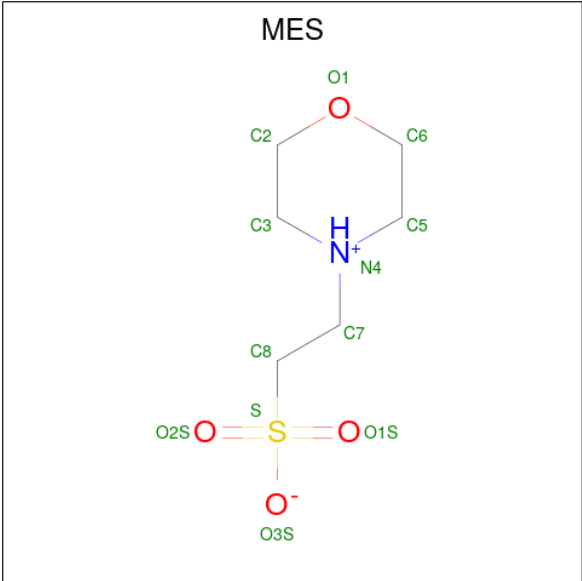
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	F	H	N	O	0	0
			44	19	1	19	4	1		
8	D	1	Total	C	F	H	N	O	0	0
			44	19	1	19	4	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



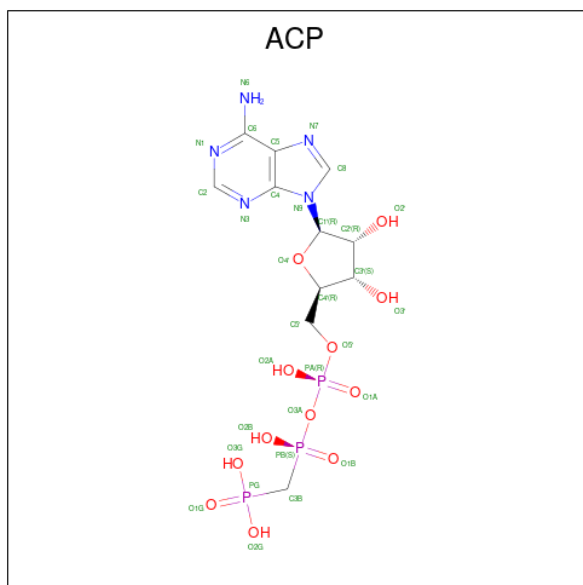
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

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

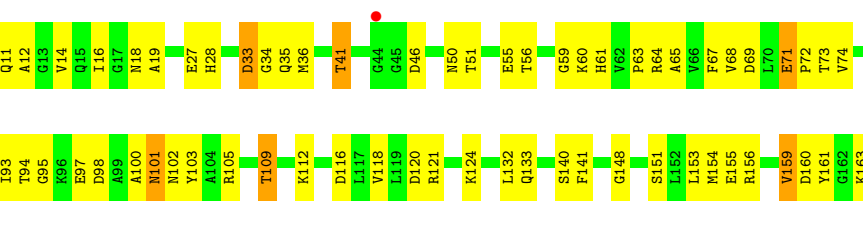
- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
11	F	1	45	11	14	5	12	45	0

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.

- Chain A: 

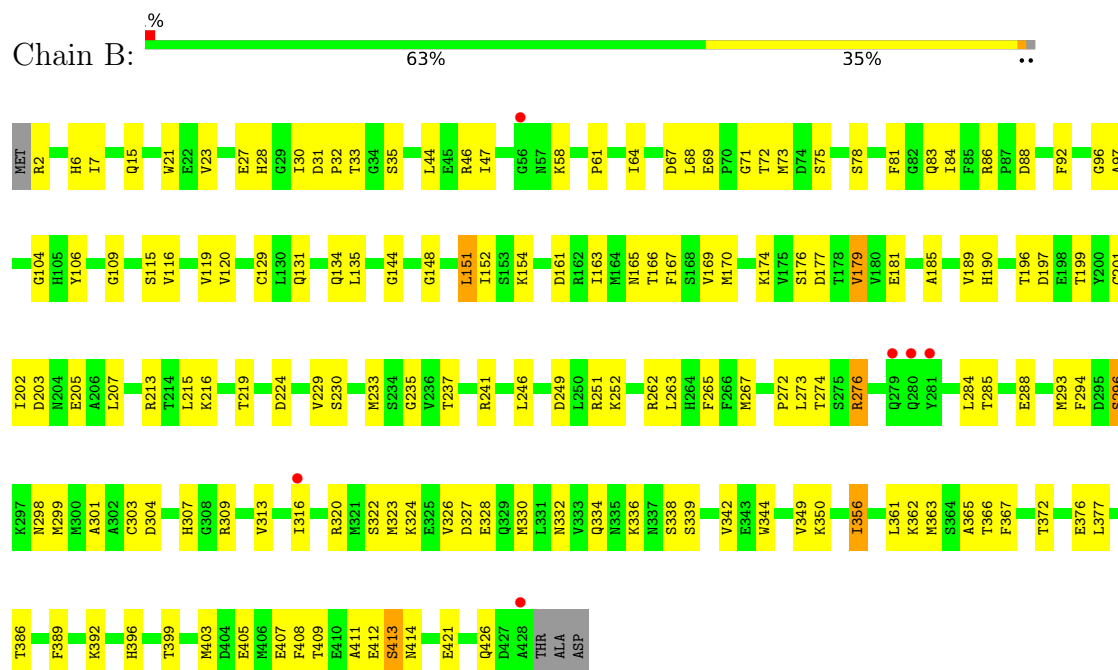


Heatmap visualization for Chain A. The chart displays a grid of colored cells (green, yellow, orange, red) representing different states or categories. The columns are labeled with IDs (M1, R2, E3, V9, G10, Q11, A12, G13, V14, Q15, I16, G17, M18, A19, E27, H28, D33, G34, Q35, M36, T41, G44, G45, D46, N50, T51, E55, T56, G59, K60, H61, V62, P63, R64, A65, V66, F67, V68, D69, L70, E71, P72, T73, V74, V78, G81, R84, Q85, L86, F87, H88, P89, E90, Q91, L92, I93, T94, G95, K96, E97, D98, A99, M100, I101, M102, Y103, A104, R105, T109, K112, D116, L117, V118, G119, D120, R121, K124, L132, Q133, S140, F141, H142, G148, S151, L152, A153, M154, E155, R156, V159, D160, Y161, G162, K163, K164, S165, T166, S170, I171, Y172, P173, Q176, T179, A180, E183, P184, S187, I188, L189, H192, T193, Y194, L195, E196, H197, I209, C213, R214, L217, D218, I219, E220, R221, T222, T223, L227, L230, Q233, I234, T238, T239, A240, S241, L242, R243, N249, V250, E254, F255, Q256, T257, N258, L259, V260, P261, Y265, H266, L269, A281, Y282, Q285, L286, S287, E290, L291, T292, N293, P298, Q301, M302, A314, C315, C316, Y319, R320, V323, A333, T334, I335, K336, R339, S340, I341, D345, W346, F351, K352, I355, B356, Y357, T361, L368, A369, K370, V371, Q372, R373, S376, R390, L391, F395, Y399, A400, K401, R402, V405, E411, G412, M413, E414, E415, G416, E417, F418, A421, R422, E423, D424, M425, A426, A427, Y432, V437, ASP, SER, VAL.

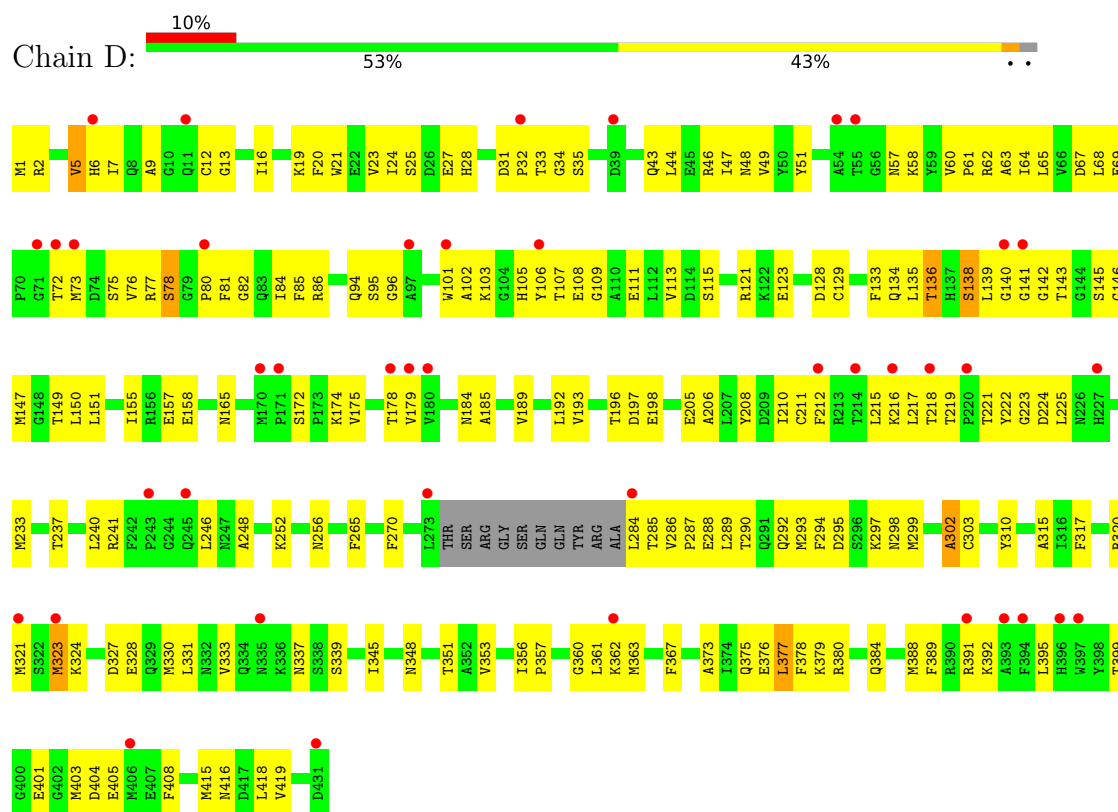
- Chain C: 

Label	Color
M1	Red
R2	Red
E3	Red
C4	Red
H28	Red
M36	Red
D46	Red
D47	Red
S48	Red
S54	Red
K60	Red
H61	Red
V62	Red
P63	Red
F67	Red
V68	Red
E71	Red
P72	Red
T73	Red
V74	Red
I75	Red
Q85	Red
L86	Red
F87	Red
H88	Red
P89	Red
E90	Red
T93	Red
T94	Red
K95	Red
K96	Red
E97	Red
D98	Red
N101	Red
R105	Red
T109	Red
L115	Red
L117	Red
V118	Red
L119	Red
D120	Red
R121	Red
K124	Red
T126	Red
G131	Green
L132	Green
L136	Green
F141	Green
S151	Green
E155	Green
R156	Green
Y161	Green
G162	Green
S165	Green
K166	Green
S170	Green
I171	Green
V177	Green
S178	Green
T179	Green
A180	Green
E183	Green
I188	Green
H192	Green
H197	Green
I209	Green
Y210	Green
D211	Green
R214	Green
R215	Green
K216	Green
L217	Green
D218	Green
I219	Green
E220	Green
R221	Green
P222	Green
L227	Green
L230	Green
Q233	Green
T234	Green
R243	Green
L248	Green
N249	Green

- Molecule 2: Tubulin beta chain

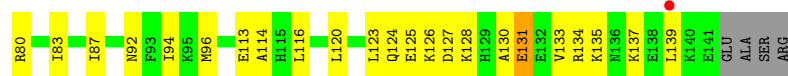
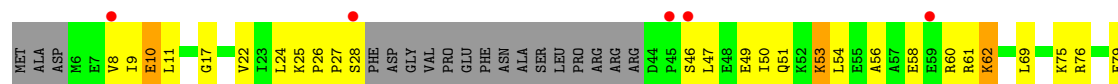


- Molecule 2: Tubulin beta chain

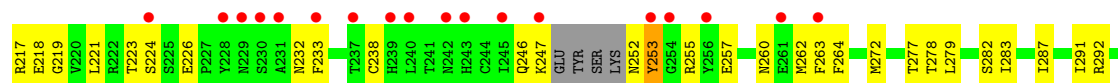
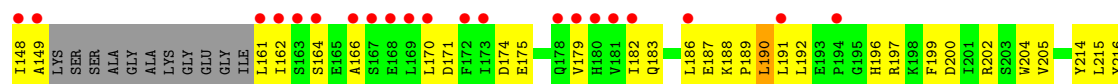
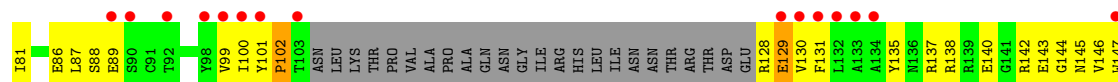
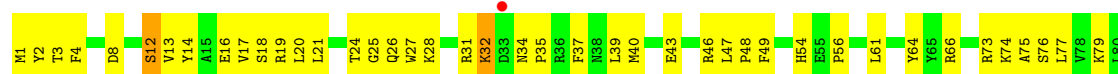


- Molecule 3: Stathmin-4





• 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	105.15Å 157.26Å 181.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 2.71 39.70 – 2.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.70-2.71) 99.9 (39.70-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.222 , 0.286 0.222 , 0.284	Depositor DCC
R_{free} test set	2000 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17484	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: CA, A1D6E, GDP, MES, GTP, ACP, MG

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	0.41	0/3482	0.60	0/4728
1	C	0.44	0/3511	0.62	0/4768
2	B	0.42	0/3426	0.60	0/4643
2	D	0.35	0/3373	0.53	0/4570
3	E	0.41	0/1008	0.57	0/1337
4	F	0.30	0/2775	0.50	0/3752
All	All	0.39	0/17575	0.58	0/23798

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	217	LEU	Peptide
4	F	311	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3405	0	3313	149	0
1	C	3433	0	3337	86	0
2	B	3351	0	3216	136	0
2	D	3300	0	3175	198	0
3	E	1000	0	1018	48	0
4	F	2713	0	2659	171	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	25	19	0	2	0
8	D	25	19	0	1	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	24	0	24	0	0
11	F	31	14	14	0	0
All	All	17432	52	16804	756	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 22.

The worst 5 of 756 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:THR:HG22	2:D:288:GLU:HG3	1.20	1.16
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.32	1.10
2:D:290:THR:HG23	2:D:330:MET:HE3	1.47	0.95
2:D:285:THR:HG22	2:D:288:GLU:CG	1.96	0.95
2:D:294:PHE:HE1	2:D:330:MET:HE1	1.31	0.93

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	435/440 (99%)	400 (92%)	30 (7%)	5 (1%)	11	27
1	C	438/440 (100%)	414 (94%)	20 (5%)	4 (1%)	14	33
2	B	425/431 (99%)	410 (96%)	14 (3%)	1 (0%)	43	66
2	D	417/431 (97%)	389 (93%)	26 (6%)	2 (0%)	24	46
3	E	117/143 (82%)	103 (88%)	12 (10%)	2 (2%)	7	17
4	F	322/380 (85%)	296 (92%)	21 (6%)	5 (2%)	7	18
All	All	2154/2265 (95%)	2012 (93%)	123 (6%)	19 (1%)	14	33

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	ASP
1	A	109	THR
2	B	71	GLY
1	C	109	THR
3	E	10	GLU

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	366/371 (99%)	358 (98%)	8 (2%)	45	72
1	C	370/371 (100%)	361 (98%)	9 (2%)	43	70
2	B	367/372 (99%)	358 (98%)	9 (2%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	362/372 (97%)	348 (96%)	14 (4%)	28	56
3	E	109/127 (86%)	106 (97%)	3 (3%)	38	67
4	F	295/338 (87%)	291 (99%)	4 (1%)	59	80
All	All	1869/1951 (96%)	1822 (98%)	47 (2%)	42	69

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	57	ASN
2	D	178	THR
2	D	78	SER
2	D	115	SER
2	D	339	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	48	ASN
3	E	103	GLN
4	F	242	ASN
3	E	108	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 5 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
9	GDP	B	502	7	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
5	GTP	C	501	7	33,34,34	0.98	2 (6%)	50,54,54	1.57	8 (16%)
11	ACP	F	401	-	31,33,33	0.52	1 (3%)	47,52,52	1.18	2 (4%)
8	A1D6E	B	501	-	28,28,28	3.00	9 (32%)	35,40,40	1.84	12 (34%)
10	MES	B	504	-	12,12,12	2.32	1 (8%)	15,16,16	1.87	2 (13%)
5	GTP	A	501	7	33,34,34	0.96	1 (3%)	50,54,54	1.57	8 (16%)
8	A1D6E	D	502	-	28,28,28	2.93	6 (21%)	35,40,40	1.99	8 (22%)
10	MES	B	503	-	12,12,12	2.33	1 (8%)	15,16,16	1.83	3 (20%)
9	GDP	D	501	-	29,30,30	1.17	2 (6%)	45,47,47	1.75	6 (13%)

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	GDP	B	502	7	-	5/16/32/32	0/3/3/3
5	GTP	C	501	7	-	10/22/38/38	0/3/3/3
11	ACP	F	401	-	-	5/19/38/38	0/3/3/3
8	A1D6E	B	501	-	-	5/8/18/18	0/4/4/4
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	7	-	9/22/38/38	0/3/3/3
8	A1D6E	D	502	-	-	5/8/18/18	0/4/4/4
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
9	GDP	D	501	-	-	3/16/32/32	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	A1D6E	C09-N11	12.68	1.44	1.34
8	D	502	A1D6E	C09-N11	12.55	1.44	1.34
10	B	503	MES	C8-S	-7.82	1.66	1.77
10	B	504	MES	C8-S	-7.79	1.66	1.77
8	D	502	A1D6E	C18-N13	5.15	1.49	1.40

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	PB-O3A-PA	-6.74	110.36	132.37
8	D	502	A1D6E	C07-C05-C04	6.30	119.65	115.47
9	B	502	GDP	C5-C4-N3	-6.07	118.73	128.39
9	D	501	GDP	C5-C4-N3	-5.82	119.12	128.39
5	C	501	GTP	C5-C4-N3	-5.02	120.41	128.39

There are no chirality outliers.

5 of 50 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-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G

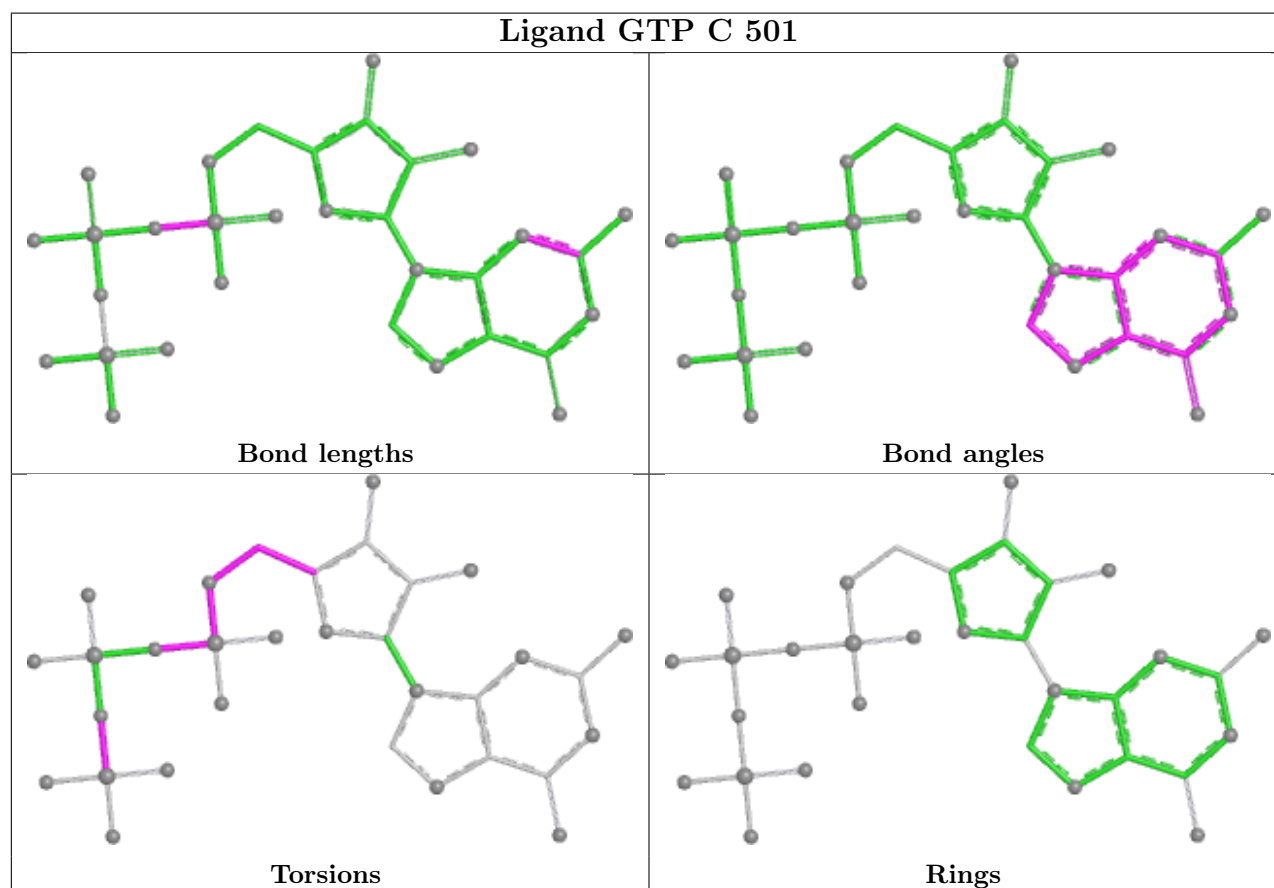
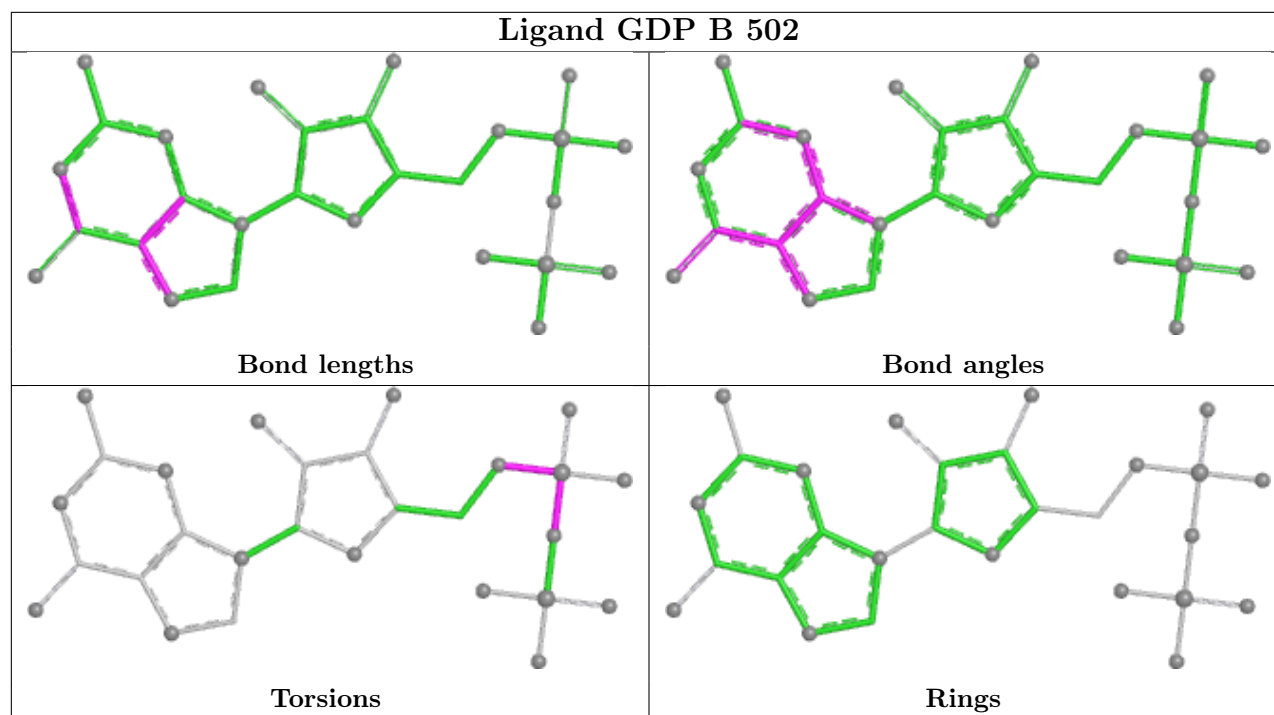
There are no ring outliers.

2 monomers are involved in 3 short contacts:

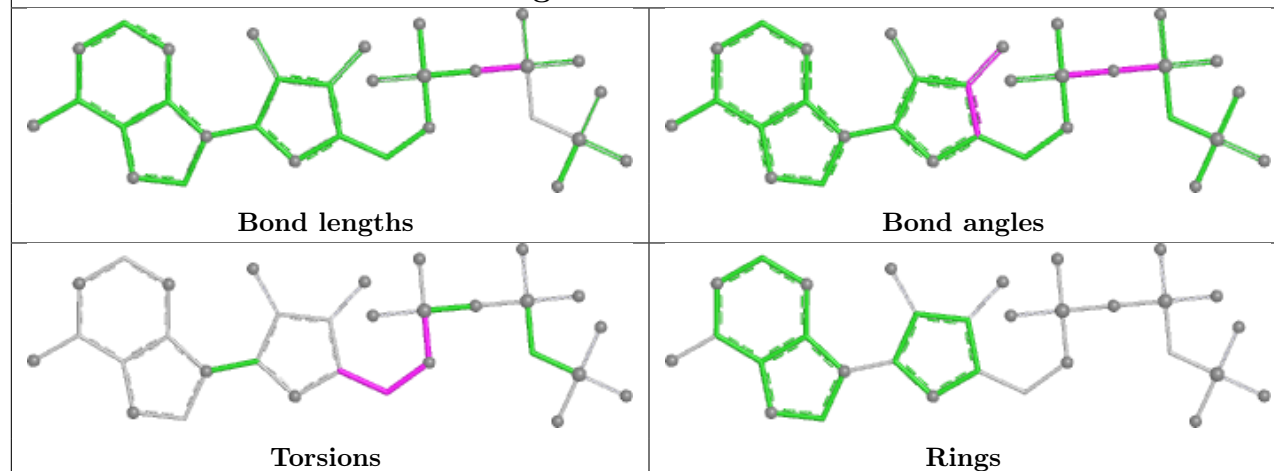
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	A1D6E	2	0
8	D	502	A1D6E	1	0

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

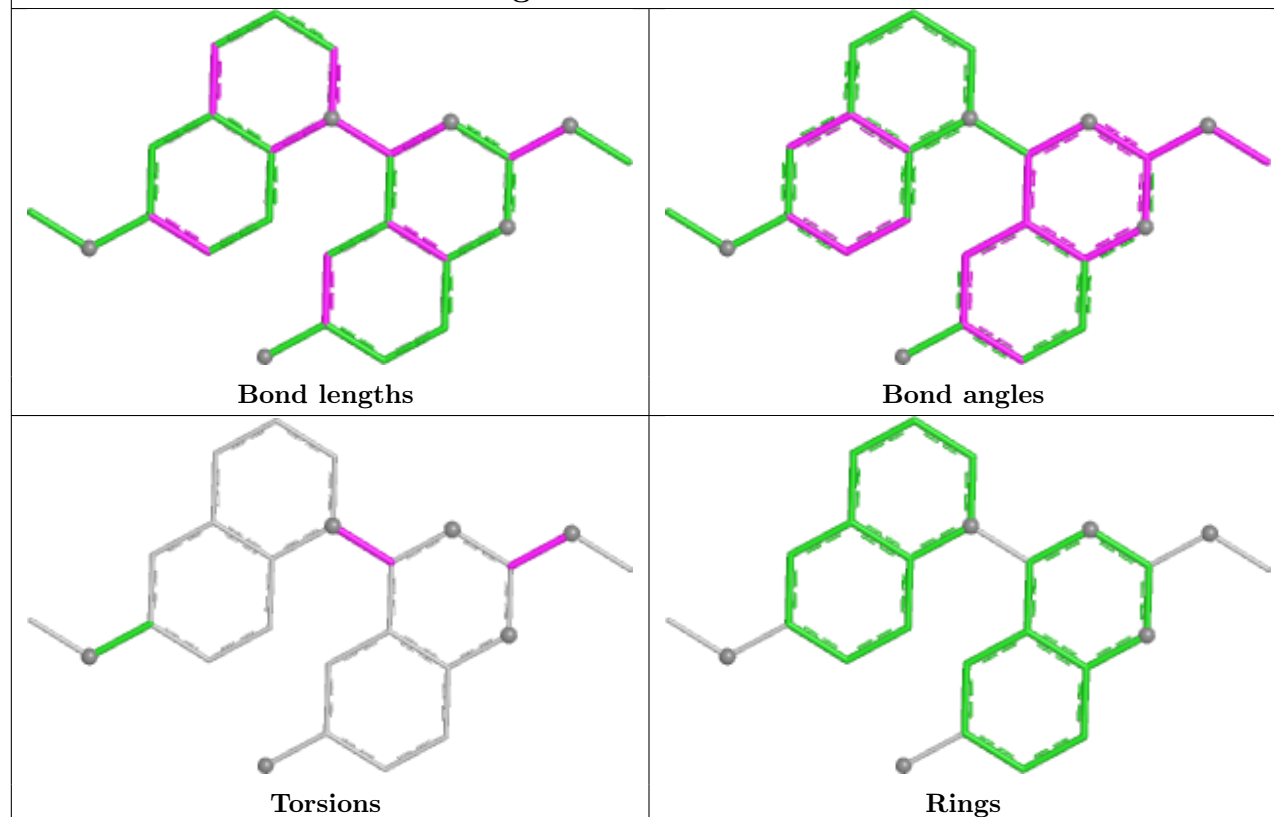
equivalents in the CSD to analyse the geometry.

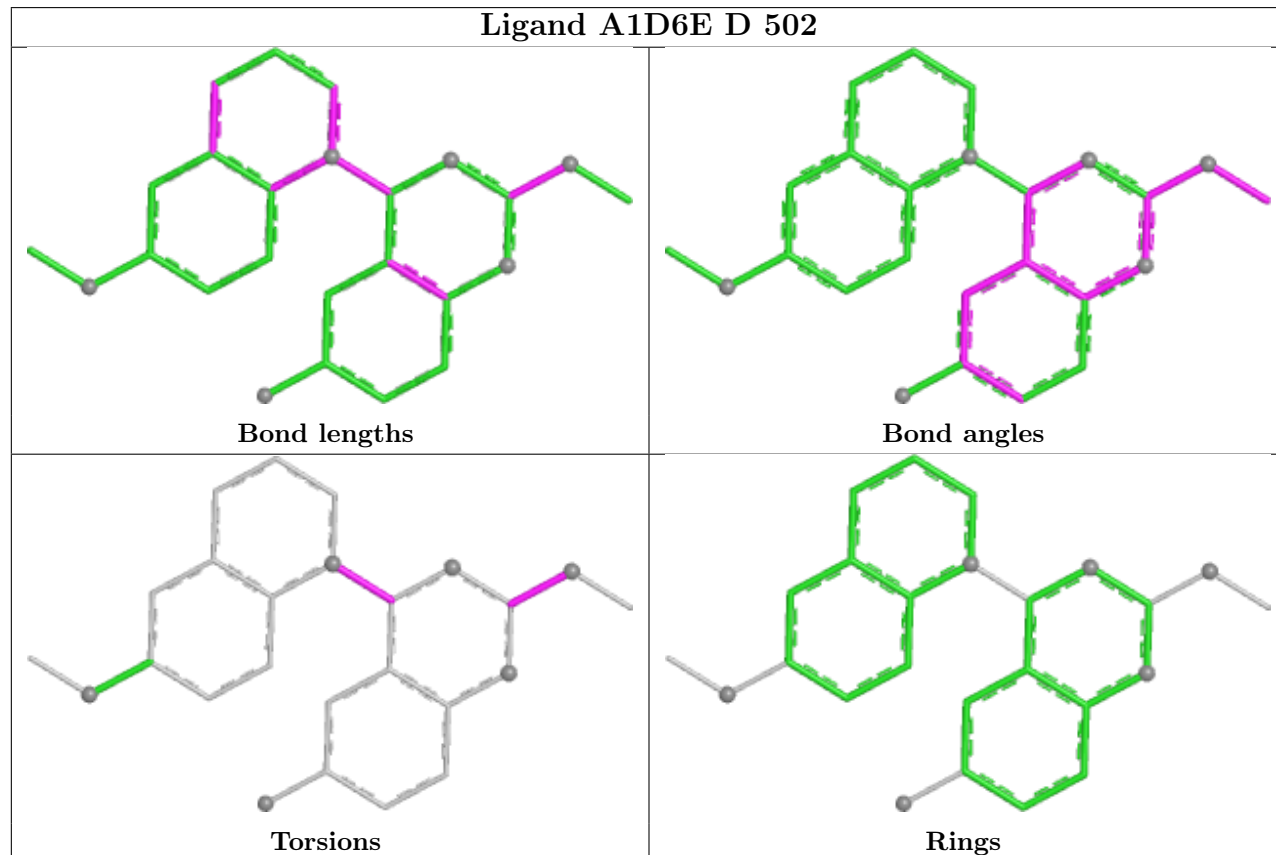
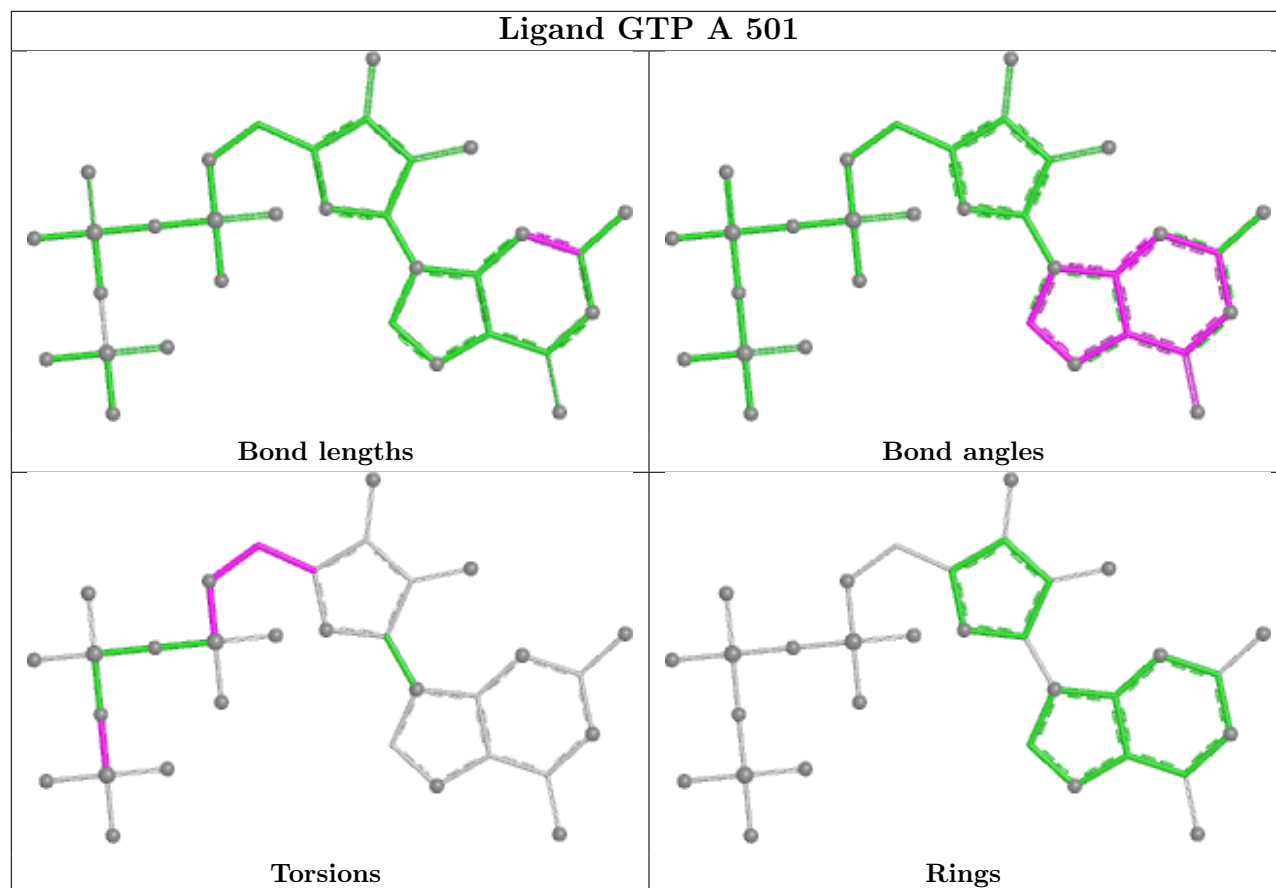


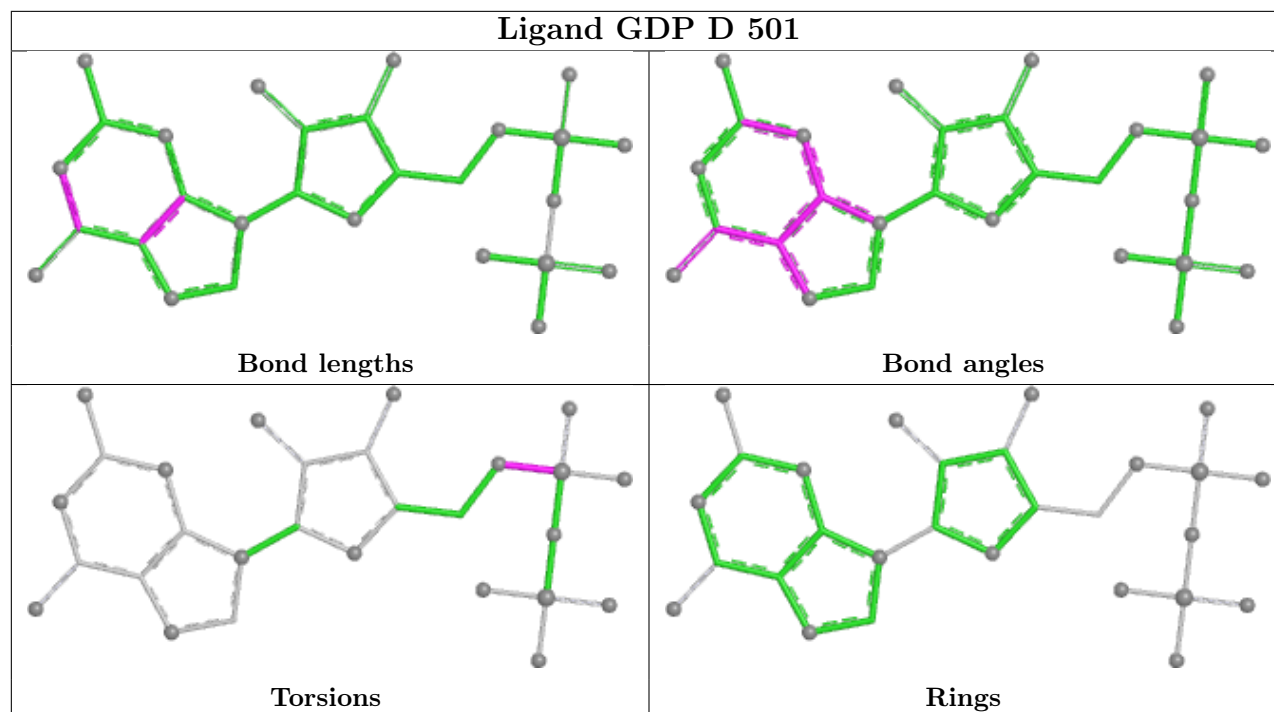
Ligand ACP F 401



Ligand A1D6E B 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/440 (99%)	0.11	6 (1%) 73 71	35, 52, 73, 112	0
1	C	440/440 (100%)	-0.22	4 (0%) 81 80	28, 41, 63, 76	0
2	B	427/431 (99%)	-0.01	6 (1%) 73 71	31, 49, 78, 125	0
2	D	421/431 (97%)	0.79	41 (9%) 13 11	39, 72, 103, 124	0
3	E	121/143 (84%)	0.49	6 (4%) 34 31	41, 62, 92, 114	0
4	F	332/380 (87%)	0.95	60 (18%) 3 3	45, 77, 141, 155	0
All	All	2178/2265 (96%)	0.30	123 (5%) 30 27	28, 56, 105, 155	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	141	GLY	6.5
4	F	173	ILE	4.6
2	D	73	MET	4.1
4	F	132	LEU	4.1
4	F	237	THR	4.1

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

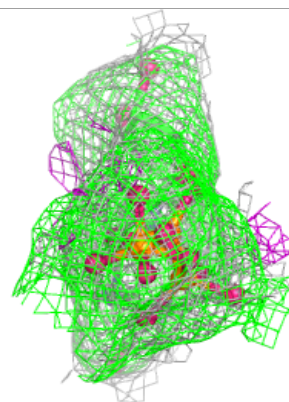
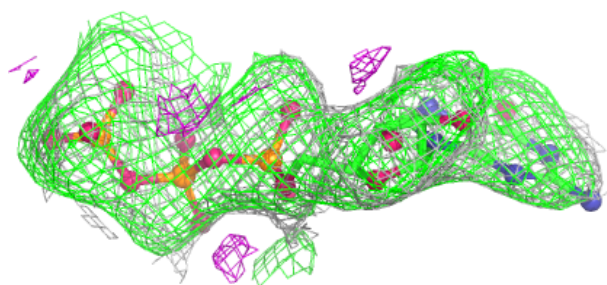
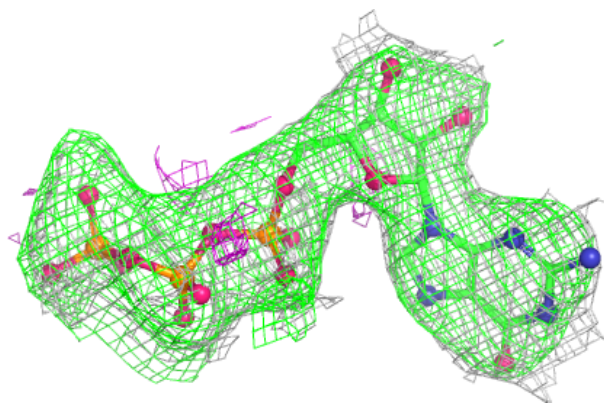
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	A	501	32/32	-	-	40,42,47,48	32
5	GTP	C	501	32/32	-	-	32,35,39,40	32
6	CA	A	502	1/1	-	-	71,71,71,71	1
6	CA	C	502	1/1	-	-	59,59,59,59	1
7	MG	A	503	1/1	-	-	46,46,46,46	1
7	MG	B	505	1/1	-	-	45,45,45,45	1
7	MG	C	503	1/1	-	-	39,39,39,39	1
8	A1D6E	B	501	25/25	0.93	0.10	36,50,63,65	0
8	A1D6E	D	502	25/25	0.93	0.10	42,56,69,70	0
9	GDP	B	502	28/28	-	-	35,38,40,41	28
9	GDP	D	501	28/28	-	-	71,79,86,87	28
10	MES	B	503	12/12	-	-	42,43,45,45	12
10	MES	B	504	12/12	-	-	57,62,63,64	12
11	ACP	F	401	31/31	-	-	99,107,130,130	45

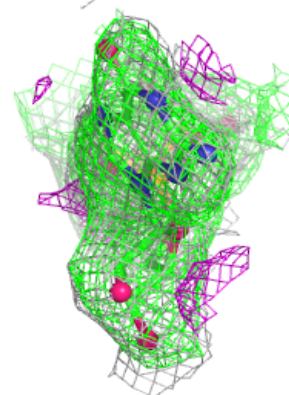
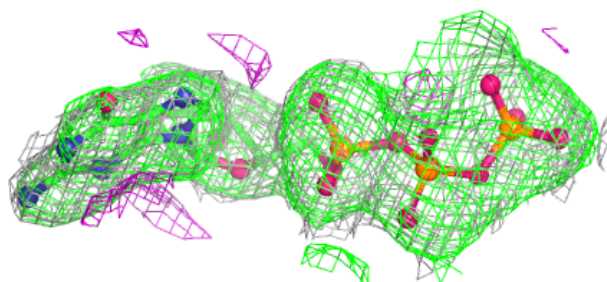
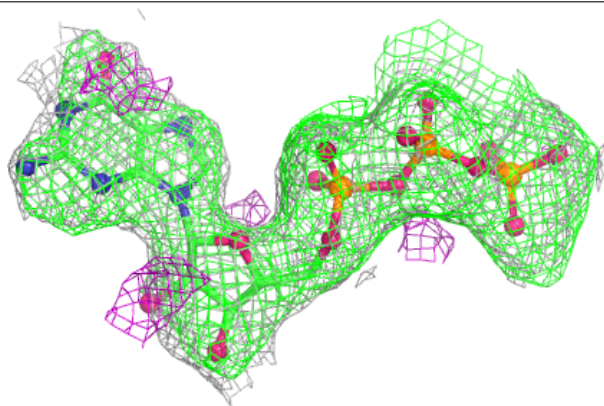
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP 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)

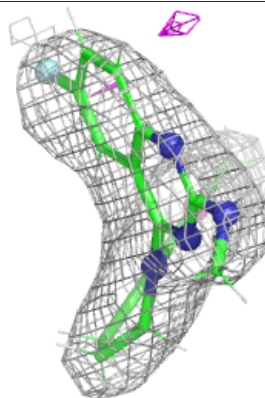
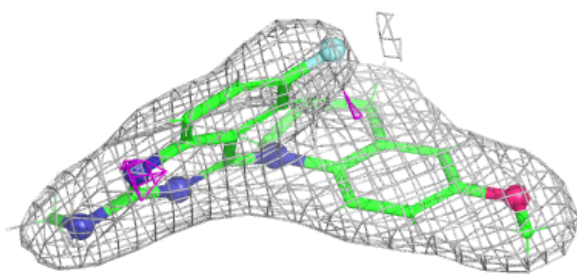
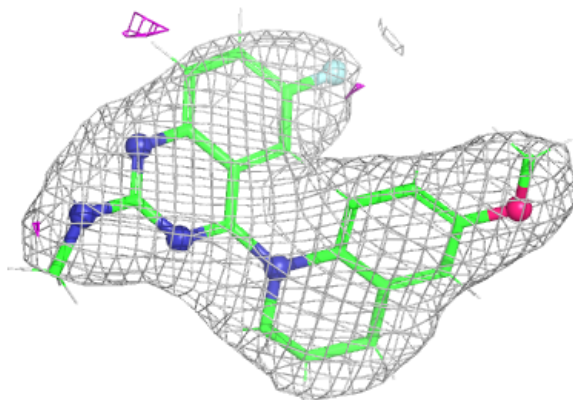
**Electron density around GTP C 501:**

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

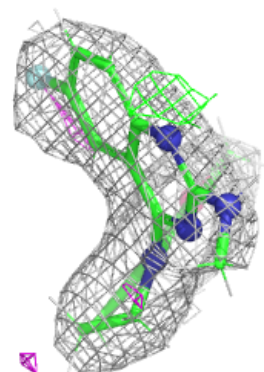
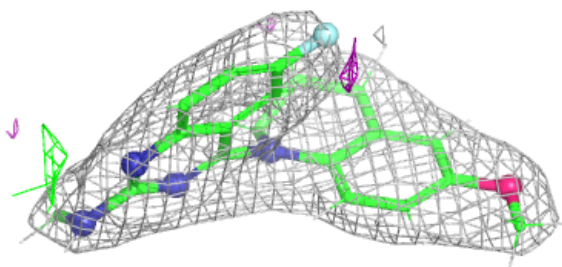
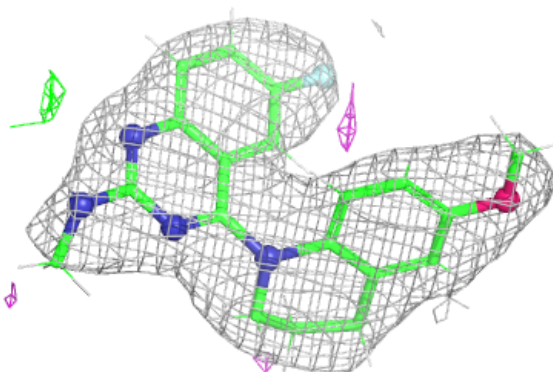


Electron density around A1D6E B 501:

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

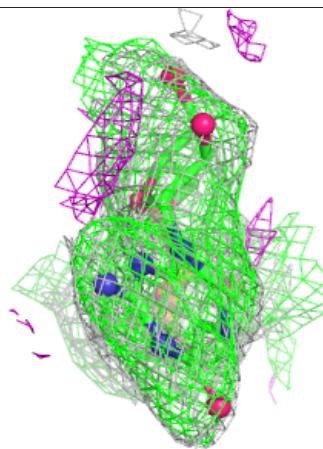
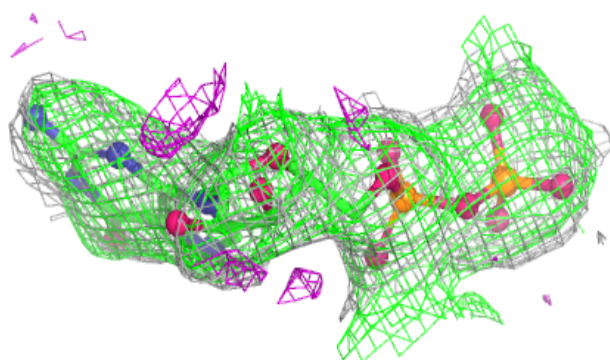
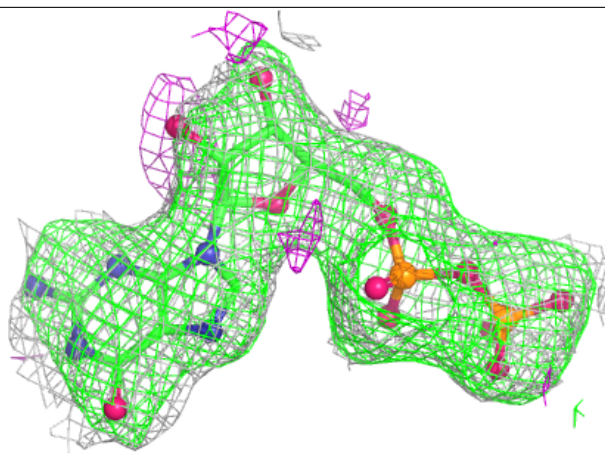
**Electron density around A1D6E D 502:**

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



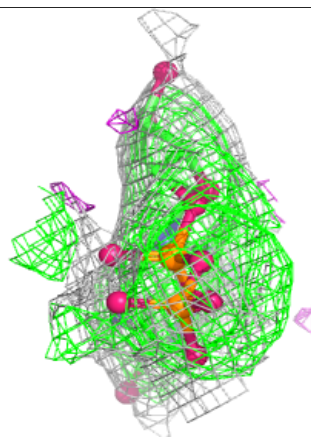
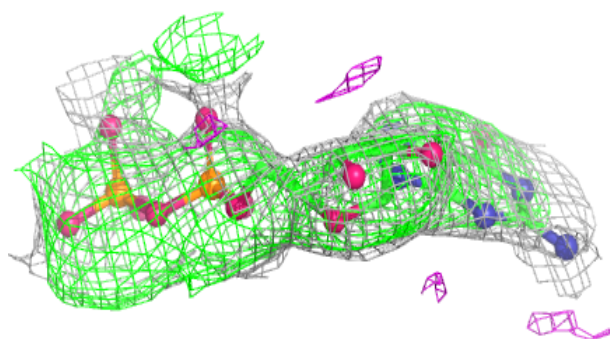
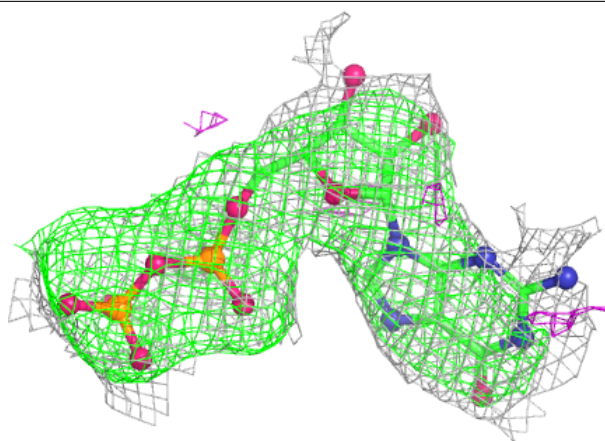
Electron density around GDP B 502:

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

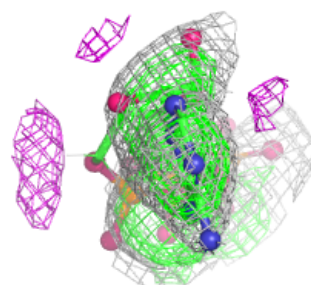
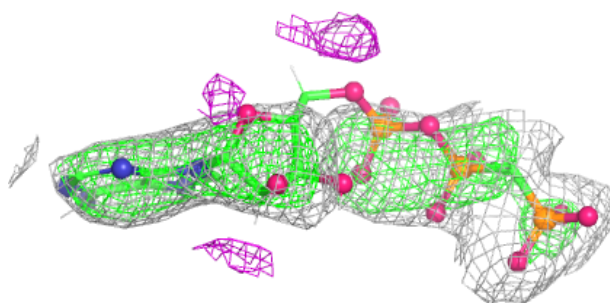
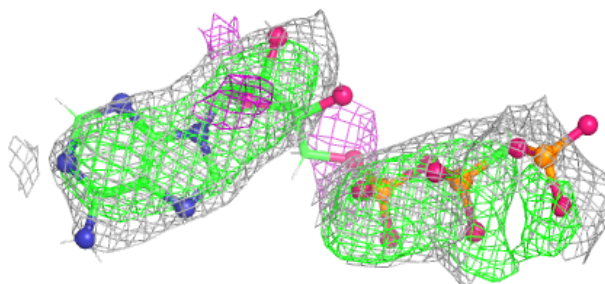


Electron density around GDP D 501:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.