



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 20, 2026 – 09:12 PM JST

PDB ID : 9VYP / pdb_00009vyp
Title : Crystal structure of T2R-TTL-TZ2 complex
Authors : Lun, T.; Chengyong, W.
Deposited on : 2025-07-21
Resolution : 2.52 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

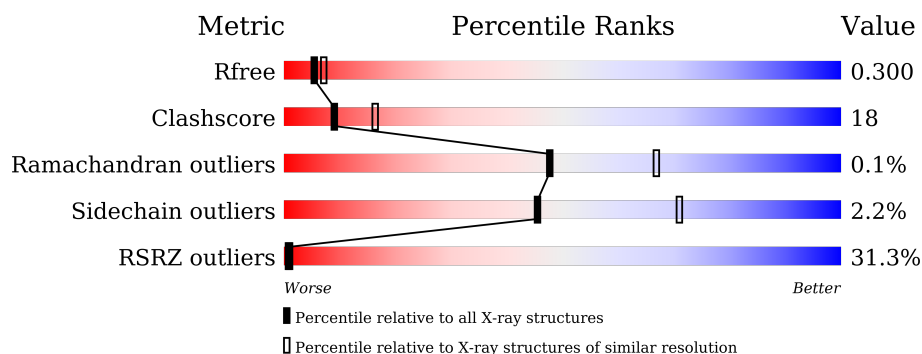
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	440	
1	C	440	
2	B	431	
2	D	431	
3	E	136	
4	F	380	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	A1EU1	D	502	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17464 atoms, of which 38 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			

- 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 35 discrepancies between the modelled and reference sequences:

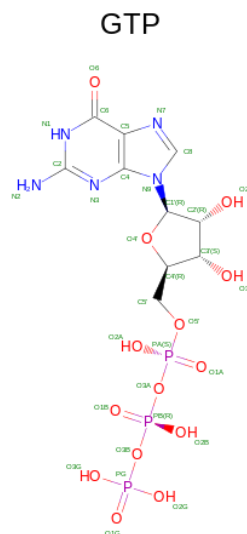
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0

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

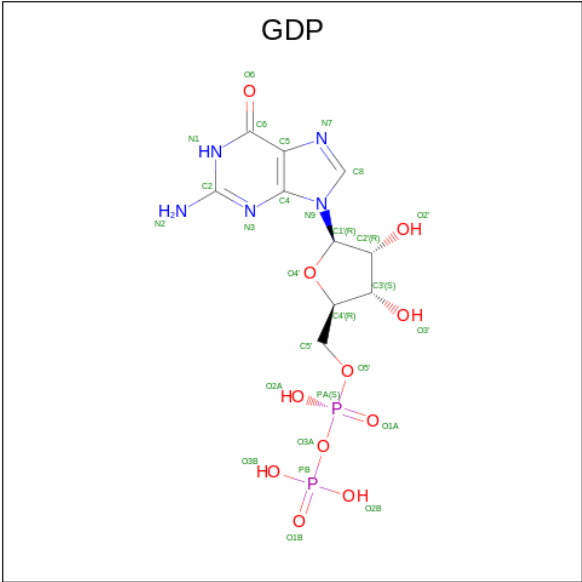
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

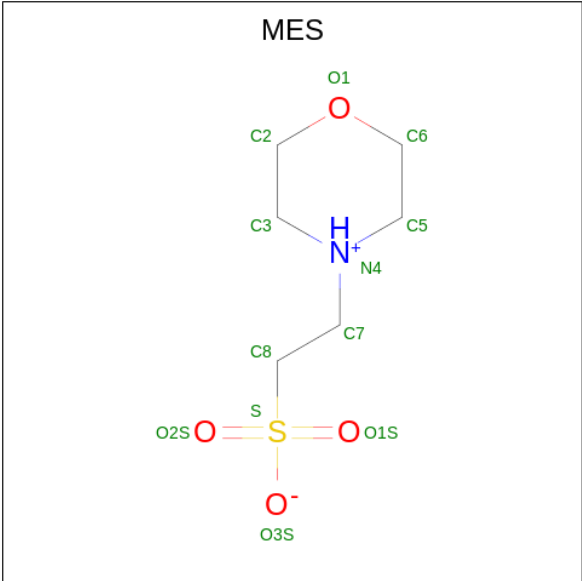
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	1	0
7	B	1	Total Mg 1 1	1	0
7	C	1	Total Mg 1 1	1	0

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



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

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



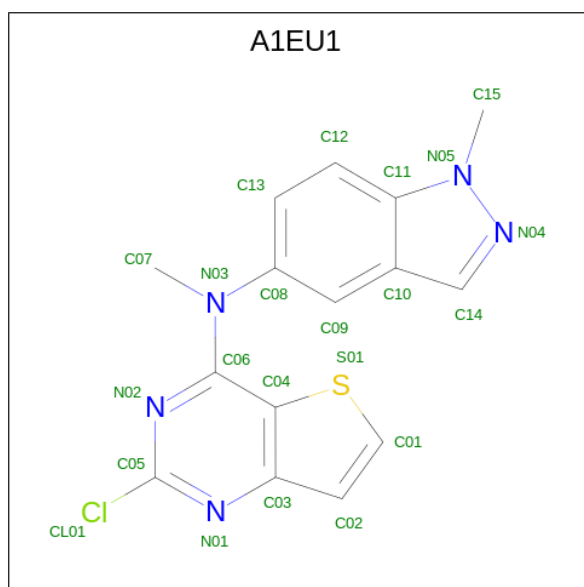
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

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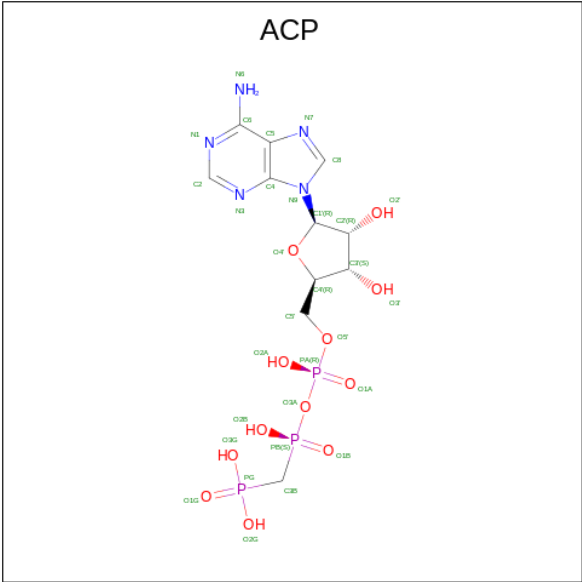
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

- Molecule 10 is 2-chloranyl- {N}-methyl- {N}-(1-methylindazol-5-yl)thieno[3,2-d]pyrimidin-4-amine (CCD ID: A1EU1) (formula: C₁₅H₁₂ClN₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	Cl	H	N	S	0	0
			34	15	1	12	5	1		
10	D	1	Total	C	Cl	H	N	S	0	0
			34	15	1	12	5	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).

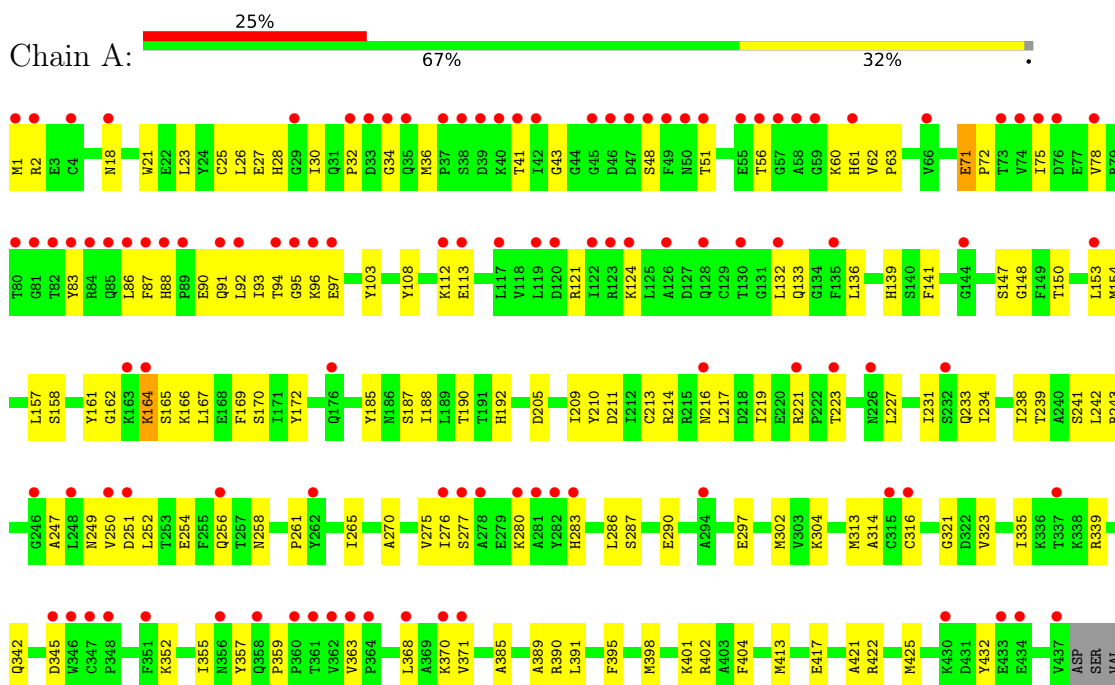


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	
			45	11	14	5	12	3	

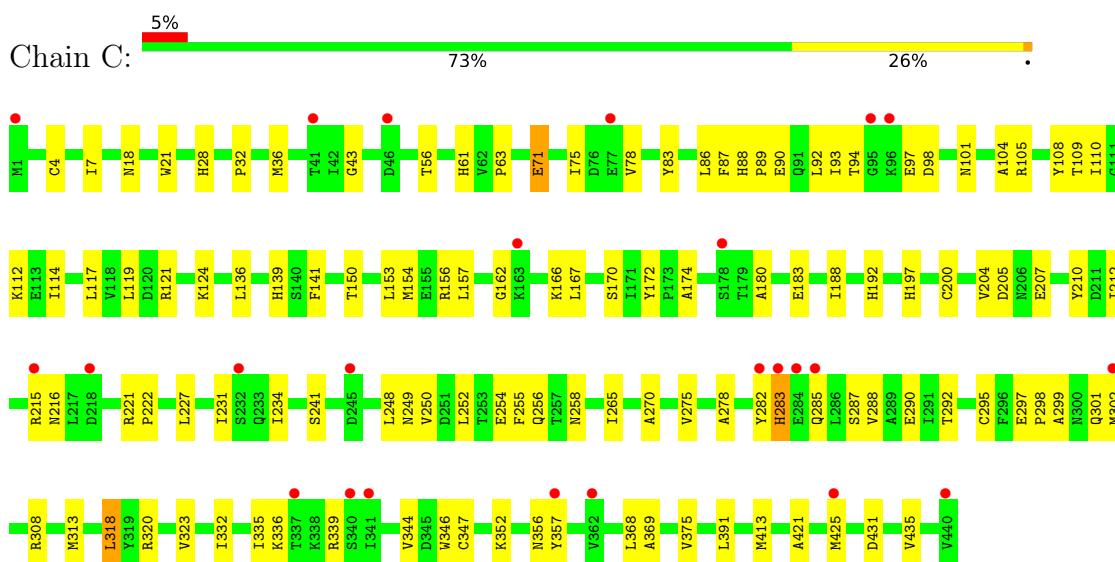
3 Residue-property plots [i](#)

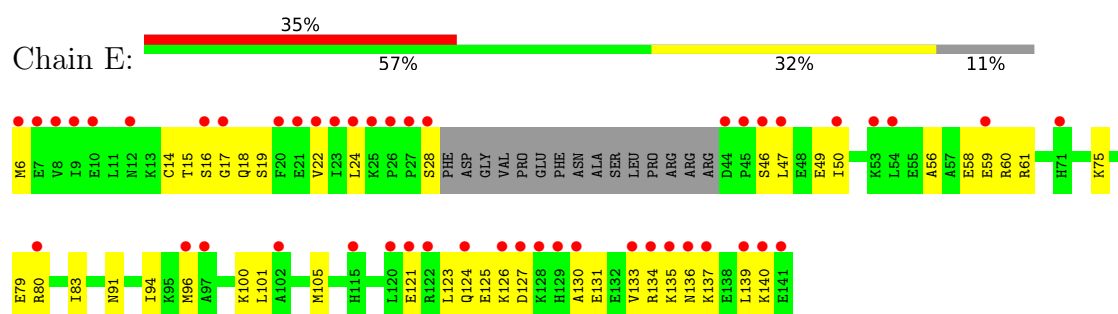
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Detyrosinated tubulin alpha-1B chain

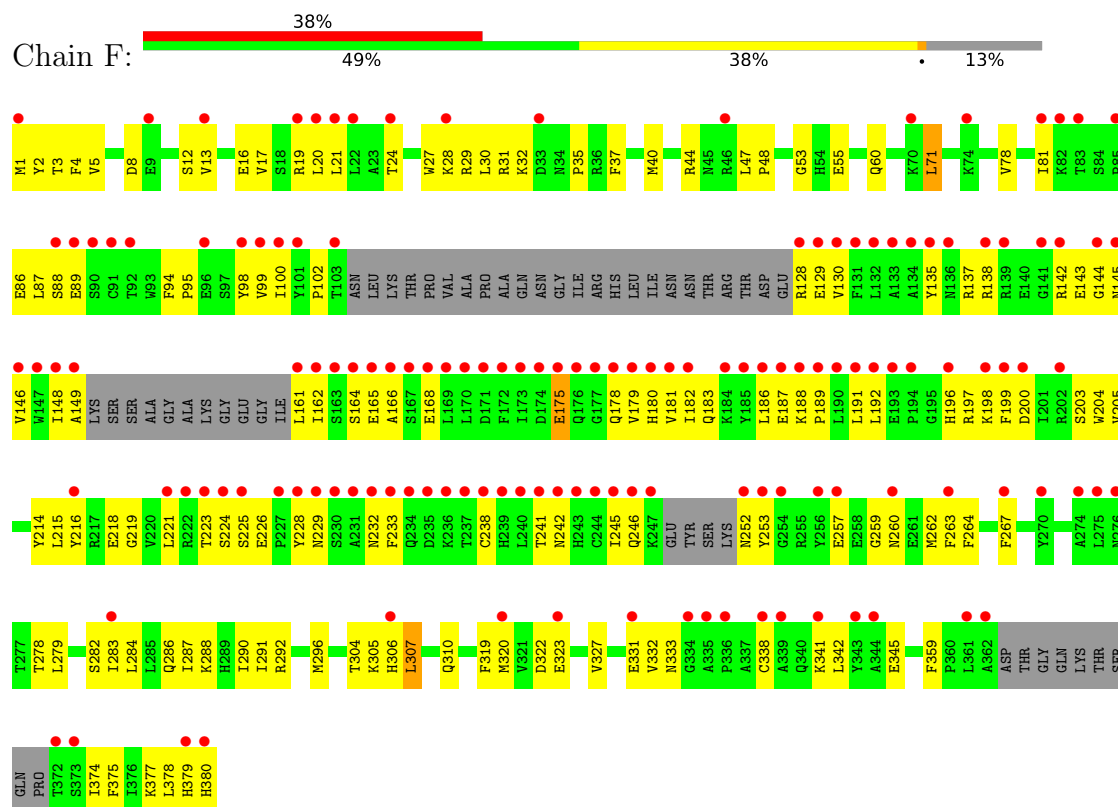


• Molecule 1: Detyrosinated tubulin alpha-1B chain





• 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	104.74Å 157.26Å 179.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.05 – 2.52 56.05 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.05-2.52) 99.8 (56.05-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.51Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.268 , 0.300 0.269 , 0.300	Depositor DCC
R_{free} test set	5121 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.4	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	0.91	EDS
Total number of atoms	17464	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, ACP, GDP, A1EU1, MG, MES, GTP

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	0.24	0/3482	0.44	0/4728
1	C	0.23	0/3511	0.42	0/4768
2	B	0.34	3/3426 (0.1%)	0.45	1/4643 (0.0%)
2	D	0.23	0/3373	0.40	0/4570
3	E	0.18	0/1008	0.33	0/1337
4	F	0.18	0/2775	0.34	0/3752
All	All	0.25	3/17575 (0.0%)	0.41	1/23798 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	323	MET	SD-CE	11.49	2.08	1.79
2	B	332	ASN	CB-CG	-6.26	1.36	1.52
2	B	336	LYS	CD-CE	-5.20	1.36	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	323	MET	CG-SD-CE	-8.42	82.37	100.90

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	3405	0	3312	121	0
1	C	3433	0	3337	98	2
2	B	3351	0	3216	128	1
2	D	3300	0	3176	139	0
3	E	1000	0	1018	40	1
4	F	2713	0	2659	124	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	28	0	12	0	0
8	D	28	0	12	0	0
9	B	24	0	26	0	0
10	B	22	12	0	5	0
10	D	22	12	0	5	0
11	F	31	14	14	0	0
All	All	17426	38	16806	626	2

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 18.

The worst 5 of 626 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:323:MET:SD	2:B:323:MET:CE	2.08	1.41
1:A:209:ILE:HD11	1:A:302:MET:HE1	1.12	1.12
3:E:46:SER:HB3	3:E:49:GLU:HG3	1.44	0.98
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.44	0.98
2:D:350:LYS:HB2	10:D:502:A1EU1:C14	1.94	0.97

All (2) 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:B:401:GLU:OE1	1:C:282:TYR:OH[4_445]	2.06	0.14
1:C:285:GLN:NE2	3:E:91:ASN:OD1[4_545]	2.14	0.06

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	435/440 (99%)	426 (98%)	8 (2%)	1 (0%)	43	62
1	C	438/440 (100%)	425 (97%)	13 (3%)	0	100	100
2	B	425/431 (99%)	417 (98%)	8 (2%)	0	100	100
2	D	417/431 (97%)	408 (98%)	8 (2%)	1 (0%)	43	62
3	E	117/136 (86%)	114 (97%)	3 (3%)	0	100	100
4	F	322/380 (85%)	305 (95%)	16 (5%)	1 (0%)	36	53
All	All	2154/2258 (95%)	2095 (97%)	56 (3%)	3 (0%)	48	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
2	D	302	ALA
4	F	129	GLU

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	366/371 (99%)	359 (98%)	7 (2%)	50	74
1	C	370/371 (100%)	366 (99%)	4 (1%)	65	83
2	B	367/372 (99%)	361 (98%)	6 (2%)	55	78
2	D	362/372 (97%)	350 (97%)	12 (3%)	33	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	109/122 (89%)	105 (96%)	4 (4%)	30	54
4	F	295/338 (87%)	286 (97%)	9 (3%)	35	60
All	All	1869/1946 (96%)	1827 (98%)	42 (2%)	45	71

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	406	MET
4	F	89	GLU
3	E	14	CYS
3	E	18	GLN
4	F	179	VAL

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

Mol	Chain	Res	Type
2	B	332	ASN
2	B	423	GLN
2	B	426	GLN
2	D	298	ASN
4	F	180	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
10	A1EU1	D	502	-	25,25,25	3.66	14 (56%)	34,37,37	6.27	16 (47%)
10	A1EU1	B	505	-	25,25,25	3.68	15 (60%)	34,37,37	6.32	13 (38%)
5	GTP	C	501	7	30,34,34	0.83	1 (3%)	46,54,54	1.74	10 (21%)
9	MES	B	503	-	12,12,12	1.11	1 (8%)	14,16,16	0.85	0
8	GDP	D	501	-	28,30,30	1.14	3 (10%)	44,47,47	1.84	8 (18%)
9	MES	B	502	-	12,12,12	1.13	1 (8%)	14,16,16	0.91	2 (14%)
8	GDP	B	501	7	28,30,30	1.14	3 (10%)	44,47,47	1.80	7 (15%)
11	ACP	F	401	-	30,33,33	1.90	2 (6%)	45,52,52	1.14	3 (6%)
5	GTP	A	501	7	30,34,34	0.85	1 (3%)	46,54,54	1.76	10 (21%)

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
10	A1EU1	D	502	-	-	0/8/8/8	0/4/4/4
10	A1EU1	B	505	-	-	0/8/8/8	0/4/4/4
5	GTP	C	501	7	-	6/22/38/38	0/3/3/3
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
8	GDP	D	501	-	-	3/16/32/32	0/3/3/3
9	MES	B	502	-	-	3/6/14/14	0/1/1/1
8	GDP	B	501	7	-	3/16/32/32	0/3/3/3
11	ACP	F	401	-	-	4/19/38/38	0/3/3/3
5	GTP	A	501	7	-	6/22/38/38	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	A1EU1	N05-N04	-11.09	1.31	1.37
10	B	505	A1EU1	N05-N04	-10.75	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	9.37	1.68	1.58
10	D	502	A1EU1	C04-S01	8.75	1.88	1.73
10	B	505	A1EU1	C04-S01	8.71	1.88	1.73

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	A1EU1	C10-C11-N05	-23.00	98.35	106.68
10	D	502	A1EU1	C10-C11-N05	-21.25	98.99	106.68
10	B	505	A1EU1	C11-N05-N04	19.78	122.47	111.62
10	D	502	A1EU1	C11-N05-N04	19.73	122.44	111.62
10	D	502	A1EU1	C10-C14-N04	10.92	120.34	112.06

There are no chirality outliers.

5 of 25 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-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G

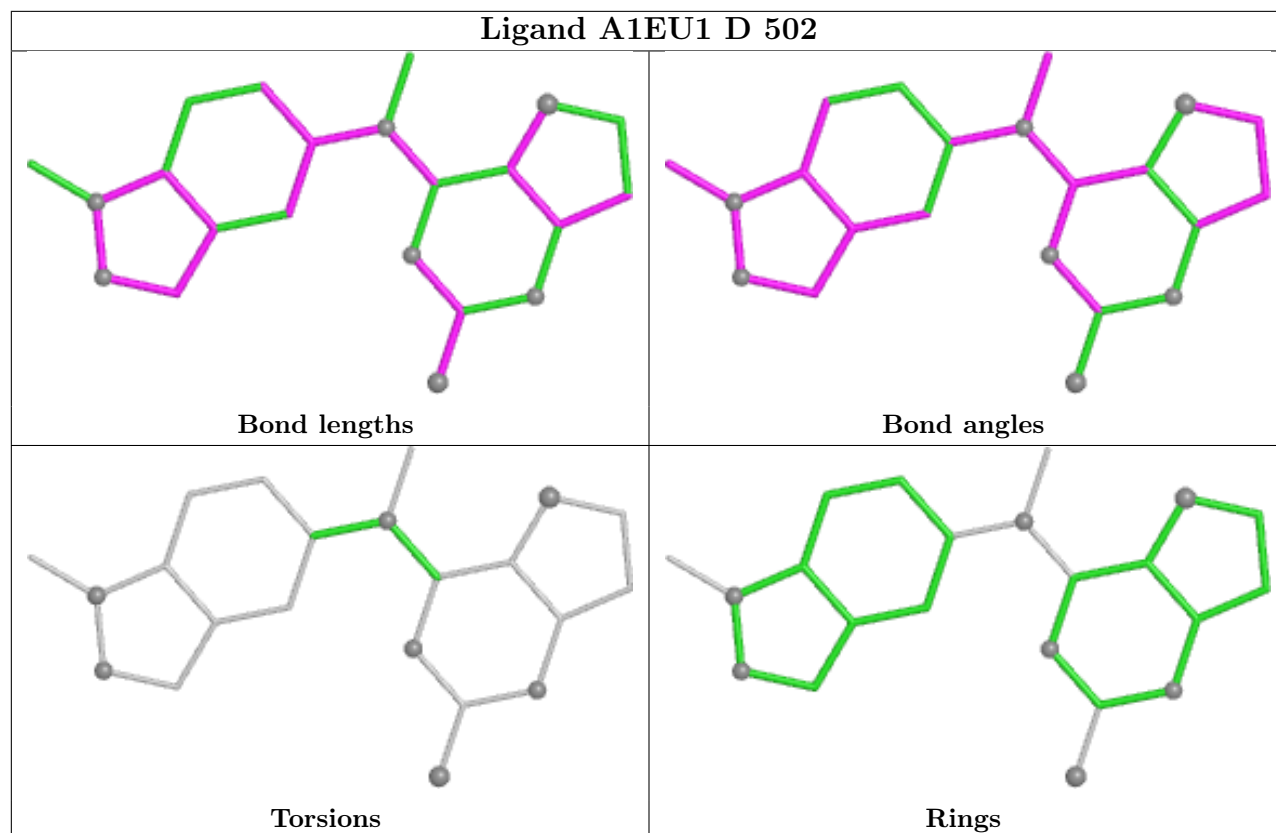
There are no ring outliers.

2 monomers are involved in 10 short contacts:

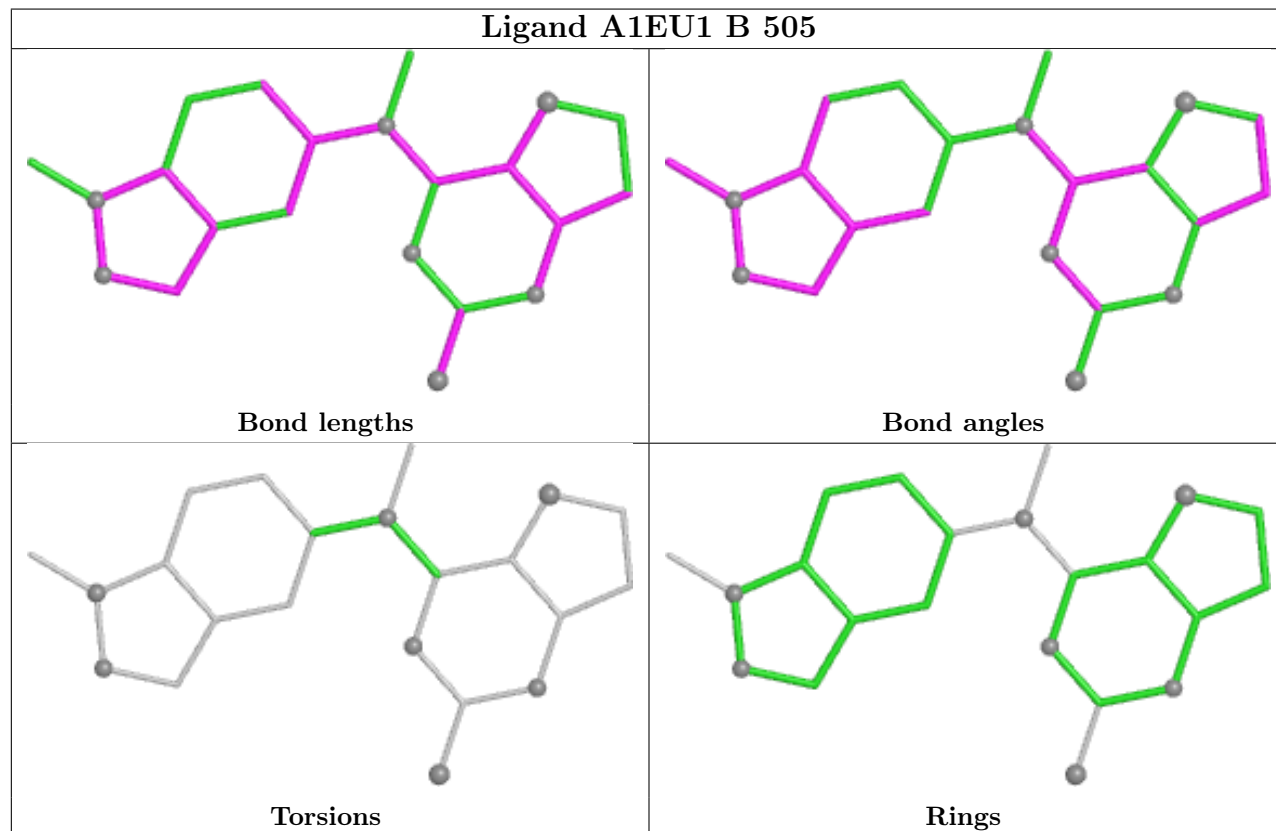
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	A1EU1	5	0
10	B	505	A1EU1	5	0

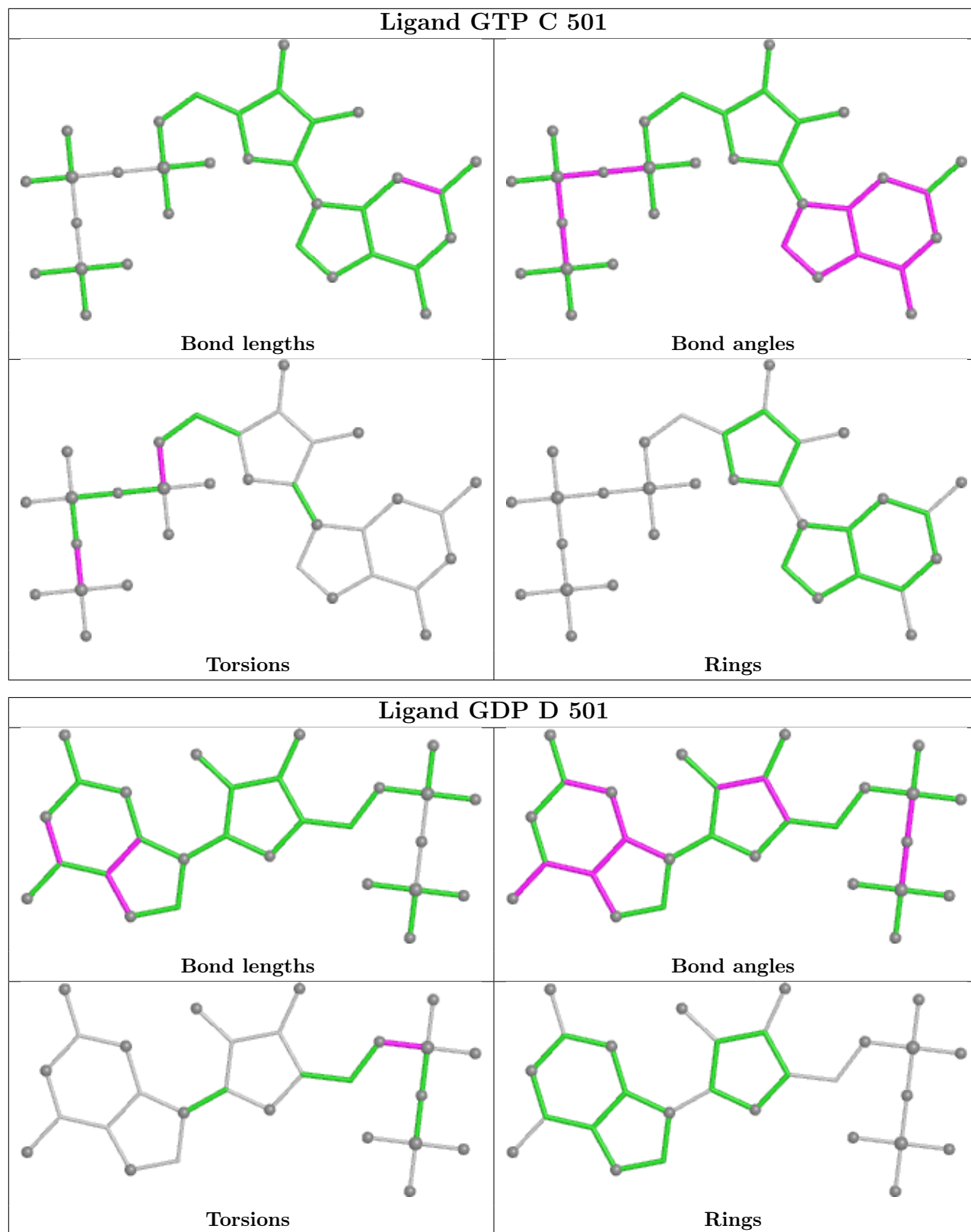
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

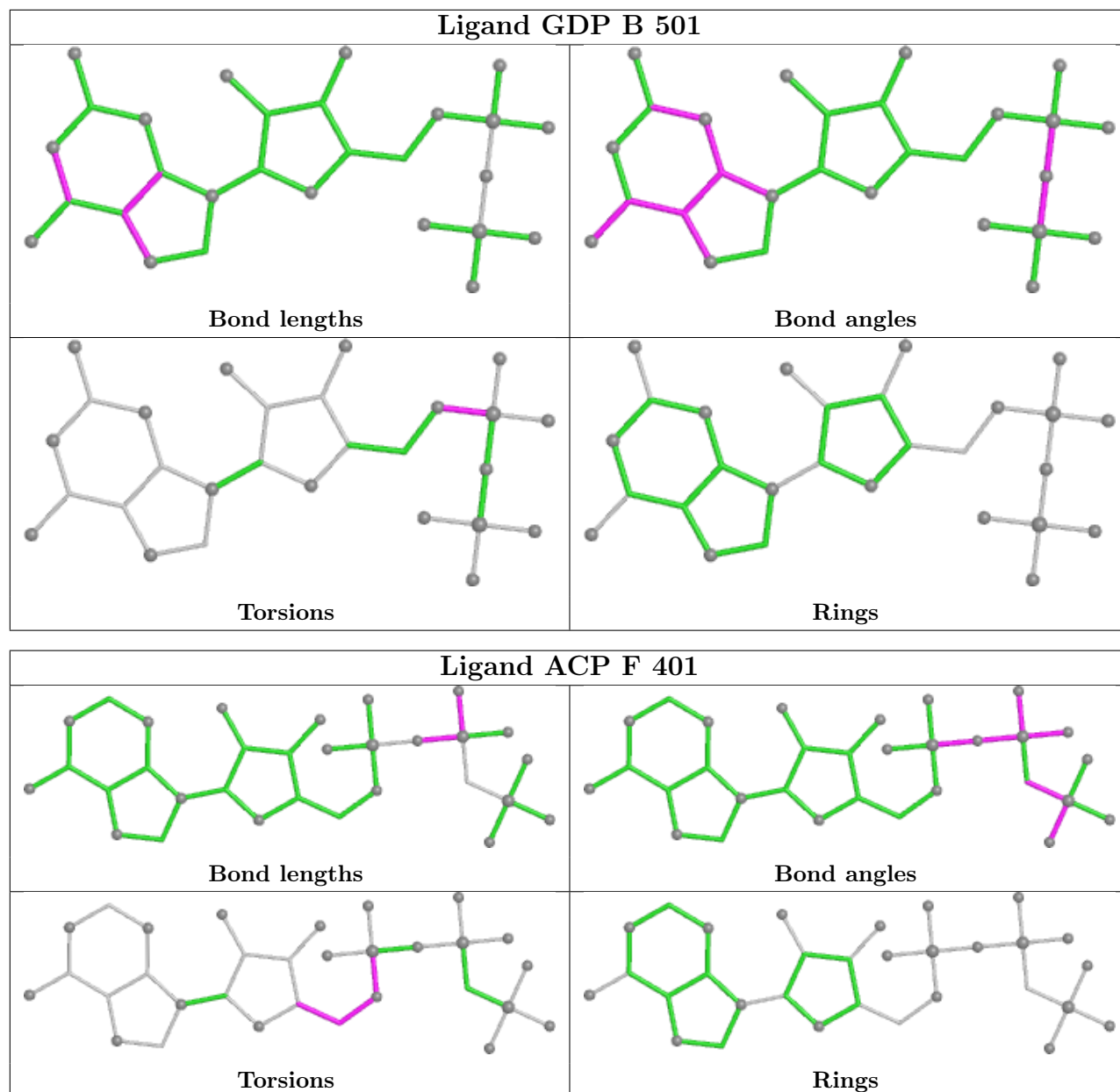
Ligand A1EU1 D 502

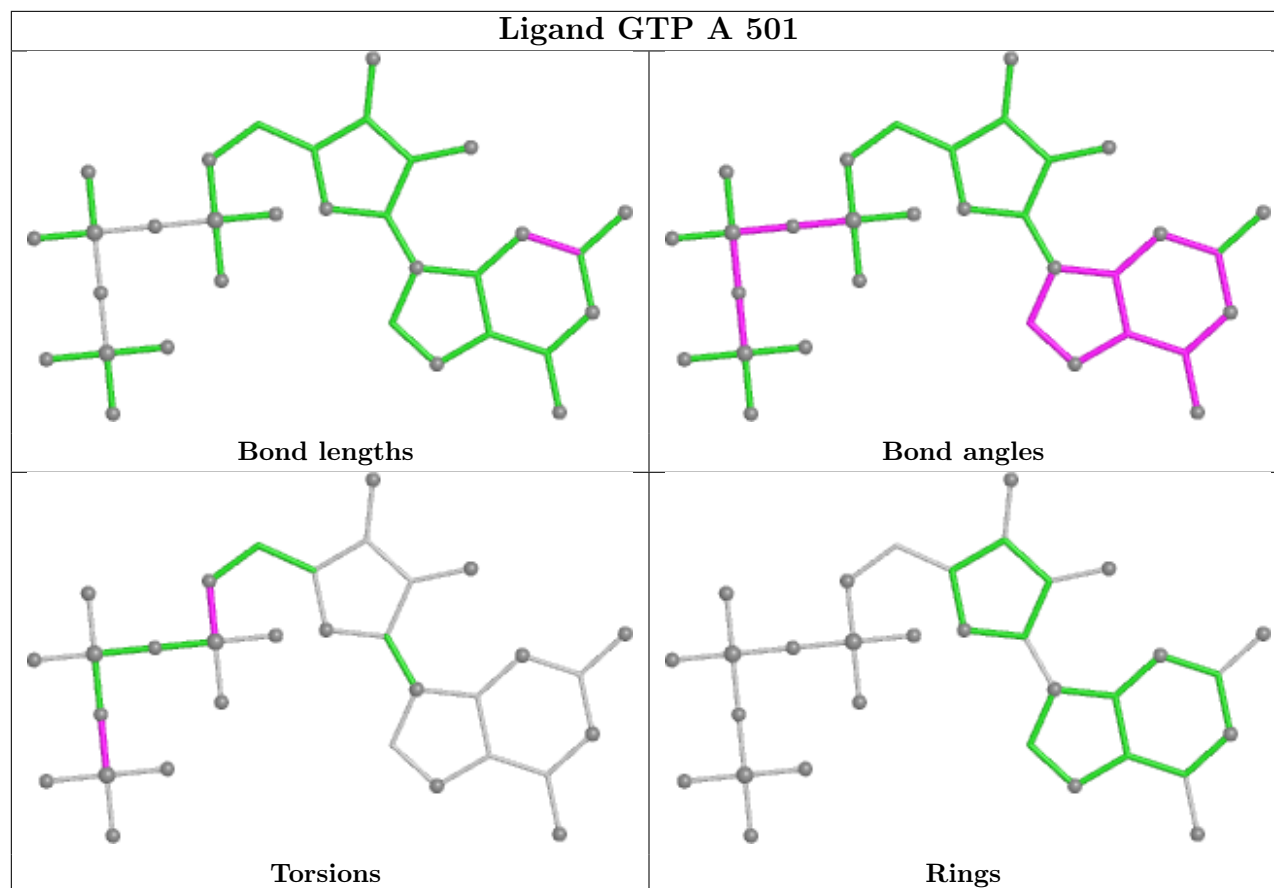


Ligand A1EU1 B 505









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%)	1.34	109 (24%) 2 1	42, 58, 84, 125	0
1	C	440/440 (100%)	0.52	24 (5%) 30 27	34, 49, 67, 87	0
2	B	427/431 (99%)	1.01	53 (12%) 8 7	39, 56, 86, 138	0
2	D	421/431 (97%)	2.91	305 (72%) 0 0	47, 84, 119, 137	0
3	E	121/136 (88%)	1.71	48 (39%) 1 0	49, 71, 102, 119	0
4	F	332/380 (87%)	2.04	143 (43%) 0 0	49, 81, 153, 169	0
All	All	2178/2258 (96%)	1.54	682 (31%) 1 1	34, 63, 116, 169	0

The worst 5 of 682 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	141	GLY	7.8
2	D	42	LEU	6.8
2	D	85	PHE	6.8
2	D	273	LEU	6.7
4	F	148	ILE	6.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

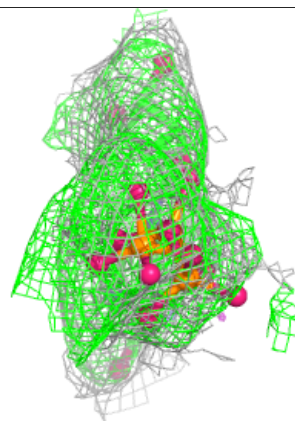
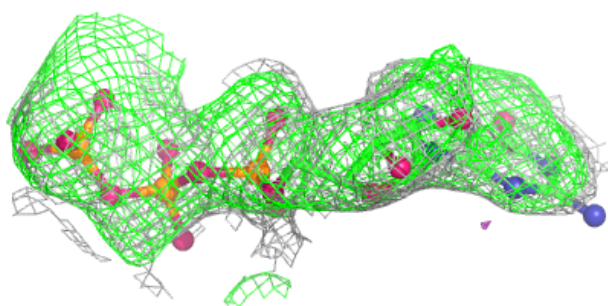
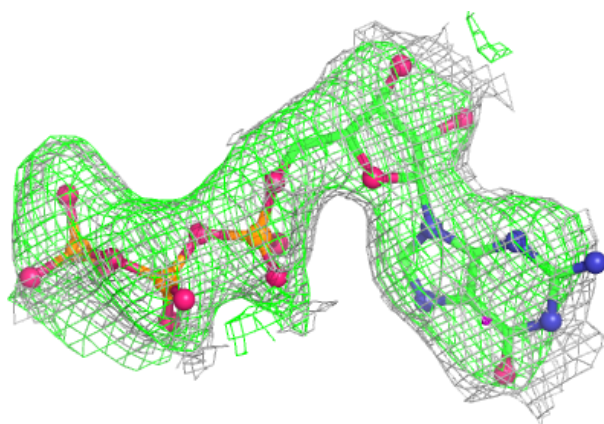
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GTP	A	501	32/32	-	-	46,48,50,50	32
5	GTP	C	501	32/32	-	-	39,43,46,47	32
6	CA	A	502	1/1	-	-	85,85,85,85	1
6	CA	C	502	1/1	-	-	61,61,61,61	1
7	MG	A	503	1/1	-	-	50,50,50,50	1
7	MG	B	504	1/1	-	-	56,56,56,56	1
7	MG	C	503	1/1	-	-	44,44,44,44	1
8	GDP	B	501	28/28	-	-	45,49,51,52	28
8	GDP	D	501	28/28	-	-	83,91,98,99	28
9	MES	B	502	12/12	-	-	47,48,51,51	12
9	MES	B	503	12/12	-	-	64,66,68,70	12
10	A1EU1	D	502	22/22	0.76	0.20	56,69,77,87	0
10	A1EU1	B	505	22/22	0.87	0.18	42,57,70,185	0
11	ACP	F	401	31/31	-	-	107,118,142,146	45

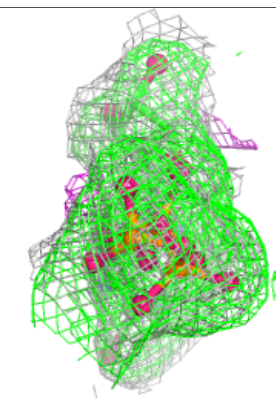
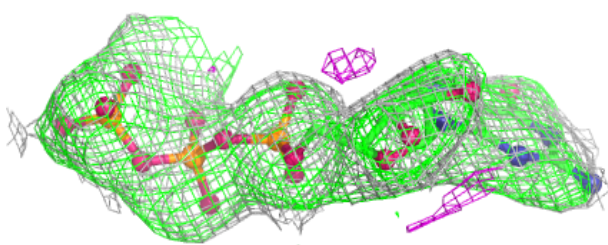
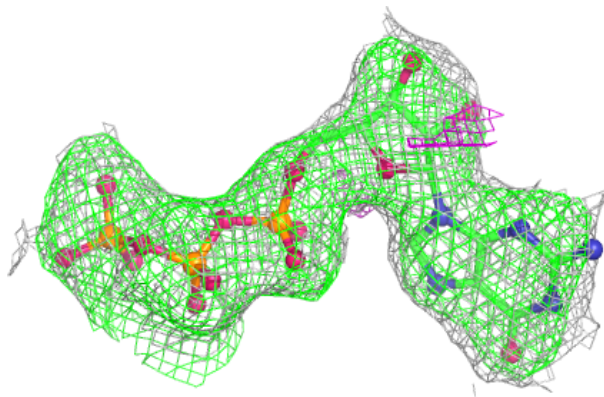
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

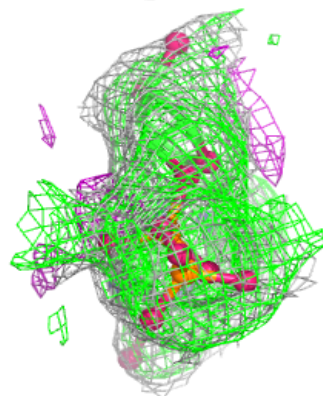
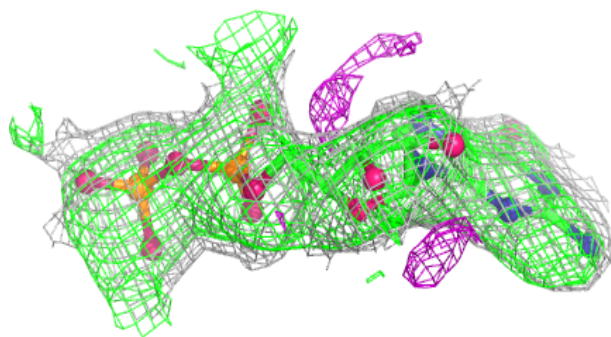
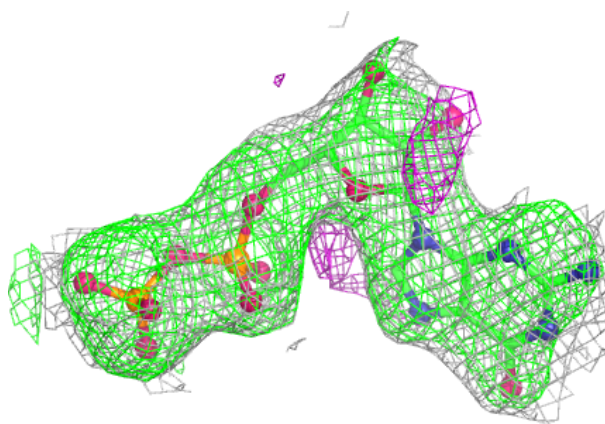
**Electron density around GTP C 501:**

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



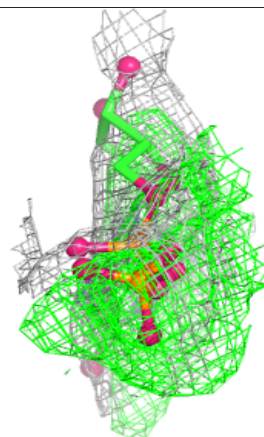
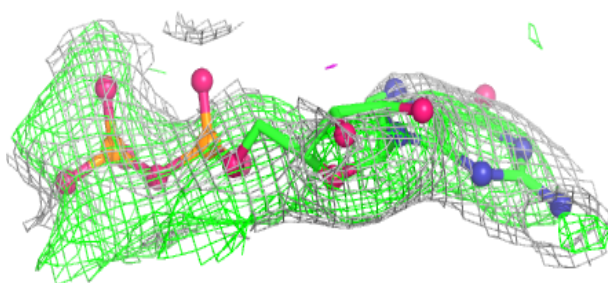
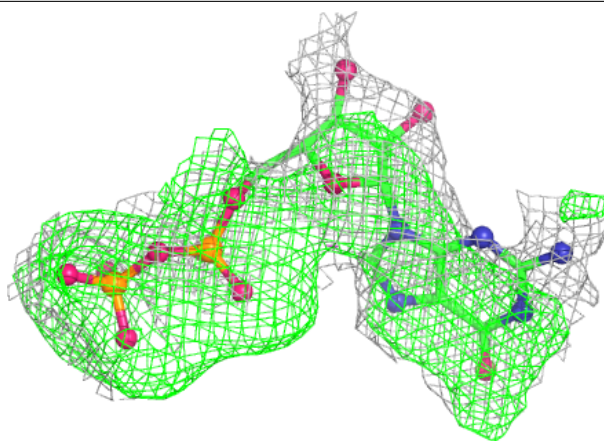
Electron density around GDP B 501:

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

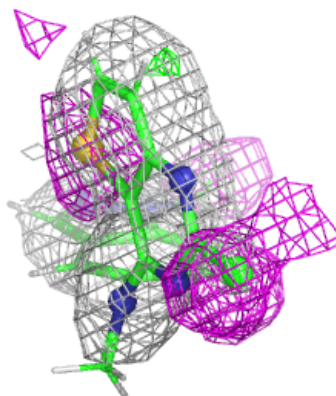
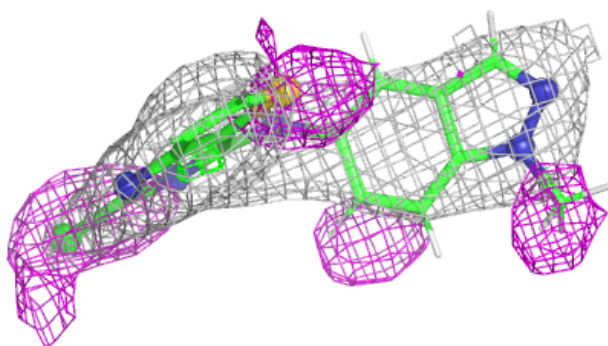
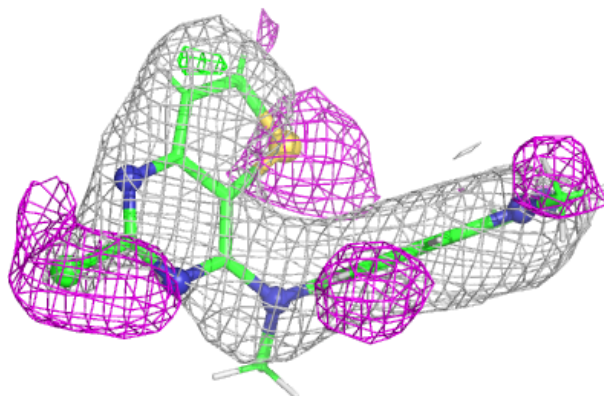


Electron density around GDP D 501:

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

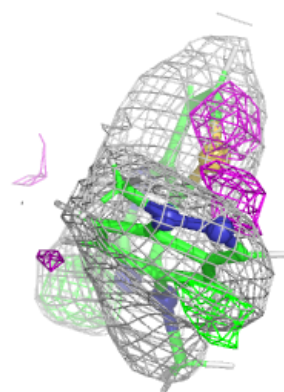
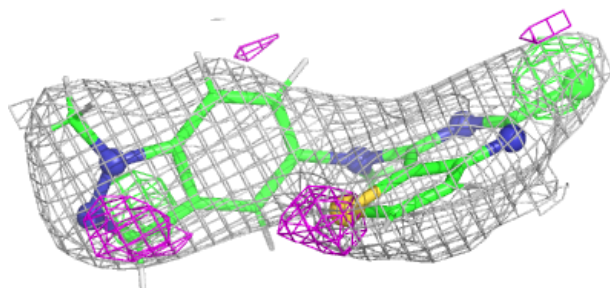
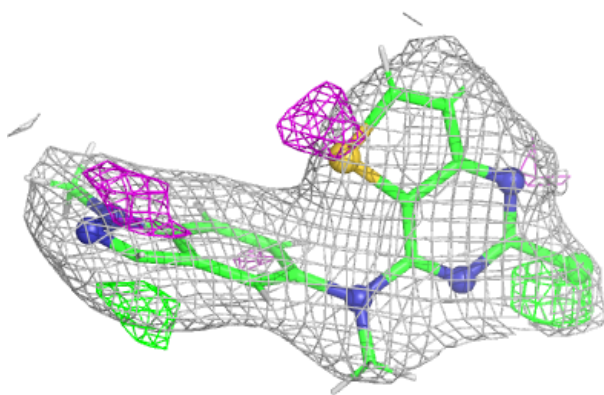
**Electron density around A1EU1 D 502:**

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

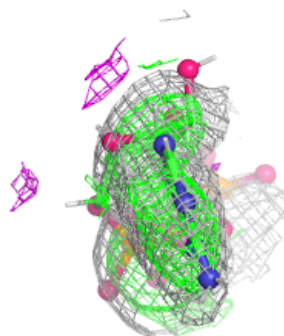
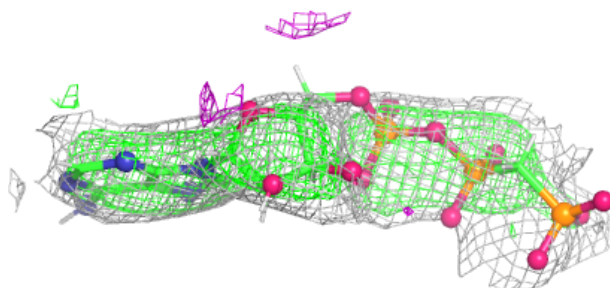
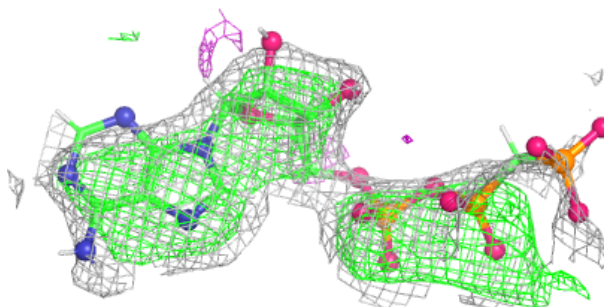


Electron density around A1EU1 B 505:

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

**Electron density around 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.