



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:30 PM UTC

PDB ID : 8R6O / pdb_00008r6o
Title : Tubulin-4AZA2996 complex
Authors : Herman, J.; Vanstreels, E.; Bardiot, D.; Protá, A.E.; Olieric, N.; Gao, L.-J.; Vercruysse, T.; Daems, T.; Waer, M.; Herdewijn, P.; Louat, T.; Steinmetz, M.O.; De Jonghe, S.; Sprangers, B.; Daelemans, D.
Deposited on : 2023-11-22
Resolution : 2.20 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

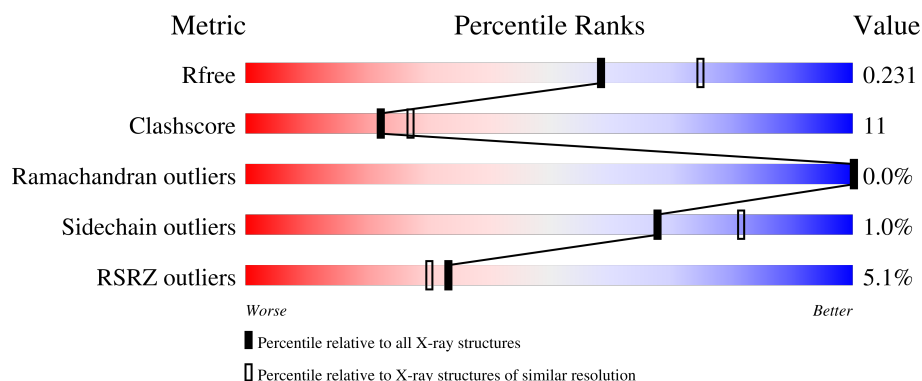
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

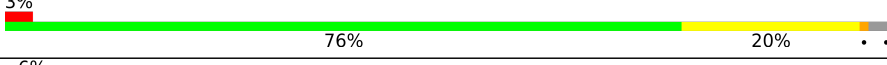
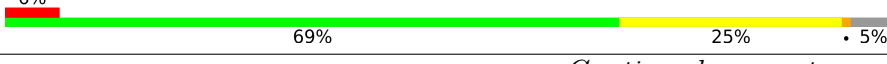
The reported resolution of this entry is 2.20 Å.

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.



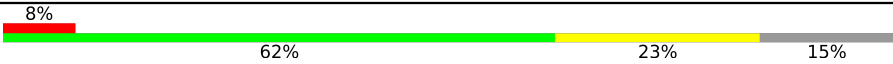
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	
1	C	451	
2	B	445	
2	D	445	

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Mol	Chain	Length	Quality of chain
3	E	143	
4	F	384	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17733 atoms, of which 46 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	2	0
			3422	2167	581	650	24			
1	C	440	Total	C	N	O	S	0	4	0
			3451	2184	585	658	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3357	2110	573	647	27			
2	D	422	Total	C	N	O	S	0	0	0
			3316	2084	563	642	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

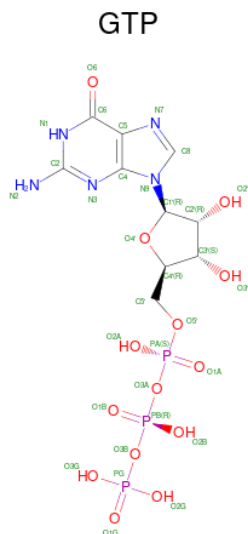
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	314	Total	C	N	O	S	0	0	0
			2576	1662	432	468	14			

There are 39 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
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
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	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	0	0
5	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

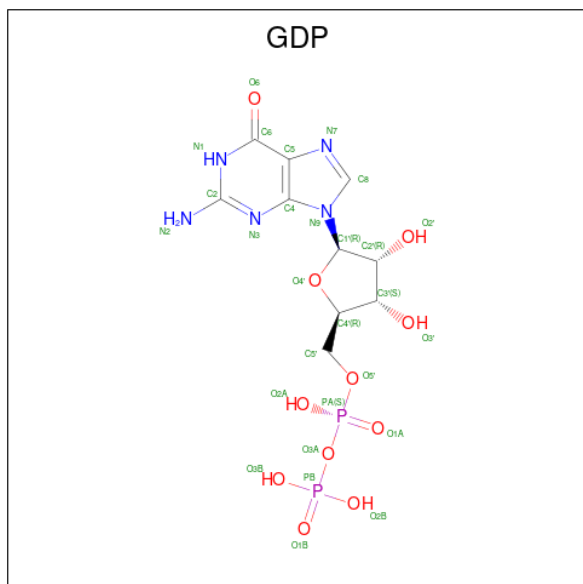
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0

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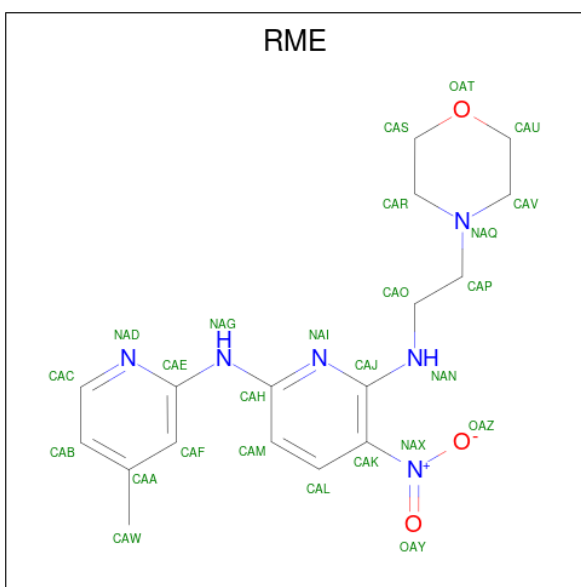
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

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



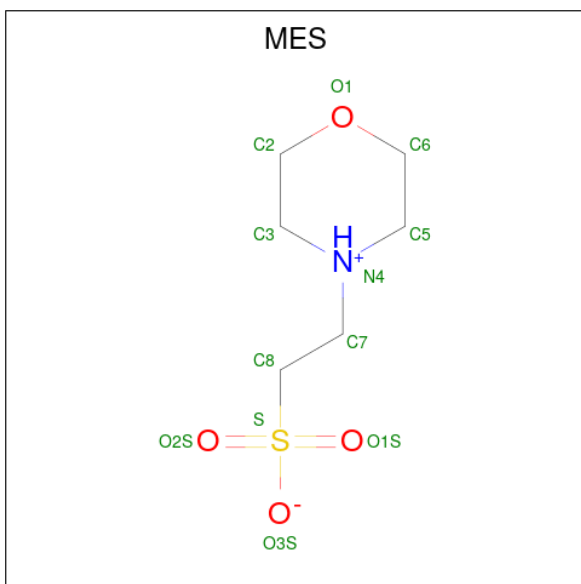
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is N6-(4-methylpyridin-2-yl)-N2-(2-morpholinoethyl)-3-nitropyridine-2,6-diamine (CCD ID: RME) (formula: $C_{17}H_{22}N_6O_3$) (labeled as "Ligand of Interest" by depositor).



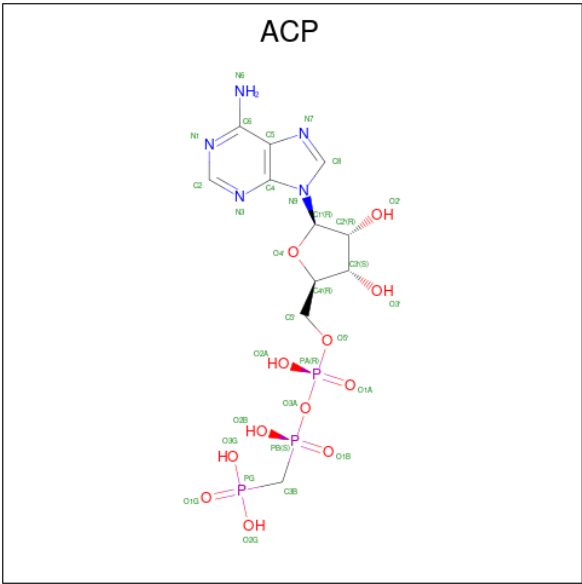
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 49	C 17	H 23	N 6	O 3	0	0
9	D	1	Total 49	C 17	H 23	N 6	O 3	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



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

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



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

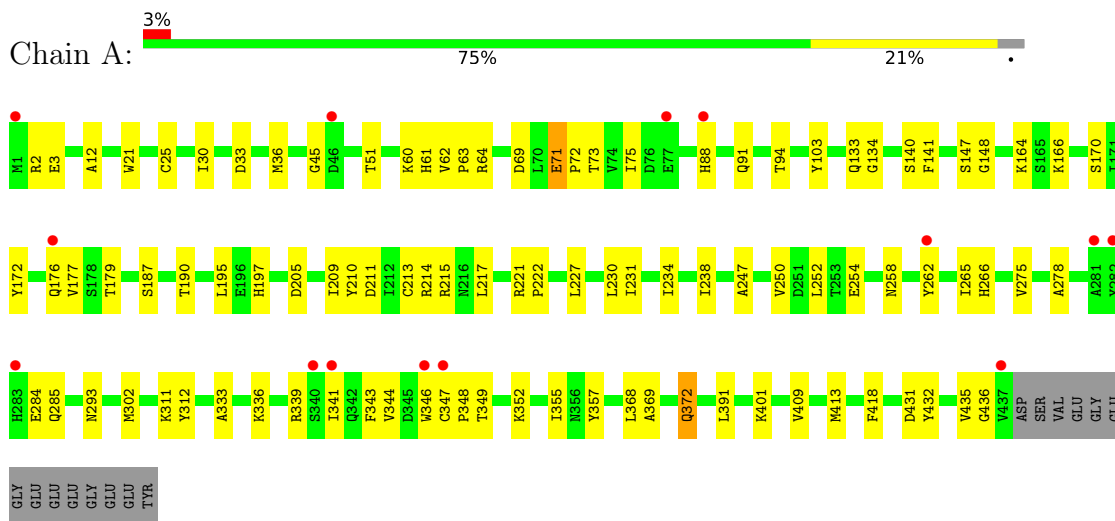
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	53	Total	O	0	0
			53	53		
12	B	76	Total	O	0	0
			76	76		
12	C	150	Total	O	0	0
			150	150		
12	D	26	Total	O	0	0
			26	26		
12	E	14	Total	O	0	0
			14	14		
12	F	23	Total	O	0	0
			23	23		

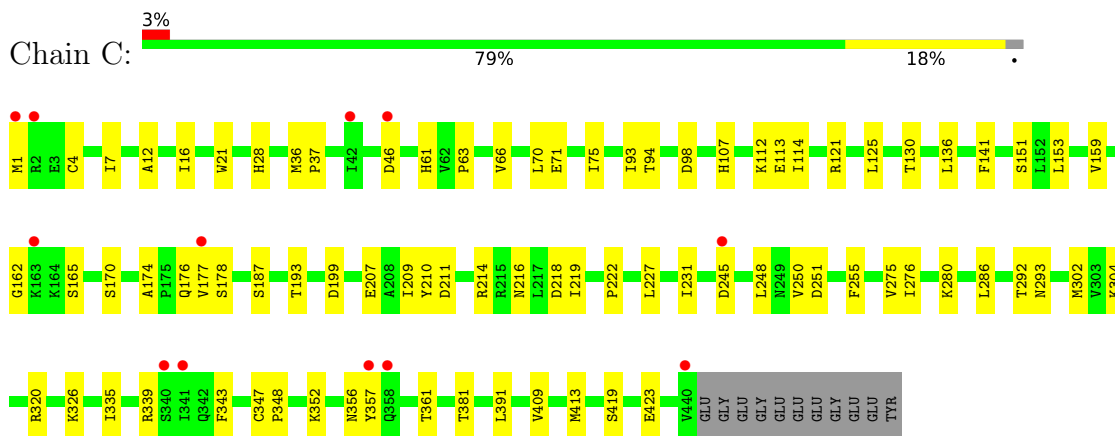
3 Residue-property plots [i](#)

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.

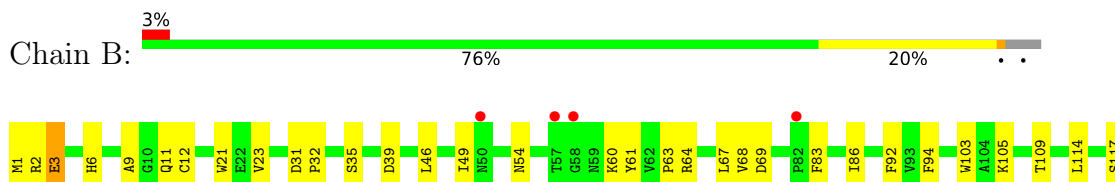
• Molecule 1: Detyrosinated tubulin alpha-1B chain

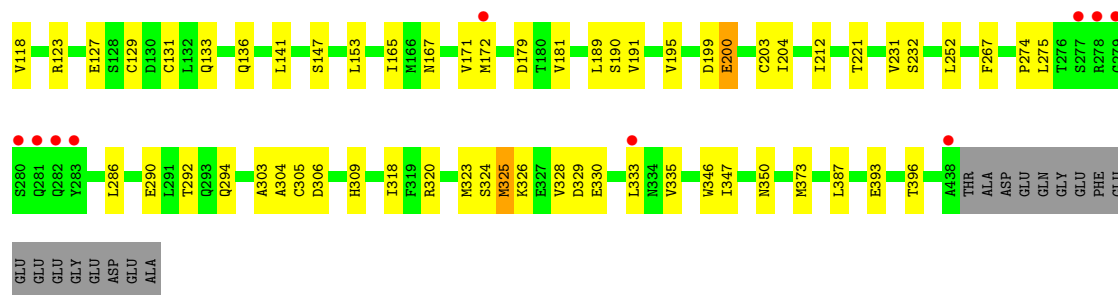


• Molecule 1: Detyrosinated tubulin alpha-1B chain

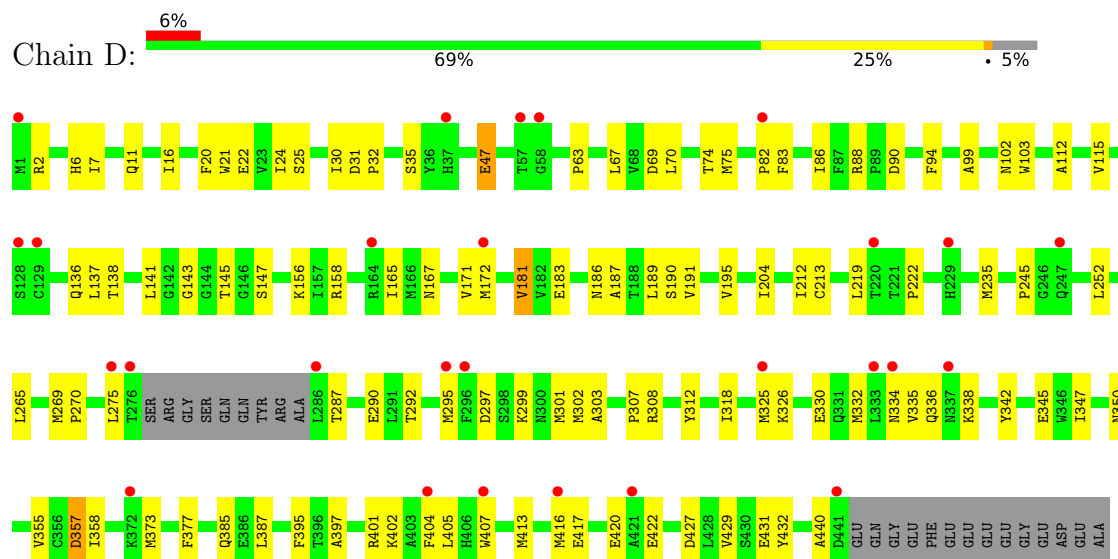


• Molecule 2: Tubulin beta-2B chain

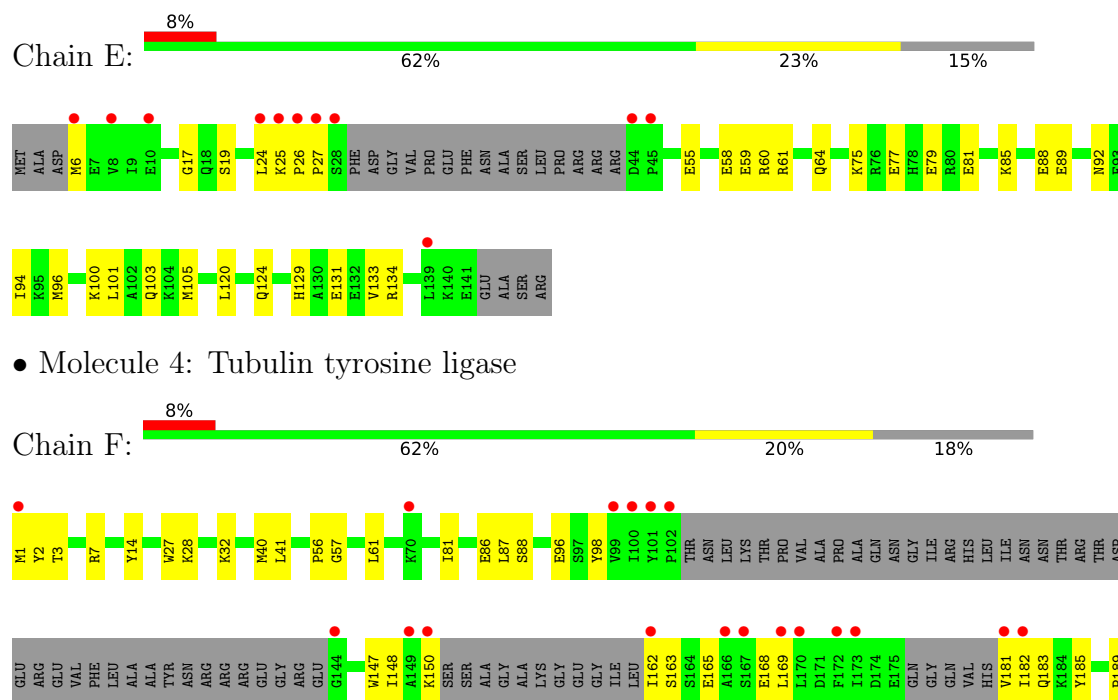




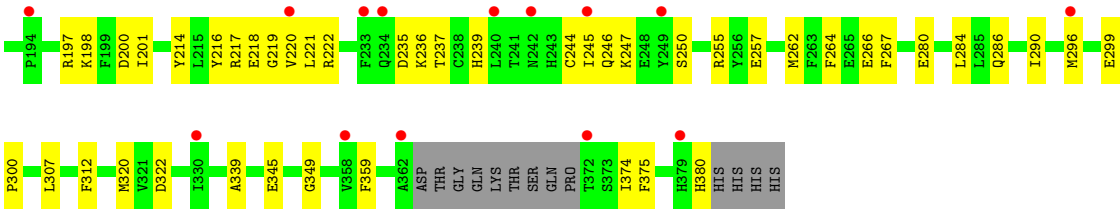
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.33Å 158.18Å 182.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 2.20 48.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.9 (48.20-2.20) 99.2 (48.20-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.208 , 0.233 0.205 , 0.231	Depositor DCC
R_{free} test set	7684 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17733	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: MES, CA, MG, RME, GTP, GDP, 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	0.09	0/3506	0.28	0/4759
1	C	0.10	0/3541	0.28	0/4808
2	B	0.09	0/3432	0.27	0/4650
2	D	0.09	0/3389	0.26	0/4591
3	E	0.08	0/1008	0.21	0/1337
4	F	0.08	0/2636	0.27	0/3562
All	All	0.09	0/17512	0.27	0/23707

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	3422	0	3340	80	0
1	C	3451	0	3369	58	0
2	B	3357	0	3227	71	0
2	D	3316	0	3196	86	0
3	E	1000	0	1018	30	0
4	F	2576	0	2552	57	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
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
8	B	28	0	12	1	0
8	D	28	0	12	3	0
9	B	26	23	0	1	0
9	D	26	23	0	1	0
10	B	12	0	12	0	0
11	F	31	0	14	0	0
12	A	53	0	0	2	0
12	B	76	0	0	1	0
12	C	150	0	0	2	0
12	D	26	0	0	3	0
12	E	14	0	0	0	0
12	F	23	0	0	0	0
All	All	17687	46	16776	361	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 11.

The worst 5 of 361 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:C:209:ILE:HG22	1:C:227:LEU:HD22	1.48	0.95
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.55	0.87
2:B:292:THR:HG22	2:B:335:VAL:HG11	1.57	0.85
2:B:1:MET:N	2:B:131:CYS:SG	2.48	0.85
2:B:323:MET:HE2	2:B:373:MET:HE2	1.62	0.82

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/451 (97%)	428 (98%)	9 (2%)	0	100	100
1	C	442/451 (98%)	433 (98%)	9 (2%)	0	100	100
2	B	426/445 (96%)	417 (98%)	8 (2%)	1 (0%)	43	51
2	D	418/445 (94%)	411 (98%)	7 (2%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	304/384 (79%)	295 (97%)	9 (3%)	0	100	100
All	All	2144/2319 (92%)	2101 (98%)	42 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	304	ALA

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	370/379 (98%)	366 (99%)	4 (1%)	65	79
1	C	375/379 (99%)	370 (99%)	5 (1%)	61	76
2	B	366/383 (96%)	362 (99%)	4 (1%)	65	79
2	D	365/383 (95%)	361 (99%)	4 (1%)	65	79
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	285/342 (83%)	284 (100%)	1 (0%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1870/1993 (94%)	1852 (99%)	18 (1%)	68 81

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	181	VAL
4	F	255	ARG
2	D	358	ILE
1	C	71	GLU
2	D	47	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	59	ASN
2	D	436	GLN
2	D	101	ASN
3	E	51	GLN
2	B	331	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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	ACP	F	701	6	31,33,33	1.35	4 (12%)	47,52,52	2.08	9 (19%)
9	RME	B	503	-	28,28,28	1.89	6 (21%)	33,37,37	2.11	10 (30%)
5	GTP	C	501	6	33,34,34	0.96	2 (6%)	50,54,54	1.52	9 (18%)
10	MES	B	504	-	12,12,12	2.27	1 (8%)	15,16,16	1.93	3 (20%)
5	GTP	A	501	6	33,34,34	1.01	4 (12%)	50,54,54	1.53	8 (16%)
8	GDP	D	501	6	29,30,30	1.18	3 (10%)	45,47,47	1.74	6 (13%)
9	RME	D	503	-	28,28,28	1.92	8 (28%)	33,37,37	2.03	9 (27%)
8	GDP	B	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.73	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
11	ACP	F	701	6	-	6/19/38/38	0/3/3/3
9	RME	B	503	-	-	0/11/22/22	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
8	GDP	D	501	6	-	4/16/32/32	0/3/3/3
9	RME	D	503	-	-	0/11/22/22	0/3/3/3
8	GDP	B	501	-	-	5/16/32/32	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-7.59	1.66	1.77
9	D	503	RME	CAK-NAX	-6.72	1.33	1.45
9	B	503	RME	CAK-NAX	-6.51	1.33	1.45
9	D	503	RME	CAW-CAA	-4.22	1.38	1.51
9	B	503	RME	CAW-CAA	-4.21	1.38	1.51

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	701	ACP	PB-O3A-PA	-7.45	108.06	132.37
8	D	501	GDP	C5-C4-N3	-6.04	118.78	128.39
8	B	501	GDP	C5-C4-N3	-5.99	118.86	128.39
11	F	701	ACP	C5-C4-N3	-5.84	118.67	126.72
9	B	503	RME	CAL-CAK-NAX	5.59	122.44	116.47

There are no chirality outliers.

5 of 34 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	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A

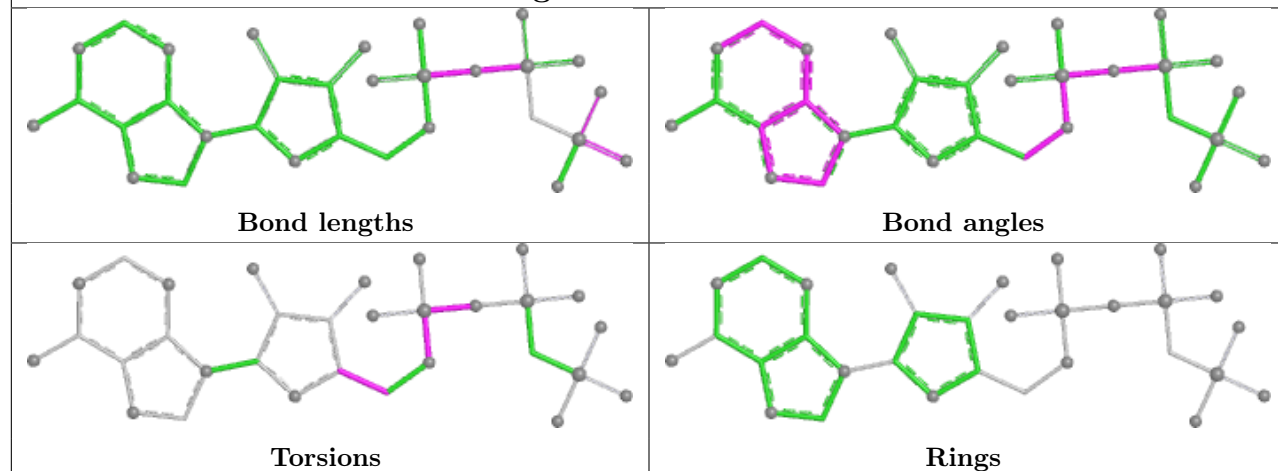
There are no ring outliers.

4 monomers are involved in 6 short contacts:

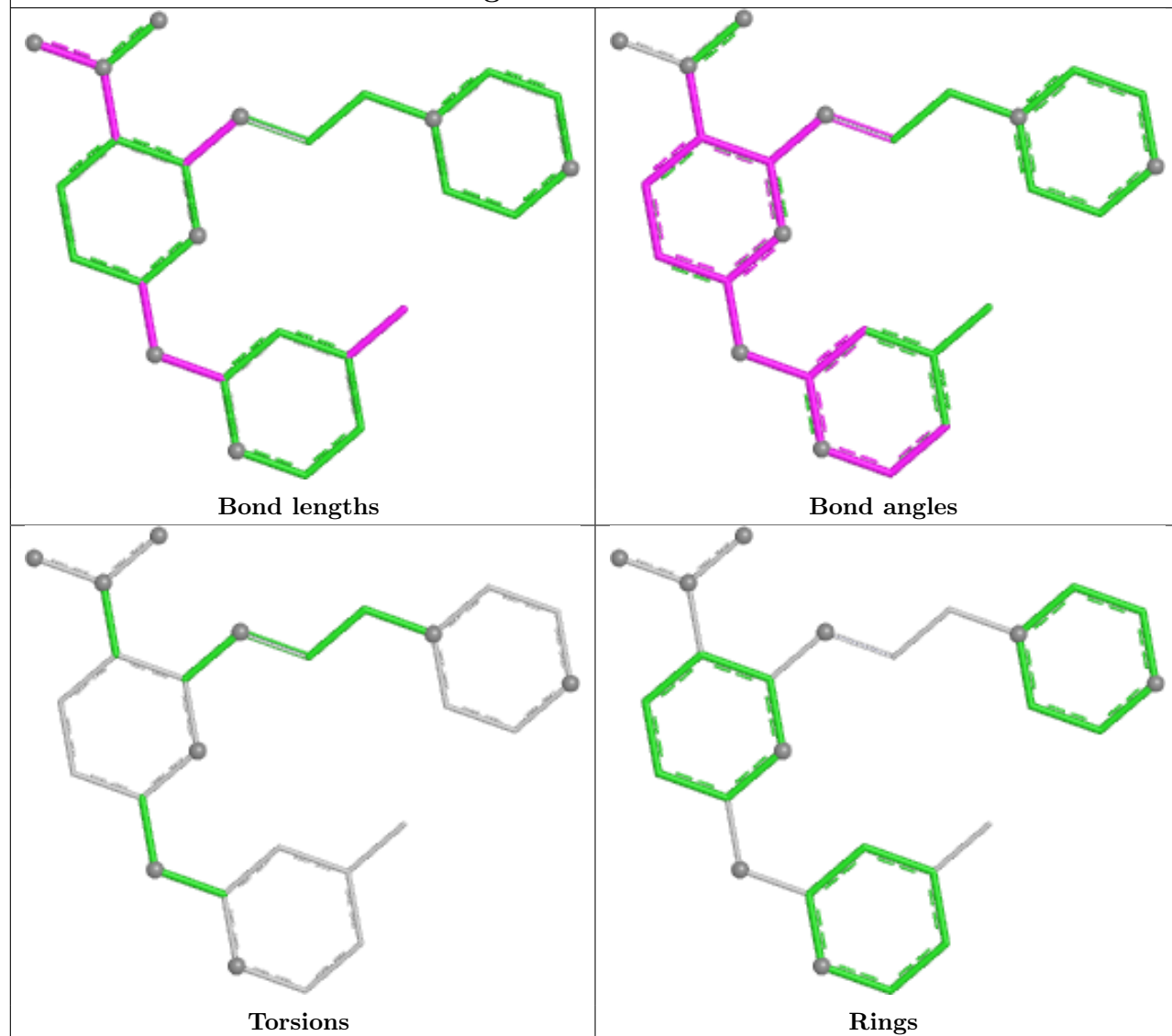
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	RME	1	0
8	D	501	GDP	3	0
9	D	503	RME	1	0
8	B	501	GDP	1	0

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.

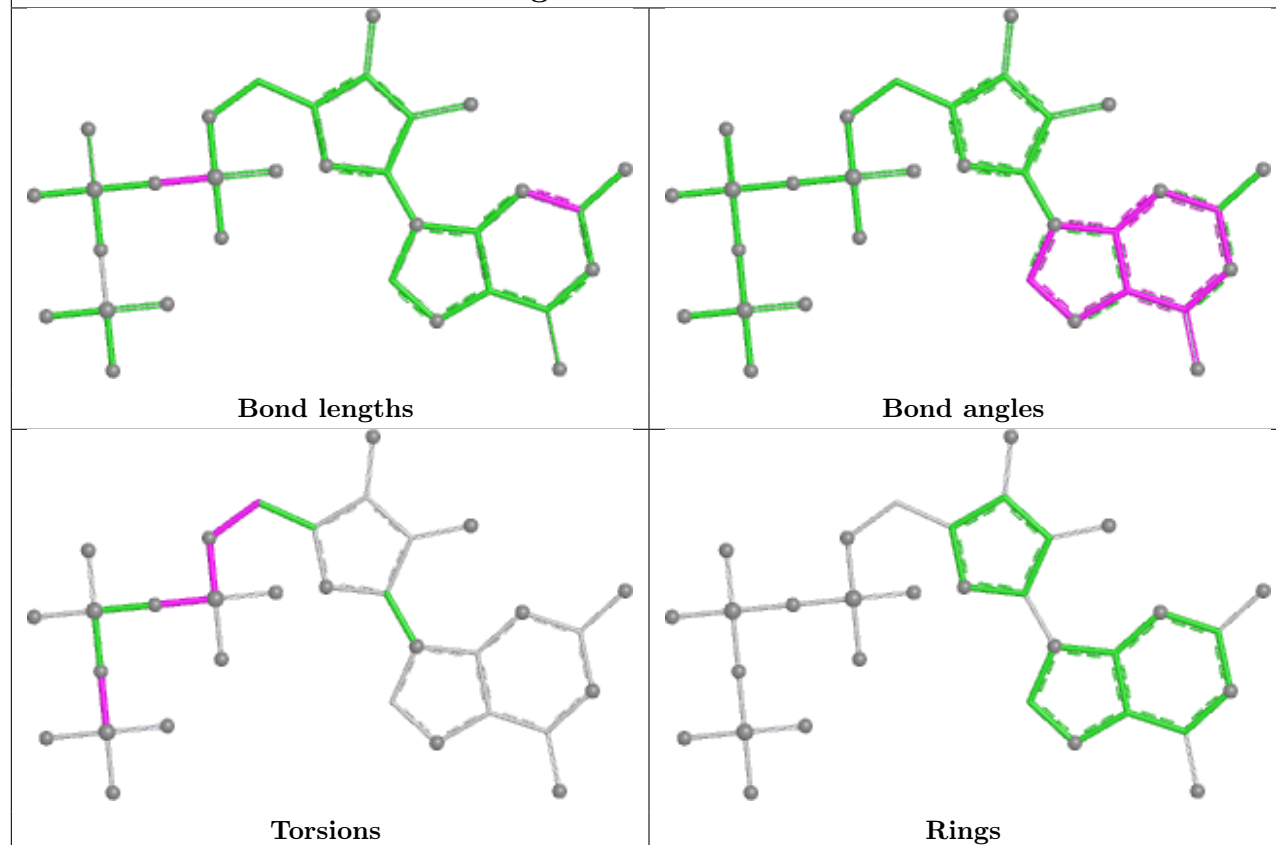
Ligand ACP F 701



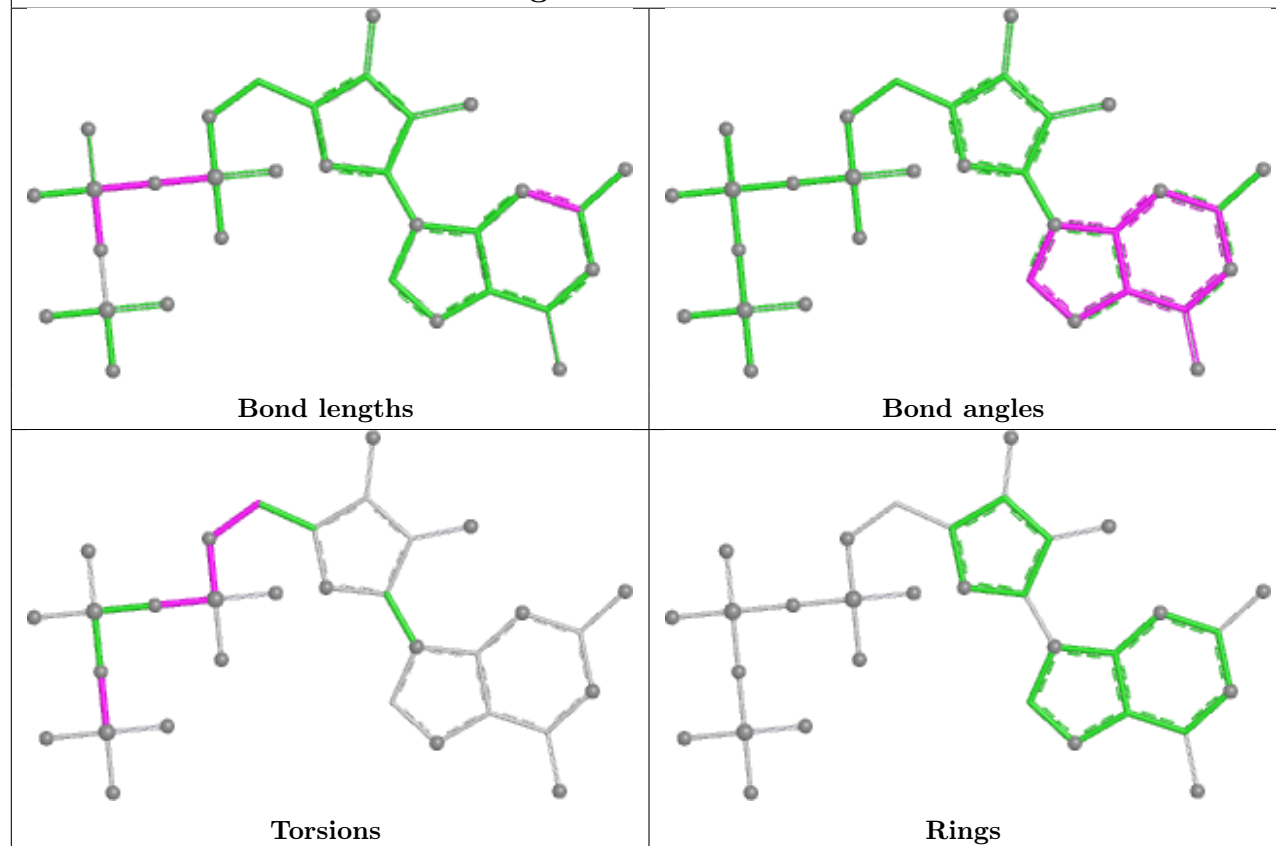
Ligand RME B 503

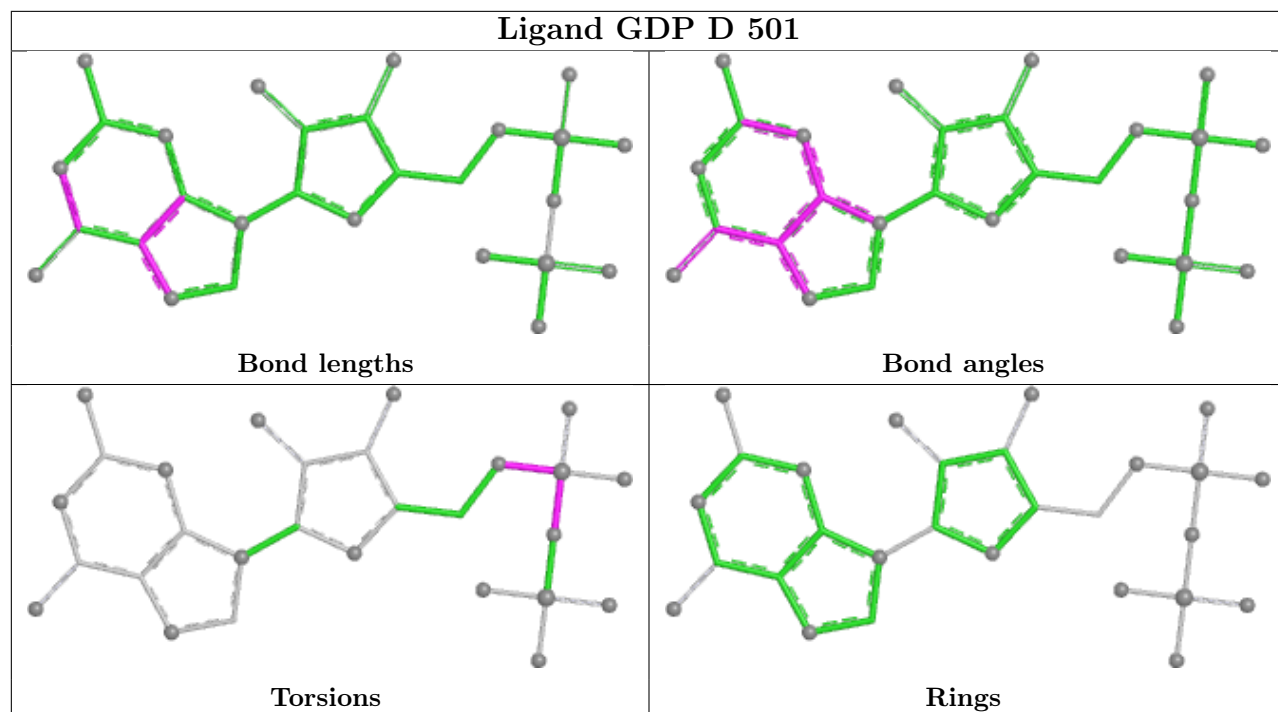


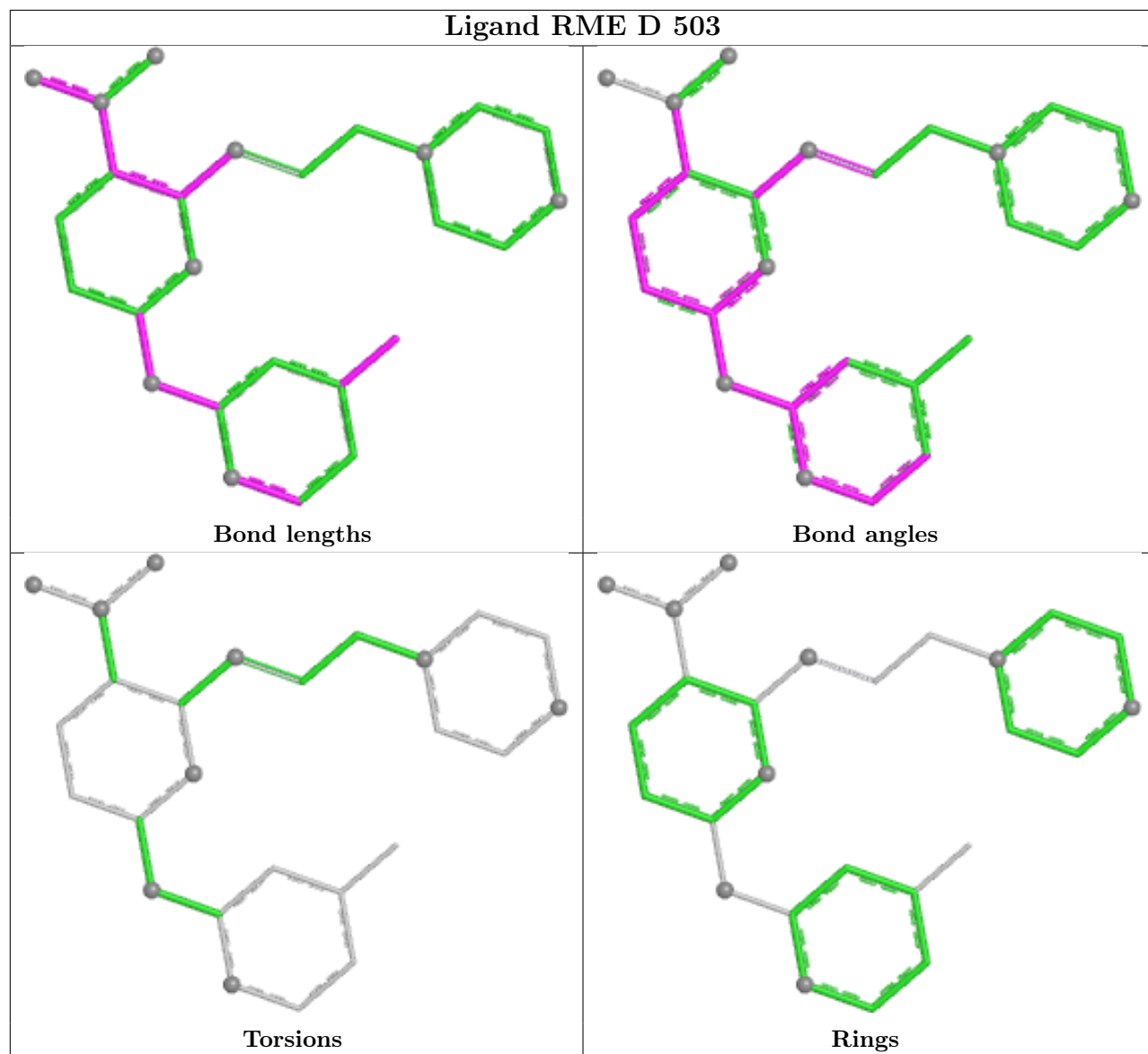
Ligand GTP C 501

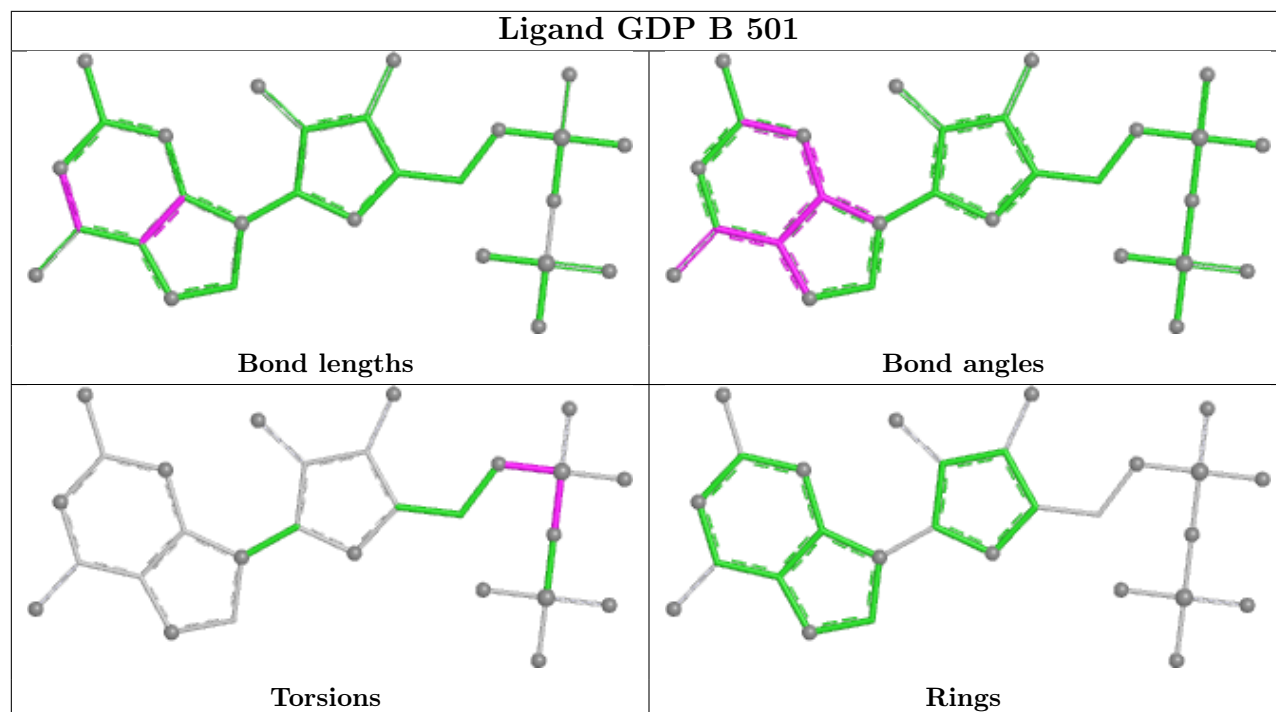


Ligand GTP A 501









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	437/451 (96%)	0.31	14 (3%)	50	47	37, 64, 102, 175	2 (0%)
1	C	440/451 (97%)	-0.06	12 (2%)	56	53	28, 48, 76, 109	4 (0%)
2	B	428/445 (96%)	0.18	14 (3%)	49	46	37, 56, 89, 138	0
2	D	422/445 (94%)	0.61	27 (6%)	25	22	44, 78, 110, 156	0
3	E	121/143 (84%)	0.73	11 (9%)	15	12	47, 74, 123, 145	0
4	F	314/384 (81%)	0.83	32 (10%)	12	9	56, 89, 156, 177	0
All	All	2162/2319 (93%)	0.37	110 (5%)	33	30	28, 65, 115, 177	6 (0%)

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	4.9
1	A	340	SER	4.5
4	F	362	ALA	4.3
4	F	102	PRO	4.0
2	B	57	THR	3.8

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 ⓘ

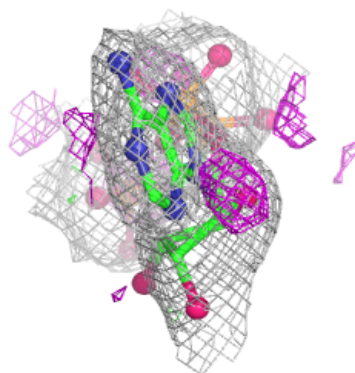
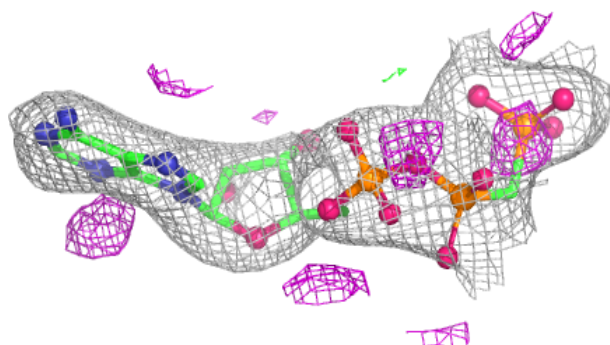
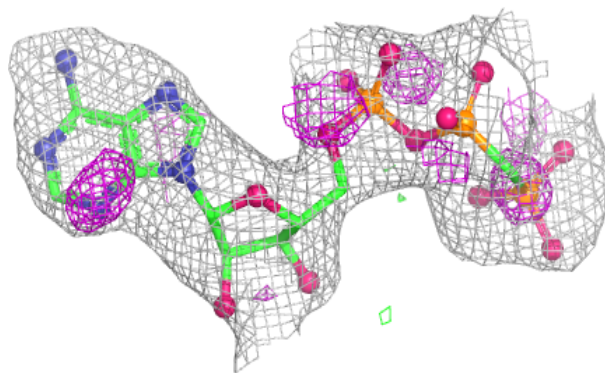
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	F	702	1/1	0.67	0.16	93,93,93,93	0
6	MG	D	502	1/1	0.72	0.24	80,80,80,80	0
11	ACP	F	701	31/31	0.83	0.14	101,109,115,117	0
8	GDP	D	501	28/28	0.92	0.13	70,75,80,81	0
7	CA	B	505	1/1	0.92	0.11	92,92,92,92	0
10	MES	B	504	12/12	0.95	0.09	48,56,63,66	0
6	MG	B	502	1/1	0.96	0.07	57,57,57,57	0
9	RME	D	503	26/26	0.96	0.07	45,54,64,65	0
9	RME	B	503	26/26	0.97	0.07	44,48,57,58	0
5	GTP	C	501	32/32	0.97	0.06	34,38,43,45	0
8	GDP	B	501	28/28	0.97	0.07	37,43,47,49	0
5	GTP	A	501	32/32	0.97	0.07	39,46,51,56	0
7	CA	A	503	1/1	0.98	0.05	96,96,96,96	0
7	CA	C	503	1/1	0.98	0.04	74,74,74,74	0
6	MG	A	502	1/1	0.99	0.03	51,51,51,51	0
6	MG	C	502	1/1	1.00	0.02	40,40,40,40	0

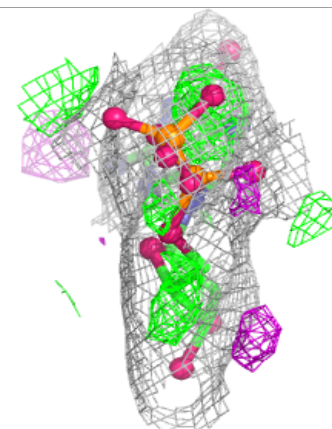
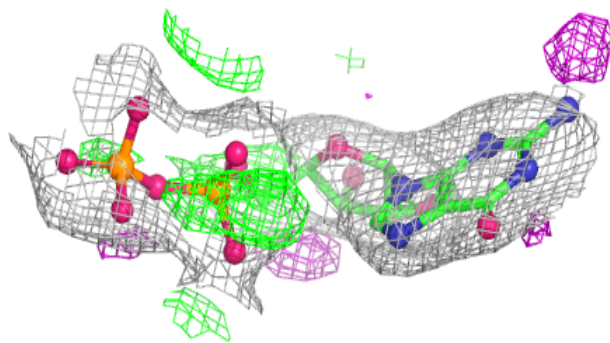
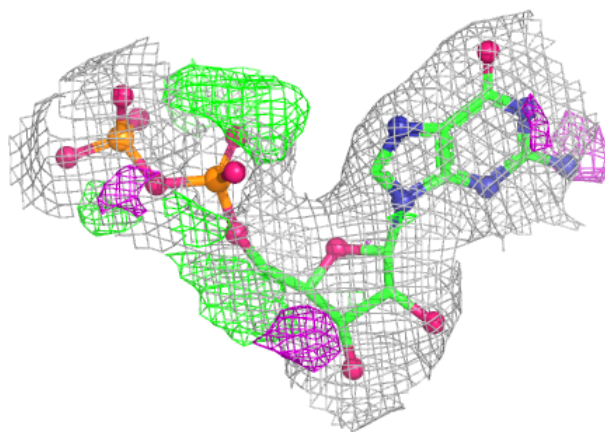
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 701:

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

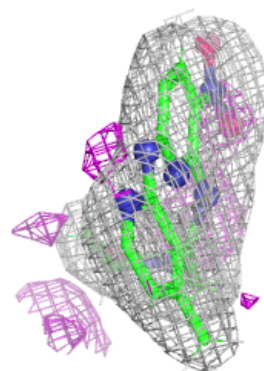
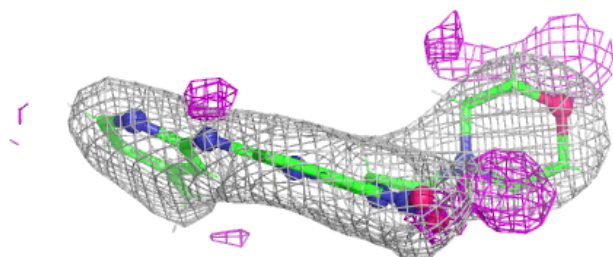
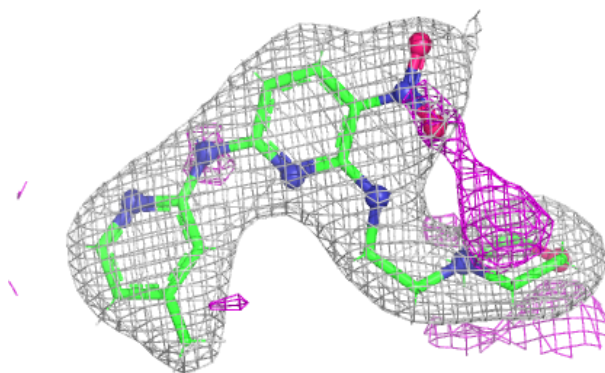
**Electron density around GDP D 501:**

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

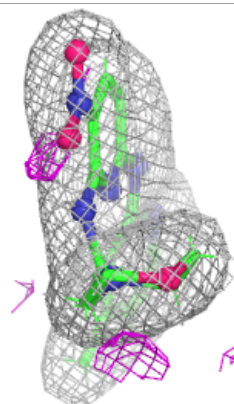
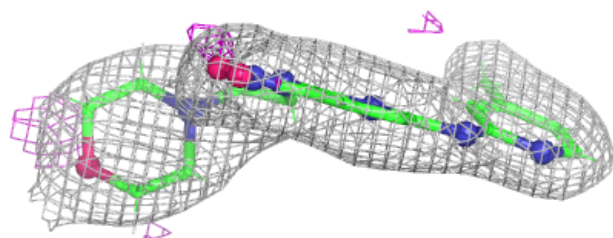
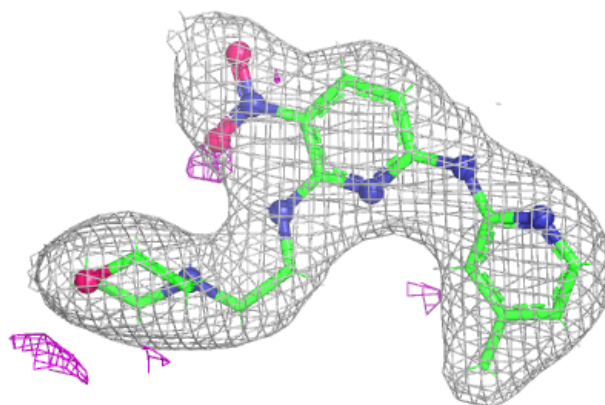


Electron density around RME D 503:

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

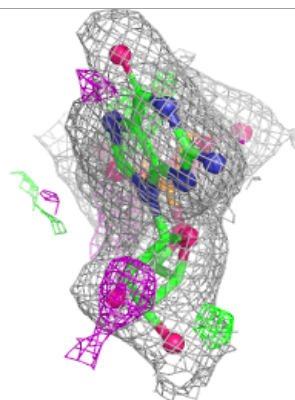
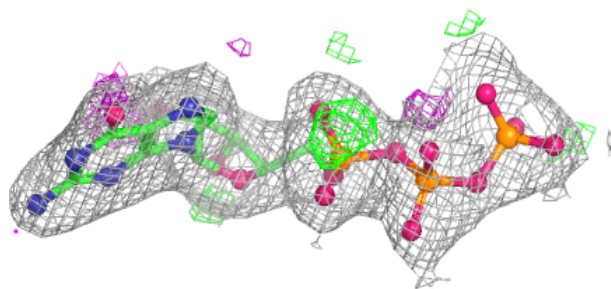
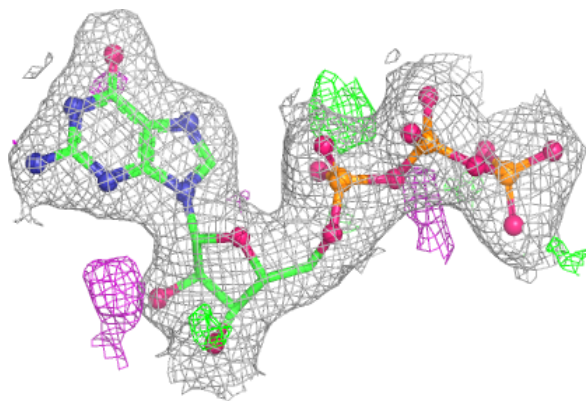
**Electron density around RME B 503:**

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



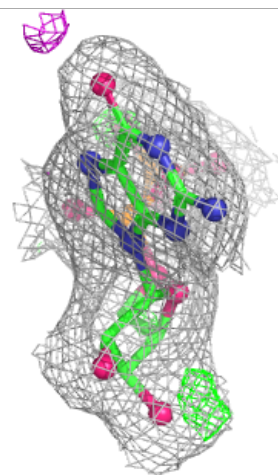
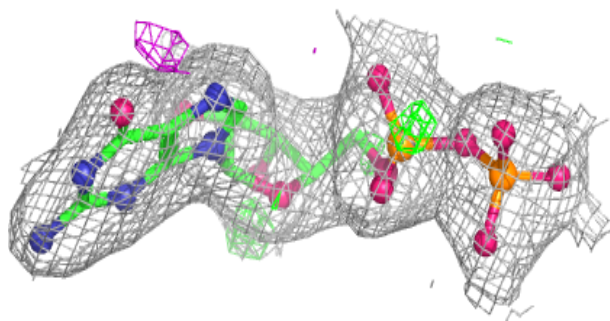
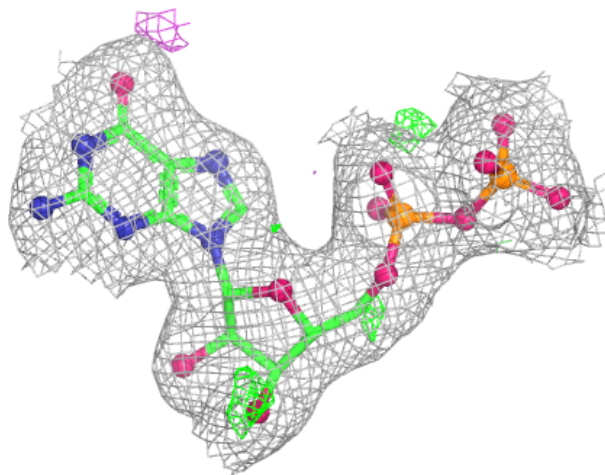
Electron density around GTP C 501:

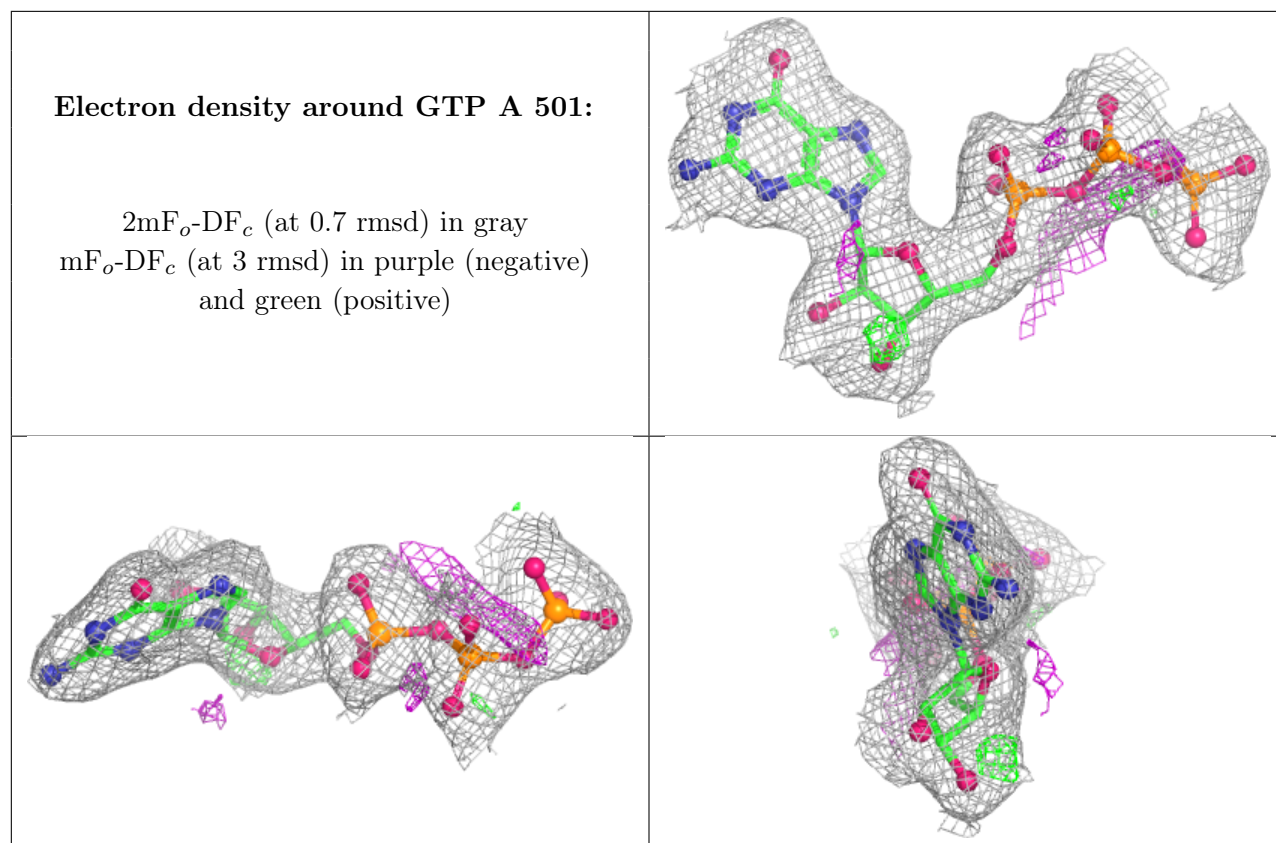
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.