



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 1, 2025 – 12:33 pm BST

PDB ID : 9GMY / pdb_00009gmy
Title : Tubulin in complex with an oxathiane analog of zampanolide
Authors : Oliva, M.A.; Diaz, J.F.; Altmann, K.H.
Deposited on : 2024-08-30
Resolution : 1.97 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

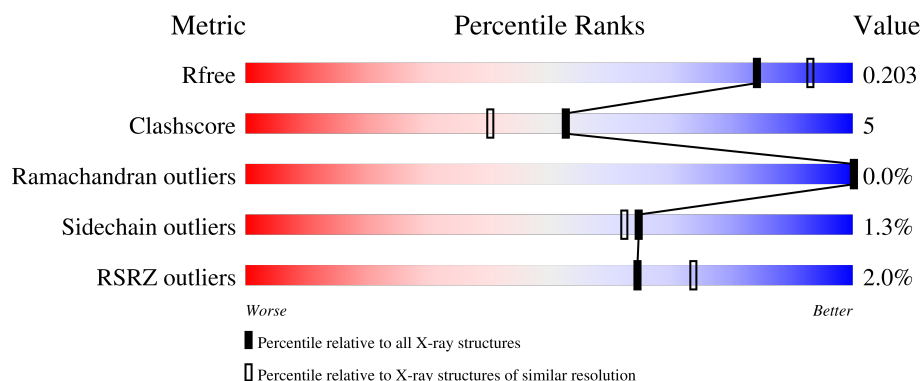
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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}	164625	1356 (1.98-1.98)
Clashscore	180529	1437 (1.98-1.98)
Ramachandran outliers	177936	1426 (1.98-1.98)
Sidechain outliers	177891	1426 (1.98-1.98)
RSRZ outliers	164620	1356 (1.98-1.98)

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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 88%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 88% 8% </div> </div>
1	C	451	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 82%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 82% 15% </div> </div>
2	B	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 81%, grey 12%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 81% 12% 6% </div> </div>
2	D	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 82%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 82% 12% </div> </div>
3	E	189	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 53%, grey 7%, grey 39%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 53% 7% 39% </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>3%</div><div>70%</div><div>9%</div><div>19%</div></div>

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 36165 atoms, of which 17209 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	434	Total	C	H	N	O	S	107	8	0
			6815	2177	3374	583	656	25			
1	C	439	Total	C	H	N	O	S	111	18	0
			7031	2245	3468	605	687	26			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	419	Total	C	H	N	O	S	101	15	0
			6703	2141	3294	579	661	28			
2	D	427	Total	C	H	N	O	S	104	8	0
			6737	2148	3312	584	663	30			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	115	Total	C	H	N	O	S	15	4	0
			1994	608	1011	181	189	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	311	Total	C	H	N	O	S	79	4	0
			5164	1659	2582	445	464	14			

There are 39 discrepancies between the modelled and reference sequences:

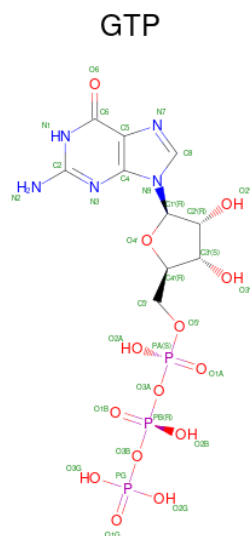
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0

Continued on next page...

Continued from previous page...

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
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: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 44	C 10	H 12	N 5	O 14	P 3	2	0
5	C	1	Total 44	C 10	H 12	N 5	O 14	P 3	2	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

Continued on next page...

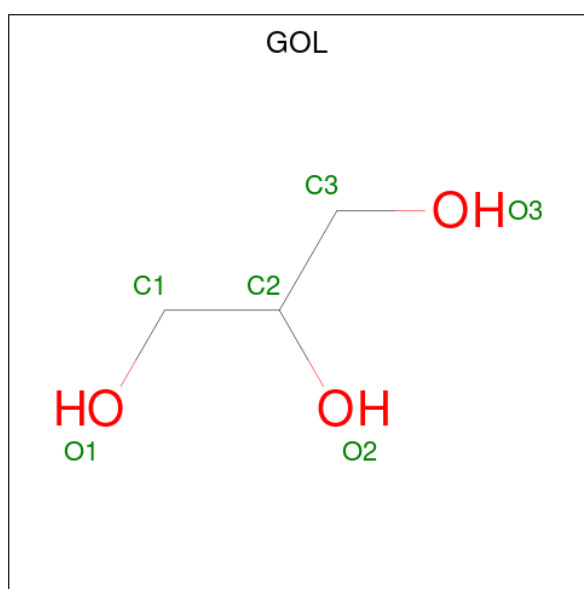
Continued from previous page...

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

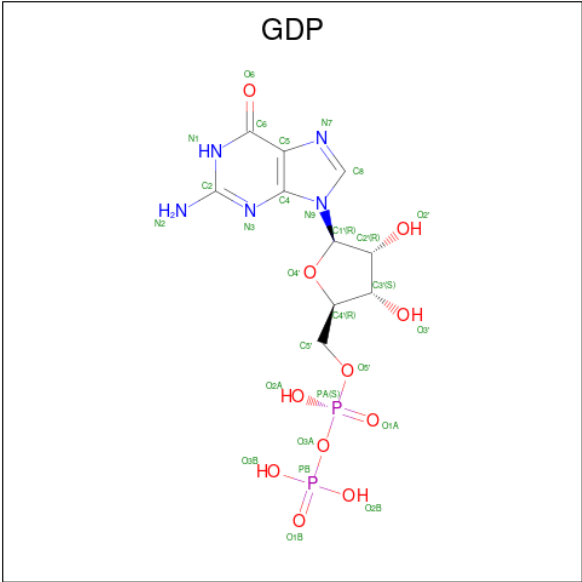
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



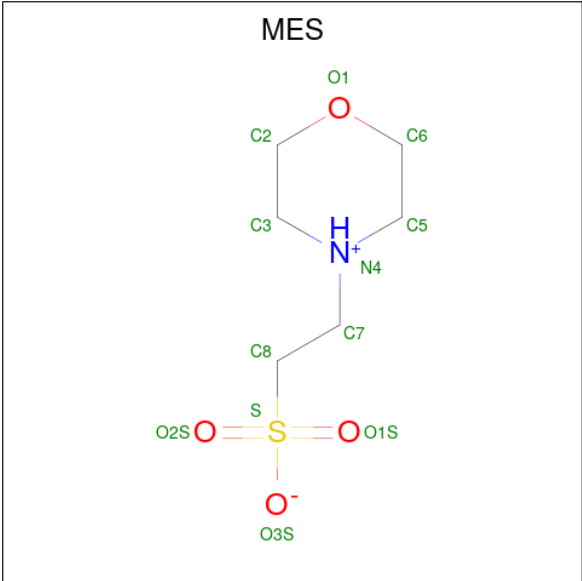
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	3	0
			14	3	8	3		
9	B	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



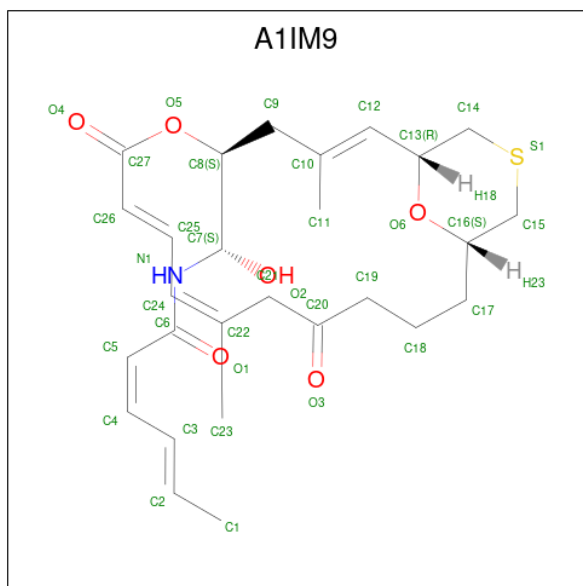
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total 40	C 10	H 12	N 5	O 11	P 2	2	0
10	D	1	Total 40	C 10	H 12	N 5	O 11	P 2	0	0

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



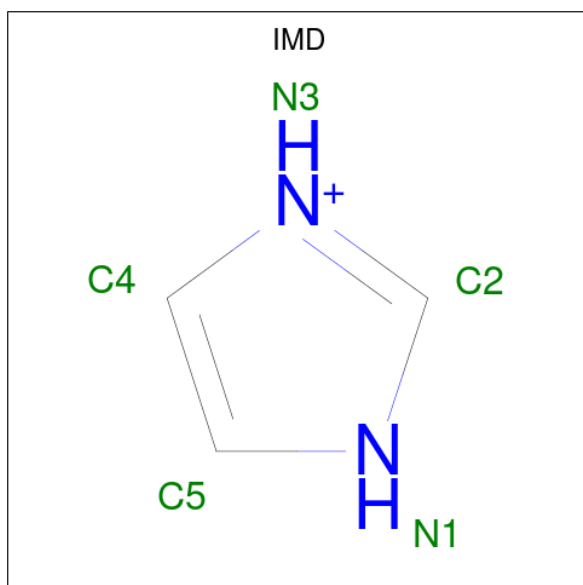
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 12 is (2Z,4E)-N-[(S)-[(1R,2E,5S,8E,10Z,17S)-3,11-dimethyl-7,13-bis(oxidanylidene)-6,21-dioxa-19-thiabicyclo[15.3.1]henicosa-2,8,10-trien-5-yl]-oxidanyl-methyl]hexa-2,4-dienamide (CCD ID: A1IM9) (formula: $C_{27}H_{37}NO_6S$) (labeled as "Ligand of Interest" by depositor).



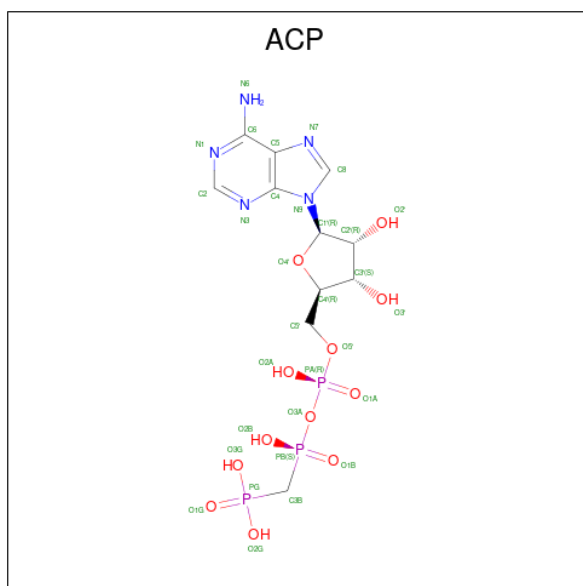
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	S	10	0
			71	27	36	1	6	1		
12	D	1	Total	C	H	N	O	S	10	0
			71	27	36	1	6	1		

- Molecule 13 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	H	N	0	0
			10	3	5	2		

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	F	1	Total	C	H	N	O	P	2	0
			45	11	14	5	12	3		

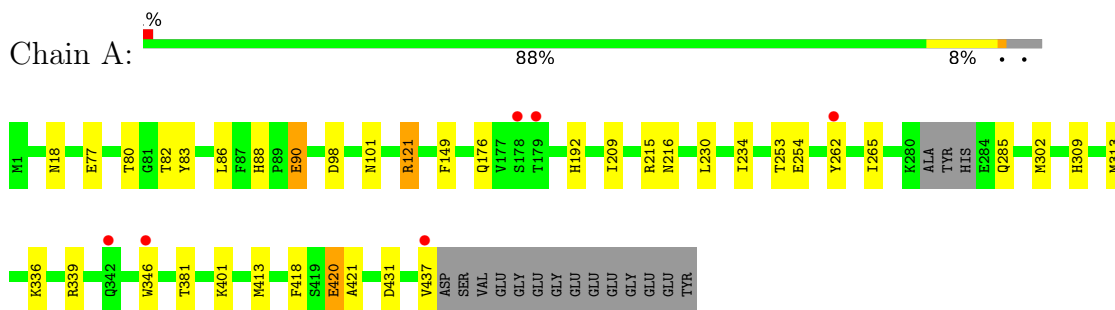
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	260	Total	O	0	0
			260	260		
15	B	220	Total	O	0	0
			220	220		
15	C	382	Total	O	0	0
			382	382		
15	D	234	Total	O	0	0
			234	234		
15	E	76	Total	O	0	0
			76	76		
15	F	122	Total	O	0	0
			122	122		

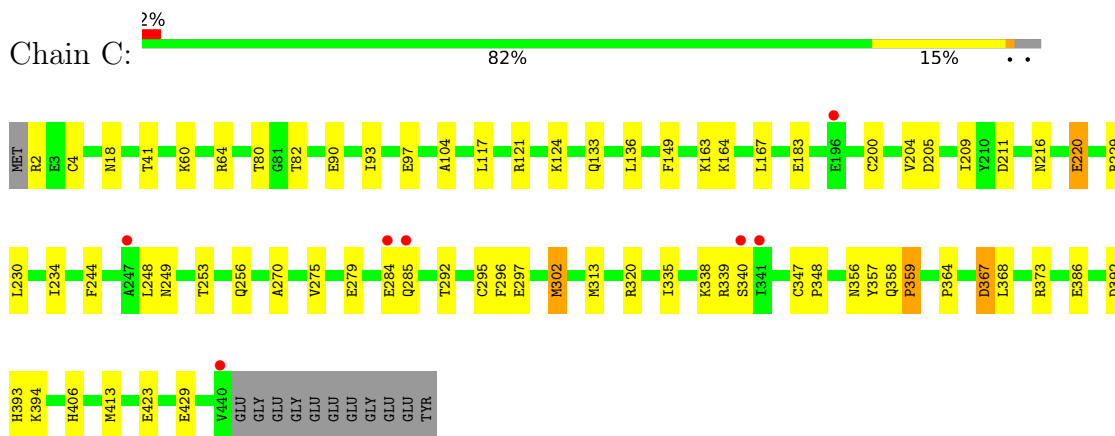
3 Residue-property plots

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.

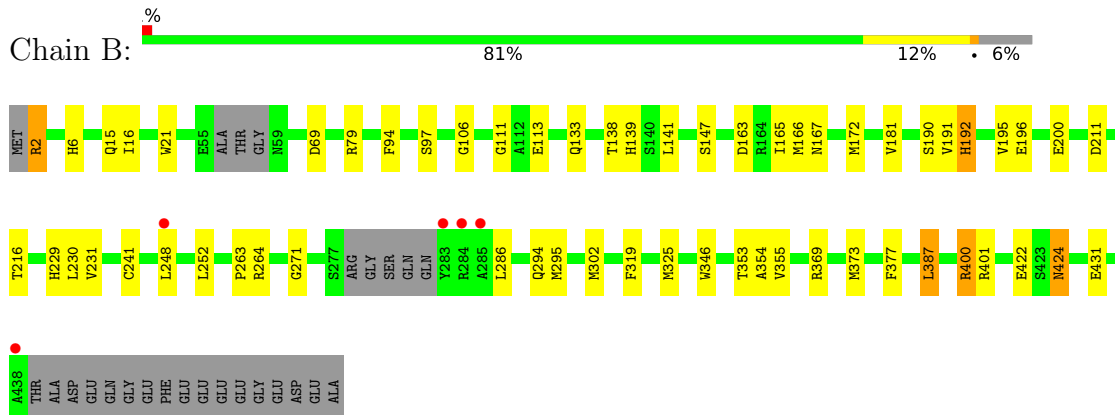
- Molecule 1: Tubulin alpha-1B chain



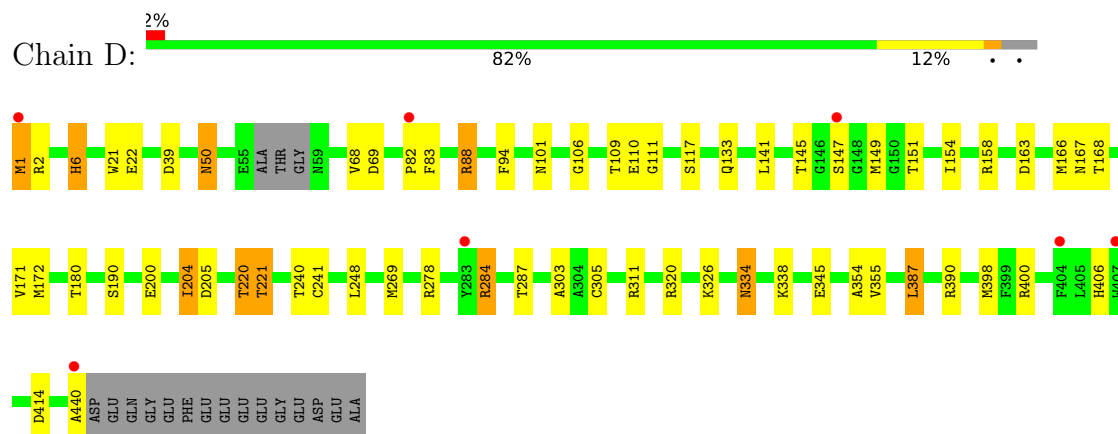
- Molecule 1: Tubulin alpha-1B chain



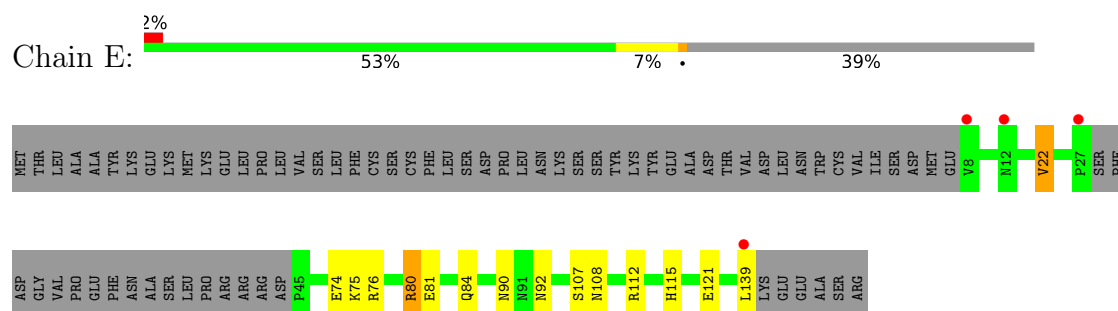
- Molecule 2: Tubulin beta-2B chain



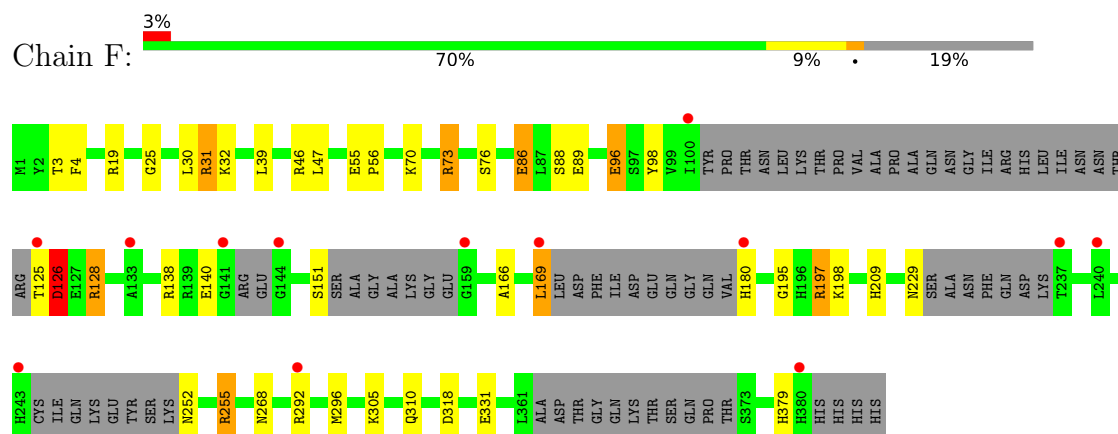
• Molecule 2: Tubulin beta-2B chain



• 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	104.91Å 158.35Å 178.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 1.97 49.31 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.31-1.97) 99.9 (49.31-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.160 , 0.202 0.161 , 0.203	Depositor DCC
R_{free} test set	10427 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36165	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, CL, IMD, A1IM9, ACP, GTP, GOL, MES, MG, CA

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	0.95	1/3522 (0.0%)	1.33	17/4778 (0.4%)
1	C	1.05	5/3642 (0.1%)	1.37	25/4946 (0.5%)
2	B	0.97	4/3494 (0.1%)	1.34	13/4729 (0.3%)
2	D	1.01	5/3499 (0.1%)	1.36	23/4737 (0.5%)
3	E	0.96	0/995	1.57	10/1320 (0.8%)
4	F	0.81	0/2640	1.31	12/3559 (0.3%)
All	All	0.97	15/17792 (0.1%)	1.36	100/24069 (0.4%)

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	A	0	1
1	C	0	2
2	B	0	2
2	D	0	4
3	E	0	1
4	F	0	7
All	All	0	17

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	406	HIS	CG-CD2	18.66	1.56	1.35
2	D	406	HIS	CE1-NE2	14.37	1.47	1.32
2	D	406	HIS	ND1-CE1	9.93	1.42	1.32
2	B	229	HIS	CE1-NE2	8.24	1.40	1.32
1	C	367	ASP	CG-OD2	6.83	1.38	1.25

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	345	GLU	CB-CG-CD	9.99	129.58	112.60
1	A	18	ASN	CB-CA-C	-8.83	97.02	110.88
2	D	414	ASP	CA-CB-CG	8.71	121.31	112.60
1	A	121	ARG	CD-NE-CZ	8.60	136.44	124.40
2	B	133	GLN	CB-CA-C	-8.29	94.45	110.11

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	339	ARG	Sidechain
2	B	2	ARG	Sidechain
2	B	79	ARG	Sidechain
1	C	2	ARG	Sidechain
1	C	339	ARG	Sidechain

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	3441	3374	3359	15	0
1	C	3563	3468	3438	44	0
2	B	3409	3294	3280	46	0
2	D	3425	3312	3296	36	0
3	E	983	1011	1003	9	0
4	F	2582	2582	2563	23	0
5	A	32	12	12	0	0
5	C	32	12	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
9	A	6	8	8	0	0
9	B	6	8	8	2	0
10	B	28	12	12	0	0
10	D	28	12	12	0	0
11	B	12	13	13	0	0
12	B	35	36	0	0	0
12	D	35	36	0	0	0
13	C	5	5	5	0	0
14	F	31	14	14	2	0
15	A	260	0	0	6	0
15	B	220	0	0	16	1
15	C	382	0	0	14	1
15	D	234	0	0	9	0
15	E	76	0	0	6	0
15	F	122	0	0	6	0
All	All	18956	17209	17035	170	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 5.

The worst 5 of 170 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:16[B]:ILE:HD11	2:B:138[B]:THR:HG23	1.37	1.06
2:B:424:ASN:HB3	15:B:772:HOH:O	1.56	1.02
2:B:16[B]:ILE:HD11	2:B:138[B]:THR:CG2	1.93	0.97
2:B:16[B]:ILE:HG13	2:B:138[B]:THR:HG21	1.55	0.86
2:B:97:SER:HB2	15:B:738:HOH:O	1.78	0.82

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)
15:B:606:HOH:O	15:C:649:HOH:O[4_555]	2.08	0.12

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	438/451 (97%)	431 (98%)	7 (2%)	0	100	100
1	C	455/451 (101%)	445 (98%)	10 (2%)	0	100	100
2	B	428/445 (96%)	422 (99%)	6 (1%)	0	100	100
2	D	431/445 (97%)	426 (99%)	5 (1%)	0	100	100
3	E	115/189 (61%)	113 (98%)	2 (2%)	0	100	100
4	F	299/384 (78%)	294 (98%)	4 (1%)	1 (0%)	37	27
All	All	2166/2365 (92%)	2131 (98%)	34 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	88	SER

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	374/379 (99%)	370 (99%)	4 (1%)	70	68
1	C	388/379 (102%)	384 (99%)	4 (1%)	73	72
2	B	379/383 (99%)	377 (100%)	2 (0%)	86	86
2	D	378/383 (99%)	373 (99%)	5 (1%)	65	62
3	E	107/171 (63%)	104 (97%)	3 (3%)	38	28
4	F	284/342 (83%)	277 (98%)	7 (2%)	42	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1910/2037 (94%)	1885 (99%)	25 (1%)	65 62

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	387	LEU
3	E	139	LEU
4	F	169	LEU
3	E	107	SER
4	F	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	283	HIS
1	C	309	HIS
4	F	269	GLN
3	E	64	GLN
3	E	90	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 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 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
12	A1IM9	D	503	2	34,36,36	0.87	1 (2%)	35,46,46	1.53	9 (25%)
5	GTP	A	501	6	26,34,34	1.08	1 (3%)	32,54,54	1.13	3 (9%)
5	GTP	C	501	6	26,34,34	1.17	3 (11%)	32,54,54	1.04	1 (3%)
9	GOL	B	503	-	5,5,5	0.26	0	5,5,5	0.43	0
10	GDP	B	501	6	24,30,30	1.05	1 (4%)	30,47,47	0.89	1 (3%)
10	GDP	D	501	6	24,30,30	1.20	2 (8%)	30,47,47	0.90	1 (3%)
11	MES	B	504	-	12,12,12	0.85	0	14,16,16	1.13	1 (7%)
14	ACP	F	401	6	27,33,33	1.09	2 (7%)	32,52,52	1.55	6 (18%)
9	GOL	A	505	-	5,5,5	0.18	0	5,5,5	0.64	0
12	A1IM9	B	506	2	34,36,36	0.80	1 (2%)	35,46,46	1.88	8 (22%)
13	IMD	C	504	-	3,5,5	0.44	0	4,5,5	0.83	0

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
12	A1IM9	D	503	2	-	3/41/51/51	0/1/2/2
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
9	GOL	B	503	-	-	4/4/4/4	-
10	GDP	B	501	6	-	5/12/32/32	0/3/3/3
10	GDP	D	501	6	-	3/12/32/32	0/3/3/3
11	MES	B	504	-	-	0/6/14/14	0/1/1/1
14	ACP	F	401	6	-	3/15/38/38	0/3/3/3
9	GOL	A	505	-	-	0/4/4/4	-
12	A1IM9	B	506	2	-	6/41/51/51	0/1/2/2
13	IMD	C	504	-	-	-	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	501	GDP	C5-C6	-3.78	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	401	ACP	PG-O3G	3.53	1.63	1.54
10	D	501	GDP	C5-C6	-3.01	1.41	1.47
5	C	501	GTP	C6-N1	2.86	1.42	1.37
5	A	501	GTP	C5-C6	-2.80	1.41	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	506	A1IM9	C7-N1-C6	5.87	128.04	121.30
12	B	506	A1IM9	O1-C6-N1	-4.91	115.86	122.35
14	F	401	ACP	O2G-PG-C3B	-4.66	95.09	106.40
11	B	504	MES	O3S-S-C8	-3.70	99.78	105.77
12	B	506	A1IM9	C18-C19-C20	3.43	123.42	114.60

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

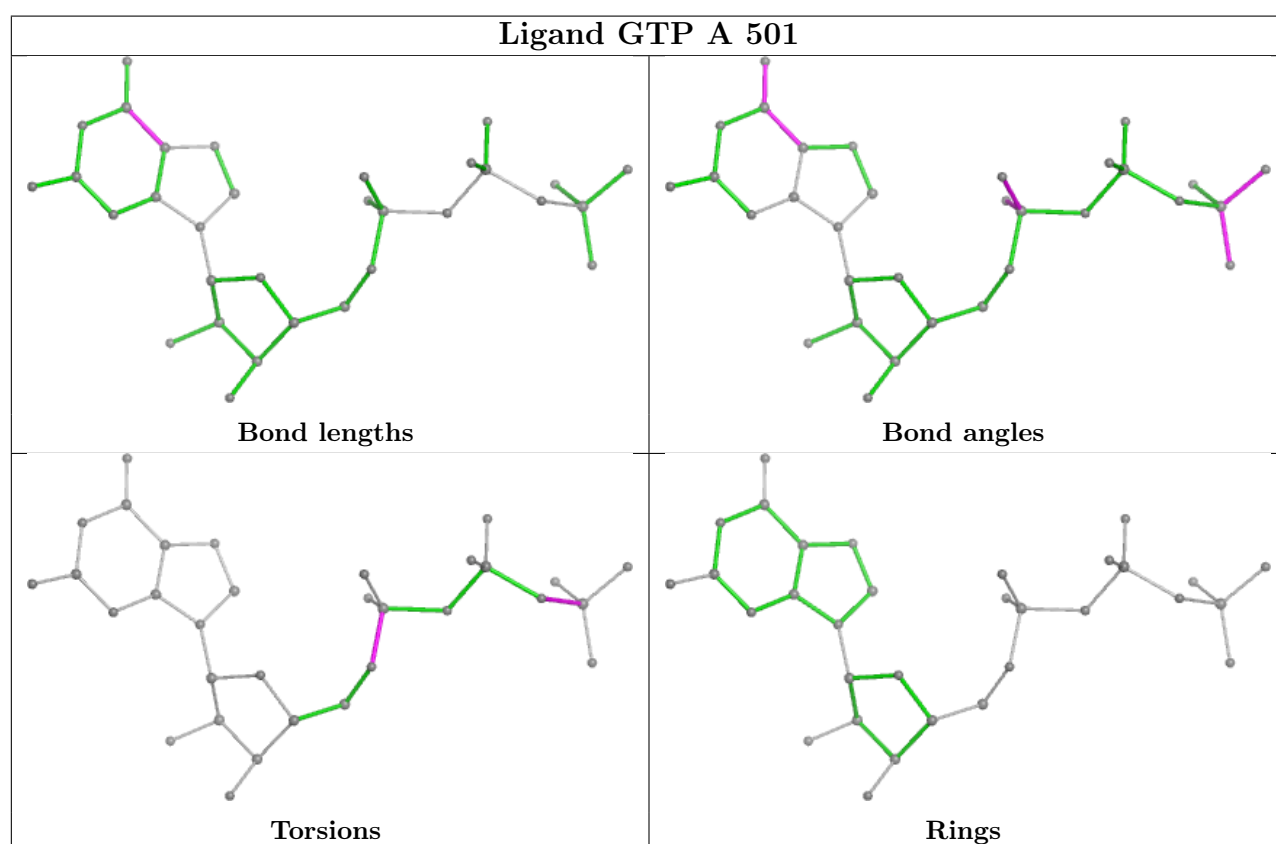
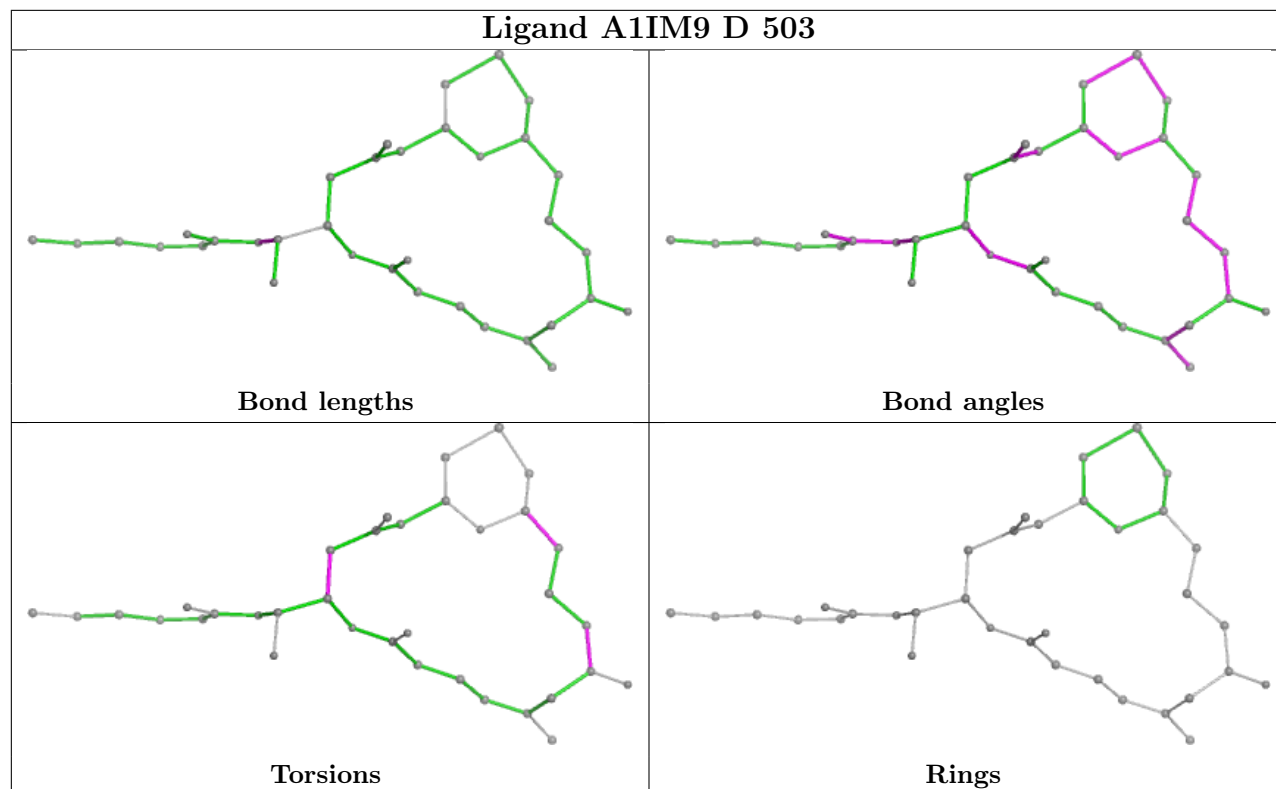
There are no ring outliers.

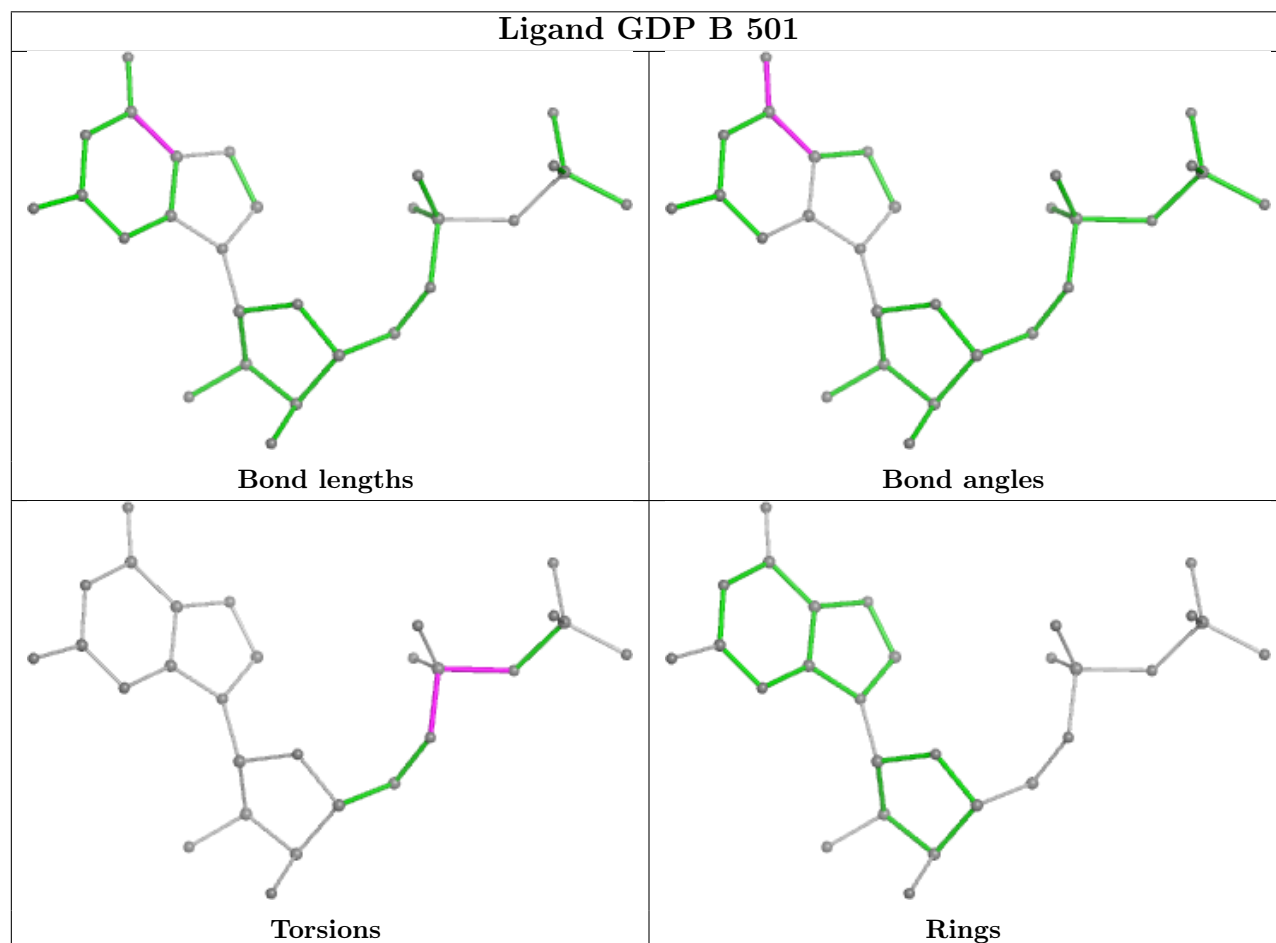
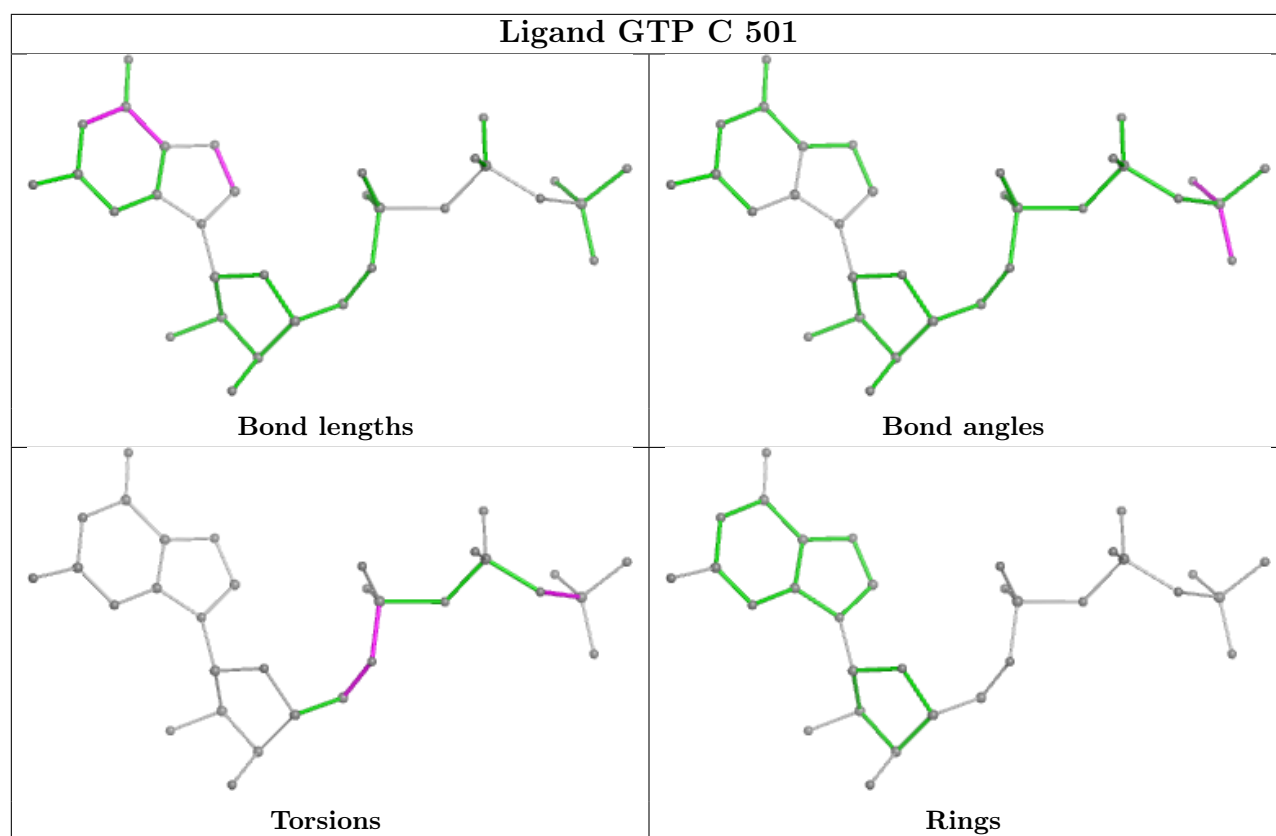
2 monomers are involved in 4 short contacts:

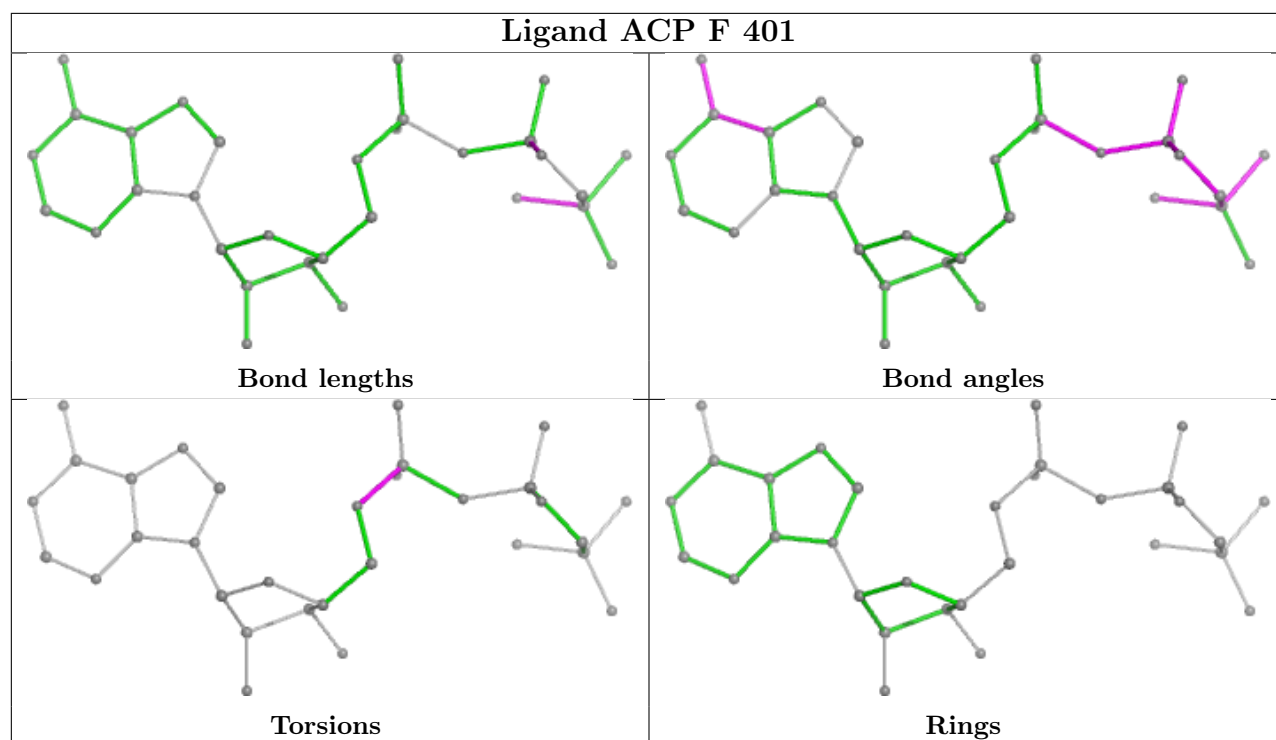
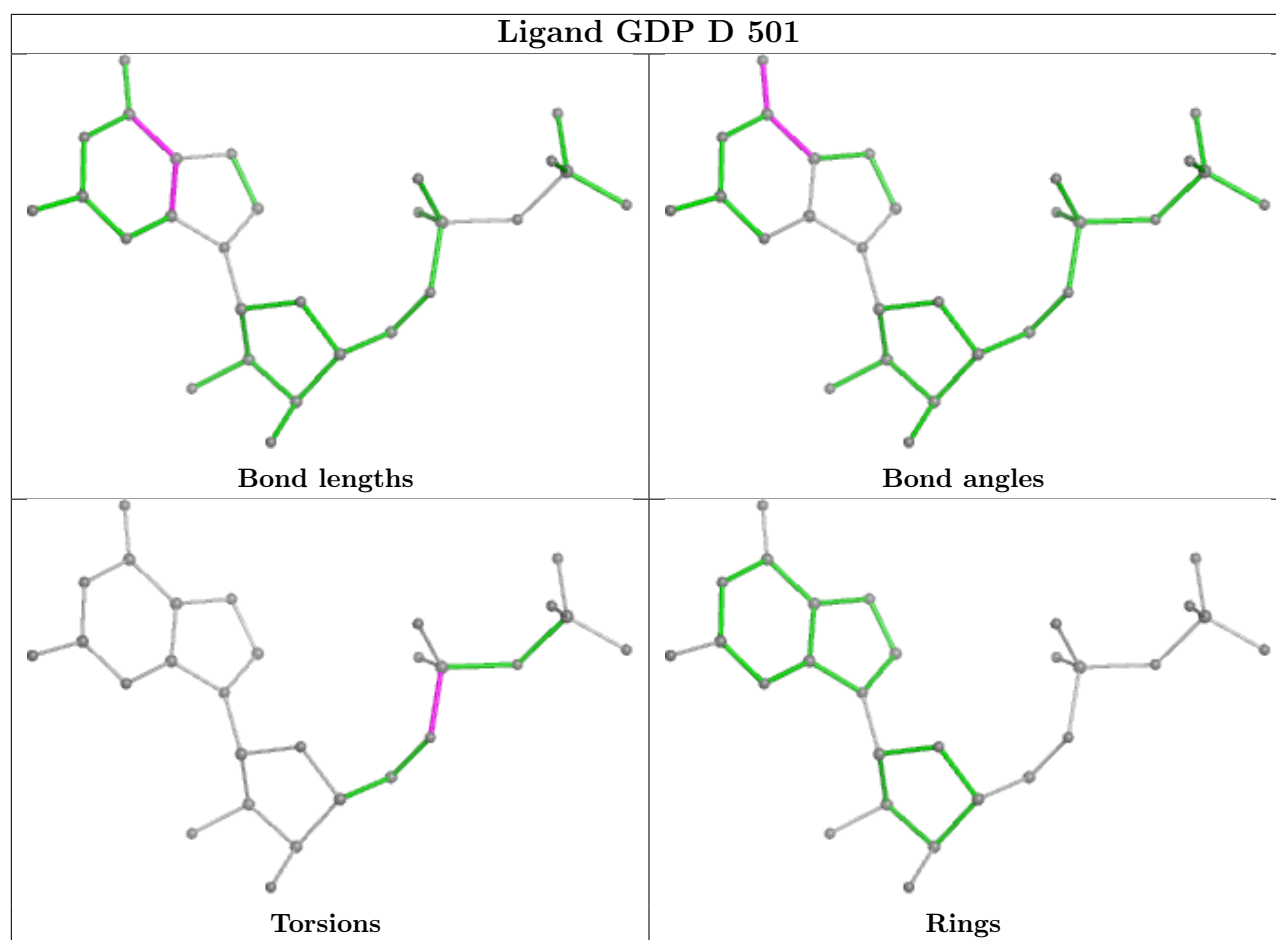
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	GOL	2	0
14	F	401	ACP	2	0

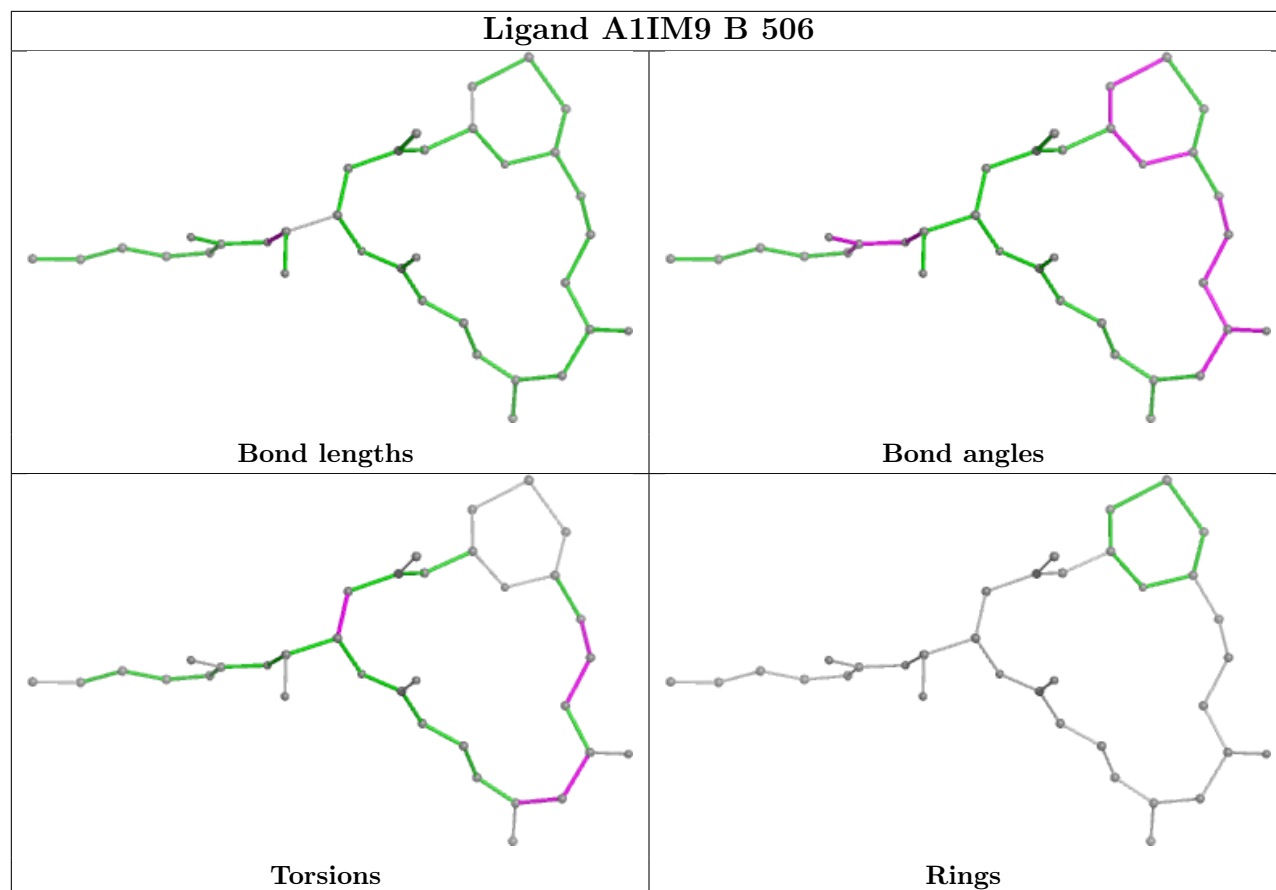
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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	434/451 (96%)	-0.44	6 (1%) 73 81	18, 44, 70, 94	8 (1%)
1	C	439/451 (97%)	-0.55	7 (1%) 70 78	14, 37, 62, 84	18 (4%)
2	B	419/445 (94%)	-0.33	5 (1%) 76 83	13, 45, 78, 116	16 (3%)
2	D	427/445 (95%)	-0.37	7 (1%) 70 78	17, 46, 72, 97	14 (3%)
3	E	115/189 (60%)	0.01	4 (3%) 47 58	19, 54, 80, 94	4 (3%)
4	F	311/384 (80%)	-0.12	13 (4%) 41 52	22, 57, 87, 104	4 (1%)
All	All	2145/2365 (90%)	-0.36	42 (1%) 64 74	13, 45, 77, 116	64 (2%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	139	LEU	5.6
4	F	141	GLY	4.4
1	A	437	VAL	4.4
4	F	159	GLY	4.1
1	A	346	TRP	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

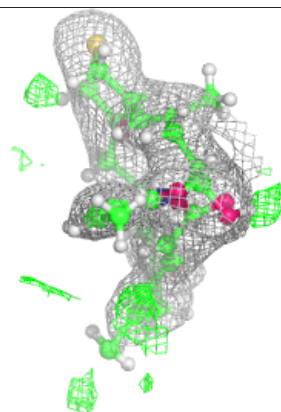
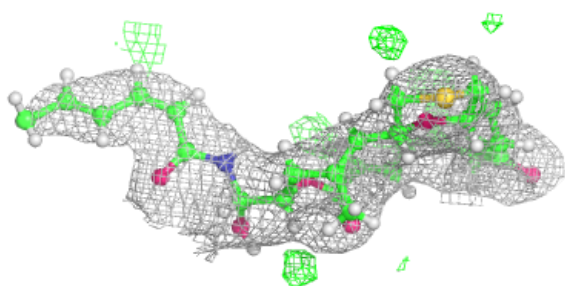
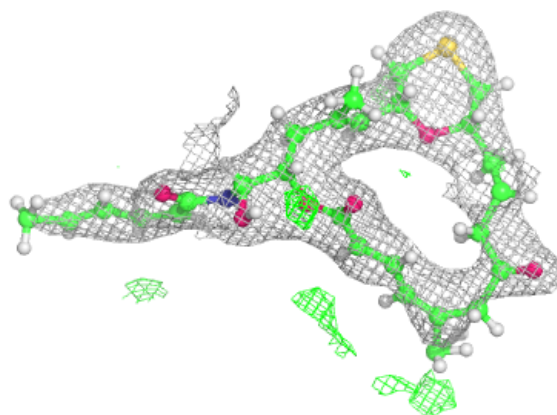
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	IMD	C	504	5/5	0.85	0.18	53,65,70,72	0
6	MG	F	402	1/1	0.92	0.10	52,52,52,52	0
12	A1IM9	B	506	35/35	0.93	0.12	30,69,80,85	10
9	GOL	A	505	6/6	0.93	0.11	30,60,73,84	3
9	GOL	B	503	6/6	0.94	0.12	30,63,69,70	3
14	ACP	F	401	31/31	0.94	0.07	30,60,92,96	2
11	MES	B	504	12/12	0.95	0.09	51,57,65,77	0
7	CA	B	505	1/1	0.97	0.07	85,85,85,85	0
12	A1IM9	D	503	35/35	0.97	0.07	30,47,57,69	10
10	GDP	D	501	28/28	0.98	0.04	42,46,50,50	0
6	MG	D	502	1/1	0.98	0.04	52,52,52,52	0
10	GDP	B	501	28/28	0.99	0.03	30,34,37,40	2
7	CA	A	503	1/1	0.99	0.04	55,55,55,55	0
6	MG	B	502	1/1	0.99	0.08	26,26,26,26	0
7	CA	C	503	1/1	0.99	0.02	48,48,48,48	0
8	CL	A	504	1/1	0.99	0.05	64,64,64,64	0
5	GTP	A	501	32/32	0.99	0.04	29,33,36,37	2
5	GTP	C	501	32/32	0.99	0.03	26,30,32,35	2
6	MG	C	502	1/1	1.00	0.06	30,30,30,30	0
6	MG	A	502	1/1	1.00	0.04	32,32,32,32	0

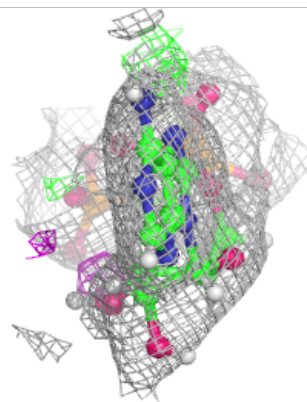
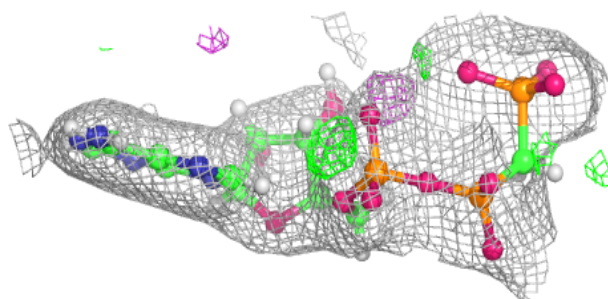
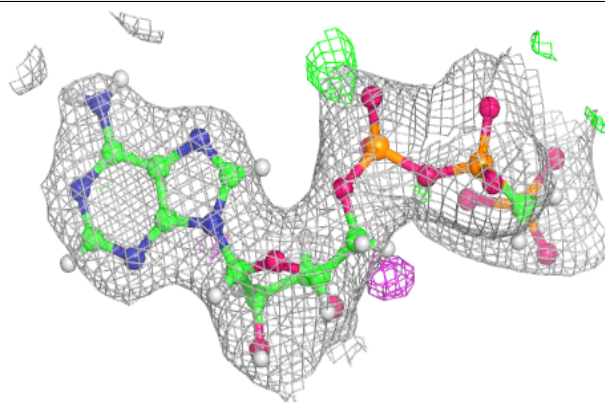
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IM9 B 506:

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

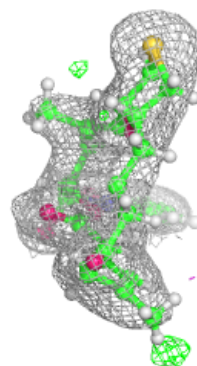
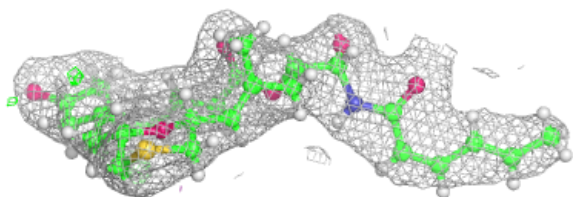
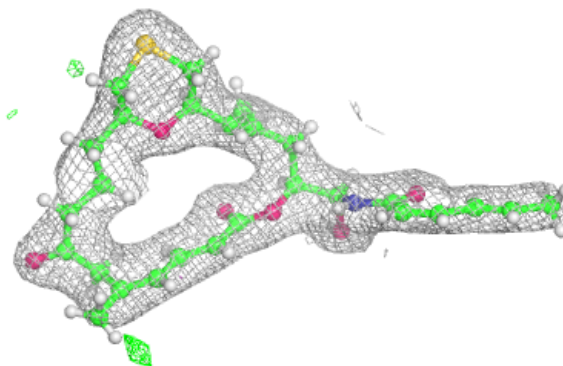
**Electron density around ACP F 401:**

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



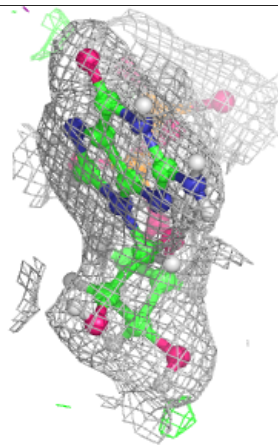
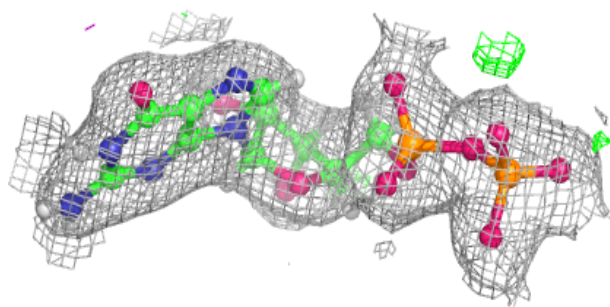
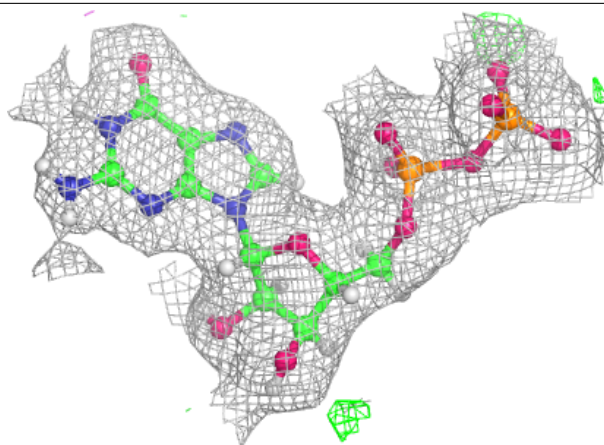
Electron density around A1IM9 D 503:

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



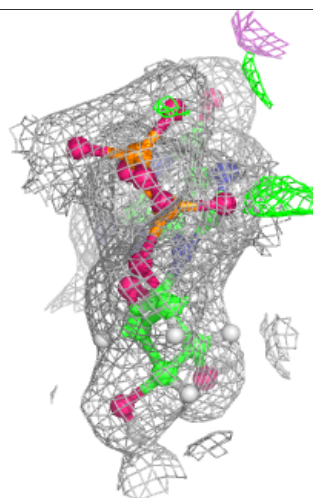
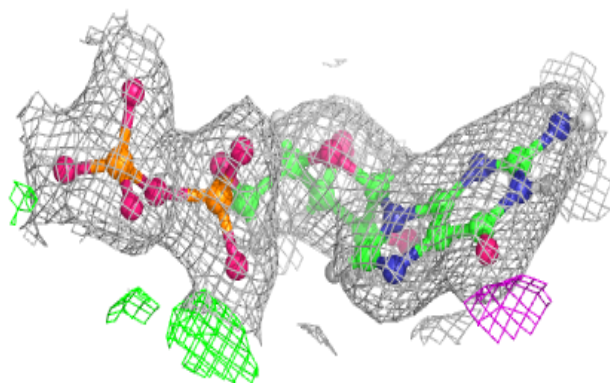
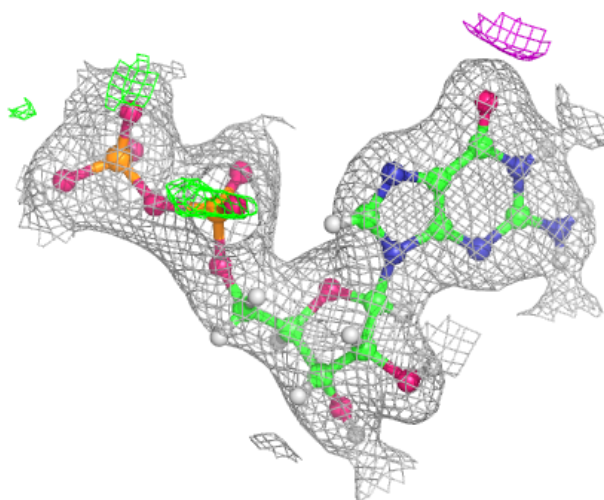
Electron density around GDP D 501:

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



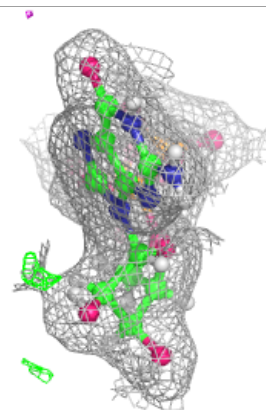
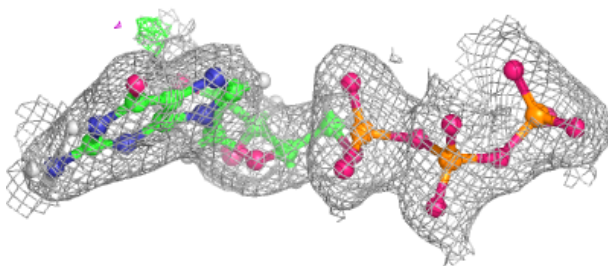
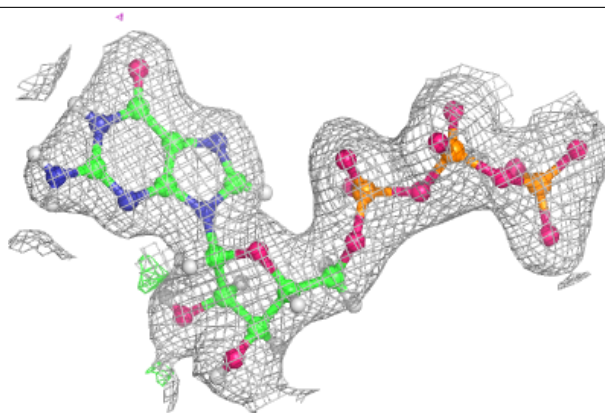
Electron density around GDP B 501:

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

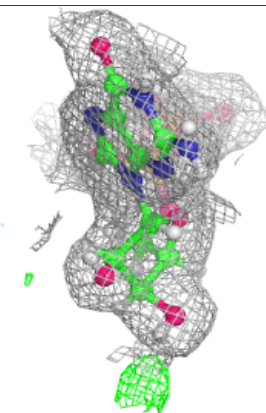
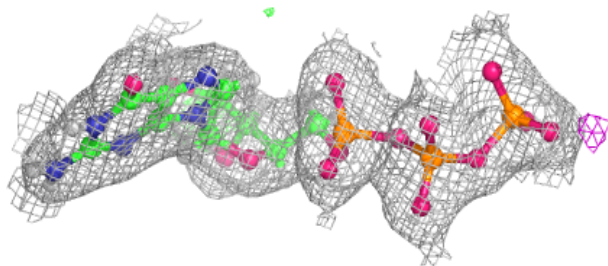
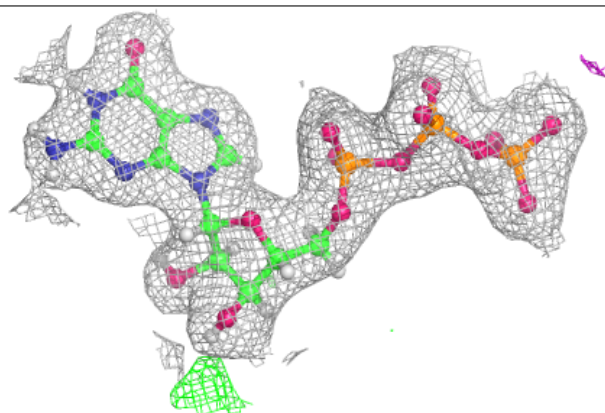


Electron density around GTP A 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.