



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 01:23 PM UTC

PDB ID : 2XKB / pdb_00002xkb
Title : Crystal structure of GDP-form protofilaments of *Bacillus thuringiensis* serovar israelensis TubZ
Authors : Aylett, C.H.S.; Lowe, J.
Deposited on : 2010-07-07
Resolution : 3.00 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

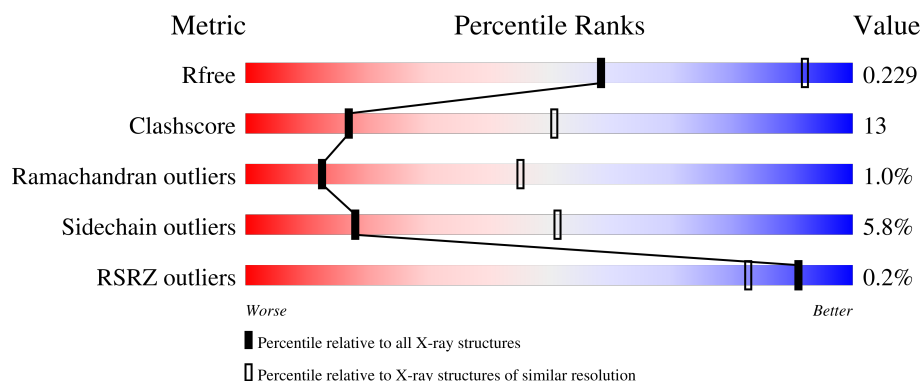
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	427	 58% 30% • 8%
1	B	427	 68% 24% • 5%
1	C	427	 66% 23% • 9%
1	D	427	 67% 23% • 8%
1	E	427	 70% 20% • 7%

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Mol	Chain	Length	Quality of chain
1	F	427	 64%25%• 8%
1	G	427	 65%27%• 5%
1	H	427	 66%25%• 8%
1	I	427	 64%27%• 5%
1	J	427	 65%24%• 8%
1	K	427	 66%26%• 6%
1	L	427	 64%23%• 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37877 atoms, of which 0 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 FTSZ/TUBULIN-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3095	1952	526	604	13			
1	B	405	Total	C	N	O	S	0	0	0
			3209	2022	544	630	13			
1	C	389	Total	C	N	O	S	0	0	0
			3095	1949	532	601	13			
1	D	391	Total	C	N	O	S	0	0	0
			3094	1949	528	604	13			
1	E	395	Total	C	N	O	S	0	0	0
			3137	1976	534	614	13			
1	F	391	Total	C	N	O	S	0	0	0
			3095	1949	529	605	12			
1	G	404	Total	C	N	O	S	0	0	0
			3198	2016	543	626	13			
1	H	394	Total	C	N	O	S	0	0	0
			3143	1983	533	614	13			
1	I	404	Total	C	N	O	S	0	0	0
			3202	2018	543	628	13			
1	J	393	Total	C	N	O	S	0	0	0
			3114	1963	531	608	12			
1	K	400	Total	C	N	O	S	0	0	0
			3182	2003	545	622	12			
1	L	379	Total	C	N	O	S	0	0	0
			3001	1897	507	585	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	HIS	-	expression tag	UNP Q8KNP3
A	423	HIS	-	expression tag	UNP Q8KNP3
A	424	HIS	-	expression tag	UNP Q8KNP3
A	425	HIS	-	expression tag	UNP Q8KNP3
A	426	HIS	-	expression tag	UNP Q8KNP3

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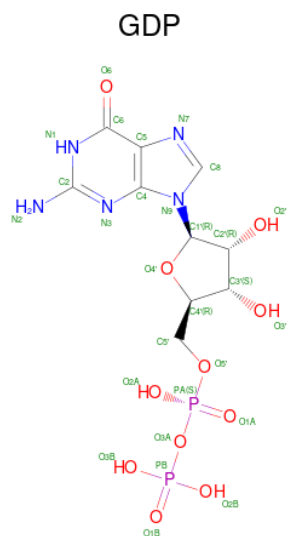
Chain	Residue	Modelled	Actual	Comment	Reference
A	427	HIS	-	expression tag	UNP Q8KNP3
A	2	VAL	LEU	engineered mutation	UNP Q8KNP3
B	422	HIS	-	expression tag	UNP Q8KNP3
B	423	HIS	-	expression tag	UNP Q8KNP3
B	424	HIS	-	expression tag	UNP Q8KNP3
B	425	HIS	-	expression tag	UNP Q8KNP3
B	426	HIS	-	expression tag	UNP Q8KNP3
B	427	HIS	-	expression tag	UNP Q8KNP3
B	2	VAL	LEU	engineered mutation	UNP Q8KNP3
C	422	HIS	-	expression tag	UNP Q8KNP3
C	423	HIS	-	expression tag	UNP Q8KNP3
C	424	HIS	-	expression tag	UNP Q8KNP3
C	425	HIS	-	expression tag	UNP Q8KNP3
C	426	HIS	-	expression tag	UNP Q8KNP3
C	427	HIS	-	expression tag	UNP Q8KNP3
C	2	VAL	LEU	engineered mutation	UNP Q8KNP3
D	422	HIS	-	expression tag	UNP Q8KNP3
D	423	HIS	-	expression tag	UNP Q8KNP3
D	424	HIS	-	expression tag	UNP Q8KNP3
D	425	HIS	-	expression tag	UNP Q8KNP3
D	426	HIS	-	expression tag	UNP Q8KNP3
D	427	HIS	-	expression tag	UNP Q8KNP3
D	2	VAL	LEU	engineered mutation	UNP Q8KNP3
E	422	HIS	-	expression tag	UNP Q8KNP3
E	423	HIS	-	expression tag	UNP Q8KNP3
E	424	HIS	-	expression tag	UNP Q8KNP3
E	425	HIS	-	expression tag	UNP Q8KNP3
E	426	HIS	-	expression tag	UNP Q8KNP3
E	427	HIS	-	expression tag	UNP Q8KNP3
E	2	VAL	LEU	engineered mutation	UNP Q8KNP3
F	422	HIS	-	expression tag	UNP Q8KNP3
F	423	HIS	-	expression tag	UNP Q8KNP3
F	424	HIS	-	expression tag	UNP Q8KNP3
F	425	HIS	-	expression tag	UNP Q8KNP3
F	426	HIS	-	expression tag	UNP Q8KNP3
F	427	HIS	-	expression tag	UNP Q8KNP3
F	2	VAL	LEU	engineered mutation	UNP Q8KNP3
G	422	HIS	-	expression tag	UNP Q8KNP3
G	423	HIS	-	expression tag	UNP Q8KNP3
G	424	HIS	-	expression tag	UNP Q8KNP3
G	425	HIS	-	expression tag	UNP Q8KNP3
G	426	HIS	-	expression tag	UNP Q8KNP3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	427	HIS	-	expression tag	UNP Q8KNP3
G	2	VAL	LEU	engineered mutation	UNP Q8KNP3
H	422	HIS	-	expression tag	UNP Q8KNP3
H	423	HIS	-	expression tag	UNP Q8KNP3
H	424	HIS	-	expression tag	UNP Q8KNP3
H	425	HIS	-	expression tag	UNP Q8KNP3
H	426	HIS	-	expression tag	UNP Q8KNP3
H	427	HIS	-	expression tag	UNP Q8KNP3
H	2	VAL	LEU	engineered mutation	UNP Q8KNP3
I	422	HIS	-	expression tag	UNP Q8KNP3
I	423	HIS	-	expression tag	UNP Q8KNP3
I	424	HIS	-	expression tag	UNP Q8KNP3
I	425	HIS	-	expression tag	UNP Q8KNP3
I	426	HIS	-	expression tag	UNP Q8KNP3
I	427	HIS	-	expression tag	UNP Q8KNP3
I	2	VAL	LEU	engineered mutation	UNP Q8KNP3
J	422	HIS	-	expression tag	UNP Q8KNP3
J	423	HIS	-	expression tag	UNP Q8KNP3
J	424	HIS	-	expression tag	UNP Q8KNP3
J	425	HIS	-	expression tag	UNP Q8KNP3
J	426	HIS	-	expression tag	UNP Q8KNP3
J	427	HIS	-	expression tag	UNP Q8KNP3
J	2	VAL	LEU	engineered mutation	UNP Q8KNP3
K	422	HIS	-	expression tag	UNP Q8KNP3
K	423	HIS	-	expression tag	UNP Q8KNP3
K	424	HIS	-	expression tag	UNP Q8KNP3
K	425	HIS	-	expression tag	UNP Q8KNP3
K	426	HIS	-	expression tag	UNP Q8KNP3
K	427	HIS	-	expression tag	UNP Q8KNP3
K	2	VAL	LEU	engineered mutation	UNP Q8KNP3
L	422	HIS	-	expression tag	UNP Q8KNP3
L	423	HIS	-	expression tag	UNP Q8KNP3
L	424	HIS	-	expression tag	UNP Q8KNP3
L	425	HIS	-	expression tag	UNP Q8KNP3
L	426	HIS	-	expression tag	UNP Q8KNP3
L	427	HIS	-	expression tag	UNP Q8KNP3
L	2	VAL	LEU	engineered mutation	UNP Q8KNP3

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	C	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	D	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	E	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	F	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	G	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	I	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	J	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	K	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	L	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

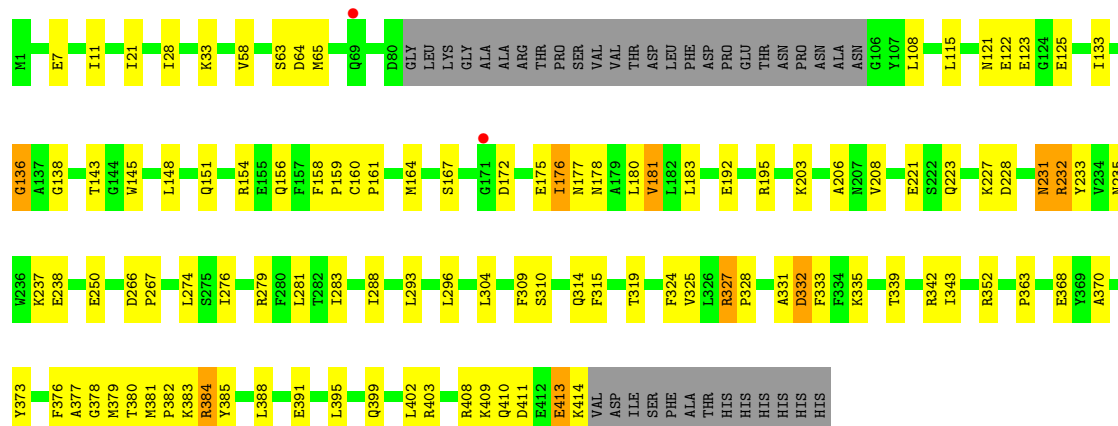
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

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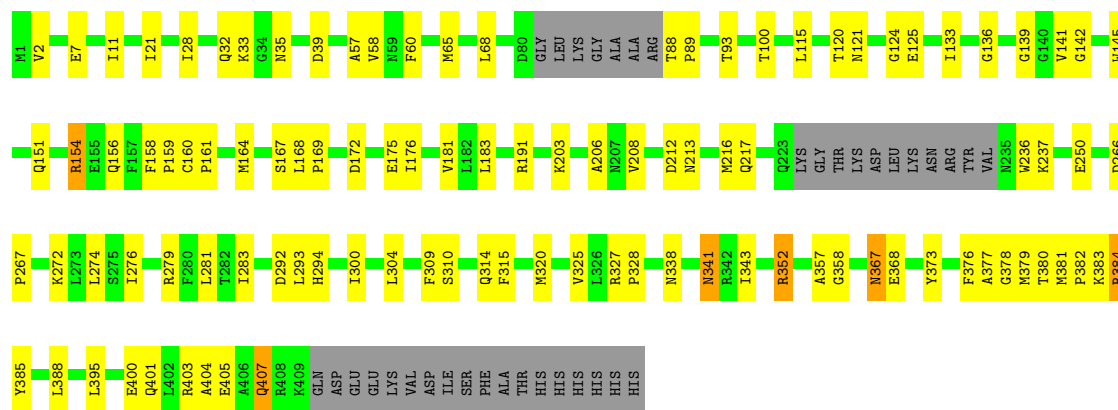
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	I	1	Total 1	Mg 1	0	0

Chain C:  66% 23% 9%



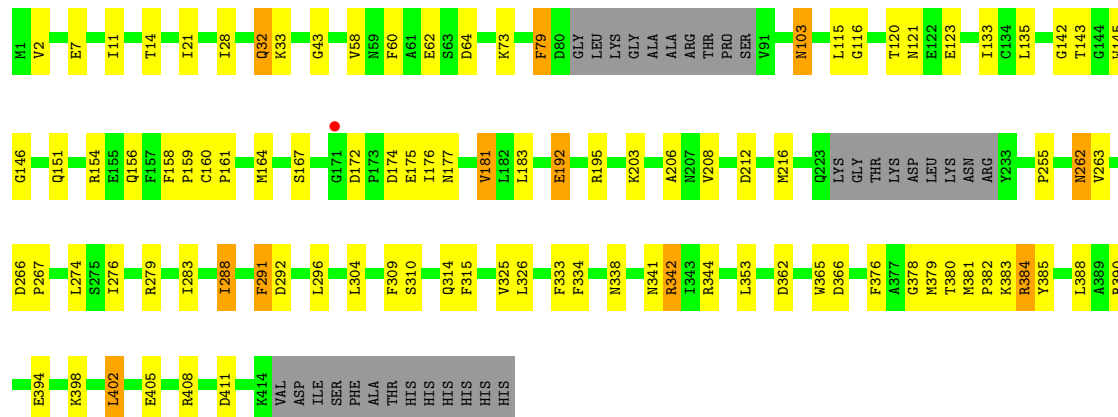
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain D:  67% 23% 8%



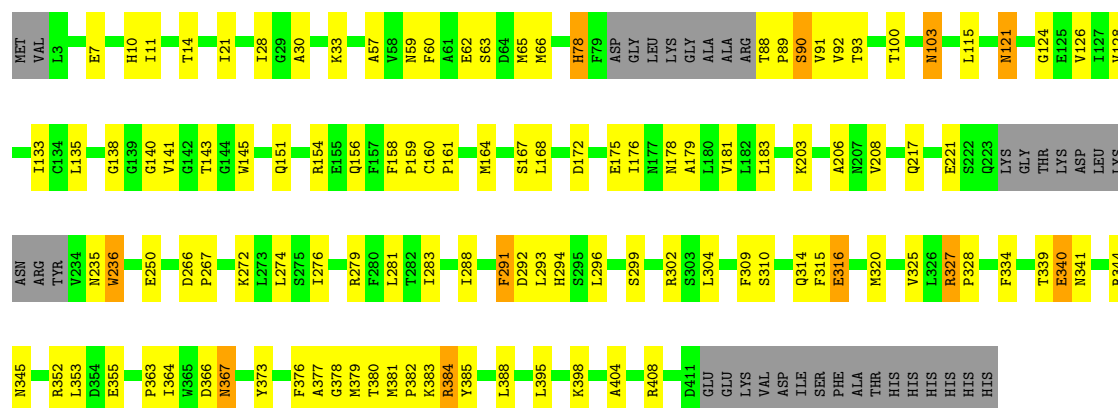
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain E:  70% 20% 7%



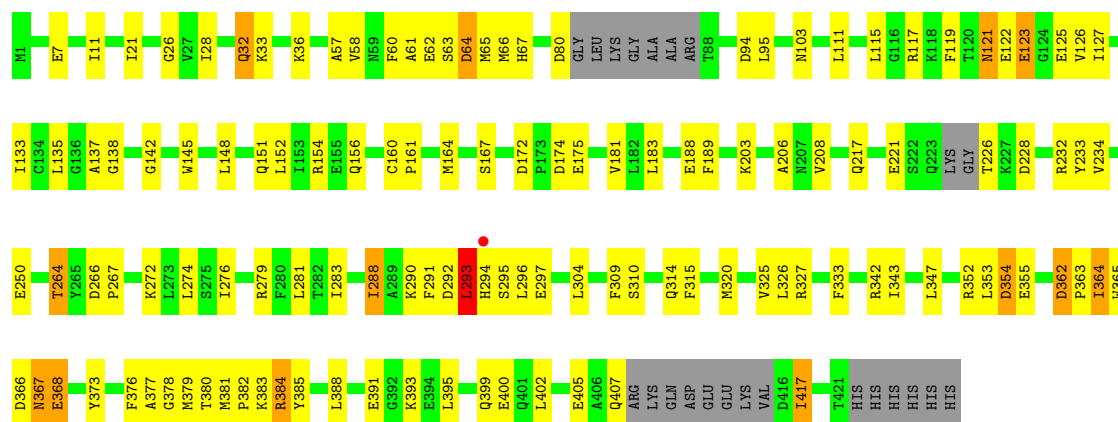
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain F:  64% 25% 8%



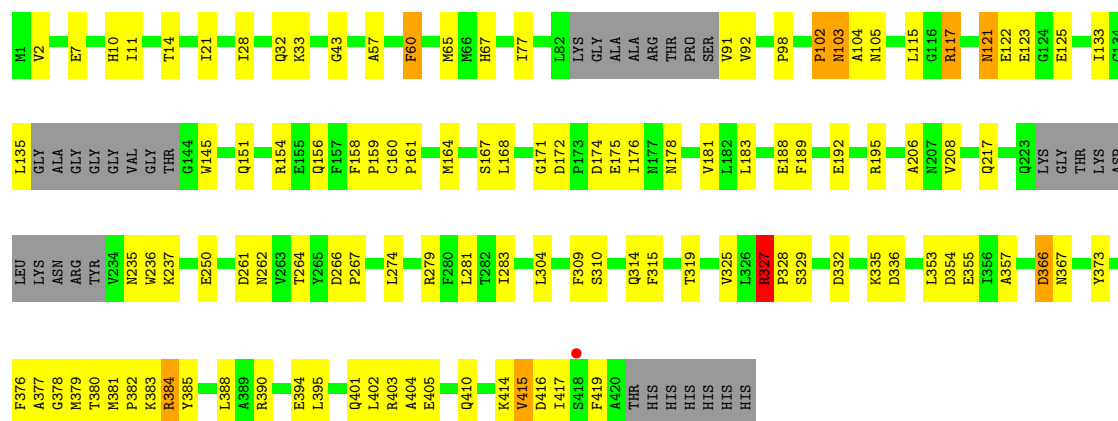
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain G:  65% 27% 5%



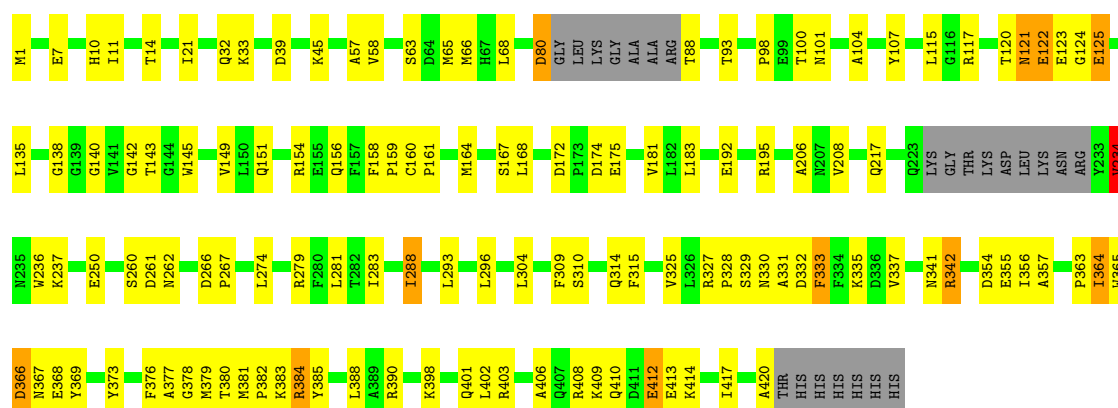
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain H:  66% 25% 8%



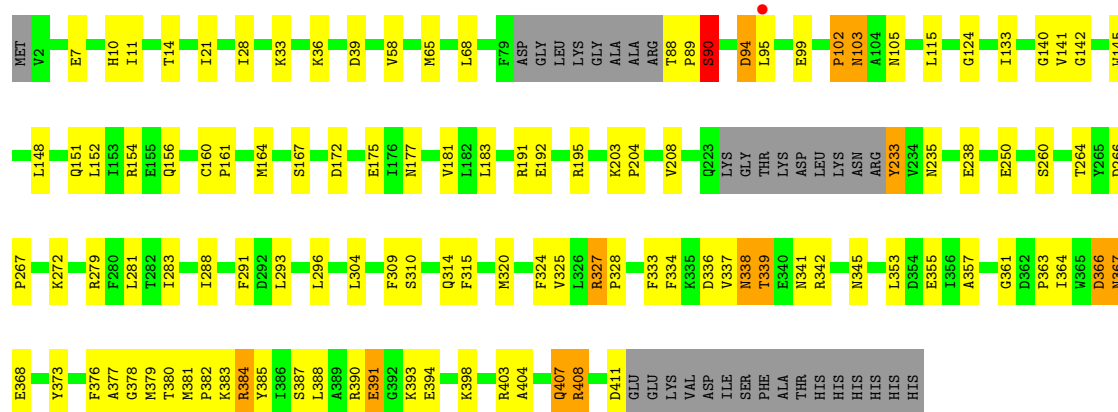
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain I:  64% 27% 5%



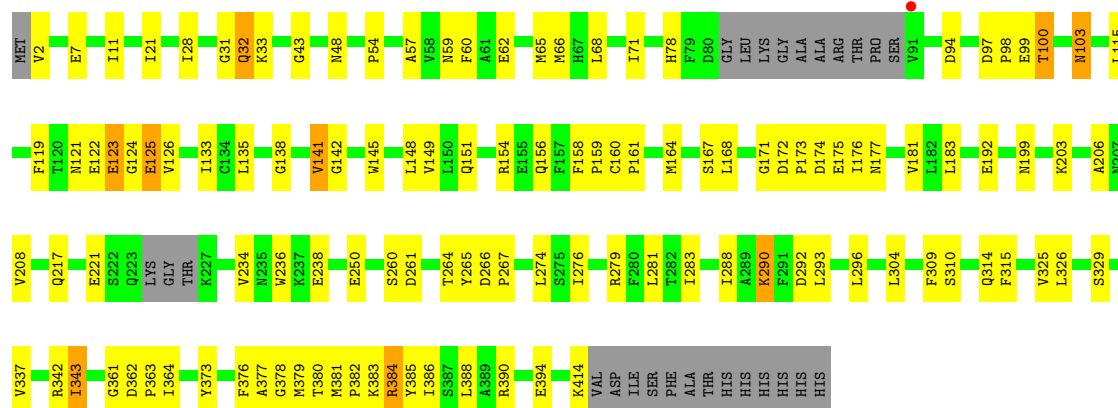
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain J:  65% 24% 8%



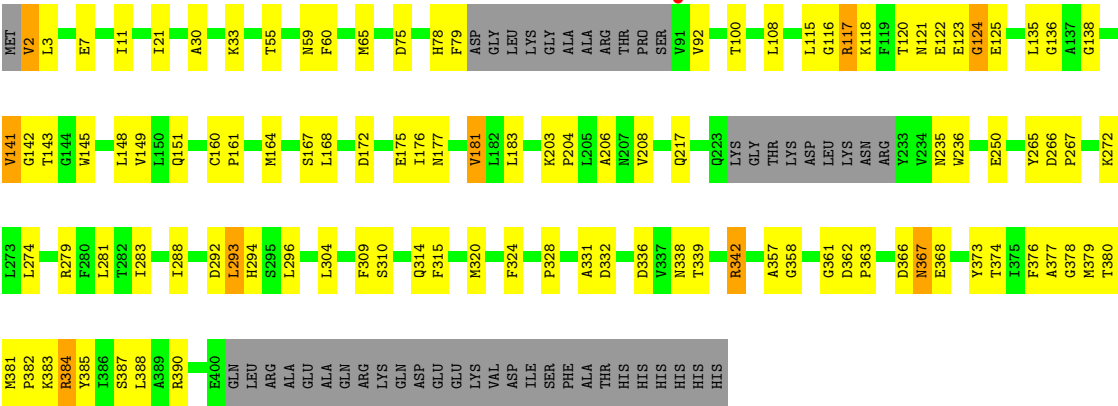
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain K:  66% 26% 6%



• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain L: 64% 23% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.95Å 541.10Å 86.13Å 90.00° 92.51° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.9 (50.00-3.00) 92.9 (50.00-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.294 (Not available) , 0.229	Depositor DCC
R_{free} test set	4465 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	37877	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: MG, GDP

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	0.61	0/3155	0.91	3/4268 (0.1%)
1	B	0.63	0/3270	0.93	4/4422 (0.1%)
1	C	0.63	0/3152	0.93	1/4252 (0.0%)
1	D	0.68	3/3153 (0.1%)	0.97	6/4263 (0.1%)
1	E	0.60	1/3196 (0.0%)	0.91	0/4319
1	F	0.63	0/3154	0.96	5/4265 (0.1%)
1	G	0.64	1/3258 (0.0%)	0.91	1/4405 (0.0%)
1	H	0.63	0/3201	0.94	7/4325 (0.2%)
1	I	0.64	1/3263 (0.0%)	0.94	5/4412 (0.1%)
1	J	0.62	0/3174	0.94	1/4293 (0.0%)
1	K	0.60	0/3241	0.95	3/4378 (0.1%)
1	L	0.62	0/3060	0.94	4/4140 (0.1%)
All	All	0.63	6/38277 (0.0%)	0.94	40/51742 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	154	ARG	CZ-NH1	10.88	1.48	1.32
1	D	154	ARG	NE-CZ	10.85	1.45	1.33
1	D	154	ARG	CD-NE	8.68	1.58	1.46
1	G	264	THR	CA-CB	6.10	1.61	1.53
1	I	262	ASN	CA-C	5.47	1.55	1.52

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	ARG	CD-NE-CZ	-10.88	109.17	124.40
1	D	154	ARG	NH1-CZ-NH2	10.16	132.50	119.30
1	F	316	GLU	CA-CB-CG	10.04	134.18	114.10
1	D	154	ARG	NE-CZ-NH1	-9.81	111.69	121.50
1	J	339	THR	N-CA-C	-8.84	101.60	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	223	GLN	Peptide

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	3095	0	3006	104	0
1	B	3209	0	3114	80	0
1	C	3095	0	3026	75	1
1	D	3094	0	3009	74	0
1	E	3137	0	3045	65	1
1	F	3095	0	3005	79	0
1	G	3198	0	3108	94	0
1	H	3143	0	3056	83	0
1	I	3202	0	3107	93	1
1	J	3114	0	3023	87	0
1	K	3182	0	3093	87	1
1	L	3001	0	2910	81	0
2	A	28	0	12	2	0
2	B	28	0	12	1	0
2	C	28	0	12	0	0
2	D	28	0	12	3	0
2	E	28	0	12	0	0
2	F	28	0	12	0	0
2	G	28	0	12	0	0
2	I	28	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	28	0	12	0	0
2	K	28	0	12	0	0
2	L	28	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	37877	0	36634	946	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 13.

The worst 5 of 946 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:L:315:PHE:HA	1:L:379:MET:HE2	1.31	1.12
1:L:117:ARG:HH11	1:L:117:ARG:HG2	1.04	1.12
1:H:117:ARG:HG2	1:H:117:ARG:HH11	1.14	1.10
1:D:176:ILE:HD12	1:D:388:LEU:HD11	1.34	1.09
1:B:315:PHE:HA	1:B:379:MET:HE2	1.34	1.08

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)
1:E:73:LYS:NZ	1:K:48:ASN:O[1_655]	1.73	0.47
1:C:232:ARG:NH2	1:I:124:GLY:O[1_655]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/427 (90%)	355 (92%)	24 (6%)	6 (2%)	7	34
1	B	399/427 (93%)	371 (93%)	25 (6%)	3 (1%)	16	50
1	C	385/427 (90%)	357 (93%)	26 (7%)	2 (0%)	24	60
1	D	385/427 (90%)	356 (92%)	28 (7%)	1 (0%)	36	70
1	E	389/427 (91%)	364 (94%)	22 (6%)	3 (1%)	16	50
1	F	385/427 (90%)	347 (90%)	33 (9%)	5 (1%)	9	38
1	G	396/427 (93%)	356 (90%)	35 (9%)	5 (1%)	9	38
1	H	386/427 (90%)	349 (90%)	32 (8%)	5 (1%)	9	38
1	I	398/427 (93%)	365 (92%)	30 (8%)	3 (1%)	16	50
1	J	387/427 (91%)	353 (91%)	28 (7%)	6 (2%)	7	34
1	K	394/427 (92%)	368 (93%)	24 (6%)	2 (0%)	24	60
1	L	373/427 (87%)	342 (92%)	26 (7%)	5 (1%)	9	38
All	All	4662/5124 (91%)	4283 (92%)	333 (7%)	46 (1%)	12	45

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	B	102	PRO
1	B	413	GLU
1	E	60	PHE
1	F	121	ASN

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	339/369 (92%)	317 (94%)	22 (6%)	15	47
1	B	352/369 (95%)	331 (94%)	21 (6%)	17	50
1	C	337/369 (91%)	318 (94%)	19 (6%)	19	52
1	D	339/369 (92%)	322 (95%)	17 (5%)	22	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	343/369 (93%)	329 (96%)	14 (4%)	27	61
1	F	339/369 (92%)	320 (94%)	19 (6%)	19	52
1	G	351/369 (95%)	327 (93%)	24 (7%)	14	45
1	H	346/369 (94%)	329 (95%)	17 (5%)	22	56
1	I	351/369 (95%)	325 (93%)	26 (7%)	13	42
1	J	341/369 (92%)	320 (94%)	21 (6%)	16	49
1	K	348/369 (94%)	326 (94%)	22 (6%)	16	48
1	L	329/369 (89%)	314 (95%)	15 (5%)	24	58
All	All	4115/4428 (93%)	3878 (94%)	237 (6%)	18	51

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	80	ASP
1	K	414	LYS
1	H	181	VAL
1	K	364	ILE
1	L	384	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	78	HIS
1	K	231	ASN
1	G	314	GLN
1	K	215	GLN
1	L	101	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 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
2	GDP	F	900	-	29,30,30	1.22	3 (10%)	45,47,47	1.77	6 (13%)
2	GDP	A	900	3	29,30,30	1.16	3 (10%)	45,47,47	1.82	6 (13%)
2	GDP	D	900	-	29,30,30	1.18	2 (6%)	45,47,47	1.76	7 (15%)
2	GDP	L	900	-	29,30,30	1.20	3 (10%)	45,47,47	1.97	11 (24%)
2	GDP	G	900	3	29,30,30	1.10	2 (6%)	45,47,47	1.78	7 (15%)
2	GDP	B	900	3	29,30,30	1.28	3 (10%)	45,47,47	1.84	10 (22%)
2	GDP	I	900	3	29,30,30	1.40	2 (6%)	45,47,47	1.88	8 (17%)
2	GDP	K	900	-	29,30,30	1.21	2 (6%)	45,47,47	1.71	7 (15%)
2	GDP	C	900	-	29,30,30	1.25	3 (10%)	45,47,47	1.97	11 (24%)
2	GDP	J	900	-	29,30,30	1.24	3 (10%)	45,47,47	1.74	6 (13%)
2	GDP	E	900	-	29,30,30	1.30	3 (10%)	45,47,47	1.86	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
2	GDP	F	900	-	-	4/16/32/32	0/3/3/3
2	GDP	A	900	3	-	6/16/32/32	0/3/3/3
2	GDP	D	900	-	-	2/16/32/32	0/3/3/3
2	GDP	L	900	-	-	4/16/32/32	0/3/3/3
2	GDP	G	900	3	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	B	900	3	-	1/16/32/32	0/3/3/3
2	GDP	I	900	3	-	4/16/32/32	0/3/3/3
2	GDP	K	900	-	-	2/16/32/32	0/3/3/3
2	GDP	C	900	-	-	7/16/32/32	0/3/3/3
2	GDP	J	900	-	-	4/16/32/32	0/3/3/3
2	GDP	E	900	-	-	2/16/32/32	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	900	GDP	PA-O3A	4.30	1.64	1.59
2	L	900	GDP	C5-C4	3.79	1.49	1.38
2	B	900	GDP	C5-C4	3.63	1.48	1.38
2	K	900	GDP	C5-C4	3.44	1.48	1.38
2	C	900	GDP	C5-C4	3.44	1.48	1.38

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	900	GDP	C5-C4-N3	-6.61	117.87	128.39
2	B	900	GDP	C5-C4-N3	-6.39	118.21	128.39
2	I	900	GDP	C5-C4-N3	-6.32	118.33	128.39
2	A	900	GDP	C5-C4-N3	-6.31	118.34	128.39
2	G	900	GDP	C5-C4-N3	-6.27	118.41	128.39

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	GDP	PA-O3A-PB-O3B
2	A	900	GDP	C5'-O5'-PA-O3A
2	A	900	GDP	O4'-C4'-C5'-O5'
2	B	900	GDP	C5'-O5'-PA-O3A
2	C	900	GDP	PA-O3A-PB-O2B

There are no ring outliers.

5 monomers are involved in 8 short contacts:

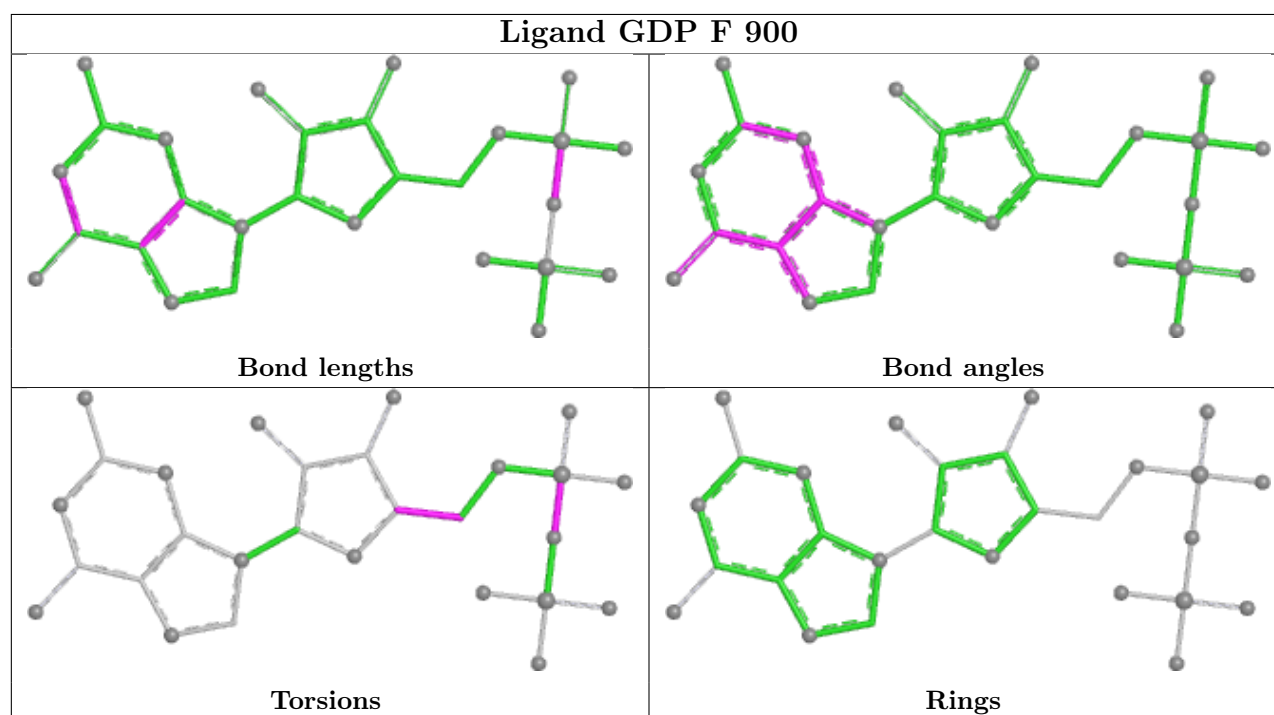
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	GDP	2	0

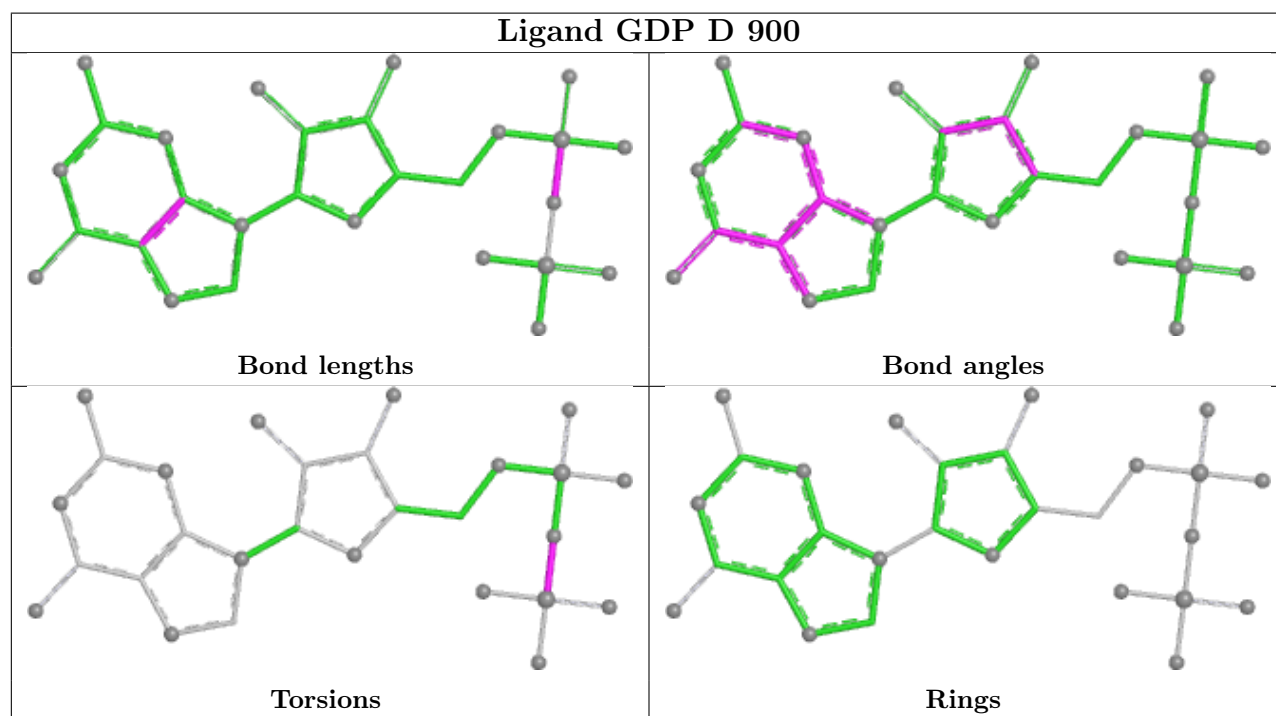
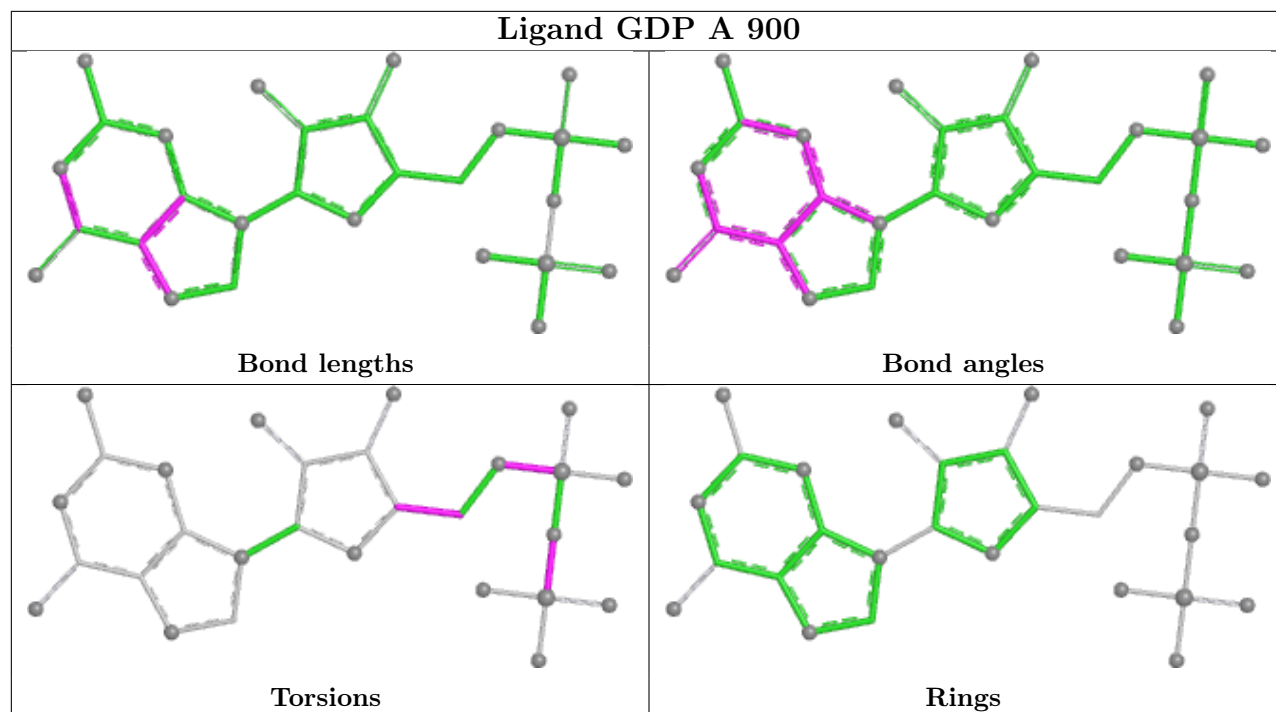
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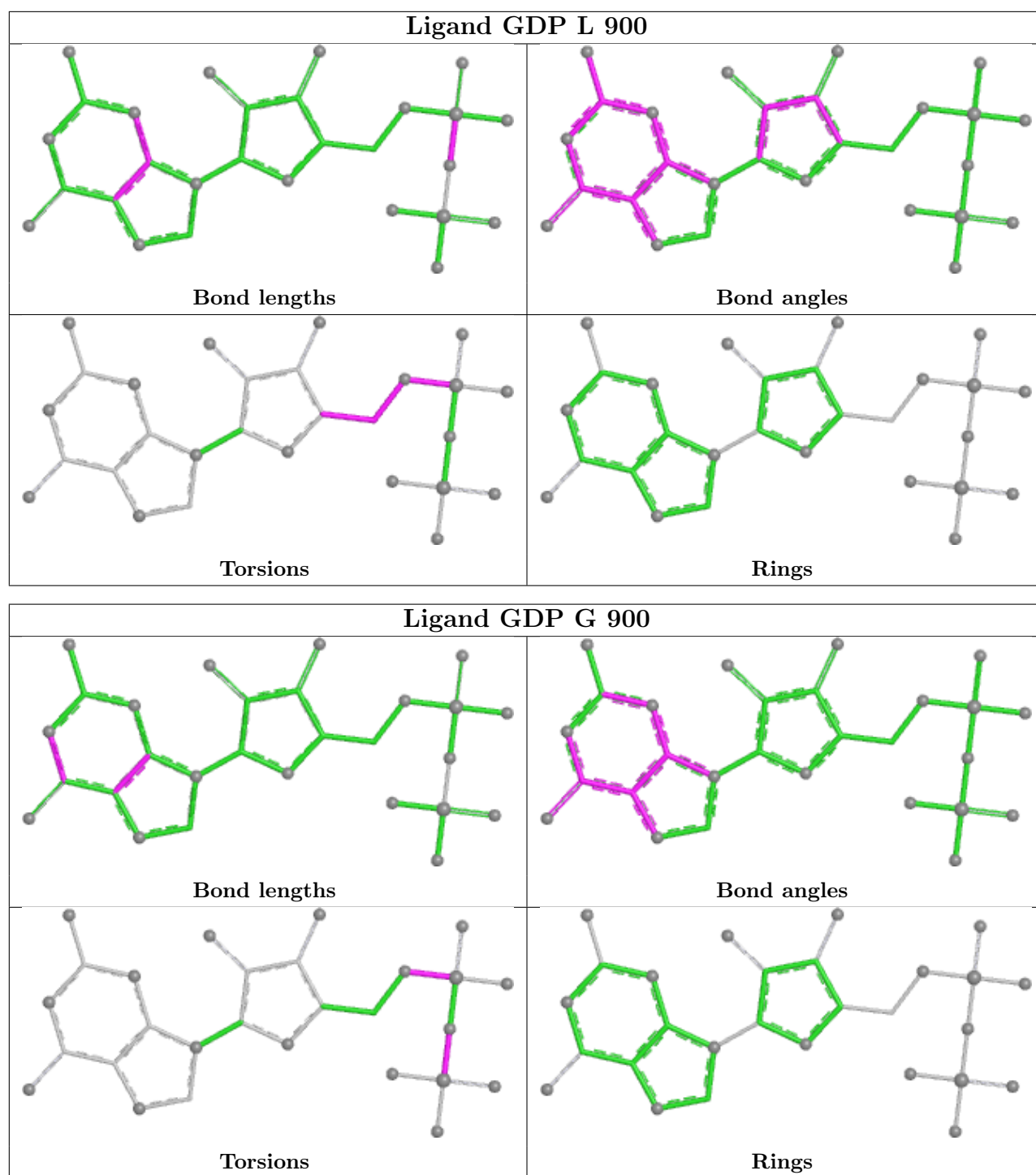
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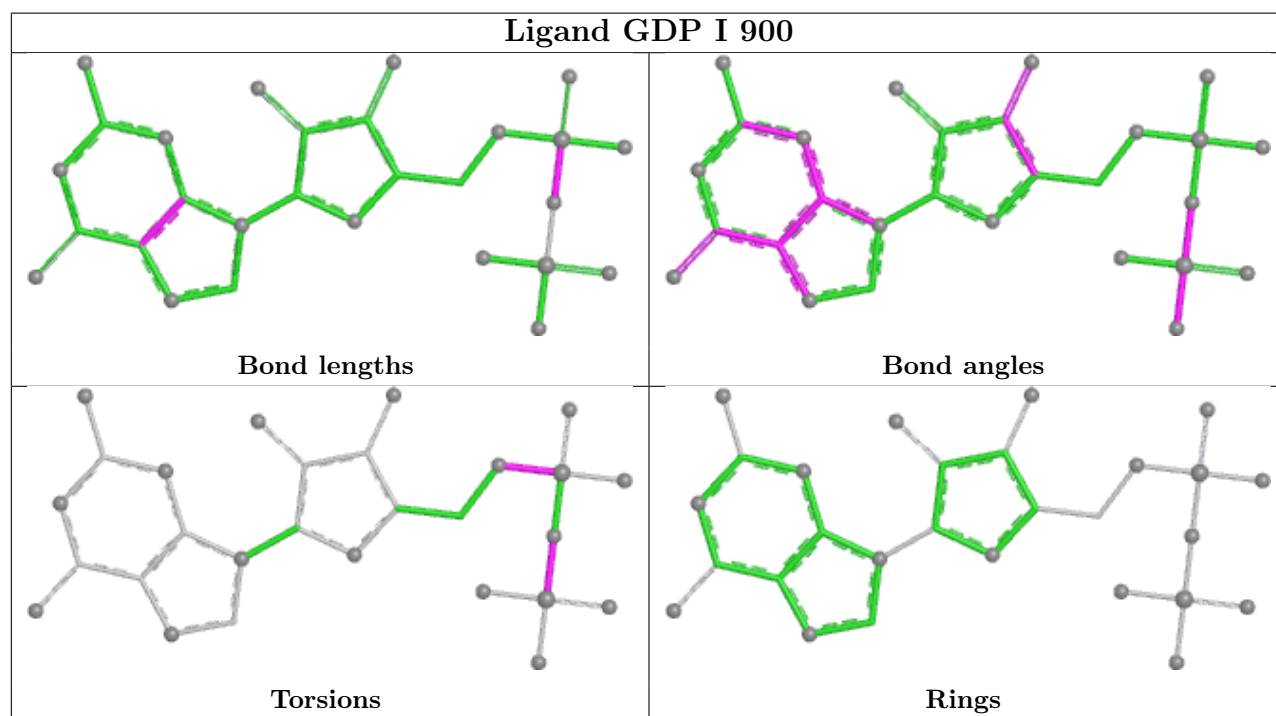
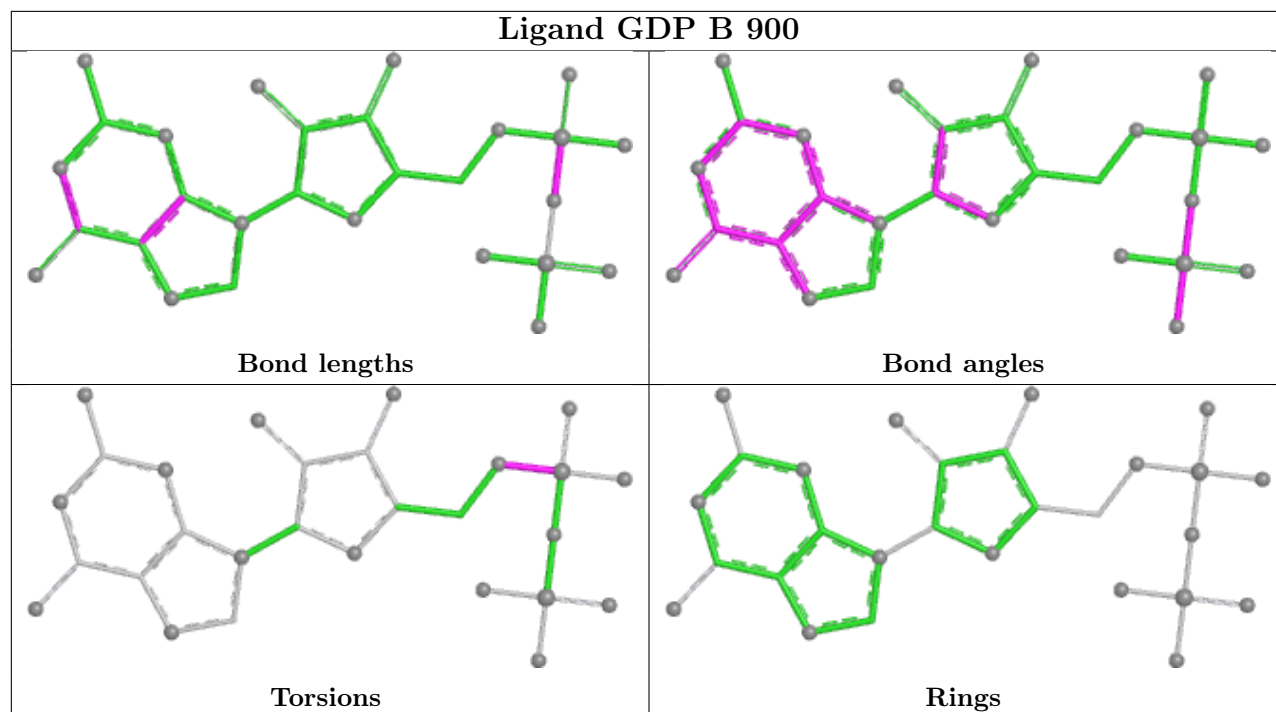
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	GDP	3	0
2	L	900	GDP	1	0
2	B	900	GDP	1	0
2	I	900	GDP	1	0

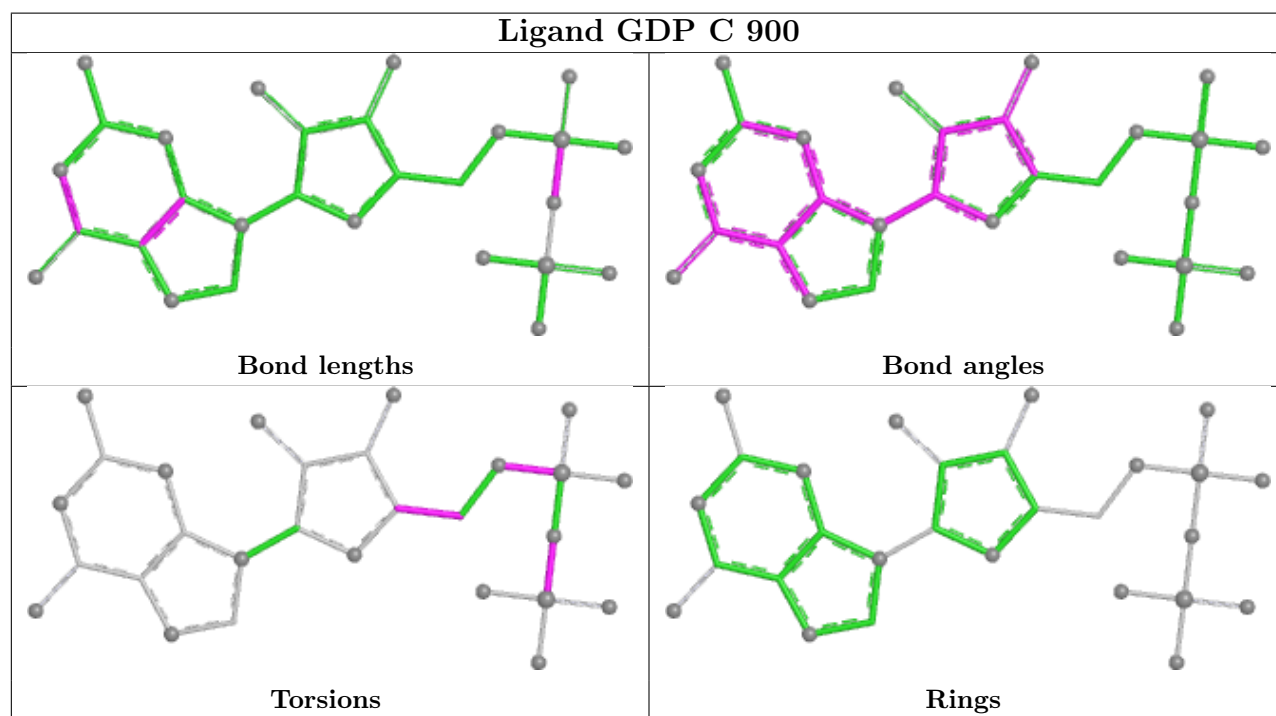
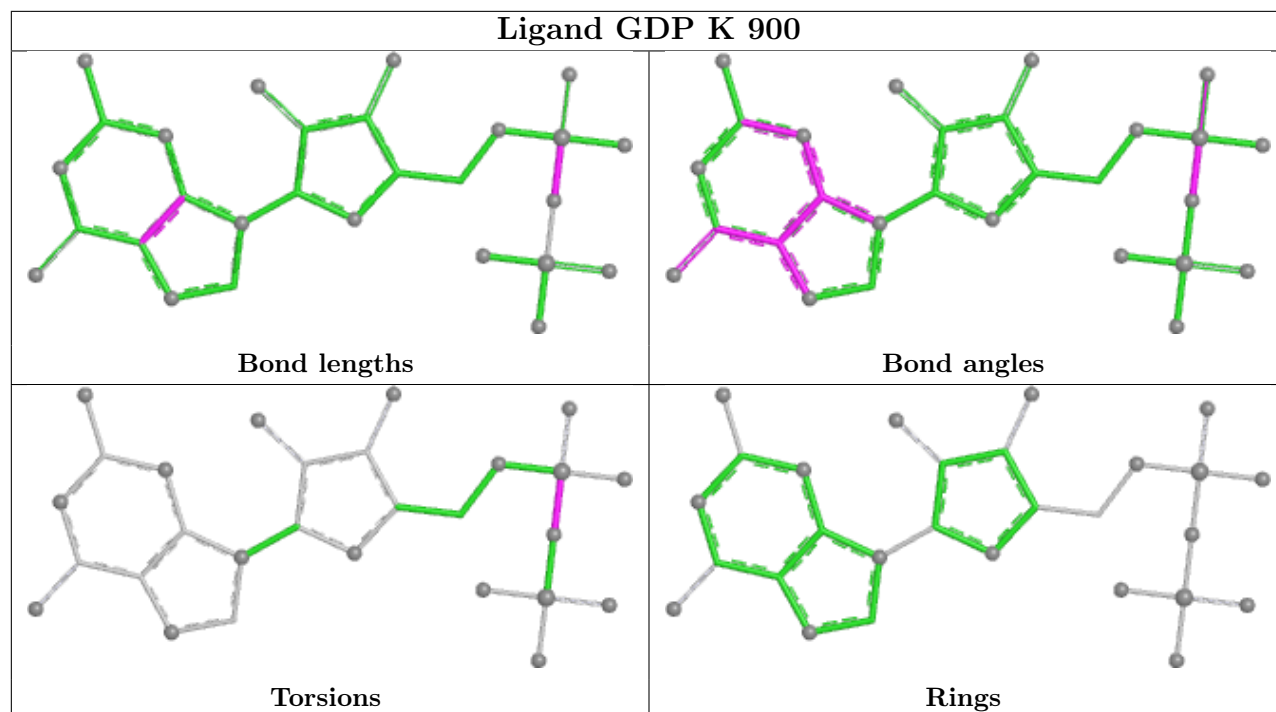
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

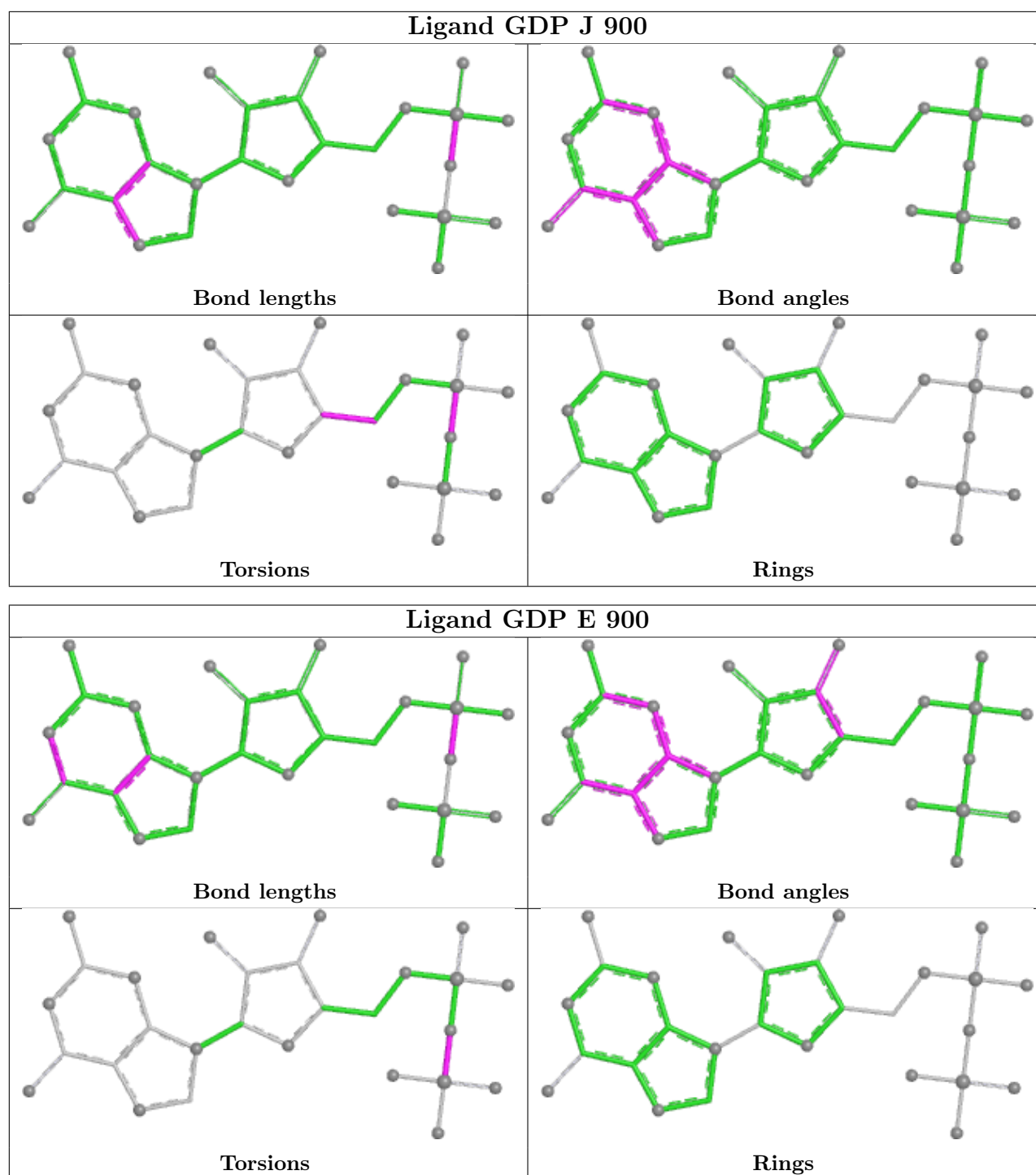












5.7 Other polymers [i](#)

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	391/427 (91%)	-0.10	2 (0%) 87 72	35, 54, 77, 83	0
1	B	405/427 (94%)	-0.04	0 100 100	18, 53, 84, 92	0
1	C	389/427 (91%)	-0.20	2 (0%) 87 72	35, 54, 68, 85	0
1	D	391/427 (91%)	-0.14	0 100 100	35, 56, 87, 95	0
1	E	395/427 (92%)	-0.16	1 (0%) 90 79	35, 54, 72, 103	0
1	F	391/427 (91%)	-0.12	0 100 100	35, 55, 78, 87	0
1	G	404/427 (94%)	0.04	1 (0%) 91 83	35, 56, 82, 88	0
1	H	394/427 (92%)	-0.05	1 (0%) 90 79	35, 53, 71, 82	0
1	I	404/427 (94%)	-0.04	0 100 100	35, 55, 91, 105	0
1	J	393/427 (92%)	-0.19	1 (0%) 90 79	35, 55, 79, 108	0
1	K	400/427 (93%)	-0.18	1 (0%) 90 79	35, 55, 75, 115	0
1	L	379/427 (88%)	-0.10	1 (0%) 90 79	35, 55, 78, 104	0
All	All	4736/5124 (92%)	-0.11	10 (0%) 91 83	18, 55, 79, 115	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	91	VAL	3.6
1	C	171	GLY	2.9
1	A	171	GLY	2.8
1	A	406	ALA	2.4
1	K	91	VAL	2.4

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 [i](#)

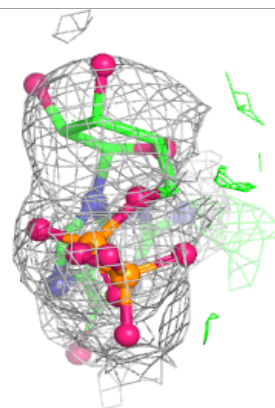
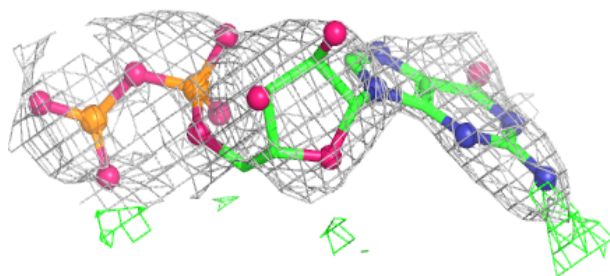
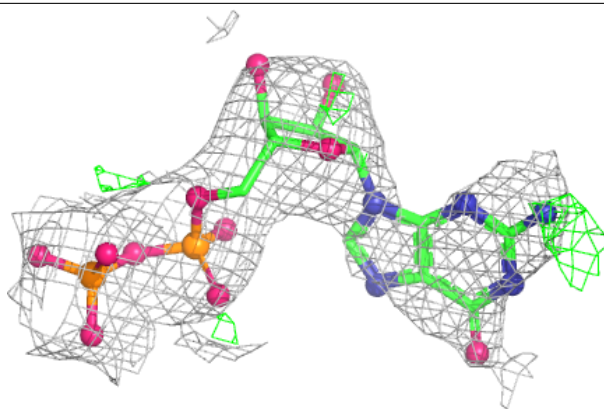
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GDP	L	900	28/28	0.80	0.13	110,112,115,115	0
2	GDP	D	900	28/28	0.81	0.13	107,110,111,111	0
2	GDP	F	900	28/28	0.85	0.12	107,107,110,110	0
2	GDP	J	900	28/28	0.87	0.10	89,91,92,93	0
3	MG	B	999	1/1	0.88	0.10	13,13,13,13	0
3	MG	A	999	1/1	0.91	0.14	12,12,12,12	0
2	GDP	K	900	28/28	0.92	0.09	67,70,70,70	0
2	GDP	C	900	28/28	0.93	0.07	37,42,43,43	0
3	MG	I	999	1/1	0.93	0.18	17,17,17,17	0
2	GDP	E	900	28/28	0.94	0.07	36,45,52,52	0
2	GDP	B	900	28/28	0.94	0.07	36,37,39,40	0
2	GDP	A	900	28/28	0.95	0.07	47,49,50,51	0
2	GDP	G	900	28/28	0.96	0.06	35,39,44,44	0
3	MG	G	999	1/1	0.96	0.13	17,17,17,17	0
2	GDP	I	900	28/28	0.96	0.06	26,30,34,34	0

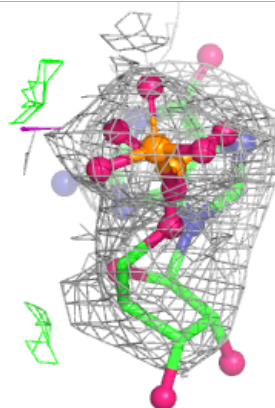
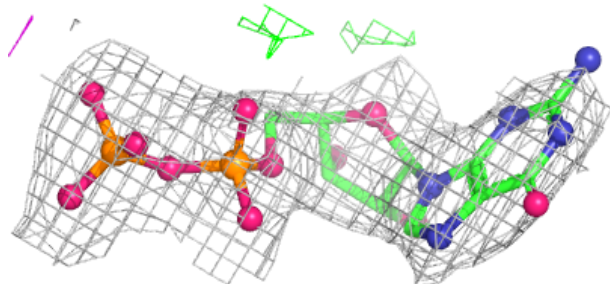
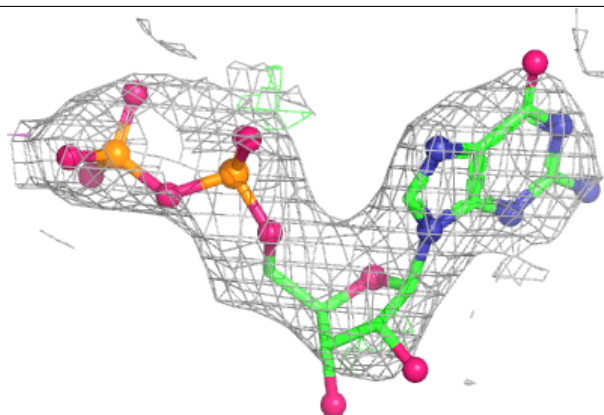
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP L 900:

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

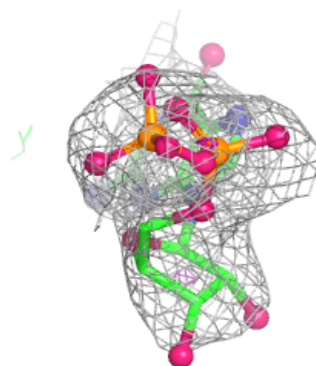
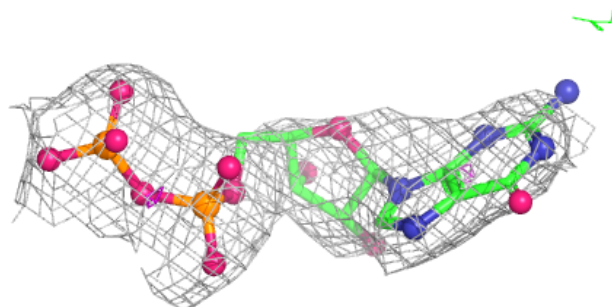
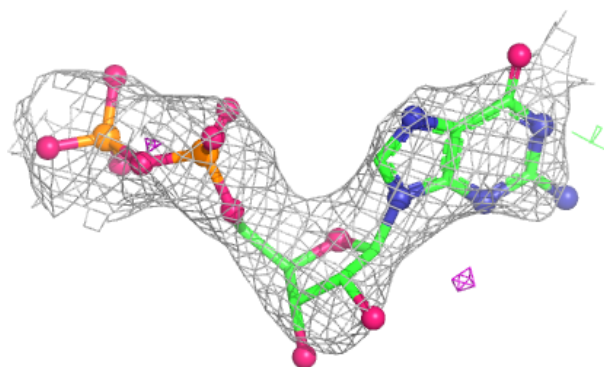
**Electron density around GDP D 900:**

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and green (positive)

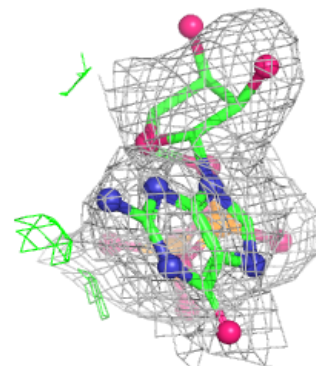
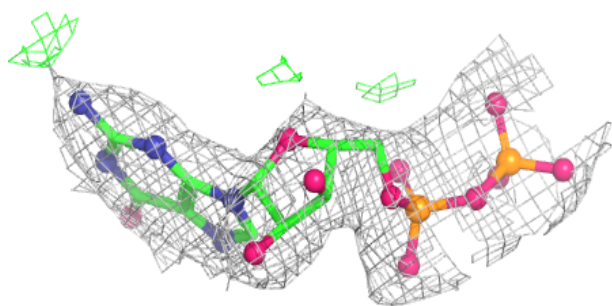
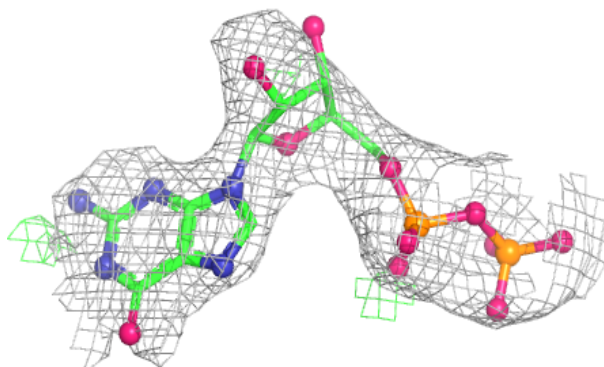


Electron density around GDP F 900:

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and green (positive)

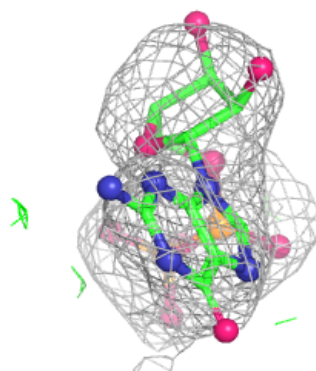
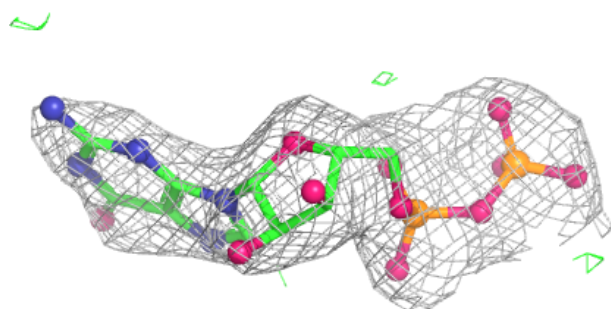
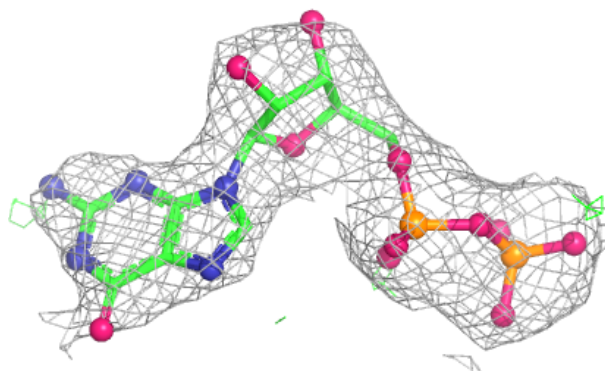
**Electron density around GDP J 900:**

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and green (positive)

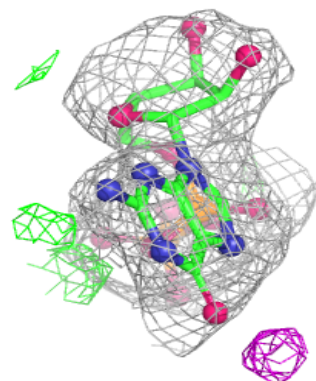
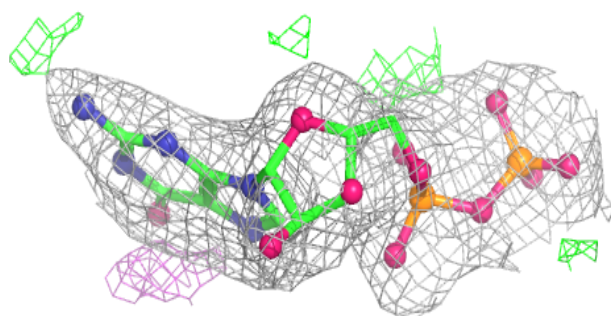
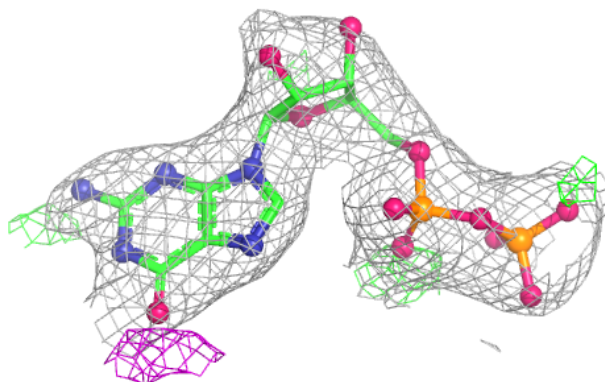


Electron density around GDP K 900:

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

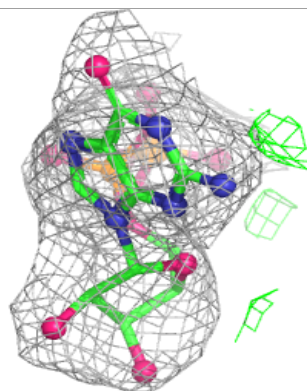
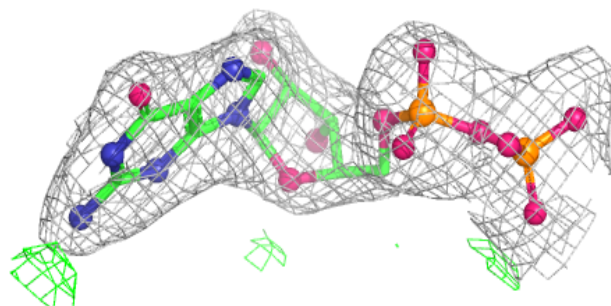
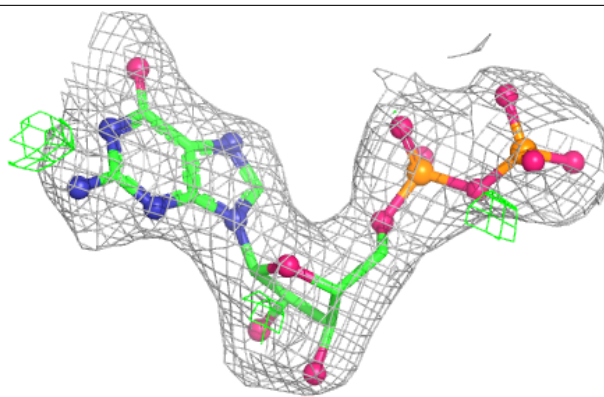
**Electron density around GDP C 900:**

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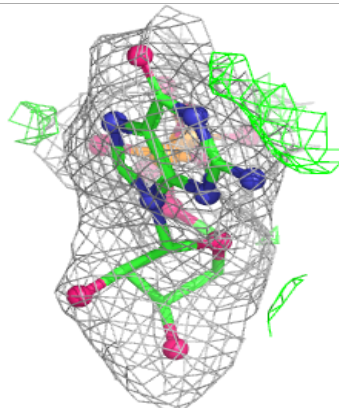
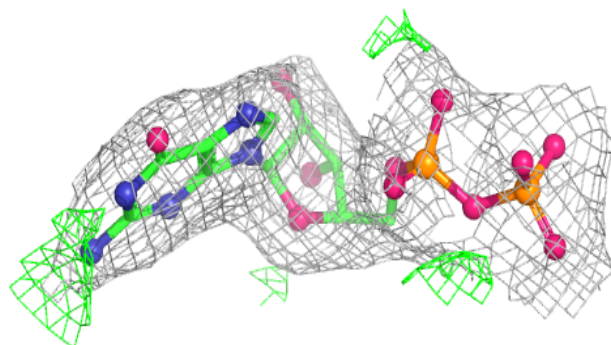
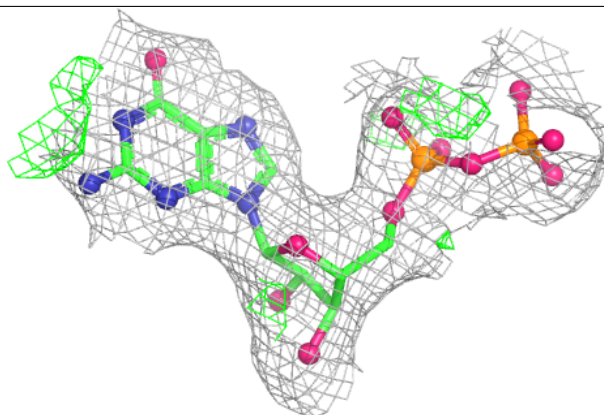


Electron density around GDP E 900:

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and green (positive)

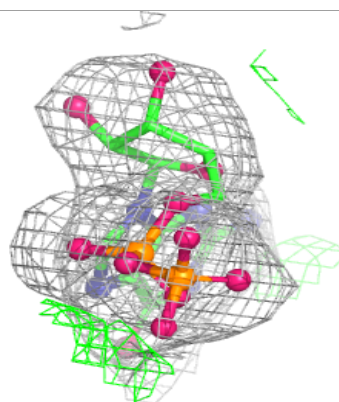
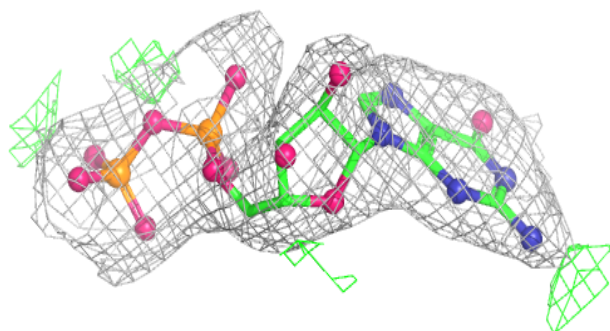
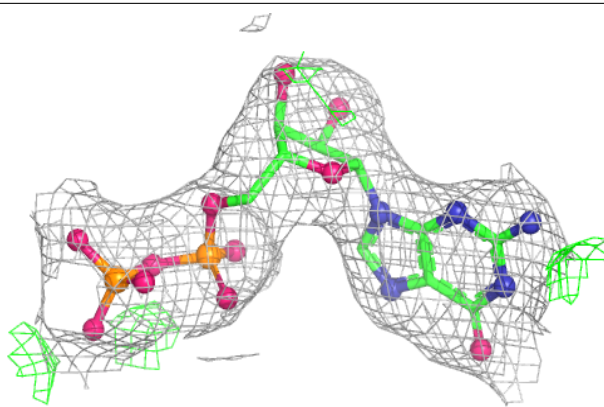
**Electron density around GDP B 900:**

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

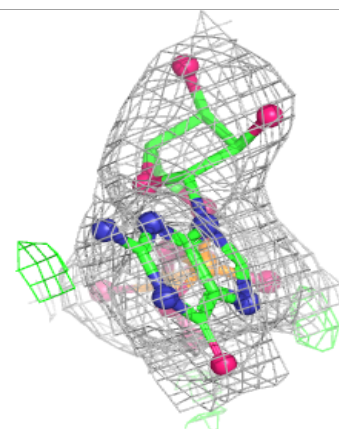
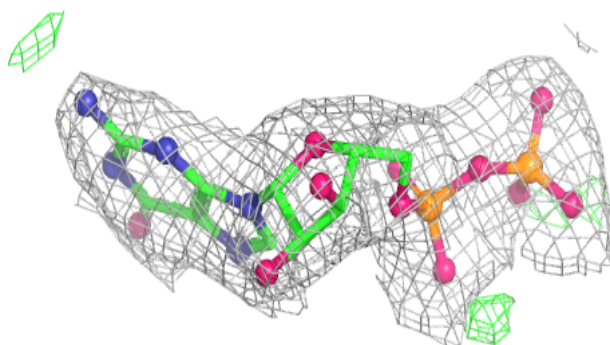
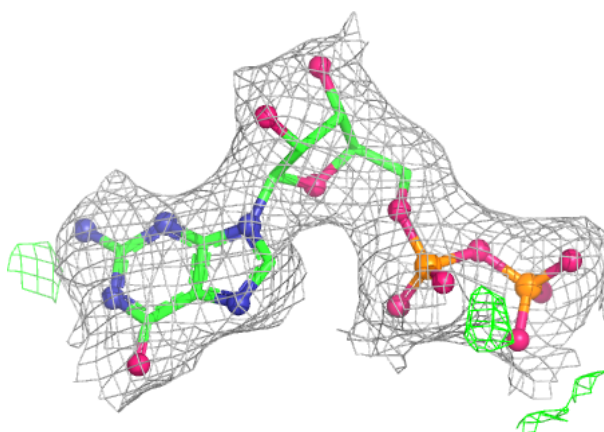


Electron density around GDP A 900:

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

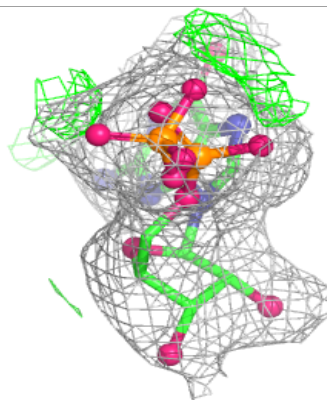
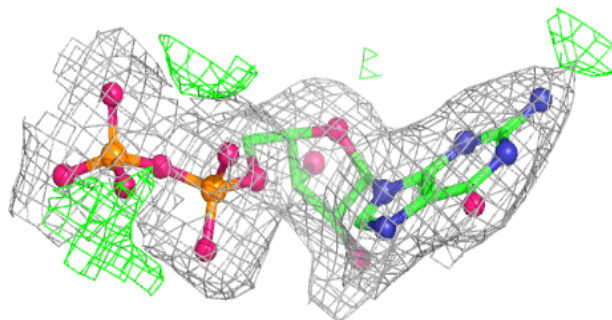
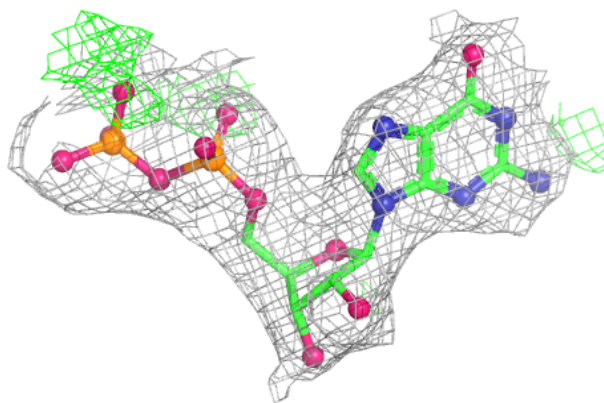
**Electron density around GDP G 900:**

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



Electron density around GDP I 900:

$2mF_o-DF_c$ (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.