



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:25 PM UTC

PDB ID : 3FI0 / pdb_00003fi0
Title : Crystal Structure Analysis of B. stearothermophilus Tryptophanyl-tRNA Synthetase Complexed with Tryptophan, AMP, and Inorganic Phosphate
Authors : Laowanapiban, P.; Kapustina, M.; Vonnrhein, C.; Delarue, M.; Koehl, P.; Carter Jr., C.W.
Deposited on : 2008-12-10
Resolution : 2.70 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:

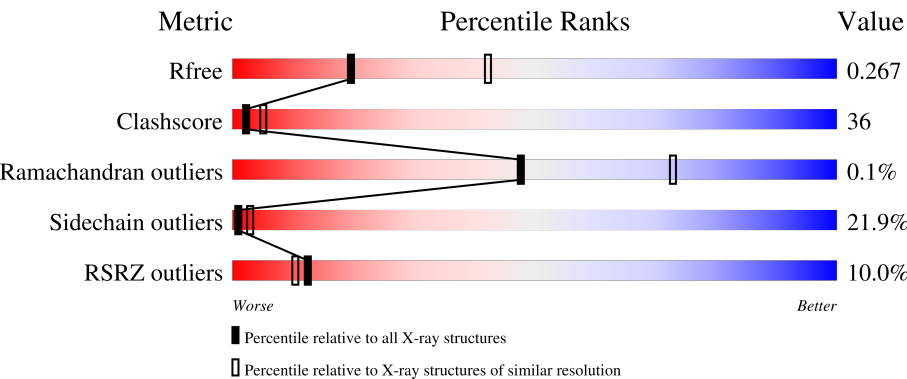
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	2% 46%35%10%9%
1	B	326	7% 36%42%13%10%
1	C	326	4% 44%39%9%9%
1	D	326	2% 49%34%9%8%

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Mol	Chain	Length	Quality of chain
1	E	326	
1	F	326	
1	G	326	
1	H	326	
1	I	326	
1	J	326	
1	K	326	
1	L	326	
1	M	326	
1	N	326	
1	O	326	
1	P	326	
1	Q	326	
1	R	326	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	E	1002	-	-	X	-
3	PO4	F	1002	-	-	X	-
3	PO4	H	1002	-	-	X	-
3	PO4	M	1002	-	-	X	-
3	PO4	N	1002	-	-	X	-
3	PO4	O	1002	-	-	X	-
3	PO4	P	1002	-	-	X	-
4	AMP	A	1003	-	-	X	-
4	AMP	E	1003	-	-	-	X
4	AMP	G	1003	-	-	X	-
4	AMP	H	1003	-	-	-	X
4	AMP	K	1003	-	-	-	X
4	AMP	O	1003	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AMP	P	1003	-	-	X	X
4	AMP	R	1003	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43727 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	Se	0	0	0
			2383	1512	410	448	3	10			
1	B	295	Total	C	N	O	S	Se	0	0	0
			2370	1505	408	444	3	10			
1	C	297	Total	C	N	O	S	Se	0	0	0
			2383	1512	410	448	3	10			
1	D	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	E	293	Total	C	N	O	S	Se	0	0	0
			2342	1484	405	440	3	10			
1	F	296	Total	C	N	O	S	Se	0	0	0
			2368	1502	410	443	3	10			
1	G	302	Total	C	N	O	S	Se	0	0	0
			2416	1534	416	453	3	10			
1	H	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	I	298	Total	C	N	O	S	Se	0	0	0
			2377	1507	409	448	3	10			
1	J	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	K	296	Total	C	N	O	S	Se	0	0	0
			2367	1504	408	442	3	10			
1	L	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	M	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	N	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	O	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	P	295	Total	C	N	O	S	Se	0	0	0
			2361	1499	407	442	3	10			

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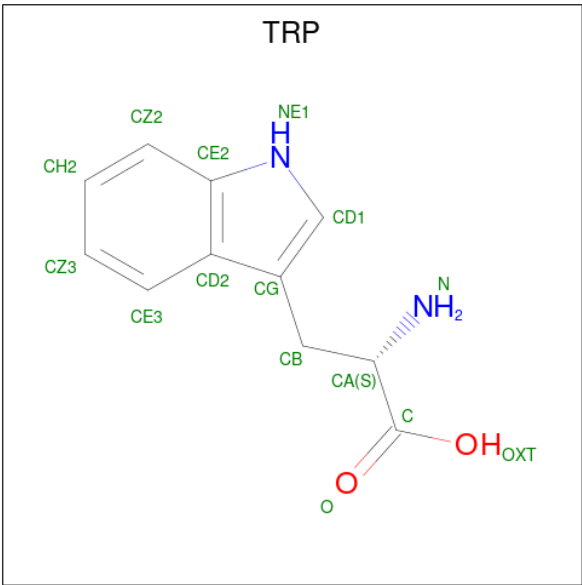
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	R	290	Total	C	N	O	S	Se	0	0	0
			2322	1473	399	437	3	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	LYS	conflict	UNP P00953
D	64	LEU	LYS	conflict	UNP P00953
B	64	LEU	LYS	conflict	UNP P00953
C	64	LEU	LYS	conflict	UNP P00953
E	64	LEU	LYS	conflict	UNP P00953
F	64	LEU	LYS	conflict	UNP P00953
G	64	LEU	LYS	conflict	UNP P00953
H	64	LEU	LYS	conflict	UNP P00953
I	64	LEU	LYS	conflict	UNP P00953
J	64	LEU	LYS	conflict	UNP P00953
K	64	LEU	LYS	conflict	UNP P00953
L	64	LEU	LYS	conflict	UNP P00953
M	64	LEU	LYS	conflict	UNP P00953
N	64	LEU	LYS	conflict	UNP P00953
O	64	LEU	LYS	conflict	UNP P00953
P	64	LEU	LYS	conflict	UNP P00953
Q	64	LEU	LYS	conflict	UNP P00953
R	64	LEU	LYS	conflict	UNP P00953

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



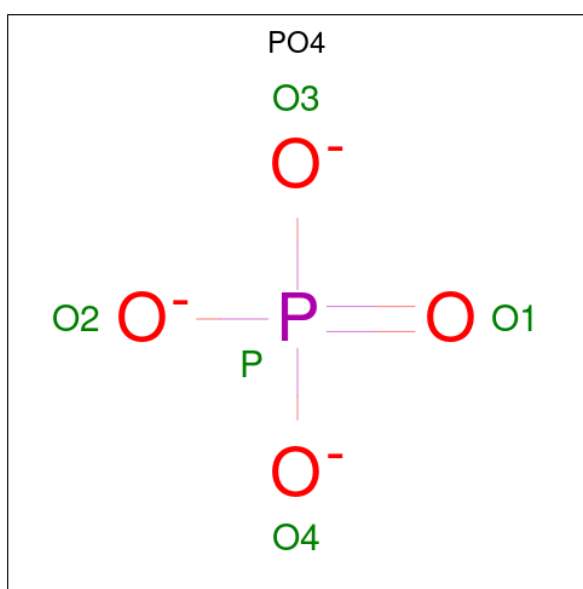
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	F	1	Total	C	N	O	0	0
			15	11	2	2		
2	G	1	Total	C	N	O	0	0
			15	11	2	2		
2	H	1	Total	C	N	O	0	0
			15	11	2	2		
2	I	1	Total	C	N	O	0	0
			15	11	2	2		
2	J	1	Total	C	N	O	0	0
			15	11	2	2		
2	K	1	Total	C	N	O	0	0
			15	11	2	2		
2	L	1	Total	C	N	O	0	0
			15	11	2	2		
2	M	1	Total	C	N	O	0	0
			15	11	2	2		
2	N	1	Total	C	N	O	0	0
			15	11	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	N	O	0	0
			15	11	2	2		
2	P	1	Total	C	N	O	0	0
			15	11	2	2		
2	Q	1	Total	C	N	O	0	0
			15	11	2	2		
2	R	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



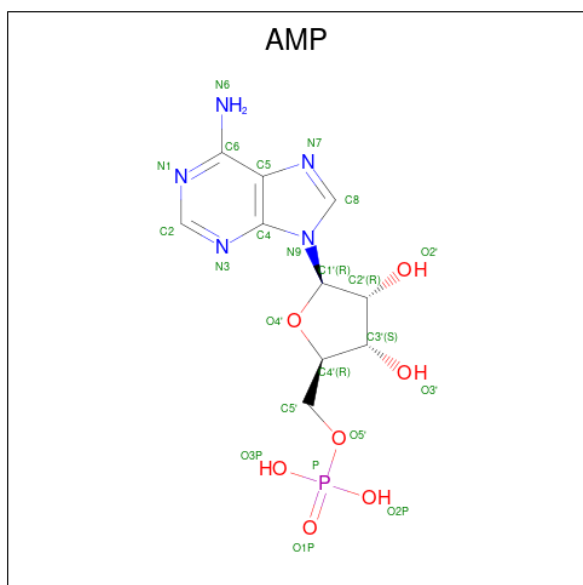
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		
3	N	1	Total	O	P	0	0
			5	4	1		
3	O	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	R	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).

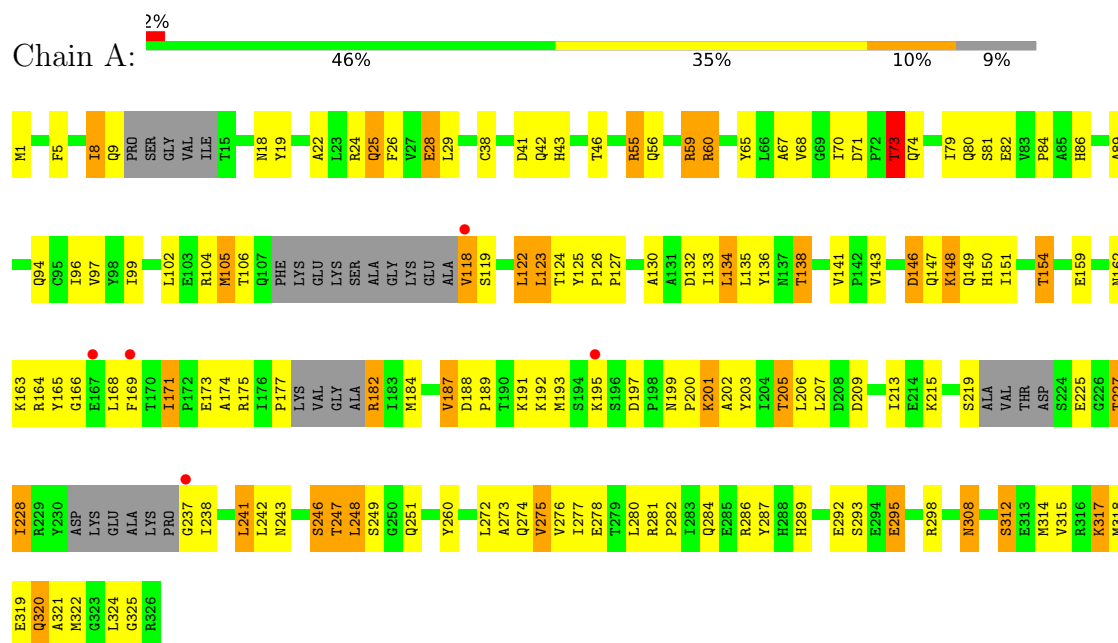


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	D	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	E	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	F	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	G	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	H	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	I	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	J	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	K	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	L	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	M	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	N	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	O	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	P	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	R	1	Total 23	C 10	N 5	O 7	P 1	0	0

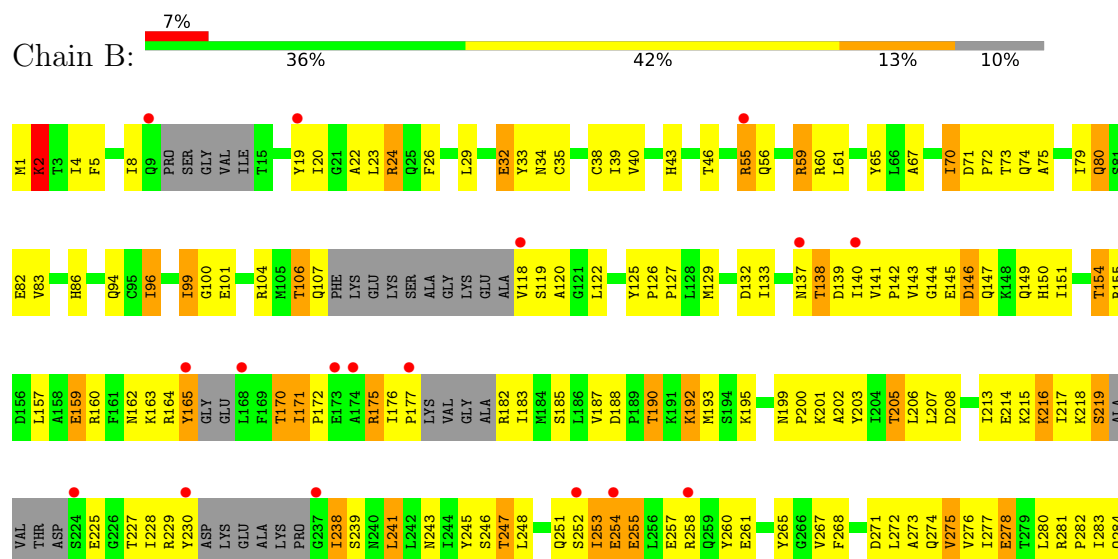
3 Residue-property plots

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: Tryptophanyl-tRNA synthetase

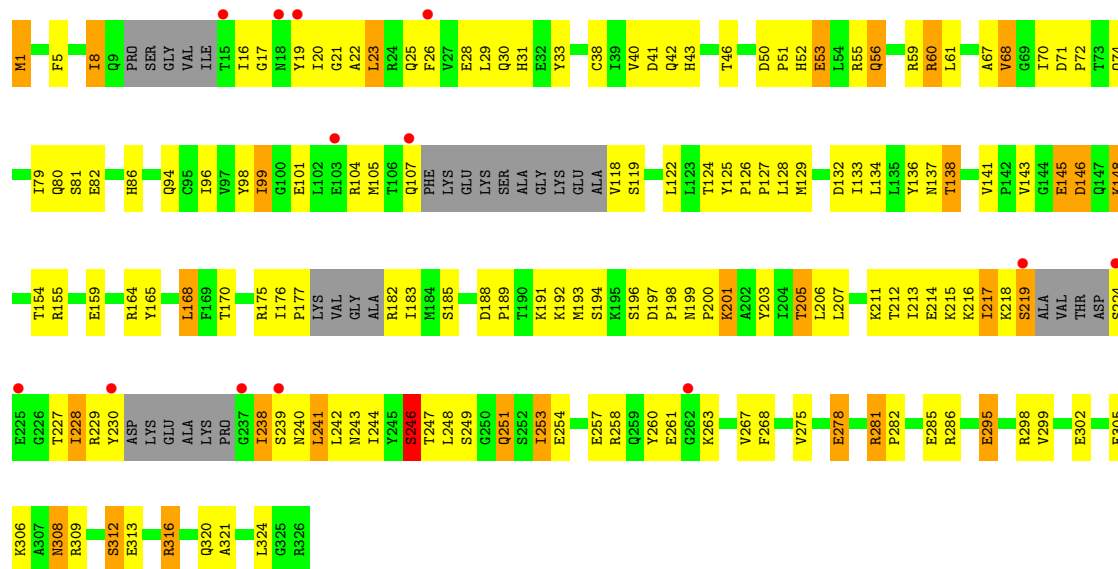
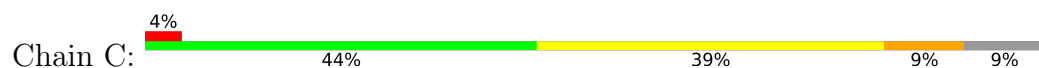


• Molecule 1: Tryptophanyl-tRNA synthetase

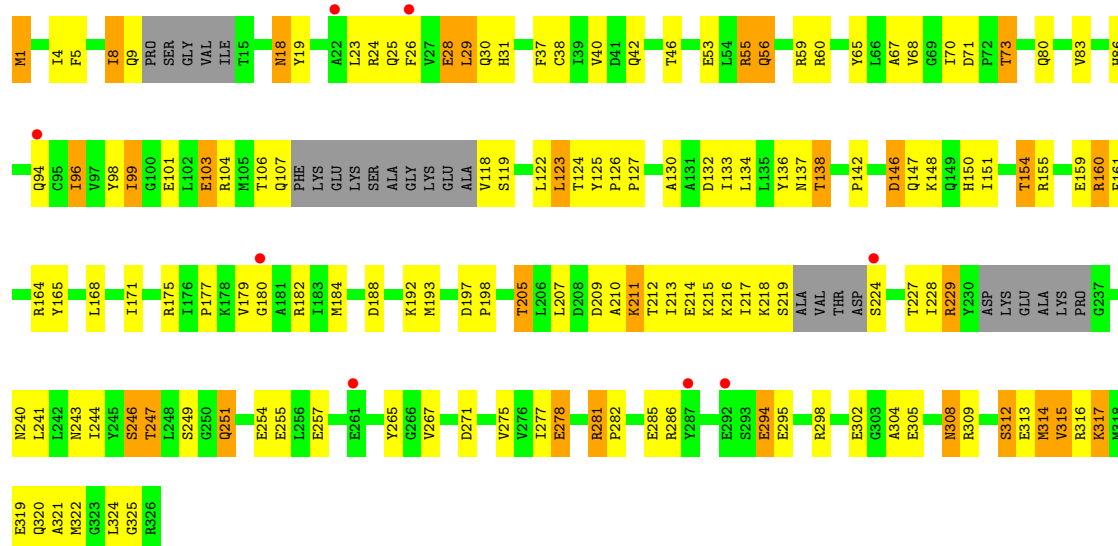




• Molecule 1: Tryptophanyl-tRNA synthetase

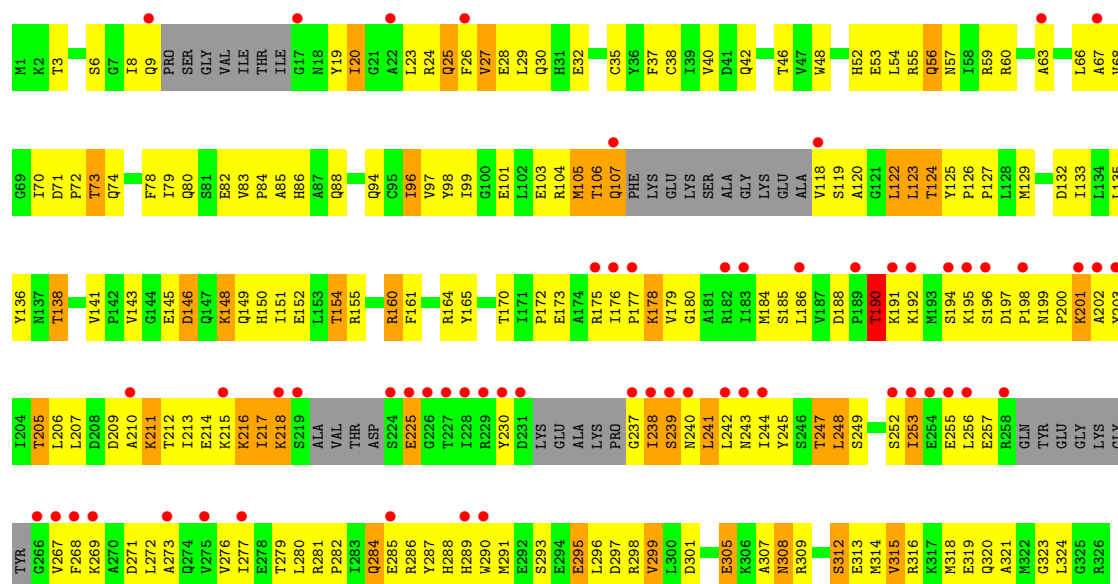


• Molecule 1: Tryptophanyl-tRNA synthetase

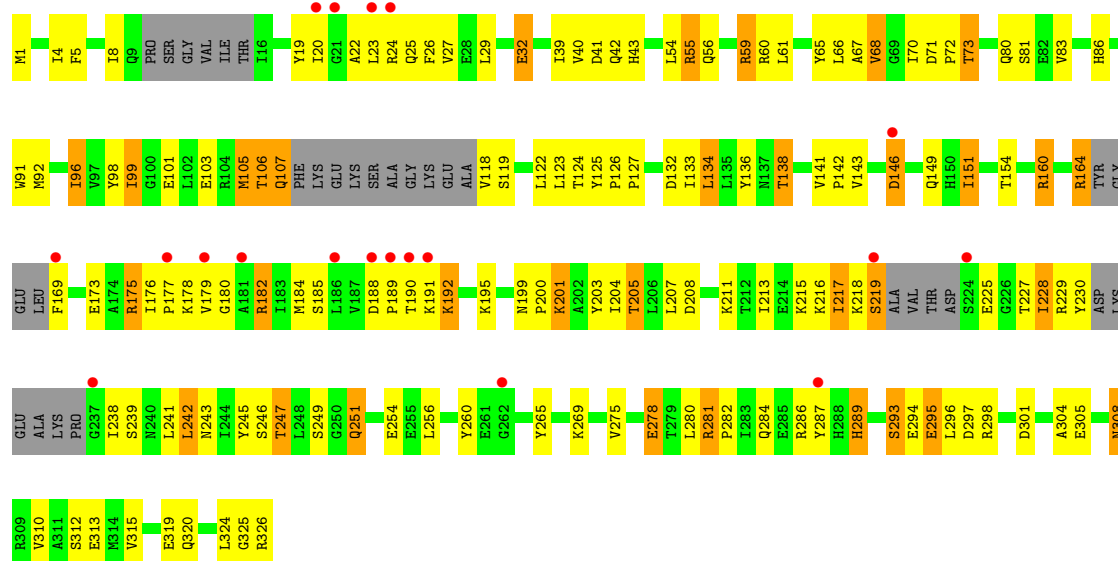
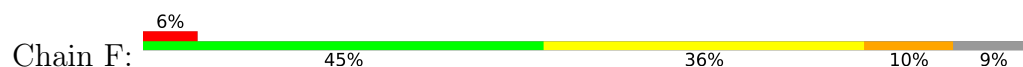


• Molecule 1: Tryptophanyl-tRNA synthetase

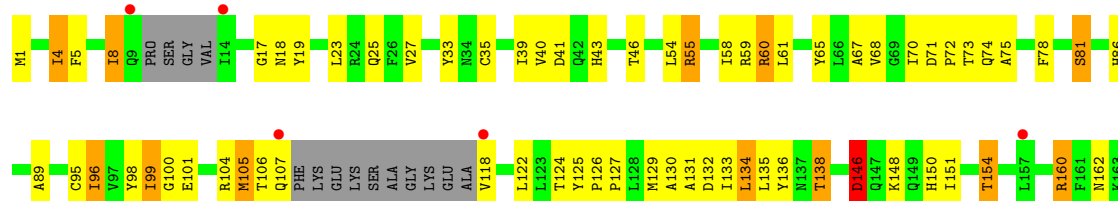


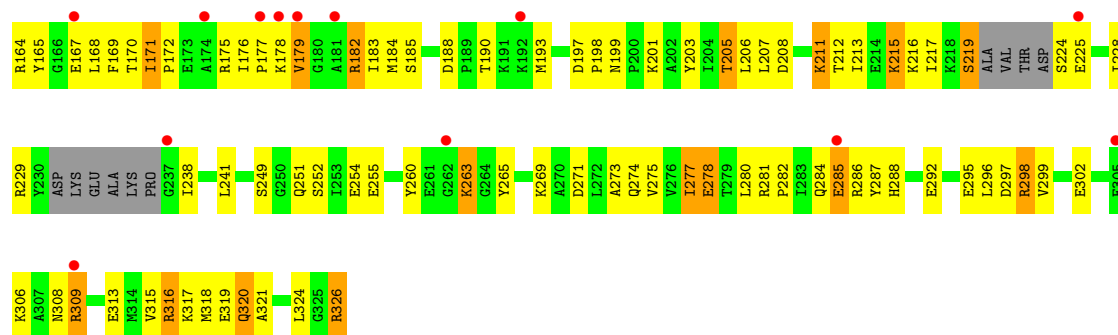


• Molecule 1: Tryptophanyl-tRNA synthetase

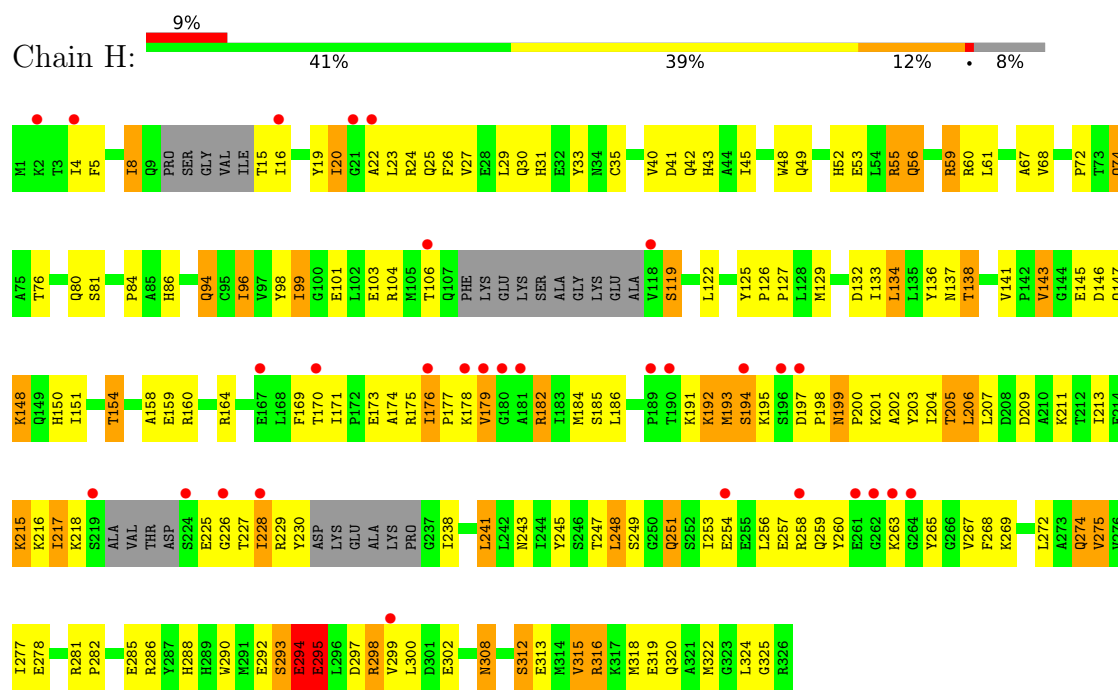


• Molecule 1: Tryptophanyl-tRNA synthetase

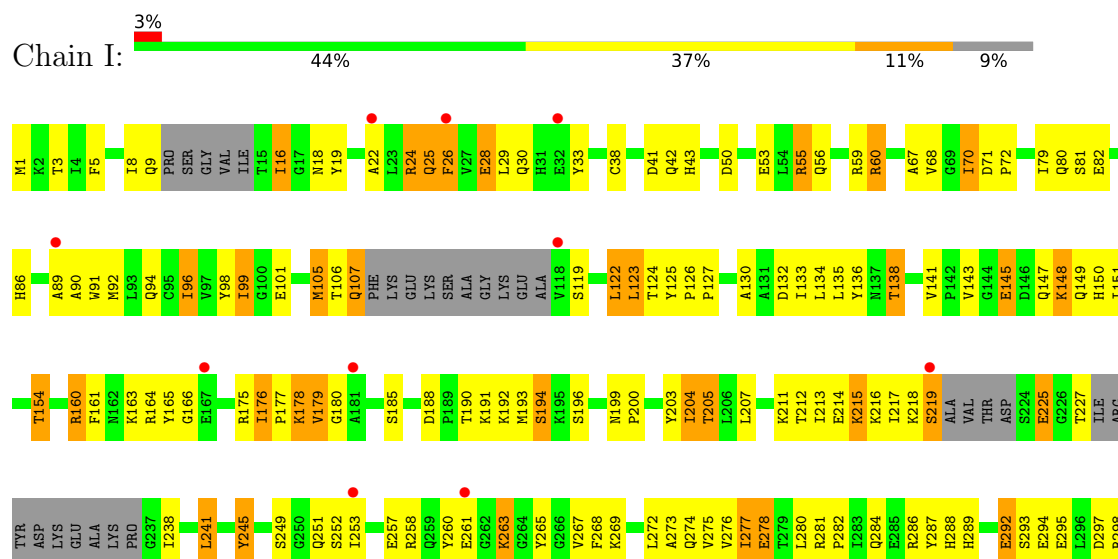




• Molecule 1: Tryptophanyl-tRNA synthetase

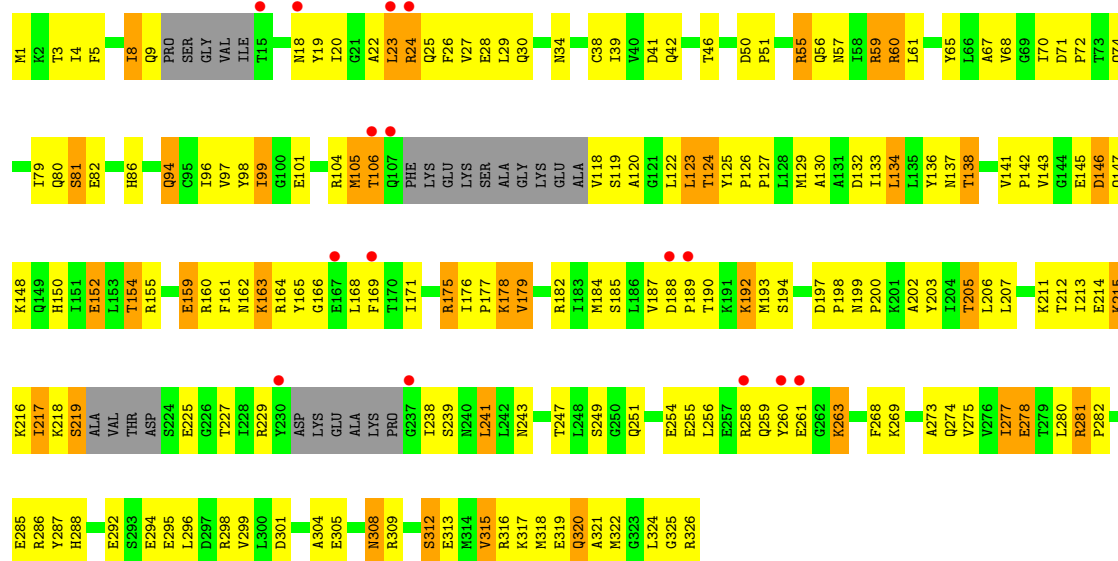


• Molecule 1: Tryptophanyl-tRNA synthetase

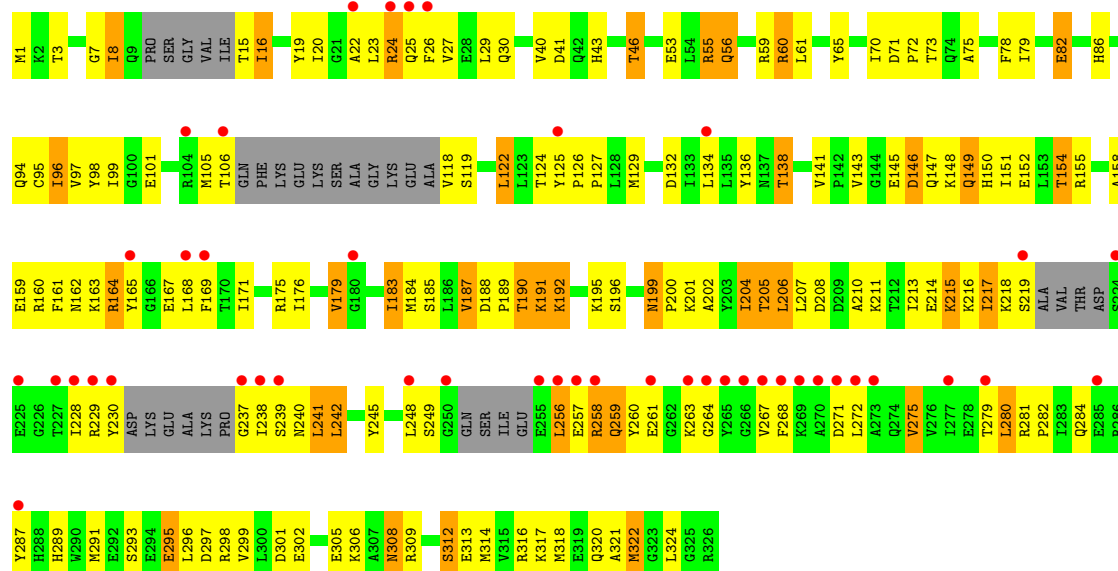




• Molecule 1: Tryptophanyl-tRNA synthetase

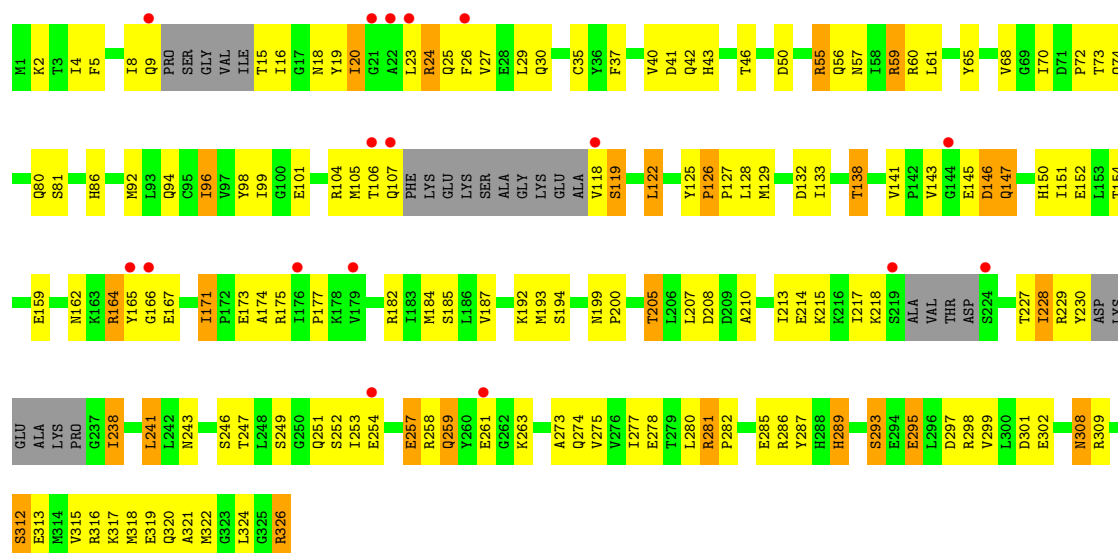


• Molecule 1: Tryptophanyl-tRNA synthetase

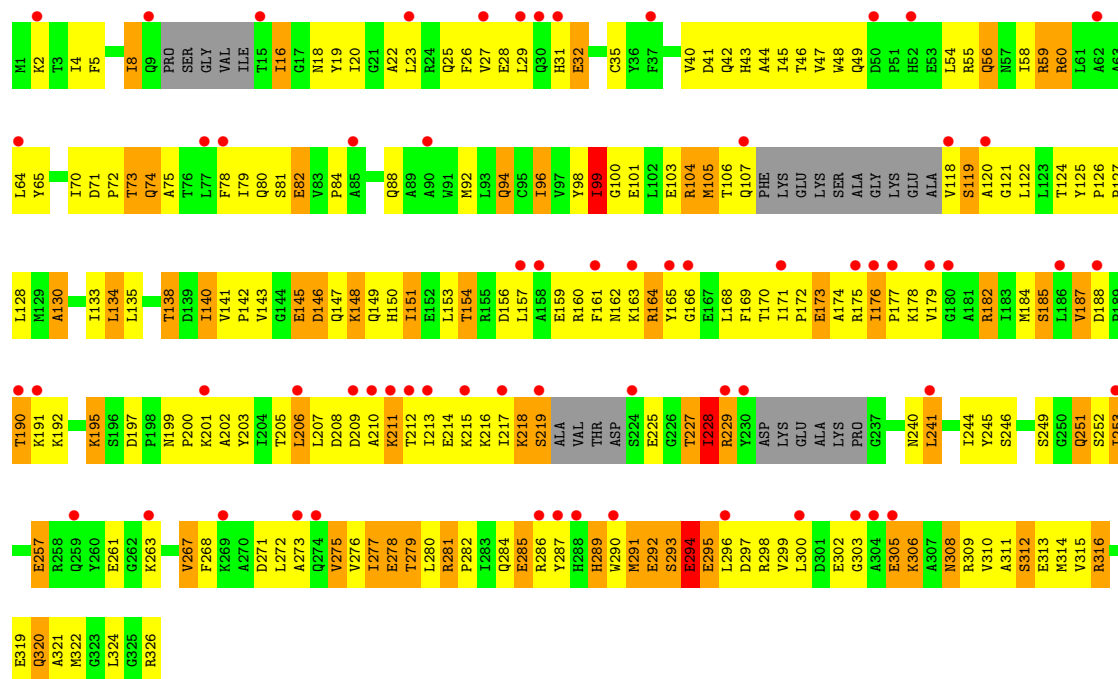


• Molecule 1: Tryptophanyl-tRNA synthetase

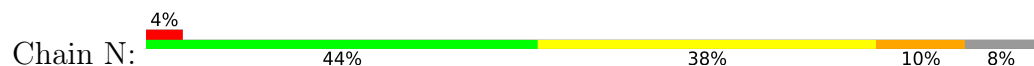


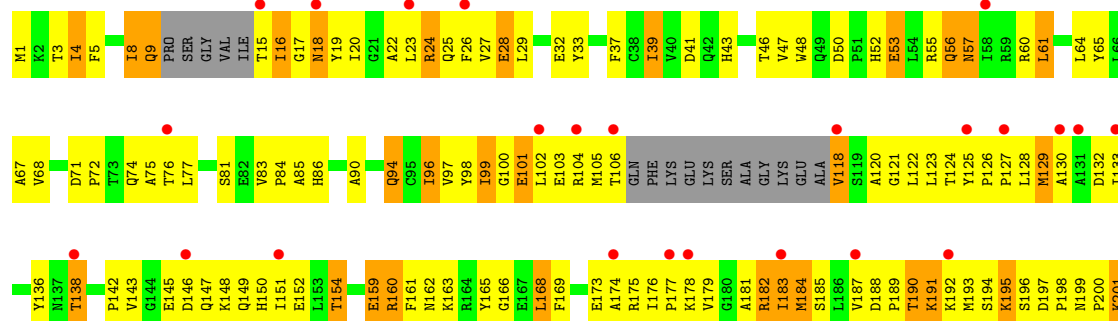


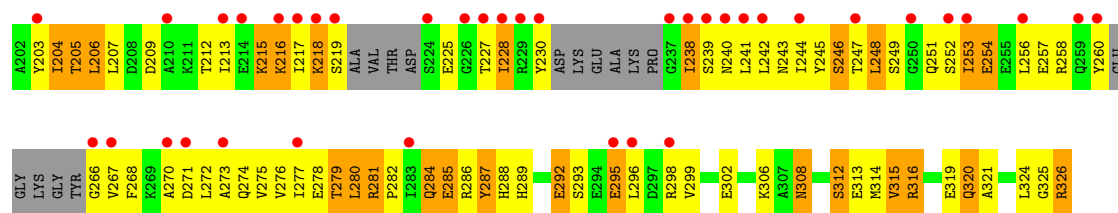
• Molecule 1: Tryptophanyl-tRNA synthetase



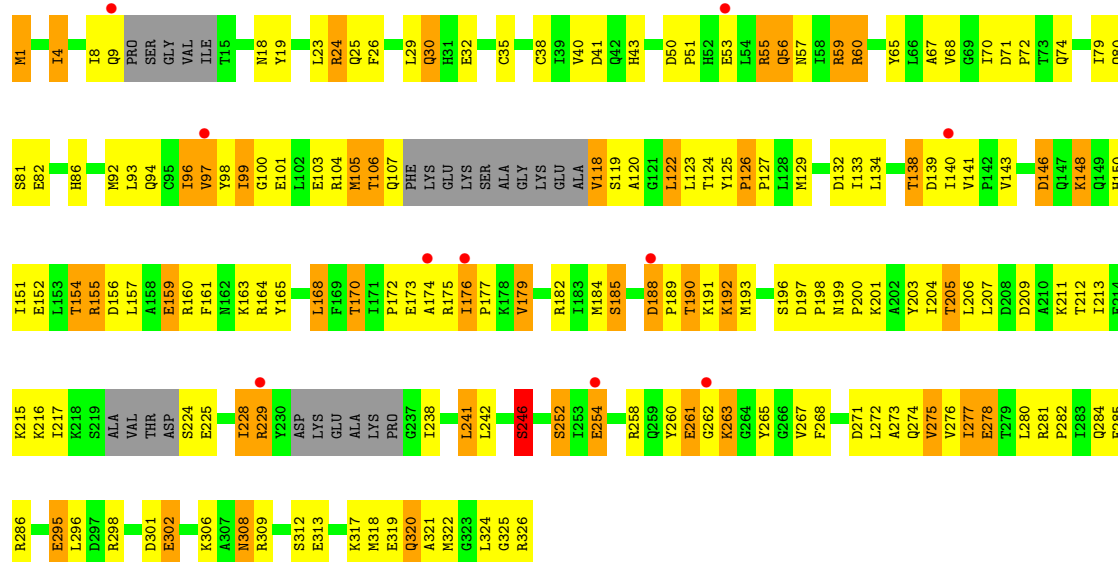
• Molecule 1: Tryptophanyl-tRNA synthetase



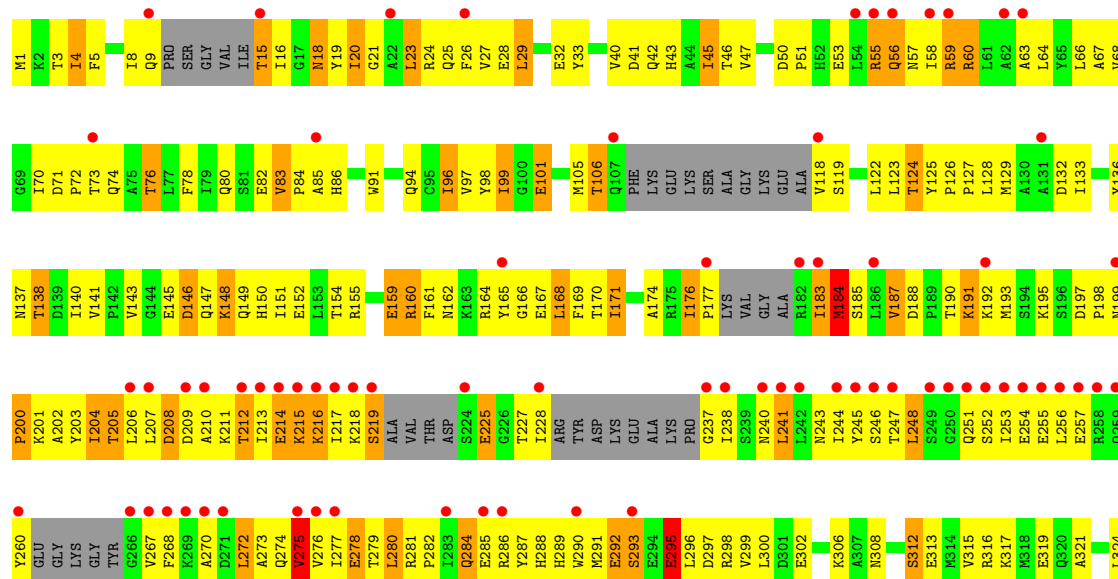




● Molecule 1: Tryptophanyl-tRNA synthetase



● Molecule 1: Tryptophanyl-tRNA synthetase



C325
R326

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.03Å 122.40Å 122.34Å 79.90° 80.52° 79.81°	Depositor
Resolution (Å)	25.00 – 2.70 25.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (25.00-2.70) 98.8 (25.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.72Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0019	Depositor
R, R_{free}	0.190 , 0.220 0.254 , 0.267	Depositor DCC
R_{free} test set	9262 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for l,h,k 0.048 for k,l,h 0.000 for -l,-k,-h 0.000 for -k,-h,-l 0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	43727	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.9719e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, AMP

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	0.46	0/2414	0.89	6/3242 (0.2%)
1	B	0.37	0/2400	0.87	4/3222 (0.1%)
1	C	0.40	0/2414	0.92	5/3242 (0.2%)
1	D	0.40	0/2440	0.90	7/3278 (0.2%)
1	E	0.37	0/2371	0.91	8/3184 (0.3%)
1	F	0.36	0/2398	0.87	1/3219 (0.0%)
1	G	0.37	0/2448	0.91	5/3289 (0.2%)
1	H	0.37	0/2440	0.90	7/3278 (0.2%)
1	I	0.39	0/2408	0.91	6/3235 (0.2%)
1	J	0.38	0/2440	0.88	2/3278 (0.1%)
1	K	0.35	0/2398	0.88	6/3220 (0.2%)
1	L	0.39	0/2440	0.93	7/3278 (0.2%)
1	M	0.36	0/2440	0.91	11/3278 (0.3%)
1	N	0.38	0/2440	0.91	9/3278 (0.3%)
1	O	0.37	0/2440	0.94	9/3278 (0.3%)
1	P	0.33	0/2391	0.95	12/3212 (0.4%)
1	Q	0.39	0/2440	0.96	9/3278 (0.3%)
1	R	0.36	0/2350	0.90	11/3156 (0.3%)
All	All	0.38	0/43512	0.91	125/58445 (0.2%)

There are no bond length outliers.

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	225	GLU	N-CA-C	8.88	120.96	111.28
1	P	190	THR	N-CA-C	-8.71	103.73	112.97
1	P	295	GLU	N-CA-C	-8.15	103.32	113.18
1	K	73	THR	N-CA-C	-7.84	102.82	111.36
1	I	294	GLU	N-CA-C	-7.56	104.08	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2383	0	2390	141	0
1	B	2370	0	2380	202	0
1	C	2383	0	2390	130	0
1	D	2408	0	2421	131	0
1	E	2342	0	2355	227	0
1	F	2368	0	2384	140	0
1	G	2416	0	2432	141	0
1	H	2408	0	2421	160	0
1	I	2377	0	2388	142	0
1	J	2408	0	2421	146	0
1	K	2367	0	2382	210	0
1	L	2408	0	2421	123	0
1	M	2408	0	2421	269	0
1	N	2408	0	2421	146	0
1	O	2408	0	2421	202	0
1	P	2361	0	2378	365	0
1	Q	2408	0	2421	178	0
1	R	2322	0	2333	285	0
2	A	15	0	9	0	0
2	B	15	0	9	1	0
2	C	15	0	9	2	0
2	D	15	0	9	0	0
2	E	15	0	9	0	0
2	F	15	0	9	0	0
2	G	15	0	9	2	0
2	H	15	0	9	1	0
2	I	15	0	9	0	0
2	J	15	0	9	2	0
2	K	15	0	9	0	0
2	L	15	0	9	0	0
2	M	15	0	9	0	0
2	N	15	0	9	0	0
2	O	15	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	15	0	9	0	0
2	Q	15	0	9	1	0
2	R	15	0	9	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	3	0
3	F	5	0	0	2	0
3	G	5	0	0	1	0
3	H	5	0	0	2	0
3	I	5	0	0	1	0
3	J	5	0	0	1	0
3	K	5	0	0	1	0
3	L	5	0	0	0	0
3	M	5	0	0	3	0
3	N	5	0	0	2	0
3	O	5	0	0	2	0
3	P	5	0	0	7	0
3	Q	5	0	0	0	0
3	R	5	0	0	1	0
4	A	23	0	12	7	0
4	B	23	0	12	4	0
4	C	23	0	12	2	0
4	D	23	0	12	3	0
4	E	23	0	12	1	0
4	F	23	0	12	2	0
4	G	23	0	12	7	0
4	H	23	0	12	0	0
4	I	23	0	12	3	0
4	J	23	0	12	3	0
4	K	23	0	12	1	0
4	L	23	0	12	0	0
4	M	23	0	12	5	0
4	N	23	0	12	1	0
4	O	23	0	12	17	0
4	P	23	0	12	7	0
4	Q	23	0	12	2	0
4	R	23	0	12	3	0
All	All	43727	0	43558	3170	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 36.

The worst 5 of 3170 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:Q:140:ILE:CD1	1:Q:175:ARG:HG3	1.54	1.36
1:M:23:LEU:HD21	1:M:65:TYR:CE1	1.72	1.24
1:I:199:ASN:ND2	1:I:200:PRO:HD2	1.54	1.23
1:Q:140:ILE:HD11	1:Q:175:ARG:CG	1.69	1.22
1:B:94:GLN:NE2	1:E:124:THR:HG21	1.55	1.20

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/326 (87%)	273 (96%)	11 (4%)	1 (0%)	30	54
1	B	281/326 (86%)	266 (95%)	14 (5%)	1 (0%)	30	54
1	C	285/326 (87%)	273 (96%)	12 (4%)	0	100	100
1	D	291/326 (89%)	282 (97%)	9 (3%)	0	100	100
1	E	281/326 (86%)	252 (90%)	29 (10%)	0	100	100
1	F	284/326 (87%)	276 (97%)	8 (3%)	0	100	100
1	G	292/326 (90%)	272 (93%)	20 (7%)	0	100	100
1	H	291/326 (89%)	278 (96%)	12 (4%)	1 (0%)	36	60
1	I	288/326 (88%)	279 (97%)	9 (3%)	0	100	100
1	J	291/326 (89%)	277 (95%)	14 (5%)	0	100	100
1	K	284/326 (87%)	269 (95%)	15 (5%)	0	100	100
1	L	291/326 (89%)	283 (97%)	8 (3%)	0	100	100
1	M	291/326 (89%)	269 (92%)	19 (6%)	3 (1%)	12	32
1	N	291/326 (89%)	281 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	291/326 (89%)	277 (95%)	14 (5%)	0	100	100
1	P	283/326 (87%)	256 (90%)	27 (10%)	0	100	100
1	Q	291/326 (89%)	277 (95%)	14 (5%)	0	100	100
1	R	276/326 (85%)	260 (94%)	16 (6%)	0	100	100
All	All	5167/5868 (88%)	4900 (95%)	261 (5%)	6 (0%)	48	73

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	GLY
1	H	193	MSE
1	M	291	MSE
1	A	246	SER
1	M	105	MSE

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	257/268 (96%)	210 (82%)	47 (18%)	2	5
1	B	256/268 (96%)	194 (76%)	62 (24%)	1	2
1	C	257/268 (96%)	206 (80%)	51 (20%)	1	4
1	D	259/268 (97%)	205 (79%)	54 (21%)	1	3
1	E	253/268 (94%)	197 (78%)	56 (22%)	1	3
1	F	255/268 (95%)	197 (77%)	58 (23%)	1	3
1	G	260/268 (97%)	212 (82%)	48 (18%)	1	4
1	H	259/268 (97%)	206 (80%)	53 (20%)	1	3
1	I	256/268 (96%)	196 (77%)	60 (23%)	1	2
1	J	259/268 (97%)	198 (76%)	61 (24%)	1	2
1	K	254/268 (95%)	203 (80%)	51 (20%)	1	4
1	L	259/268 (97%)	212 (82%)	47 (18%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	259/268 (97%)	194 (75%)	65 (25%)	0	2
1	N	259/268 (97%)	210 (81%)	49 (19%)	1	4
1	O	259/268 (97%)	188 (73%)	71 (27%)	0	1
1	P	255/268 (95%)	194 (76%)	61 (24%)	1	2
1	Q	259/268 (97%)	196 (76%)	63 (24%)	1	2
1	R	252/268 (94%)	191 (76%)	61 (24%)	1	2
All	All	4627/4824 (96%)	3609 (78%)	1018 (22%)	1	3

5 of 1018 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	196	SER
1	P	296	LEU
1	K	187	VAL
1	P	252	SER
1	Q	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	31	HIS
1	M	94	GLN
1	R	42	GLN
1	K	56	GLN
1	L	94	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 ⓘ

54 ligands are modelled in this entry.

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
3	PO4	B	1002	-	4,4,4	2.04	1 (25%)	6,6,6	0.55	0
4	AMP	C	1003	-	25,25,25	0.67	0	37,38,38	0.74	0
2	TRP	N	1001	-	15,16,16	0.66	0	18,22,22	0.40	0
2	TRP	H	1001	-	15,16,16	0.72	0	18,22,22	0.41	0
4	AMP	Q	1003	-	25,25,25	0.66	0	37,38,38	0.74	0
2	TRP	C	1001	-	15,16,16	0.67	0	18,22,22	0.40	0
2	TRP	P	1001	-	15,16,16	0.76	0	18,22,22	0.43	0
3	PO4	F	1002	-	4,4,4	1.91	1 (25%)	6,6,6	0.49	0
4	AMP	L	1003	-	25,25,25	0.64	0	37,38,38	0.77	0
4	AMP	K	1003	-	25,25,25	0.63	0	37,38,38	0.80	0
3	PO4	C	1002	-	4,4,4	2.05	1 (25%)	6,6,6	0.49	0
4	AMP	O	1003	-	25,25,25	0.74	0	37,38,38	1.29	5 (13%)
3	PO4	I	1002	-	4,4,4	2.03	1 (25%)	6,6,6	0.39	0
2	TRP	F	1001	-	15,16,16	0.76	0	18,22,22	0.41	0
4	AMP	I	1003	-	25,25,25	0.63	1 (4%)	37,38,38	0.86	1 (2%)
4	AMP	R	1003	-	25,25,25	0.66	0	37,38,38	0.76	0
2	TRP	E	1001	-	15,16,16	0.69	0	18,22,22	0.40	0
3	PO4	J	1002	-	4,4,4	2.15	1 (25%)	6,6,6	0.77	0
3	PO4	Q	1002	-	4,4,4	2.01	1 (25%)	6,6,6	0.42	0
4	AMP	B	1003	-	25,25,25	0.68	0	37,38,38	0.69	0
3	PO4	R	1002	-	4,4,4	1.84	1 (25%)	6,6,6	0.44	0
4	AMP	N	1003	-	25,25,25	0.83	1 (4%)	37,38,38	1.06	2 (5%)
2	TRP	G	1001	-	15,16,16	0.66	0	18,22,22	0.39	0
2	TRP	Q	1001	-	15,16,16	0.66	0	18,22,22	0.39	0
3	PO4	N	1002	-	4,4,4	2.02	1 (25%)	6,6,6	0.50	0
2	TRP	M	1001	-	15,16,16	0.67	0	18,22,22	0.40	0
2	TRP	K	1001	-	15,16,16	0.68	0	18,22,22	0.38	0
3	PO4	H	1002	-	4,4,4	2.07	1 (25%)	6,6,6	0.49	0
4	AMP	P	1003	-	25,25,25	0.62	0	37,38,38	1.23	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	M	1002	-	4,4,4	1.80	1 (25%)	6,6,6	0.85	0
2	TRP	B	1001	-	15,16,16	0.75	0	18,22,22	0.41	0
2	TRP	A	1001	-	15,16,16	0.68	0	18,22,22	0.39	0
4	AMP	A	1003	-	25,25,25	0.88	1 (4%)	37,38,38	1.17	6 (16%)
4	AMP	H	1003	-	25,25,25	0.78	0	37,38,38	1.47	6 (16%)
4	AMP	J	1003	-	25,25,25	0.57	0	37,38,38	0.75	0
2	TRP	D	1001	-	15,16,16	0.78	0	18,22,22	0.44	0
3	PO4	G	1002	-	4,4,4	2.02	1 (25%)	6,6,6	0.49	0
4	AMP	E	1003	-	25,25,25	0.68	0	37,38,38	0.83	1 (2%)
3	PO4	L	1002	-	4,4,4	2.06	1 (25%)	6,6,6	0.66	0
2	TRP	L	1001	-	15,16,16	0.66	0	18,22,22	0.41	0
4	AMP	G	1003	-	25,25,25	0.69	1 (4%)	37,38,38	0.69	0
4	AMP	M	1003	-	25,25,25	1.34	4 (16%)	37,38,38	2.22	17 (45%)
2	TRP	I	1001	-	15,16,16	0.66	0	18,22,22	0.39	0
2	TRP	O	1001	-	15,16,16	0.65	0	18,22,22	0.41	0
3	PO4	A	1002	-	4,4,4	2.01	1 (25%)	6,6,6	0.62	0
3	PO4	E	1002	-	4,4,4	2.20	1 (25%)	6,6,6	0.57	0
3	PO4	K	1002	-	4,4,4	1.93	1 (25%)	6,6,6	0.52	0
4	AMP	D	1003	-	25,25,25	0.65	0	37,38,38	0.66	0
3	PO4	O	1002	-	4,4,4	2.02	1 (25%)	6,6,6	0.49	0
3	PO4	D	1002	-	4,4,4	1.92	1 (25%)	6,6,6	0.43	0
4	AMP	F	1003	-	25,25,25	0.69	0	37,38,38	0.79	1 (2%)
2	TRP	J	1001	-	15,16,16	0.67	0	18,22,22	0.41	0
2	TRP	R	1001	-	15,16,16	0.67	0	18,22,22	0.40	0
3	PO4	P	1002	-	4,4,4	1.88	1 (25%)	6,6,6	0.95	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
4	AMP	C	1003	-	-	4/10/26/26	0/3/3/3
2	TRP	N	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	H	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	Q	1003	-	-	3/10/26/26	0/3/3/3
2	TRP	C	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	P	1001	-	-	2/8/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AMP	L	1003	-	-	6/10/26/26	0/3/3/3
4	AMP	K	1003	-	-	3/10/26/26	0/3/3/3
4	AMP	O	1003	-	-	2/10/26/26	0/3/3/3
2	TRP	F	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	I	1003	-	-	4/10/26/26	0/3/3/3
4	AMP	R	1003	-	-	2/10/26/26	0/3/3/3
2	TRP	E	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	B	1003	-	-	5/10/26/26	0/3/3/3
4	AMP	N	1003	-	-	3/10/26/26	0/3/3/3
2	TRP	G	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	Q	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	M	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	K	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	P	1003	-	-	6/10/26/26	0/3/3/3
2	TRP	B	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	A	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	A	1003	-	-	6/10/26/26	0/3/3/3
4	AMP	H	1003	-	-	6/10/26/26	0/3/3/3
4	AMP	J	1003	-	-	5/10/26/26	0/3/3/3
2	TRP	D	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	E	1003	-	-	1/10/26/26	0/3/3/3
2	TRP	L	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	G	1003	-	-	4/10/26/26	0/3/3/3
4	AMP	M	1003	-	-	4/10/26/26	0/3/3/3
2	TRP	I	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	O	1001	-	-	2/8/8/8	0/2/2/2
4	AMP	D	1003	-	-	6/10/26/26	0/3/3/3
4	AMP	F	1003	-	-	5/10/26/26	0/3/3/3
2	TRP	J	1001	-	-	2/8/8/8	0/2/2/2
2	TRP	R	1001	-	-	2/8/8/8	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1003	AMP	C5-C4	3.72	1.45	1.39
3	E	1002	PO4	P-O1	3.58	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1002	PO4	P-O1	3.56	1.58	1.50
3	L	1002	PO4	P-O1	3.43	1.58	1.50
3	H	1002	PO4	P-O1	3.43	1.58	1.50

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1003	AMP	C4'-O4'-C1'	-4.66	99.17	109.47
4	M	1003	AMP	C5-C4-N3	-4.62	120.35	126.72
4	M	1003	AMP	C4-N9-C8	4.40	110.36	105.74
4	M	1003	AMP	N3-C4-N9	4.39	134.63	127.17
4	P	1003	AMP	O3P-P-O5'	4.31	117.91	106.67

There are no chirality outliers.

5 of 111 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	AMP	C5'-O5'-P-O1P
4	A	1003	AMP	C5'-O5'-P-O2P
4	A	1003	AMP	C5'-O5'-P-O3P
4	B	1003	AMP	C5'-O5'-P-O1P
4	B	1003	AMP	C5'-O5'-P-O2P

There are no ring outliers.

36 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	PO4	1	0
4	C	1003	AMP	2	0
2	H	1001	TRP	1	0
4	Q	1003	AMP	2	0
2	C	1001	TRP	2	0
3	F	1002	PO4	2	0
4	K	1003	AMP	1	0
4	O	1003	AMP	17	0
3	I	1002	PO4	1	0
4	I	1003	AMP	3	0
4	R	1003	AMP	3	0
3	J	1002	PO4	1	0
4	B	1003	AMP	4	0
3	R	1002	PO4	1	0

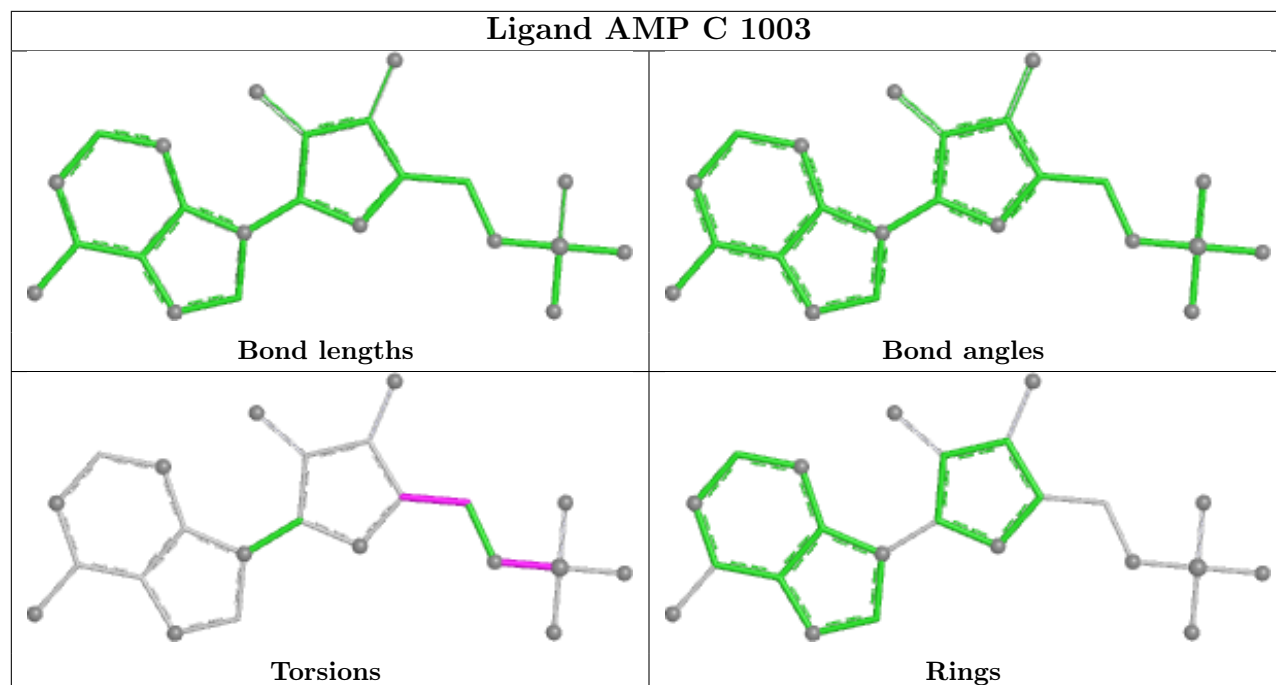
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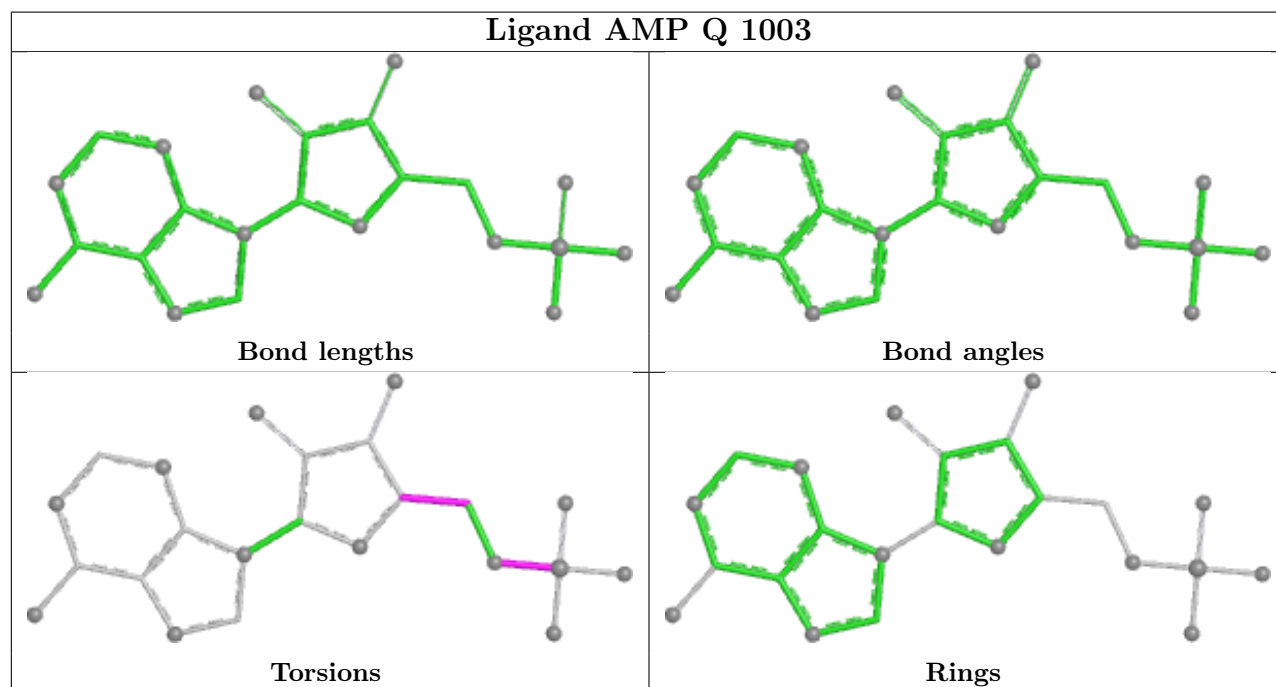
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1003	AMP	1	0
2	G	1001	TRP	2	0
2	Q	1001	TRP	1	0
3	N	1002	PO4	2	0
3	H	1002	PO4	2	0
4	P	1003	AMP	7	0
3	M	1002	PO4	3	0
2	B	1001	TRP	1	0
4	A	1003	AMP	7	0
4	J	1003	AMP	3	0
3	G	1002	PO4	1	0
4	E	1003	AMP	1	0
4	G	1003	AMP	7	0
4	M	1003	AMP	5	0
3	A	1002	PO4	1	0
3	E	1002	PO4	3	0
3	K	1002	PO4	1	0
4	D	1003	AMP	3	0
3	O	1002	PO4	2	0
4	F	1003	AMP	2	0
2	J	1001	TRP	2	0
3	P	1002	PO4	7	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.

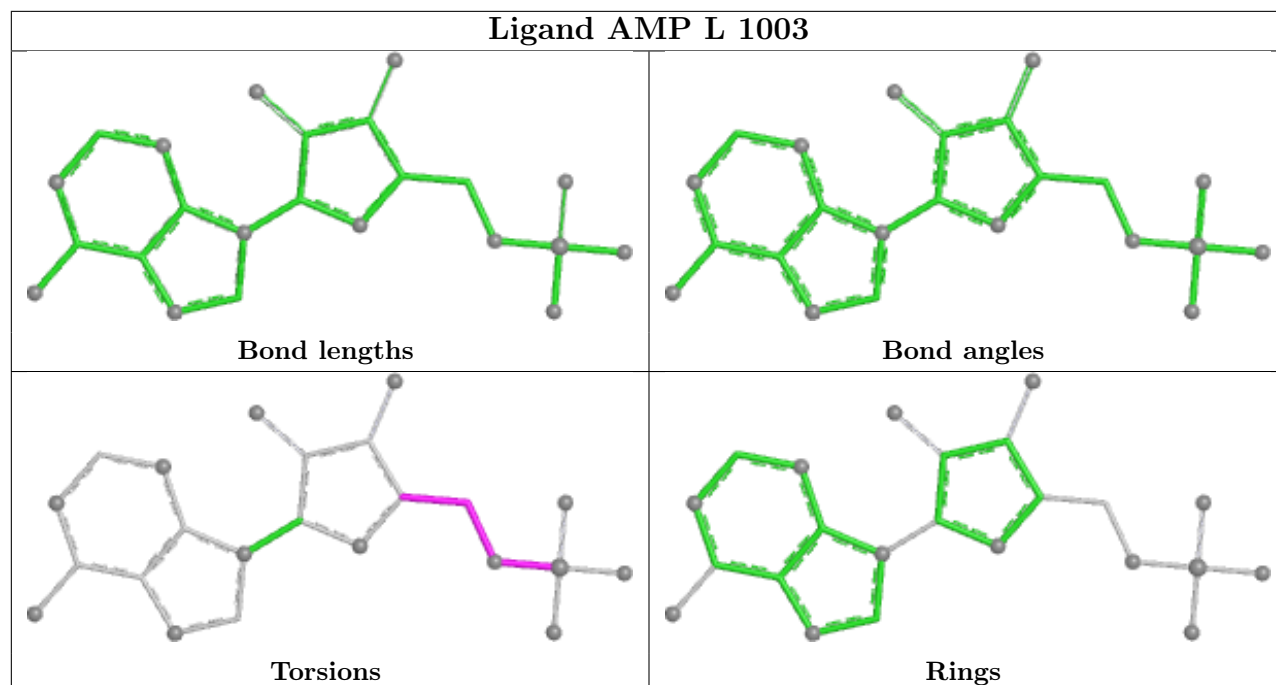
Ligand AMP C 1003



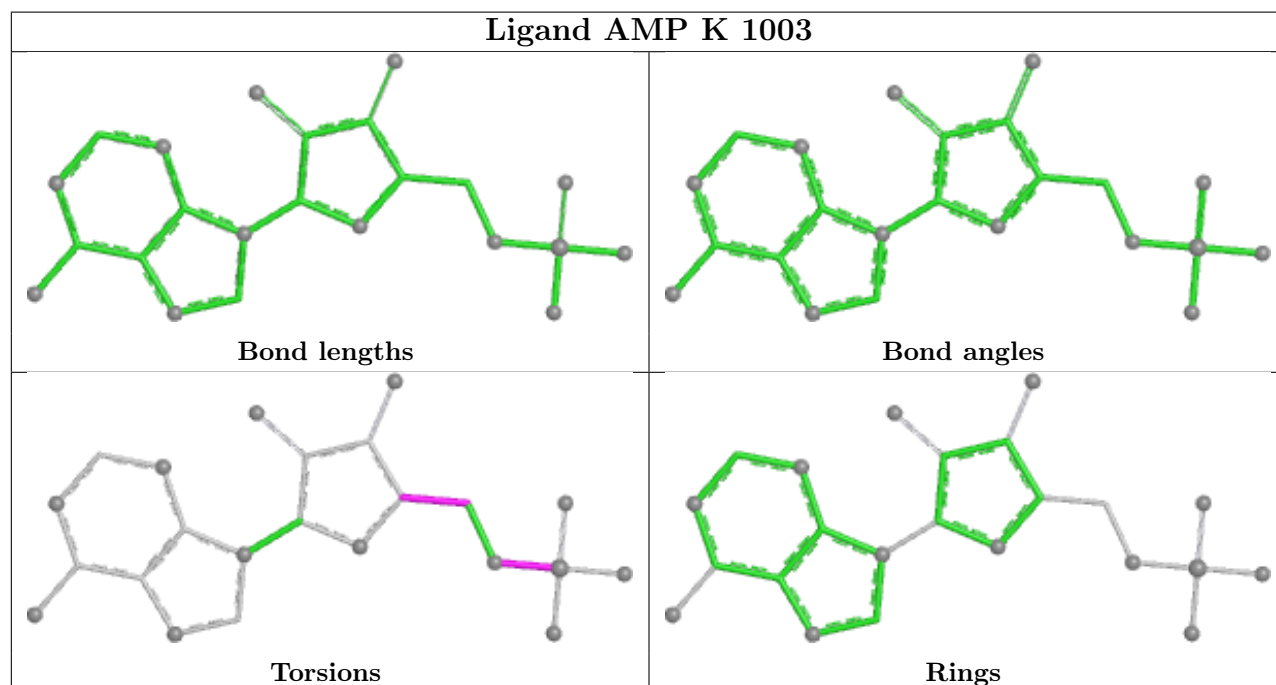
Ligand AMP Q 1003



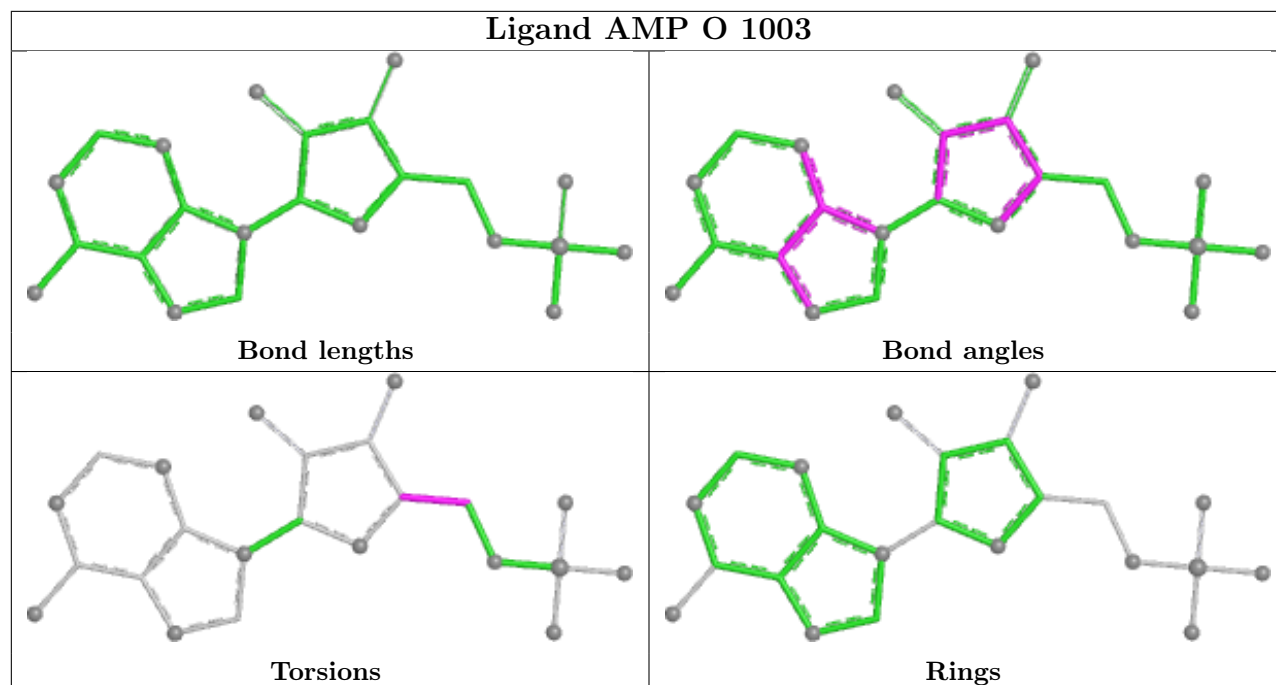
Ligand AMP L 1003



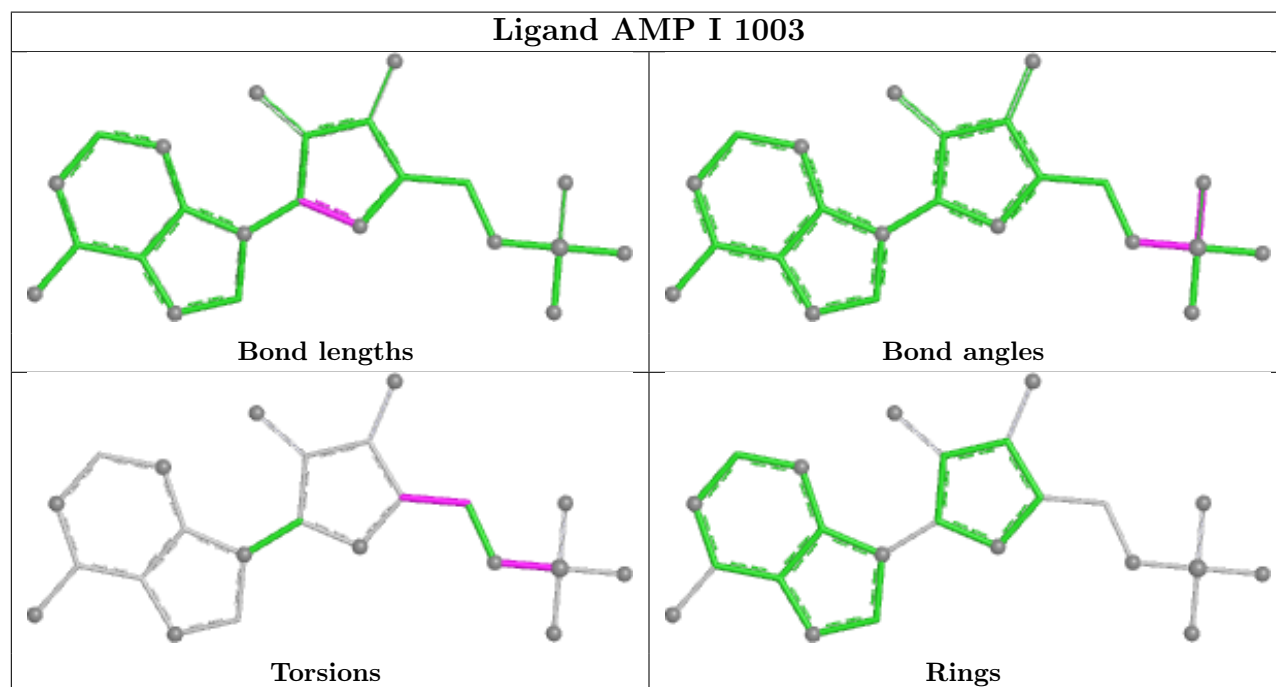
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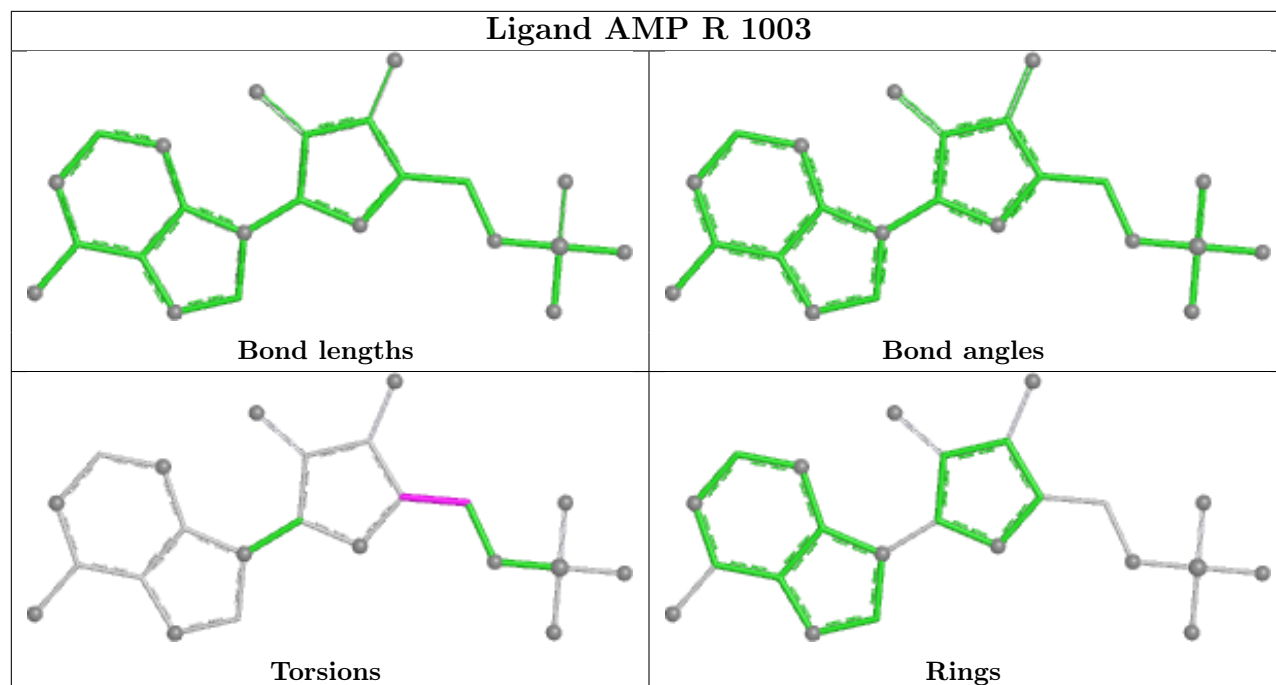
Ligand AMP O 1003



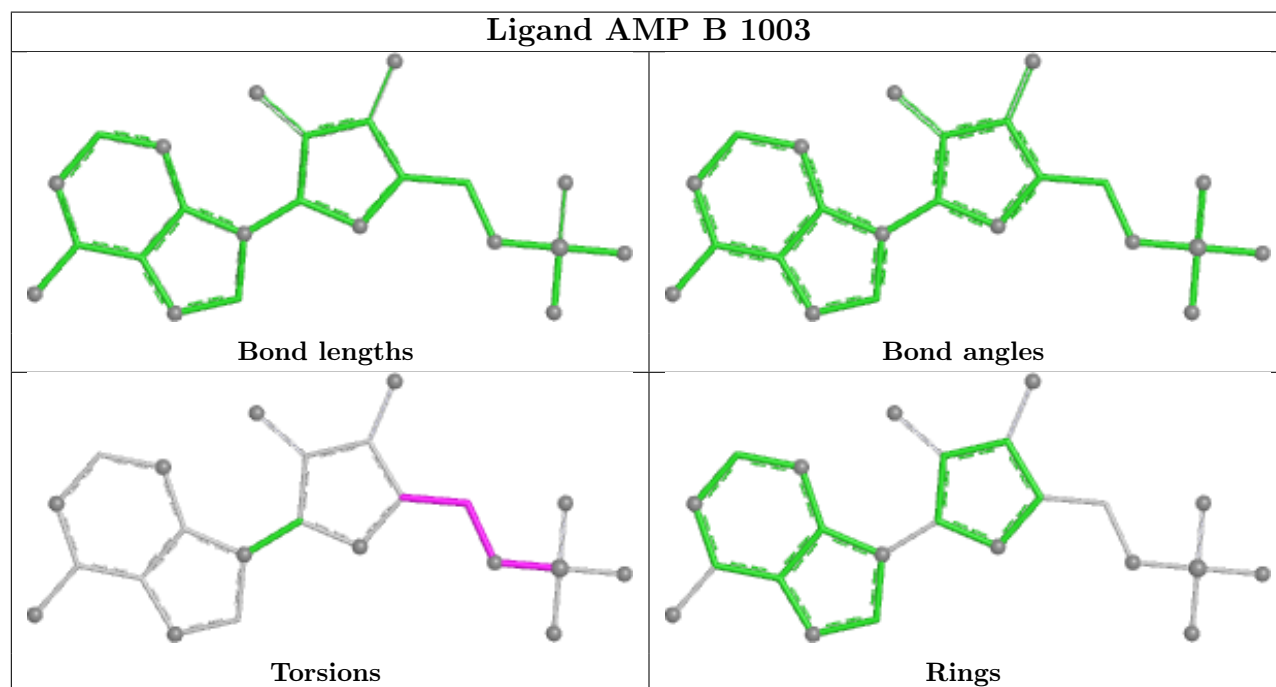
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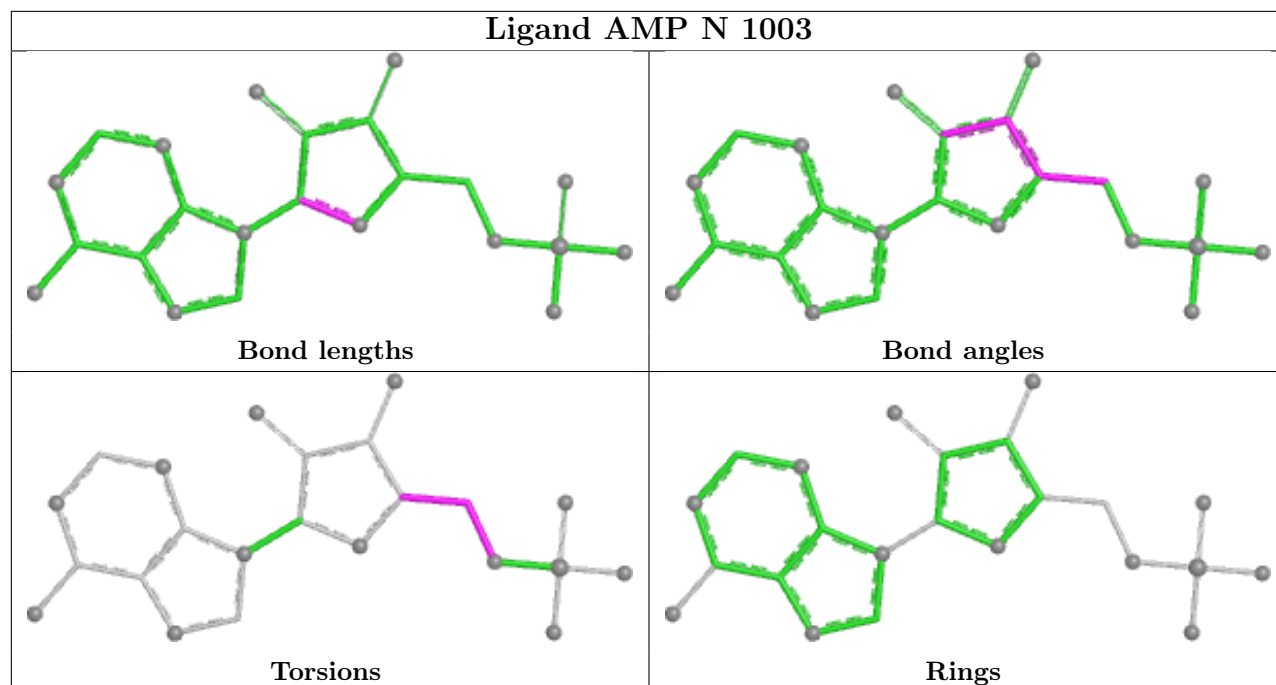
Ligand AMP R 1003



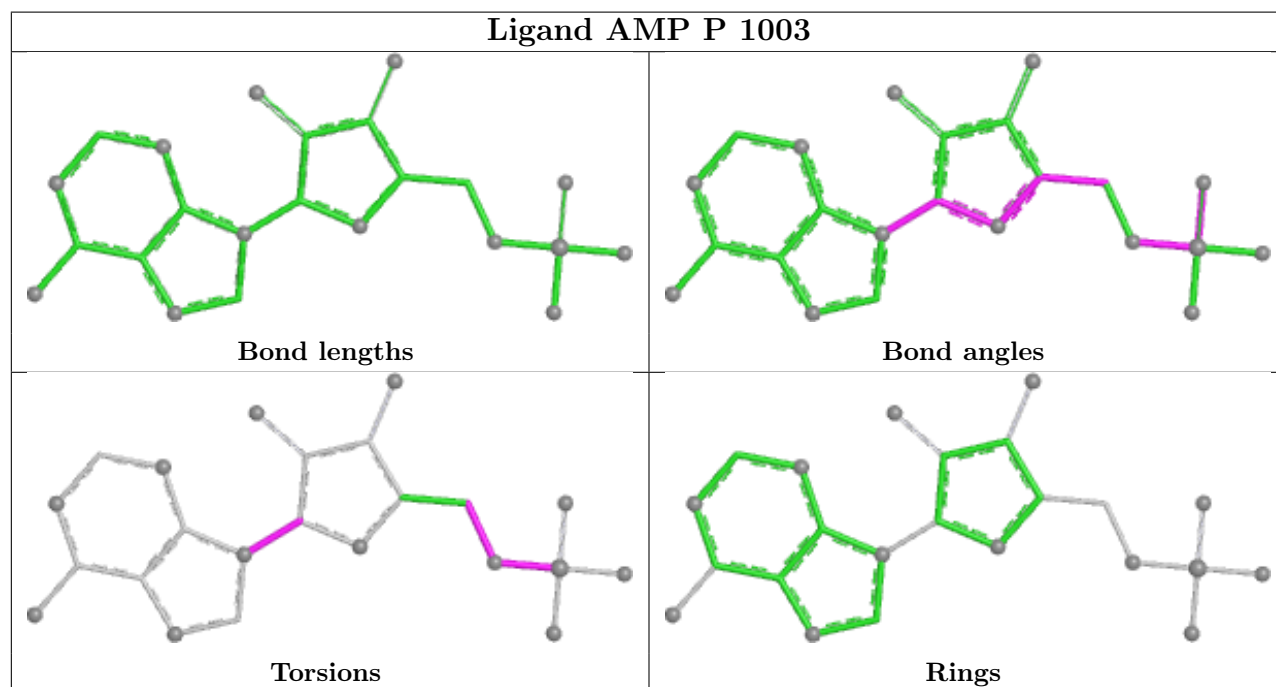
Ligand AMP B 1003



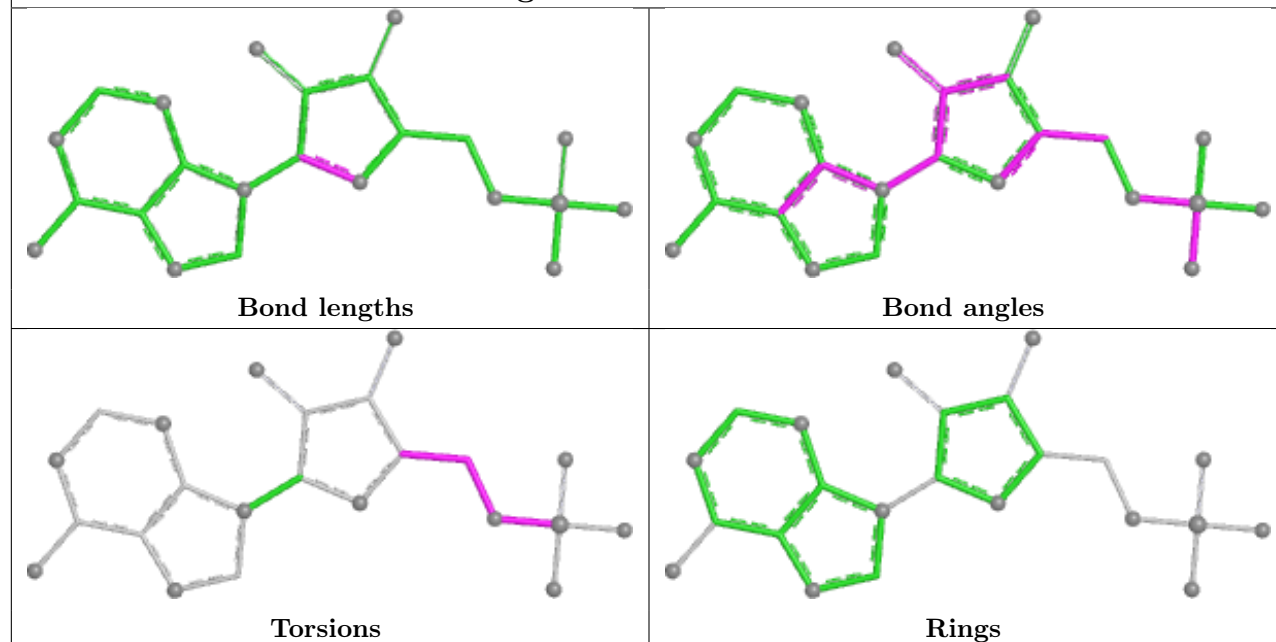
Ligand AMP N 1003



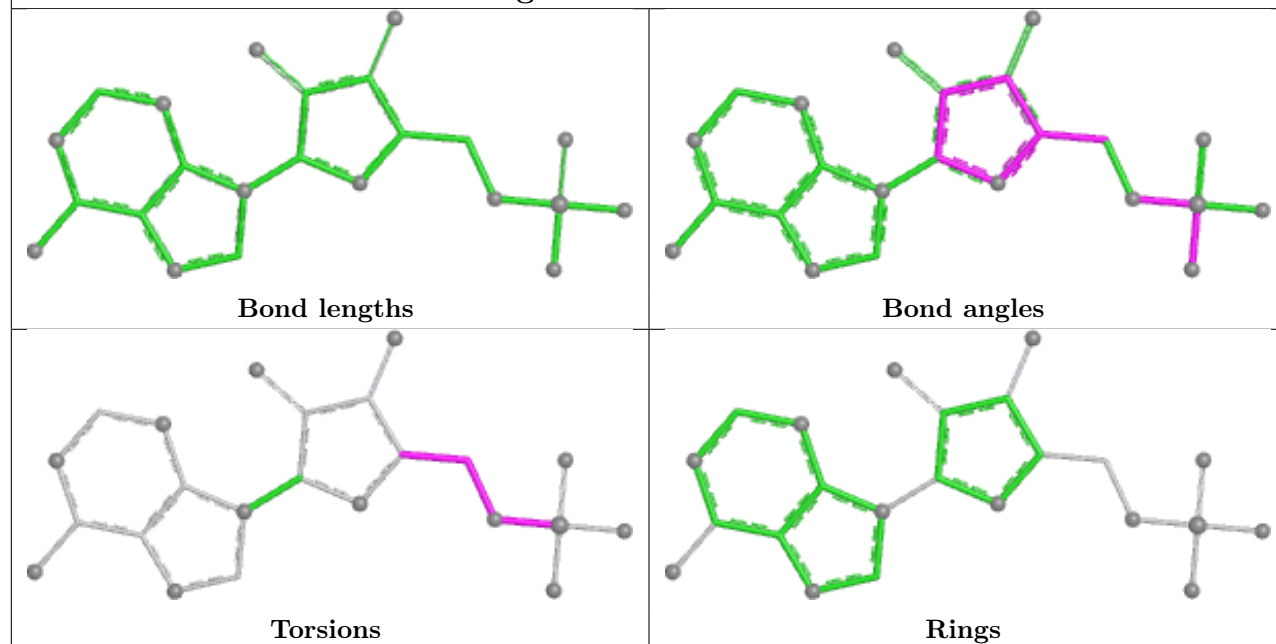
Ligand AMP P 1003



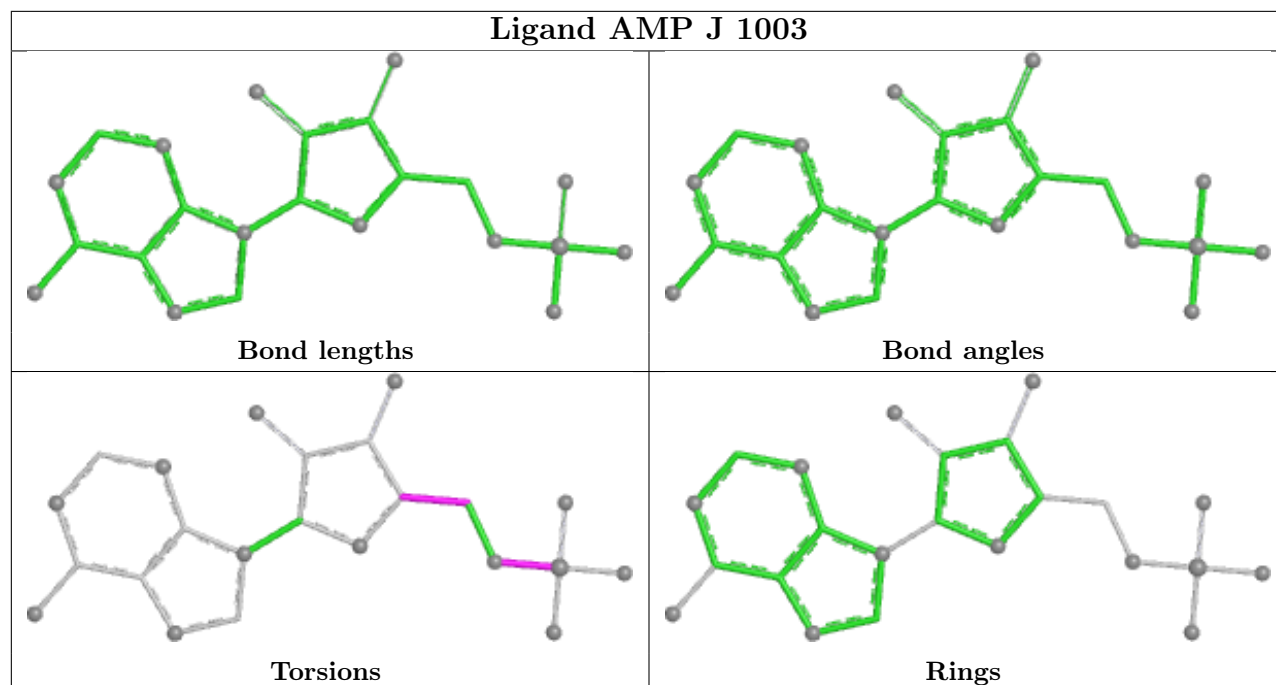
Ligand AMP A 1003



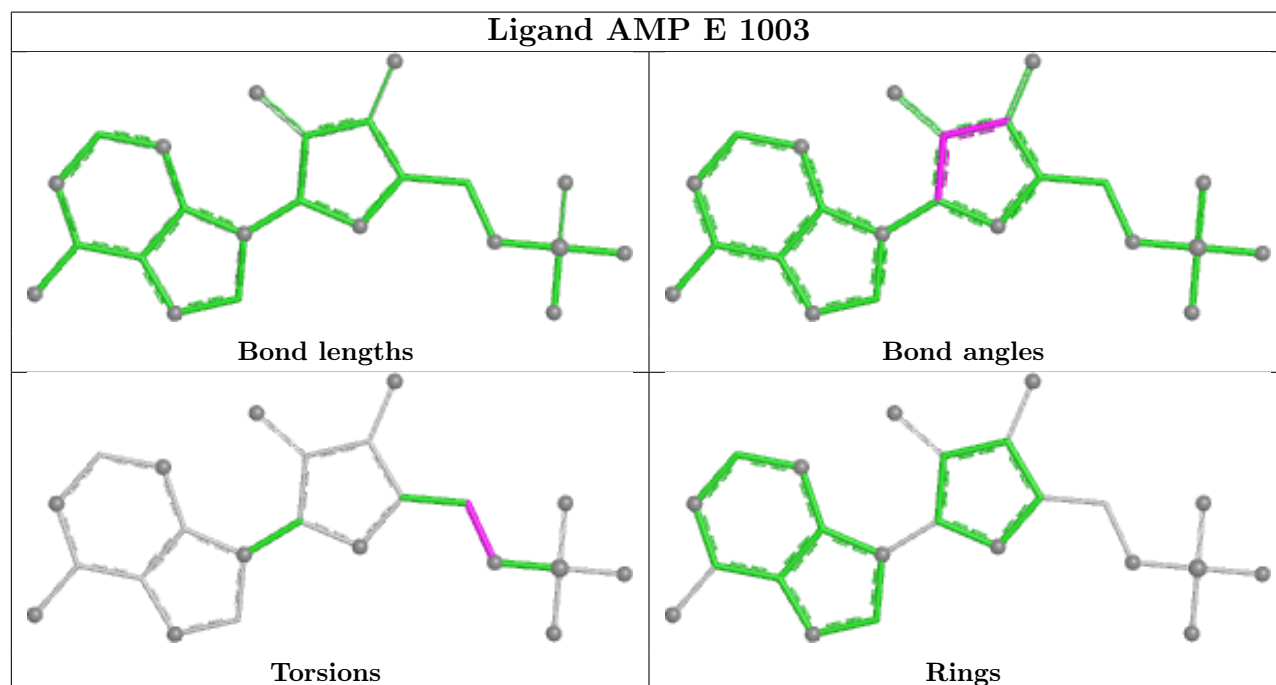
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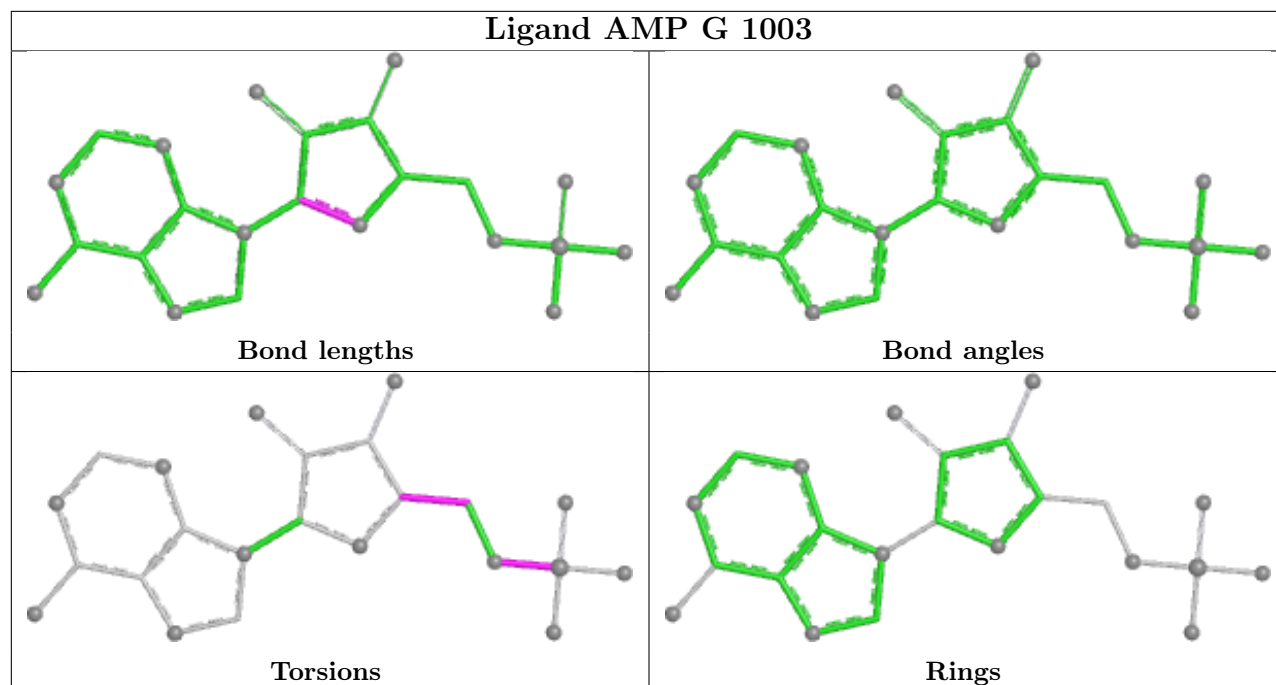
Ligand AMP J 1003



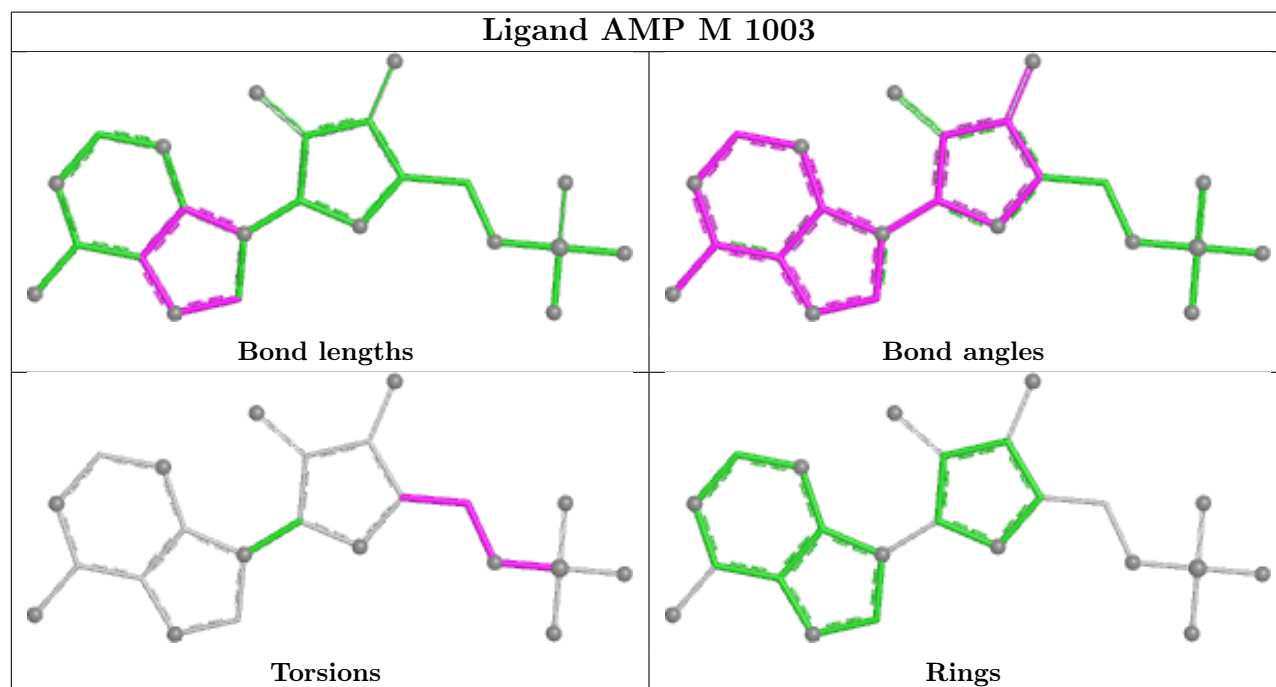
Ligand AMP E 1003

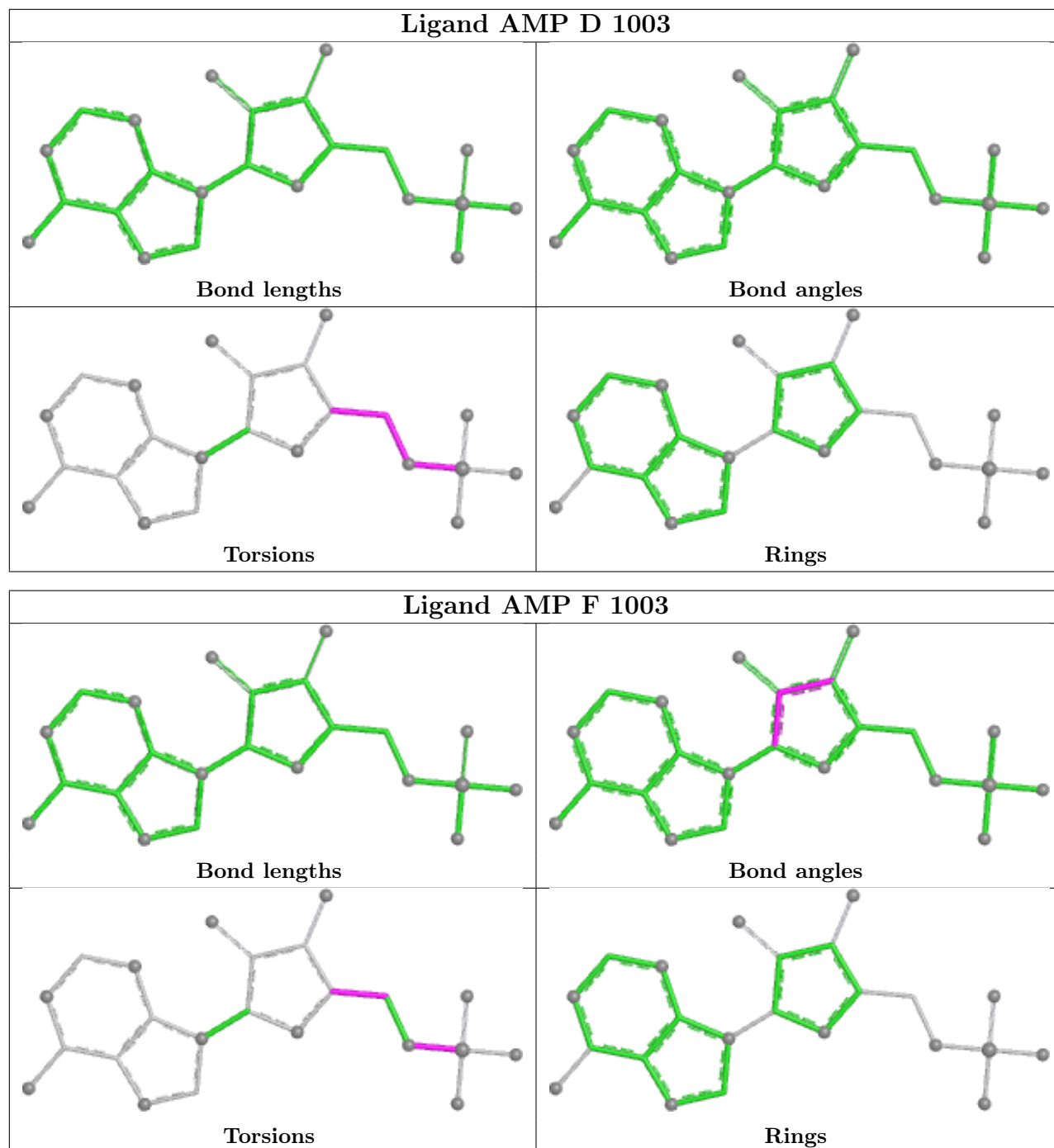


Ligand AMP G 1003



Ligand AMP M 1003





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

6.1 Protein, DNA and RNA chains

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	287/326 (88%)	0.28	5 (1%) 69 67	23, 45, 67, 89	0
1	B	285/326 (87%)	0.77	22 (7%) 19 17	41, 56, 80, 95	0
1	C	287/326 (88%)	0.30	13 (4%) 38 34	28, 43, 63, 86	0
1	D	291/326 (89%)	0.33	8 (2%) 56 53	29, 43, 66, 87	0
1	E	283/326 (86%)	1.13	59 (20%) 2 2	37, 63, 100, 125	0
1	F	286/326 (87%)	0.57	19 (6%) 24 21	32, 50, 73, 91	0
1	G	292/326 (89%)	0.51	18 (6%) 26 23	36, 51, 76, 92	0
1	H	291/326 (89%)	0.73	30 (10%) 12 10	26, 54, 79, 96	0
1	I	288/326 (88%)	0.31	10 (3%) 47 43	28, 44, 69, 89	0
1	J	291/326 (89%)	0.31	15 (5%) 33 29	31, 44, 67, 91	0
1	K	286/326 (87%)	0.90	44 (15%) 5 4	29, 58, 95, 120	0
1	L	291/326 (89%)	0.32	17 (5%) 29 25	24, 42, 68, 83	0
1	M	291/326 (89%)	1.34	65 (22%) 2 2	49, 69, 93, 106	0
1	N	291/326 (89%)	0.33	13 (4%) 38 34	25, 43, 65, 92	0
1	O	291/326 (89%)	0.92	35 (12%) 9 7	44, 60, 85, 98	0
1	P	285/326 (87%)	1.24	62 (21%) 2 2	44, 69, 110, 135	0
1	Q	291/326 (89%)	0.34	10 (3%) 48 44	28, 43, 68, 86	0
1	R	280/326 (85%)	1.47	72 (25%) 1 1	27, 67, 118, 137	0
All	All	5187/5868 (88%)	0.67	517 (9%) 12 10	23, 52, 88, 137	0

The worst 5 of 517 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	252	SER	8.5
1	E	237	GLY	7.2
1	R	255	GLU	7.1

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Mol	Chain	Res	Type	RSRZ
1	R	256	LEU	6.5
1	P	237	GLY	6.2

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($\text{\AA}^2$)	Q<0.9
4	AMP	M	1003	23/23	0.56	0.18	20,20,20,20	0
3	PO4	P	1002	5/5	0.62	0.23	104,107,110,111	5
4	AMP	O	1003	23/23	0.62	0.34	34,41,47,48	23
4	AMP	R	1003	23/23	0.64	0.52	49,56,66,68	23
4	AMP	K	1003	23/23	0.69	0.52	47,55,60,61	23
4	AMP	F	1003	23/23	0.72	0.34	39,47,56,58	23
3	PO4	R	1002	5/5	0.73	0.16	76,79,82,83	5
4	AMP	H	1003	23/23	0.73	0.41	45,50,52,53	23
4	AMP	B	1003	23/23	0.74	0.28	34,43,47,49	23
4	AMP	E	1003	23/23	0.74	0.49	42,50,56,57	23
4	AMP	P	1003	23/23	0.75	0.52	54,60,69,70	23
4	AMP	N	1003	23/23	0.76	0.26	19,29,47,48	23
4	AMP	I	1003	23/23	0.76	0.29	22,28,41,42	23
4	AMP	D	1003	23/23	0.77	0.31	33,42,54,56	23
4	AMP	Q	1003	23/23	0.78	0.21	22,37,51,53	23
4	AMP	C	1003	23/23	0.78	0.28	21,30,43,44	23
3	PO4	E	1002	5/5	0.80	0.15	75,78,80,81	5
4	AMP	J	1003	23/23	0.81	0.29	29,37,48,49	23
3	PO4	O	1002	5/5	0.82	0.16	41,44,46,47	5
4	AMP	L	1003	23/23	0.82	0.24	24,37,46,47	23
3	PO4	K	1002	5/5	0.85	0.13	64,67,70,71	5

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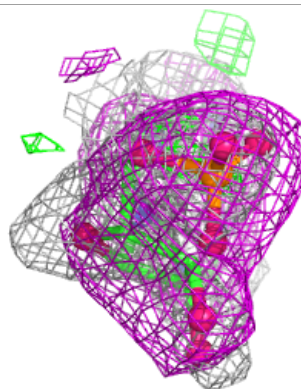
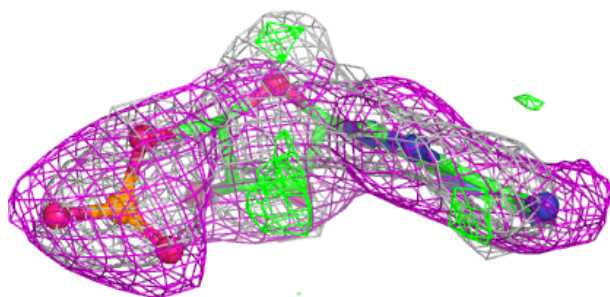
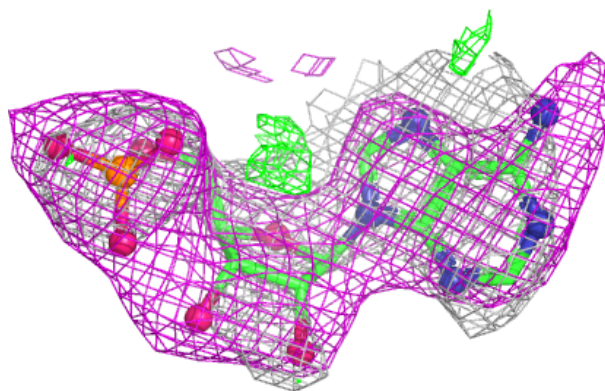
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AMP	A	1003	23/23	0.85	0.24	38,41,48,50	23
2	TRP	B	1001	15/15	0.86	0.16	29,44,76,106	15
2	TRP	O	1001	15/15	0.86	0.15	24,42,70,106	15
2	TRP	M	1001	15/15	0.87	0.14	21,34,65,103	15
4	AMP	G	1003	23/23	0.88	0.19	41,47,51,53	23
2	TRP	R	1001	15/15	0.88	0.15	12,44,70,106	15
3	PO4	F	1002	5/5	0.89	0.10	51,54,58,60	0
3	PO4	G	1002	5/5	0.89	0.11	50,53,56,56	5
2	TRP	A	1001	15/15	0.89	0.14	22,34,61,104	15
2	TRP	L	1001	15/15	0.89	0.14	20,35,69,101	15
2	TRP	E	1001	15/15	0.90	0.13	5,25,52,93	15
3	PO4	H	1002	5/5	0.90	0.15	46,49,52,54	5
3	PO4	C	1002	5/5	0.90	0.13	42,45,48,49	5
2	TRP	P	1001	15/15	0.91	0.14	18,32,70,99	15
3	PO4	I	1002	5/5	0.91	0.10	47,50,53,53	5
2	TRP	H	1001	15/15	0.91	0.12	20,36,73,103	15
2	TRP	D	1001	15/15	0.91	0.12	11,32,64,100	15
2	TRP	F	1001	15/15	0.92	0.11	12,37,65,99	15
3	PO4	B	1002	5/5	0.92	0.10	48,51,54,54	5
2	TRP	N	1001	15/15	0.92	0.12	14,29,61,100	15
2	TRP	Q	1001	15/15	0.93	0.11	20,34,69,98	15
2	TRP	I	1001	15/15	0.93	0.10	16,37,63,103	15
2	TRP	J	1001	15/15	0.93	0.12	16,30,62,95	15
2	TRP	K	1001	15/15	0.93	0.11	16,32,62,101	15
3	PO4	J	1002	5/5	0.93	0.08	65,68,71,72	0
2	TRP	G	1001	15/15	0.93	0.11	23,46,73,106	15
3	PO4	N	1002	5/5	0.93	0.08	52,55,57,59	0
2	TRP	C	1001	15/15	0.94	0.10	20,37,69,101	15
3	PO4	M	1002	5/5	0.94	0.30	20,20,20,20	0
3	PO4	D	1002	5/5	0.94	0.10	51,54,56,59	0
3	PO4	L	1002	5/5	0.95	0.07	57,60,62,63	0
3	PO4	A	1002	5/5	0.95	0.13	39,43,45,45	5
3	PO4	Q	1002	5/5	0.96	0.07	34,37,40,42	5

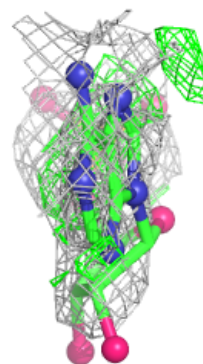
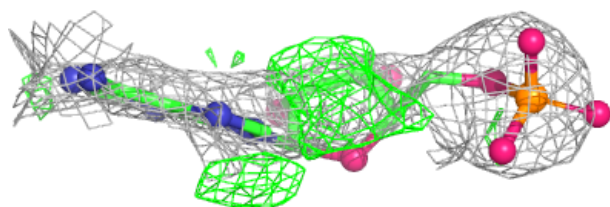
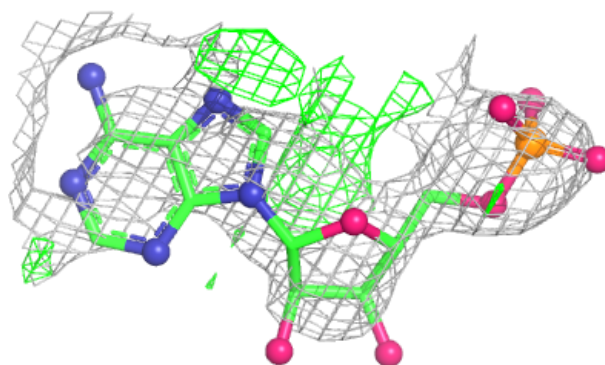
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP M 1003:

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

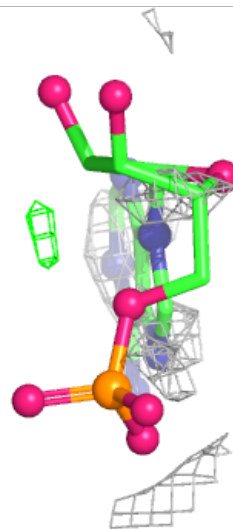
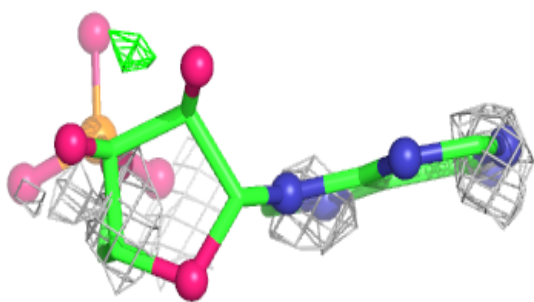
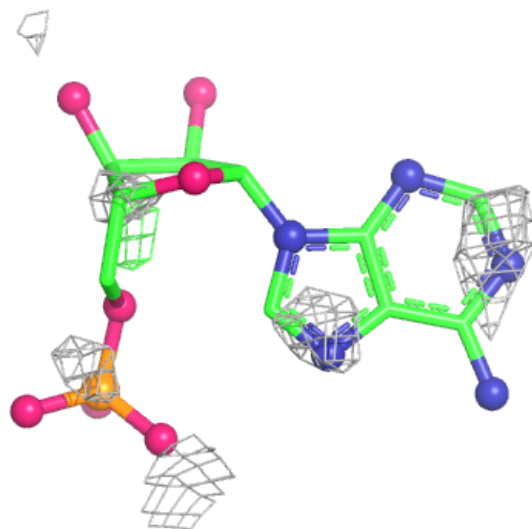
**Electron density around AMP O 1003:**

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



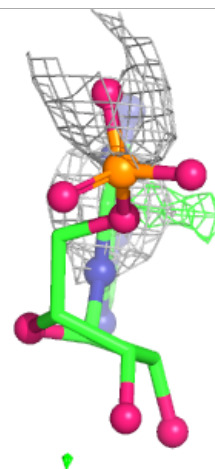
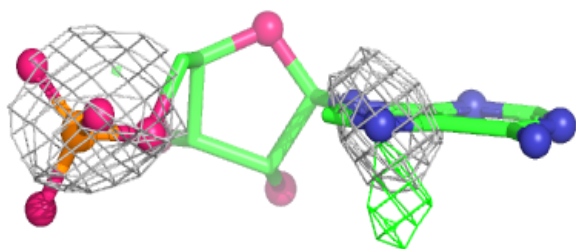
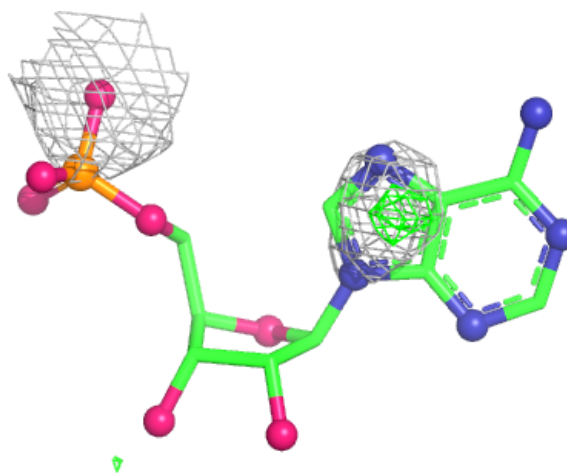
Electron density around AMP R 1003:

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



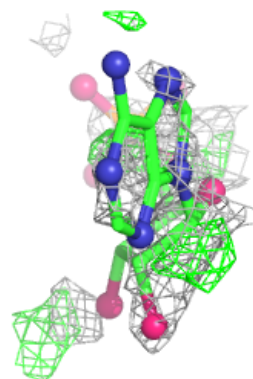
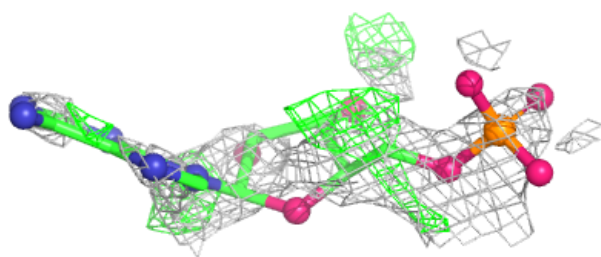
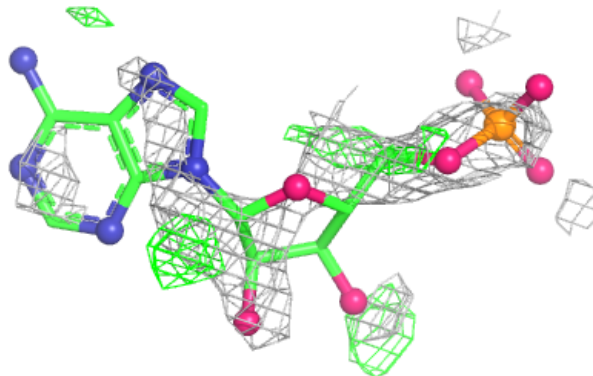
Electron density around AMP K 1003:

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



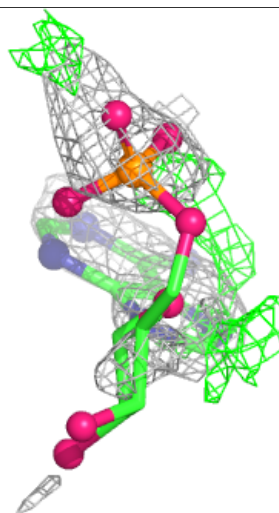
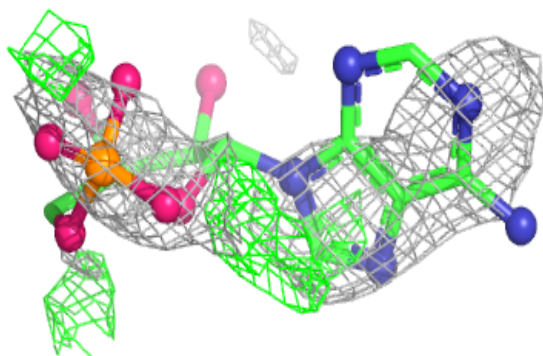
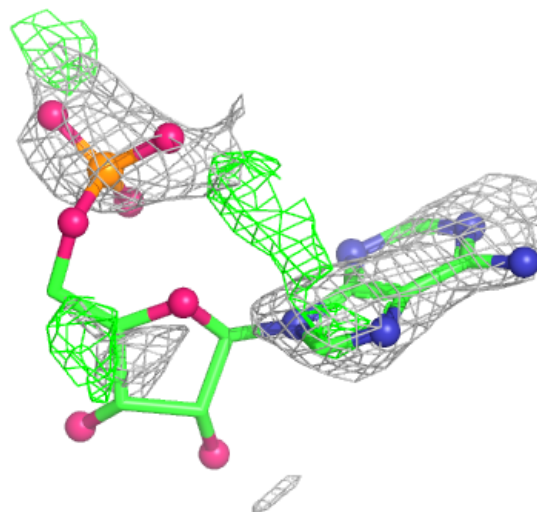
Electron density around AMP F 1003:

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



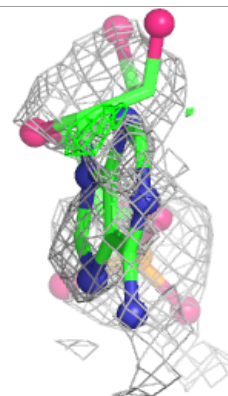
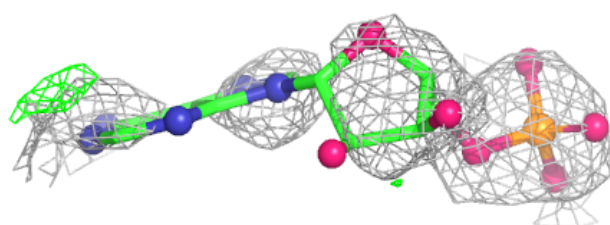
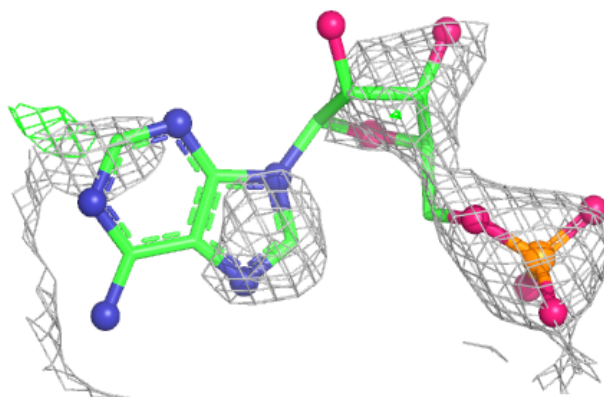
Electron density around AMP H 1003:

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

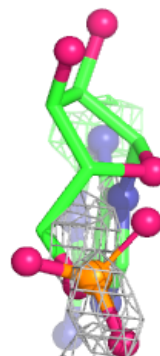
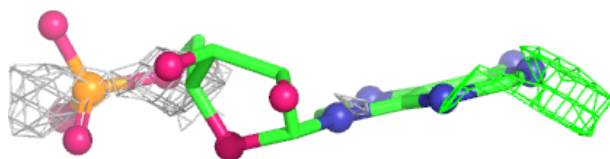
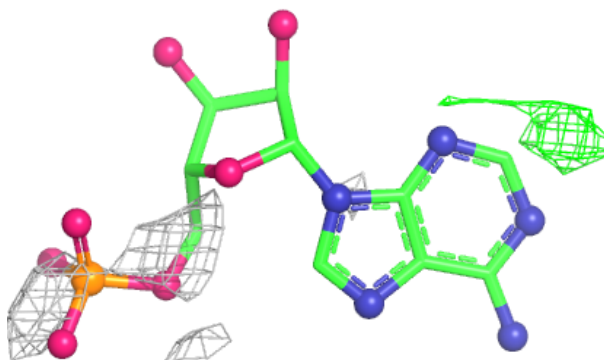


Electron density around AMP B 1003:

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and green (positive)

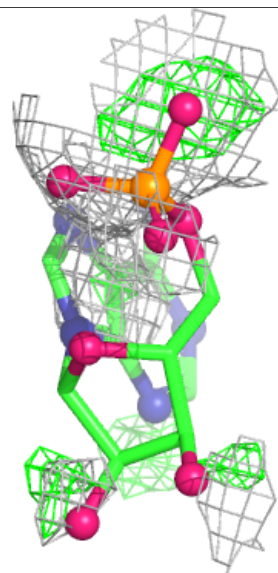
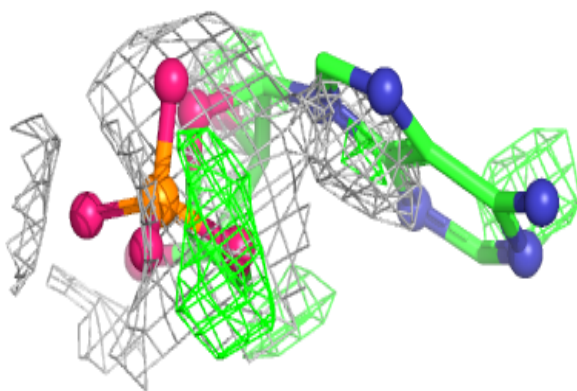
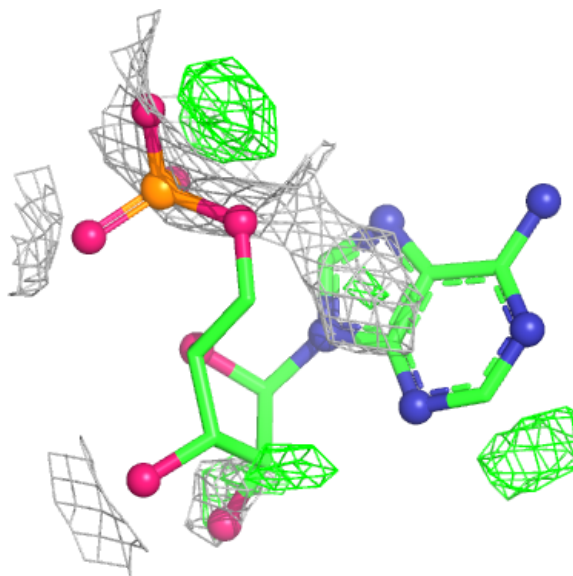
**Electron density around AMP E 1003:**

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and green (positive)



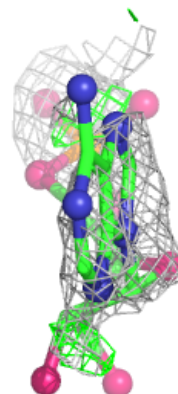
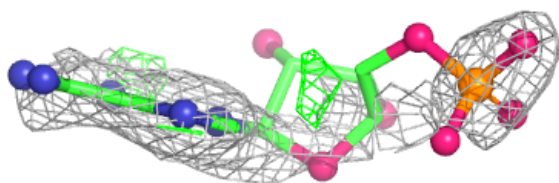
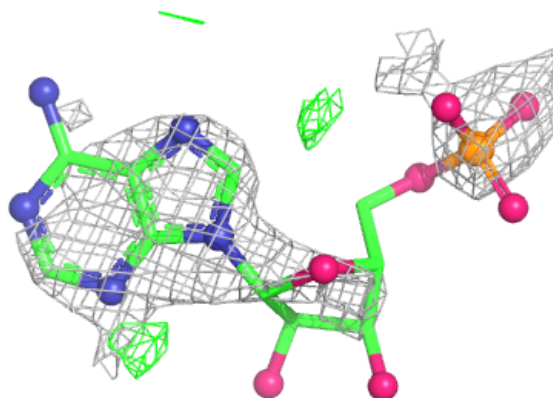
Electron density around AMP P 1003:

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

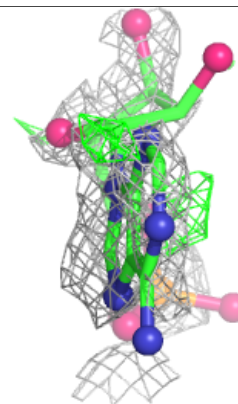
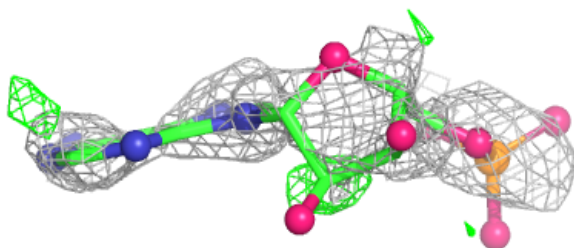
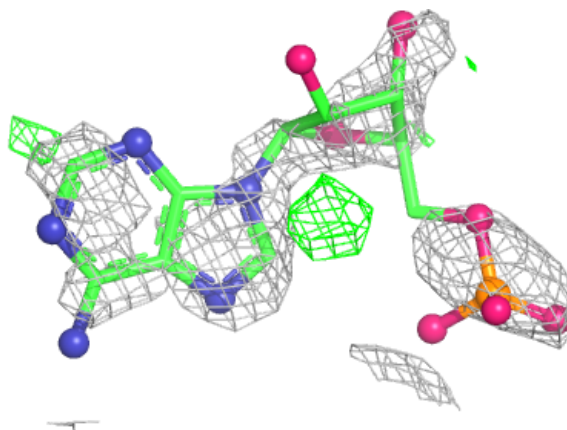


Electron density around AMP N 1003:

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

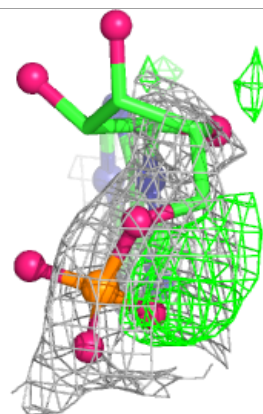
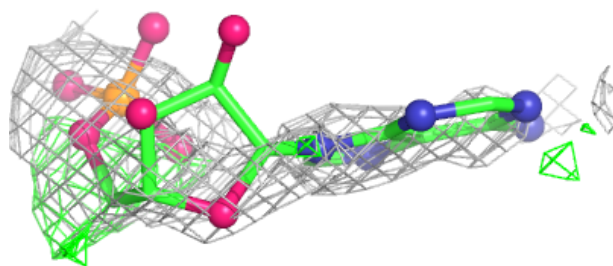
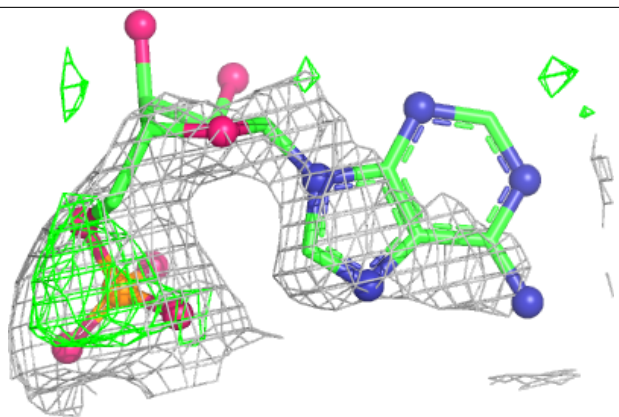
**Electron density around AMP I 1003:**

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

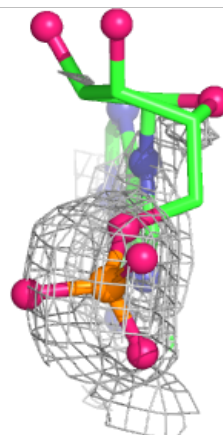
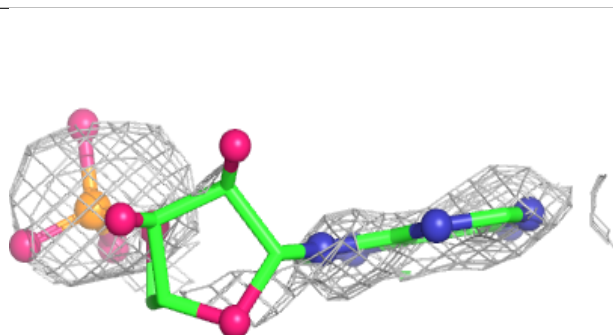
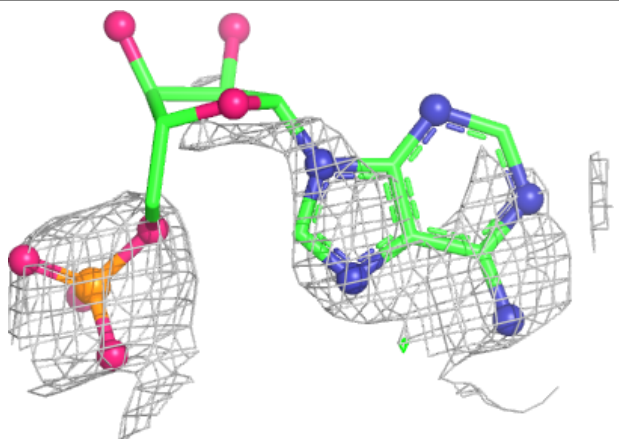


Electron density around AMP D 1003:

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

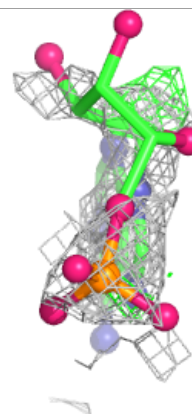
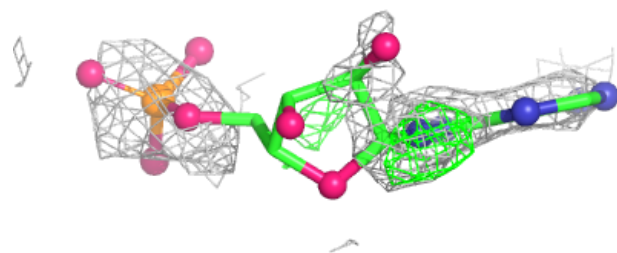
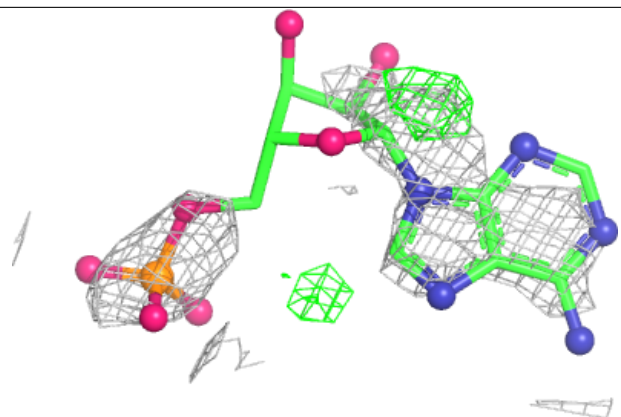
**Electron density around AMP Q 1003:**

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

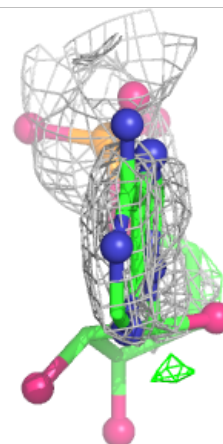
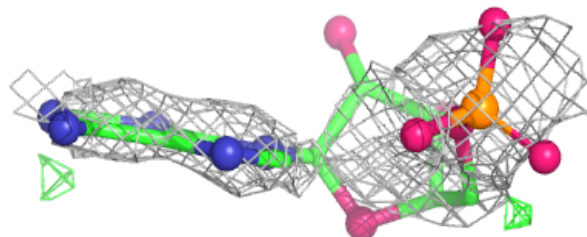
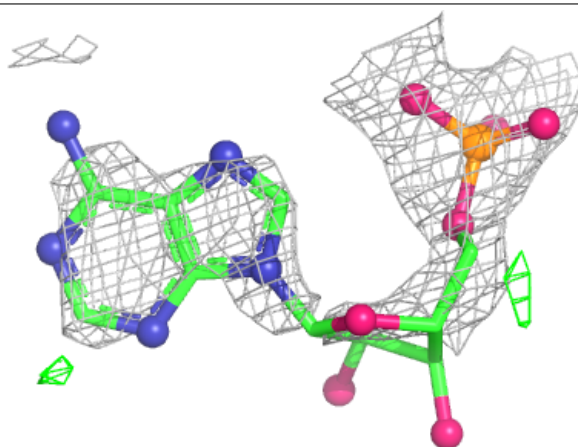


Electron density around AMP C 1003:

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

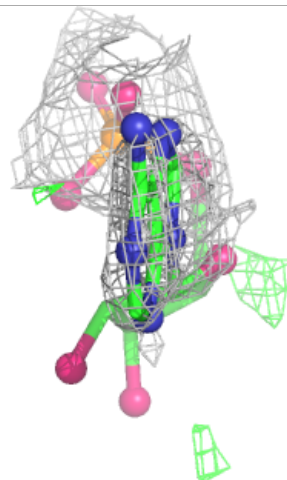
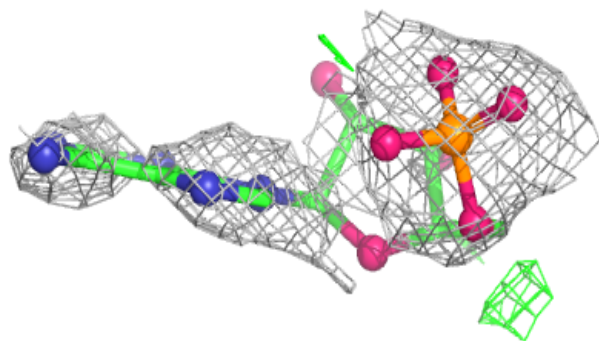
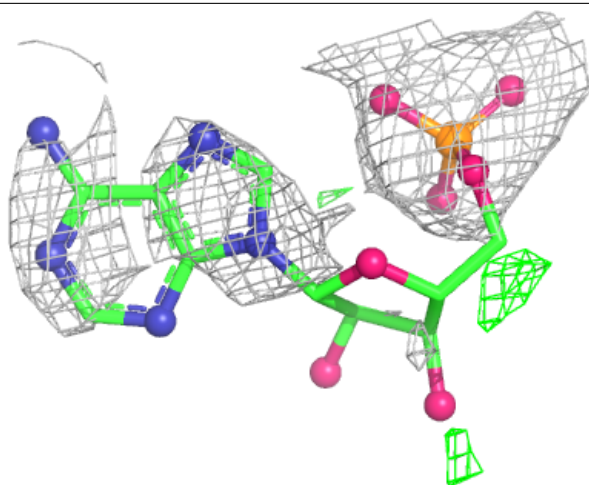
**Electron density around AMP J 1003:**

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



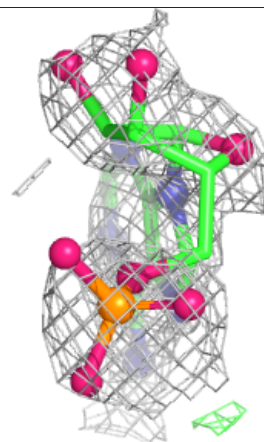
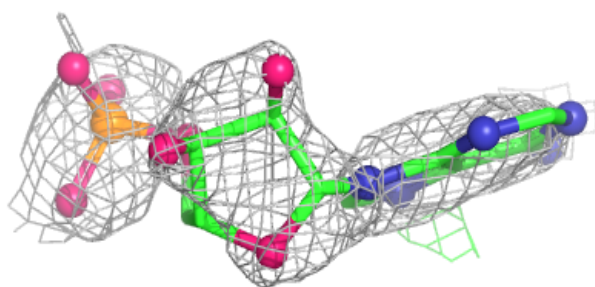
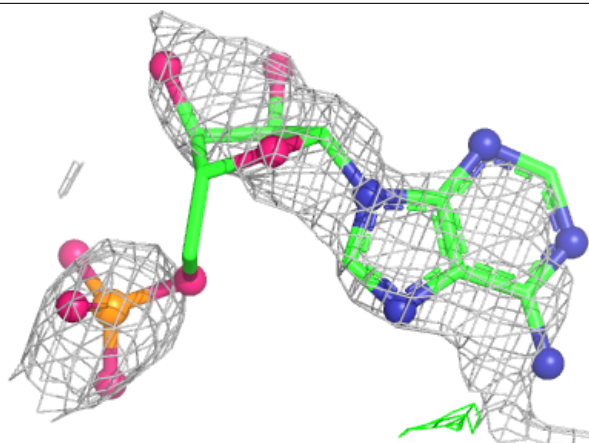
Electron density around AMP L 1003:

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

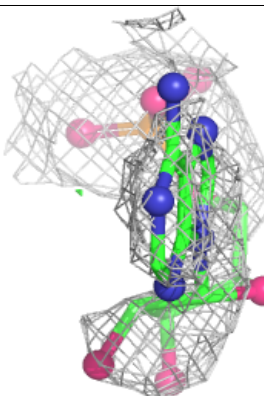
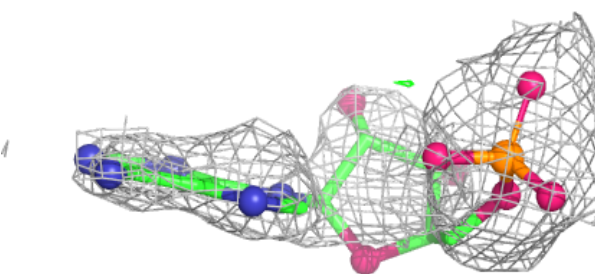
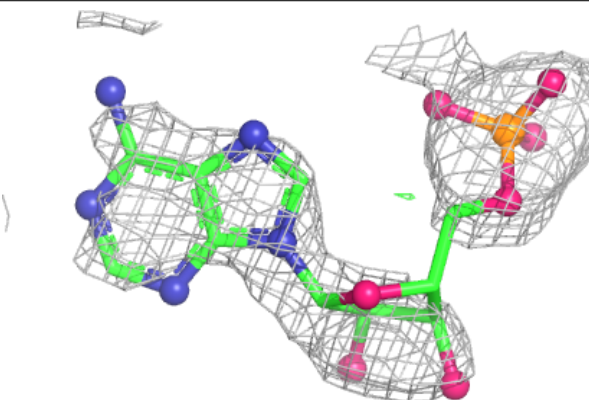


Electron density around AMP A 1003:

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

**Electron density around AMP G 1003:**

$2mF_o-DF_c$ (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.