



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 08:58 pm BST

PDB ID : 3FI0
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

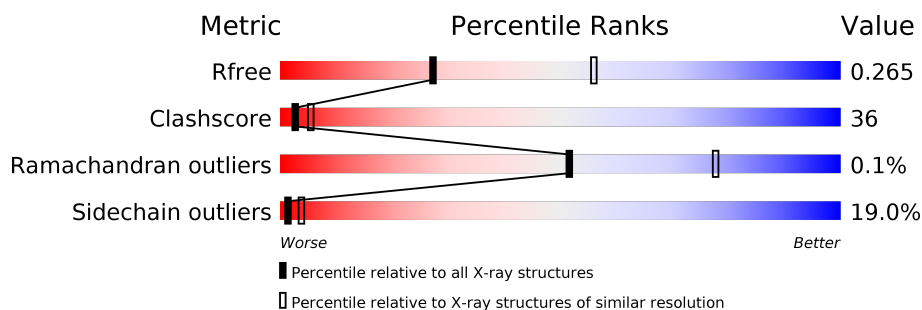
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 on 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	326	<div> <div>48%</div> <div>36%</div> <div>8%</div> <div>9%</div> </div>
1	B	326	<div> <div>38%</div> <div>41%</div> <div>11%</div> <div>10%</div> </div>
1	C	326	<div> <div>45%</div> <div>39%</div> <div>7%</div> <div>9%</div> </div>
1	D	326	<div> <div>52%</div> <div>34%</div> <div>6%</div> <div>8%</div> </div>
1	E	326	<div> <div>36%</div> <div>44%</div> <div>10%</div> <div>10%</div> </div>
1	F	326	<div> <div>47%</div> <div>33%</div> <div>10%</div> <div>9%</div> </div>
1	G	326	<div> <div>48%</div> <div>36%</div> <div>8%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
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	B	1003	-	-	X	-
4	AMP	G	1003	-	-	X	-
4	AMP	I	1003	-	-	X	-
4	AMP	O	1003	-	-	X	-
4	AMP	P	1003	-	-	X	-
4	AMP	Q	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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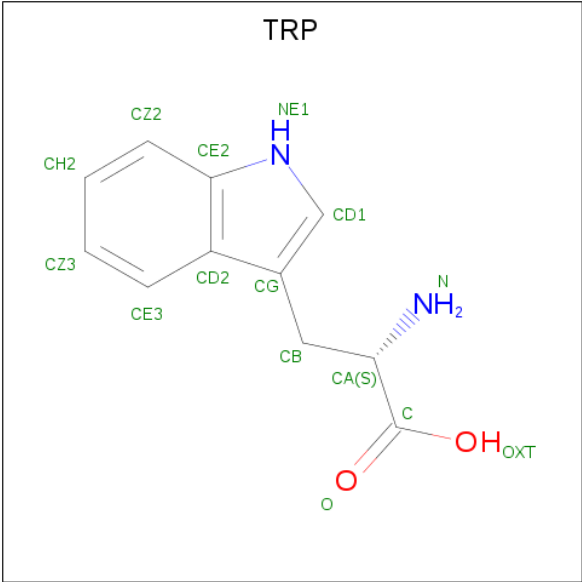
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	301	Total	C	N	O	S	Se	0	0	0
			2408	1528	415	452	3	10			
1	R	290	Total	C	N	O	S	Se	0	0	0
			2322	1473	399	437	3	10			

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 (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂).



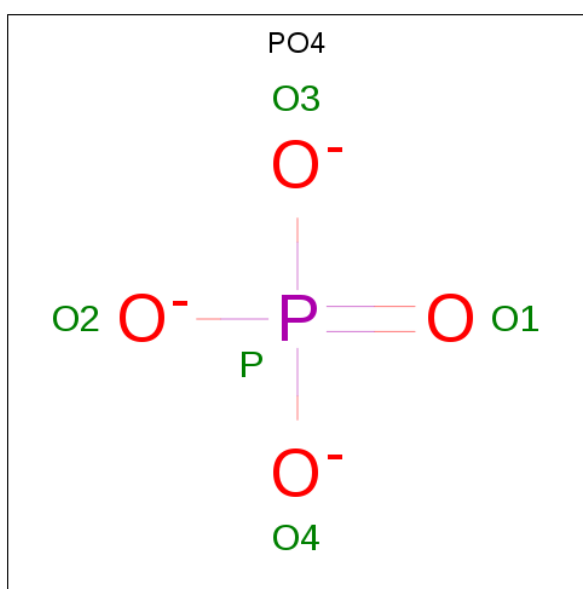
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	F	1	Total	C	N	O	0	0
			15	11	2	2		
2	G	1	Total	C	N	O	0	0
			15	11	2	2		
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 (three-letter code: PO4) (formula: O₄P).



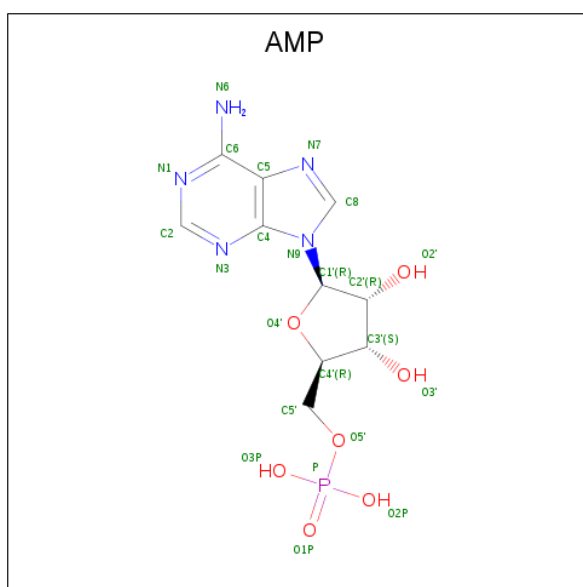
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		

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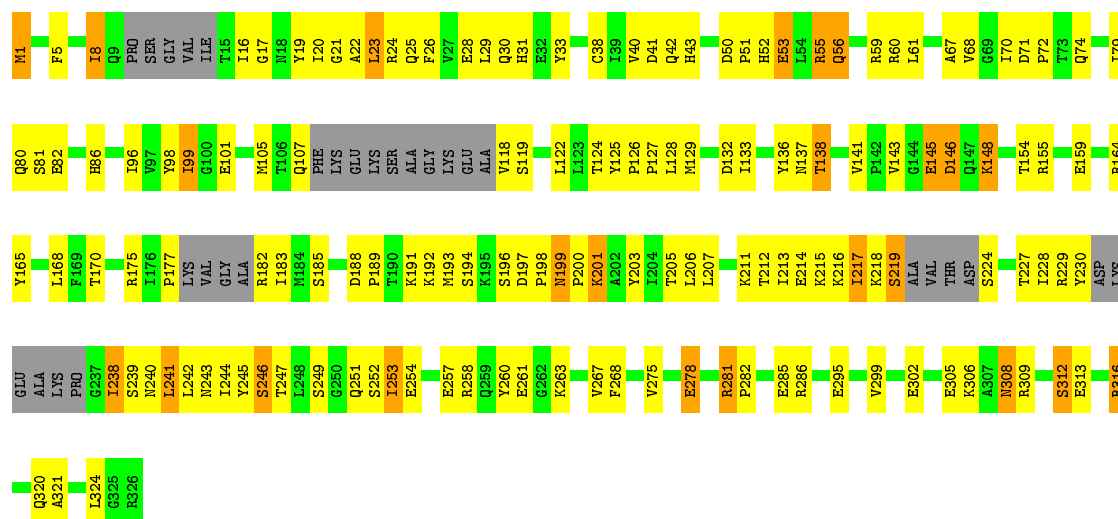
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		
3	N	1	Total	O	P	0	0
			5	4	1		
3	O	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	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 (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



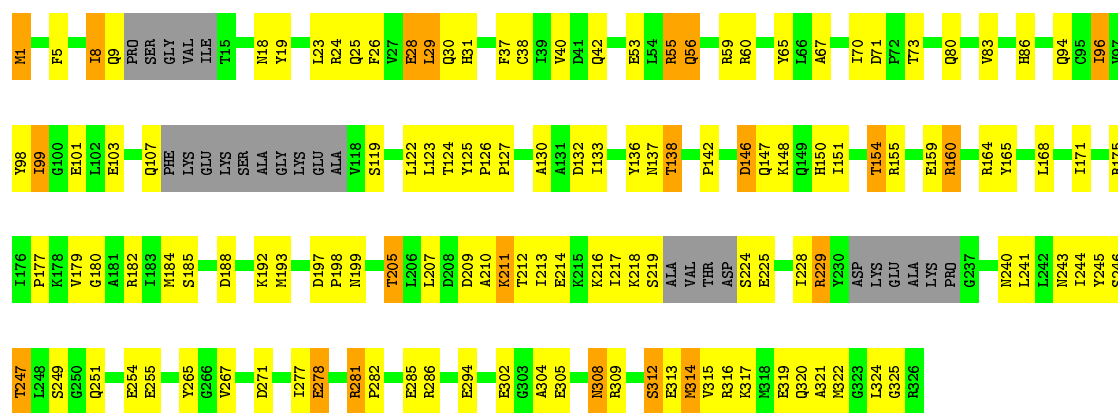
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	D	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	E	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	F	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	G	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	H	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

Chain C: 



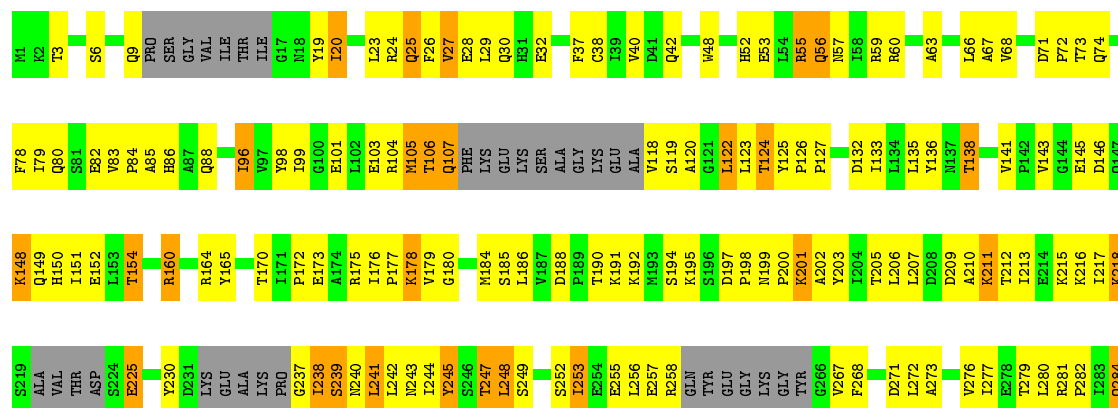
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain D: 



• Molecule 1: Tryptophanyl-tRNA synthetase

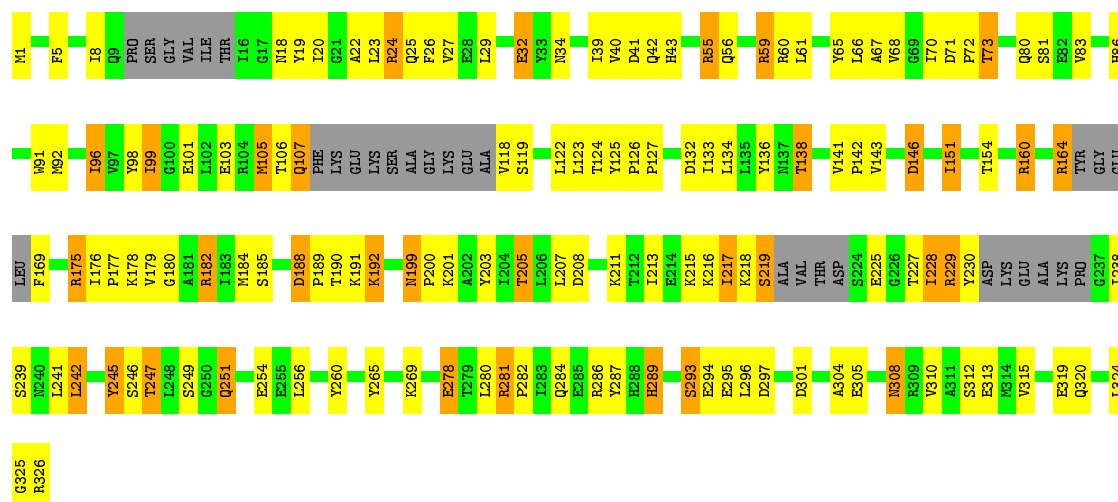
Chain E: 





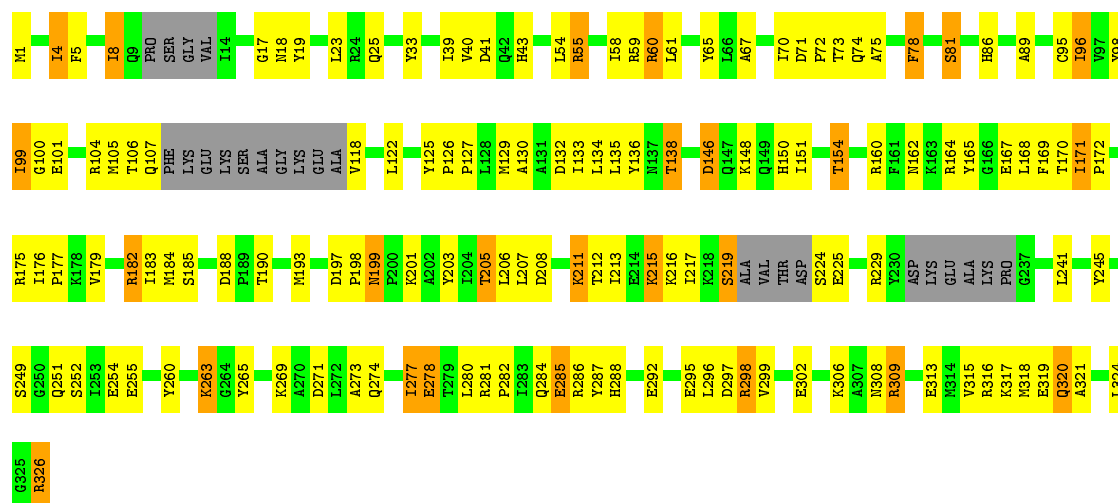
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain F: 47% 33% 10% 9%



• Molecule 1: Tryptophanyl-tRNA synthetase

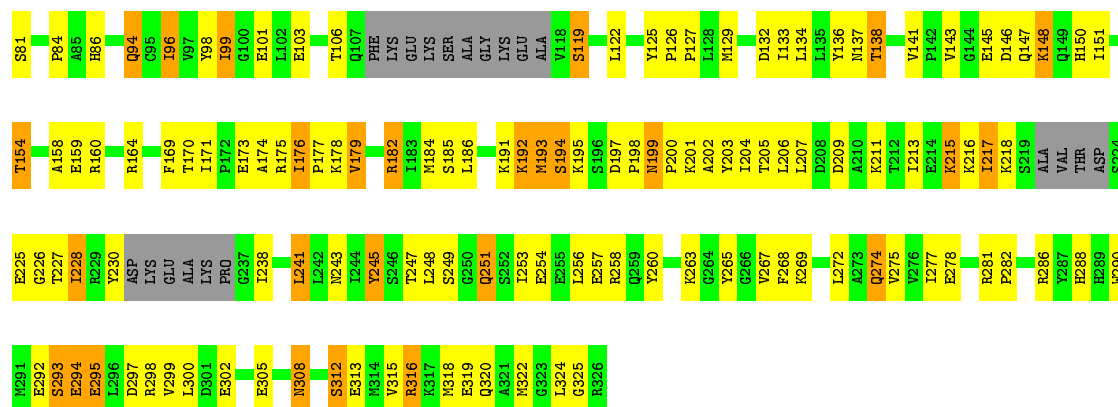
Chain G: 48% 36% 8% 7%



• Molecule 1: Tryptophanyl-tRNA synthetase

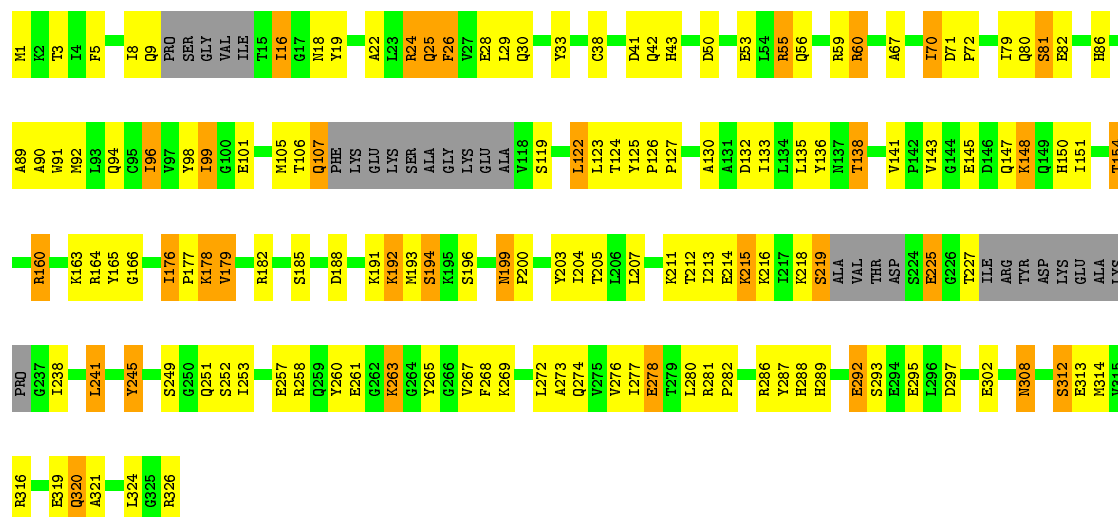
Chain H: 42% 41% 10% 8%





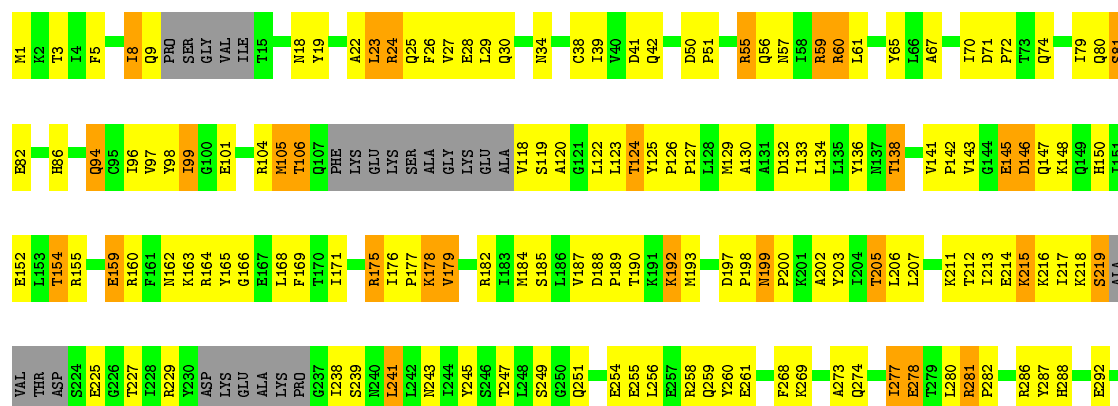
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain I: 47% 34% 10% 9%



• Molecule 1: Tryptophanyl-tRNA synthetase

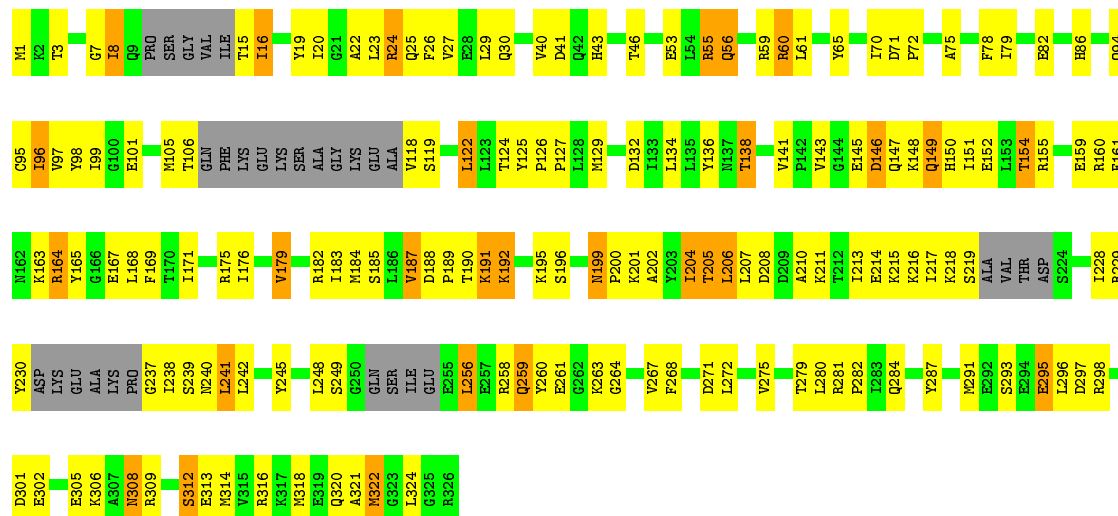
Chain J: 40% 42% 10% 8%

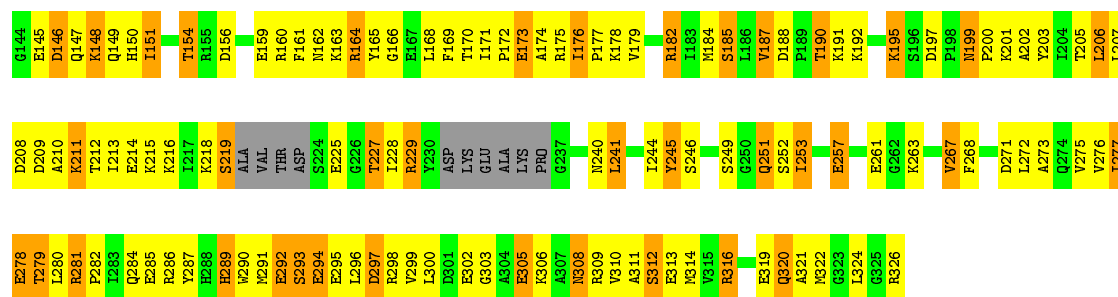




• Molecule 1: Tryptophanyl-tRNA synthetase

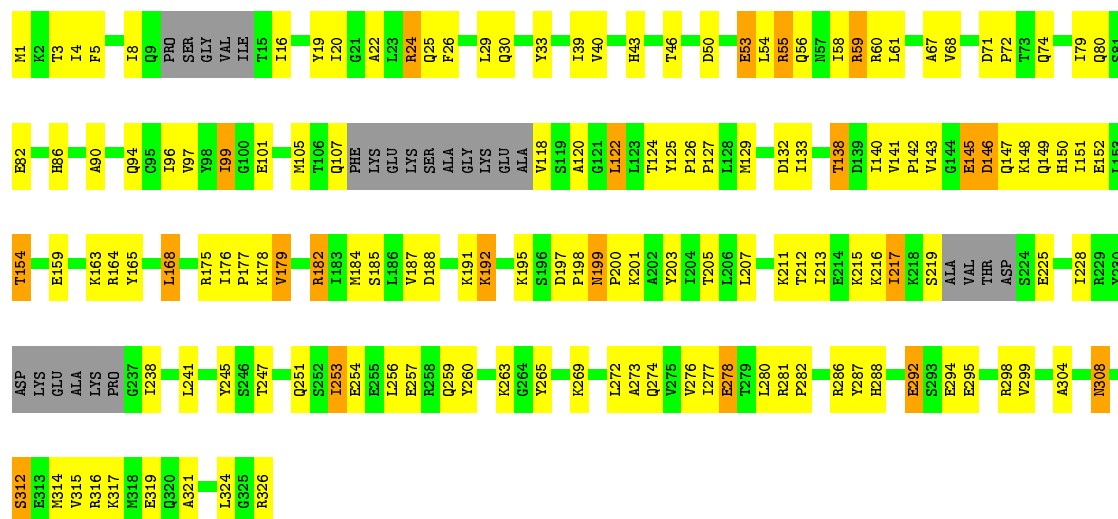
Chain K: 41% 41% 9% 9%





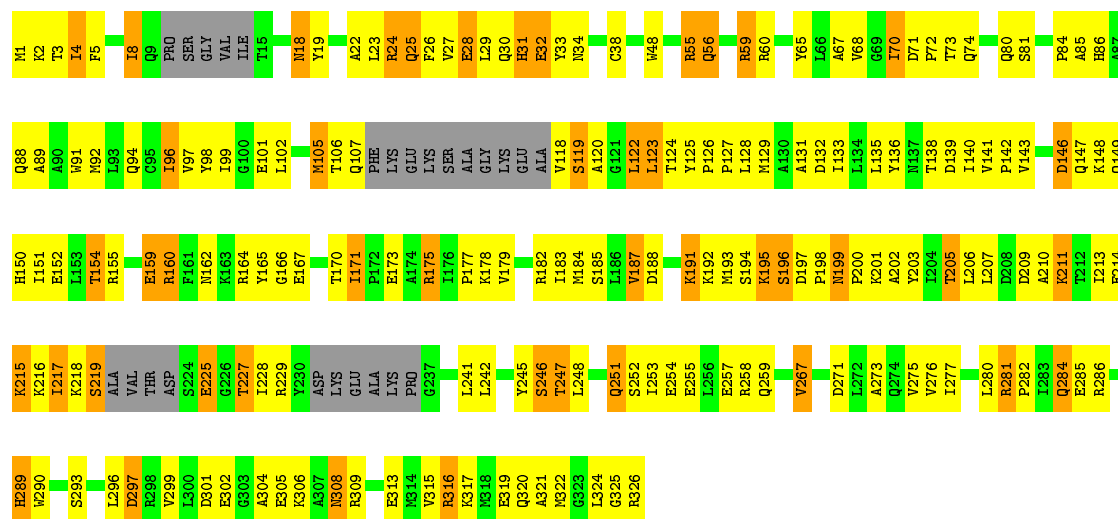
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain N: 48% 38% 6% 8%



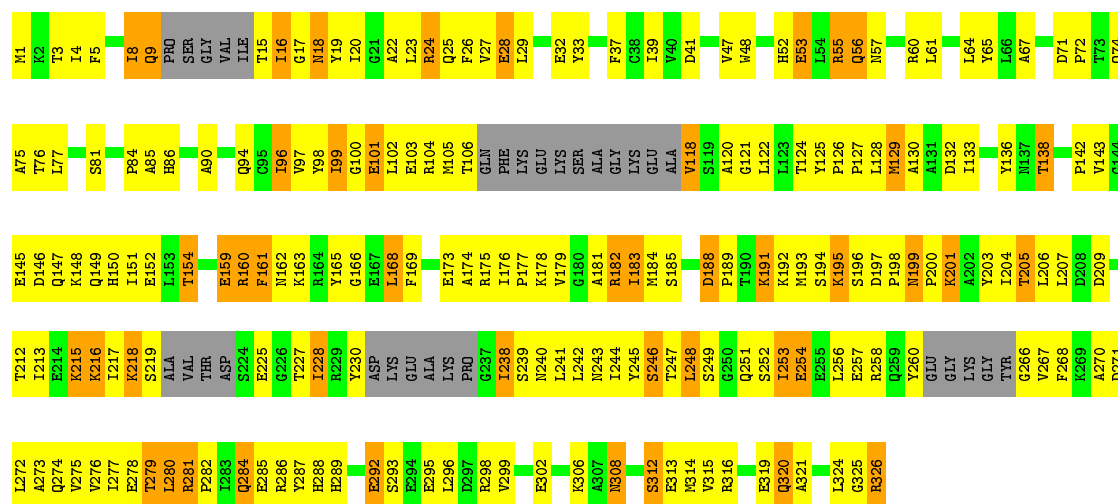
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain O: 36% 43% 14% 8%



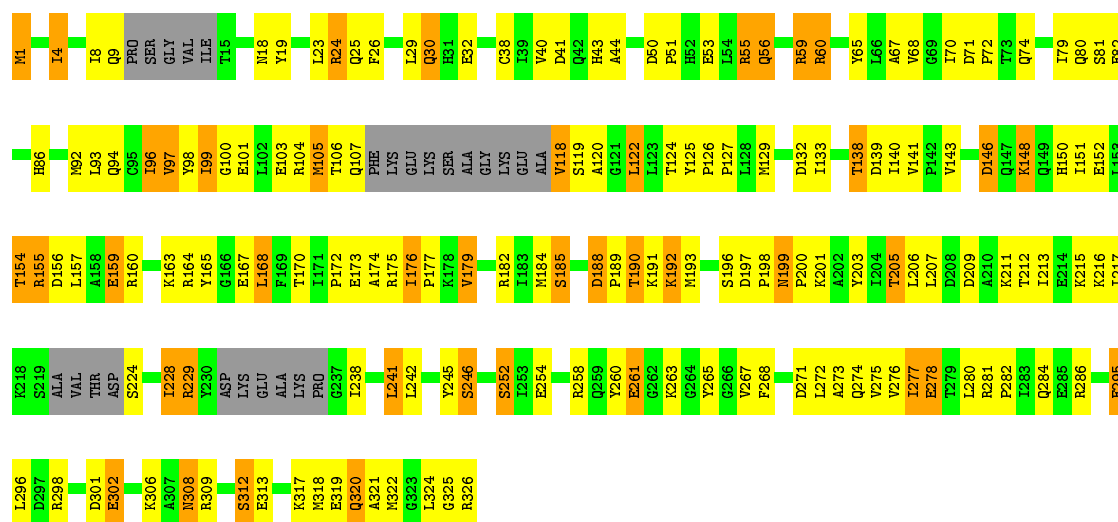
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain P: 



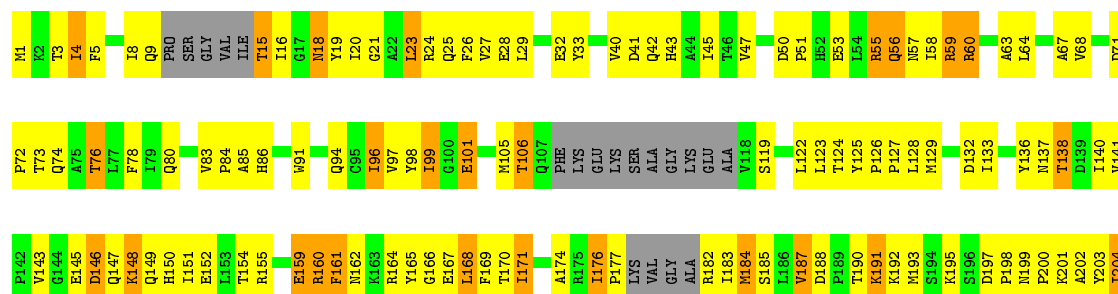
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain Q: 



• Molecule 1: Tryptophanyl-tRNA synthetase

Chain R: 



T206	T207	D208	D209	A210	K211	T212	I213	E214	K215	K216	I217	K218	S219	ALA	VAL	THR	ASP	S224	E225	G226	T227	I228	ARG	THR	ASP	LYS	GLU	ALA	LYS	PRO	G237	I238	S239	N240	I241	L242	N243	I244	Y245	S246	T247	L248		Q251	S252	I253	E254	E255	L256	E257		Y260	GLU	GLY	LYS	GLY	TYR	G266
V267	F268	K269	A270	L271	A272	A273	Q274	V275	V276	I277	E278	T279	L280	R281	P282	I283	Q284	E285	R286	Y287	H288	H289	W290	W291	E292	S293	E294	E295	L296	D297	R298	V299	L300	D301	E302		K306	A307	N308		S312	E313	K314	V315	R316		E319	Q320	A321		L324	G325	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 24.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (25.00-2.70) 99.0 (24.96-2.70)	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 0.252 , 0.265	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)	0.36 , 63.8	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: AMP, PO4

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	0.38	0/2414	0.52	0/3242
1	B	0.30	0/2400	0.51	0/3222
1	C	0.31	0/2414	0.56	0/3242
1	D	0.32	0/2440	0.53	0/3278
1	E	0.29	0/2371	0.54	0/3184
1	F	0.29	0/2398	0.51	0/3219
1	G	0.30	0/2448	0.55	0/3289
1	H	0.29	0/2440	0.54	0/3278
1	I	0.31	0/2408	0.54	0/3235
1	J	0.30	0/2440	0.54	0/3278
1	K	0.28	0/2398	0.52	0/3220
1	L	0.31	0/2440	0.55	0/3278
1	M	0.28	0/2440	0.56	2/3278 (0.1%)
1	N	0.30	0/2440	0.56	0/3278
1	O	0.30	0/2440	0.56	0/3278
1	P	0.27	0/2391	0.57	1/3212 (0.0%)
1	Q	0.31	0/2440	0.57	1/3278 (0.0%)
1	R	0.29	0/2350	0.55	0/3156
All	All	0.30	0/43512	0.54	4/58445 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	44	ALA	CB-CA-C	-5.73	101.51	110.10
1	P	188	ASP	C-N-CD	-5.51	108.48	120.60
1	M	252	SER	N-CA-CB	-5.37	102.44	110.50
1	M	99	ILE	CB-CA-C	-5.31	100.98	111.60

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	197	0
1	C	2383	0	2390	129	0
1	D	2408	0	2421	130	0
1	E	2342	0	2355	219	0
1	F	2368	0	2384	141	0
1	G	2416	0	2432	139	0
1	H	2408	0	2421	158	0
1	I	2377	0	2388	138	0
1	J	2408	0	2421	137	0
1	K	2367	0	2382	207	0
1	L	2408	0	2421	123	0
1	M	2408	0	2421	264	0
1	N	2408	0	2421	143	0
1	O	2408	0	2421	198	0
1	P	2361	0	2378	355	0
1	Q	2408	0	2421	172	0
1	R	2322	0	2333	283	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
2	P	15	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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	10	0
4	B	23	0	12	8	0
4	C	23	0	12	3	0
4	D	23	0	12	5	0
4	E	23	0	12	4	0
4	F	23	0	12	2	0
4	G	23	0	12	9	0
4	H	23	0	12	1	0
4	I	23	0	12	7	0
4	J	23	0	12	3	0
4	K	23	0	12	4	0
4	L	23	0	12	1	0
4	M	23	0	12	5	0
4	N	23	0	12	6	0
4	O	23	0	12	17	0
4	P	23	0	12	12	0
4	Q	23	0	12	7	0
4	R	23	0	12	4	0
All	All	43727	0	43558	3147	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 3147 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%)	34	60
1	B	281/326 (86%)	266 (95%)	14 (5%)	1 (0%)	34	60
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%)	41	66
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%)	15	37
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%)	51	78

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%)	219 (85%)	38 (15%)	3	7
1	B	256/268 (96%)	202 (79%)	54 (21%)	1	3
1	C	257/268 (96%)	211 (82%)	46 (18%)	2	4
1	D	259/268 (97%)	216 (83%)	43 (17%)	2	5
1	E	253/268 (94%)	208 (82%)	45 (18%)	2	4
1	F	255/268 (95%)	203 (80%)	52 (20%)	1	3
1	G	260/268 (97%)	219 (84%)	41 (16%)	2	6
1	H	259/268 (97%)	214 (83%)	45 (17%)	2	5
1	I	256/268 (96%)	203 (79%)	53 (21%)	1	3
1	J	259/268 (97%)	207 (80%)	52 (20%)	1	3
1	K	254/268 (95%)	210 (83%)	44 (17%)	2	5
1	L	259/268 (97%)	219 (85%)	40 (15%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	259/268 (97%)	202 (78%)	57 (22%)	1	2
1	N	259/268 (97%)	221 (85%)	38 (15%)	3	7
1	O	259/268 (97%)	194 (75%)	65 (25%)	0	1
1	P	255/268 (95%)	200 (78%)	55 (22%)	1	3
1	Q	259/268 (97%)	199 (77%)	60 (23%)	1	2
1	R	252/268 (94%)	196 (78%)	56 (22%)	1	2
All	All	4627/4824 (96%)	3743 (81%)	884 (19%)	1	4

5 of 884 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	215	LYS
1	K	195	LYS
1	Q	261	GLU
1	I	295	GLU
1	J	192	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 191 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	18	ASN
1	K	43	HIS
1	Q	308	ASN
1	I	43	HIS
1	J	43	HIS

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 carbohydrates 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	N	1002	-	4,4,4	1.95	1 (25%)	6,6,6	0.47	0
4	AMP	K	1003	-	22,25,25	1.03	1 (4%)	25,38,38	1.01	2 (8%)
3	PO4	Q	1002	-	4,4,4	1.94	1 (25%)	6,6,6	0.40	0
4	AMP	C	1003	-	22,25,25	1.14	2 (9%)	25,38,38	0.87	1 (4%)
3	PO4	G	1002	-	4,4,4	1.95	1 (25%)	6,6,6	0.46	0
4	AMP	E	1003	-	22,25,25	1.11	2 (9%)	25,38,38	1.05	1 (4%)
4	AMP	G	1003	-	22,25,25	1.15	2 (9%)	25,38,38	0.94	2 (8%)
3	PO4	F	1002	-	4,4,4	1.84	1 (25%)	6,6,6	0.46	0
3	PO4	R	1002	-	4,4,4	1.78	1 (25%)	6,6,6	0.41	0
4	AMP	M	1003	-	22,25,25	0.80	0	25,38,38	1.80	8 (32%)
3	PO4	H	1002	-	4,4,4	2.00	1 (25%)	6,6,6	0.46	0
4	AMP	O	1003	-	22,25,25	1.16	2 (9%)	25,38,38	1.51	3 (12%)
3	PO4	I	1002	-	4,4,4	1.96	1 (25%)	6,6,6	0.37	0
3	PO4	P	1002	-	4,4,4	1.81	1 (25%)	6,6,6	0.91	0
4	AMP	Q	1003	-	22,25,25	1.13	2 (9%)	25,38,38	1.07	2 (8%)
4	AMP	D	1003	-	22,25,25	1.11	2 (9%)	25,38,38	0.88	1 (4%)
3	PO4	J	1002	-	4,4,4	2.08	1 (25%)	6,6,6	0.73	0
4	AMP	L	1003	-	22,25,25	1.08	2 (9%)	25,38,38	1.07	1 (4%)
3	PO4	O	1002	-	4,4,4	1.95	1 (25%)	6,6,6	0.46	0
4	AMP	N	1003	-	22,25,25	1.38	3 (13%)	25,38,38	1.35	4 (16%)
4	AMP	H	1003	-	22,25,25	1.11	2 (9%)	25,38,38	1.82	6 (24%)
4	AMP	P	1003	-	22,25,25	0.96	2 (9%)	25,38,38	1.44	5 (20%)
4	AMP	R	1003	-	22,25,25	1.12	2 (9%)	25,38,38	1.00	1 (4%)
3	PO4	B	1002	-	4,4,4	1.96	1 (25%)	6,6,6	0.52	0
4	AMP	F	1003	-	22,25,25	1.16	2 (9%)	25,38,38	1.10	1 (4%)
3	PO4	E	1002	-	4,4,4	2.12	1 (25%)	6,6,6	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	C	1002	-	4,4,4	1.98	1 (25%)	6,6,6	0.46	0
4	AMP	B	1003	-	22,25,25	1.11	2 (9%)	25,38,38	0.97	1 (4%)
3	PO4	L	1002	-	4,4,4	1.99	1 (25%)	6,6,6	0.63	0
4	AMP	I	1003	-	22,25,25	1.13	2 (9%)	25,38,38	1.21	3 (12%)
3	PO4	M	1002	-	4,4,4	1.75	0	6,6,6	0.81	0
3	PO4	K	1002	-	4,4,4	1.86	1 (25%)	6,6,6	0.48	0
4	AMP	J	1003	-	22,25,25	1.06	1 (4%)	25,38,38	0.97	1 (4%)
4	AMP	A	1003	-	22,25,25	1.33	2 (9%)	25,38,38	1.52	3 (12%)
3	PO4	D	1002	-	4,4,4	1.85	1 (25%)	6,6,6	0.41	0
3	PO4	A	1002	-	4,4,4	1.94	1 (25%)	6,6,6	0.58	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	N	1003	-	-	3/6/26/26	0/3/3/3
4	AMP	M	1003	-	-	4/6/26/26	0/3/3/3
4	AMP	H	1003	-	-	6/6/26/26	0/3/3/3
4	AMP	O	1003	-	-	2/6/26/26	0/3/3/3
4	AMP	J	1003	-	-	5/6/26/26	0/3/3/3
4	AMP	I	1003	-	-	4/6/26/26	0/3/3/3
4	AMP	P	1003	-	-	4/6/26/26	0/3/3/3
4	AMP	R	1003	-	-	2/6/26/26	0/3/3/3
4	AMP	Q	1003	-	-	3/6/26/26	0/3/3/3
4	AMP	C	1003	-	-	4/6/26/26	0/3/3/3
4	AMP	D	1003	-	-	6/6/26/26	0/3/3/3
4	AMP	K	1003	-	-	3/6/26/26	0/3/3/3
4	AMP	F	1003	-	-	5/6/26/26	0/3/3/3
4	AMP	E	1003	-	-	1/6/26/26	0/3/3/3
4	AMP	G	1003	-	-	4/6/26/26	0/3/3/3
4	AMP	B	1003	-	-	5/6/26/26	0/3/3/3
4	AMP	A	1003	-	-	6/6/26/26	0/3/3/3
4	AMP	L	1003	-	-	6/6/26/26	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	AMP	O4'-C1'	4.30	1.47	1.41
4	N	1003	AMP	O4'-C1'	4.26	1.47	1.41
4	I	1003	AMP	O4'-C1'	4.02	1.46	1.41
4	G	1003	AMP	O4'-C1'	4.00	1.46	1.41
4	Q	1003	AMP	O4'-C1'	3.88	1.46	1.41

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1003	AMP	O4'-C1'-C2'	-5.72	98.56	106.93
4	A	1003	AMP	P-O5'-C5'	-4.40	106.17	118.30
4	P	1003	AMP	O3P-P-O5'	4.20	117.91	106.73
4	O	1003	AMP	C4-C5-N7	4.17	113.75	109.40
4	M	1003	AMP	N3-C2-N1	-4.04	122.36	128.68

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1003	AMP	C5'-O5'-P-O1P
4	E	1003	AMP	C4'-C5'-O5'-P
4	G	1003	AMP	C5'-O5'-P-O2P
4	G	1003	AMP	C5'-O5'-P-O3P
4	M	1003	AMP	C4'-C5'-O5'-P

There are no ring outliers.

31 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1002	PO4	2	0
4	K	1003	AMP	4	0
4	C	1003	AMP	3	0
3	G	1002	PO4	1	0
4	E	1003	AMP	4	0
4	G	1003	AMP	9	0
3	F	1002	PO4	2	0
3	R	1002	PO4	1	0
4	M	1003	AMP	5	0
3	H	1002	PO4	2	0
4	O	1003	AMP	17	0
3	I	1002	PO4	1	0
3	P	1002	PO4	7	0

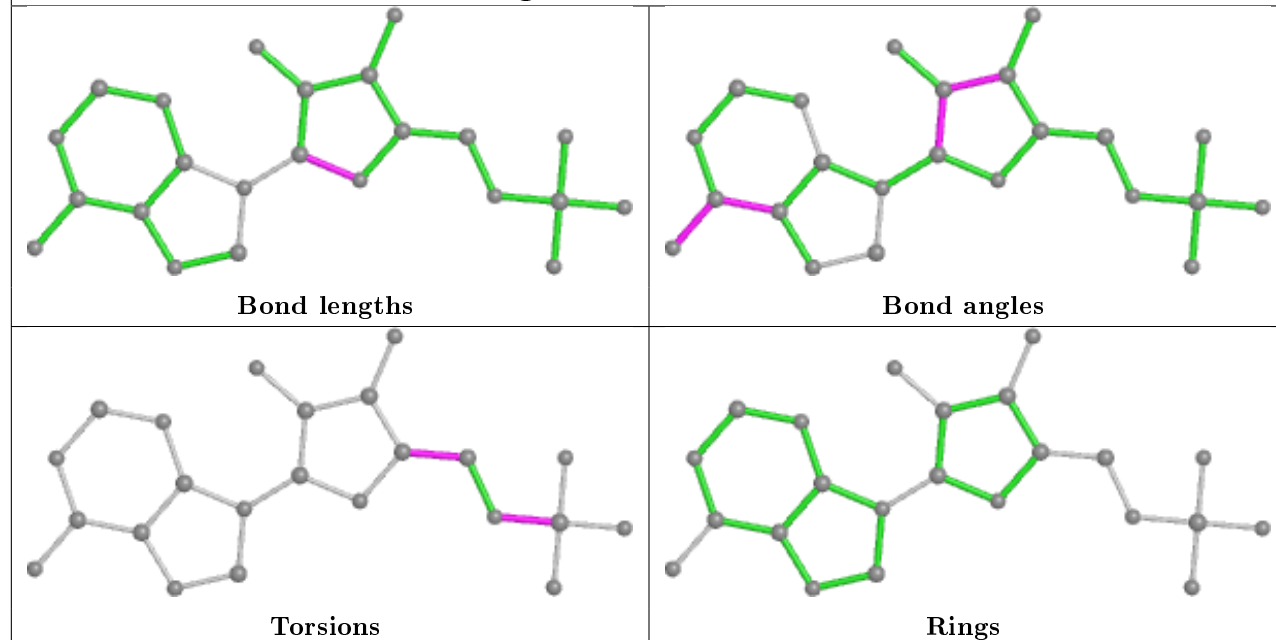
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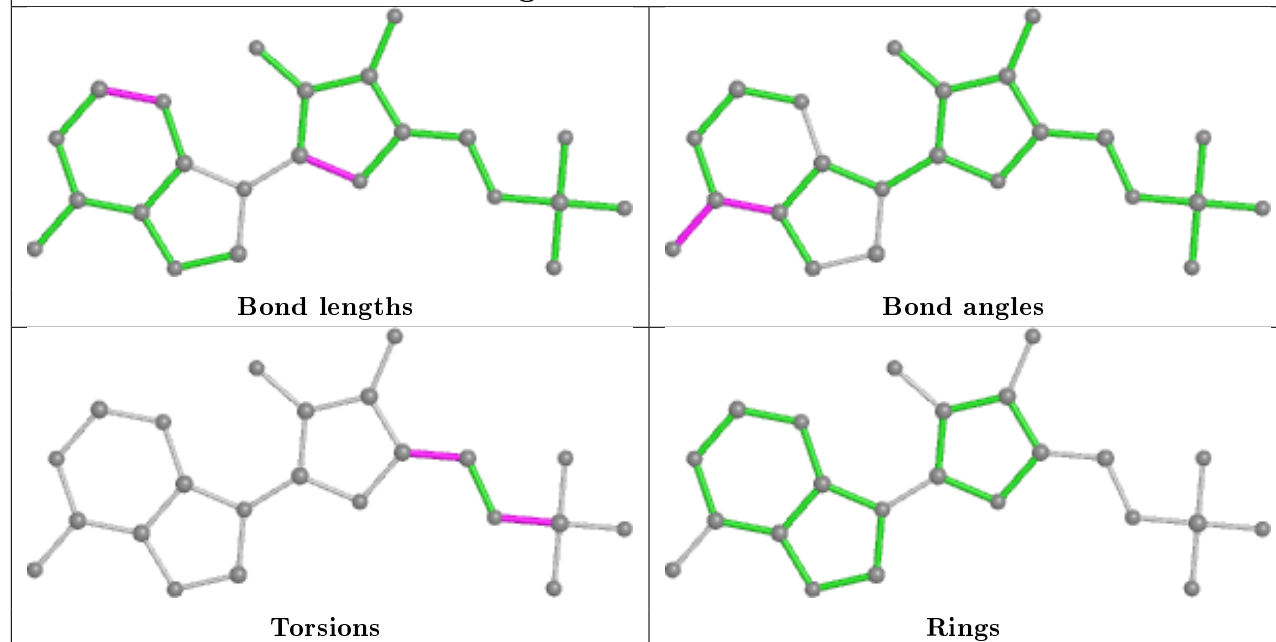
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	1003	AMP	7	0
4	D	1003	AMP	5	0
4	L	1003	AMP	1	0
3	O	1002	PO4	2	0
4	N	1003	AMP	6	0
4	H	1003	AMP	1	0
4	P	1003	AMP	12	0
4	R	1003	AMP	4	0
3	B	1002	PO4	1	0
4	F	1003	AMP	2	0
3	E	1002	PO4	3	0
4	B	1003	AMP	8	0
4	I	1003	AMP	7	0
3	M	1002	PO4	3	0
3	K	1002	PO4	1	0
4	J	1003	AMP	3	0
4	A	1003	AMP	10	0
3	A	1002	PO4	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.

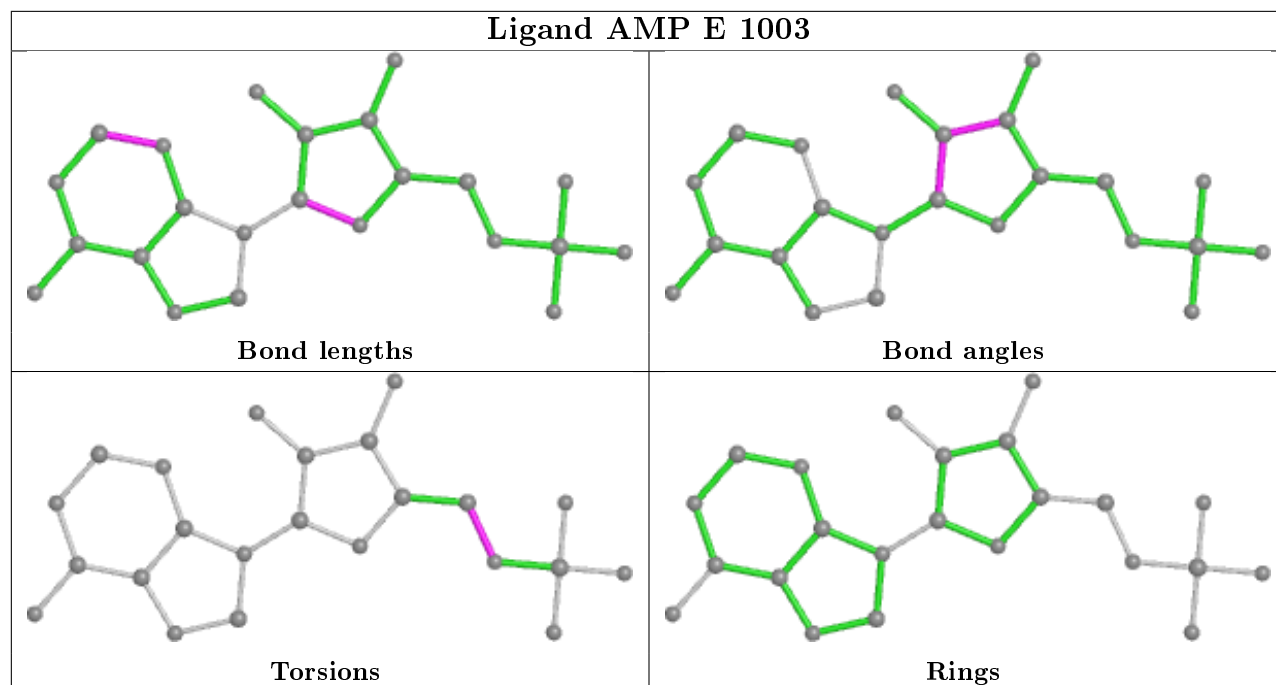
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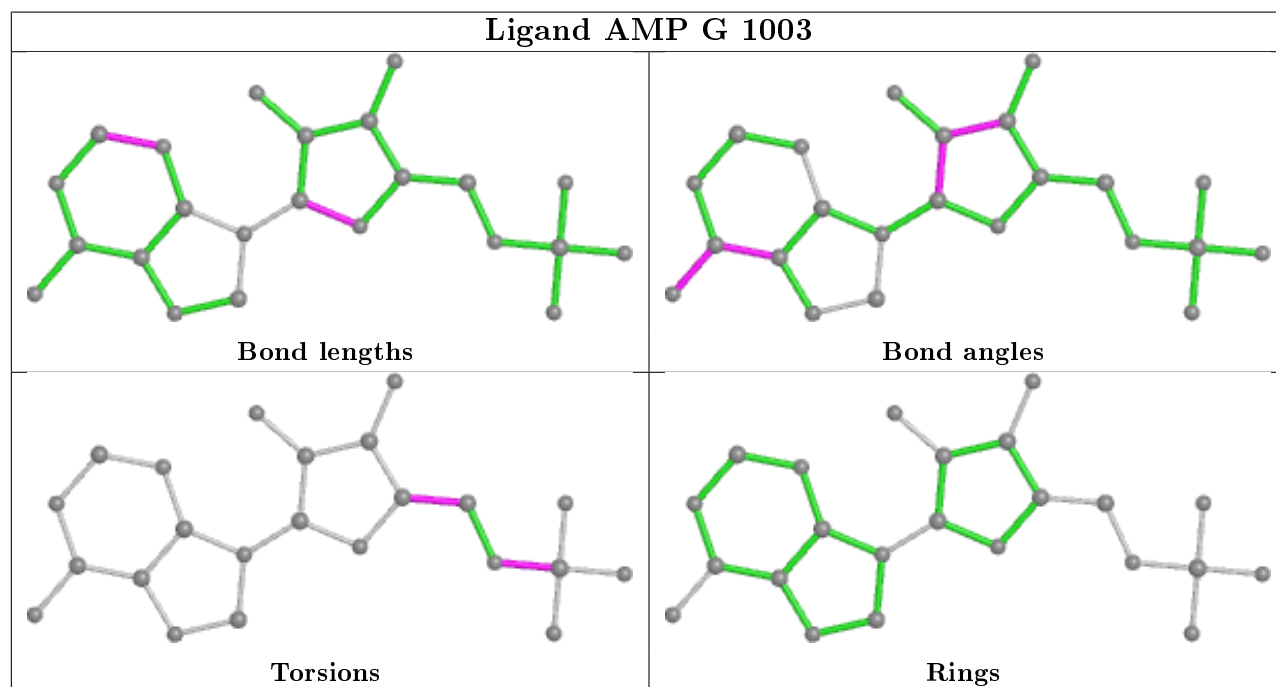
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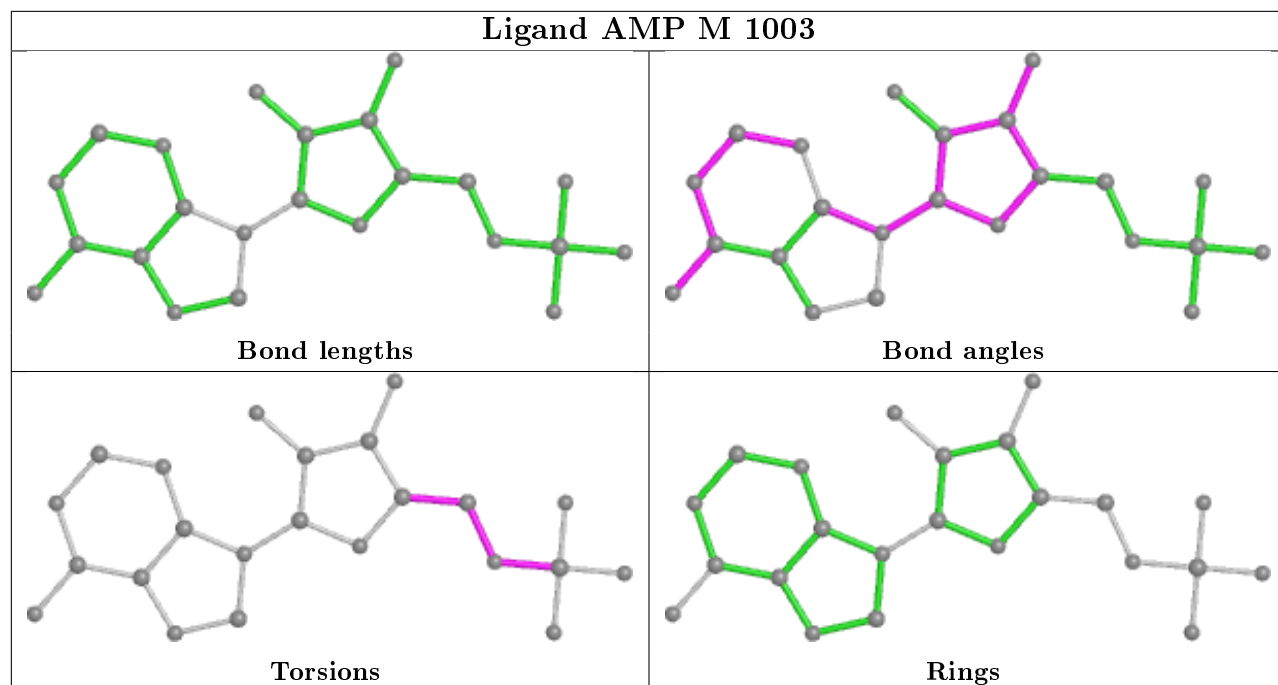
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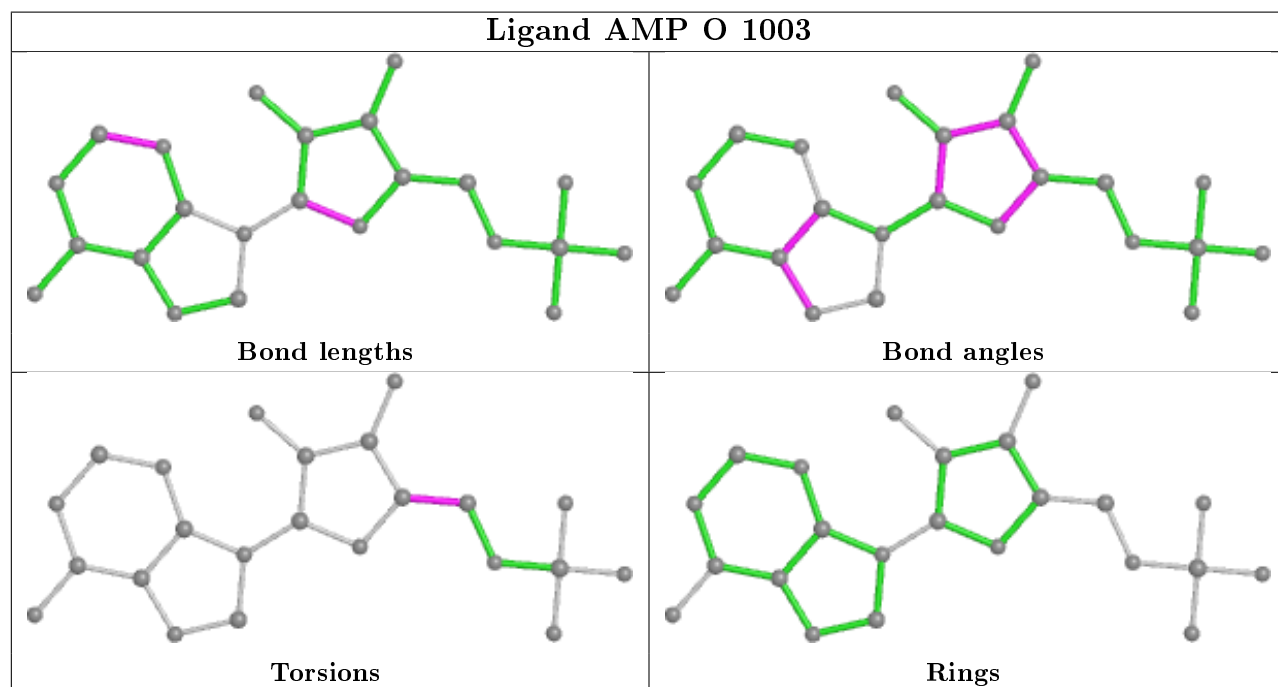
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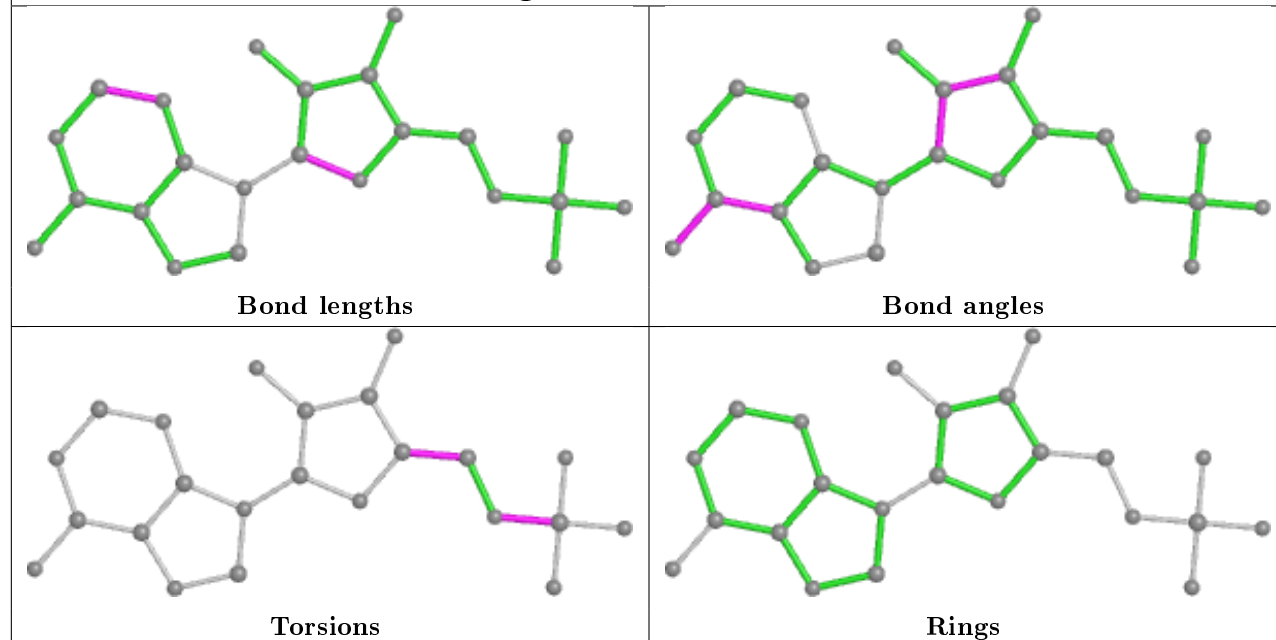
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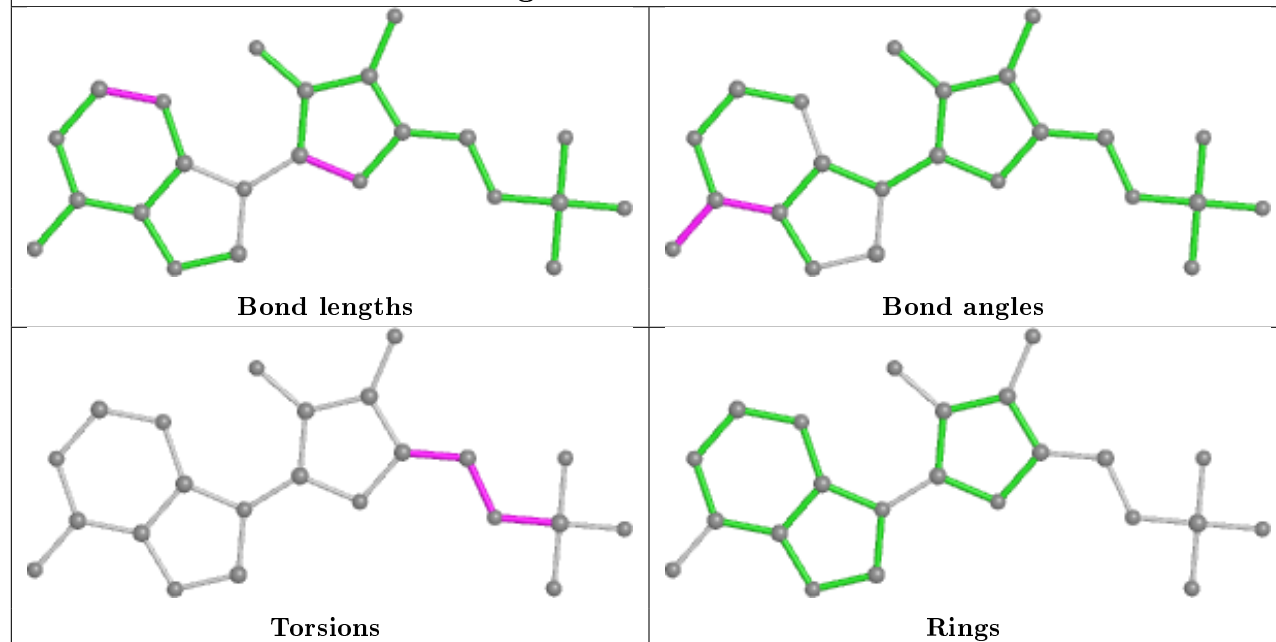
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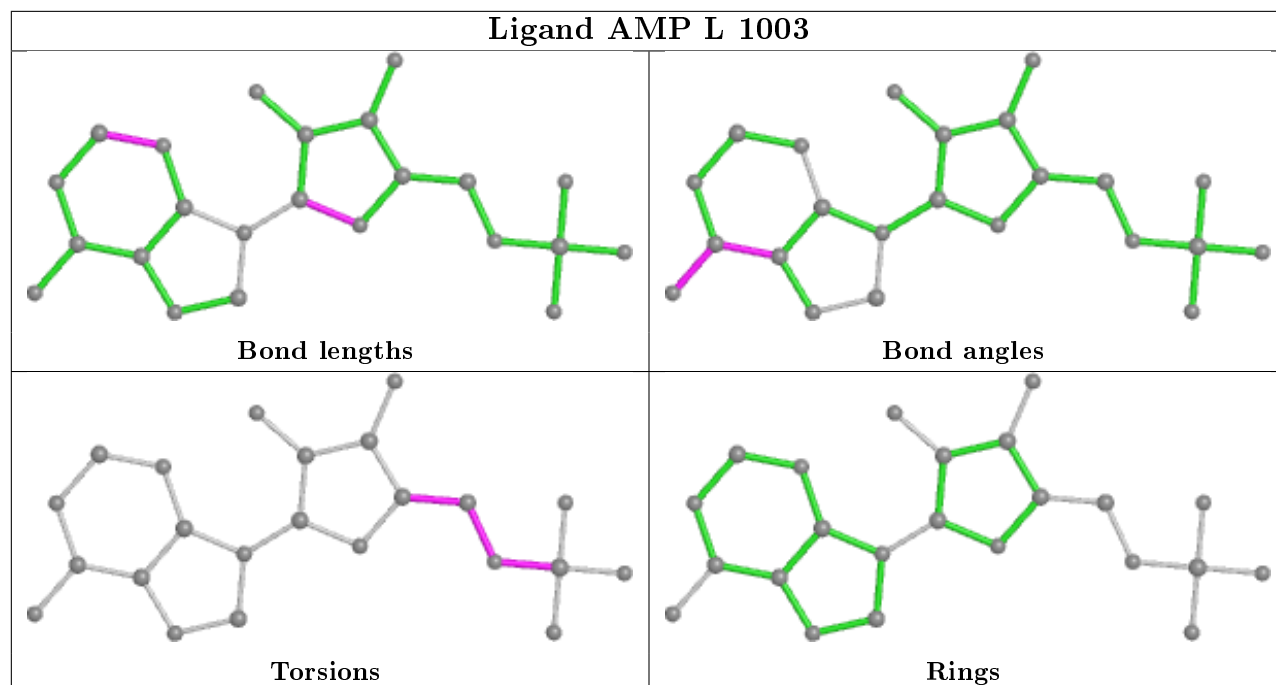
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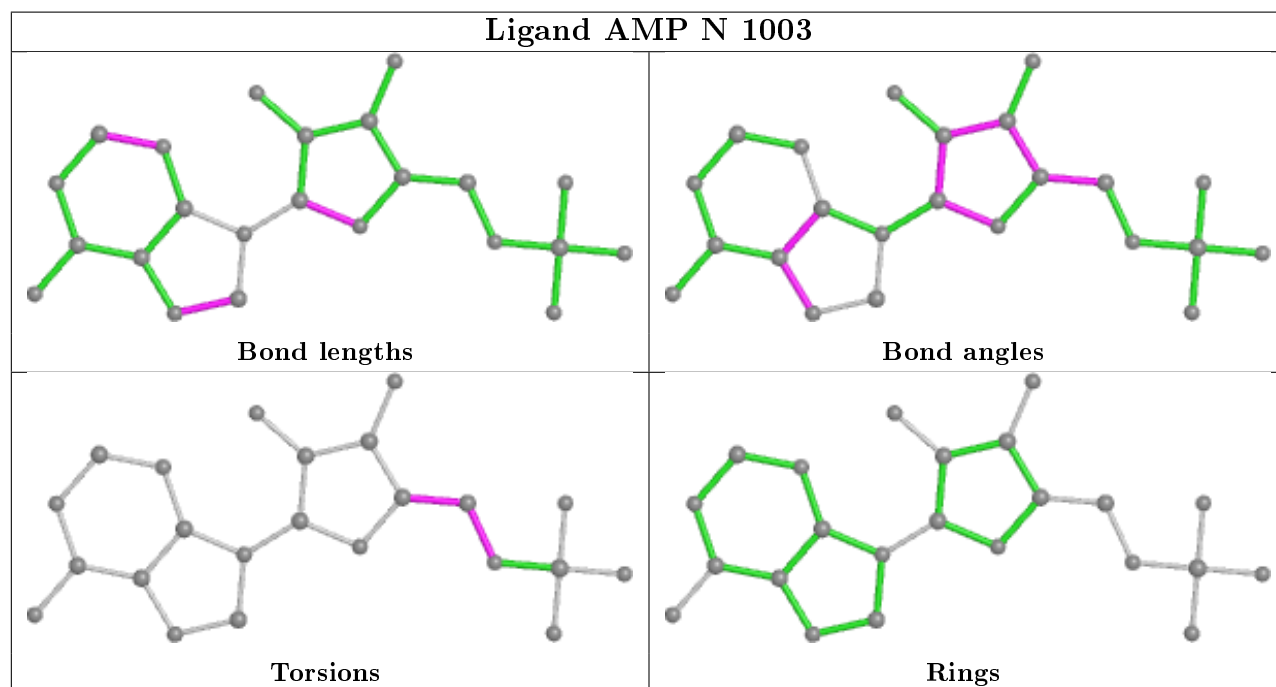
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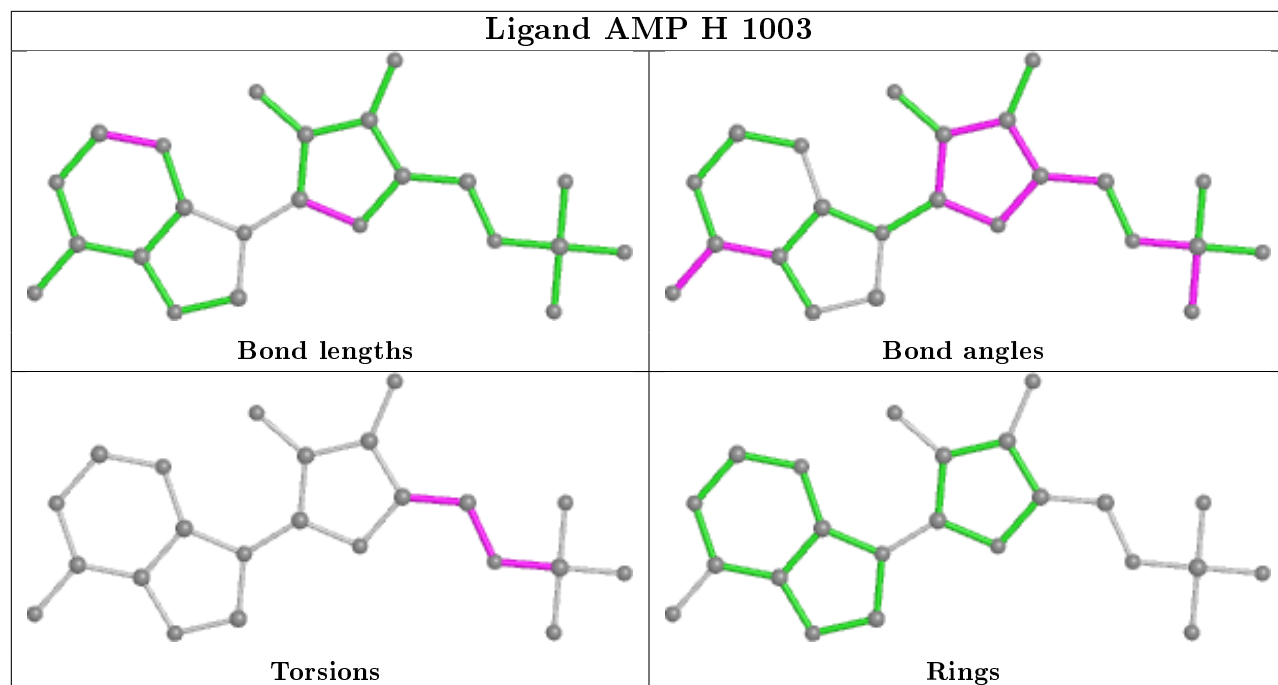
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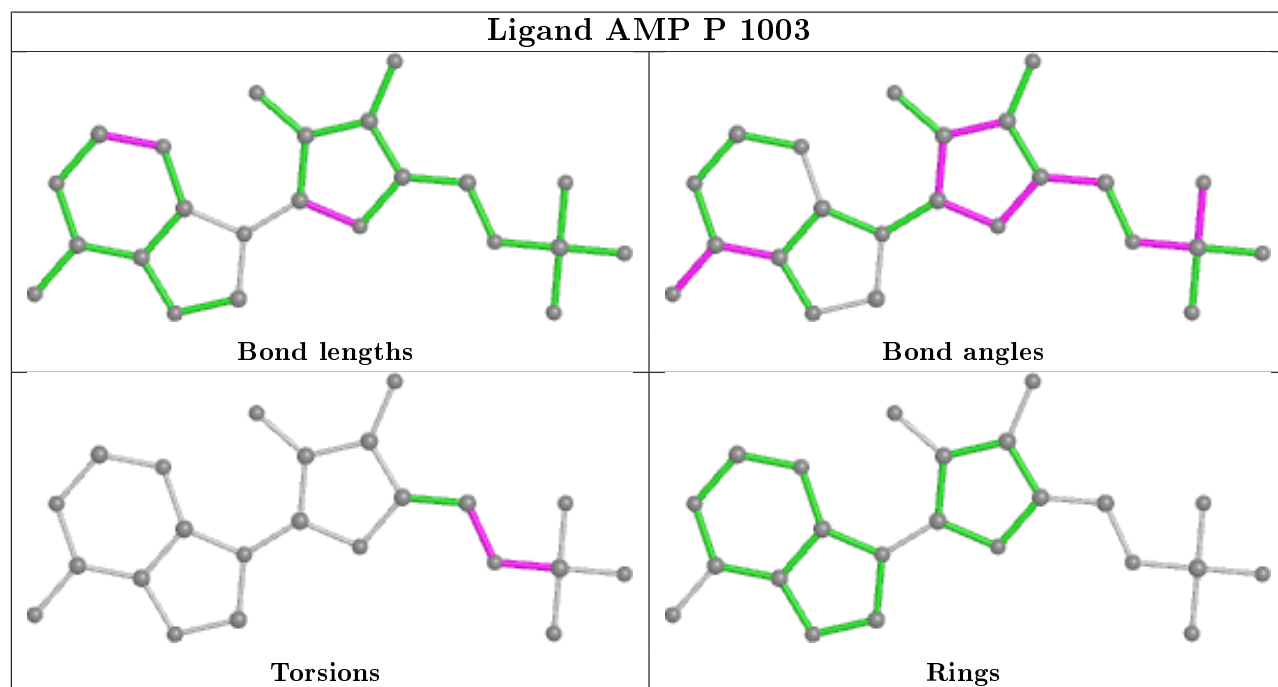
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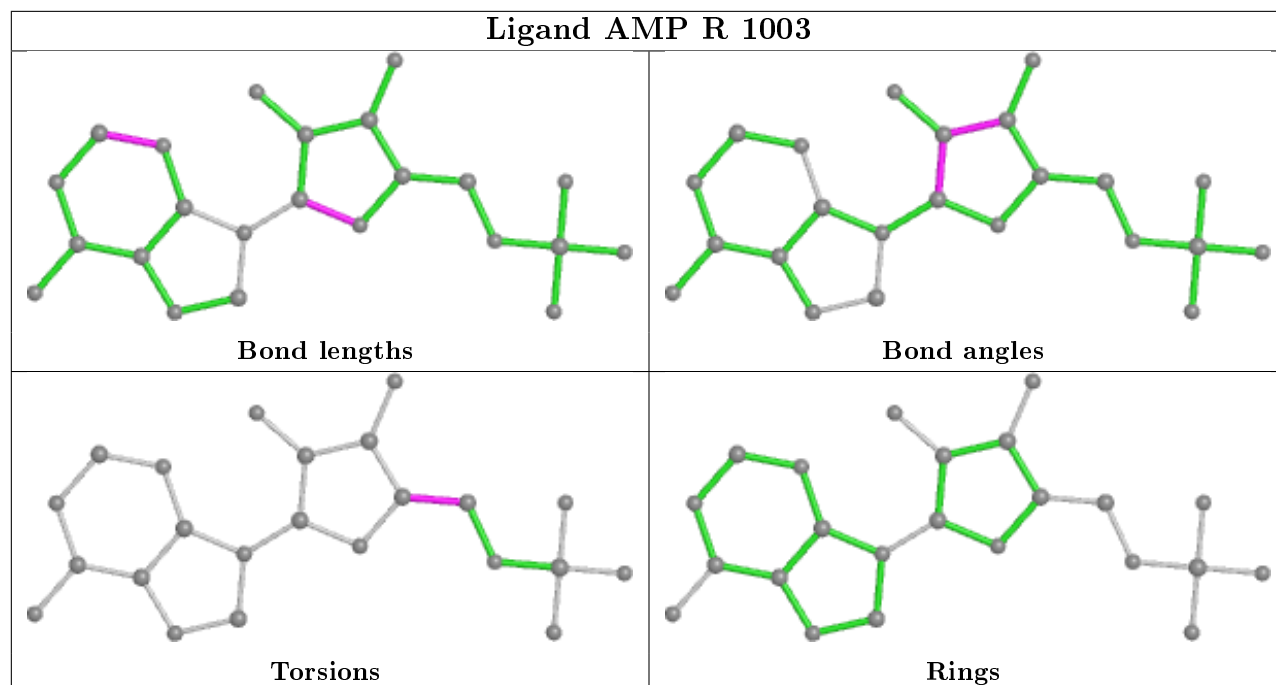
Ligand AMP H 1003



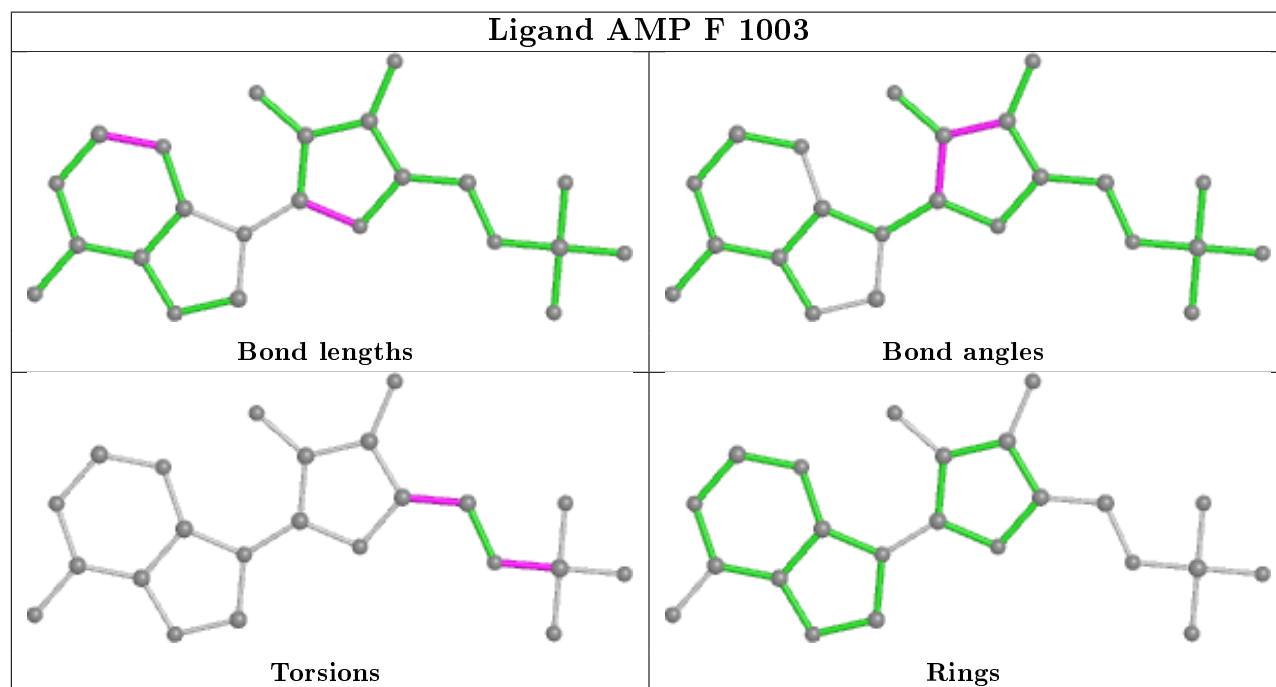
Ligand AMP P 1003



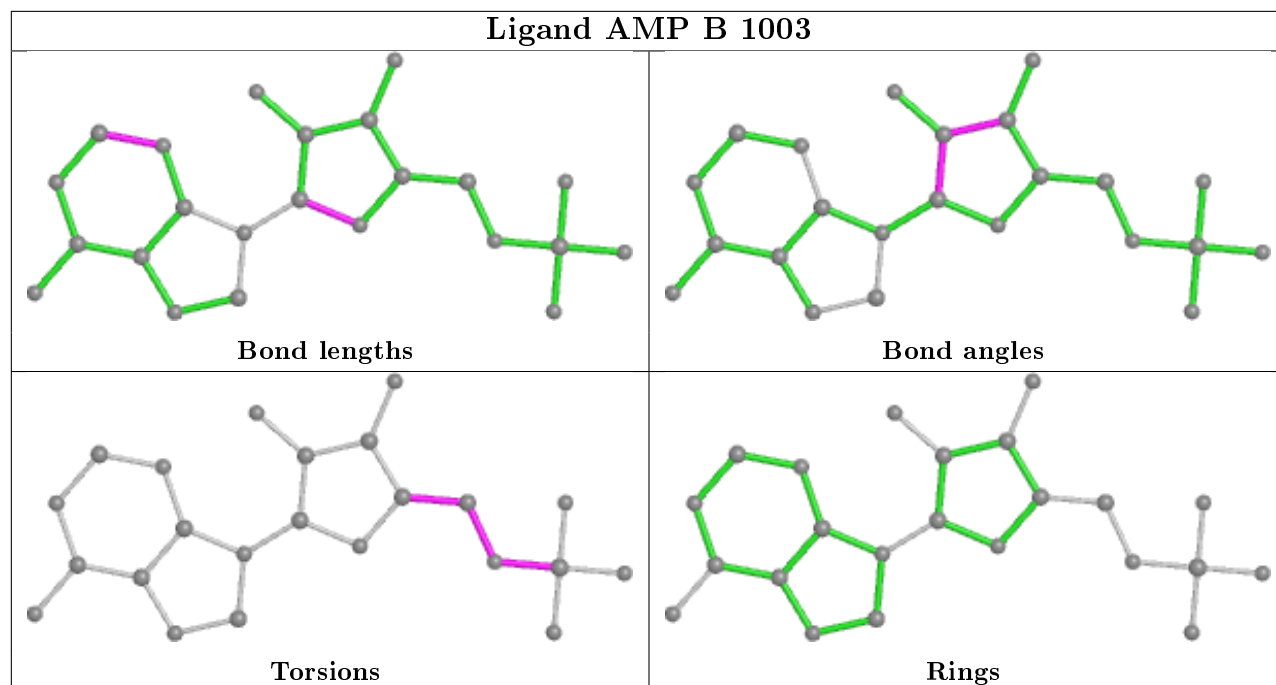
Ligand AMP R 1003



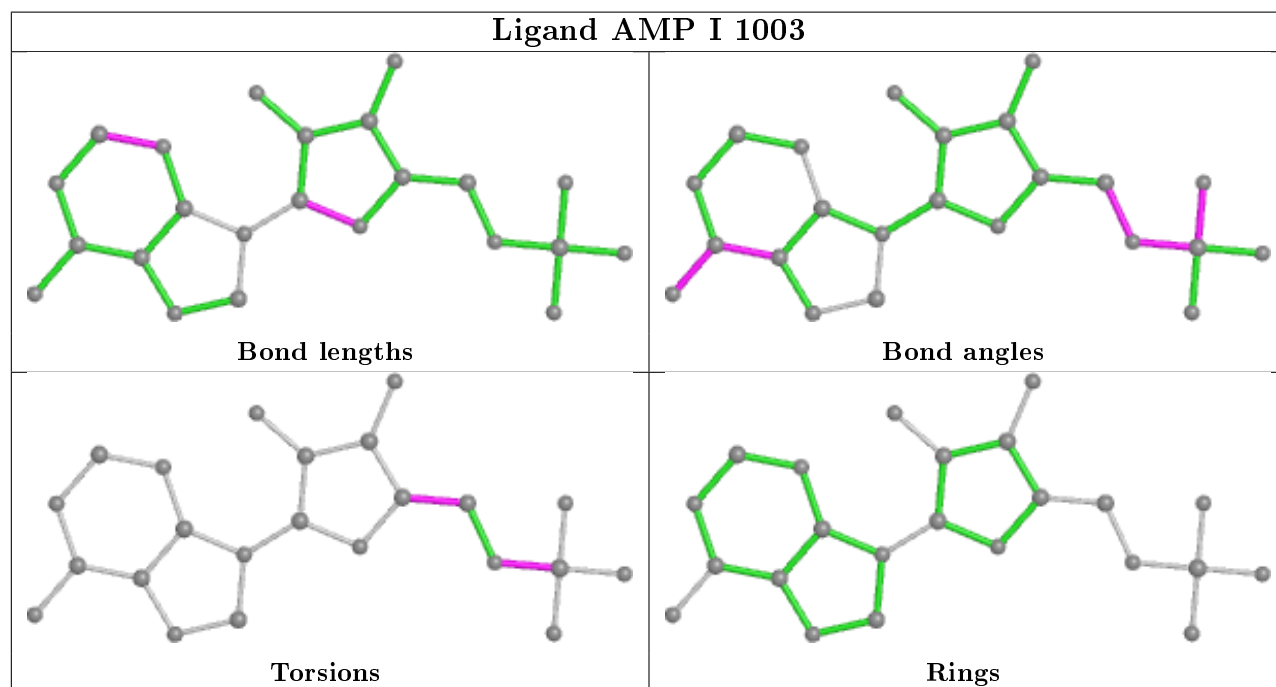
Ligand AMP F 1003

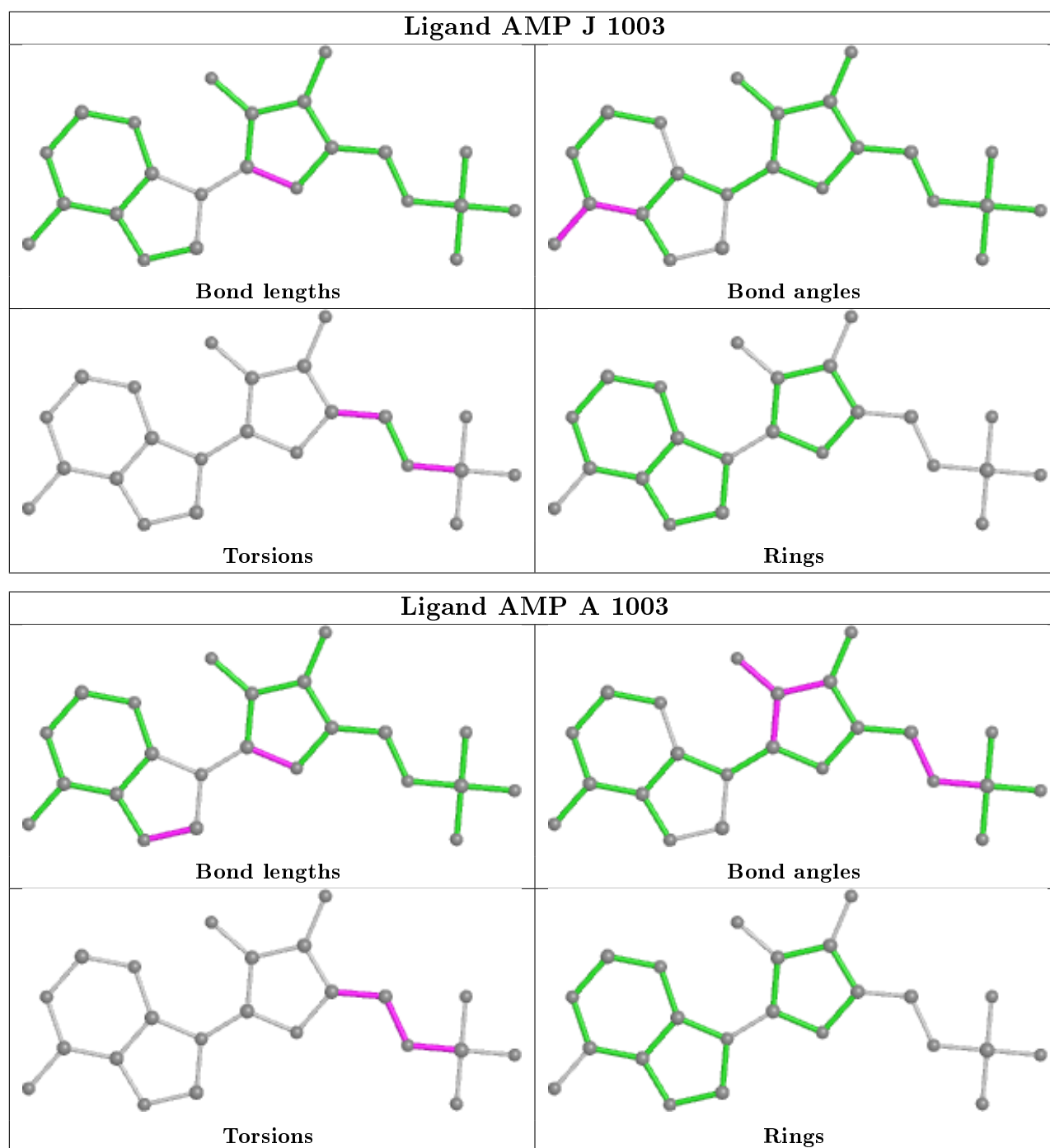


Ligand AMP B 1003



Ligand AMP I 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

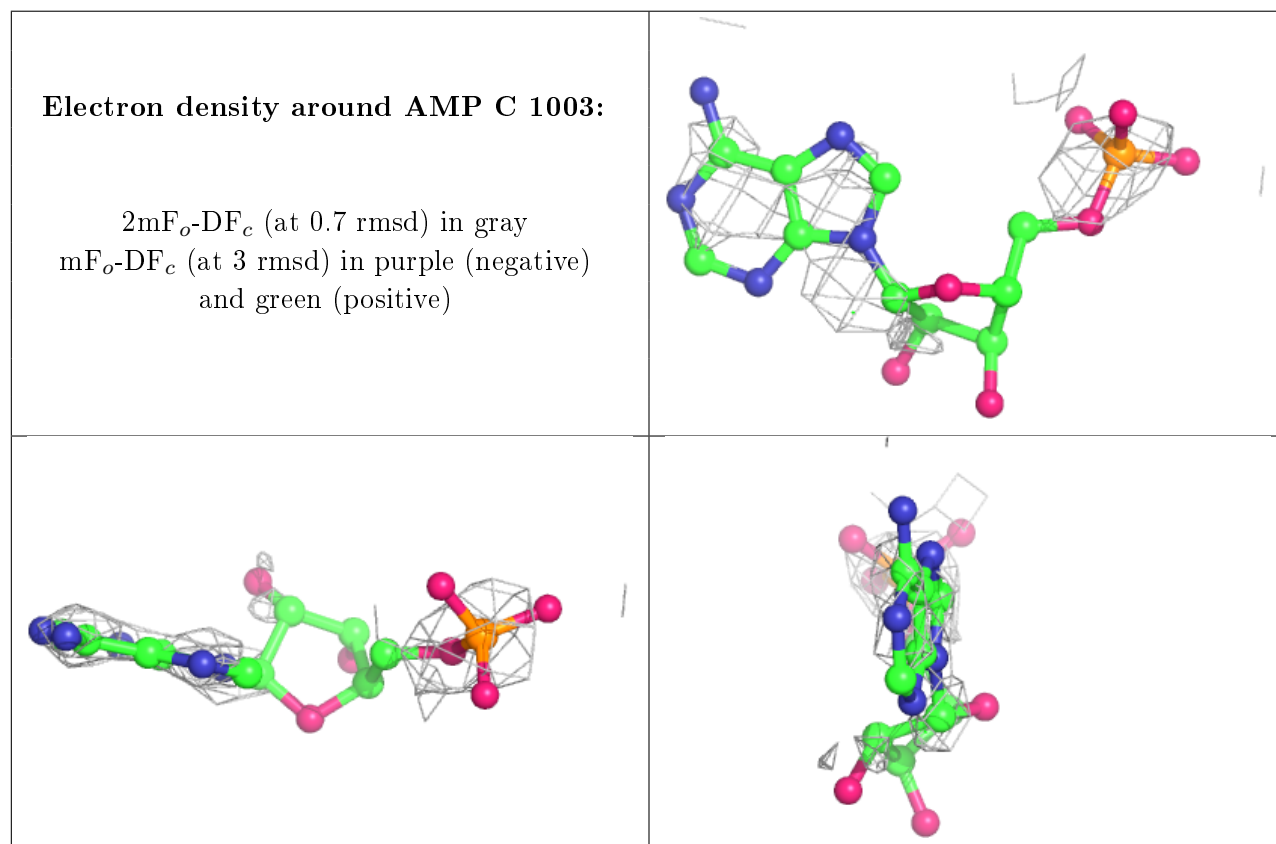
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

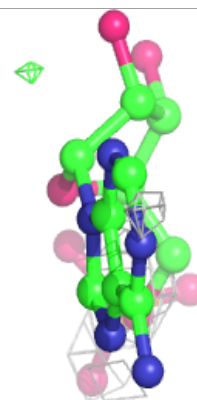
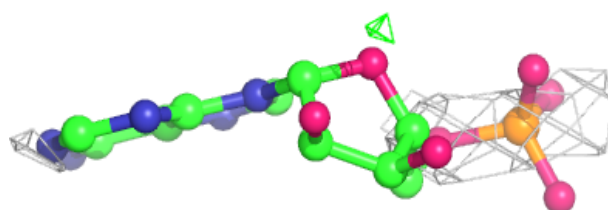
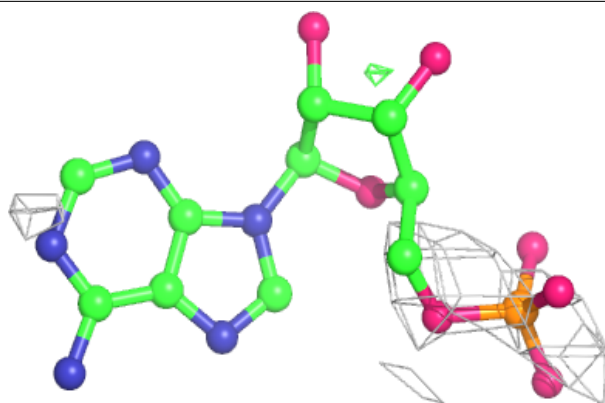
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

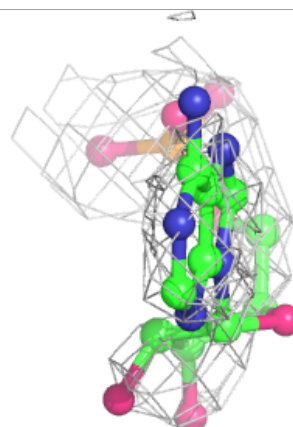
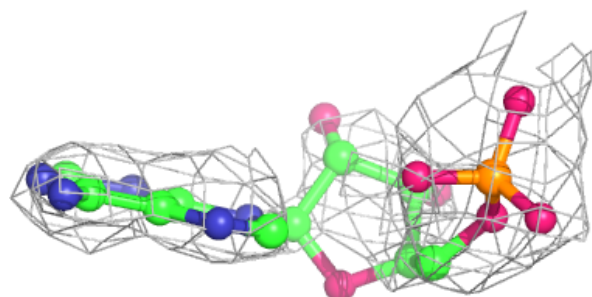
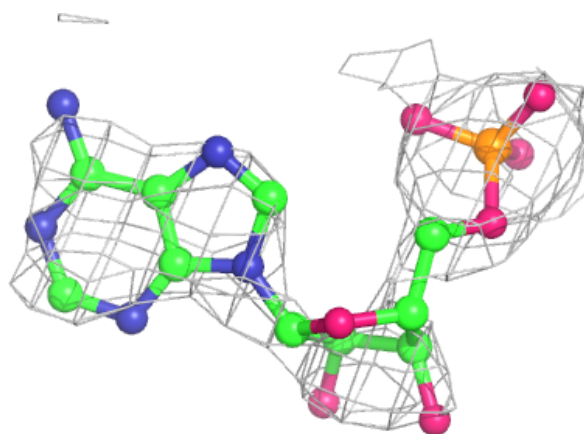


Electron density around AMP E 1003:

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

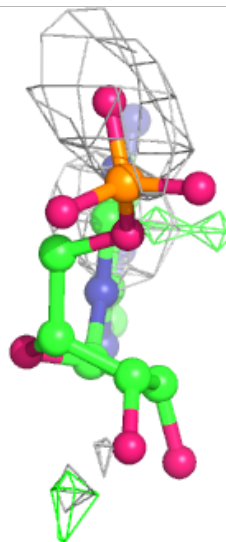
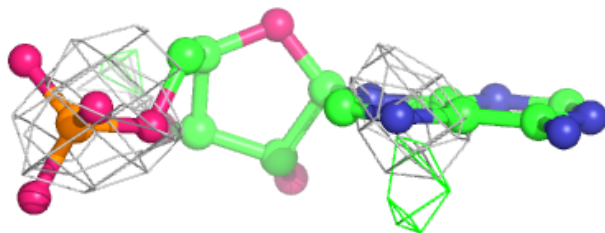
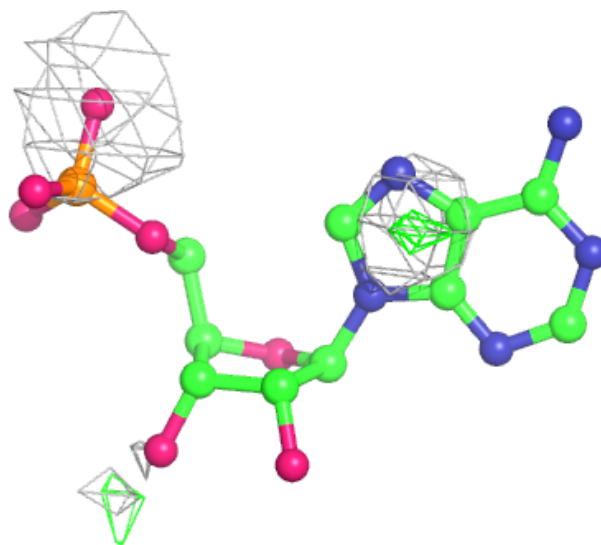
**Electron density around AMP G 1003:**

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



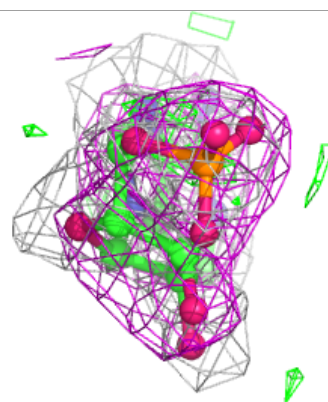
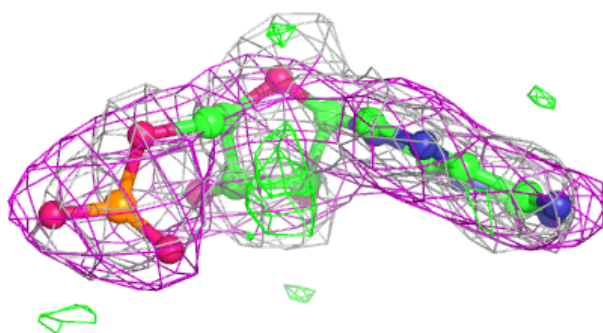
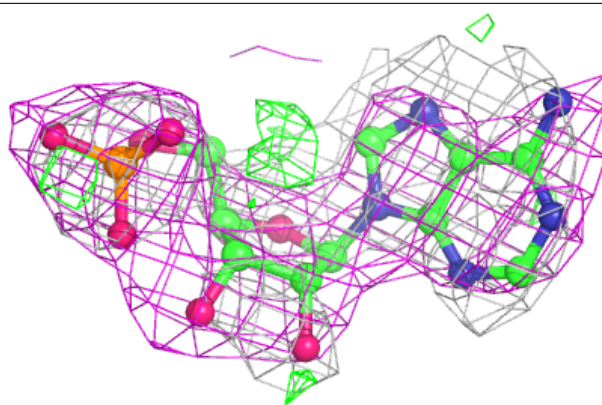
Electron density around AMP K 1003:

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

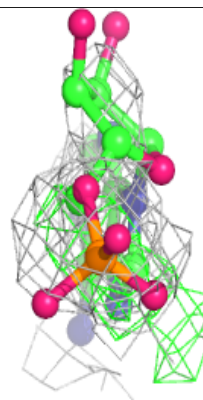
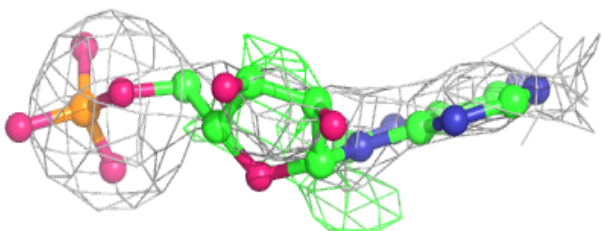
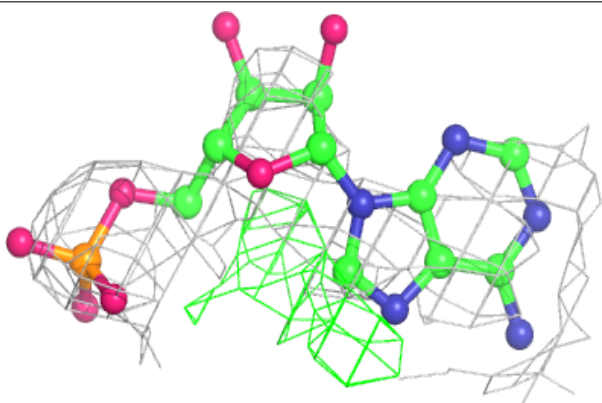


Electron density around AMP M 1003:

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

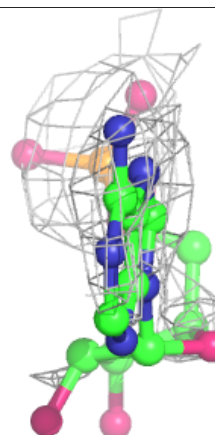
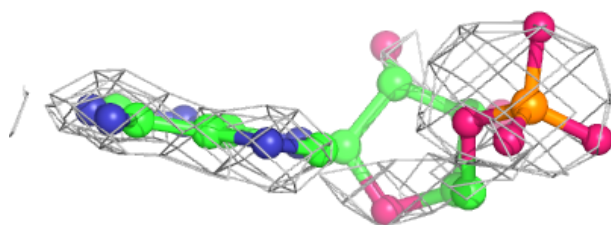
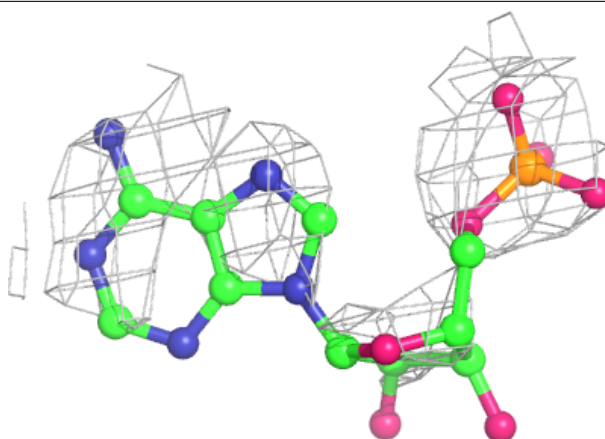
**Electron density around AMP O 1003:**

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

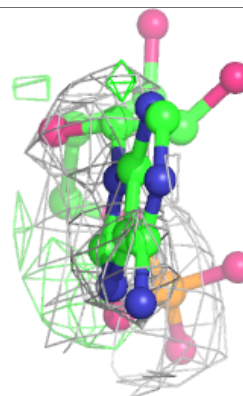
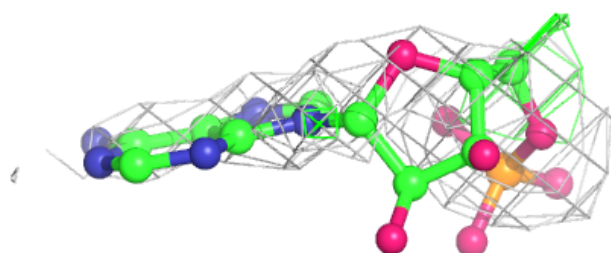
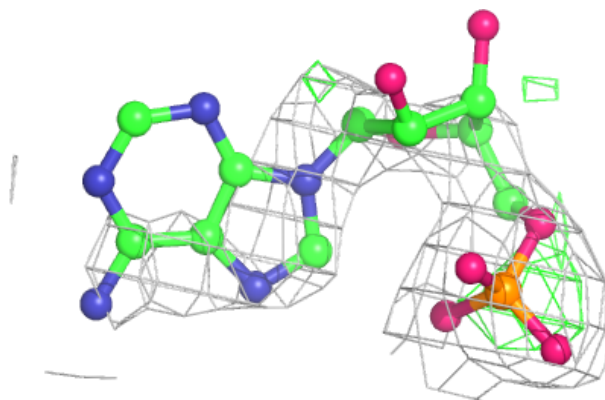


Electron density around AMP Q 1003:

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

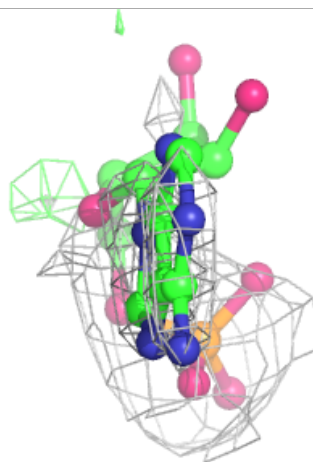
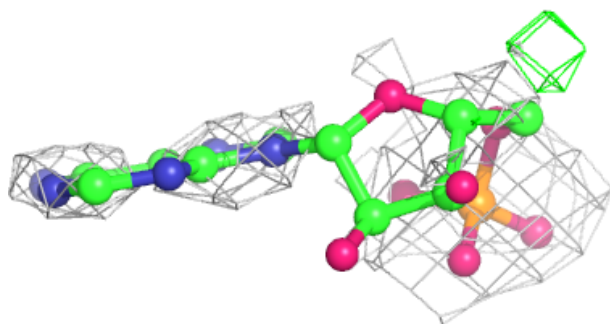
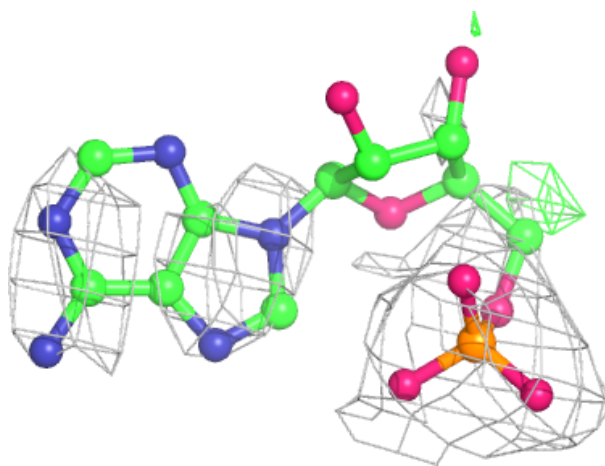
**Electron density around AMP D 1003:**

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



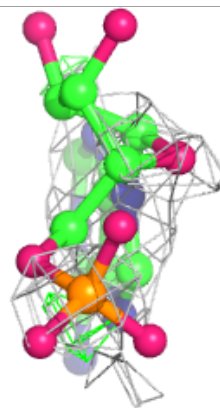
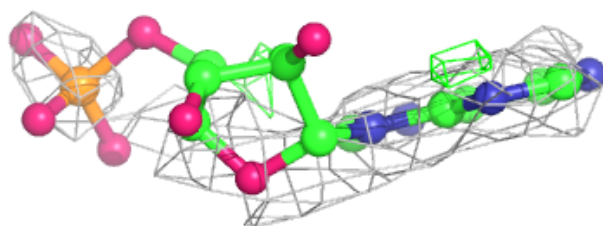
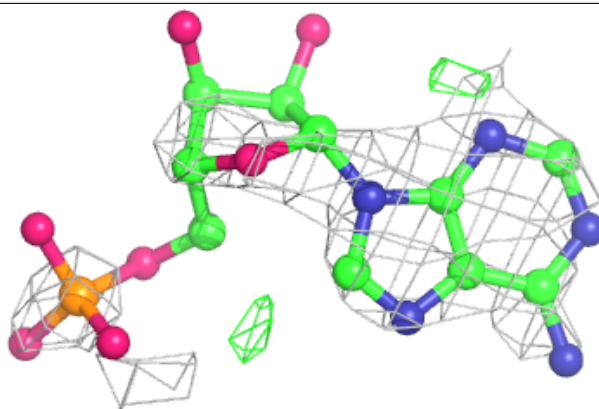
Electron density around AMP L 1003:

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



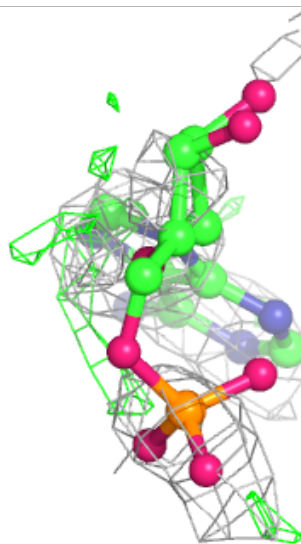
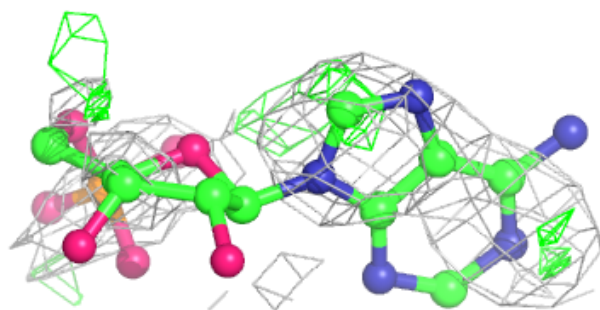
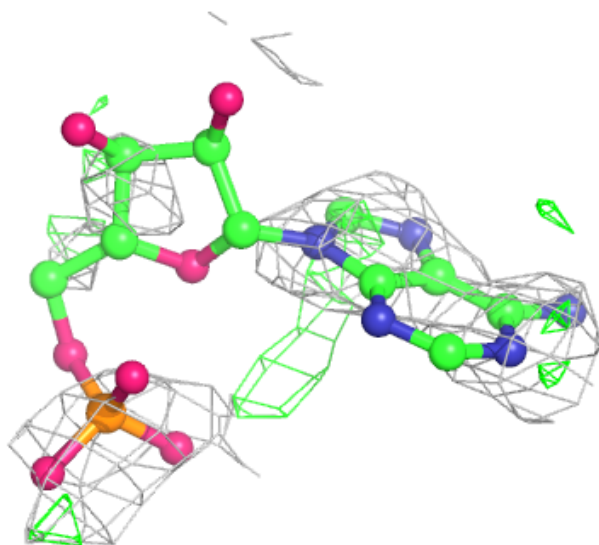
Electron density around AMP N 1003:

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



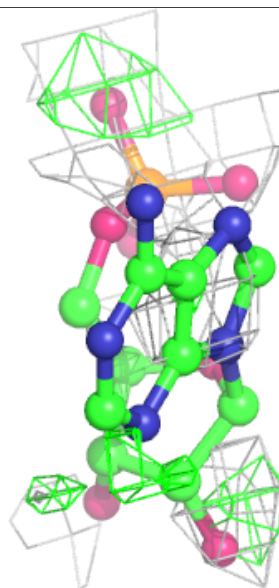
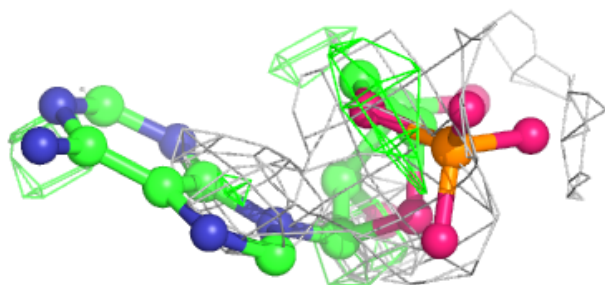
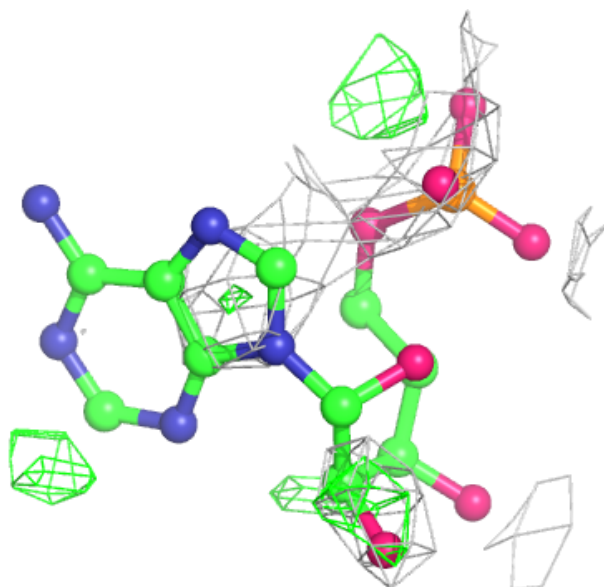
Electron density around AMP H 1003:

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



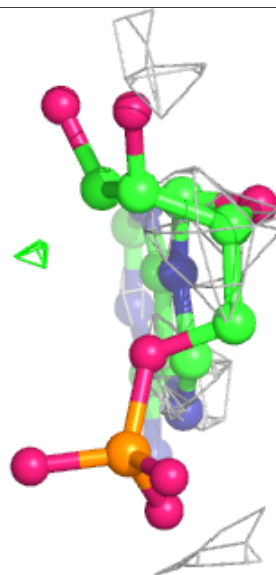
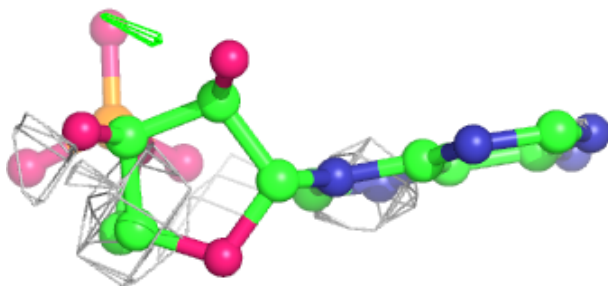
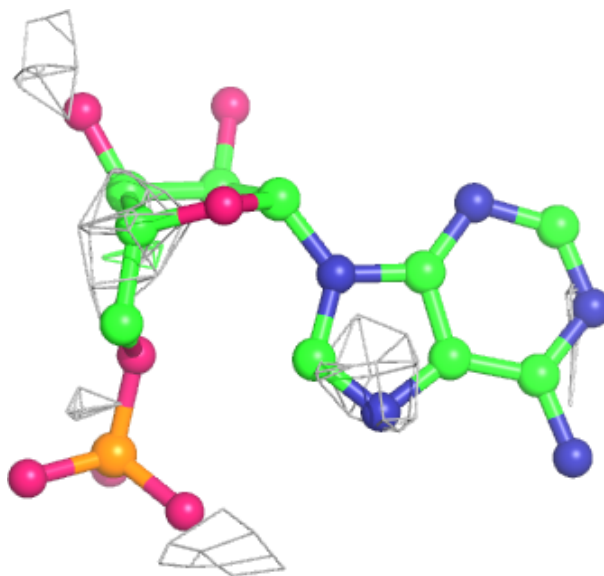
Electron density around AMP P 1003:

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



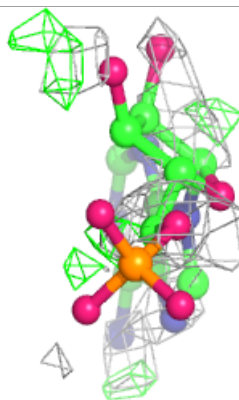
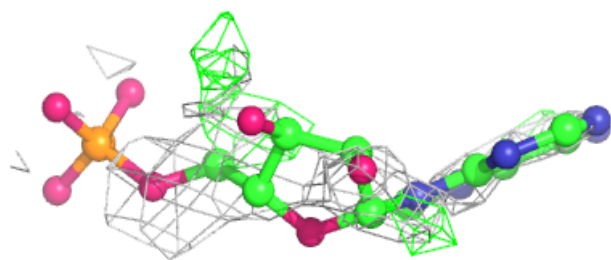
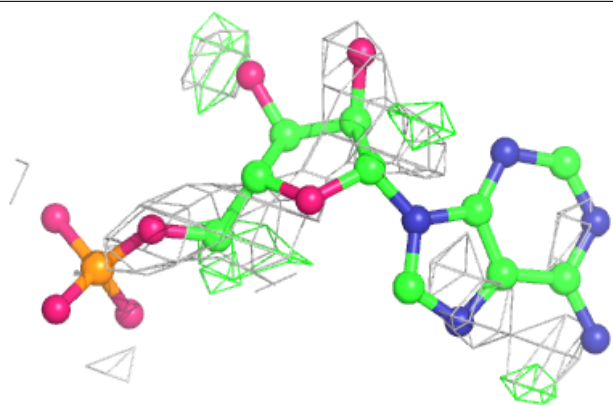
Electron density around AMP R 1003:

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

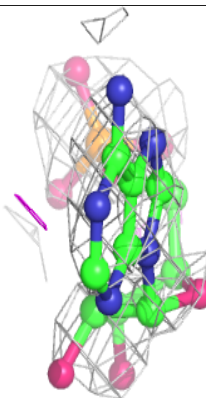
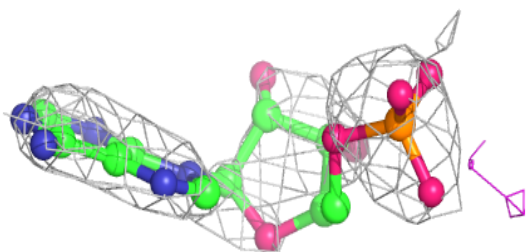
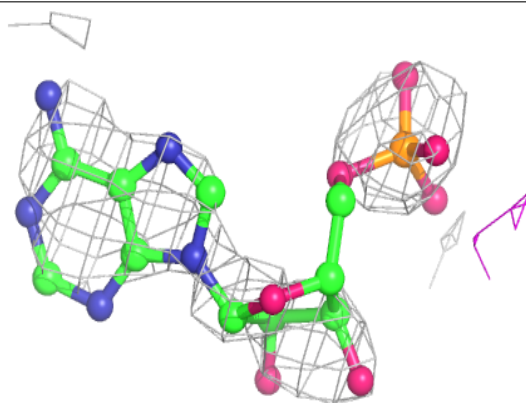


Electron density around AMP F 1003:

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

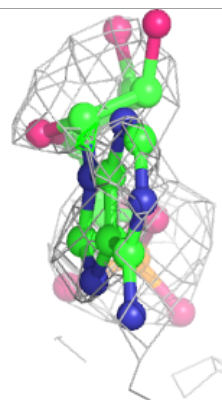
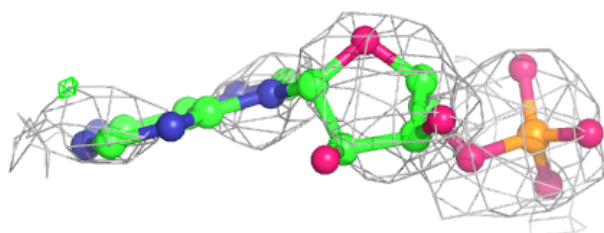
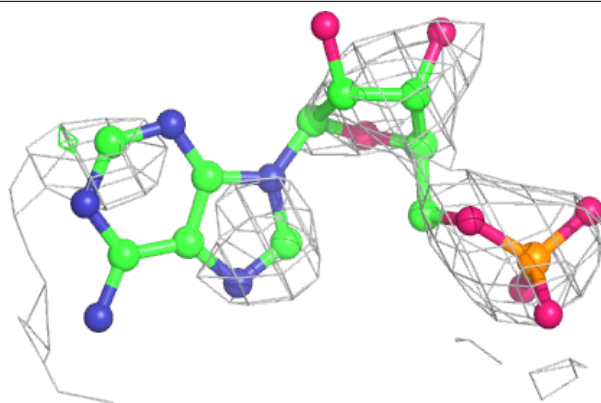
**Electron density around AMP A 1003:**

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

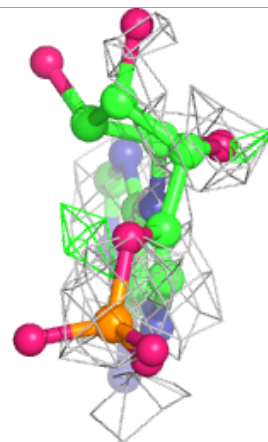
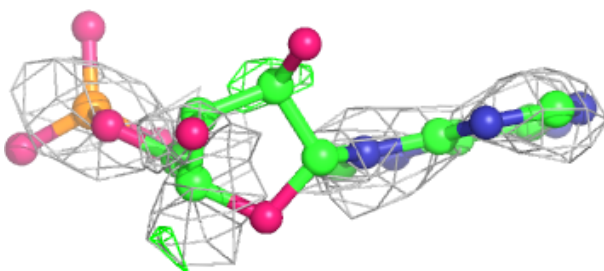
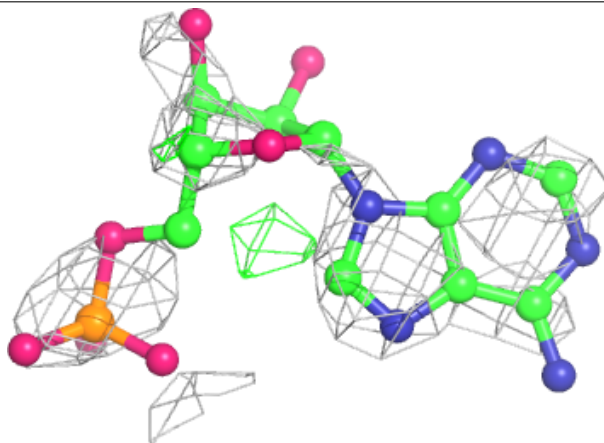


Electron density around AMP B 1003:

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

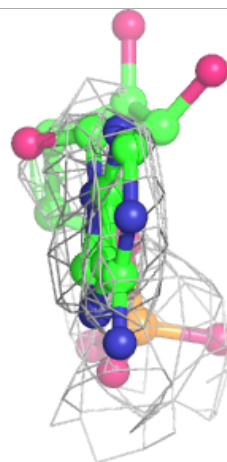
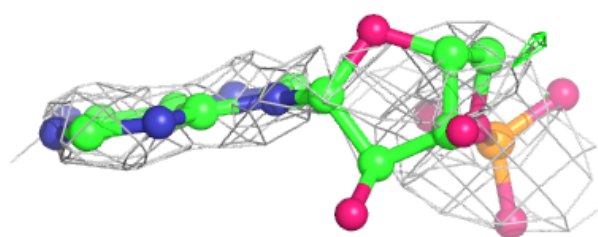
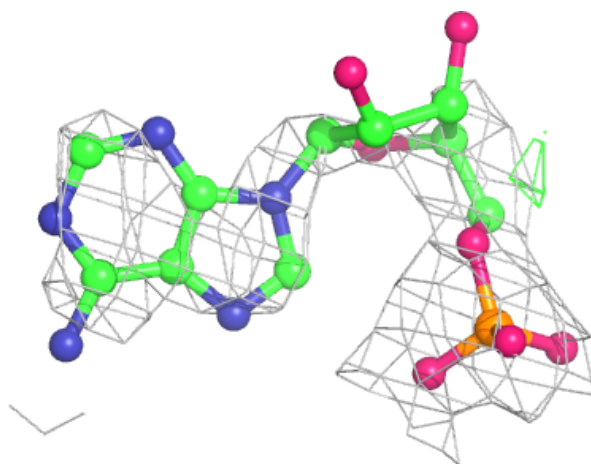
**Electron density around AMP I 1003:**

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



Electron density around AMP 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)



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.