



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 08:02 AM EDT

PDB ID : 4XYC  
Title : NANOMOLAR INHIBITORS OF MYCOBACTERIUM TUBERCULOSIS  
GLUTAMINE SYNTHETASE 1: SYNTHESIS, BIOLOGICAL EVALUA-  
TION AND X-RAY CRYSTALLOGRAPHIC STUDIES  
Authors : Couturier, C.; Silve, S.; Morales, R.; Ppessegue, B.; Llopart, S.; Nair, A.;  
Bauer, A.; Scheiper, B.; poeverlein, c.; Ganzhorn, A.; Lagrange, S.; Bacque,  
E.  
Deposited on : 2015-02-02  
Resolution : 3.30 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](mailto: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

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.37.1
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)

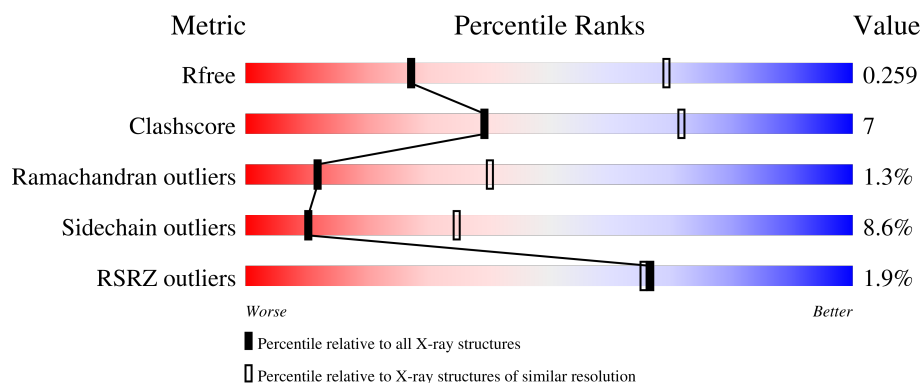
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

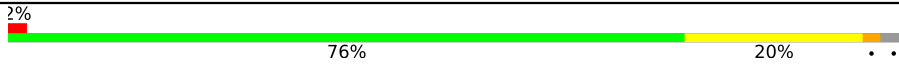

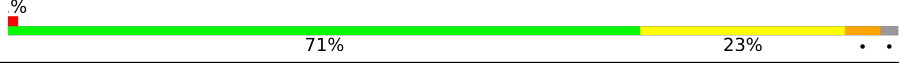
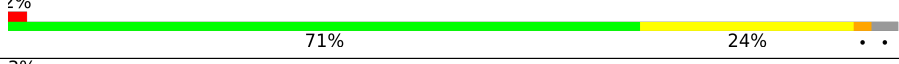

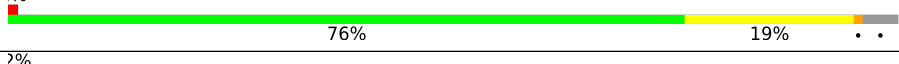


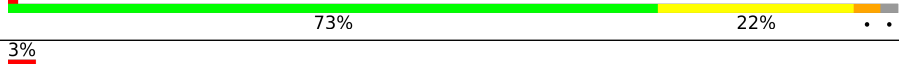


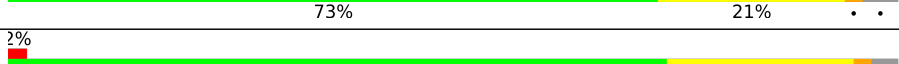

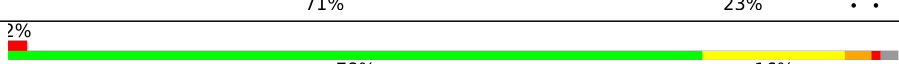
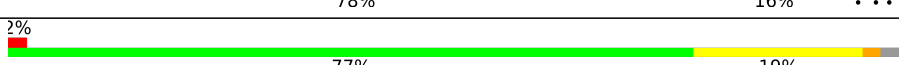
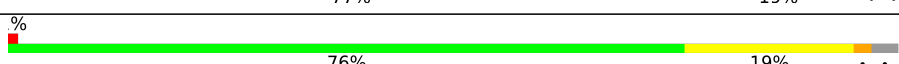
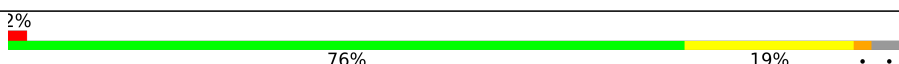
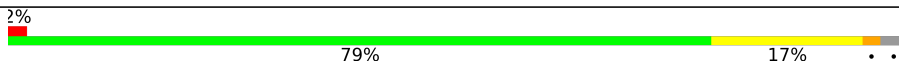
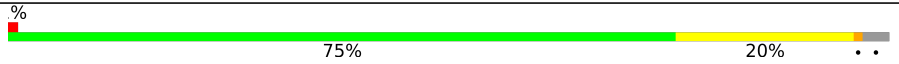


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	478	<div> <div>4%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>
1	B	478	<div> <div>3%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	C	478	<div> <div>%</div> <div>73%</div> <div>19%</div> <div>..</div> </div>

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

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Mol	Chain	Length	Quality of chain
1	D	478	
1	E	478	
1	F	478	
1	G	478	
1	H	478	
1	I	478	
1	J	478	
1	K	478	
1	L	478	
1	M	478	
1	N	478	
1	O	478	
1	P	478	
1	Q	478	
1	R	478	
1	S	478	
1	T	478	
1	U	478	
1	V	478	
1	W	478	
1	X	478	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 88848 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 Glutamine synthetase 1.

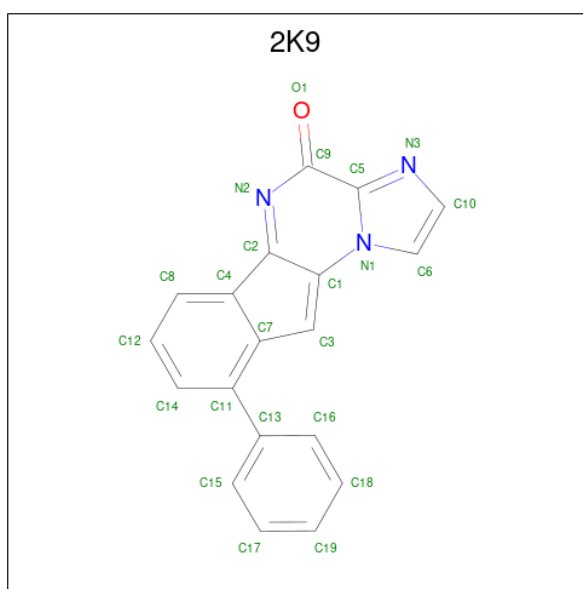
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3693	2354	618	709	12			
1	B	464	Total	C	N	O	S	0	0	0
			3674	2342	613	707	12			
1	C	460	Total	C	N	O	S	0	0	0
			3645	2325	609	699	12			
1	D	466	Total	C	N	O	S	0	0	0
			3690	2352	616	710	12			
1	E	463	Total	C	N	O	S	0	0	0
			3670	2341	613	704	12			
1	F	467	Total	C	N	O	S	0	0	0
			3702	2359	619	712	12			
1	G	466	Total	C	N	O	S	0	0	0
			3693	2354	618	709	12			
1	H	464	Total	C	N	O	S	0	0	0
			3674	2342	613	707	12			
1	I	460	Total	C	N	O	S	0	0	0
			3645	2325	609	699	12			
1	J	466	Total	C	N	O	S	0	0	0
			3690	2352	616	710	12			
1	K	463	Total	C	N	O	S	0	0	0
			3670	2341	613	704	12			
1	L	467	Total	C	N	O	S	0	0	0
			3702	2359	619	712	12			
1	M	466	Total	C	N	O	S	0	0	0
			3693	2354	618	709	12			
1	N	464	Total	C	N	O	S	0	0	0
			3674	2342	613	707	12			
1	O	460	Total	C	N	O	S	0	0	0
			3645	2325	609	699	12			
1	P	466	Total	C	N	O	S	0	0	0
			3690	2352	616	710	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	463	Total	C	N	O	S	0	0	0
			3670	2341	613	704	12			
1	R	467	Total	C	N	O	S	0	0	0
			3702	2359	619	712	12			
1	S	466	Total	C	N	O	S	0	0	0
			3693	2354	618	709	12			
1	T	464	Total	C	N	O	S	0	0	0
			3674	2342	613	707	12			
1	U	460	Total	C	N	O	S	0	0	0
			3645	2325	609	699	12			
1	V	466	Total	C	N	O	S	0	0	0
			3690	2352	616	710	12			
1	W	463	Total	C	N	O	S	0	0	0
			3670	2341	613	704	12			
1	X	467	Total	C	N	O	S	0	0	0
			3702	2359	619	712	12			

- Molecule 2 is 9-phenyl-4H-imidazo[1,2-a]indeno[1,2-e]pyrazin-4-one (three-letter code: 2K9) (formula: C<sub>19</sub>H<sub>11</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	19	3	1		
2	B	1	Total	C	N	O	0	0
			23	19	3	1		
2	C	1	Total	C	N	O	0	0
			23	19	3	1		

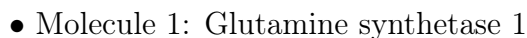
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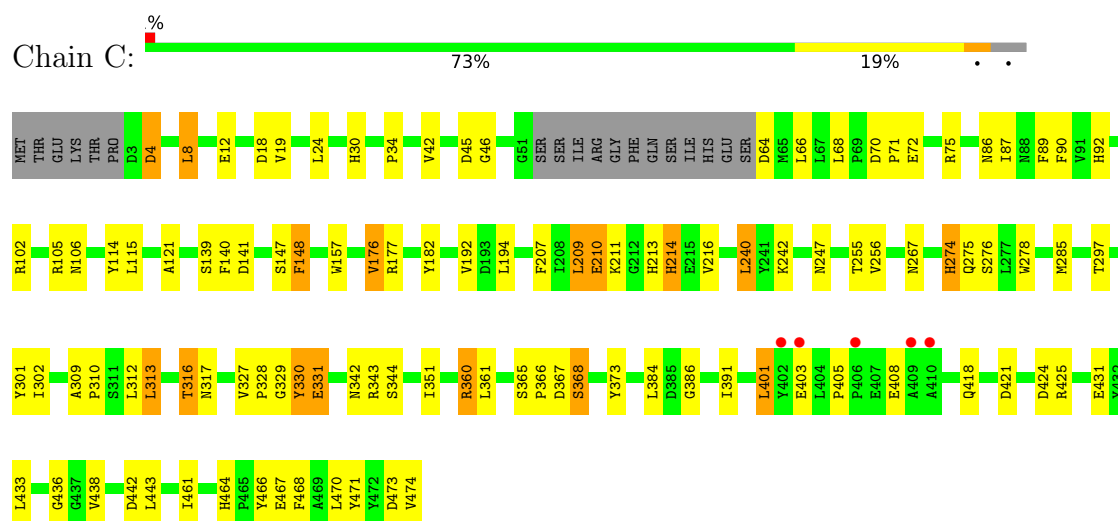
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total 23	C 19	N 3	O 1	0	0
2	E	1	Total 23	C 19	N 3	O 1	0	0
2	F	1	Total 23	C 19	N 3	O 1	0	0
2	G	1	Total 23	C 19	N 3	O 1	0	0
2	H	1	Total 23	C 19	N 3	O 1	0	0
2	I	1	Total 23	C 19	N 3	O 1	0	0
2	J	1	Total 23	C 19	N 3	O 1	0	0
2	K	1	Total 23	C 19	N 3	O 1	0	0
2	L	1	Total 23	C 19	N 3	O 1	0	0
2	M	1	Total 23	C 19	N 3	O 1	0	0
2	N	1	Total 23	C 19	N 3	O 1	0	0
2	O	1	Total 23	C 19	N 3	O 1	0	0
2	P	1	Total 23	C 19	N 3	O 1	0	0
2	Q	1	Total 23	C 19	N 3	O 1	0	0
2	R	1	Total 23	C 19	N 3	O 1	0	0
2	S	1	Total 23	C 19	N 3	O 1	0	0
2	T	1	Total 23	C 19	N 3	O 1	0	0
2	U	1	Total 23	C 19	N 3	O 1	0	0
2	V	1	Total 23	C 19	N 3	O 1	0	0
2	W	1	Total 23	C 19	N 3	O 1	0	0
2	X	1	Total 23	C 19	N 3	O 1	0	0

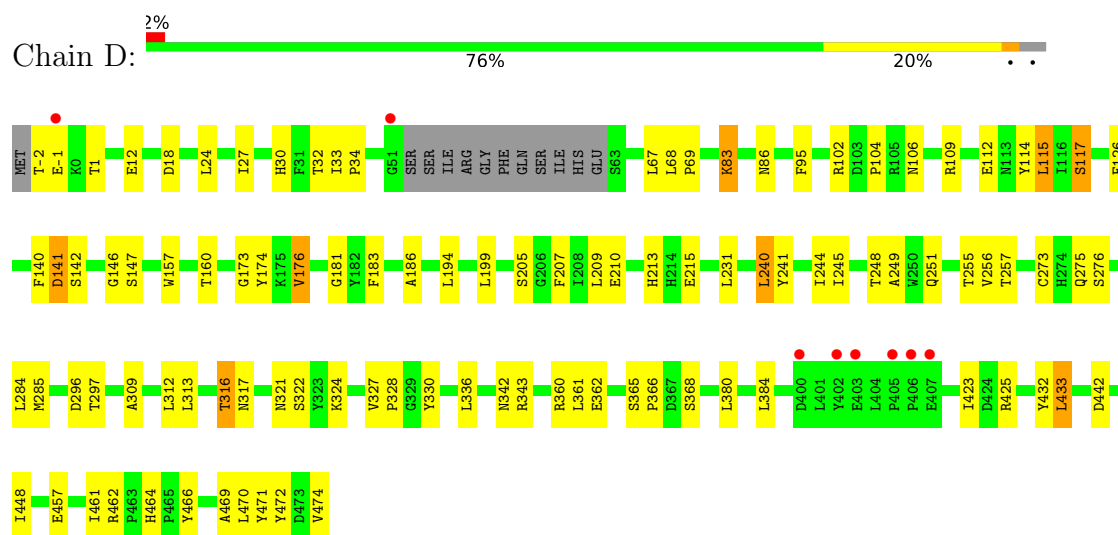


- Molecule 1: Glutamine synthetase 1

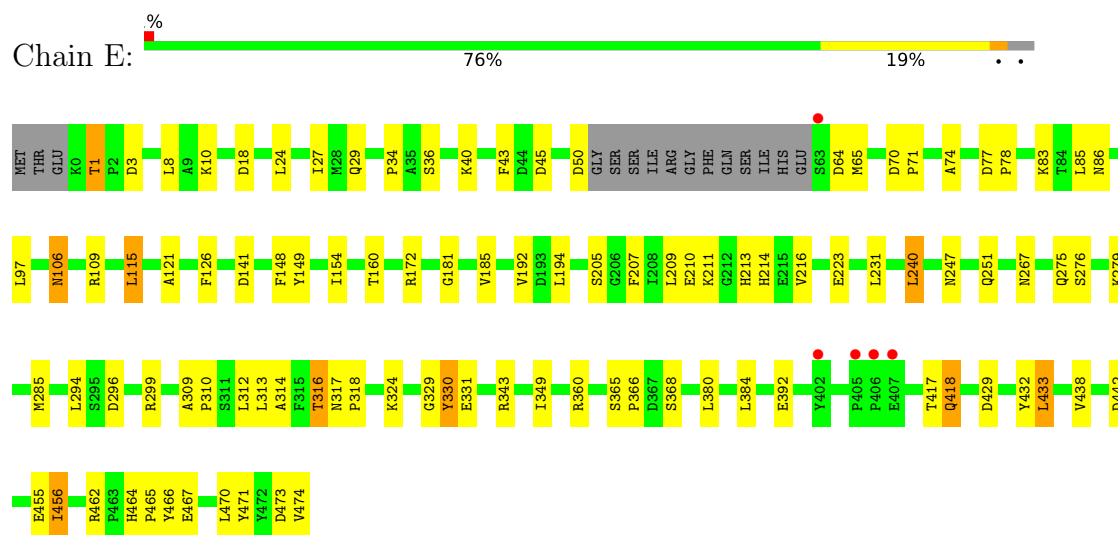




• Molecule 1: Glutamine synthetase 1

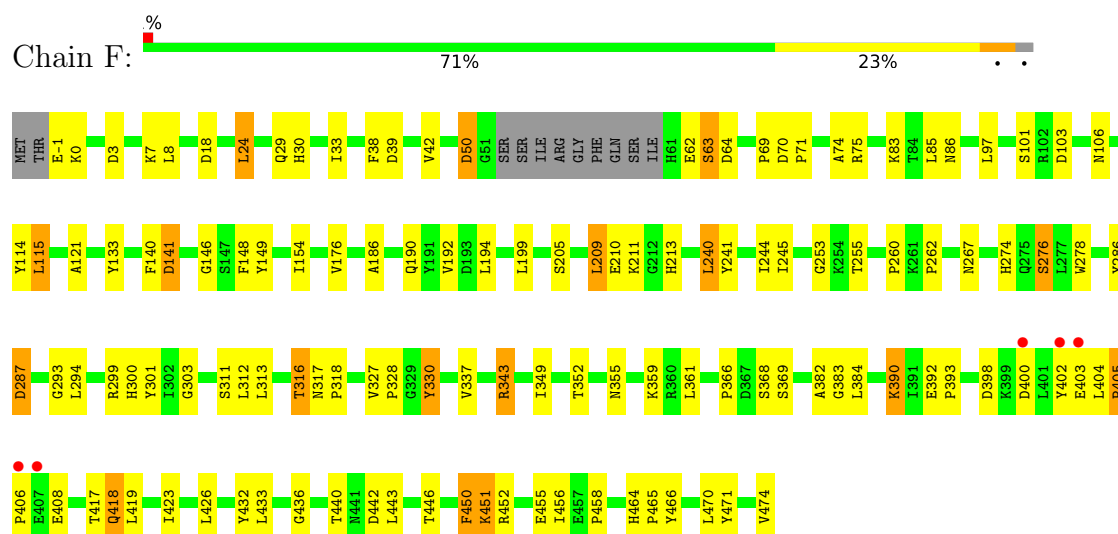


• Molecule 1: Glutamine synthetase 1

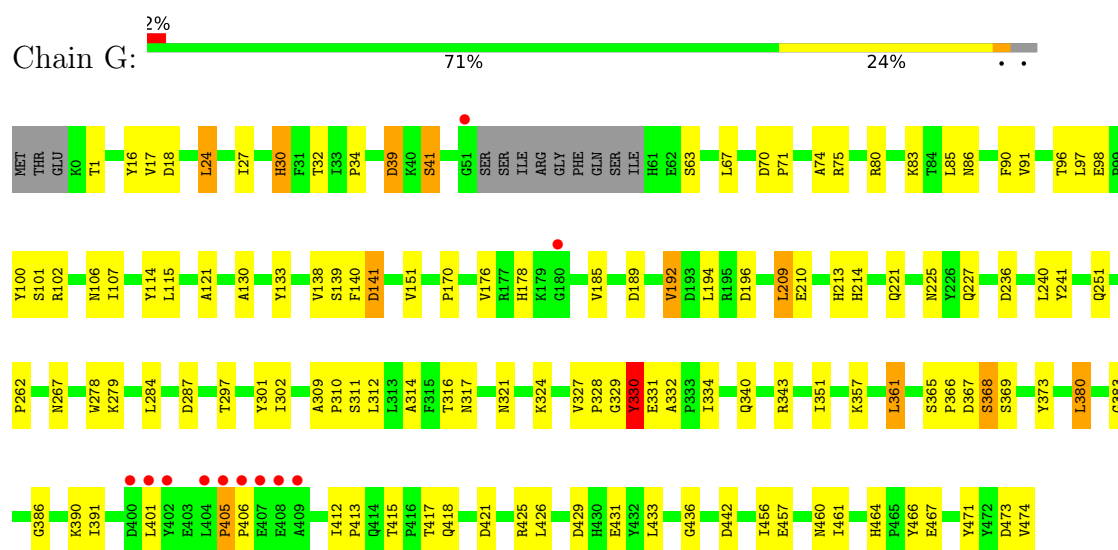


• Molecule 1: Glutamine synthetase 1

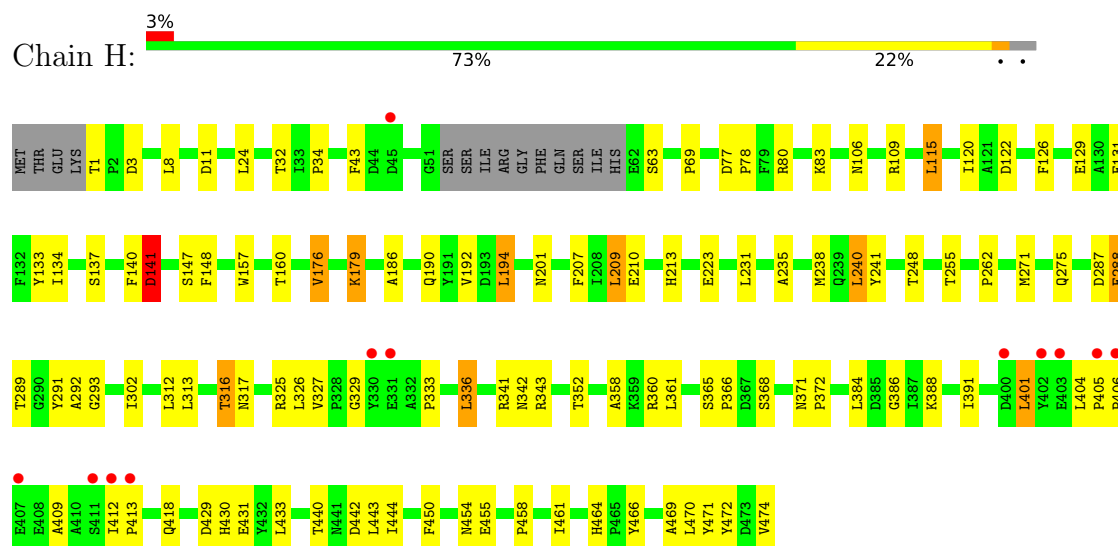




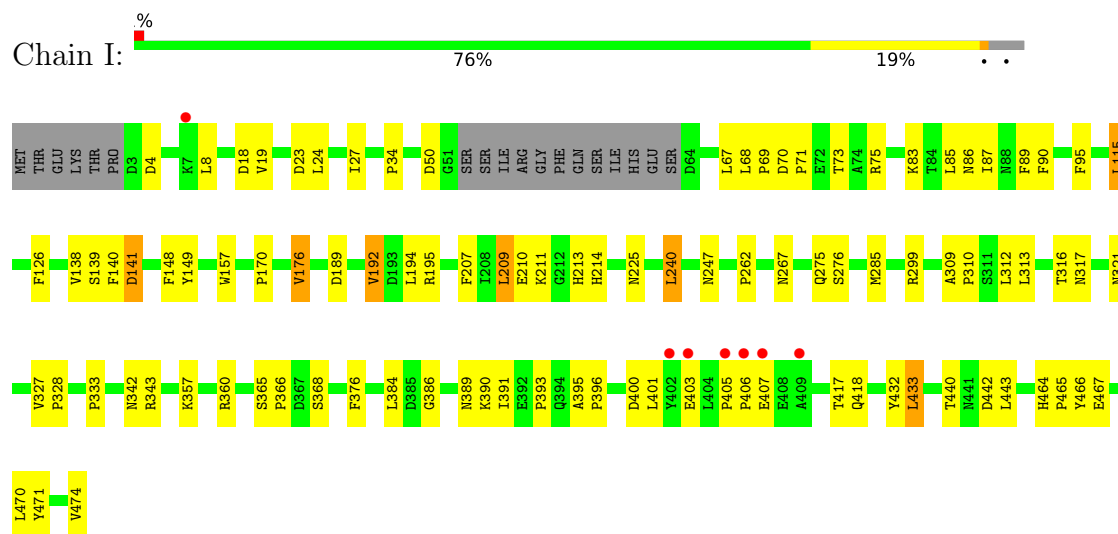
• Molecule 1: Glutamine synthetase 1



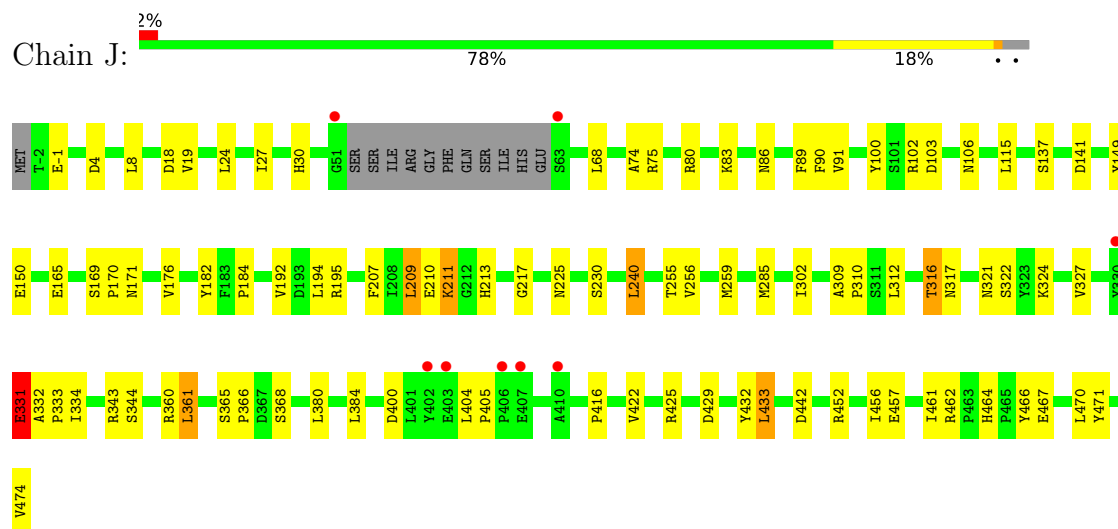
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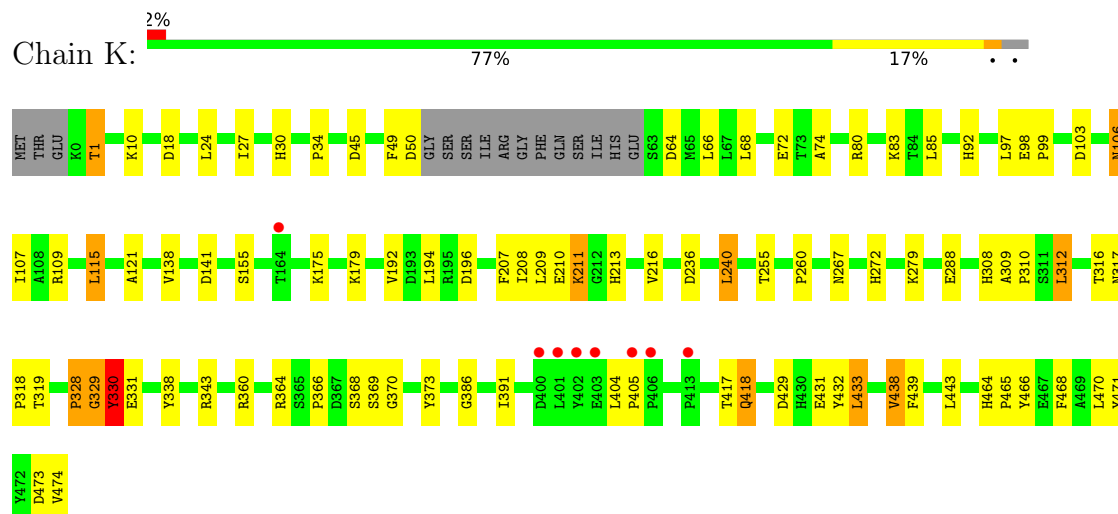
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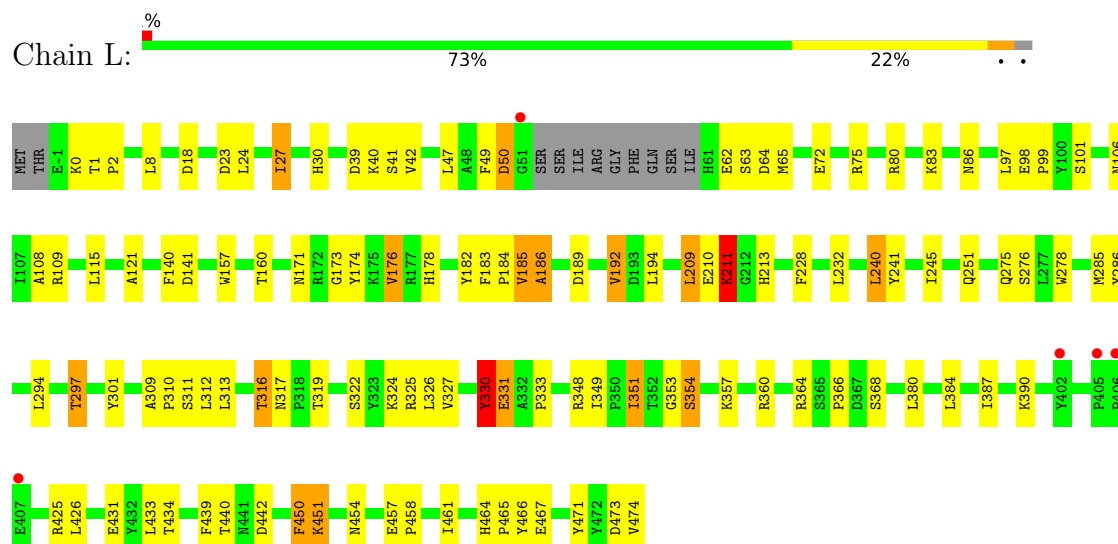
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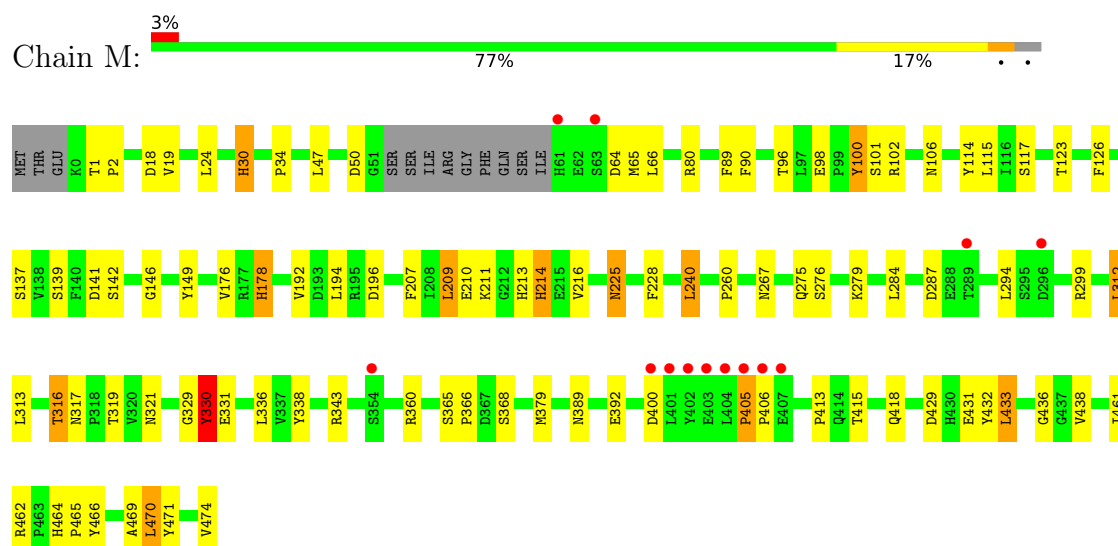
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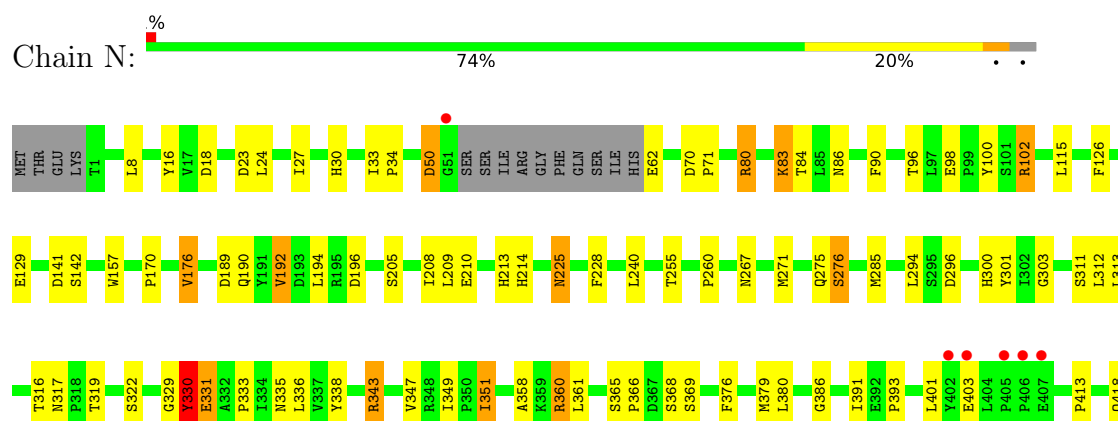
• Molecule 1: Glutamine synthetase 1



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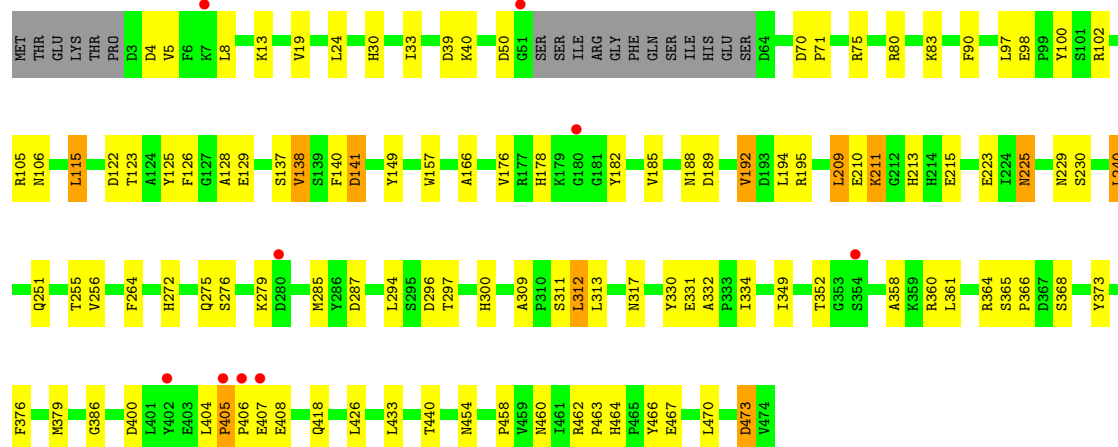
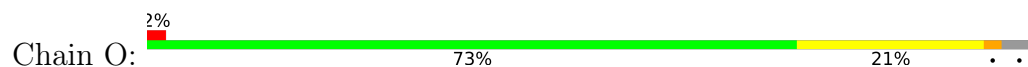


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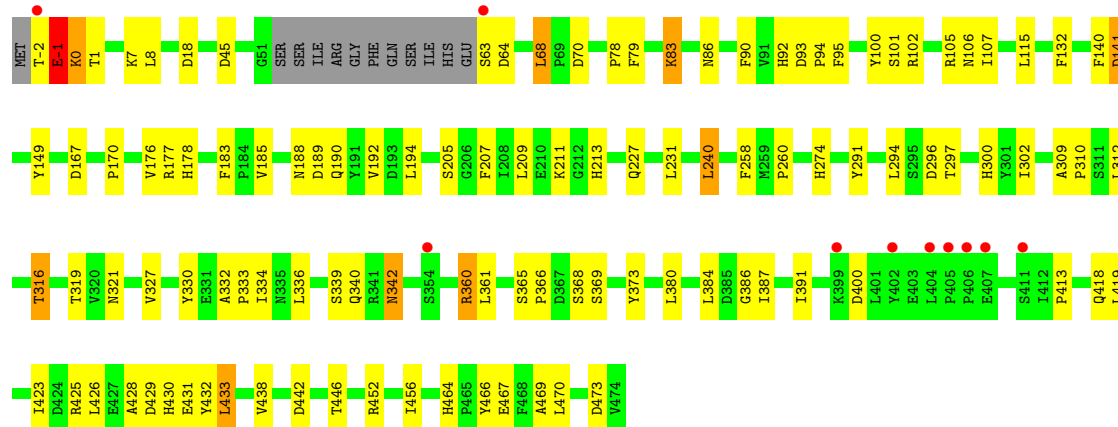
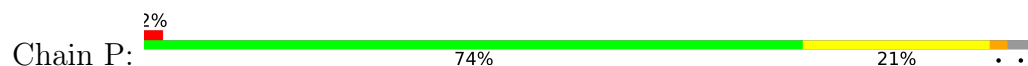




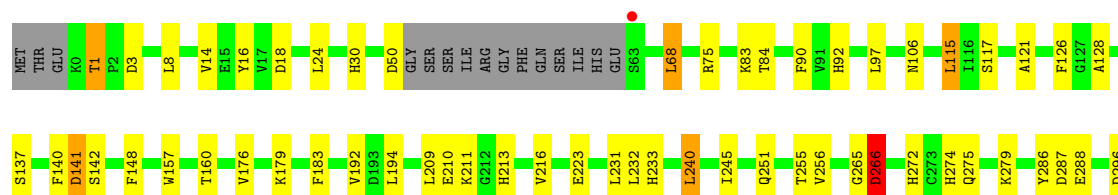
• Molecule 1: Glutamine synthetase 1

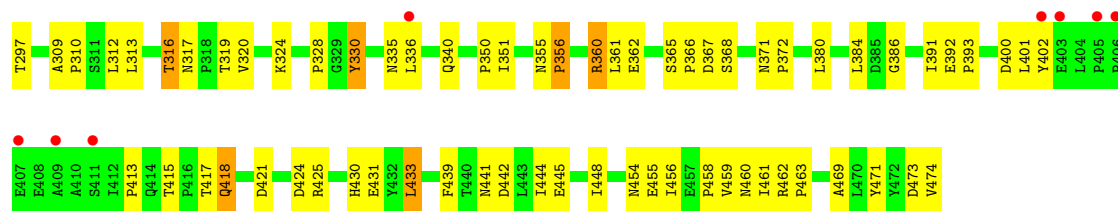


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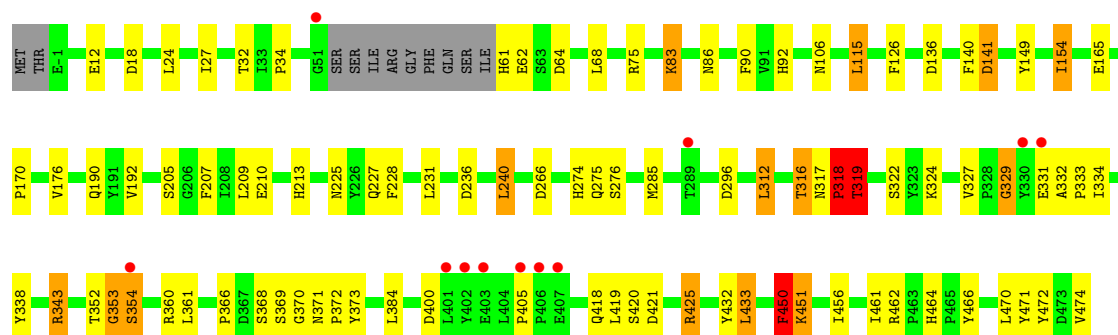
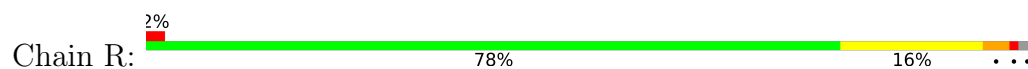


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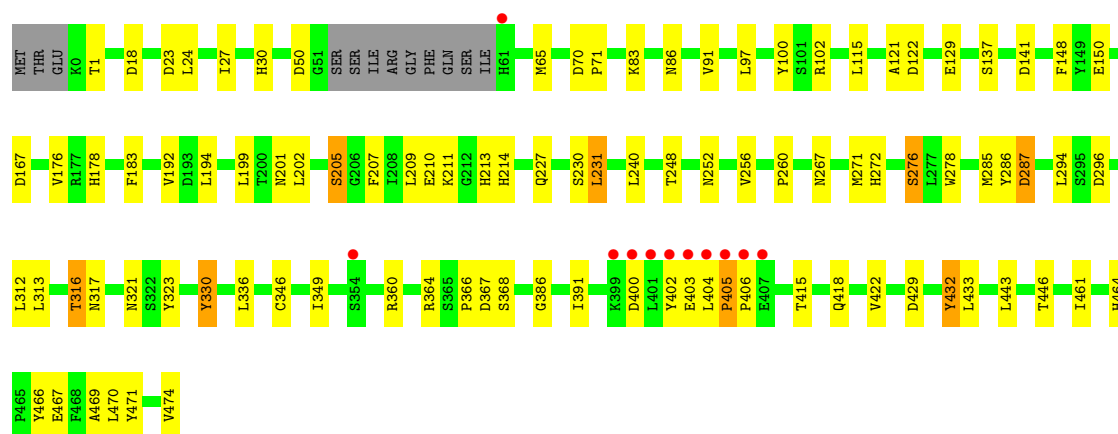
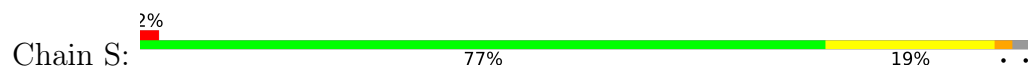




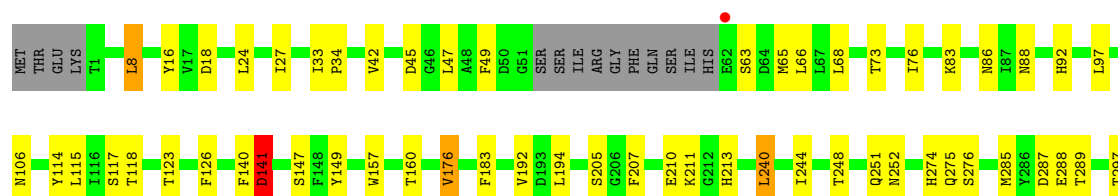
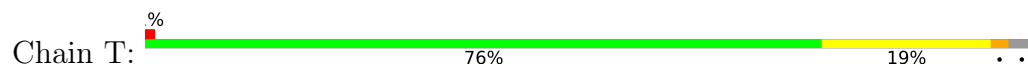
• Molecule 1: Glutamine synthetase 1

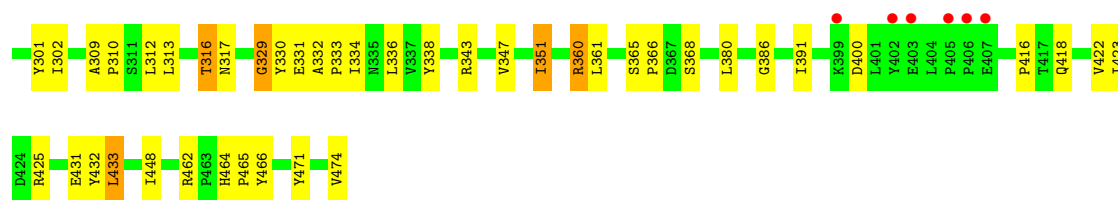


• Molecule 1: Glutamine synthetase 1

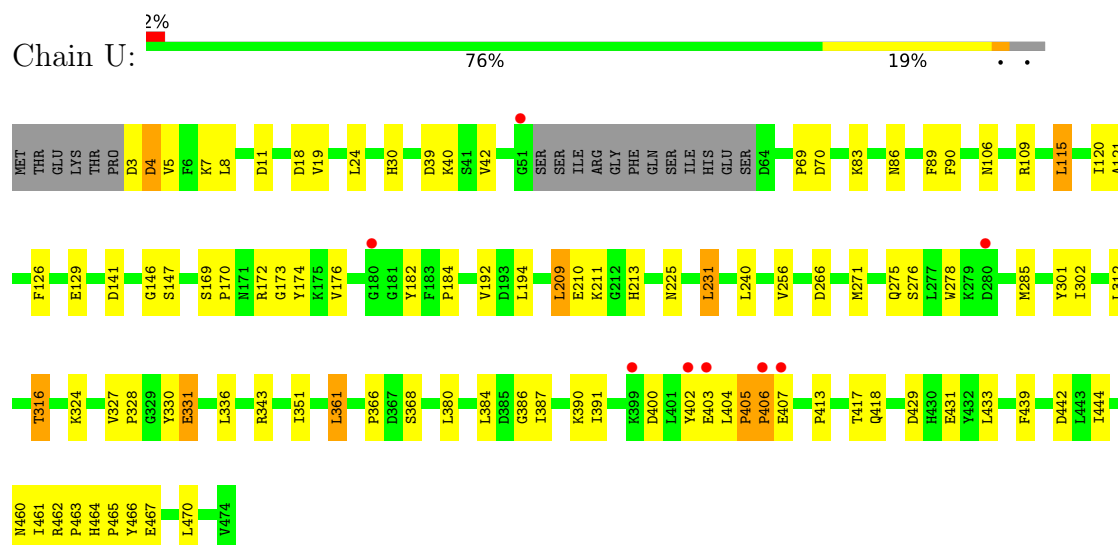


• Molecule 1: Glutamine synthetase 1

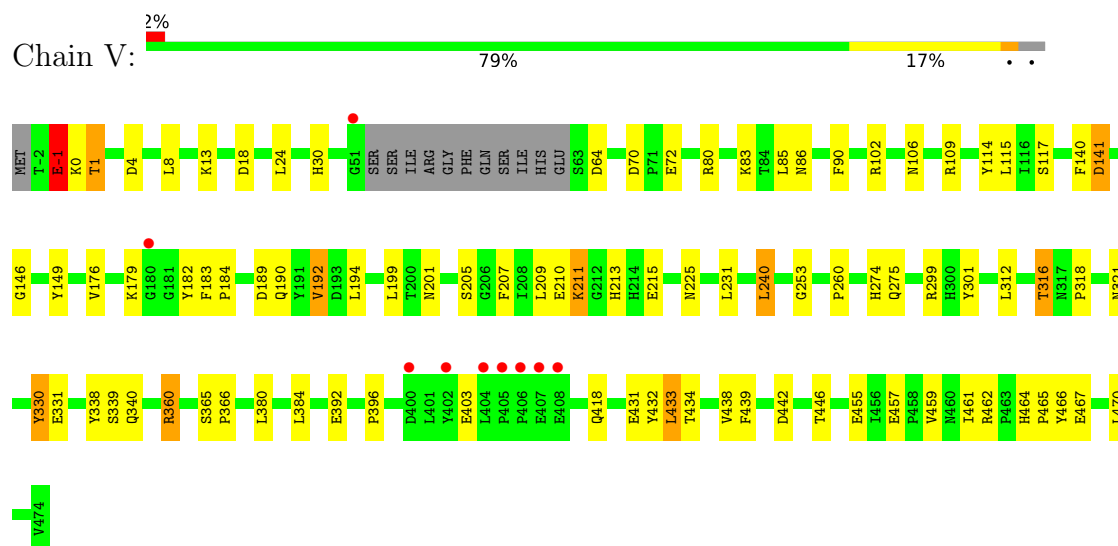




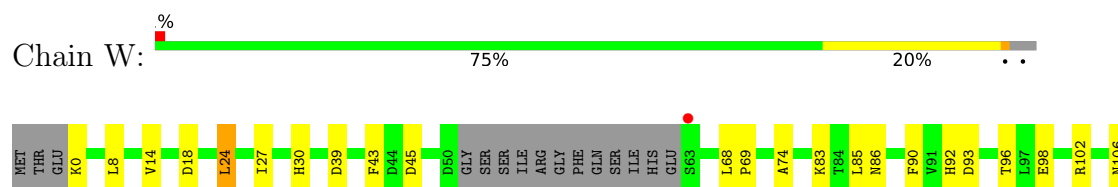
• Molecule 1: Glutamine synthetase 1



• Molecule 1: Glutamine synthetase 1



• Molecule 1: Glutamine synthetase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	260.11Å 273.50Å 207.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.30) 99.9 (49.62-3.30)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.200 , 0.265 0.197 , 0.259	Depositor DCC
$R_{free}$ test set	11105 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 22.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	88848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	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 34.86 % 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 6.3847e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: 2K9

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	0.48	0/3797	0.59	0/5161
1	B	0.59	0/3777	0.62	0/5135
1	C	0.50	0/3747	0.62	0/5093
1	D	0.47	0/3793	0.61	0/5156
1	E	0.47	0/3773	0.62	0/5129
1	F	0.52	0/3806	0.63	1/5173 (0.0%)
1	G	0.49	0/3797	0.61	1/5161 (0.0%)
1	H	0.52	0/3777	0.63	0/5135
1	I	0.49	0/3747	0.61	1/5093 (0.0%)
1	J	0.46	0/3793	0.62	1/5156 (0.0%)
1	K	0.47	0/3773	0.61	0/5129
1	L	0.49	0/3806	0.65	1/5173 (0.0%)
1	M	0.53	0/3797	0.61	1/5161 (0.0%)
1	N	0.50	0/3777	0.61	1/5135 (0.0%)
1	O	0.51	0/3747	0.62	1/5093 (0.0%)
1	P	0.51	0/3793	0.62	0/5156
1	Q	0.57	0/3773	0.63	1/5129 (0.0%)
1	R	0.48	0/3806	0.65	5/5173 (0.1%)
1	S	0.47	0/3797	0.61	0/5161
1	T	0.51	0/3777	0.60	1/5135 (0.0%)
1	U	0.50	0/3747	0.62	0/5093
1	V	0.48	0/3793	0.61	0/5156
1	W	0.49	0/3773	0.61	0/5129
1	X	0.46	0/3806	0.63	2/5173 (0.0%)
All	All	0.50	0/90772	0.62	17/123388 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	R	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	318	PRO	N-CA-C	7.49	131.58	112.10
1	R	318	PRO	C-N-CA	7.06	139.35	121.70
1	R	318	PRO	CA-C-N	5.83	130.02	117.20
1	X	380	LEU	CA-CB-CG	5.83	128.70	115.30
1	N	380	LEU	CA-CB-CG	5.74	128.50	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	185	VAL	Peptide
1	R	318	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3693	0	3523	53	0
1	B	3674	0	3503	81	0
1	C	3645	0	3475	61	0
1	D	3690	0	3523	58	0
1	E	3670	0	3507	59	0
1	F	3702	0	3529	78	0
1	G	3693	0	3523	73	0
1	H	3674	0	3503	62	0
1	I	3645	0	3475	56	0
1	J	3690	0	3523	50	0
1	K	3670	0	3507	46	0
1	L	3702	0	3529	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3693	0	3523	61	0
1	N	3674	0	3503	63	0
1	O	3645	0	3475	59	0
1	P	3690	0	3523	55	0
1	Q	3670	0	3507	64	0
1	R	3702	0	3529	62	0
1	S	3693	0	3523	47	0
1	T	3674	0	3503	58	0
1	U	3645	0	3475	50	0
1	V	3690	0	3523	49	0
1	W	3670	0	3507	56	0
1	X	3702	0	3529	58	0
2	A	23	0	11	0	0
2	B	23	0	11	1	0
2	C	23	0	11	0	0
2	D	23	0	11	0	0
2	E	23	0	11	0	0
2	F	23	0	11	2	0
2	G	23	0	11	0	0
2	H	23	0	11	0	0
2	I	23	0	11	0	0
2	J	23	0	11	0	0
2	K	23	0	11	0	0
2	L	23	0	11	0	0
2	M	23	0	11	2	0
2	N	23	0	11	1	0
2	O	23	0	11	0	0
2	P	23	0	11	1	0
2	Q	23	0	11	0	0
2	R	23	0	11	1	0
2	S	23	0	11	0	0
2	T	23	0	11	0	0
2	U	23	0	11	0	0
2	V	23	0	11	0	0
2	W	23	0	11	0	0
2	X	23	0	11	0	0
All	All	88848	0	84504	1283	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 7.

The worst 5 of 1283 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:H:313:LEU:HG	1:H:317:ASN:HD22	1.29	0.98
1:P:68:LEU:HD23	1:P:92:HIS:CD2	1.99	0.96
1:R:318:PRO:HG2	1:R:370:GLY:HA2	1.48	0.96
1:J:464:HIS:HD2	1:J:466:TYR:H	1.14	0.95
1:I:210:GLU:H	1:I:213:HIS:HD2	1.12	0.95

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	462/478 (97%)	432 (94%)	25 (5%)	5 (1%)	14	45
1	B	460/478 (96%)	414 (90%)	40 (9%)	6 (1%)	12	40
1	C	456/478 (95%)	408 (90%)	44 (10%)	4 (1%)	17	48
1	D	462/478 (97%)	430 (93%)	30 (6%)	2 (0%)	34	66
1	E	459/478 (96%)	421 (92%)	32 (7%)	6 (1%)	12	40
1	F	463/478 (97%)	419 (90%)	38 (8%)	6 (1%)	12	40
1	G	462/478 (97%)	426 (92%)	28 (6%)	8 (2%)	9	35
1	H	460/478 (96%)	424 (92%)	30 (6%)	6 (1%)	12	40
1	I	456/478 (95%)	421 (92%)	30 (7%)	5 (1%)	14	45
1	J	462/478 (97%)	432 (94%)	26 (6%)	4 (1%)	17	48
1	K	459/478 (96%)	418 (91%)	34 (7%)	7 (2%)	10	38
1	L	463/478 (97%)	424 (92%)	29 (6%)	10 (2%)	6	30
1	M	462/478 (97%)	425 (92%)	32 (7%)	5 (1%)	14	45
1	N	460/478 (96%)	422 (92%)	34 (7%)	4 (1%)	17	48
1	O	456/478 (95%)	421 (92%)	29 (6%)	6 (1%)	12	40
1	P	462/478 (97%)	418 (90%)	35 (8%)	9 (2%)	8	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	459/478 (96%)	420 (92%)	31 (7%)	8 (2%)	9	35
1	R	463/478 (97%)	422 (91%)	32 (7%)	9 (2%)	8	34
1	S	462/478 (97%)	424 (92%)	32 (7%)	6 (1%)	12	40
1	T	460/478 (96%)	420 (91%)	34 (7%)	6 (1%)	12	40
1	U	456/478 (95%)	425 (93%)	27 (6%)	4 (1%)	17	48
1	V	462/478 (97%)	429 (93%)	26 (6%)	7 (2%)	10	38
1	W	459/478 (96%)	426 (93%)	29 (6%)	4 (1%)	17	48
1	X	463/478 (97%)	428 (92%)	28 (6%)	7 (2%)	10	38
All	All	11048/11472 (96%)	10149 (92%)	755 (7%)	144 (1%)	12	40

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	LYS
1	C	330	TYR
1	D	-1	GLU
1	F	287	ASP
1	F	451	LYS

### 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	394/405 (97%)	368 (93%)	26 (7%)	16	46
1	B	392/405 (97%)	360 (92%)	32 (8%)	11	36
1	C	388/405 (96%)	349 (90%)	39 (10%)	7	27
1	D	394/405 (97%)	361 (92%)	33 (8%)	11	35
1	E	392/405 (97%)	359 (92%)	33 (8%)	11	35
1	F	395/405 (98%)	351 (89%)	44 (11%)	6	23
1	G	394/405 (97%)	361 (92%)	33 (8%)	11	35
1	H	392/405 (97%)	358 (91%)	34 (9%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	388/405 (96%)	363 (94%)	25 (6%)	17	46
1	J	394/405 (97%)	363 (92%)	31 (8%)	12	37
1	K	392/405 (97%)	356 (91%)	36 (9%)	9	31
1	L	395/405 (98%)	363 (92%)	32 (8%)	11	36
1	M	394/405 (97%)	360 (91%)	34 (9%)	10	35
1	N	392/405 (97%)	353 (90%)	39 (10%)	8	28
1	O	388/405 (96%)	351 (90%)	37 (10%)	8	29
1	P	394/405 (97%)	359 (91%)	35 (9%)	9	32
1	Q	392/405 (97%)	357 (91%)	35 (9%)	9	32
1	R	395/405 (98%)	364 (92%)	31 (8%)	12	38
1	S	394/405 (97%)	360 (91%)	34 (9%)	10	35
1	T	392/405 (97%)	362 (92%)	30 (8%)	13	38
1	U	388/405 (96%)	350 (90%)	38 (10%)	8	29
1	V	394/405 (97%)	364 (92%)	30 (8%)	13	39
1	W	392/405 (97%)	358 (91%)	34 (9%)	10	34
1	X	395/405 (98%)	360 (91%)	35 (9%)	9	32
All	All	9420/9720 (97%)	8610 (91%)	810 (9%)	10	35

5 of 810 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	361	LEU
1	Q	424	ASP
1	X	316	THR
1	O	98	GLU
1	N	360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 288 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	92	HIS
1	X	317	ASN
1	T	275	GLN
1	V	225	ASN
1	I	86	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

24 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
2	2K9	C	900	-	25,27,27	2.09	4 (16%)	26,40,40	2.40	7 (26%)
2	2K9	K	900	-	25,27,27	2.03	3 (12%)	26,40,40	2.13	4 (15%)
2	2K9	M	900	-	25,27,27	2.04	4 (16%)	26,40,40	2.28	6 (23%)
2	2K9	V	900	-	25,27,27	2.00	4 (16%)	26,40,40	2.36	5 (19%)
2	2K9	A	900	-	25,27,27	1.89	3 (12%)	26,40,40	2.32	5 (19%)
2	2K9	G	900	-	25,27,27	2.01	4 (16%)	26,40,40	2.33	5 (19%)
2	2K9	L	900	-	25,27,27	2.01	3 (12%)	26,40,40	2.16	3 (11%)
2	2K9	I	900	-	25,27,27	2.04	4 (16%)	26,40,40	2.34	4 (15%)
2	2K9	E	900	-	25,27,27	2.02	3 (12%)	26,40,40	2.24	4 (15%)
2	2K9	N	900	-	25,27,27	2.09	4 (16%)	26,40,40	2.39	5 (19%)
2	2K9	S	900	-	25,27,27	1.99	4 (16%)	26,40,40	2.30	4 (15%)
2	2K9	P	900	-	25,27,27	2.11	4 (16%)	26,40,40	2.30	5 (19%)
2	2K9	R	900	-	25,27,27	2.02	4 (16%)	26,40,40	2.25	3 (11%)
2	2K9	U	900	-	25,27,27	2.10	4 (16%)	26,40,40	2.33	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2K9	D	900	-	25,27,27	1.99	4 (16%)	26,40,40	2.31	5 (19%)
2	2K9	X	900	-	25,27,27	2.03	4 (16%)	26,40,40	2.26	4 (15%)
2	2K9	F	900	-	25,27,27	1.99	3 (12%)	26,40,40	2.30	5 (19%)
2	2K9	W	900	-	25,27,27	2.08	3 (12%)	26,40,40	2.20	4 (15%)
2	2K9	O	900	-	25,27,27	1.96	3 (12%)	26,40,40	2.23	4 (15%)
2	2K9	B	900	-	25,27,27	2.06	4 (16%)	26,40,40	2.21	3 (11%)
2	2K9	H	900	-	25,27,27	1.99	4 (16%)	26,40,40	2.31	5 (19%)
2	2K9	Q	900	-	25,27,27	2.04	3 (12%)	26,40,40	2.17	3 (11%)
2	2K9	T	900	-	25,27,27	2.00	4 (16%)	26,40,40	2.30	4 (15%)
2	2K9	J	900	-	25,27,27	1.95	4 (16%)	26,40,40	2.29	4 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2K9	C	900	-	-	0/4/12/12	0/4/5/5
2	2K9	K	900	-	-	0/4/12/12	0/4/5/5
2	2K9	M	900	-	-	0/4/12/12	0/4/5/5
2	2K9	V	900	-	-	0/4/12/12	0/4/5/5
2	2K9	A	900	-	-	0/4/12/12	0/4/5/5
2	2K9	G	900	-	-	0/4/12/12	0/4/5/5
2	2K9	L	900	-	-	0/4/12/12	0/4/5/5
2	2K9	I	900	-	-	0/4/12/12	0/4/5/5
2	2K9	E	900	-	-	0/4/12/12	0/4/5/5
2	2K9	N	900	-	-	0/4/12/12	0/4/5/5
2	2K9	S	900	-	-	0/4/12/12	0/4/5/5
2	2K9	P	900	-	-	0/4/12/12	0/4/5/5
2	2K9	R	900	-	-	0/4/12/12	0/4/5/5
2	2K9	U	900	-	-	0/4/12/12	0/4/5/5
2	2K9	D	900	-	-	0/4/12/12	0/4/5/5
2	2K9	X	900	-	-	0/4/12/12	0/4/5/5
2	2K9	F	900	-	-	0/4/12/12	0/4/5/5
2	2K9	W	900	-	-	0/4/12/12	0/4/5/5
2	2K9	O	900	-	-	0/4/12/12	0/4/5/5
2	2K9	B	900	-	-	3/4/12/12	0/4/5/5
2	2K9	H	900	-	-	1/4/12/12	0/4/5/5
2	2K9	Q	900	-	-	0/4/12/12	0/4/5/5
2	2K9	T	900	-	-	0/4/12/12	0/4/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2K9	J	900	-	-	0/4/12/12	0/4/5/5

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	900	2K9	C3-C1	6.72	1.48	1.37
2	C	900	2K9	C3-C1	6.60	1.47	1.37
2	W	900	2K9	C3-C1	6.50	1.47	1.37
2	Q	900	2K9	C3-C1	6.49	1.47	1.37
2	U	900	2K9	C3-C1	6.45	1.47	1.37

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	900	2K9	C9-C5-N3	9.92	135.19	119.92
2	T	900	2K9	C9-C5-N3	9.90	135.15	119.92
2	N	900	2K9	C9-C5-N3	9.85	135.09	119.92
2	H	900	2K9	C9-C5-N3	9.81	135.02	119.92
2	S	900	2K9	C9-C5-N3	9.79	134.98	119.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	2K9	C7-C11-C13-C16
2	H	900	2K9	C7-C11-C13-C16
2	B	900	2K9	C7-C11-C13-C15
2	B	900	2K9	C14-C11-C13-C16

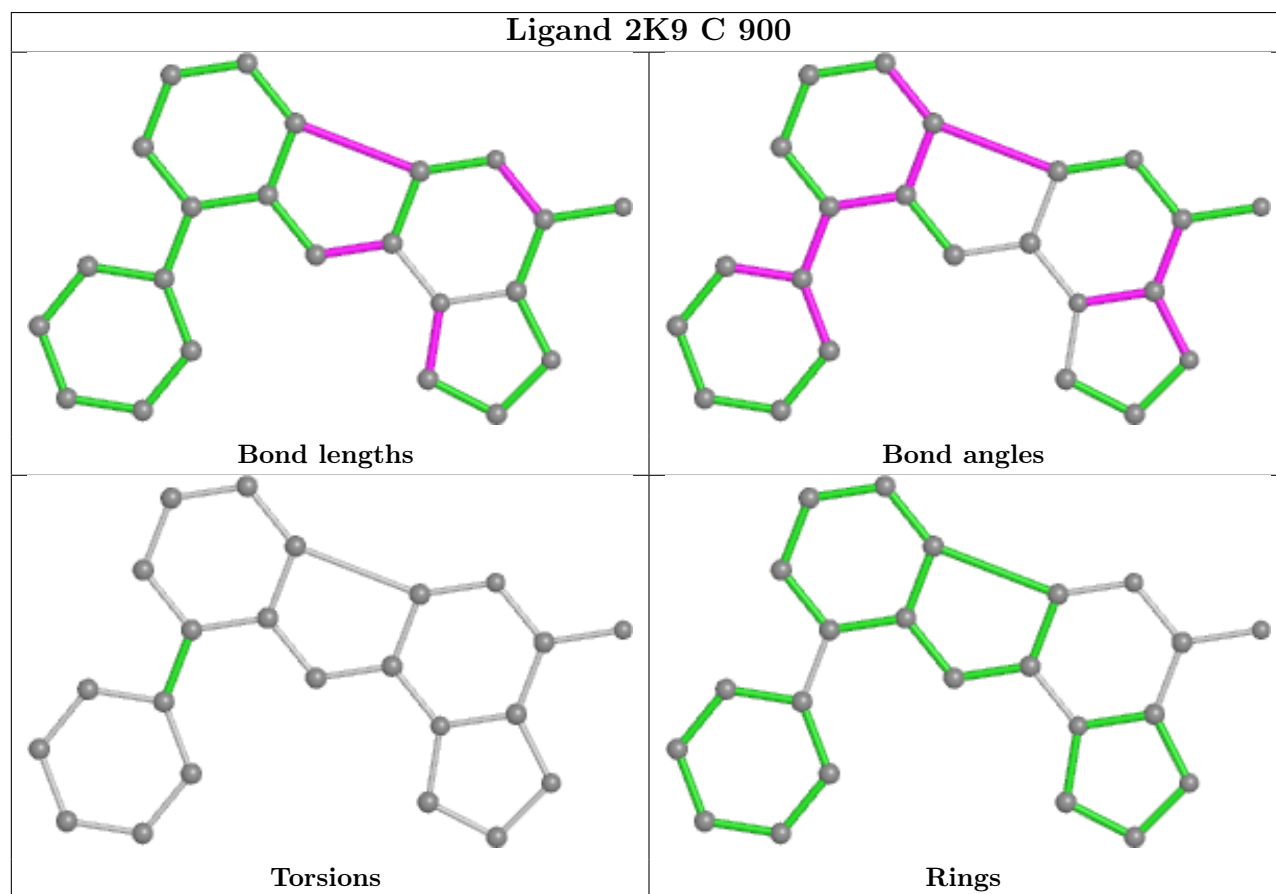
There are no ring outliers.

6 monomers are involved in 8 short contacts:

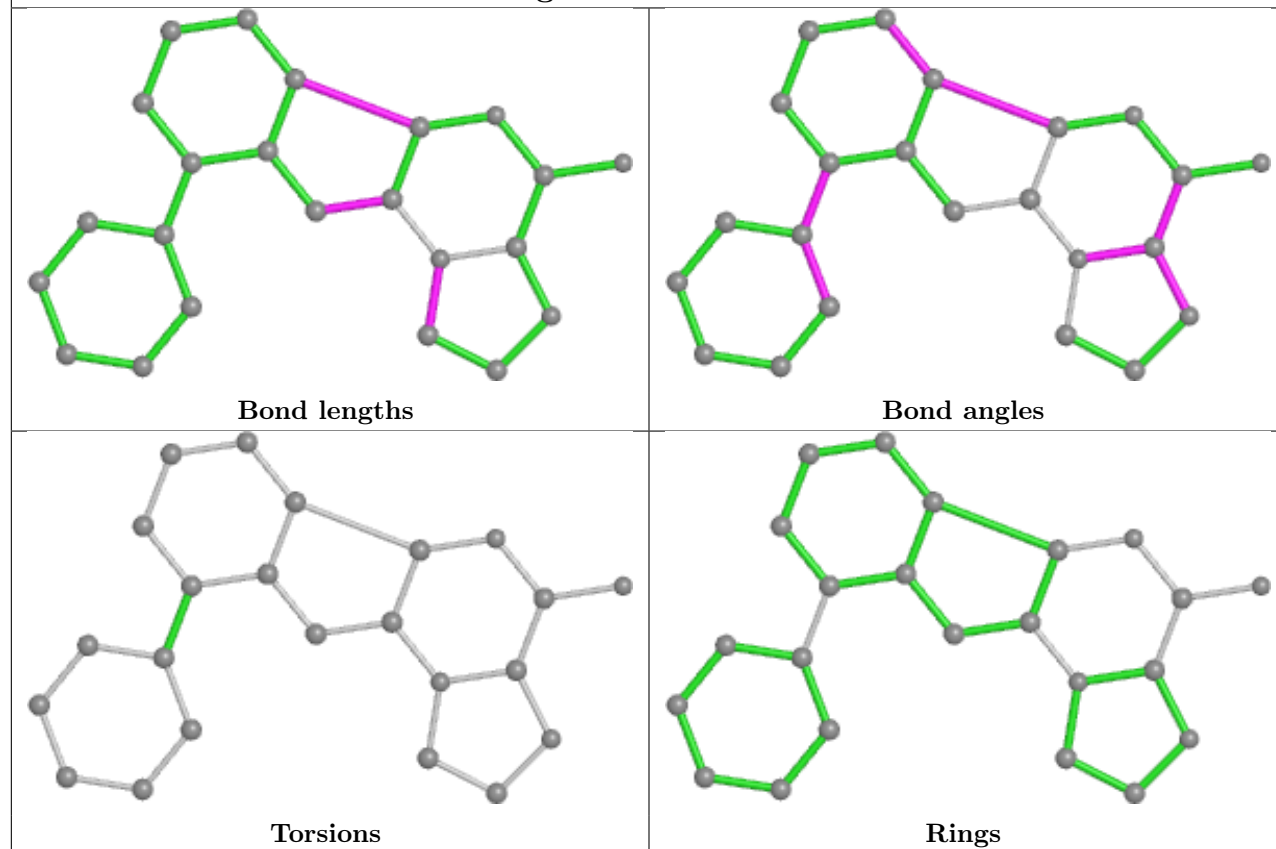
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	900	2K9	2	0
2	N	900	2K9	1	0
2	P	900	2K9	1	0
2	R	900	2K9	1	0
2	F	900	2K9	2	0
2	B	900	2K9	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

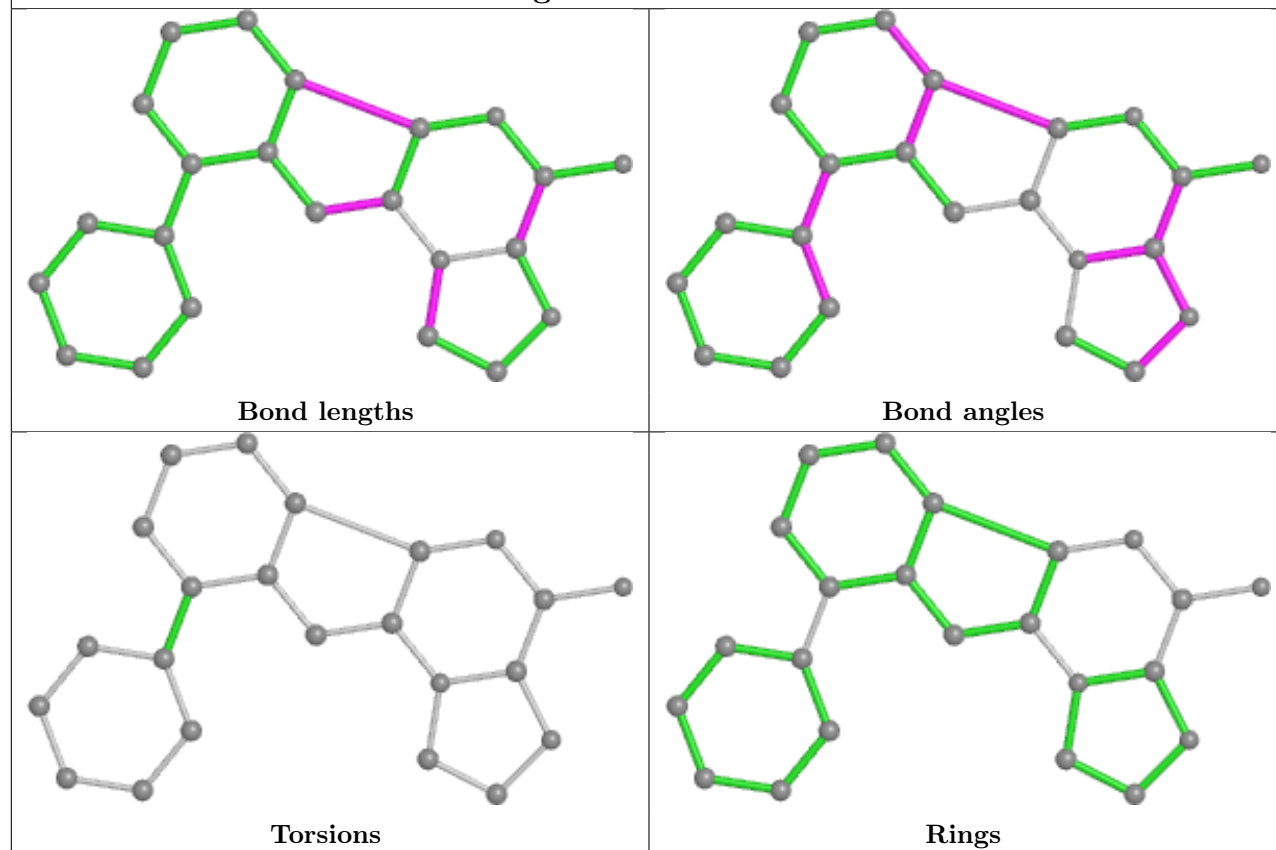
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



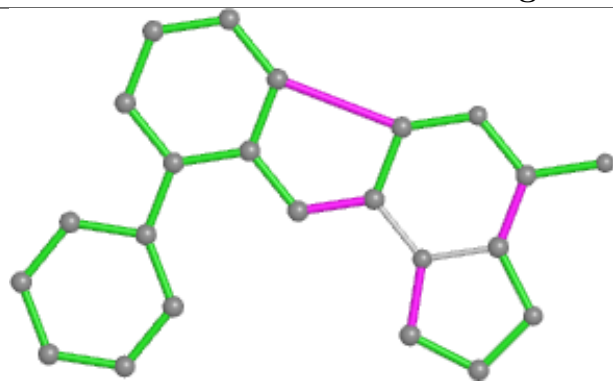
## Ligand 2K9 K 900



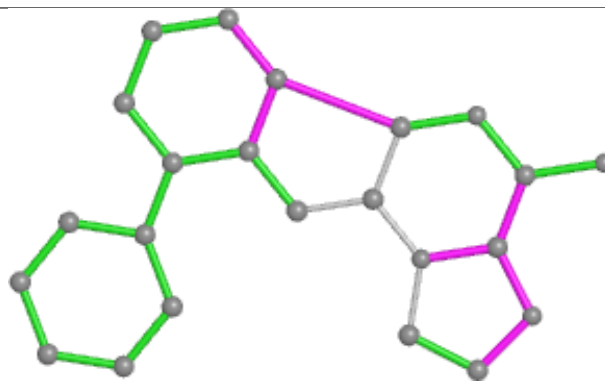
## Ligand 2K9 M 900



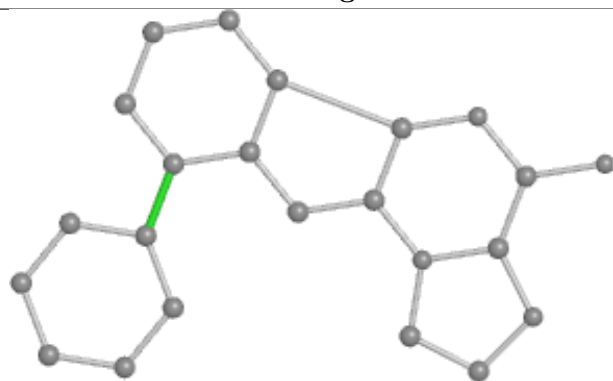
## Ligand 2K9 V 900



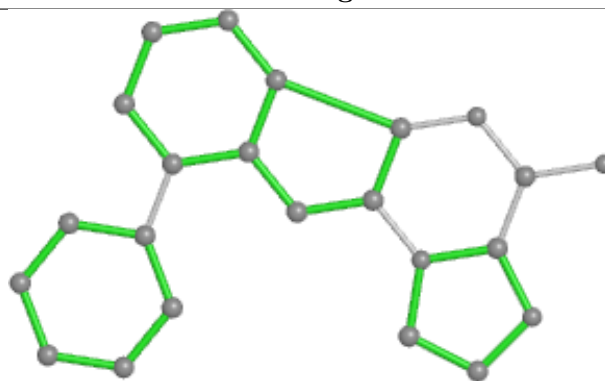
Bond lengths



Bond angles

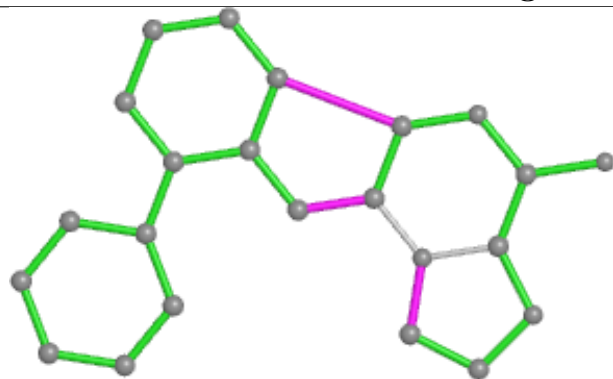


Torsions

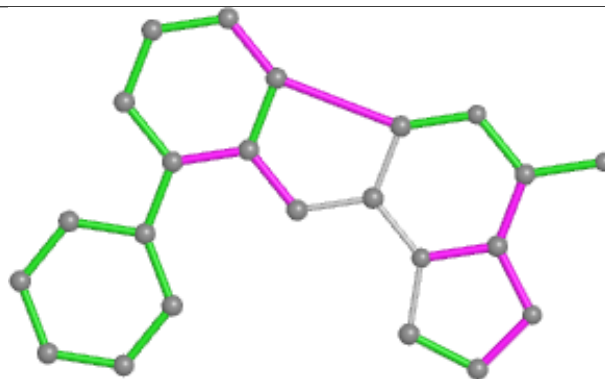


Rings

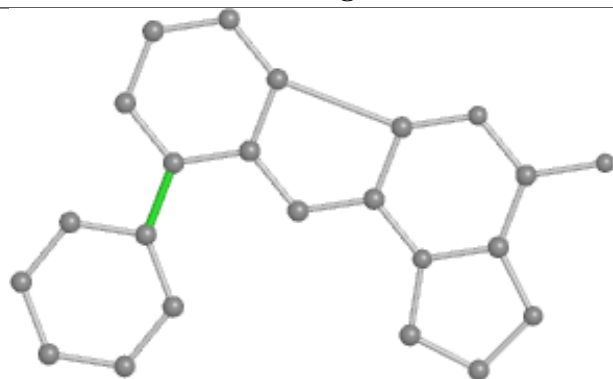
## Ligand 2K9 A 900



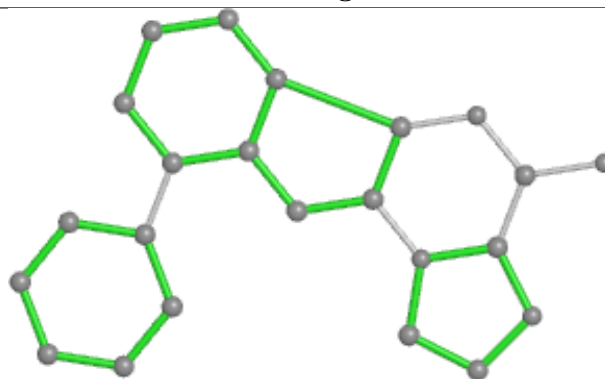
Bond lengths



Bond angles

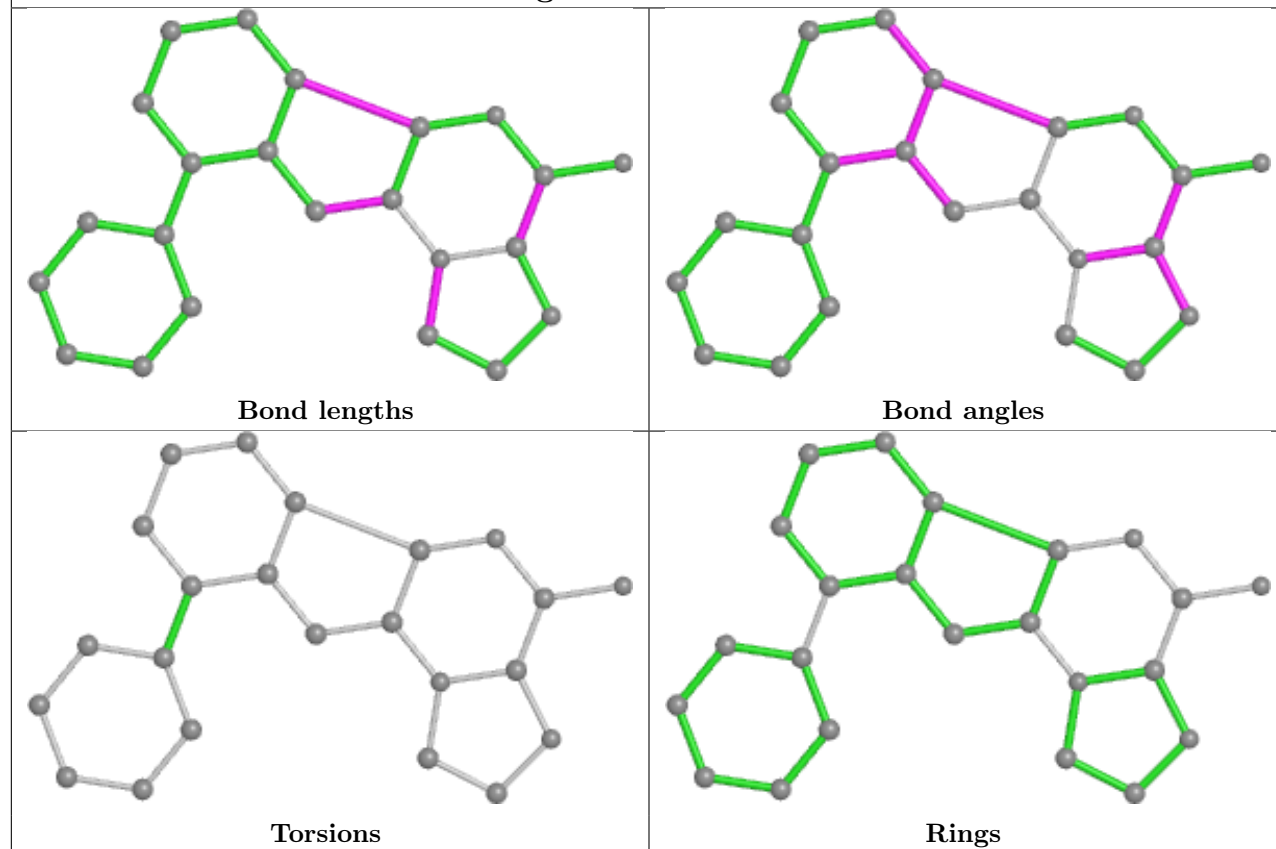


Torsions

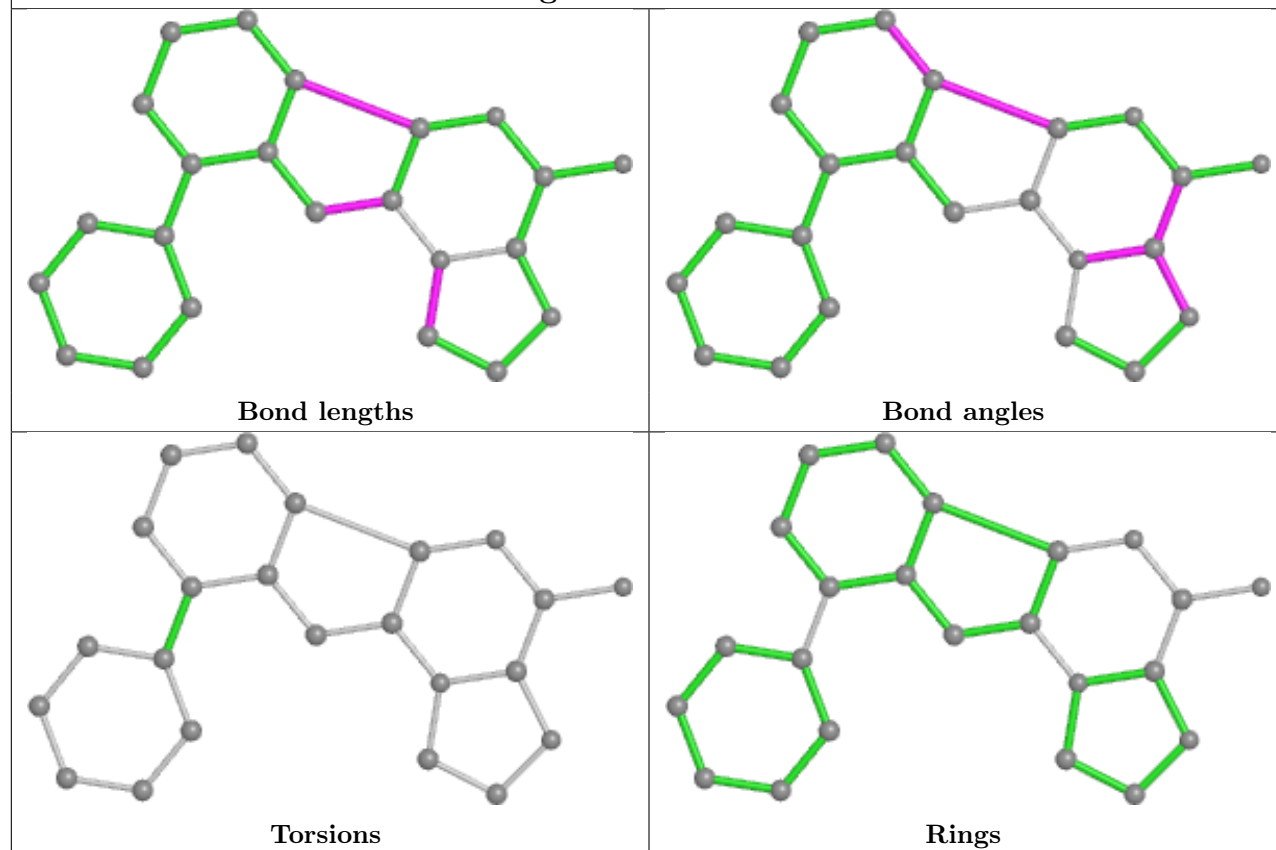


Rings

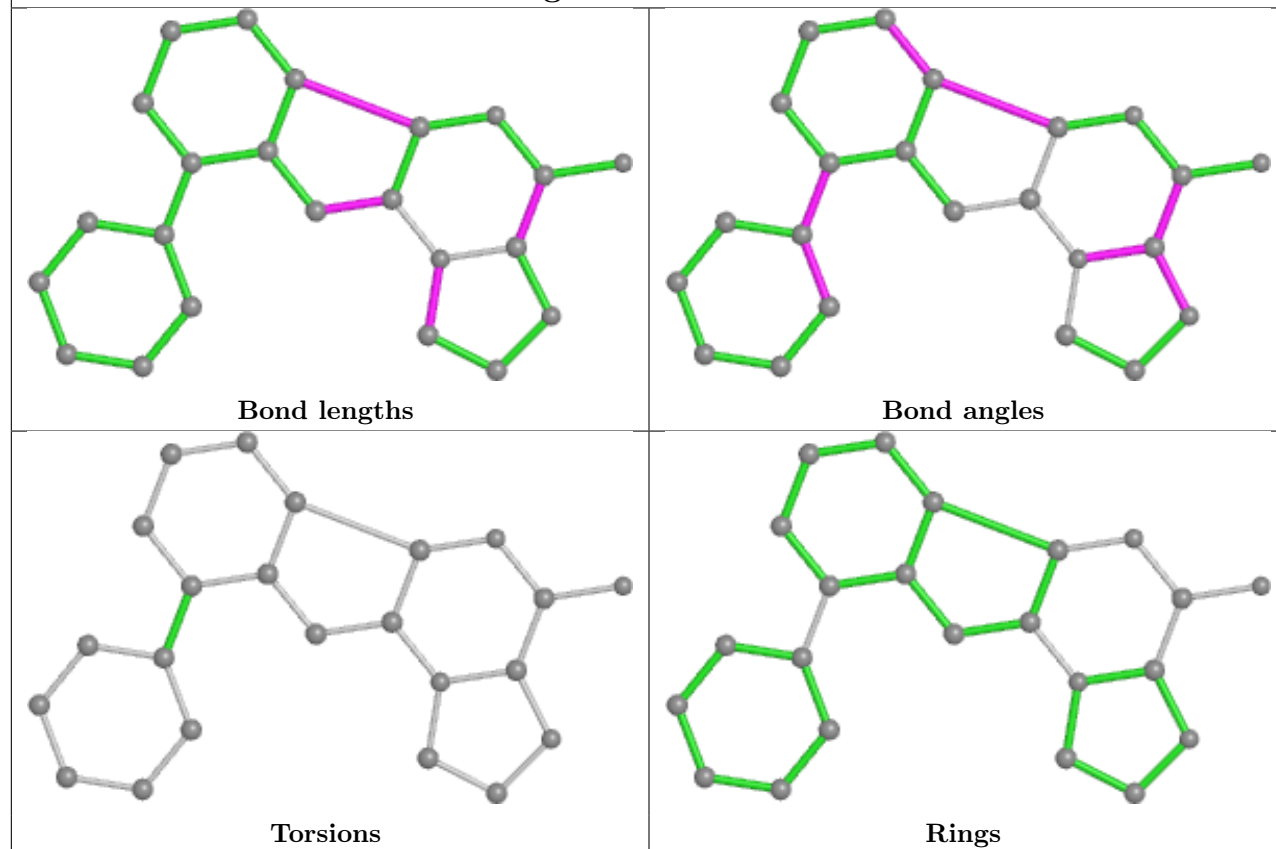
## Ligand 2K9 G 900



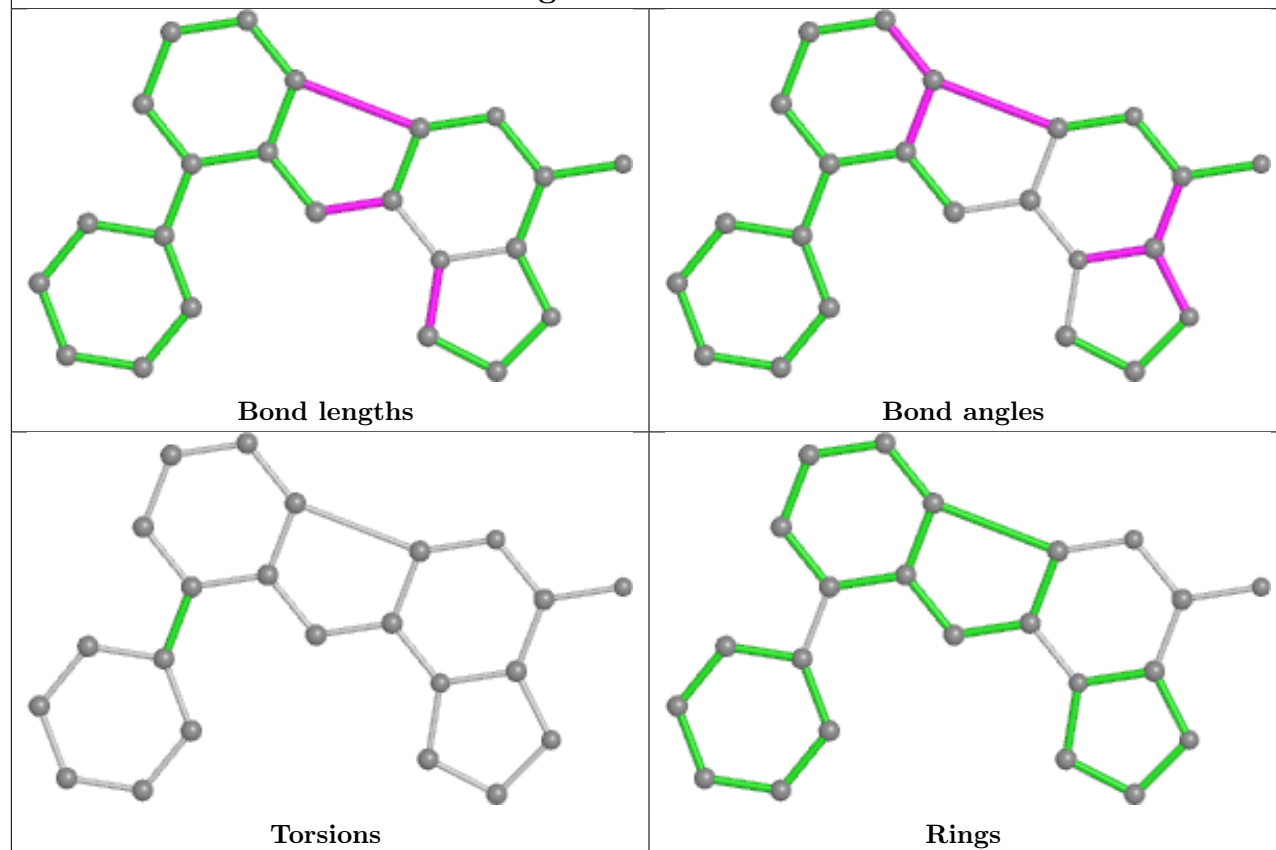
## Ligand 2K9 L 900



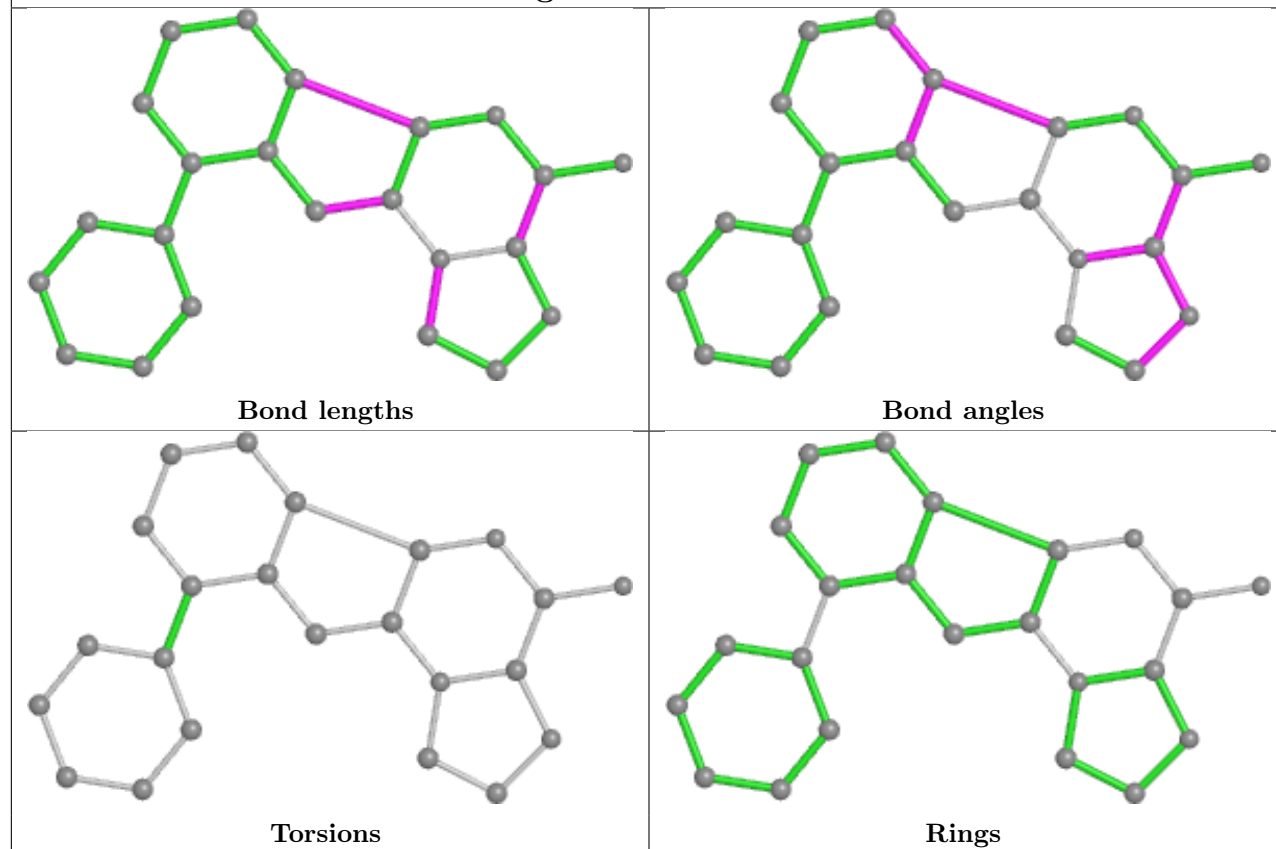
## Ligand 2K9 I 900



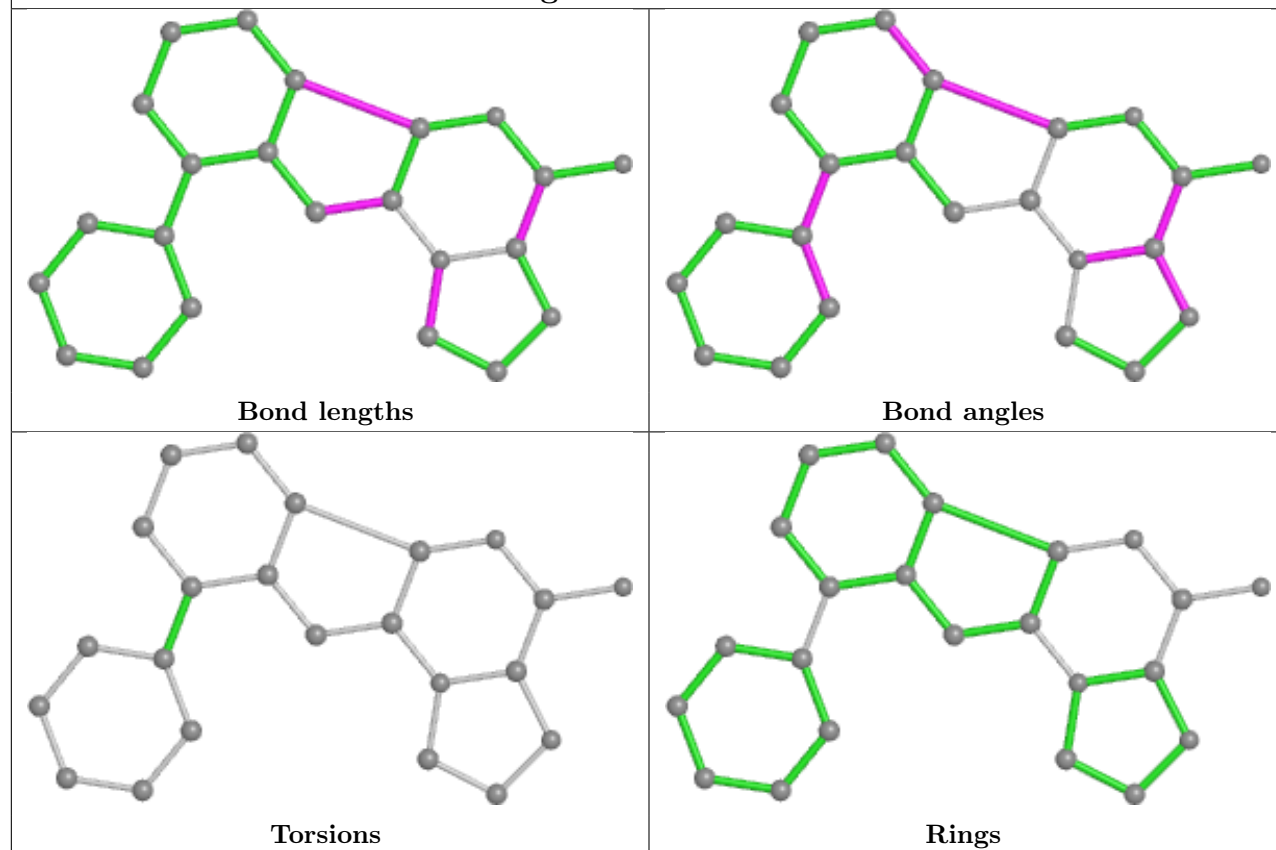
## Ligand 2K9 E 900



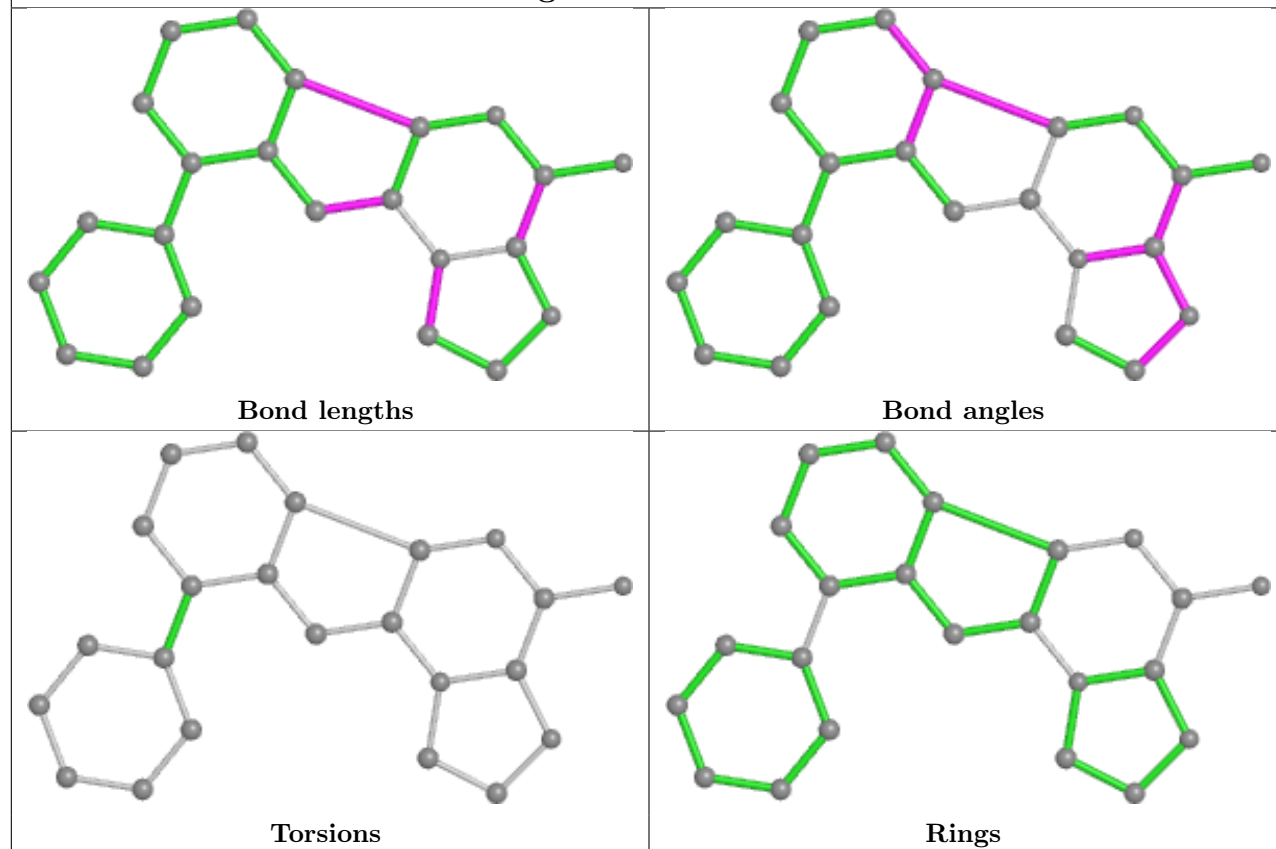
## Ligand 2K9 N 900



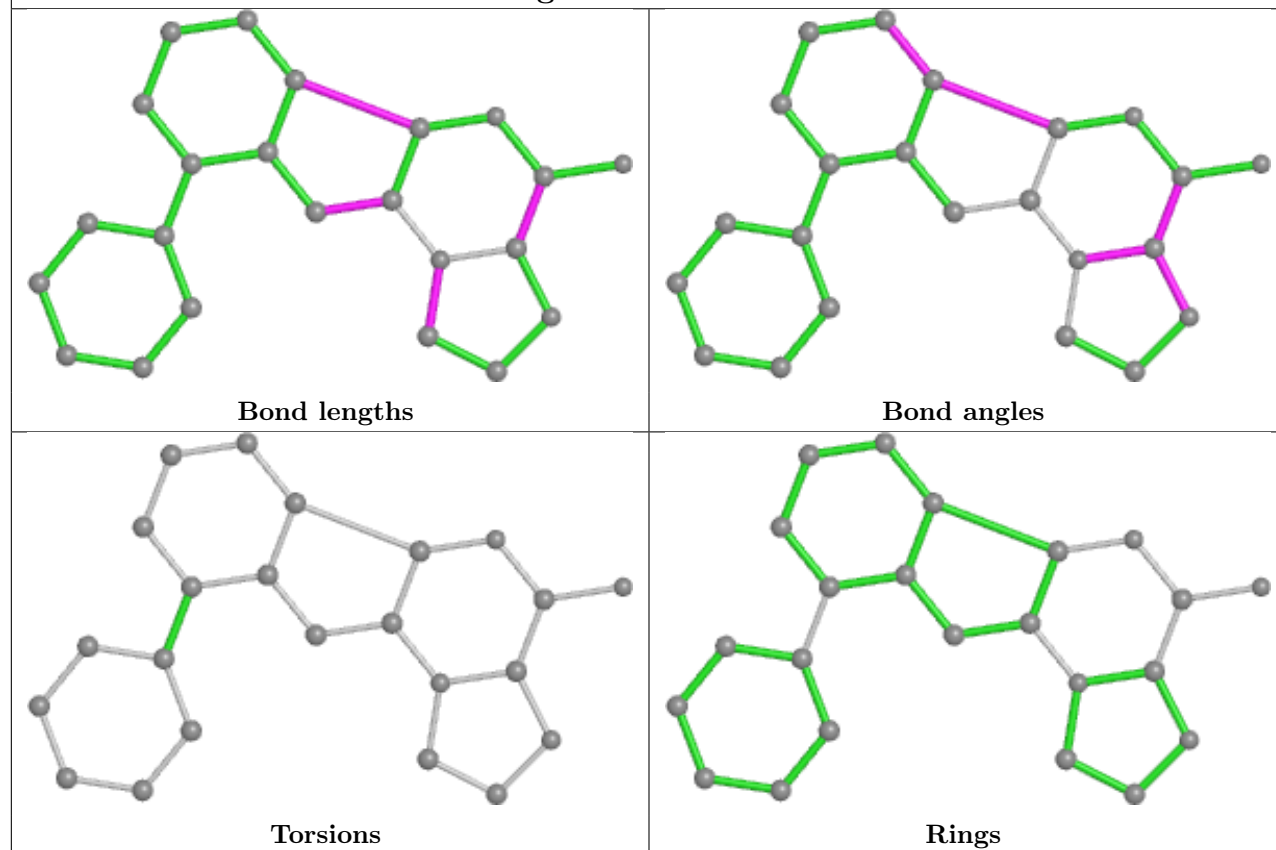
## Ligand 2K9 S 900



## Ligand 2K9 P 900

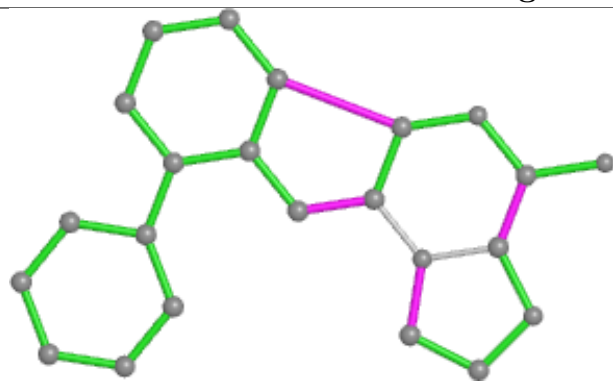


## Ligand 2K9 R 900

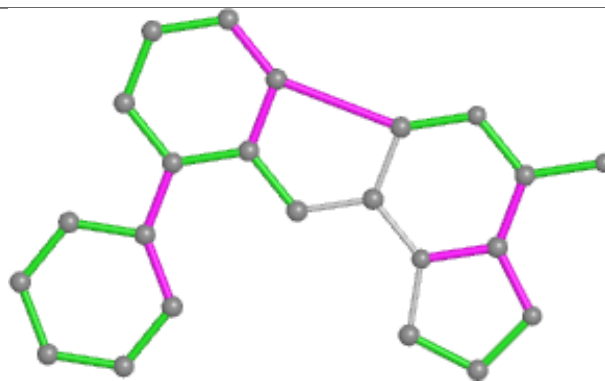




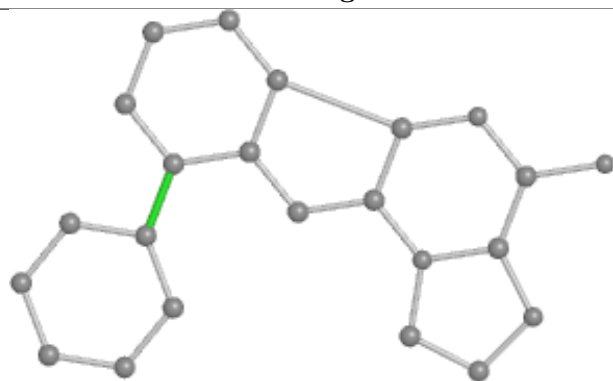
## Ligand 2K9 U 900



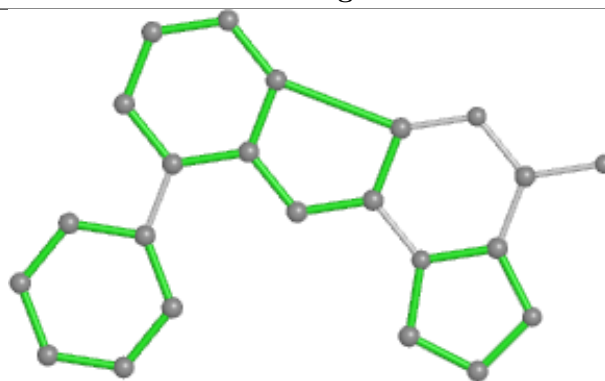
Bond lengths



Bond angles

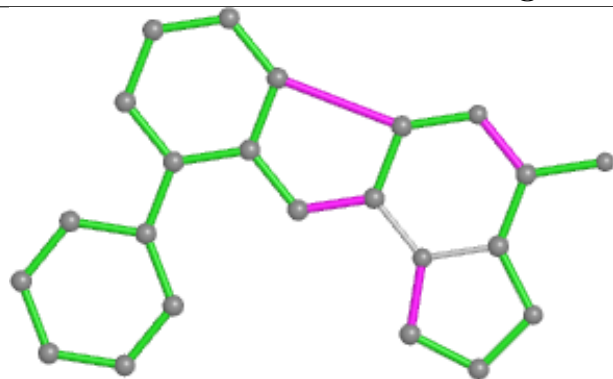


Torsions

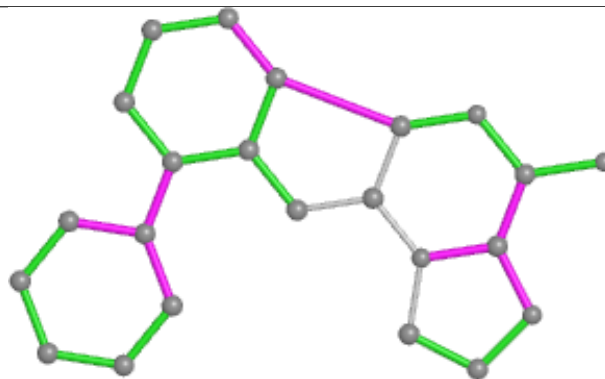


Rings

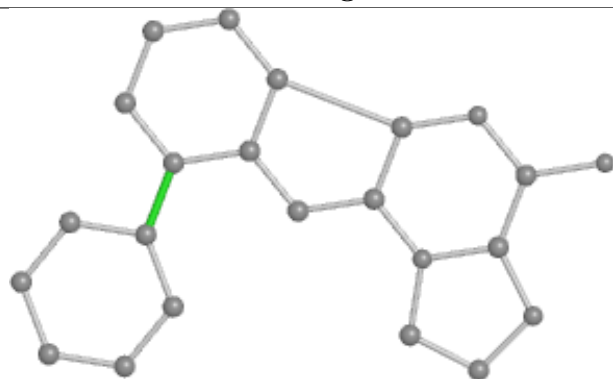
## Ligand 2K9 D 900



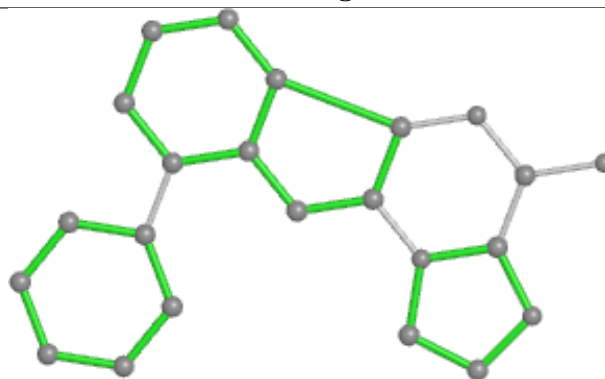
Bond lengths



Bond angles

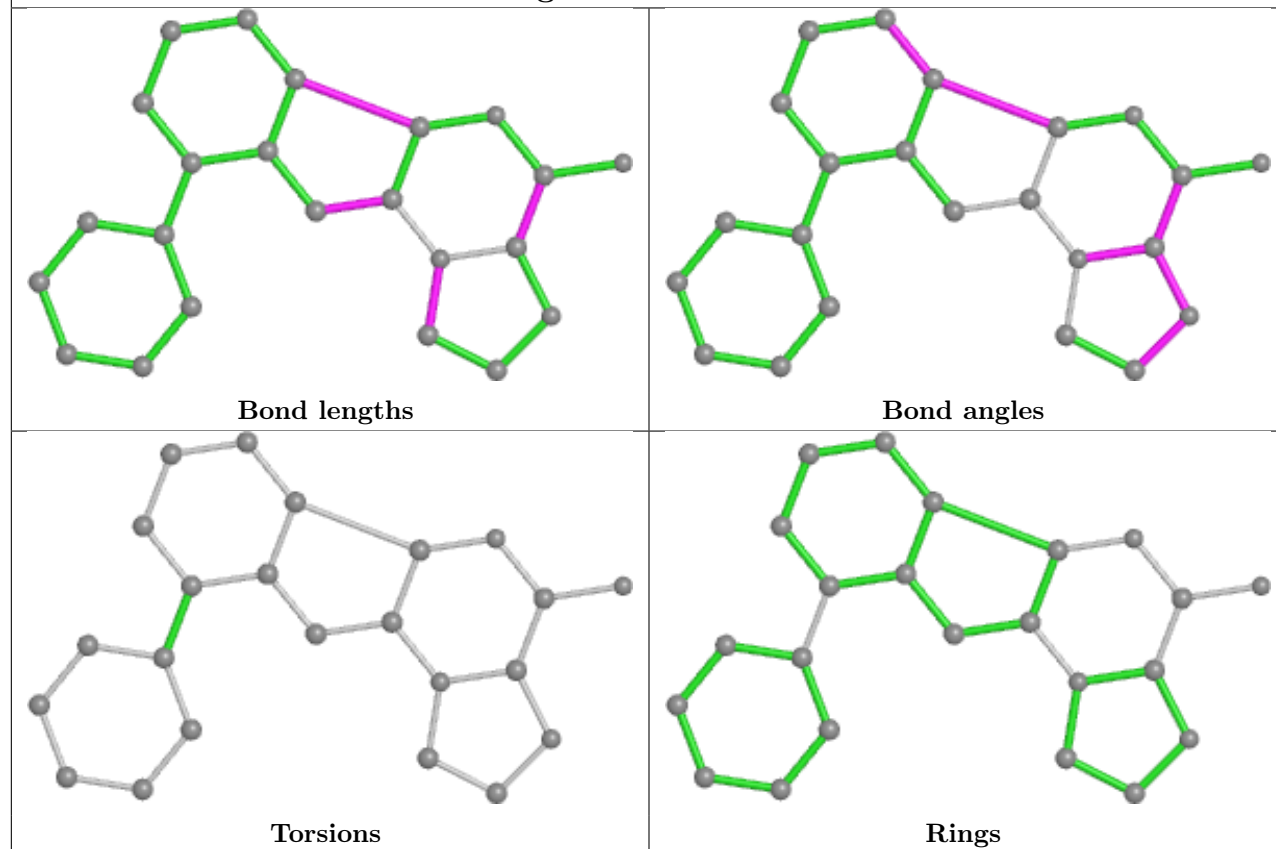


Torsions

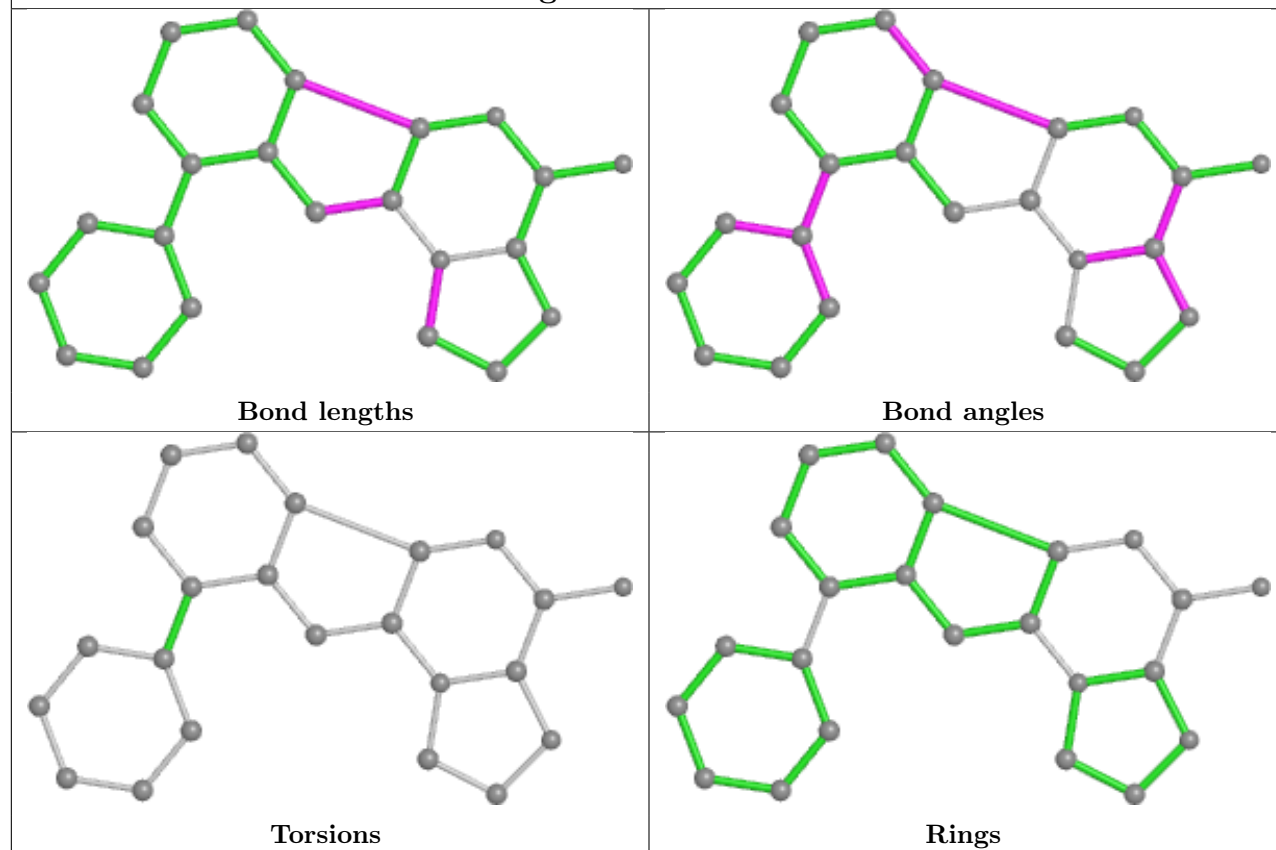


Rings

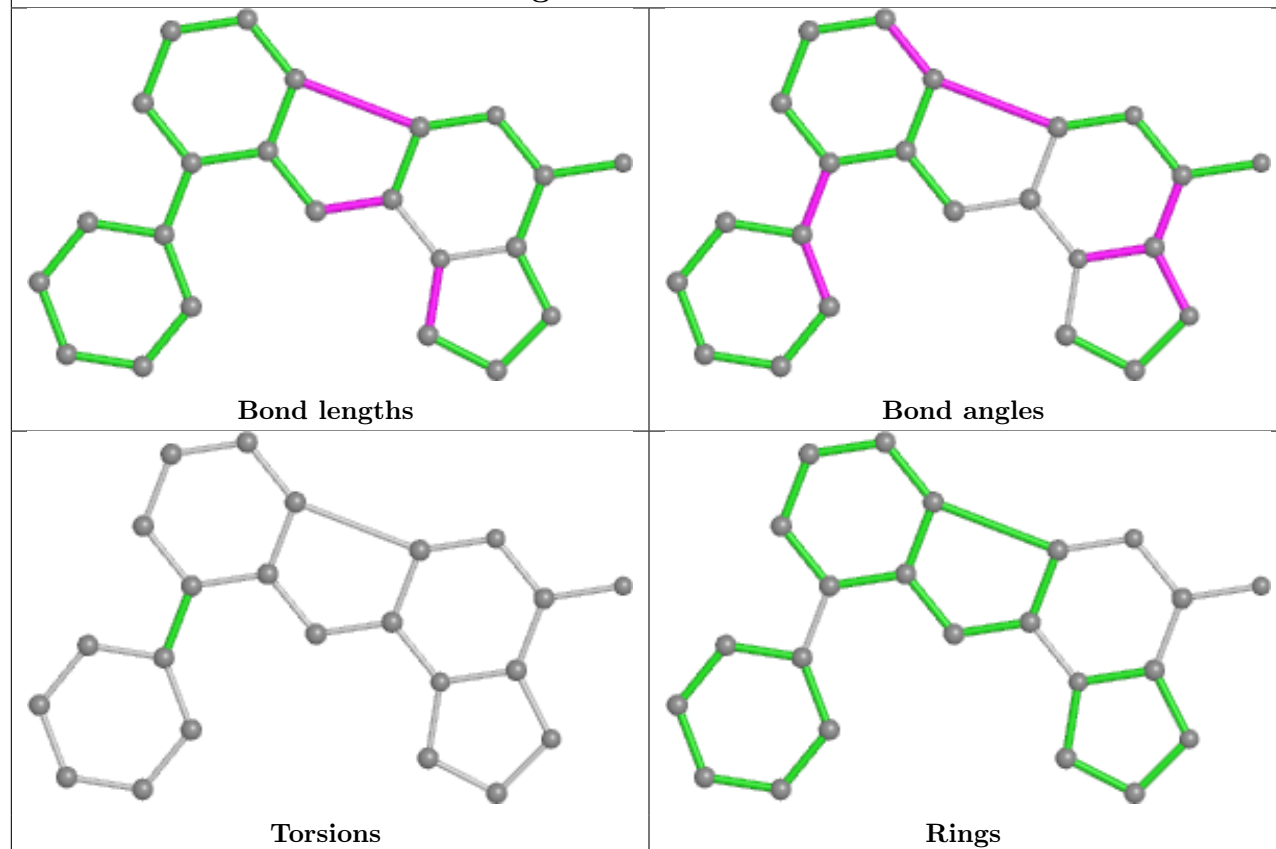
## Ligand 2K9 X 900



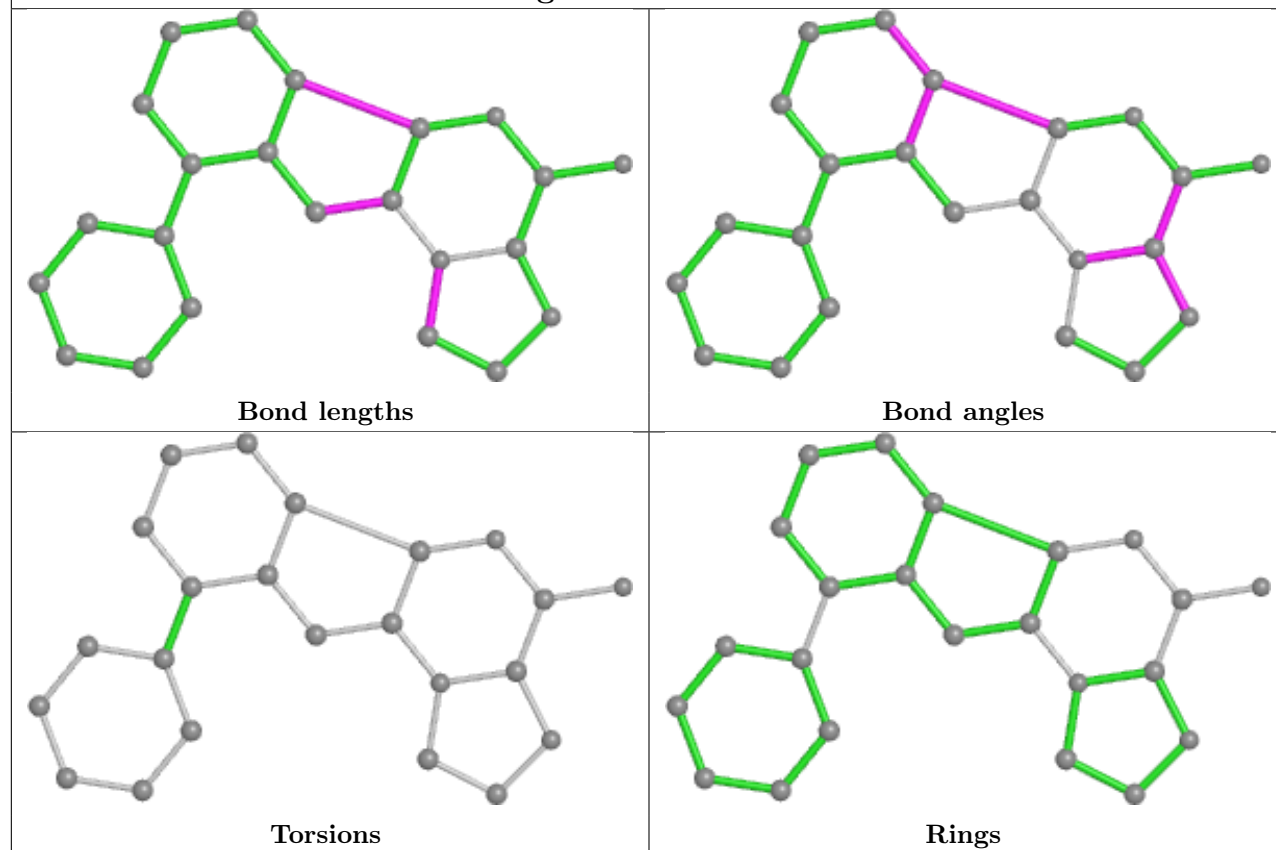
## Ligand 2K9 F 900



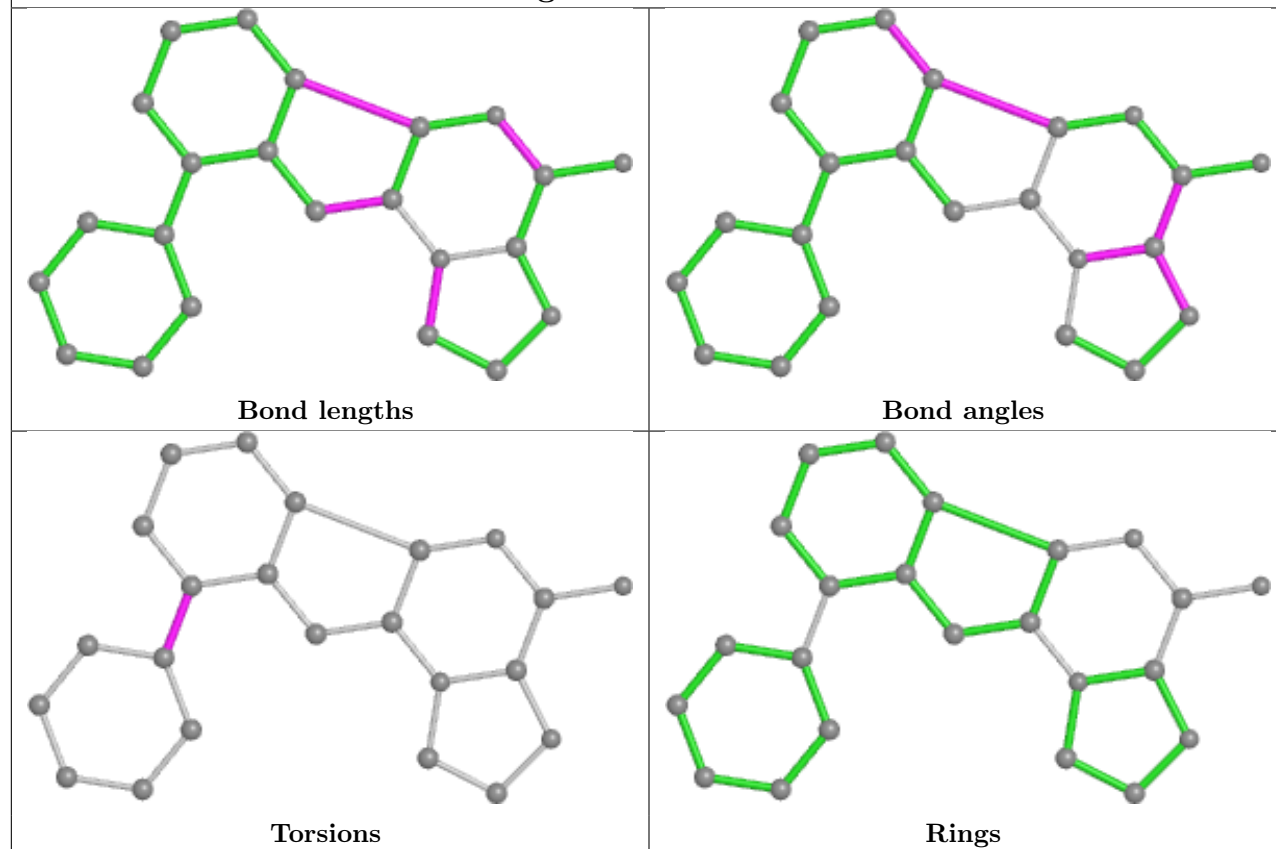
## Ligand 2K9 W 900



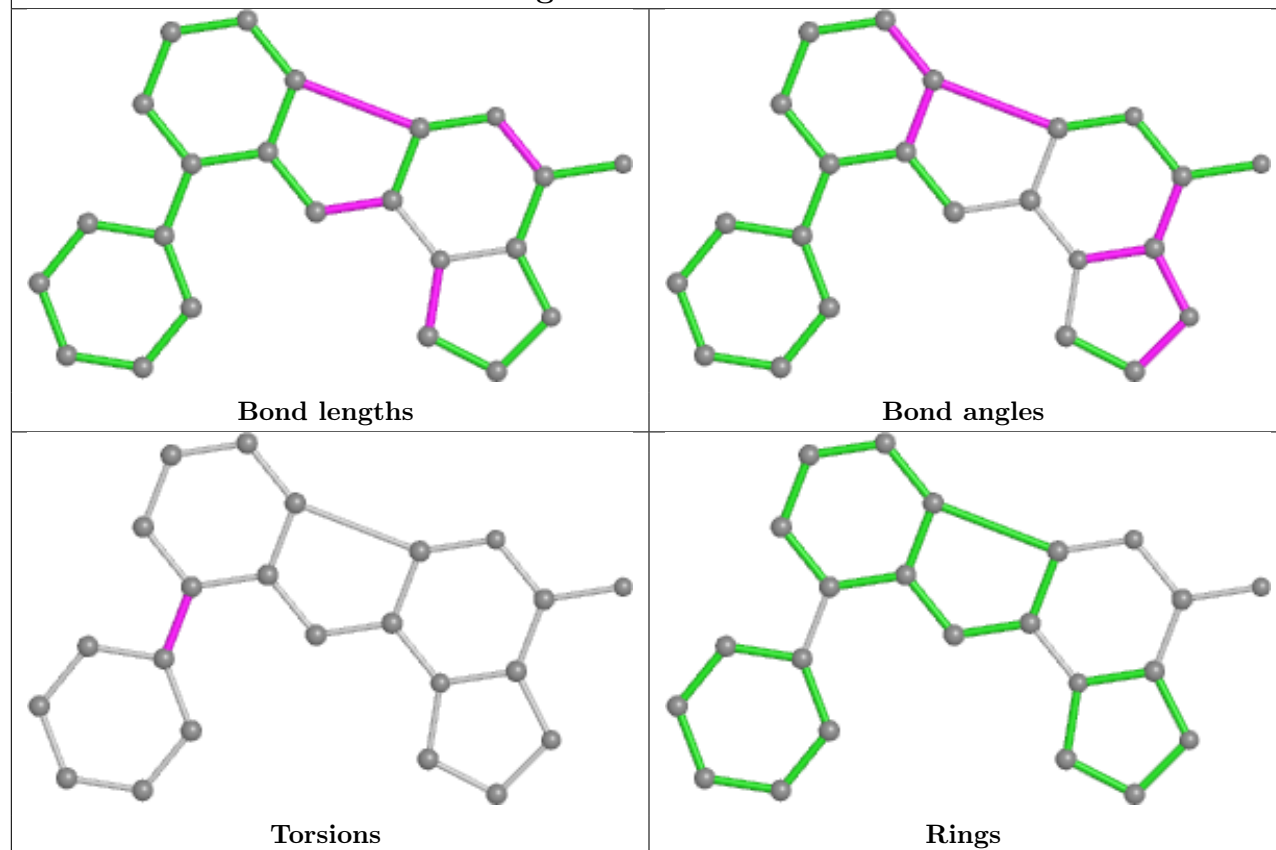
## Ligand 2K9 O 900



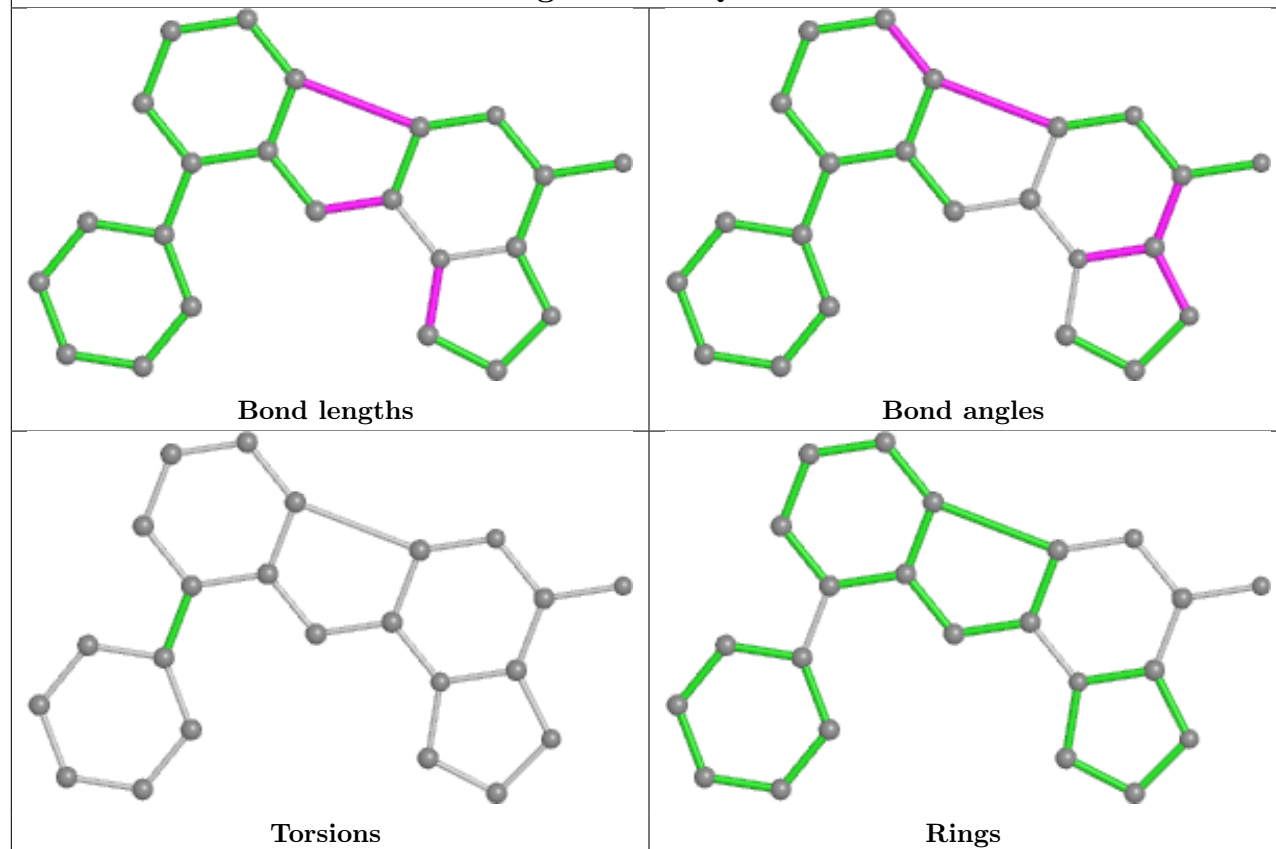
## Ligand 2K9 B 900



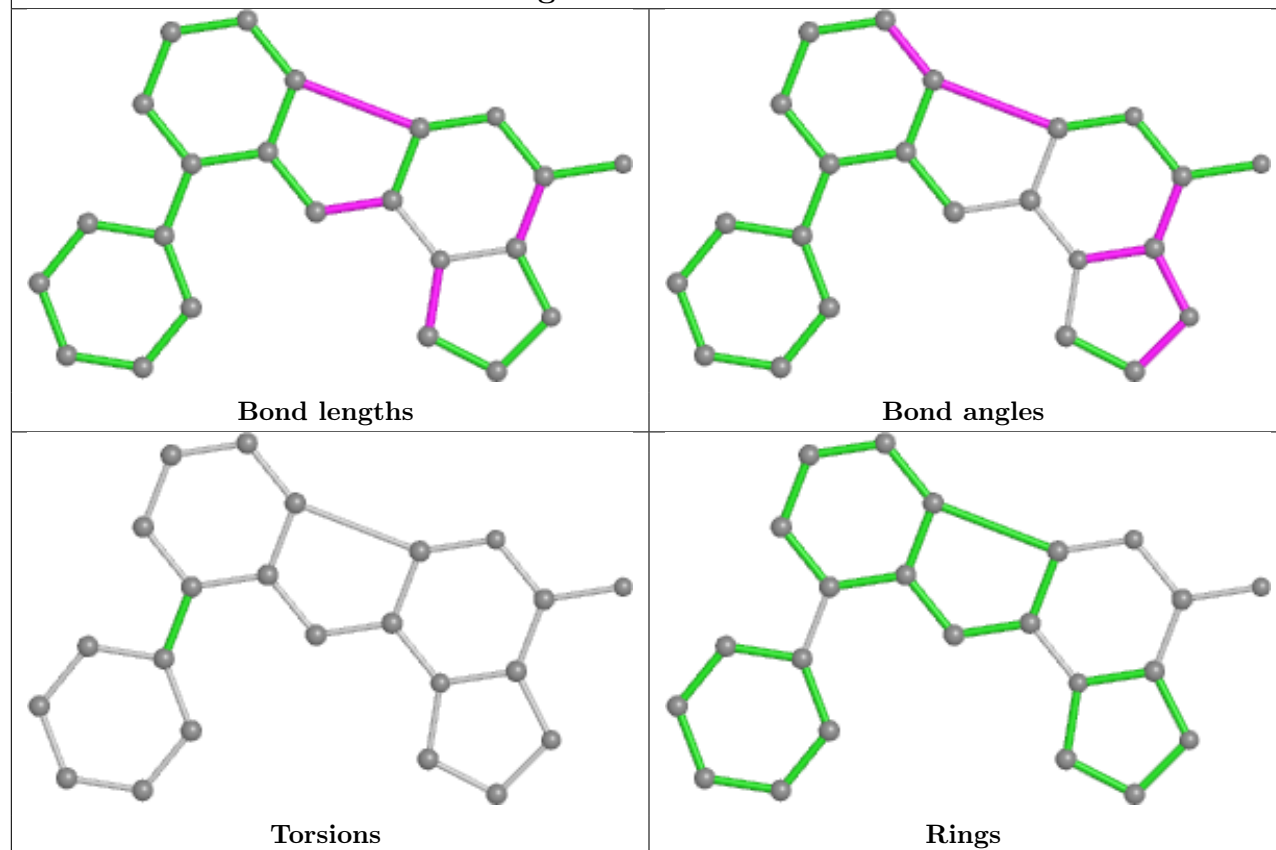
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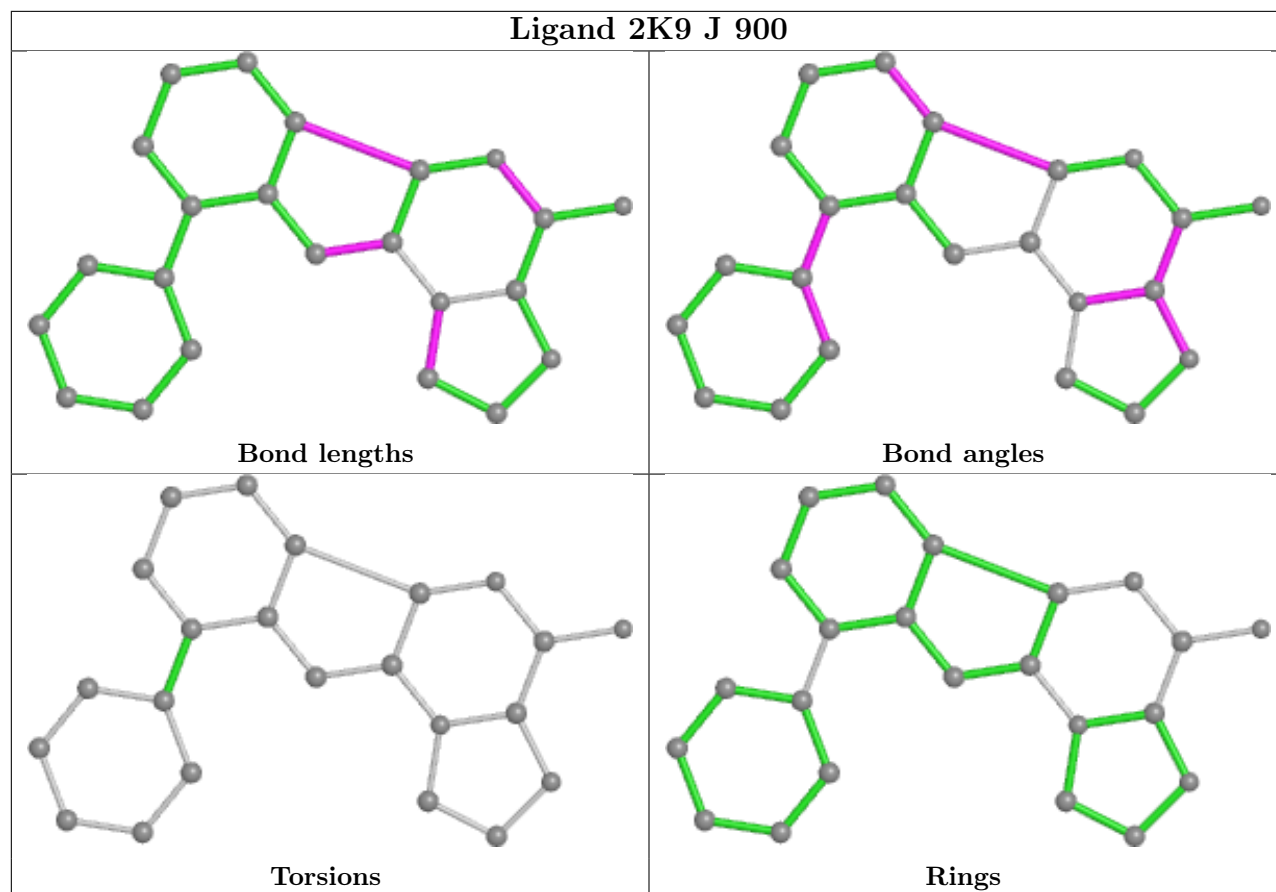


## Ligand 2K9 Q 900



## Ligand 2K9 T 900





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	466/478 (97%)	-0.18	17 (3%) 42 40	31, 54, 85, 128	0
1	B	464/478 (97%)	-0.11	15 (3%) 47 46	33, 55, 85, 125	0
1	C	460/478 (96%)	-0.20	5 (1%) 80 81	32, 53, 83, 124	0
1	D	466/478 (97%)	-0.17	8 (1%) 70 68	31, 52, 82, 124	0
1	E	463/478 (96%)	-0.21	5 (1%) 80 81	31, 52, 82, 124	0
1	F	467/478 (97%)	-0.19	5 (1%) 80 81	31, 54, 85, 124	0
1	G	466/478 (97%)	-0.18	11 (2%) 59 56	31, 54, 84, 124	0
1	H	464/478 (97%)	-0.20	12 (2%) 56 53	32, 54, 84, 124	0
1	I	460/478 (96%)	-0.26	7 (1%) 73 72	32, 53, 82, 124	0
1	J	466/478 (97%)	-0.25	8 (1%) 70 68	31, 52, 82, 124	0
1	K	463/478 (96%)	-0.16	8 (1%) 70 68	31, 53, 82, 124	0
1	L	467/478 (97%)	-0.25	5 (1%) 80 81	32, 53, 84, 124	0
1	M	466/478 (97%)	-0.10	13 (2%) 53 51	33, 54, 85, 124	0
1	N	464/478 (97%)	-0.23	6 (1%) 77 77	32, 53, 83, 124	0
1	O	460/478 (96%)	-0.20	9 (1%) 65 64	32, 54, 83, 124	0
1	P	466/478 (97%)	-0.23	10 (2%) 63 62	32, 54, 83, 124	0
1	Q	463/478 (96%)	-0.17	9 (1%) 66 65	34, 55, 83, 125	0
1	R	467/478 (97%)	-0.20	11 (2%) 59 56	32, 53, 84, 124	0
1	S	466/478 (97%)	-0.17	11 (2%) 59 56	33, 54, 84, 124	0
1	T	464/478 (97%)	-0.22	7 (1%) 73 72	32, 54, 83, 124	0
1	U	460/478 (96%)	-0.22	8 (1%) 70 68	32, 53, 83, 124	0
1	V	466/478 (97%)	-0.28	9 (1%) 66 65	31, 53, 82, 124	0
1	W	463/478 (96%)	-0.25	6 (1%) 77 77	33, 54, 82, 124	0
1	X	467/478 (97%)	-0.22	9 (1%) 66 65	31, 53, 84, 124	0

*Continued on next page...*

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	11144/11472 (97%)	-0.20	214 (1%) 66 65	31, 54, 84, 128	0

The worst 5 of 214 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	402	TYR	6.6
1	O	406	PRO	5.6
1	M	405	PRO	4.7
1	M	406	PRO	4.6
1	A	61	HIS	4.6

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	2K9	F	900	23/23	0.90	0.27	64,67,67,68	0
2	2K9	O	900	23/23	0.90	0.44	82,85,88,88	0
2	2K9	M	900	23/23	0.91	0.27	85,86,87,88	0
2	2K9	Q	900	23/23	0.92	0.24	113,114,114,114	0
2	2K9	W	900	23/23	0.92	0.22	76,77,77,78	0
2	2K9	B	900	23/23	0.93	0.26	100,102,103,104	0
2	2K9	S	900	23/23	0.93	0.22	67,69,71,72	0
2	2K9	U	900	23/23	0.93	0.32	69,73,75,77	0
2	2K9	P	900	23/23	0.93	0.27	64,65,66,67	0
2	2K9	H	900	23/23	0.94	0.27	90,90,91,92	0
2	2K9	G	900	23/23	0.94	0.26	54,54,56,57	0
2	2K9	N	900	23/23	0.94	0.24	58,60,61,62	0
2	2K9	R	900	23/23	0.95	0.31	57,58,59,59	0

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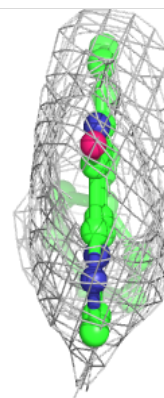
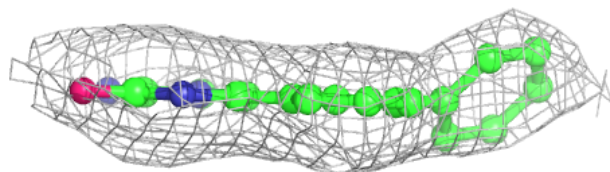
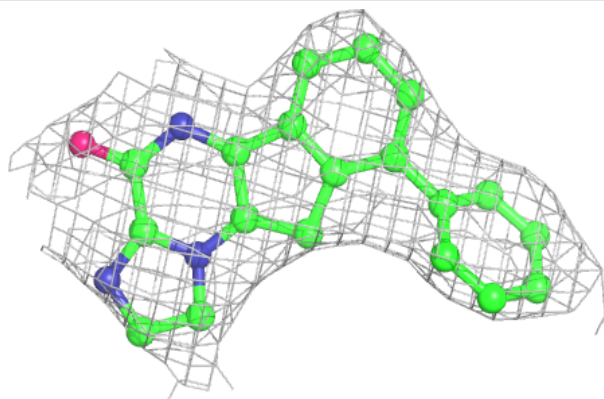
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2K9	K	900	23/23	0.95	0.20	46,48,49,50	0
2	2K9	D	900	23/23	0.95	0.22	47,51,53,54	0
2	2K9	V	900	23/23	0.95	0.23	39,43,45,47	0
2	2K9	I	900	23/23	0.95	0.19	54,55,57,57	0
2	2K9	X	900	23/23	0.95	0.28	60,61,61,62	0
2	2K9	A	900	23/23	0.96	0.27	58,60,62,62	0
2	2K9	L	900	23/23	0.96	0.24	50,51,52,53	0
2	2K9	J	900	23/23	0.96	0.24	56,58,60,60	0
2	2K9	T	900	23/23	0.96	0.24	75,75,76,76	0
2	2K9	E	900	23/23	0.97	0.25	43,44,46,46	0
2	2K9	C	900	23/23	0.97	0.20	47,48,49,50	0

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

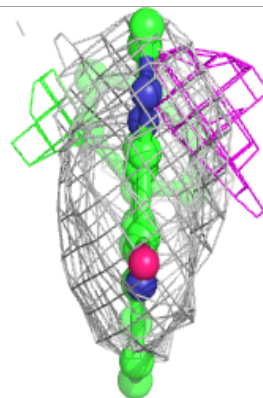
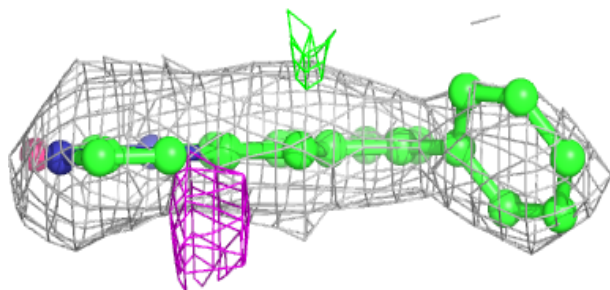
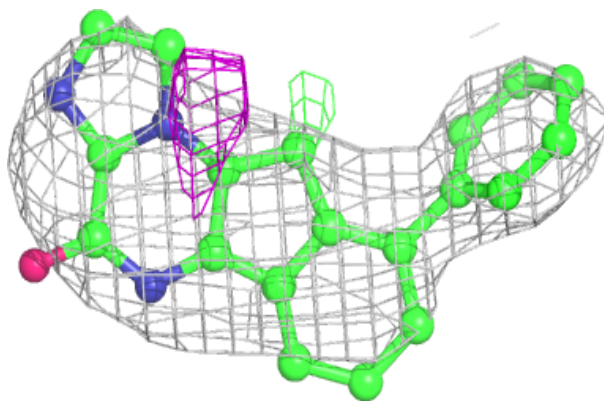
**Electron density around 2K9 F 900:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

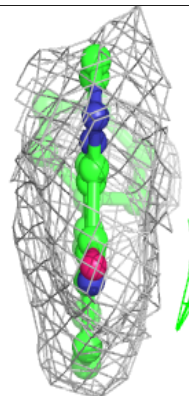
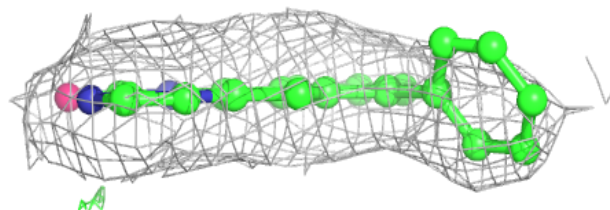
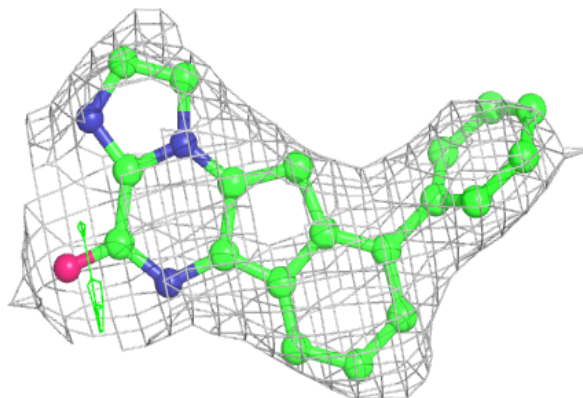


**Electron density around 2K9 O 900:**

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

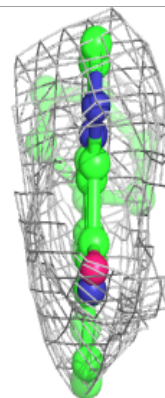
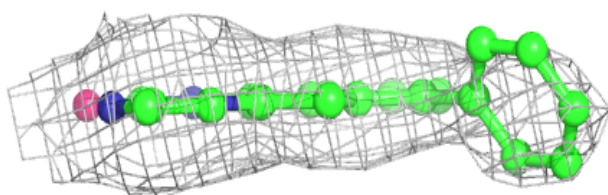
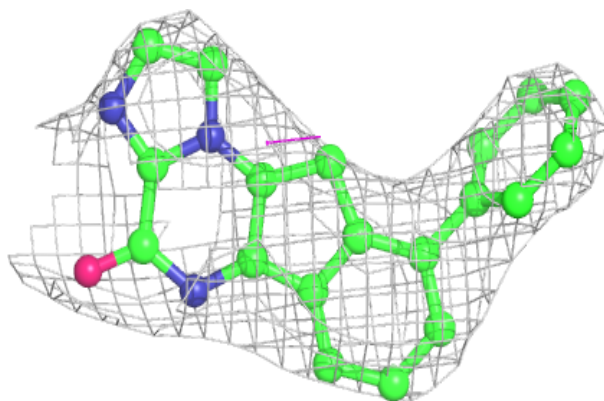
**Electron density around 2K9 M 900:**

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and green (positive)

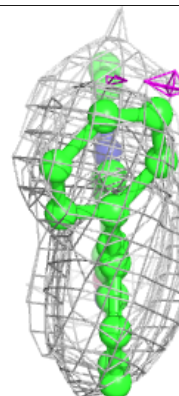
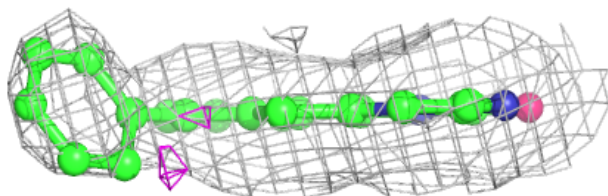
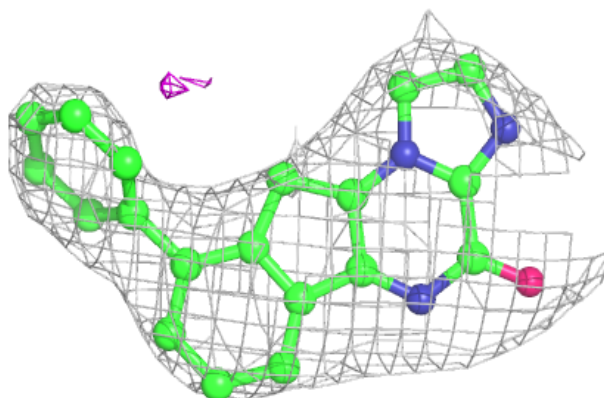


**Electron density around 2K9 Q 900:**

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and green (positive)

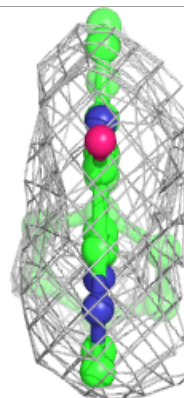
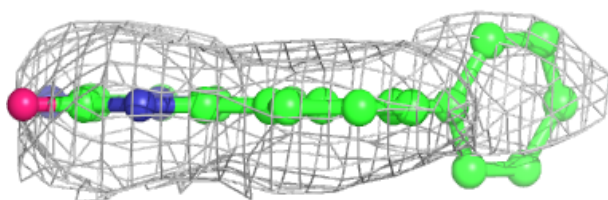
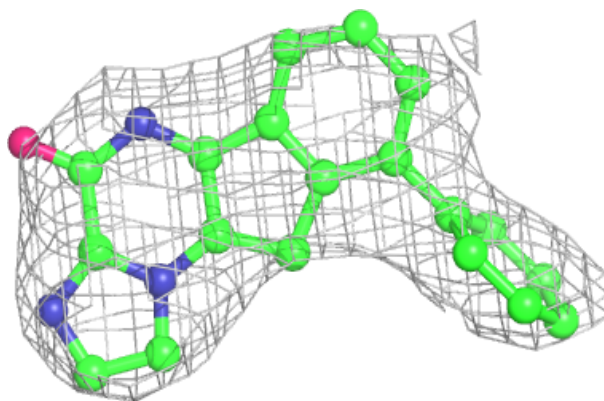
**Electron density around 2K9 W 900:**

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and green (positive)

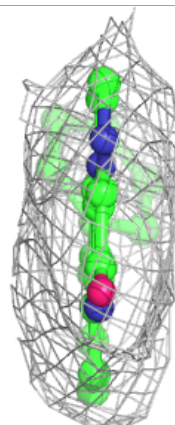
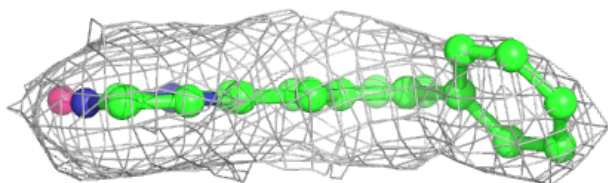
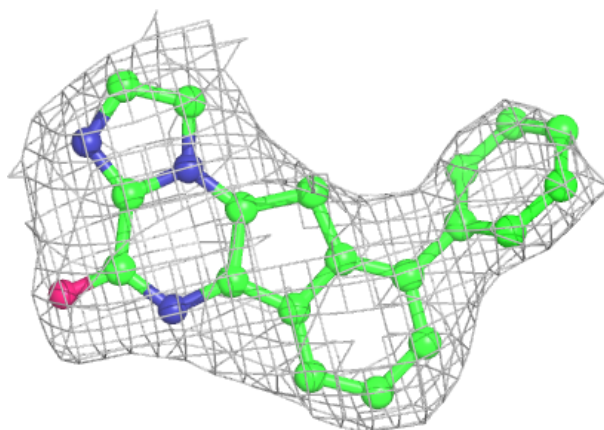


**Electron density around 2K9 B 900:**

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

**Electron density around 2K9 S 900:**

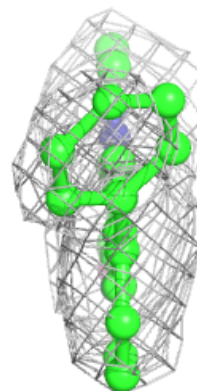
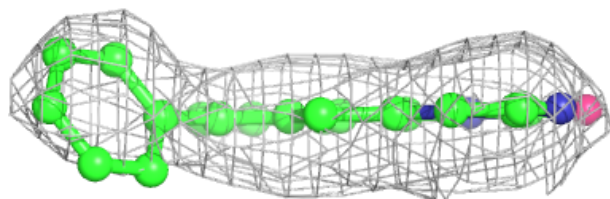
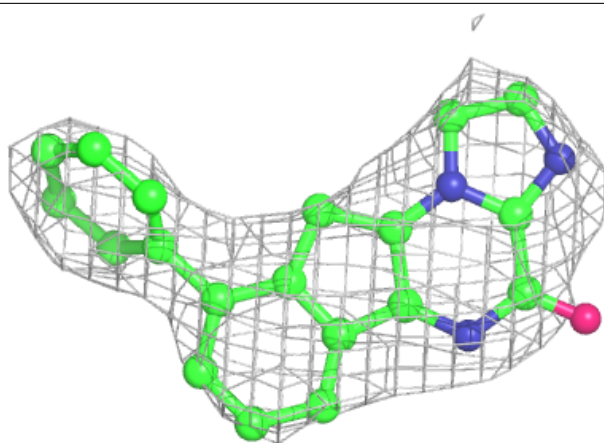
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



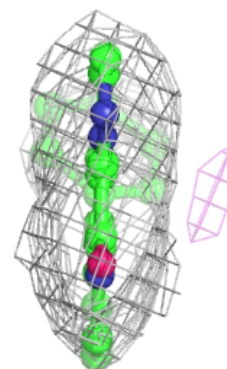
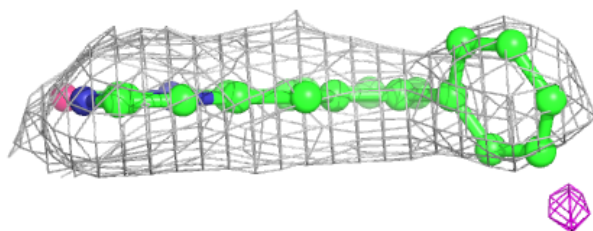
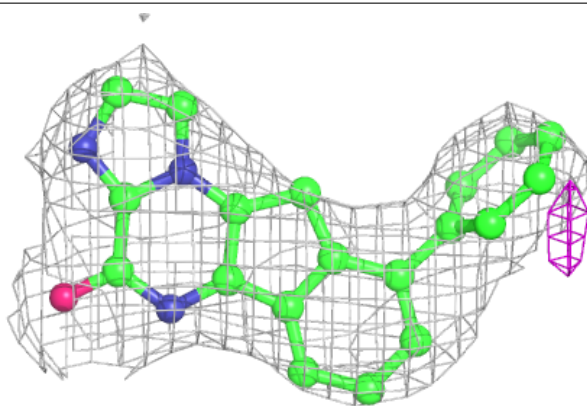


**Electron density around 2K9 U 900:**

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and green (positive)

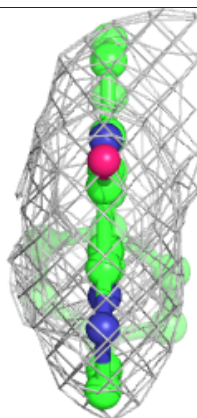
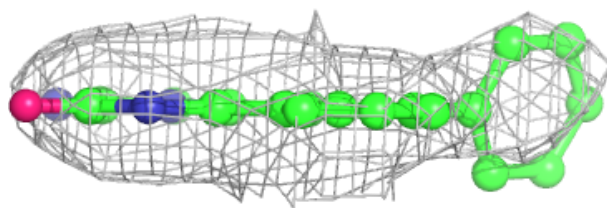
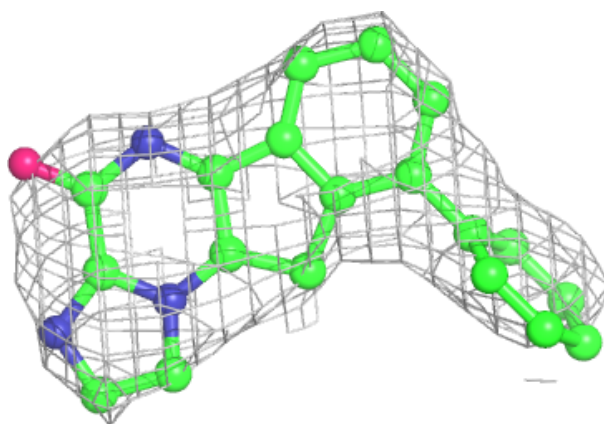
**Electron density around 2K9 P 900:**

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and green (positive)



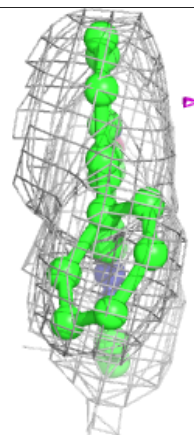
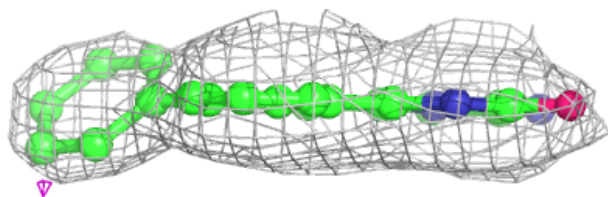
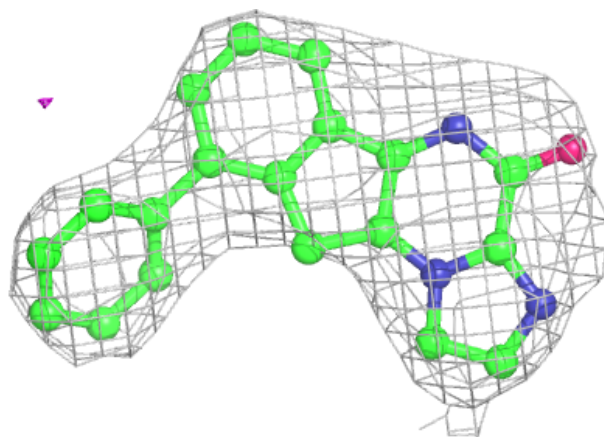
**Electron density around 2K9 H 900:**

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and green (positive)

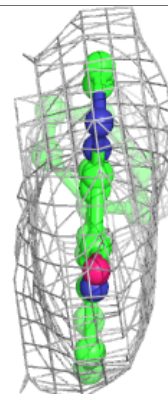
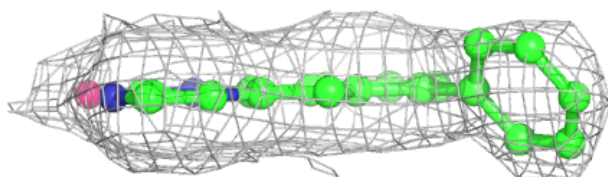
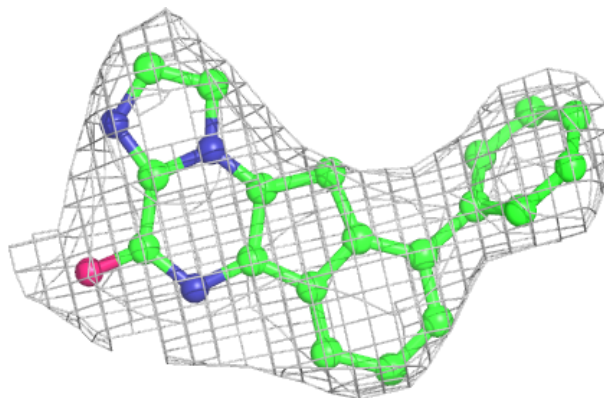


**Electron density around 2K9 G 900:**

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

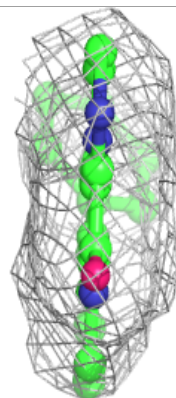
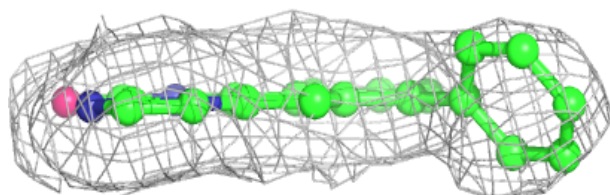
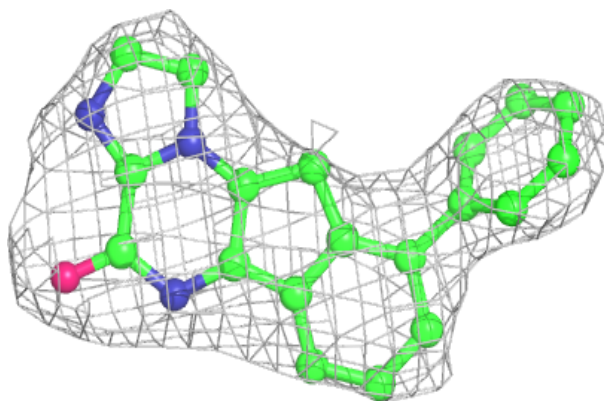
**Electron density around 2K9 N 900:**

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

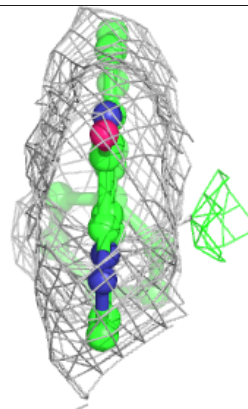
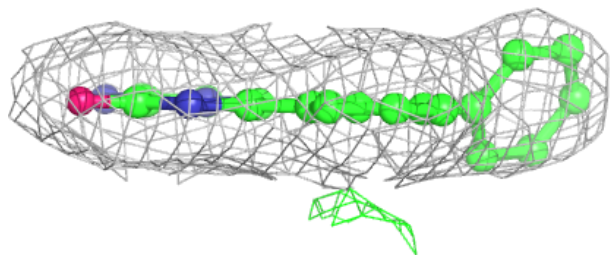
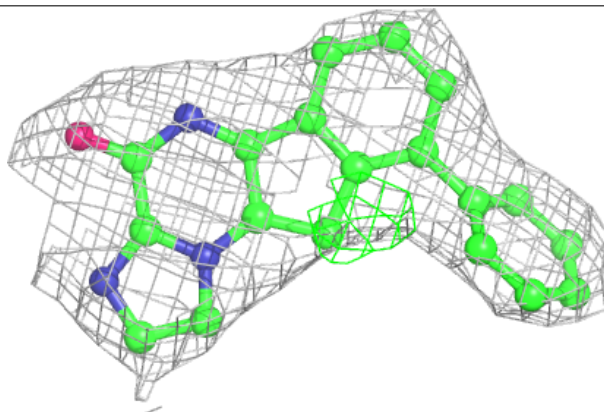


**Electron density around 2K9 R 900:**

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

**Electron density around 2K9 K 900:**

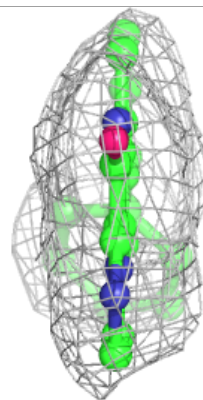
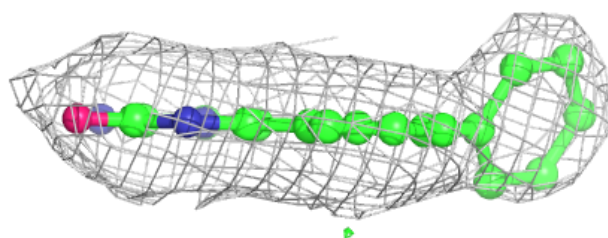
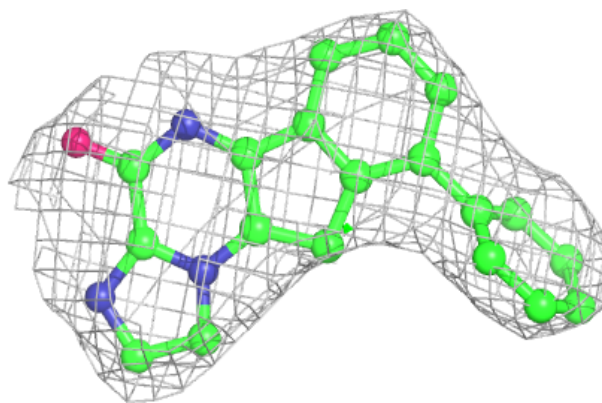
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



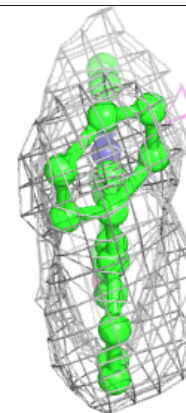
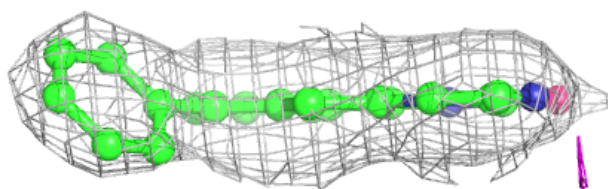
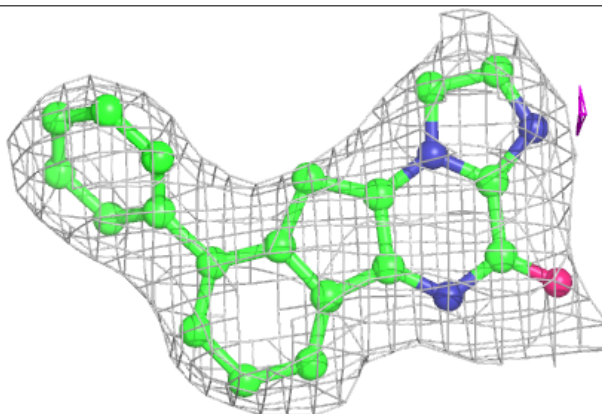


**Electron density around 2K9 D 900:**

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

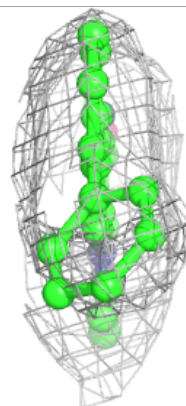
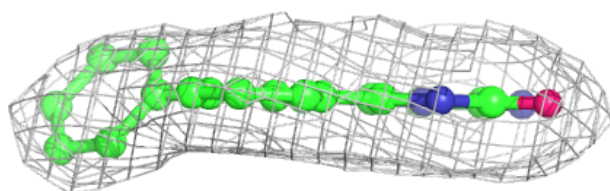
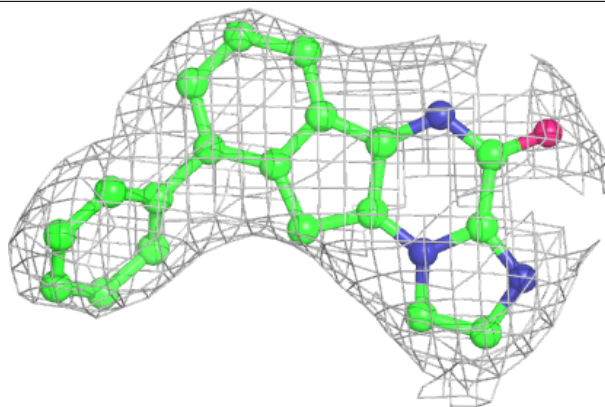
**Electron density around 2K9 V 900:**

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

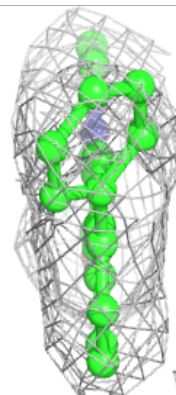
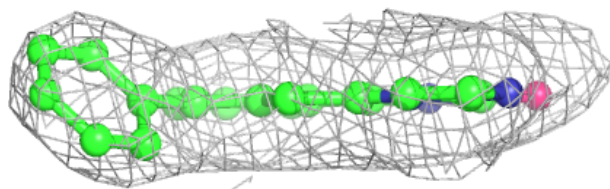
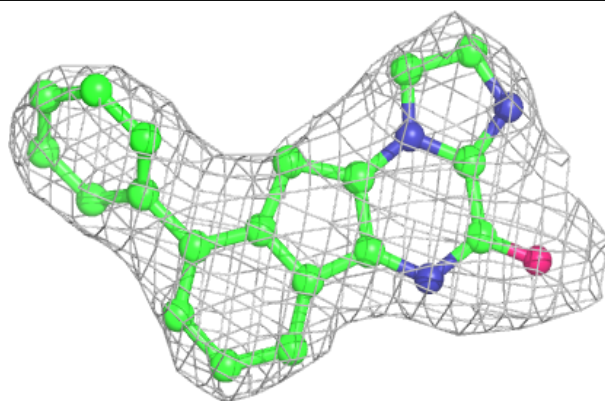


**Electron density around 2K9 I 900:**

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

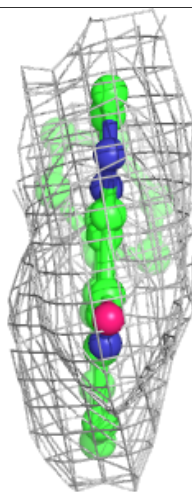
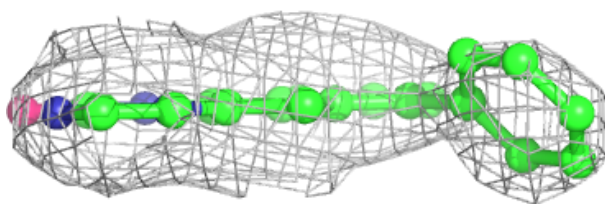
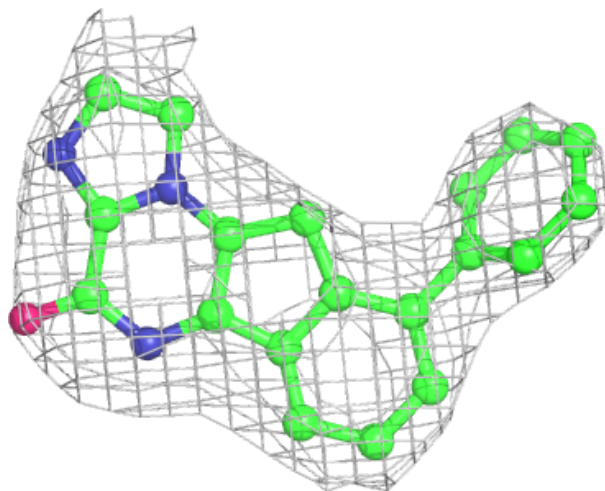
**Electron density around 2K9 X 900:**

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



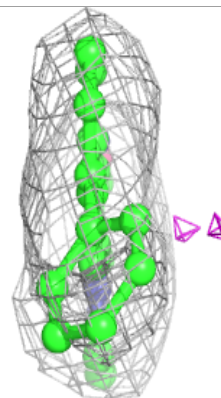
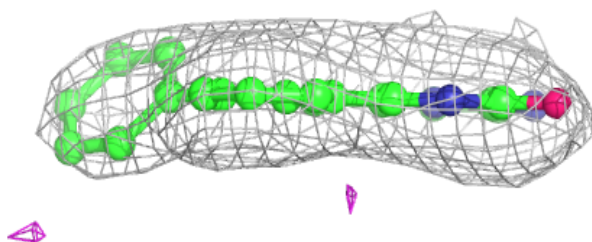
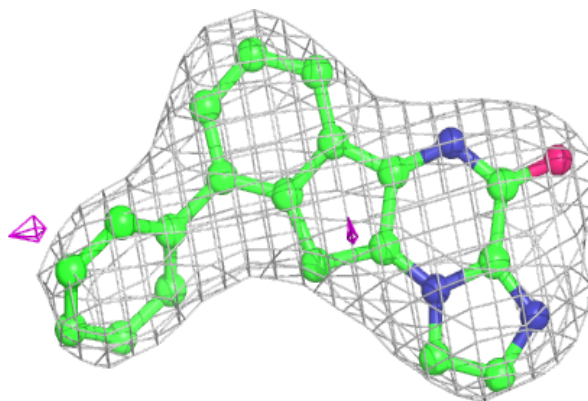
**Electron density around 2K9 A 900:**

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

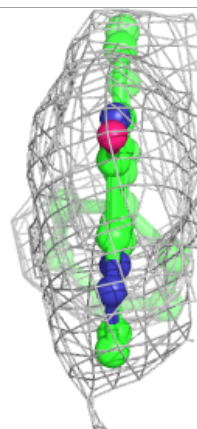
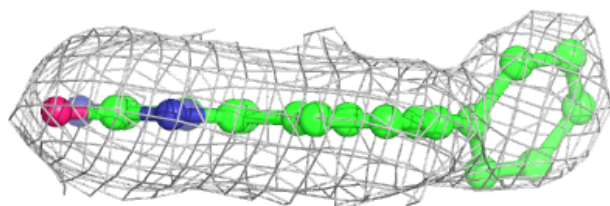
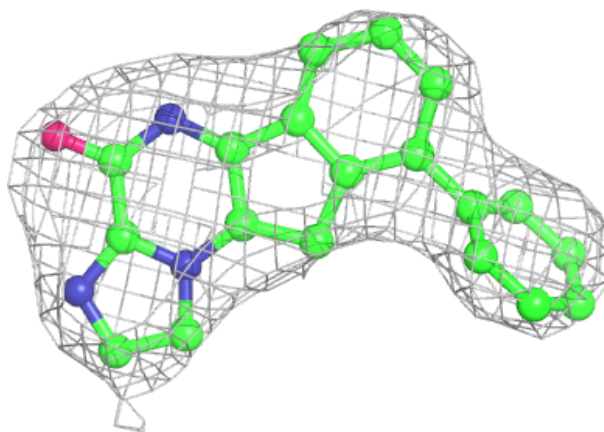


**Electron density around 2K9 L 900:**

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

**Electron density around 2K9 J 900:**

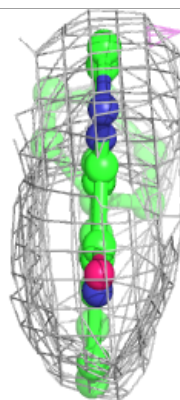
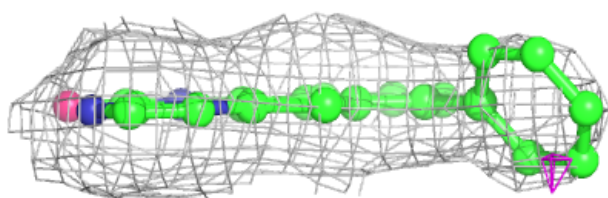
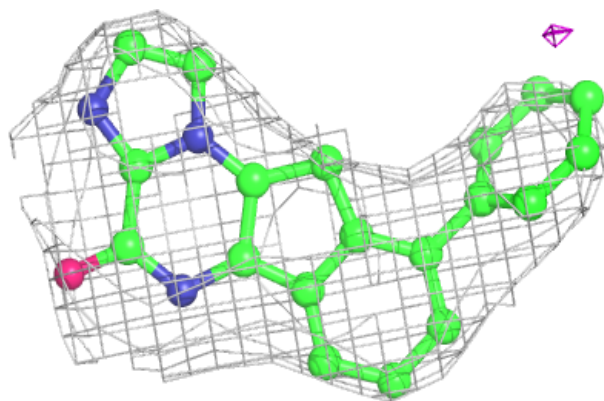
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



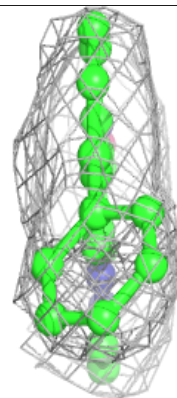
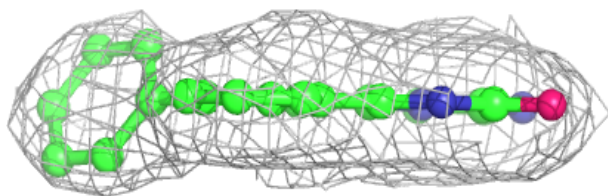
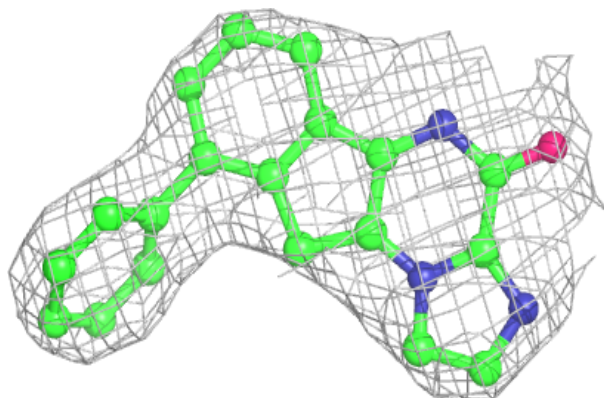


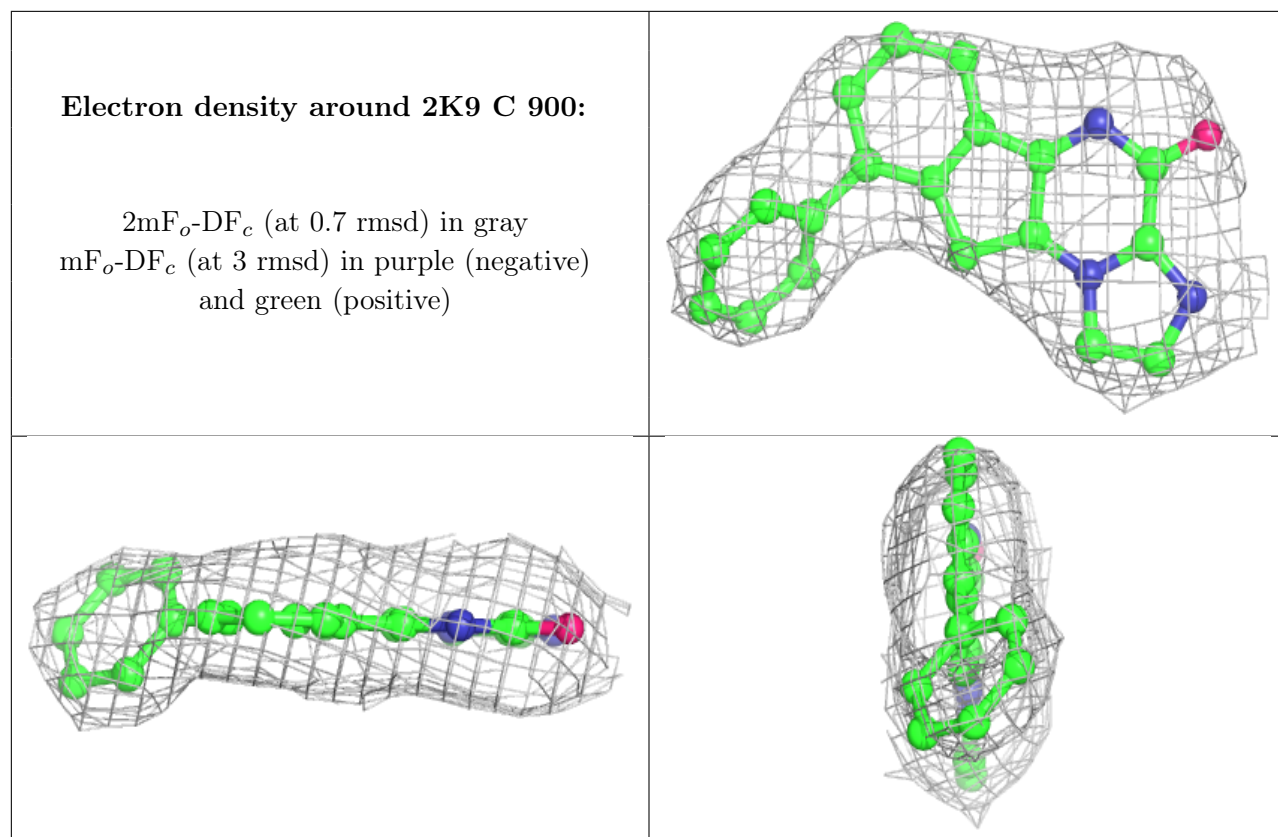
**Electron density around 2K9 T 900:**

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

**Electron density around 2K9 E 900:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.