



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 05:24 pm BST

PDB ID : 5K3I
Title : Crystal structure of Acyl-CoA oxidase-1 in *Caenorhabditis elegans* complexed with FAD and ATP
Authors : Zhang, X.; Li, K.; Jones, R.A.; Bruner, S.D.; Butcher, R.A.
Deposited on : 2016-05-19
Resolution : 2.68 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

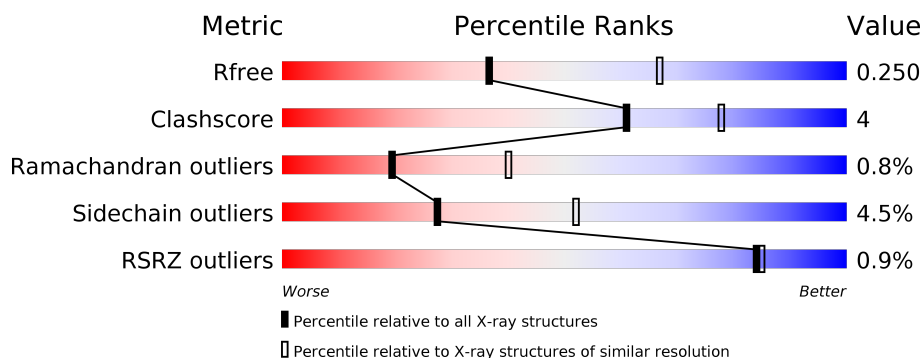
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 $\leq 5\%$. 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	684	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• •</div> </div> </div>
1	B	684	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>
1	C	684	<div> <div></div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• 5%</div> </div> </div>
1	D	684	<div> <div></div> <div> <div></div> <div>84%</div> <div>10%</div> <div>• 5%</div> </div> </div>
1	E	684	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• •</div> </div> </div>
1	F	684	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	684	<div><div>%</div><div><div></div><div>83%</div><div>11%</div><div>• 5%</div></div></div>
1	H	684	<div><div>%</div><div><div></div><div>84%</div><div>11%</div><div>• •</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42900 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 Acyl-coenzyme A oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5236	3321	921	966	28			
1	B	657	Total	C	N	O	S	0	0	0
			5211	3307	916	960	28			
1	C	650	Total	C	N	O	S	0	0	0
			5166	3281	907	950	28			
1	D	653	Total	C	N	O	S	0	0	0
			5188	3294	911	955	28			
1	E	661	Total	C	N	O	S	0	0	0
			5236	3321	921	966	28			
1	F	651	Total	C	N	O	S	0	0	0
			5164	3275	906	955	28			
1	G	653	Total	C	N	O	S	0	0	0
			5182	3288	911	955	28			
1	H	661	Total	C	N	O	S	0	0	0
			5236	3321	921	966	28			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	ALA	GLU	engineered mutation	UNP O62140
A	675	HIS	-	expression tag	UNP O62140
A	676	HIS	-	expression tag	UNP O62140
A	677	HIS	-	expression tag	UNP O62140
A	678	HIS	-	expression tag	UNP O62140
A	679	HIS	-	expression tag	UNP O62140
A	680	HIS	-	expression tag	UNP O62140
A	681	HIS	-	expression tag	UNP O62140
A	682	HIS	-	expression tag	UNP O62140
A	683	HIS	-	expression tag	UNP O62140
A	684	HIS	-	expression tag	UNP O62140
B	434	ALA	GLU	engineered mutation	UNP O62140
B	675	HIS	-	expression tag	UNP O62140

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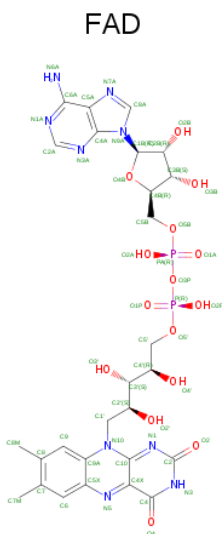
Chain	Residue	Modelled	Actual	Comment	Reference
B	676	HIS	-	expression tag	UNP O62140
B	677	HIS	-	expression tag	UNP O62140
B	678	HIS	-	expression tag	UNP O62140
B	679	HIS	-	expression tag	UNP O62140
B	680	HIS	-	expression tag	UNP O62140
B	681	HIS	-	expression tag	UNP O62140
B	682	HIS	-	expression tag	UNP O62140
B	683	HIS	-	expression tag	UNP O62140
B	684	HIS	-	expression tag	UNP O62140
C	434	ALA	GLU	engineered mutation	UNP O62140
C	675	HIS	-	expression tag	UNP O62140
C	676	HIS	-	expression tag	UNP O62140
C	677	HIS	-	expression tag	UNP O62140
C	678	HIS	-	expression tag	UNP O62140
C	679	HIS	-	expression tag	UNP O62140
C	680	HIS	-	expression tag	UNP O62140
C	681	HIS	-	expression tag	UNP O62140
C	682	HIS	-	expression tag	UNP O62140
C	683	HIS	-	expression tag	UNP O62140
C	684	HIS	-	expression tag	UNP O62140
D	434	ALA	GLU	engineered mutation	UNP O62140
D	675	HIS	-	expression tag	UNP O62140
D	676	HIS	-	expression tag	UNP O62140
D	677	HIS	-	expression tag	UNP O62140
D	678	HIS	-	expression tag	UNP O62140
D	679	HIS	-	expression tag	UNP O62140
D	680	HIS	-	expression tag	UNP O62140
D	681	HIS	-	expression tag	UNP O62140
D	682	HIS	-	expression tag	UNP O62140
D	683	HIS	-	expression tag	UNP O62140
D	684	HIS	-	expression tag	UNP O62140
E	434	ALA	GLU	engineered mutation	UNP O62140
E	675	HIS	-	expression tag	UNP O62140
E	676	HIS	-	expression tag	UNP O62140
E	677	HIS	-	expression tag	UNP O62140
E	678	HIS	-	expression tag	UNP O62140
E	679	HIS	-	expression tag	UNP O62140
E	680	HIS	-	expression tag	UNP O62140
E	681	HIS	-	expression tag	UNP O62140
E	682	HIS	-	expression tag	UNP O62140
E	683	HIS	-	expression tag	UNP O62140
E	684	HIS	-	expression tag	UNP O62140

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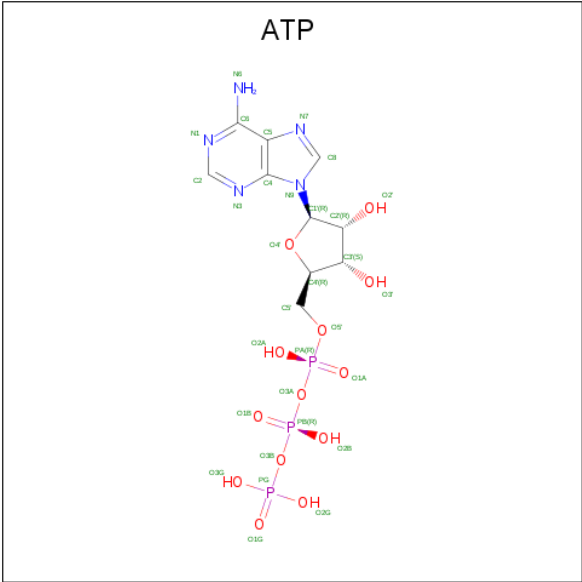
Chain	Residue	Modelled	Actual	Comment	Reference
F	434	ALA	GLU	engineered mutation	UNP O62140
F	675	HIS	-	expression tag	UNP O62140
F	676	HIS	-	expression tag	UNP O62140
F	677	HIS	-	expression tag	UNP O62140
F	678	HIS	-	expression tag	UNP O62140
F	679	HIS	-	expression tag	UNP O62140
F	680	HIS	-	expression tag	UNP O62140
F	681	HIS	-	expression tag	UNP O62140
F	682	HIS	-	expression tag	UNP O62140
F	683	HIS	-	expression tag	UNP O62140
F	684	HIS	-	expression tag	UNP O62140
G	434	ALA	GLU	engineered mutation	UNP O62140
G	675	HIS	-	expression tag	UNP O62140
G	676	HIS	-	expression tag	UNP O62140
G	677	HIS	-	expression tag	UNP O62140
G	678	HIS	-	expression tag	UNP O62140
G	679	HIS	-	expression tag	UNP O62140
G	680	HIS	-	expression tag	UNP O62140
G	681	HIS	-	expression tag	UNP O62140
G	682	HIS	-	expression tag	UNP O62140
G	683	HIS	-	expression tag	UNP O62140
G	684	HIS	-	expression tag	UNP O62140
H	434	ALA	GLU	engineered mutation	UNP O62140
H	675	HIS	-	expression tag	UNP O62140
H	676	HIS	-	expression tag	UNP O62140
H	677	HIS	-	expression tag	UNP O62140
H	678	HIS	-	expression tag	UNP O62140
H	679	HIS	-	expression tag	UNP O62140
H	680	HIS	-	expression tag	UNP O62140
H	681	HIS	-	expression tag	UNP O62140
H	682	HIS	-	expression tag	UNP O62140
H	683	HIS	-	expression tag	UNP O62140
H	684	HIS	-	expression tag	UNP O62140

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Id	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	G	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	H	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0

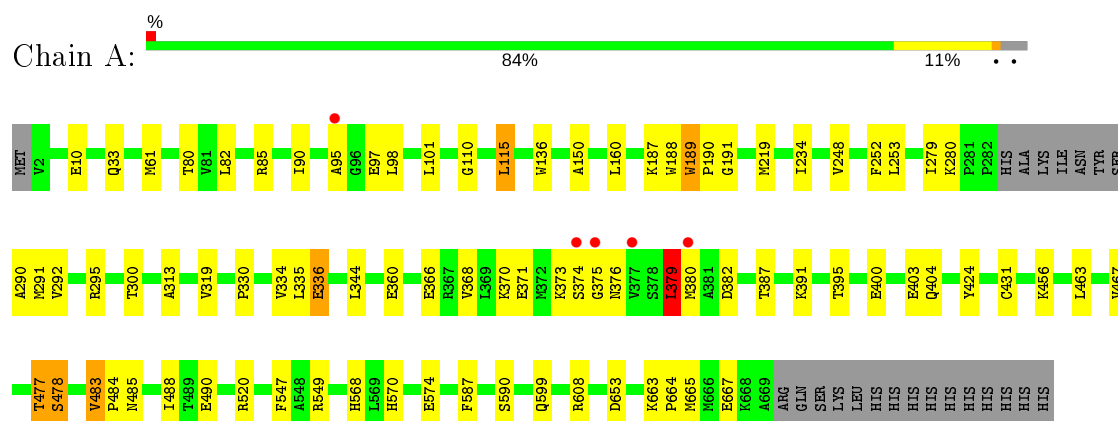
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	102	Total 102	O 102	0	0
5	B	69	Total 69	O 69	0	0
5	C	58	Total 58	O 58	0	0
5	D	76	Total 76	O 76	0	0
5	E	82	Total 82	O 82	0	0
5	F	58	Total 58	O 58	0	0
5	G	71	Total 71	O 71	0	0
5	H	85	Total 85	O 85	0	0

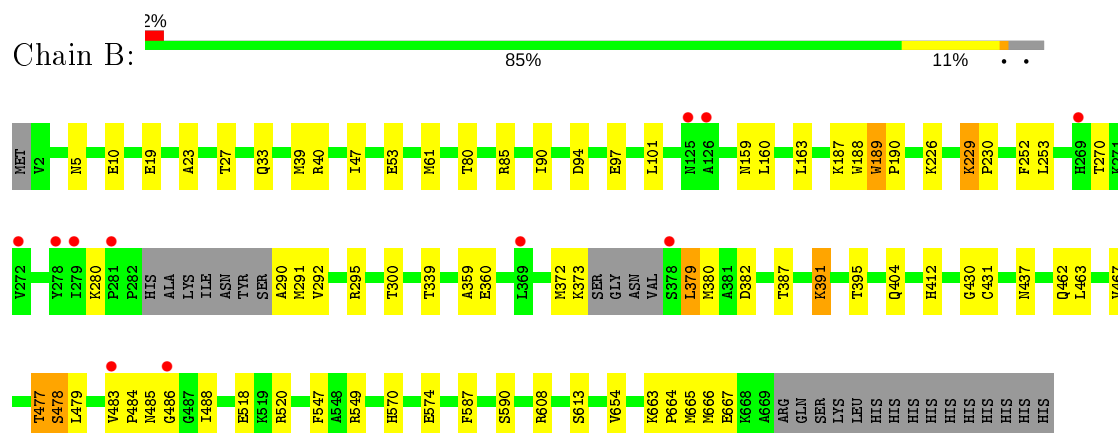
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

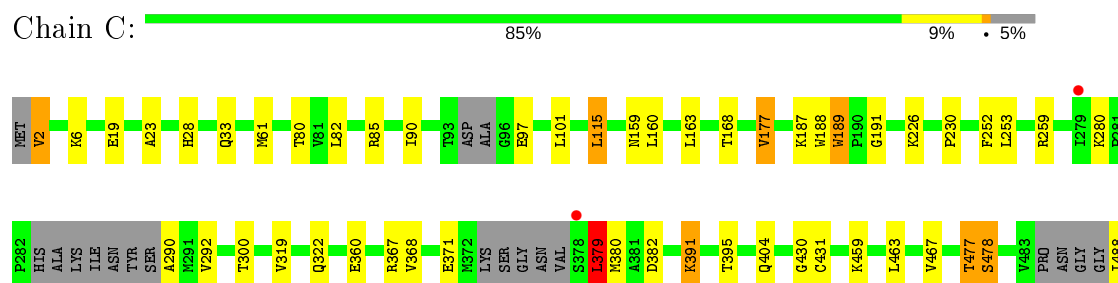
• Molecule 1: Acyl-coenzyme A oxidase



• Molecule 1: Acyl-coenzyme A oxidase



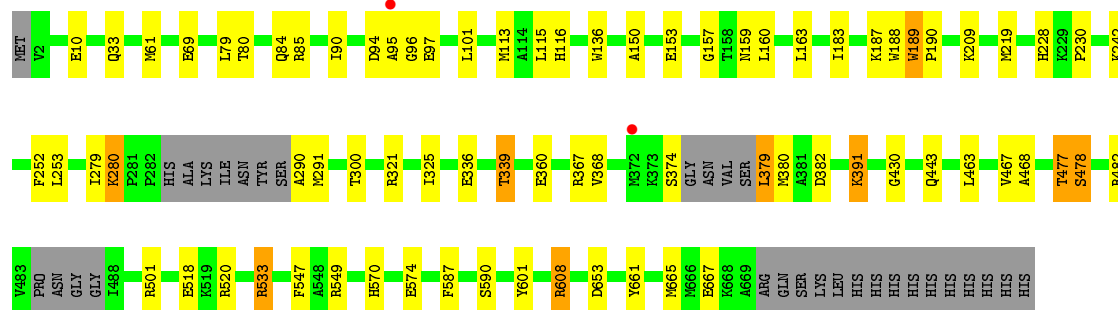
• Molecule 1: Acyl-coenzyme A oxidase





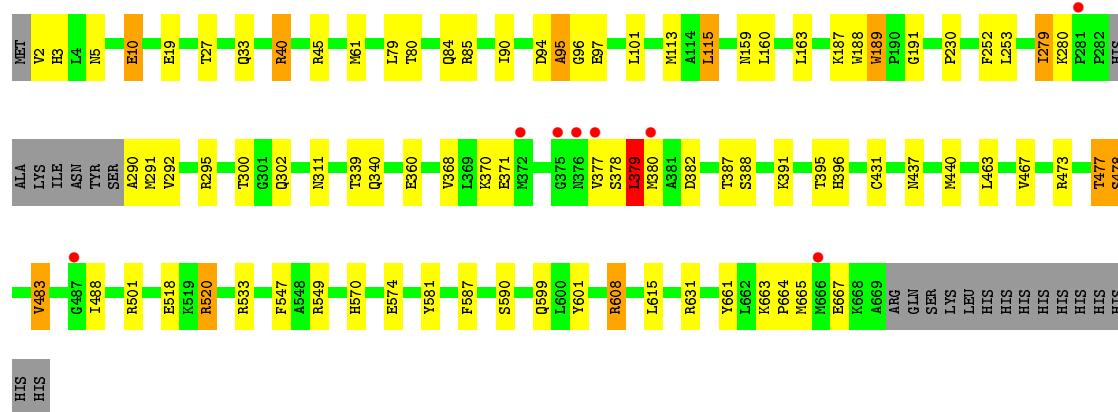
• Molecule 1: Acyl-coenzyme A oxidase

Chain D: 84% 10% • 5%



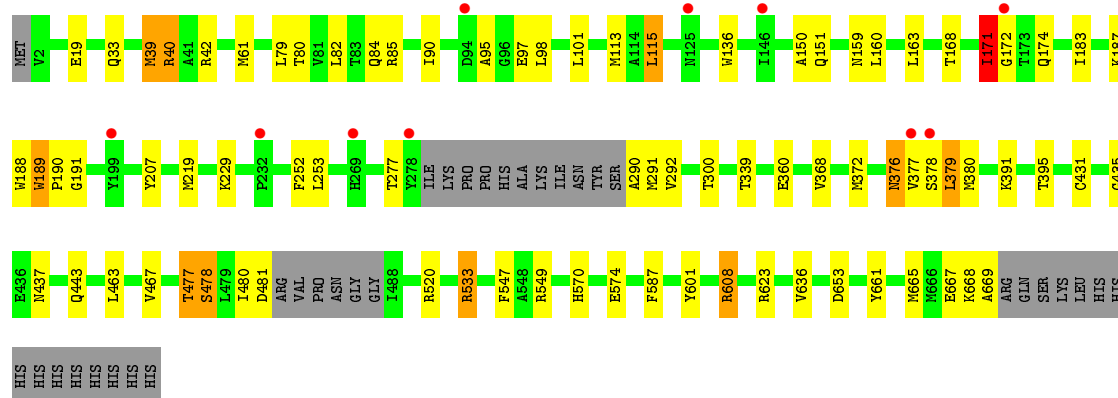
• Molecule 1: Acyl-coenzyme A oxidase

Chain E: 84% 11% • 5%

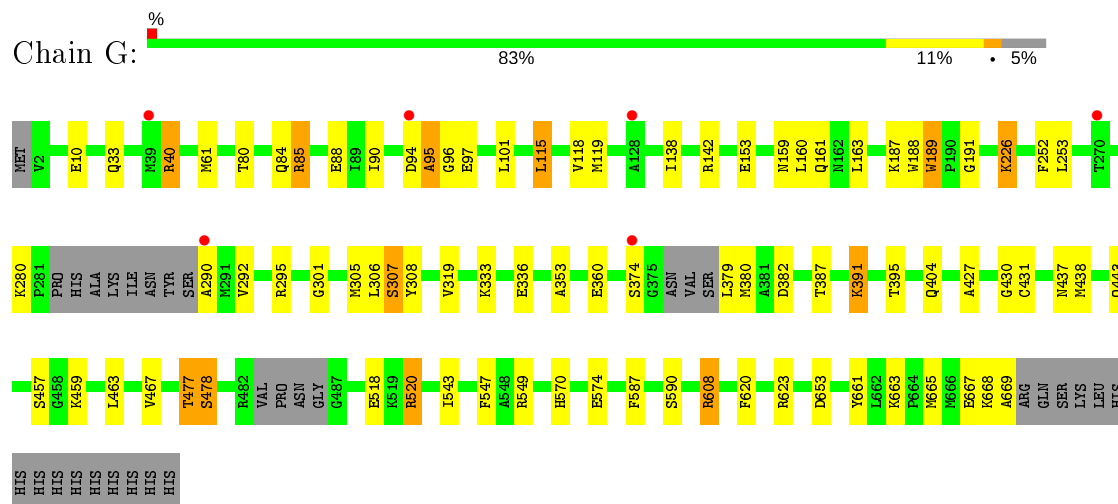


• Molecule 1: Acyl-coenzyme A oxidase

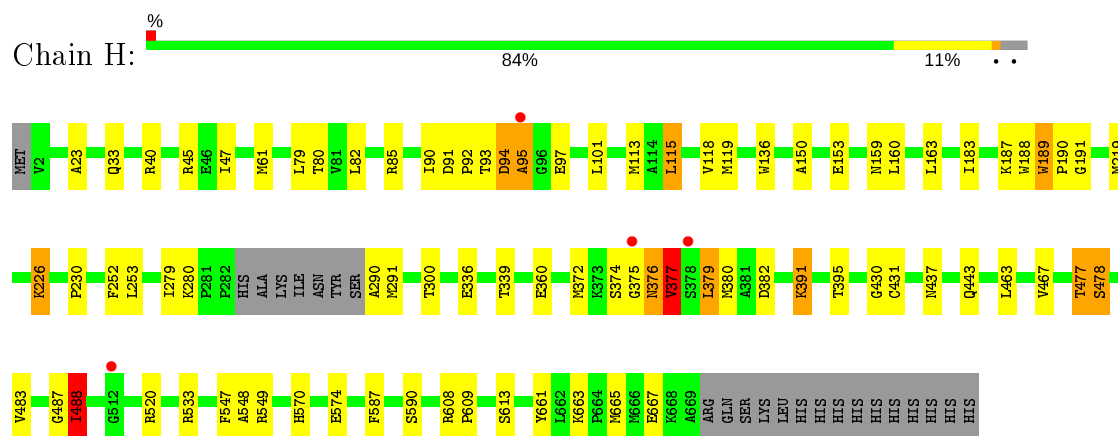
Chain F: 83% 10% • 5%



- Molecule 1: Acyl-coenzyme A oxidase



- Molecule 1: Acyl-coenzyme A oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.34Å 141.50Å 154.97Å 90.00° 116.76° 90.00°	Depositor
Resolution (Å)	38.74 – 2.68 38.74 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.74-2.68) 94.1 (38.74-2.68)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.217 , 0.232 0.236 , 0.250	Depositor DCC
R_{free} test set	8015 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 2.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.176 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	42900	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 52.22 % 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 5.0142e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FAD, ATP

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	0.32	0/5343	0.58	0/7224
1	B	0.32	0/5317	0.56	0/7187
1	C	0.31	0/5269	0.57	0/7119
1	D	0.31	0/5292	0.52	0/7151
1	E	0.31	0/5343	0.54	0/7224
1	F	0.31	0/5267	0.54	0/7118
1	G	0.30	0/5285	0.55	0/7139
1	H	0.31	0/5343	0.54	0/7224
All	All	0.31	0/42459	0.55	0/57386

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	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	95	ALA	Peptide

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	5236	0	5260	49	0
1	B	5211	0	5236	43	0
1	C	5166	0	5193	55	0
1	D	5188	0	5216	47	0
1	E	5236	0	5260	56	0
1	F	5164	0	5180	55	0
1	G	5182	0	5206	52	0
1	H	5236	0	5260	53	0
2	A	53	0	29	1	0
2	B	53	0	30	1	0
2	C	53	0	30	1	0
2	D	53	0	30	1	0
2	E	53	0	30	0	0
2	F	53	0	30	4	0
2	G	53	0	30	0	0
2	H	53	0	30	2	0
3	A	31	0	12	2	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	1	0
3	E	31	0	12	0	0
3	F	31	0	12	0	0
3	G	31	0	12	2	0
3	H	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	102	0	0	4	0
5	B	69	0	0	3	0
5	C	58	0	0	7	0
5	D	76	0	0	5	0
5	E	82	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	58	0	0	4	0
5	G	71	0	0	5	0
5	H	85	0	0	1	0
All	All	42900	0	42146	378	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 4.

The worst 5 of 378 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:C:520:ARG:NH2	1:E:483:VAL:HG13	1.48	1.26
1:C:520:ARG:HH21	1:E:483:VAL:HG13	1.05	1.00
1:B:47:ILE:HD11	1:B:97:GLU:HG2	1.43	0.99
1:F:171:ILE:HG23	1:F:172:GLY:H	1.23	0.99
1:C:520:ARG:NH2	1:E:483:VAL:CG1	2.33	0.91

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	657/684 (96%)	619 (94%)	30 (5%)	8 (1%)	13	29
1	B	651/684 (95%)	619 (95%)	27 (4%)	5 (1%)	19	40
1	C	640/684 (94%)	613 (96%)	23 (4%)	4 (1%)	25	47
1	D	645/684 (94%)	616 (96%)	25 (4%)	4 (1%)	25	47
1	E	657/684 (96%)	622 (95%)	29 (4%)	6 (1%)	17	37
1	F	645/684 (94%)	613 (95%)	28 (4%)	4 (1%)	25	47
1	G	645/684 (94%)	620 (96%)	21 (3%)	4 (1%)	25	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	657/684 (96%)	622 (95%)	27 (4%)	8 (1%)	13	29
All	All	5197/5472 (95%)	4944 (95%)	210 (4%)	43 (1%)	19	40

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	TRP
1	A	488	ILE
1	B	189	TRP
1	C	189	TRP
1	D	189	TRP

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	556/578 (96%)	534 (96%)	22 (4%)	31	57
1	B	553/578 (96%)	530 (96%)	23 (4%)	30	55
1	C	549/578 (95%)	529 (96%)	20 (4%)	35	61
1	D	551/578 (95%)	525 (95%)	26 (5%)	26	50
1	E	556/578 (96%)	530 (95%)	26 (5%)	26	50
1	F	548/578 (95%)	521 (95%)	27 (5%)	25	49
1	G	549/578 (95%)	522 (95%)	27 (5%)	25	49
1	H	556/578 (96%)	529 (95%)	27 (5%)	25	49
All	All	4418/4624 (96%)	4220 (96%)	198 (4%)	27	52

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	608	ARG
1	E	483	VAL
1	H	376	ASN
1	E	33	GLN

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Mol	Chain	Res	Type
1	E	300	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	570	HIS
1	G	462	GLN
1	E	462	GLN
1	B	384	HIS
1	F	174	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	F	701	-	51,58,58	4.60	19 (37%)	60,89,89	2.69	16 (26%)
2	FAD	A	701	-	51,58,58	4.61	18 (35%)	60,89,89	2.85	18 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	G	701	-	51,58,58	4.58	20 (39%)	60,89,89	2.66	14 (23%)
2	FAD	E	701	-	51,58,58	4.64	20 (39%)	60,89,89	2.74	15 (25%)
3	ATP	H	702	4	26,33,33	0.97	2 (7%)	31,52,52	1.44	4 (12%)
3	ATP	C	703	4	26,33,33	0.99	1 (3%)	31,52,52	1.47	4 (12%)
3	ATP	B	703	4	26,33,33	0.93	1 (3%)	31,52,52	1.55	5 (16%)
3	ATP	E	703	4	26,33,33	0.95	2 (7%)	31,52,52	1.49	5 (16%)
3	ATP	A	702	4	26,33,33	1.03	2 (7%)	31,52,52	1.51	5 (16%)
3	ATP	G	703	4	26,33,33	1.00	2 (7%)	31,52,52	1.56	6 (19%)
3	ATP	D	801	4	26,33,33	0.89	1 (3%)	31,52,52	1.43	5 (16%)
3	ATP	F	702	4	26,33,33	1.00	1 (3%)	31,52,52	1.46	5 (16%)
2	FAD	H	701	-	51,58,58	4.62	20 (39%)	60,89,89	2.72	14 (23%)
2	FAD	D	803	-	51,58,58	4.69	18 (35%)	60,89,89	2.33	12 (20%)
2	FAD	B	702	-	51,58,58	4.58	18 (35%)	60,89,89	2.66	15 (25%)
2	FAD	C	701	-	51,58,58	4.58	17 (33%)	60,89,89	2.58	16 (26%)

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	FAD	F	701	-	-	7/30/50/50	0/6/6/6
2	FAD	A	701	-	-	1/30/50/50	0/6/6/6
2	FAD	G	701	-	-	6/30/50/50	0/6/6/6
2	FAD	E	701	-	-	6/30/50/50	0/6/6/6
3	ATP	H	702	4	-	3/18/38/38	0/3/3/3
3	ATP	C	703	4	-	3/18/38/38	0/3/3/3
3	ATP	B	703	4	-	2/18/38/38	0/3/3/3
3	ATP	E	703	4	-	3/18/38/38	0/3/3/3
3	ATP	A	702	4	-	5/18/38/38	0/3/3/3
3	ATP	G	703	4	-	4/18/38/38	0/3/3/3
3	ATP	D	801	4	-	4/18/38/38	0/3/3/3
3	ATP	F	702	4	-	2/18/38/38	0/3/3/3
2	FAD	H	701	-	-	5/30/50/50	0/6/6/6
2	FAD	D	803	-	-	5/30/50/50	0/6/6/6
2	FAD	B	702	-	-	4/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	701	-	-	5/30/50/50	0/6/6/6

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FAD	O4B-C1B	15.97	1.63	1.41
2	E	701	FAD	O4B-C1B	15.94	1.63	1.41
2	B	702	FAD	O4B-C1B	15.92	1.63	1.41
2	G	701	FAD	C2B-C1B	-15.70	1.29	1.53
2	H	701	FAD	C2B-C1B	-15.60	1.30	1.53

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	701	FAD	C5A-C6A-N6A	11.55	137.90	120.35
2	A	701	FAD	C5A-C6A-N6A	11.42	137.70	120.35
2	E	701	FAD	C5A-C6A-N6A	11.28	137.49	120.35
2	F	701	FAD	C5A-C6A-N6A	11.24	137.44	120.35
2	B	702	FAD	C5A-C6A-N6A	11.11	137.23	120.35

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	701	FAD	C5B-O5B-PA-O1A
3	A	702	ATP	PB-O3B-PG-O3G
2	D	803	FAD	C5B-O5B-PA-O2A
2	D	803	FAD	C5B-O5B-PA-O3P
2	D	803	FAD	C5'-O5'-P-O1P

There are no ring outliers.

10 monomers are involved in 16 short contacts:

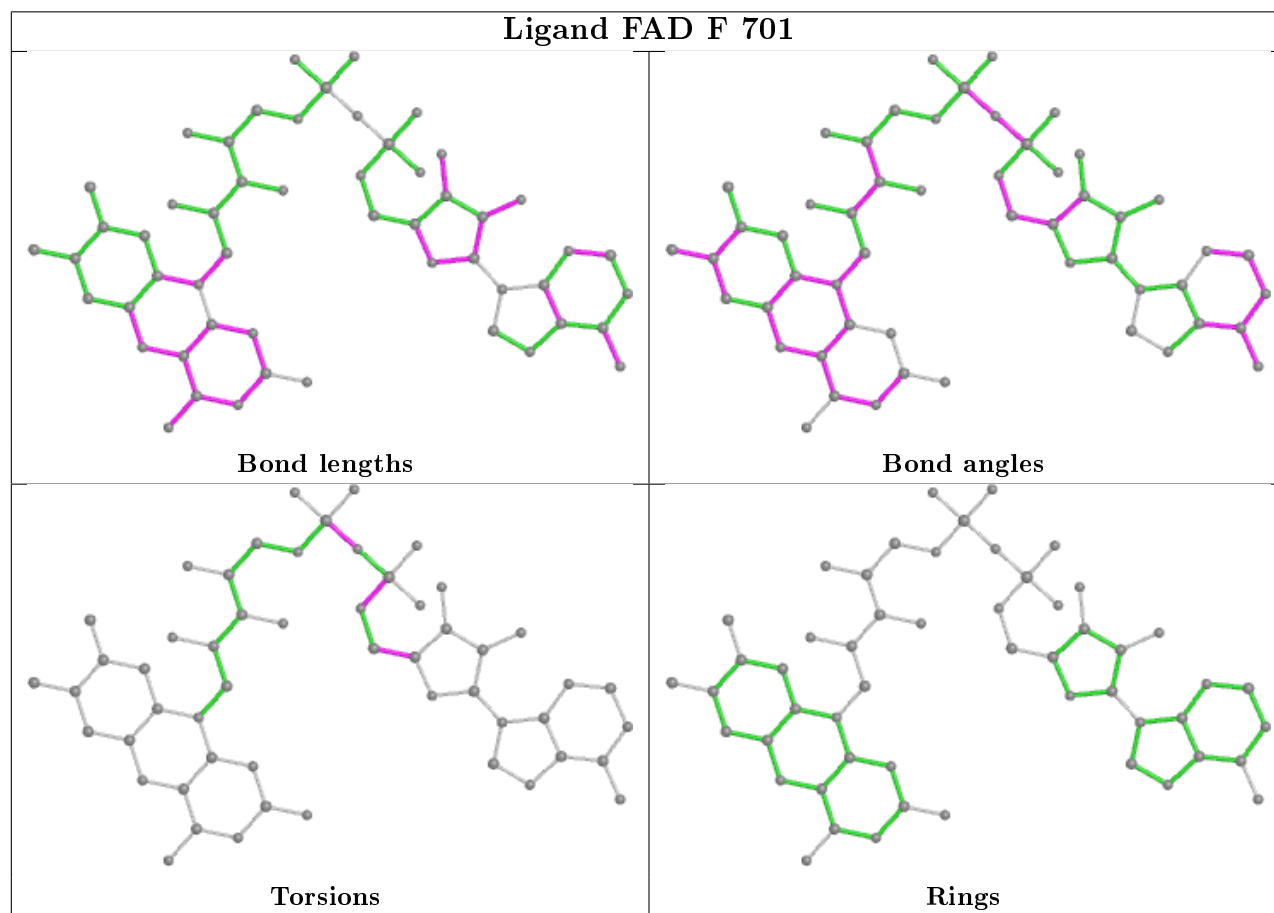
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	FAD	4	0
2	A	701	FAD	1	0
3	H	702	ATP	1	0
3	A	702	ATP	2	0
3	G	703	ATP	2	0
3	D	801	ATP	1	0
2	H	701	FAD	2	0

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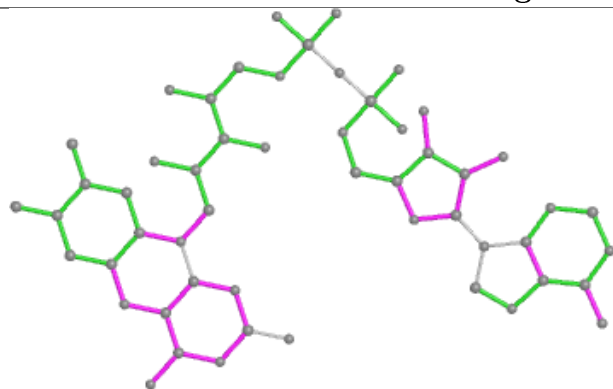
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	803	FAD	1	0
2	B	702	FAD	1	0
2	C	701	FAD	1	0

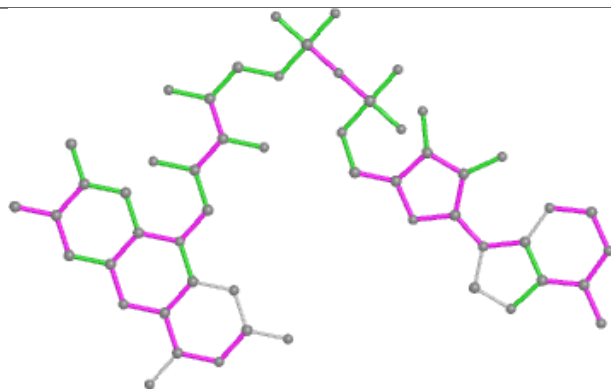
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



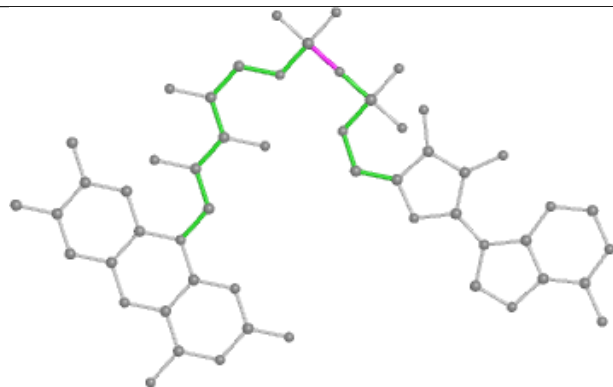
Ligand FAD A 701



Bond lengths



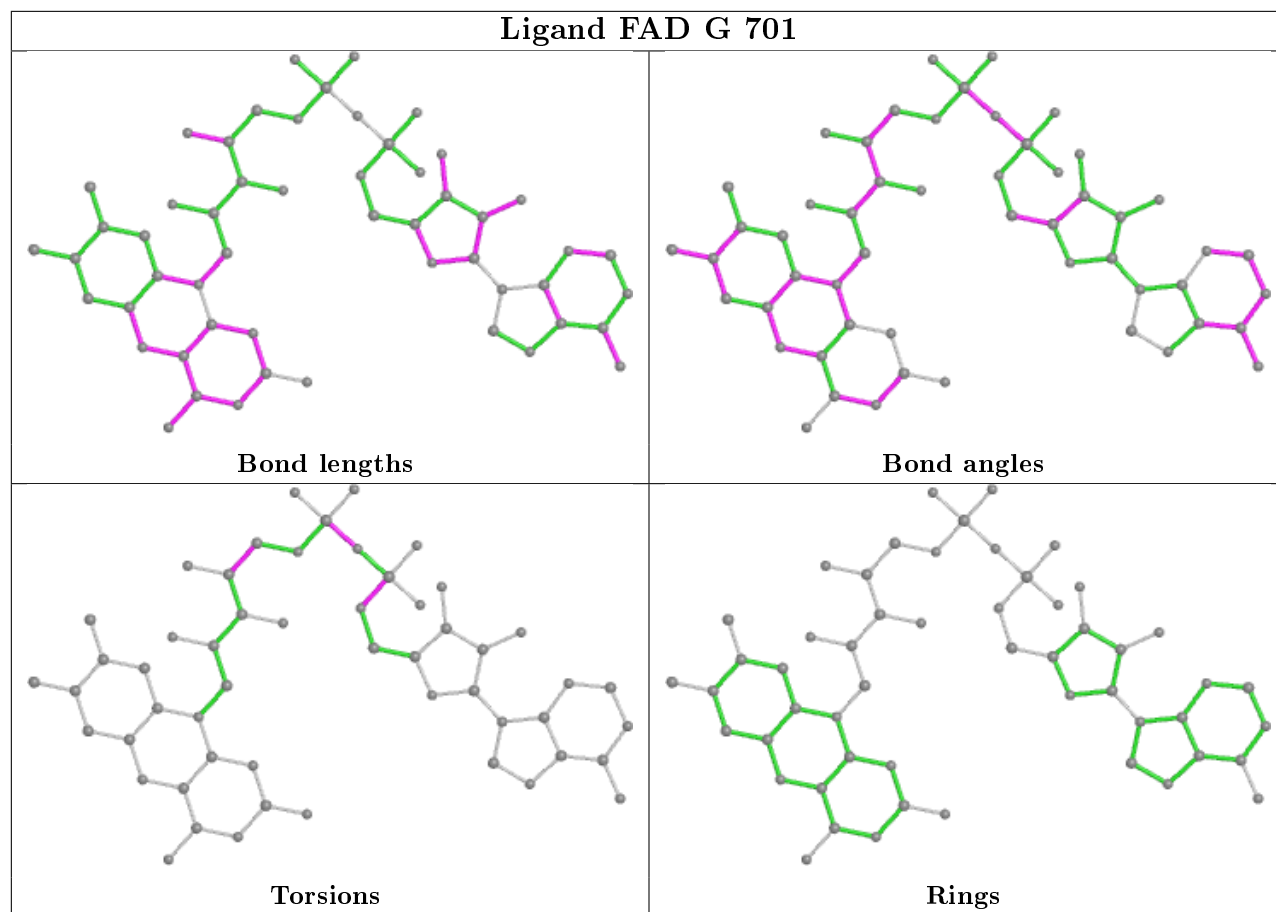
Bond angles



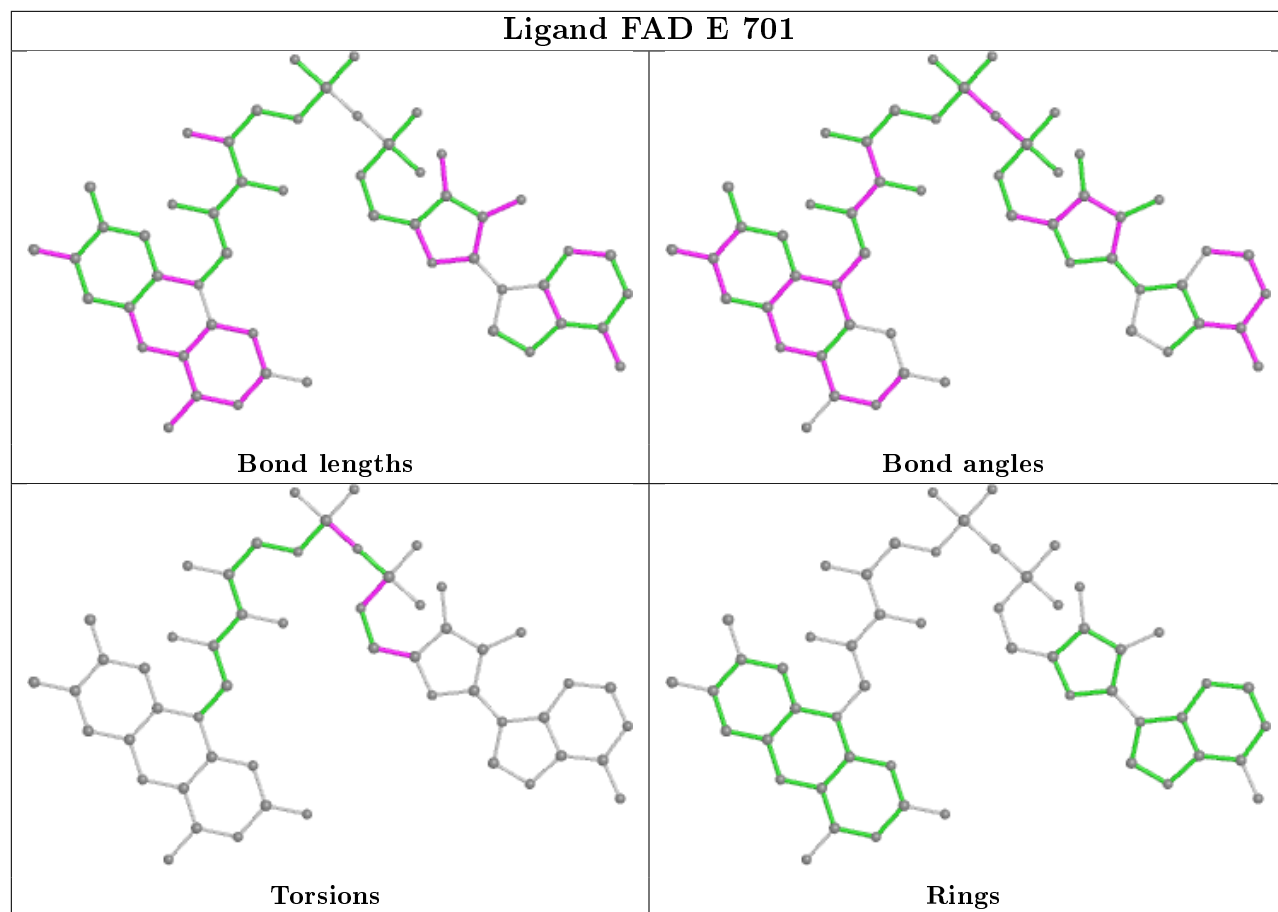
Torsions

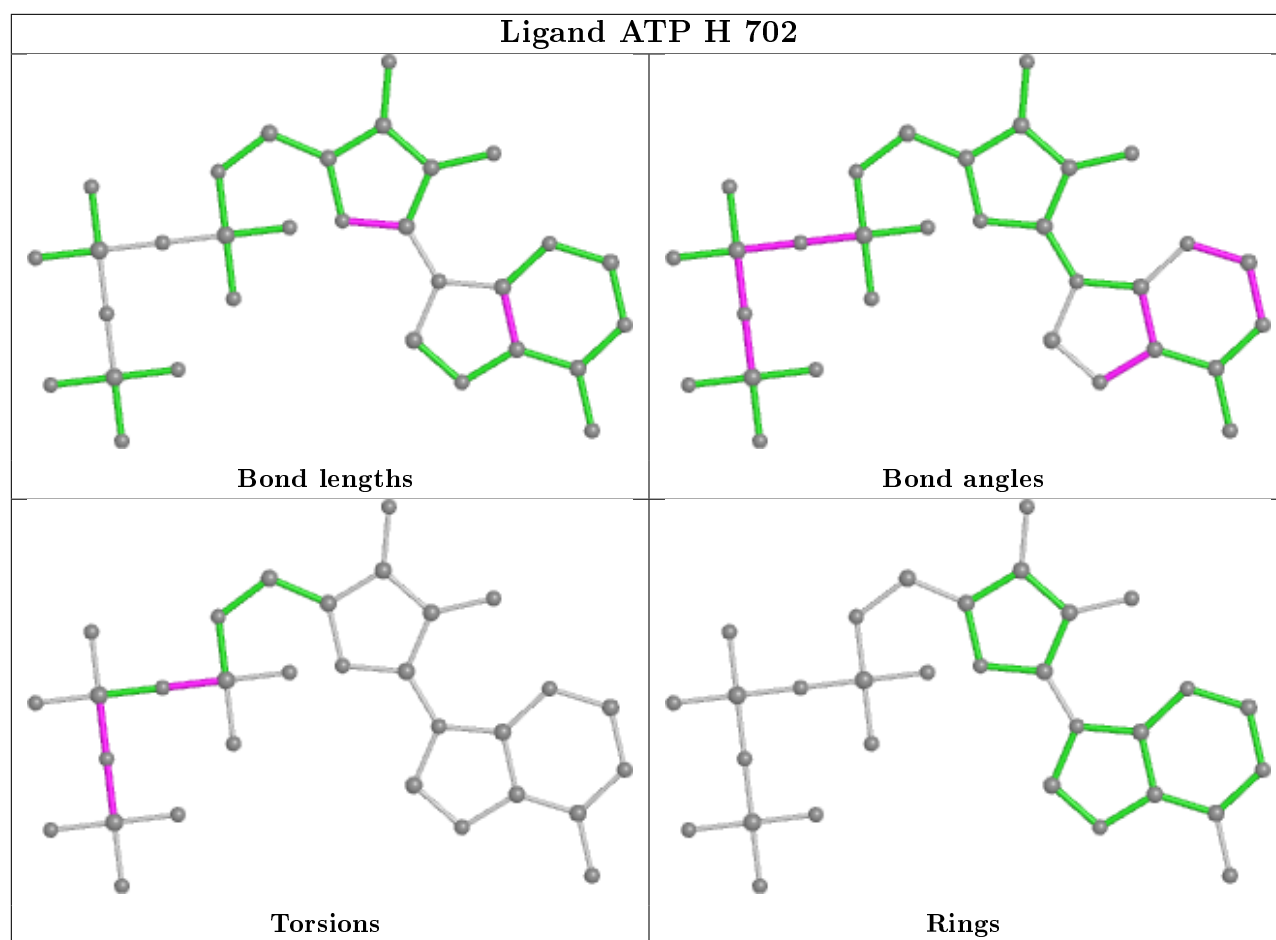


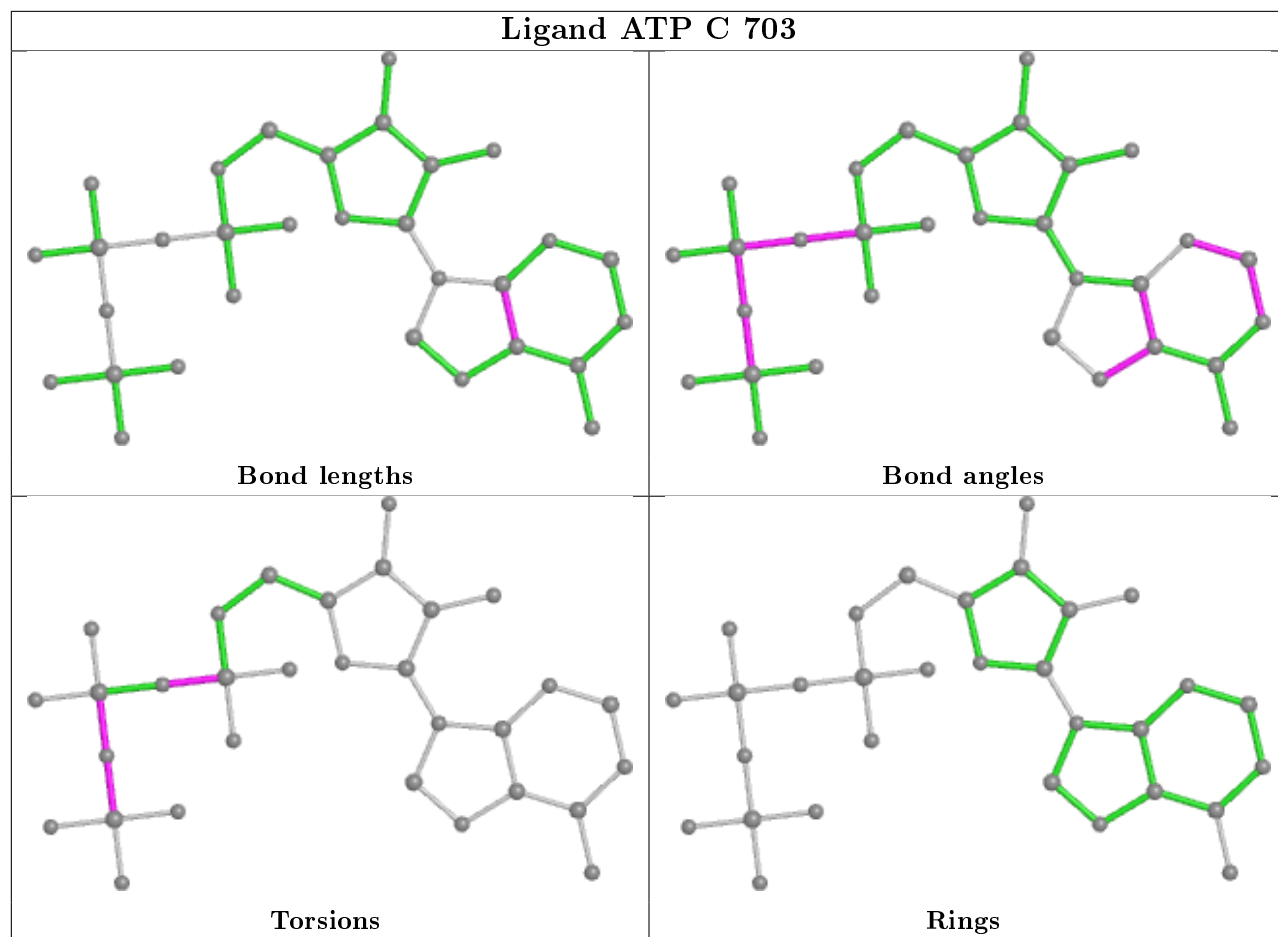
Rings



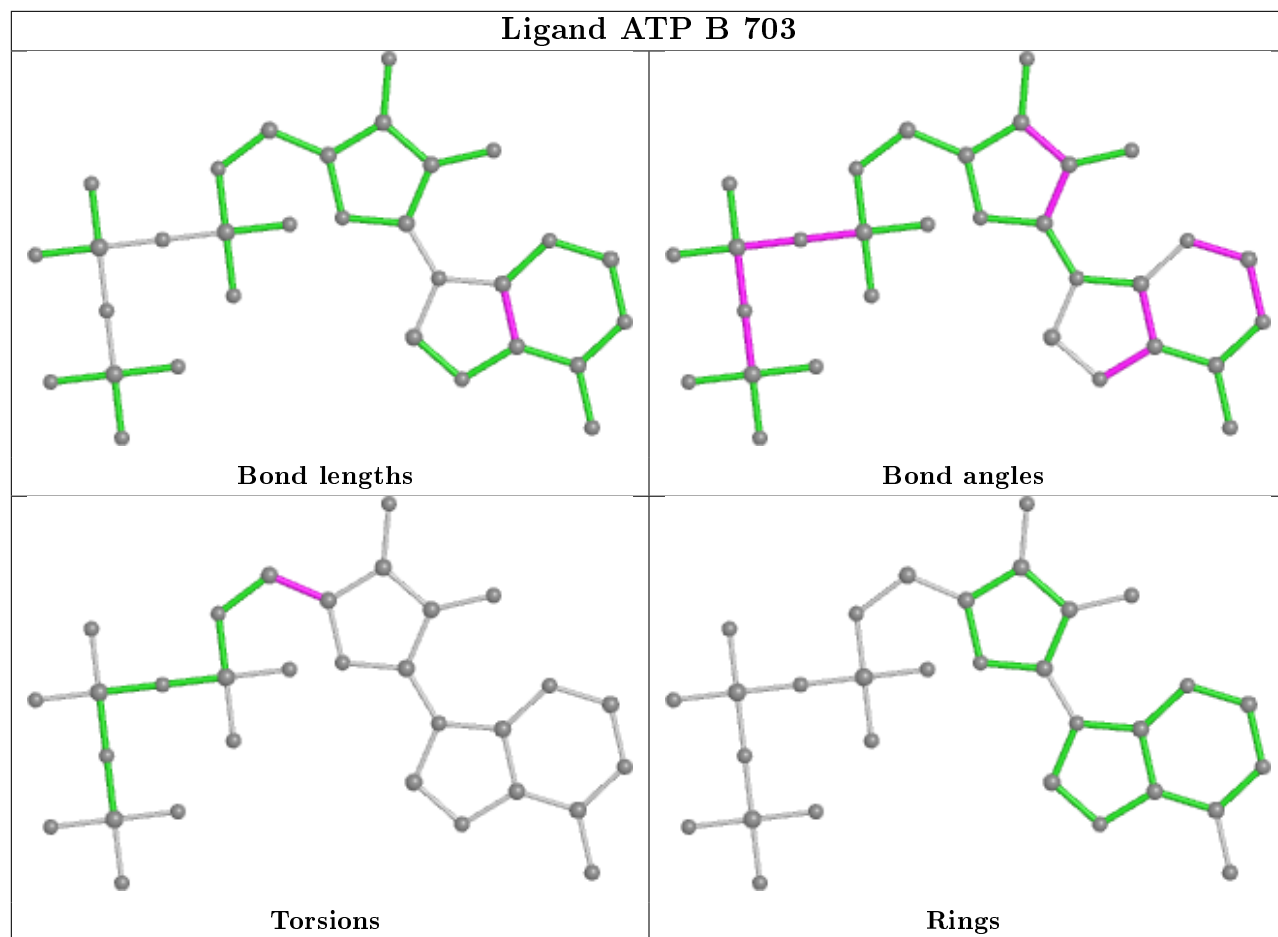
Ligand FAD E 701



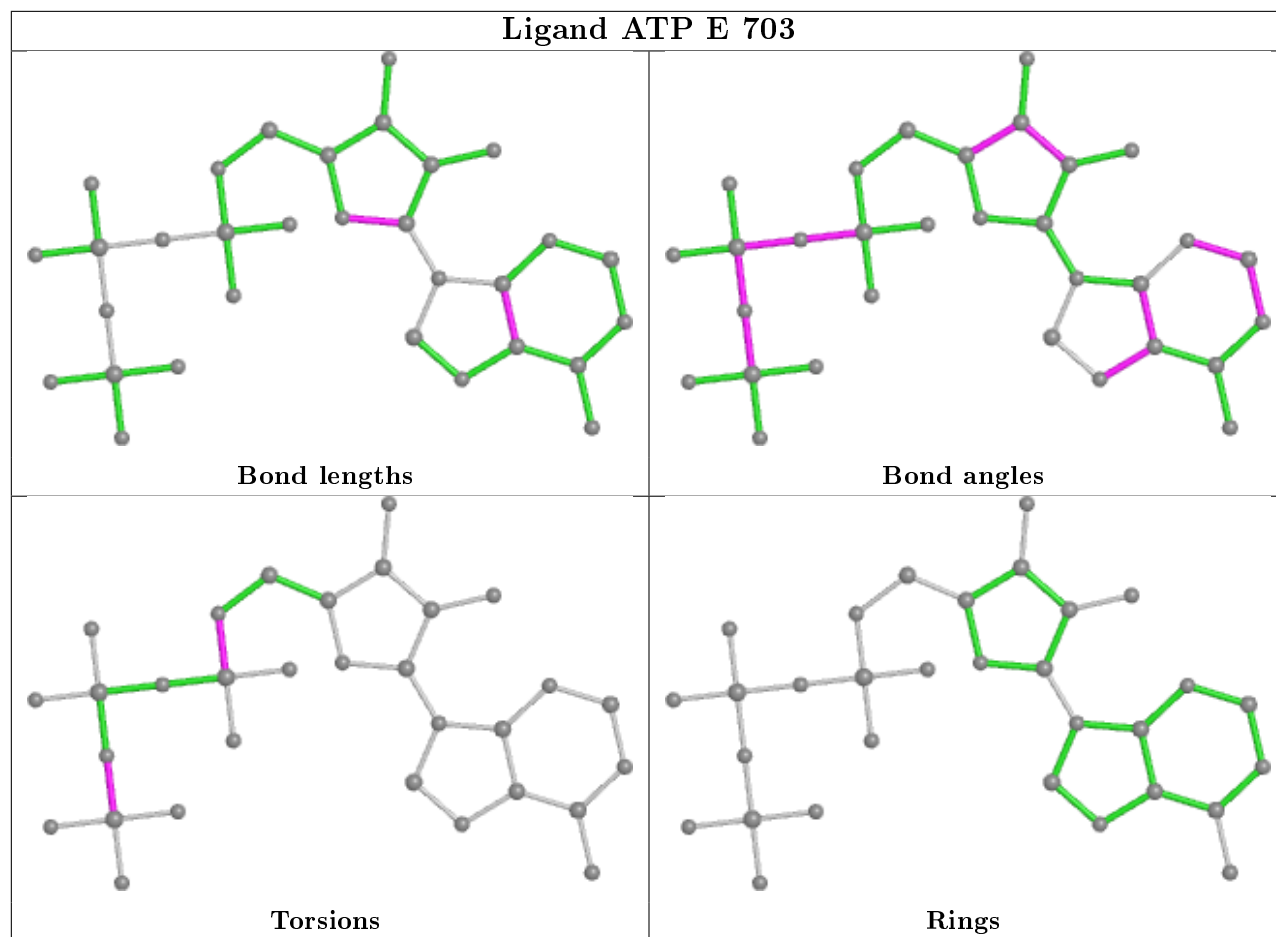


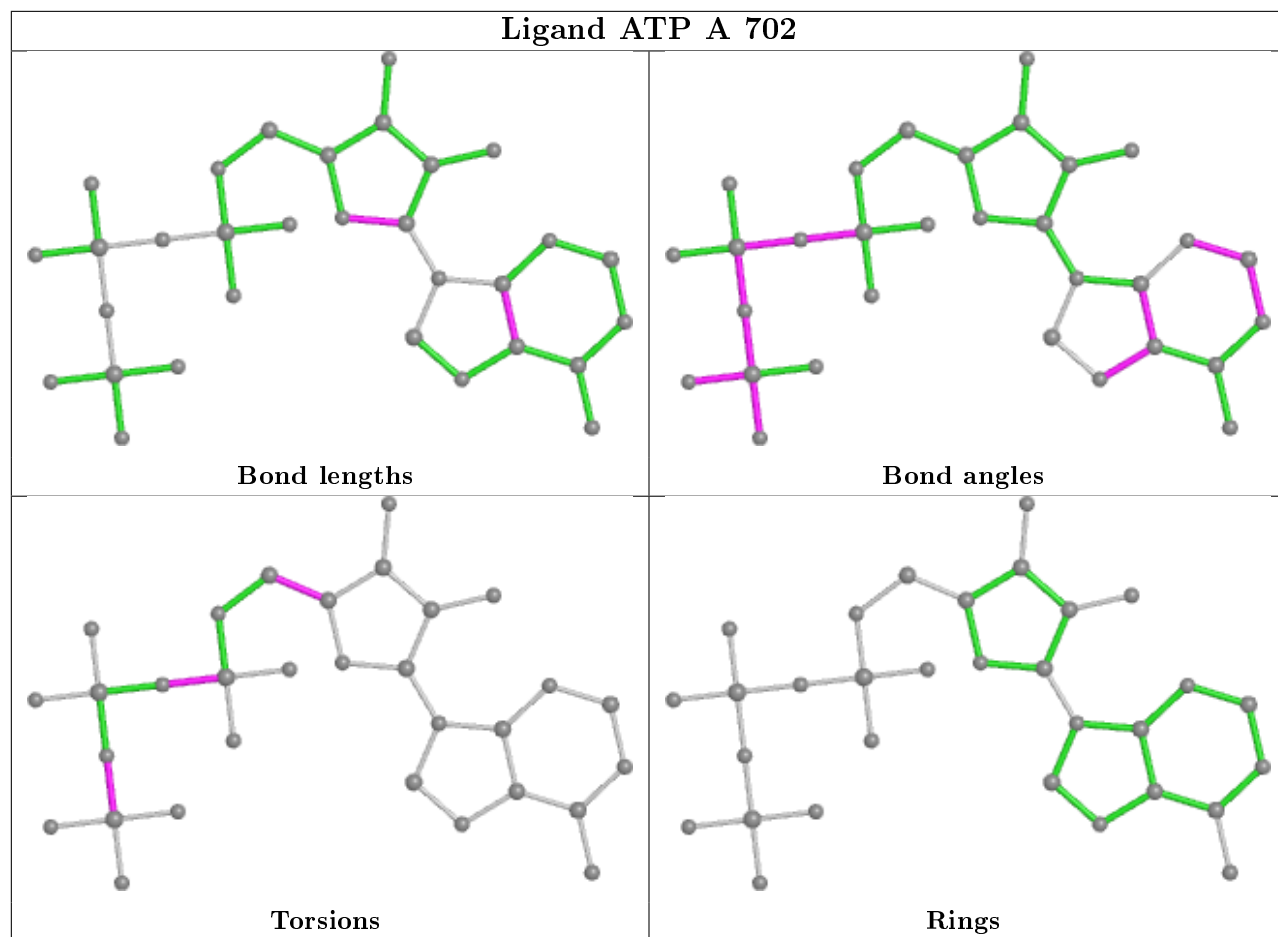


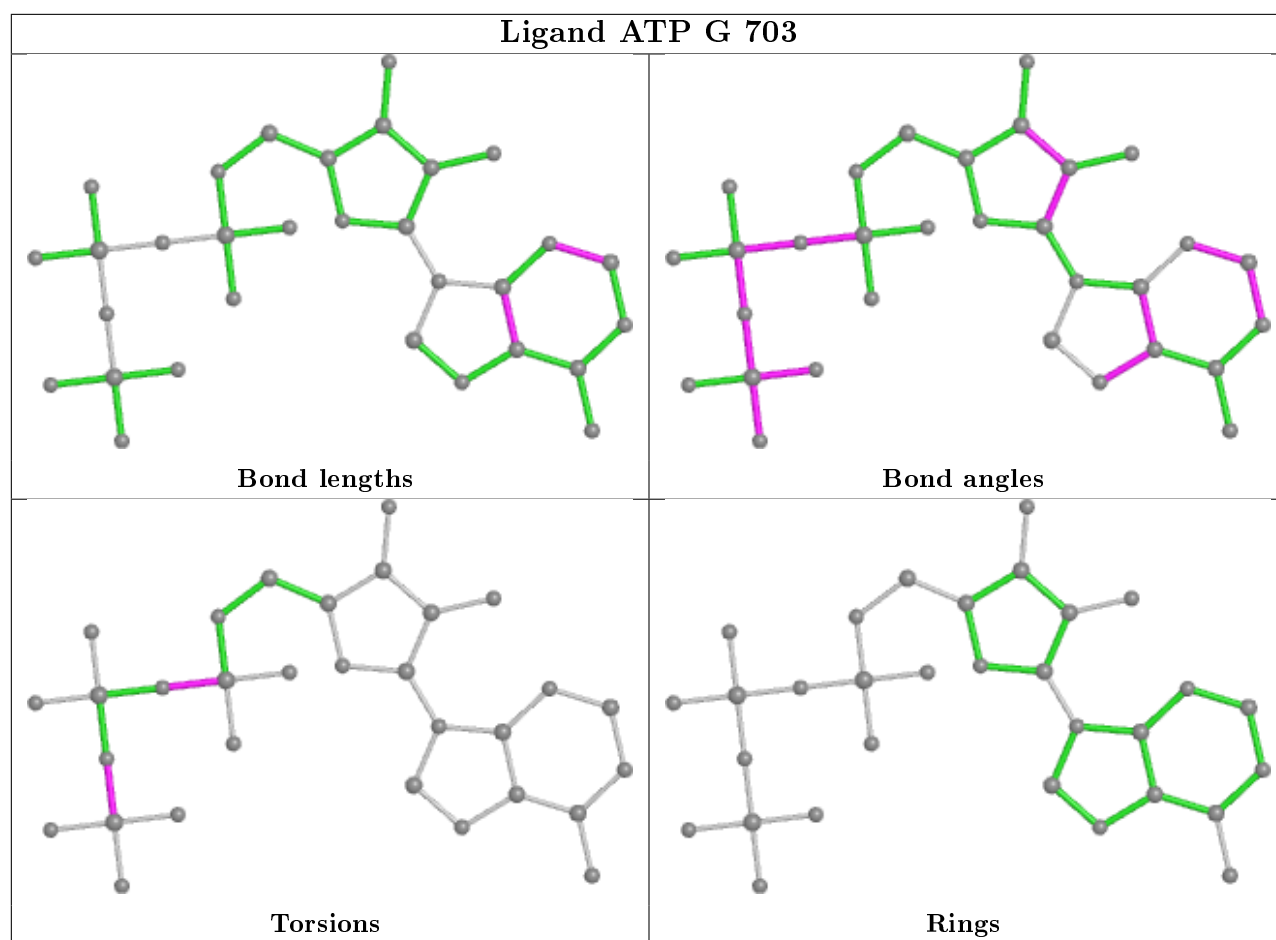
Ligand ATP B 703

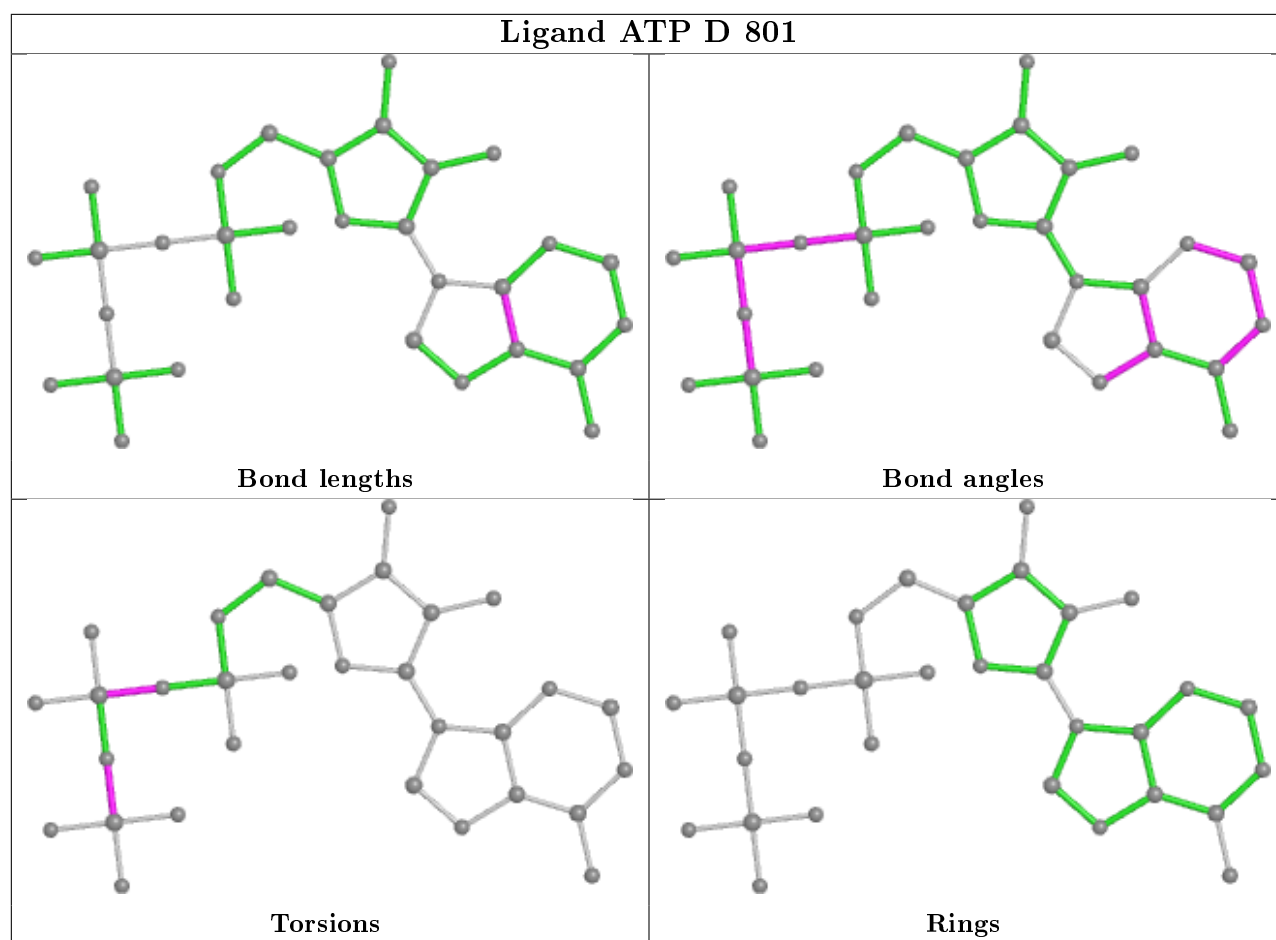


Ligand ATP E 703

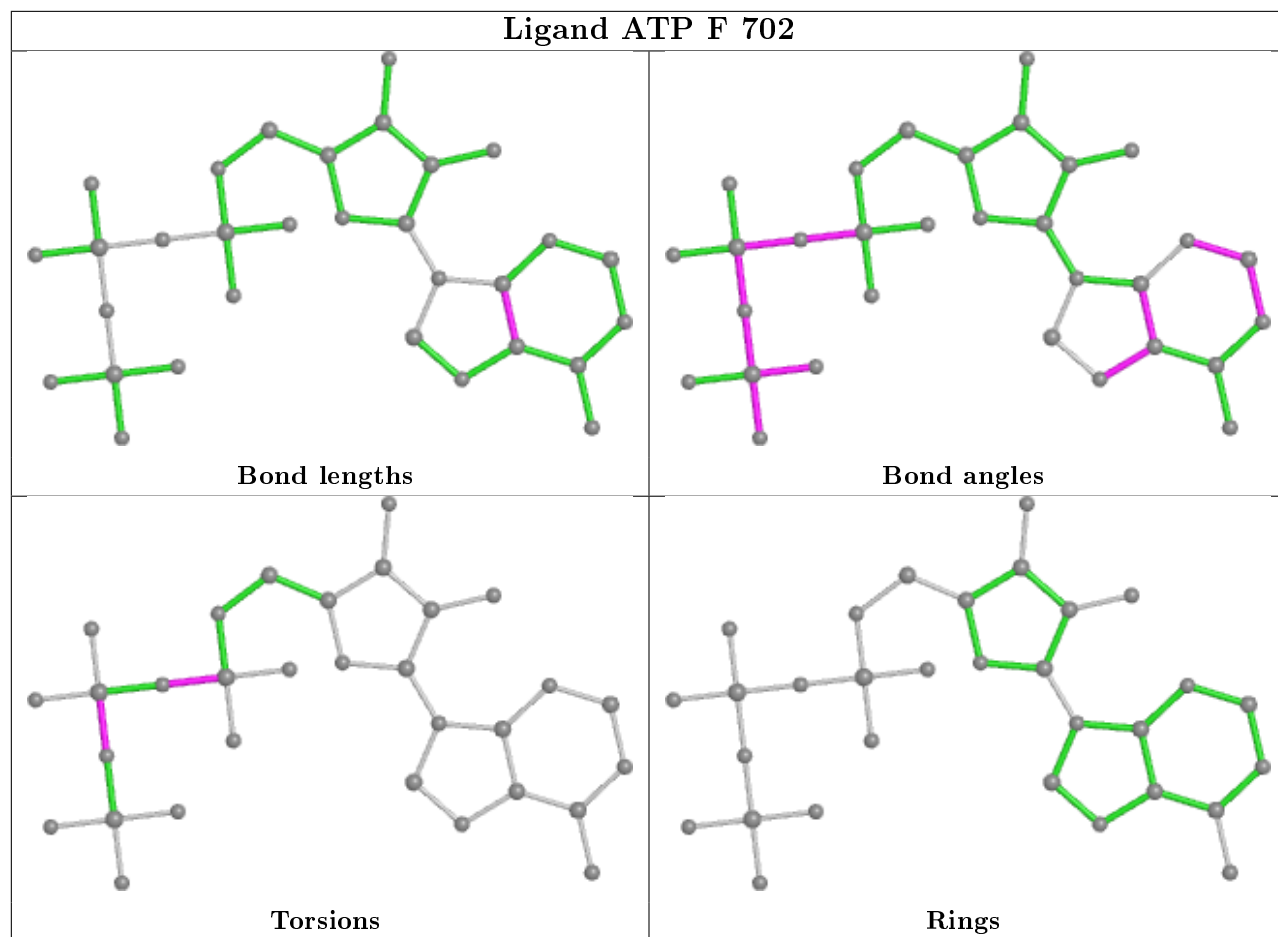


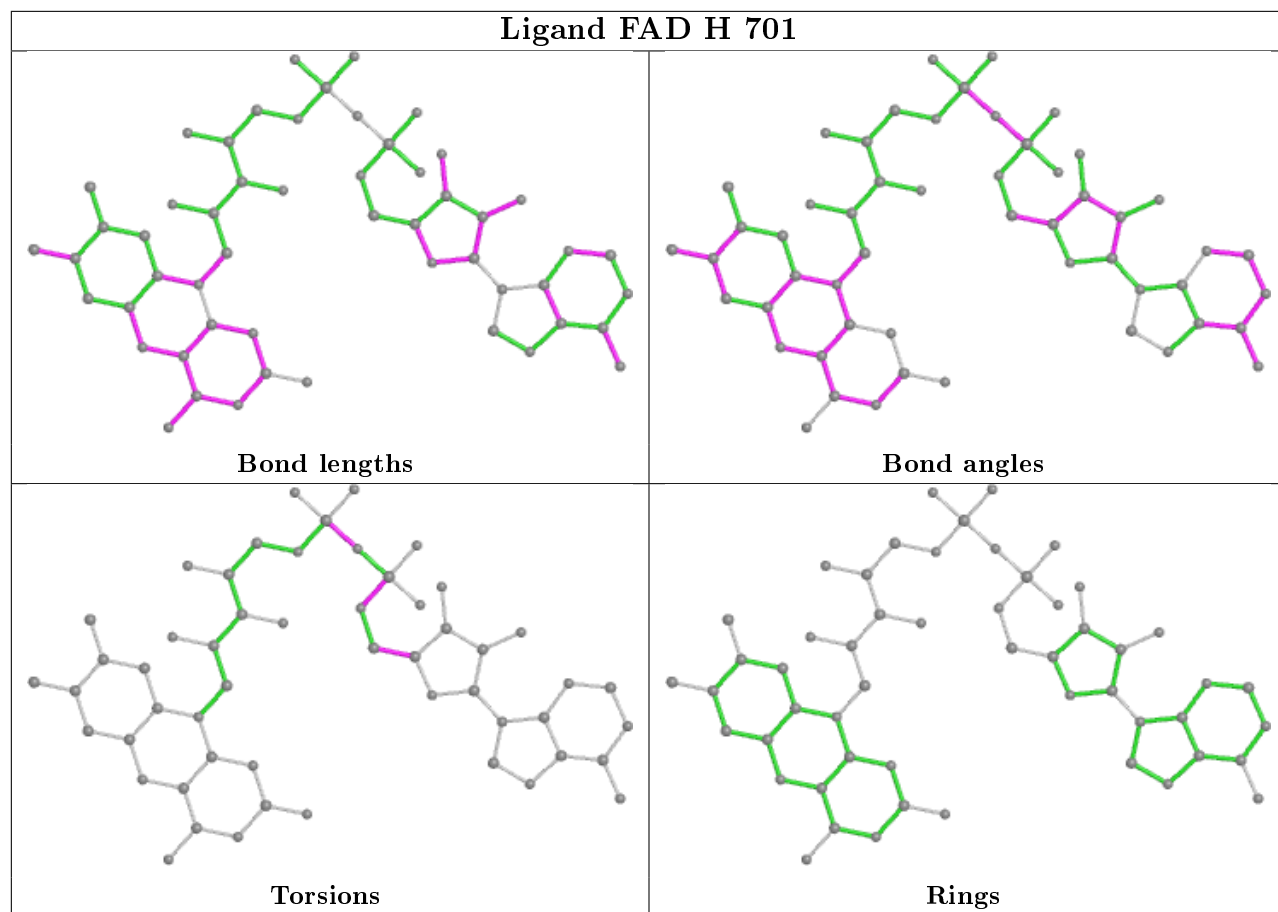


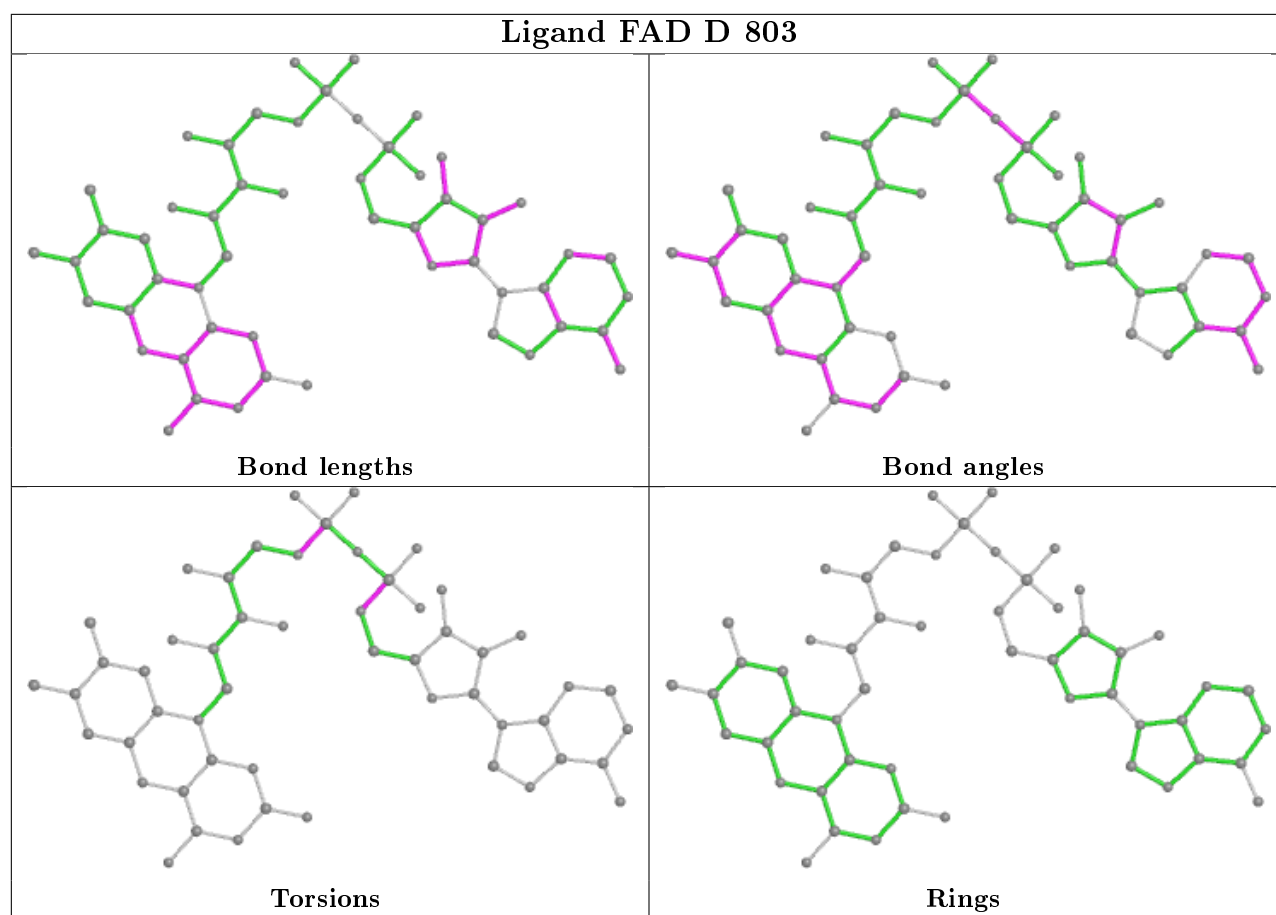


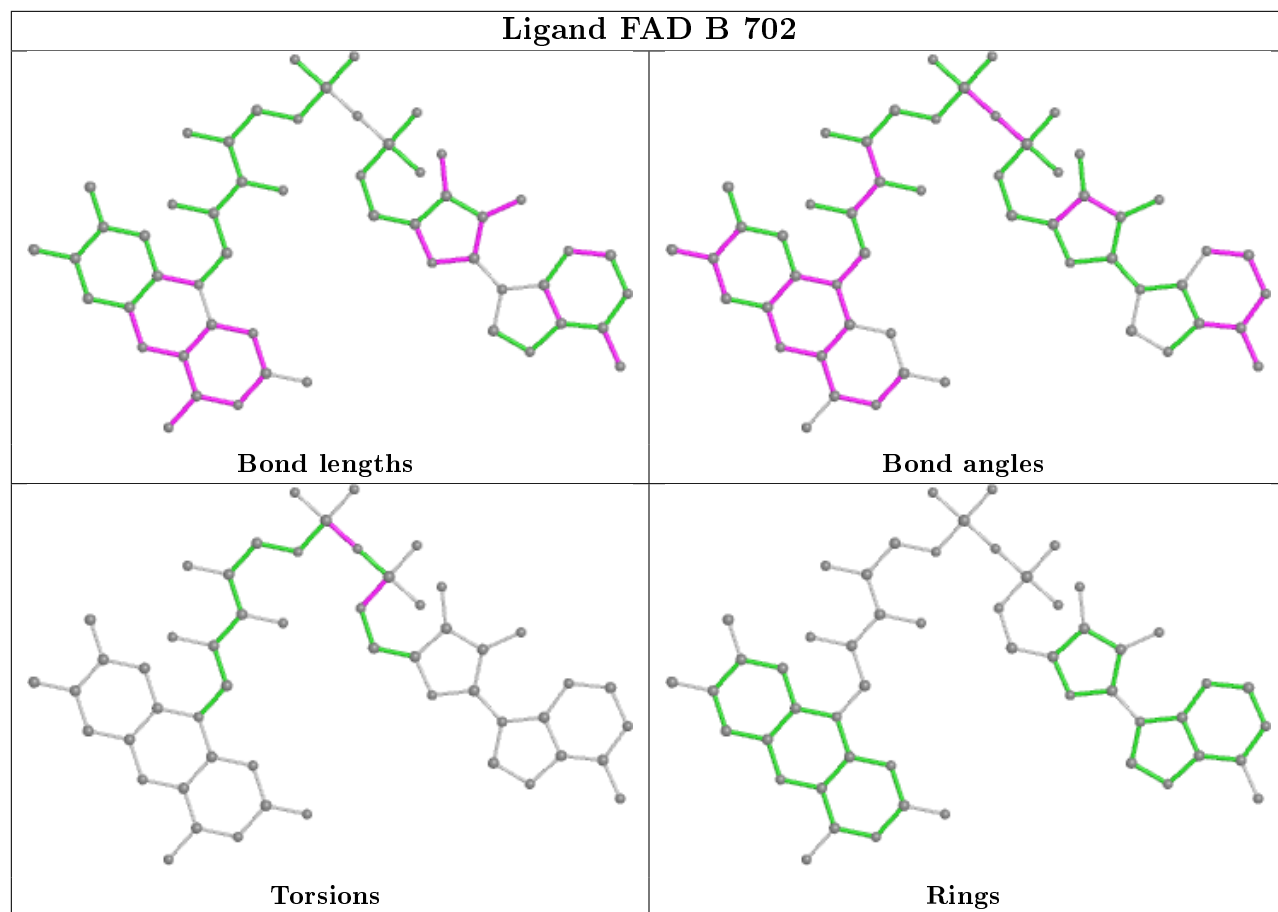


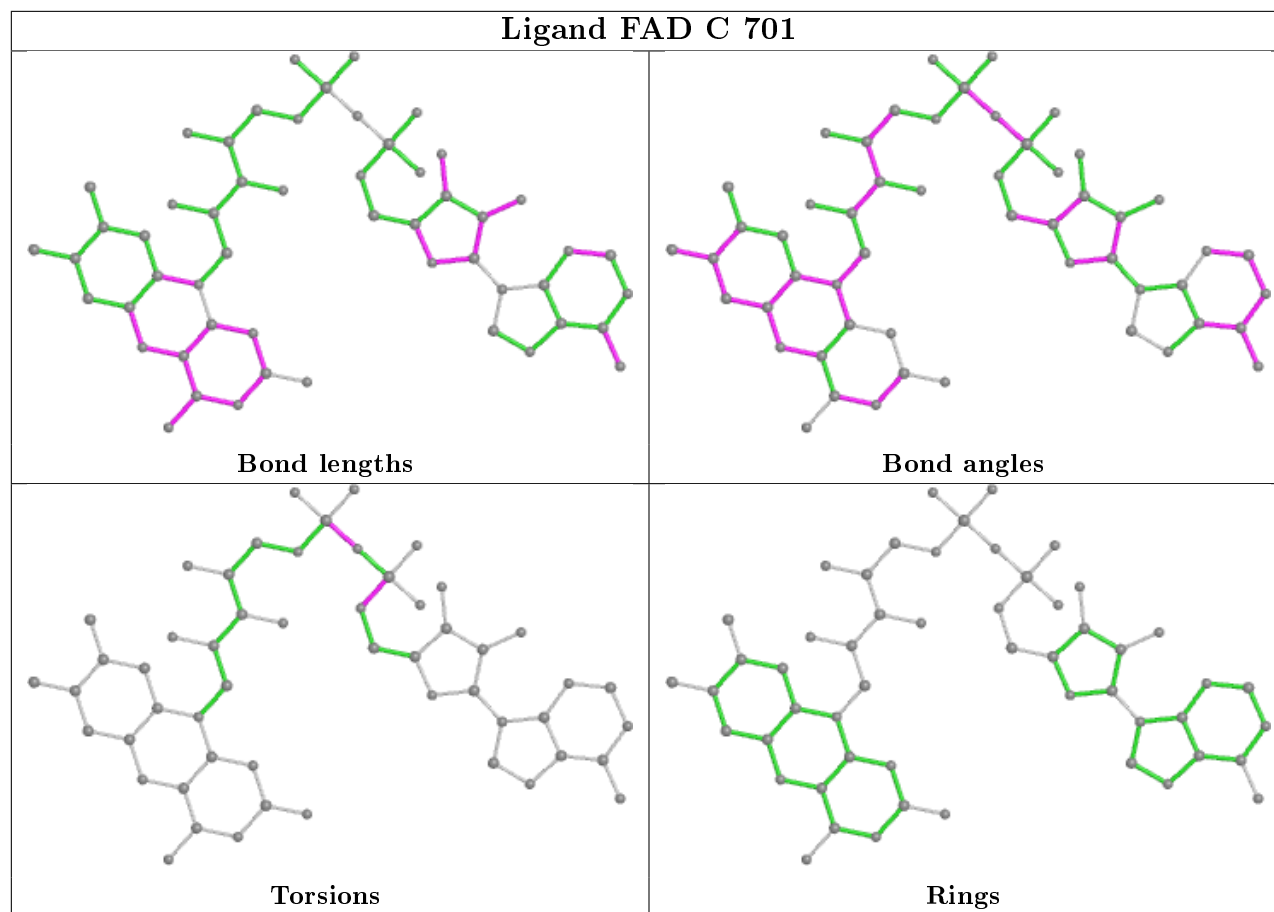
Ligand ATP F 702











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	661/684 (96%)	-0.39	5 (0%) 86 86	17, 27, 47, 73	0
1	B	657/684 (96%)	-0.26	11 (1%) 70 71	17, 32, 65, 80	0
1	C	650/684 (95%)	-0.26	2 (0%) 94 95	20, 34, 56, 72	0
1	D	653/684 (95%)	-0.38	2 (0%) 94 95	18, 30, 49, 66	0
1	E	661/684 (96%)	-0.25	8 (1%) 79 79	20, 33, 57, 77	0
1	F	651/684 (95%)	-0.16	10 (1%) 73 74	22, 36, 66, 84	0
1	G	653/684 (95%)	-0.25	6 (0%) 84 85	20, 33, 63, 74	0
1	H	661/684 (96%)	-0.38	4 (0%) 89 90	18, 27, 48, 67	0
All	All	5247/5472 (95%)	-0.29	48 (0%) 84 85	17, 31, 59, 84	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	377	VAL	7.2
1	F	378	SER	3.9
1	B	126	ALA	3.6
1	E	375	GLY	3.6
1	B	378	SER	3.4

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 carbohydrates in this entry.

6.4 Ligands ⓘ

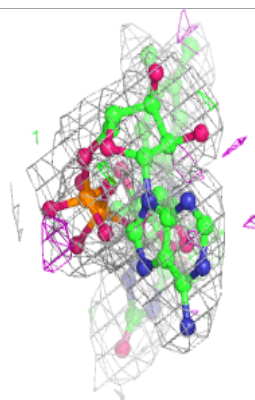
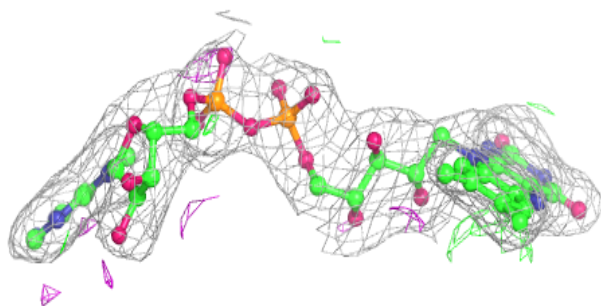
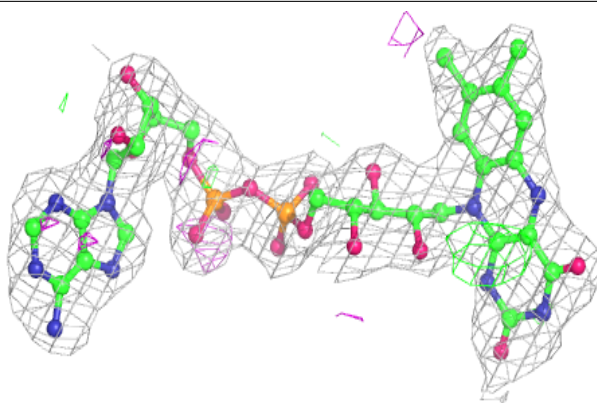
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	F	701	53/53	0.94	0.14	21,25,27,28	0
4	MG	H	703	1/1	0.94	0.16	14,14,14,14	0
3	ATP	B	703	31/31	0.95	0.14	16,18,19,19	0
2	FAD	D	803	53/53	0.95	0.14	21,22,23,23	0
2	FAD	A	701	53/53	0.95	0.14	20,21,23,25	0
2	FAD	H	701	53/53	0.95	0.16	19,23,25,26	0
4	MG	F	703	1/1	0.95	0.16	23,23,23,23	0
4	MG	D	802	1/1	0.95	0.23	23,23,23,23	0
2	FAD	B	702	53/53	0.96	0.13	21,24,25,26	0
3	ATP	D	801	31/31	0.96	0.13	20,21,23,23	0
2	FAD	E	701	53/53	0.96	0.13	22,25,28,28	0
3	ATP	F	702	31/31	0.96	0.13	21,22,23,23	0
2	FAD	G	701	53/53	0.96	0.14	24,25,26,26	0
4	MG	A	703	1/1	0.96	0.17	18,18,18,18	0
2	FAD	C	701	53/53	0.96	0.13	22,26,29,31	0
3	ATP	E	703	31/31	0.97	0.13	19,21,22,23	0
3	ATP	G	703	31/31	0.97	0.12	18,19,19,19	0
4	MG	B	701	1/1	0.97	0.21	14,14,14,14	0
3	ATP	A	702	31/31	0.97	0.13	16,16,17,17	0
4	MG	G	702	1/1	0.97	0.20	22,22,22,22	0
3	ATP	H	702	31/31	0.97	0.12	19,22,24,26	0
3	ATP	C	703	31/31	0.97	0.12	19,21,22,22	0
4	MG	C	702	1/1	0.98	0.17	20,20,20,20	0
4	MG	E	702	1/1	0.98	0.18	22,22,22,22	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.

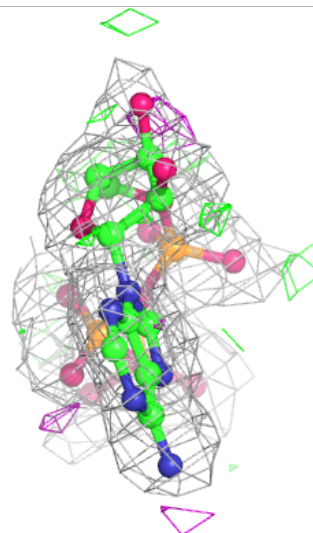
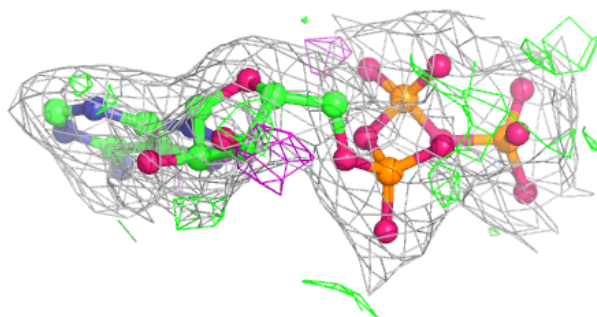
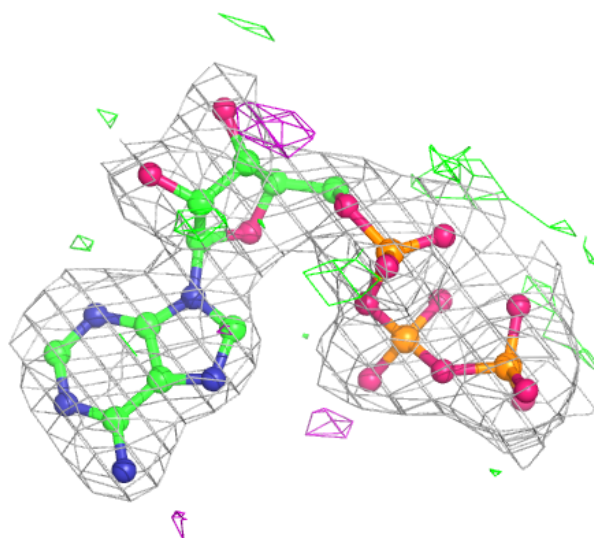
Electron density around FAD F 701:

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



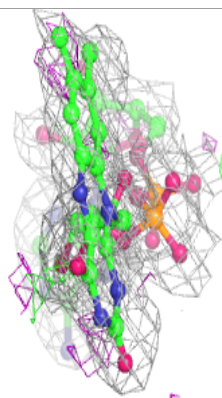
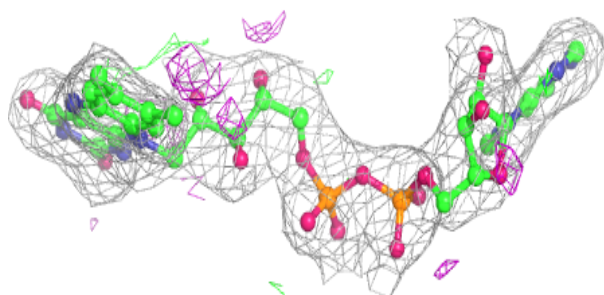
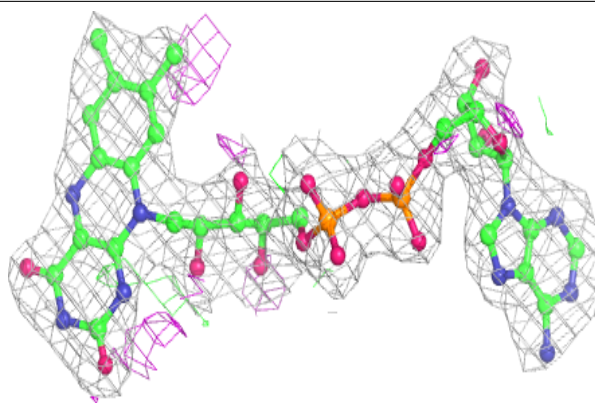
Electron density around ATP B 703:

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

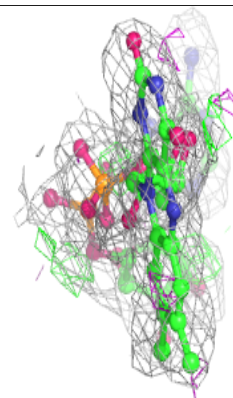
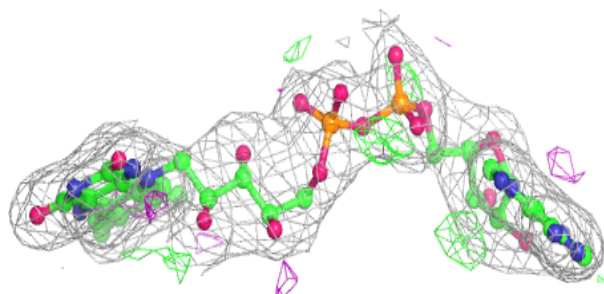
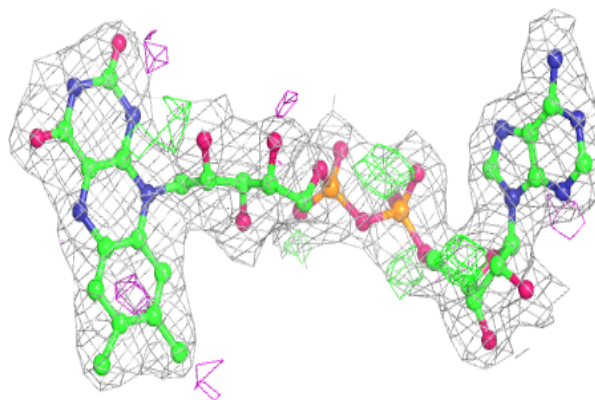


Electron density around FAD D 803:

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

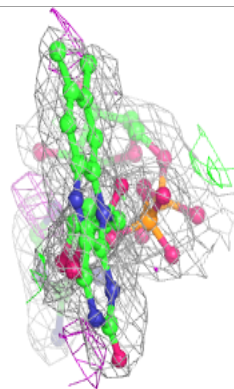
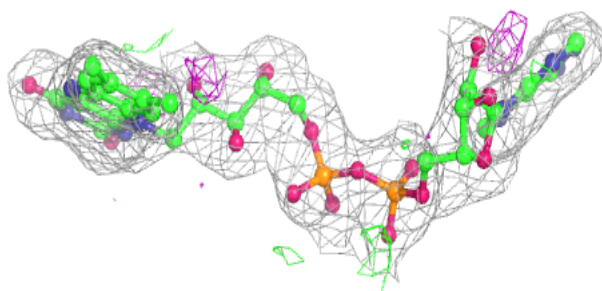
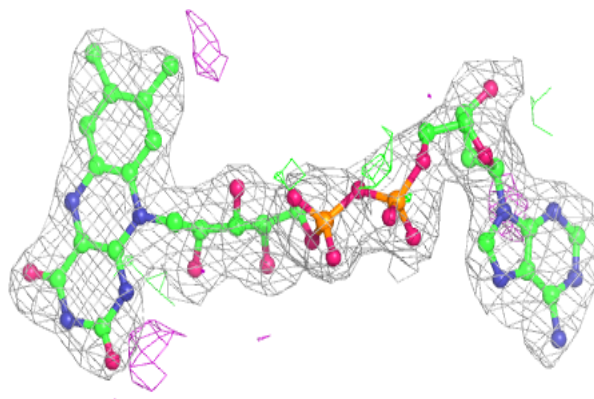
**Electron density around FAD A 701:**

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

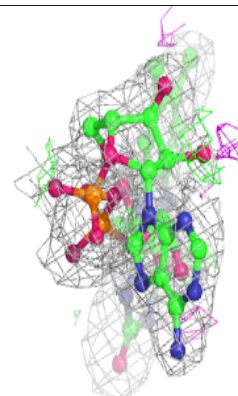
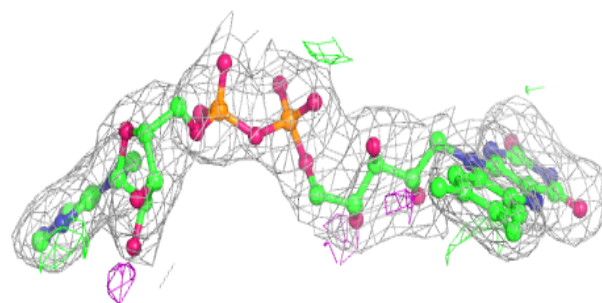
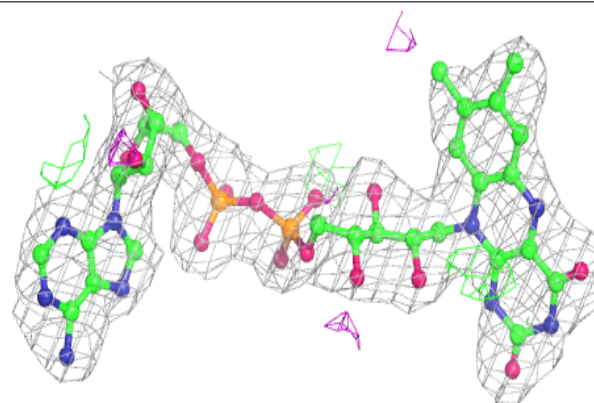


Electron density around FAD H 701:

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

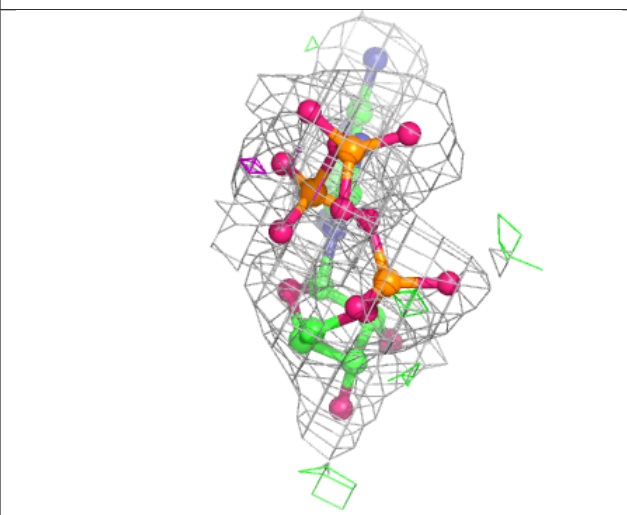
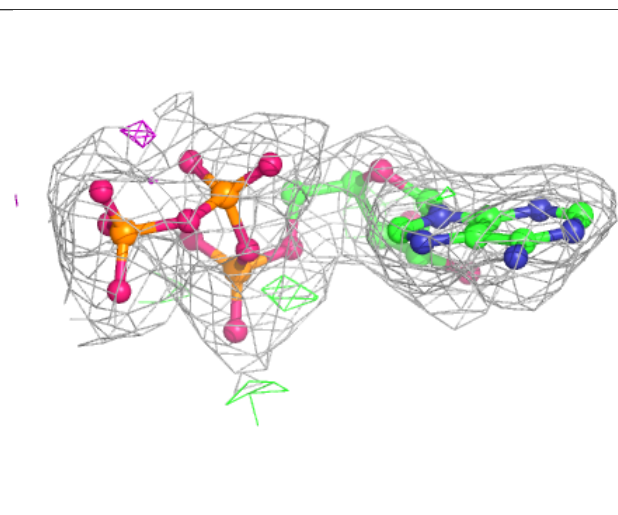
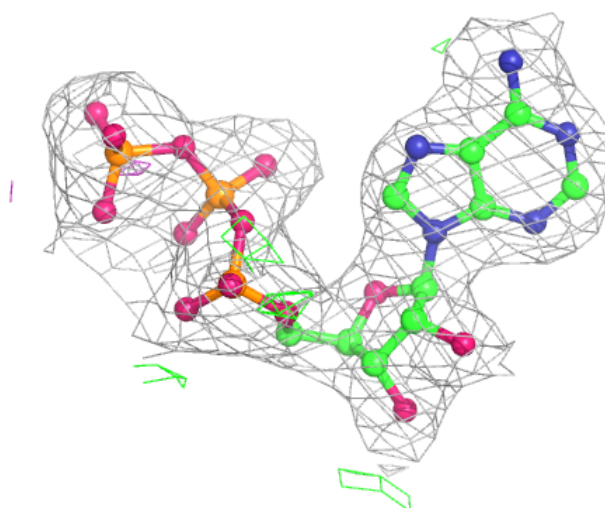
**Electron density around FAD B 702:**

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



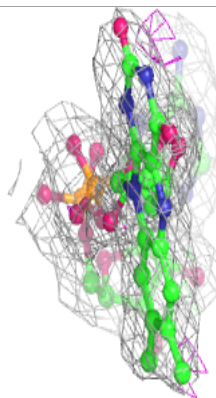
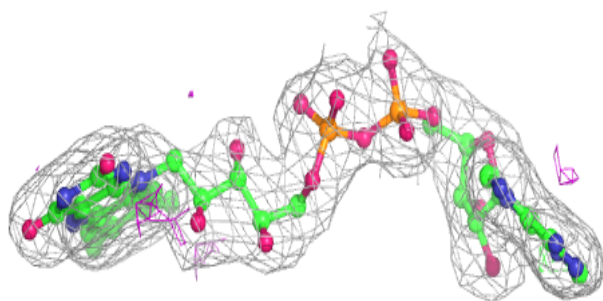
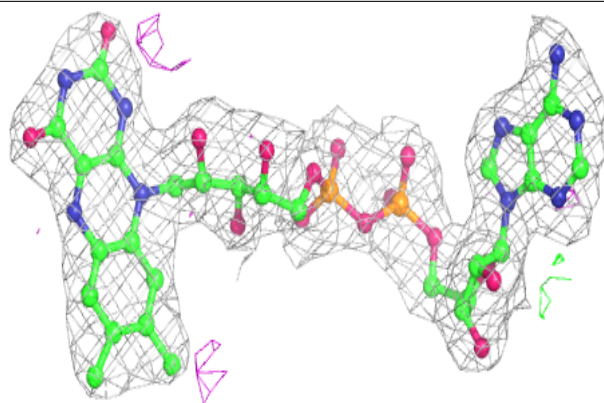
Electron density around ATP D 801:

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



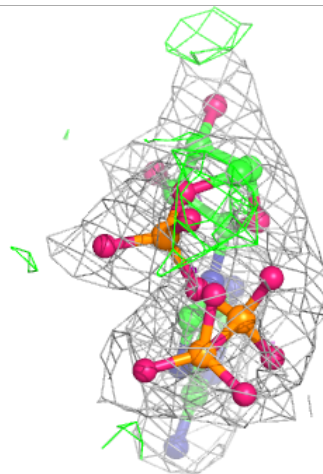
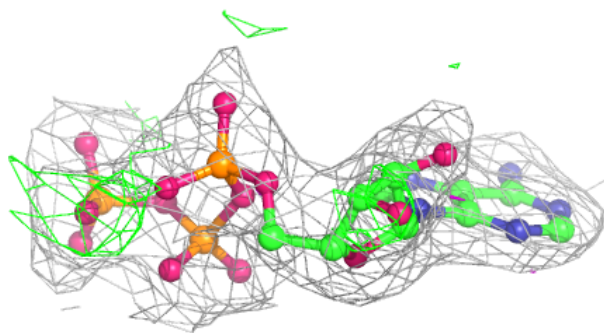
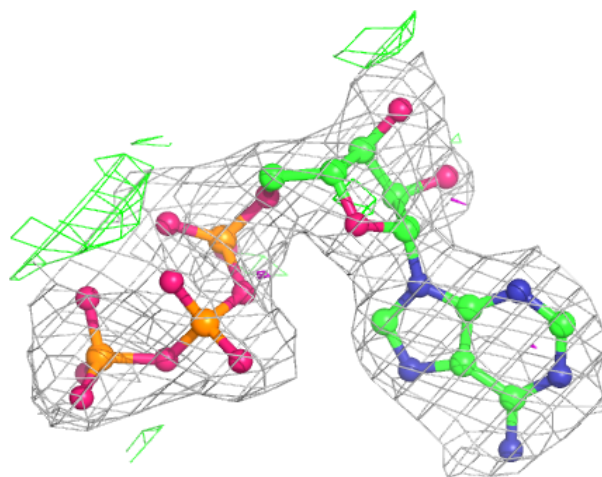
Electron density around FAD E 701:

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



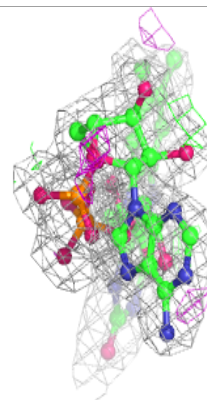
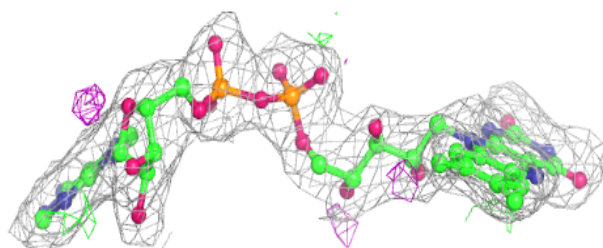
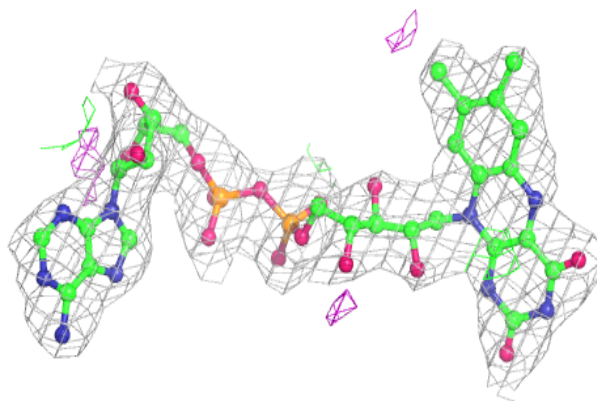
Electron density around ATP F 702:

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

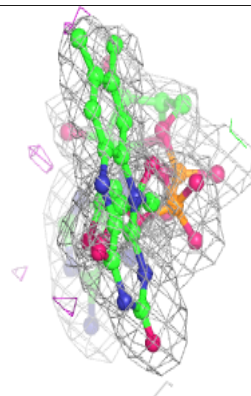
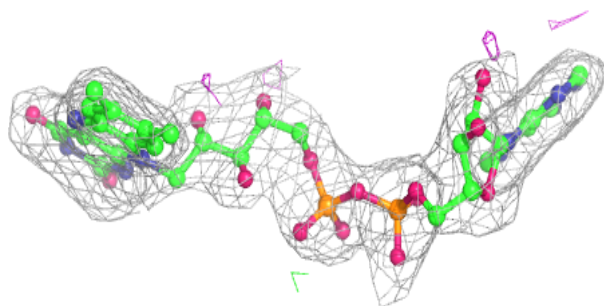
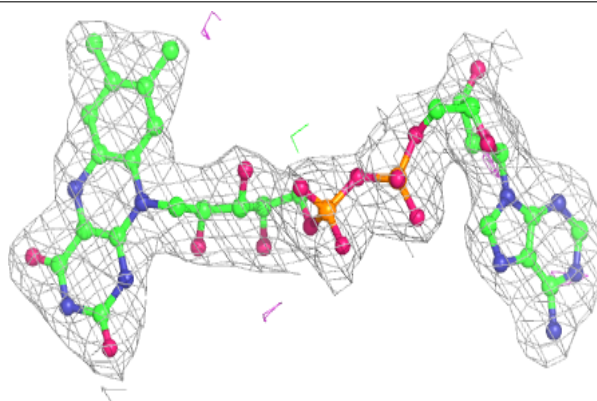


Electron density around FAD G 701:

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

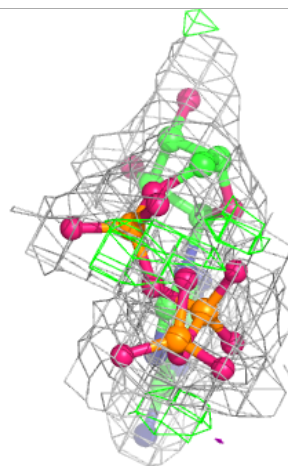
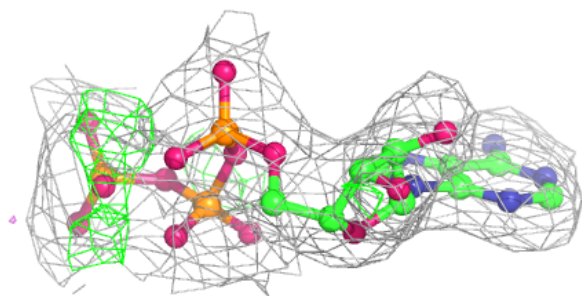
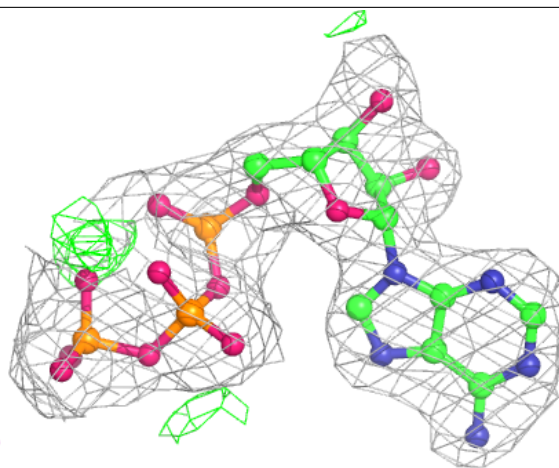
**Electron density around FAD C 701:**

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



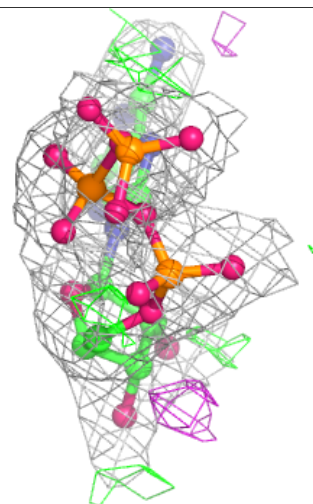
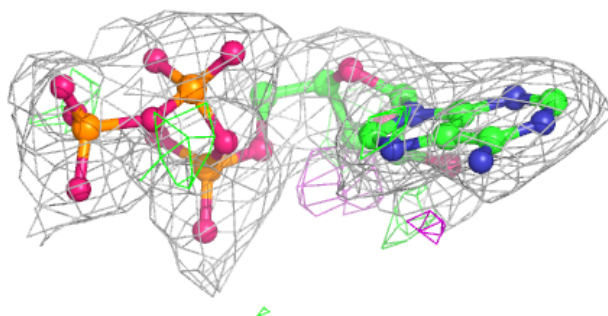
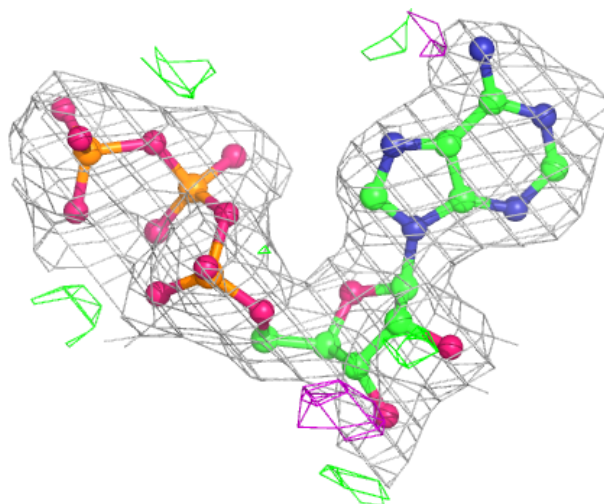
Electron density around ATP E 703:

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



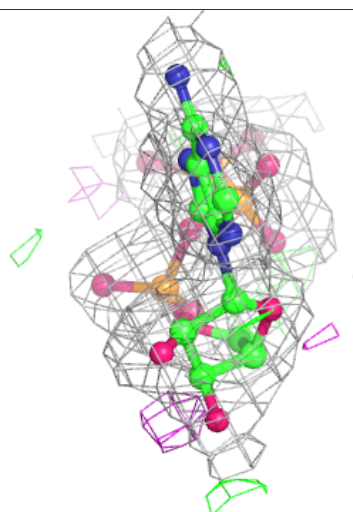
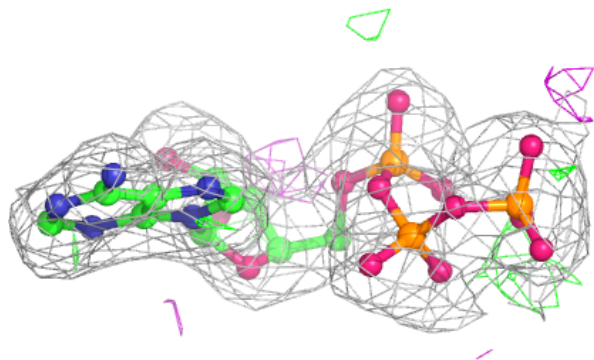
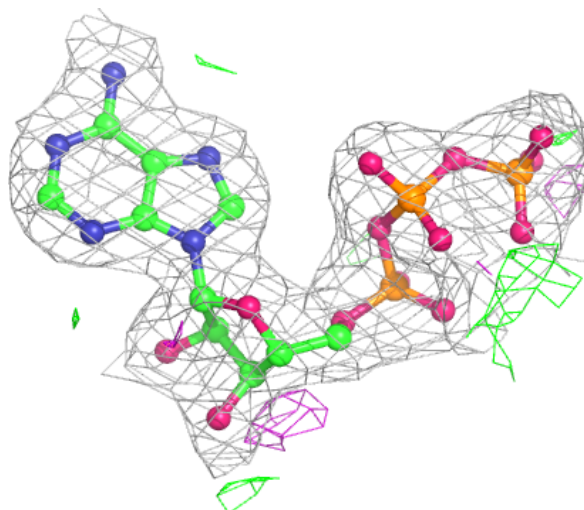
Electron density around ATP G 703:

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



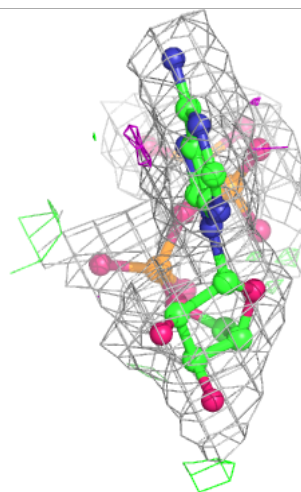
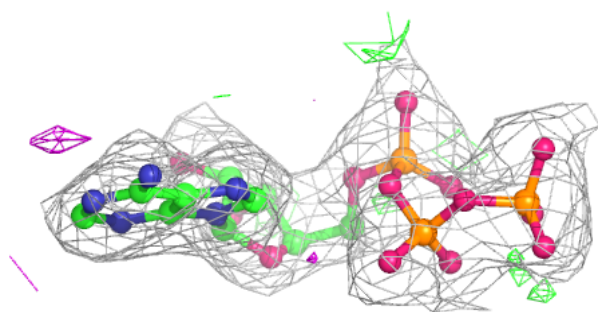
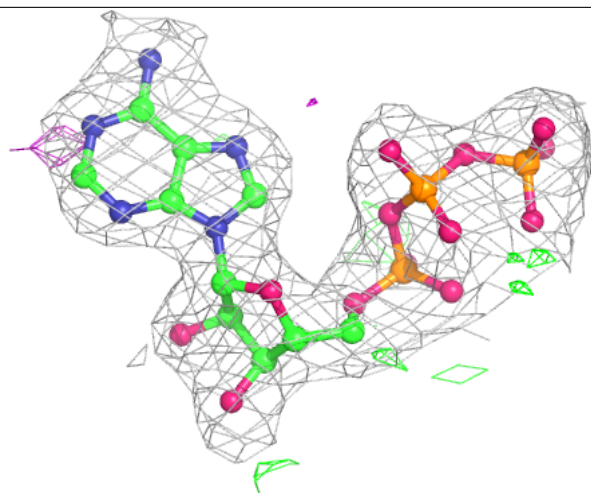
Electron density around ATP A 702:

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



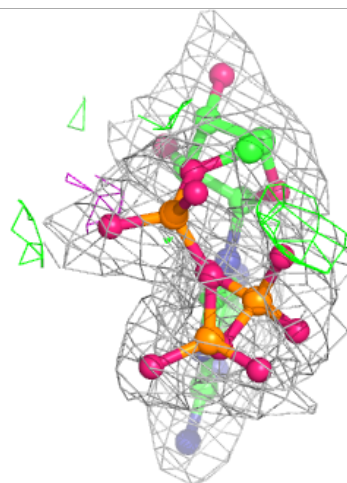
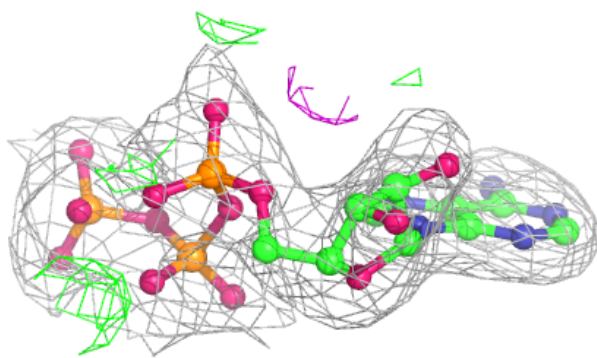
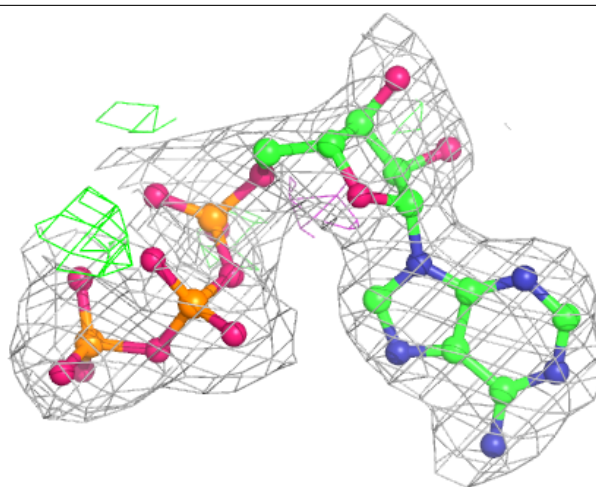
Electron density around ATP H 702:

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



Electron density around ATP C 703:

$2mF_o-DF_c$ (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.