



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2026 – 07:13 PM UTC

PDB ID : 3OAA / pdb\_00003oaa  
Title : Structure of the E.coli F1-ATP synthase inhibited by subunit Epsilon  
Authors : Cingolani, G.; Duncan, T.M.  
Deposited on : 2010-08-05  
Resolution : 3.26 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

<http://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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

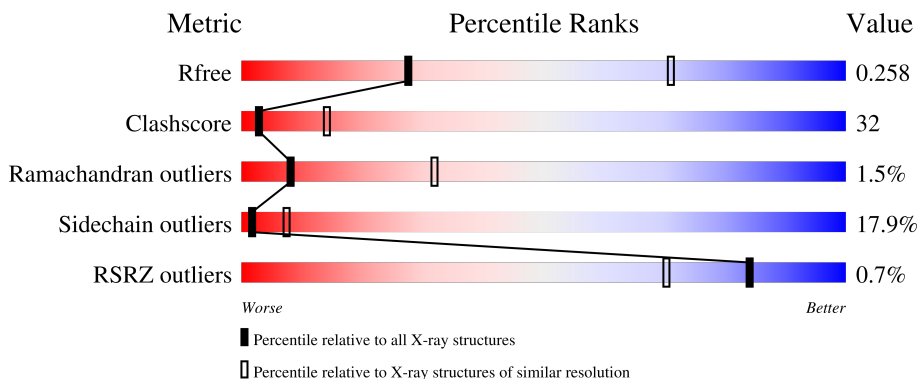
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






The reported resolution of this entry is 3.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





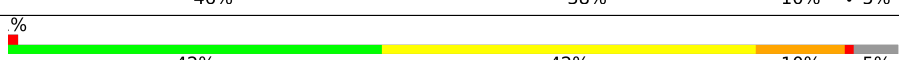

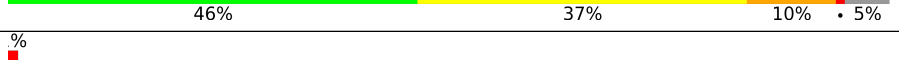
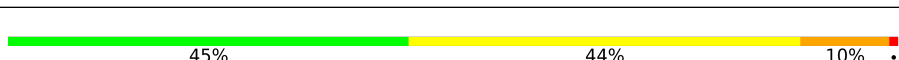
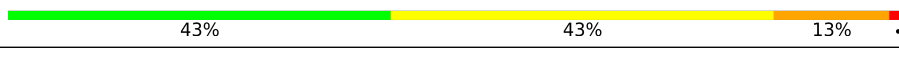
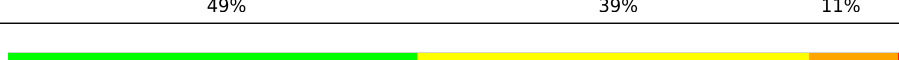


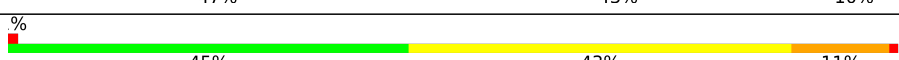



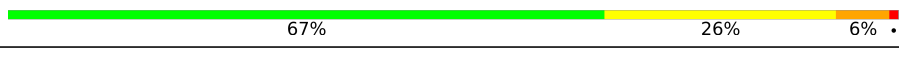
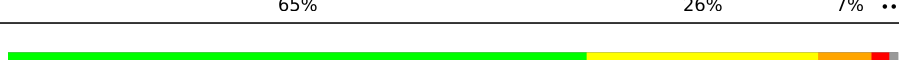





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	513	
1	B	513	
1	C	513	
1	I	513	
1	J	513	



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Mol	Chain	Length	Quality of chain
1	K	513	
1	Q	513	
1	R	513	
1	S	513	
1	Y	513	
1	Z	513	
1	a	513	
2	D	459	
2	E	459	
2	F	459	
2	L	459	
2	M	459	
2	N	459	
2	T	459	
2	U	459	
2	V	459	
2	b	459	
2	c	459	
2	d	459	
3	G	286	
3	O	286	
3	W	286	
3	e	286	
4	H	138	
4	P	138	

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Mol	Chain	Length	Quality of chain
4	X	138	 66% 28% 6%
4	f	138	 % 64% 28% 7%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 99573 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	488	3667	2301	648	705	13	0	0	0
1	B	486	3627	2278	642	694	13	0	0	0
1	C	487	3646	2288	646	699	13	0	0	0
1	I	488	3667	2301	648	705	13	0	0	0
1	J	486	3627	2278	642	694	13	0	0	0
1	K	487	3646	2288	646	699	13	0	0	0
1	Q	488	3667	2301	648	705	13	0	0	0
1	R	486	3627	2278	642	694	13	0	0	0
1	S	487	3646	2288	646	699	13	0	0	0
1	Y	488	3667	2301	648	705	13	0	0	0
1	Z	486	3627	2278	642	694	13	0	0	0
1	a	487	3646	2288	646	699	13	0	0	0

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	458	3521	2218	601	687	15	0	0	0
2	E	458	3521	2218	601	687	15	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	458	3521	2218	601	687	15	0	0	0
2	L	458	3521	2218	601	687	15	0	0	0
2	M	458	3521	2218	601	687	15	0	0	0
2	N	458	3521	2218	601	687	15	0	0	0
2	T	458	3521	2218	601	687	15	0	0	0
2	U	458	3521	2218	601	687	15	0	0	0
2	V	458	3521	2218	601	687	15	0	0	0
2	b	458	3521	2218	601	687	15	0	0	0
2	c	458	3521	2218	601	687	15	0	0	0
2	d	458	3521	2218	601	687	15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	81	GLU	LYS	engineered mutation	UNP C9QXA4
E	81	GLU	LYS	engineered mutation	UNP C9QXA4
F	81	GLU	LYS	engineered mutation	UNP C9QXA4
L	81	GLU	LYS	engineered mutation	UNP C9QXA4
M	81	GLU	LYS	engineered mutation	UNP C9QXA4
N	81	GLU	LYS	engineered mutation	UNP C9QXA4
T	81	GLU	LYS	engineered mutation	UNP C9QXA4
U	81	GLU	LYS	engineered mutation	UNP C9QXA4
V	81	GLU	LYS	engineered mutation	UNP C9QXA4
b	81	GLU	LYS	engineered mutation	UNP C9QXA4
c	81	GLU	LYS	engineered mutation	UNP C9QXA4
d	81	GLU	LYS	engineered mutation	UNP C9QXA4

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	284	2182	1369	382	417	14	0	0	0

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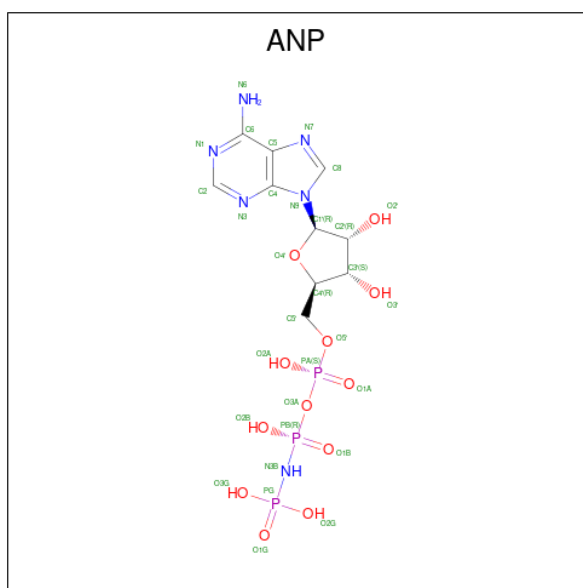
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			
3	W	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			
3	e	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	P	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	X	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	f	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	I	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	J	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	K	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	Q	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	R	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	S	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	Y	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	Z	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	a	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

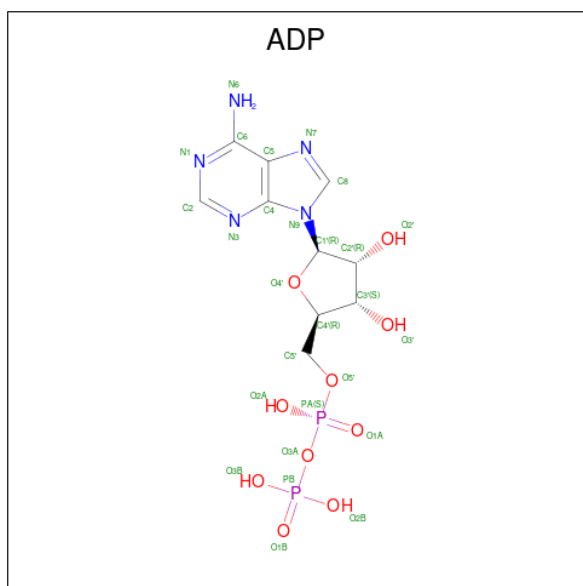
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Mg 1	0	0
6	B	1	Total 1	Mg 1	0	0
6	C	1	Total 1	Mg 1	0	0
6	D	1	Total 1	Mg 1	0	0
6	I	1	Total 1	Mg 1	0	0
6	J	1	Total 1	Mg 1	0	0
6	K	1	Total 1	Mg 1	0	0
6	L	1	Total 1	Mg 1	0	0
6	Q	1	Total 1	Mg 1	0	0

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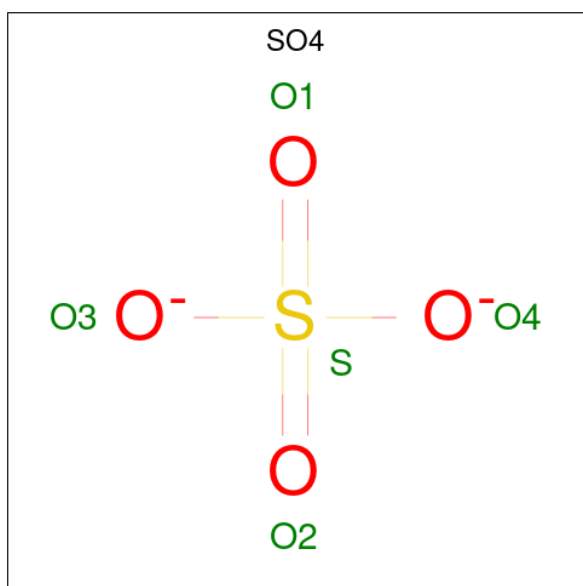
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	R	1	Total Mg 1 1	0	0
6	S	1	Total Mg 1 1	0	0
6	T	1	Total Mg 1 1	0	0
6	Y	1	Total Mg 1 1	0	0
6	Z	1	Total Mg 1 1	0	0
6	a	1	Total Mg 1 1	0	0
6	b	1	Total Mg 1 1	0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C N O P 27 10 5 10 2	0	0
7	L	1	Total C N O P 27 10 5 10 2	0	0
7	T	1	Total C N O P 27 10 5 10 2	0	0
7	b	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		
8	G	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	N	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		
8	P	1	Total	O	S	0	0
			5	4	1		
8	T	1	Total	O	S	0	0
			5	4	1		
8	U	1	Total	O	S	0	0
			5	4	1		
8	V	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	W	1	Total 5	O 4	S 1	0	0
8	b	1	Total 5	O 4	S 1	0	0
8	c	1	Total 5	O 4	S 1	0	0
8	d	1	Total 5	O 4	S 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total 3	O 3	0	0
9	B	2	Total 2	O 2	0	0
9	C	2	Total 2	O 2	0	0
9	D	8	Total 8	O 8	0	0
9	E	1	Total 1	O 1	0	0
9	F	5	Total 5	O 5	0	0
9	G	10	Total 10	O 10	0	0
9	H	4	Total 4	O 4	0	0
9	J	3	Total 3	O 3	0	0
9	L	6	Total 6	O 6	0	0
9	N	3	Total 3	O 3	0	0
9	O	5	Total 5	O 5	0	0
9	P	2	Total 2	O 2	0	0
9	Q	1	Total 1	O 1	0	0
9	R	1	Total 1	O 1	0	0

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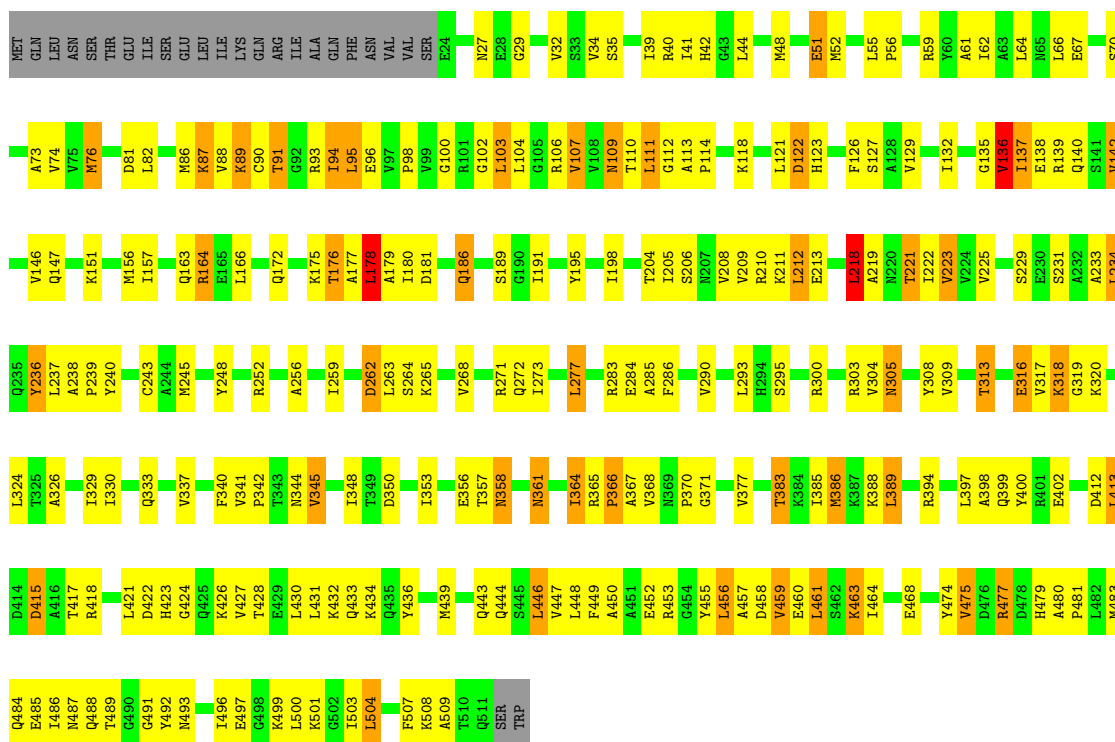
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
9	S	1	Total O 1 1	0	0
9	V	2	Total O 2 2	0	0
9	X	1	Total O 1 1	0	0
9	a	1	Total O 1 1	0	0
9	b	1	Total O 1 1	0	0
9	d	2	Total O 2 2	0	0

### 3 Residue-property plots i

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

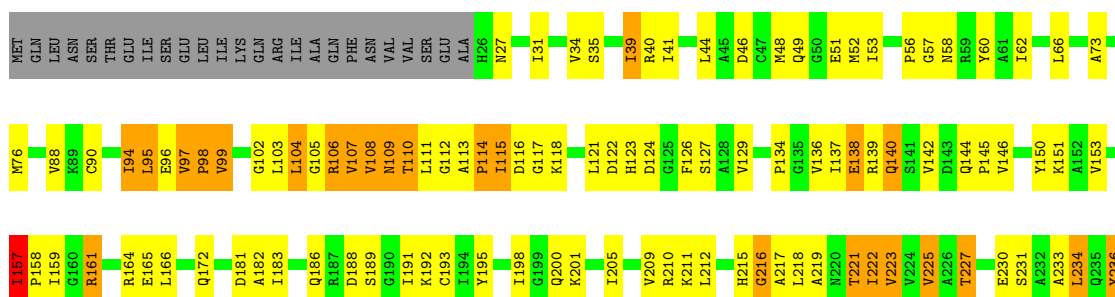
- Molecule 1: ATP synthase subunit alpha

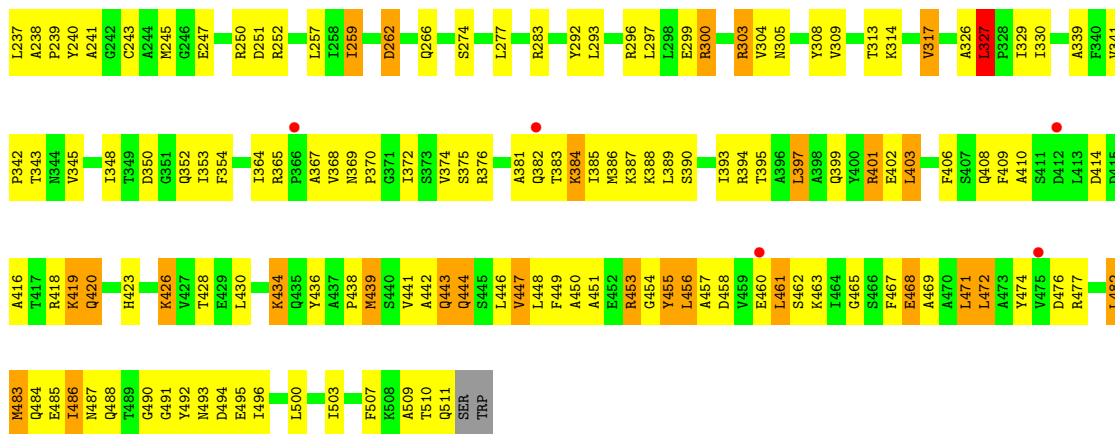
Chain A: 



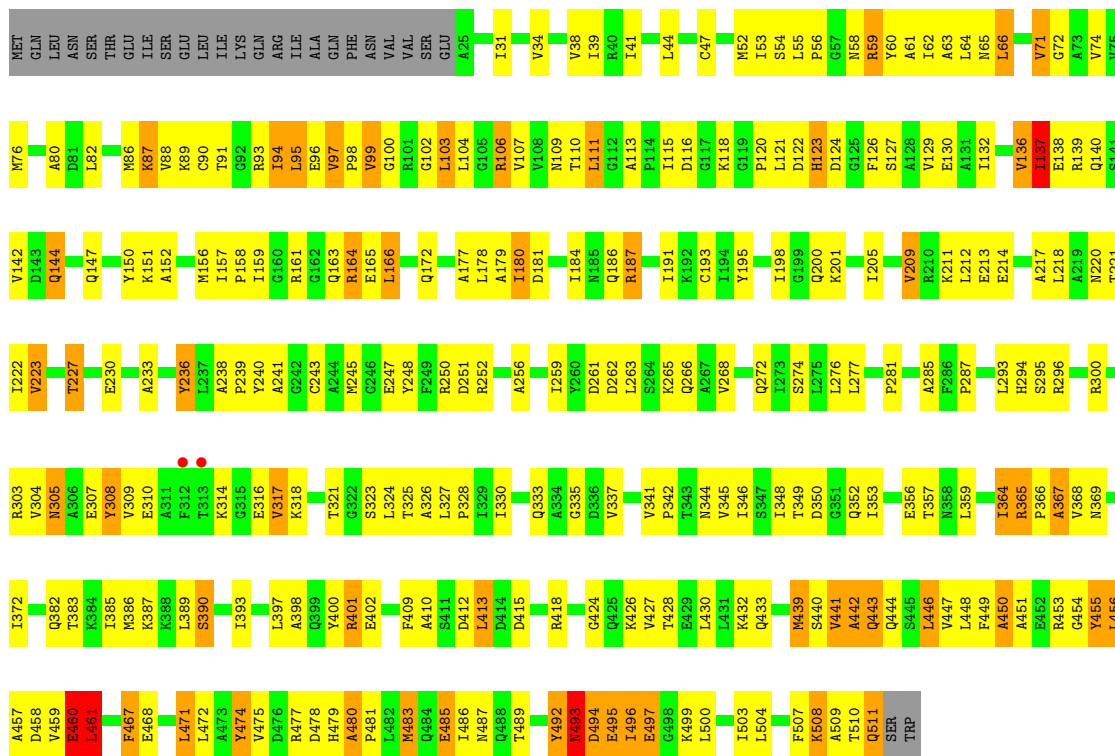
- Molecule 1: ATP synthase subunit alpha

Chain B: 

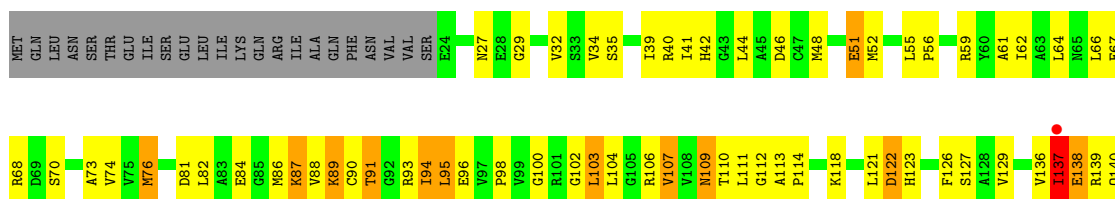


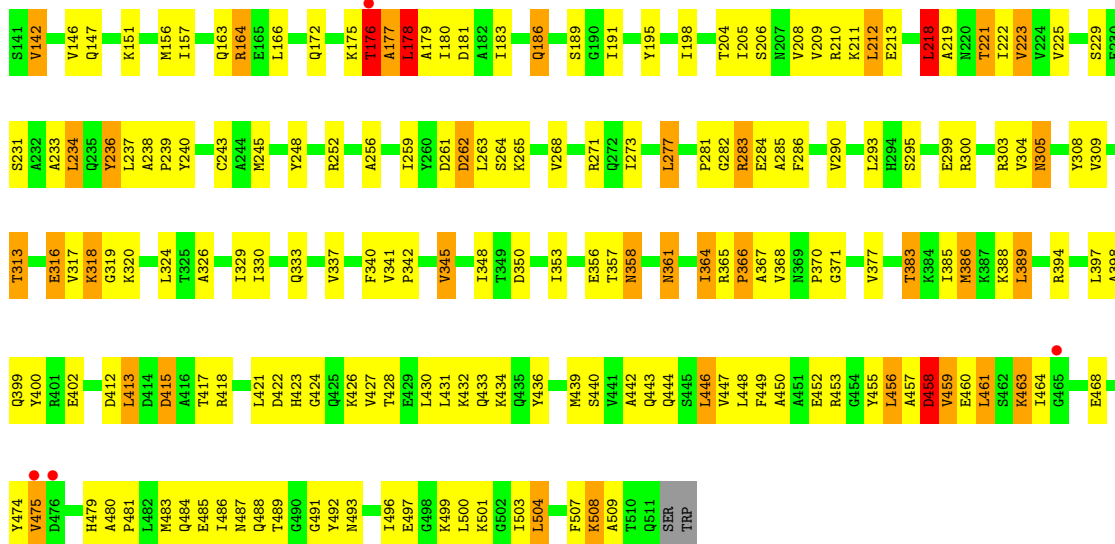


• Molecule 1: ATP synthase subunit alpha

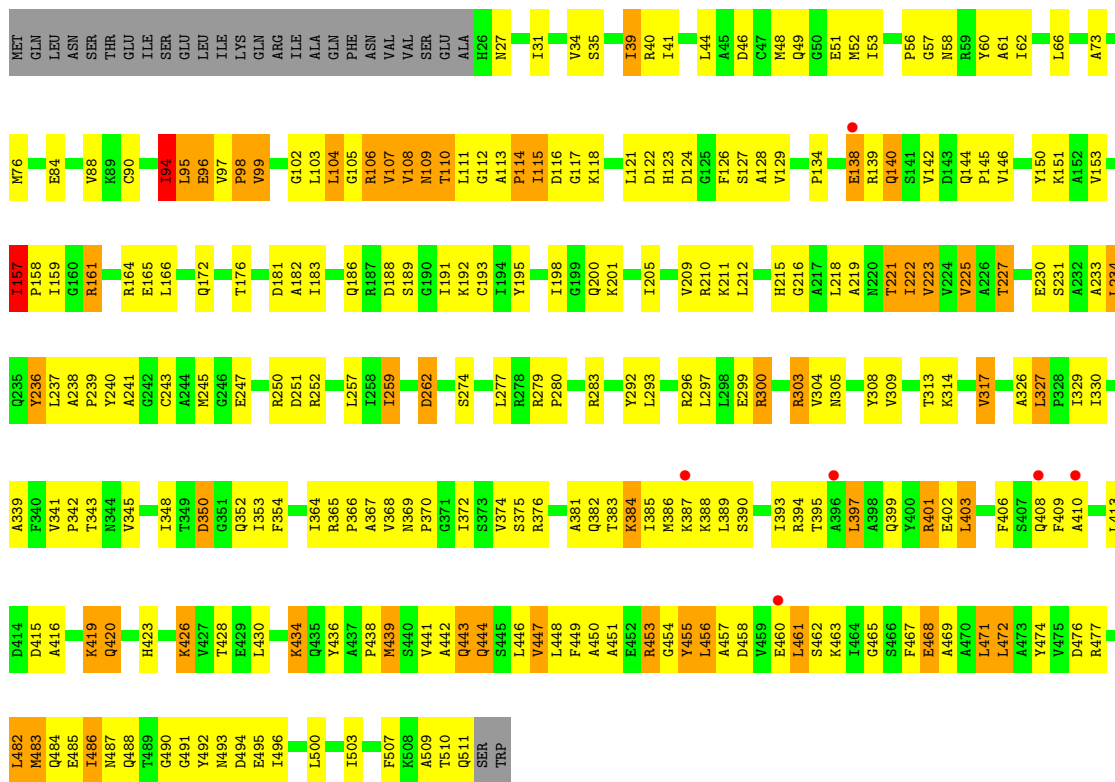


• Molecule 1: ATP synthase subunit alpha

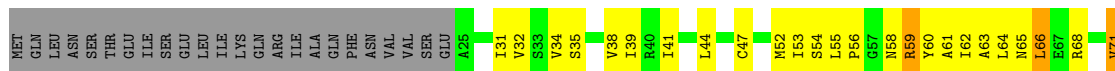
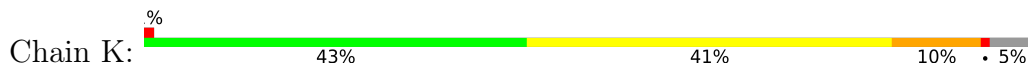


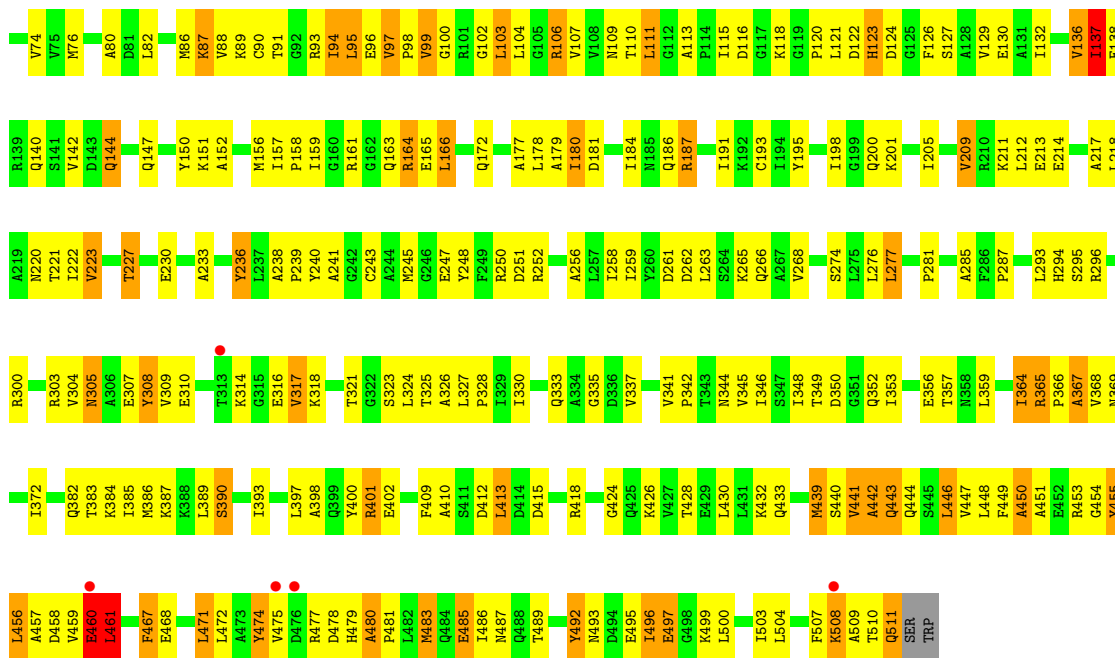


• Molecule 1: ATP synthase subunit alpha

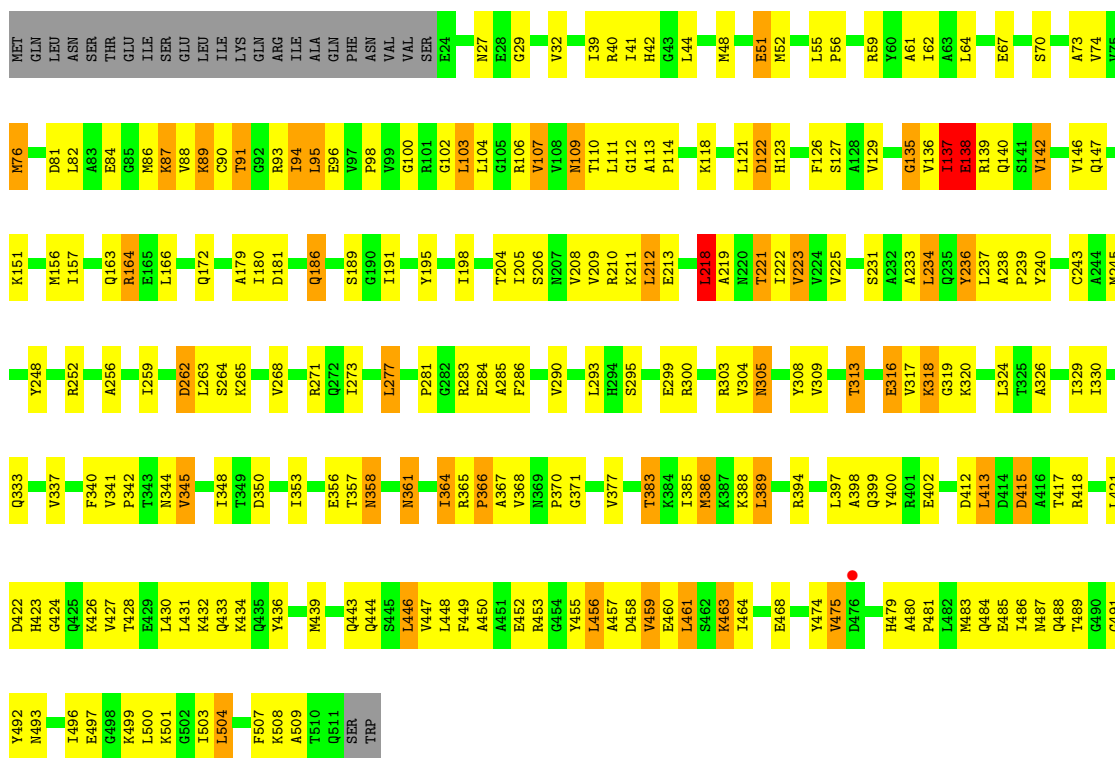


• Molecule 1: ATP synthase subunit alpha



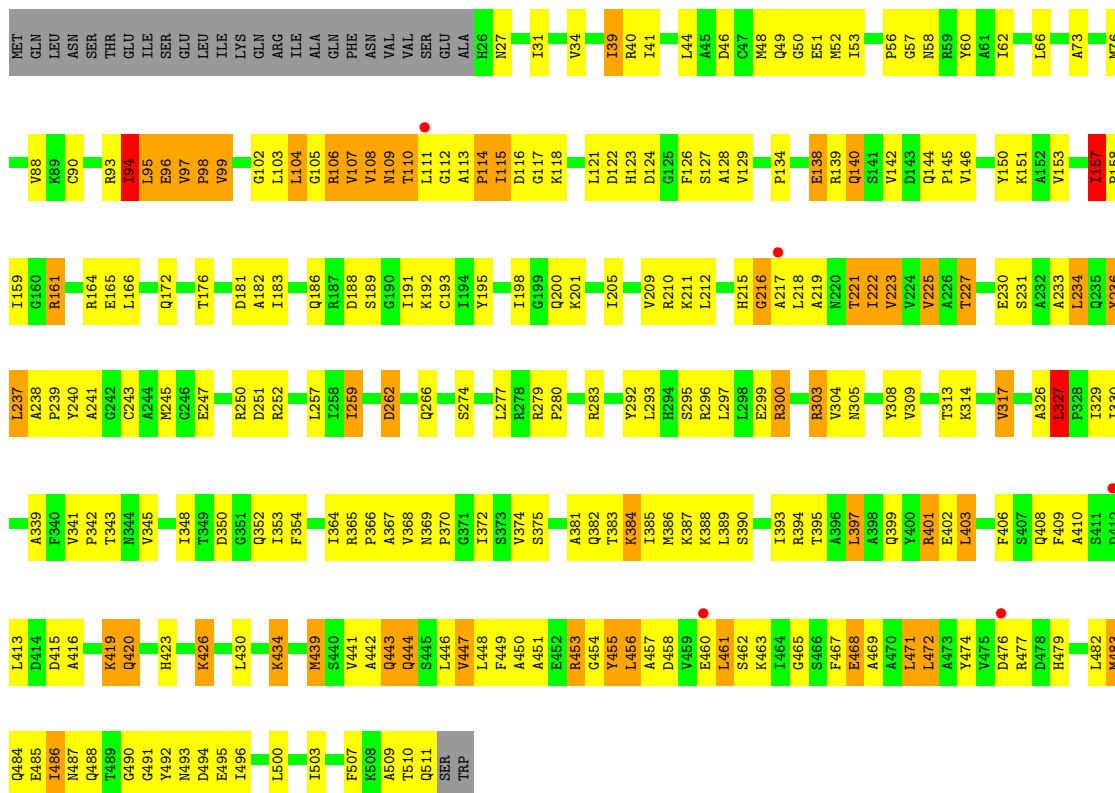


• Molecule 1: ATP synthase subunit alpha

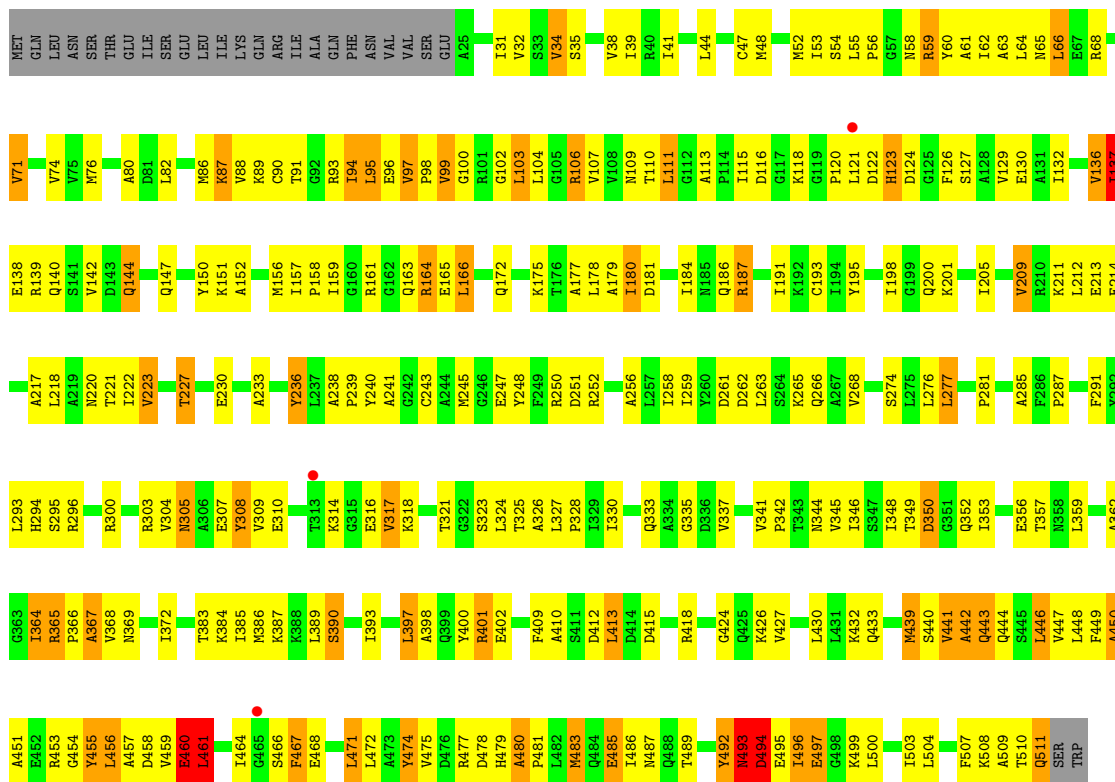
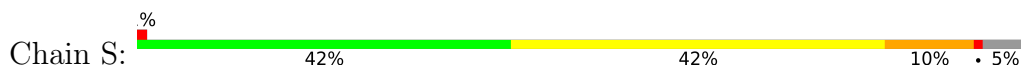


• Molecule 1: ATP synthase subunit alpha

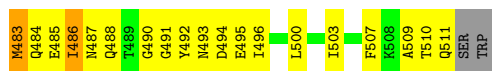




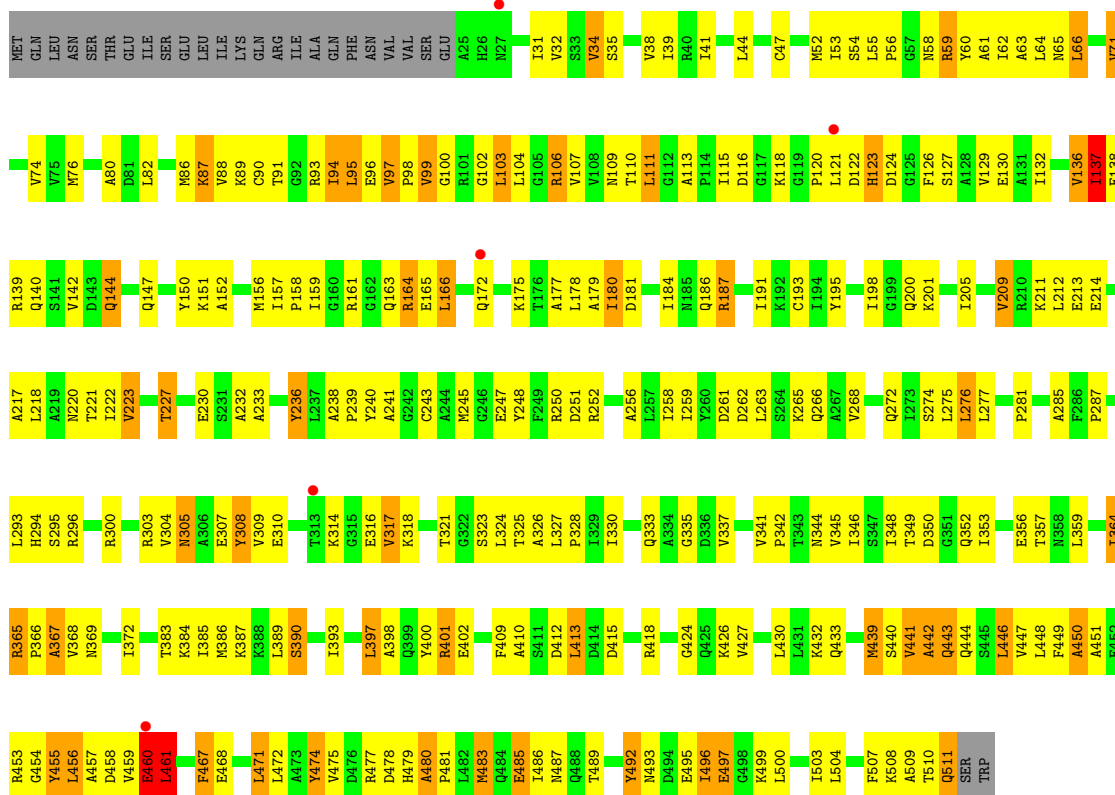
• Molecule 1: ATP synthase subunit alpha



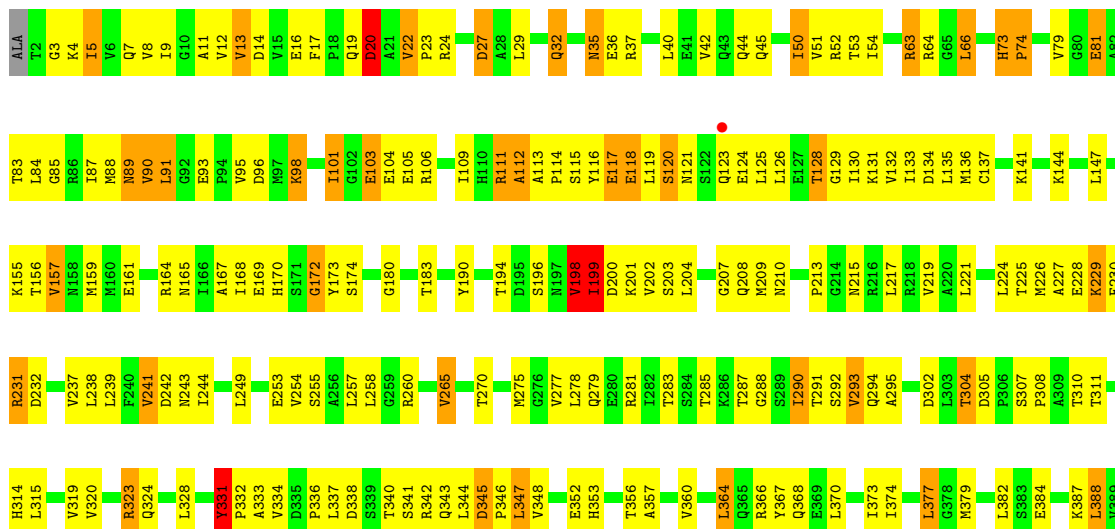


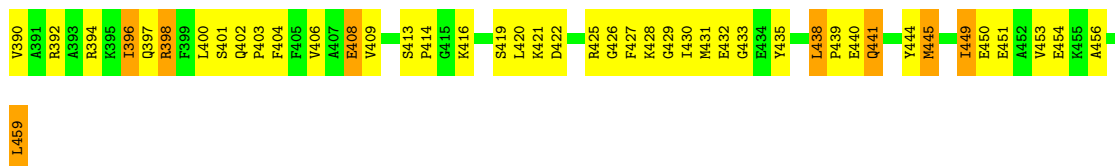


● Molecule 1: ATP synthase subunit alpha



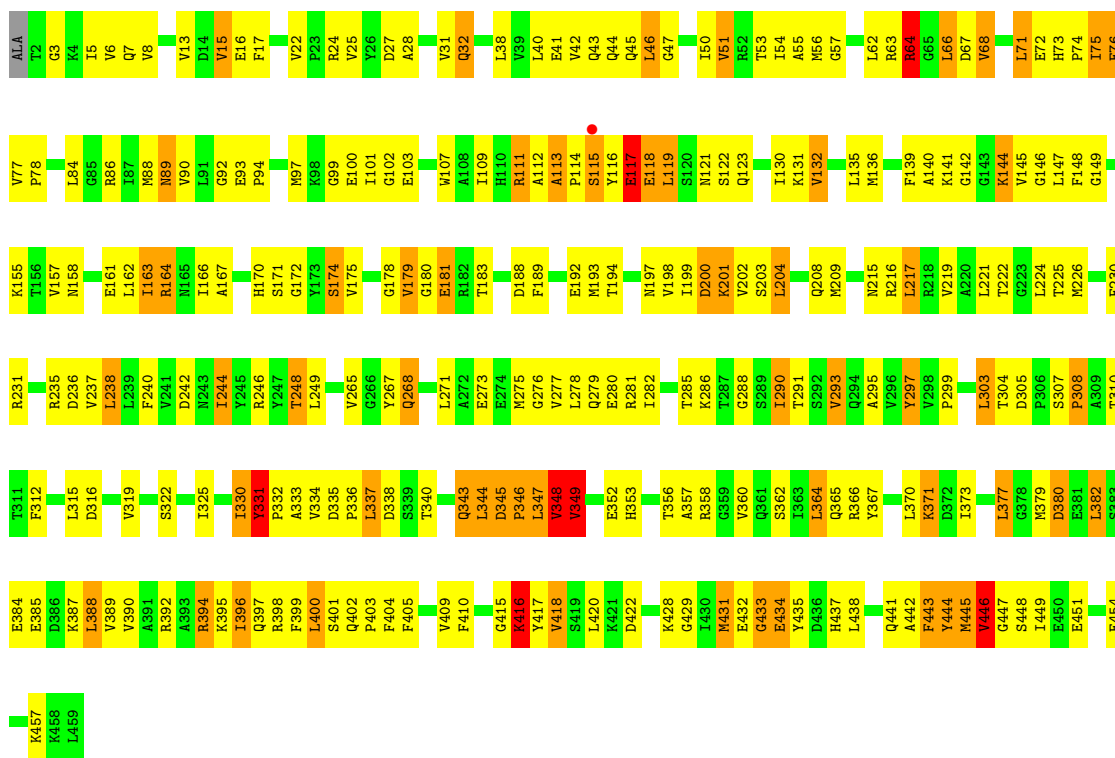
● Molecule 2: ATP synthase subunit beta





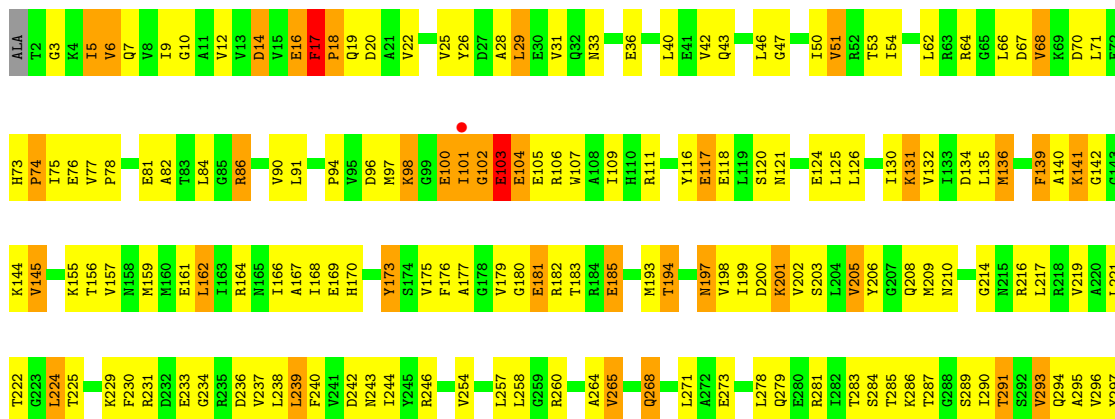
- Molecule 2: ATP synthase subunit beta

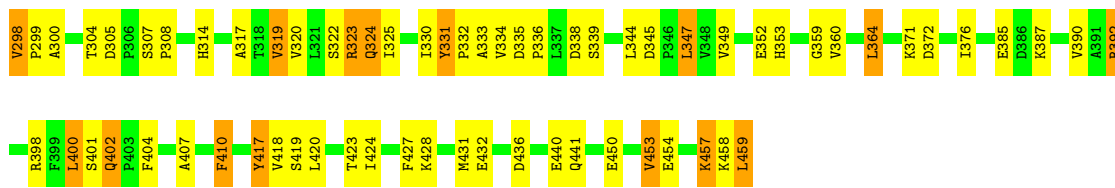
Chain E: 43% 43% 13%



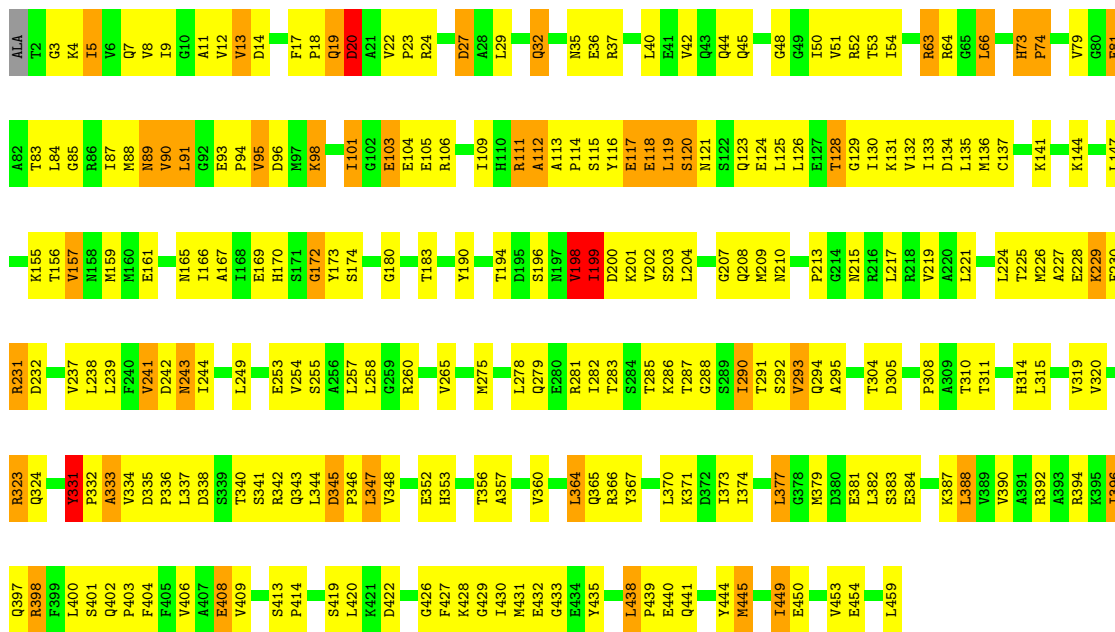
- Molecule 2: ATP synthase subunit beta

Chain F: 49% 39% 11%

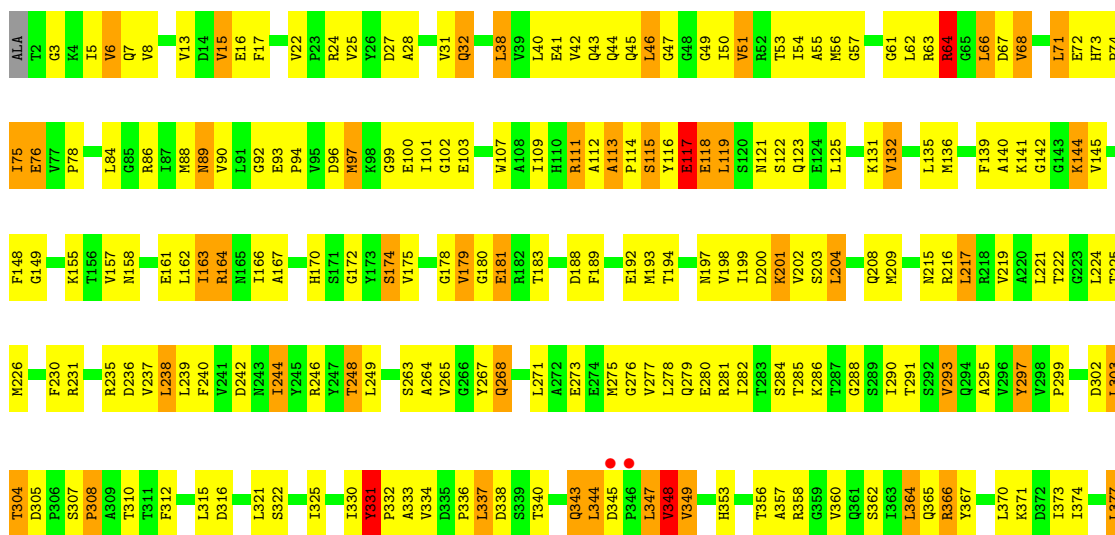


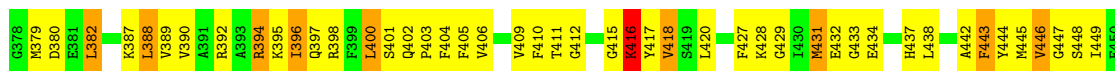


• Molecule 2: ATP synthase subunit beta

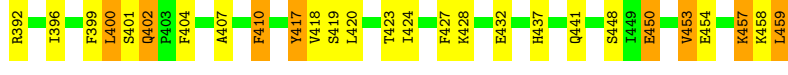
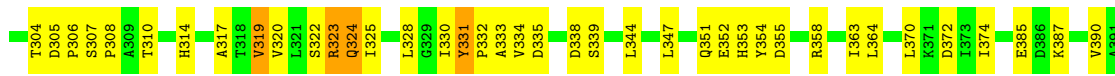
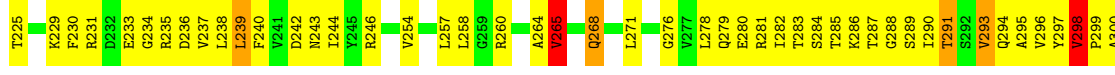
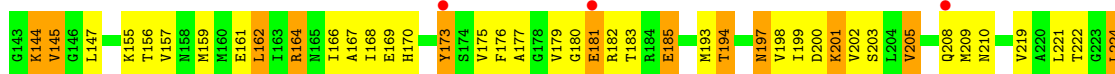
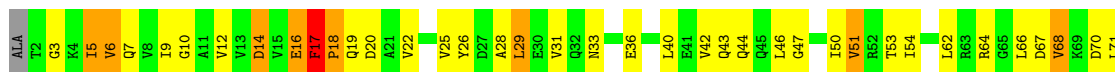


• Molecule 2: ATP synthase subunit beta

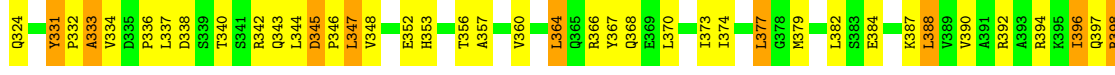
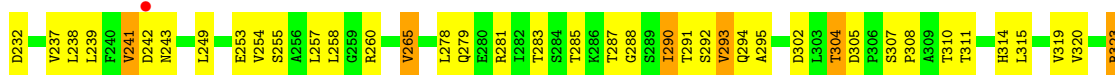
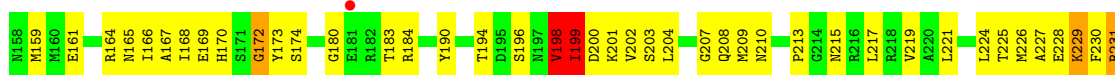
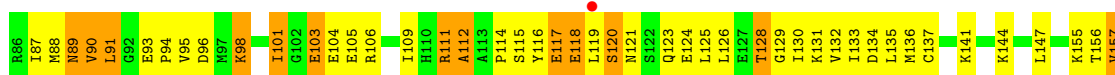




• Molecule 2: ATP synthase subunit beta

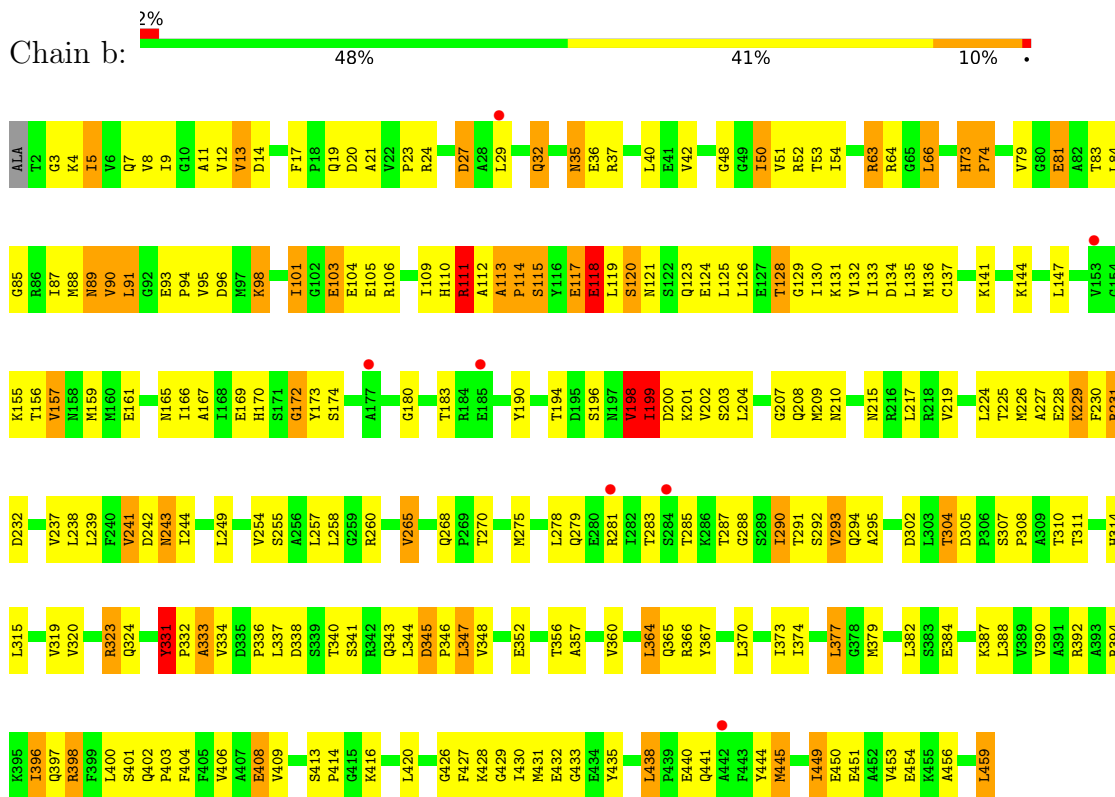


• Molecule 2: ATP synthase subunit beta

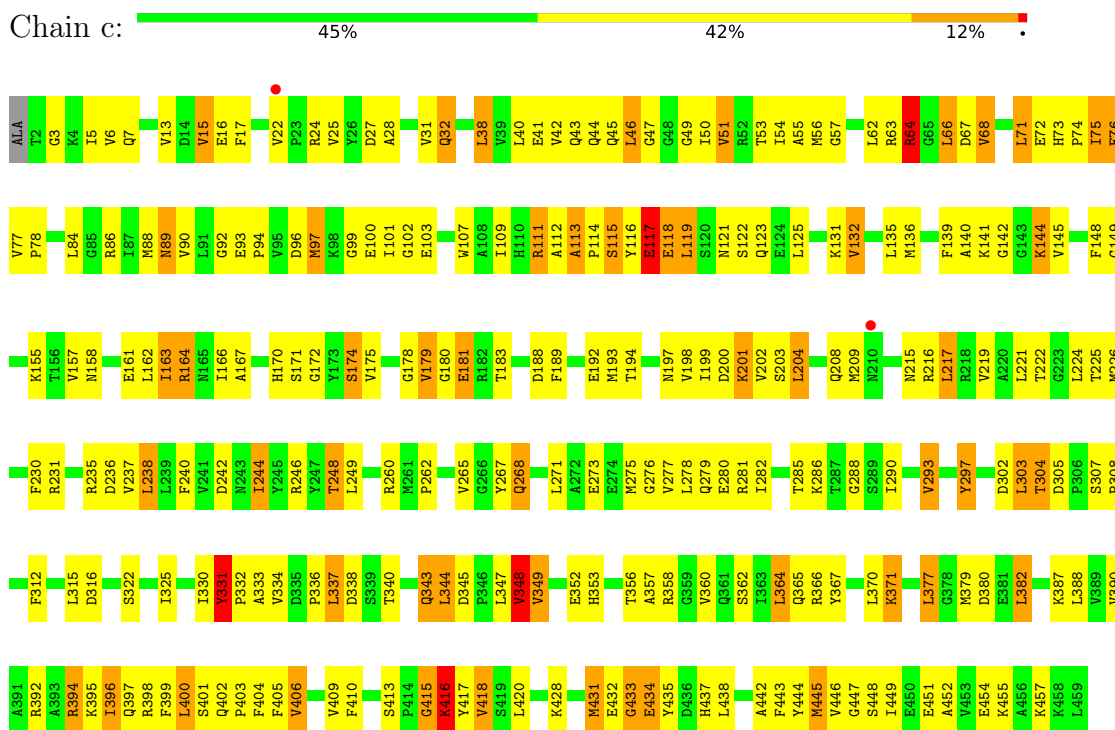




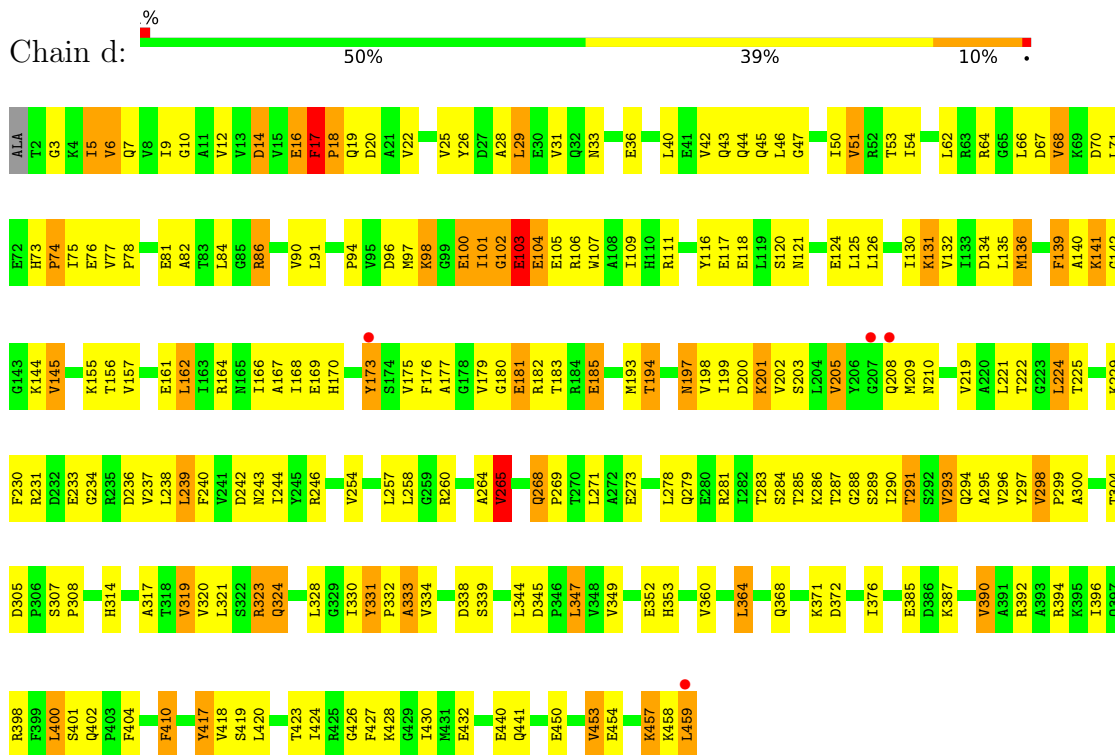
- Molecule 2: ATP synthase subunit beta



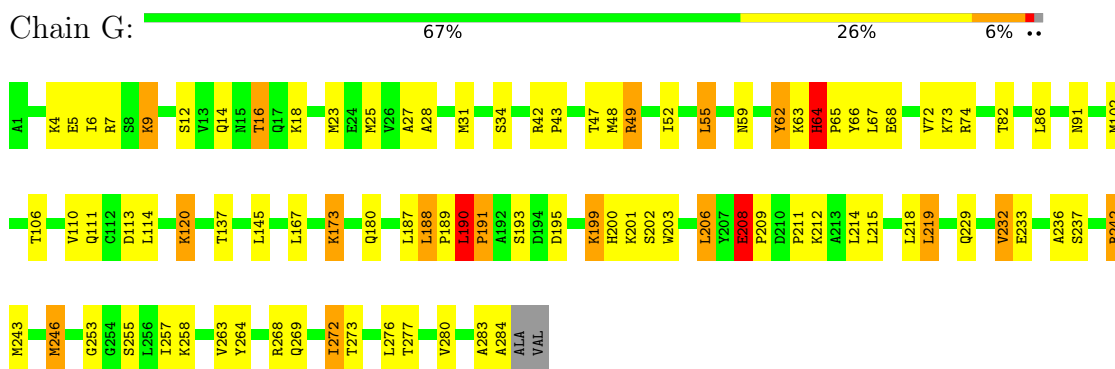
- Molecule 2: ATP synthase subunit beta



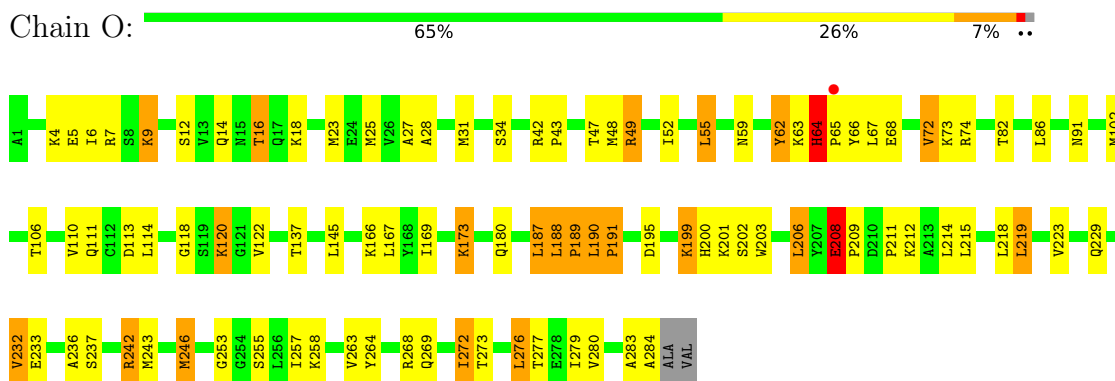
- Molecule 2: ATP synthase subunit beta



• Molecule 3: ATP synthase gamma chain

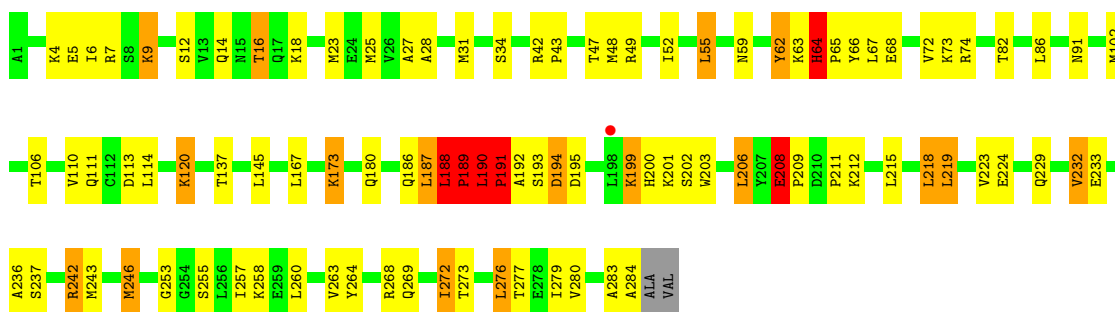


• Molecule 3: ATP synthase gamma chain



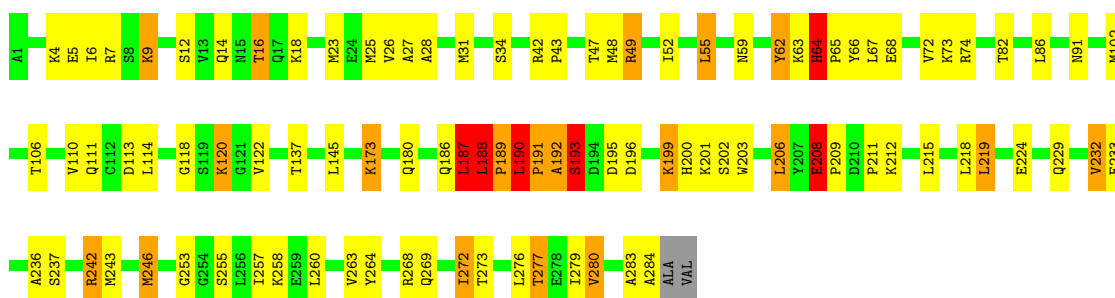
• Molecule 3: ATP synthase gamma chain

Chain W:  65% 26% 6% ..



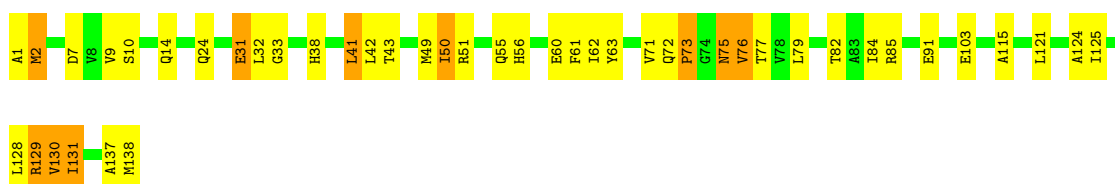
- Molecule 3: ATP synthase gamma chain

Chain e:  65% 26% 7% ..



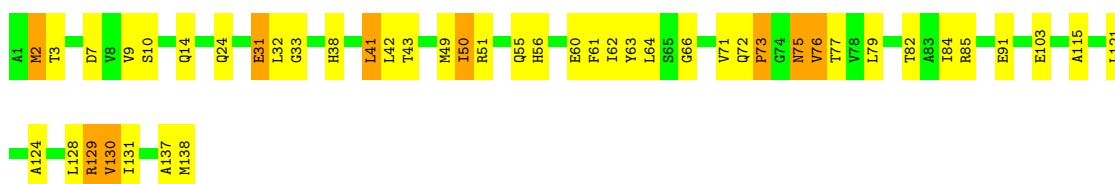
- Molecule 4: ATP synthase epsilon chain

Chain H:  67% 25% 7%



- Molecule 4: ATP synthase epsilon chain

Chain P:  67% 27% 7%



- Molecule 4: ATP synthase epsilon chain

Chain X:  66% 28% 6%



- Molecule 4: ATP synthase epsilon chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	435.97Å 183.00Å 225.39Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	15.00 – 3.26 15.00 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-3.26) 97.0 (15.00-3.26)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 3.26Å)	Xtrriage
Refinement program	PHENIX 1.6.3_473	Depositor
R, $R_{free}$	0.243 , 0.265 0.239 , 0.258	Depositor DCC
$R_{free}$ test set	2000 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.5	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 82.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	99573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ANP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/3720	0.80	5/5032 (0.1%)
1	B	0.33	0/3679	0.80	6/4979 (0.1%)
1	C	0.32	0/3699	0.81	6/5005 (0.1%)
1	I	0.38	0/3720	0.87	8/5032 (0.2%)
1	J	0.33	0/3679	0.79	4/4979 (0.1%)
1	K	0.33	1/3699 (0.0%)	0.81	6/5005 (0.1%)
1	Q	0.33	0/3720	0.77	3/5032 (0.1%)
1	R	0.33	0/3679	0.81	8/4979 (0.2%)
1	S	0.31	0/3699	0.81	7/5005 (0.1%)
1	Y	0.29	0/3720	0.94	5/5032 (0.1%)
1	Z	0.32	0/3679	0.80	6/4979 (0.1%)
1	a	0.30	0/3699	0.81	6/5005 (0.1%)
2	D	0.33	0/3578	0.79	7/4843 (0.1%)
2	E	0.36	1/3578 (0.0%)	0.84	8/4843 (0.2%)
2	F	0.30	0/3578	0.81	7/4843 (0.1%)
2	L	0.32	0/3578	0.81	8/4843 (0.2%)
2	M	0.33	0/3578	0.83	6/4843 (0.1%)
2	N	0.31	0/3578	0.83	9/4843 (0.2%)
2	T	0.30	0/3578	0.82	7/4843 (0.1%)
2	U	0.32	0/3578	0.83	6/4843 (0.1%)
2	V	0.29	0/3578	0.82	9/4843 (0.2%)
2	b	0.33	0/3578	0.80	7/4843 (0.1%)
2	c	0.31	0/3578	0.83	9/4843 (0.2%)
2	d	0.29	0/3578	0.81	6/4843 (0.1%)
3	G	0.44	0/2213	0.81	6/2984 (0.2%)
3	O	0.39	0/2213	0.79	5/2984 (0.2%)
3	W	0.34	0/2213	0.78	5/2984 (0.2%)
3	e	0.35	1/2213 (0.0%)	0.80	6/2984 (0.2%)
4	H	0.27	0/1062	1.00	3/1432 (0.2%)
4	P	0.28	0/1062	0.67	1/1432 (0.1%)
4	X	0.29	0/1062	0.68	1/1432 (0.1%)
4	f	0.29	0/1062	1.01	3/1432 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.33	3/100428 (0.0%)	0.82	189/135844 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	I	1	1
1	J	0	1
1	K	0	1
1	Q	0	1
1	R	0	1
1	S	0	2
1	Y	1	1
1	Z	0	2
1	a	0	1
2	D	0	2
2	E	0	4
2	F	0	1
2	L	0	2
2	M	0	1
2	N	0	1
2	T	0	1
2	U	0	1
2	V	0	1
2	b	0	5
2	c	0	1
2	d	0	1
3	G	0	2
3	O	0	2
3	W	0	4
3	e	0	4
All	All	2	47

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	e	188	LEU	CA-C	-6.37	1.49	1.53
1	K	136	VAL	CA-CB	-5.72	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	446	VAL	CA-CB	-5.21	1.47	1.54

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	ALA	CB-CA-C	27.19	151.29	110.50
4	f	1	ALA	CB-CA-C	27.17	151.26	110.50
1	Y	137	ILE	CA-C-N	-24.43	80.11	121.64
1	Y	137	ILE	C-N-CA	-24.43	80.11	121.64
1	Y	137	ILE	N-CA-C	16.23	143.09	109.34

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	I	138	GLU	CA
1	Y	137	ILE	CA

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	GLY	Peptide
1	C	460	GLU	Peptide
1	C	493	ASN	Peptide
2	D	119	LEU	Peptide
2	D	20	ASP	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	3667	0	3702	258	0
1	B	3627	0	3650	264	0
1	C	3646	0	3669	257	0
1	I	3667	0	3702	274	0
1	J	3627	0	3650	271	0
1	K	3646	0	3669	257	0
1	Q	3667	0	3702	234	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	3627	0	3650	277	0
1	S	3646	0	3669	262	0
1	Y	3667	0	3702	239	0
1	Z	3627	0	3650	264	0
1	a	3646	0	3669	256	0
2	D	3521	0	3523	270	0
2	E	3521	0	3524	330	0
2	F	3521	0	3524	217	0
2	L	3521	0	3523	249	0
2	M	3521	0	3524	294	0
2	N	3521	0	3524	215	0
2	T	3521	0	3523	235	0
2	U	3521	0	3524	265	0
2	V	3521	0	3524	218	0
2	b	3521	0	3523	265	0
2	c	3521	0	3524	268	0
2	d	3521	0	3524	209	0
3	G	2182	0	2227	86	0
3	O	2182	0	2227	95	0
3	W	2182	0	2227	132	0
3	e	2182	0	2227	106	0
4	H	1047	0	1058	37	0
4	P	1047	0	1058	45	0
4	X	1047	0	1058	46	0
4	f	1047	0	1058	39	0
5	A	31	0	12	2	0
5	B	31	0	12	3	0
5	C	31	0	12	3	0
5	I	31	0	12	4	0
5	J	31	0	12	3	0
5	K	31	0	12	2	0
5	Q	31	0	12	2	0
5	R	31	0	12	3	0
5	S	31	0	12	2	0
5	Y	31	0	12	3	0
5	Z	31	0	12	3	0
5	a	31	0	12	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
6	Y	1	0	0	0	0
6	Z	1	0	0	0	0
6	a	1	0	0	0	0
6	b	1	0	0	0	0
7	D	27	0	11	5	0
7	L	27	0	11	5	0
7	T	27	0	11	4	0
7	b	27	0	11	4	0
8	D	5	0	0	1	0
8	E	5	0	0	0	0
8	F	5	0	0	1	0
8	G	5	0	0	0	0
8	H	5	0	0	0	0
8	L	5	0	0	1	0
8	M	5	0	0	0	0
8	N	5	0	0	1	0
8	O	5	0	0	0	0
8	P	5	0	0	0	0
8	T	5	0	0	0	0
8	U	5	0	0	0	0
8	V	5	0	0	0	0
8	W	5	0	0	1	0
8	b	5	0	0	1	0
8	c	5	0	0	1	0
8	d	5	0	0	0	0
9	A	3	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	8	0	0	0	0
9	E	1	0	0	0	0
9	F	5	0	0	0	0
9	G	10	0	0	0	0
9	H	4	0	0	0	0
9	J	3	0	0	0	0
9	L	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	3	0	0	0	0
9	O	5	0	0	0	0
9	P	2	0	0	0	0
9	Q	1	0	0	0	0
9	R	1	0	0	0	0
9	S	1	0	0	0	0
9	V	2	0	0	0	0
9	X	1	0	0	0	0
9	a	1	0	0	0	0
9	b	1	0	0	0	0
9	d	2	0	0	0	0
All	All	99573	0	99696	6463	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 32.

The worst 5 of 6463 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:A:137:ILE:HD13	1:A:138:GLU:CA	1.35	1.50
4:P:2:MET:HE1	2:c:197:ASN:CB	1.46	1.45
1:R:50:GLY:O	1:R:94:ILE:CG2	1.63	1.45
3:W:186:GLN:NE2	3:W:189:PRO:HG2	1.31	1.45
1:R:95:LEU:CD2	1:R:129:VAL:HG22	1.44	1.42

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	486/513 (95%)	433 (89%)	48 (10%)	5 (1%)	<b>12</b> 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	484/513 (94%)	421 (87%)	54 (11%)	9 (2%)	6	28
1	C	485/513 (94%)	429 (88%)	48 (10%)	8 (2%)	7	30
1	I	486/513 (95%)	433 (89%)	49 (10%)	4 (1%)	16	44
1	J	484/513 (94%)	419 (87%)	56 (12%)	9 (2%)	6	28
1	K	485/513 (94%)	428 (88%)	49 (10%)	8 (2%)	7	30
1	Q	486/513 (95%)	433 (89%)	47 (10%)	6 (1%)	10	36
1	R	484/513 (94%)	417 (86%)	58 (12%)	9 (2%)	6	28
1	S	485/513 (94%)	429 (88%)	48 (10%)	8 (2%)	7	30
1	Y	486/513 (95%)	431 (89%)	49 (10%)	6 (1%)	10	36
1	Z	484/513 (94%)	418 (86%)	57 (12%)	9 (2%)	6	28
1	a	485/513 (94%)	427 (88%)	50 (10%)	8 (2%)	7	30
2	D	456/459 (99%)	397 (87%)	54 (12%)	5 (1%)	11	38
2	E	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	4	21
2	F	456/459 (99%)	411 (90%)	40 (9%)	5 (1%)	11	38
2	L	456/459 (99%)	398 (87%)	53 (12%)	5 (1%)	11	38
2	M	456/459 (99%)	405 (89%)	41 (9%)	10 (2%)	5	25
2	N	456/459 (99%)	413 (91%)	37 (8%)	6 (1%)	9	34
2	T	456/459 (99%)	402 (88%)	48 (10%)	6 (1%)	9	34
2	U	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	4	21
2	V	456/459 (99%)	410 (90%)	40 (9%)	6 (1%)	9	34
2	b	456/459 (99%)	398 (87%)	51 (11%)	7 (2%)	8	32
2	c	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	4	21
2	d	456/459 (99%)	411 (90%)	39 (9%)	6 (1%)	9	34
3	G	282/286 (99%)	265 (94%)	17 (6%)	0	100	100
3	O	282/286 (99%)	266 (94%)	15 (5%)	1 (0%)	30	59
3	W	282/286 (99%)	264 (94%)	16 (6%)	2 (1%)	18	48
3	e	282/286 (99%)	265 (94%)	15 (5%)	2 (1%)	18	48
4	H	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	32
4	P	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	32
4	X	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	32
4	f	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	12964/13360 (97%)	11533 (89%)	1237 (10%)	194 (2%)	8 32

5 of 194 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	455	TYR
1	B	491	GLY
1	C	137	ILE
2	E	333	ALA
2	E	348	VAL

### 5.3.2 Protein sidechains [i](#)

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	380/407 (93%)	316 (83%)	64 (17%)	2 10
1	B	371/407 (91%)	302 (81%)	69 (19%)	1 7
1	C	375/407 (92%)	299 (80%)	76 (20%)	1 5
1	I	380/407 (93%)	314 (83%)	66 (17%)	2 8
1	J	371/407 (91%)	302 (81%)	69 (19%)	1 7
1	K	375/407 (92%)	303 (81%)	72 (19%)	1 6
1	Q	380/407 (93%)	317 (83%)	63 (17%)	2 10
1	R	371/407 (91%)	301 (81%)	70 (19%)	1 6
1	S	375/407 (92%)	300 (80%)	75 (20%)	1 5
1	Y	380/407 (93%)	318 (84%)	62 (16%)	2 10
1	Z	371/407 (91%)	301 (81%)	70 (19%)	1 6
1	a	375/407 (92%)	302 (80%)	73 (20%)	1 6
2	D	380/380 (100%)	317 (83%)	63 (17%)	2 10
2	E	380/380 (100%)	297 (78%)	83 (22%)	1 4
2	F	380/380 (100%)	307 (81%)	73 (19%)	1 6
2	L	380/380 (100%)	320 (84%)	60 (16%)	2 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	380/380 (100%)	302 (80%)	78 (20%)	1	5
2	N	380/380 (100%)	305 (80%)	75 (20%)	1	6
2	T	380/380 (100%)	320 (84%)	60 (16%)	2	11
2	U	380/380 (100%)	303 (80%)	77 (20%)	1	5
2	V	380/380 (100%)	307 (81%)	73 (19%)	1	6
2	b	380/380 (100%)	321 (84%)	59 (16%)	2	12
2	c	380/380 (100%)	303 (80%)	77 (20%)	1	5
2	d	380/380 (100%)	307 (81%)	73 (19%)	1	6
3	G	236/239 (99%)	202 (86%)	34 (14%)	3	14
3	O	236/239 (99%)	202 (86%)	34 (14%)	3	14
3	W	236/239 (99%)	199 (84%)	37 (16%)	2	11
3	e	236/239 (99%)	200 (85%)	36 (15%)	3	12
4	H	109/109 (100%)	96 (88%)	13 (12%)	5	20
4	P	109/109 (100%)	96 (88%)	13 (12%)	5	20
4	X	109/109 (100%)	97 (89%)	12 (11%)	6	23
4	f	109/109 (100%)	96 (88%)	13 (12%)	5	20
All	All	10444/10836 (96%)	8572 (82%)	1872 (18%)	2	7

5 of 1872 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	O	276	LEU
2	d	141	LYS
1	S	494	ASP
2	d	17	PHE
1	a	446	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 390 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	186	GLN
3	W	172	ASN
1	S	382	GLN
2	U	351	GLN
1	Y	266	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 16 are monoatomic - leaving 33 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
8	SO4	P	200	-	4,4,4	0.37	0	6,6,6	0.49	0
5	ANP	Y	600	6	33,33,33	2.94	11 (33%)	45,52,52	2.82	14 (31%)
5	ANP	I	600	6	33,33,33	2.93	12 (36%)	45,52,52	2.82	14 (31%)
5	ANP	C	600	6	33,33,33	2.93	12 (36%)	45,52,52	2.81	14 (31%)
5	ANP	B	600	6	33,33,33	2.57	11 (33%)	45,52,52	2.90	17 (37%)
8	SO4	N	530	-	4,4,4	0.24	0	6,6,6	0.10	0
8	SO4	T	630	6	4,4,4	0.22	0	6,6,6	0.11	0
8	SO4	U	530	-	4,4,4	0.23	0	6,6,6	0.08	0
5	ANP	R	600	6	33,33,33	2.56	11 (33%)	45,52,52	2.91	17 (37%)
5	ANP	Z	600	6	33,33,33	2.57	11 (33%)	45,52,52	2.94	17 (37%)
8	SO4	E	530	-	4,4,4	0.22	0	6,6,6	0.10	0
7	ADP	L	600	6	28,29,29	2.12	8 (28%)	43,45,45	1.94	12 (27%)
5	ANP	A	600	6	33,33,33	2.94	12 (36%)	45,52,52	2.82	14 (31%)
8	SO4	b	630	6	4,4,4	0.25	0	6,6,6	0.10	0
8	SO4	d	530	-	4,4,4	0.22	0	6,6,6	0.13	0
5	ANP	J	600	6	33,33,33	2.56	11 (33%)	45,52,52	2.91	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ADP	b	600	6	28,29,29	2.09	8 (28%)	43,45,45	1.97	12 (27%)
8	SO4	W	300	-	4,4,4	0.22	0	6,6,6	0.28	0
7	ADP	T	600	6	28,29,29	2.09	9 (32%)	43,45,45	1.94	11 (25%)
8	SO4	G	300	-	4,4,4	0.47	0	6,6,6	0.40	0
7	ADP	D	600	6	28,29,29	2.13	8 (28%)	43,45,45	1.94	12 (27%)
5	ANP	K	600	6	33,33,33	2.94	12 (36%)	45,52,52	2.85	14 (31%)
5	ANP	a	600	6	33,33,33	2.96	12 (36%)	45,52,52	2.81	13 (28%)
8	SO4	O	300	-	4,4,4	0.43	0	6,6,6	0.60	0
5	ANP	Q	600	6	33,33,33	2.93	12 (36%)	45,52,52	2.82	14 (31%)
8	SO4	D	630	6	4,4,4	0.22	0	6,6,6	0.09	0
8	SO4	F	530	-	4,4,4	0.22	0	6,6,6	0.10	0
8	SO4	V	530	-	4,4,4	0.21	0	6,6,6	0.12	0
8	SO4	c	530	-	4,4,4	0.21	0	6,6,6	0.08	0
8	SO4	M	530	-	4,4,4	0.22	0	6,6,6	0.10	0
8	SO4	L	630	6	4,4,4	0.22	0	6,6,6	0.10	0
8	SO4	H	200	-	4,4,4	0.40	0	6,6,6	0.35	0
5	ANP	S	600	6	33,33,33	2.95	11 (33%)	45,52,52	2.83	13 (28%)

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
5	ANP	J	600	6	-	6/18/38/38	0/3/3/3
7	ADP	b	600	6	-	4/16/32/32	0/3/3/3
5	ANP	R	600	6	-	6/18/38/38	0/3/3/3
7	ADP	L	600	6	-	4/16/32/32	0/3/3/3
5	ANP	Y	600	6	-	2/18/38/38	0/3/3/3
7	ADP	T	600	6	-	4/16/32/32	0/3/3/3
5	ANP	Z	600	6	-	6/18/38/38	0/3/3/3
7	ADP	D	600	6	-	4/16/32/32	0/3/3/3
5	ANP	I	600	6	-	2/18/38/38	0/3/3/3
5	ANP	K	600	6	-	2/18/38/38	0/3/3/3
5	ANP	C	600	6	-	2/18/38/38	0/3/3/3
5	ANP	B	600	6	-	6/18/38/38	0/3/3/3
5	ANP	A	600	6	-	2/18/38/38	0/3/3/3
5	ANP	a	600	6	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	S	600	6	-	2/18/38/38	0/3/3/3
5	ANP	Q	600	6	-	2/18/38/38	0/3/3/3

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	600	ANP	PB-O1B	9.13	1.60	1.46
5	S	600	ANP	PB-O1B	8.96	1.59	1.46
5	A	600	ANP	PB-O1B	8.94	1.59	1.46
5	C	600	ANP	PB-O1B	8.94	1.59	1.46
5	Y	600	ANP	PB-O1B	8.94	1.59	1.46

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	600	ANP	O1B-PB-N3B	-11.49	94.85	111.77
5	C	600	ANP	O1B-PB-N3B	-11.38	95.02	111.77
5	I	600	ANP	O1B-PB-N3B	-11.37	95.03	111.77
5	A	600	ANP	O1B-PB-N3B	-11.36	95.05	111.77
5	Q	600	ANP	O1B-PB-N3B	-11.35	95.05	111.77

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	ANP	PB-N3B-PG-O1G
5	A	600	ANP	PG-N3B-PB-O1B
5	B	600	ANP	PG-N3B-PB-O1B
5	B	600	ANP	C5'-O5'-PA-O1A
5	B	600	ANP	O4'-C4'-C5'-O5'

There are no ring outliers.

23 monomers are involved in 54 short contacts:

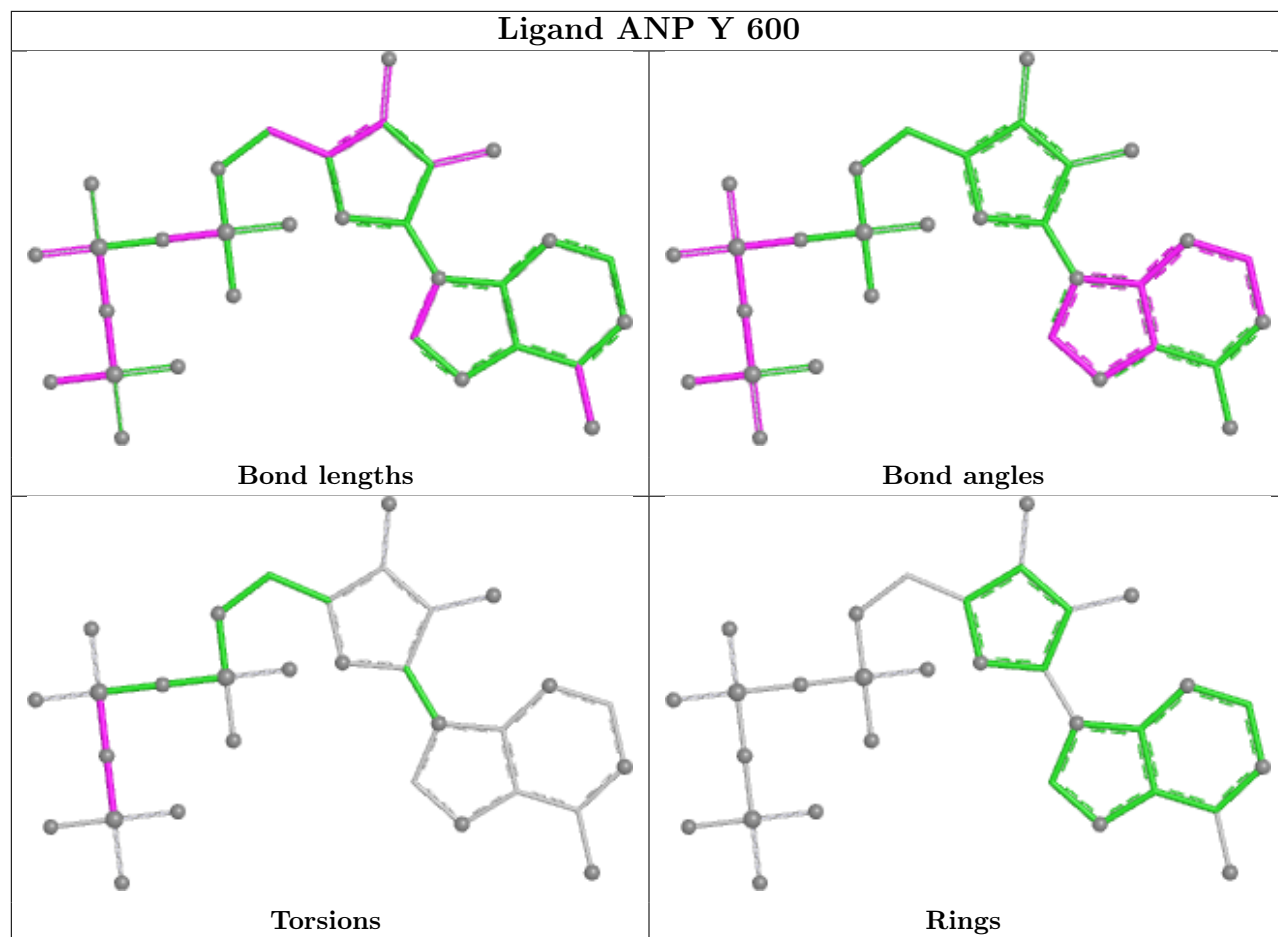
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	600	ANP	3	0
5	I	600	ANP	4	0
5	C	600	ANP	3	0
5	B	600	ANP	3	0
8	N	530	SO4	1	0

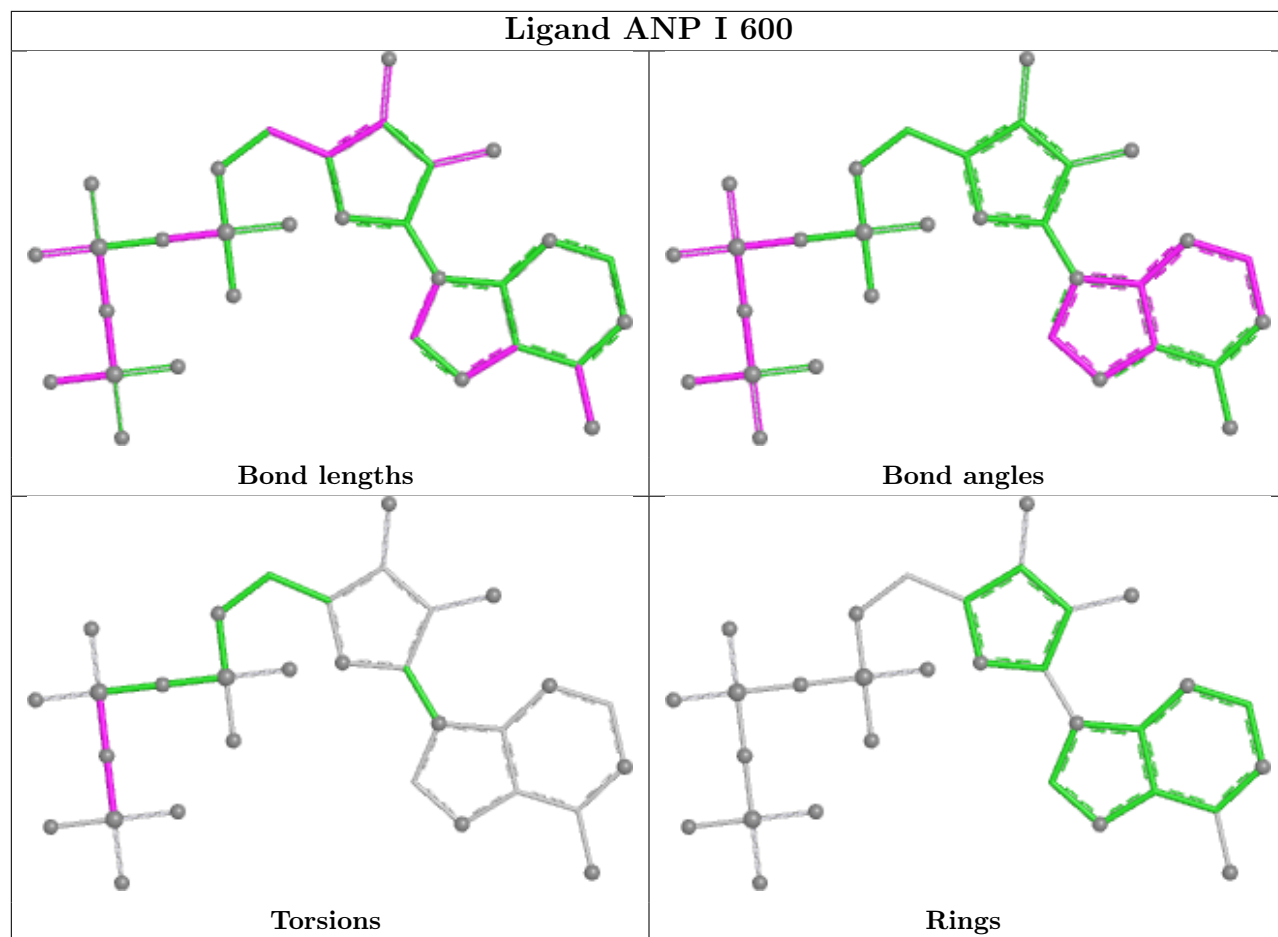
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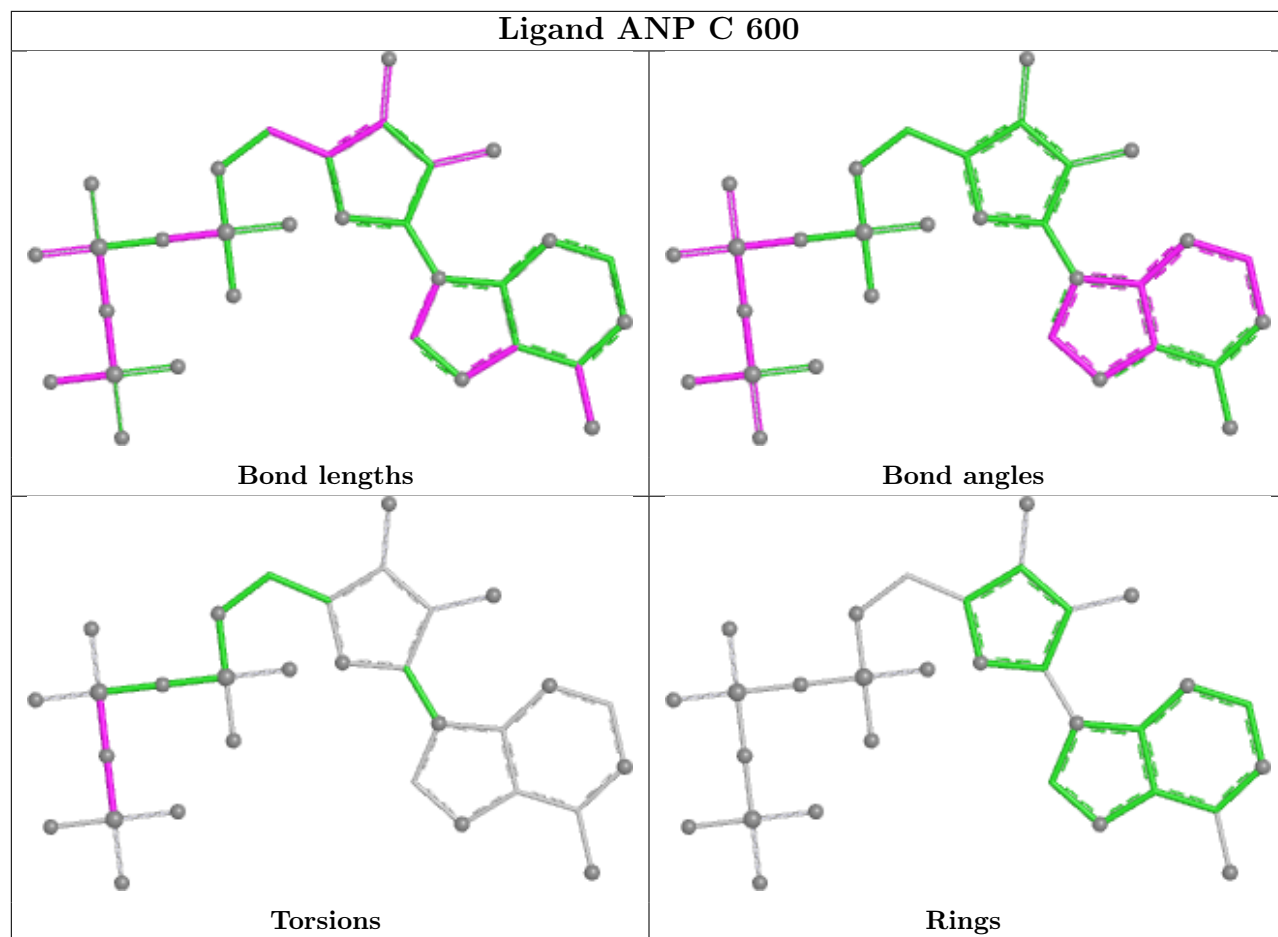
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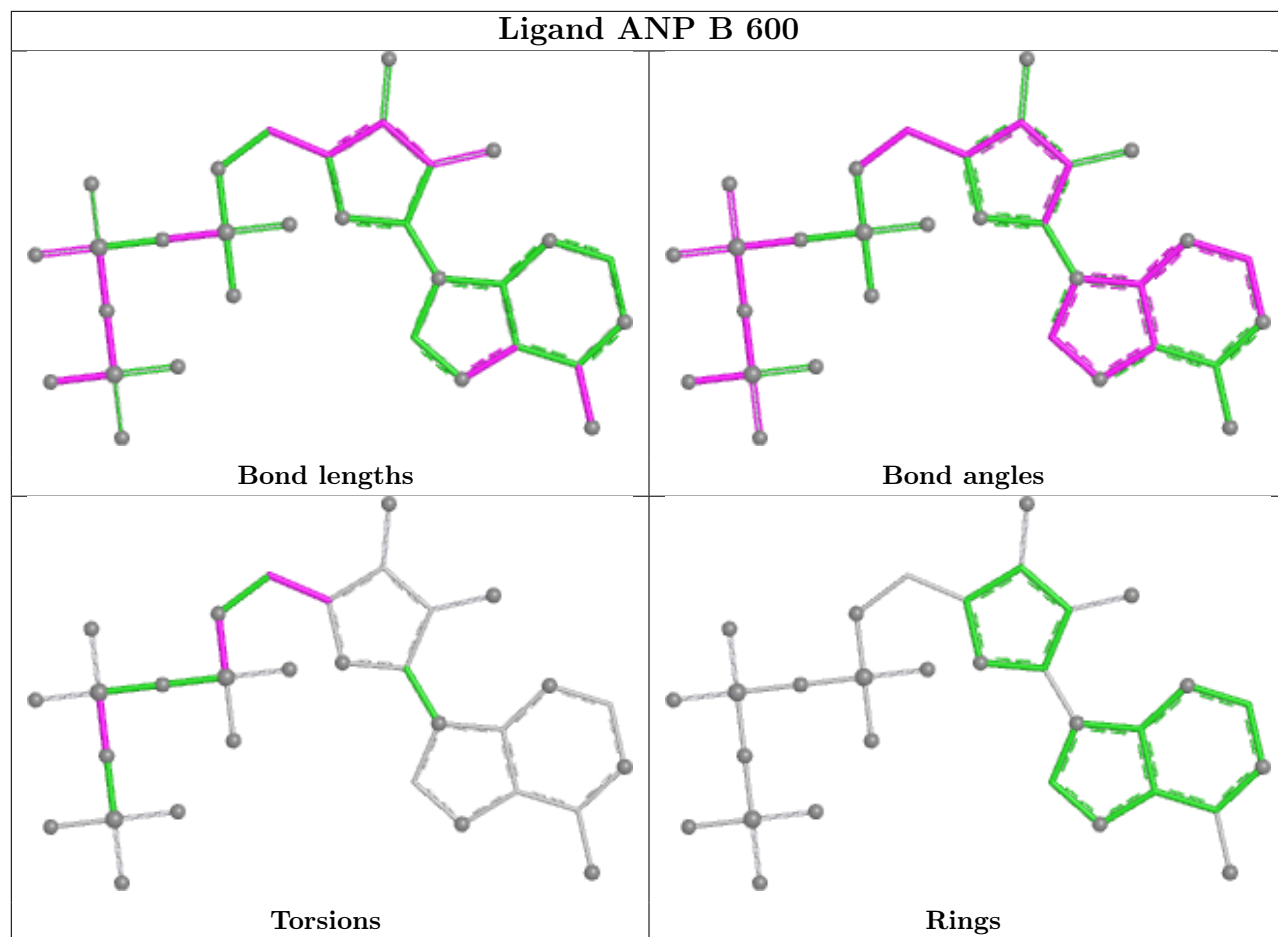
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	600	ANP	3	0
5	Z	600	ANP	3	0
7	L	600	ADP	5	0
5	A	600	ANP	2	0
8	b	630	SO4	1	0
5	J	600	ANP	3	0
7	b	600	ADP	4	0
8	W	300	SO4	1	0
7	T	600	ADP	4	0
7	D	600	ADP	5	0
5	K	600	ANP	2	0
5	a	600	ANP	2	0
5	Q	600	ANP	2	0
8	D	630	SO4	1	0
8	F	530	SO4	1	0
8	c	530	SO4	1	0
8	L	630	SO4	1	0
5	S	600	ANP	2	0

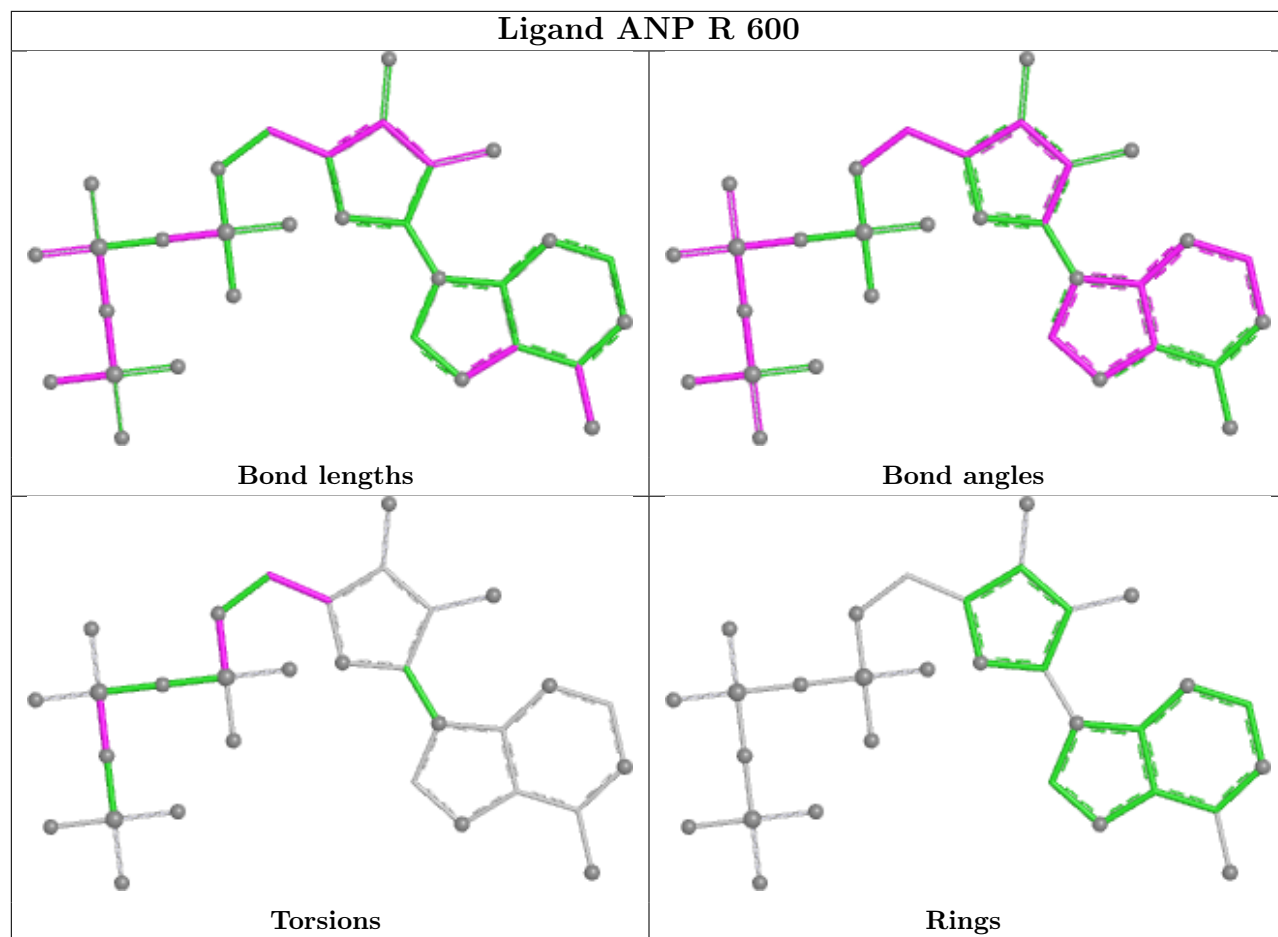
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

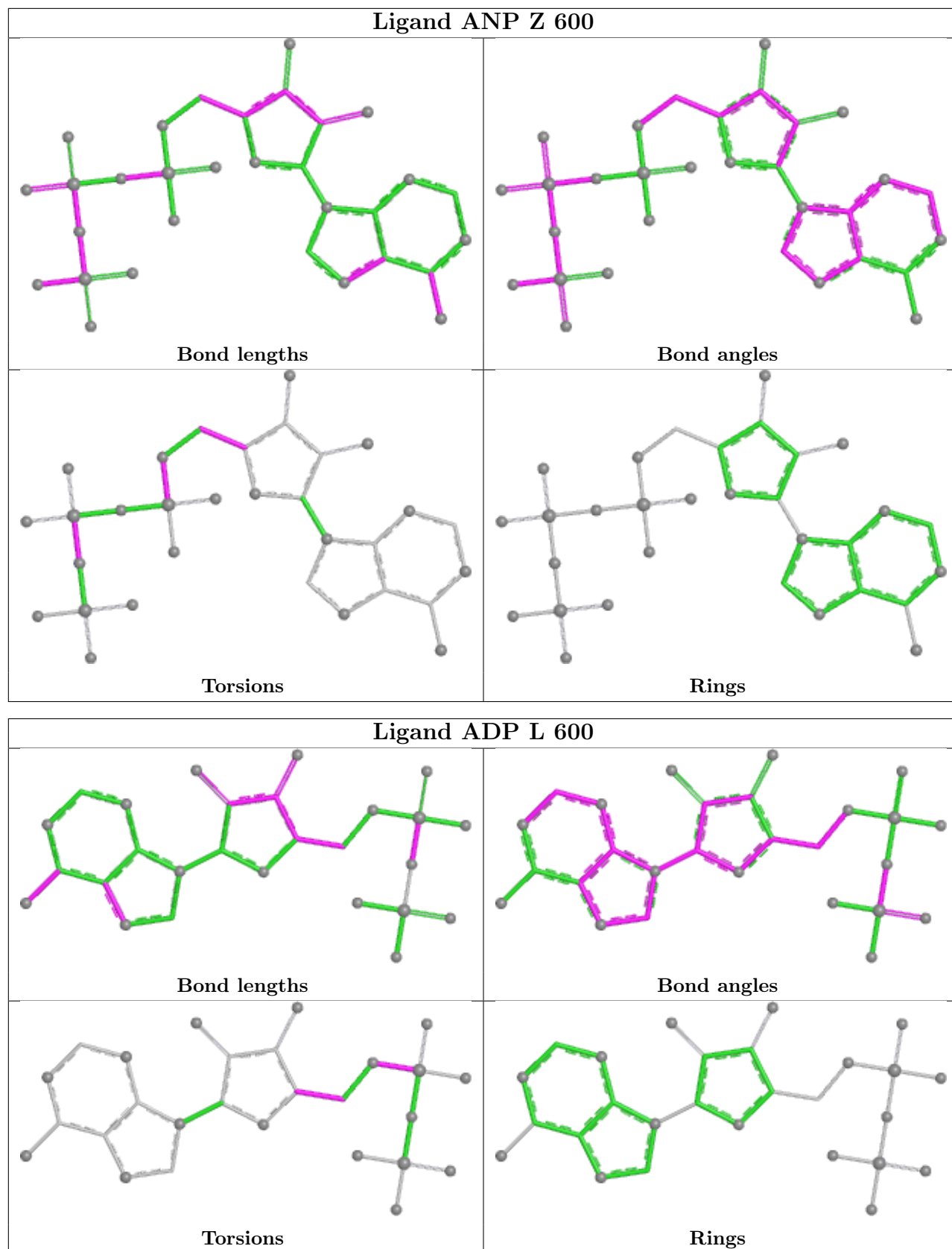


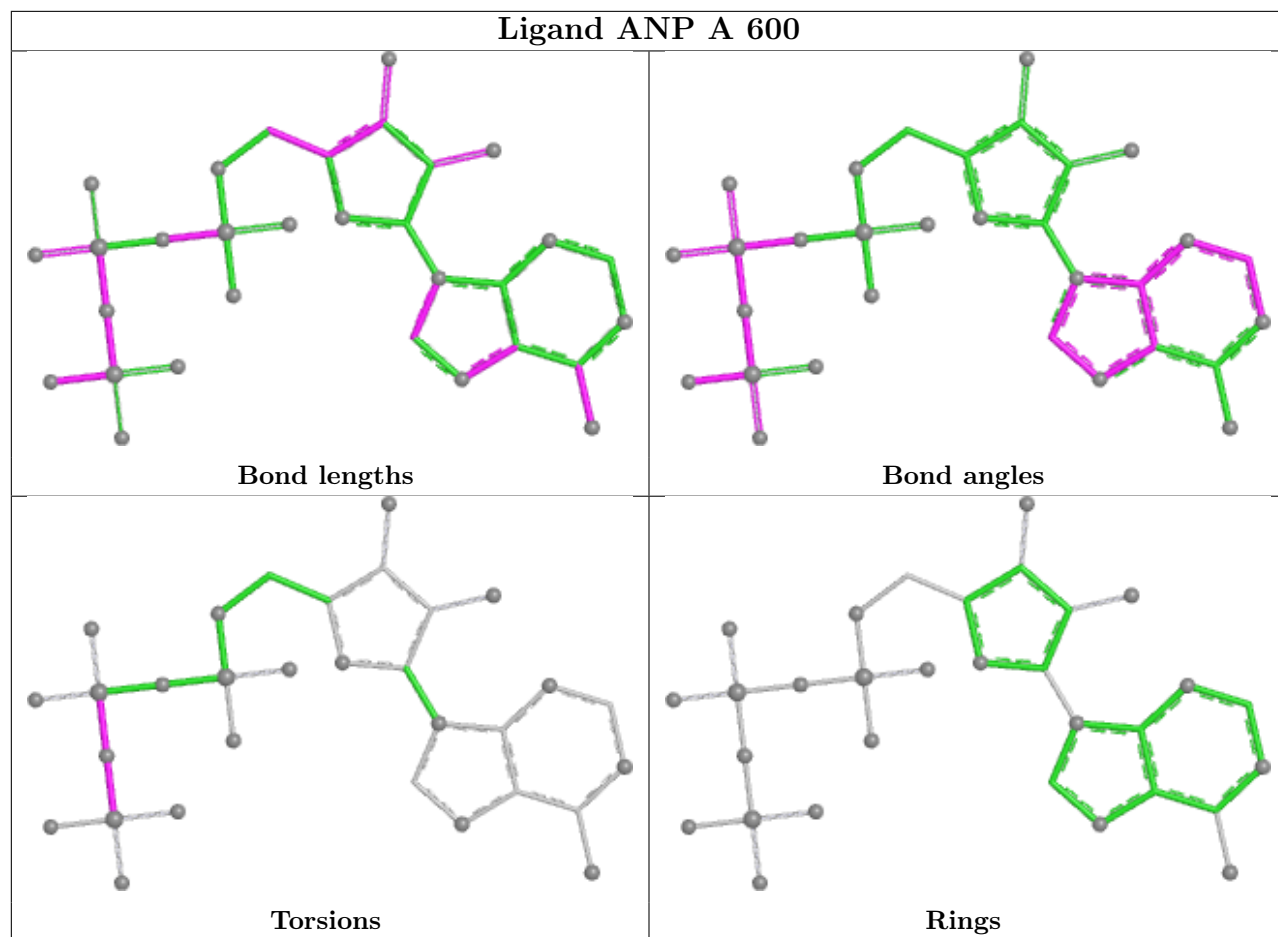


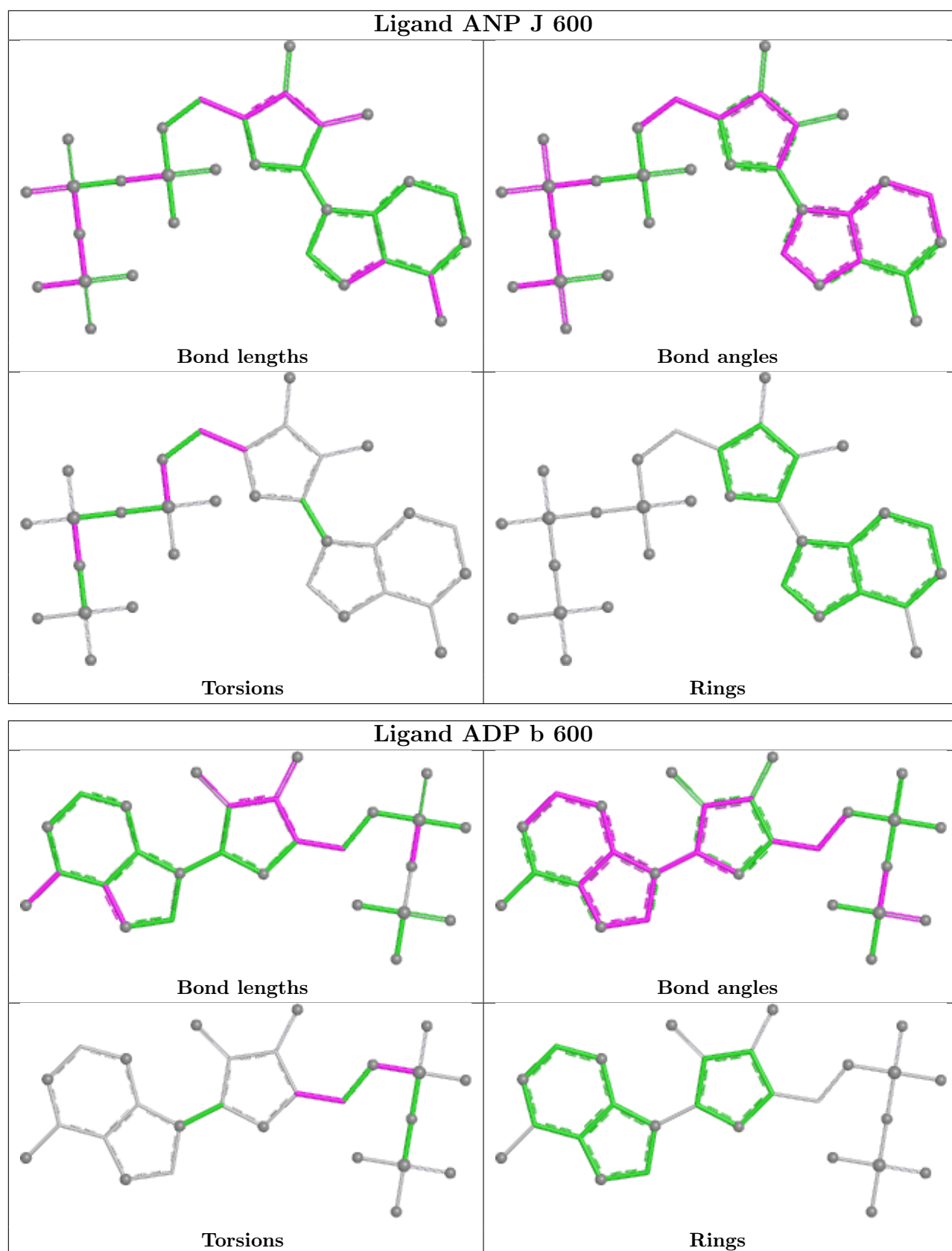


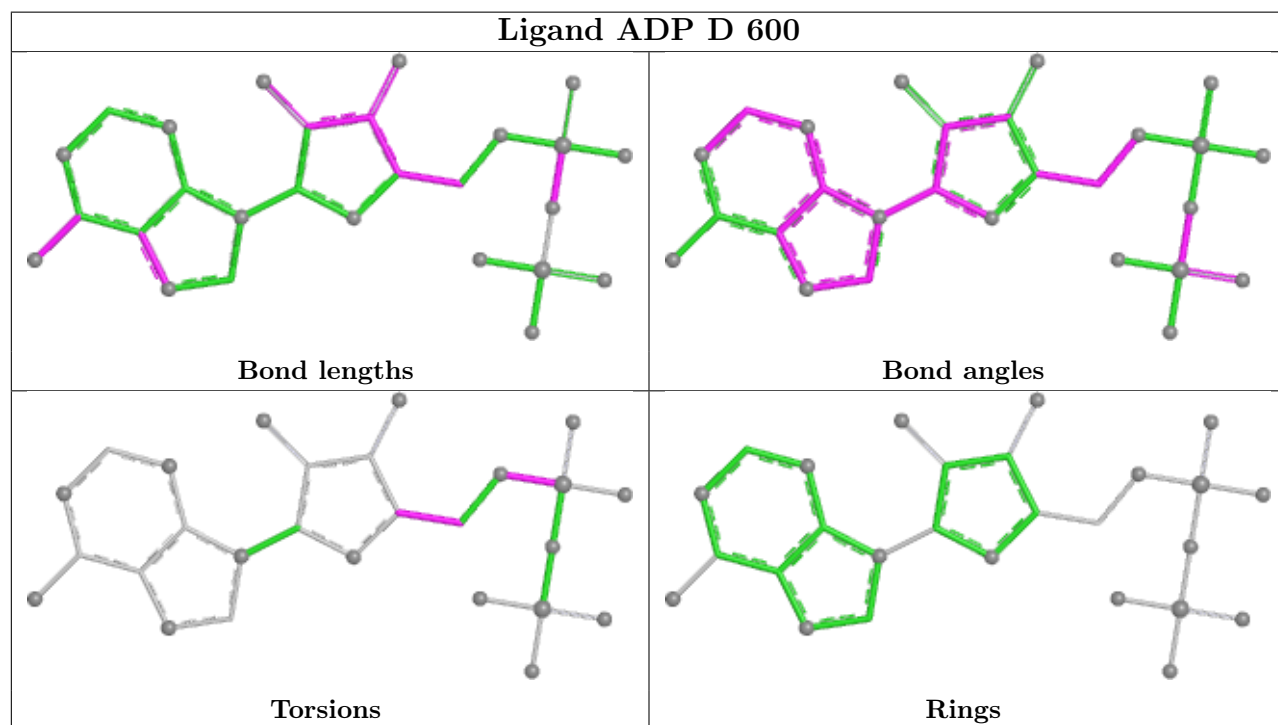
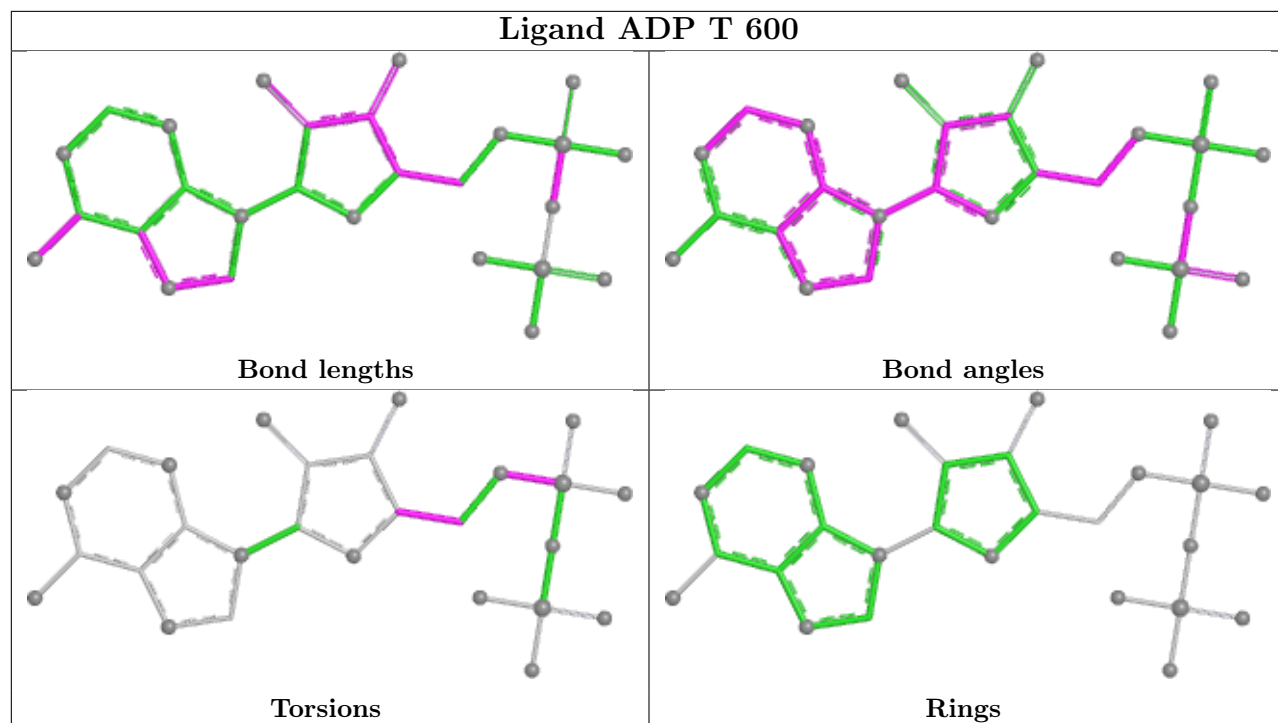


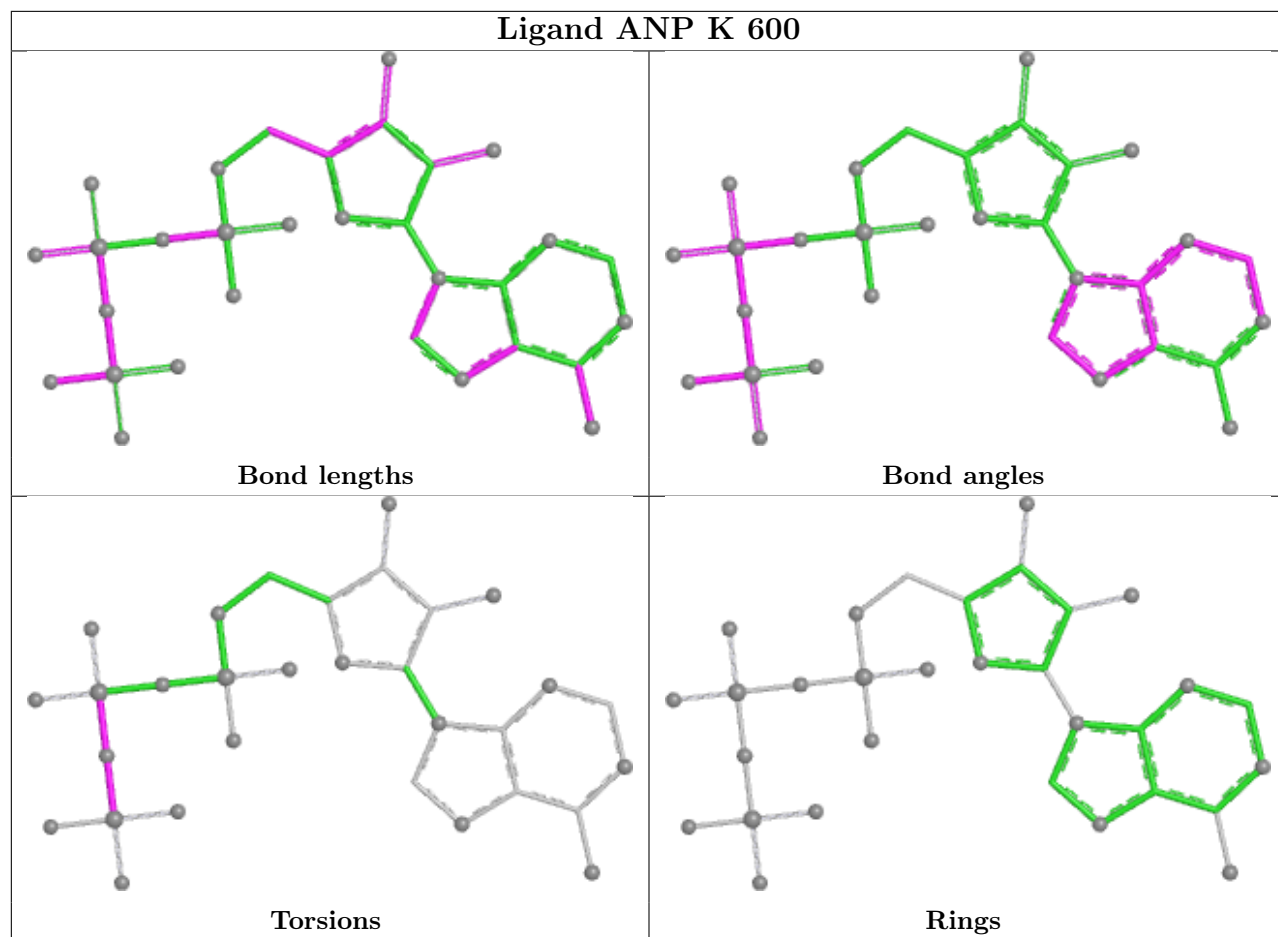


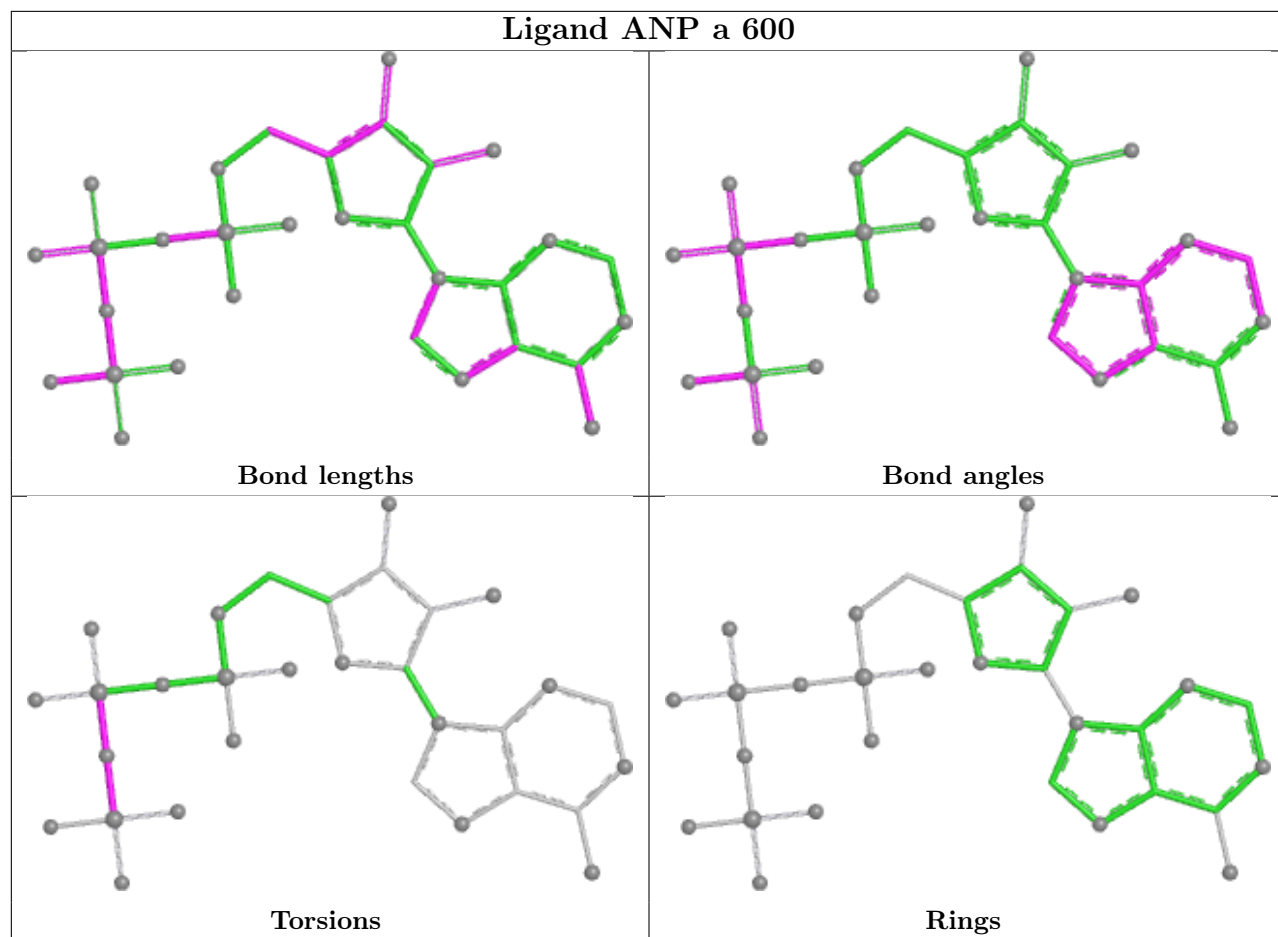


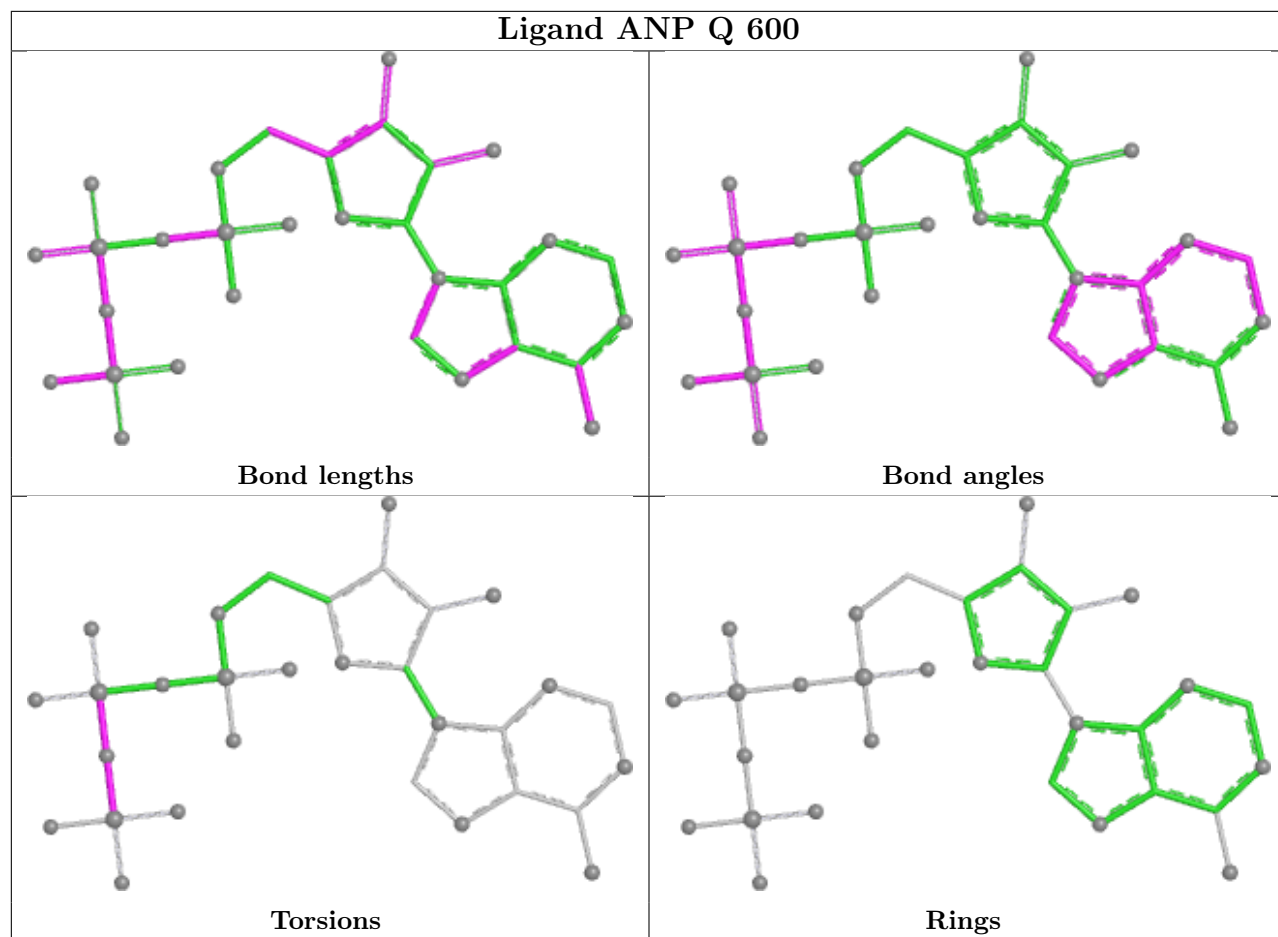


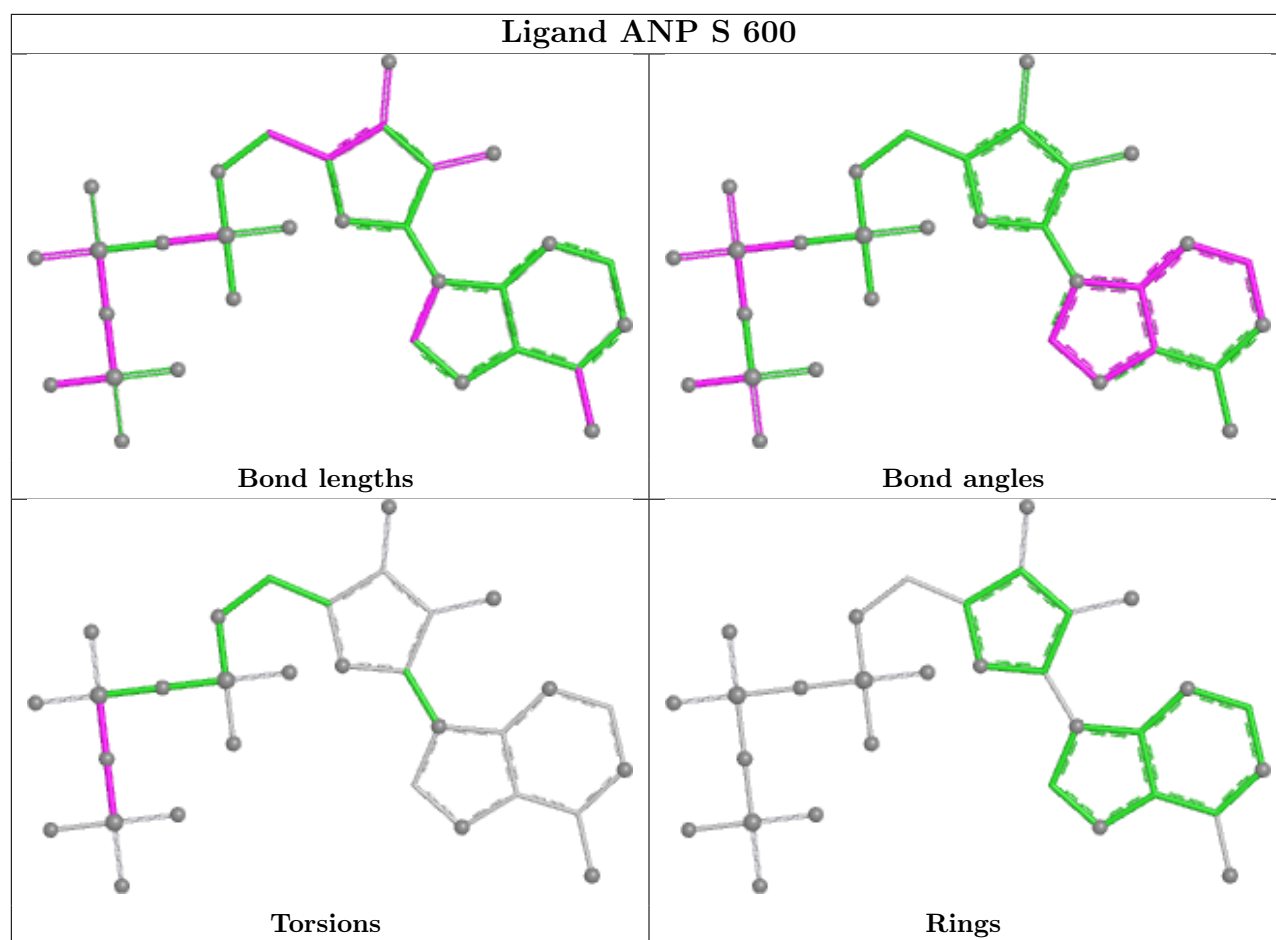












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	488/513 (95%)	-0.31	0 <b>100</b> <b>100</b>	49, 93, 144, 177	0
1	B	486/513 (94%)	-0.18	5 (1%) 79 62	55, 116, 181, 216	0
1	C	487/513 (94%)	-0.24	2 (0%) 88 78	51, 102, 151, 231	0
1	I	488/513 (95%)	-0.18	5 (1%) 79 62	66, 120, 167, 205	0
1	J	486/513 (94%)	-0.13	6 (1%) 76 58	47, 103, 183, 223	0
1	K	487/513 (94%)	-0.20	5 (1%) 79 62	46, 91, 149, 211	0
1	Q	488/513 (95%)	-0.25	1 (0%) 91 85	50, 104, 153, 214	0
1	R	486/513 (94%)	0.08	5 (1%) 79 62	66, 123, 195, 227	0
1	S	487/513 (94%)	-0.05	3 (0%) 85 73	78, 131, 180, 226	0
1	Y	488/513 (95%)	0.02	1 (0%) 91 85	79, 142, 184, 224	0
1	Z	486/513 (94%)	0.26	8 (1%) 70 52	76, 152, 215, 254	0
1	a	487/513 (94%)	0.11	5 (1%) 79 62	89, 146, 200, 249	0
2	D	458/459 (99%)	-0.38	1 (0%) 91 85	44, 92, 142, 186	0
2	E	458/459 (99%)	-0.39	1 (0%) 91 85	53, 102, 152, 184	0
2	F	458/459 (99%)	-0.38	1 (0%) 91 85	41, 103, 158, 216	0
2	L	458/459 (99%)	-0.17	0 <b>100</b> <b>100</b>	46, 111, 167, 217	0
2	M	458/459 (99%)	-0.22	2 (0%) 88 78	55, 114, 161, 219	0
2	N	458/459 (99%)	-0.29	6 (1%) 75 56	33, 73, 131, 186	0
2	T	458/459 (99%)	-0.17	3 (0%) 84 70	73, 124, 181, 229	0
2	U	458/459 (99%)	-0.16	3 (0%) 84 70	54, 102, 170, 232	0
2	V	458/459 (99%)	0.01	8 (1%) 69 50	67, 124, 180, 233	0
2	b	458/459 (99%)	0.27	7 (1%) 72 53	102, 158, 204, 240	0
2	c	458/459 (99%)	-0.04	2 (0%) 88 78	68, 119, 174, 213	0
2	d	458/459 (99%)	0.12	4 (0%) 81 65	92, 151, 200, 243	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	G	284/286 (99%)	-0.49	0 100 100	29, 54, 137, 200	0
3	O	284/286 (99%)	-0.40	1 (0%) 88 78	26, 57, 140, 209	0
3	W	284/286 (99%)	-0.15	1 (0%) 88 78	51, 116, 192, 232	0
3	e	284/286 (99%)	-0.02	0 100 100	84, 142, 205, 230	0
4	H	138/138 (100%)	-0.47	0 100 100	35, 72, 120, 144	0
4	P	138/138 (100%)	-0.36	0 100 100	43, 71, 129, 156	0
4	X	138/138 (100%)	-0.14	0 100 100	77, 136, 175, 227	0
4	f	138/138 (100%)	-0.04	1 (0%) 84 70	94, 151, 198, 217	0
All	All	13028/13360 (97%)	-0.14	87 (0%) 84 70	26, 116, 183, 254	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	101	ILE	4.4
1	R	460	GLU	4.4
2	b	284	SER	4.1
2	V	101	ILE	3.7
2	d	207	GLY	3.4

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	SO4	c	530	5/5	0.58	0.15	113,113,115,116	0
6	MG	B	601	1/1	0.69	0.08	125,125,125,125	0

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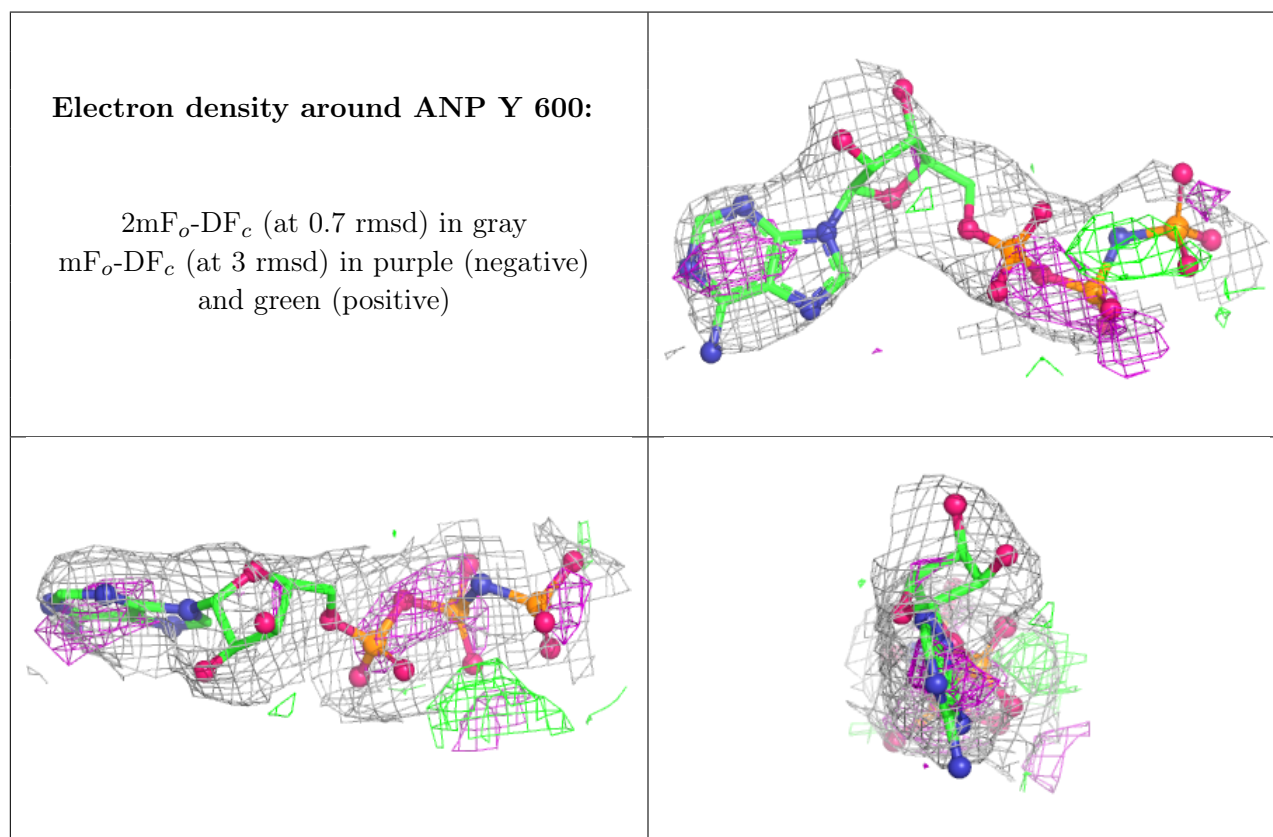
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	SO4	W	300	5/5	0.76	0.25	207,210,212,214	0
8	SO4	U	530	5/5	0.77	0.11	106,106,107,107	0
8	SO4	M	530	5/5	0.78	0.13	117,118,119,119	0
6	MG	Z	601	1/1	0.80	0.08	147,147,147,147	0
5	ANP	Y	600	31/31	0.82	0.10	87,93,109,129	0
8	SO4	E	530	5/5	0.82	0.14	109,109,109,110	0
6	MG	Q	601	1/1	0.83	0.12	64,64,64,64	0
5	ANP	Z	600	31/31	0.84	0.10	147,151,153,154	0
6	MG	R	601	1/1	0.84	0.08	118,118,118,118	0
6	MG	A	601	1/1	0.86	0.12	64,64,64,64	0
8	SO4	d	530	5/5	0.86	0.12	107,108,108,109	0
5	ANP	A	600	31/31	0.87	0.12	87,93,109,129	0
6	MG	I	601	1/1	0.88	0.09	64,64,64,64	0
5	ANP	Q	600	31/31	0.88	0.12	87,93,109,129	0
8	SO4	G	300	5/5	0.89	0.21	95,101,102,103	0
8	SO4	O	300	5/5	0.89	0.27	109,115,118,119	0
6	MG	Y	601	1/1	0.90	0.08	64,64,64,64	0
6	MG	J	601	1/1	0.90	0.06	122,122,122,122	0
6	MG	a	601	1/1	0.90	0.06	83,83,83,83	0
8	SO4	V	530	5/5	0.90	0.07	82,83,85,87	0
5	ANP	S	600	31/31	0.90	0.10	109,114,121,135	0
5	ANP	I	600	31/31	0.90	0.09	87,93,109,129	0
8	SO4	H	200	5/5	0.90	0.16	114,115,117,119	0
5	ANP	a	600	31/31	0.91	0.09	123,126,130,136	0
5	ANP	R	600	31/31	0.92	0.09	91,101,110,112	0
5	ANP	C	600	31/31	0.92	0.09	87,93,109,129	0
8	SO4	b	630	5/5	0.92	0.08	98,99,100,101	0
8	SO4	P	200	5/5	0.92	0.18	120,120,123,124	0
7	ADP	b	600	27/27	0.92	0.07	136,139,142,143	0
8	SO4	F	530	5/5	0.93	0.08	79,81,82,82	0
7	ADP	T	600	27/27	0.93	0.07	114,118,121,123	0
7	ADP	L	600	27/27	0.94	0.07	77,86,95,98	0
5	ANP	B	600	31/31	0.94	0.08	96,107,111,112	0
8	SO4	T	630	5/5	0.94	0.07	85,88,88,89	0
6	MG	L	601	1/1	0.95	0.04	66,66,66,66	0
6	MG	T	601	1/1	0.95	0.05	80,80,80,80	0
8	SO4	N	530	5/5	0.95	0.07	64,64,67,67	0
6	MG	b	601	1/1	0.95	0.08	127,127,127,127	0
7	ADP	D	600	27/27	0.95	0.06	75,81,87,90	0
5	ANP	J	600	31/31	0.95	0.08	83,96,100,103	0
5	ANP	K	600	31/31	0.96	0.08	63,81,109,131	0
6	MG	C	601	1/1	0.96	0.05	64,64,64,64	0

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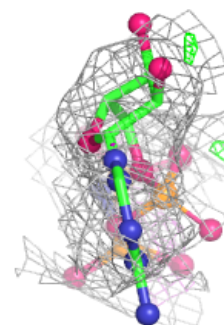
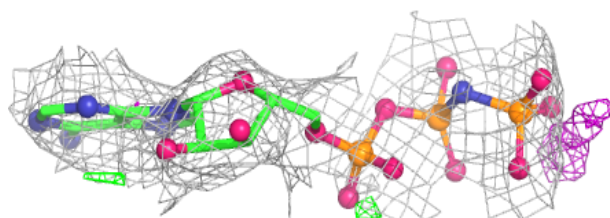
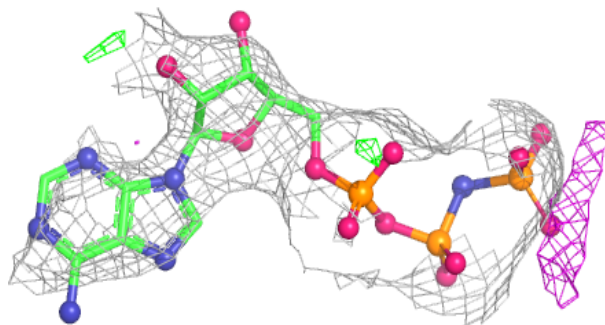
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SO4	D	630	5/5	0.96	0.05	72,74,75,77	0
6	MG	S	601	1/1	0.97	0.04	60,60,60,60	0
8	SO4	L	630	5/5	0.98	0.06	81,83,84,85	0
6	MG	K	601	1/1	0.98	0.05	44,44,44,44	0
6	MG	D	601	1/1	0.99	0.06	51,51,51,51	0

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.

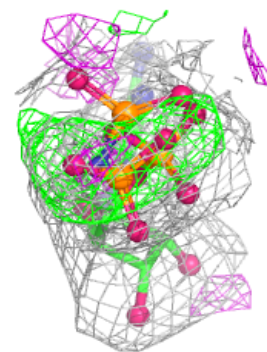
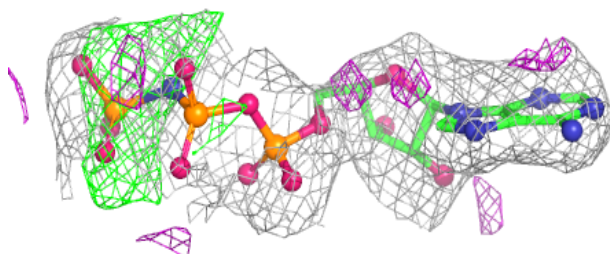
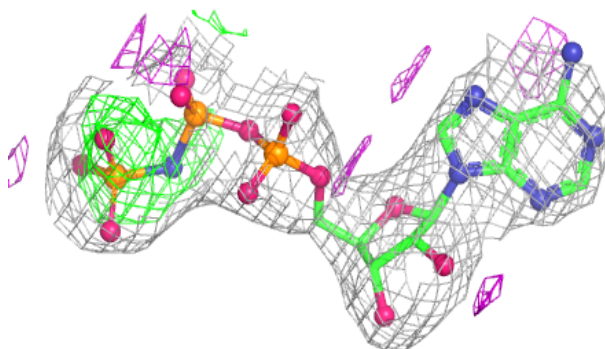


**Electron density around ANP Z 600:**

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

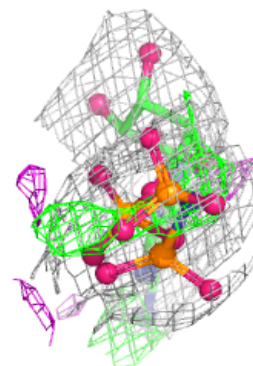
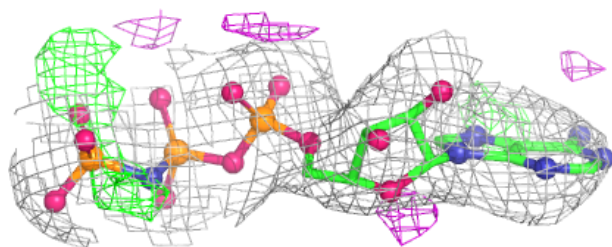
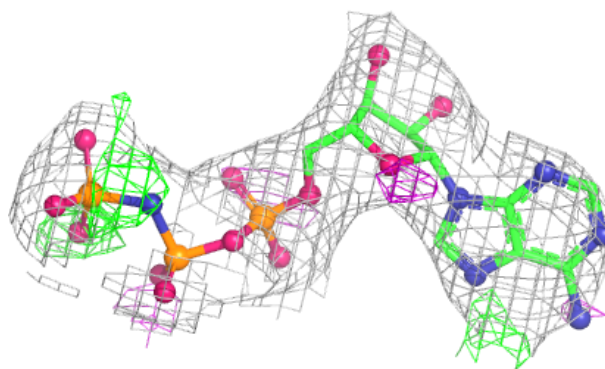
**Electron density around ANP A 600:**

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

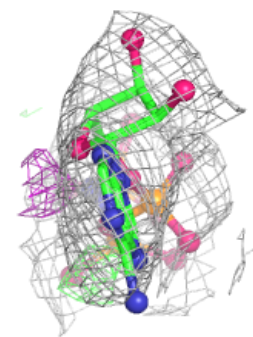
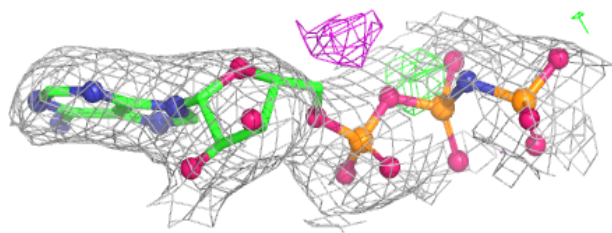
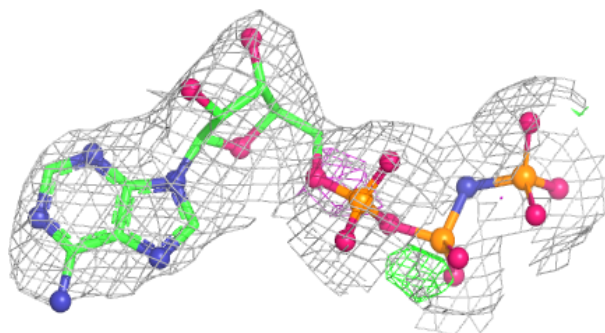


**Electron density around ANP Q 600:**

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

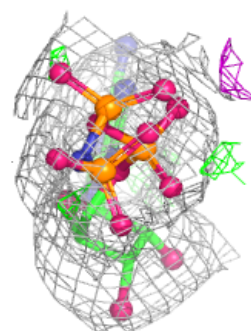
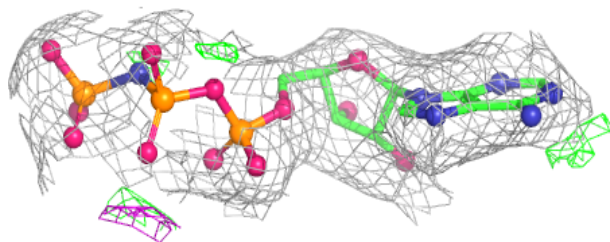
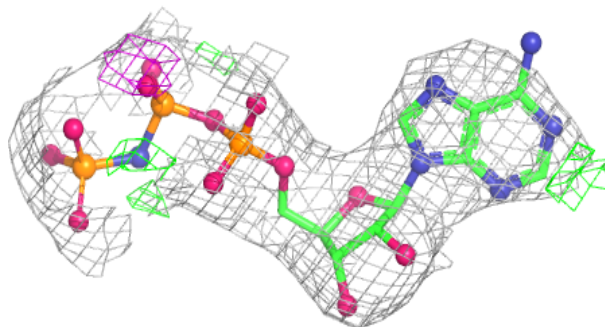
**Electron density around ANP S 600:**

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

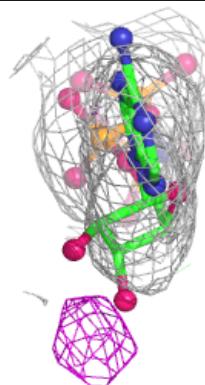
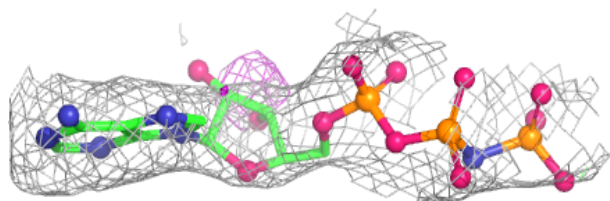
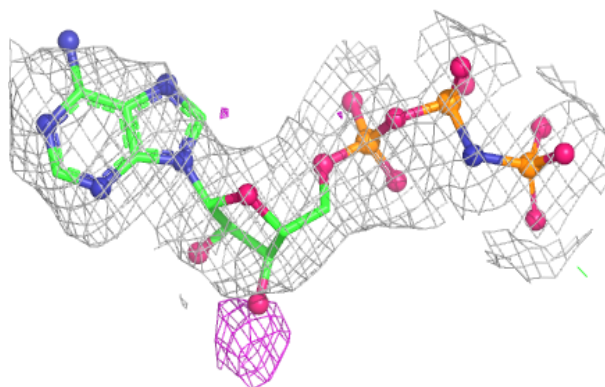


**Electron density around ANP I 600:**

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

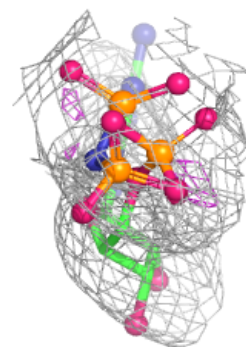
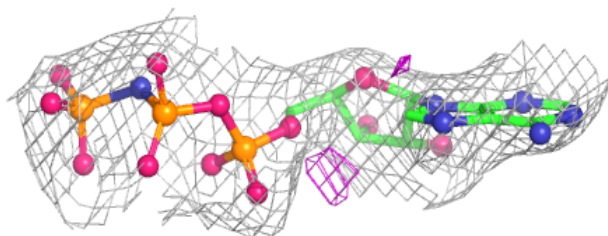
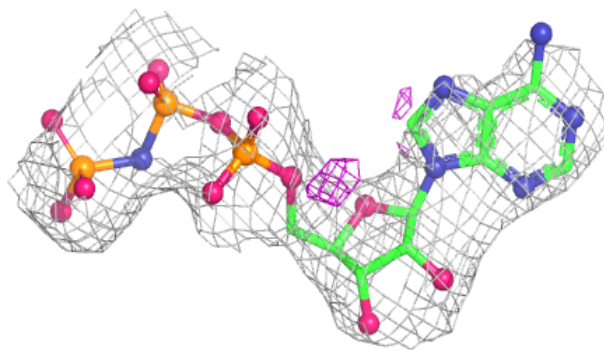
**Electron density around ANP a 600:**

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and green (positive)

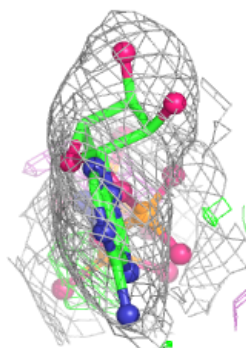
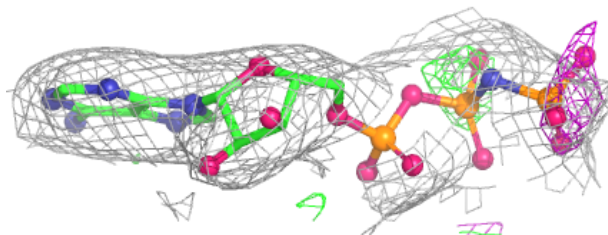
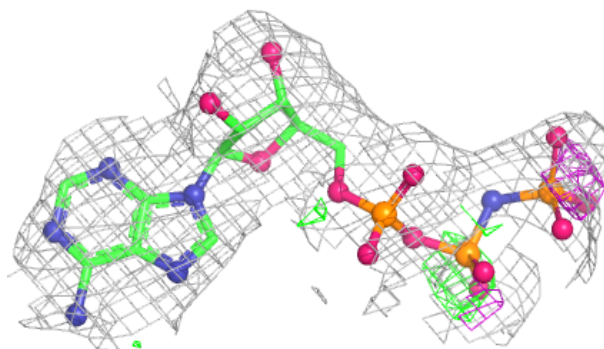


**Electron density around ANP R 600:**

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

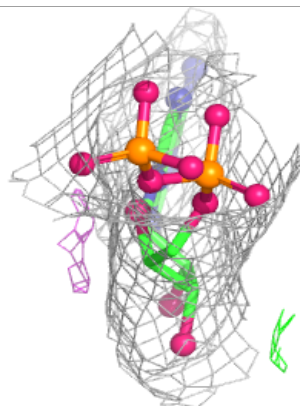
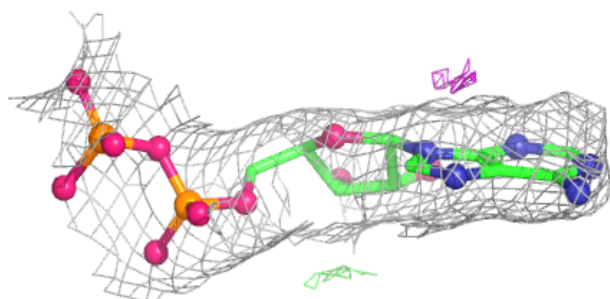
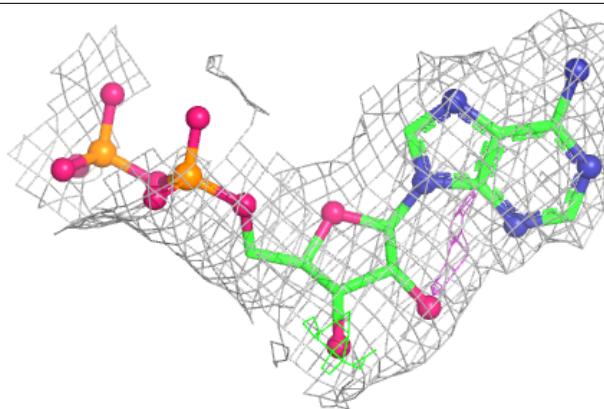
**Electron density around ANP C 600:**

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

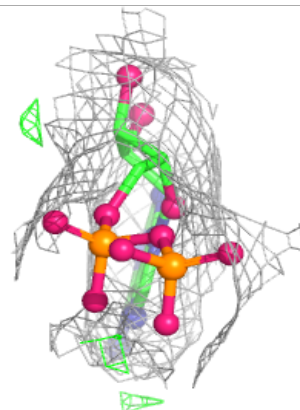
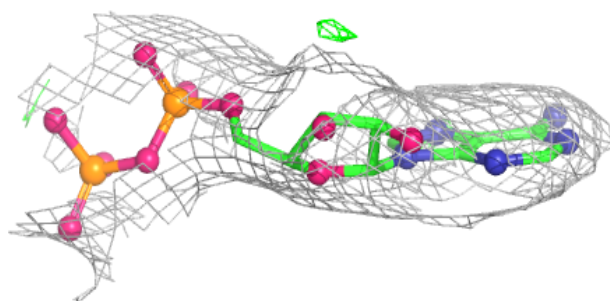
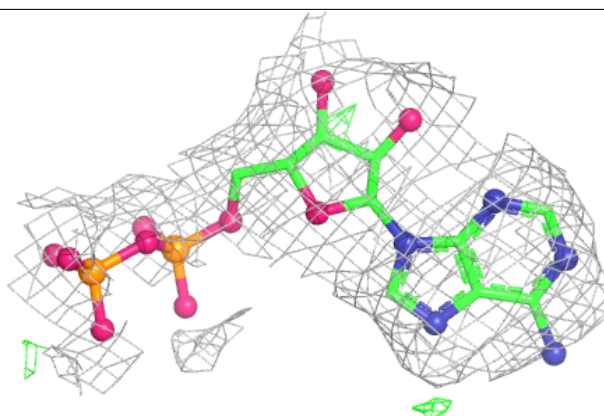


**Electron density around ADP b 600:**

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

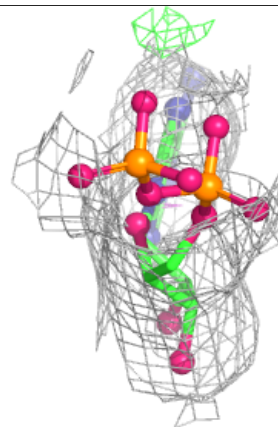
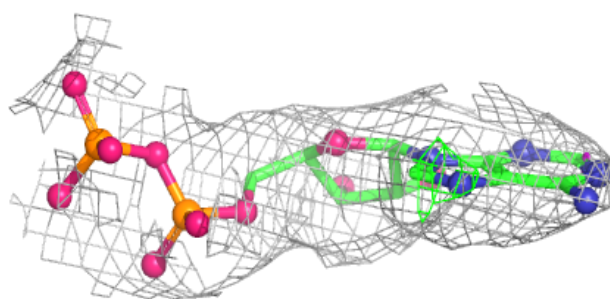
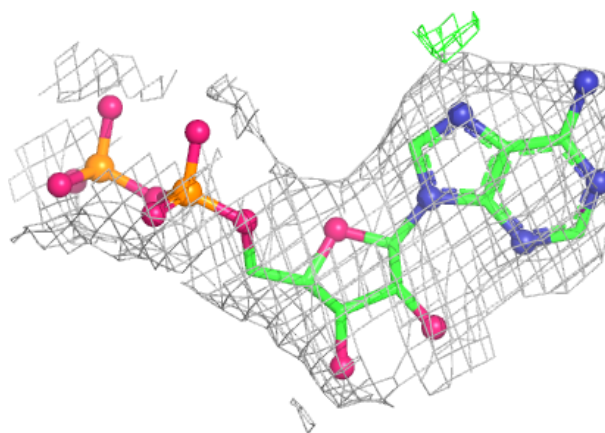
**Electron density around ADP T 600:**

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

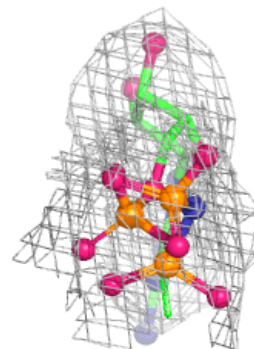
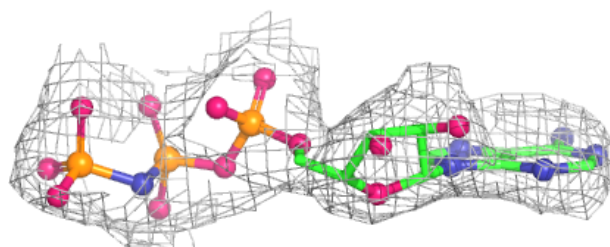
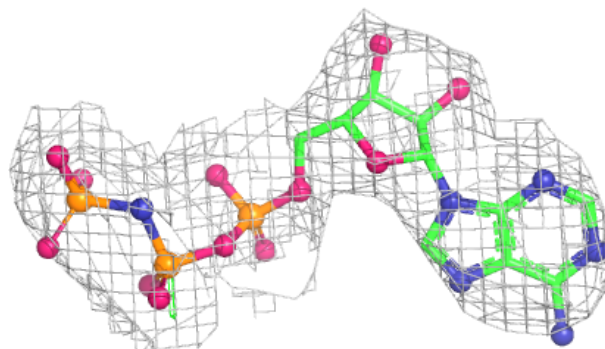


**Electron density around ADP L 600:**

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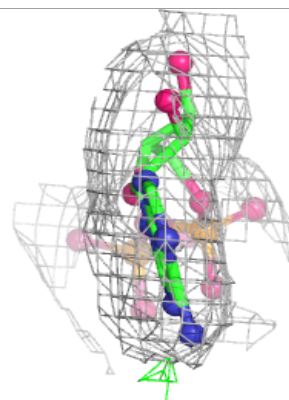
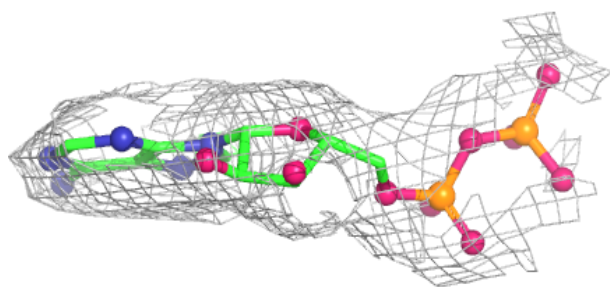
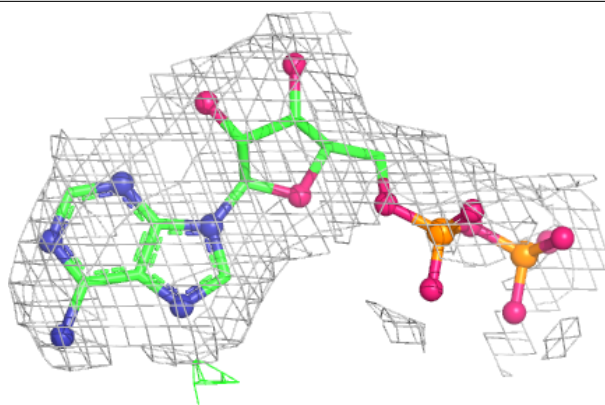
**Electron density around ANP B 600:**

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

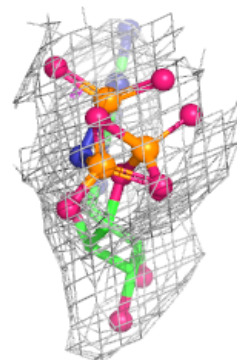
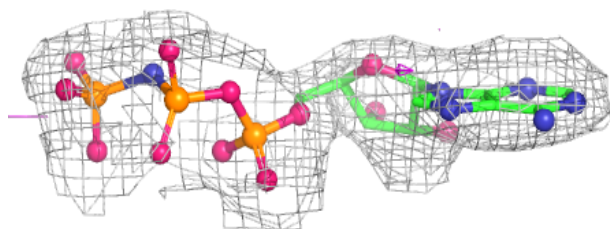
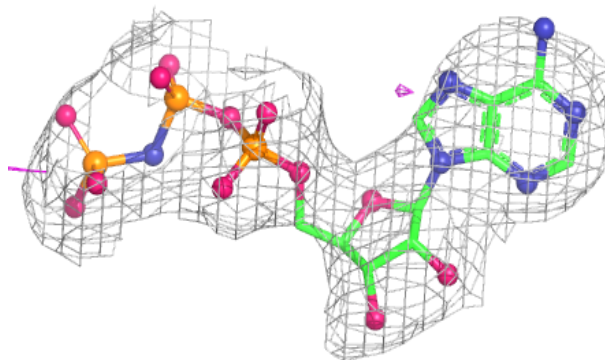


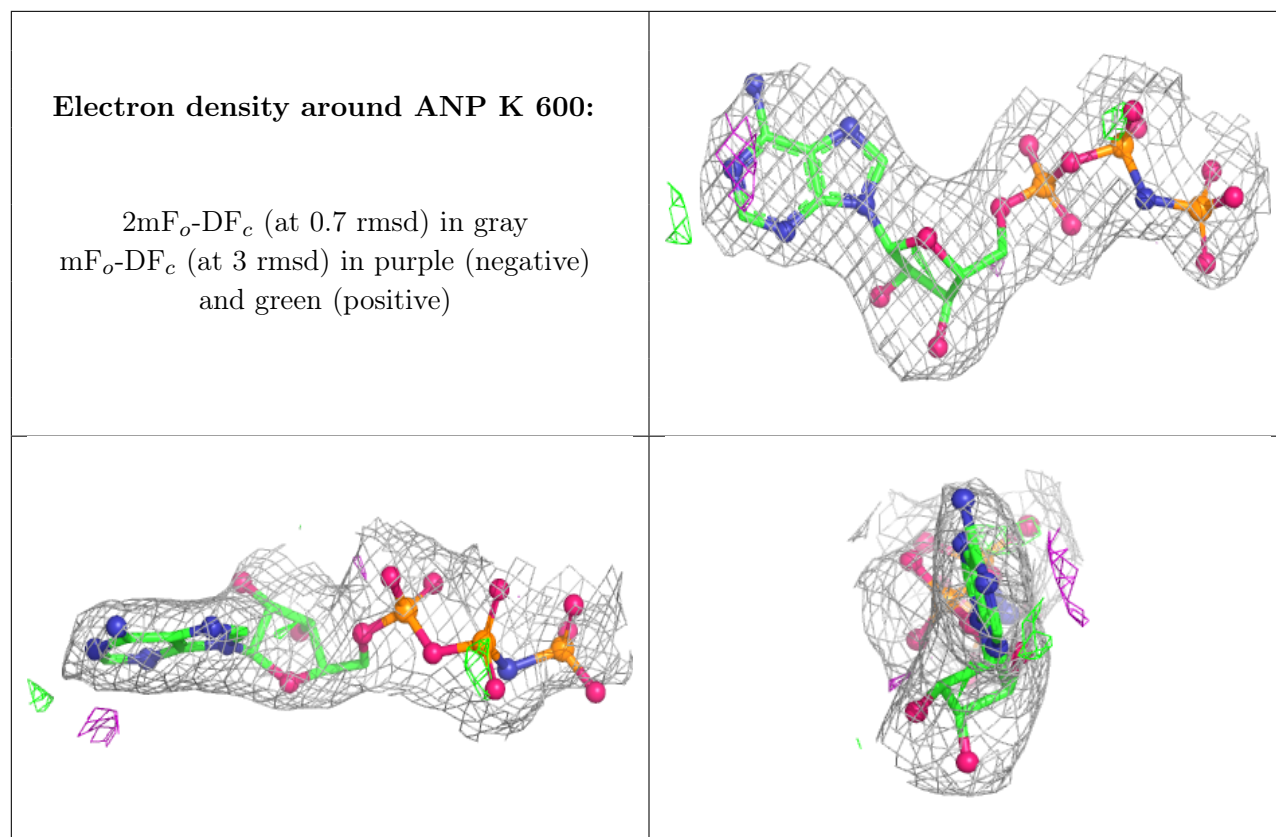
**Electron density around ADP D 600:**

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

**Electron density around ANP J 600:**

$2mF_o-DF_c$  (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.