



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 07:06 PM UTC

PDB ID : 3OEE / pdb_00003oe
Title : Structure of four mutant forms of yeast F1 ATPase: alpha-F405S
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.
Deposited on : 2010-08-12
Resolution : 2.74 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

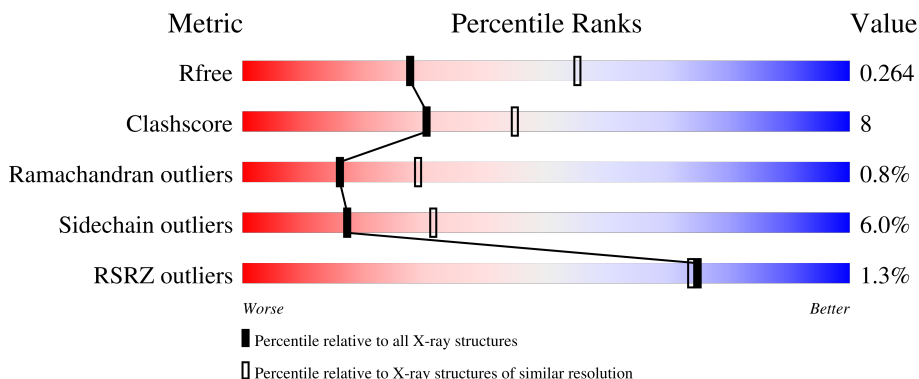
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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

Mol	Chain	Length	Quality of chain
1	A	510	 75% 18% • 5%
1	B	510	 75% 19% • 5%
1	C	510	 75% 18% • 5%
1	J	510	 % 76% 18% • 6%
1	K	510	 73% 21% •• 5%

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Mol	Chain	Length	Quality of chain
1	L	510	74% 18% • 5%
1	S	510	66% 26% • 6%
1	T	510	72% 21% • 6%
1	U	510	64% 27% • 6%
2	D	484	75% 21% • •
2	E	484	76% 17% • •
2	F	484	77% 17% • •
2	M	484	73% 23% • •
2	N	484	73% 23% • •
2	O	484	79% 17% • •
2	V	484	74% 22% • •
2	W	484	74% 20% • •
2	X	484	73% 22% • •
3	G	278	68% 24% • • •
3	P	278	60% 25% • 12%
3	Y	278	58% 13% • 28%
4	H	138	61% 25% • 12%
4	Q	138	54% 5% • 40%
4	Z	138	12% • 88%
5	I	61	66% 11% • 20%
5	R	61	56% 44%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 72675 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	482	Total 3659	C 2308	N 648	O 700	S 3	0	0	0
1	B	483	Total 3664	C 2311	N 649	O 701	S 3	0	0	0
1	C	484	Total 3675	C 2319	N 650	O 703	S 3	0	0	0
1	J	481	Total 3650	C 2303	N 646	O 698	S 3	0	0	0
1	K	486	Total 3679	C 2320	N 652	O 704	S 3	0	0	0
1	L	482	Total 3659	C 2308	N 648	O 700	S 3	0	0	0
1	S	477	Total 3622	C 2287	N 642	O 690	S 3	0	0	0
1	T	478	Total 3632	C 2293	N 643	O 693	S 3	0	0	0
1	U	481	Total 3650	C 2302	N 646	O 699	S 3	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	405	SER	PHE	engineered mutation	UNP P07251
B	405	SER	PHE	engineered mutation	UNP P07251
C	405	SER	PHE	engineered mutation	UNP P07251
J	405	SER	PHE	engineered mutation	UNP P07251
K	405	SER	PHE	engineered mutation	UNP P07251
L	405	SER	PHE	engineered mutation	UNP P07251
S	405	SER	PHE	engineered mutation	UNP P07251
T	405	SER	PHE	engineered mutation	UNP P07251
U	405	SER	PHE	engineered mutation	UNP P07251

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3545	2248	603	688	6			
2	E	468	Total	C	N	O	S	0	0	0
			3504	2223	598	677	6			
2	F	469	Total	C	N	O	S	0	0	0
			3527	2238	602	681	6			
2	M	470	Total	C	N	O	S	0	0	0
			3535	2243	600	686	6			
2	N	470	Total	C	N	O	S	0	0	0
			3541	2245	602	688	6			
2	O	468	Total	C	N	O	S	0	0	0
			3534	2242	602	684	6			
2	V	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	W	467	Total	C	N	O	S	0	0	0
			3531	2240	601	684	6			
2	X	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	ALA	-	expression tag	UNP P00830
D	-4	SER	-	expression tag	UNP P00830
D	-3	HIS	-	expression tag	UNP P00830
D	-2	HIS	-	expression tag	UNP P00830
D	-1	HIS	-	expression tag	UNP P00830
D	0	HIS	-	expression tag	UNP P00830
D	1	HIS	-	expression tag	UNP P00830
D	2	HIS	-	expression tag	UNP P00830
E	-5	ALA	-	expression tag	UNP P00830
E	-4	SER	-	expression tag	UNP P00830
E	-3	HIS	-	expression tag	UNP P00830
E	-2	HIS	-	expression tag	UNP P00830
E	-1	HIS	-	expression tag	UNP P00830
E	0	HIS	-	expression tag	UNP P00830
E	1	HIS	-	expression tag	UNP P00830
E	2	HIS	-	expression tag	UNP P00830
F	-5	ALA	-	expression tag	UNP P00830
F	-4	SER	-	expression tag	UNP P00830
F	-3	HIS	-	expression tag	UNP P00830
F	-2	HIS	-	expression tag	UNP P00830
F	-1	HIS	-	expression tag	UNP P00830
F	0	HIS	-	expression tag	UNP P00830

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	HIS	-	expression tag	UNP P00830
F	2	HIS	-	expression tag	UNP P00830
M	-5	ALA	-	expression tag	UNP P00830
M	-4	SER	-	expression tag	UNP P00830
M	-3	HIS	-	expression tag	UNP P00830
M	-2	HIS	-	expression tag	UNP P00830
M	-1	HIS	-	expression tag	UNP P00830
M	0	HIS	-	expression tag	UNP P00830
M	1	HIS	-	expression tag	UNP P00830
M	2	HIS	-	expression tag	UNP P00830
N	-5	ALA	-	expression tag	UNP P00830
N	-4	SER	-	expression tag	UNP P00830
N	-3	HIS	-	expression tag	UNP P00830
N	-2	HIS	-	expression tag	UNP P00830
N	-1	HIS	-	expression tag	UNP P00830
N	0	HIS	-	expression tag	UNP P00830
N	1	HIS	-	expression tag	UNP P00830
N	2	HIS	-	expression tag	UNP P00830
O	-5	ALA	-	expression tag	UNP P00830
O	-4	SER	-	expression tag	UNP P00830
O	-3	HIS	-	expression tag	UNP P00830
O	-2	HIS	-	expression tag	UNP P00830
O	-1	HIS	-	expression tag	UNP P00830
O	0	HIS	-	expression tag	UNP P00830
O	1	HIS	-	expression tag	UNP P00830
O	2	HIS	-	expression tag	UNP P00830
V	-5	ALA	-	expression tag	UNP P00830
V	-4	SER	-	expression tag	UNP P00830
V	-3	HIS	-	expression tag	UNP P00830
V	-2	HIS	-	expression tag	UNP P00830
V	-1	HIS	-	expression tag	UNP P00830
V	0	HIS	-	expression tag	UNP P00830
V	1	HIS	-	expression tag	UNP P00830
V	2	HIS	-	expression tag	UNP P00830
W	-5	ALA	-	expression tag	UNP P00830
W	-4	SER	-	expression tag	UNP P00830
W	-3	HIS	-	expression tag	UNP P00830
W	-2	HIS	-	expression tag	UNP P00830
W	-1	HIS	-	expression tag	UNP P00830
W	0	HIS	-	expression tag	UNP P00830
W	1	HIS	-	expression tag	UNP P00830
W	2	HIS	-	expression tag	UNP P00830

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-5	ALA	-	expression tag	UNP P00830
X	-4	SER	-	expression tag	UNP P00830
X	-3	HIS	-	expression tag	UNP P00830
X	-2	HIS	-	expression tag	UNP P00830
X	-1	HIS	-	expression tag	UNP P00830
X	0	HIS	-	expression tag	UNP P00830
X	1	HIS	-	expression tag	UNP P00830
X	2	HIS	-	expression tag	UNP P00830

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	266	Total	C	N	O	S	0	0	0
			2055	1291	359	395	10			
3	P	244	Total	C	N	O	S	0	0	0
			1850	1162	323	356	9			
3	Y	200	Total	C	N	O	S	0	0	0
			1517	944	273	291	9			

- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	122	Total	C	N	O	S	0	0	0
			795	497	138	158	2			
4	Q	83	Total	C	N	O		0	0	0
			441	267	88	86				
4	Z	17	Total	C	N	O		0	0	0
			85	51	17	17				

- Molecule 5 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	49	Total	C	N	O	0	0	0
			339	212	57	70			
5	R	34	Total	C	N	O	0	0	0
			175	104	34	37			
5	1	27	Total	C	N	O	0	0	0
			145	86	31	28			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

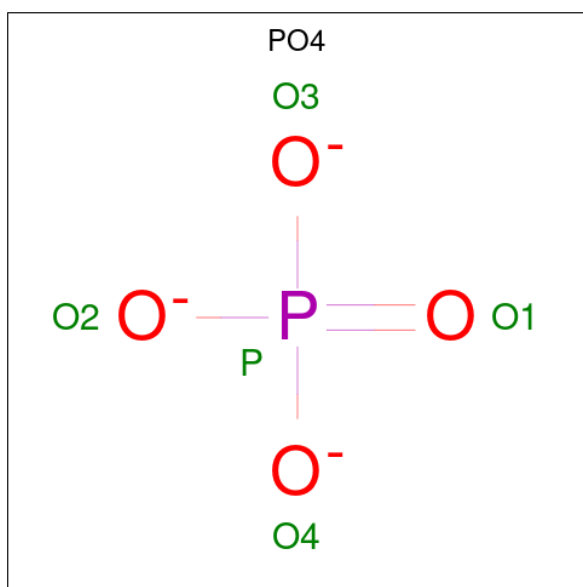
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	X	1	31	10	6	12	3	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Mg 1	0	0
7	B	1	Total 1	Mg 1	0	0
7	C	1	Total 1	Mg 1	0	0
7	D	1	Total 1	Mg 1	0	0
7	F	1	Total 1	Mg 1	0	0
7	J	1	Total 1	Mg 1	0	0
7	K	1	Total 1	Mg 1	0	0
7	L	1	Total 1	Mg 1	0	0
7	M	1	Total 1	Mg 1	0	0
7	O	1	Total 1	Mg 1	0	0
7	S	1	Total 1	Mg 1	0	0
7	T	1	Total 1	Mg 1	0	0
7	U	1	Total 1	Mg 1	0	0
7	V	1	Total 1	Mg 1	0	0
7	X	1	Total 1	Mg 1	0	0

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	O	P	0	0
			5	4	1		
8	N	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	10	Total	O	0	0
			10	10		
9	B	9	Total	O	0	0
			9	9		
9	C	3	Total	O	0	0
			3	3		
9	D	11	Total	O	0	0
			11	11		
9	E	10	Total	O	0	0
			10	10		
9	F	8	Total	O	0	0
			8	8		
9	G	2	Total	O	0	0
			2	2		
9	J	3	Total	O	0	0
			3	3		
9	K	5	Total	O	0	0
			5	5		
9	L	8	Total	O	0	0
			8	8		

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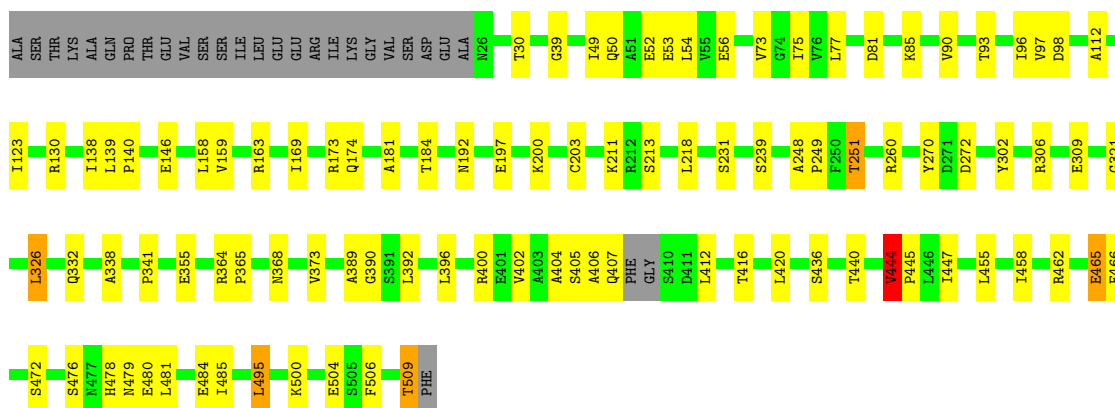
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9	M	4	Total O 4 4	0	0
9	N	3	Total O 3 3	0	0
9	O	5	Total O 5 5	0	0
9	P	2	Total O 2 2	0	0
9	X	1	Total O 1 1	0	0

3 Residue-property plots

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

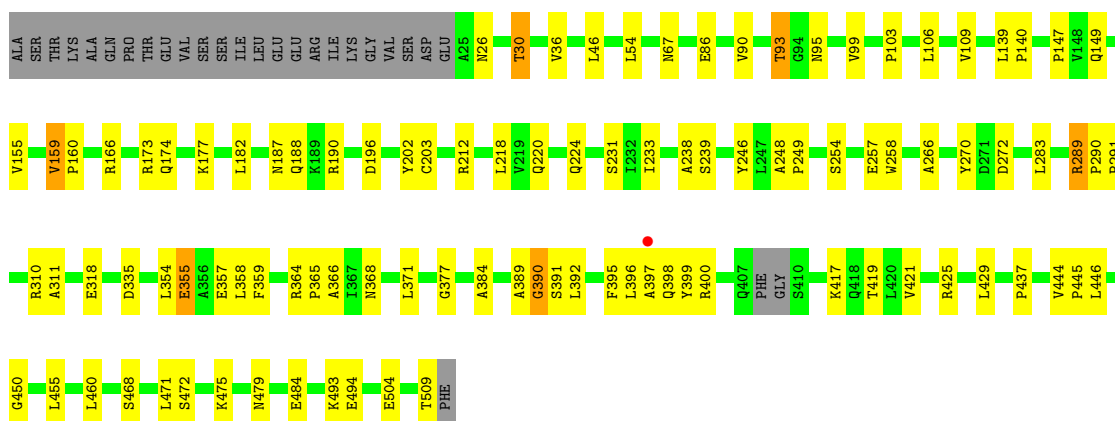
- Molecule 1: ATP synthase subunit alpha

Chain A: 



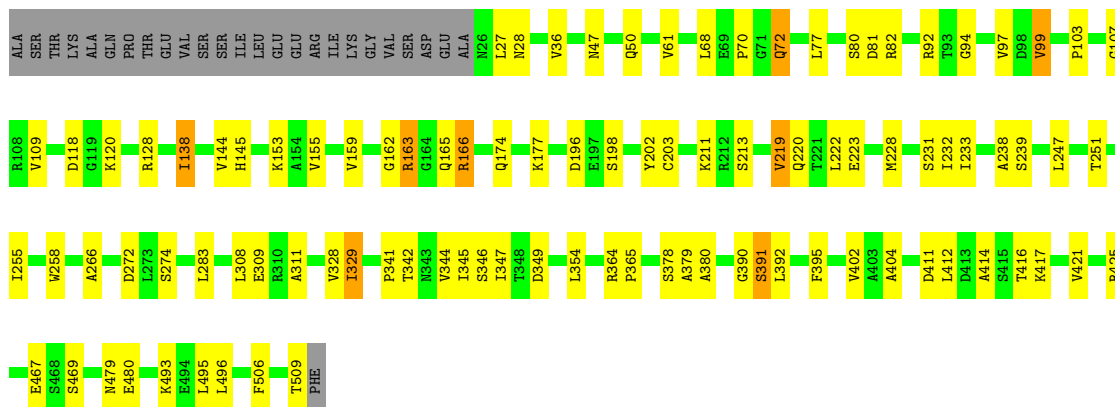
- Molecule 1: ATP synthase subunit alpha

Chain B: 

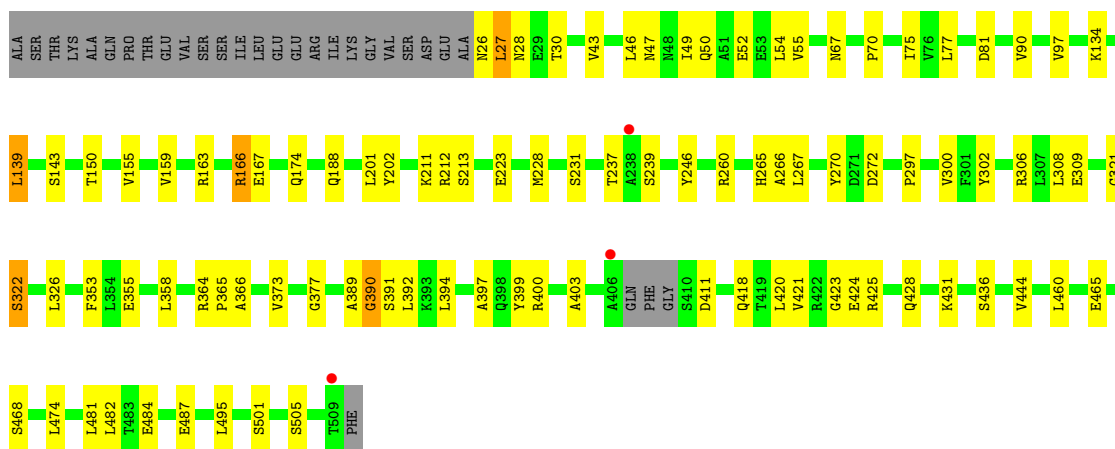
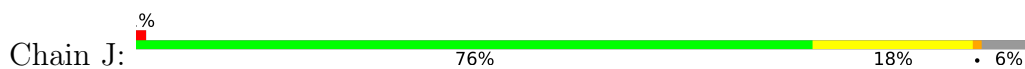


- Molecule 1: ATP synthase subunit alpha

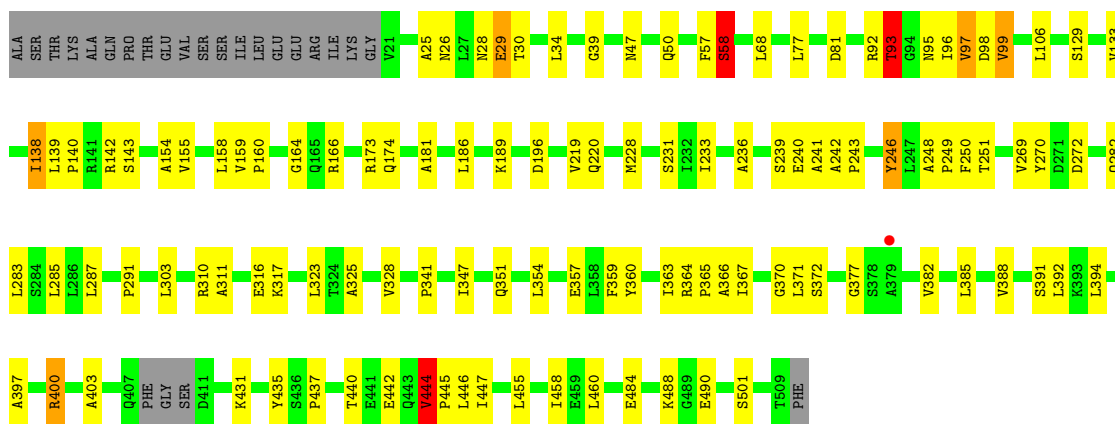
Chain C: 



• Molecule 1: ATP synthase subunit alpha

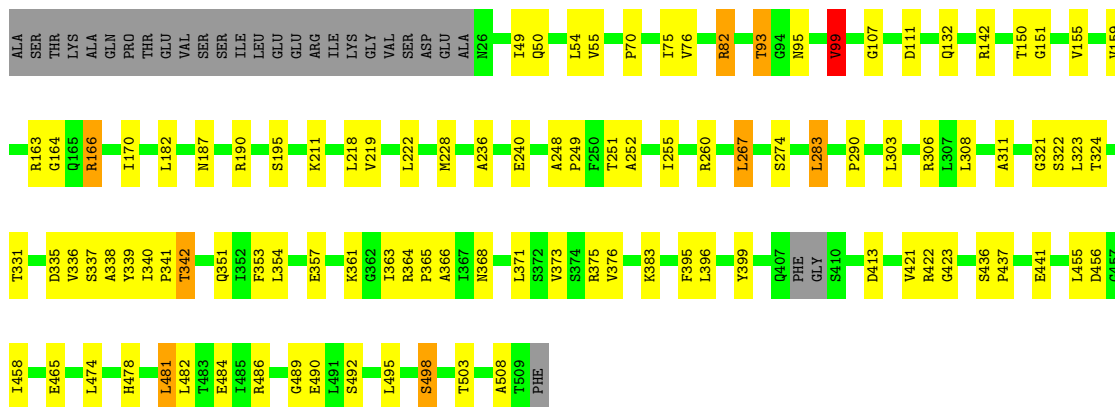


• Molecule 1: ATP synthase subunit alpha

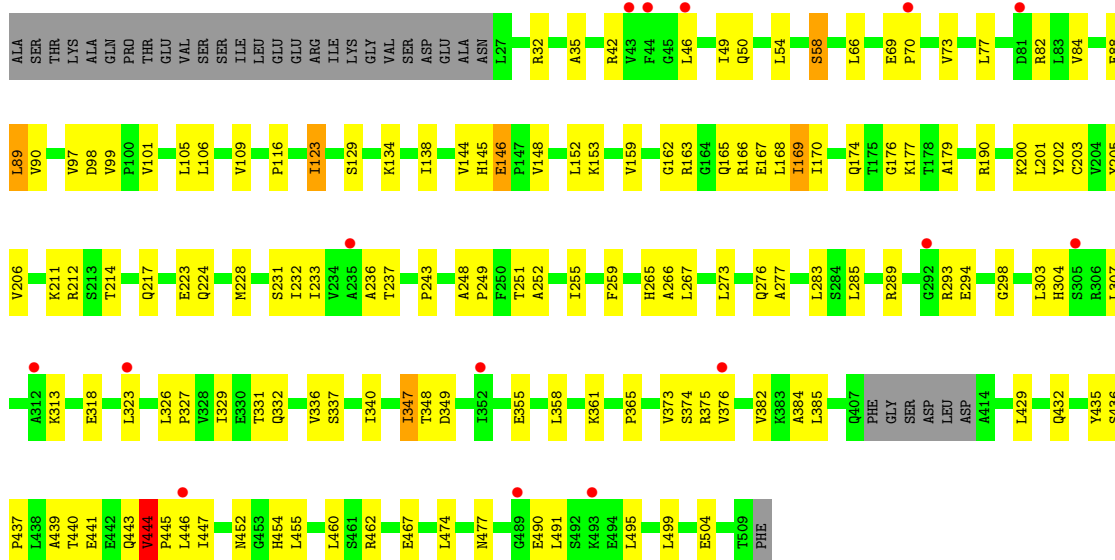


• Molecule 1: ATP synthase subunit alpha





● Molecule 1: ATP synthase subunit alpha

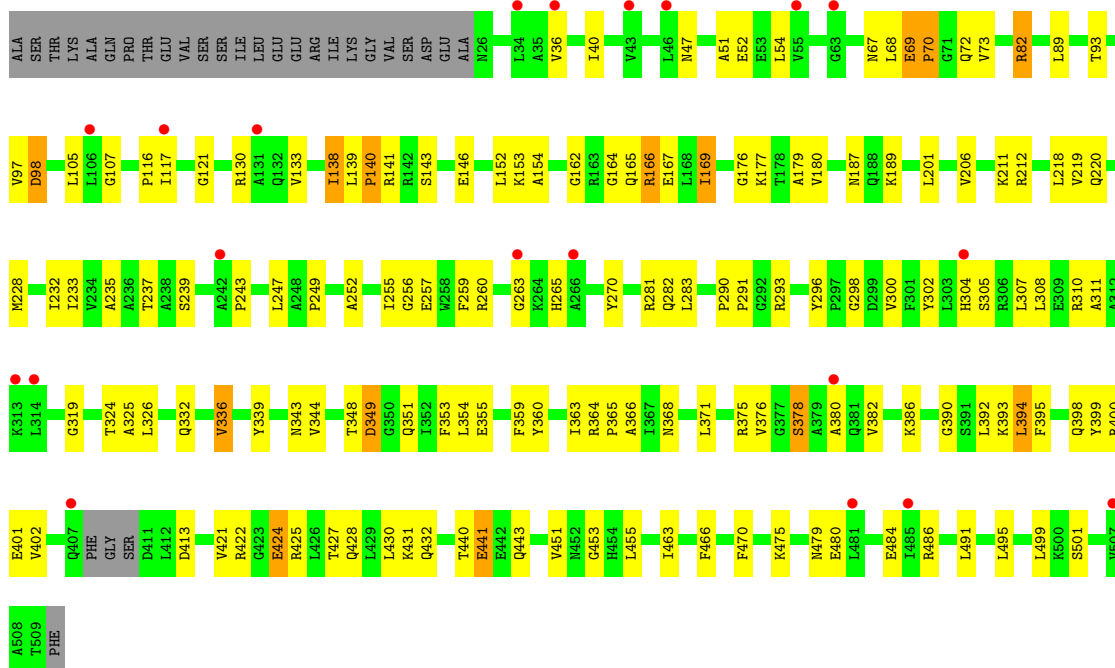


● Molecule 1: ATP synthase subunit alpha

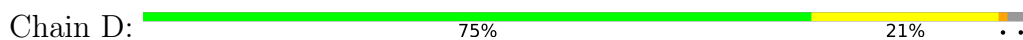




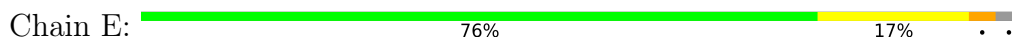
- Molecule 1: ATP synthase subunit alpha

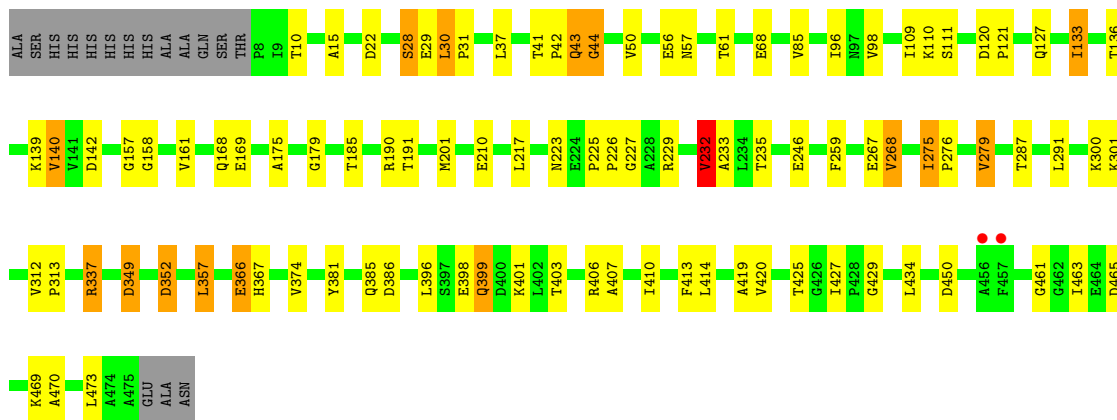


- Molecule 2: ATP synthase subunit beta

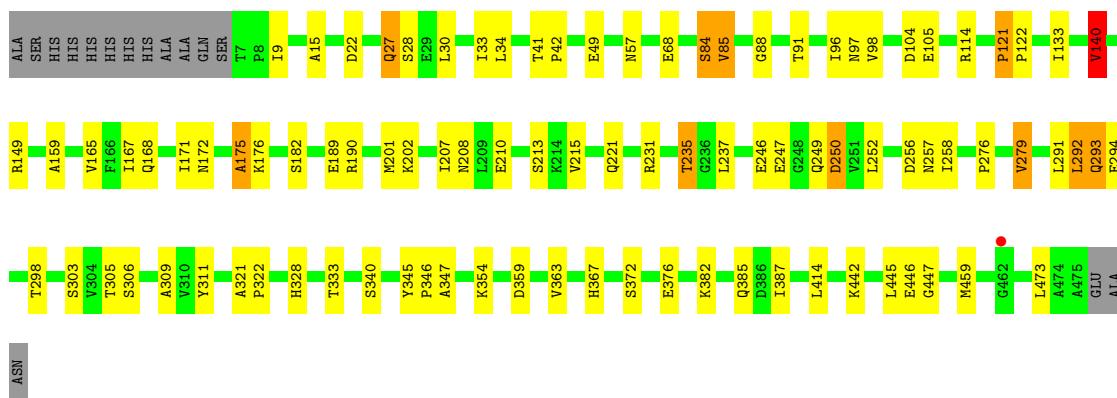
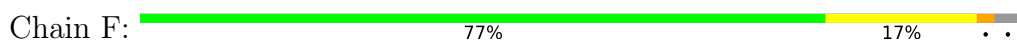


- Molecule 2: ATP synthase subunit beta

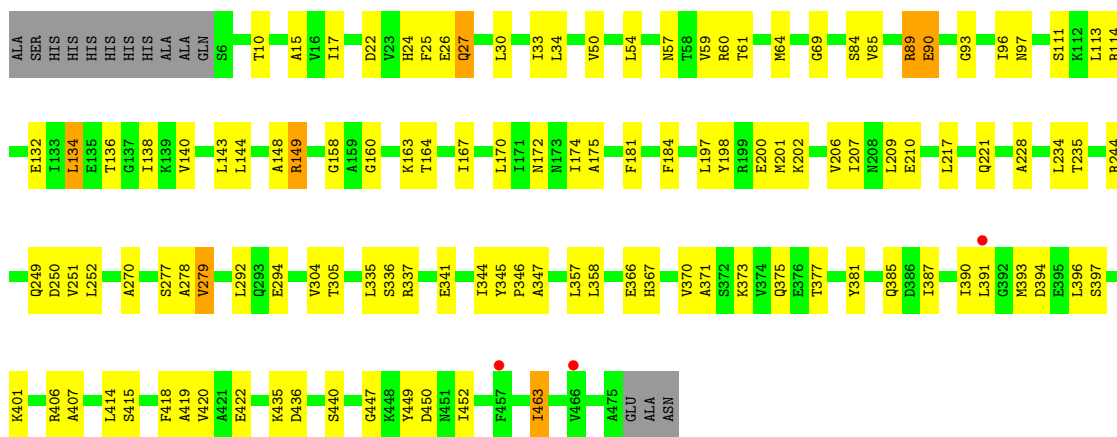
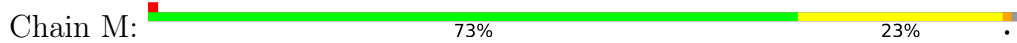




• Molecule 2: ATP synthase subunit beta

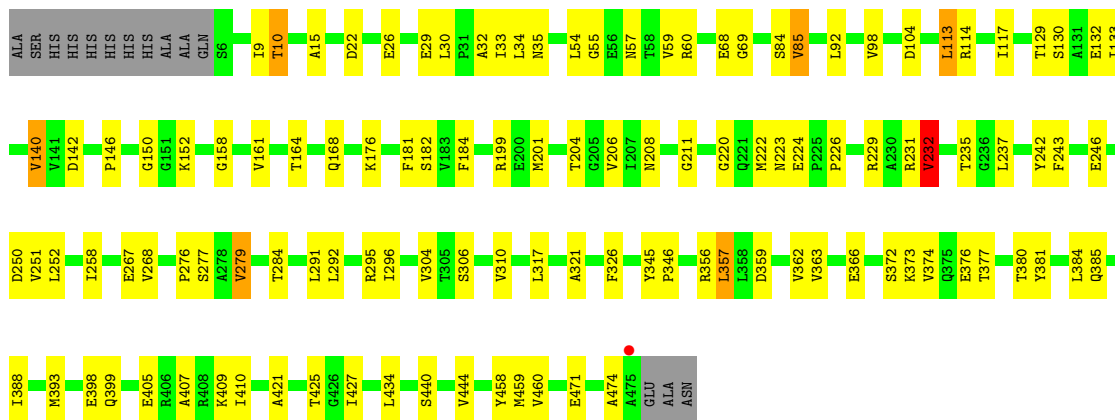


• Molecule 2: ATP synthase subunit beta

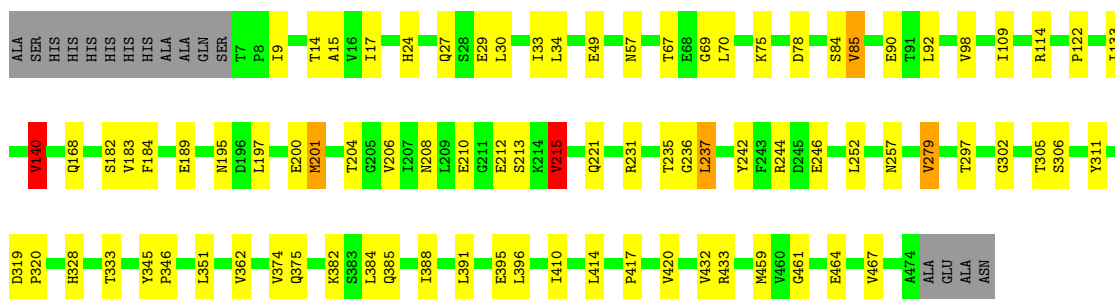
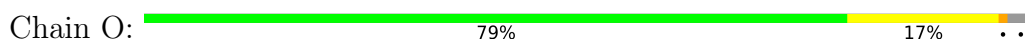


• Molecule 2: ATP synthase subunit beta

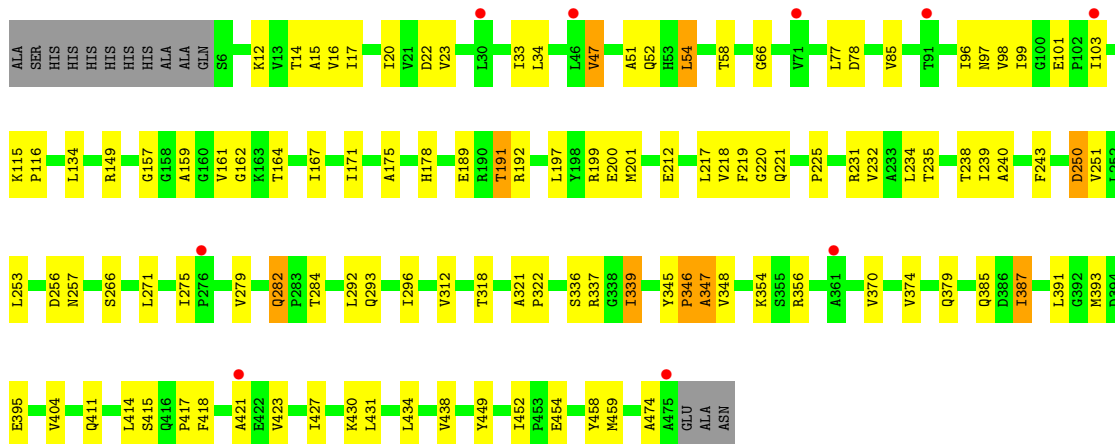
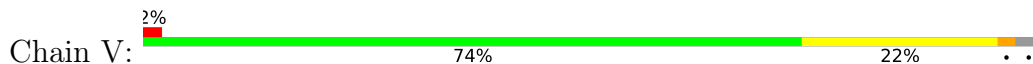




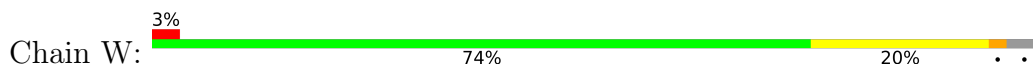
• Molecule 2: ATP synthase subunit beta

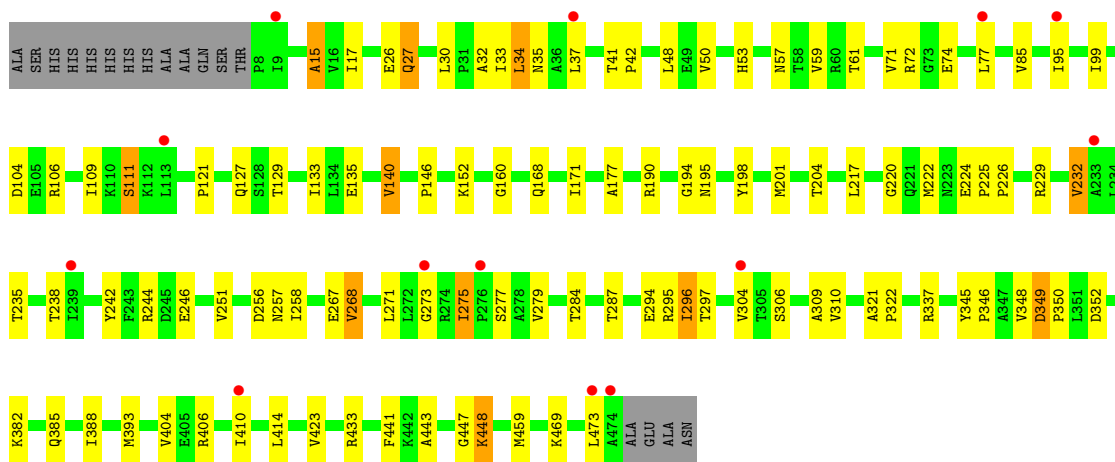


• Molecule 2: ATP synthase subunit beta

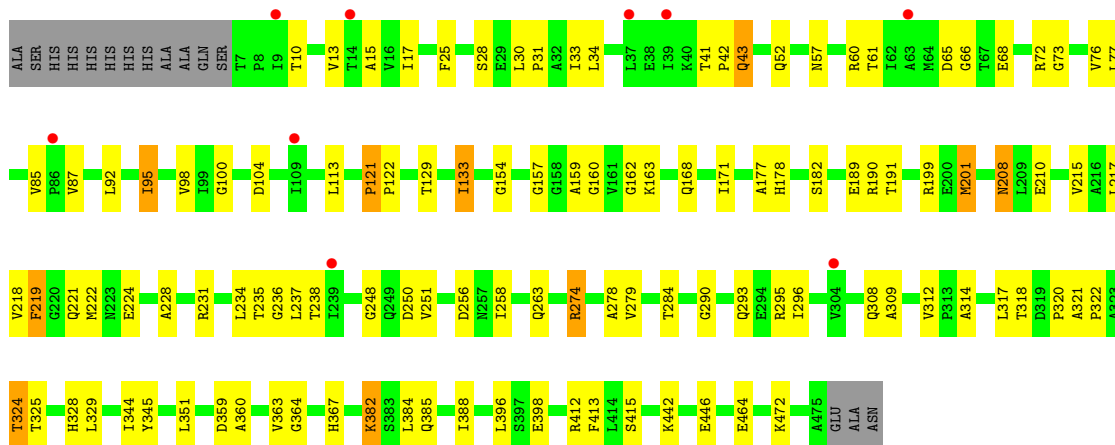
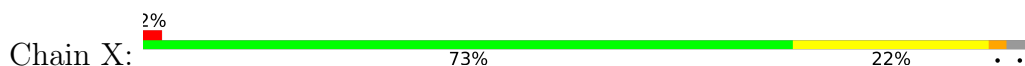


• Molecule 2: ATP synthase subunit beta

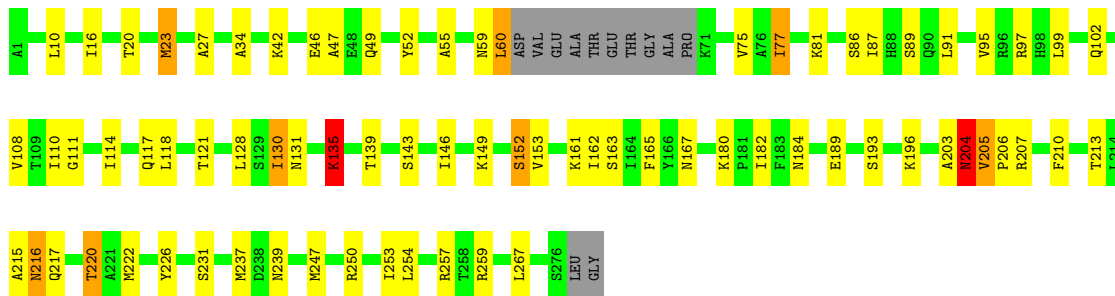




• Molecule 2: ATP synthase subunit beta

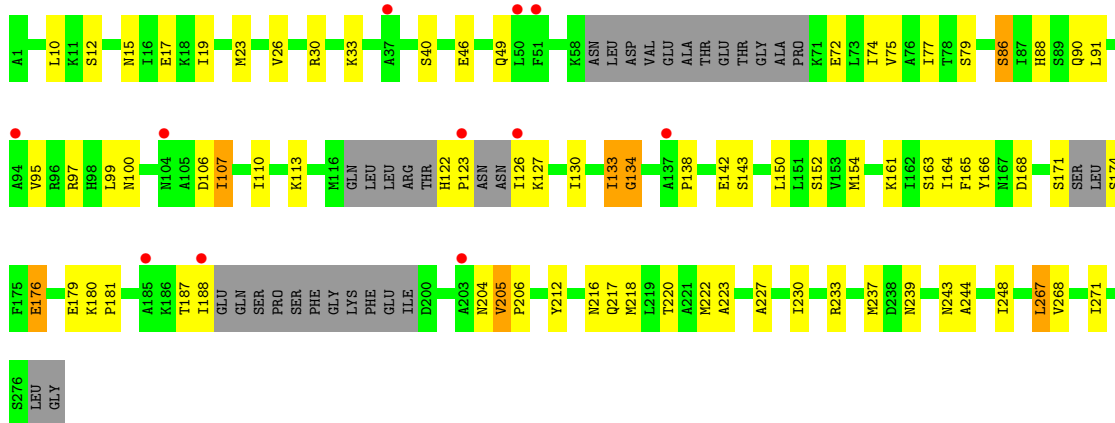


• Molecule 3: ATP synthase subunit gamma

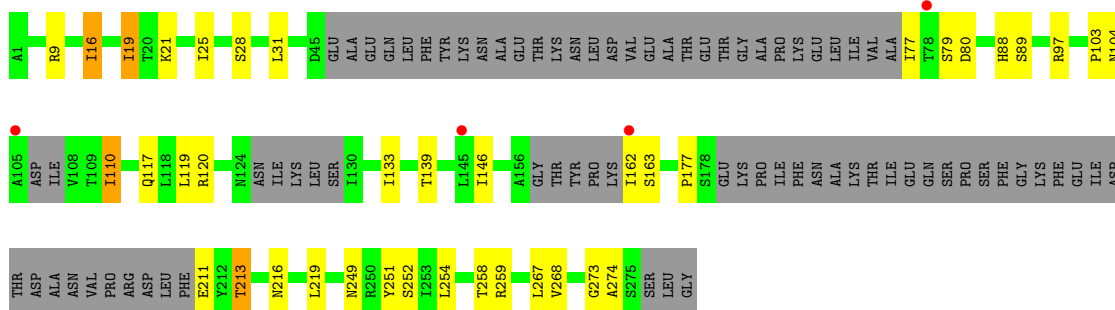


• Molecule 3: ATP synthase subunit gamma

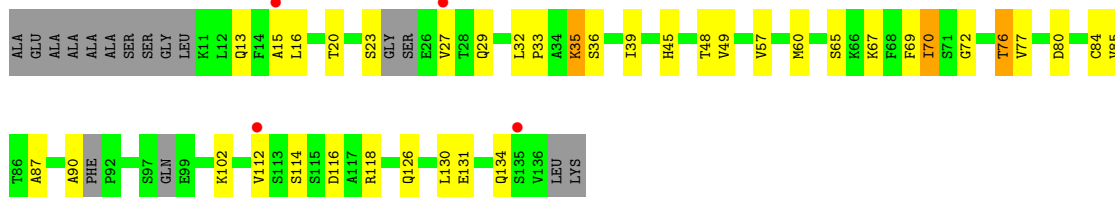




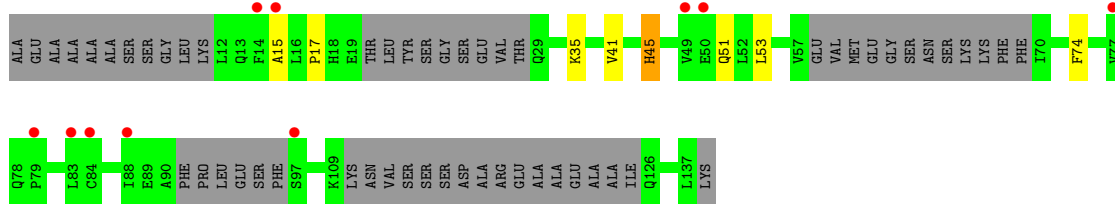
• Molecule 3: ATP synthase subunit gamma



• Molecule 4: ATP synthase subunit delta



• Molecule 4: ATP synthase subunit delta



• Molecule 4: ATP synthase subunit delta

Chain Z:  12% . 88%

ALA GLU
GLU GLY
ALA ALA
ASN ALA
SER ALA
SER ALA
LYS LYS
SER SER
PHE PHE
GLY ILE
LEU LYS
LEU LYS
GLN LYS
PHE PHE
ALA ALA
LEU LEU
VAL PRO
GLN HIS
GLU HIS
THR THR
LEU LEU
TYR TYR
GLN GLN
SER SER
GLY GLY
VAL VAL
SER SER
GLU GLU
VAL VAL
THR THR
ILE ILE
GLN GLN
ALA VAL
ASN ASN
LEU LEU
PRO PRO
ALA ALA
LYS LYS
SER SER
PHE PHE
SER SER
GLY GLY
ARG ARG
ILE ILE
GLU GLU
ASN ASN
GLY GLY
VAL VAL
LEU LEU
ASN ASN
HIS HIS
VAL VAL
PRO PRO
THR THR
VAL VAL
LYS LYS
LYS LYS
GLN GLN
VAL VAL
LEU LEU
SER SER
PRO PRO
GLY GLY
VAL VAL
ALA ALA
GLU GLU
VAL VAL
MET MET

GLU GLY
SER ASN
SER SER
SER ALA
LYS LYS
PHE PHE
PHE PHE
ILE ILE
SER SER
LEU LYS
GLY GLY
PHE PHE
ALA ALA
THR THR
VAL VAL
GLN GLN
PRO PRO
ASP ASP
SER SER
LEU LEU
TYR TYR
GLN GLN
SER SER
VAL VAL
THR THR
ALA ALA
ILE ILE
THR THR
GLN GLN
ALA VAL
PHE PHE
PRO PRO
LEU LEU
GLU GLU
ALA ALA
SER SER
PHE PHE
SER SER
SER SER
GLN GLN
ILE ILE
ASN ASN
ILE ILE
LYS LYS
LYS LYS
ASN ASN
LEU LEU
ALA ALA
PRO PRO
ALA ALA
THR THR
VAL VAL
LYS LYS
LYS LYS
ASN ASN
VAL VAL
LEU LEU
SER SER
SER SER
SER SER
ASP ASP
ALA ALA
ARG ARG
A119
A120

S135
VAL
LEU
LYS

- Molecule 5: ATP synthase subunit epsilon

Chain I:  5% 66% 11% . 20%


SER ALA
TRP TRP
ARG ARG
LYS LYS
ALA ALA
GLY GLY
I8 I8
S9 S9
Y10 Y10
L14 L14
I15 I15
V16 V16
Q19 Q19
S23 S23
SER SER
LEU LEU
K26 K26
V34 V34
L35 L35
N36 N36
R37 R37
D41 D41
H49 H49
GLY GLY
THR THR
ALA ALA
A53 A53
S54 S54
E55 E55
P56 P56
R61 R61

- Molecule 5: ATP synthase subunit epsilon

Chain R:  10% 56% 44%

SER ALA
TRP TRP
ARG ARG
LYS LYS
ALA ALA
GLY GLY
ILE ILE
SER SER
Y10 Y10
A20 A20
I21 I21
R22 R22
SER SER
SER SER
LEU LEU
THR THR
LYS LYS
T27 T27
Q30 Q30
N36 N36
Y47 Y47
LYS LYS
ASN ASN
GLY GLY
THR THR
ALA ALA
ALA ALA
SER SER
GLU GLU
PRO PRO
THR THR
PRO PRO
ILE ILE
THR THR
LYS LYS

- Molecule 5: ATP synthase subunit epsilon

Chain 1:  2% 39% 5% 56%

SER ALA
TRP TRP
ARG ARG
LYS LYS
ALA ALA
GLY GLY
ILE ILE
S9 S9
Y10 Y10
A11 A11
R22 R22
SER SER
SER SER
LEU LEU
THR THR
GLU GLU
LEU LEU
GLN GLN
THR THR
ALA ALA
S33 S33
Y34 Y34
R37 R37
T45 T45
GLN GLN
TYR TYR
LYS LYS
ASN ASN
GLY GLY
THR THR
ALA ALA
ALA ALA
SER SER
GLU GLU
PRO PRO
THR THR
PRO PRO
ILE ILE
THR THR
LYS LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.43Å 288.58Å 187.17Å 90.00° 101.37° 90.00°	Depositor
Resolution (Å)	20.00 – 2.74 20.00 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.74) 98.4 (20.00-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.73Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.212 , 0.259 0.215 , 0.264	Depositor DCC
R_{free} test set	5983 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtrriage
Anisotropy	0.248	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	72675	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.68	1/3712 (0.0%)	0.98	5/5024 (0.1%)
1	B	0.65	0/3717	0.96	1/5031 (0.0%)
1	C	0.57	0/3730	0.89	4/5049 (0.1%)
1	J	0.56	0/3703	0.90	1/5012 (0.0%)
1	K	0.61	1/3732 (0.0%)	0.93	4/5052 (0.1%)
1	L	0.59	0/3712	0.93	6/5024 (0.1%)
1	S	0.58	1/3675 (0.0%)	0.92	3/4973 (0.1%)
1	T	0.55	0/3685	0.91	3/4987 (0.1%)
1	U	0.58	0/3703	0.89	1/5013 (0.0%)
2	D	0.62	0/3601	0.92	4/4884 (0.1%)
2	E	0.66	0/3560	0.96	10/4834 (0.2%)
2	F	0.58	0/3583	0.93	3/4862 (0.1%)
2	M	0.56	0/3591	0.89	0/4872
2	N	0.64	0/3597	0.93	7/4880 (0.1%)
2	O	0.61	0/3590	0.92	2/4869 (0.0%)
2	V	0.58	0/3605	0.91	4/4889 (0.1%)
2	W	0.61	0/3587	0.90	4/4863 (0.1%)
2	X	0.57	0/3599	0.89	3/4881 (0.1%)
3	G	0.52	0/2080	0.89	1/2798 (0.0%)
3	P	0.57	0/1867	0.90	1/2509 (0.0%)
3	Y	0.52	0/1527	0.87	2/2048 (0.1%)
4	H	0.60	0/804	0.98	2/1101 (0.2%)
4	Q	0.65	0/440	0.96	1/603 (0.2%)
4	Z	0.63	0/84	1.18	0/116
5	I	0.53	0/143	0.98	0/195
5	I	0.61	0/343	0.99	0/470
5	R	0.65	0/173	1.04	0/239
All	All	0.60	3/73143 (0.0%)	0.92	72/99078 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	444	VAL	CA-CB	8.79	1.59	1.53
1	A	444	VAL	CA-CB	6.69	1.58	1.53
1	S	444	VAL	CA-CB	5.69	1.56	1.54

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	VAL	N-CA-CB	7.93	115.50	110.50
1	L	340	ILE	CA-C-N	-7.69	111.04	119.19
1	L	340	ILE	C-N-CA	-7.69	111.04	119.19
2	E	275	ILE	CA-C-N	7.66	127.67	119.78
2	E	275	ILE	C-N-CA	7.66	127.67	119.78

There are no chirality outliers.

There are no planarity outliers.

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	3659	0	3743	55	0
1	B	3664	0	3748	56	0
1	C	3675	0	3759	54	0
1	J	3650	0	3735	41	0
1	K	3679	0	3754	75	0
1	L	3659	0	3743	53	0
1	S	3622	0	3716	92	0
1	T	3632	0	3724	74	0
1	U	3650	0	3730	102	0
2	D	3545	0	3614	67	0
2	E	3504	0	3550	56	0
2	F	3527	0	3592	51	0
2	M	3535	0	3599	66	0
2	N	3541	0	3604	66	0
2	O	3534	0	3606	55	0
2	V	3549	0	3620	77	0
2	W	3531	0	3605	62	0
2	X	3543	0	3615	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2055	0	2123	48	0
3	P	1850	0	1892	52	0
3	Y	1517	0	1561	21	0
4	H	795	0	670	19	0
4	Q	441	0	234	3	0
4	Z	85	0	45	0	0
5	1	145	0	87	2	0
5	I	339	0	280	4	0
5	R	175	0	100	0	0
6	A	31	0	13	1	0
6	B	31	0	13	2	0
6	C	31	0	13	0	0
6	D	31	0	13	1	0
6	F	31	0	13	2	0
6	J	31	0	13	0	0
6	K	31	0	13	1	0
6	L	31	0	13	0	0
6	M	31	0	13	5	0
6	O	31	0	13	0	0
6	S	31	0	13	4	0
6	T	31	0	13	1	0
6	U	31	0	13	4	0
6	V	31	0	13	4	0
6	X	31	0	13	6	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	O	1	0	0	0	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
7	U	1	0	0	0	0
7	V	1	0	0	0	0
7	X	1	0	0	0	0
8	E	5	0	0	0	0
8	N	5	0	0	0	0
9	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	9	0	0	0	0
9	C	3	0	0	0	0
9	D	11	0	0	0	0
9	E	10	0	0	0	0
9	F	8	0	0	0	0
9	G	2	0	0	1	0
9	J	3	0	0	0	0
9	K	5	0	0	0	0
9	L	8	0	0	0	0
9	M	4	0	0	0	0
9	N	3	0	0	0	0
9	O	5	0	0	0	0
9	P	2	0	0	0	0
9	X	1	0	0	0	0
All	All	72675	0	73244	1228	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 8.

The worst 5 of 1228 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)
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.24	1.08
2:O:84:SER:HB3	2:O:114:ARG:HH11	1.18	1.07
1:L:336:VAL:HG11	1:L:353:PHE:HE2	1.23	1.03
1:A:112:ALA:O	1:A:251:THR:HG21	1.61	1.01
2:X:95:ILE:HD12	2:X:104:ASP:HB3	1.43	1.01

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	478/510 (94%)	456 (95%)	19 (4%)	3 (1%)	21	36
1	B	479/510 (94%)	455 (95%)	21 (4%)	3 (1%)	21	36
1	C	482/510 (94%)	448 (93%)	31 (6%)	3 (1%)	21	36
1	J	477/510 (94%)	449 (94%)	23 (5%)	5 (1%)	12	22
1	K	482/510 (94%)	446 (92%)	32 (7%)	4 (1%)	16	29
1	L	478/510 (94%)	451 (94%)	23 (5%)	4 (1%)	16	29
1	S	473/510 (93%)	434 (92%)	39 (8%)	0	100	100
1	T	474/510 (93%)	430 (91%)	42 (9%)	2 (0%)	30	47
1	U	477/510 (94%)	423 (89%)	48 (10%)	6 (1%)	9	16
2	D	468/484 (97%)	435 (93%)	30 (6%)	3 (1%)	21	36
2	E	466/484 (96%)	429 (92%)	30 (6%)	7 (2%)	8	14
2	F	467/484 (96%)	432 (92%)	34 (7%)	1 (0%)	43	62
2	M	468/484 (97%)	431 (92%)	32 (7%)	5 (1%)	11	20
2	N	468/484 (97%)	438 (94%)	27 (6%)	3 (1%)	21	36
2	O	466/484 (96%)	430 (92%)	34 (7%)	2 (0%)	30	47
2	V	468/484 (97%)	433 (92%)	31 (7%)	4 (1%)	14	26
2	W	465/484 (96%)	425 (91%)	36 (8%)	4 (1%)	14	26
2	X	467/484 (96%)	419 (90%)	45 (10%)	3 (1%)	21	36
3	G	262/278 (94%)	240 (92%)	19 (7%)	3 (1%)	11	20
3	P	232/278 (84%)	210 (90%)	20 (9%)	2 (1%)	14	26
3	Y	188/278 (68%)	173 (92%)	13 (7%)	2 (1%)	11	20
4	H	114/138 (83%)	91 (80%)	20 (18%)	3 (3%)	4	6
4	Q	73/138 (53%)	61 (84%)	9 (12%)	3 (4%)	2	3
4	Z	15/138 (11%)	10 (67%)	4 (27%)	1 (7%)	1	1
5	1	23/61 (38%)	18 (78%)	4 (17%)	1 (4%)	2	2
5	I	43/61 (70%)	39 (91%)	2 (5%)	2 (5%)	2	2
5	R	30/61 (49%)	21 (70%)	9 (30%)	0	100	100
All	All	9483/10377 (91%)	8727 (92%)	677 (7%)	79 (1%)	16	29

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	152	SER
3	G	204	ASN

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Mol	Chain	Res	Type
4	H	118	ARG
5	I	55	GLU
5	I	56	PRO

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	388/412 (94%)	368 (95%)	20 (5%)	21	38
1	B	388/412 (94%)	365 (94%)	23 (6%)	18	32
1	C	390/412 (95%)	371 (95%)	19 (5%)	22	41
1	J	387/412 (94%)	363 (94%)	24 (6%)	16	30
1	K	388/412 (94%)	365 (94%)	23 (6%)	18	32
1	L	388/412 (94%)	360 (93%)	28 (7%)	13	24
1	S	384/412 (93%)	361 (94%)	23 (6%)	17	31
1	T	386/412 (94%)	370 (96%)	16 (4%)	27	48
1	U	387/412 (94%)	355 (92%)	32 (8%)	10	19
2	D	379/390 (97%)	366 (97%)	13 (3%)	32	55
2	E	370/390 (95%)	349 (94%)	21 (6%)	18	34
2	F	375/390 (96%)	349 (93%)	26 (7%)	14	26
2	M	377/390 (97%)	356 (94%)	21 (6%)	19	35
2	N	378/390 (97%)	353 (93%)	25 (7%)	15	28
2	O	378/390 (97%)	361 (96%)	17 (4%)	24	44
2	V	380/390 (97%)	361 (95%)	19 (5%)	22	40
2	W	378/390 (97%)	352 (93%)	26 (7%)	14	26
2	X	379/390 (97%)	361 (95%)	18 (5%)	23	43
3	G	225/236 (95%)	205 (91%)	20 (9%)	9	17
3	P	197/236 (84%)	185 (94%)	12 (6%)	17	30
3	Y	163/236 (69%)	151 (93%)	12 (7%)	13	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	65/112 (58%)	57 (88%)	8 (12%)	4	8
4	Q	8/112 (7%)	8 (100%)	0	100	100
5	1	2/48 (4%)	2 (100%)	0	100	100
5	I	28/48 (58%)	23 (82%)	5 (18%)	2	2
5	R	3/48 (6%)	3 (100%)	0	100	100
All	All	7571/8294 (91%)	7120 (94%)	451 (6%)	17	31

5 of 451 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	17	ILE
3	Y	119	LEU
2	O	215	VAL
2	X	413	PHE
2	W	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	208	ASN
1	S	210	GLN
3	Y	124	ASN
2	W	172	ASN
2	O	52	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 32 ligands modelled in this entry, 15 are monoatomic - leaving 17 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
6	ANP	A	600	7	33,33,33	1.89	10 (30%)	45,52,52	2.36	15 (33%)
6	ANP	T	600	7	33,33,33	2.18	10 (30%)	45,52,52	2.07	13 (28%)
6	ANP	K	600	7	33,33,33	1.90	10 (30%)	45,52,52	1.99	12 (26%)
6	ANP	C	600	7	33,33,33	2.00	11 (33%)	45,52,52	2.27	13 (28%)
6	ANP	F	600	7	33,33,33	1.91	9 (27%)	45,52,52	2.23	14 (31%)
6	ANP	V	600	7	33,33,33	2.09	11 (33%)	45,52,52	2.21	13 (28%)
6	ANP	M	600	7	33,33,33	2.00	11 (33%)	45,52,52	2.08	11 (24%)
6	ANP	S	600	7	33,33,33	2.13	10 (30%)	45,52,52	2.25	13 (28%)
6	ANP	J	600	7	33,33,33	1.94	11 (33%)	45,52,52	2.12	10 (22%)
6	ANP	U	600	7	33,33,33	2.04	11 (33%)	45,52,52	2.19	12 (26%)
8	PO4	E	800	-	4,4,4	0.66	0	6,6,6	0.79	0
6	ANP	D	600	7	33,33,33	1.92	10 (30%)	45,52,52	1.99	14 (31%)
6	ANP	B	600	7	33,33,33	2.00	10 (30%)	45,52,52	2.16	10 (22%)
6	ANP	O	600	7	33,33,33	1.96	11 (33%)	45,52,52	2.19	13 (28%)
6	ANP	L	600	7	33,33,33	1.89	11 (33%)	45,52,52	2.16	11 (24%)
8	PO4	N	800	-	4,4,4	0.85	0	6,6,6	0.59	0
6	ANP	X	600	7	33,33,33	2.08	9 (27%)	45,52,52	2.03	10 (22%)

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
6	ANP	A	600	7	-	2/18/38/38	0/3/3/3
6	ANP	T	600	7	-	7/18/38/38	0/3/3/3
6	ANP	K	600	7	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	C	600	7	-	4/18/38/38	0/3/3/3
6	ANP	F	600	7	-	8/18/38/38	0/3/3/3
6	ANP	V	600	7	-	10/18/38/38	0/3/3/3
6	ANP	M	600	7	-	4/18/38/38	0/3/3/3
6	ANP	S	600	7	-	6/18/38/38	0/3/3/3
6	ANP	J	600	7	-	4/18/38/38	0/3/3/3
6	ANP	U	600	7	-	4/18/38/38	0/3/3/3
6	ANP	D	600	7	-	5/18/38/38	0/3/3/3
6	ANP	B	600	7	-	2/18/38/38	0/3/3/3
6	ANP	O	600	7	-	4/18/38/38	0/3/3/3
6	ANP	L	600	7	-	2/18/38/38	0/3/3/3
6	ANP	X	600	7	-	4/18/38/38	0/3/3/3

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	600	ANP	C5-C4	5.40	1.48	1.39
6	O	600	ANP	C5-C4	5.27	1.48	1.39
6	M	600	ANP	C5-C4	5.14	1.48	1.39
6	U	600	ANP	C5-C4	5.14	1.48	1.39
6	T	600	ANP	C5-C4	5.02	1.48	1.39

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	ANP	O1G-PG-N3B	-7.52	100.69	111.77
6	B	600	ANP	C5-C4-N3	-6.81	117.34	126.72
6	V	600	ANP	O1G-PG-N3B	-6.70	101.90	111.77
6	X	600	ANP	C5-C4-N3	-6.69	117.50	126.72
6	L	600	ANP	O1G-PG-N3B	-6.56	102.11	111.77

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	600	ANP	PB-N3B-PG-O1G
6	A	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	PB-N3B-PG-O1G
6	B	600	ANP	PG-N3B-PB-O1B

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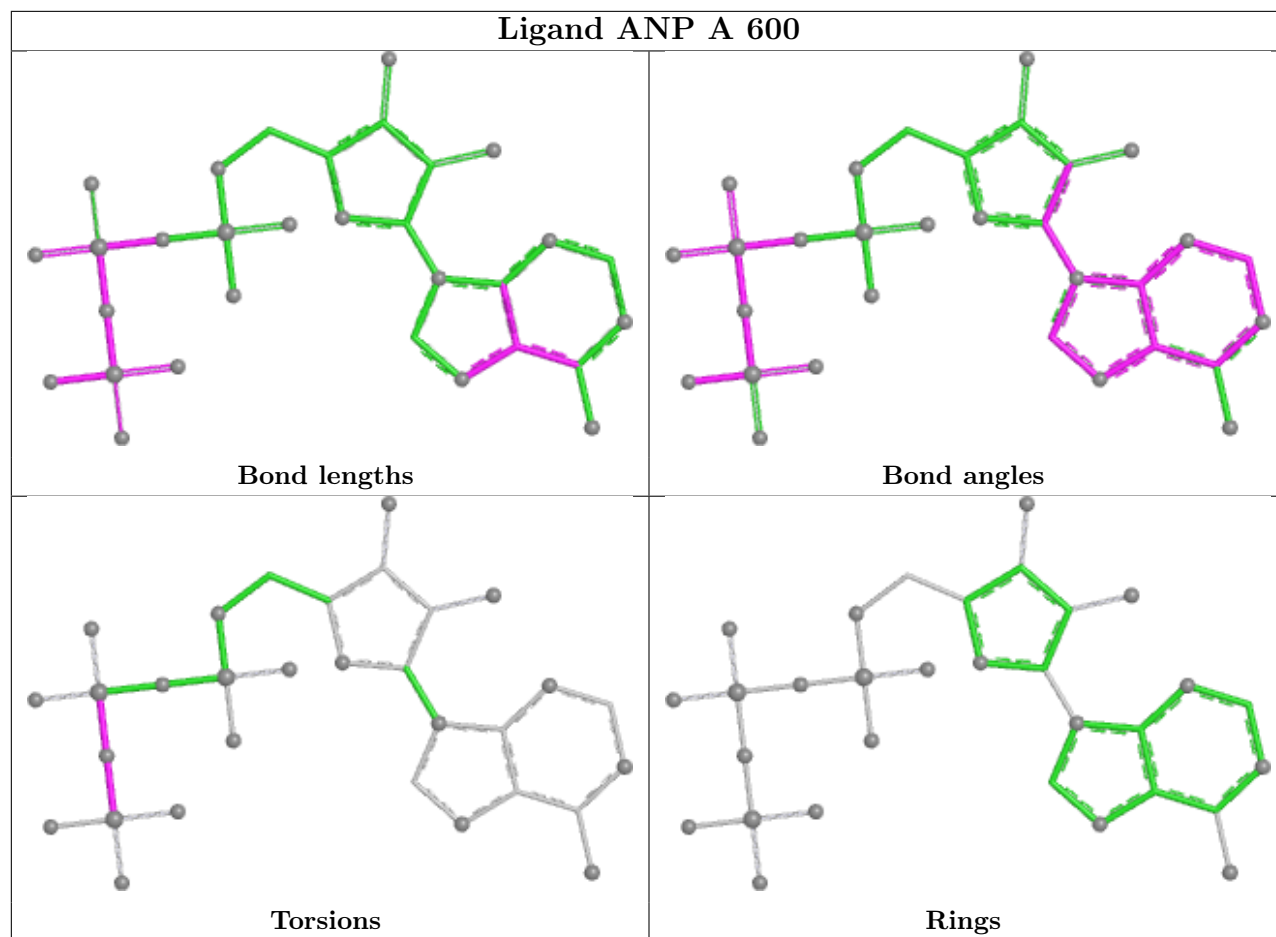
Mol	Chain	Res	Type	Atoms
6	C	600	ANP	PB-N3B-PG-O1G

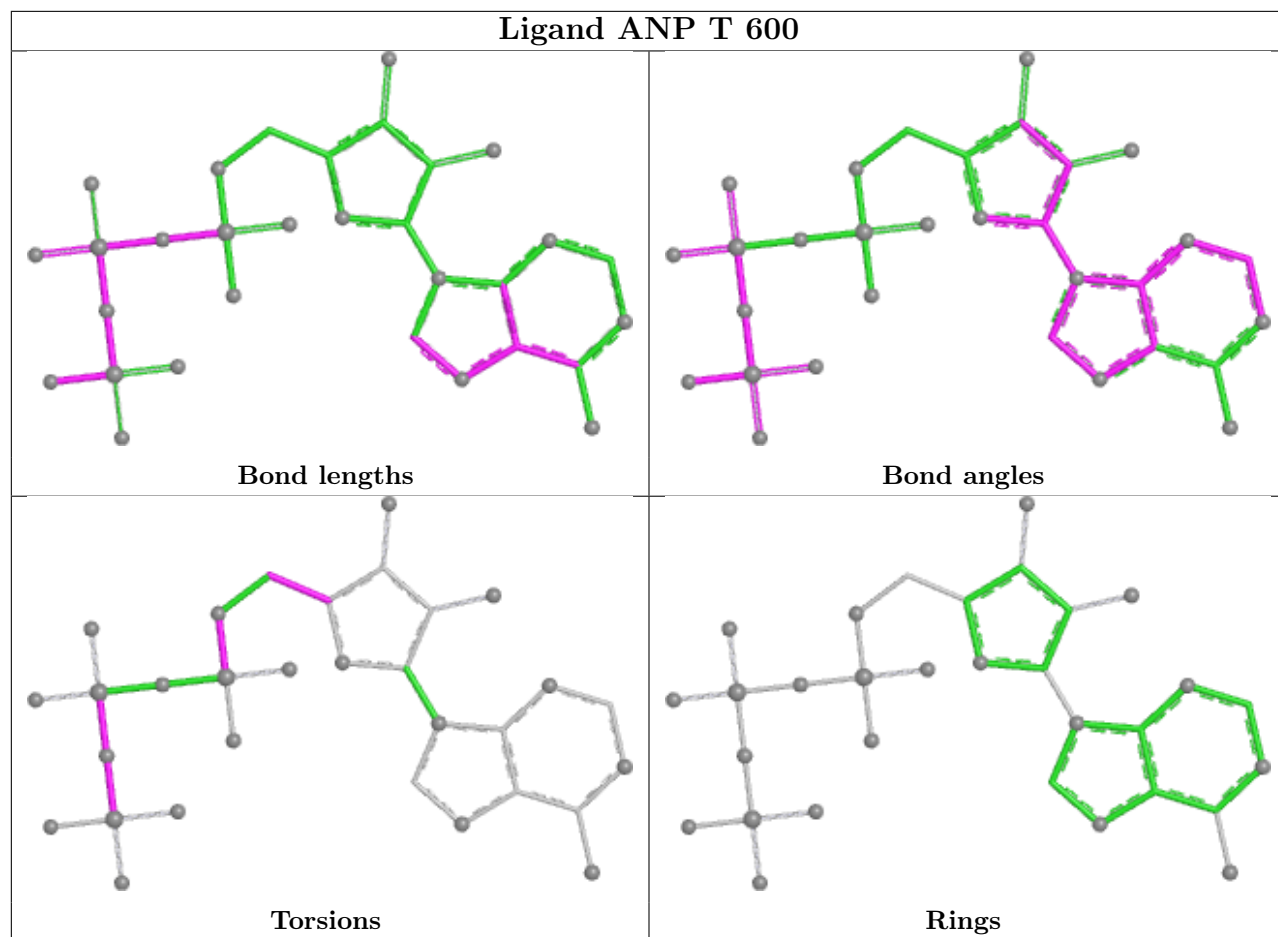
There are no ring outliers.

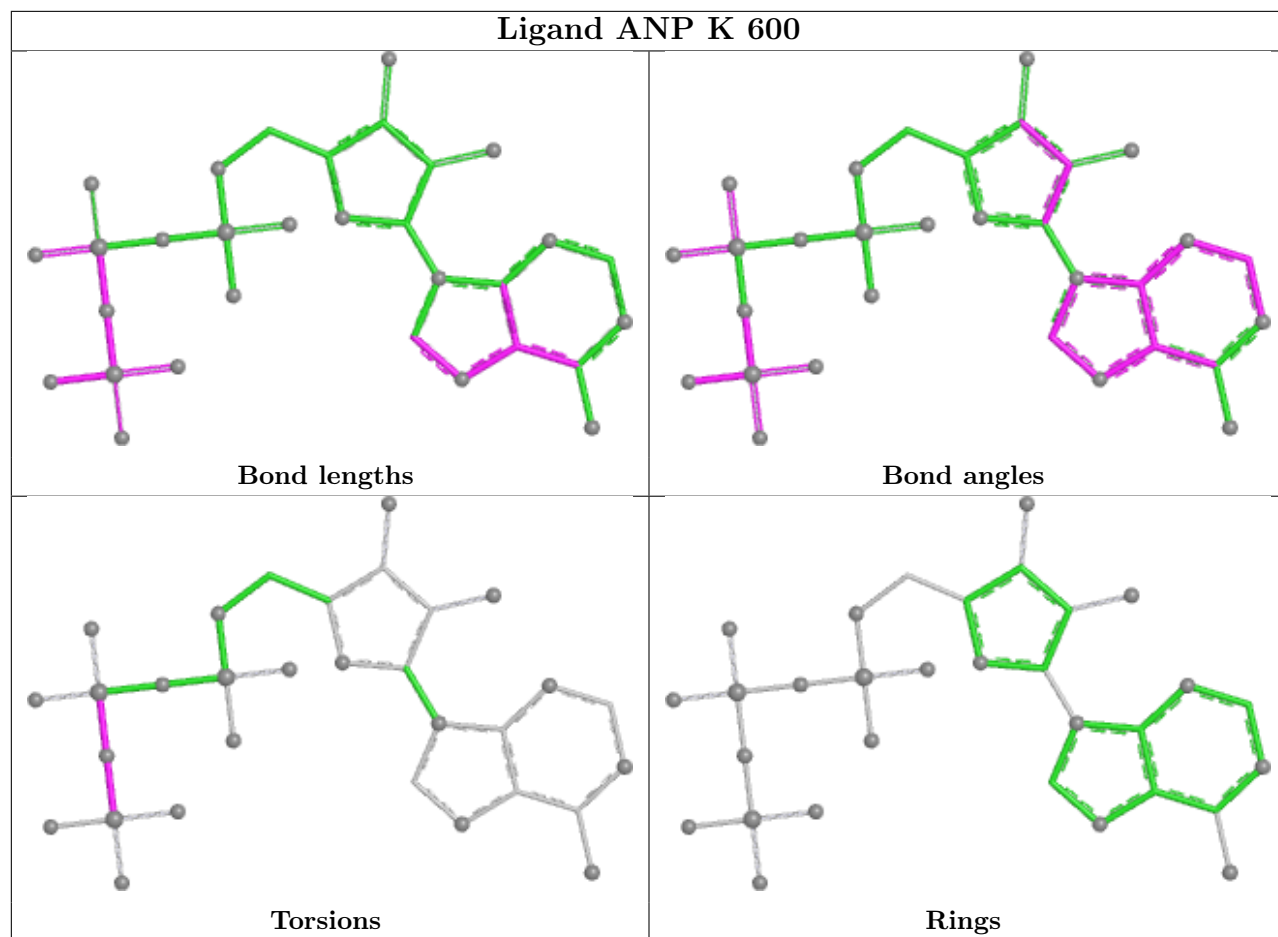
11 monomers are involved in 31 short contacts:

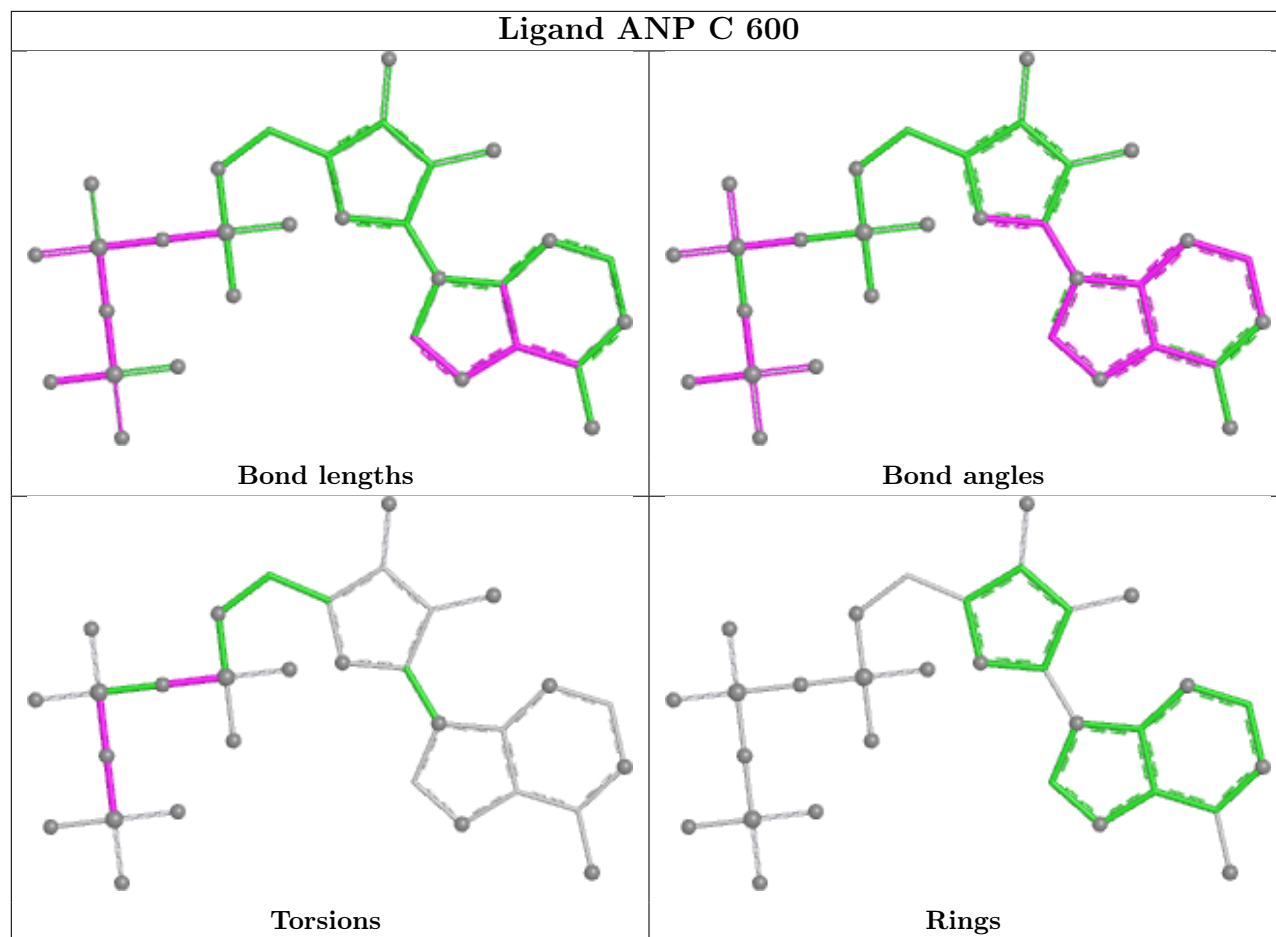
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	600	ANP	1	0
6	T	600	ANP	1	0
6	K	600	ANP	1	0
6	F	600	ANP	2	0
6	V	600	ANP	4	0
6	M	600	ANP	5	0
6	S	600	ANP	4	0
6	U	600	ANP	4	0
6	D	600	ANP	1	0
6	B	600	ANP	2	0
6	X	600	ANP	6	0

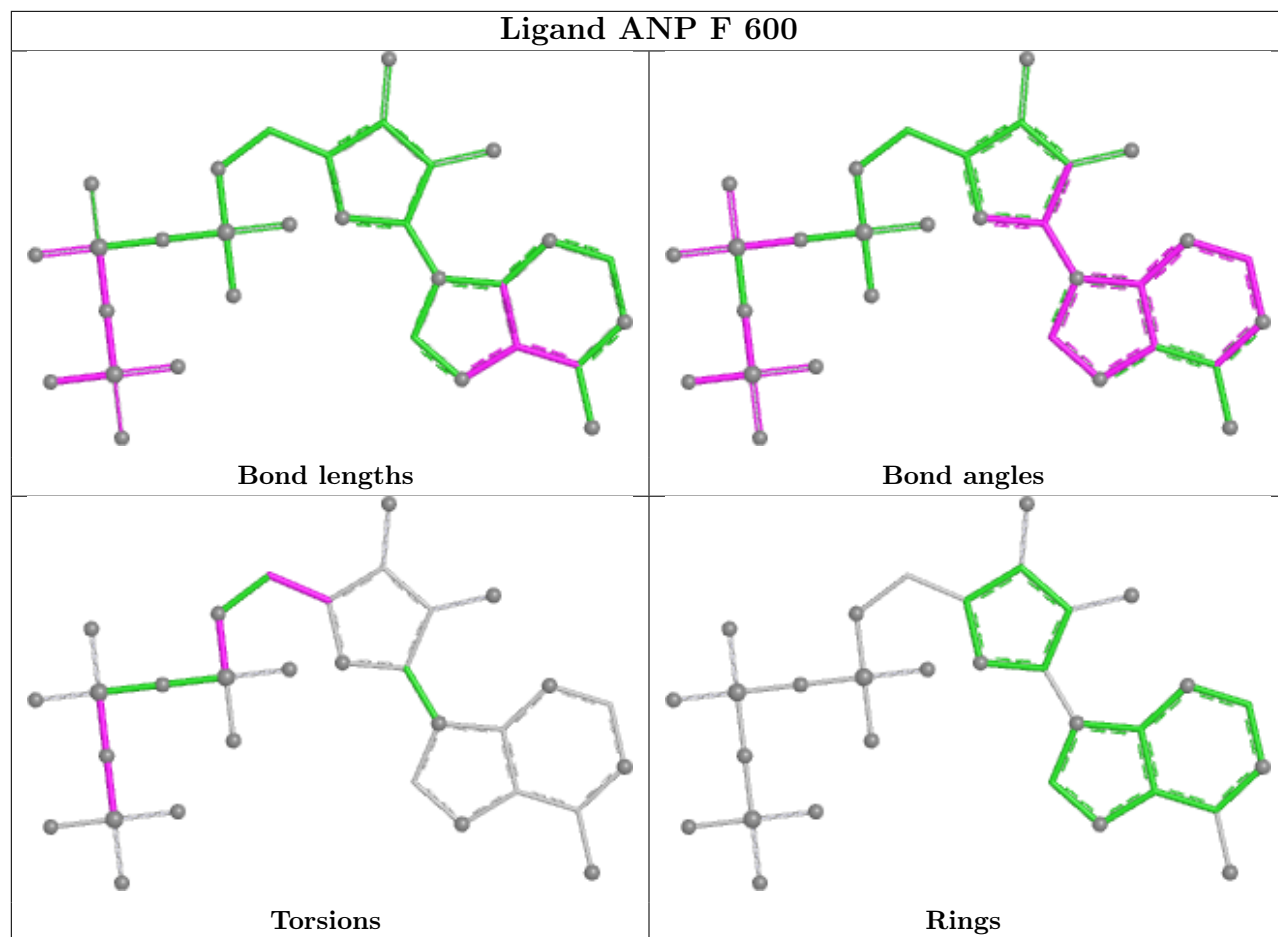
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

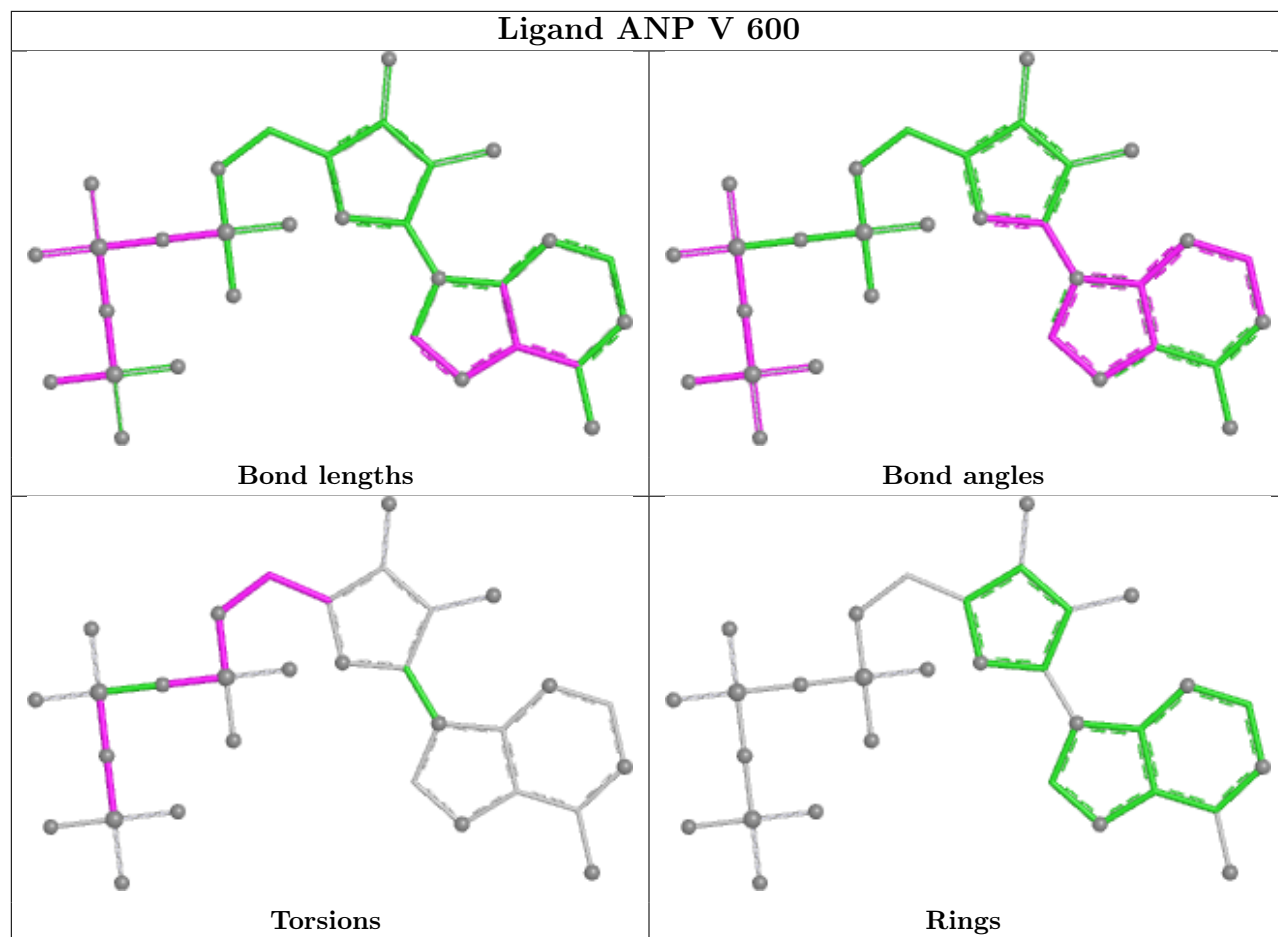


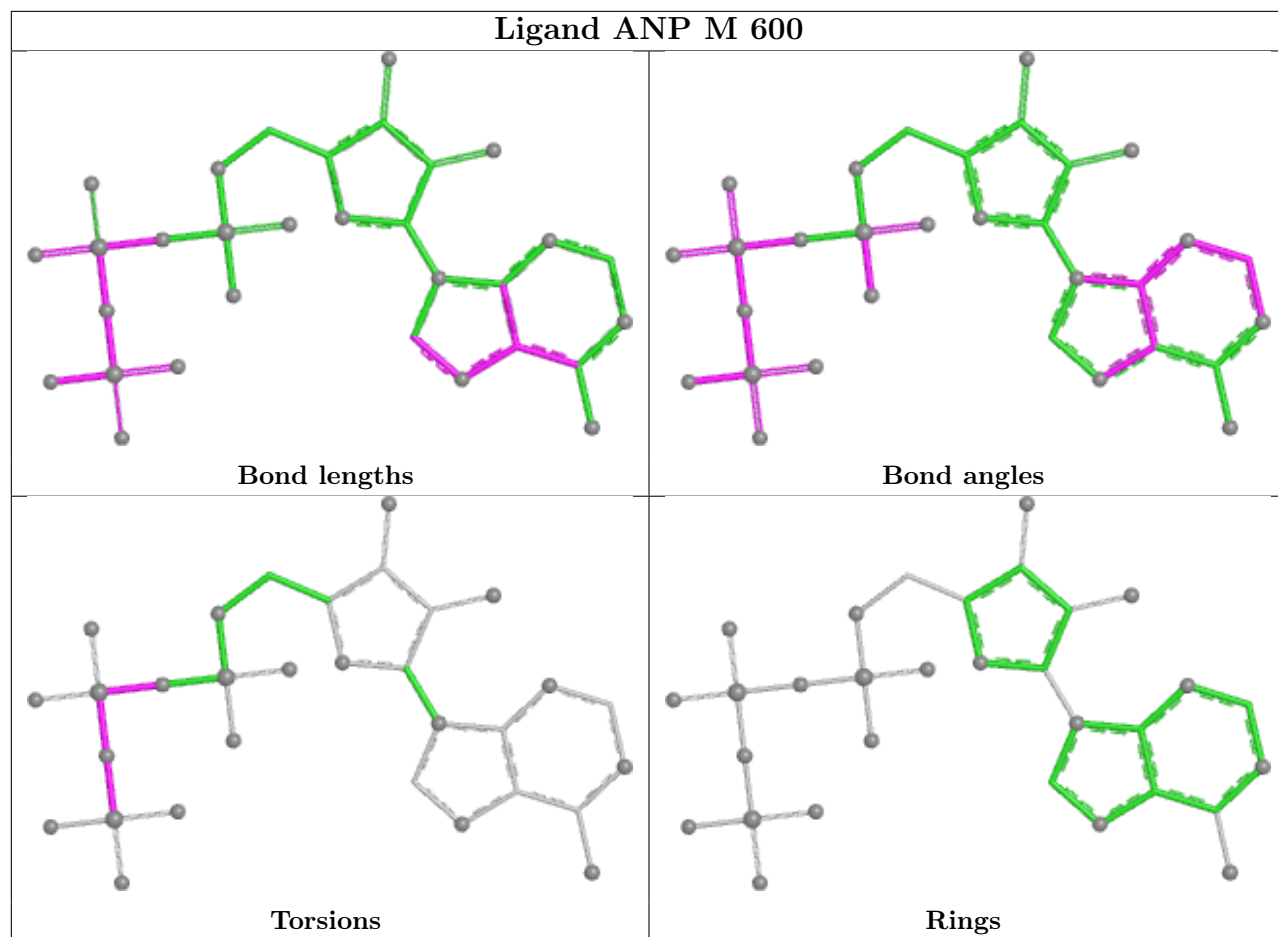


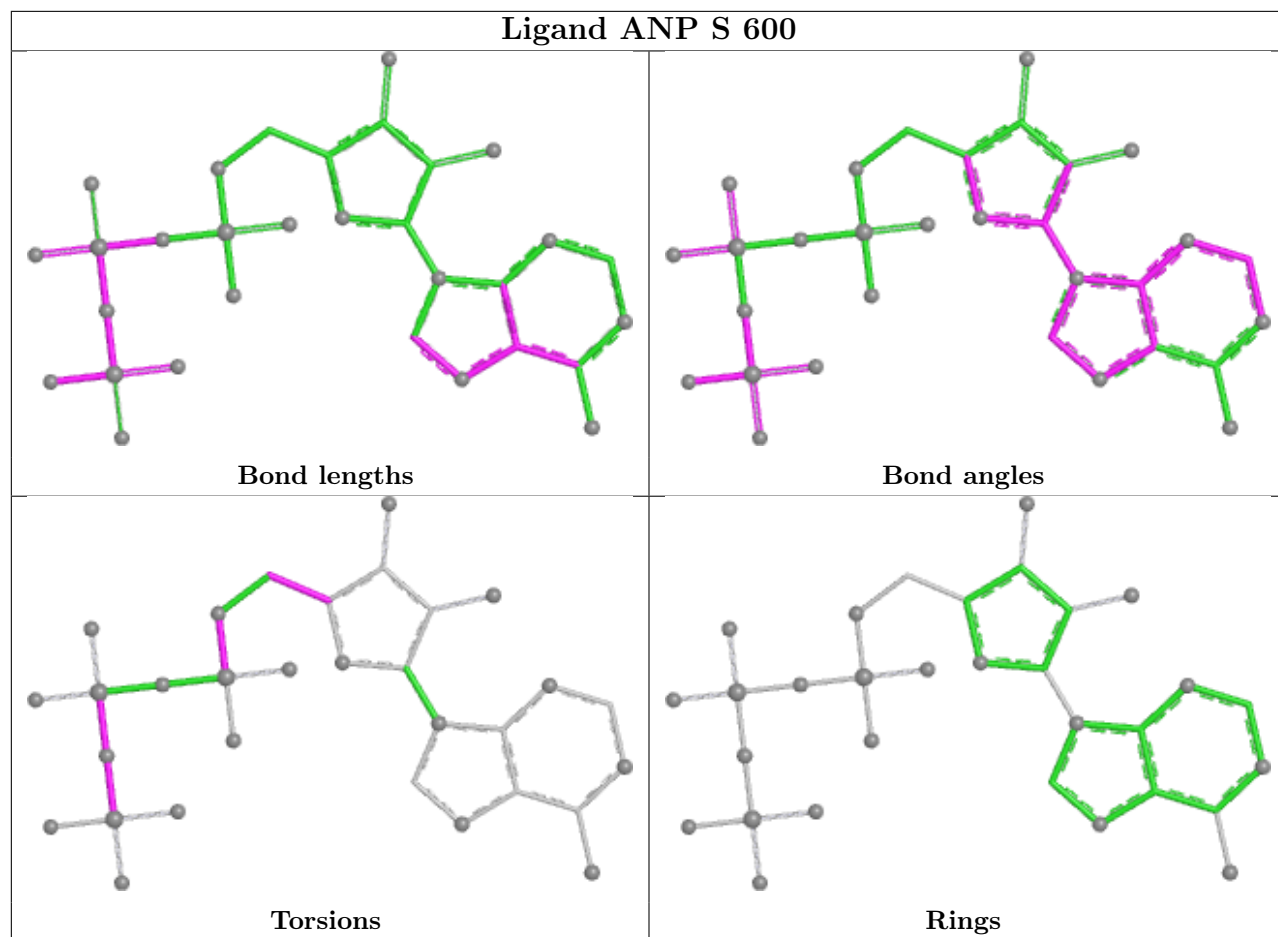


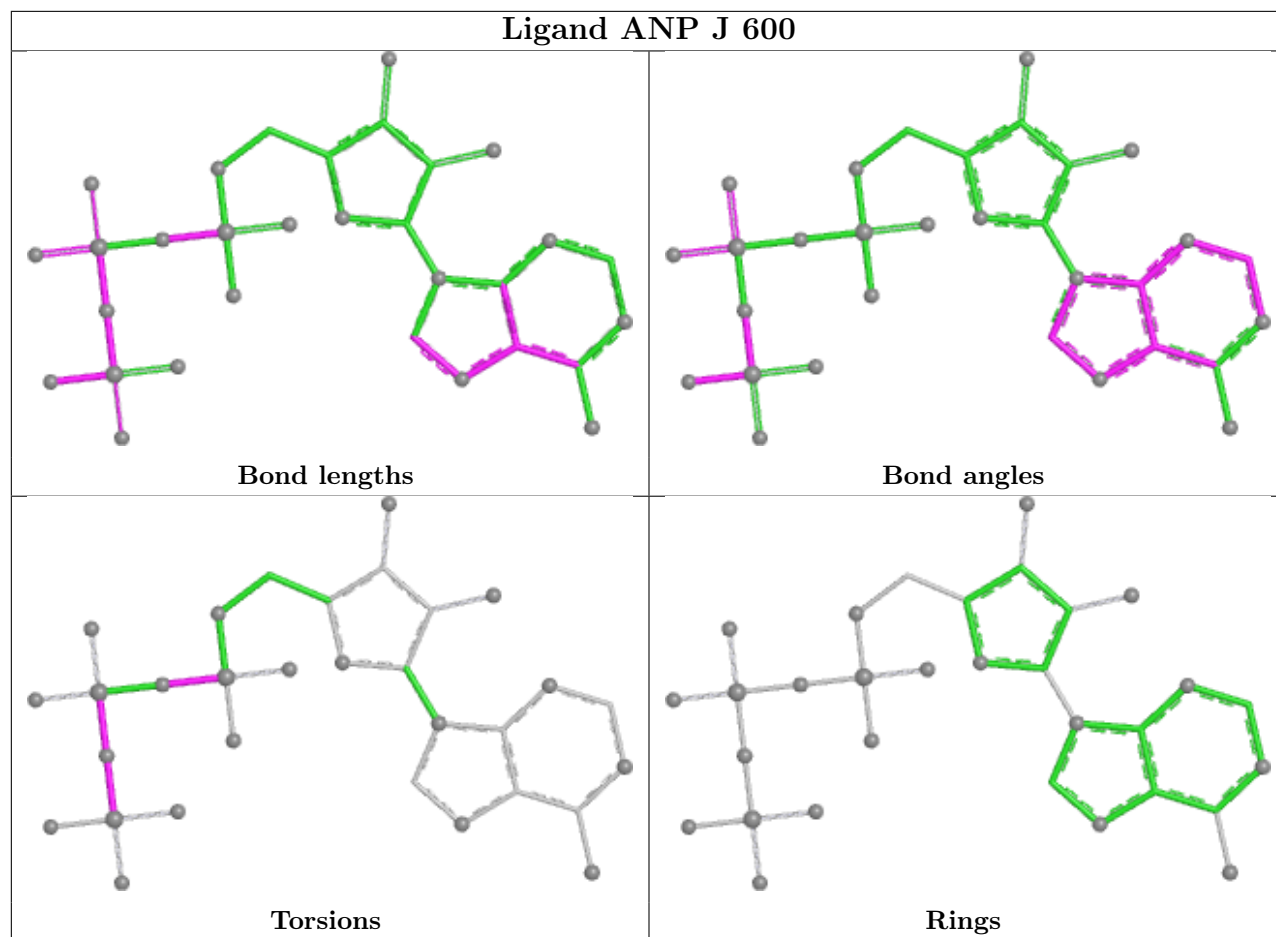


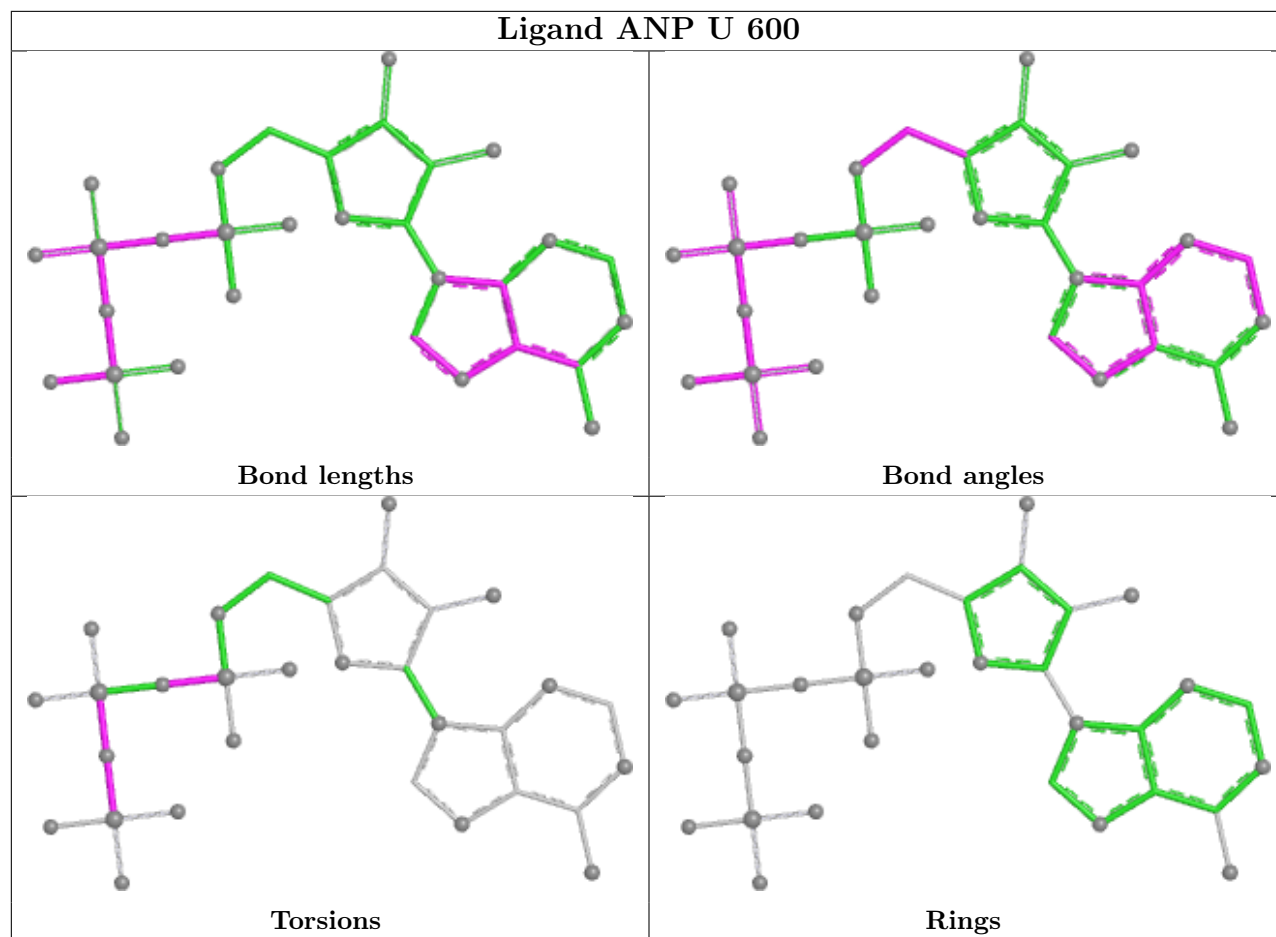


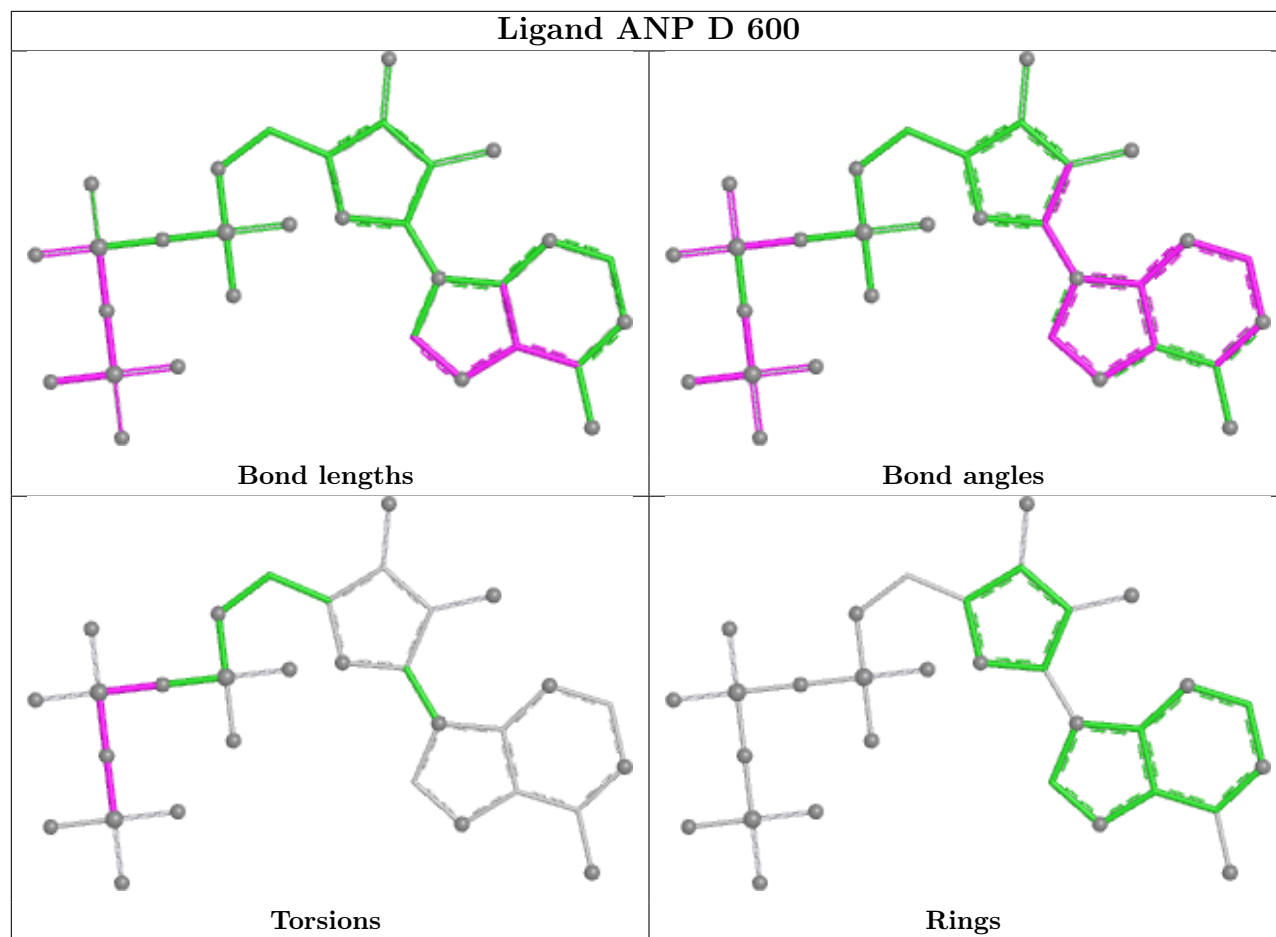


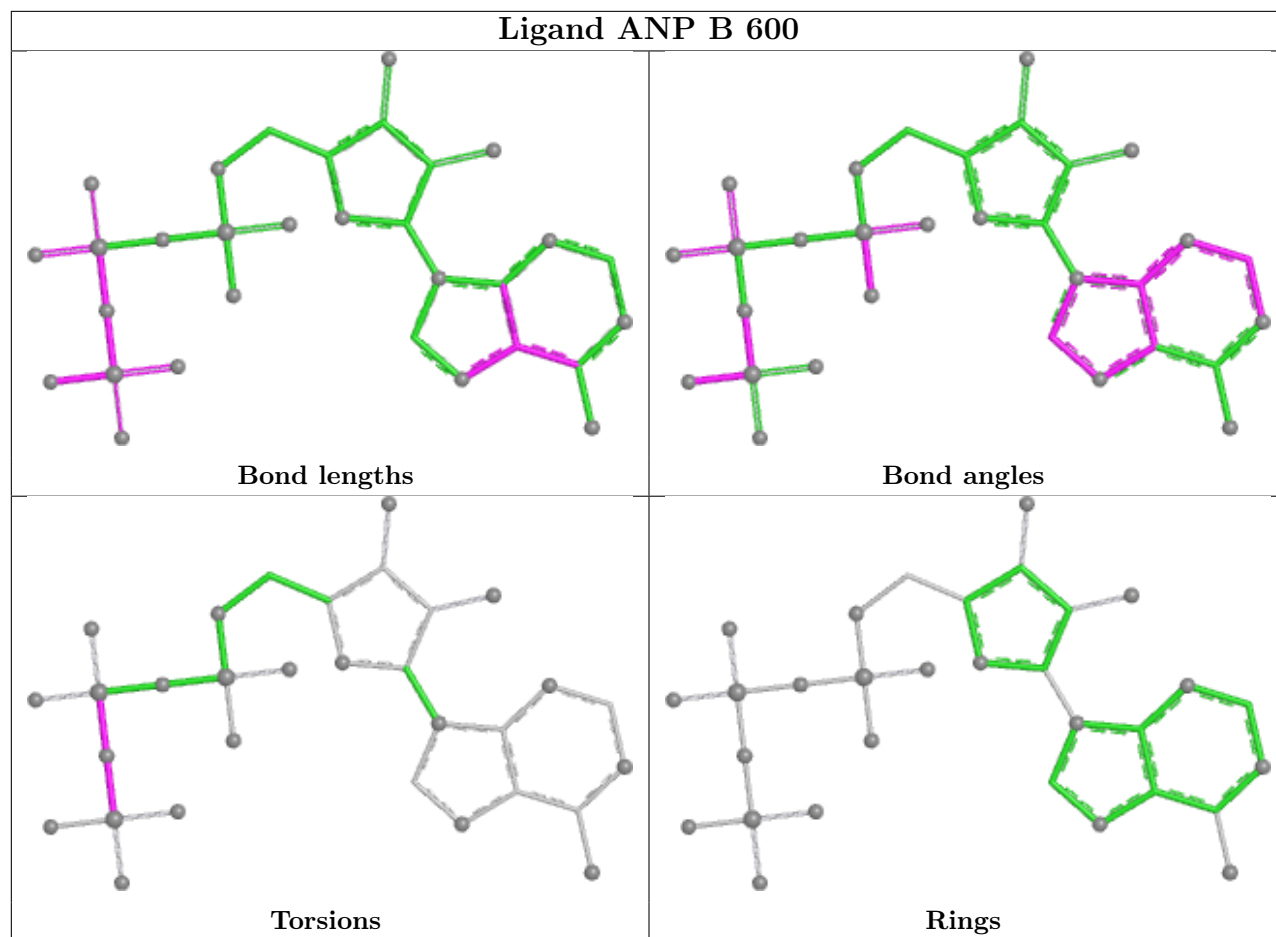


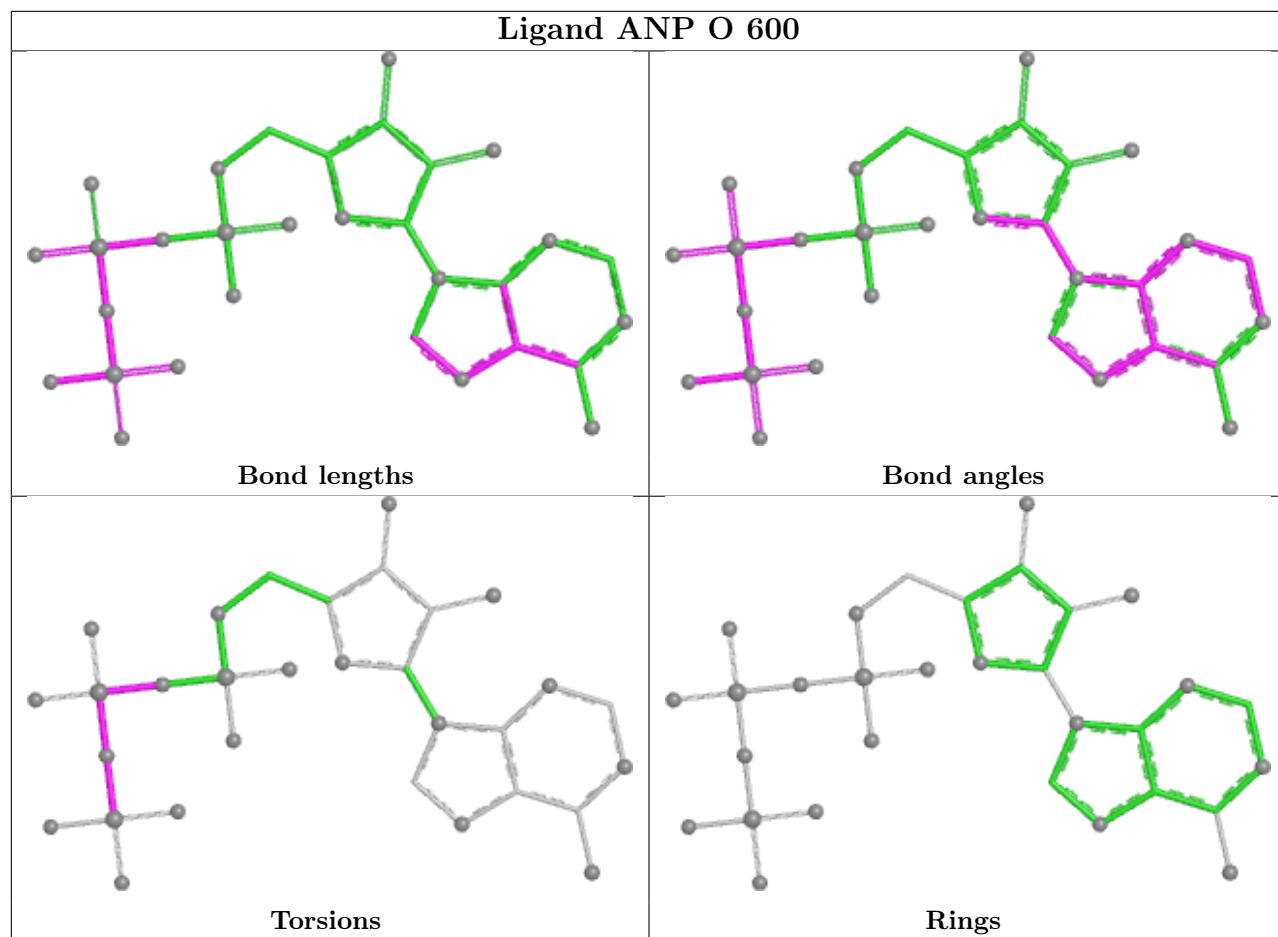


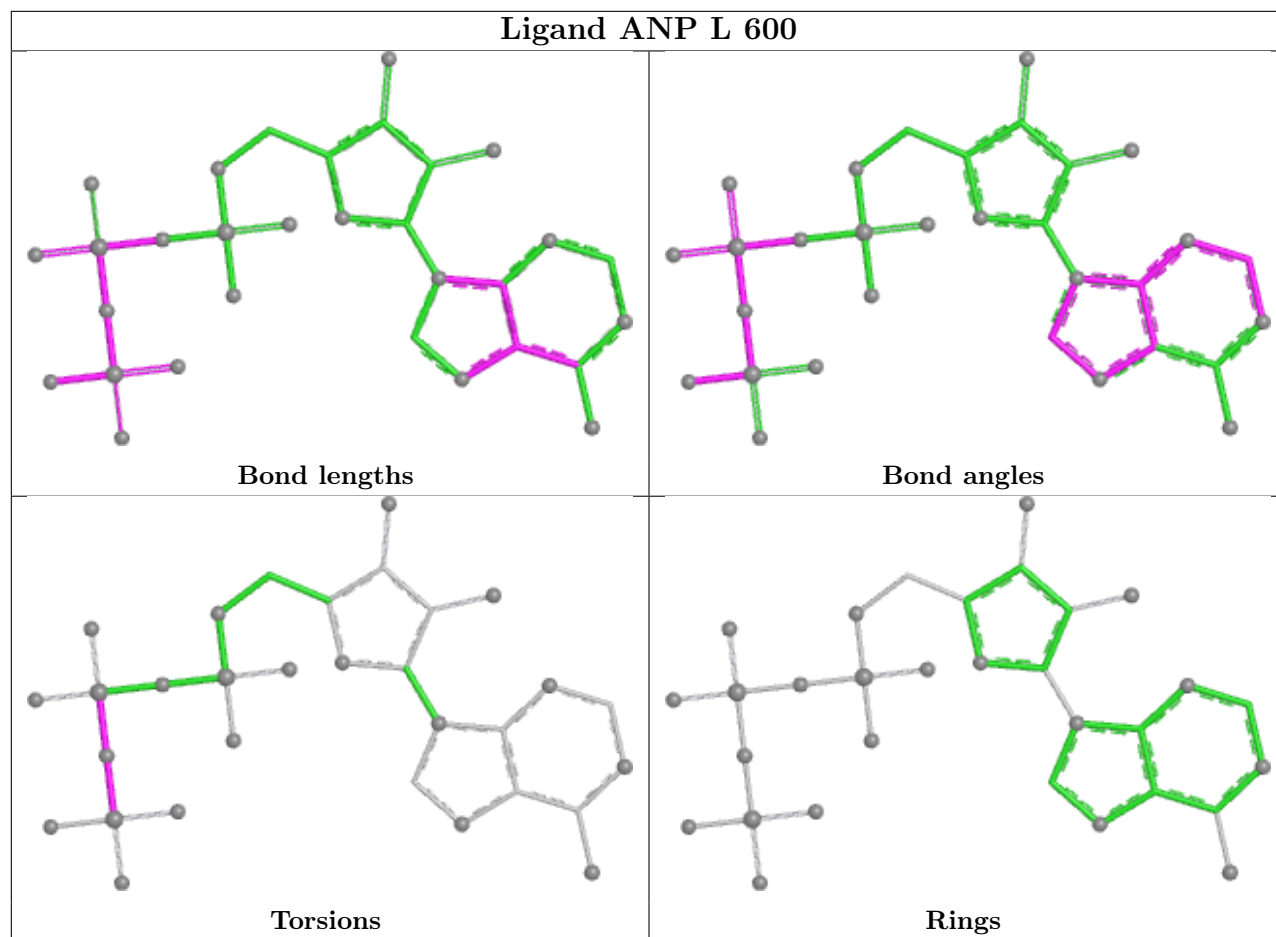


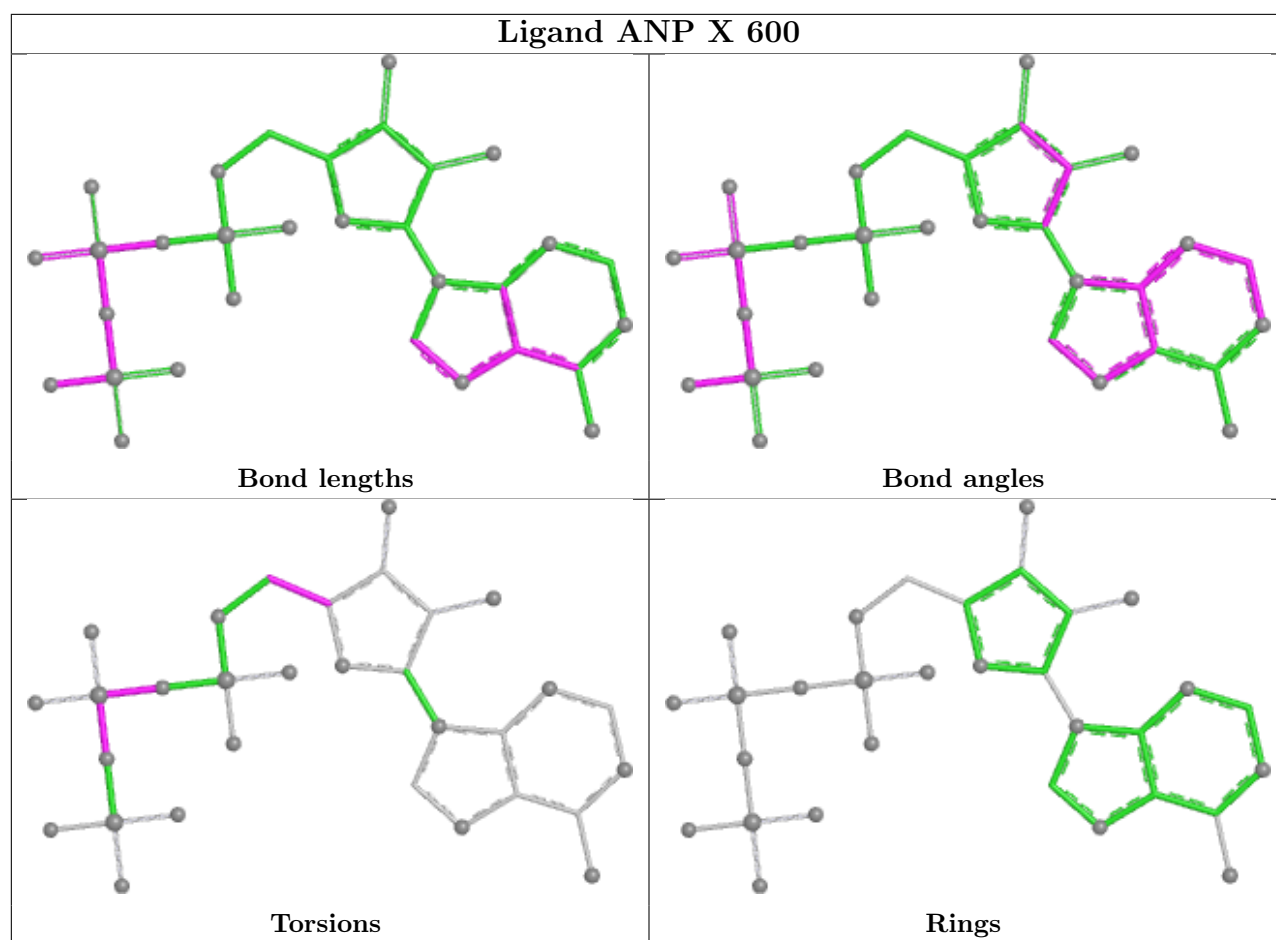












5.7 Other polymers [\(i\)](#)

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, 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	482/510 (94%)	-0.56	0 100 100	37, 55, 89, 139	0
1	B	483/510 (94%)	-0.49	1 (0%) 91 92	35, 58, 109, 138	0
1	C	484/510 (94%)	-0.34	0 100 100	47, 74, 127, 169	0
1	J	481/510 (94%)	-0.41	3 (0%) 85 85	45, 72, 114, 155	0
1	K	486/510 (95%)	-0.50	1 (0%) 91 92	41, 64, 116, 150	0
1	L	482/510 (94%)	-0.44	0 100 100	46, 62, 113, 162	0
1	S	477/510 (93%)	0.51	15 (3%) 51 49	95, 123, 165, 179	0
1	T	478/510 (93%)	0.31	11 (2%) 61 58	93, 120, 148, 167	0
1	U	481/510 (94%)	0.55	20 (4%) 40 39	85, 120, 151, 163	0
2	D	470/484 (97%)	-0.44	1 (0%) 91 92	43, 66, 102, 136	0
2	E	468/484 (96%)	-0.41	2 (0%) 88 89	36, 61, 129, 168	0
2	F	469/484 (96%)	-0.40	1 (0%) 91 92	42, 75, 98, 120	0
2	M	470/484 (97%)	-0.24	3 (0%) 85 85	51, 81, 139, 168	0
2	N	470/484 (97%)	-0.44	1 (0%) 91 92	42, 62, 117, 157	0
2	O	468/484 (96%)	-0.42	0 100 100	44, 70, 103, 129	0
2	V	470/484 (97%)	0.33	9 (1%) 66 63	85, 122, 151, 172	0
2	W	467/484 (96%)	0.35	13 (2%) 55 52	92, 107, 138, 156	0
2	X	469/484 (96%)	0.31	9 (1%) 66 63	66, 125, 158, 176	0
3	G	266/278 (95%)	0.07	0 100 100	49, 102, 128, 137	0
3	P	244/278 (87%)	0.45	11 (4%) 38 37	50, 117, 137, 152	0
3	Y	200/278 (71%)	0.38	4 (2%) 65 62	89, 116, 141, 152	0
4	H	122/138 (88%)	0.58	4 (3%) 49 47	96, 126, 153, 160	0
4	Q	83/138 (60%)	1.10	10 (12%) 9 8	113, 135, 153, 156	0
4	Z	17/138 (12%)	0.73	0 100 100	134, 138, 144, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	1	27/61 (44%)	1.02	1 (3%) 45 43	119, 126, 131, 136	0
5	I	49/61 (80%)	0.53	3 (6%) 27 26	98, 111, 131, 143	0
5	R	34/61 (55%)	1.03	6 (17%) 4 4	107, 118, 147, 152	0
All	All	9597/10377 (92%)	-0.09	129 (1%) 75 74	35, 90, 146, 179	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	15	ALA	5.2
3	Y	105	ALA	4.7
4	Q	97	SER	4.3
4	Q	84	CYS	4.0
1	U	266	ALA	4.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PO4	E	800	5/5	0.74	0.10	101,101,102,103	0
6	ANP	S	600	31/31	0.81	0.11	74,79,82,83	0
7	MG	O	700	1/1	0.85	0.12	55,55,55,55	0
8	PO4	N	800	5/5	0.85	0.09	96,97,97,97	0
6	ANP	T	600	31/31	0.88	0.09	75,82,84,85	0
7	MG	T	700	1/1	0.88	0.07	65,65,65,65	0
7	MG	F	700	1/1	0.89	0.14	56,56,56,56	0
7	MG	X	700	1/1	0.89	0.09	65,65,65,65	0
6	ANP	V	600	31/31	0.90	0.09	77,85,87,88	0

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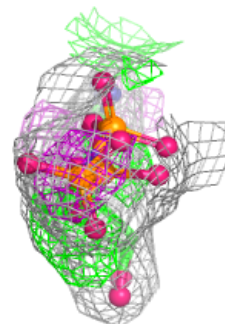
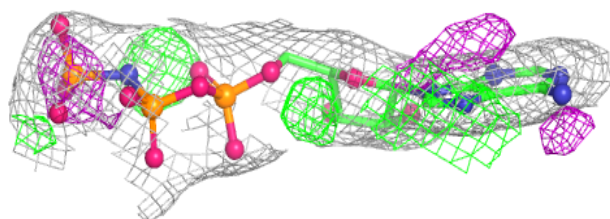
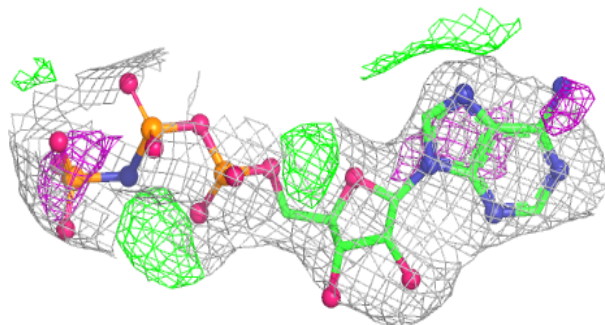
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ANP	U	600	31/31	0.91	0.10	71,74,77,79	0
7	MG	D	700	1/1	0.91	0.13	57,57,57,57	0
7	MG	C	700	1/1	0.92	0.14	56,56,56,56	0
7	MG	L	700	1/1	0.92	0.18	52,52,52,52	0
6	ANP	X	600	31/31	0.92	0.09	75,79,83,85	0
7	MG	S	700	1/1	0.92	0.07	64,64,64,64	0
6	ANP	M	600	31/31	0.93	0.09	64,77,78,78	0
7	MG	U	700	1/1	0.94	0.07	75,75,75,75	0
7	MG	B	700	1/1	0.94	0.12	50,50,50,50	0
7	MG	M	700	1/1	0.95	0.12	57,57,57,57	0
7	MG	V	700	1/1	0.95	0.12	67,67,67,67	0
7	MG	J	700	1/1	0.95	0.13	52,52,52,52	0
7	MG	K	700	1/1	0.95	0.14	47,47,47,47	0
6	ANP	C	600	31/31	0.95	0.07	60,70,72,73	0
6	ANP	A	600	31/31	0.96	0.08	50,60,62,62	0
6	ANP	D	600	31/31	0.96	0.07	62,66,69,71	0
6	ANP	F	600	31/31	0.96	0.07	58,65,69,70	0
7	MG	A	700	1/1	0.96	0.16	47,47,47,47	0
6	ANP	B	600	31/31	0.97	0.07	53,63,65,65	0
6	ANP	O	600	31/31	0.97	0.08	58,62,72,72	0
6	ANP	J	600	31/31	0.97	0.06	58,73,81,82	0
6	ANP	L	600	31/31	0.97	0.07	57,61,63,64	0
6	ANP	K	600	31/31	0.98	0.07	51,60,62,63	0

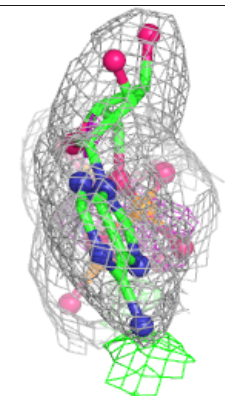
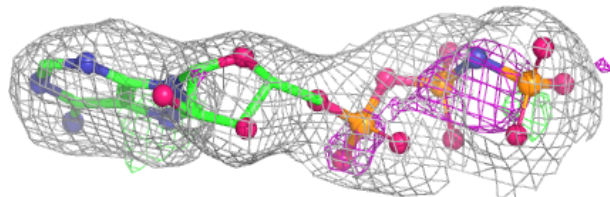
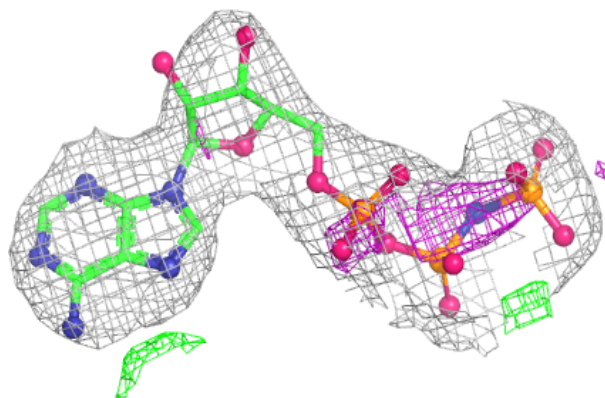
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP S 600:

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

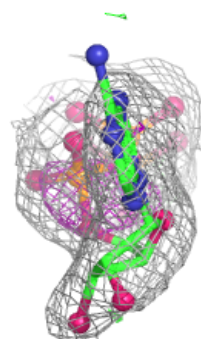
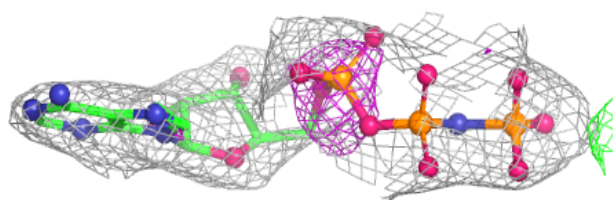
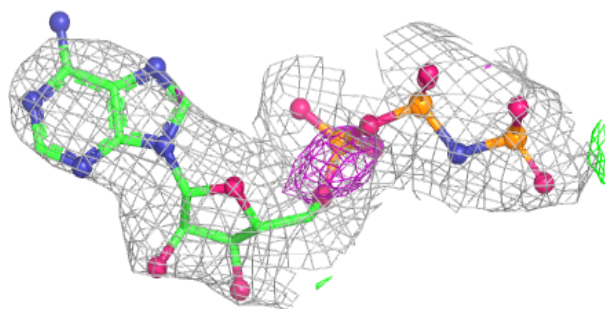
**Electron density around ANP T 600:**

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and green (positive)

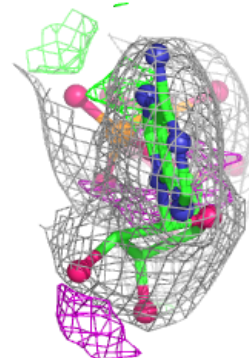
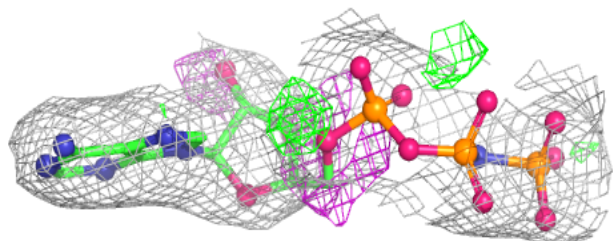
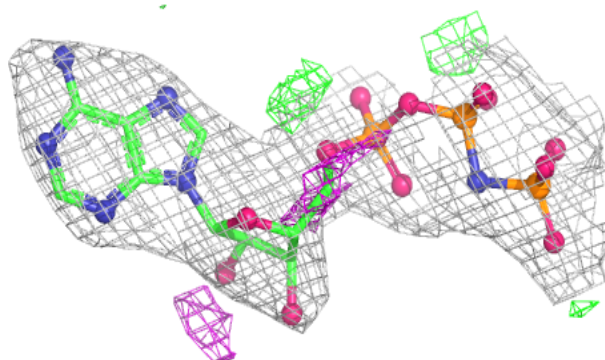


Electron density around ANP V 600:

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and green (positive)

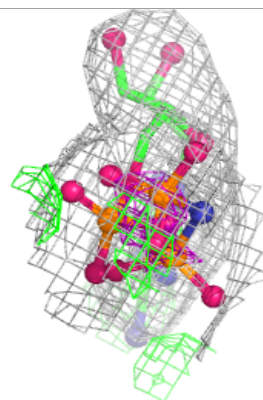
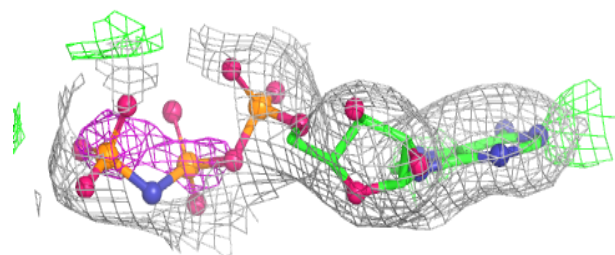
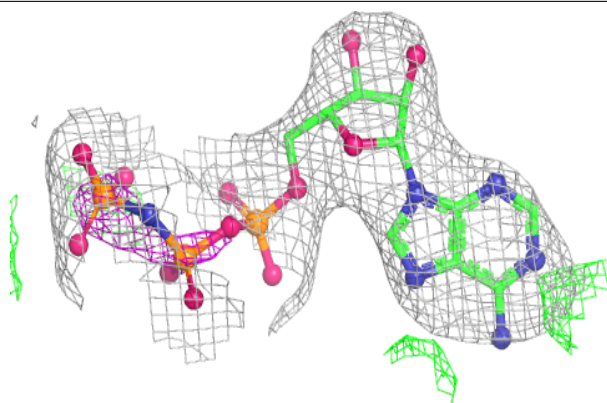
**Electron density around ANP U 600:**

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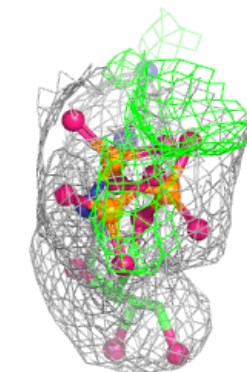
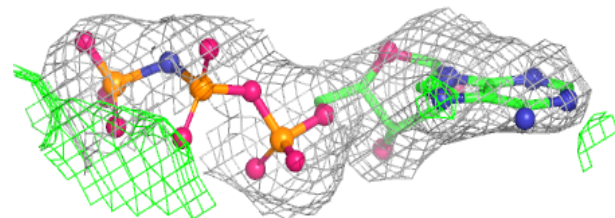
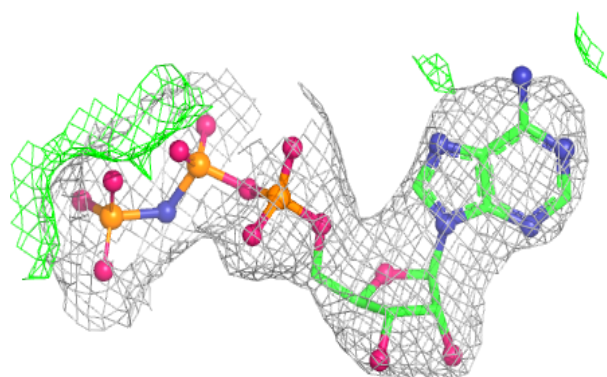


Electron density around ANP X 600:

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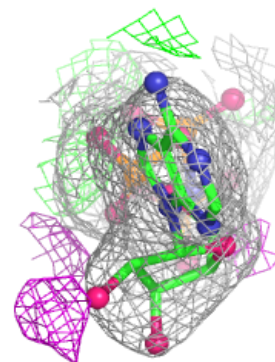
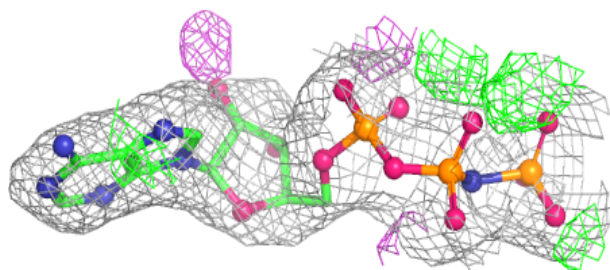
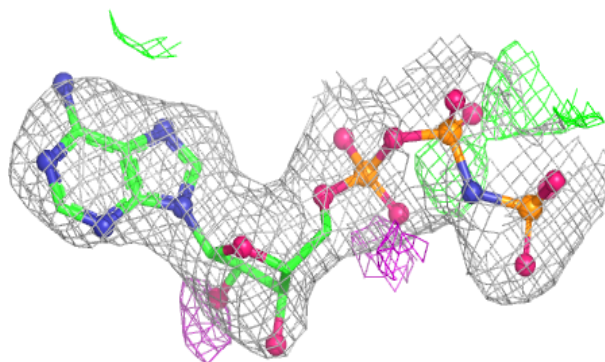
**Electron density around ANP M 600:**

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and green (positive)

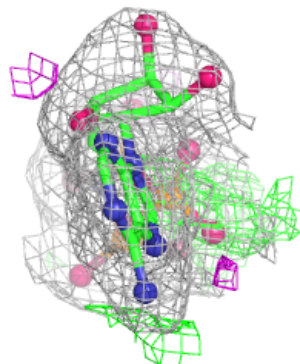
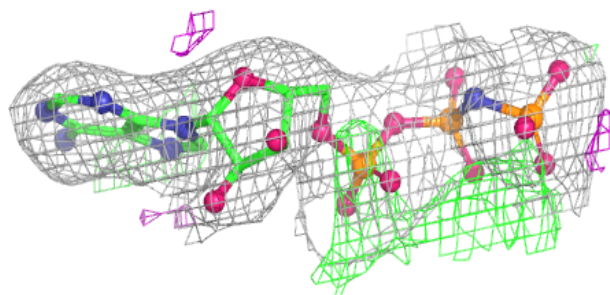
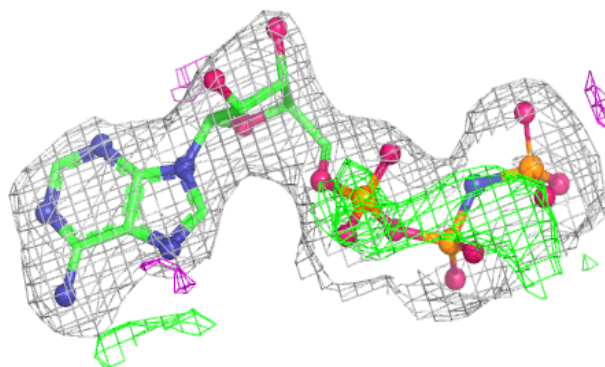


Electron density around ANP C 600:

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

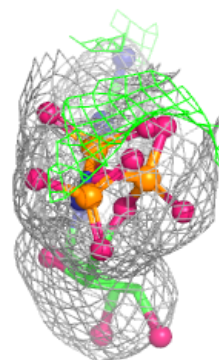
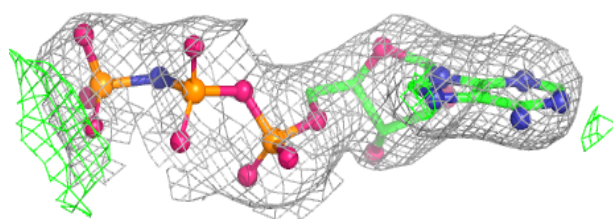
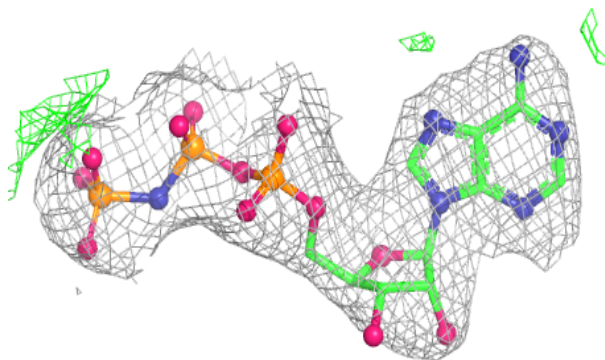
**Electron density around ANP A 600:**

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

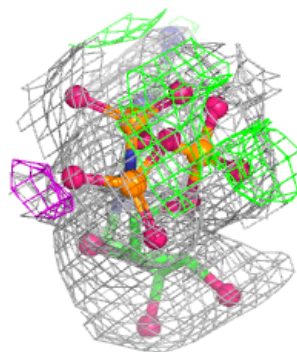
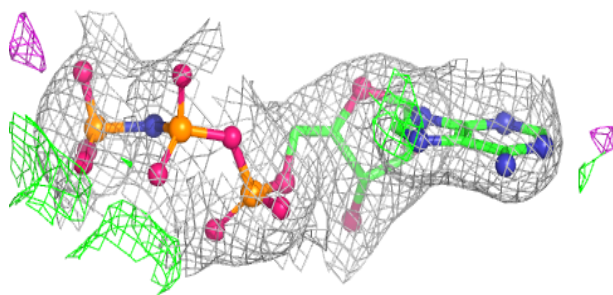
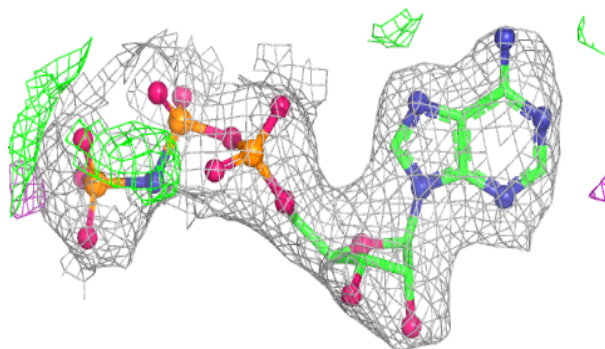


Electron density around ANP D 600:

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

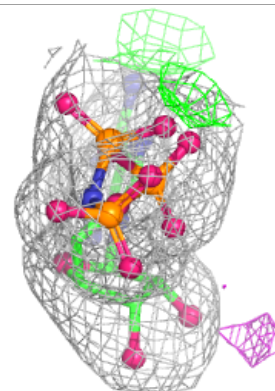
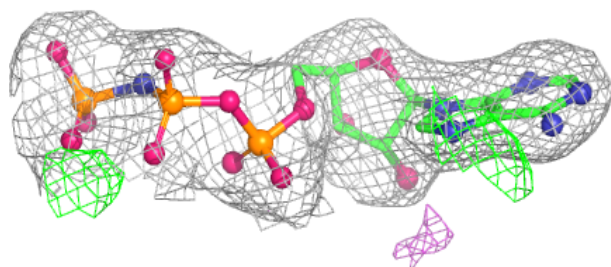
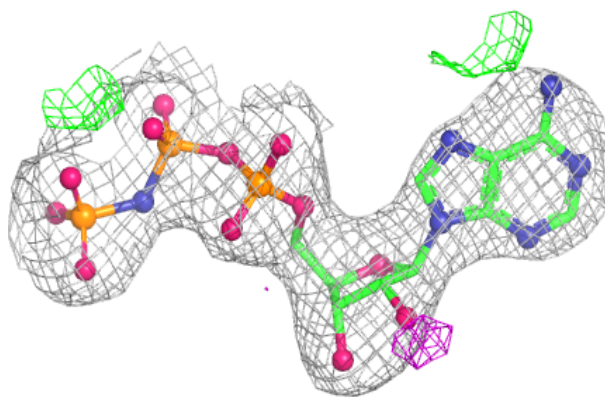
**Electron density around ANP F 600:**

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

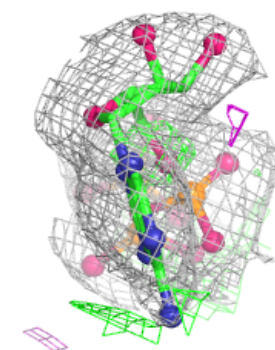
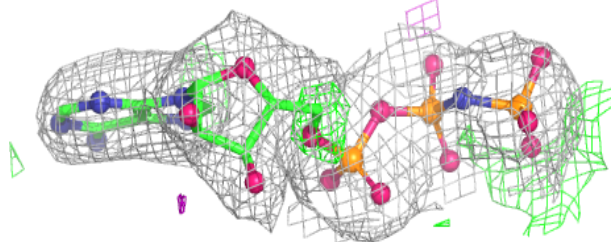
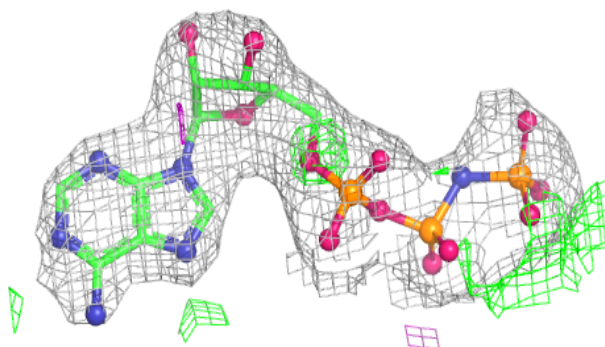


Electron density around ANP B 600:

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

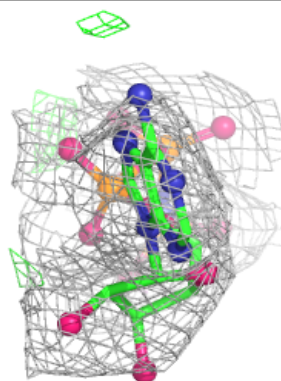
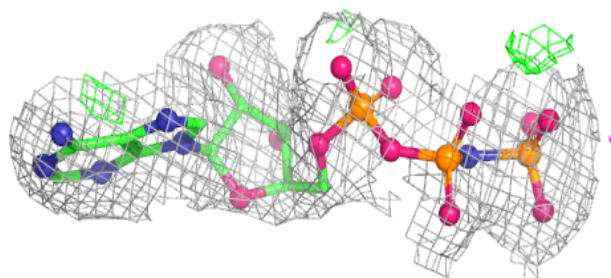
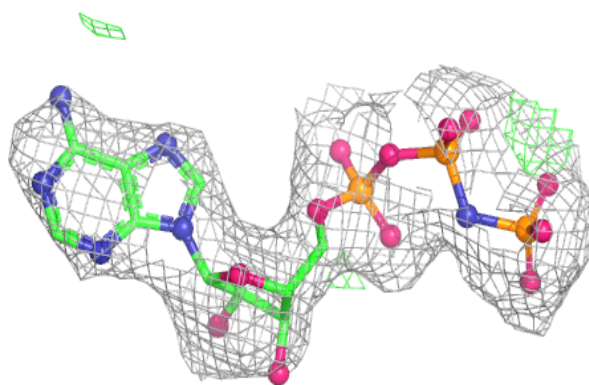
**Electron density around ANP O 600:**

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

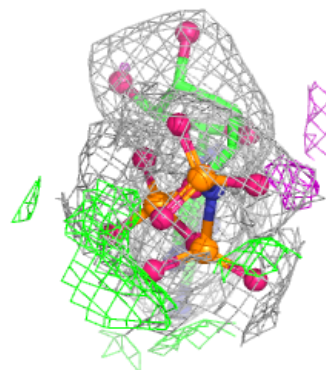
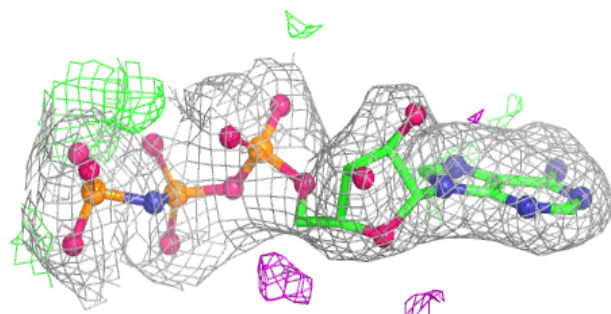
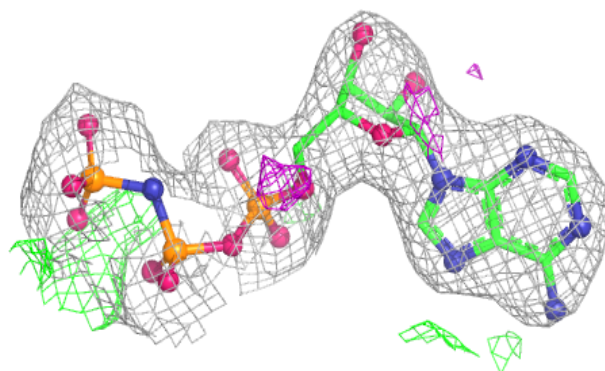


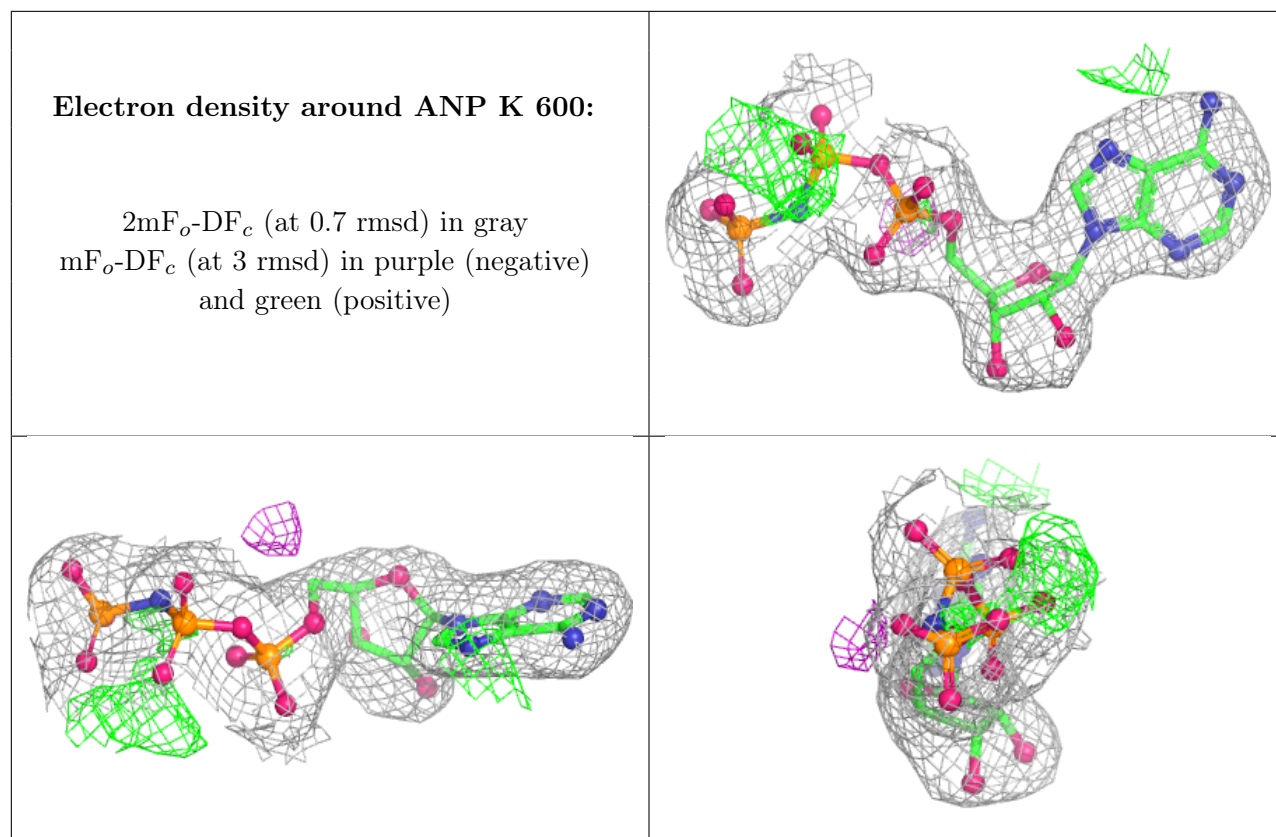
Electron density around ANP J 600:

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

**Electron density around ANP L 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.