



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 09:17 am BST

PDB ID : 3OE7
Title : Structure of four mutant forms of yeast f1 ATPase: gamma-I270T
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.
Deposited on : 2010-08-12
Resolution : 3.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

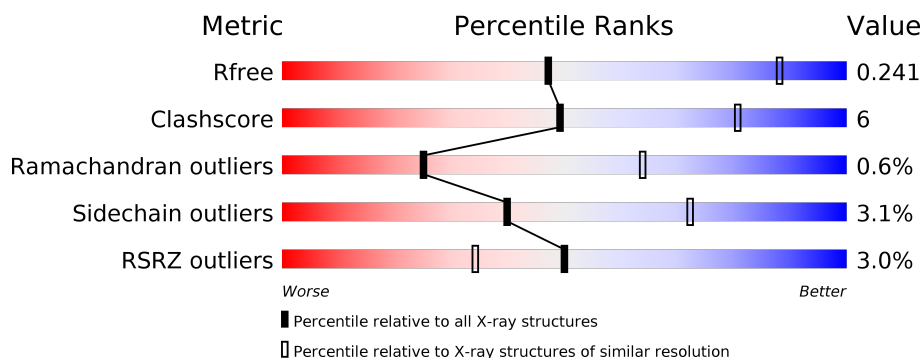
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	510	<div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div>
1	B	510	<div> <div>4%</div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>
1	C	510	<div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div>
1	J	510	<div> <div>80%</div> <div>14%</div> <div>• 6%</div> </div>
1	K	510	<div> <div>4%</div> <div>78%</div> <div>16%</div> <div>5%</div> </div>
1	L	510	<div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	S	510	
1	T	510	
1	U	510	
2	D	484	
2	E	484	
2	F	484	
2	M	484	
2	N	484	
2	O	484	
2	V	484	
2	W	484	
2	X	484	
3	G	278	
3	P	278	
3	Y	278	
4	H	137	
4	Q	137	
4	Z	137	
5	1	61	
5	I	61	
5	R	61	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 72533 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
1	A	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	B	483	Total	C	N	O	S	0	0	0
			3669	2317	649	700	3			
1	C	484	Total	C	N	O	S	0	0	0
			3674	2319	650	702	3			
1	J	481	Total	C	N	O	S	0	0	0
			3655	2309	646	697	3			
1	K	486	Total	C	N	O	S	0	0	0
			3694	2331	652	708	3			
1	L	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	S	480	Total	C	N	O	S	0	0	0
			3651	2307	645	696	3			
1	T	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			
1	U	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			

- 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
			3549	2250	604	689	6			
2	E	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	F	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			
2	M	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	N	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	468	Total	C	N	O	S	0	0	0
			3538	2244	602	686	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
3	G	265	Total	C	N	O	S	0	0	0
			2042	1282	356	394	10			
3	P	244	Total	C	N	O	S	0	0	0
			1847	1159	322	357	9			
3	Y	198	Total	C	N	O	S	0	0	0
			1356	827	250	272	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	270	THR	ILE	ENGINEERED MUTATION	UNP P38077
P	270	THR	ILE	ENGINEERED MUTATION	UNP P38077
Y	270	THR	ILE	ENGINEERED MUTATION	UNP P38077

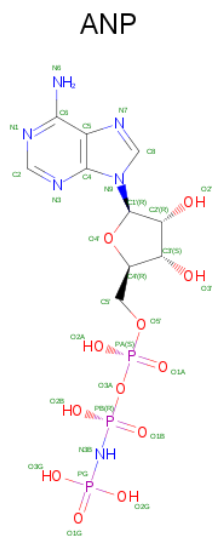
- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	120	Total	C	N	O	S	0	0	0
			775	484	135	154	2			
4	Q	84	Total	C	N	O		0	0	0
			449	271	88	90				
4	Z	15	Total	C	N	O		0	0	0
			75	45	15	15				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	48	Total	C	N	O	0	0	0
			330	204	59	67			
5	R	31	Total	C	N	O	0	0	0
			173	107	32	34			
5	1	25	Total	C	N	O	0	0	0
			125	75	25	25			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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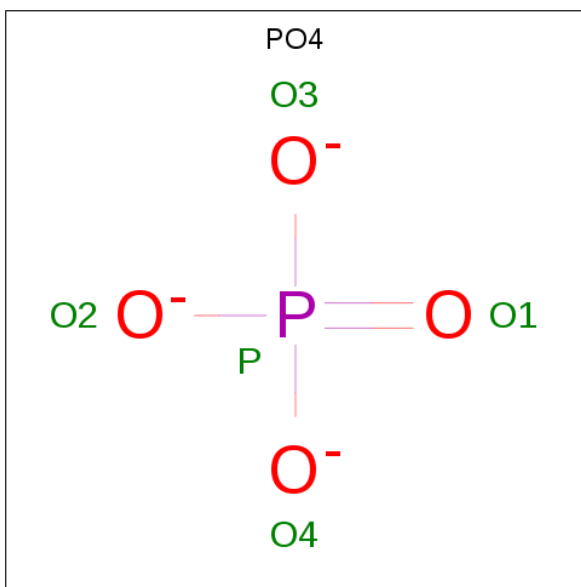
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	X	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

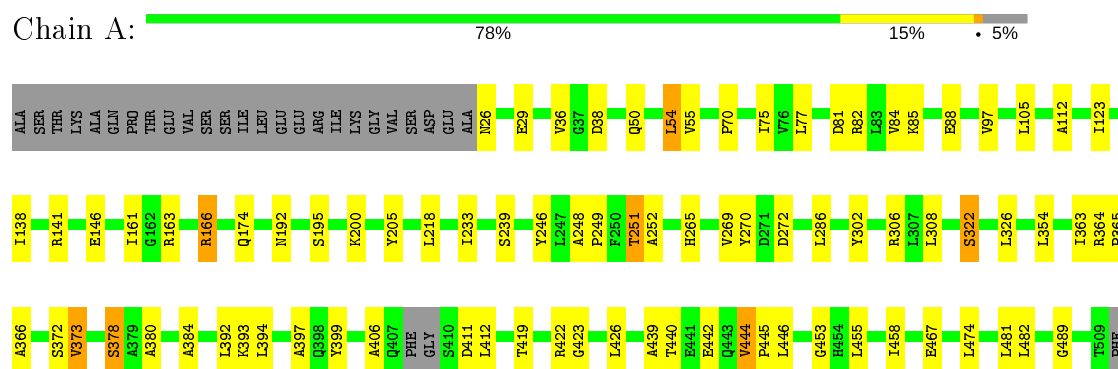


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	O	P	0	0
			5	4	1		

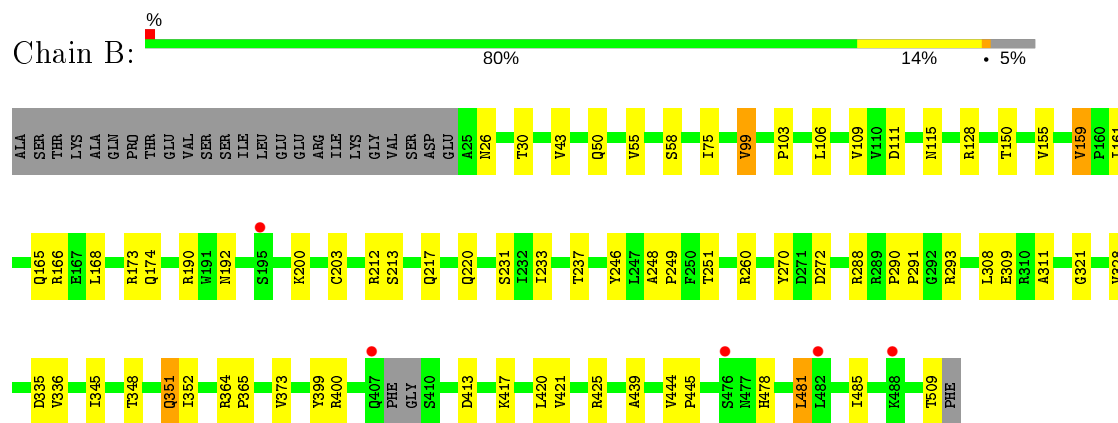
3 Residue-property plots

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

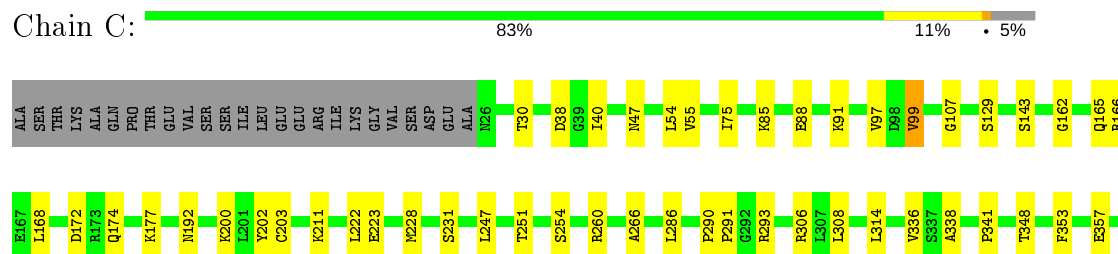
• Molecule 1: ATP synthase subunit alpha

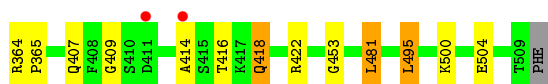


• Molecule 1: ATP synthase subunit alpha



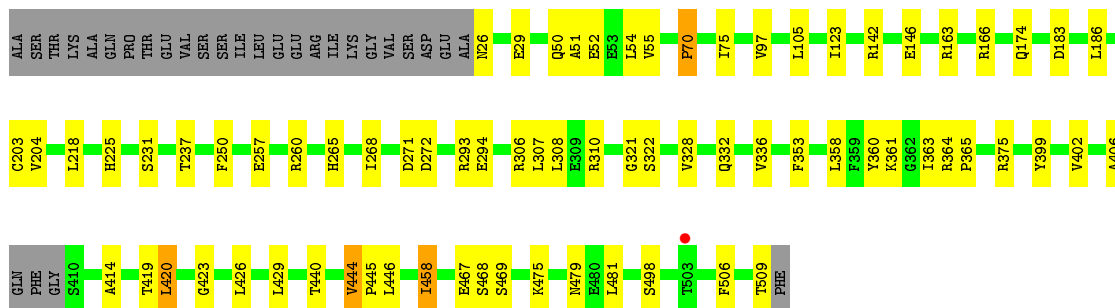
• Molecule 1: ATP synthase subunit alpha





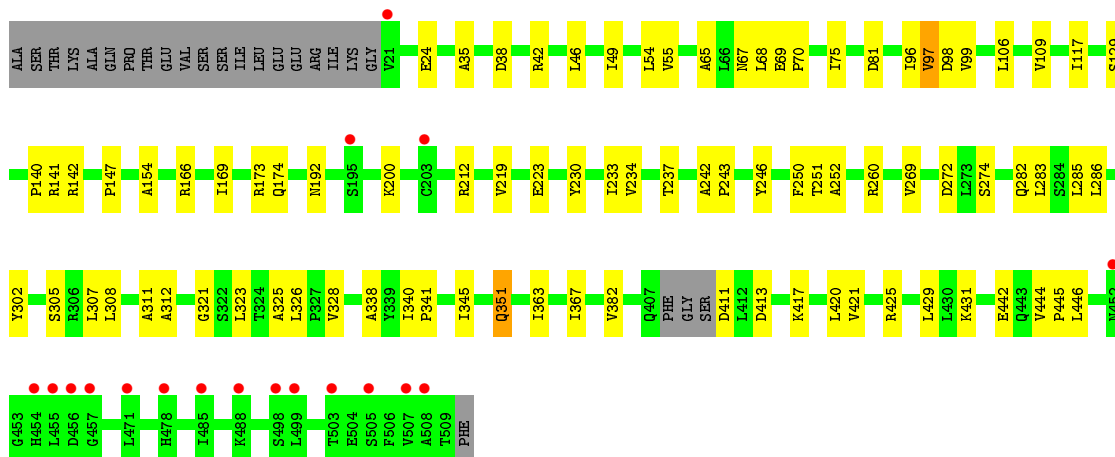
- Molecule 1: ATP synthase subunit alpha

Chain J: 80% 14% 6%



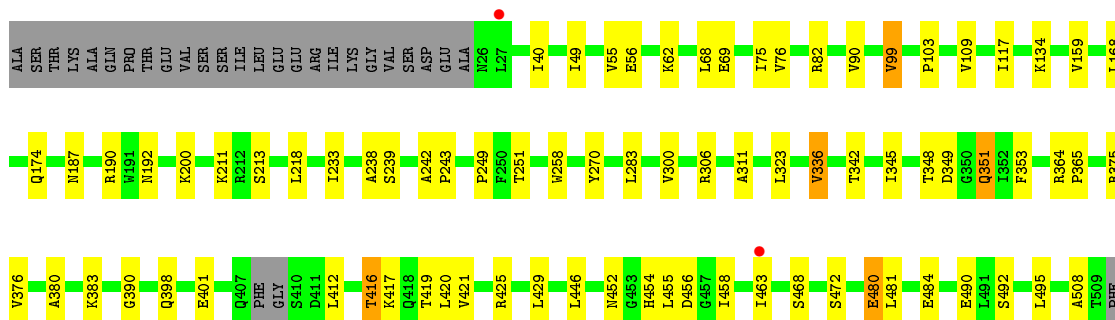
- Molecule 1: ATP synthase subunit alpha

Chain K: 4% 78% 16% 5%

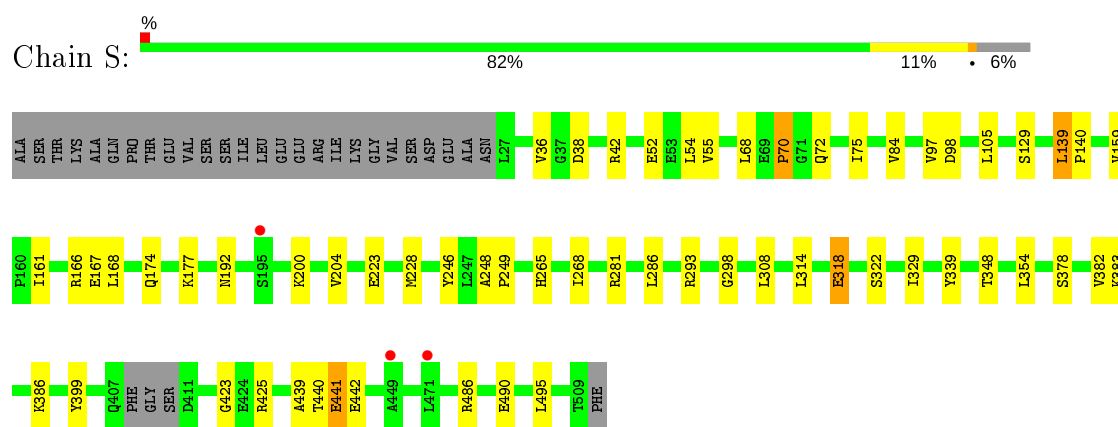


- Molecule 1: ATP synthase subunit alpha

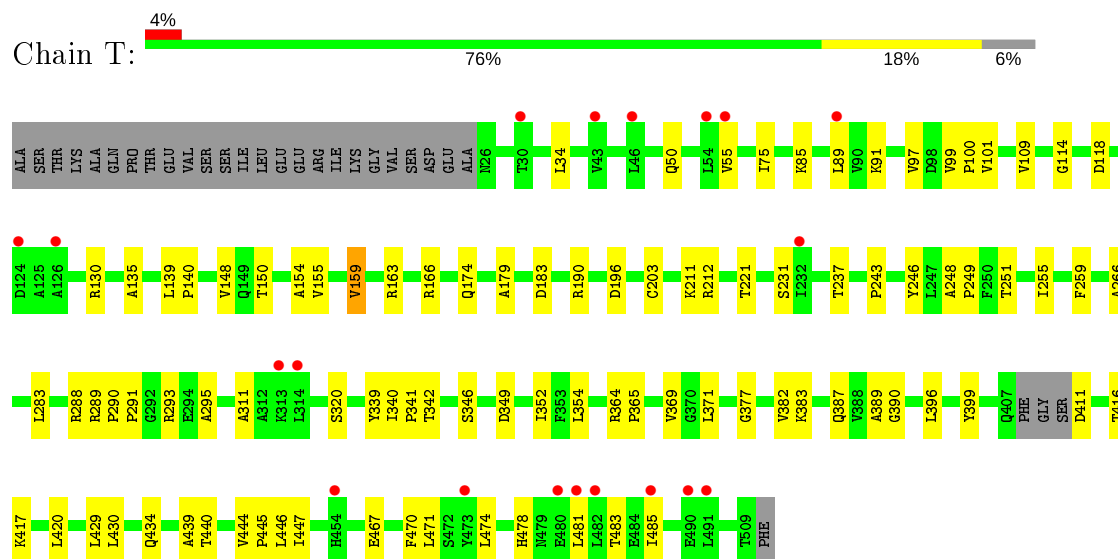
Chain L: 79% 15% 5%



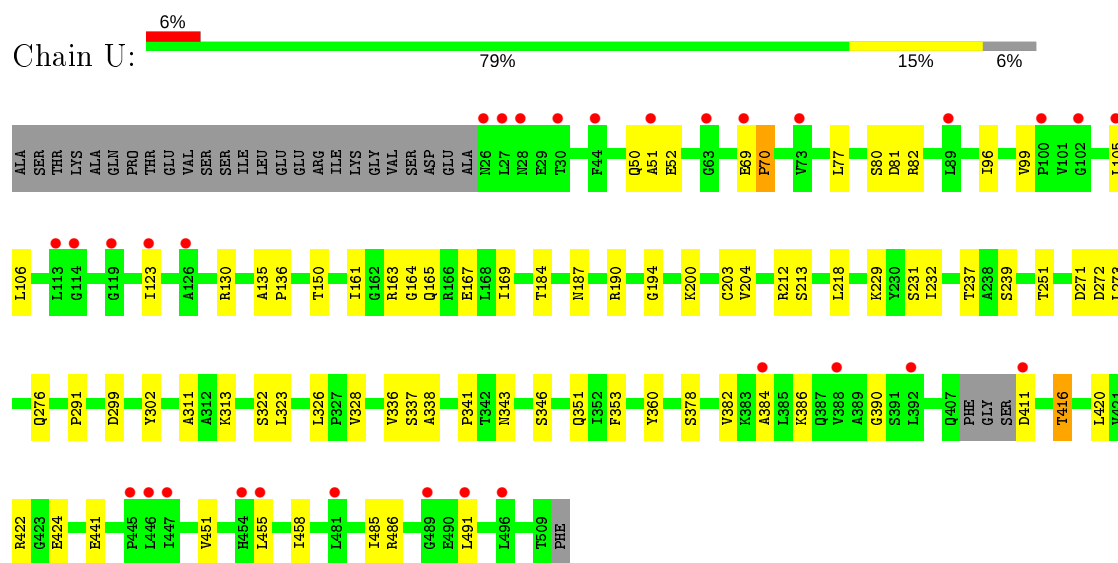
- Molecule 1: ATP synthase subunit alpha



• Molecule 1: ATP synthase subunit alpha

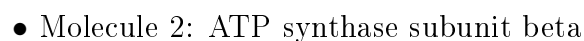


• Molecule 1: ATP synthase subunit alpha

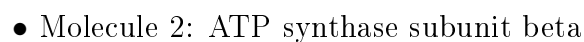


• Molecule 2: ATP synthase subunit beta

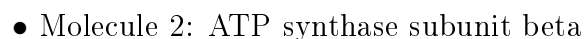
82% 14% .



Response	Percentage
Yes	3%
No	80%
Don't know	16%

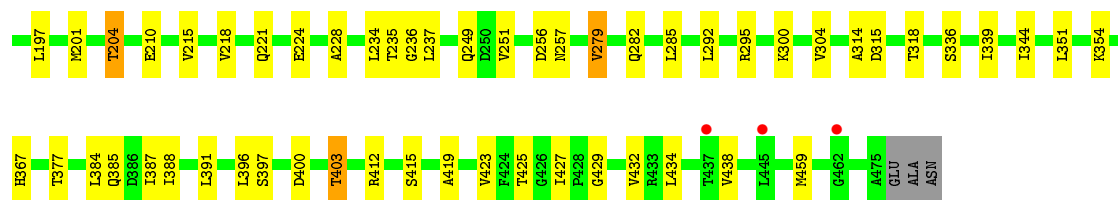


82% 15% •

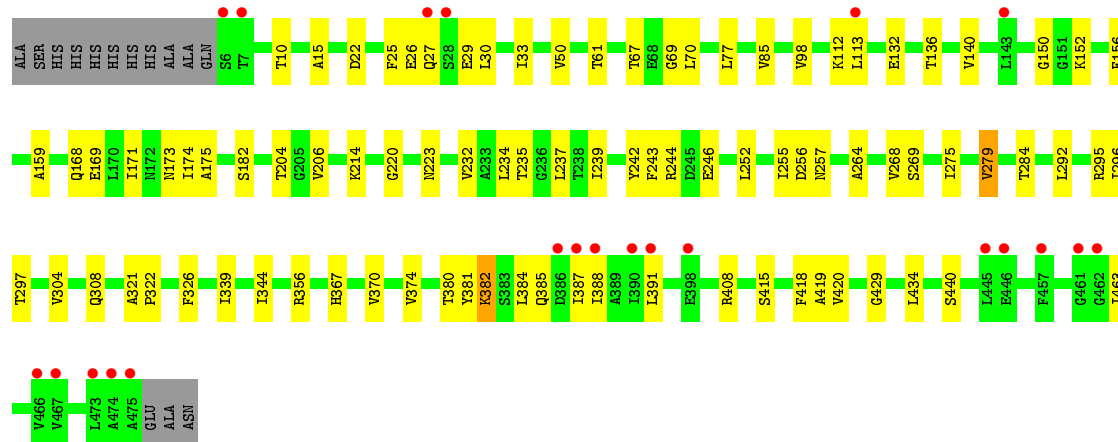
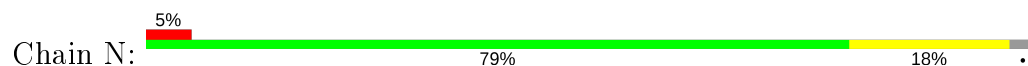


Response	Percentage
Yes	80%
No	16%

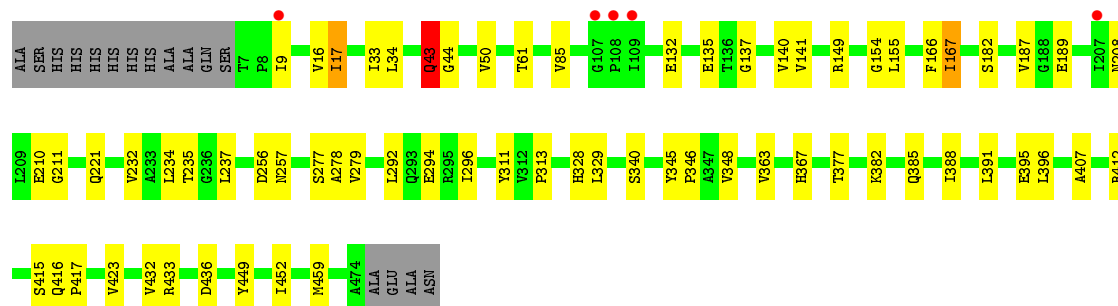
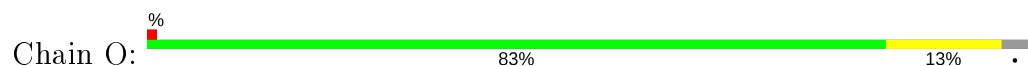




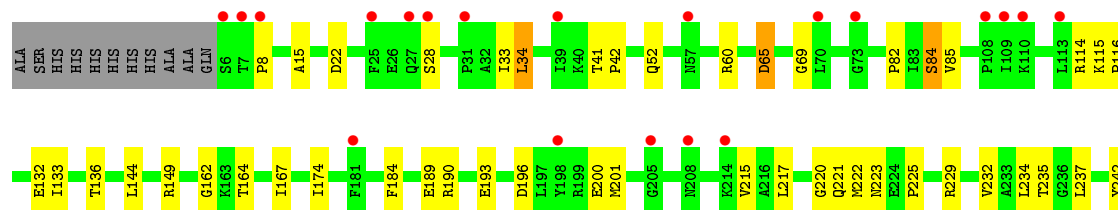
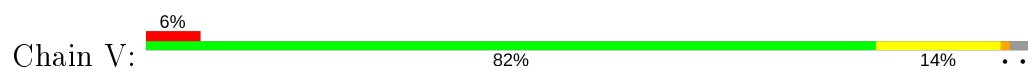
• Molecule 2: ATP synthase subunit beta

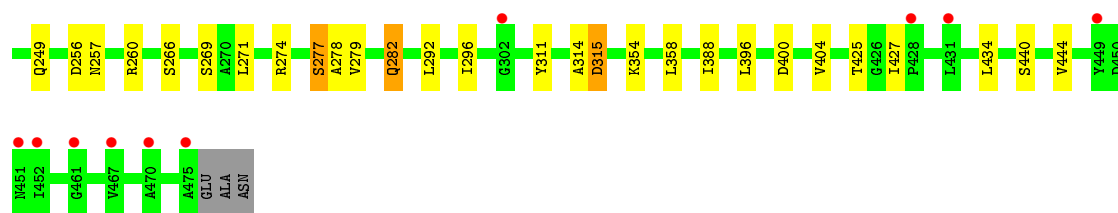


• Molecule 2: ATP synthase subunit beta

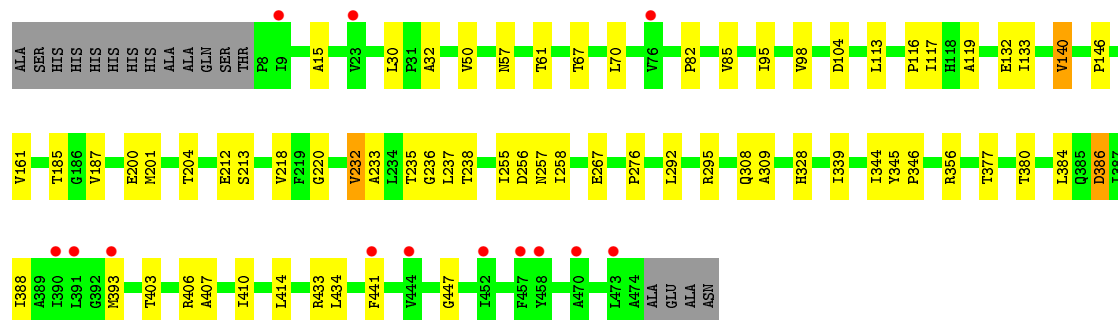
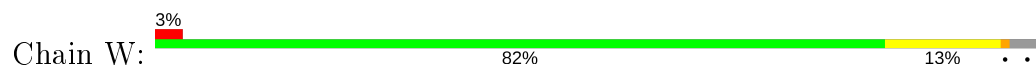


• Molecule 2: ATP synthase subunit beta

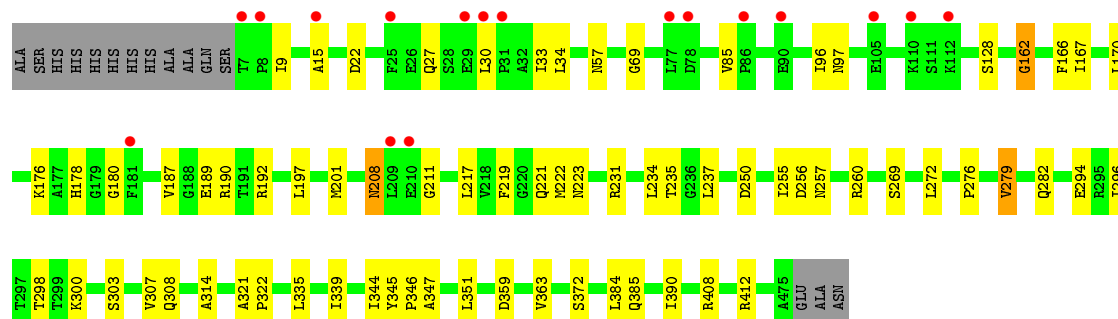
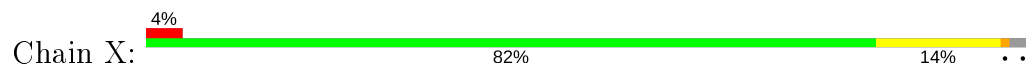




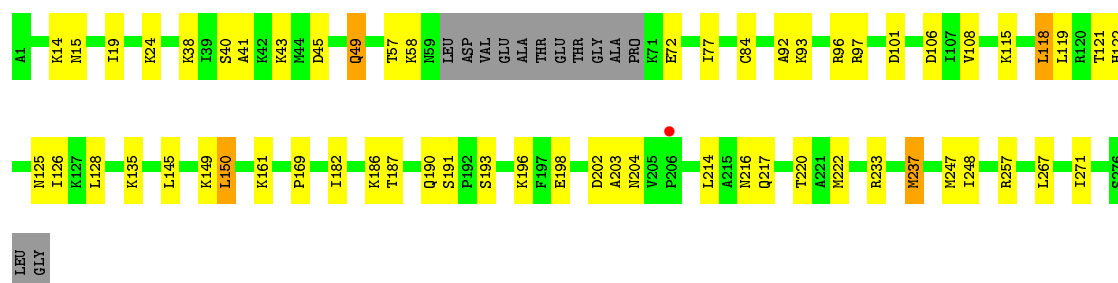
• Molecule 2: ATP synthase subunit beta



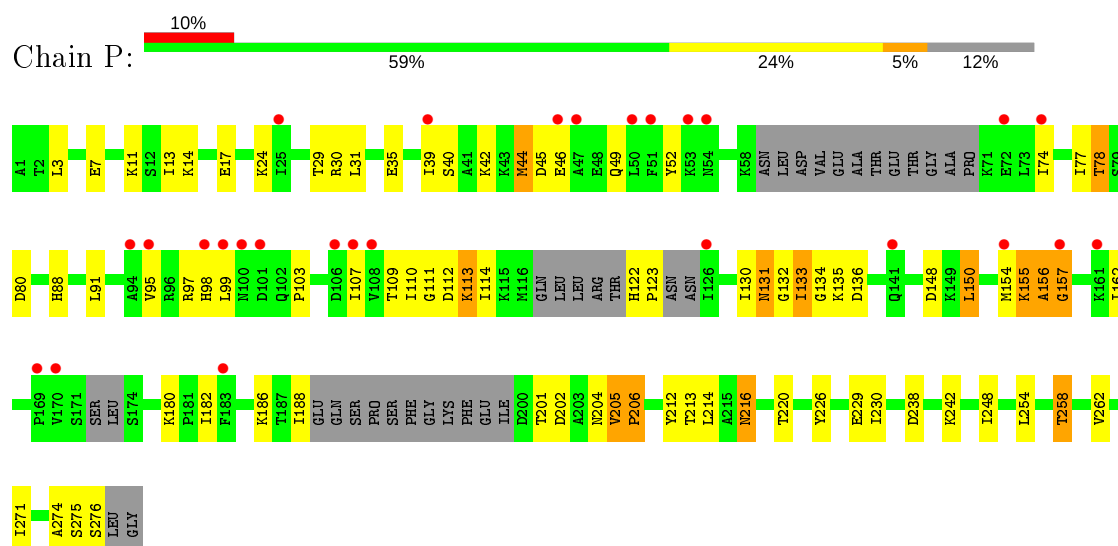
• Molecule 2: ATP synthase subunit beta



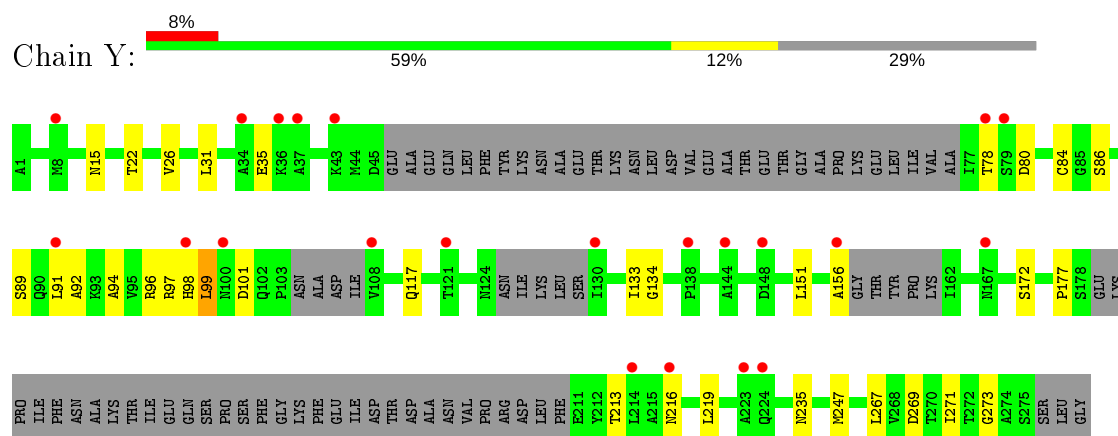
• Molecule 3: ATP synthase subunit gamma



• Molecule 3: ATP synthase subunit gamma



• Molecule 3: ATP synthase subunit gamma





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.03Å 292.21Å 189.05Å 90.00° 101.82° 90.00°	Depositor
Resolution (Å)	20.00 – 3.19 49.47 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-3.19) 95.4 (49.47-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.189 , 0.245 0.188 , 0.241	Depositor DCC
R_{free} test set	9702 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	84.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	72533	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: PO4, ANP, MG

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	0.43	0/3718	0.60	0/5032
1	B	0.38	0/3723	0.56	0/5039
1	C	0.39	0/3729	0.56	0/5048
1	J	0.36	0/3709	0.54	0/5020
1	K	0.37	0/3748	0.53	0/5073
1	L	0.40	0/3718	0.57	0/5032
1	S	0.36	0/3705	0.54	0/5014
1	T	0.36	0/3713	0.51	0/5025
1	U	0.37	0/3713	0.52	0/5025
2	D	0.41	0/3605	0.58	0/4889
2	E	0.41	0/3592	0.56	1/4870 (0.0%)
2	F	0.39	0/3599	0.56	0/4881
2	M	0.40	0/3605	0.56	0/4889
2	N	0.38	0/3605	0.53	0/4889
2	O	0.37	0/3594	0.55	0/4874
2	V	0.37	0/3605	0.53	0/4889
2	W	0.37	0/3587	0.53	0/4863
2	X	0.37	0/3599	0.53	0/4881
3	G	0.39	0/2067	0.54	0/2782
3	P	0.36	0/1865	0.52	0/2508
3	Y	0.32	0/1361	0.46	0/1843
4	H	0.40	0/783	0.54	0/1072
4	Q	0.34	0/448	0.51	0/614
4	Z	0.31	0/74	0.44	0/102
5	1	0.32	0/123	0.50	0/169
5	I	0.44	0/332	0.59	0/452
5	R	0.38	0/173	0.53	0/238
All	All	0.38	0/73093	0.55	1/99013 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	113	LEU	CA-CB-CG	5.21	127.27	115.30

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	3664	0	3747	47	0
1	B	3669	0	3752	41	0
1	C	3674	0	3756	33	0
1	J	3655	0	3739	43	0
1	K	3694	0	3774	51	0
1	L	3664	0	3747	43	0
1	S	3651	0	3739	35	0
1	T	3659	0	3745	49	0
1	U	3659	0	3745	46	0
2	D	3549	0	3620	42	0
2	E	3536	0	3610	42	0
2	F	3543	0	3616	45	0
2	M	3549	0	3620	54	0
2	N	3549	0	3621	54	0
2	O	3538	0	3610	38	0
2	V	3549	0	3620	48	0
2	W	3531	0	3605	41	0
2	X	3543	0	3616	43	0
3	G	2042	0	2102	33	0
3	P	1847	0	1873	43	0
3	Y	1356	0	1262	15	0
4	H	775	0	640	19	0
4	Q	449	0	240	4	0
4	Z	75	0	38	0	0
5	1	125	0	66	1	0
5	I	330	0	260	8	0
5	R	173	0	101	0	0
6	A	31	0	13	1	0
6	B	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	31	0	13	1	0
6	D	31	0	13	4	0
6	F	31	0	13	0	0
6	J	31	0	13	0	0
6	K	31	0	13	0	0
6	L	31	0	13	1	0
6	M	31	0	13	2	0
6	O	31	0	13	0	0
6	S	31	0	13	0	0
6	T	31	0	13	2	0
6	U	31	0	13	0	0
6	V	31	0	13	1	0
6	X	31	0	13	2	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	N	5	0	0	0	0
All	All	72533	0	73059	852	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 6.

The worst 5 of 852 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)
3:G:96:ARG:HE	3:G:121:THR:HG21	1.25	0.98
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.47	0.96
3:P:180:LYS:HZ3	3:P:220:THR:HB	1.33	0.94
1:K:99:VAL:HG11	1:K:251:THR:HB	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.51	0.92

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%)	20 (4%)	2 (0%)	34	69
1	B	479/510 (94%)	457 (95%)	22 (5%)	0	100	100
1	C	482/510 (94%)	460 (95%)	21 (4%)	1 (0%)	47	79
1	J	477/510 (94%)	460 (96%)	15 (3%)	2 (0%)	34	69
1	K	482/510 (94%)	458 (95%)	21 (4%)	3 (1%)	25	64
1	L	478/510 (94%)	454 (95%)	22 (5%)	2 (0%)	34	69
1	S	476/510 (93%)	454 (95%)	21 (4%)	1 (0%)	47	79
1	T	477/510 (94%)	452 (95%)	22 (5%)	3 (1%)	25	64
1	U	477/510 (94%)	447 (94%)	28 (6%)	2 (0%)	34	69
2	D	468/484 (97%)	444 (95%)	22 (5%)	2 (0%)	34	69
2	E	466/484 (96%)	437 (94%)	29 (6%)	0	100	100
2	F	467/484 (96%)	436 (93%)	29 (6%)	2 (0%)	34	69
2	M	468/484 (97%)	442 (94%)	23 (5%)	3 (1%)	25	64
2	N	468/484 (97%)	437 (93%)	29 (6%)	2 (0%)	34	69
2	O	466/484 (96%)	441 (95%)	23 (5%)	2 (0%)	34	69
2	V	468/484 (97%)	424 (91%)	40 (8%)	4 (1%)	17	56
2	W	465/484 (96%)	442 (95%)	23 (5%)	0	100	100
2	X	467/484 (96%)	439 (94%)	25 (5%)	3 (1%)	25	64
3	G	261/278 (94%)	244 (94%)	13 (5%)	4 (2%)	10	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	232/278 (84%)	202 (87%)	22 (10%)	8 (3%)	3	24
3	Y	186/278 (67%)	173 (93%)	12 (6%)	1 (0%)	29	67
4	H	110/137 (80%)	100 (91%)	10 (9%)	0	100	100
4	Q	74/137 (54%)	58 (78%)	11 (15%)	5 (7%)	1	9
4	Z	13/137 (10%)	10 (77%)	2 (15%)	1 (8%)	1	6
5	1	21/61 (34%)	18 (86%)	2 (10%)	1 (5%)	2	17
5	I	42/61 (69%)	32 (76%)	7 (17%)	3 (7%)	1	8
5	R	27/61 (44%)	22 (82%)	3 (11%)	2 (7%)	1	7
All	All	9475/10374 (91%)	8899 (94%)	517 (6%)	59 (1%)	25	64

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	202	ASP
1	J	414	ALA
2	M	28	SER
3	P	156	ALA
3	P	275	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/412 (94%)	373 (96%)	15 (4%)	32	67
1	B	388/412 (94%)	375 (97%)	13 (3%)	37	70
1	C	389/412 (94%)	378 (97%)	11 (3%)	43	74
1	J	387/412 (94%)	375 (97%)	12 (3%)	40	72
1	K	392/412 (95%)	387 (99%)	5 (1%)	69	87
1	L	388/412 (94%)	371 (96%)	17 (4%)	28	64
1	S	387/412 (94%)	379 (98%)	8 (2%)	53	79
1	T	388/412 (94%)	374 (96%)	14 (4%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	388/412 (94%)	381 (98%)	7 (2%)	59	82
2	D	380/390 (97%)	370 (97%)	10 (3%)	46	76
2	E	378/390 (97%)	361 (96%)	17 (4%)	27	63
2	F	379/390 (97%)	366 (97%)	13 (3%)	37	70
2	M	380/390 (97%)	372 (98%)	8 (2%)	53	79
2	N	380/390 (97%)	370 (97%)	10 (3%)	46	76
2	O	379/390 (97%)	370 (98%)	9 (2%)	49	77
2	V	380/390 (97%)	374 (98%)	6 (2%)	62	84
2	W	378/390 (97%)	366 (97%)	12 (3%)	39	71
2	X	379/390 (97%)	374 (99%)	5 (1%)	69	87
3	G	223/236 (94%)	214 (96%)	9 (4%)	31	66
3	P	196/236 (83%)	172 (88%)	24 (12%)	5	22
3	Y	126/236 (53%)	117 (93%)	9 (7%)	14	47
4	H	62/112 (55%)	60 (97%)	2 (3%)	39	71
4	Q	9/112 (8%)	9 (100%)	0	100	100
5	I	24/48 (50%)	24 (100%)	0	100	100
5	R	3/48 (6%)	2 (67%)	1 (33%)	0	0
All	All	7551/8246 (92%)	7314 (97%)	237 (3%)	40	72

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	90	VAL
2	N	10	THR
2	W	386	ASP
1	L	159	VAL
1	L	468	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	398	GLN
2	N	168	GLN
2	X	379	GLN
1	L	479	ASN

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Mol	Chain	Res	Type
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 15 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ANP	T	600	7	29,33,33	1.90	8 (27%)	31,52,52	1.88	8 (25%)
6	ANP	F	600	7	29,33,33	1.69	8 (27%)	31,52,52	1.77	7 (22%)
6	ANP	C	600	7	29,33,33	1.71	7 (24%)	31,52,52	1.85	7 (22%)
6	ANP	B	600	7	29,33,33	1.90	6 (20%)	31,52,52	1.96	6 (19%)
6	ANP	A	600	7	29,33,33	1.95	9 (31%)	31,52,52	1.70	8 (25%)
6	ANP	O	600	7	29,33,33	1.73	8 (27%)	31,52,52	1.89	9 (29%)
6	ANP	M	600	7	29,33,33	1.76	7 (24%)	31,52,52	2.03	6 (19%)
6	ANP	D	600	7	29,33,33	1.80	7 (24%)	31,52,52	1.76	8 (25%)
6	ANP	K	600	7	29,33,33	1.86	8 (27%)	31,52,52	1.91	8 (25%)
8	PO4	N	800	-	4,4,4	0.88	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ANP	U	600	7	29,33,33	1.80	7 (24%)	31,52,52	2.01	8 (25%)
6	ANP	V	600	7	29,33,33	1.81	6 (20%)	31,52,52	2.03	8 (25%)
6	ANP	J	600	7	29,33,33	1.81	7 (24%)	31,52,52	2.00	6 (19%)
6	ANP	L	600	7	29,33,33	1.76	7 (24%)	31,52,52	1.94	9 (29%)
6	ANP	S	600	7	29,33,33	1.82	7 (24%)	31,52,52	1.95	8 (25%)
6	ANP	X	600	7	29,33,33	1.79	8 (27%)	31,52,52	2.04	8 (25%)

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	T	600	7	-	4/14/38/38	0/3/3/3
6	ANP	F	600	7	-	7/14/38/38	0/3/3/3
6	ANP	C	600	7	-	3/14/38/38	0/3/3/3
6	ANP	B	600	7	-	6/14/38/38	0/3/3/3
6	ANP	A	600	7	-	2/14/38/38	0/3/3/3
6	ANP	O	600	7	-	5/14/38/38	0/3/3/3
6	ANP	M	600	7	-	4/14/38/38	0/3/3/3
6	ANP	D	600	7	-	4/14/38/38	0/3/3/3
6	ANP	K	600	7	-	5/14/38/38	0/3/3/3
6	ANP	J	600	7	-	3/14/38/38	0/3/3/3
6	ANP	V	600	7	-	6/14/38/38	0/3/3/3
6	ANP	U	600	7	-	4/14/38/38	0/3/3/3
6	ANP	L	600	7	-	3/14/38/38	0/3/3/3
6	ANP	S	600	7	-	3/14/38/38	0/3/3/3
6	ANP	X	600	7	-	9/14/38/38	0/3/3/3

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	ANP	PG-N3B	4.69	1.75	1.63
6	T	600	ANP	PB-N3B	4.54	1.75	1.63
6	S	600	ANP	PG-N3B	4.51	1.75	1.63
6	A	600	ANP	PB-N3B	4.50	1.75	1.63
6	V	600	ANP	PG-N3B	4.49	1.75	1.63

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	600	ANP	O1G-PG-N3B	-6.32	102.46	111.77
6	J	600	ANP	O1G-PG-N3B	-6.02	102.90	111.77
6	B	600	ANP	O1G-PG-N3B	-6.00	102.94	111.77
6	V	600	ANP	O1G-PG-N3B	-5.95	103.00	111.77
6	M	600	ANP	O2B-PB-O1B	5.89	122.28	109.92

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	600	ANP	PB-N3B-PG-O1G
6	F	600	ANP	PG-N3B-PB-O1B
6	F	600	ANP	C5'-O5'-PA-O2A
6	D	600	ANP	PB-N3B-PG-O1G
6	D	600	ANP	PG-N3B-PB-O1B

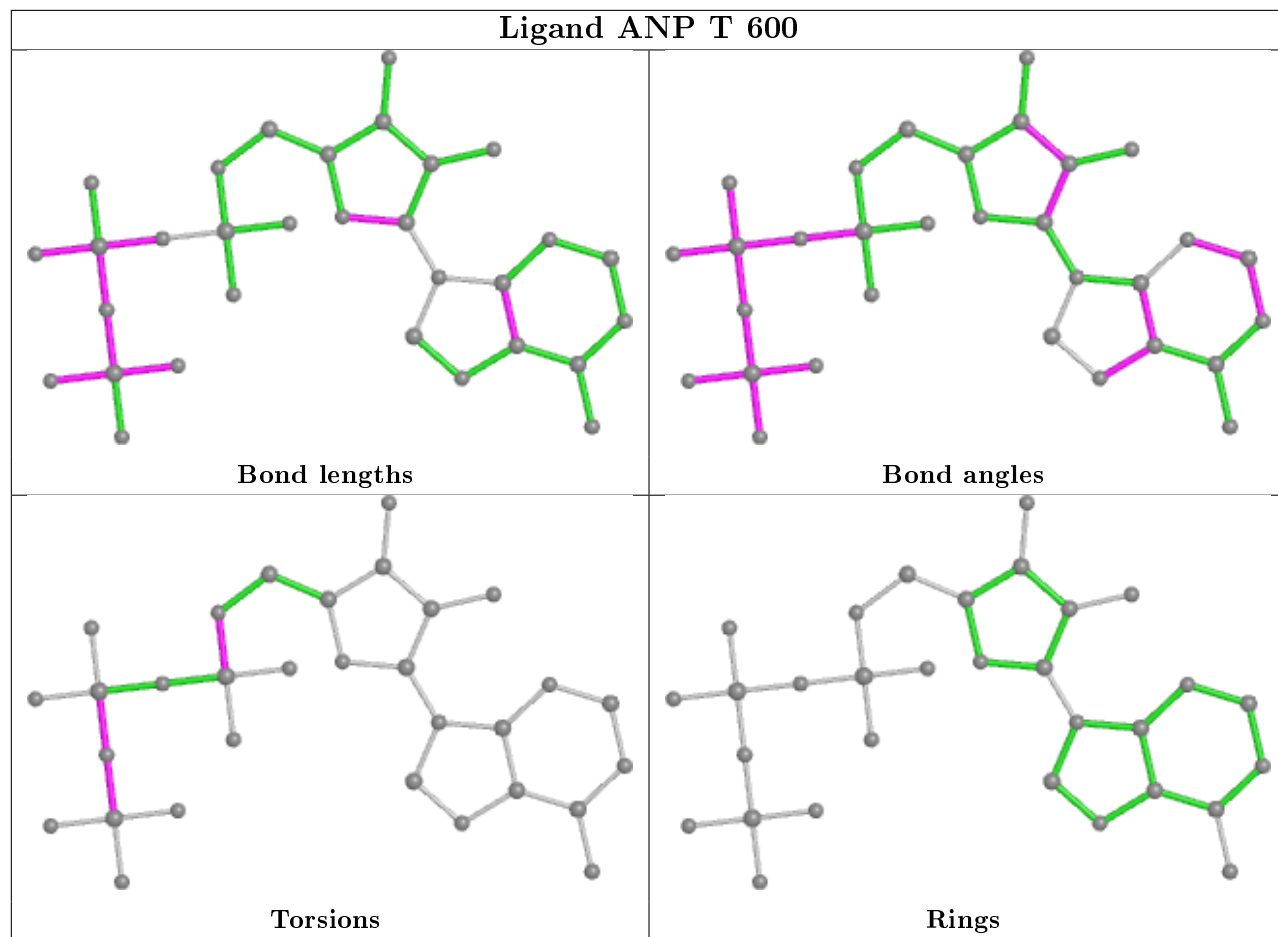
There are no ring outliers.

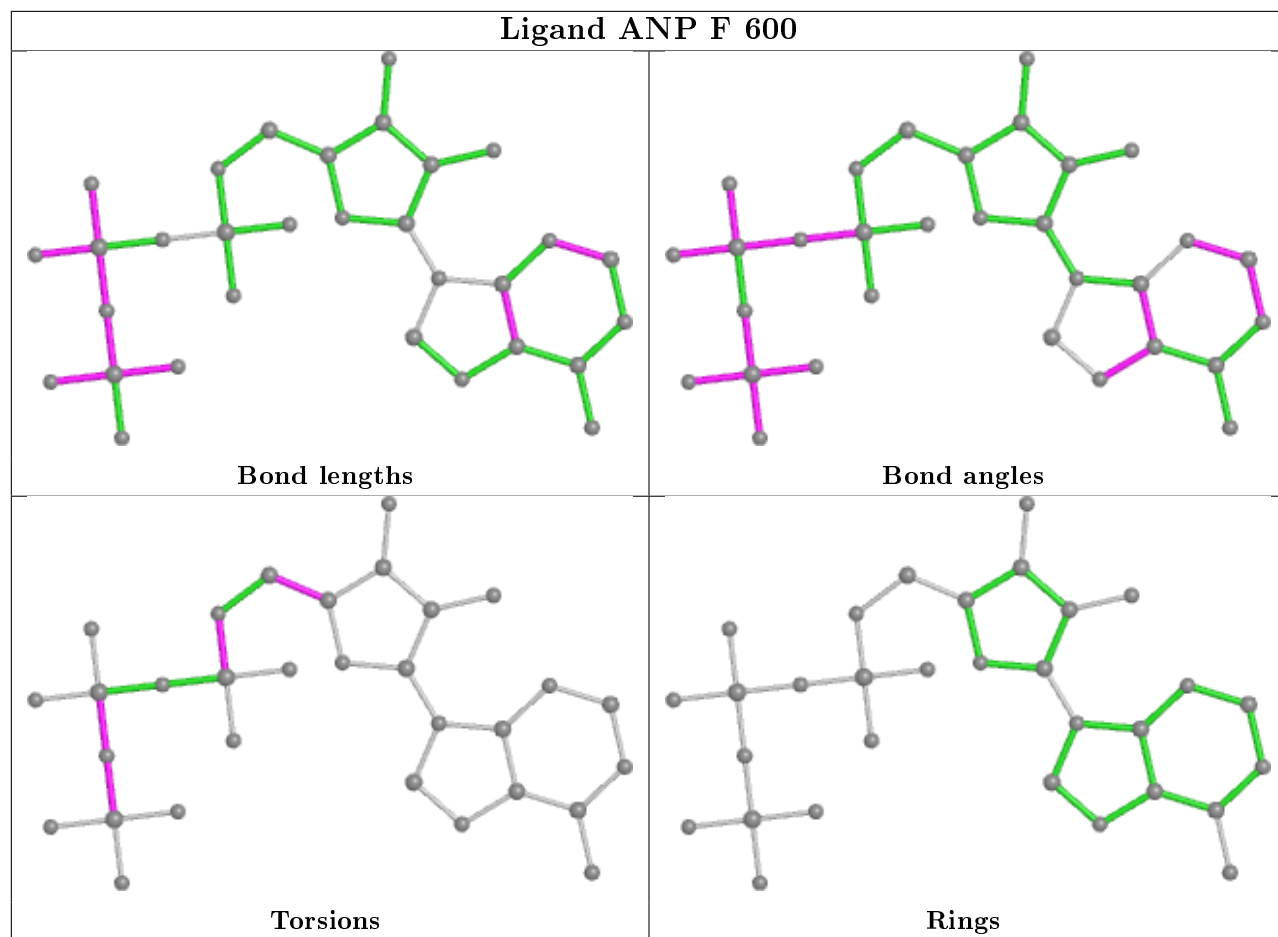
9 monomers are involved in 15 short contacts:

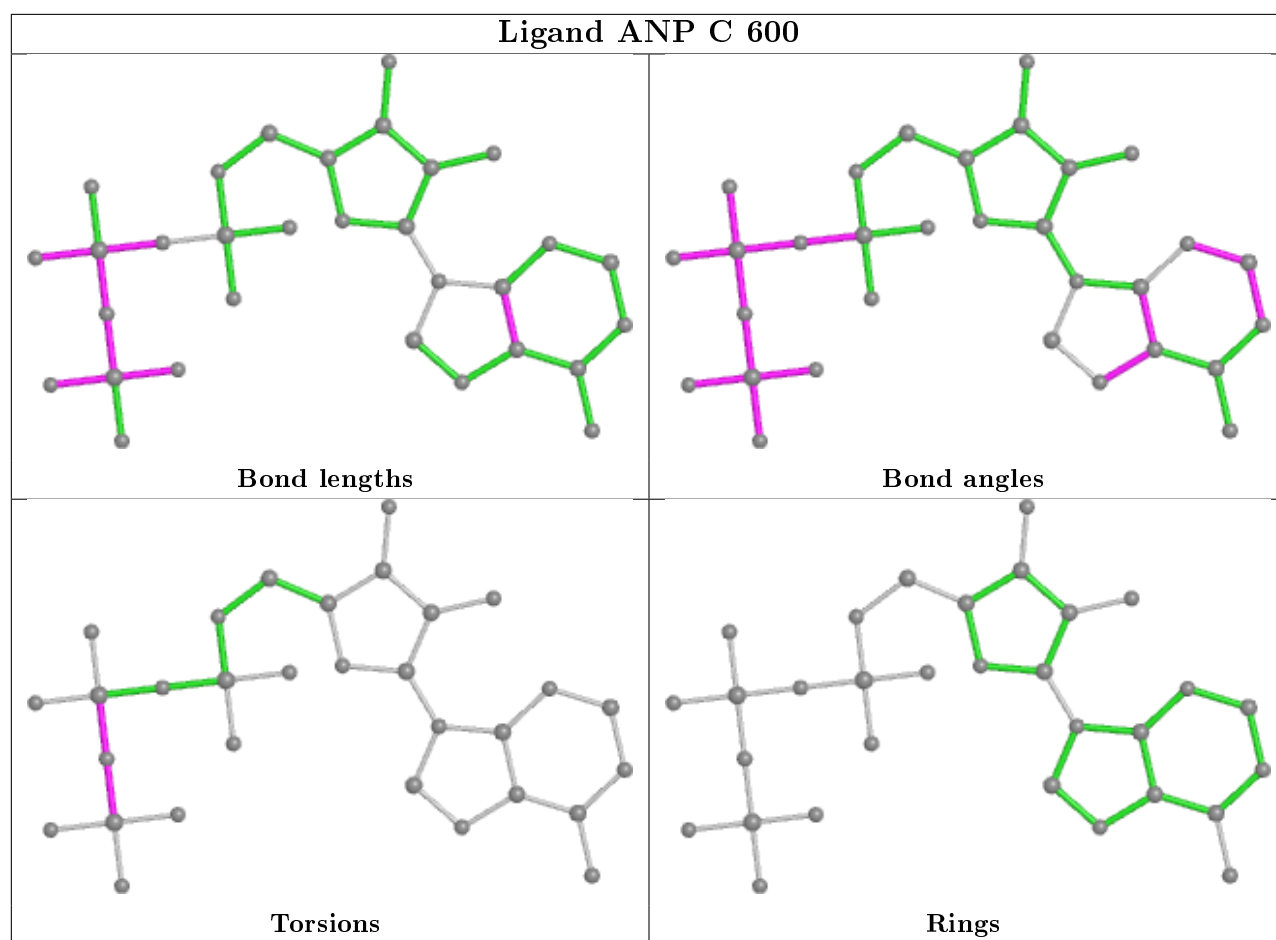
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	T	600	ANP	2	0
6	C	600	ANP	1	0
6	B	600	ANP	1	0
6	A	600	ANP	1	0
6	M	600	ANP	2	0
6	D	600	ANP	4	0
6	V	600	ANP	1	0
6	L	600	ANP	1	0
6	X	600	ANP	2	0

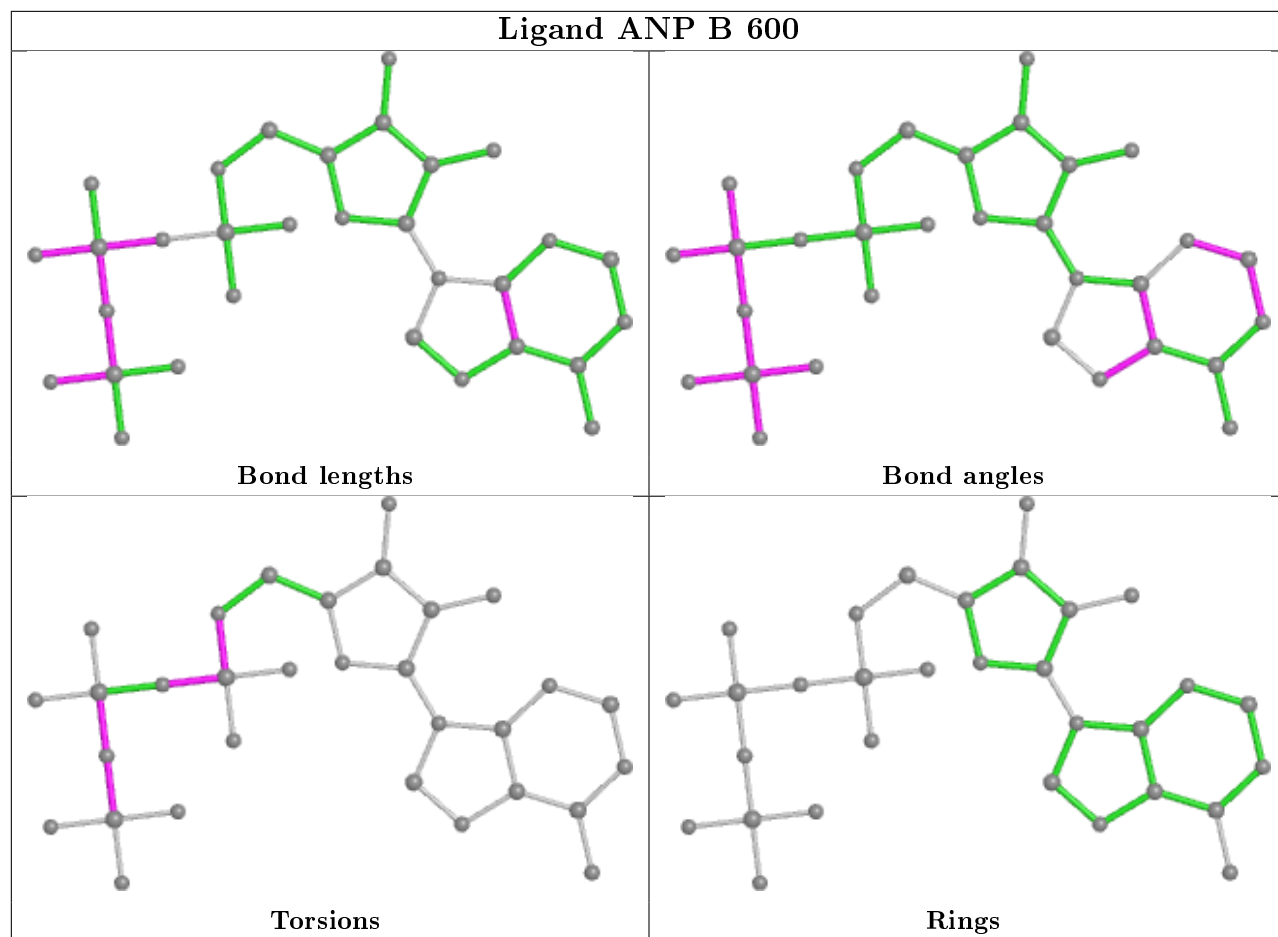
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

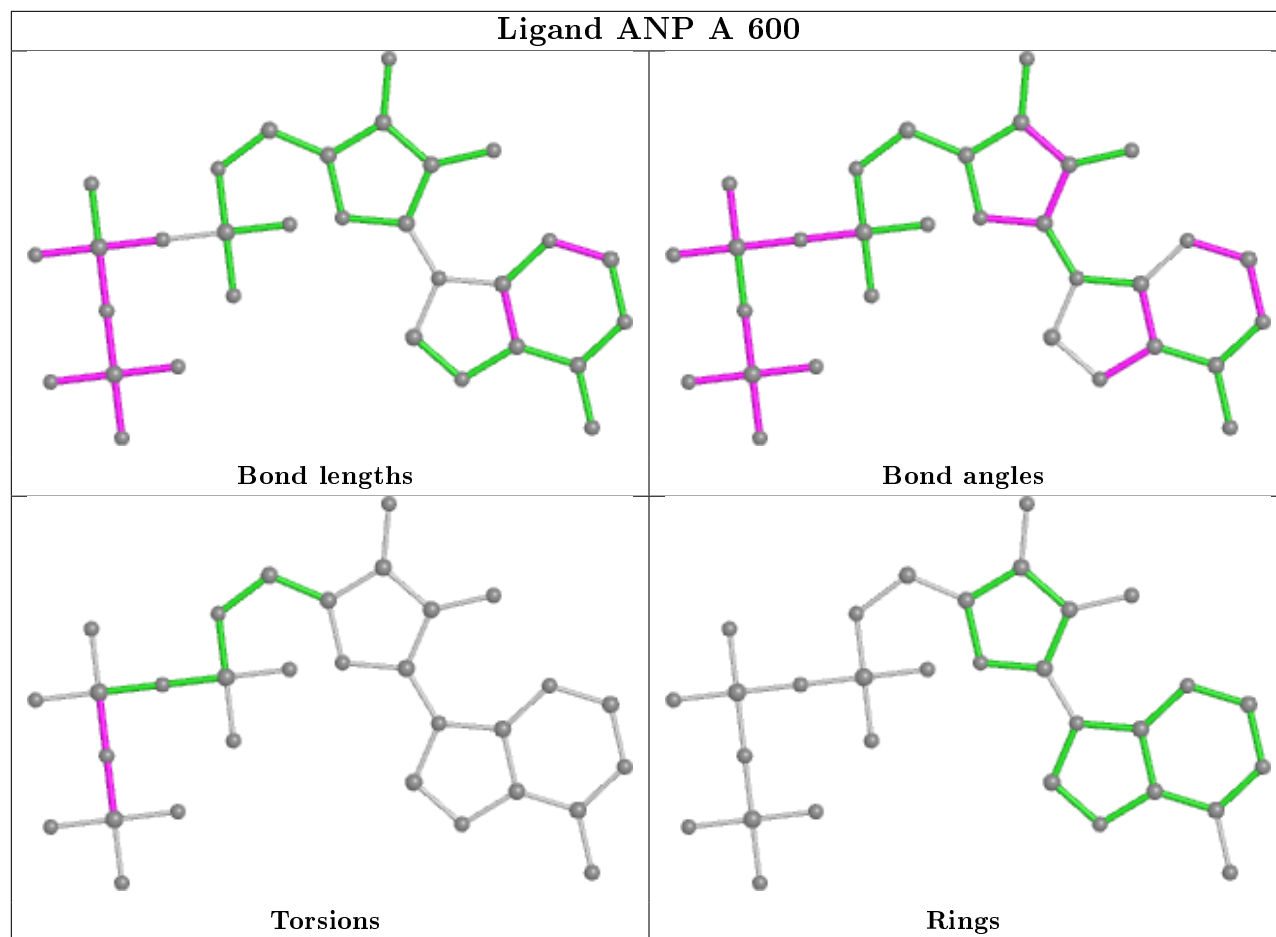
equivalents in the CSD to analyse the geometry.

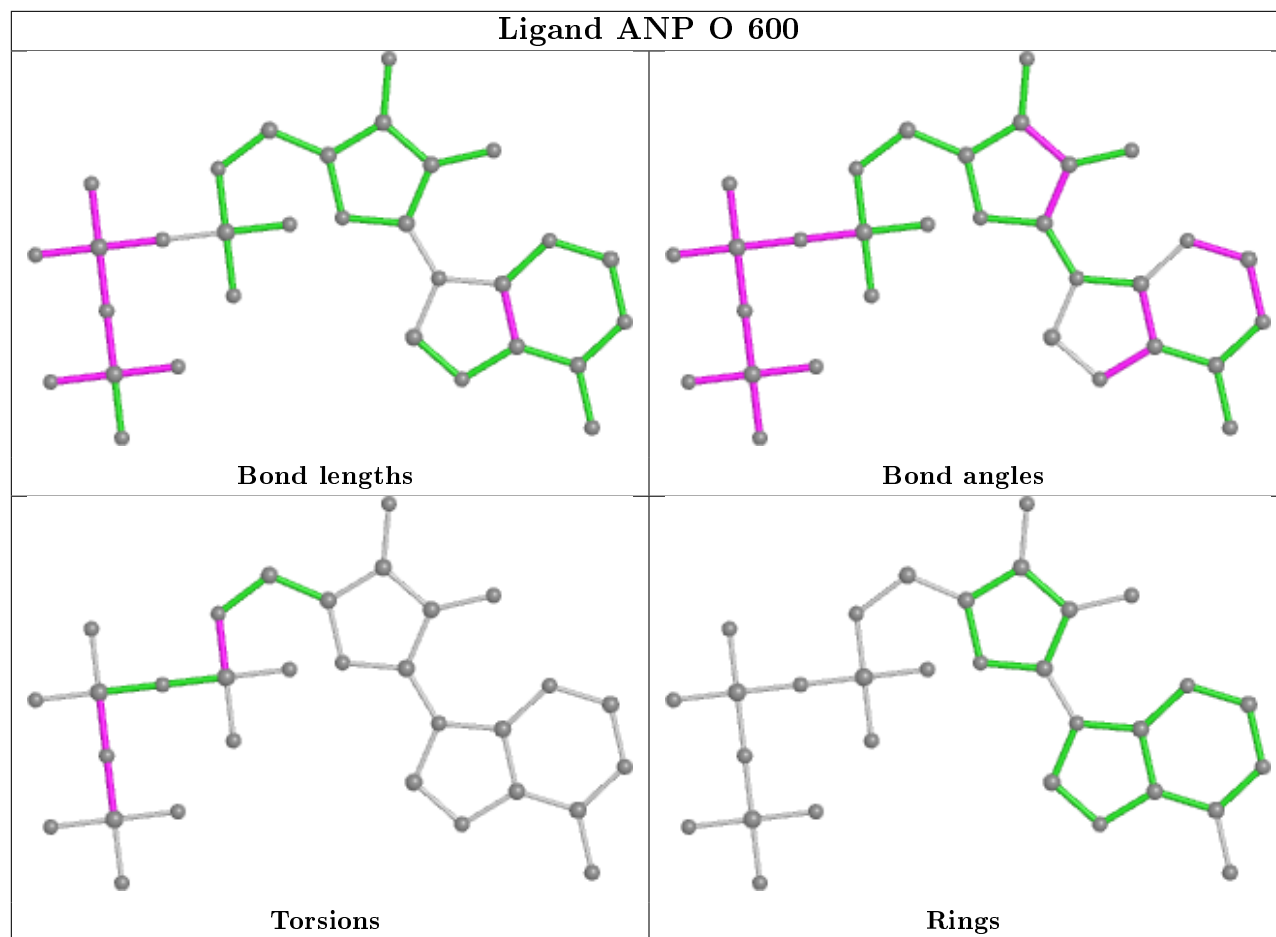


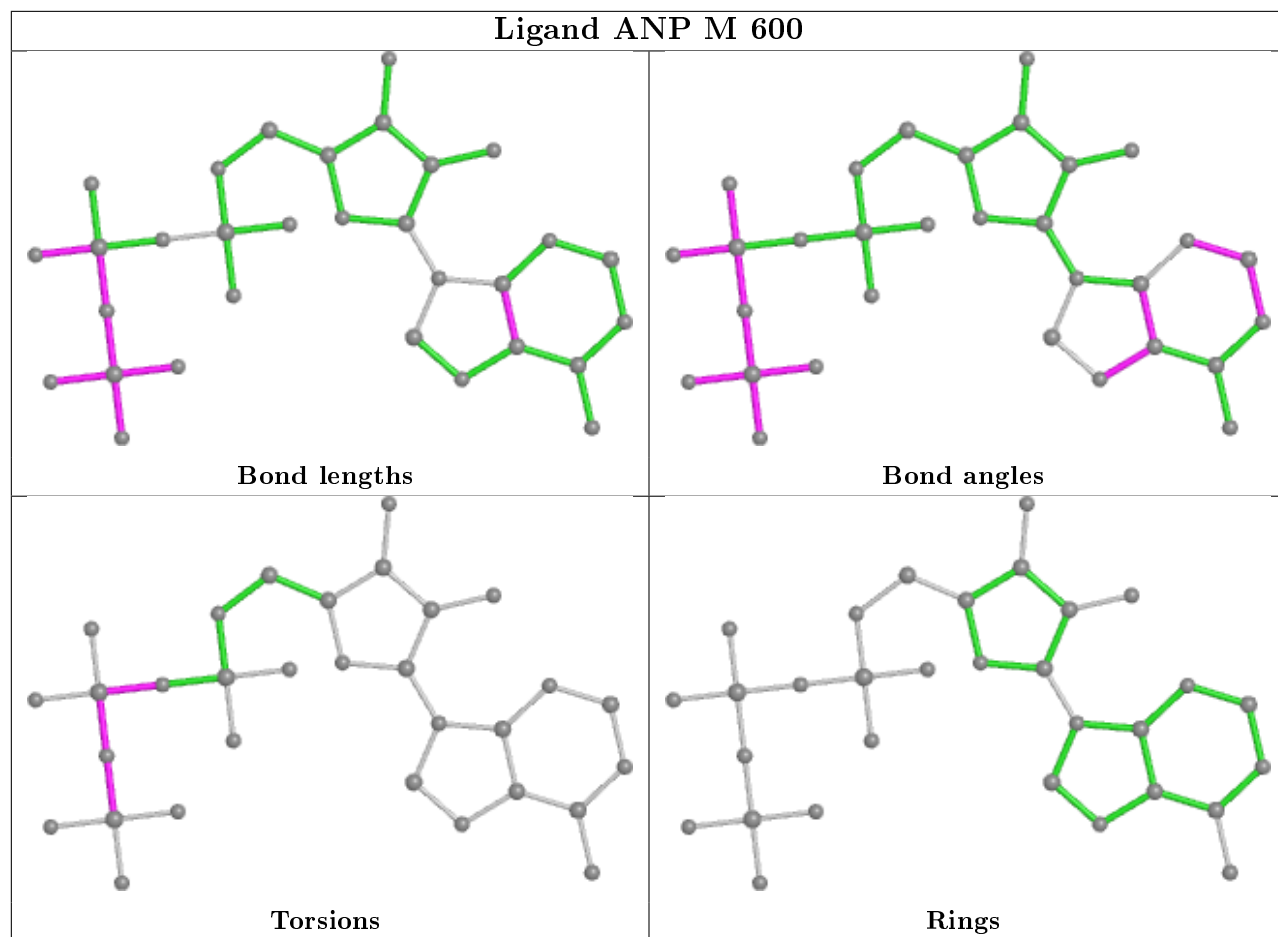


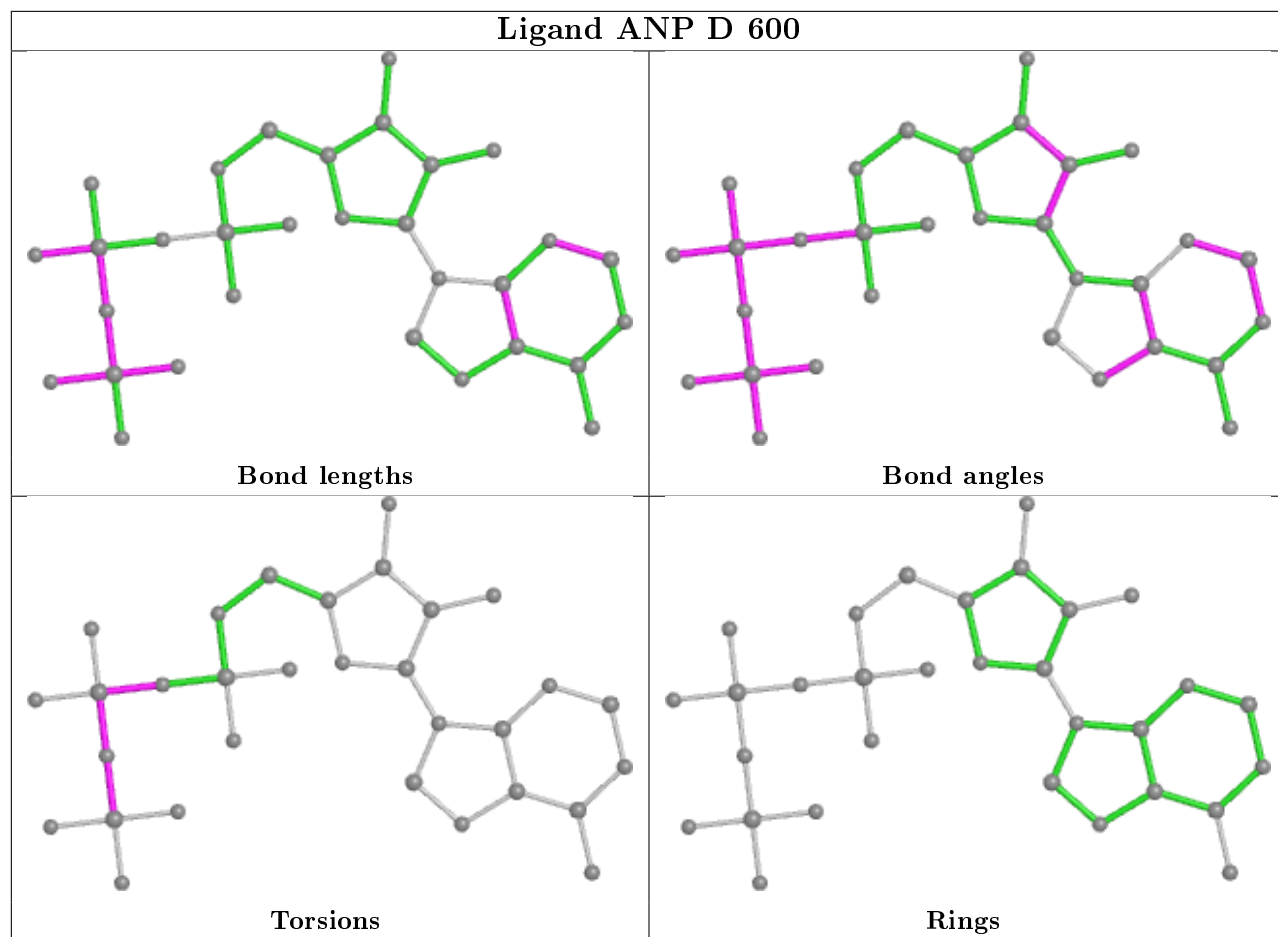


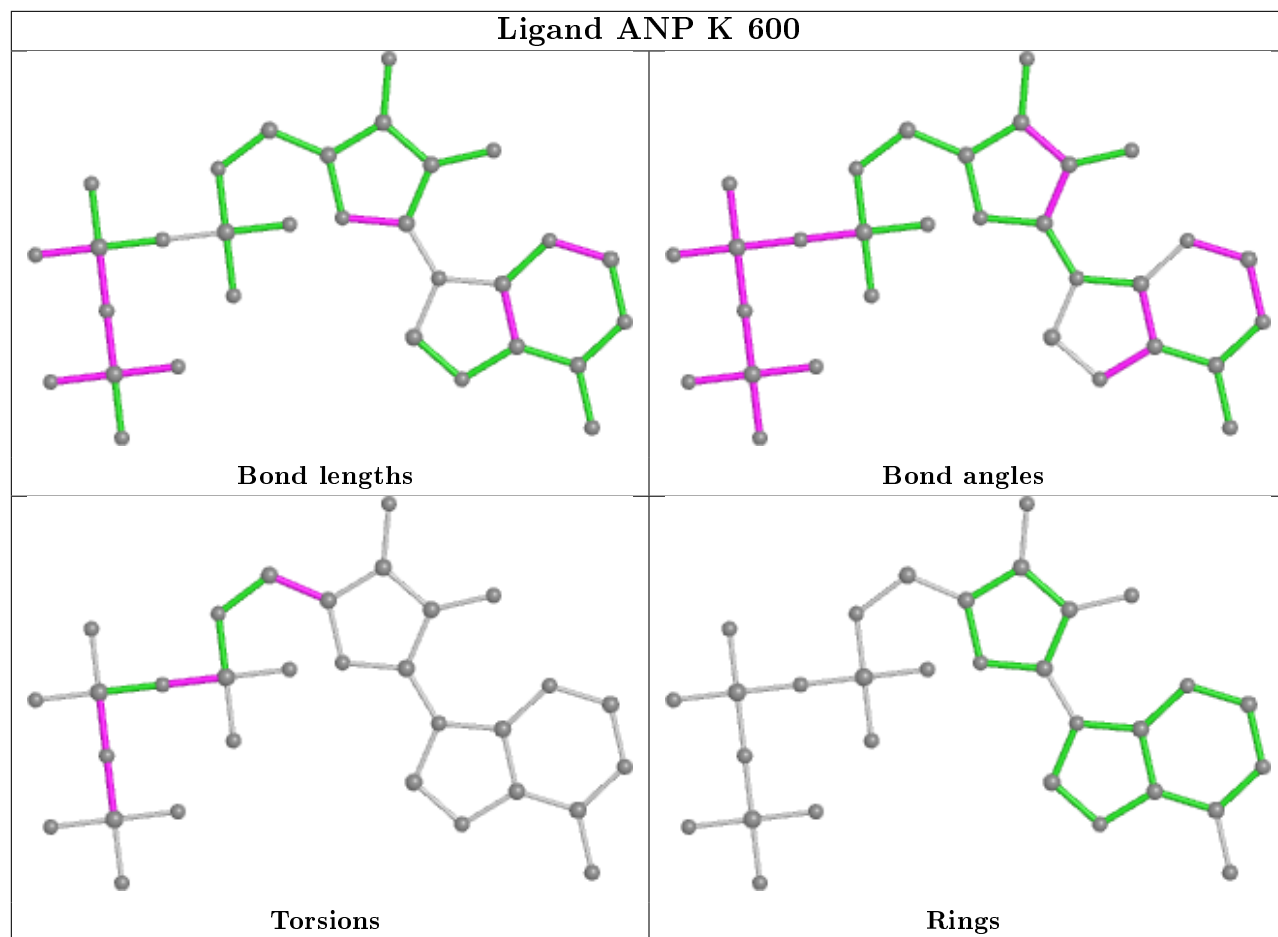


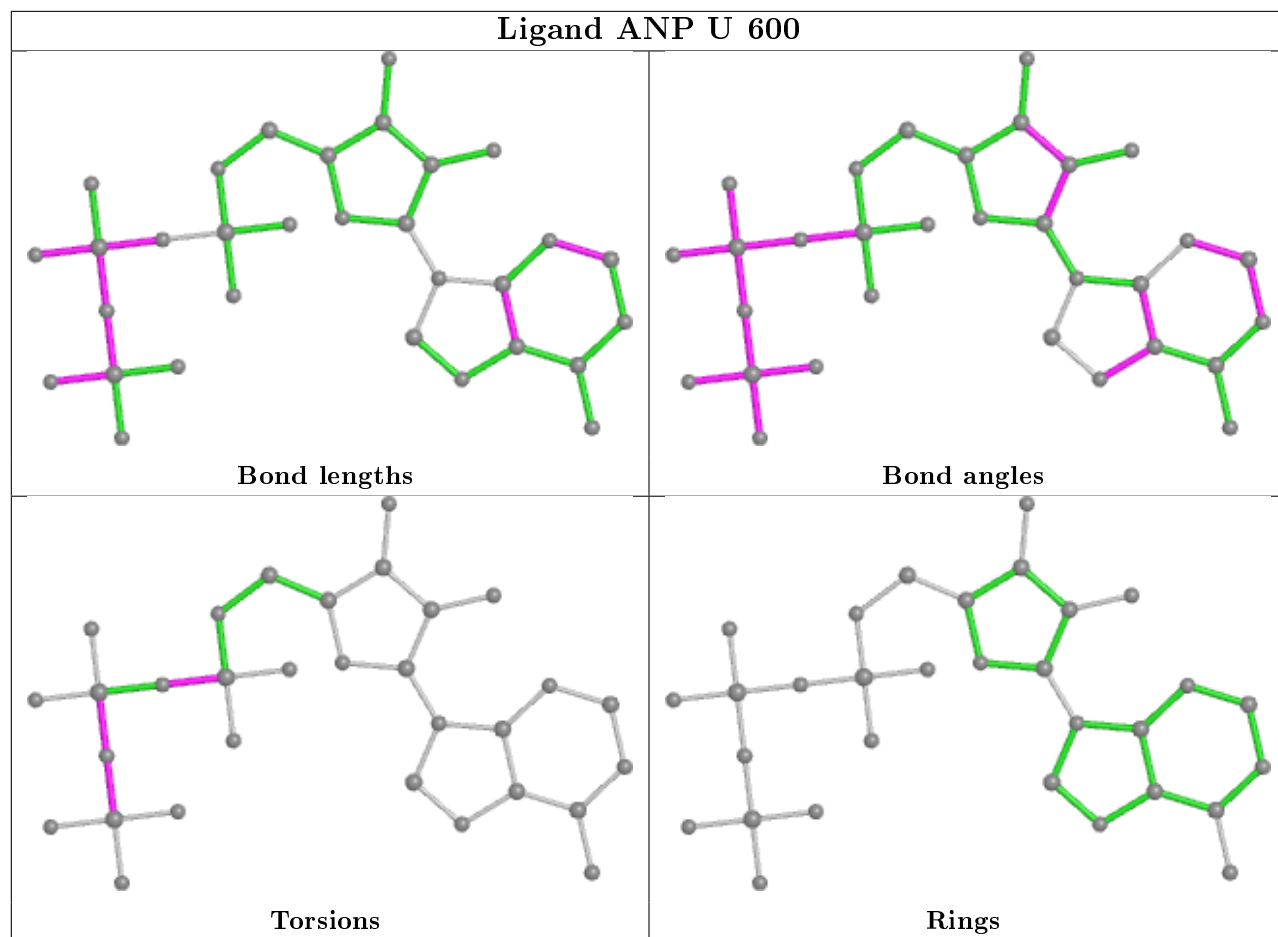


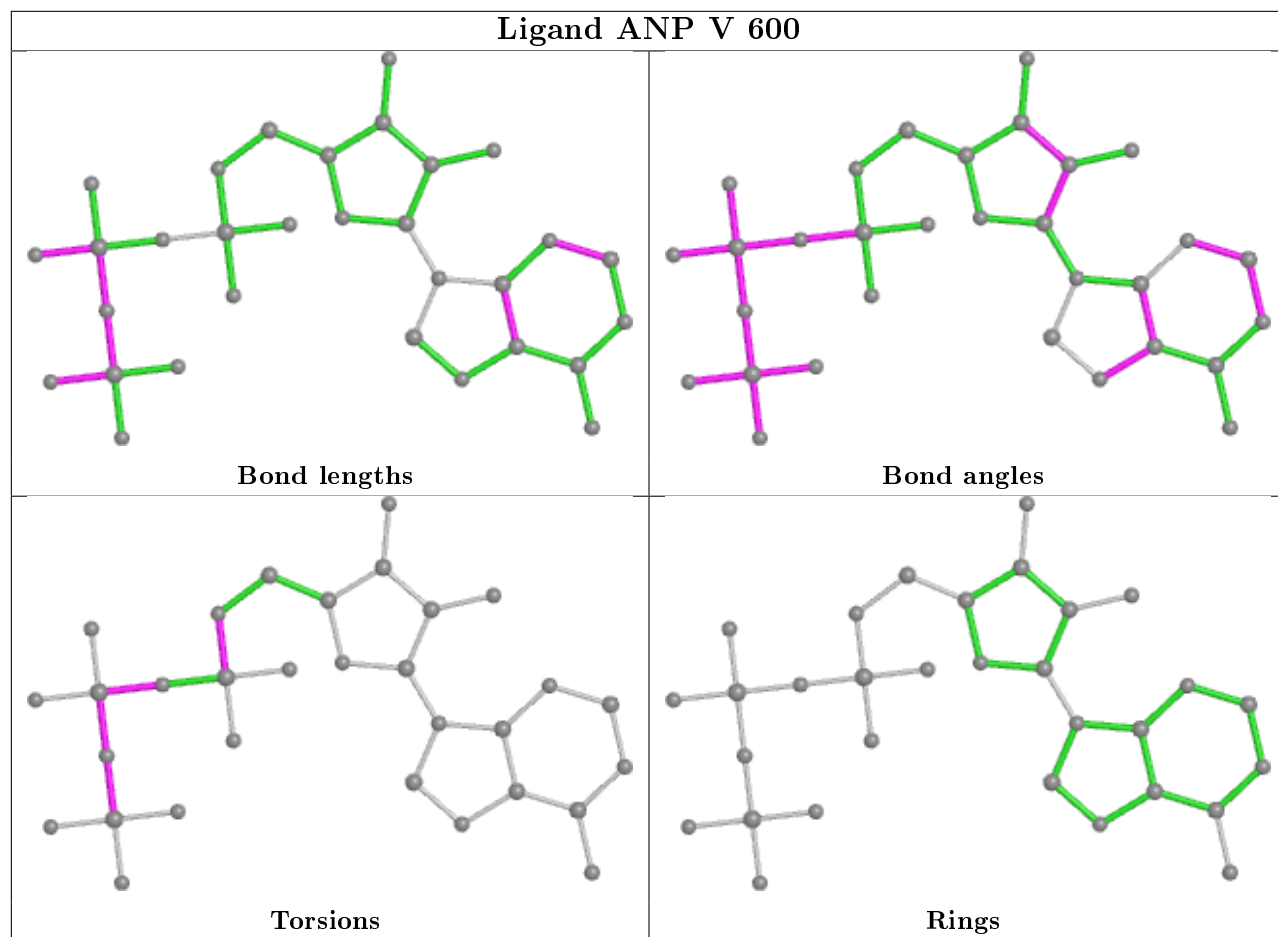




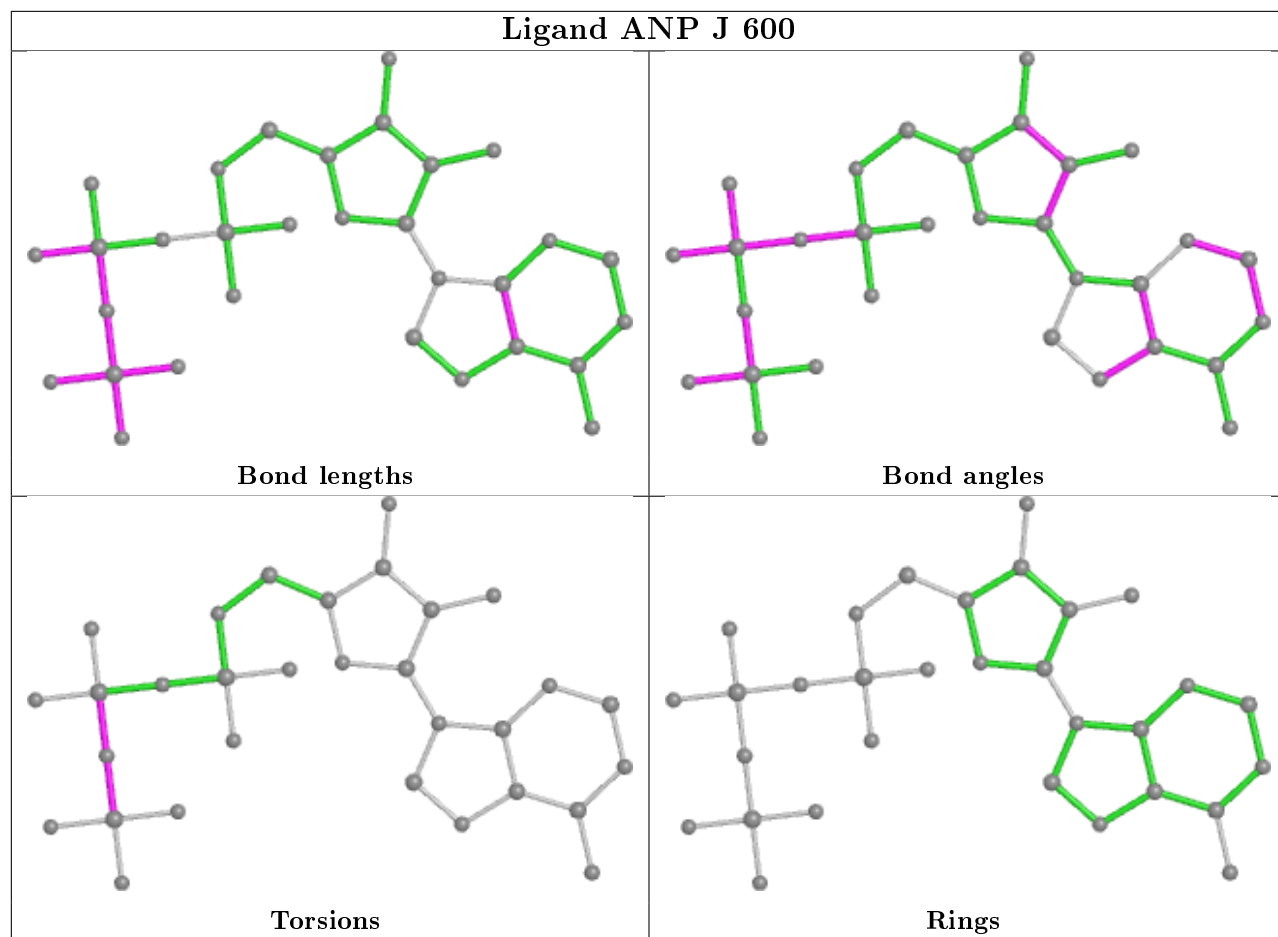


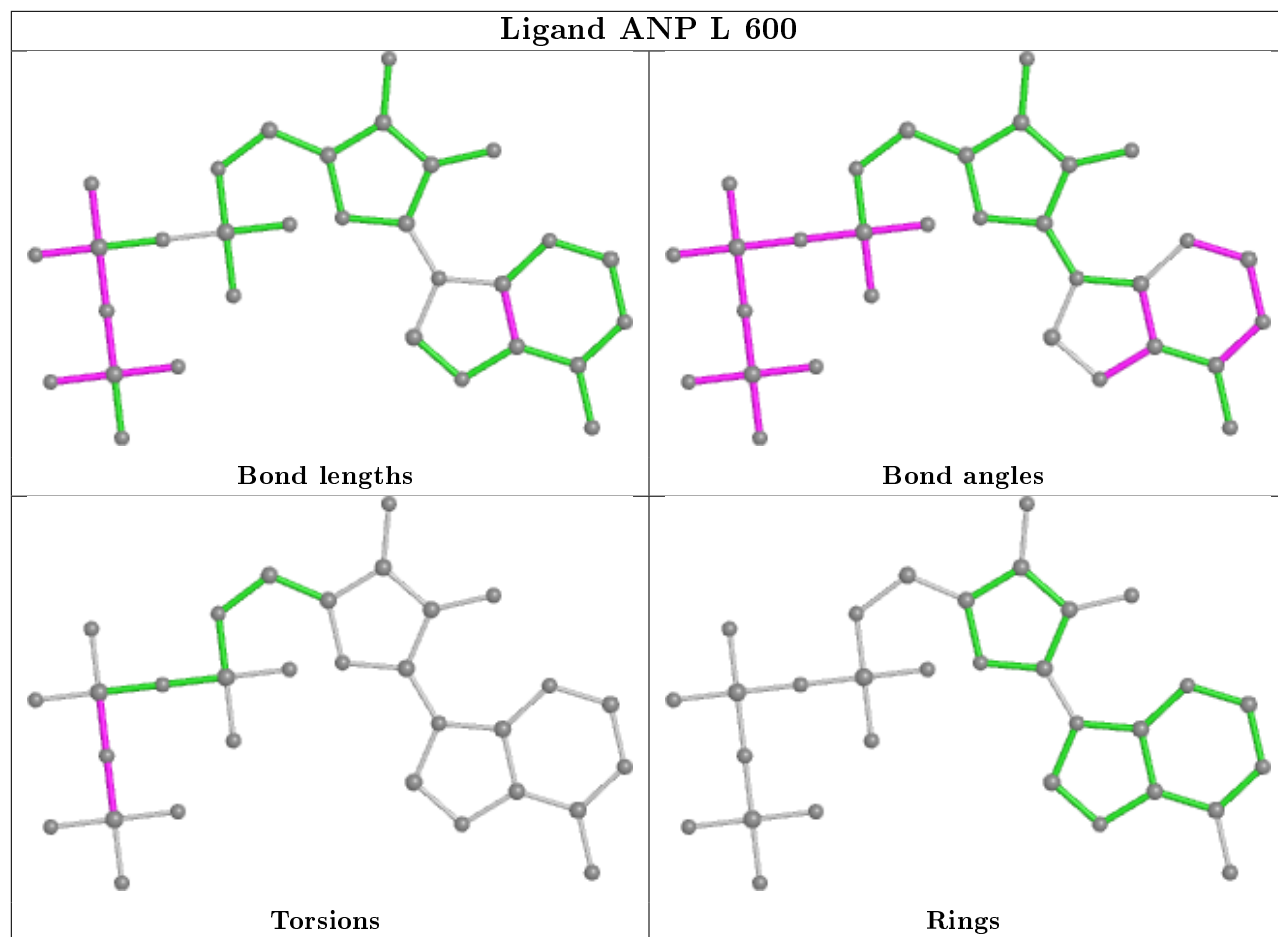


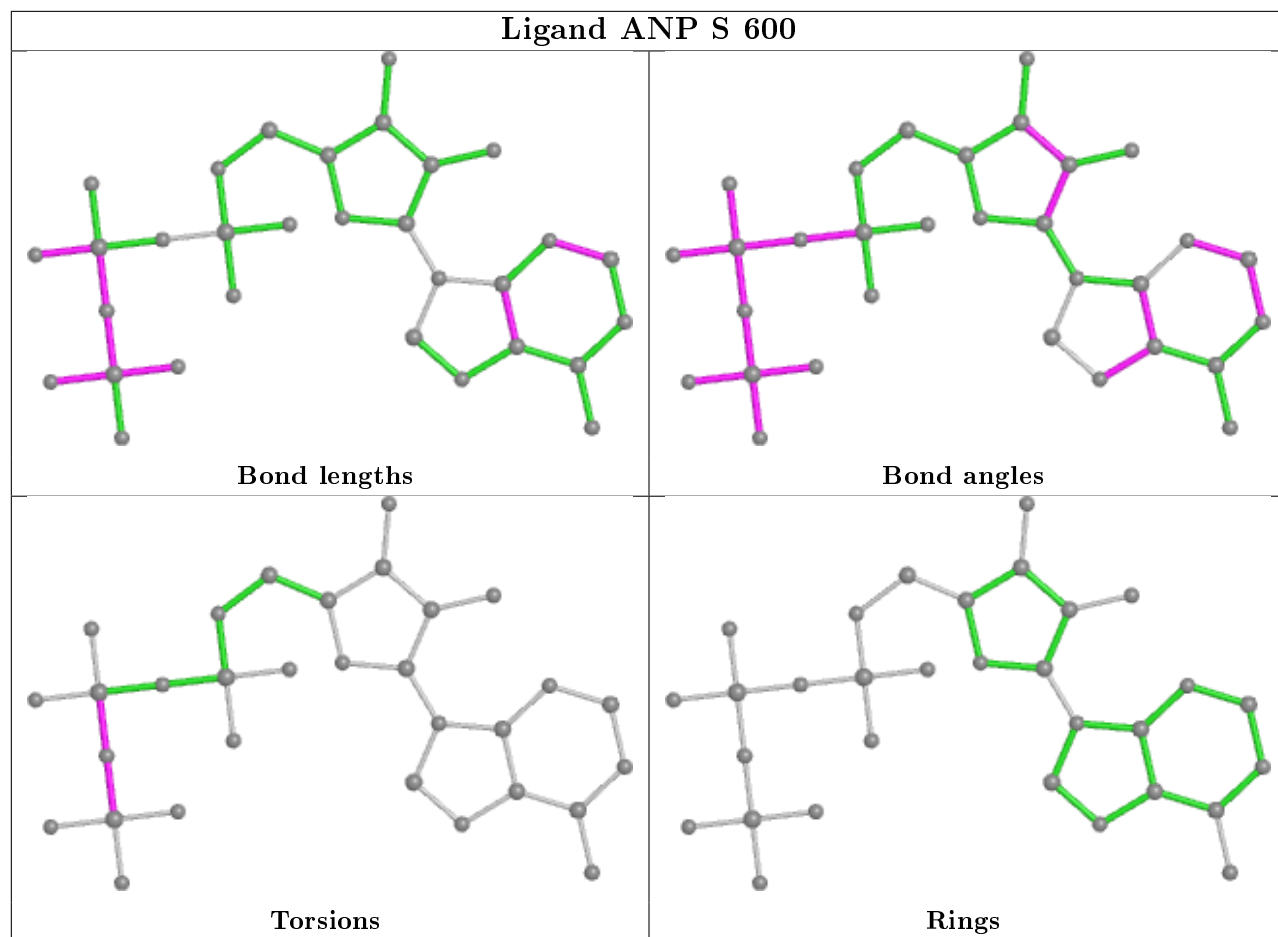


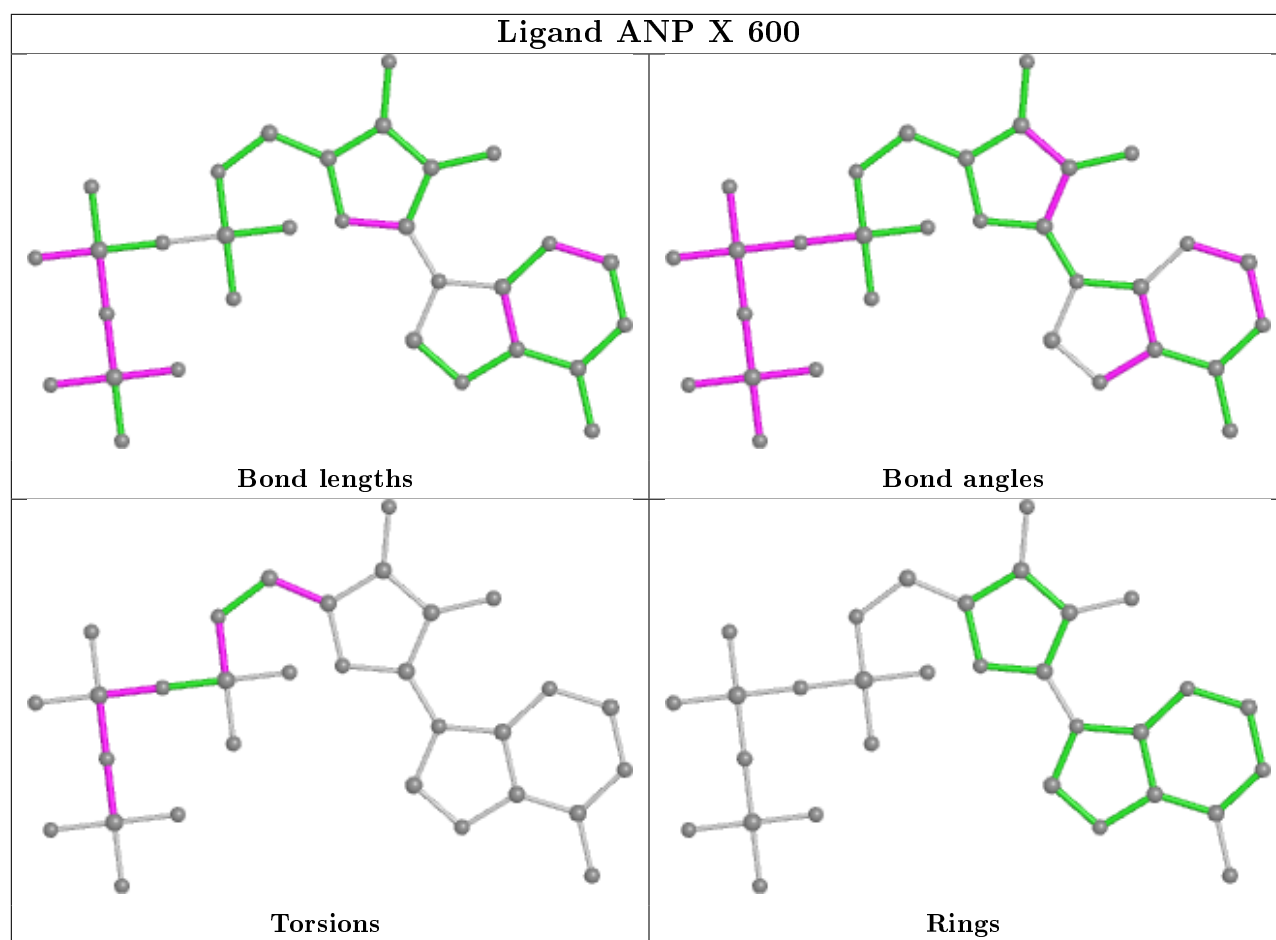


Ligand ANP J 600









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	482/510 (94%)	-0.32	0 100 100	45, 64, 100, 166	0
1	B	483/510 (94%)	-0.06	5 (1%) 82 72	48, 92, 165, 195	0
1	C	484/510 (94%)	-0.18	2 (0%) 92 89	51, 75, 138, 181	0
1	J	481/510 (94%)	-0.14	1 (0%) 95 94	59, 93, 137, 181	0
1	K	486/510 (95%)	0.03	18 (3%) 41 26	61, 107, 166, 182	0
1	L	482/510 (94%)	-0.22	2 (0%) 92 89	47, 68, 123, 164	0
1	S	480/510 (94%)	-0.08	3 (0%) 89 83	72, 106, 140, 186	0
1	T	481/510 (94%)	0.21	19 (3%) 38 25	91, 131, 153, 165	0
1	U	481/510 (94%)	0.27	31 (6%) 19 11	93, 133, 166, 194	0
2	D	470/484 (97%)	-0.26	2 (0%) 92 89	46, 72, 121, 172	0
2	E	468/484 (96%)	-0.02	16 (3%) 45 29	48, 85, 147, 186	0
2	F	469/484 (96%)	-0.17	1 (0%) 95 94	48, 84, 117, 161	0
2	M	470/484 (97%)	-0.14	6 (1%) 77 65	57, 84, 131, 172	0
2	N	470/484 (97%)	0.09	22 (4%) 31 19	64, 110, 165, 188	0
2	O	468/484 (96%)	-0.14	5 (1%) 80 69	53, 92, 128, 153	0
2	V	470/484 (97%)	0.30	30 (6%) 19 11	93, 139, 171, 189	0
2	W	467/484 (96%)	0.01	13 (2%) 53 37	76, 101, 137, 171	0
2	X	469/484 (96%)	0.11	17 (3%) 42 27	85, 121, 162, 187	0
3	G	265/278 (95%)	-0.15	1 (0%) 92 89	56, 90, 117, 134	0
3	P	244/278 (87%)	0.59	27 (11%) 5 3	64, 139, 185, 209	0
3	Y	198/278 (71%)	0.55	22 (11%) 5 3	98, 147, 190, 214	0
4	H	120/137 (87%)	0.09	6 (5%) 28 16	86, 115, 166, 176	0
4	Q	84/137 (61%)	0.90	18 (21%) 0 1	138, 163, 187, 198	0
4	Z	15/137 (10%)	1.94	9 (60%) 0 0	192, 201, 222, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	1	25/61 (40%)	1.41	9 (36%) 0 0	176, 183, 194, 202	0
5	I	48/61 (78%)	-0.30	0 100 100	92, 112, 140, 157	0
5	R	31/61 (50%)	0.08	0 100 100	136, 153, 167, 178	0
All	All	9591/10374 (92%)	0.00	285 (2%) 50 34	45, 100, 160, 222	0

The worst 5 of 285 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	83	LEU	5.4
2	M	6	SER	5.4
3	P	39	ILE	5.4
3	P	100	ASN	5.3
1	T	491	LEU	5.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	T	700	1/1	0.83	0.52	91,91,91,91	0
6	ANP	T	600	31/31	0.91	0.22	91,101,106,106	0
6	ANP	B	600	31/31	0.92	0.20	71,82,85,85	0
8	PO4	N	800	5/5	0.92	0.24	131,131,131,132	0
6	ANP	U	600	31/31	0.92	0.21	84,89,90,91	0
7	MG	D	700	1/1	0.93	0.36	64,64,64,64	0
6	ANP	V	600	31/31	0.93	0.25	102,106,109,109	0
7	MG	F	700	1/1	0.94	0.44	65,65,65,65	0
6	ANP	J	600	31/31	0.94	0.20	67,73,80,81	0

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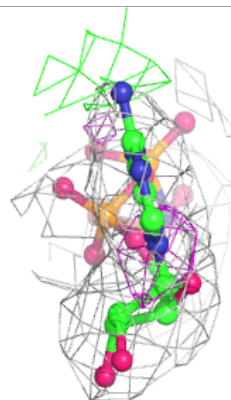
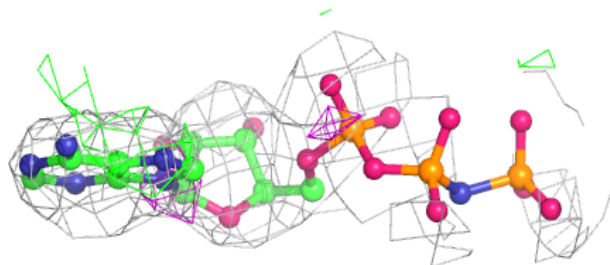
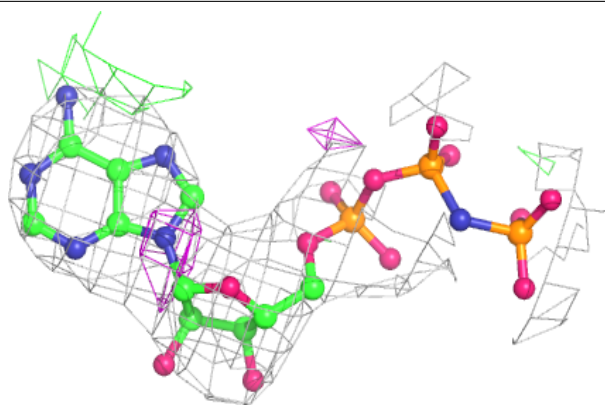
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	U	700	1/1	0.94	0.40	88,88,88,88	0
7	MG	A	700	1/1	0.94	0.43	48,48,48,48	0
6	ANP	X	600	31/31	0.94	0.24	93,94,96,97	0
6	ANP	K	600	31/31	0.94	0.17	90,97,99,100	0
7	MG	S	700	1/1	0.94	0.41	77,77,77,77	0
6	ANP	S	600	31/31	0.94	0.21	76,82,83,85	0
7	MG	K	700	1/1	0.94	0.35	90,90,90,90	0
6	ANP	C	600	31/31	0.95	0.22	58,64,68,70	0
6	ANP	F	600	31/31	0.95	0.26	66,70,78,78	0
7	MG	L	700	1/1	0.95	0.33	53,53,53,53	0
6	ANP	A	600	31/31	0.96	0.22	48,58,61,62	0
7	MG	M	700	1/1	0.96	0.42	64,64,64,64	0
7	MG	B	700	1/1	0.96	0.41	72,72,72,72	0
6	ANP	O	600	31/31	0.96	0.23	84,88,92,92	0
6	ANP	L	600	31/31	0.96	0.21	53,59,62,62	0
7	MG	X	700	1/1	0.97	0.43	96,96,96,96	0
6	ANP	M	600	31/31	0.97	0.24	64,68,70,71	0
6	ANP	D	600	31/31	0.97	0.22	62,65,68,69	0
7	MG	C	700	1/1	0.97	0.45	58,58,58,58	0
7	MG	J	700	1/1	0.97	0.46	67,67,67,67	0
7	MG	O	700	1/1	0.98	0.43	83,83,83,83	0
7	MG	V	700	1/1	0.98	0.35	107,107,107,107	0

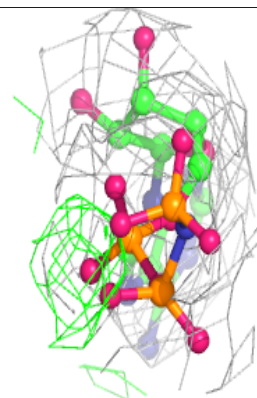
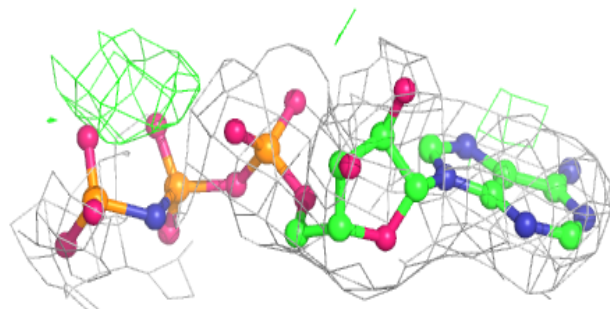
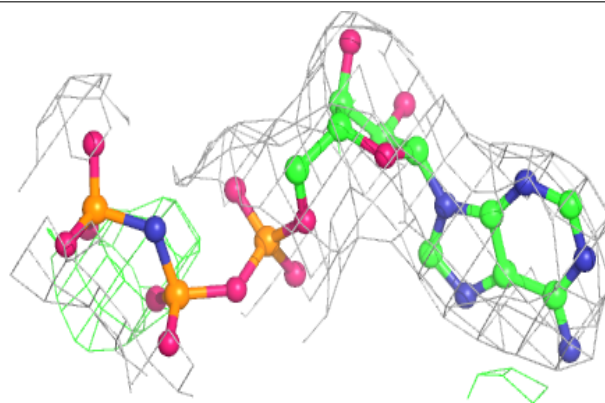
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP 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)

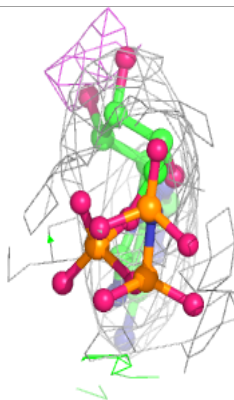
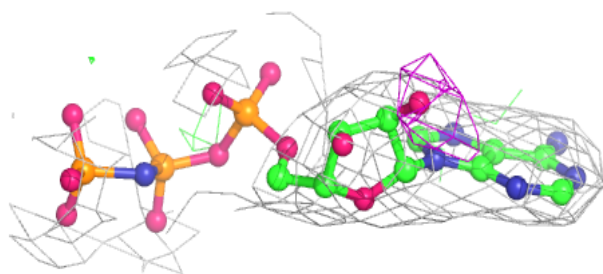
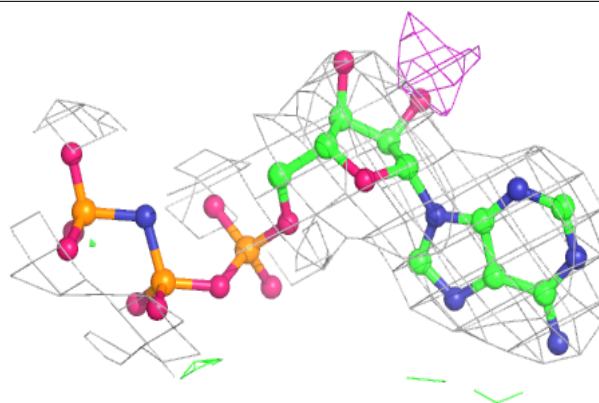
**Electron density around ANP B 600:**

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

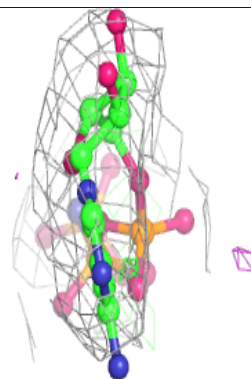
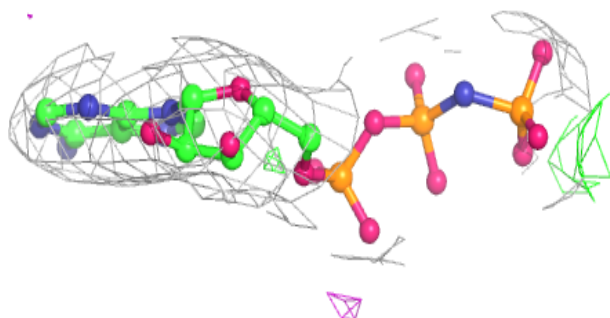
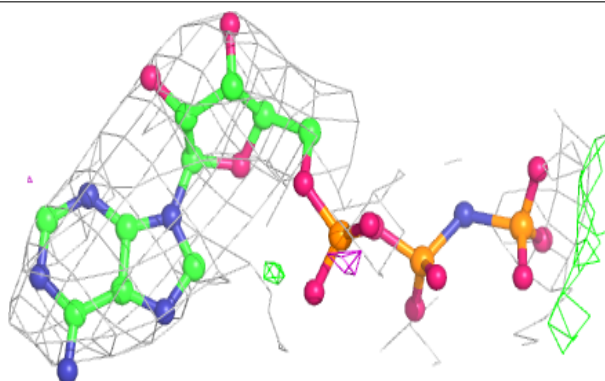


Electron density around ANP U 600:

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

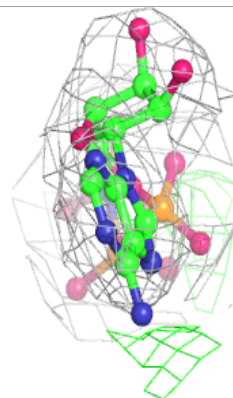
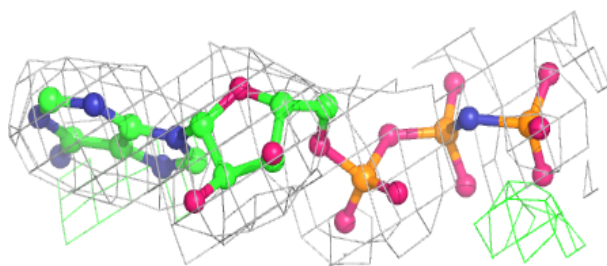
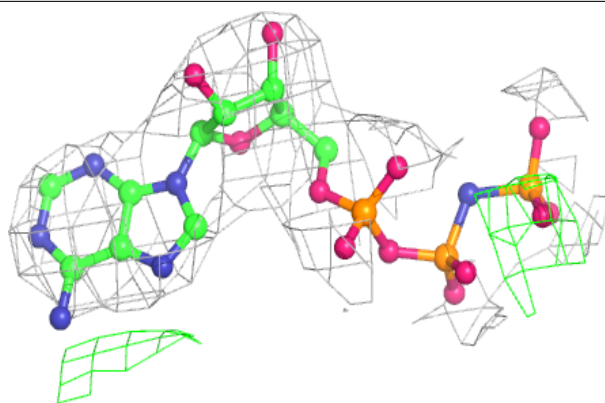
**Electron density around ANP V 600:**

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

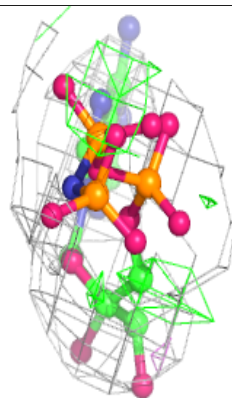
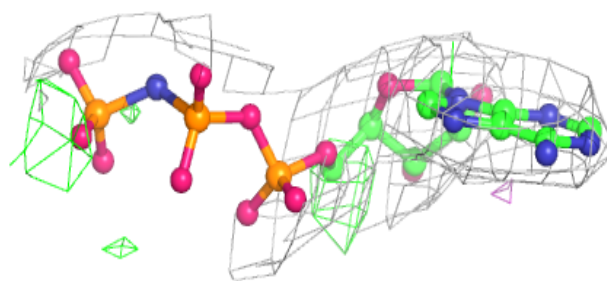
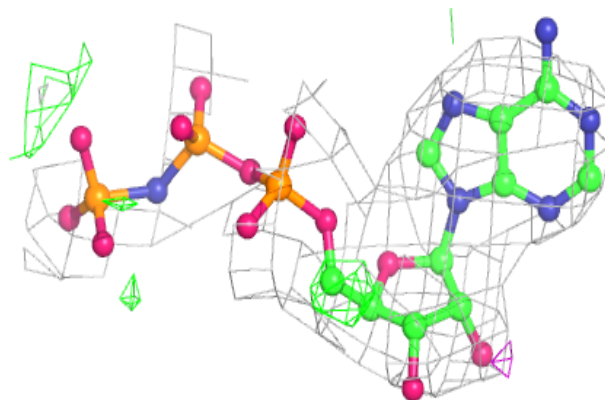


Electron density around ANP J 600:

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

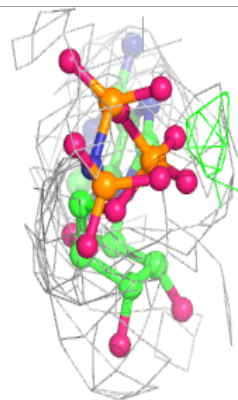
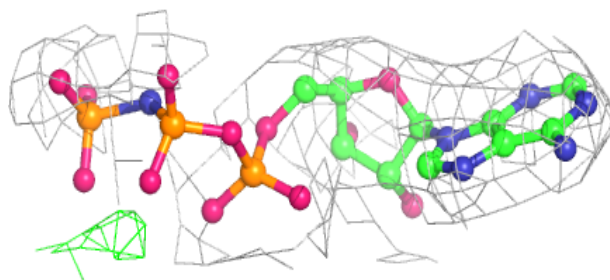
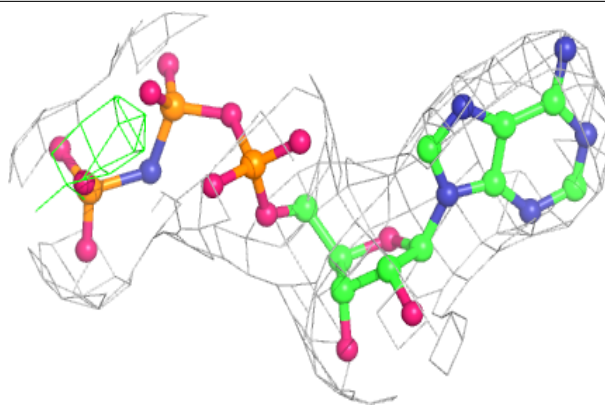
**Electron density around ANP X 600:**

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

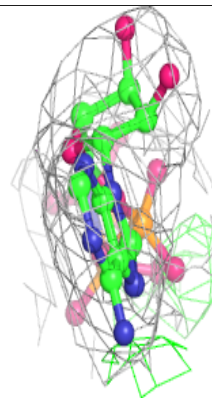
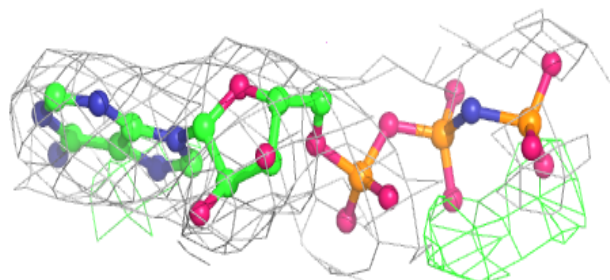
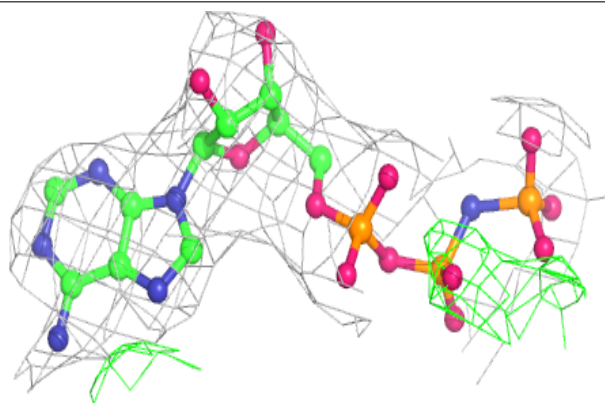


Electron density around ANP K 600:

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

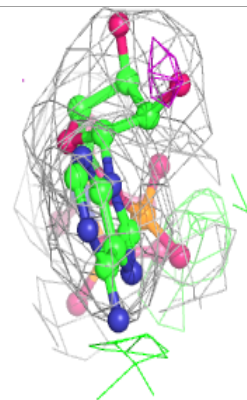
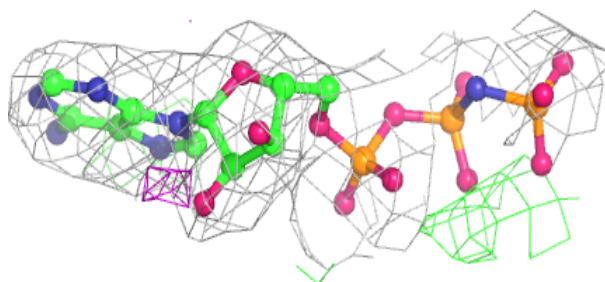
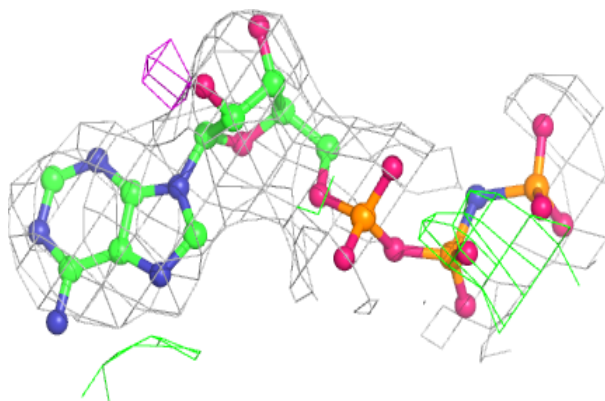
**Electron density around ANP S 600:**

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

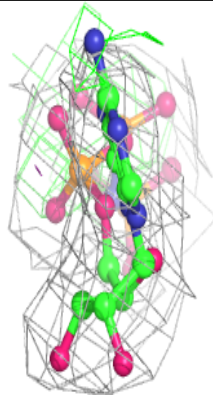
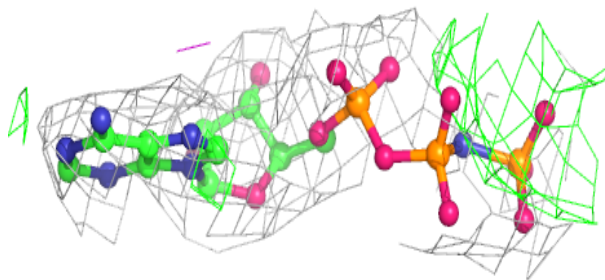
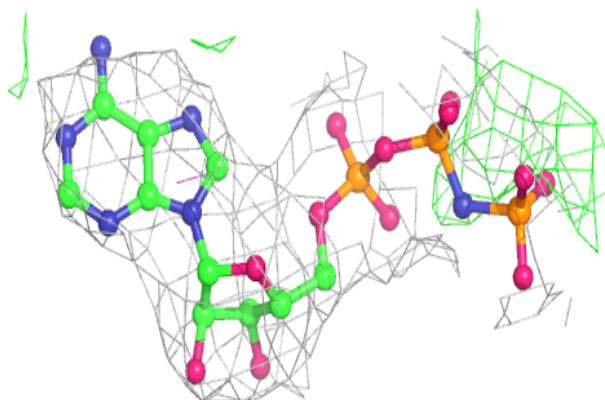


Electron density around ANP C 600:

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and green (positive)

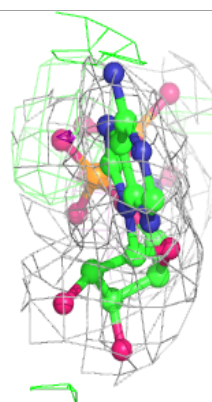
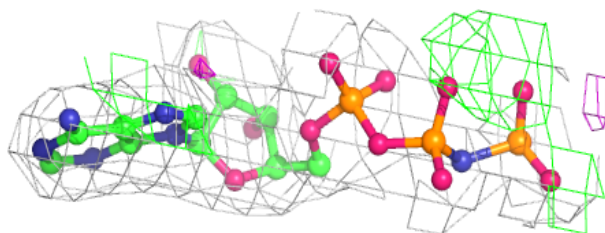
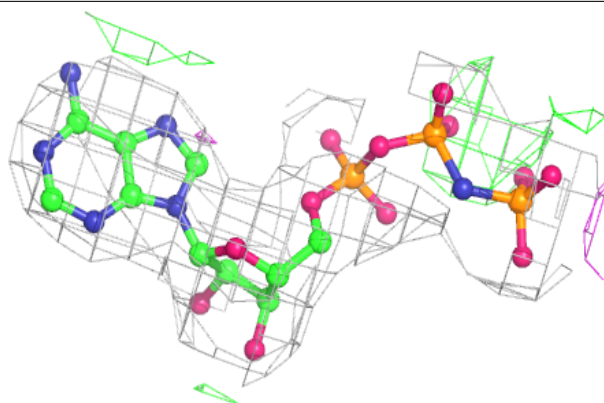
**Electron density around ANP F 600:**

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and green (positive)

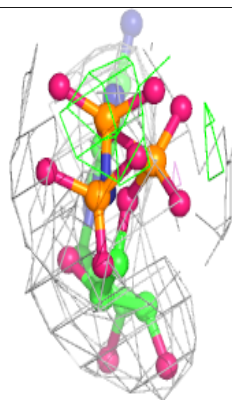
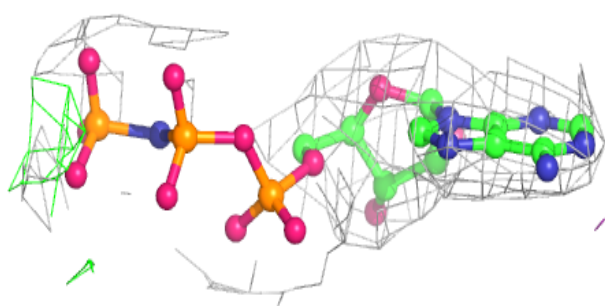
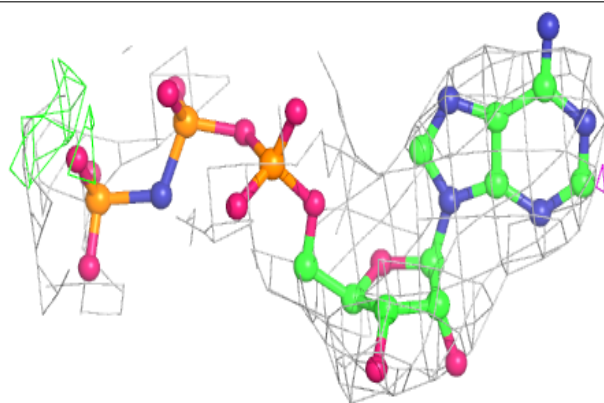


Electron density around ANP A 600:

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

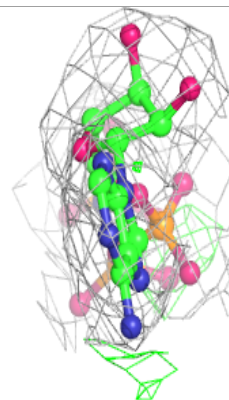
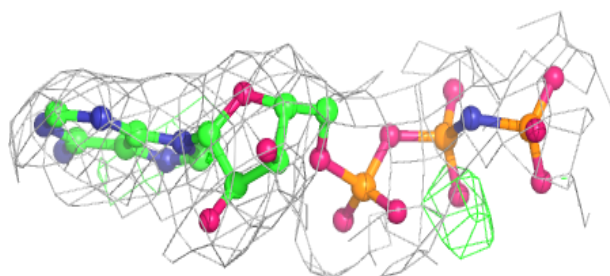
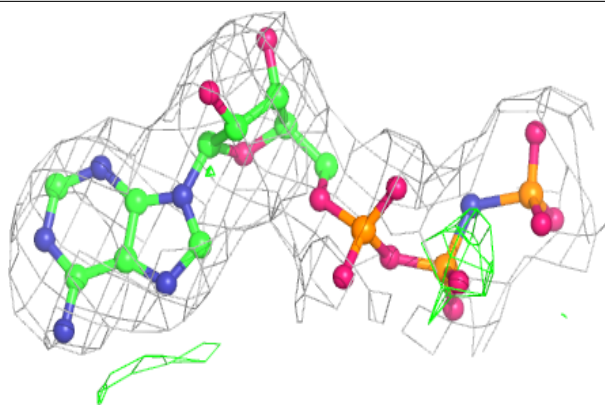
**Electron density around ANP O 600:**

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

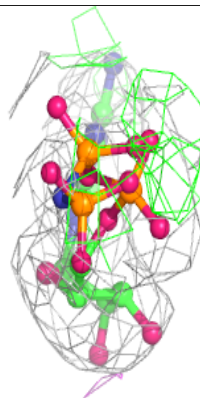
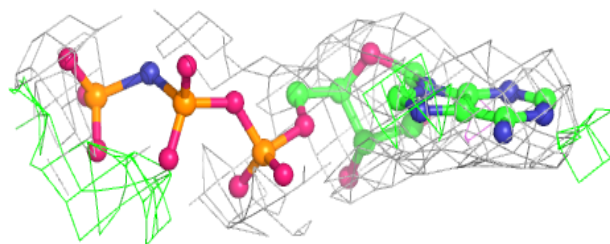
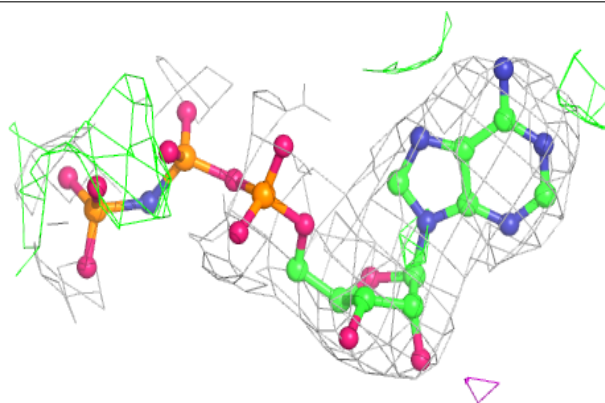


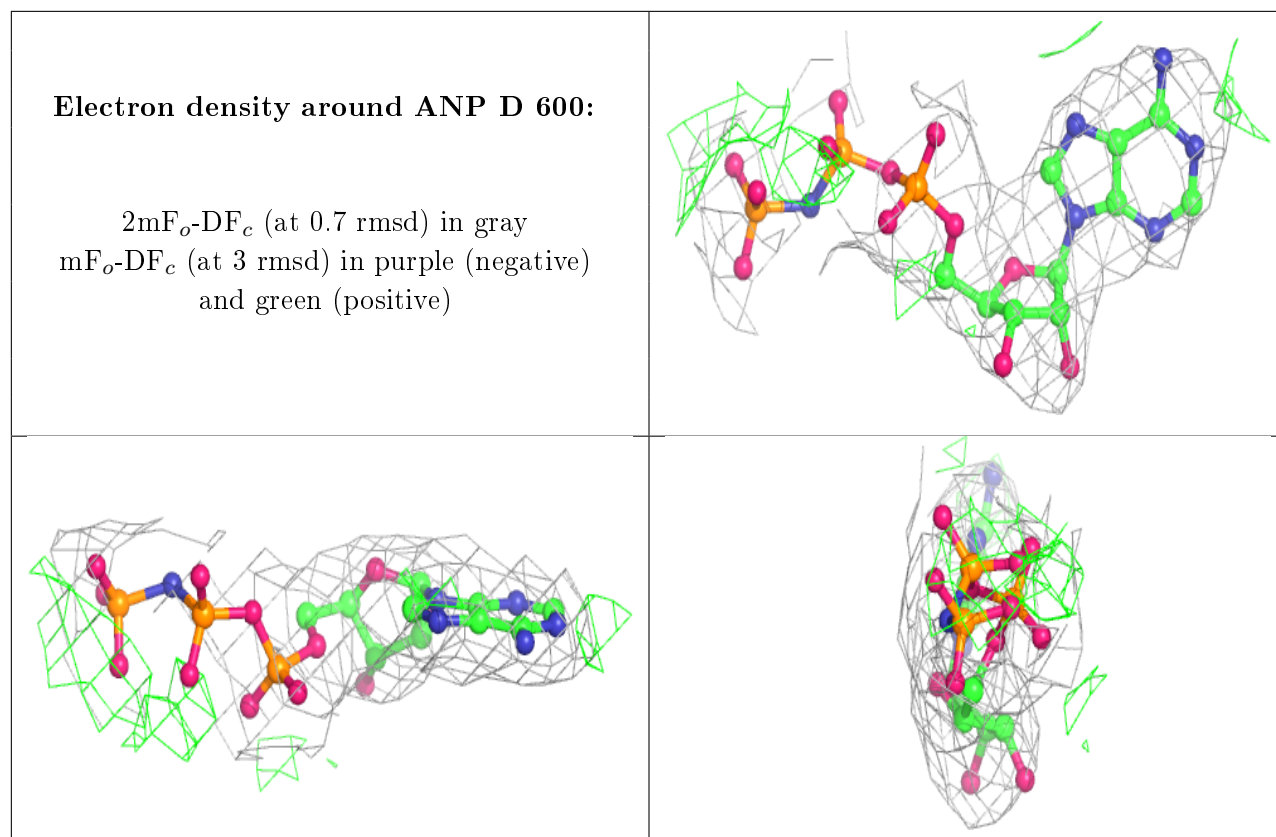
Electron density around ANP L 600:

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

**Electron density around ANP M 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.