



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 03:15 pm BST

PDB ID : 2JJ2  
Title : The Structure of F1-ATPase inhibited by quercetin.  
Authors : Gledhill, J.R.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2007-07-03  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

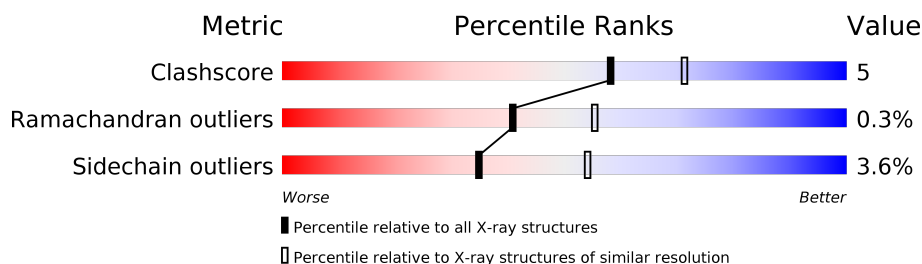
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	510	85% 10% • 5%
1	B	510	83% 10% • 6%
1	C	510	82% 13% • •
1	H	510	83% 12% • 5%
1	I	510	81% 12% • 6%
1	J	510	81% 14% • •
2	D	482	88% 9% • •
2	E	482	81% 13% • •
2	F	482	84% 12% • •

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Mol	Chain	Length	Quality of chain
2	K	482	
2	L	482	
2	M	482	
3	G	272	
3	N	272	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	1513	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48794 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 HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3658	2305	647	694	12			
1	C	495	Total	C	N	O	S	0	0	0
			3768	2374	664	718	12			
1	H	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	I	479	Total	C	N	O	S	0	0	0
			3658	2305	647	694	12			
1	J	495	Total	C	N	O	S	0	0	0
			3768	2374	664	718	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	SEE REMARK 999	UNP P19483
B	1	GLU	GLN	SEE REMARK 999	UNP P19483
C	1	GLU	GLN	SEE REMARK 999	UNP P19483
H	1	GLU	GLN	SEE REMARK 999	UNP P19483
I	1	GLU	GLN	SEE REMARK 999	UNP P19483
J	1	GLU	GLN	SEE REMARK 999	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

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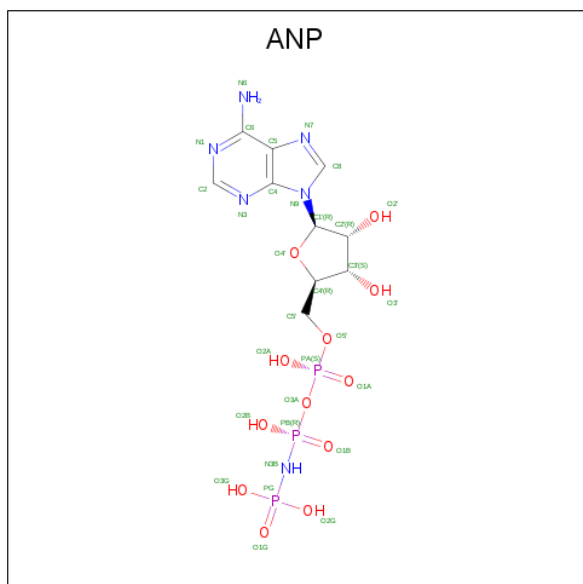
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	L	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	M	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	167	Total	C	N	O	S	0	0	0
			1296	810	237	242	7			
3	N	167	Total	C	N	O	S	0	0	0
			1296	810	237	242	7			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	M	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

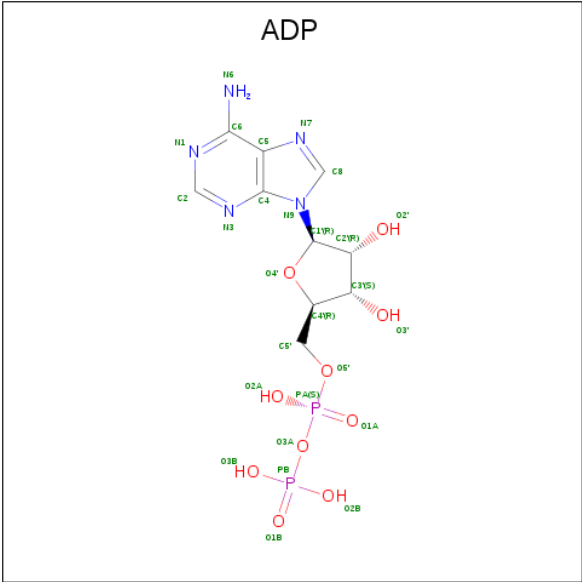
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



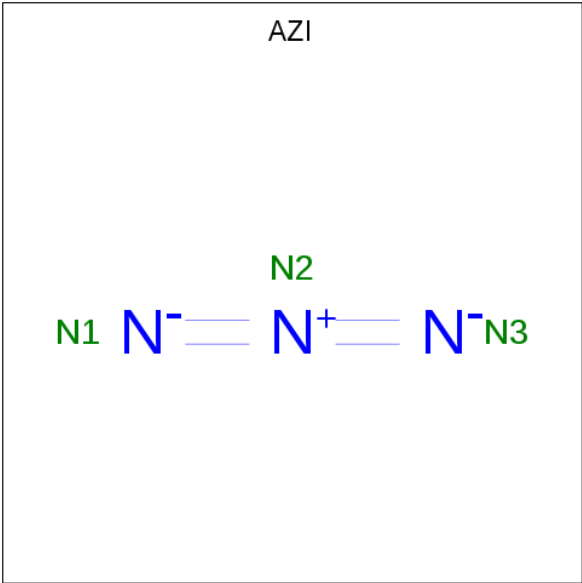
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	J	1	Total	C	O	0	0
			6	3	3		
6	K	1	Total	C	O	0	0
			6	3	3		
6	K	1	Total	C	O	0	0
			6	3	3		

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



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

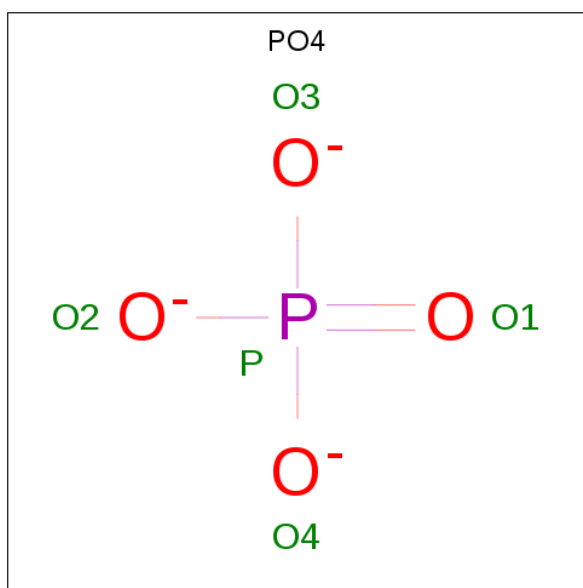
- Molecule 8 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	N	0	0
			3	3		
8	K	1	Total	N	0	0
			3	3		

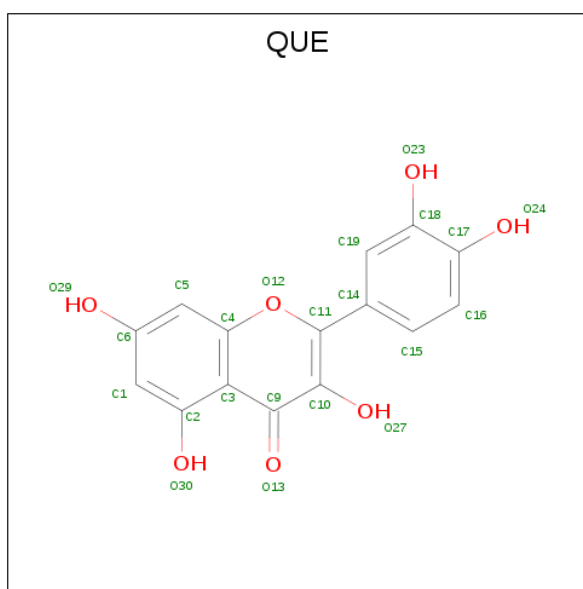


- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	O	P	0	0
			5	4	1		
9	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula:  $C_{15}H_{10}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	1
			44	30	14		
10	N	1	Total	C	O	0	1
			44	30	14		

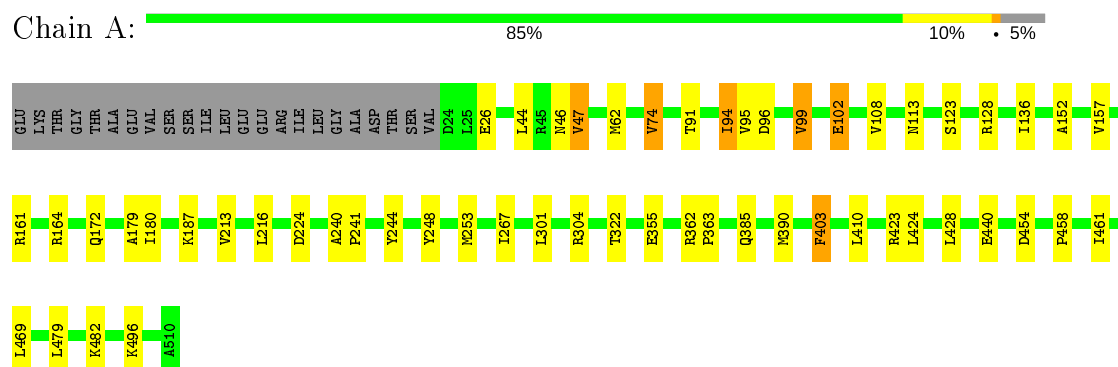
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	180	Total	O	0	0
			180	180		
11	B	153	Total	O	0	0
			153	153		
11	C	229	Total	O	0	0
			229	229		
11	D	179	Total	O	0	0
			179	179		
11	E	114	Total	O	0	0
			114	114		
11	F	205	Total	O	0	0
			205	205		
11	G	40	Total	O	0	0
			40	40		
11	H	207	Total	O	0	0
			207	207		
11	I	153	Total	O	0	0
			153	153		
11	J	236	Total	O	0	0
			236	236		
11	K	175	Total	O	0	0
			175	175		
11	L	122	Total	O	0	0
			122	122		
11	M	202	Total	O	0	0
			202	202		
11	N	39	Total	O	0	0
			39	39		

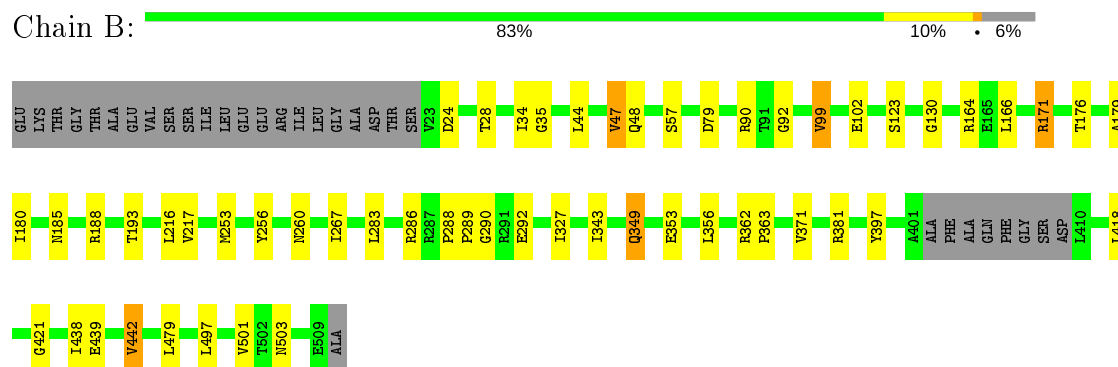
### 3 Residue-property plots

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. 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. 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.

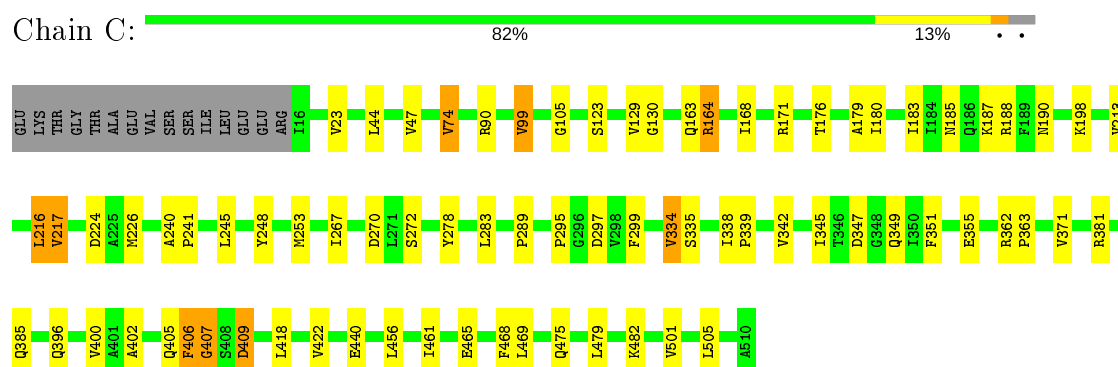
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



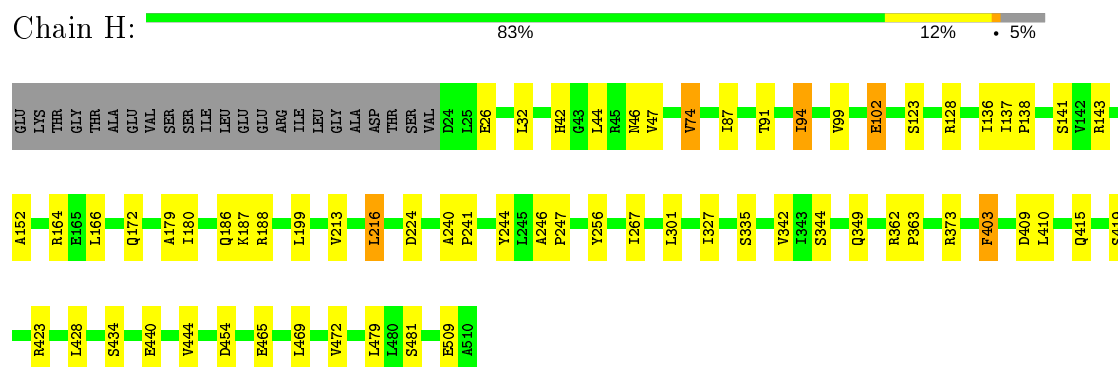
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



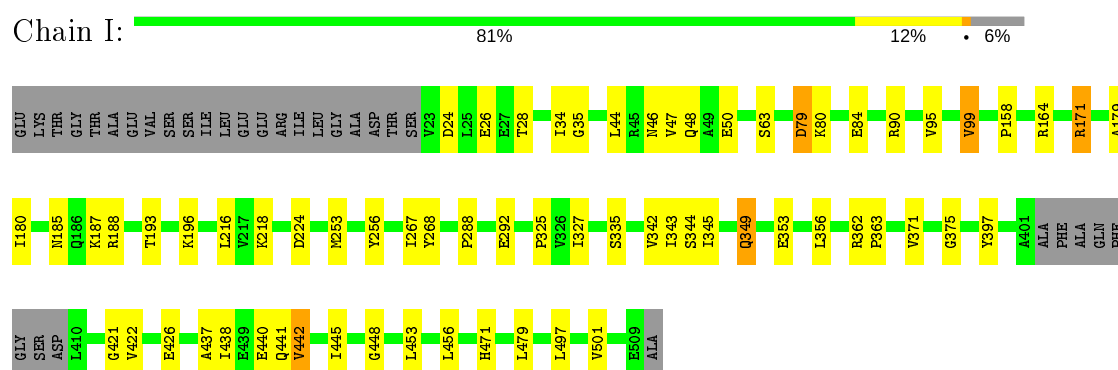
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



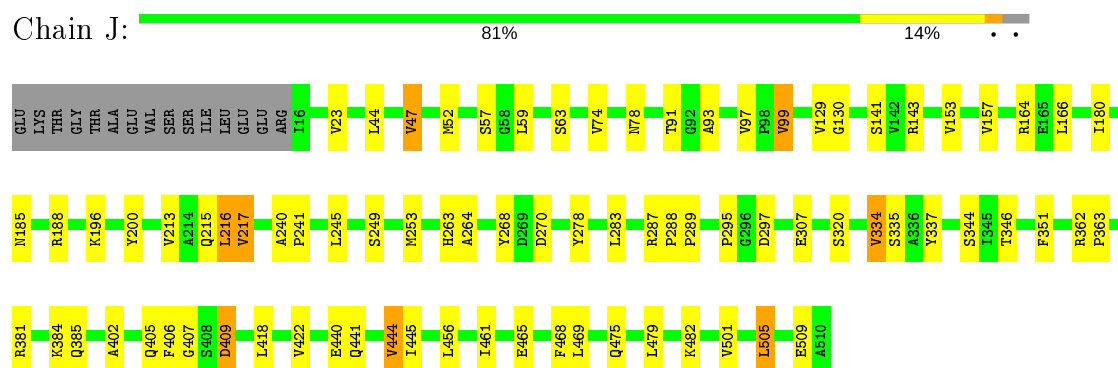
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



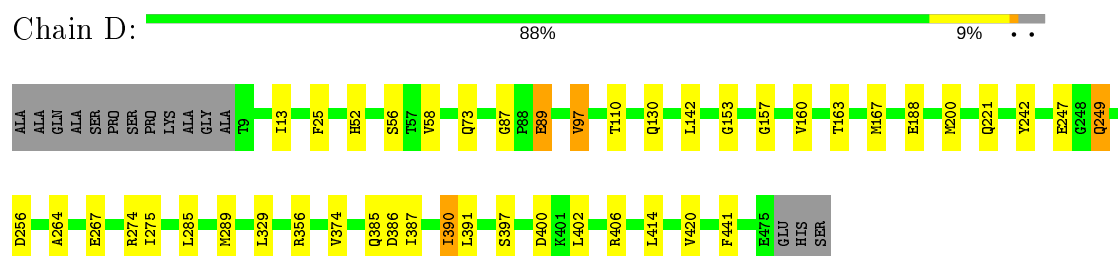
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM




- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

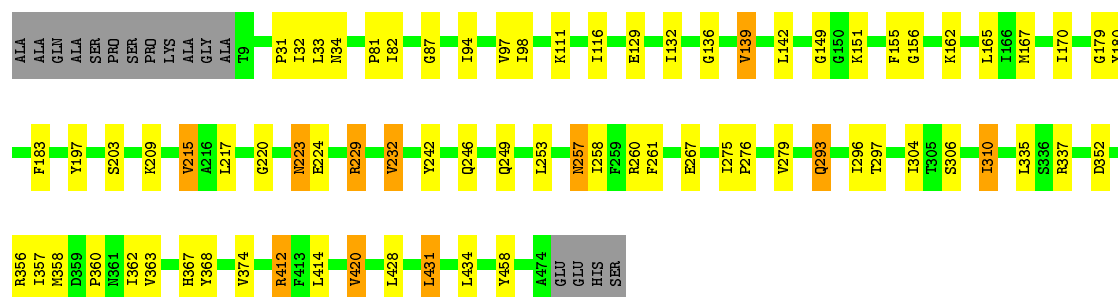


- Molecule 2: ATP SYNTHASE SUBUNIT BETA




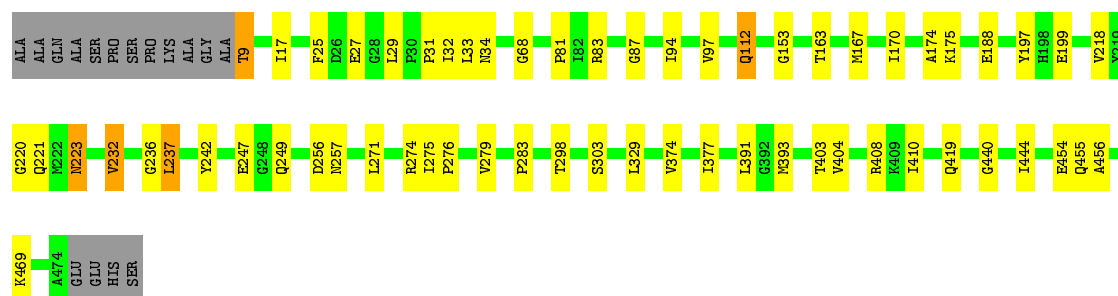
- Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain E:  81% 13% . .



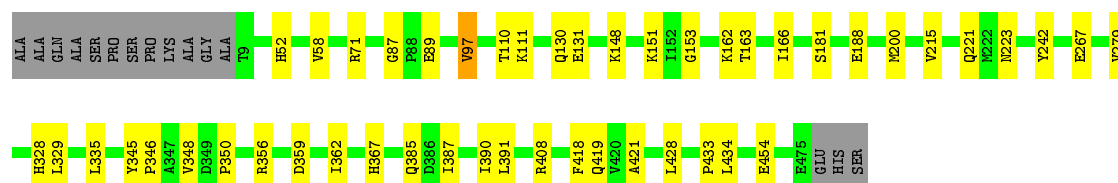
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain F:  84% 12% . .




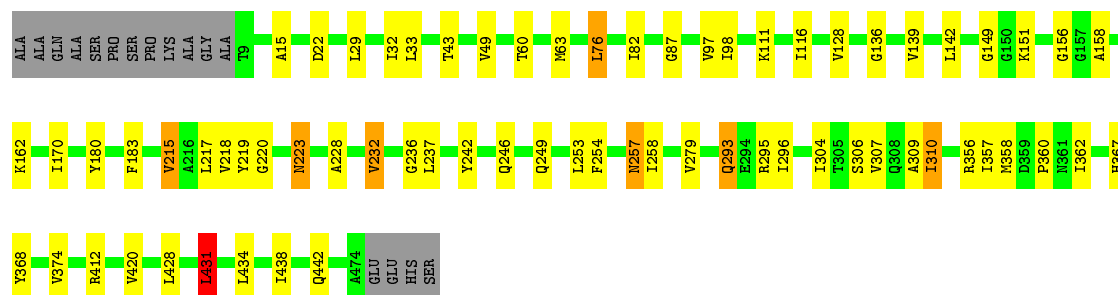
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain K:  87% 10% .




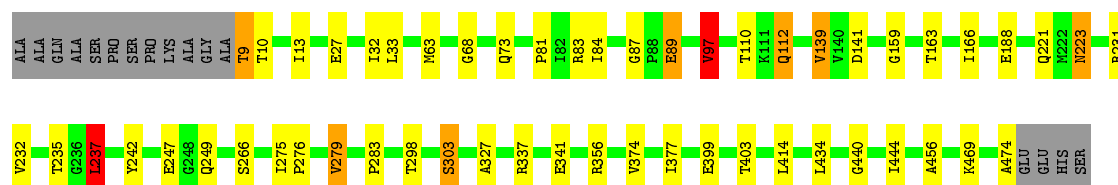
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain L:  82% 13% . .



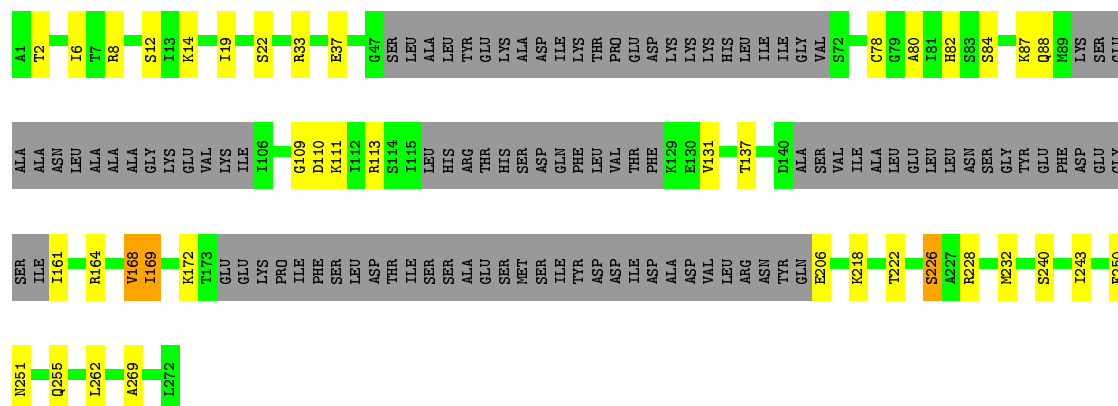
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain M:  85% 9% ..



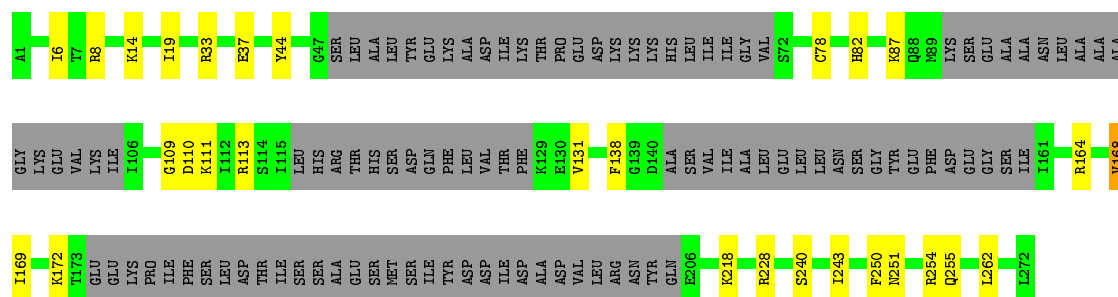
• Molecule 3: ATP SYNTHASE GAMMA CHAIN

Chain G:  47% 13% • 39%



• Molecule 3: ATP SYNTHASE GAMMA CHAIN

Chain N:  51% 10% 39%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.40Å 282.02Å 138.09Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	80.58 – 2.40 80.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.1 (80.58-2.40) 92.1 (80.48-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.188 , 0.238 0.188 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.328 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	48794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.41	0/3766	0.56	0/5080
1	B	0.40	0/3706	0.57	0/4998
1	C	0.43	0/3819	0.59	0/5153
1	H	0.40	0/3766	0.56	0/5080
1	I	0.41	0/3706	0.56	0/4998
1	J	0.43	0/3819	0.60	1/5153 (0.0%)
2	D	0.42	0/3596	0.57	1/4879 (0.0%)
2	E	0.39	0/3587	0.56	1/4867 (0.0%)
2	F	0.41	0/3587	0.58	1/4867 (0.0%)
2	K	0.42	0/3596	0.57	1/4879 (0.0%)
2	L	0.38	0/3587	0.57	2/4867 (0.0%)
2	M	0.42	0/3587	0.59	2/4867 (0.0%)
3	G	0.36	0/1304	0.48	0/1737
3	N	0.36	0/1304	0.49	0/1737
All	All	0.41	0/46730	0.57	9/63162 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	237	LEU	CA-CB-CG	7.28	132.04	115.30
2	M	237	LEU	CA-CB-CG	6.81	130.96	115.30
2	L	431	LEU	CA-CB-CG	6.09	129.30	115.30
2	D	97	VAL	CB-CA-C	-5.67	100.62	111.40
1	J	216	LEU	CA-CB-CG	5.67	128.35	115.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3715	0	3812	33	0
1	B	3658	0	3767	36	0
1	C	3768	0	3867	45	0
1	H	3715	0	3812	43	0
1	I	3658	0	3767	40	0
1	J	3768	0	3867	42	0
2	D	3539	0	3592	31	0
2	E	3530	0	3587	47	0
2	F	3530	0	3586	33	0
2	K	3539	0	3592	26	0
2	L	3530	0	3587	37	0
2	M	3530	0	3586	31	0
3	G	1296	0	1365	19	0
3	N	1296	0	1365	13	0
4	A	31	0	13	1	0
4	B	31	0	13	0	0
4	C	31	0	13	0	0
4	F	31	0	13	0	0
4	H	31	0	13	0	0
4	I	31	0	13	0	0
4	J	31	0	13	0	0
4	M	31	0	13	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	M	1	0	0	0	0
6	A	12	0	16	4	0
6	B	12	0	16	2	0
6	C	6	0	8	2	0
6	D	6	0	8	0	0
6	H	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	6	0	8	0	0
6	J	6	0	8	2	0
6	K	12	0	16	0	0
7	D	27	0	12	0	0
7	K	27	0	12	0	0
8	D	3	0	0	0	0
8	K	3	0	0	1	0
9	E	5	0	0	0	0
9	L	5	0	0	0	0
10	G	44	0	12	4	0
10	N	44	0	15	2	0
11	A	180	0	0	3	0
11	B	153	0	0	3	0
11	C	229	0	0	2	0
11	D	179	0	0	3	0
11	E	114	0	0	1	0
11	F	205	0	0	4	0
11	G	40	0	0	3	0
11	H	207	0	0	5	0
11	I	153	0	0	4	0
11	J	236	0	0	2	0
11	K	175	0	0	2	0
11	L	122	0	0	0	0
11	M	202	0	0	5	0
11	N	39	0	0	1	0
All	All	48794	0	47403	453	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 5.

The worst 5 of 453 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:E:223:ASN:H	2:E:223:ASN:HD22	1.25	0.83
1:B:290:GLY:HA3	6:B:1513:GOL:H12	1.62	0.81
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.15	0.81
2:L:183:PHE:HB3	2:L:217:LEU:HD23	1.64	0.78
1:J:180:ILE:HD11	1:J:216:LEU:HD21	1.66	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/510 (95%)	469 (97%)	15 (3%)	1 (0%)	47	62
1	B	475/510 (93%)	458 (96%)	16 (3%)	1 (0%)	47	62
1	C	493/510 (97%)	481 (98%)	10 (2%)	2 (0%)	34	48
1	H	485/510 (95%)	469 (97%)	16 (3%)	0	100	100
1	I	475/510 (93%)	462 (97%)	12 (2%)	1 (0%)	47	62
1	J	493/510 (97%)	480 (97%)	10 (2%)	3 (1%)	25	36
2	D	465/482 (96%)	441 (95%)	23 (5%)	1 (0%)	47	62
2	E	464/482 (96%)	444 (96%)	17 (4%)	3 (1%)	25	36
2	F	464/482 (96%)	446 (96%)	18 (4%)	0	100	100
2	K	465/482 (96%)	442 (95%)	21 (4%)	2 (0%)	34	48
2	L	464/482 (96%)	446 (96%)	16 (3%)	2 (0%)	34	48
2	M	464/482 (96%)	445 (96%)	18 (4%)	1 (0%)	47	62
3	G	155/272 (57%)	152 (98%)	3 (2%)	0	100	100
3	N	155/272 (57%)	151 (97%)	4 (3%)	0	100	100
All	All	6002/6496 (92%)	5786 (96%)	199 (3%)	17 (0%)	41	55

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
1	J	407	GLY
1	C	409	ASP
1	J	409	ASP
1	A	385	GLN

### 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	393/413 (95%)	379 (96%)	14 (4%)	35	54
1	B	389/413 (94%)	377 (97%)	12 (3%)	40	60
1	C	399/413 (97%)	384 (96%)	15 (4%)	33	51
1	H	393/413 (95%)	379 (96%)	14 (4%)	35	54
1	I	389/413 (94%)	377 (97%)	12 (3%)	40	60
1	J	399/413 (97%)	383 (96%)	16 (4%)	31	49
2	D	377/386 (98%)	372 (99%)	5 (1%)	69	84
2	E	376/386 (97%)	358 (95%)	18 (5%)	25	41
2	F	376/386 (97%)	364 (97%)	12 (3%)	39	59
2	K	377/386 (98%)	371 (98%)	6 (2%)	62	79
2	L	376/386 (97%)	360 (96%)	16 (4%)	29	46
2	M	376/386 (97%)	360 (96%)	16 (4%)	29	46
3	G	140/230 (61%)	126 (90%)	14 (10%)	7	11
3	N	140/230 (61%)	132 (94%)	8 (6%)	20	33
All	All	4900/5254 (93%)	4722 (96%)	178 (4%)	35	54

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	110	ASP
1	H	403	PHE
2	M	249	GLN
3	G	137	THR
1	H	74	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	443	GLN

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Mol	Chain	Res	Type
1	I	48	GLN
2	M	419	GLN
3	G	15	ASN
3	G	211	ASN

### 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 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	$\# Z  > 2$
9	PO4	L	1475	-	4,4,4	0.91	0	6,6,6	0.39	0
9	PO4	E	1475	-	4,4,4	0.89	0	6,6,6	0.40	0
7	ADP	K	1476	5	24,29,29	1.12	2 (8%)	29,45,45	1.24	3 (10%)
6	GOL	B	1512	-	5,5,5	0.38	0	5,5,5	0.36	0
6	GOL	A	1513	-	5,5,5	0.36	0	5,5,5	0.55	0
4	ANP	B	1510	5	29,33,33	1.90	9 (31%)	31,52,52	1.71	7 (22%)
6	GOL	I	1512	-	5,5,5	0.40	0	5,5,5	0.33	0
4	ANP	J	1511	5	29,33,33	1.77	8 (27%)	31,52,52	1.80	6 (19%)
6	GOL	K	1480	-	5,5,5	0.36	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ANP	I	1510	5	29,33,33	1.84	8 (27%)	31,52,52	2.14	6 (19%)
10	QUE	N	1273[A]	-	21,24,24	2.22	5 (23%)	28,36,36	1.53	3 (10%)
10	QUE	N	1273[B]	-	21,24,24	2.16	5 (23%)	28,36,36	1.43	3 (10%)
6	GOL	H	1514	-	5,5,5	0.40	0	5,5,5	0.36	0
10	QUE	G	1273[A]	-	21,24,24	2.22	5 (23%)	28,36,36	1.55	4 (14%)
4	ANP	F	1475	5	29,33,33	1.93	10 (34%)	31,52,52	2.00	7 (22%)
6	GOL	A	1514	-	5,5,5	0.35	0	5,5,5	0.70	0
10	QUE	G	1273[B]	-	21,24,24	2.14	5 (23%)	28,36,36	1.42	3 (10%)
8	AZI	D	1478	-	0,2,2	0.00	-	0,1,1	0.00	-
4	ANP	M	1475	5	29,33,33	1.89	11 (37%)	31,52,52	1.98	7 (22%)
6	GOL	K	1479	-	5,5,5	0.42	0	5,5,5	0.30	0
4	ANP	C	1511	5	29,33,33	1.80	9 (31%)	31,52,52	1.73	6 (19%)
8	AZI	K	1478	-	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	C	1513	-	5,5,5	0.37	0	5,5,5	0.22	0
6	GOL	J	1513	-	5,5,5	0.39	0	5,5,5	0.44	0
6	GOL	H	1513	-	5,5,5	0.40	0	5,5,5	0.41	0
6	GOL	B	1513	-	5,5,5	0.35	0	5,5,5	0.44	0
4	ANP	H	1511	5	29,33,33	1.84	8 (27%)	31,52,52	1.52	5 (16%)
6	GOL	D	1479	-	5,5,5	0.37	0	5,5,5	0.39	0
4	ANP	A	1511	5	29,33,33	1.91	10 (34%)	31,52,52	1.88	6 (19%)
7	ADP	D	1476	5	24,29,29	1.11	1 (4%)	29,45,45	1.18	2 (6%)

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
7	ADP	K	1476	5	-	3/12/32/32	0/3/3/3
6	GOL	B	1512	-	-	2/4/4/4	-
6	GOL	A	1513	-	-	2/4/4/4	-
4	ANP	B	1510	5	-	2/14/38/38	0/3/3/3
6	GOL	I	1512	-	-	2/4/4/4	-
4	ANP	J	1511	5	-	3/14/38/38	0/3/3/3
6	GOL	K	1480	-	-	3/4/4/4	-
4	ANP	I	1510	5	-	2/14/38/38	0/3/3/3
10	QUE	N	1273[A]	-	-	2/4/4/4	0/3/3/3
10	QUE	N	1273[B]	-	-	3/4/4/4	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	H	1514	-	-	2/4/4/4	-
10	QUE	G	1273[A]	-	-	2/4/4/4	0/3/3/3
4	ANP	F	1475	5	-	2/14/38/38	0/3/3/3
6	GOL	A	1514	-	-	2/4/4/4	-
10	QUE	G	1273[B]	-	-	2/4/4/4	0/3/3/3
4	ANP	M	1475	5	-	4/14/38/38	0/3/3/3
6	GOL	K	1479	-	-	2/4/4/4	-
4	ANP	C	1511	5	-	3/14/38/38	0/3/3/3
6	GOL	C	1513	-	-	0/4/4/4	-
6	GOL	J	1513	-	-	1/4/4/4	-
6	GOL	H	1513	-	-	2/4/4/4	-
6	GOL	B	1513	-	-	4/4/4/4	-
4	ANP	H	1511	5	-	3/14/38/38	0/3/3/3
6	GOL	D	1479	-	-	2/4/4/4	-
4	ANP	A	1511	5	-	3/14/38/38	0/3/3/3
7	ADP	D	1476	5	-	3/12/32/32	0/3/3/3

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	1273[A]	QUE	C3-C4	6.05	1.49	1.41
10	N	1273[A]	QUE	C3-C4	6.05	1.49	1.41
10	N	1273[B]	QUE	C3-C4	5.91	1.49	1.41
10	G	1273[B]	QUE	C3-C4	5.87	1.49	1.41
10	N	1273[A]	QUE	C18-C17	5.83	1.49	1.40

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1475	ANP	O1G-PG-N3B	-7.53	100.67	111.77
4	I	1510	ANP	O1G-PG-N3B	-7.32	101.00	111.77
4	M	1475	ANP	O1G-PG-N3B	-7.12	101.28	111.77
4	A	1511	ANP	O1G-PG-N3B	-5.81	103.22	111.77
4	J	1511	ANP	O1G-PG-N3B	-5.57	103.57	111.77

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	1476	ADP	PA-O3A-PB-O2B
4	A	1511	ANP	PB-N3B-PG-O1G
4	A	1511	ANP	PG-N3B-PB-O1B
4	A	1511	ANP	PG-N3B-PB-O3A
6	A	1513	GOL	C1-C2-C3-O3

There are no ring outliers.

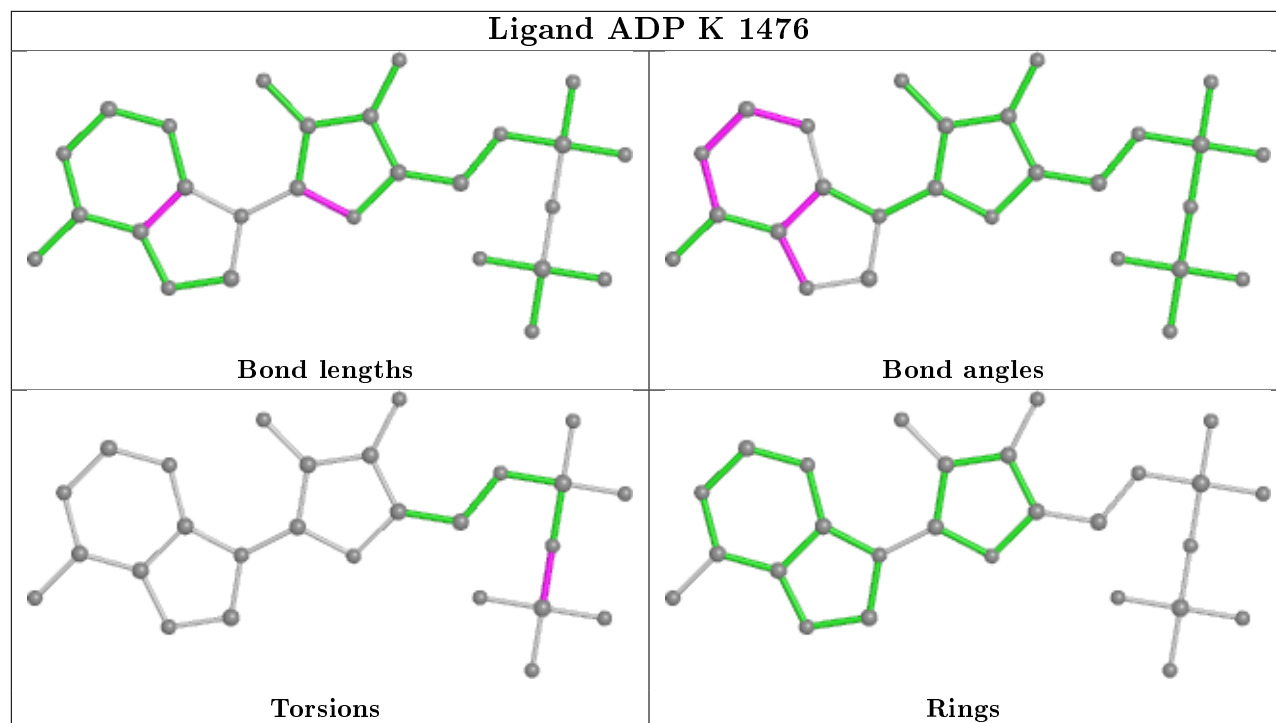
11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1512	GOL	1	0
6	A	1513	GOL	4	0
10	N	1273[A]	QUE	2	0
10	G	1273[A]	QUE	3	0
10	G	1273[B]	QUE	1	0
4	M	1475	ANP	2	0
8	K	1478	AZI	1	0
6	C	1513	GOL	2	0
6	J	1513	GOL	2	0
6	B	1513	GOL	1	0
4	A	1511	ANP	1	0

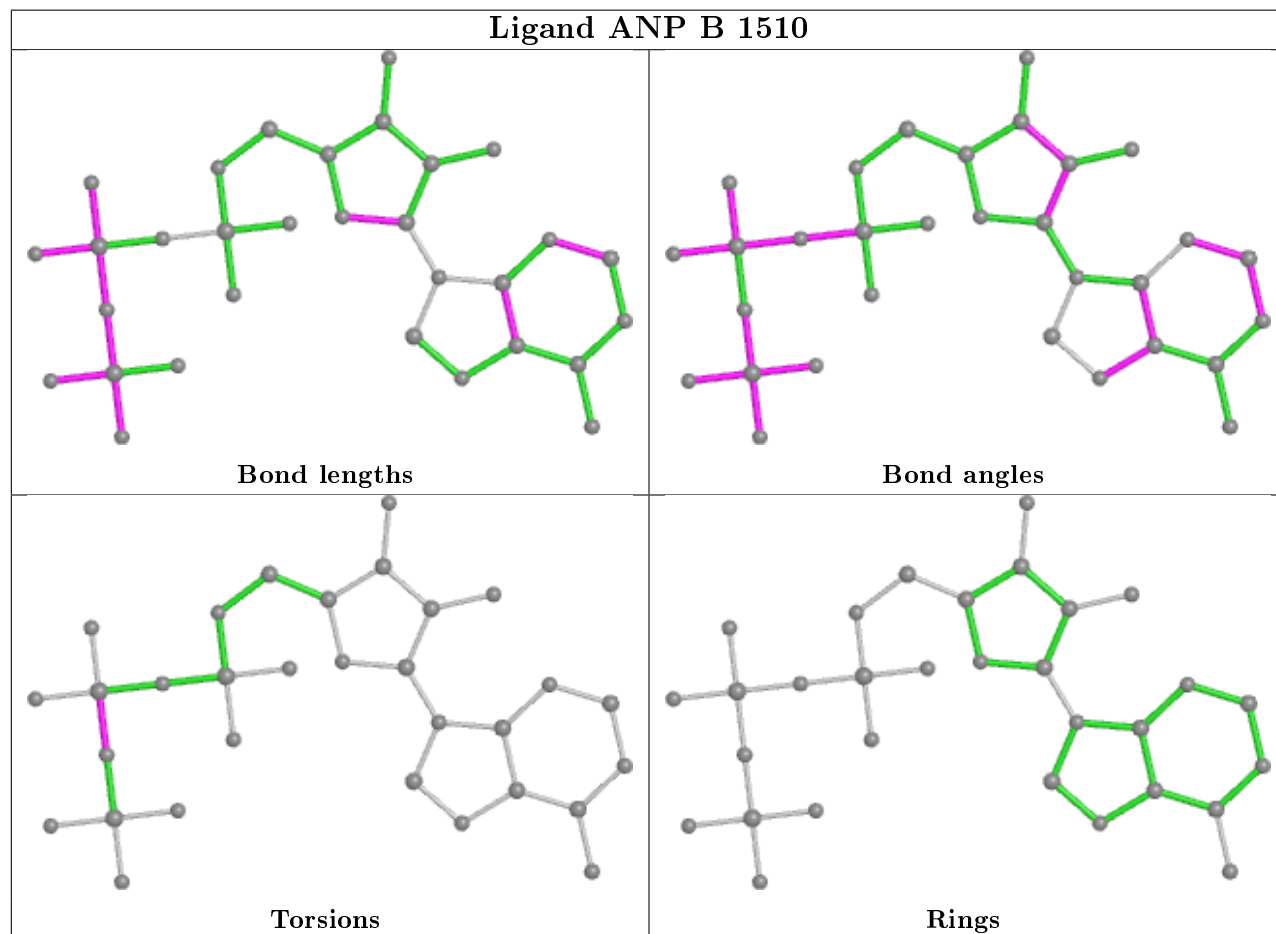
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

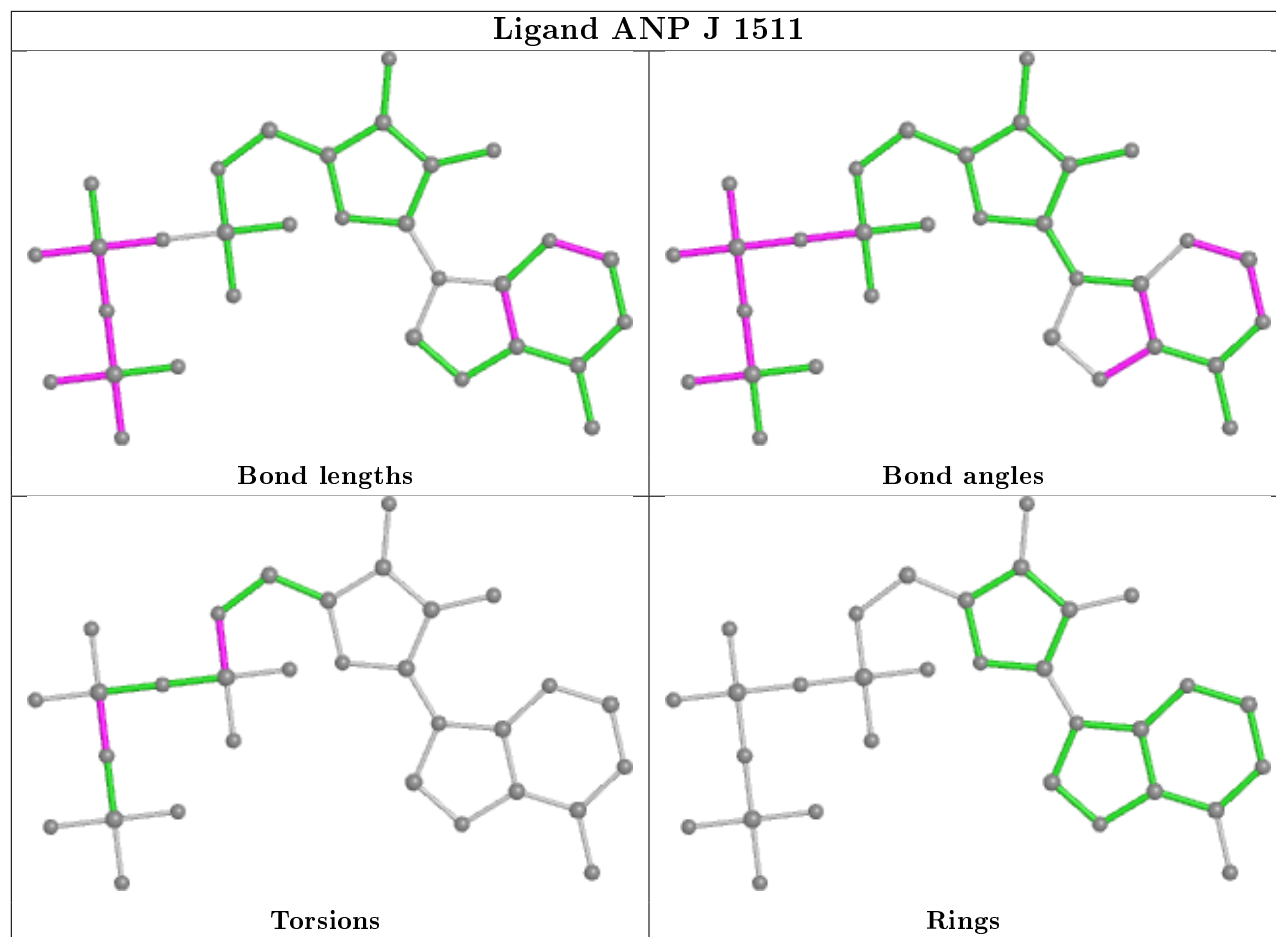


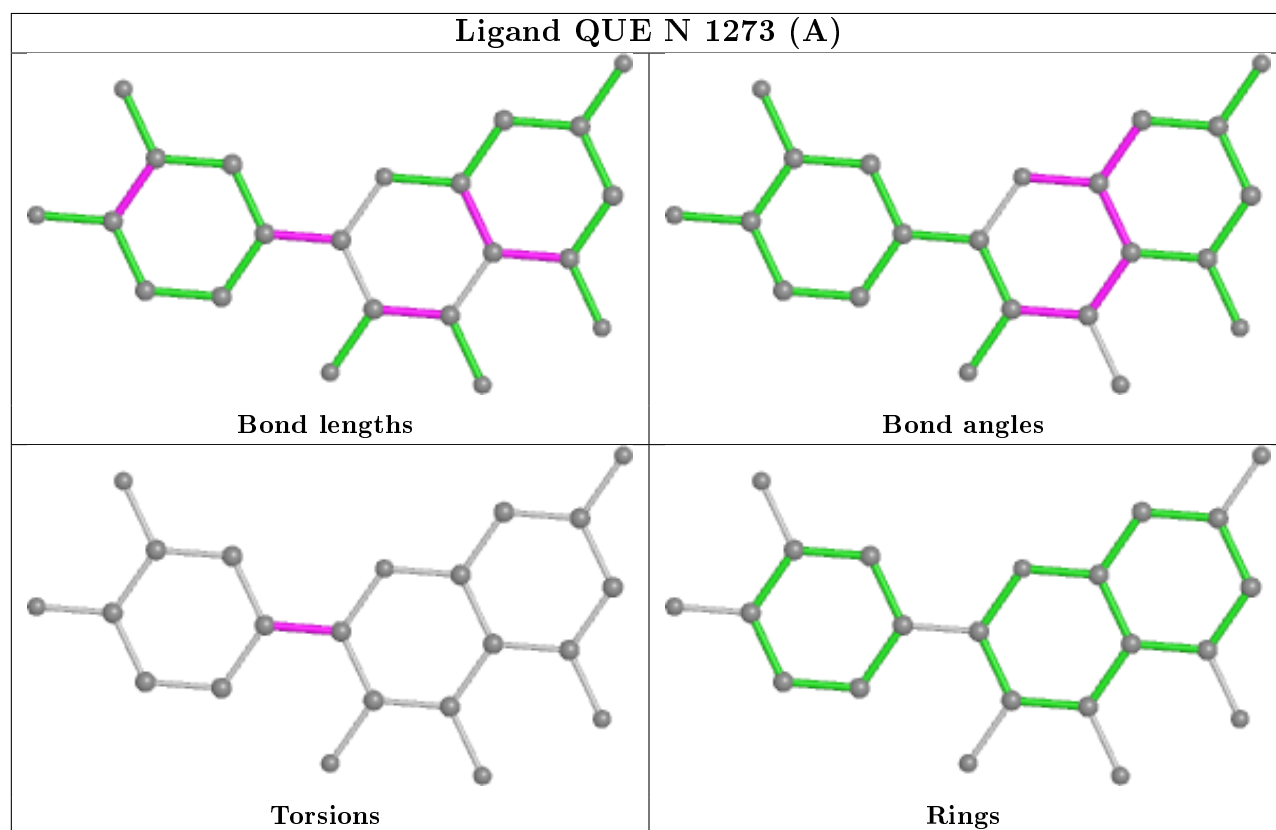
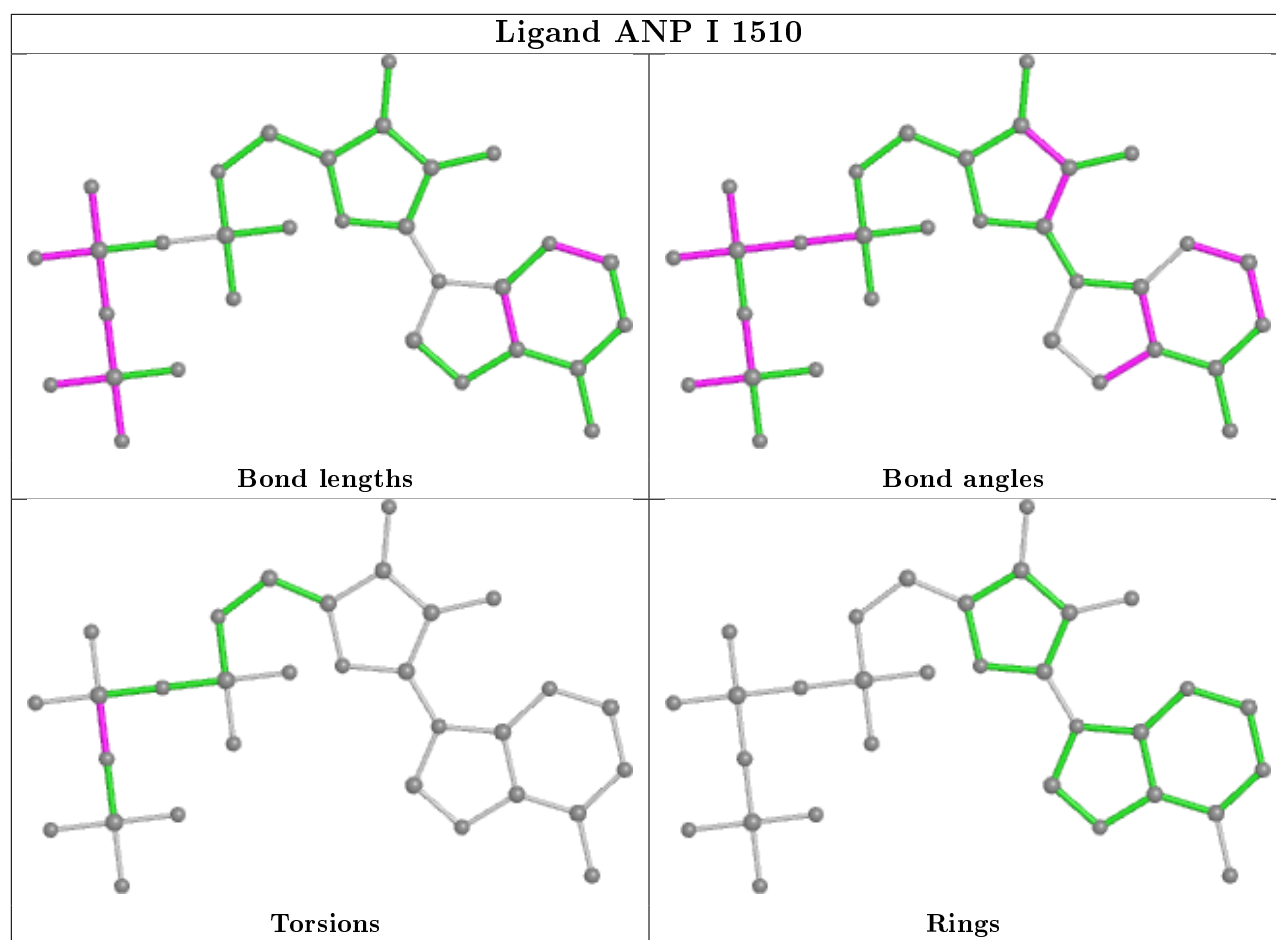
## Ligand ADP K 1476



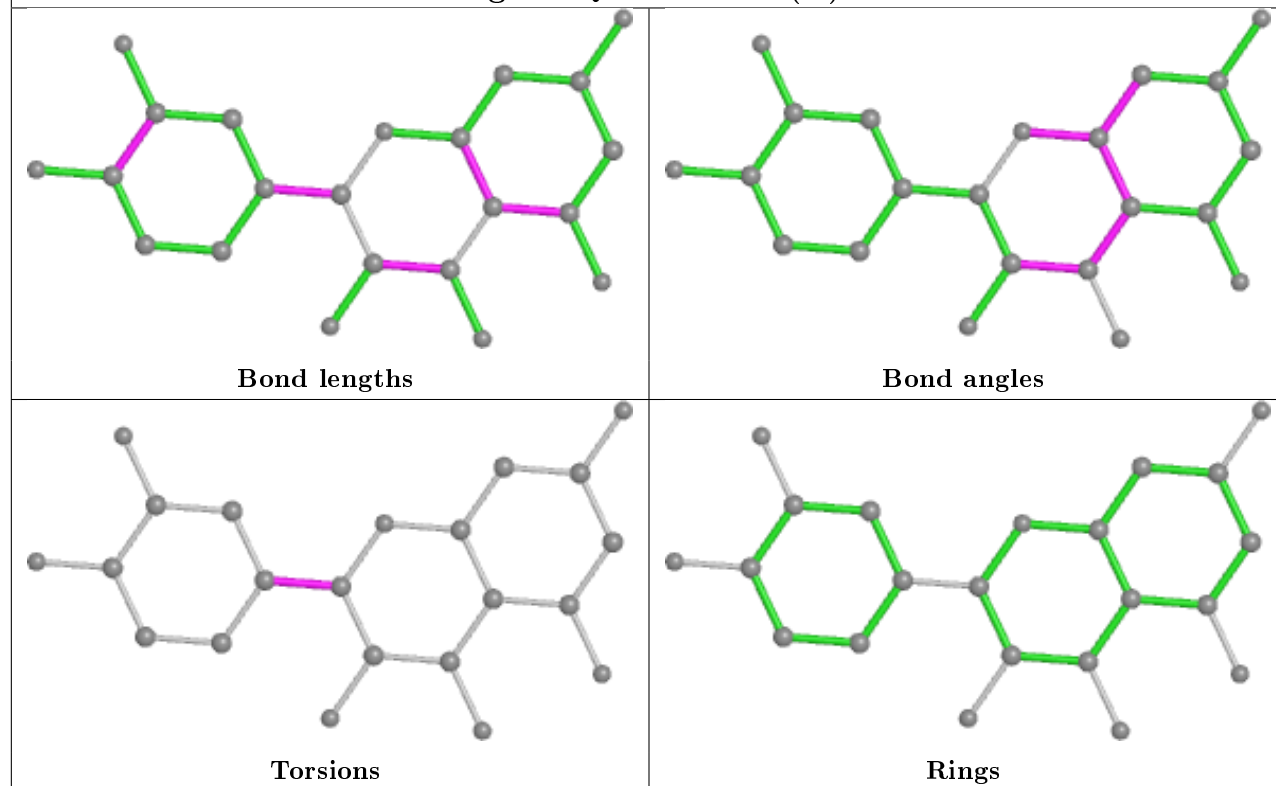
## Ligand ANP B 1510



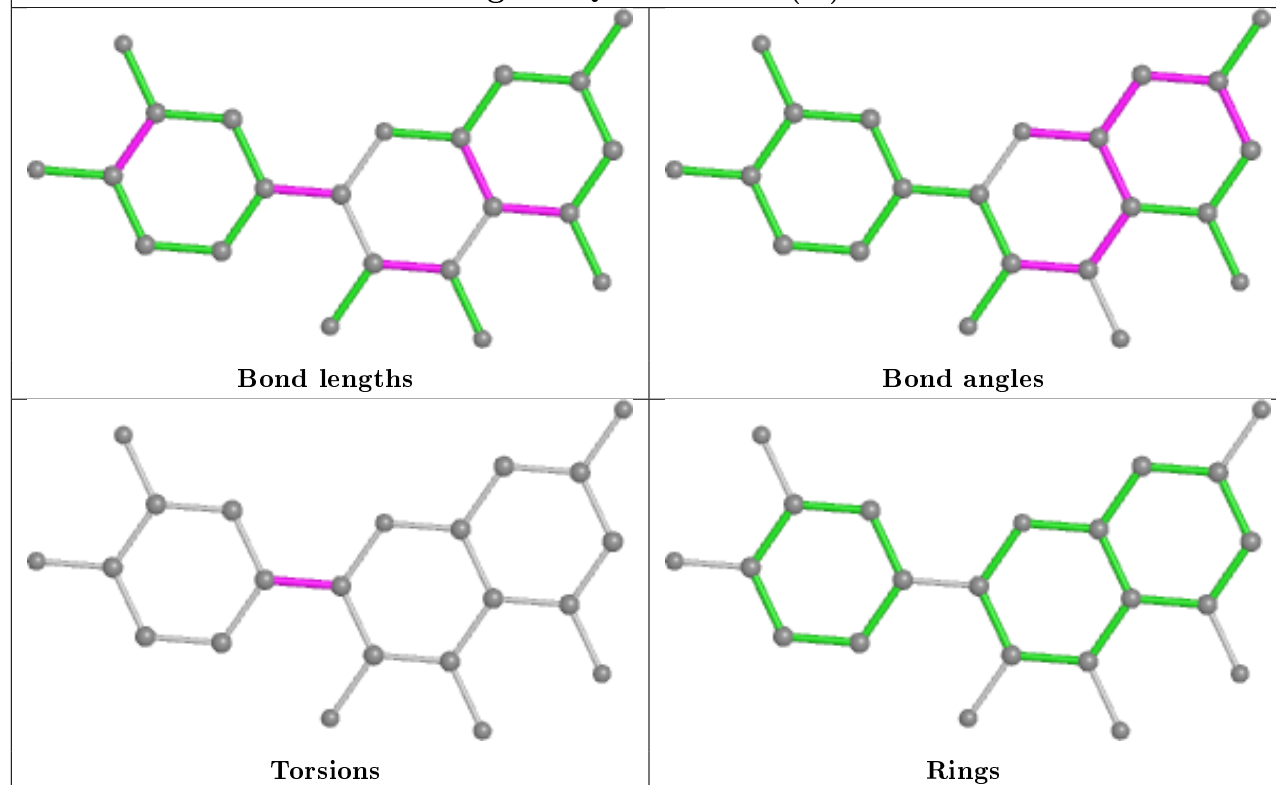




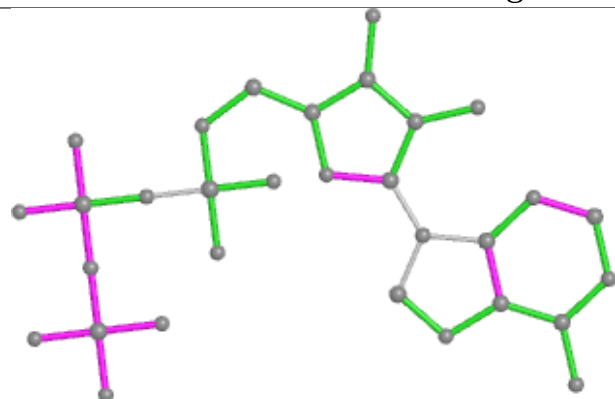
## Ligand QUE N 1273 (B)



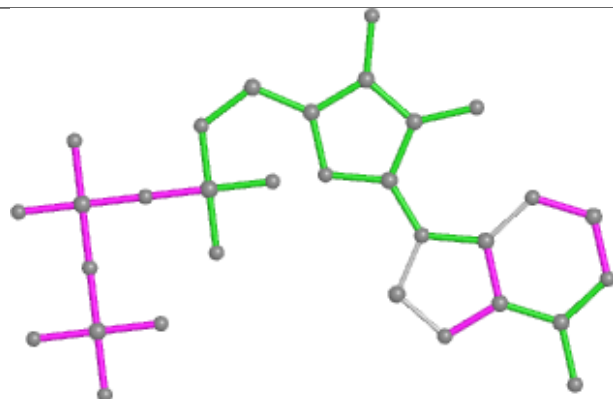
## Ligand QUE G 1273 (A)



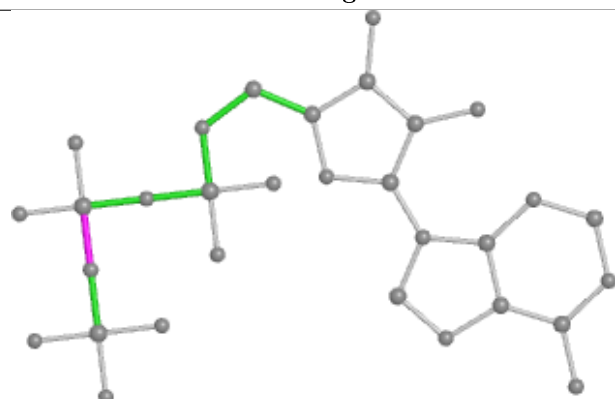
## Ligand ANP F 1475



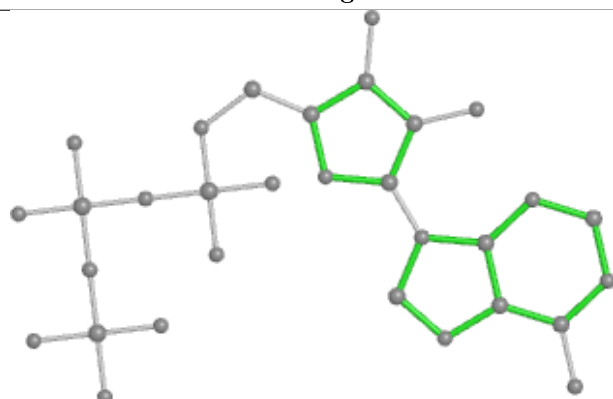
Bond lengths



Bond angles

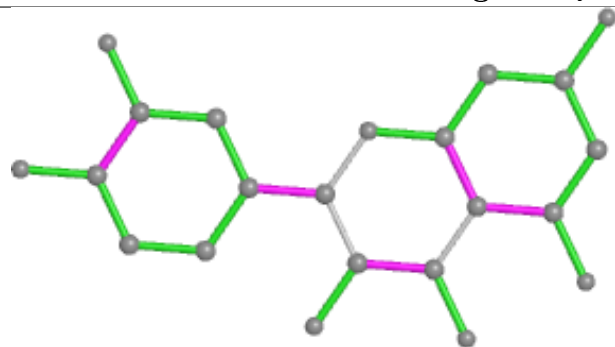


Torsions

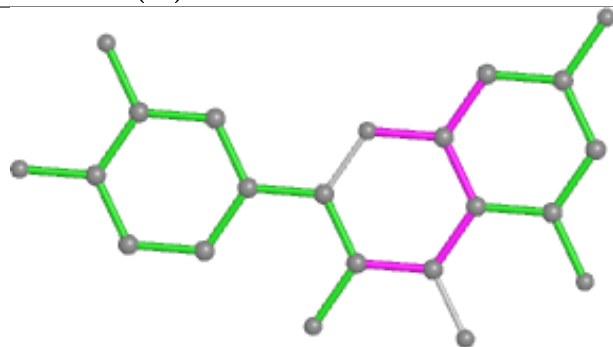


Rings

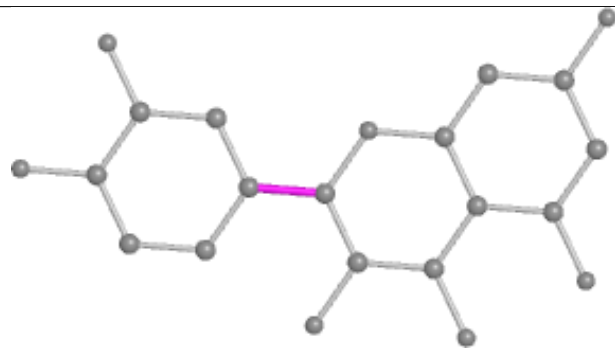
## Ligand QUE G 1273 (B)



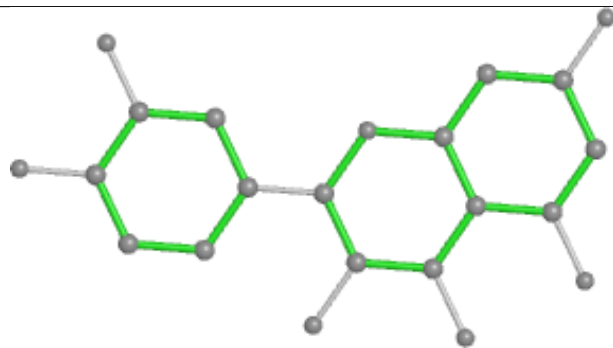
Bond lengths



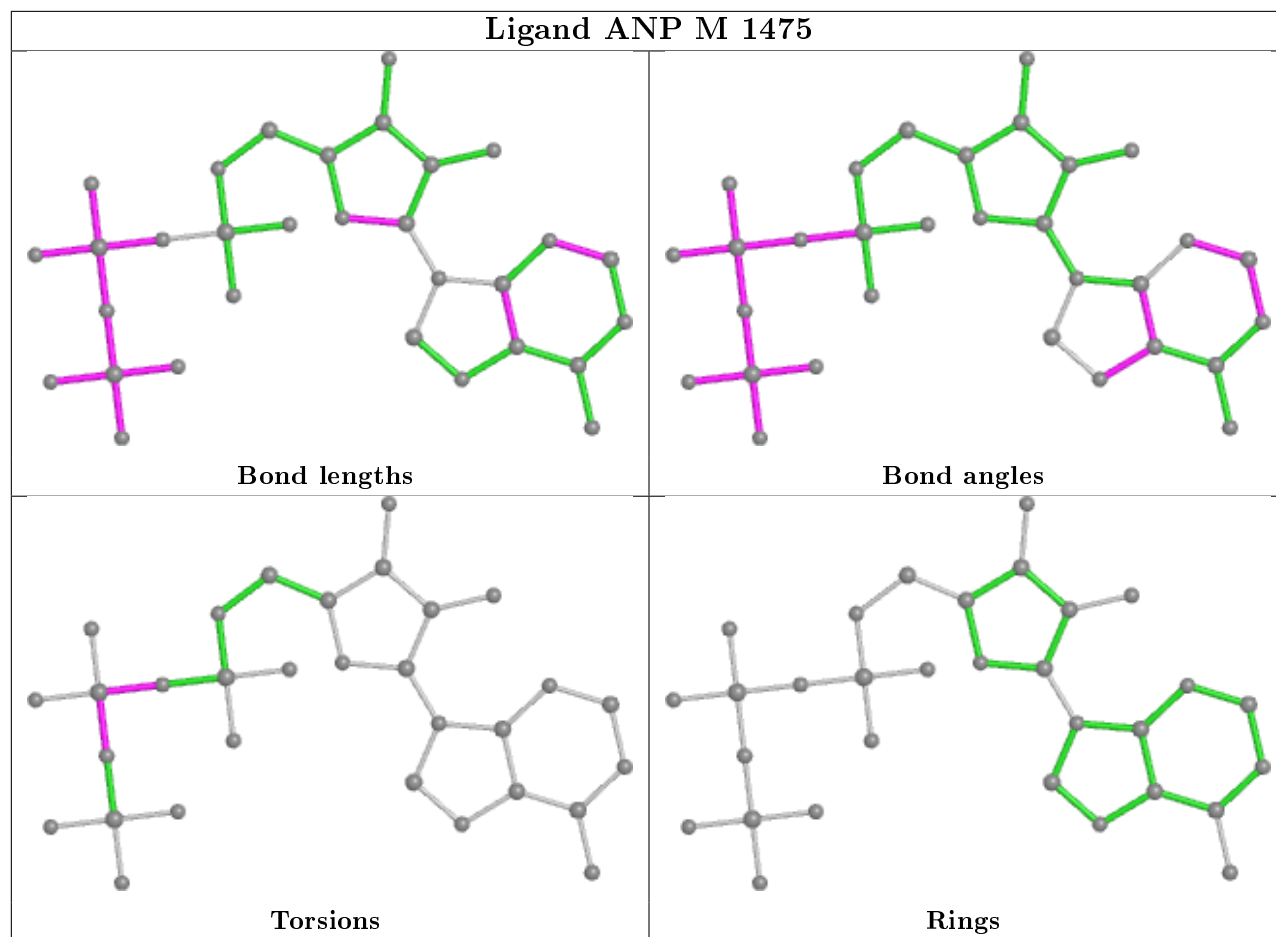
Bond angles

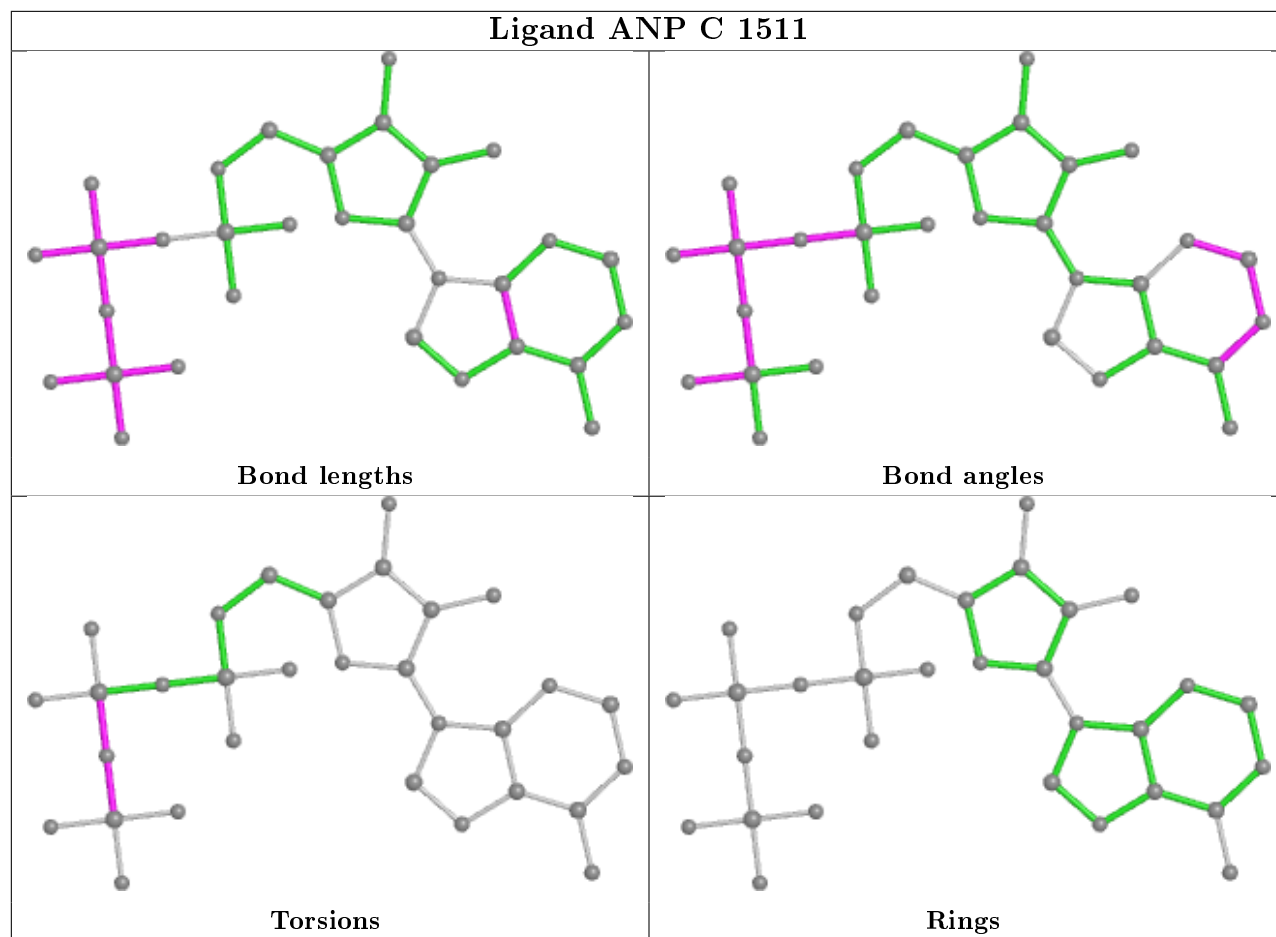


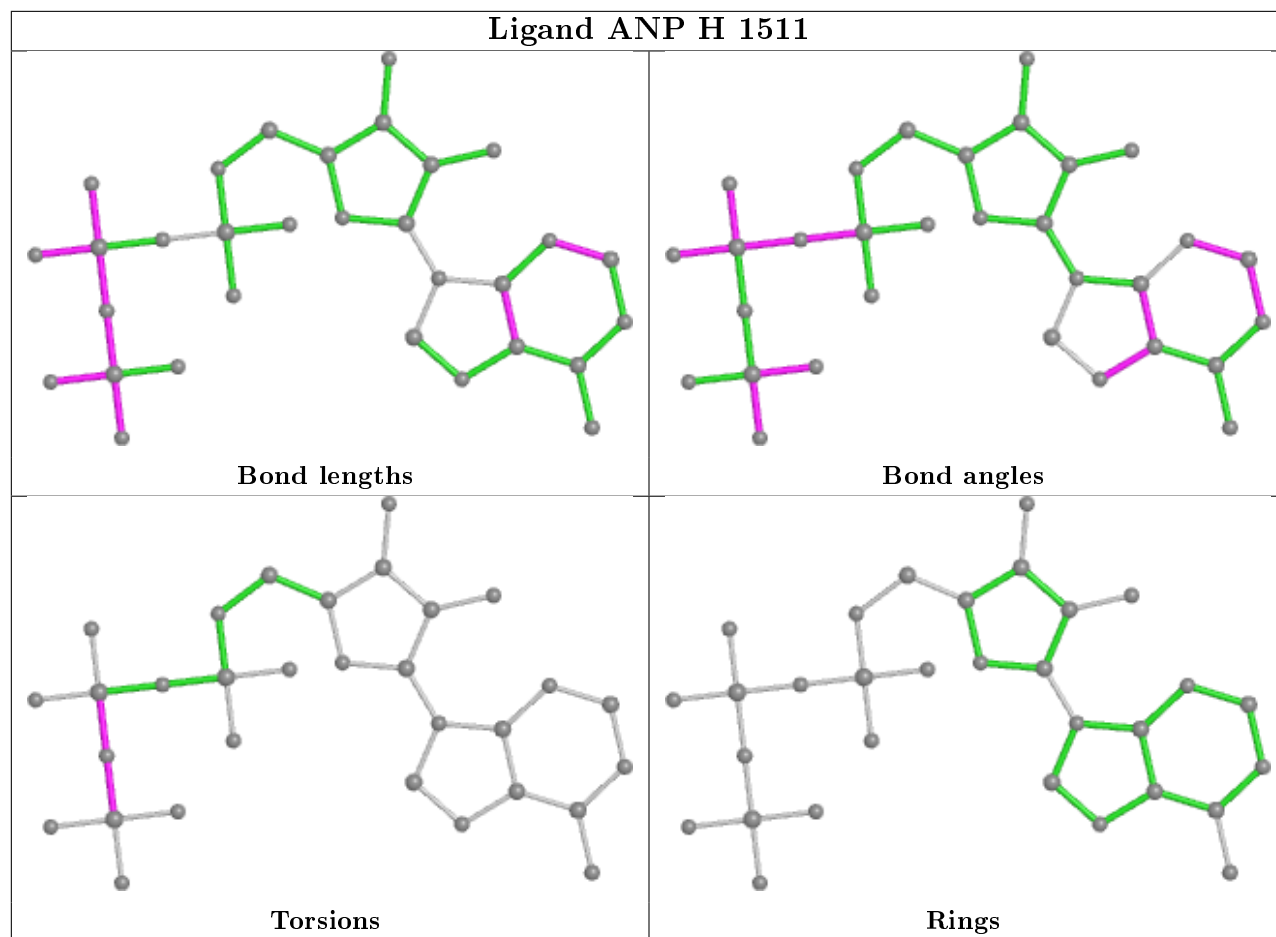
Torsions



Rings

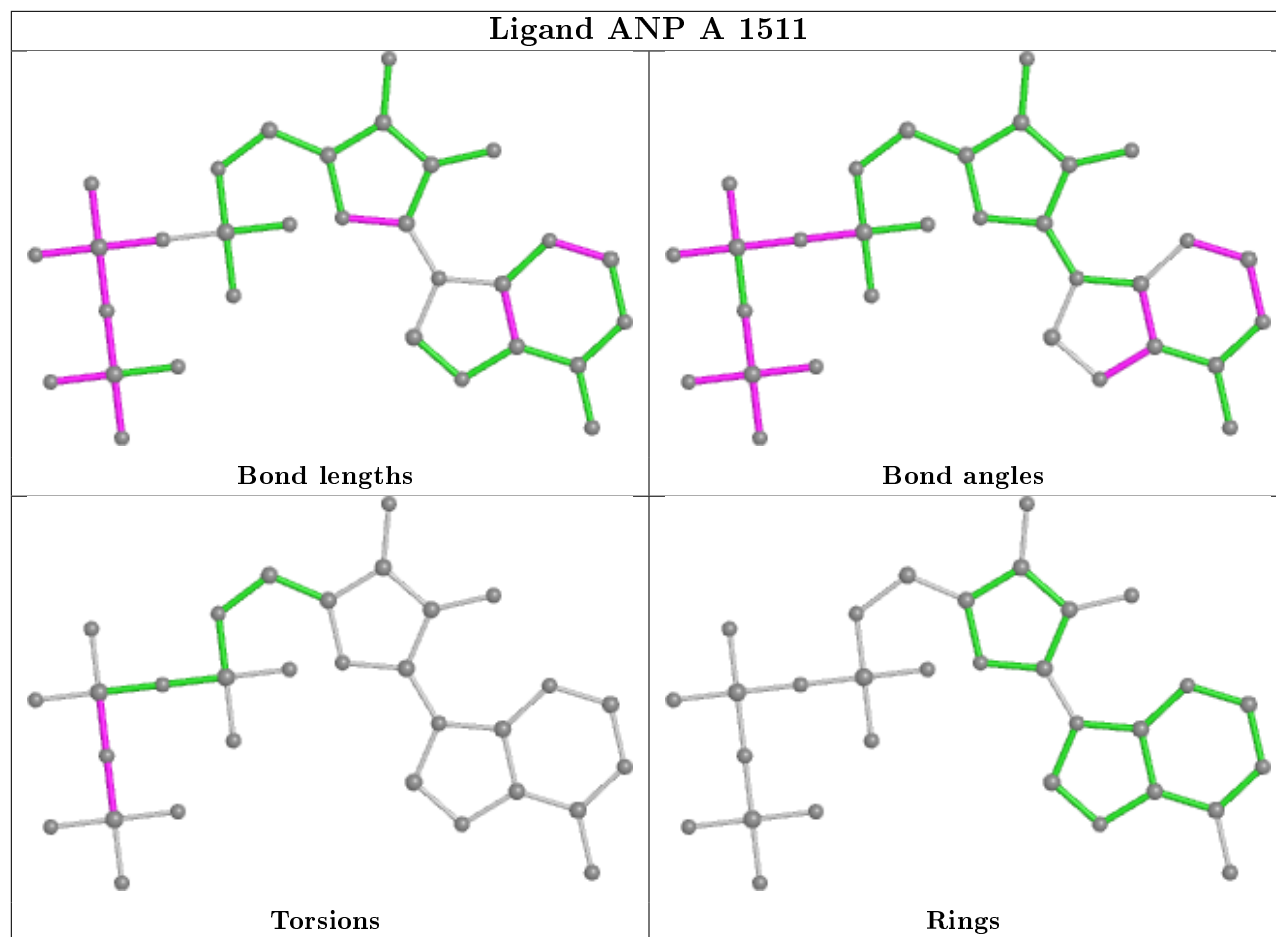




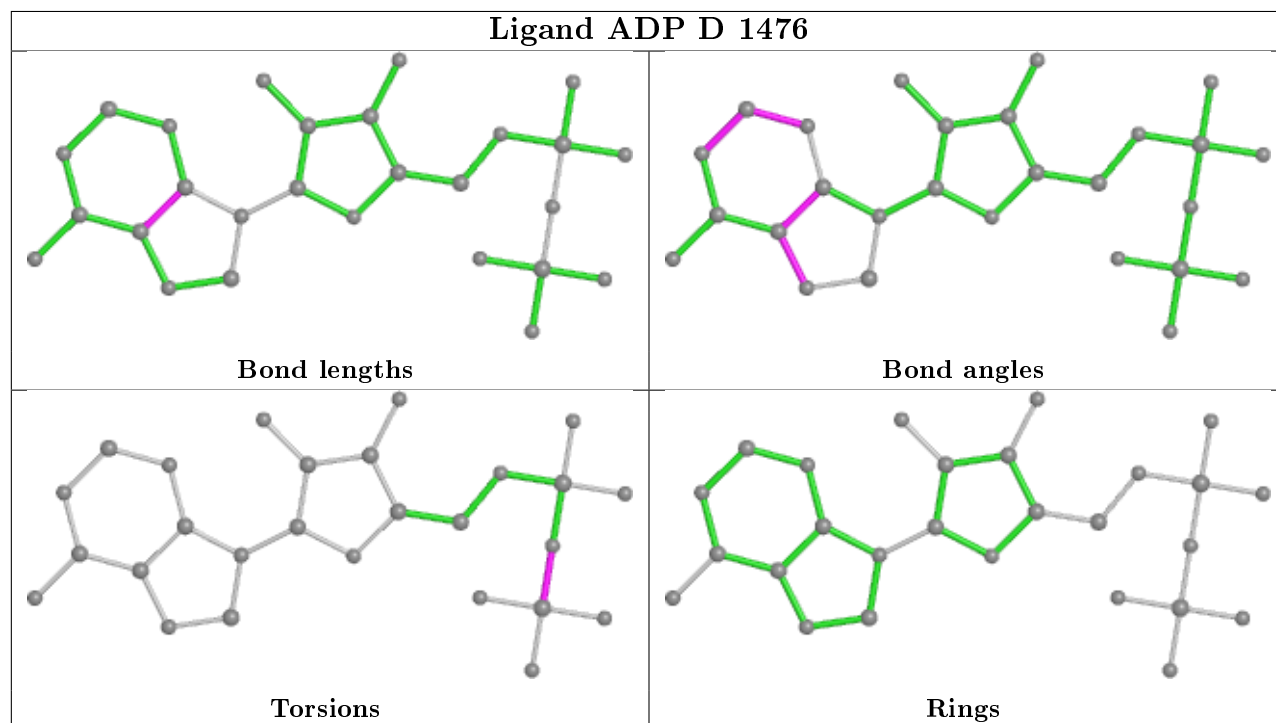




## Ligand ANP A 1511



## Ligand ADP D 1476



## 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

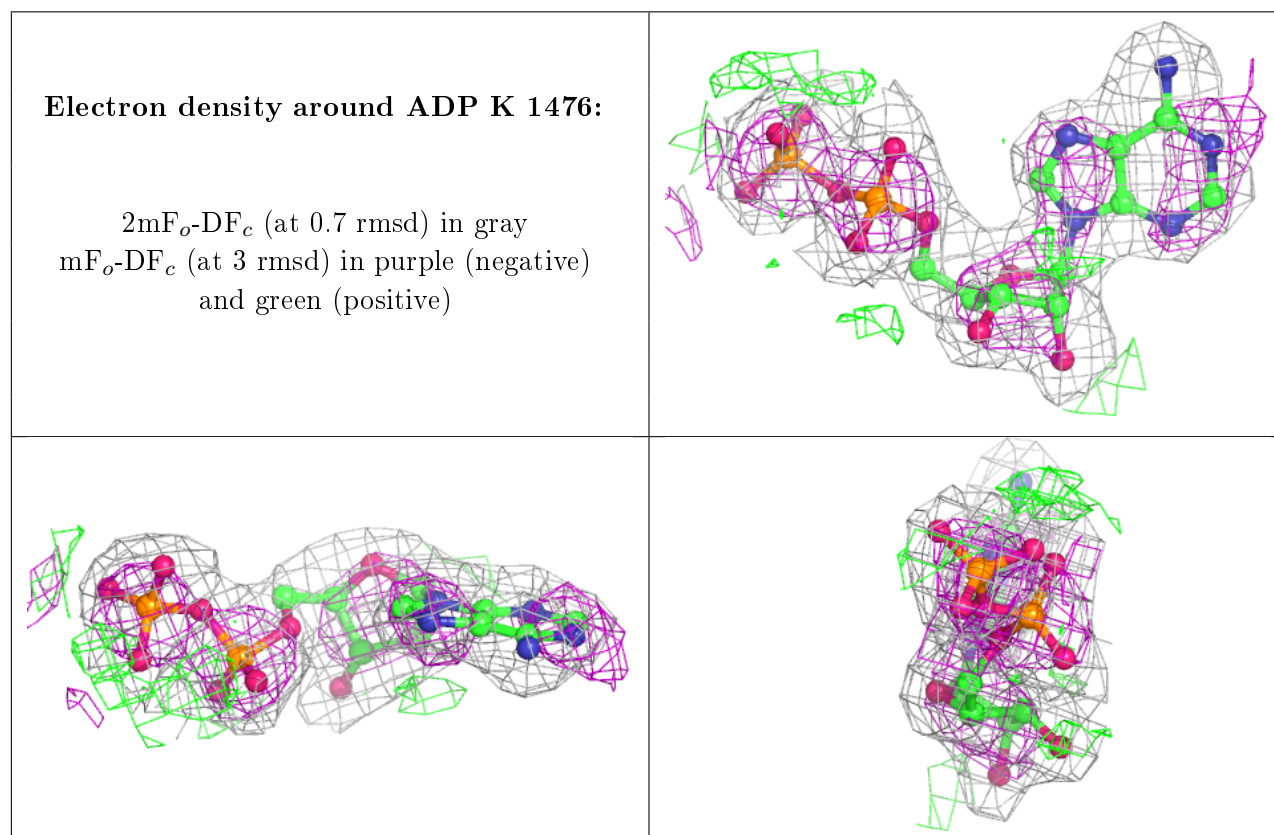
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

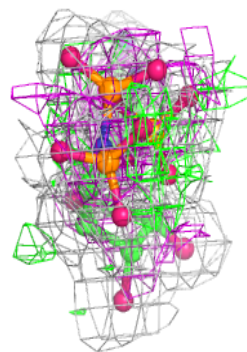
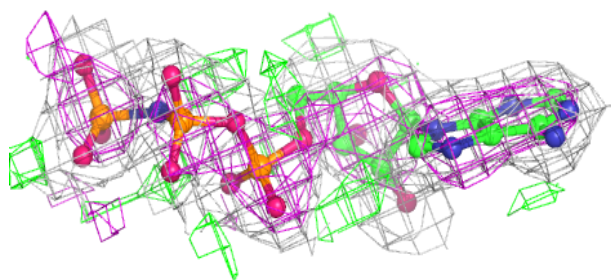
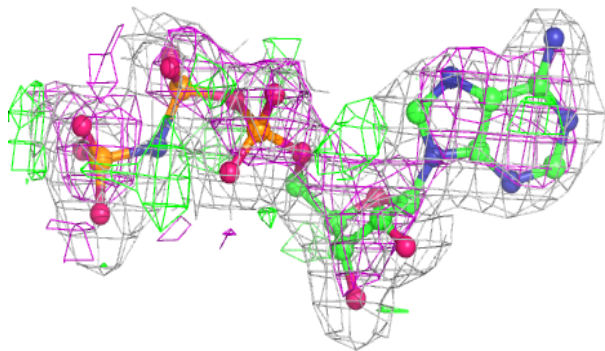
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

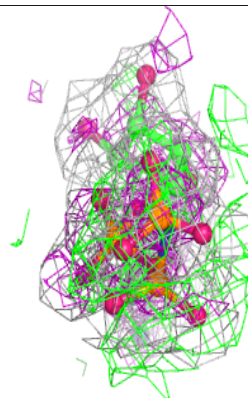
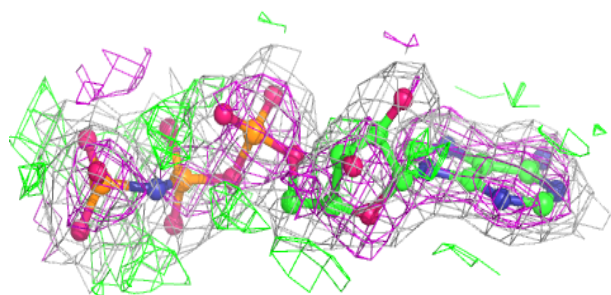
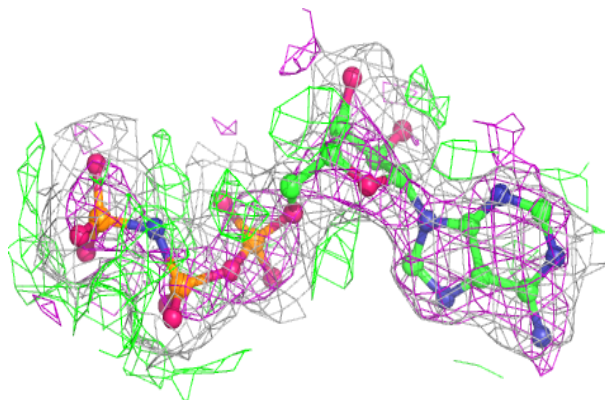


**Electron density around ANP A 1511:**

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

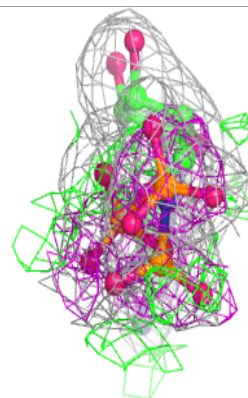
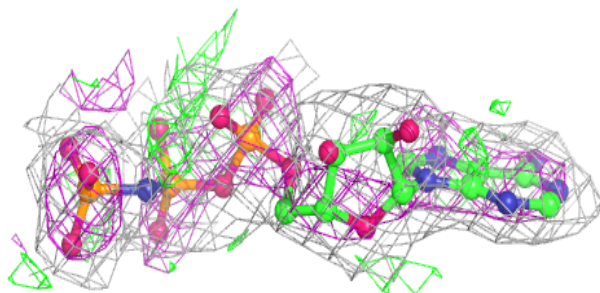
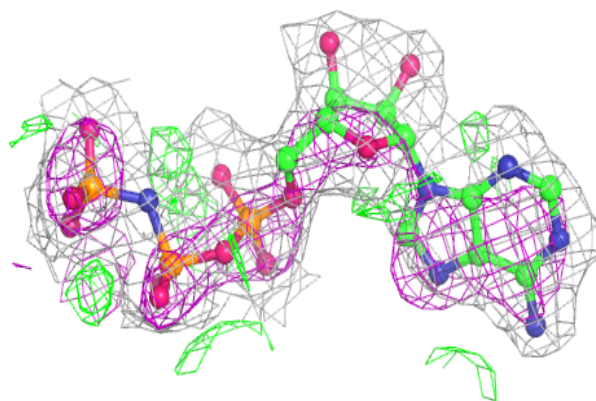
**Electron density around ANP J 1511:**

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

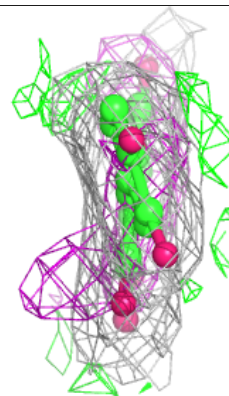
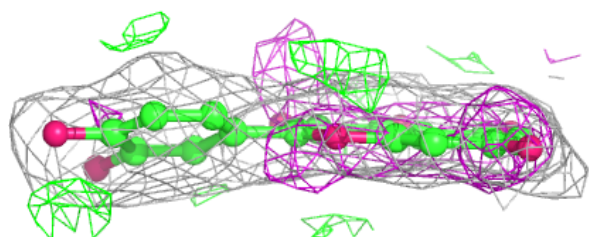
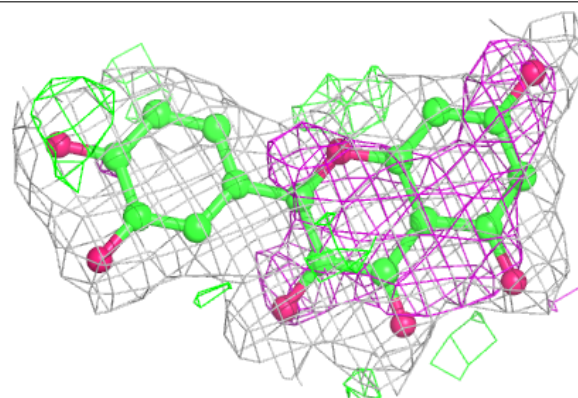


**Electron density around ANP I 1510:**

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

**Electron density around QUE N 1273 (A):**

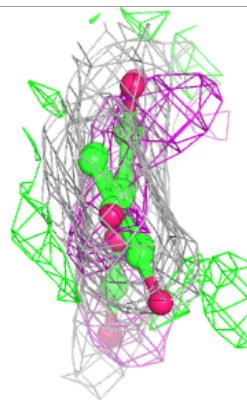
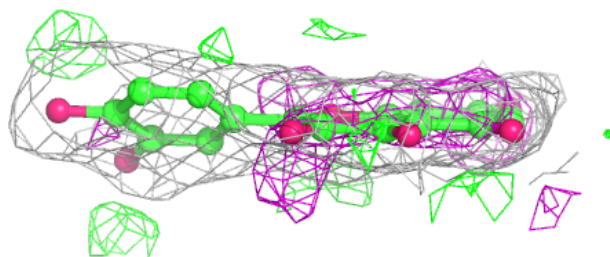
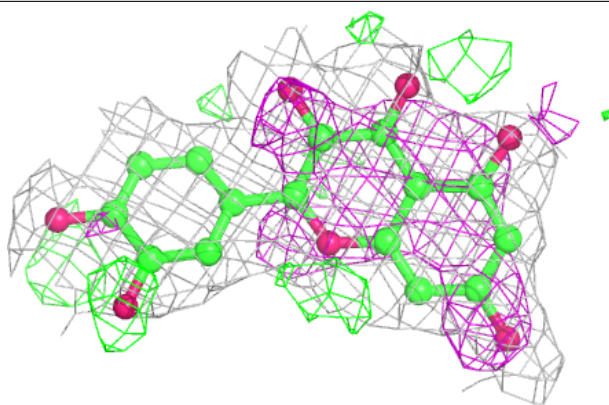
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



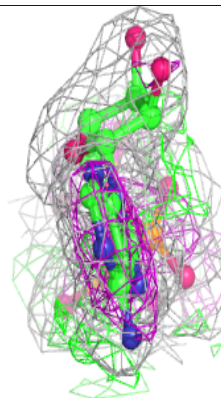
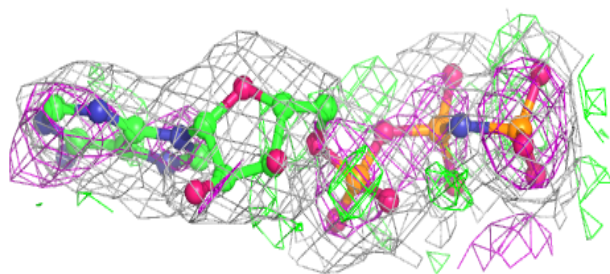
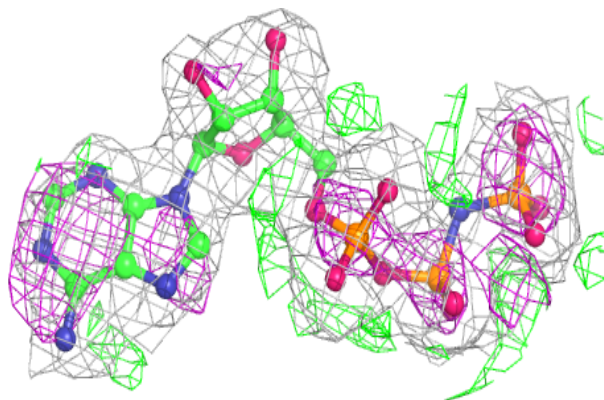


**Electron density around QUE N 1273 (B):**

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

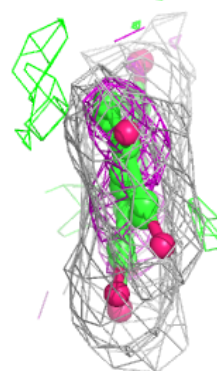
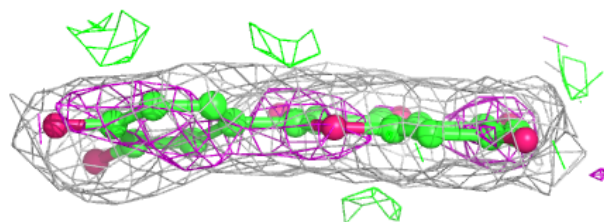
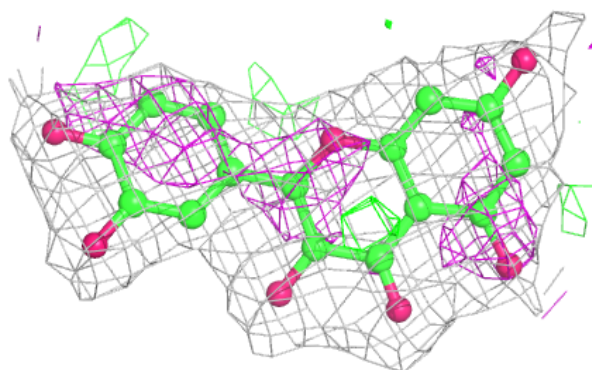
**Electron density around ANP B 1510:**

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

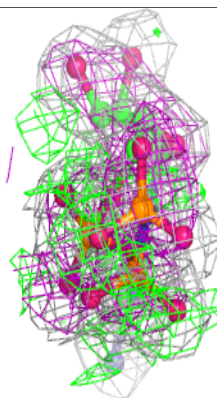
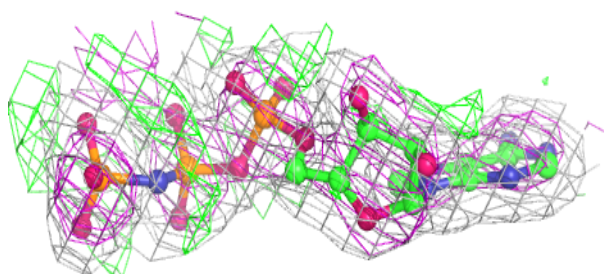
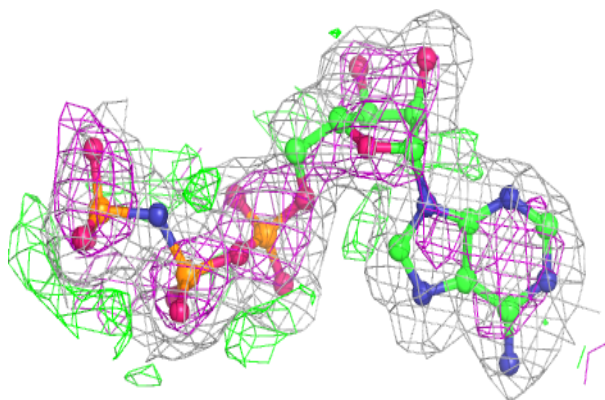


**Electron density around QUE G 1273 (A):**

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

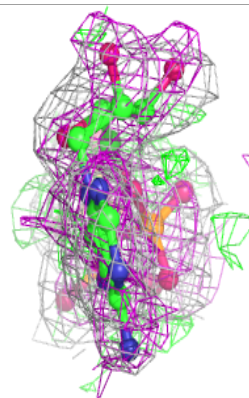
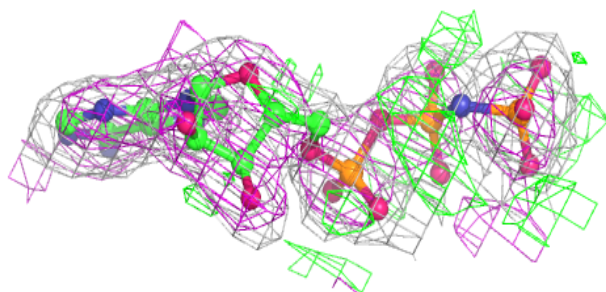
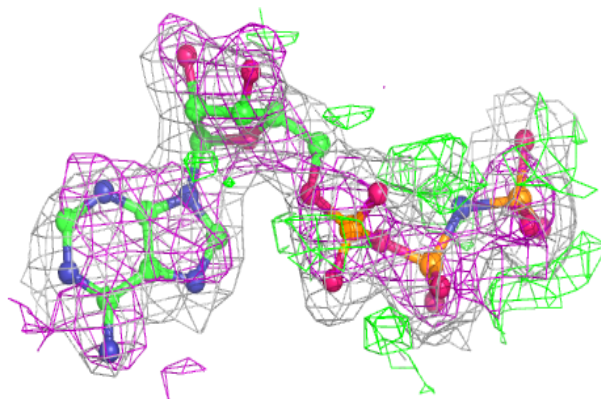
**Electron density around ANP F 1475:**

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

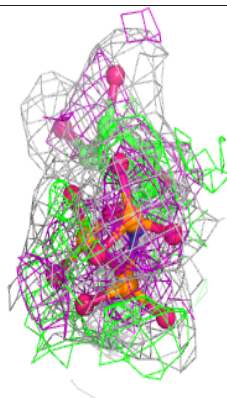
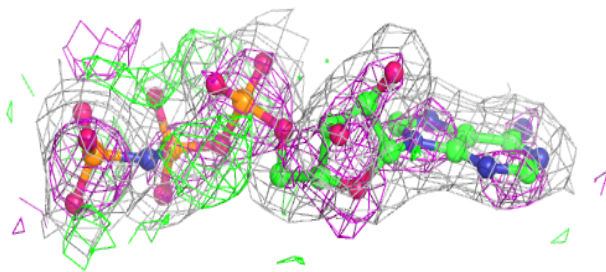
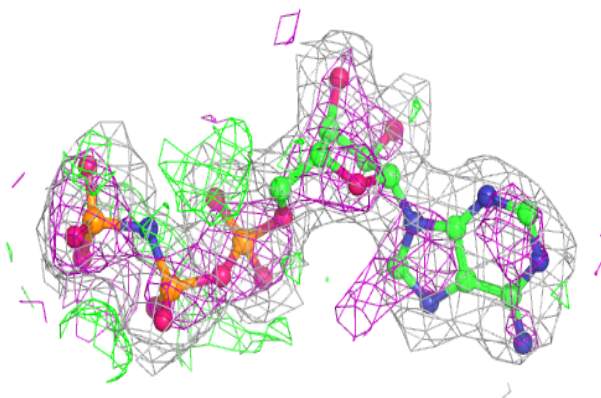


**Electron density around ANP M 1475:**

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

**Electron density around ANP C 1511:**

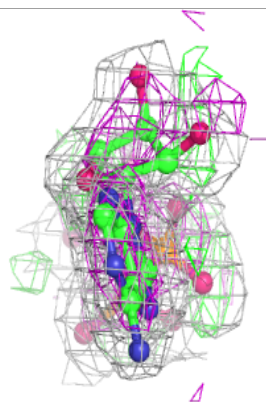
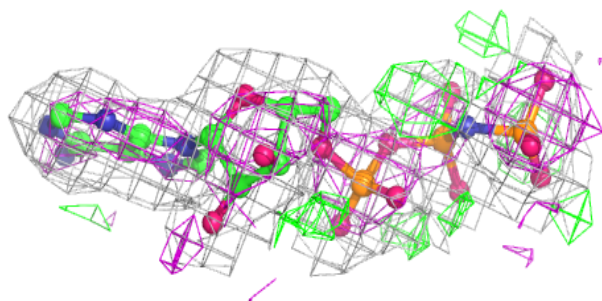
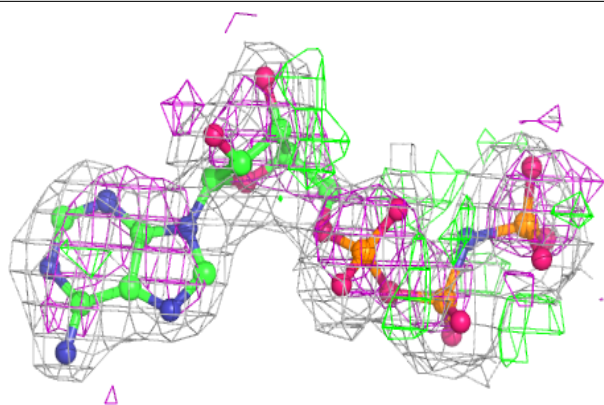
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



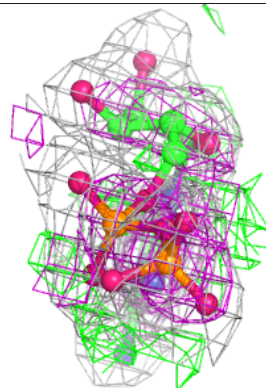
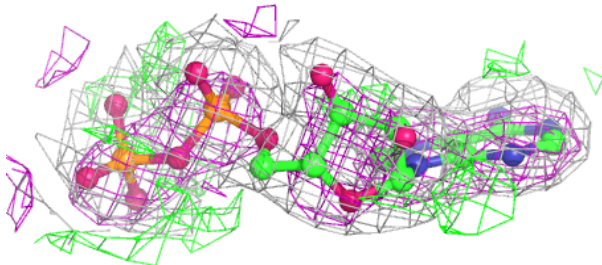
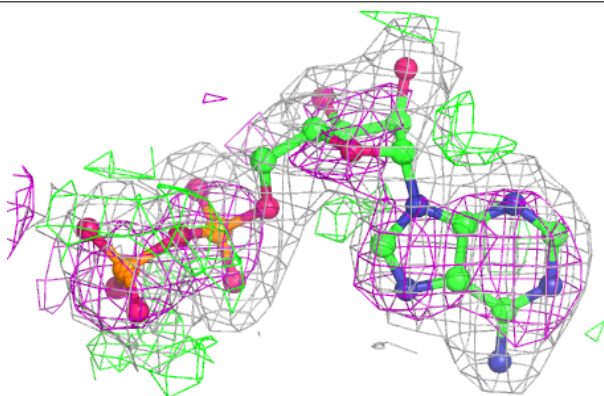


**Electron density around ANP H 1511:**

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

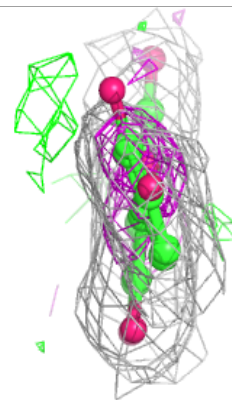
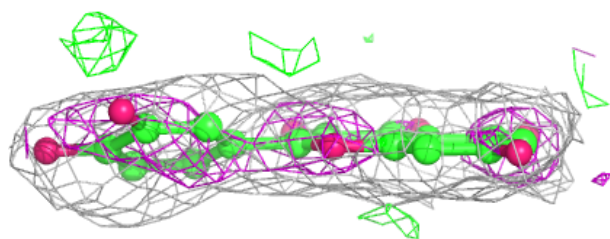
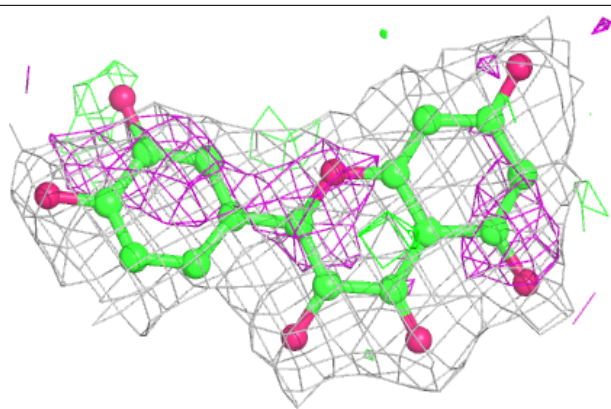
**Electron density around ADP D 1476:**

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



**Electron density around QUE G 1273 (B):**

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



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.