



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:20 AM UTC

PDB ID : 2JJ2 / pdb_00002jj2
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

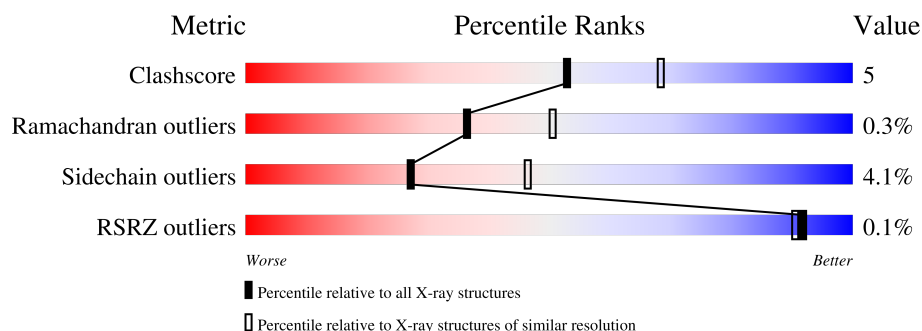
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



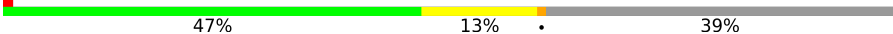
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
1	H	510	
1	I	510	
1	J	510	

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Mol	Chain	Length	Quality of chain
2	D	482	
2	E	482	
2	F	482	
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	-
8	AZI	D	1478	-	X	-	-
8	AZI	K	1478	-	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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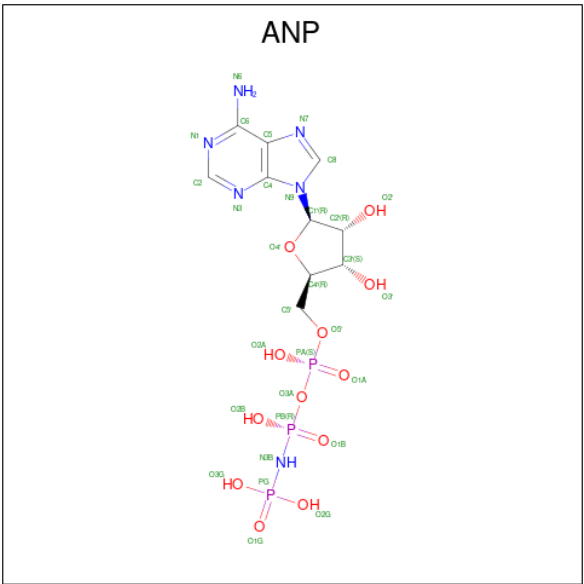
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	L	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	M	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- 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 (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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 (CCD ID: MG) (formula: Mg).

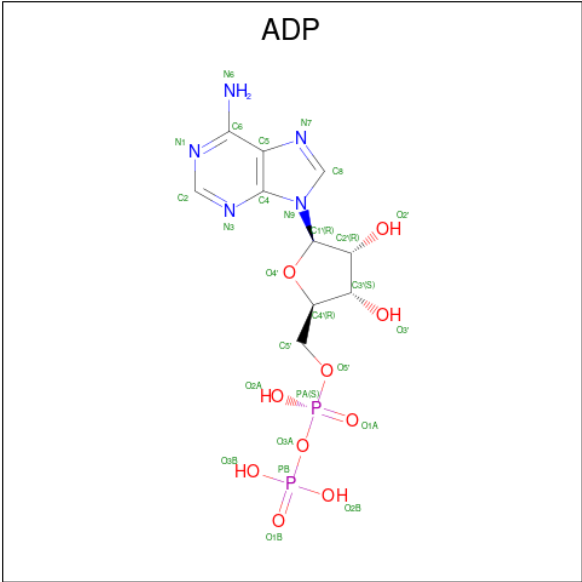
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	M	1	Total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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



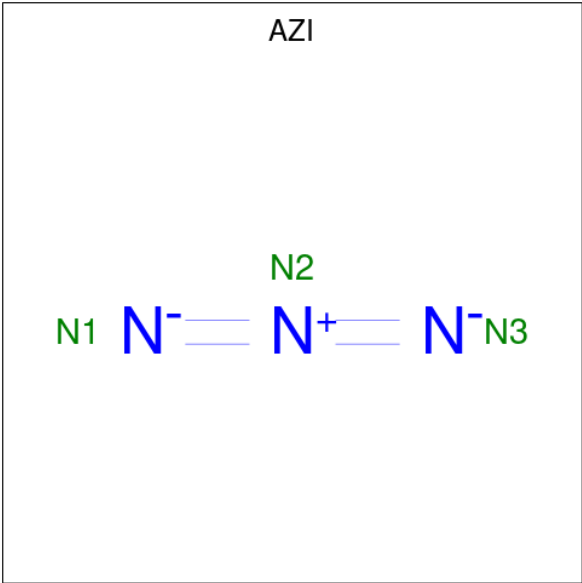
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



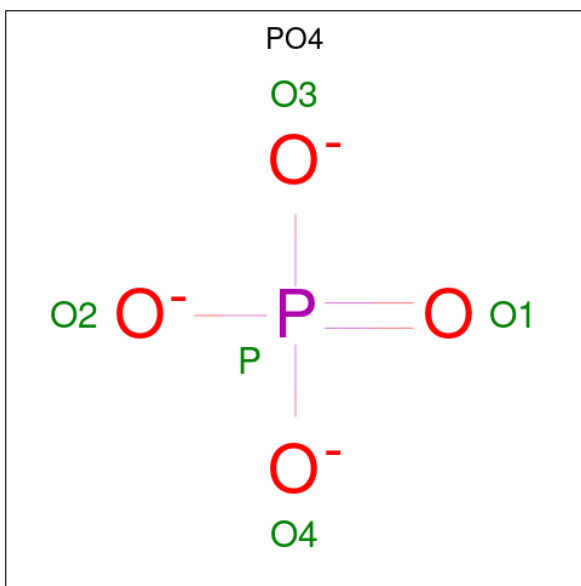
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is AZIDE ION (CCD ID: AZI) (formula: N₃).



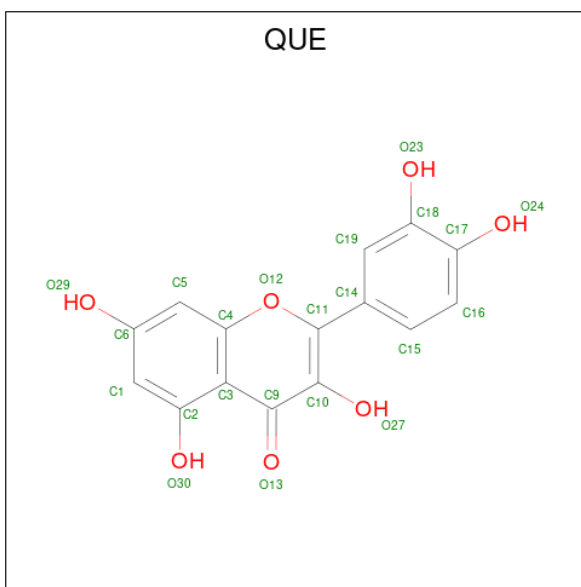
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	N	0	0
			3	3		
8	K	1	Total	N	0	0
			3	3		

- Molecule 9 is PHOSPHATE ION (CCD ID: 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 (CCD ID: 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.

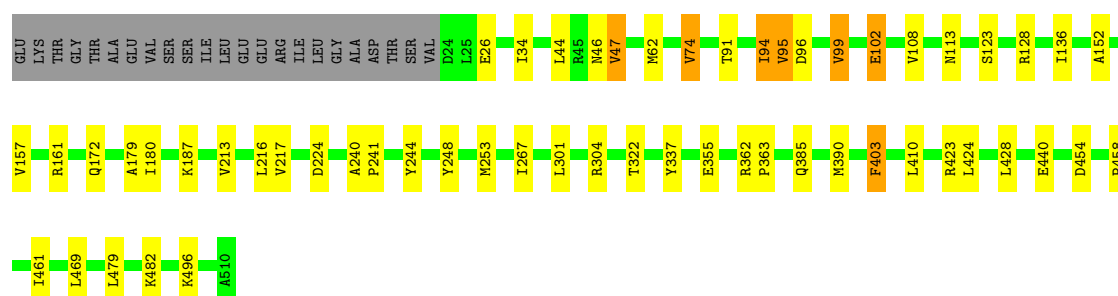
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	180	Total	O		0	0
			180	180			
11	B	153	Total	O		0	0
			153	153			
11	C	229	Total	O		0	0
			229	229			
11	D	179	Total	O		0	0
			179	179			
11	E	114	Total	O		0	0
			114	114			
11	F	205	Total	O		0	0
			205	205			
11	G	40	Total	O		0	0
			40	40			
11	H	207	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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

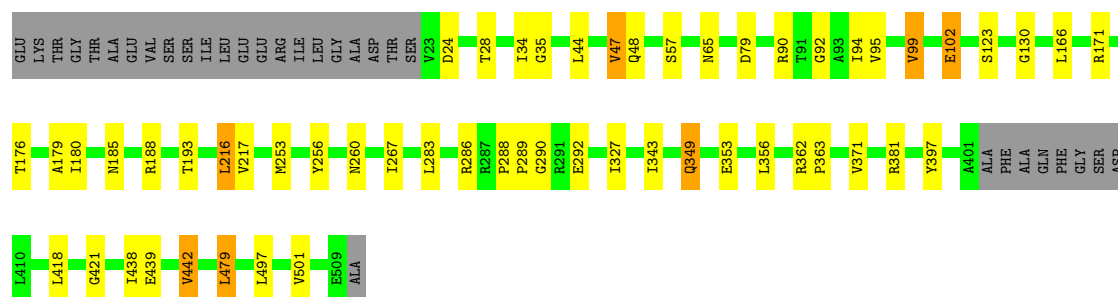
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

Chain A: 



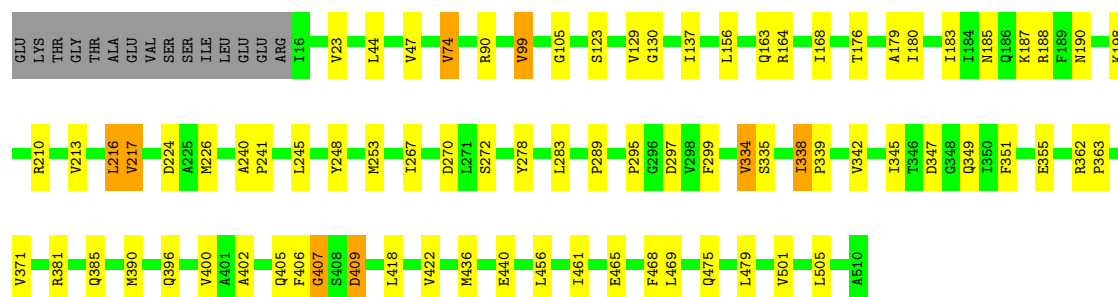
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

Chain B: 

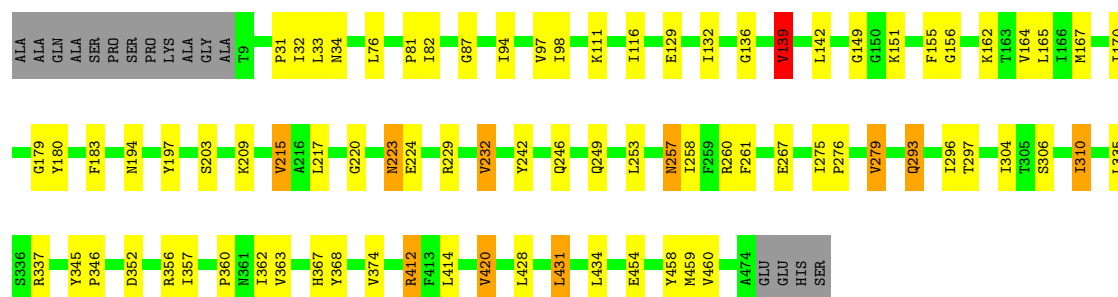


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

Chain C: 

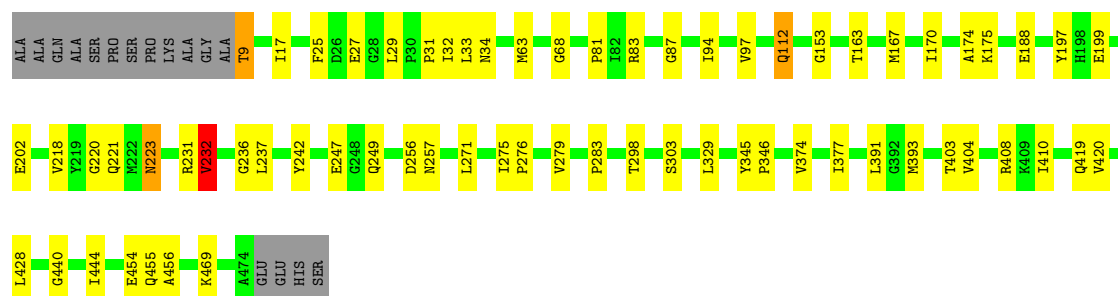


Chain E:  80% 15% . .



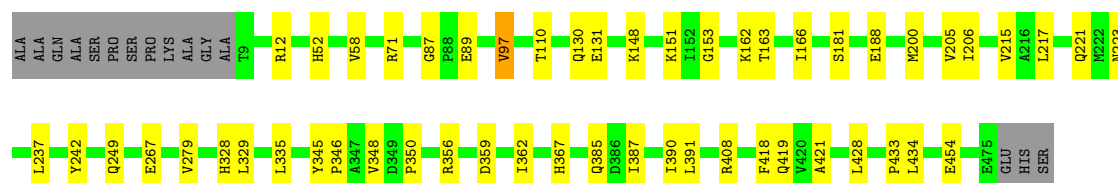
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain F:  83% 13% . .



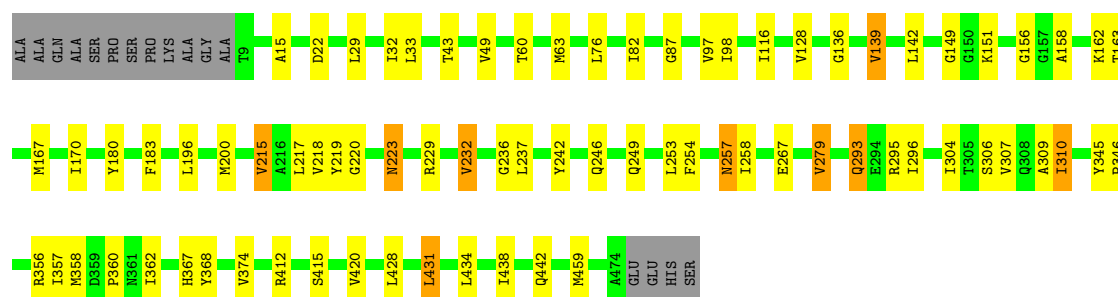
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain K:  86% 11% .



• Molecule 2: ATP SYNTHASE SUBUNIT BETA

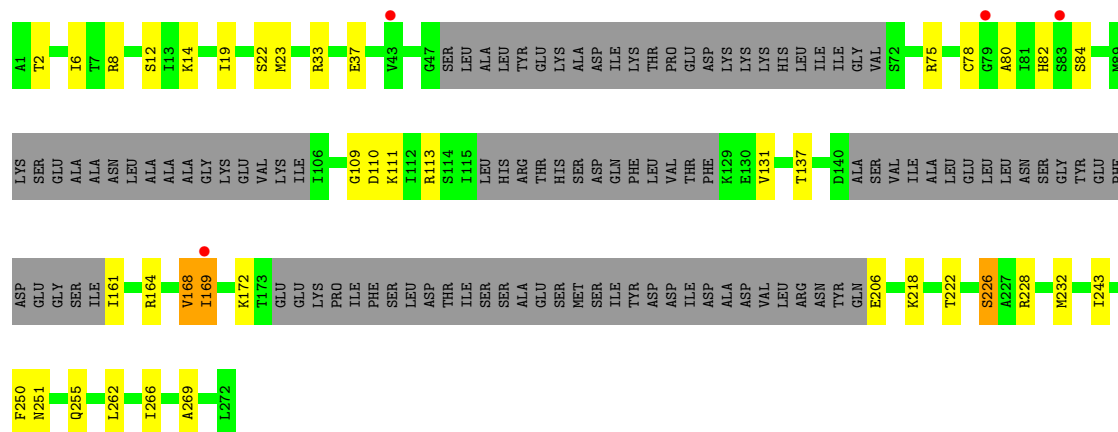
Chain L:  81% 14% . .



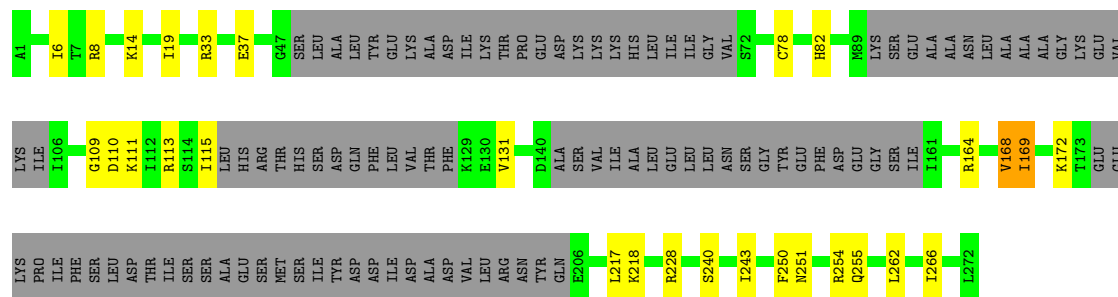
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

A474	Q221	Q222	Q223	R231	V232	T235	G236	L237	Y242	E247	G248	Q249	S266	I275	P276	V279	P283	T298	S303	A327	R337	E341	R356	V374	I377	E399	T403	L414	L428	L434	G440	I444	A456	K459									
ALA	ALA	GLN	ALA	SER	PRO	SER	PRO	LYS	ALA	GLY	ALA	ALA	T9	T10	I13	E27	I32	L33	M63	G88	Q73	P81	I82	R83	I84	G87	P88	E89	V97	K109	T110	K111	Q112	V139	V140	D141	G159	T163	I166	M167	E188	L196	F202

Chain G: %



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, α , β , γ	106.40Å 282.02Å 138.09Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	80.58 – 2.40 80.58 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.1 (80.58-2.40) 92.1 (80.58-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	37.7	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.328 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	48794	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: MG, ADP, AZI, PO4, QUE, ANP, GOL

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	0.52	0/3766	0.84	1/5080 (0.0%)
1	B	0.54	0/3706	0.83	0/4998
1	C	0.56	1/3819 (0.0%)	0.85	1/5153 (0.0%)
1	H	0.52	0/3766	0.83	0/5080
1	I	0.54	0/3706	0.82	0/4998
1	J	0.57	1/3819 (0.0%)	0.87	1/5153 (0.0%)
2	D	0.55	0/3596	0.84	4/4879 (0.1%)
2	E	0.50	0/3587	0.82	1/4867 (0.0%)
2	F	0.54	0/3587	0.84	1/4867 (0.0%)
2	K	0.55	0/3596	0.83	1/4879 (0.0%)
2	L	0.51	0/3587	0.82	1/4867 (0.0%)
2	M	0.55	0/3587	0.87	3/4867 (0.1%)
3	G	0.49	0/1304	0.85	0/1737
3	N	0.49	0/1304	0.82	0/1737
All	All	0.54	2/46730 (0.0%)	0.84	14/63162 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	137	ILE	CA-CB	6.13	1.57	1.54
1	C	137	ILE	CA-CB	5.10	1.57	1.54

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	97	VAL	CB-CA-C	-8.72	100.62	112.04
2	K	97	VAL	CB-CA-C	-8.21	101.28	112.04
2	M	97	VAL	CB-CA-C	-7.88	101.72	112.04
2	M	232	VAL	CB-CA-C	-6.18	103.95	112.04
2	M	139	VAL	CB-CA-C	-6.05	104.13	111.88

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	38	0
1	C	3768	0	3867	47	0
1	H	3715	0	3812	43	0
1	I	3658	0	3767	40	0
1	J	3768	0	3867	44	0
2	D	3539	0	3592	32	0
2	E	3530	0	3587	48	0
2	F	3530	0	3586	35	0
2	K	3539	0	3592	27	0
2	L	3530	0	3587	43	0
2	M	3530	0	3586	34	0
3	G	1296	0	1365	20	0
3	N	1296	0	1365	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	473	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 473 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:M:63:MET:HE1	2:M:231:ARG:HB2	1.50	0.94
2:E:223:ASN:HD22	2:E:223:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:183:PHE:HB3	2:L:217:LEU:HD23	1.64	0.78

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	485/510 (95%)	469 (97%)	15 (3%)	1 (0%)	43	58
1	B	475/510 (93%)	458 (96%)	16 (3%)	1 (0%)	43	58
1	C	493/510 (97%)	481 (98%)	10 (2%)	2 (0%)	30	43
1	H	485/510 (95%)	469 (97%)	16 (3%)	0	100	100
1	I	475/510 (93%)	462 (97%)	12 (2%)	1 (0%)	43	58
1	J	493/510 (97%)	480 (97%)	10 (2%)	3 (1%)	21	32
2	D	465/482 (96%)	441 (95%)	23 (5%)	1 (0%)	43	58
2	E	464/482 (96%)	444 (96%)	17 (4%)	3 (1%)	21	32
2	F	464/482 (96%)	446 (96%)	18 (4%)	0	100	100
2	K	465/482 (96%)	442 (95%)	21 (4%)	2 (0%)	30	43
2	L	464/482 (96%)	446 (96%)	16 (3%)	2 (0%)	30	43
2	M	464/482 (96%)	445 (96%)	18 (4%)	1 (0%)	43	58
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%)	36	50

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY

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Mol	Chain	Res	Type
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%)	377 (96%)	16 (4%)	27	46
1	B	389/413 (94%)	376 (97%)	13 (3%)	33	55
1	C	399/413 (97%)	387 (97%)	12 (3%)	36	58
1	H	393/413 (95%)	373 (95%)	20 (5%)	21	37
1	I	389/413 (94%)	378 (97%)	11 (3%)	38	60
1	J	399/413 (97%)	380 (95%)	19 (5%)	23	40
2	D	377/386 (98%)	370 (98%)	7 (2%)	50	71
2	E	376/386 (97%)	353 (94%)	23 (6%)	17	30
2	F	376/386 (97%)	362 (96%)	14 (4%)	30	51
2	K	377/386 (98%)	368 (98%)	9 (2%)	43	65
2	L	376/386 (97%)	360 (96%)	16 (4%)	26	44
2	M	376/386 (97%)	357 (95%)	19 (5%)	21	37
3	G	140/230 (61%)	128 (91%)	12 (9%)	10	16
3	N	140/230 (61%)	129 (92%)	11 (8%)	11	19
All	All	4900/5254 (93%)	4698 (96%)	202 (4%)	27	46

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	479	LEU
1	J	479	LEU
3	N	240	SER

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Mol	Chain	Res	Type
1	I	80	LYS
1	J	63	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	249	GLN
2	M	443	GLN
2	L	293	GLN
2	M	112	GLN
3	N	225	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
6	GOL	A	1513	-	5,5,5	0.37	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ANP	I	1510	5	33,33,33	2.04	12 (36%)	45,52,52	2.21	12 (26%)
9	PO4	E	1475	-	4,4,4	0.93	0	6,6,6	0.43	0
6	GOL	B	1513	-	5,5,5	0.35	0	5,5,5	0.47	0
6	GOL	H	1514	-	5,5,5	0.40	0	5,5,5	0.39	0
4	ANP	H	1511	5	33,33,33	2.05	10 (30%)	45,52,52	1.94	12 (26%)
6	GOL	C	1513	-	5,5,5	0.38	0	5,5,5	0.25	0
4	ANP	C	1511	5	33,33,33	2.02	13 (39%)	45,52,52	2.00	12 (26%)
9	PO4	L	1475	-	4,4,4	0.96	0	6,6,6	0.42	0
6	GOL	B	1512	-	5,5,5	0.39	0	5,5,5	0.40	0
10	QUE	N	1273[A]	-	24,24,24	3.61	5 (20%)	36,36,36	1.81	7 (19%)
6	GOL	J	1513	-	5,5,5	0.39	0	5,5,5	0.47	0
4	ANP	B	1510	5	33,33,33	2.09	11 (33%)	45,52,52	1.97	12 (26%)
7	ADP	K	1476	5	28,29,29	1.61	5 (17%)	43,45,45	1.75	9 (20%)
10	QUE	G	1273[A]	-	24,24,24	3.60	4 (16%)	36,36,36	1.75	6 (16%)
6	GOL	I	1512	-	5,5,5	0.41	0	5,5,5	0.34	0
4	ANP	A	1511	5	33,33,33	2.13	11 (33%)	45,52,52	2.17	12 (26%)
4	ANP	M	1475	5	33,33,33	2.03	11 (33%)	45,52,52	2.22	13 (28%)
8	AZI	K	1478	-	2,2,2	3.04	2 (100%)	0,1,1	-	-
4	ANP	F	1475	5	33,33,33	2.11	12 (36%)	45,52,52	2.26	13 (28%)
6	GOL	A	1514	-	5,5,5	0.36	0	5,5,5	0.76	0
10	QUE	N	1273[B]	-	24,24,24	3.51	4 (16%)	36,36,36	1.72	6 (16%)
4	ANP	J	1511	5	33,33,33	2.06	11 (33%)	45,52,52	2.04	11 (24%)
8	AZI	D	1478	-	2,2,2	2.83	2 (100%)	0,1,1	-	-
7	ADP	D	1476	5	28,29,29	1.61	4 (14%)	43,45,45	1.79	8 (18%)
6	GOL	K	1479	-	5,5,5	0.43	0	5,5,5	0.34	0
6	GOL	D	1479	-	5,5,5	0.37	0	5,5,5	0.43	0
6	GOL	K	1480	-	5,5,5	0.37	0	5,5,5	0.38	0
10	QUE	G	1273[B]	-	24,24,24	3.51	4 (16%)	36,36,36	1.65	5 (13%)
6	GOL	H	1513	-	5,5,5	0.40	0	5,5,5	0.45	0

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	GOL	A	1513	-	-	2/4/4/4	-
4	ANP	I	1510	5	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	1513	-	-	4/4/4/4	-
6	GOL	H	1514	-	-	2/4/4/4	-
4	ANP	H	1511	5	-	3/18/38/38	0/3/3/3
6	GOL	C	1513	-	-	0/4/4/4	-
4	ANP	C	1511	5	-	3/18/38/38	0/3/3/3
6	GOL	B	1512	-	-	2/4/4/4	-
10	QUE	N	1273[A]	-	-	0/4/4/4	0/3/3/3
6	GOL	J	1513	-	-	1/4/4/4	-
4	ANP	B	1510	5	-	2/18/38/38	0/3/3/3
7	ADP	K	1476	5	-	3/16/32/32	0/3/3/3
10	QUE	G	1273[A]	-	-	0/4/4/4	0/3/3/3
6	GOL	I	1512	-	-	2/4/4/4	-
4	ANP	A	1511	5	-	3/18/38/38	0/3/3/3
4	ANP	M	1475	5	-	4/18/38/38	0/3/3/3
4	ANP	F	1475	5	-	2/18/38/38	0/3/3/3
6	GOL	A	1514	-	-	2/4/4/4	-
10	QUE	N	1273[B]	-	-	0/4/4/4	0/3/3/3
4	ANP	J	1511	5	-	3/18/38/38	0/3/3/3
7	ADP	D	1476	5	-	3/16/32/32	0/3/3/3
6	GOL	K	1479	-	-	2/4/4/4	-
6	GOL	D	1479	-	-	2/4/4/4	-
6	GOL	K	1480	-	-	3/4/4/4	-
10	QUE	G	1273[B]	-	-	0/4/4/4	0/3/3/3
6	GOL	H	1513	-	-	2/4/4/4	-

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	1273[A]	QUE	C10-C11	14.66	1.50	1.36
10	G	1273[A]	QUE	C10-C11	14.62	1.50	1.36
10	G	1273[B]	QUE	C10-C11	14.34	1.50	1.36
10	N	1273[B]	QUE	C10-C11	14.33	1.50	1.36
10	N	1273[A]	QUE	C18-C17	5.61	1.49	1.40

The worst 5 of 138 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	F	1475	ANP	C5-C4-N3	-6.09	118.34	126.72
4	M	1475	ANP	C5-C4-N3	-5.99	118.47	126.72

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1511	ANP	PB-N3B-PG-O1G
4	A	1511	ANP	PG-N3B-PB-O1B
4	A	1511	ANP	PG-N3B-PB-O3A
4	B	1510	ANP	PG-N3B-PB-O1B
4	B	1510	ANP	PG-N3B-PB-O3A

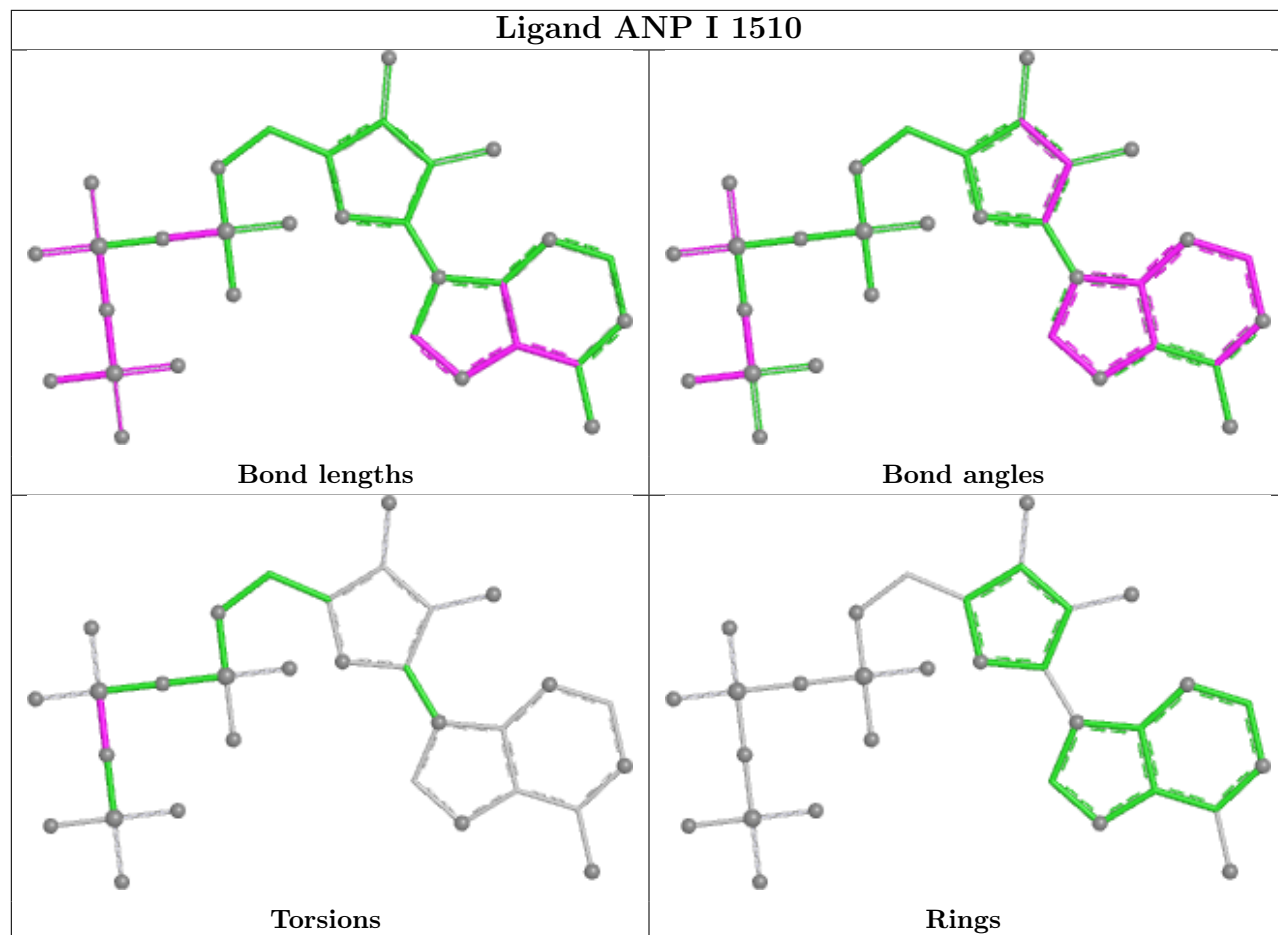
There are no ring outliers.

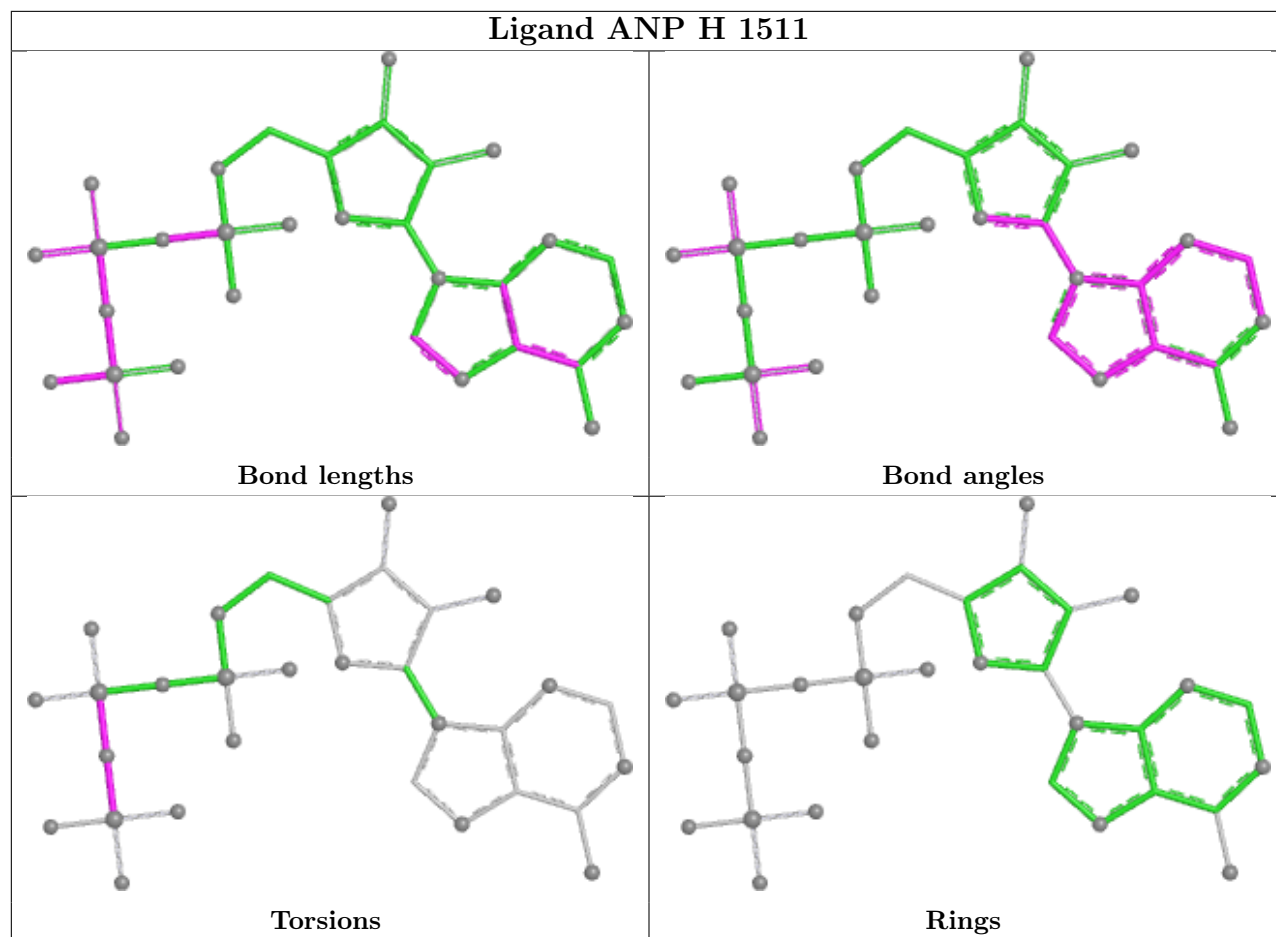
11 monomers are involved in 20 short contacts:

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

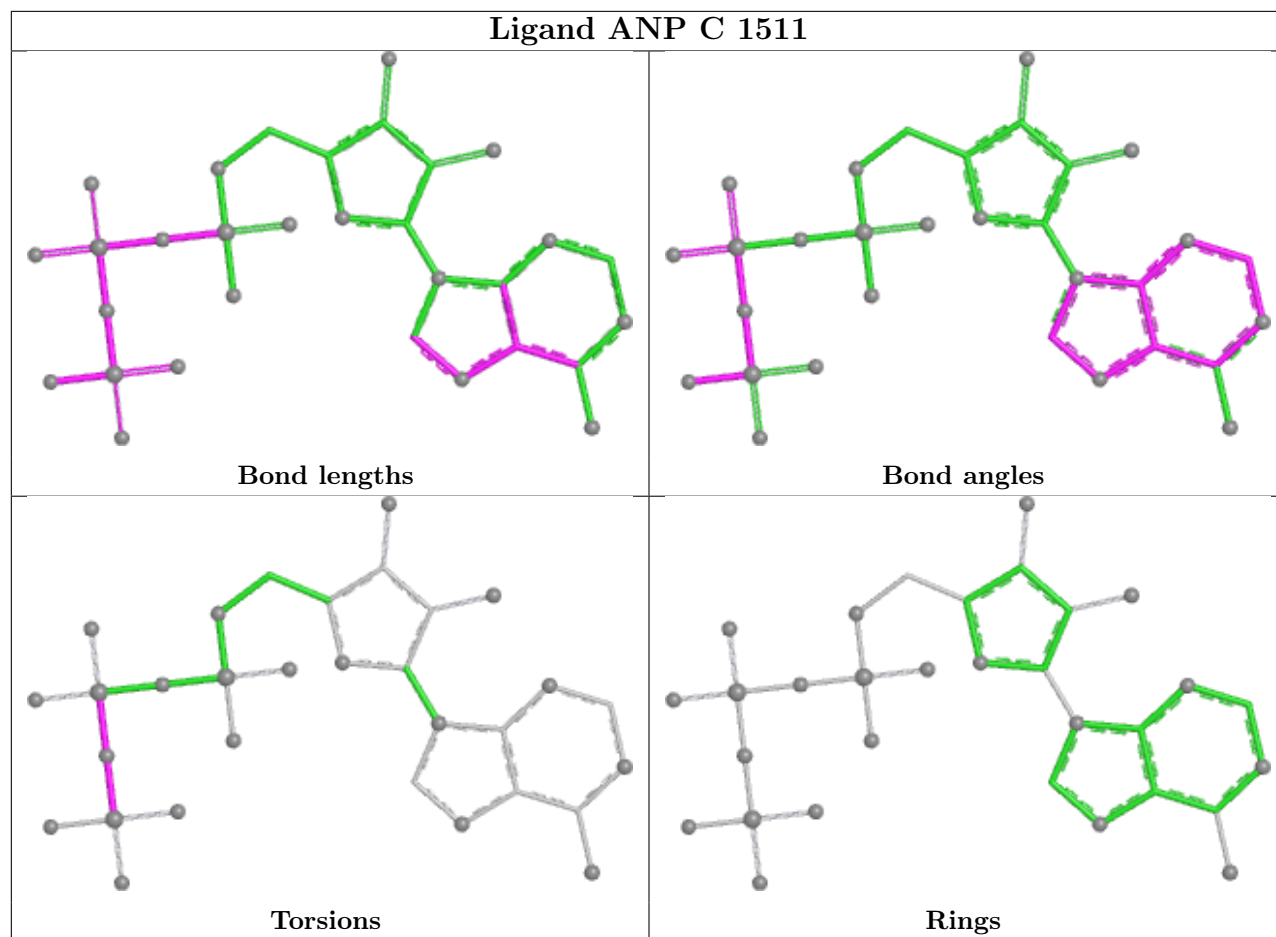
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

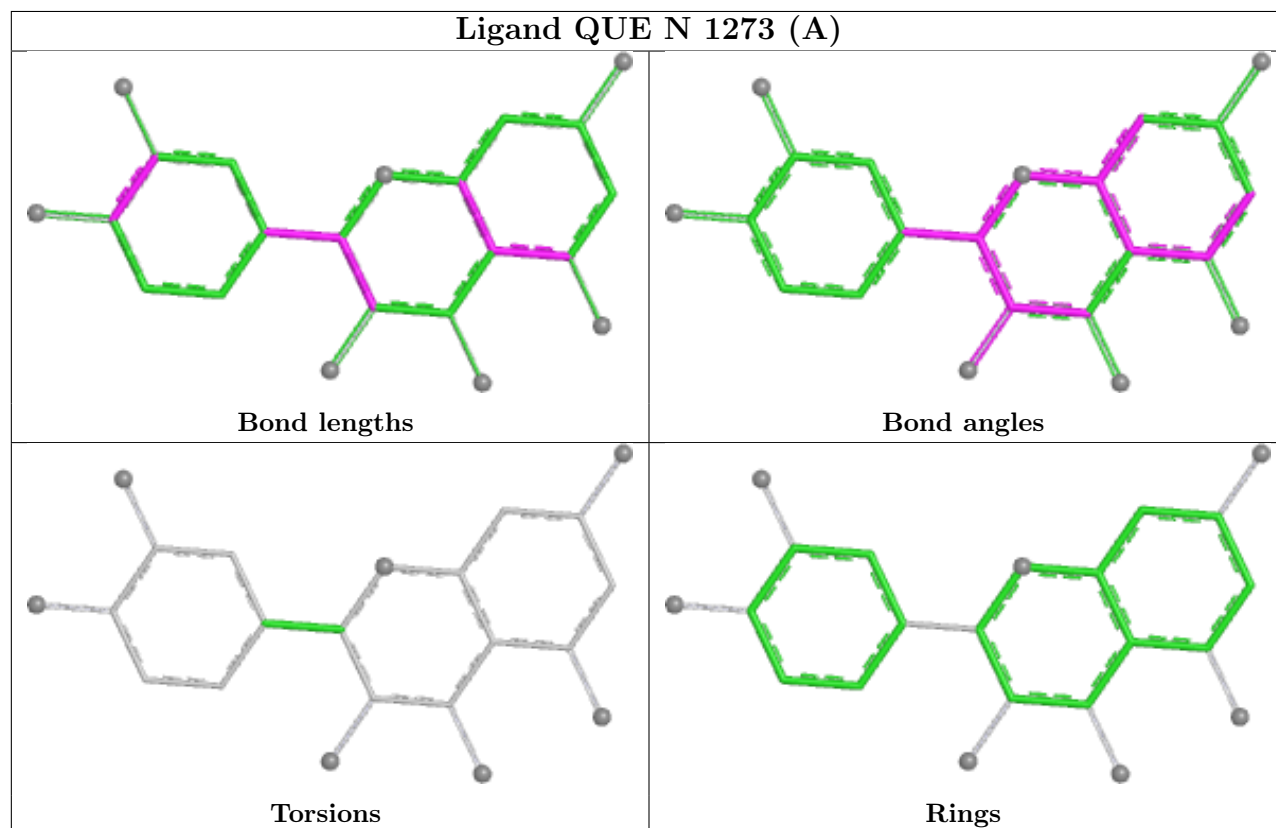




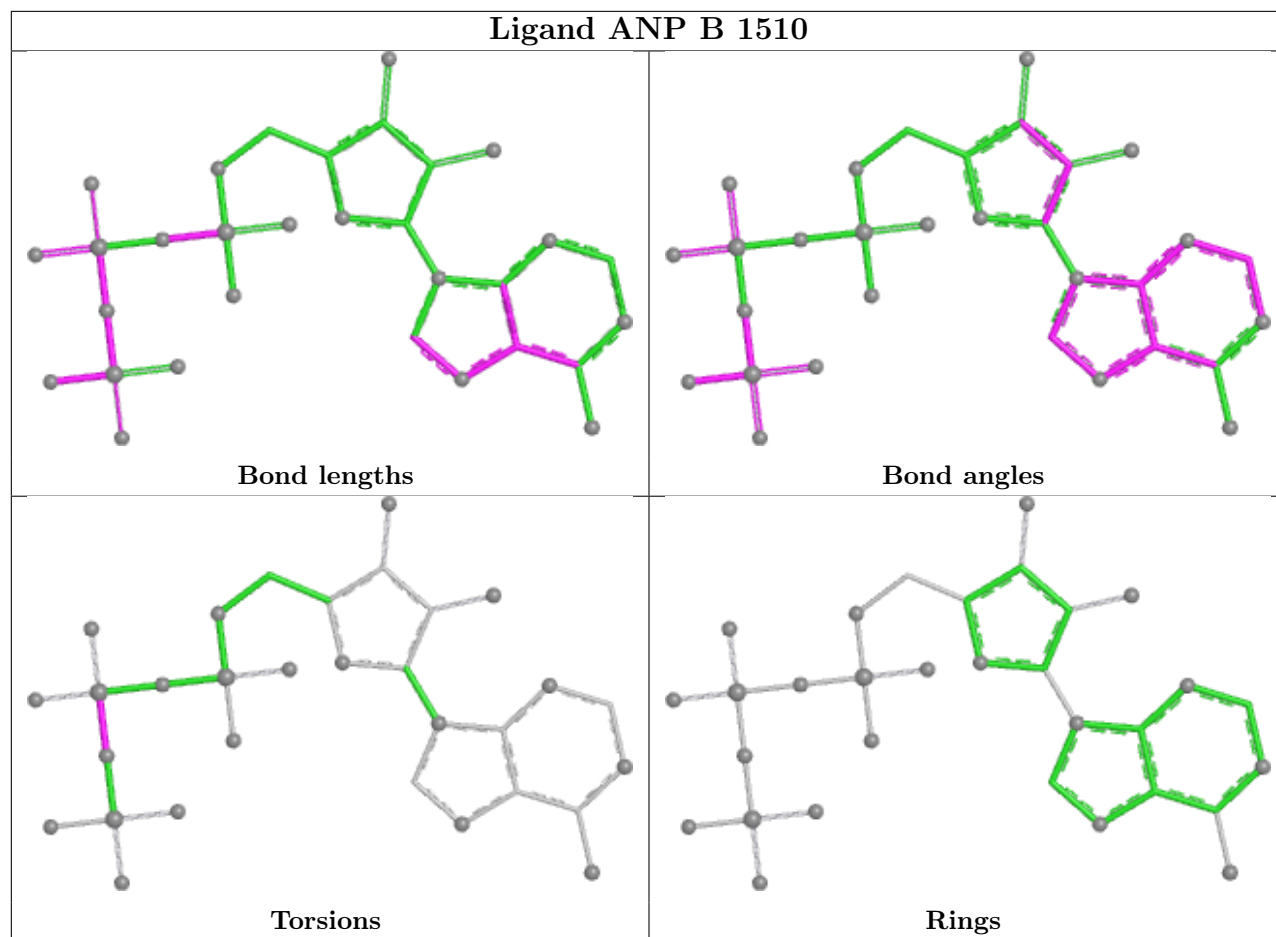
Ligand ANP C 1511



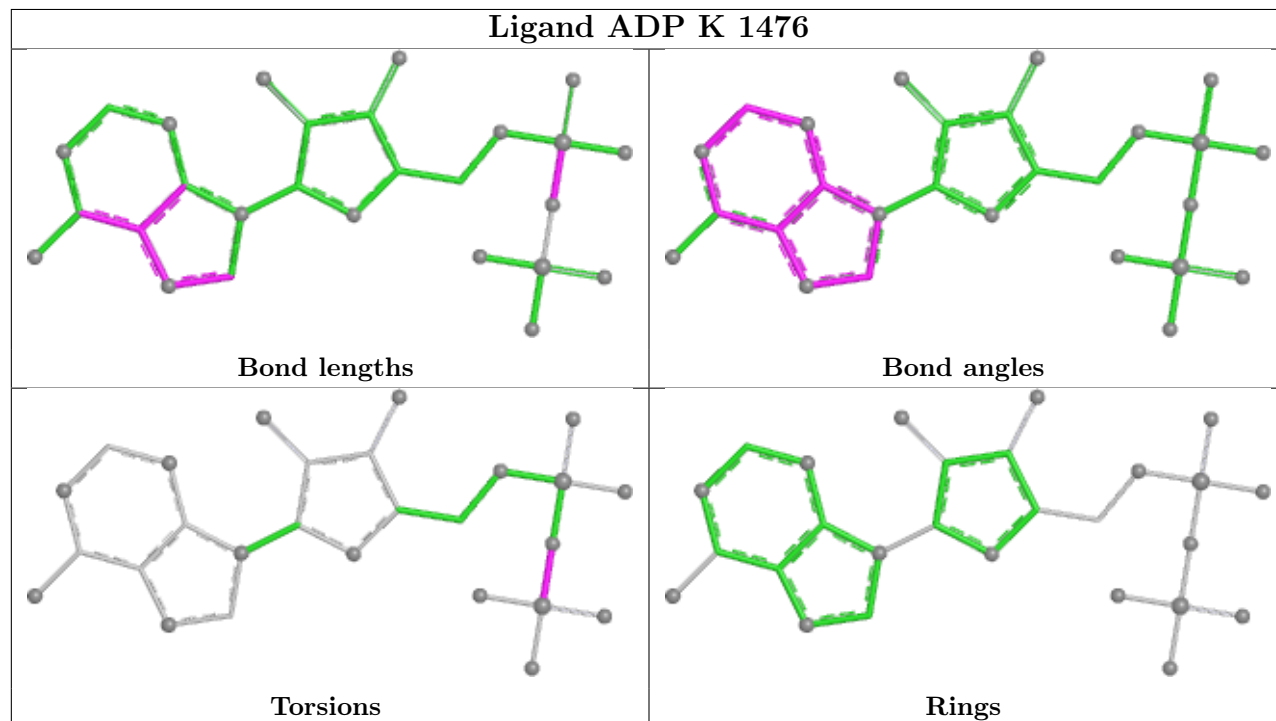
Ligand QUE N 1273 (A)



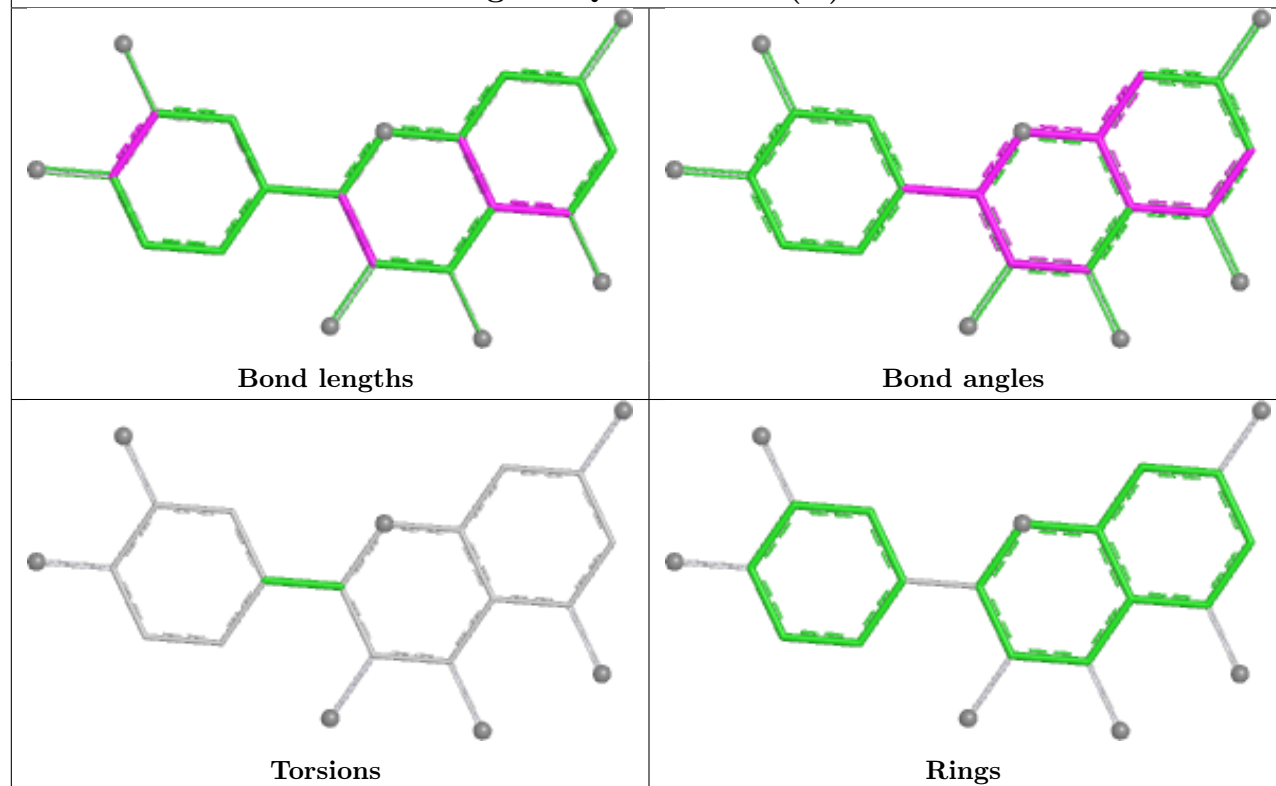
Ligand ANP B 1510



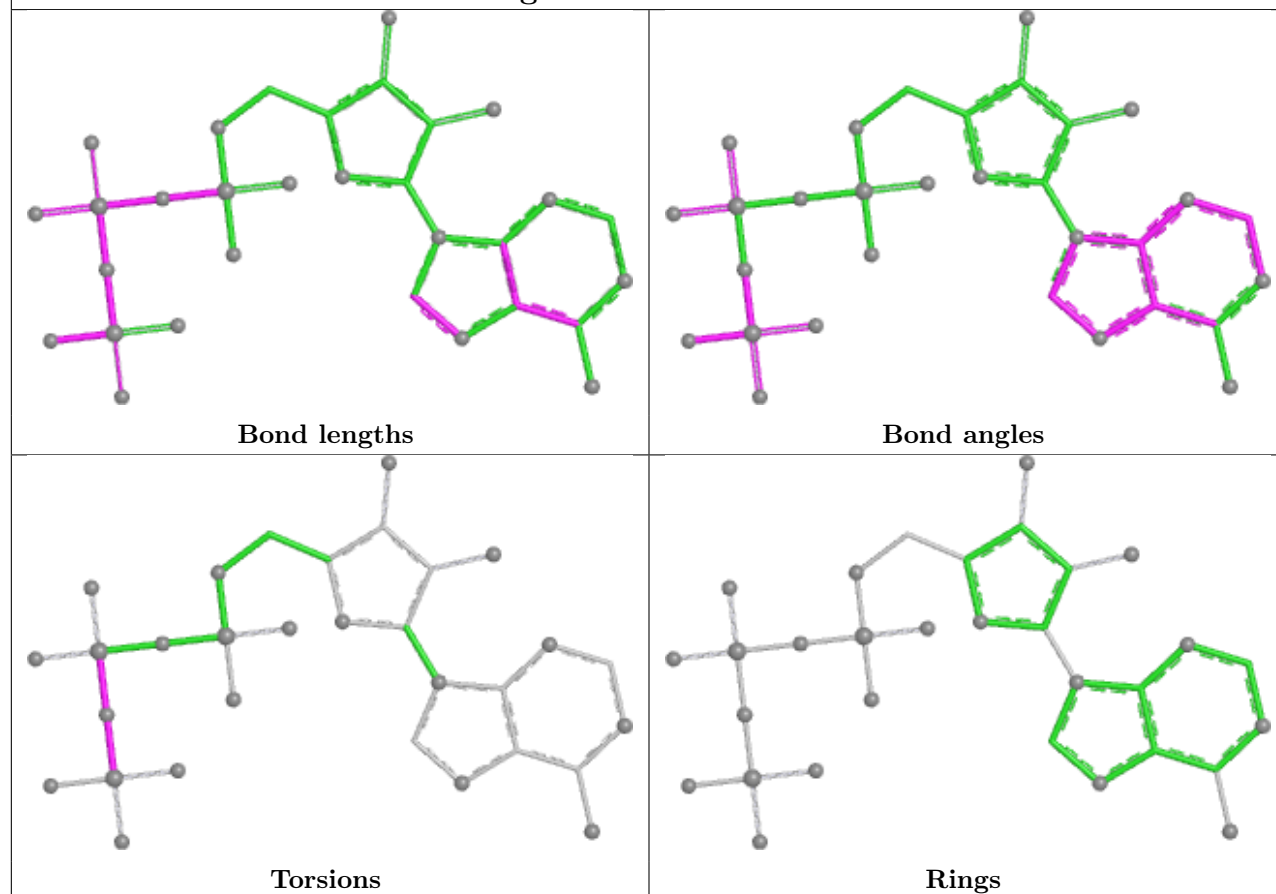
Ligand ADP K 1476



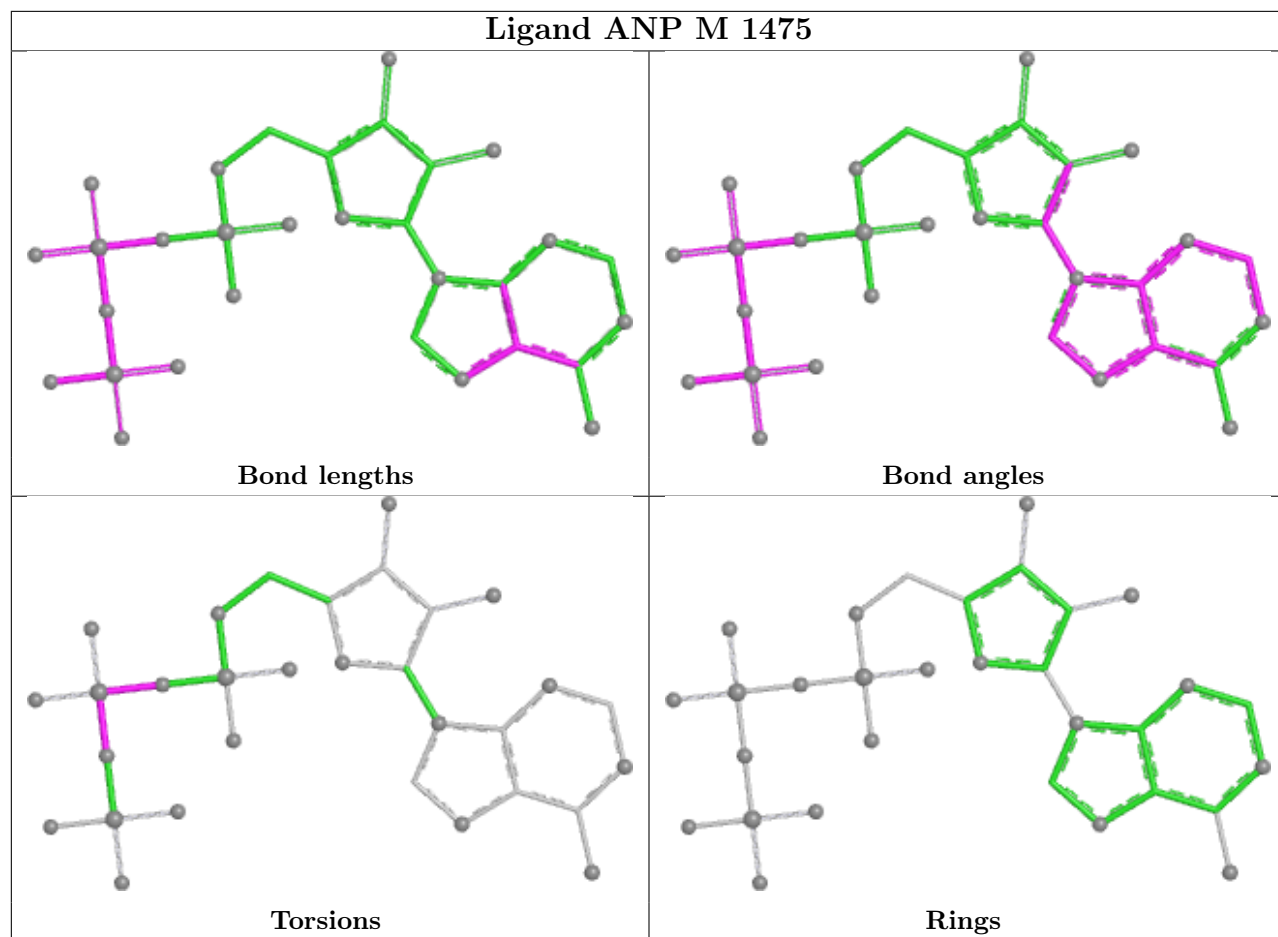
Ligand QUE G 1273 (A)



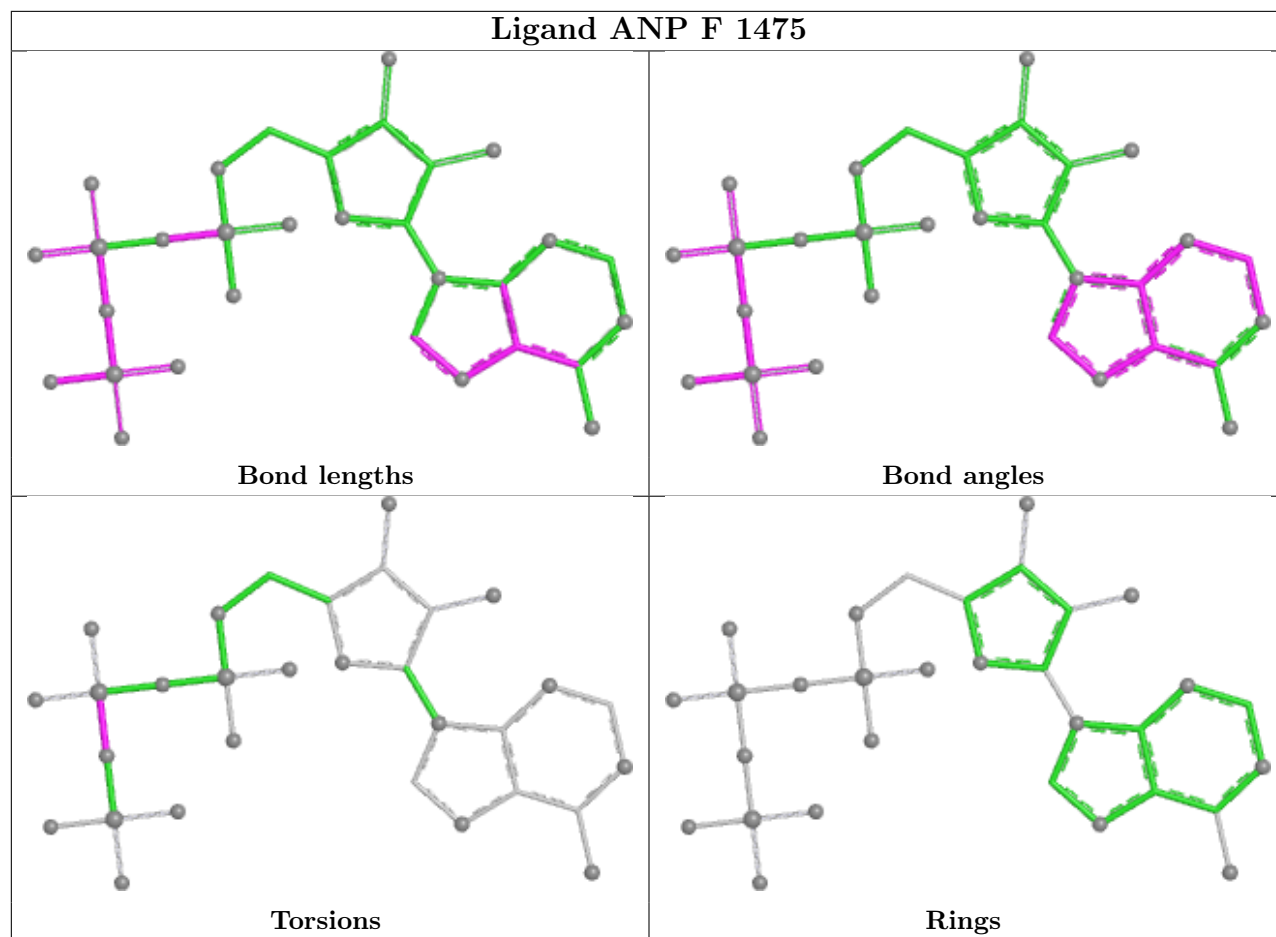
Ligand ANP A 1511



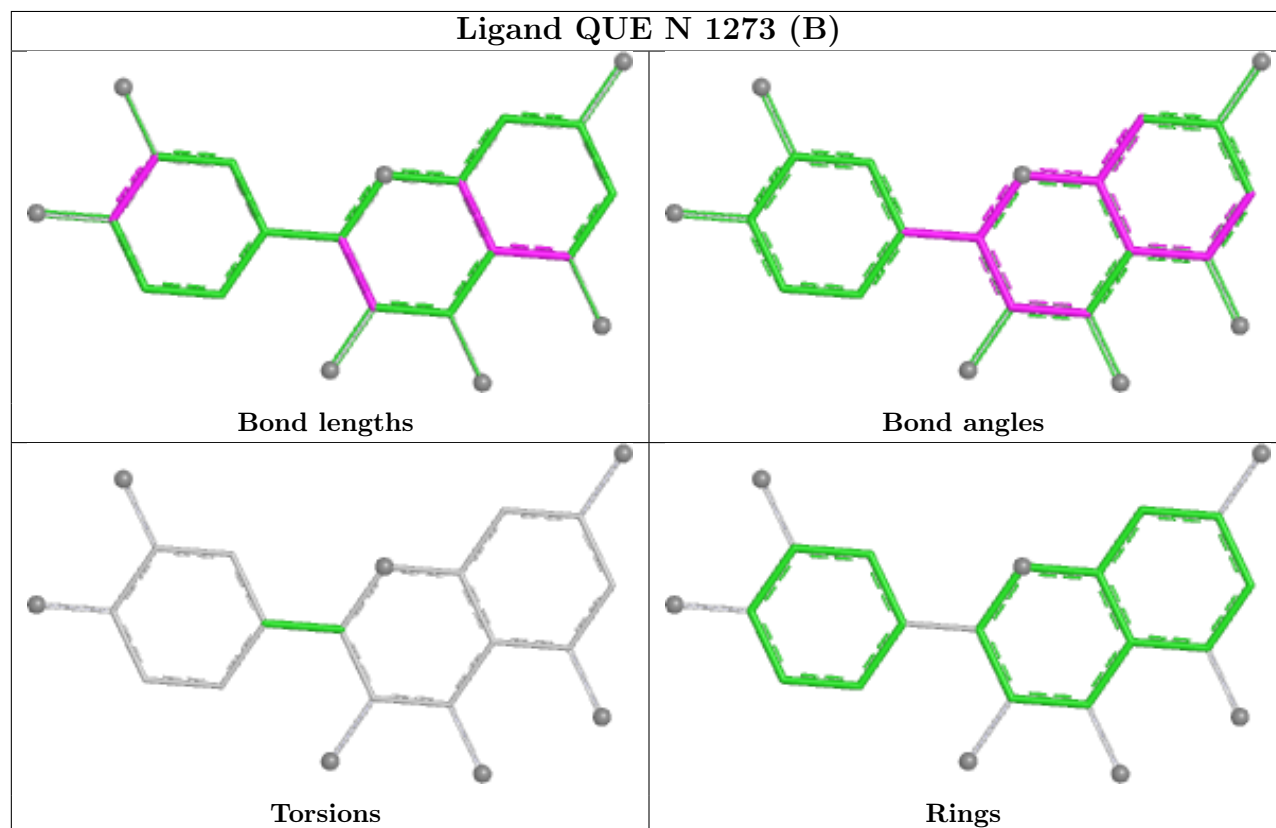
Ligand ANP M 1475



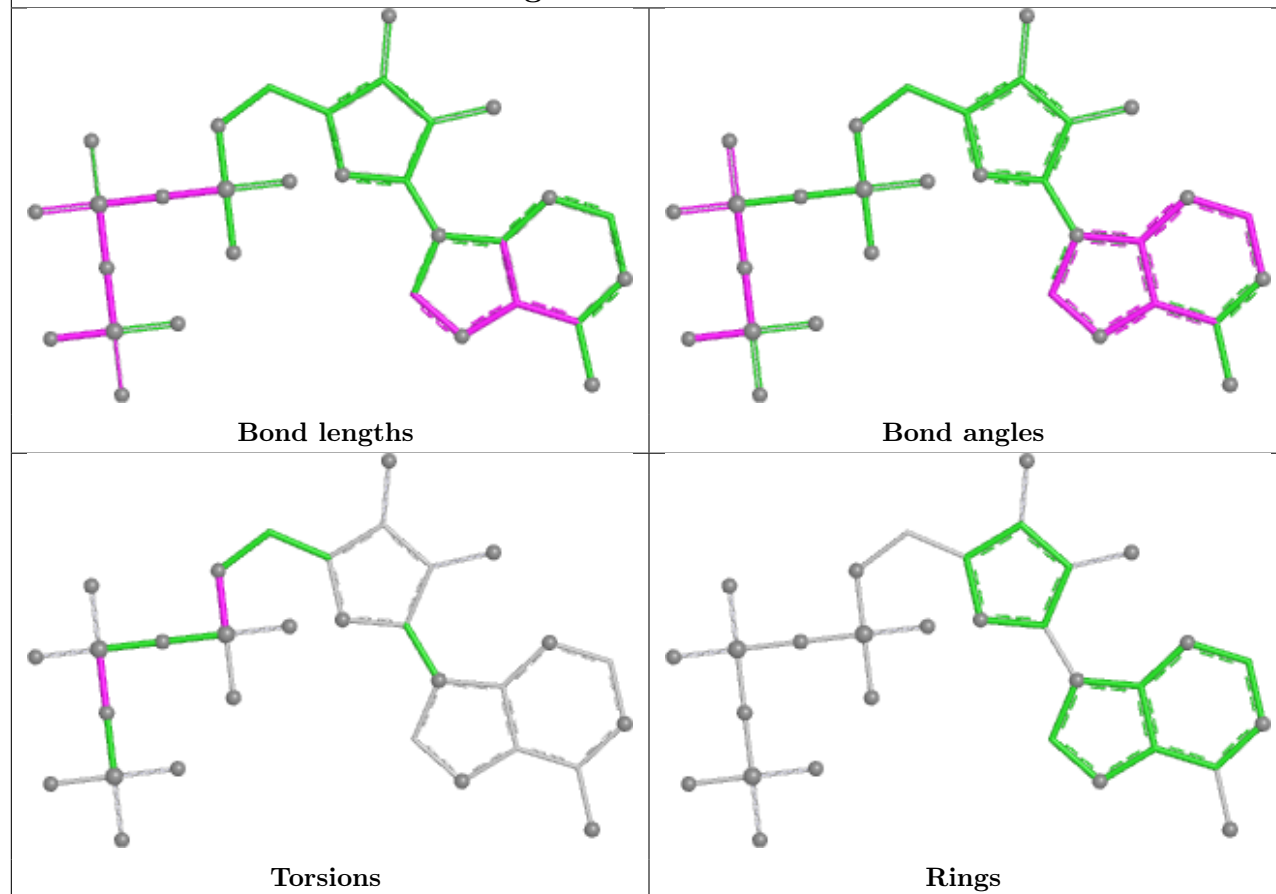
Ligand ANP F 1475



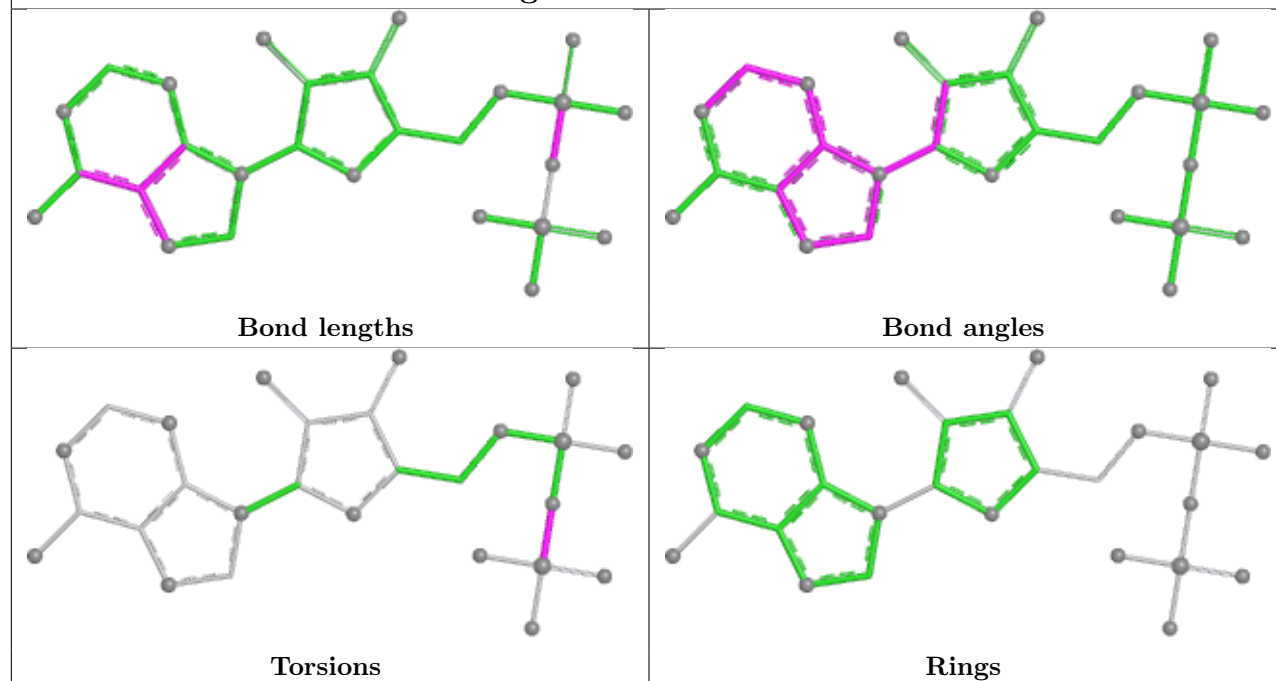
Ligand QUE N 1273 (B)

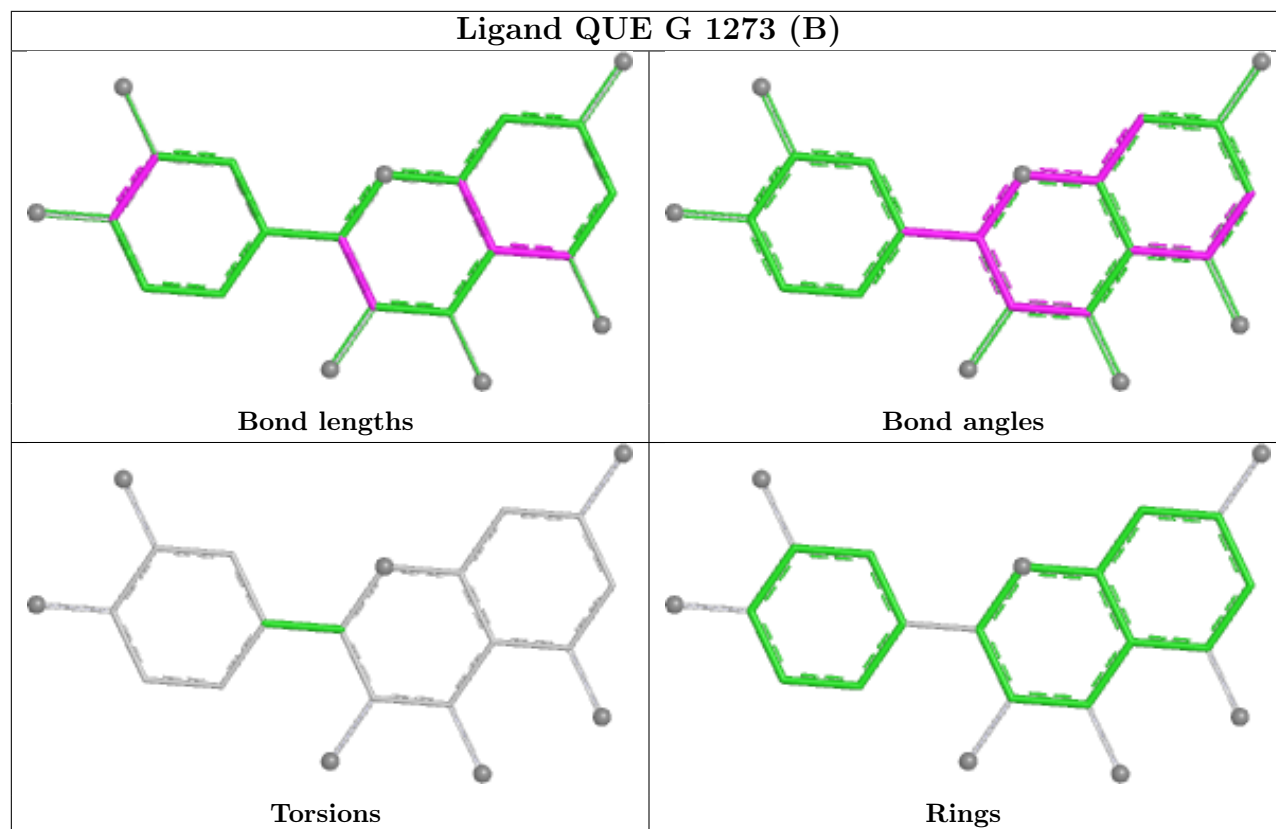


Ligand ANP J 1511



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

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	487/510 (95%)	-1.48	0	100	100	19, 38, 62, 98	0
1	B	479/510 (93%)	-1.34	0	100	100	16, 37, 90, 105	0
1	C	495/510 (97%)	-1.55	0	100	100	14, 32, 54, 94	0
1	H	487/510 (95%)	-1.48	0	100	100	17, 38, 61, 100	0
1	I	479/510 (93%)	-1.34	0	100	100	16, 37, 90, 104	0
1	J	495/510 (97%)	-1.56	0	100	100	17, 32, 53, 94	0
2	D	467/482 (96%)	-1.48	0	100	100	16, 33, 65, 92	0
2	E	466/482 (96%)	-1.17	0	100	100	19, 46, 90, 117	0
2	F	466/482 (96%)	-1.53	0	100	100	13, 31, 57, 73	0
2	K	467/482 (96%)	-1.45	0	100	100	17, 33, 65, 92	0
2	L	466/482 (96%)	-1.19	0	100	100	20, 46, 89, 117	0
2	M	466/482 (96%)	-1.55	0	100	100	15, 30, 57, 74	0
3	G	167/272 (61%)	-0.36	4 (2%)	59	55	16, 78, 123, 128	0
3	N	167/272 (61%)	-0.73	0	100	100	18, 76, 124, 129	0
All	All	6054/6496 (93%)	-1.38	4 (0%)	92	90	13, 37, 87, 129	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	43	VAL	2.3
3	G	169	ILE	2.2
3	G	83	SER	2.0
3	G	79	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	1513	6/6	0.99	0.04	39,41,46,48	0
6	GOL	A	1514	6/6	0.99	0.07	32,38,46,54	0
6	GOL	B	1512	6/6	0.99	0.06	20,23,24,31	0
6	GOL	B	1513	6/6	0.99	0.04	28,38,39,42	0
6	GOL	C	1513	6/6	0.99	0.04	36,38,41,47	0
6	GOL	D	1479	6/6	0.99	0.04	29,37,40,43	0
6	GOL	H	1513	6/6	0.99	0.04	44,46,49,53	0
6	GOL	H	1514	6/6	0.99	0.07	36,45,46,53	0
6	GOL	I	1512	6/6	0.99	0.05	19,27,28,37	0
6	GOL	J	1513	6/6	0.99	0.05	31,33,37,37	0
6	GOL	K	1479	6/6	0.99	0.04	38,41,44,49	0
6	GOL	K	1480	6/6	0.99	0.07	38,45,47,50	0
8	AZI	D	1478	3/3	0.99	0.08	10,10,12,22	0
9	PO4	E	1475	5/5	0.99	0.04	70,70,71,71	0
9	PO4	L	1475	5/5	0.99	0.04	84,84,85,86	0
10	QUE	G	1273[A]	22/22	0.99	0.03	37,41,43,43	22
10	QUE	G	1273[B]	22/22	0.99	0.03	65,65,66,66	22
10	QUE	N	1273[A]	22/22	0.99	0.03	34,42,44,45	22
10	QUE	N	1273[B]	22/22	0.99	0.03	49,51,51,51	22
4	ANP	B	1510	31/31	1.00	0.03	22,36,42,48	0
4	ANP	C	1511	31/31	1.00	0.03	18,24,32,34	0
4	ANP	F	1475	31/31	1.00	0.03	13,22,35,36	0
4	ANP	H	1511	31/31	1.00	0.03	20,29,34,36	0
4	ANP	I	1510	31/31	1.00	0.03	20,37,44,52	0
4	ANP	J	1511	31/31	1.00	0.03	14,26,28,30	0
4	ANP	M	1475	31/31	1.00	0.03	18,25,30,33	0
5	MG	A	1512	1/1	1.00	0.05	28,28,28,28	0

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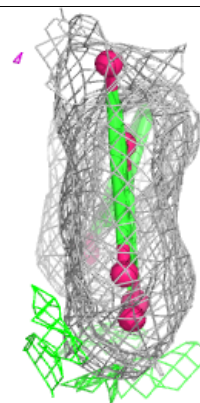
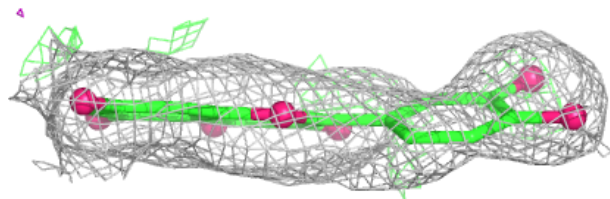
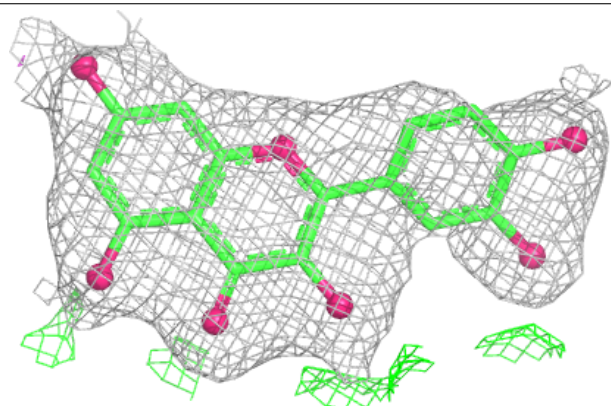
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	1511	1/1	1.00	0.09	29,29,29,29	0
5	MG	C	1512	1/1	1.00	0.06	14,14,14,14	0
5	MG	D	1477	1/1	1.00	0.06	18,18,18,18	0
7	ADP	D	1476	27/27	1.00	0.02	13,25,29,29	0
7	ADP	K	1476	27/27	1.00	0.03	20,26,29,30	0
5	MG	F	1476	1/1	1.00	0.06	18,18,18,18	0
8	AZI	K	1478	3/3	1.00	0.07	6,6,12,18	0
5	MG	H	1512	1/1	1.00	0.05	25,25,25,25	0
5	MG	I	1511	1/1	1.00	0.07	29,29,29,29	0
5	MG	J	1512	1/1	1.00	0.05	18,18,18,18	0
5	MG	K	1477	1/1	1.00	0.06	22,22,22,22	0
5	MG	M	1476	1/1	1.00	0.05	16,16,16,16	0
4	ANP	A	1511	31/31	1.00	0.03	18,25,32,33	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.

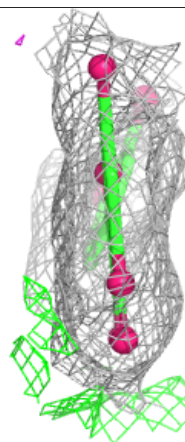
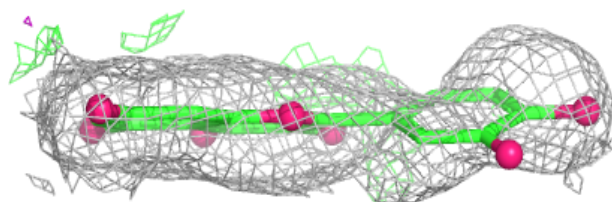
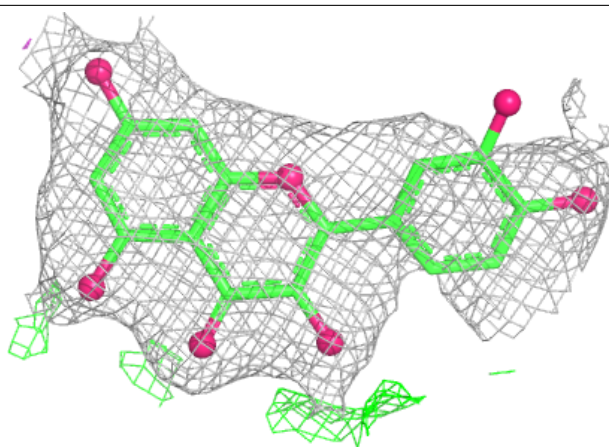
Electron density around QUE G 1273 (A):

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

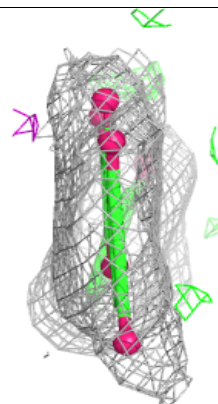
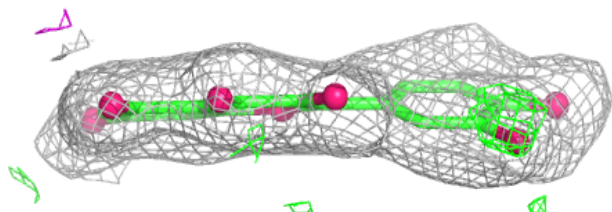
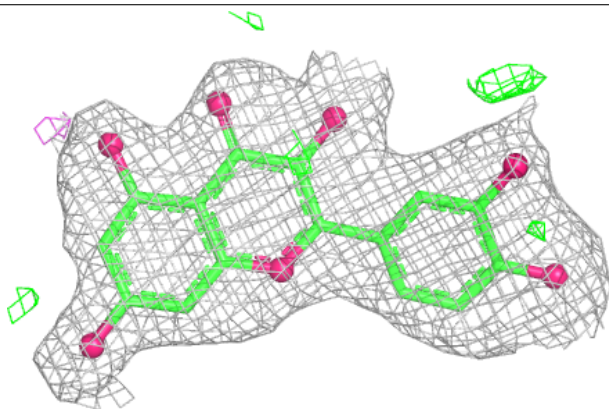


Electron density around QUE G 1273 (B):

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

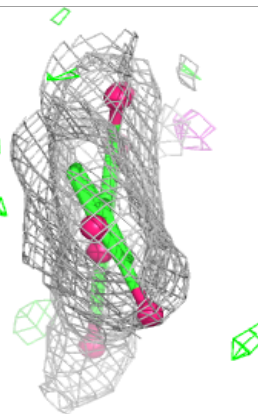
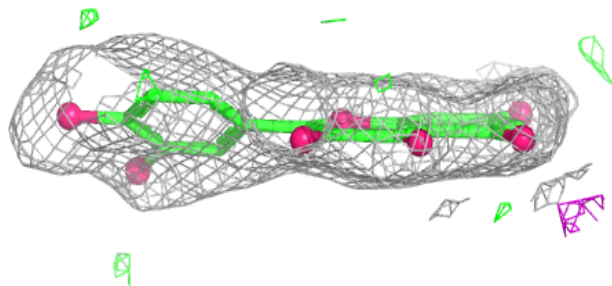
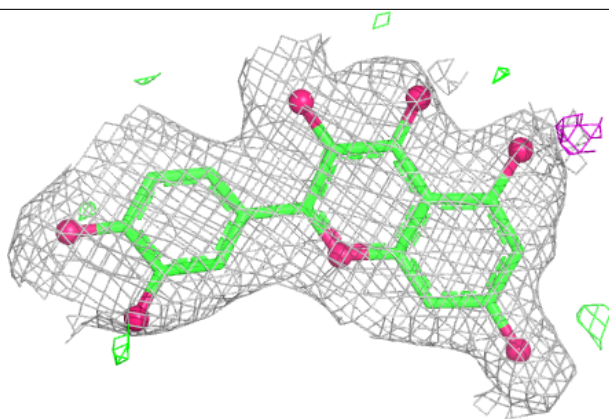
**Electron density around QUE N 1273 (A):**

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

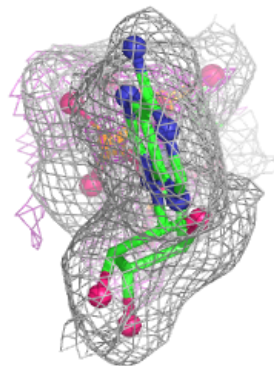
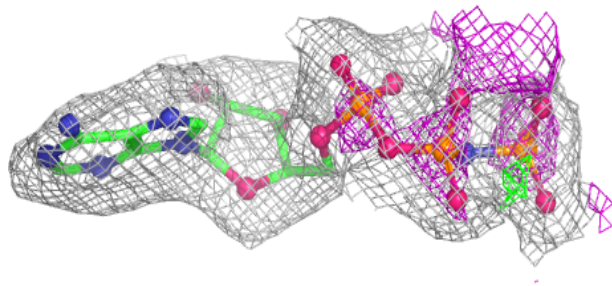
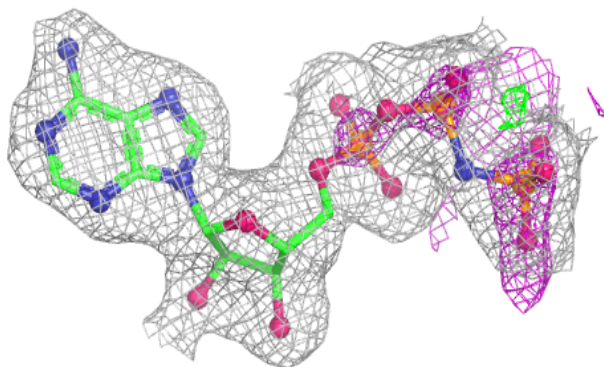


Electron density around QUE N 1273 (B):

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

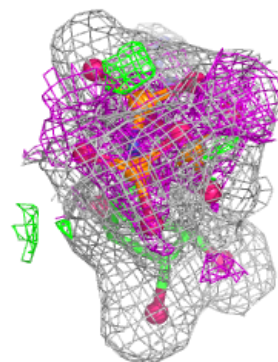
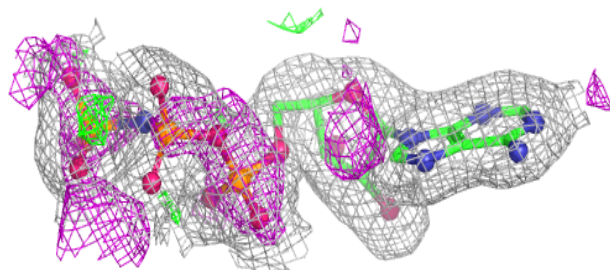
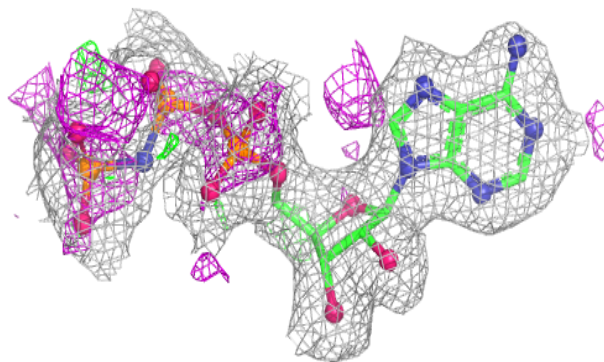
**Electron density around ANP B 1510:**

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

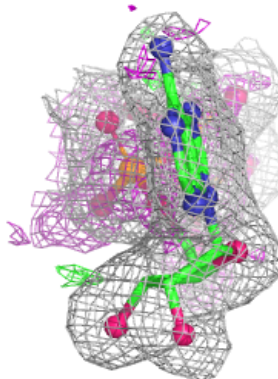
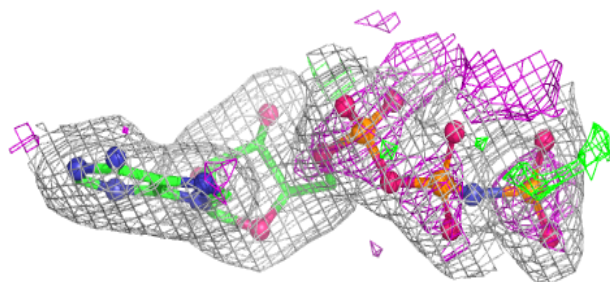
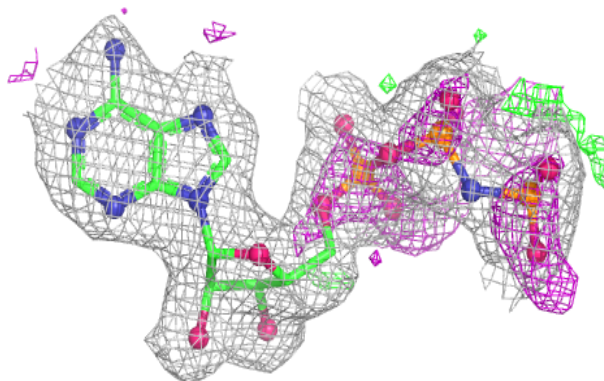


Electron density around ANP C 1511:

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

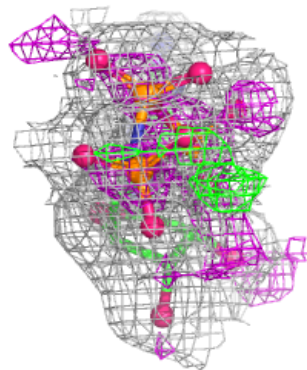
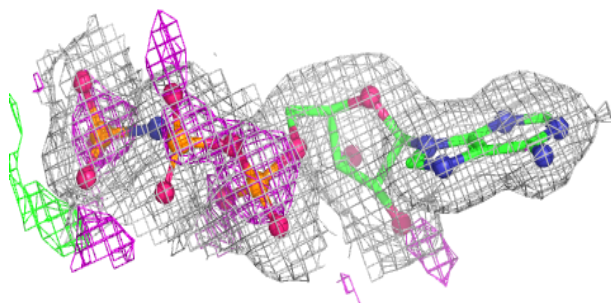
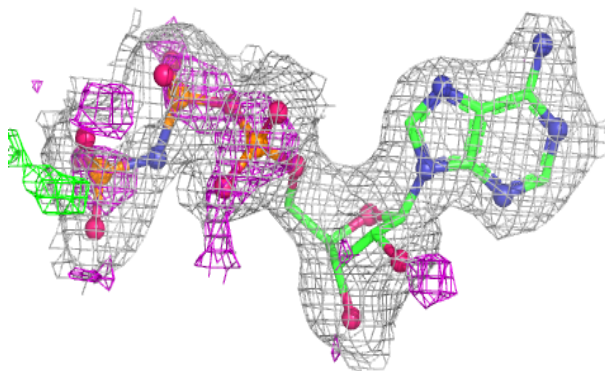
**Electron density around ANP F 1475:**

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

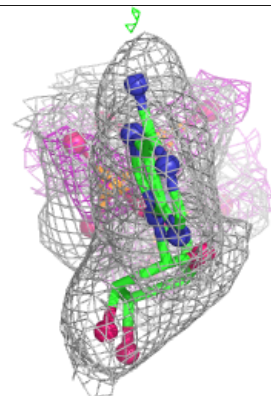
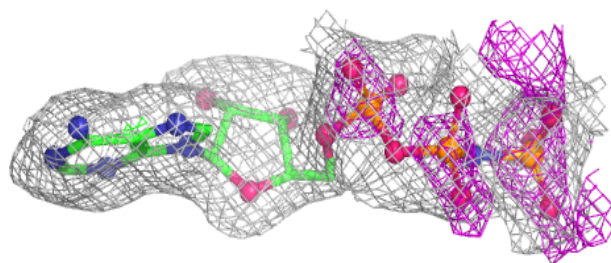
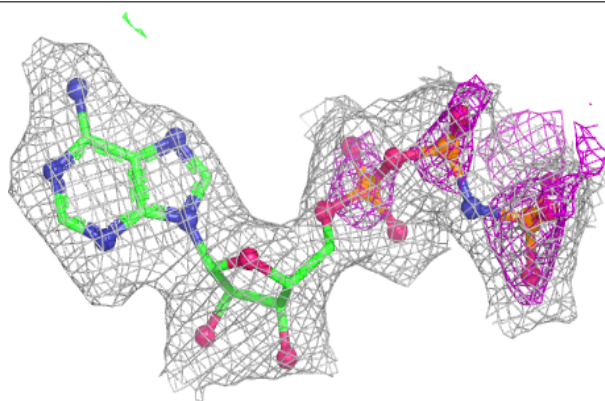


Electron density around ANP H 1511:

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

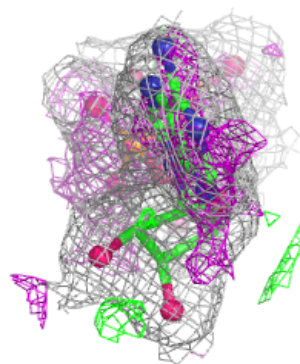
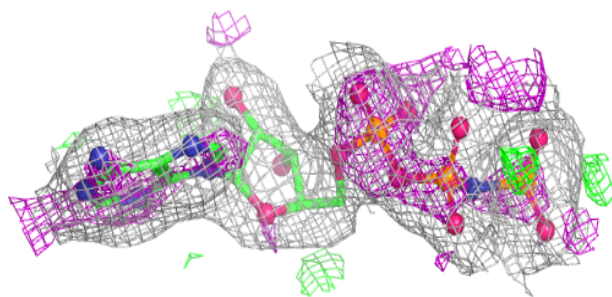
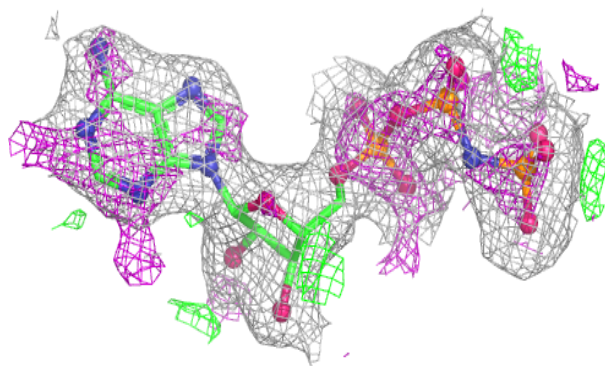
**Electron density around ANP I 1510:**

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

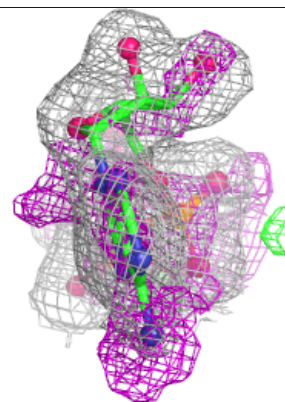
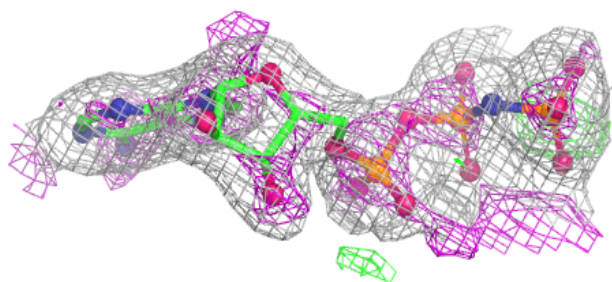
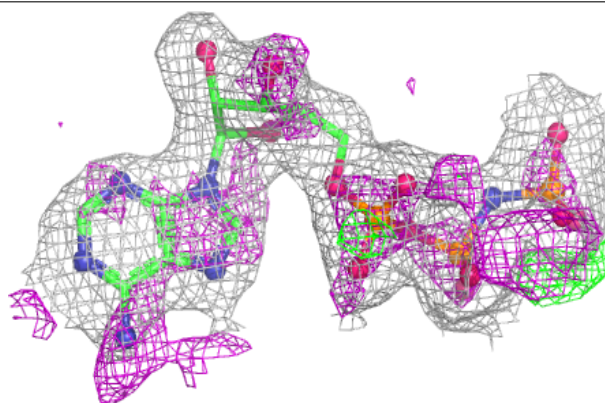


Electron density around ANP J 1511:

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

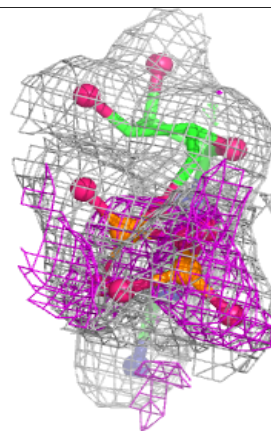
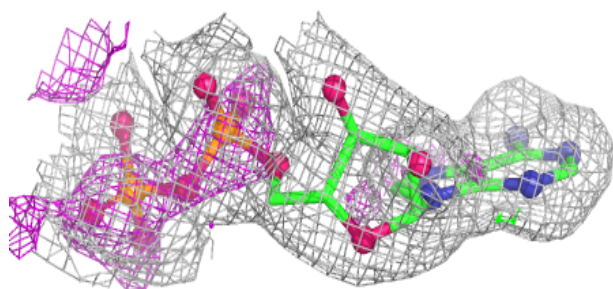
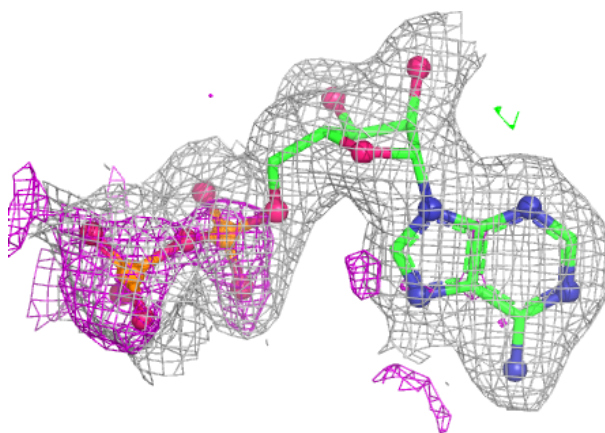
**Electron density around ANP M 1475:**

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



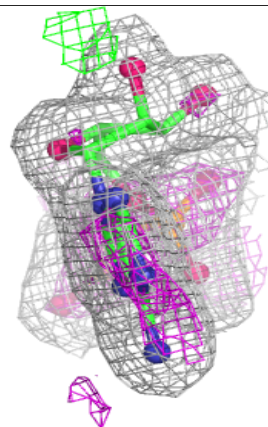
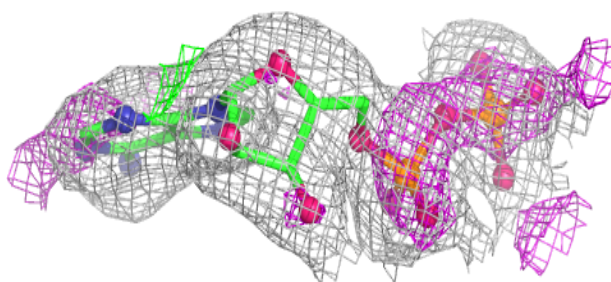
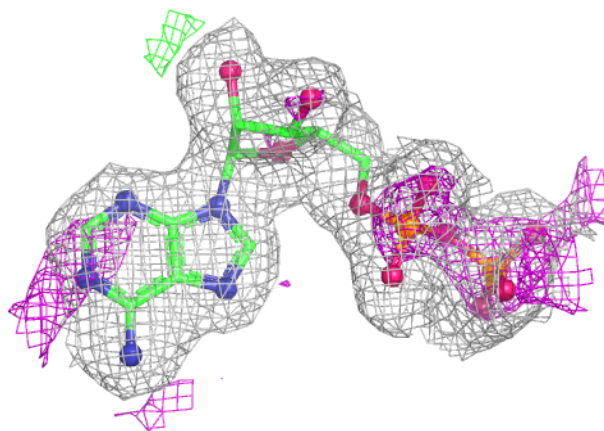
Electron density around ADP D 1476:

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

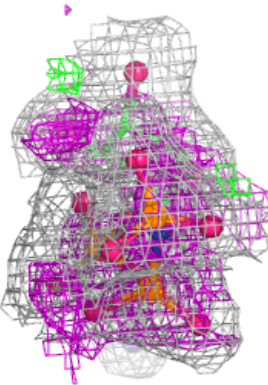
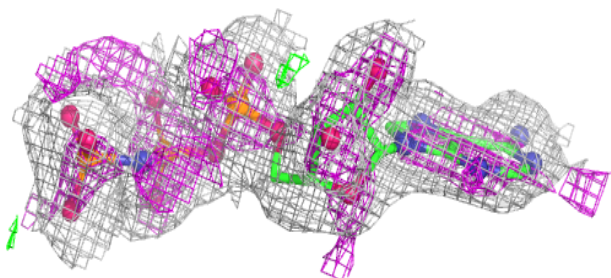
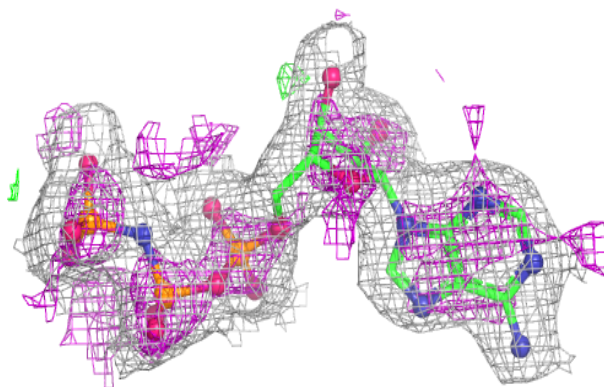


Electron density around ADP K 1476:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.