



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 02:41 am BST

PDB ID : 5OPX  
Title : Crystal structure of the GroEL mutant A109C in complex with GroES and ADP BeF<sub>2</sub>  
Authors : Yan, X.; Shi, Q.; Bracher, A.; Milicic, G.; Singh, A.K.; Hartl, F.U.; Hayer-Hartl, M.  
Deposited on : 2017-08-10  
Resolution : 3.64 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

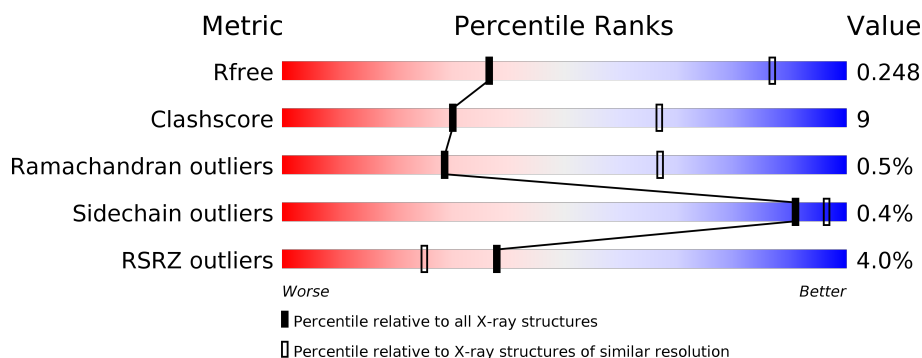
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.64 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	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)

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  $\leq 5\%$ . 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	548	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 77%; height: 10px; background-color: green;"></div> <div style="width: 16%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> </div> <div>79% 16% 5%</div> </div>
1	B	548	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 77%; height: 10px; background-color: green;"></div> <div style="width: 18%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> </div> <div>77% 18% 5%</div> </div>
1	C	548	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 78%; height: 10px; background-color: green;"></div> <div style="width: 17%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> </div> <div>78% 17% 5%</div> </div>
1	D	548	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 77%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> </div> <div>3% 80% 15% 5%</div> </div>
1	E	548	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 78%; height: 10px; background-color: green;"></div> <div style="width: 16%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> </div> <div>2% 78% 16% 5%</div> </div>
1	F	548	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 77%; height: 10px; background-color: green;"></div> <div style="width: 17%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> </div> <div>2% 77% 17% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	548	
1	H	548	
1	I	548	
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	
2	1	97	
2	2	97	
2	O	97	
2	P	97	
2	Q	97	
2	R	97	
2	S	97	
2	T	97	
2	U	97	
2	V	97	
2	W	97	
2	X	97	
2	Y	97	
2	Z	97	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 63865 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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	B	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	C	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	D	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	E	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	F	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	G	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	H	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	I	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	J	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	K	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	L	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	M	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			
1	N	520	Total	C	N	O	S	0	0	0
			3835	2386	661	767	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	CYS	ALA	engineered mutation	UNP P0A6F5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	109	CYS	ALA	engineered mutation	UNP P0A6F5
C	109	CYS	ALA	engineered mutation	UNP P0A6F5
D	109	CYS	ALA	engineered mutation	UNP P0A6F5
E	109	CYS	ALA	engineered mutation	UNP P0A6F5
F	109	CYS	ALA	engineered mutation	UNP P0A6F5
G	109	CYS	ALA	engineered mutation	UNP P0A6F5
H	109	CYS	ALA	engineered mutation	UNP P0A6F5
I	109	CYS	ALA	engineered mutation	UNP P0A6F5
J	109	CYS	ALA	engineered mutation	UNP P0A6F5
K	109	CYS	ALA	engineered mutation	UNP P0A6F5
L	109	CYS	ALA	engineered mutation	UNP P0A6F5
M	109	CYS	ALA	engineered mutation	UNP P0A6F5
N	109	CYS	ALA	engineered mutation	UNP P0A6F5

- Molecule 2 is a protein called 10 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			
2	2	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			
2	O	93	Total	C	N	O	S	0	0	0
			701	437	122	140	2			
2	P	94	Total	C	N	O	S	0	0	0
			707	440	123	142	2			
2	Q	90	Total	C	N	O	S	0	0	0
			675	421	118	135	1			
2	R	92	Total	C	N	O	S	0	0	0
			691	431	120	139	1			
2	S	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			
2	T	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			
2	U	92	Total	C	N	O	S	0	0	0
			690	430	121	138	1			
2	V	93	Total	C	N	O	S	0	0	0
			699	435	122	141	1			
2	W	93	Total	C	N	O	S	0	0	0
			699	435	122	141	1			
2	X	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			
2	Y	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	92	Total	C	N	O	S	0	0	0
			693	432	121	139	1			



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0	0



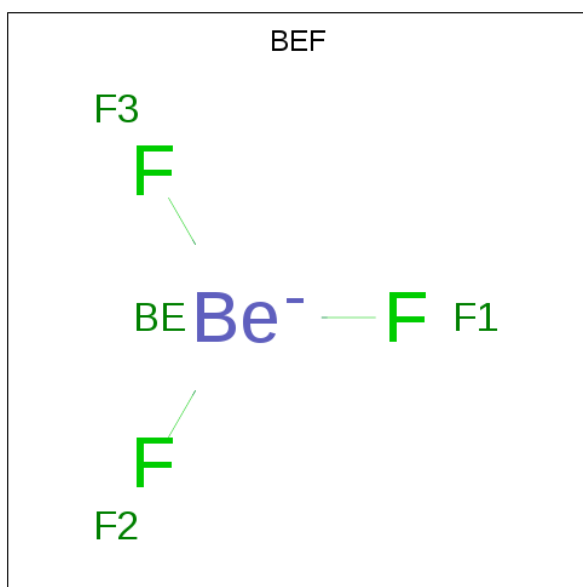
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	N	1	Total	Mg	0	0
			1	1		
4	L	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	Be 1	F 3	0	0
5	B	1	Total 4	Be 1	F 3	0	0
5	C	1	Total 4	Be 1	F 3	0	0
5	D	1	Total 4	Be 1	F 3	0	0
5	E	1	Total 4	Be 1	F 3	0	0
5	F	1	Total 4	Be 1	F 3	0	0
5	G	1	Total 4	Be 1	F 3	0	0
5	H	1	Total 4	Be 1	F 3	0	0
5	I	1	Total 4	Be 1	F 3	0	0
5	J	1	Total 4	Be 1	F 3	0	0
5	K	1	Total 4	Be 1	F 3	0	0
5	L	1	Total 4	Be 1	F 3	0	0
5	M	1	Total 4	Be 1	F 3	0	0
5	N	1	Total 4	Be 1	F 3	0	0



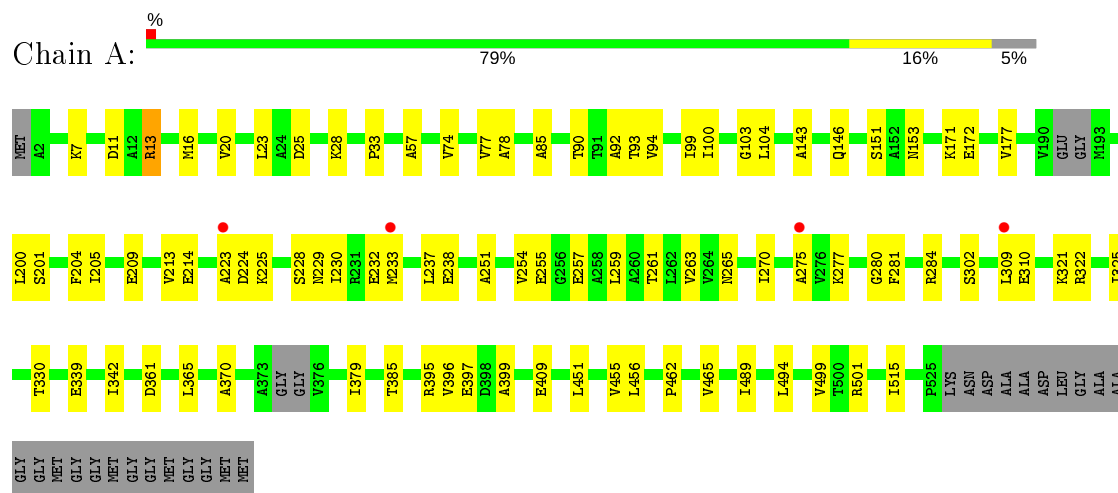
- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total 1	K 1	0	0
6	J	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0
6	K	1	Total 1	K 1	0	0
6	E	1	Total 1	K 1	0	0
6	H	1	Total 1	K 1	0	0
6	B	1	Total 1	K 1	0	0
6	I	1	Total 1	K 1	0	0
6	C	1	Total 1	K 1	0	0
6	A	1	Total 1	K 1	0	0
6	N	1	Total 1	K 1	0	0
6	L	1	Total 1	K 1	0	0
6	F	1	Total 1	K 1	0	0
6	M	1	Total 1	K 1	0	0

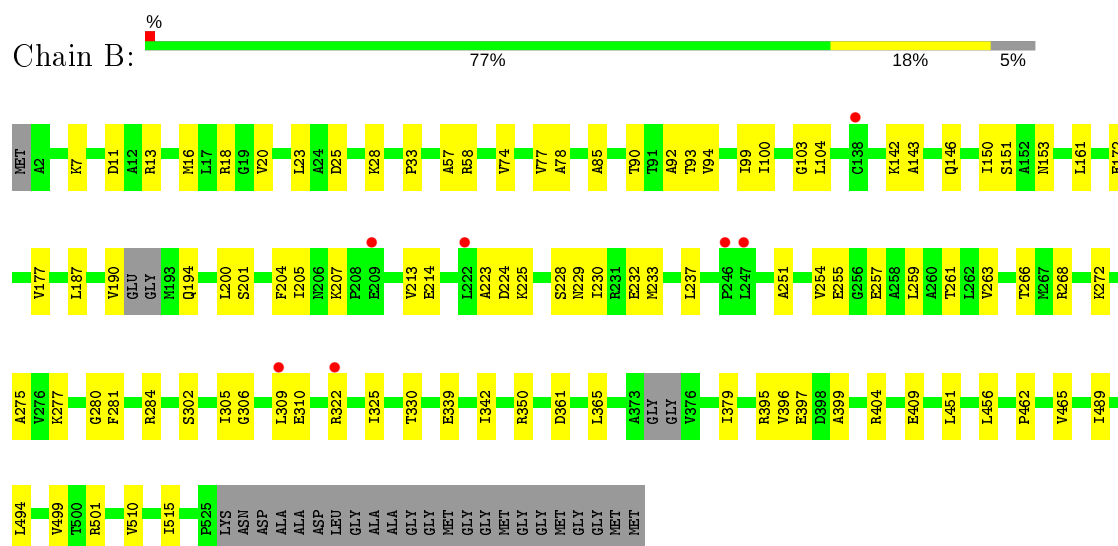
### 3 Residue-property plots [i](#)

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.

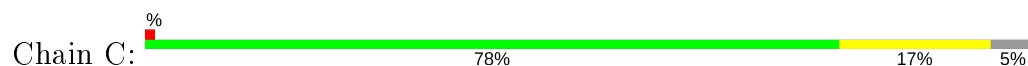
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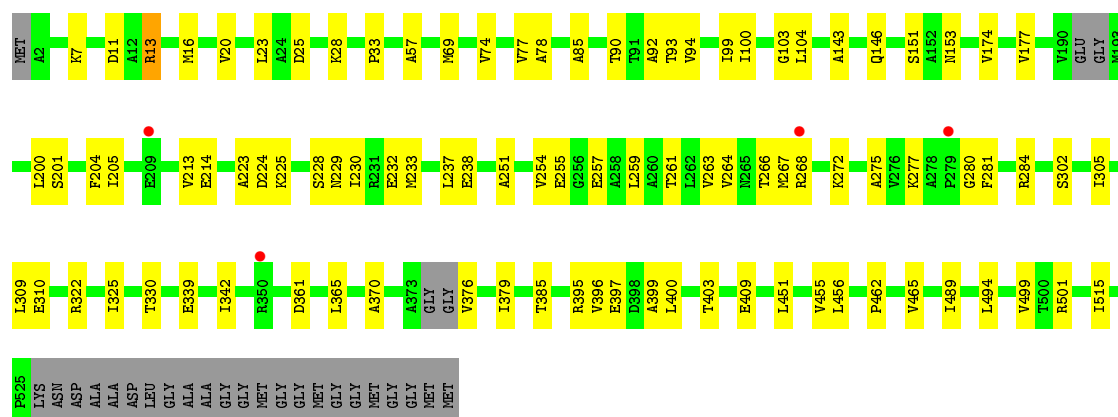


#### • Molecule 1: 60 kDa chaperonin

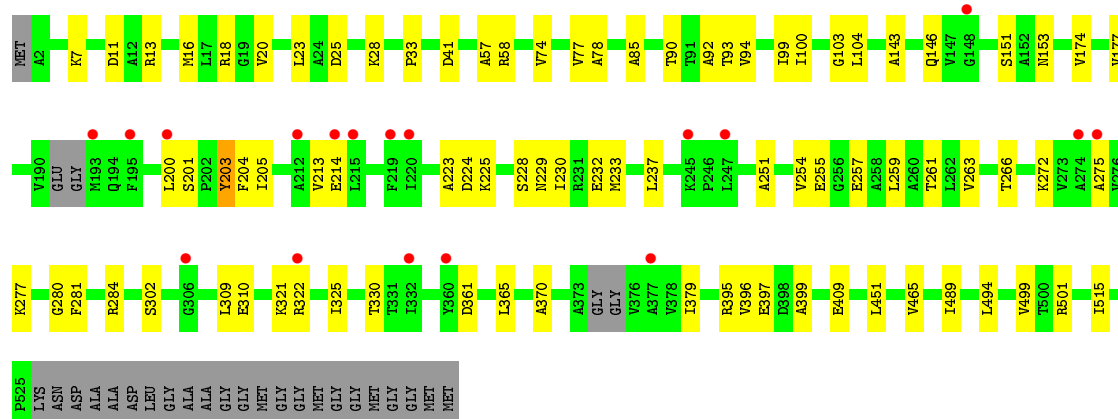
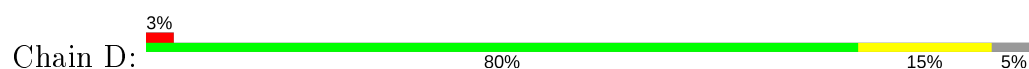


#### • Molecule 1: 60 kDa chaperonin

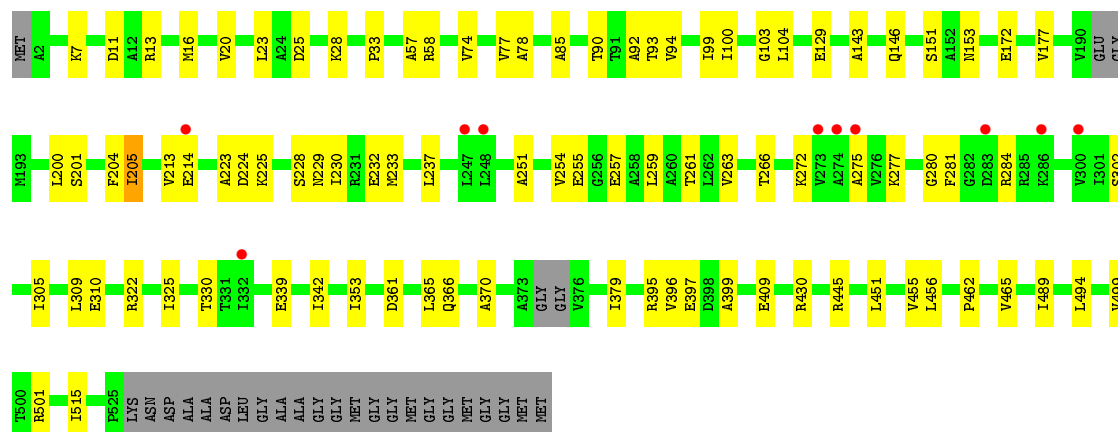
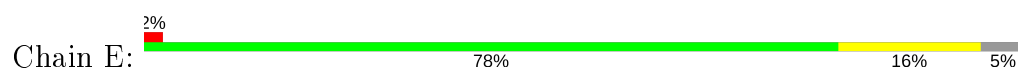




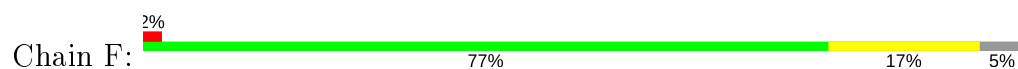
• Molecule 1: 60 kDa chaperonin

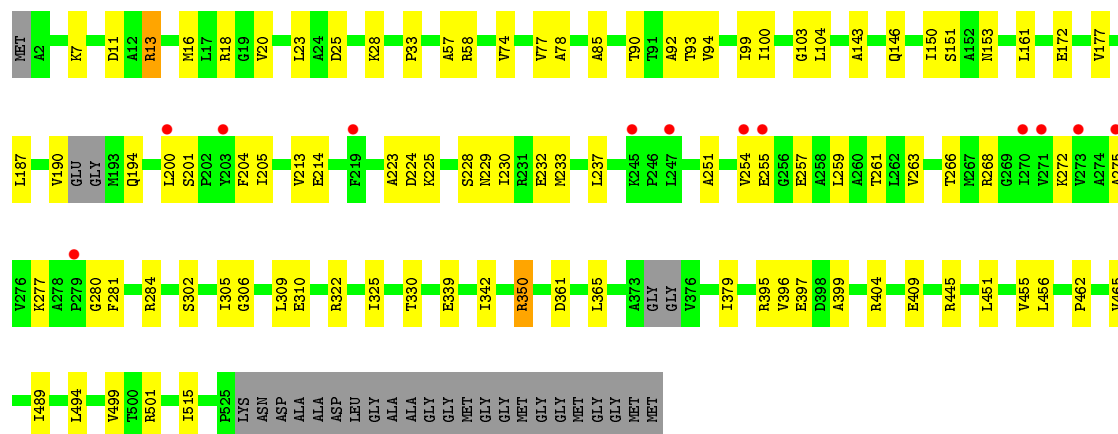


• Molecule 1: 60 kDa chaperonin

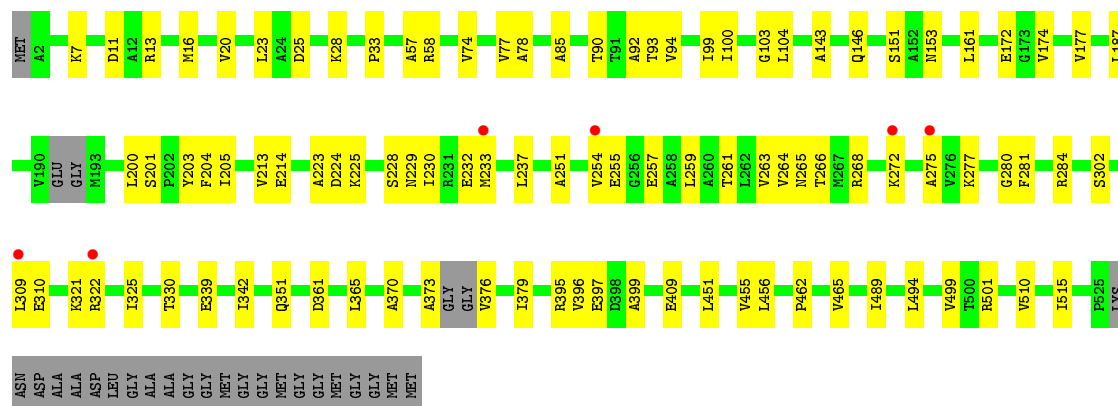
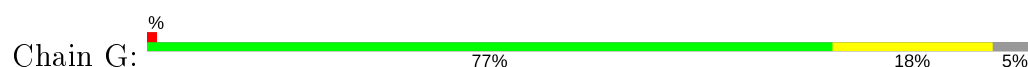


• Molecule 1: 60 kDa chaperonin

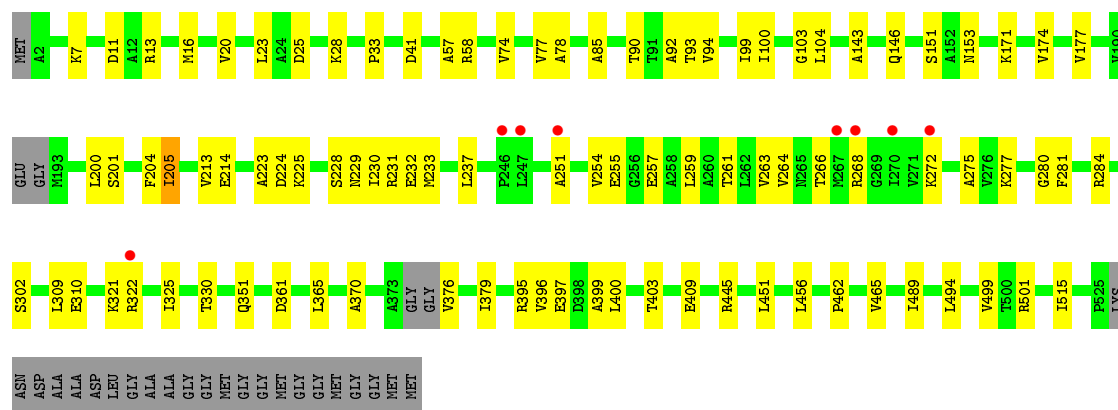
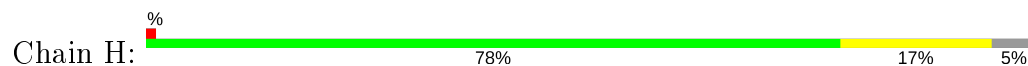




• Molecule 1: 60 kDa chaperonin

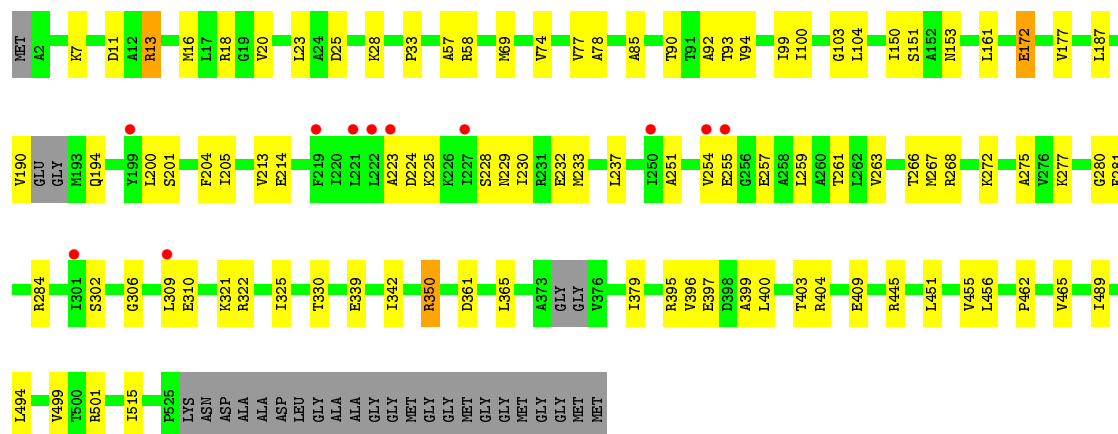


• Molecule 1: 60 kDa chaperonin

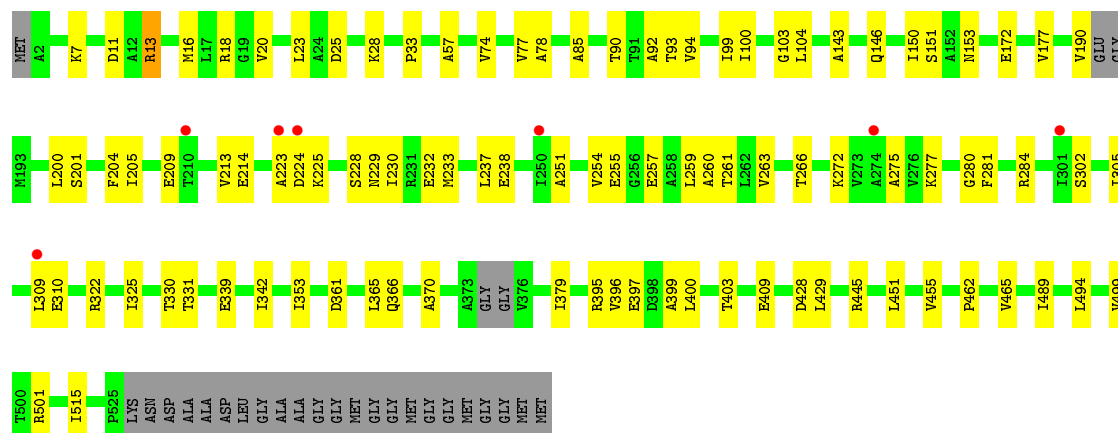
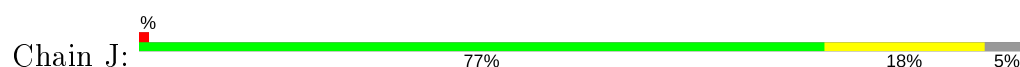


• Molecule 1: 60 kDa chaperonin

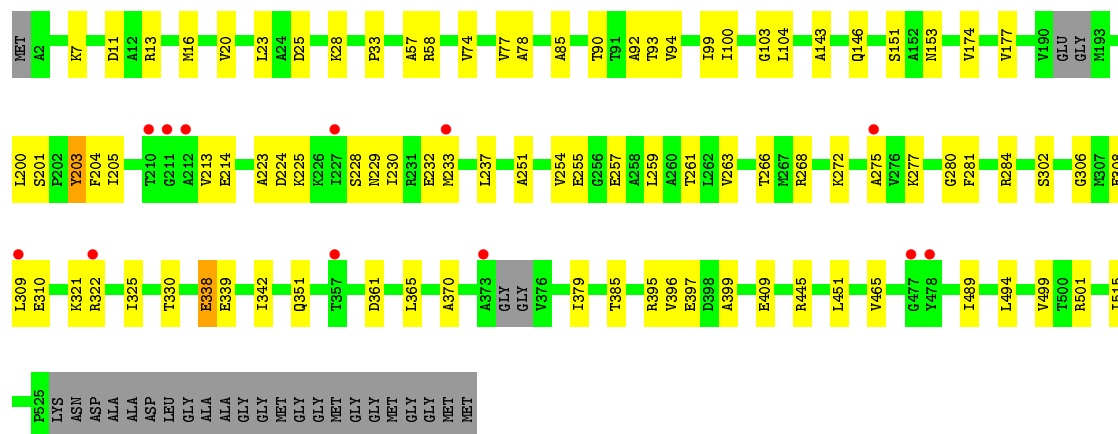
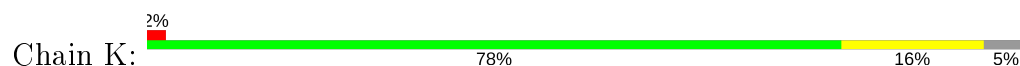




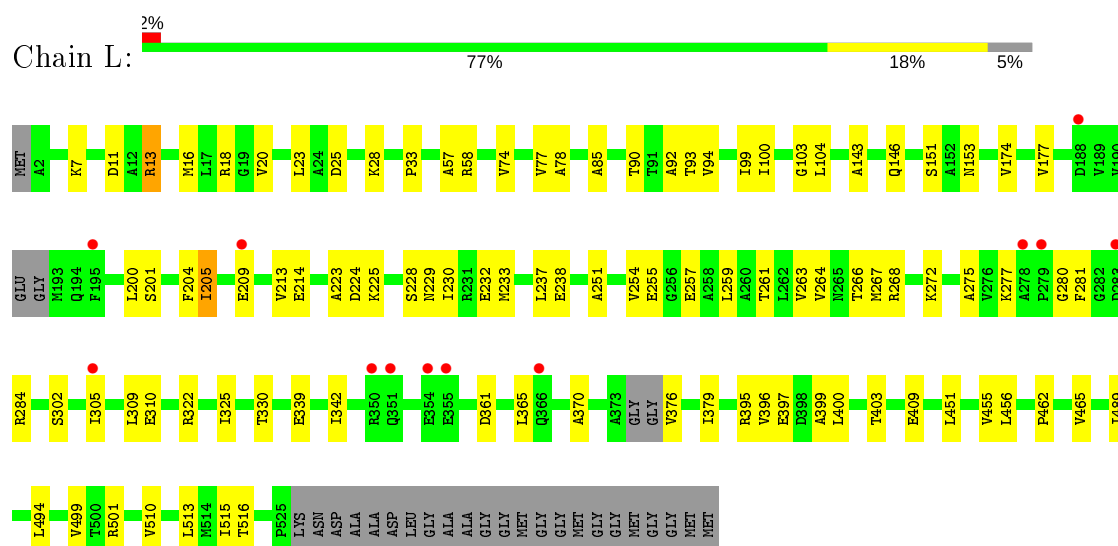
• Molecule 1: 60 kDa chaperonin



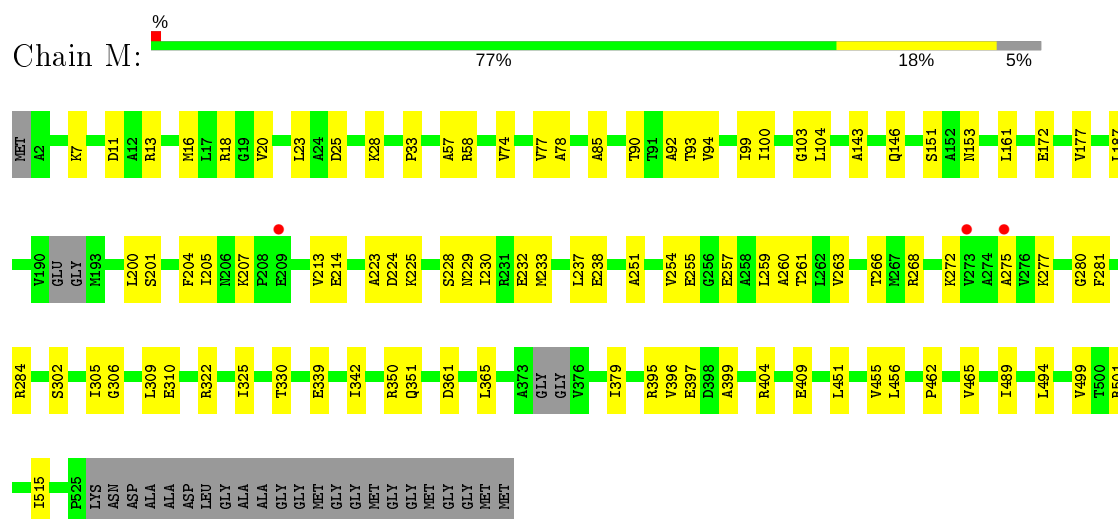
• Molecule 1: 60 kDa chaperonin



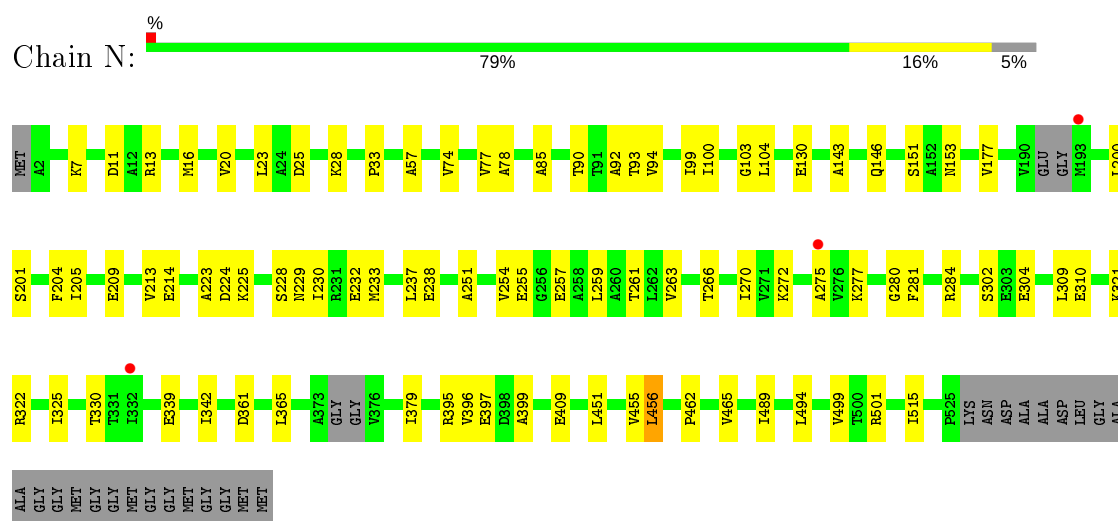
• Molecule 1: 60 kDa chaperonin



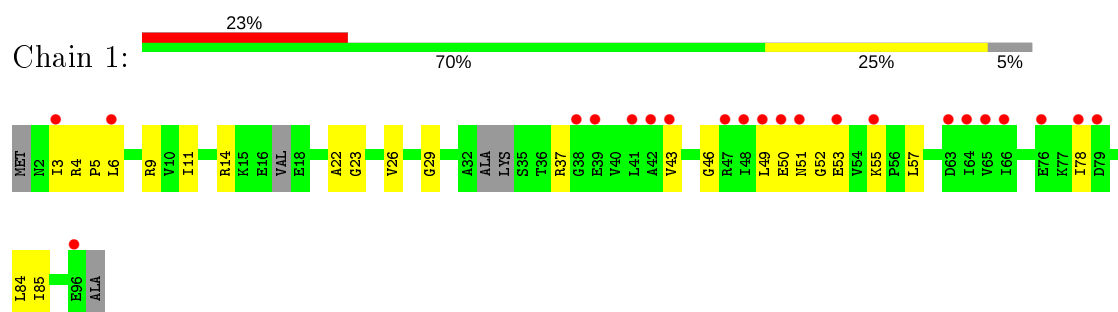
- Molecule 1: 60 kDa chaperonin



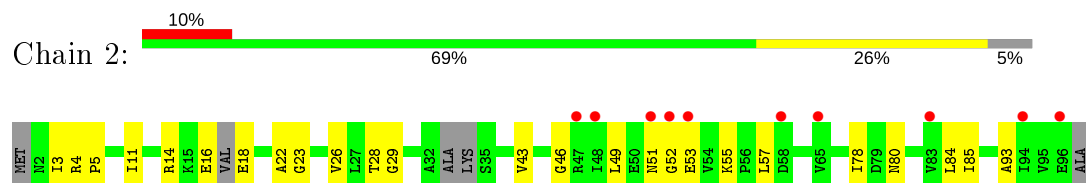
- Molecule 1: 60 kDa chaperonin



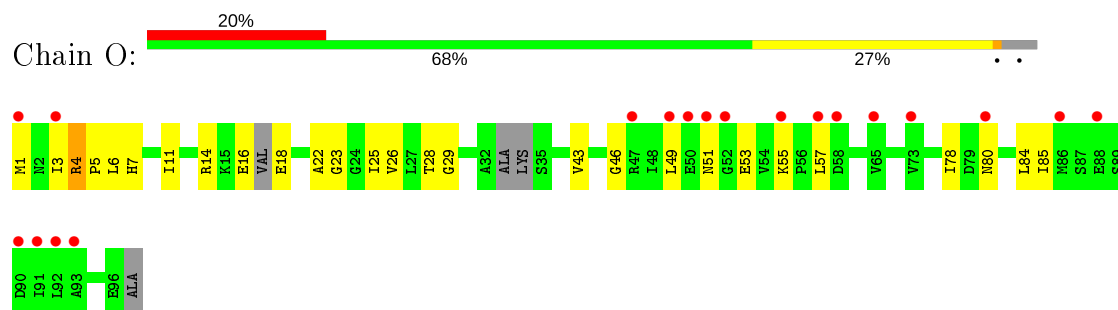
- Molecule 2: 10 kDa chaperonin



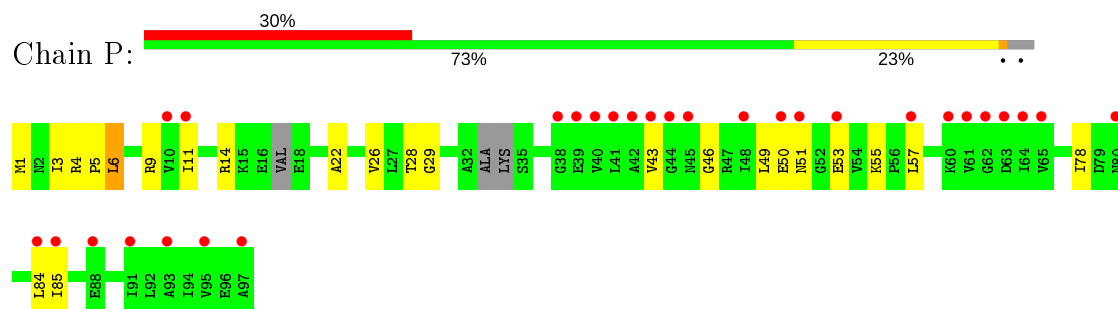
- Molecule 2: 10 kDa chaperonin



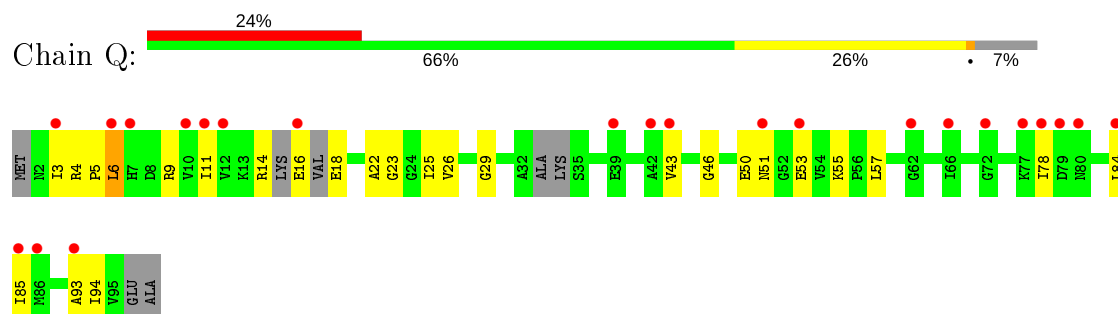
- Molecule 2: 10 kDa chaperonin



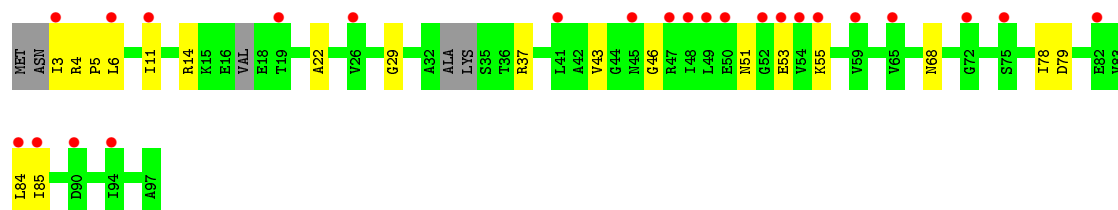
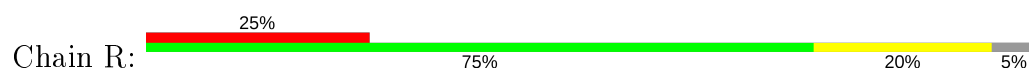
- Molecule 2: 10 kDa chaperonin



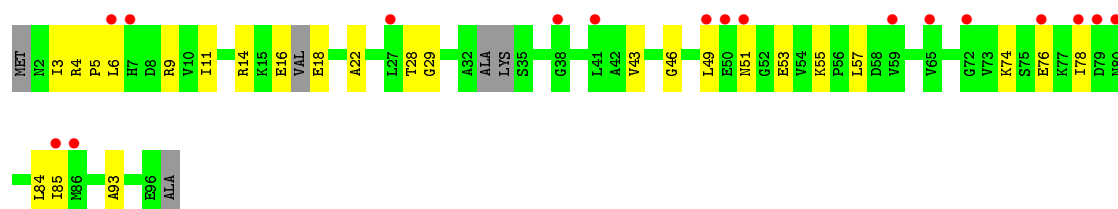
- Molecule 2: 10 kDa chaperonin



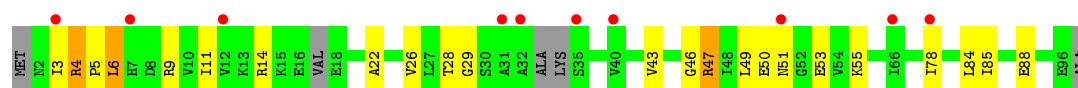
- Molecule 2: 10 kDa chaperonin



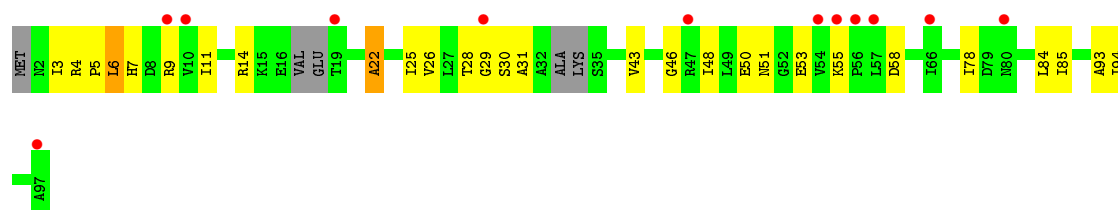
- Molecule 2: 10 kDa chaperonin



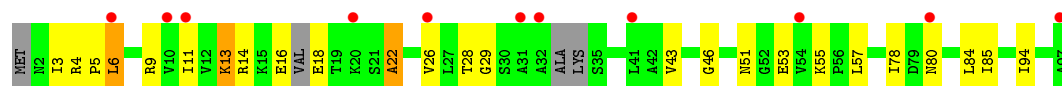
- Molecule 2: 10 kDa chaperonin



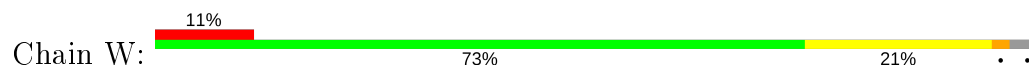
- Molecule 2: 10 kDa chaperonin



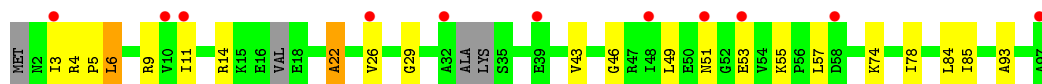
- Molecule 2: 10 kDa chaperonin



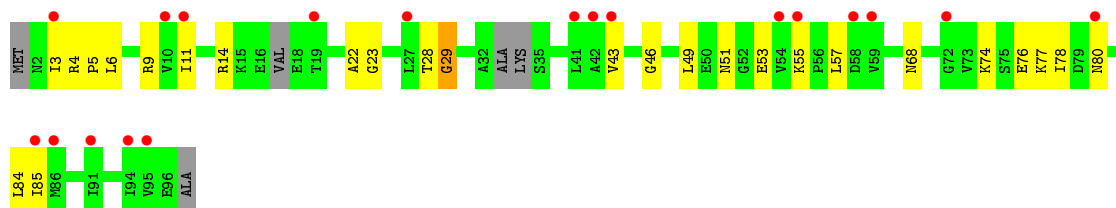
- Molecule 2: 10 kDa chaperonin



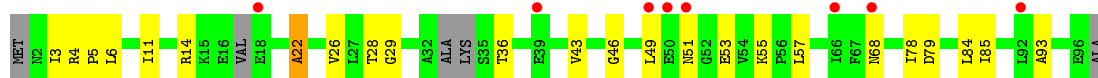




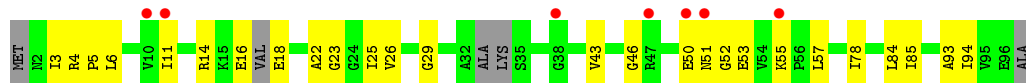
- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.57Å 230.50Å 235.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.64 49.01 – 3.64	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.01-3.64) 99.7 (49.01-3.64)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.231 , 0.256 0.227 , 0.248	Depositor DCC
$R_{free}$ test set	6583 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.3	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 81.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	63865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1222e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.57	0/3861	0.82	3/5211 (0.1%)
1	B	0.56	0/3861	0.82	5/5211 (0.1%)
1	C	0.55	0/3861	0.82	3/5211 (0.1%)
1	D	0.57	0/3861	0.82	3/5211 (0.1%)
1	E	0.57	0/3861	0.82	5/5211 (0.1%)
1	F	0.57	0/3861	0.83	9/5211 (0.2%)
1	G	0.56	0/3861	0.82	3/5211 (0.1%)
1	H	0.58	0/3861	0.82	4/5211 (0.1%)
1	I	0.57	1/3861 (0.0%)	0.82	9/5211 (0.2%)
1	J	0.56	0/3861	0.81	4/5211 (0.1%)
1	K	0.58	0/3861	0.83	4/5211 (0.1%)
1	L	0.56	0/3861	0.82	5/5211 (0.1%)
1	M	0.56	0/3861	0.82	5/5211 (0.1%)
1	N	0.58	0/3861	0.82	3/5211 (0.1%)
2	1	0.53	0/695	0.82	1/932 (0.1%)
2	2	0.50	0/695	0.80	0/932
2	O	0.58	0/703	0.83	1/942 (0.1%)
2	P	0.51	0/709	0.80	0/949
2	Q	0.52	0/676	0.83	0/906
2	R	0.54	0/693	0.81	0/928
2	S	0.50	0/695	0.78	0/932
2	T	0.54	0/695	0.84	1/932 (0.1%)
2	U	0.64	0/692	0.85	0/927
2	V	0.56	0/701	0.82	1/939 (0.1%)
2	W	0.52	0/701	0.81	0/939
2	X	0.51	0/695	0.79	0/932
2	Y	0.59	0/695	0.80	0/932
2	Z	0.55	0/695	0.83	0/932
All	All	0.56	1/63794 (0.0%)	0.82	69/86008 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	172	GLU	CD-OE2	-5.20	1.20	1.25

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	58	ARG	NE-CZ-NH2	-7.77	116.42	120.30
2	O	4	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	I	395	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	H	395	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	M	58	ARG	NE-CZ-NH2	-6.92	116.84	120.30

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	3835	0	3956	75	0
1	B	3835	0	3958	73	2
1	C	3835	0	3956	80	0
1	D	3835	0	3958	68	0
1	E	3835	0	3958	67	7
1	F	3835	0	3957	74	0
1	G	3835	0	3958	80	0
1	H	3835	0	3958	72	0
1	I	3835	0	3958	73	0
1	J	3835	0	3958	76	5
1	K	3835	0	3957	74	0
1	L	3835	0	3958	85	0
1	M	3835	0	3957	74	1
1	N	3835	0	3958	72	1
2	1	693	0	716	20	0
2	2	693	0	716	25	0
2	O	701	0	728	29	0
2	P	707	0	733	14	0
2	Q	675	0	696	17	0
2	R	691	0	715	12	5

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	693	0	716	17	0
2	T	693	0	716	18	0
2	U	690	0	715	29	0
2	V	699	0	721	23	0
2	W	699	0	721	19	0
2	X	693	0	716	22	0
2	Y	693	0	716	23	7
2	Z	693	0	716	20	0
3	A	27	0	12	1	0
3	B	27	0	12	3	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
3	G	27	0	12	1	0
3	H	27	0	12	1	0
3	I	27	0	12	2	0
3	J	27	0	12	2	0
3	K	27	0	12	1	0
3	L	27	0	12	1	0
3	M	27	0	12	1	0
3	N	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	4	0	0	1	0
5	B	4	0	0	1	0
5	C	4	0	0	1	0
5	D	4	0	0	1	0
5	E	4	0	0	1	0
5	F	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	4	0	0	1	0
5	H	4	0	0	1	0
5	I	4	0	0	1	0
5	J	4	0	0	1	0
5	K	4	0	0	1	0
5	L	4	0	0	1	0
5	M	4	0	0	1	0
5	N	4	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
All	All	63865	0	65614	1209	14

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 9.

The worst 5 of 1209 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:VAL:HG21	1:D:370:ALA:HB2	1.31	1.12
2:O:80:ASN:OD1	2:U:22:ALA:HA	1.54	1.08
2:V:80:ASN:ND2	2:W:22:ALA:HB2	1.71	1.05
1:K:203:TYR:CD2	1:L:305:ILE:HD13	1.91	1.03
1:G:229:ASN:HA	1:G:257:GLU:OE1	1.68	0.94

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:ARG:C	2:Y:79:ASP:OD1[2_454]	1.25	0.95
1:E:430:ARG:CA	2:Y:79:ASP:OD1[2_454]	1.57	0.63
1:E:430:ARG:O	2:Y:79:ASP:OD1[2_454]	1.61	0.59
1:J:429:LEU:CA	2:R:79:ASP:OD1[2_465]	1.71	0.49
1:J:428:ASP:O	2:R:79:ASP:OD2[2_465]	1.84	0.36

## 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	514/548 (94%)	491 (96%)	22 (4%)	1 (0%)	47	79
1	B	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	47	79
1	C	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	47	79
1	D	514/548 (94%)	490 (95%)	22 (4%)	2 (0%)	34	70
1	E	514/548 (94%)	492 (96%)	21 (4%)	1 (0%)	47	79
1	F	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	47	79
1	G	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	47	79
1	H	514/548 (94%)	489 (95%)	24 (5%)	1 (0%)	47	79
1	I	514/548 (94%)	491 (96%)	22 (4%)	1 (0%)	47	79
1	J	514/548 (94%)	491 (96%)	22 (4%)	1 (0%)	47	79
1	K	514/548 (94%)	491 (96%)	21 (4%)	2 (0%)	34	70
1	L	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	47	79
1	M	514/548 (94%)	490 (95%)	23 (4%)	1 (0%)	47	79
1	N	514/548 (94%)	491 (96%)	22 (4%)	1 (0%)	47	79
2	1	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	6	37
2	2	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	6	37
2	O	87/97 (90%)	81 (93%)	4 (5%)	2 (2%)	6	37
2	P	88/97 (91%)	82 (93%)	4 (4%)	2 (2%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	83/97 (86%)	77 (93%)	4 (5%)	2 (2%)	6	36
2	R	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	6	37
2	S	86/97 (89%)	81 (94%)	3 (4%)	2 (2%)	6	37
2	T	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	6	37
2	U	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	6	37
2	V	87/97 (90%)	81 (93%)	4 (5%)	2 (2%)	6	37
2	W	87/97 (90%)	81 (93%)	4 (5%)	2 (2%)	6	37
2	X	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	6	37
2	Y	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	6	37
2	Z	86/97 (89%)	80 (93%)	4 (5%)	2 (2%)	6	37
All	All	8402/9030 (93%)	7989 (95%)	369 (4%)	44 (0%)	29	67

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U	22	ALA
2	W	29	GLY
2	Y	22	ALA
2	1	22	ALA
2	2	22	ALA

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/416 (97%)	402 (100%)	2 (0%)	88	95
1	B	404/416 (97%)	404 (100%)	0	100	100
1	C	404/416 (97%)	404 (100%)	0	100	100
1	D	404/416 (97%)	403 (100%)	1 (0%)	93	98
1	E	404/416 (97%)	404 (100%)	0	100	100
1	F	404/416 (97%)	404 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	404/416 (97%)	403 (100%)	1 (0%)	93	98
1	H	404/416 (97%)	402 (100%)	2 (0%)	88	95
1	I	404/416 (97%)	403 (100%)	1 (0%)	93	98
1	J	404/416 (97%)	404 (100%)	0	100	100
1	K	404/416 (97%)	402 (100%)	2 (0%)	88	95
1	L	404/416 (97%)	404 (100%)	0	100	100
1	M	404/416 (97%)	404 (100%)	0	100	100
1	N	404/416 (97%)	403 (100%)	1 (0%)	93	98
2	1	77/80 (96%)	77 (100%)	0	100	100
2	2	77/80 (96%)	77 (100%)	0	100	100
2	O	78/80 (98%)	76 (97%)	2 (3%)	46	73
2	P	78/80 (98%)	76 (97%)	2 (3%)	46	73
2	Q	75/80 (94%)	74 (99%)	1 (1%)	69	85
2	R	76/80 (95%)	75 (99%)	1 (1%)	69	85
2	S	77/80 (96%)	77 (100%)	0	100	100
2	T	77/80 (96%)	75 (97%)	2 (3%)	46	73
2	U	76/80 (95%)	75 (99%)	1 (1%)	69	85
2	V	77/80 (96%)	75 (97%)	2 (3%)	46	73
2	W	77/80 (96%)	76 (99%)	1 (1%)	69	85
2	X	77/80 (96%)	77 (100%)	0	100	100
2	Y	77/80 (96%)	76 (99%)	1 (1%)	69	85
2	Z	77/80 (96%)	76 (99%)	1 (1%)	69	85
All	All	6732/6944 (97%)	6708 (100%)	24 (0%)	91	96

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	1	MET
2	P	6	LEU
2	Y	6	LEU
2	O	6	LEU
2	P	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	21	ASN
1	I	453	GLN
2	O	68	ASN
1	H	146	GLN
1	H	457	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 56 ligands modelled in this entry, 28 are monoatomic - leaving 28 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	$\# Z  > 2$
3	ADP	D	600	5,4,6	24,29,29	0.98	2 (8%)	29,45,45	1.90	8 (27%)
3	ADP	G	600	5,4,6	24,29,29	1.15	2 (8%)	29,45,45	1.91	9 (31%)
5	BEF	K	602	3	0,3,3	0.00	-	-		
5	BEF	I	602	3	0,3,3	0.00	-	-		
3	ADP	L	600	5,4,6	24,29,29	1.02	1 (4%)	29,45,45	1.86	10 (34%)
5	BEF	C	602	3	0,3,3	0.00	-	-		
3	ADP	F	600	5,4,6	24,29,29	0.93	1 (4%)	29,45,45	1.86	5 (17%)
5	BEF	H	602	3	0,3,3	0.00	-	-		
5	BEF	M	602	3	0,3,3	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BEF	G	602	3	0,3,3	0.00	-	-		
5	BEF	E	602	3	0,3,3	0.00	-	-		
5	BEF	L	602	3	0,3,3	0.00	-	-		
3	ADP	I	600	5,4,6	24,29,29	0.91	1 (4%)	29,45,45	1.87	8 (27%)
5	BEF	D	602	3	0,3,3	0.00	-	-		
3	ADP	N	600	5,4,6	24,29,29	1.03	0	29,45,45	1.76	7 (24%)
5	BEF	B	602	3	0,3,3	0.00	-	-		
3	ADP	C	600	5,4,6	24,29,29	0.90	1 (4%)	29,45,45	1.80	6 (20%)
3	ADP	A	600	5,4,6	24,29,29	0.82	1 (4%)	29,45,45	1.88	8 (27%)
3	ADP	H	600	5,4,6	24,29,29	0.96	1 (4%)	29,45,45	1.93	11 (37%)
3	ADP	K	600	5,4,6	24,29,29	0.96	1 (4%)	29,45,45	1.81	8 (27%)
5	BEF	J	602	3	0,3,3	0.00	-	-		
5	BEF	F	602	3	0,3,3	0.00	-	-		
3	ADP	B	600	5,4,6	24,29,29	1.01	2 (8%)	29,45,45	2.06	10 (34%)
3	ADP	E	600	5,4,6	24,29,29	0.85	0	29,45,45	1.91	7 (24%)
3	ADP	J	600	5,4,6	24,29,29	0.93	1 (4%)	29,45,45	1.90	10 (34%)
3	ADP	M	600	5,4,6	24,29,29	0.95	1 (4%)	29,45,45	1.92	9 (31%)
5	BEF	A	602	3	0,3,3	0.00	-	-		
5	BEF	N	602	3	0,3,3	0.00	-	-		

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
3	ADP	D	600	5,4,6	-	7/12/32/32	0/3/3/3
3	ADP	G	600	5,4,6	-	7/12/32/32	0/3/3/3
3	ADP	B	600	5,4,6	-	7/12/32/32	0/3/3/3
3	ADP	E	600	5,4,6	-	7/12/32/32	0/3/3/3
3	ADP	C	600	5,4,6	-	6/12/32/32	0/3/3/3
3	ADP	A	600	5,4,6	-	7/12/32/32	0/3/3/3
3	ADP	L	600	5,4,6	-	7/12/32/32	0/3/3/3
3	ADP	J	600	5,4,6	-	6/12/32/32	0/3/3/3
3	ADP	M	600	5,4,6	-	7/12/32/32	0/3/3/3
3	ADP	H	600	5,4,6	-	6/12/32/32	0/3/3/3
3	ADP	K	600	5,4,6	-	6/12/32/32	0/3/3/3
3	ADP	F	600	5,4,6	-	7/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	I	600	5,4,6	-	7/12/32/32	0/3/3/3
3	ADP	N	600	5,4,6	-	7/12/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	600	ADP	C2'-C1'	-3.14	1.49	1.53
3	L	600	ADP	C2'-C1'	-3.10	1.49	1.53
3	K	600	ADP	C2'-C1'	-2.72	1.49	1.53
3	M	600	ADP	C2'-C1'	-2.68	1.49	1.53
3	J	600	ADP	C2'-C1'	-2.58	1.49	1.53

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	600	ADP	C1'-N9-C4	-5.05	117.77	126.64
3	B	600	ADP	N3-C2-N1	-5.00	120.86	128.68
3	F	600	ADP	C1'-N9-C4	-4.72	118.36	126.64
3	M	600	ADP	C1'-N9-C4	-4.66	118.45	126.64
3	L	600	ADP	N3-C2-N1	-4.63	121.44	128.68

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	600	ADP	C5'-O5'-PA-O1A
3	D	600	ADP	C5'-O5'-PA-O2A
3	G	600	ADP	C5'-O5'-PA-O1A
3	G	600	ADP	C5'-O5'-PA-O2A
3	L	600	ADP	PA-O3A-PB-O2B

There are no ring outliers.

28 monomers are involved in 19 short contacts:

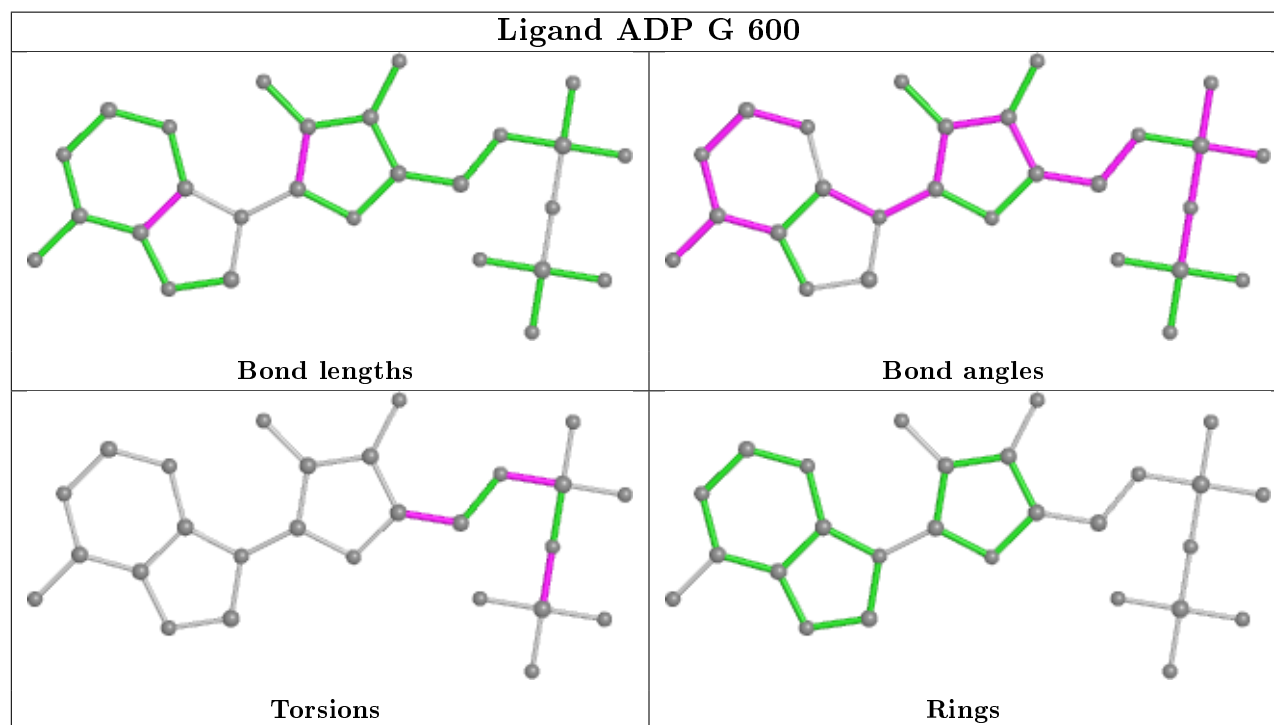
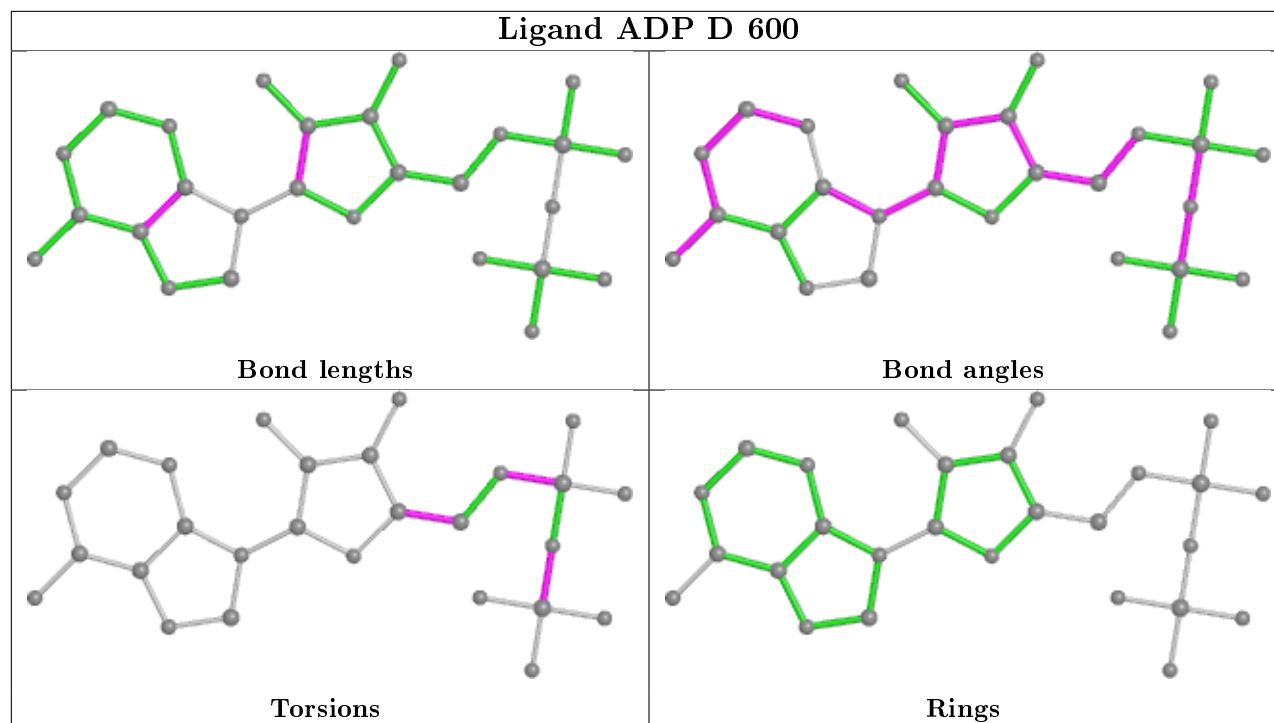
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	600	ADP	1	0
3	G	600	ADP	1	0
5	K	602	BEF	1	0
5	I	602	BEF	1	0
3	L	600	ADP	1	0

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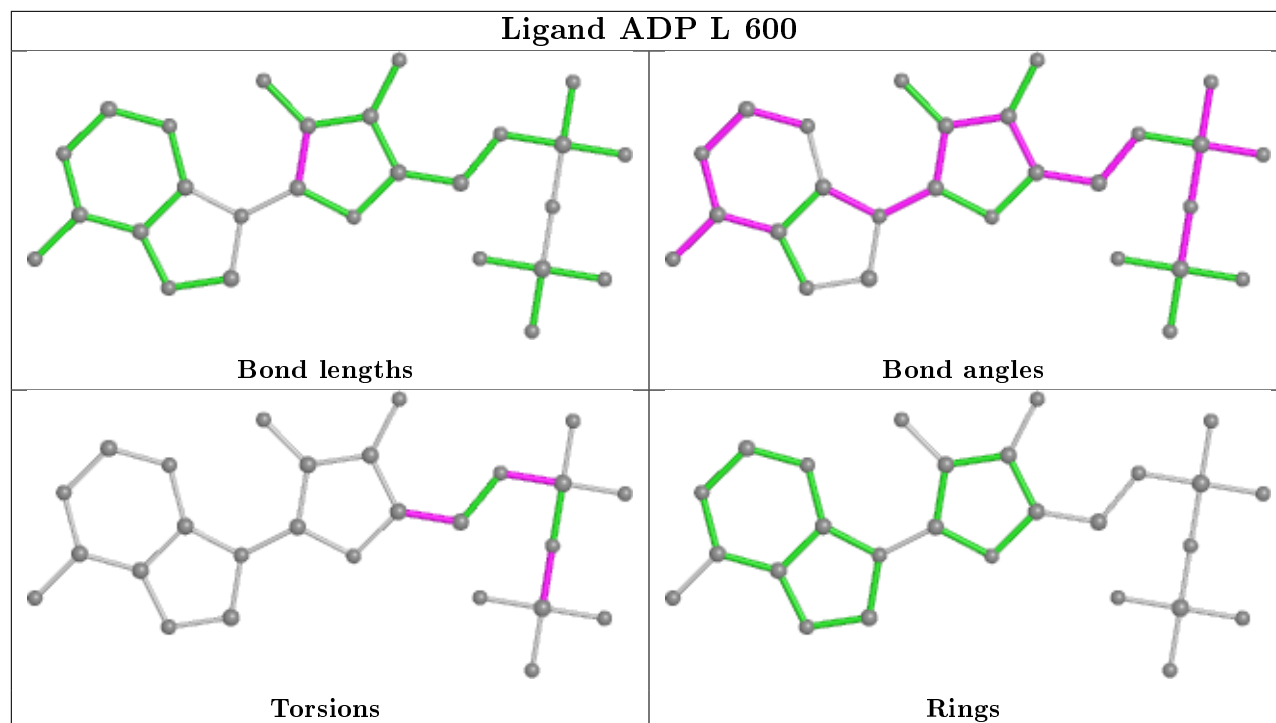
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	602	BEF	1	0
3	F	600	ADP	2	0
5	H	602	BEF	1	0
5	M	602	BEF	1	0
5	G	602	BEF	1	0
5	E	602	BEF	1	0
5	L	602	BEF	1	0
3	I	600	ADP	2	0
5	D	602	BEF	1	0
3	N	600	ADP	1	0
5	B	602	BEF	1	0
3	C	600	ADP	1	0
3	A	600	ADP	1	0
3	H	600	ADP	1	0
3	K	600	ADP	1	0
5	J	602	BEF	1	0
5	F	602	BEF	1	0
3	B	600	ADP	3	0
3	E	600	ADP	1	0
3	J	600	ADP	2	0
3	M	600	ADP	1	0
5	A	602	BEF	1	0
5	N	602	BEF	1	0

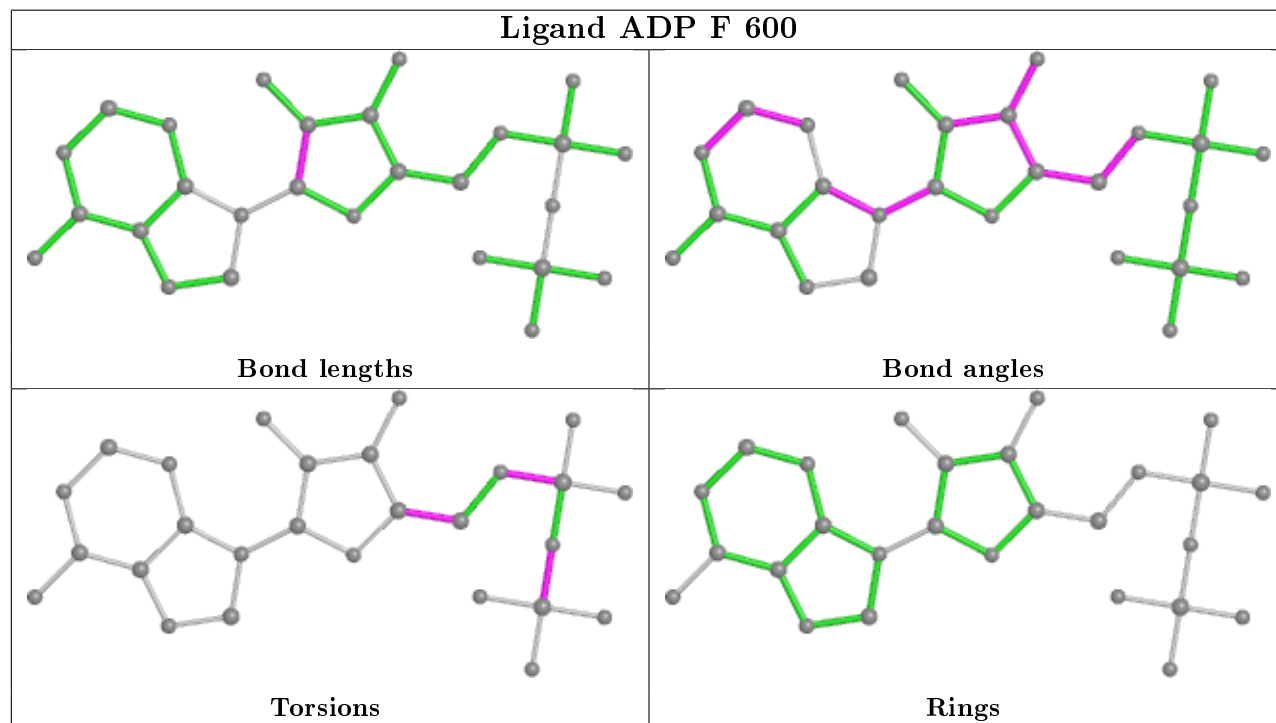
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



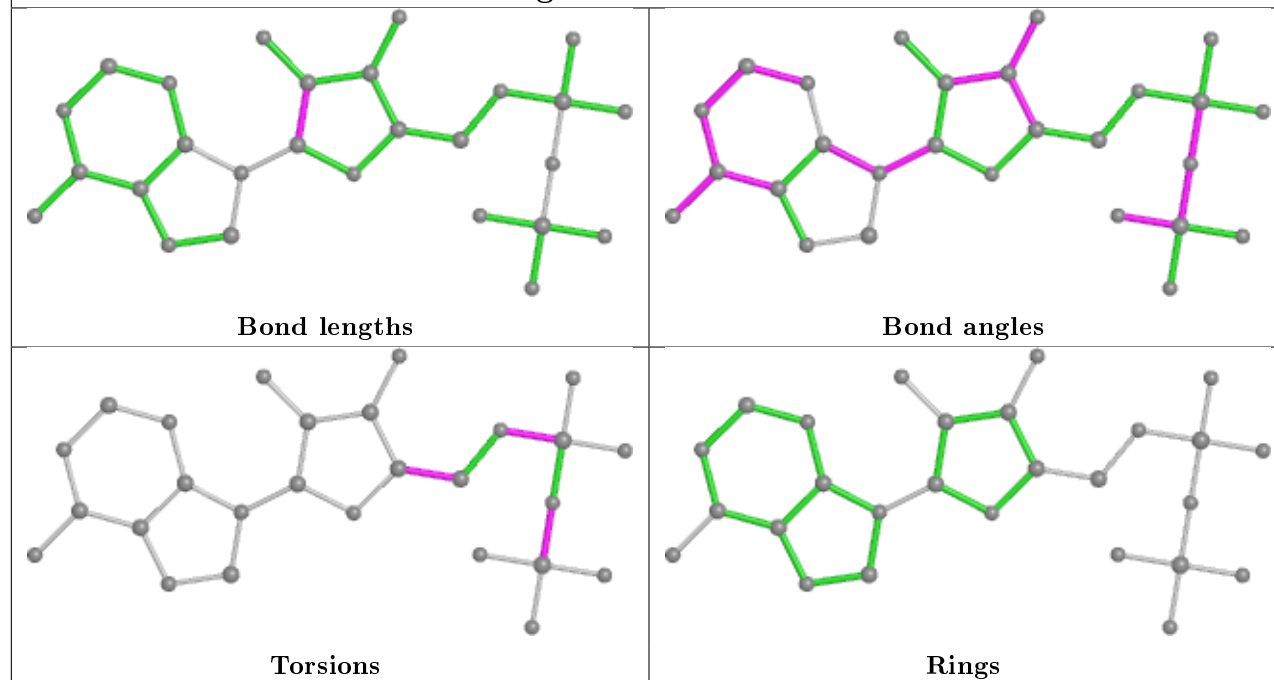
## Ligand ADP L 600



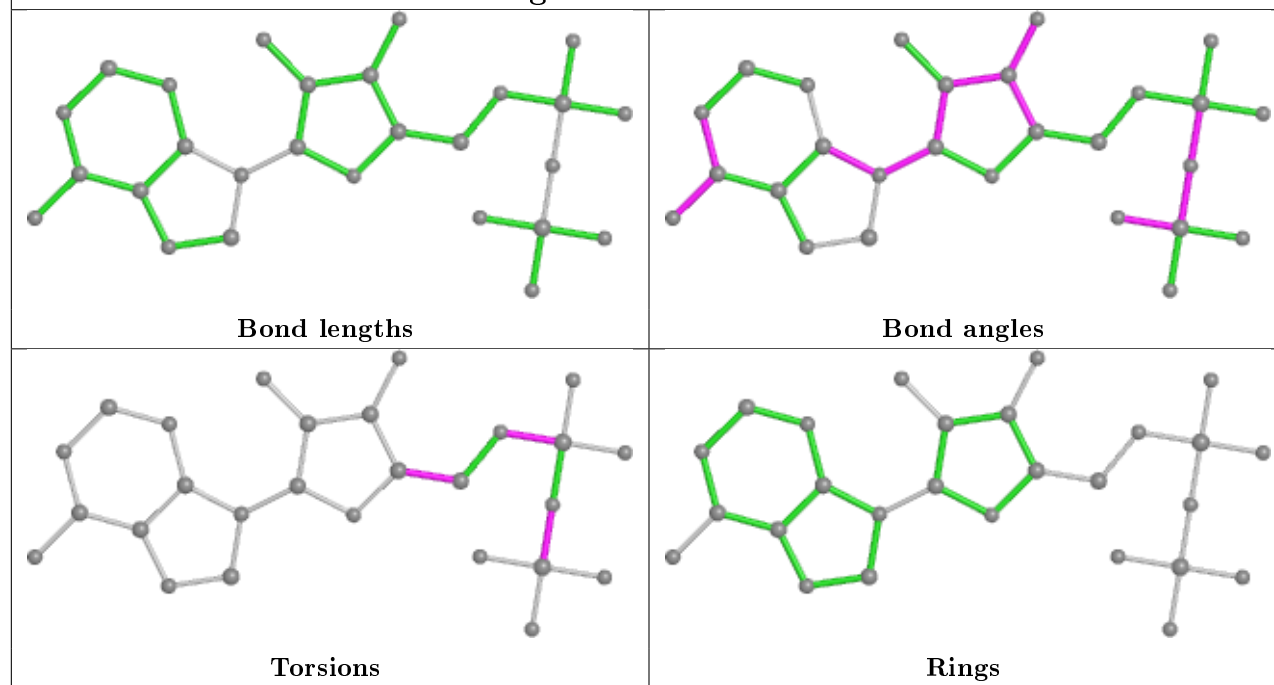
## Ligand ADP F 600



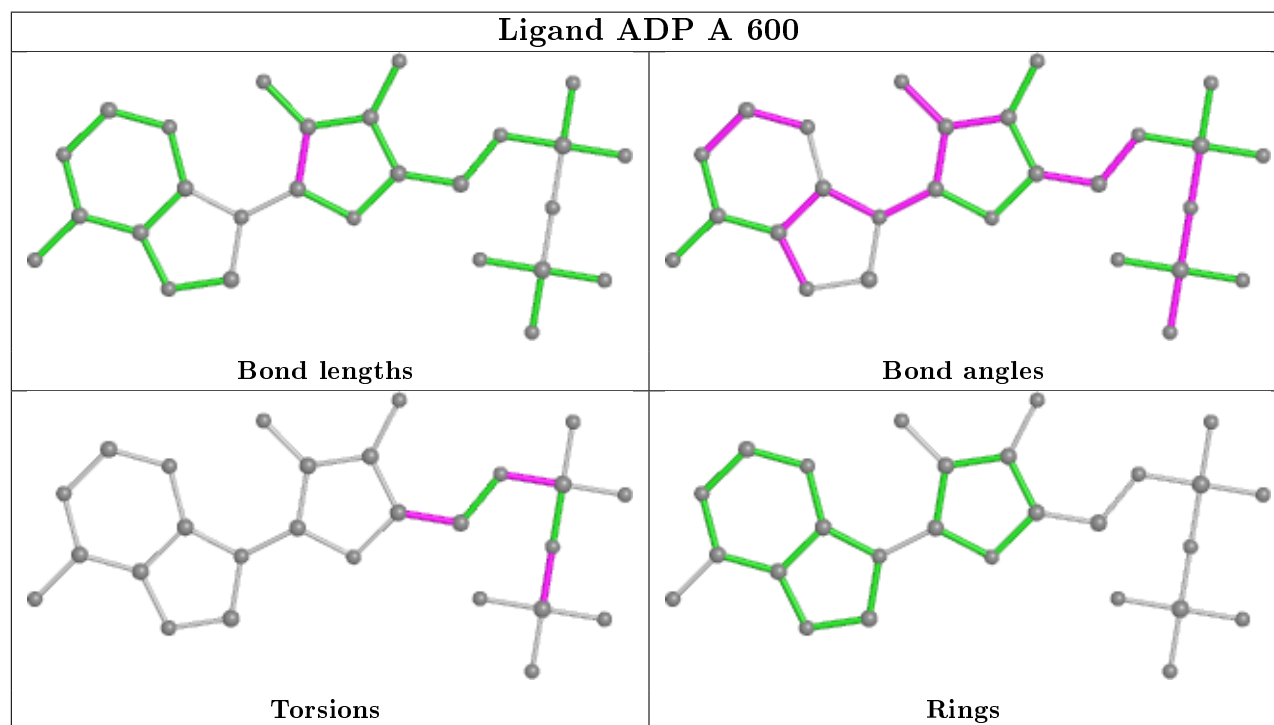
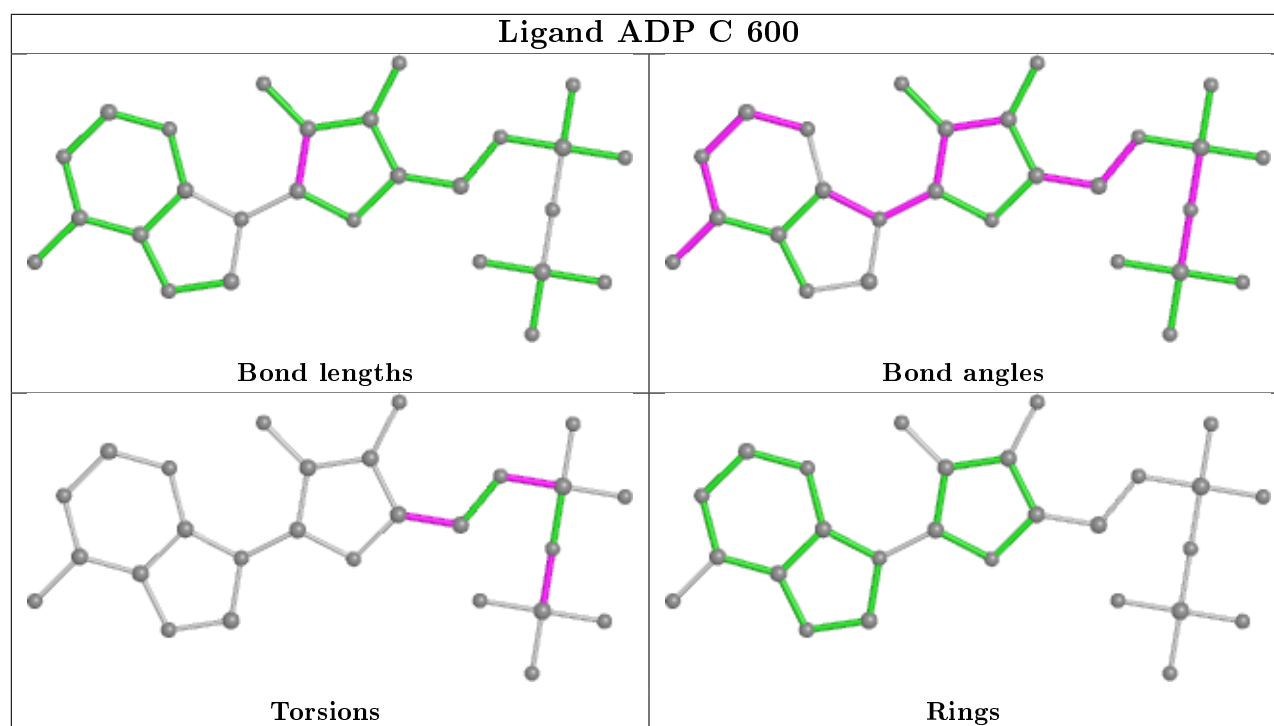
## Ligand ADP I 600

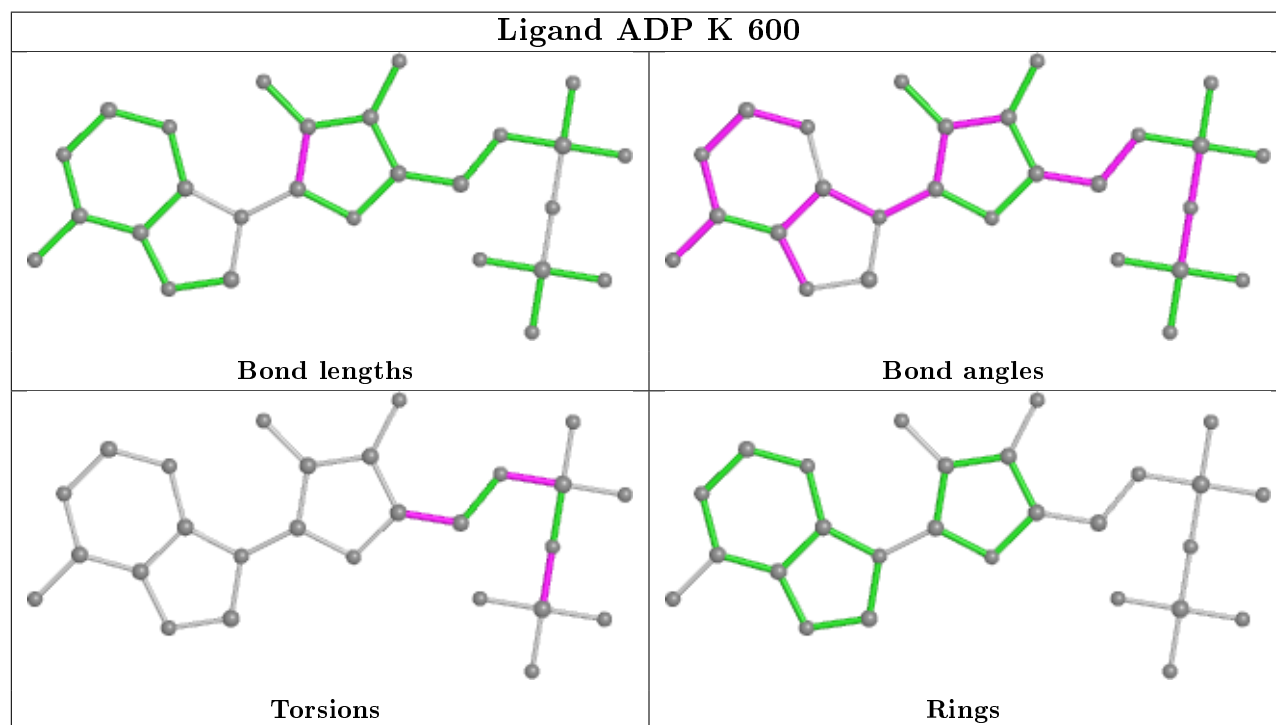
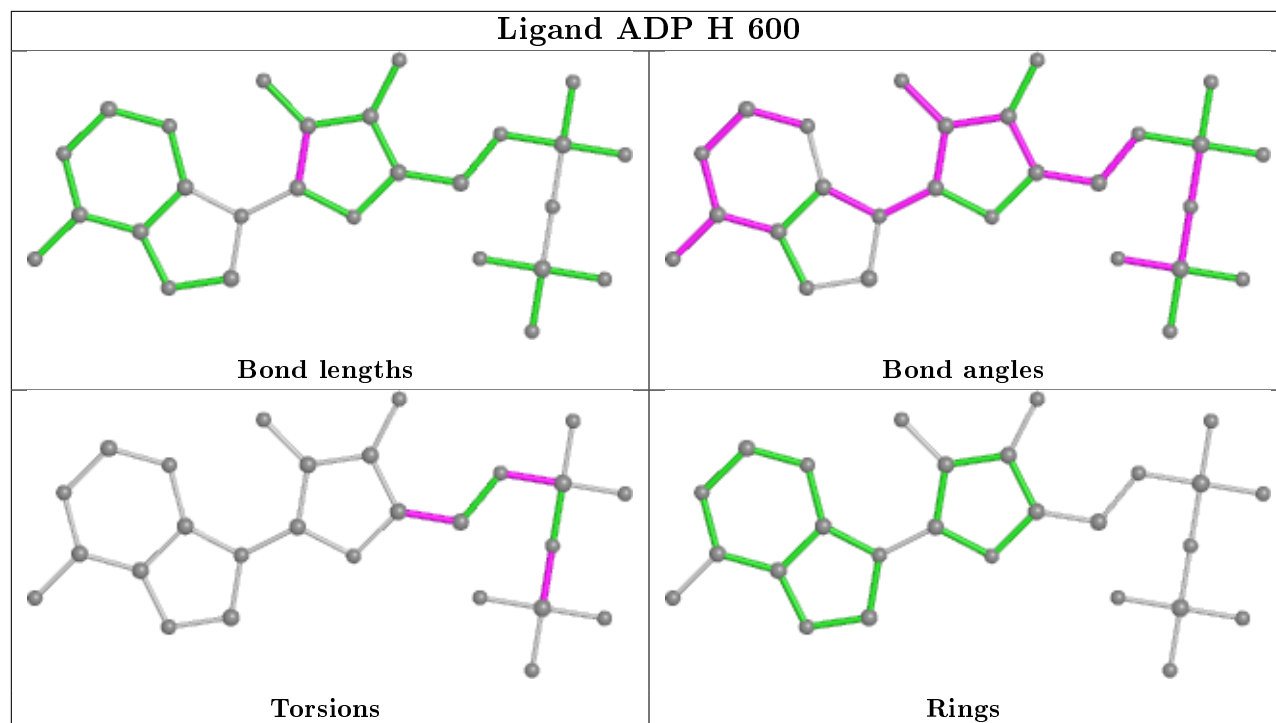


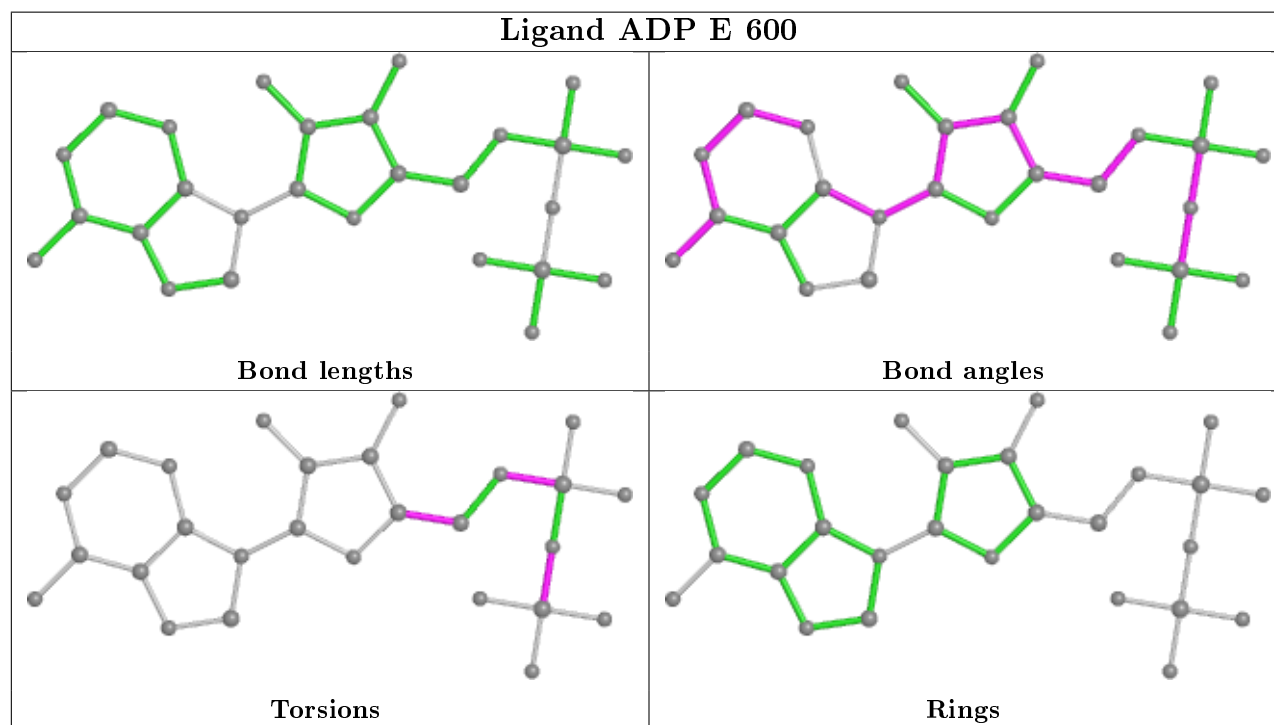
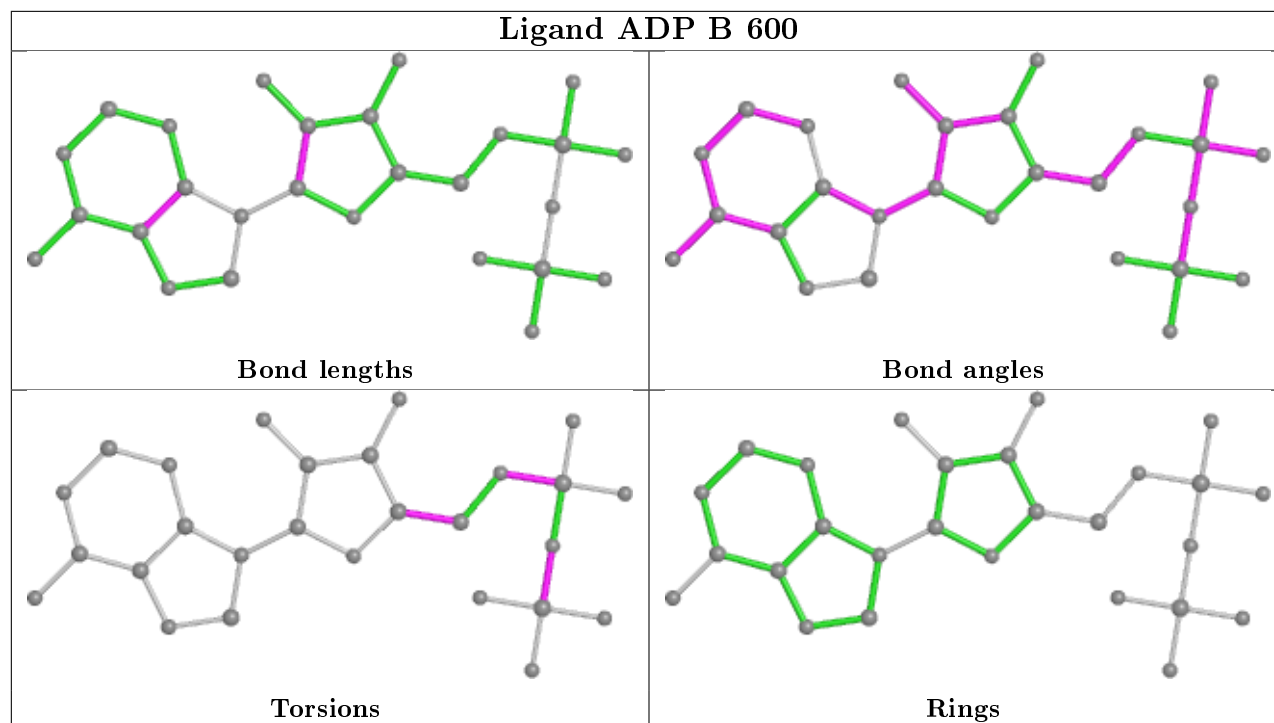
## Ligand ADP N 600

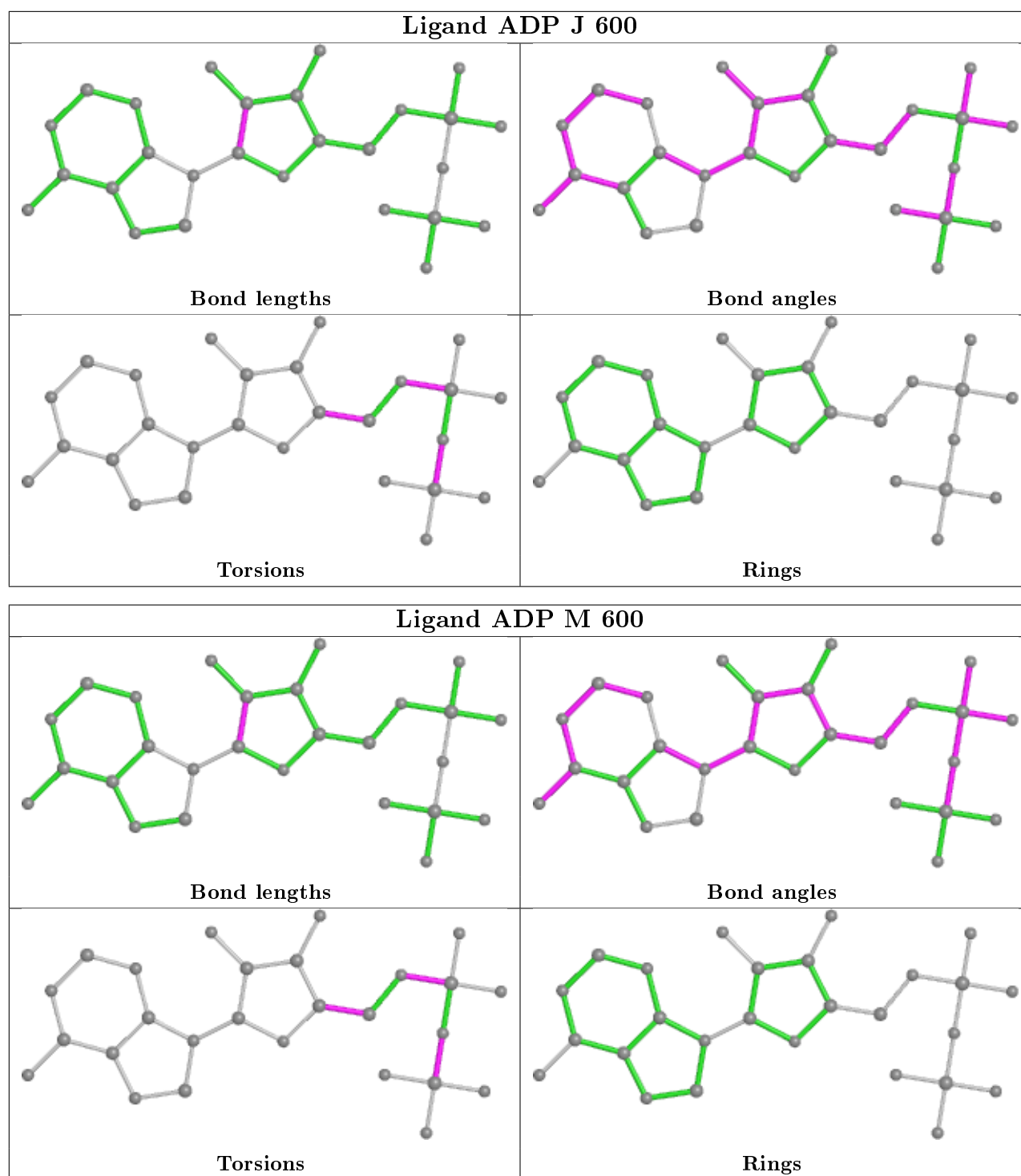












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	520/548 (94%)	-0.03	4 (0%) 86 76	59, 109, 191, 228	0
1	B	520/548 (94%)	-0.01	7 (1%) 77 64	61, 107, 198, 222	0
1	C	520/548 (94%)	0.05	4 (0%) 86 76	74, 124, 231, 257	0
1	D	520/548 (94%)	0.10	18 (3%) 44 29	76, 133, 234, 259	0
1	E	520/548 (94%)	0.04	10 (1%) 66 52	60, 116, 203, 258	0
1	F	520/548 (94%)	0.05	12 (2%) 60 44	58, 109, 188, 213	0
1	G	520/548 (94%)	-0.03	6 (1%) 79 66	58, 113, 206, 228	0
1	H	520/548 (94%)	-0.02	8 (1%) 73 60	55, 109, 200, 241	0
1	I	520/548 (94%)	0.06	11 (2%) 63 48	60, 107, 191, 212	0
1	J	520/548 (94%)	0.03	7 (1%) 77 64	63, 118, 192, 222	0
1	K	520/548 (94%)	0.06	12 (2%) 60 44	74, 134, 201, 239	0
1	L	520/548 (94%)	0.04	12 (2%) 60 44	73, 121, 222, 270	0
1	M	520/548 (94%)	0.01	3 (0%) 89 81	61, 108, 195, 220	0
1	N	520/548 (94%)	-0.08	3 (0%) 89 81	56, 100, 182, 226	0
2	1	92/97 (94%)	1.28	22 (23%) 0 0	133, 170, 220, 238	0
2	2	92/97 (94%)	0.71	10 (10%) 5 3	132, 170, 212, 237	0
2	O	93/97 (95%)	1.02	19 (20%) 1 0	158, 178, 241, 293	0
2	P	94/97 (96%)	1.48	29 (30%) 0 0	173, 194, 233, 243	0
2	Q	90/97 (92%)	1.35	23 (25%) 0 0	162, 200, 235, 253	0
2	R	92/97 (94%)	1.32	24 (26%) 0 0	198, 220, 246, 257	0
2	S	92/97 (94%)	1.29	17 (18%) 1 0	167, 205, 227, 249	0
2	T	92/97 (94%)	1.04	10 (10%) 5 3	162, 189, 224, 234	0
2	U	92/97 (94%)	0.99	12 (13%) 3 2	162, 186, 222, 232	0
2	V	93/97 (95%)	0.66	11 (11%) 4 3	139, 180, 219, 239	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	W	93/97 (95%)	1.01	11 (11%) 4 3	148, 170, 206, 214	0
2	X	92/97 (94%)	1.18	19 (20%) 1 0	163, 180, 216, 235	0
2	Y	92/97 (94%)	0.74	8 (8%) 10 6	128, 160, 220, 248	0
2	Z	92/97 (94%)	0.75	7 (7%) 13 8	124, 154, 200, 231	0
All	All	8571/9030 (94%)	0.18	339 (3%) 38 25	55, 130, 214, 293	0

The worst 5 of 339 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	32	ALA	6.5
2	W	32	ALA	5.4
2	S	51	ASN	5.1
2	Q	85	ILE	5.1
2	P	64	ILE	4.9

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	K	K	603	1/1	0.89	0.17	87,87,87,87	0
5	BEF	G	602	4/4	0.93	0.18	68,69,70,73	0
5	BEF	D	602	4/4	0.93	0.19	106,106,107,107	0
6	K	G	603	1/1	0.93	0.16	69,69,69,69	0
3	ADP	K	600	27/27	0.94	0.20	89,93,98,99	0
6	K	D	603	1/1	0.94	0.14	89,89,89,89	0
3	ADP	N	600	27/27	0.95	0.21	62,68,72,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	A	600	27/27	0.95	0.20	69,77,84,88	0
5	BEF	E	602	4/4	0.95	0.12	96,96,97,98	0
5	BEF	L	602	4/4	0.95	0.20	91,92,92,95	0
5	BEF	F	602	4/4	0.95	0.19	84,88,90,91	0
3	ADP	E	600	27/27	0.95	0.20	83,87,94,96	0
5	BEF	C	602	4/4	0.95	0.18	101,103,103,107	0
3	ADP	D	600	27/27	0.95	0.20	88,95,103,106	0
3	ADP	L	600	27/27	0.96	0.20	81,86,91,93	0
3	ADP	H	600	27/27	0.96	0.20	64,70,75,77	0
3	ADP	F	600	27/27	0.96	0.21	73,77,84,86	0
6	K	L	603	1/1	0.96	0.23	80,80,80,80	0
3	ADP	I	600	27/27	0.96	0.20	70,74,82,86	0
3	ADP	B	600	27/27	0.96	0.20	63,73,79,81	0
3	ADP	G	600	27/27	0.96	0.18	64,69,75,78	0
3	ADP	J	600	27/27	0.96	0.20	83,88,93,96	0
3	ADP	M	600	27/27	0.96	0.21	65,69,74,75	0
6	K	M	603	1/1	0.96	0.17	86,86,86,86	0
3	ADP	C	600	27/27	0.96	0.21	82,86,91,95	0
6	K	N	603	1/1	0.97	0.12	83,83,83,83	0
6	K	E	603	1/1	0.97	0.07	91,91,91,91	0
6	K	I	603	1/1	0.97	0.12	67,67,67,67	0
6	K	C	603	1/1	0.97	0.22	81,81,81,81	0
5	BEF	M	602	4/4	0.97	0.19	75,78,79,81	0
5	BEF	N	602	4/4	0.97	0.15	74,78,79,79	0
5	BEF	H	602	4/4	0.97	0.16	82,85,86,87	0
5	BEF	A	602	4/4	0.98	0.15	78,79,79,81	0
6	K	J	603	1/1	0.98	0.08	97,97,97,97	0
5	BEF	J	602	4/4	0.98	0.13	81,82,83,84	0
6	K	B	603	1/1	0.98	0.12	84,84,84,84	0
4	MG	J	601	1/1	0.98	0.14	52,52,52,52	0
6	K	H	603	1/1	0.98	0.15	69,69,69,69	0
5	BEF	I	602	4/4	0.98	0.17	76,80,80,83	0
6	K	A	603	1/1	0.98	0.12	94,94,94,94	0
4	MG	B	601	1/1	0.99	0.23	48,48,48,48	0
4	MG	E	601	1/1	0.99	0.13	62,62,62,62	0
4	MG	A	601	1/1	0.99	0.16	59,59,59,59	0
5	BEF	B	602	4/4	0.99	0.18	85,89,90,91	0
4	MG	C	601	1/1	0.99	0.21	57,57,57,57	0
4	MG	I	601	1/1	0.99	0.21	52,52,52,52	0
5	BEF	K	602	4/4	0.99	0.18	80,83,83,85	0
4	MG	K	601	1/1	0.99	0.24	68,68,68,68	0
4	MG	G	601	1/1	0.99	0.21	57,57,57,57	0

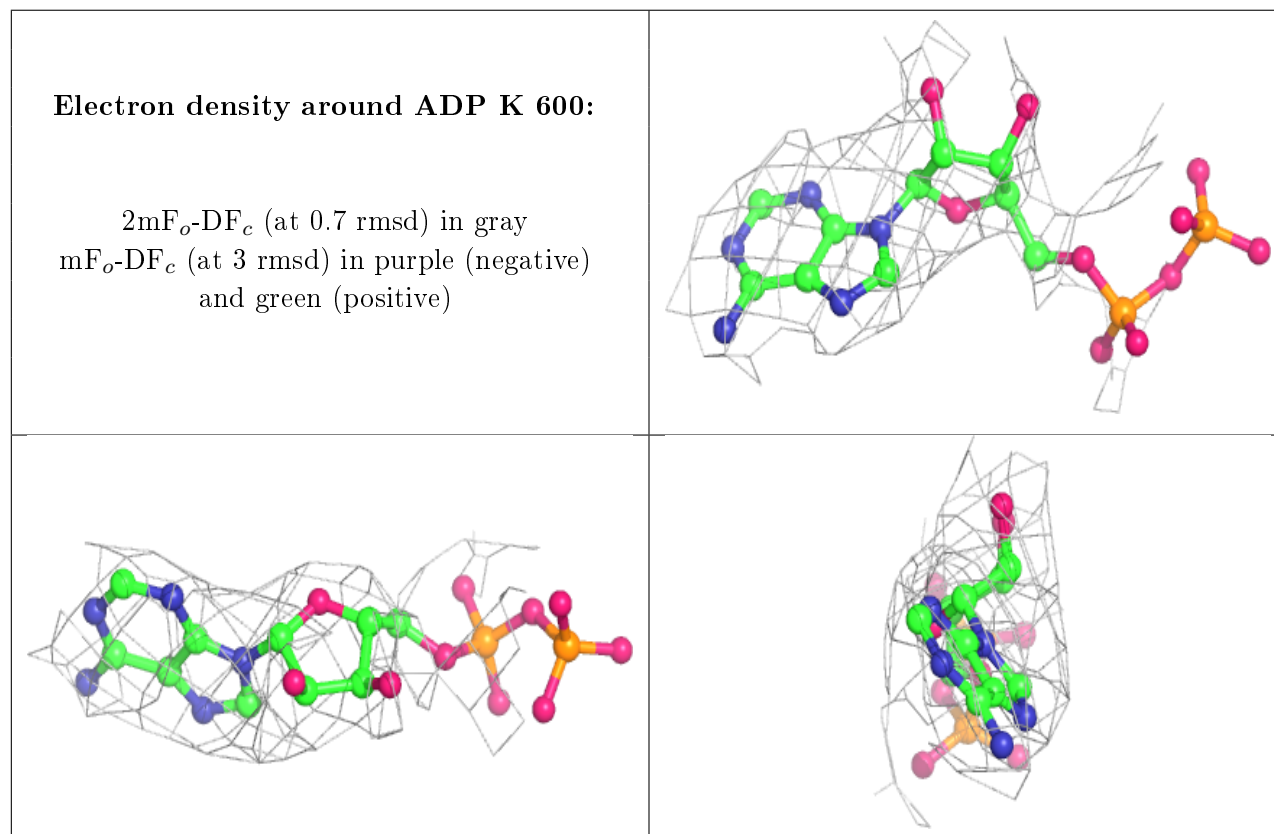
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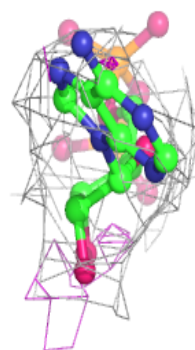
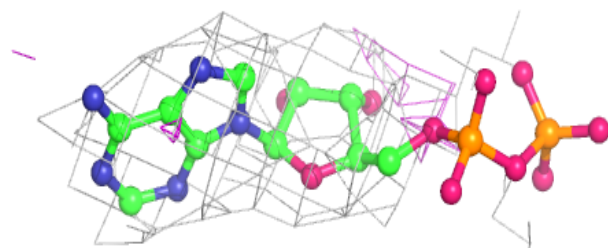
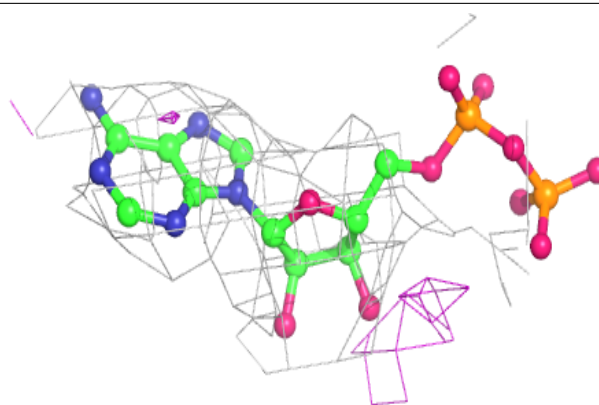
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	K	F	603	1/1	0.99	0.14	80,80,80,80	0
4	MG	D	601	1/1	0.99	0.20	78,78,78,78	0
4	MG	M	601	1/1	0.99	0.21	52,52,52,52	0
4	MG	F	601	1/1	0.99	0.20	59,59,59,59	0
4	MG	N	601	1/1	0.99	0.19	46,46,46,46	0
4	MG	H	601	1/1	0.99	0.21	47,47,47,47	0
4	MG	L	601	1/1	0.99	0.19	56,56,56,56	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.

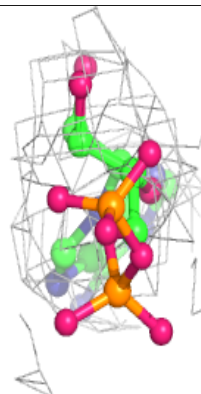
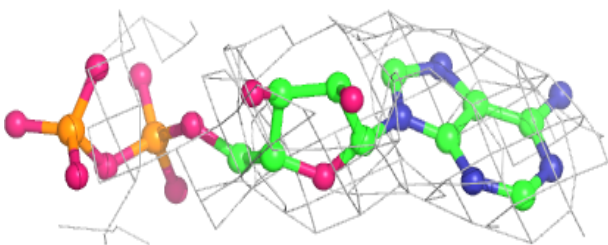
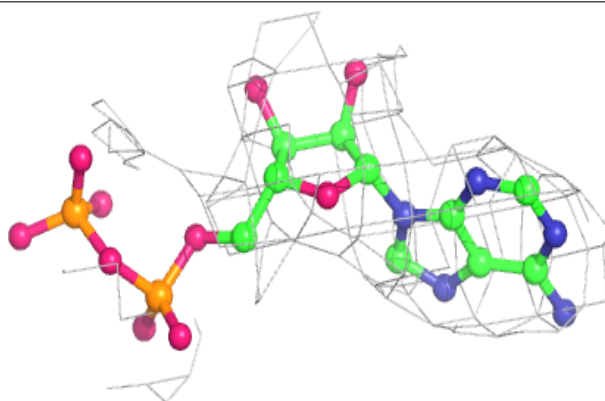


**Electron density around ADP N 600:**

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

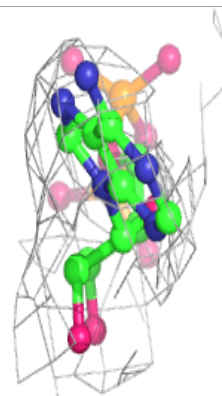
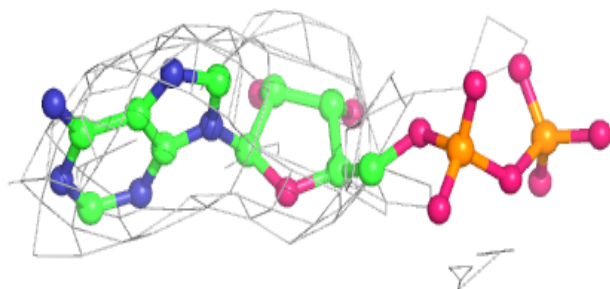
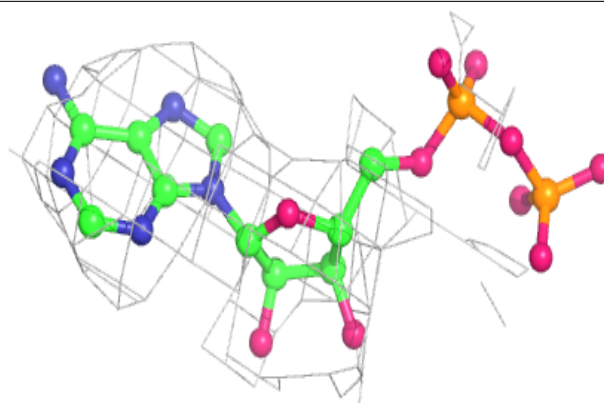
**Electron density around ADP A 600:**

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and green (positive)

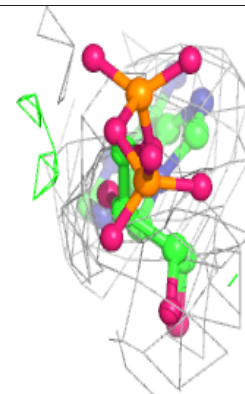
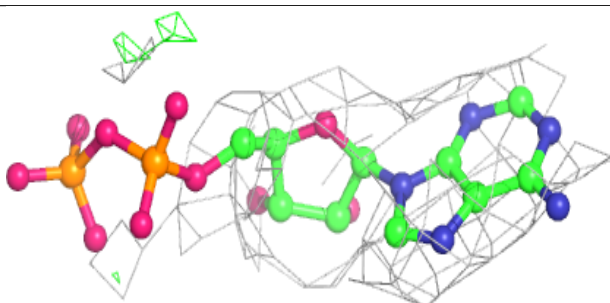
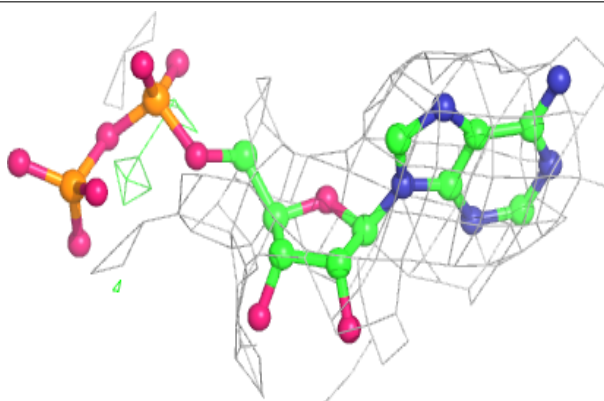


**Electron density around ADP E 600:**

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

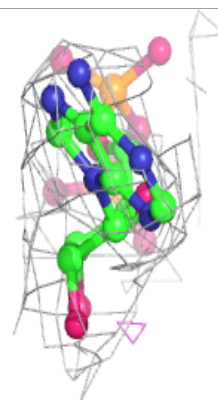
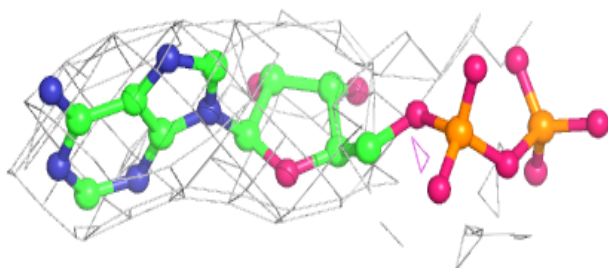
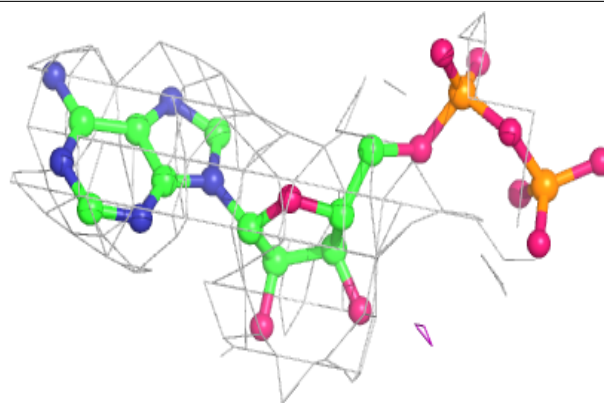
**Electron density around ADP D 600:**

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

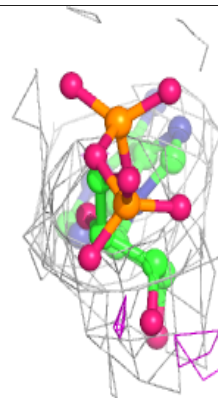
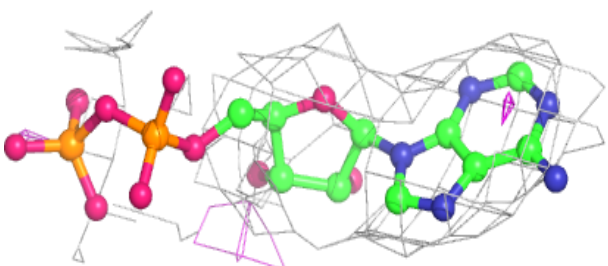
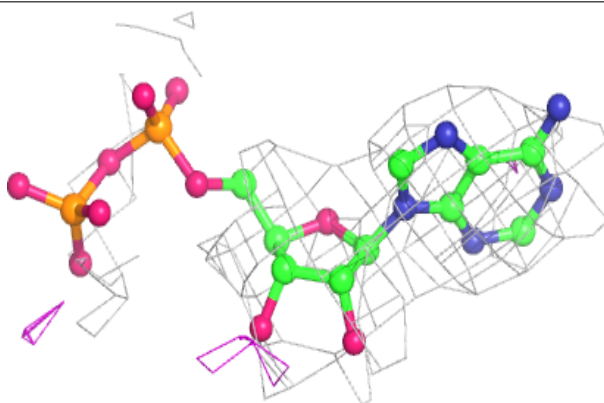


**Electron density around ADP L 600:**

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

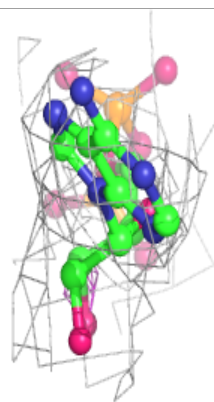
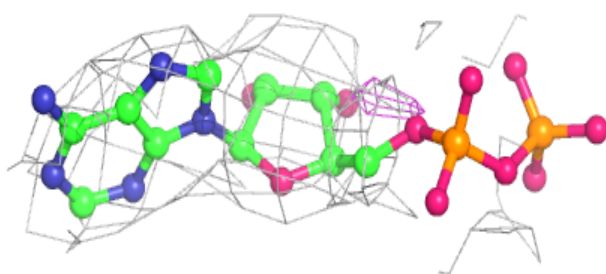
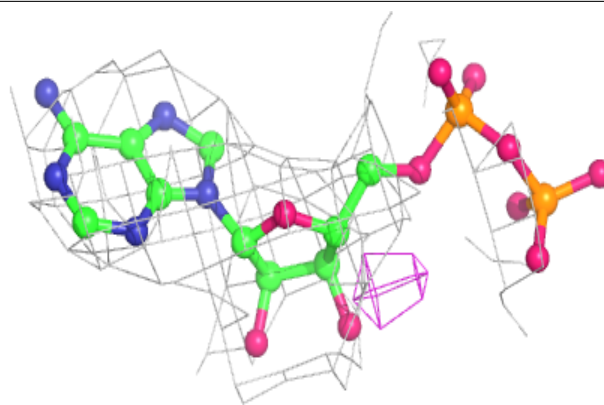
**Electron density around ADP H 600:**

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

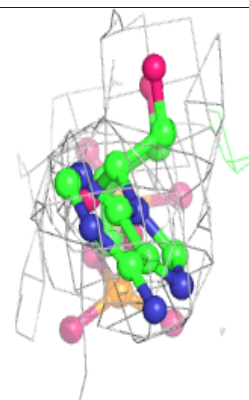
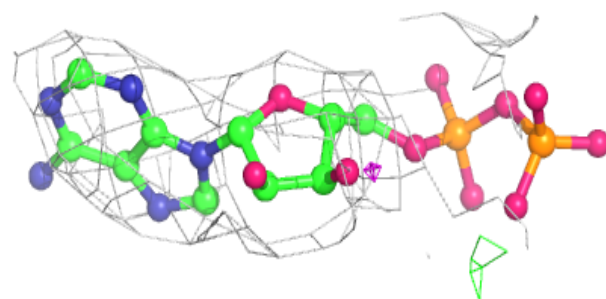
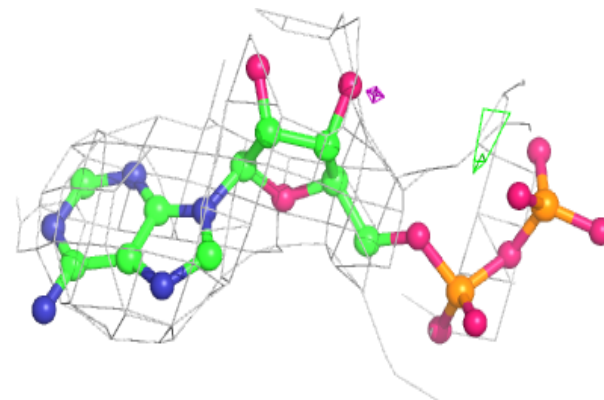


**Electron density around ADP F 600:**

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

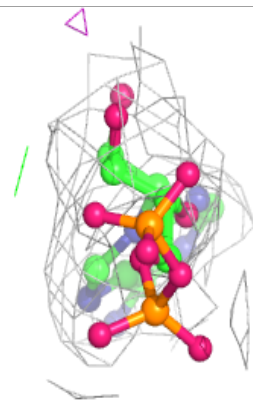
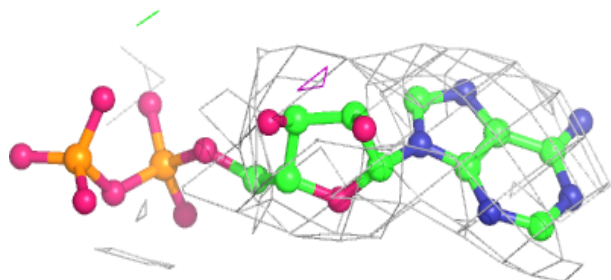
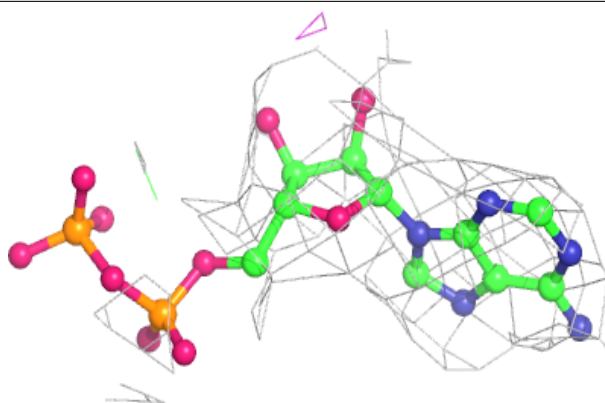
**Electron density around ADP I 600:**

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

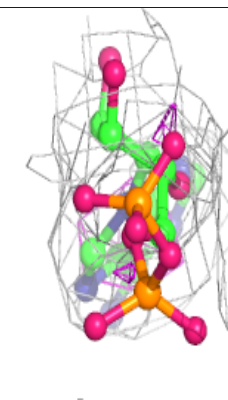
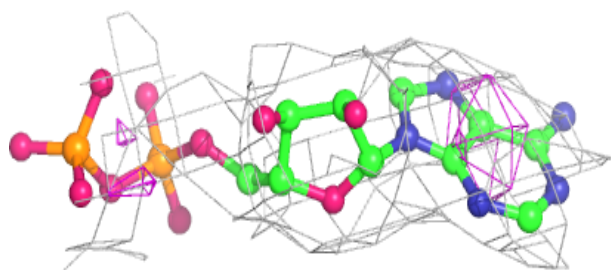
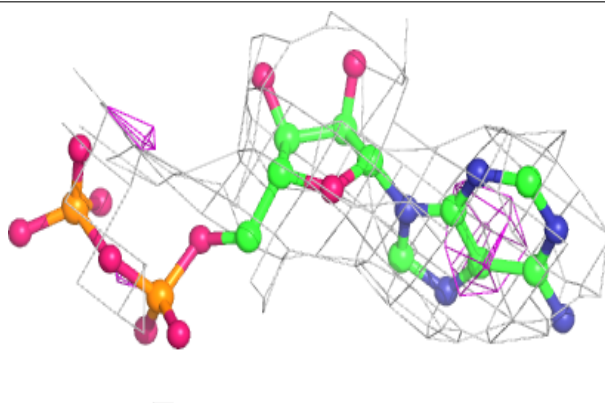


**Electron density around ADP B 600:**

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

**Electron density around ADP G 600:**

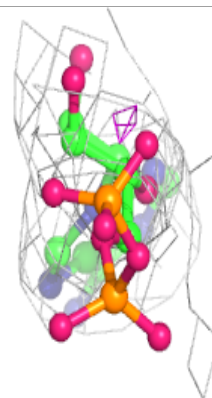
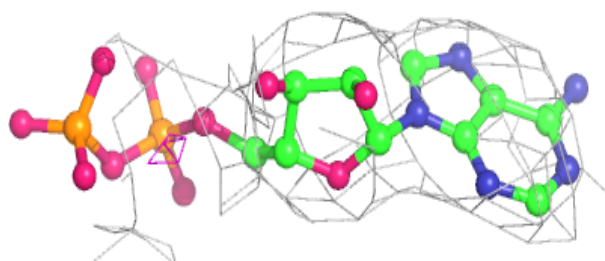
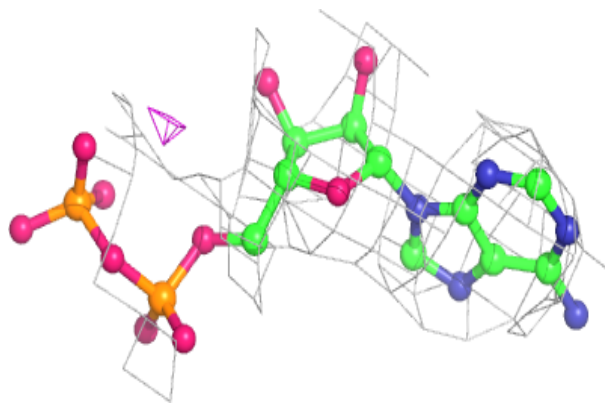
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



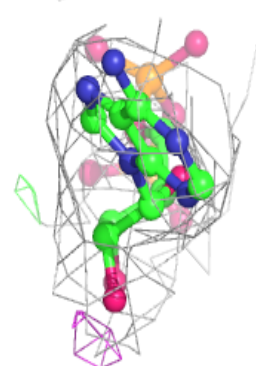
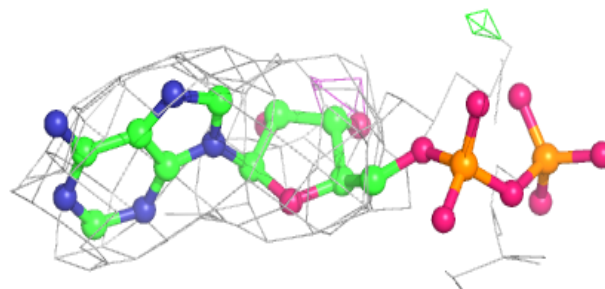
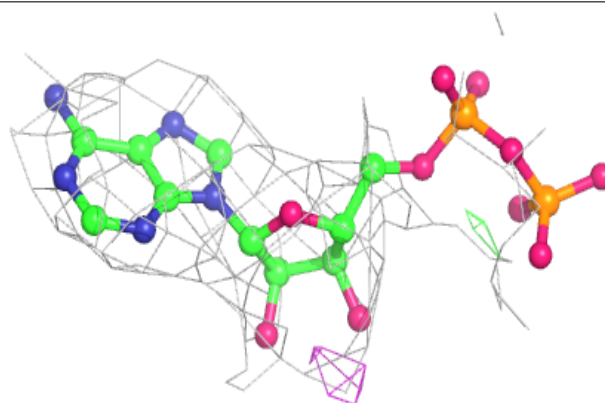


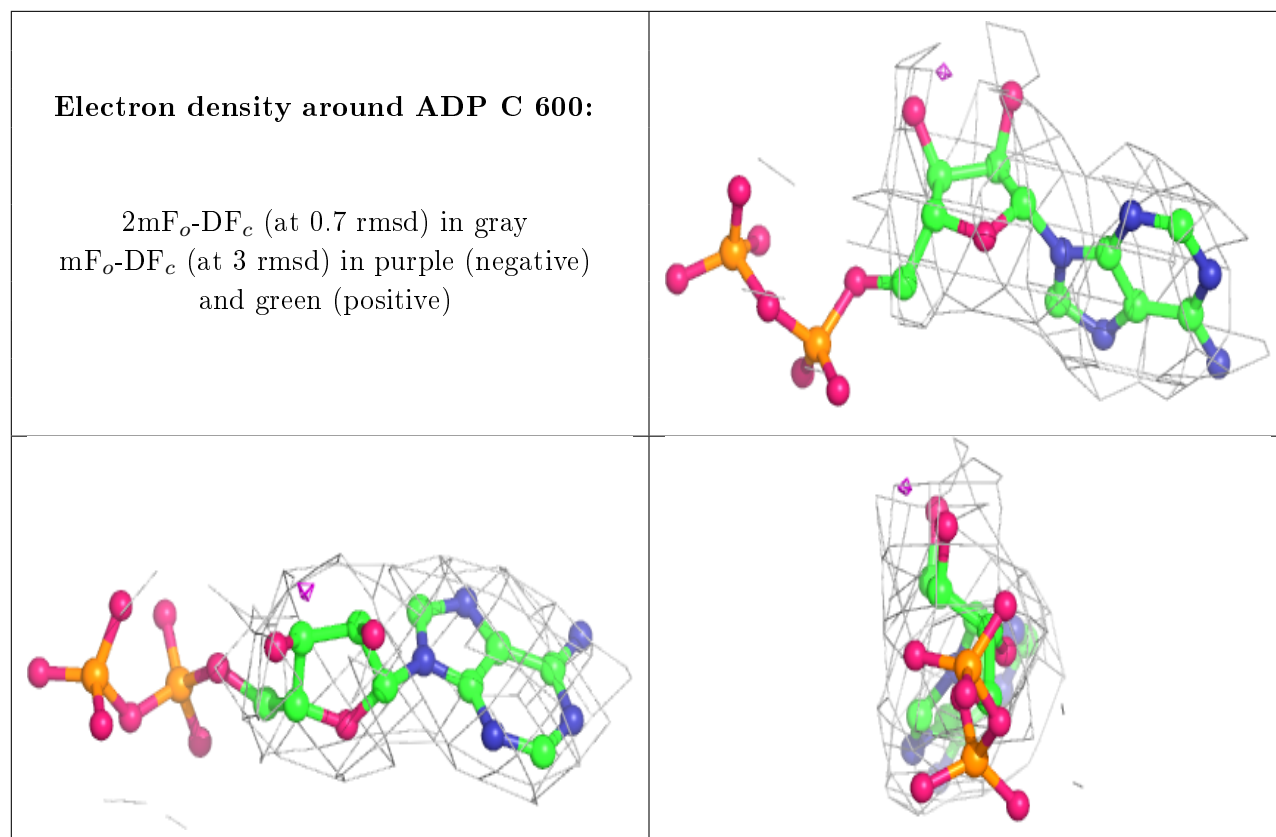
**Electron density around ADP J 600:**

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

**Electron density around ADP 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.