



wwPDB X-ray Structure Validation Summary Report

Mar 12, 2026 – 07:18 PM UTC

PDB ID : 6HT7 / pdb_00006ht7
Title : Crystal structure of the WT human mitochondrial chaperonin (ADP:BeF3)14 complex
Authors : Jebara, F.; Patra, M.; Azem, A.; Hirsch, J.
Deposited on : 2018-10-03
Resolution : 3.70 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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

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

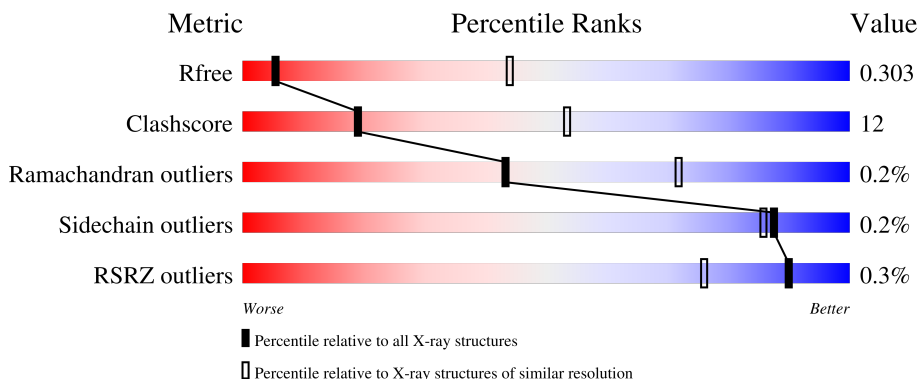
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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


























Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	549	73% (green), 23% (yellow), . (grey)
1	B	549	70% (green), 26% (yellow), . (grey)
1	C	549	75% (green), 21% (yellow), . (grey)
1	D	549	72% (green), 24% (yellow), . . (grey)
1	E	549	72% (green), 23% (yellow), . . (grey)

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Mol	Chain	Length	Quality of chain
1	F	549	 70% 26% ..
1	G	549	 72% 24% .
1	H	549	 % 70% 26% .
1	I	549	 68% 28% ..
1	J	549	 68% 28% .
1	K	549	 73% 23% .
1	L	549	 71% 24% ..
1	M	549	 % 70% 25% ..
1	N	549	 74% 22% .
2	1	102	 76% 21% ..
2	2	102	 75% 23% .
2	O	102	 77% 21% .
2	P	102	 69% 29% .
2	Q	102	 73% 25% .
2	R	102	 72% 26% .
2	S	102	 75% 24% .
2	T	102	 71% 27% .
2	U	102	 69% 29% .
2	V	102	 79% 19% .
2	W	102	 75% 23% .
2	X	102	 76% 22% .
2	Y	102	 72% 26% .
2	Z	102	 75% 24% .

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
4	BEF	B	602	-	-	X	-
4	BEF	C	602	-	-	X	-
4	BEF	D	602	-	-	X	-
4	BEF	E	602	-	-	X	-
4	BEF	F	602	-	-	X	-
4	BEF	G	602	-	-	X	-
4	BEF	H	602	-	-	X	-
4	BEF	I	602	-	-	X	-
4	BEF	J	602	-	-	X	-
4	BEF	L	602	-	-	X	-
4	BEF	N	602	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 134311 atoms, of which 68273 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 heat shock protein, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	J	528	8037	2465	4105	672	781	14	0	0	0
1	I	528	8030	2465	4098	672	781	14	0	0	0
1	H	528	8035	2465	4103	672	781	14	0	0	0
1	N	528	8035	2465	4103	672	781	14	0	0	0
1	M	528	8037	2465	4105	672	781	14	0	0	0
1	L	528	8012	2465	4080	672	781	14	0	0	0
1	K	528	8032	2465	4100	672	781	14	0	0	0
1	G	528	8036	2465	4104	672	781	14	0	0	0
1	F	528	8037	2465	4105	672	781	14	0	0	0
1	E	528	8037	2465	4105	672	781	14	0	0	0
1	D	528	8034	2465	4102	672	781	14	0	0	0
1	C	528	8035	2465	4103	672	781	14	0	0	0
1	B	528	8037	2465	4105	672	781	14	0	0	0
1	A	528	8037	2465	4105	672	781	14	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	GLY	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
J	2	SER	-	expression tag	UNP P10809
I	1	GLY	-	expression tag	UNP P10809
I	2	SER	-	expression tag	UNP P10809
H	1	GLY	-	expression tag	UNP P10809
H	2	SER	-	expression tag	UNP P10809
N	1	GLY	-	expression tag	UNP P10809
N	2	SER	-	expression tag	UNP P10809
M	1	GLY	-	expression tag	UNP P10809
M	2	SER	-	expression tag	UNP P10809
L	1	GLY	-	expression tag	UNP P10809
L	2	SER	-	expression tag	UNP P10809
K	1	GLY	-	expression tag	UNP P10809
K	2	SER	-	expression tag	UNP P10809
G	1	GLY	-	expression tag	UNP P10809
G	2	SER	-	expression tag	UNP P10809
F	1	GLY	-	expression tag	UNP P10809
F	2	SER	-	expression tag	UNP P10809
E	1	GLY	-	expression tag	UNP P10809
E	2	SER	-	expression tag	UNP P10809
D	1	GLY	-	expression tag	UNP P10809
D	2	SER	-	expression tag	UNP P10809
C	1	GLY	-	expression tag	UNP P10809
C	2	SER	-	expression tag	UNP P10809
B	1	GLY	-	expression tag	UNP P10809
B	2	SER	-	expression tag	UNP P10809
A	1	GLY	-	expression tag	UNP P10809
A	2	SER	-	expression tag	UNP P10809

- Molecule 2 is a protein called 10 kDa heat shock protein, mitochondrial.

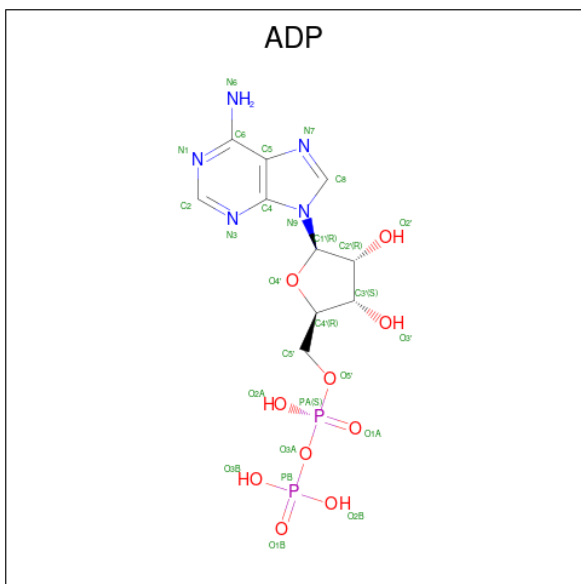
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	X	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	W	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	V	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	2	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	1	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	Z	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	Y	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	U	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	T	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	S	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	R	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	Q	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	P	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			
2	O	100	Total	C	H	N	O	S	0	0	0
			1527	483	775	126	142	1			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



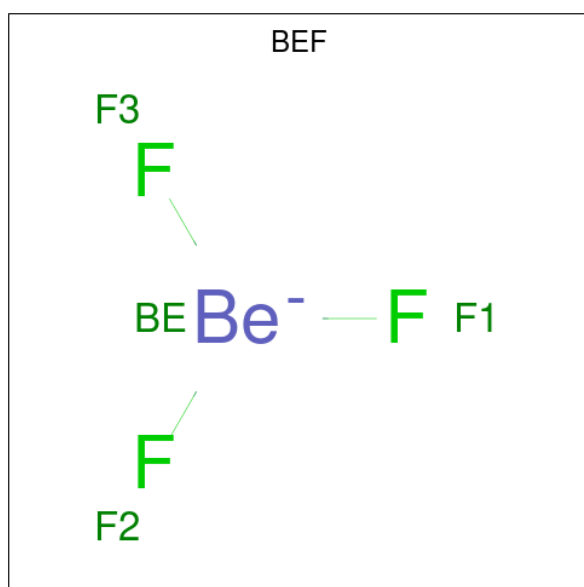
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	N	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		
5	L	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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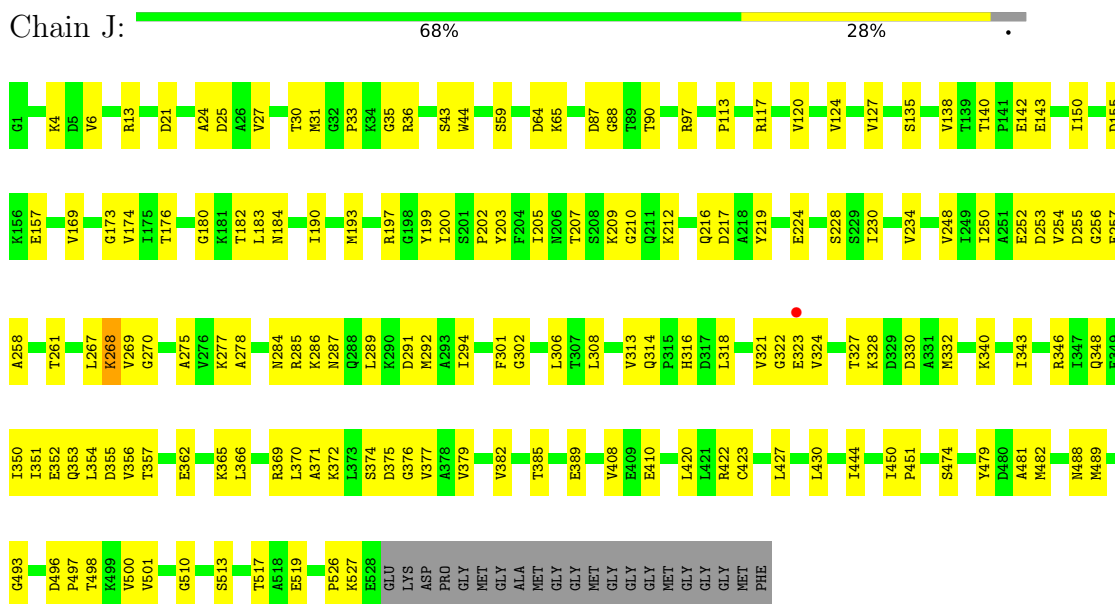
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total K 1 1	0	0
6	B	1	Total K 1 1	0	0
6	A	1	Total K 1 1	0	0

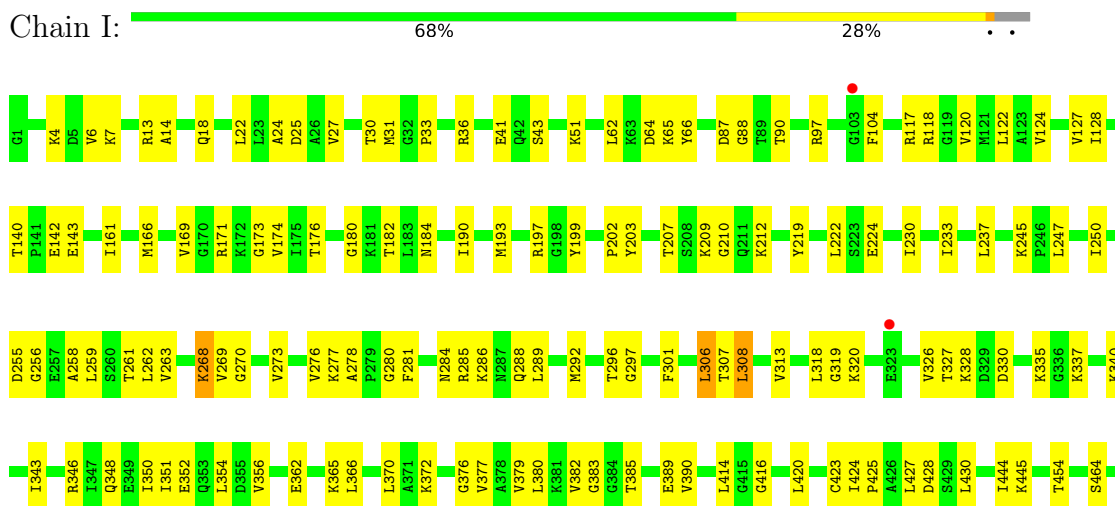
3 Residue-property plots

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

- Molecule 1: 60 kDa heat shock protein, mitochondrial

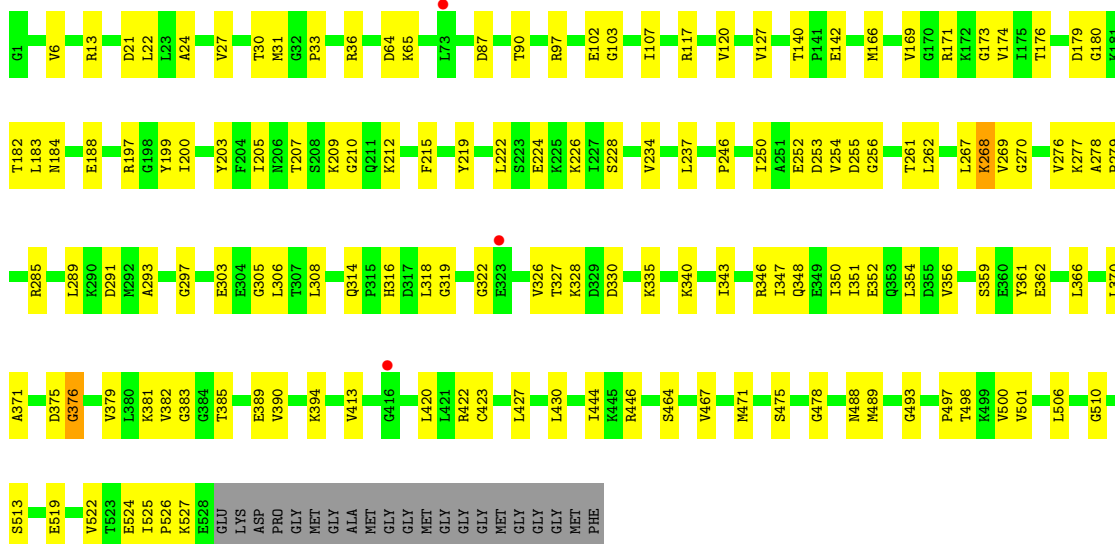


- Molecule 1: 60 kDa heat shock protein, mitochondrial

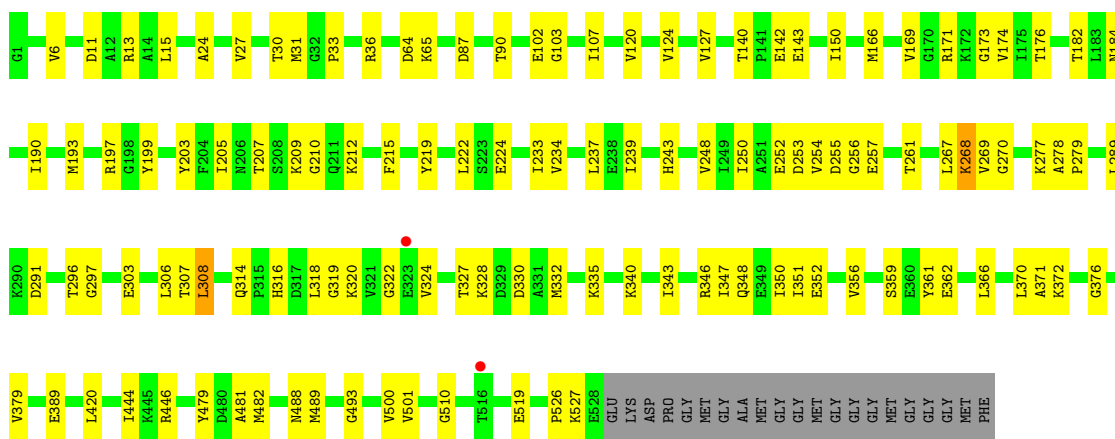




• Molecule 1: 60 kDa heat shock protein, mitochondrial

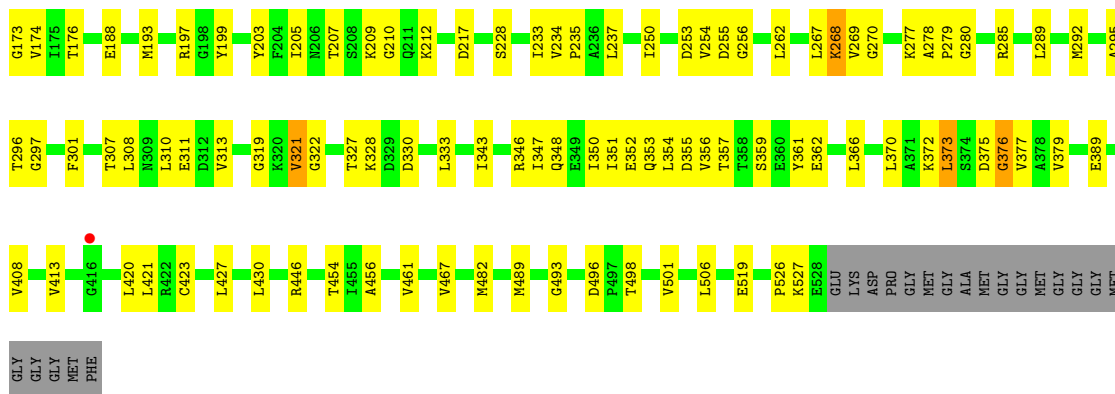


• Molecule 1: 60 kDa heat shock protein, mitochondrial

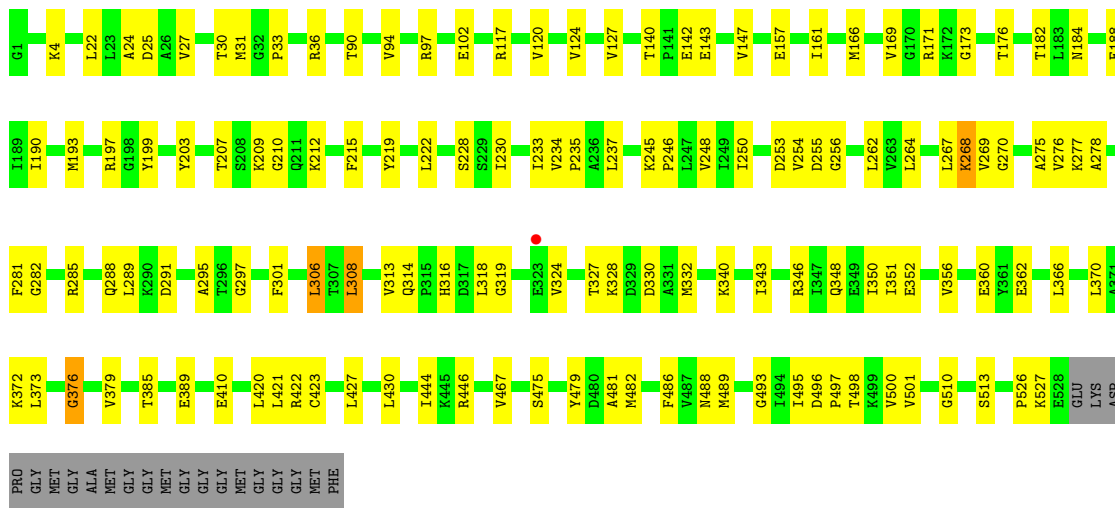


• Molecule 1: 60 kDa heat shock protein, mitochondrial

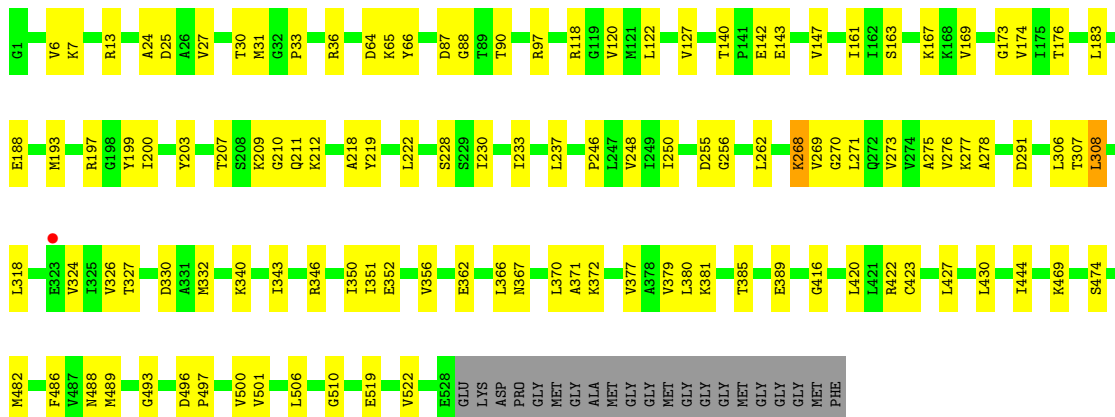




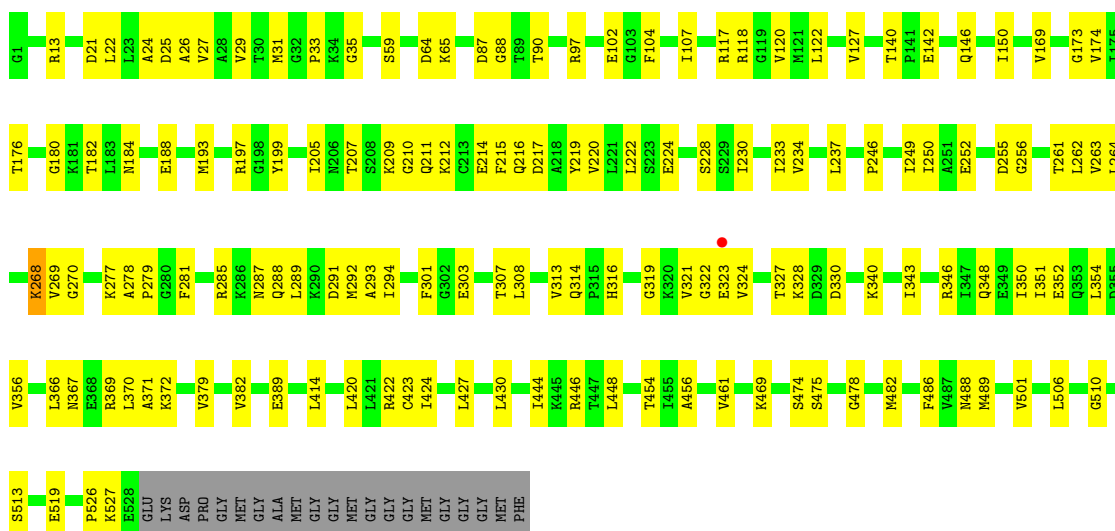
• Molecule 1: 60 kDa heat shock protein, mitochondrial



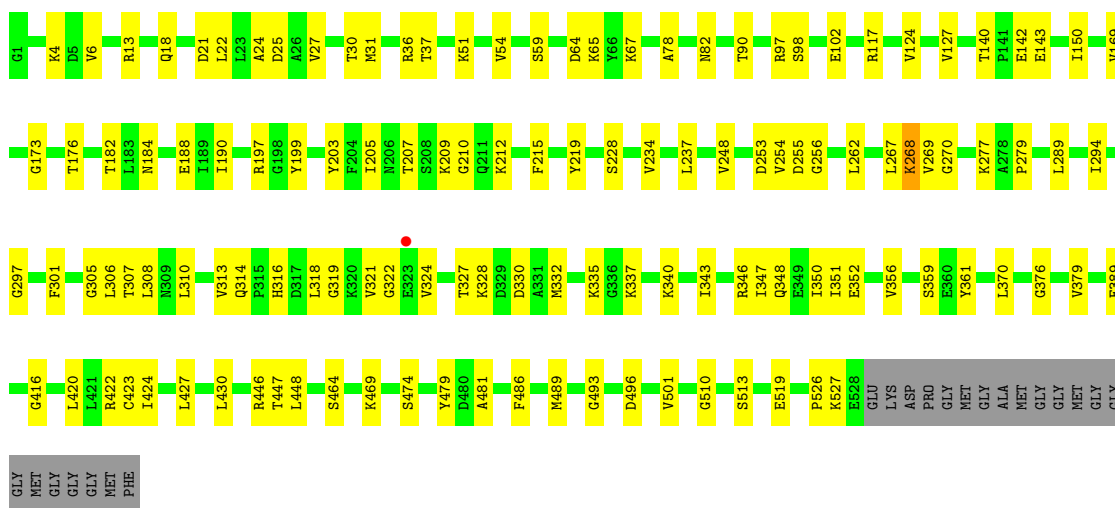
• Molecule 1: 60 kDa heat shock protein, mitochondrial




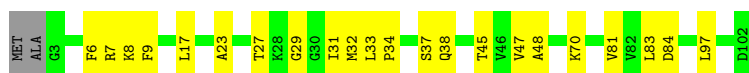
• Molecule 1: 60 kDa heat shock protein, mitochondrial

Chain B:  70% 26%


- Molecule 1: 60 kDa heat shock protein, mitochondrial

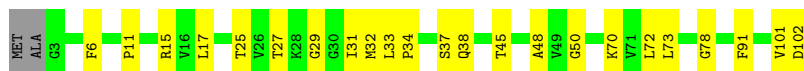
Chain A:  73% 23%

- Molecule 2: 10 kDa heat shock protein, mitochondrial

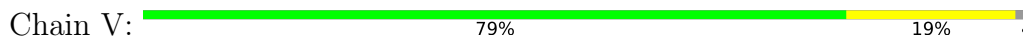
Chain X:  76% 22%

- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain W:  75% 23%



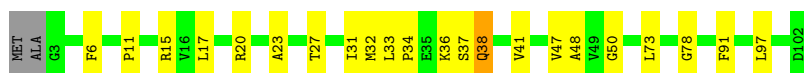
- Molecule 2: 10 kDa heat shock protein, mitochondrial



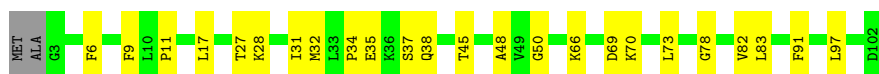
- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial



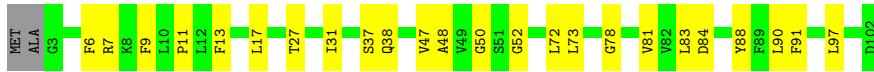
- Molecule 2: 10 kDa heat shock protein, mitochondrial





- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain S:



- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain R:



- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain Q:



- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain P:



- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain O:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.59Å 295.78Å 326.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 3.70 48.95 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.95-3.70) 86.7 (48.95-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.67Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.269 , 0.303	Depositor DCC
R_{free} test set	2000 reflections (1.36%)	wwPDB-VP
Wilson B-factor (Å ²)	110.0	Xtrriage
Anisotropy	0.504	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 112.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	134311	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.75 % 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 2.9942e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, K, BEF, 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	0.29	0/3964	0.48	0/5347
1	B	0.29	0/3964	0.49	0/5347
1	C	0.31	0/3964	0.51	0/5347
1	D	0.28	0/3964	0.50	1/5347 (0.0%)
1	E	0.29	0/3964	0.49	0/5347
1	F	0.30	0/3964	0.50	0/5347
1	G	0.31	0/3964	0.51	0/5347
1	H	0.28	0/3964	0.50	0/5347
1	I	0.31	0/3964	0.52	1/5347 (0.0%)
1	J	0.29	0/3964	0.50	0/5347
1	K	0.30	0/3964	0.51	1/5347 (0.0%)
1	L	0.35	1/3964 (0.0%)	0.60	6/5347 (0.1%)
1	M	0.29	0/3964	0.51	0/5347
1	N	0.27	0/3964	0.48	0/5347
2	1	0.26	0/763	0.59	1/1026 (0.1%)
2	2	0.24	0/763	0.49	0/1026
2	O	0.25	0/763	0.54	0/1026
2	P	0.27	0/763	0.55	0/1026
2	Q	0.25	0/763	0.57	0/1026
2	R	0.28	0/763	0.58	0/1026
2	S	0.24	0/763	0.52	0/1026
2	T	0.26	0/763	0.59	0/1026
2	U	0.28	0/763	0.54	0/1026
2	V	0.24	0/763	0.55	0/1026
2	W	0.25	0/763	0.55	0/1026
2	X	0.29	0/763	0.59	0/1026
2	Y	0.25	0/763	0.50	0/1026
2	Z	0.25	0/763	0.50	0/1026
All	All	0.29	1/66178 (0.0%)	0.51	10/89222 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	2
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	455	ILE	CA-C	9.87	1.65	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	456	ALA	N-CA-C	7.20	118.78	111.07
1	L	449	LYS	CA-C-N	6.64	125.65	120.33
1	L	449	LYS	C-N-CA	6.64	125.65	120.33
1	L	454	THR	CA-C-N	5.48	131.83	121.97
1	L	454	THR	C-N-CA	5.48	131.83	121.97

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	268	LYS	Peptide
1	I	268	LYS	Peptide
1	J	268	LYS	Peptide
1	M	268	LYS	Peptide
1	N	268	LYS	Peptide

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	3932	4105	4111	85	0
1	B	3932	4105	4110	106	0
1	C	3932	4103	4111	86	0
1	D	3932	4102	4111	92	0
1	E	3932	4105	4111	83	0
1	F	3932	4105	4111	103	1
1	G	3932	4104	4110	105	0
1	H	3932	4103	4111	105	0
1	I	3932	4098	4109	111	0
1	J	3932	4105	4111	112	2
1	K	3932	4100	4111	90	0
1	L	3932	4080	4111	115	0
1	M	3932	4105	4111	102	0
1	N	3932	4103	4111	78	0
2	1	752	775	775	26	0
2	2	752	775	775	20	0
2	O	752	775	775	18	0
2	P	752	775	775	29	0
2	Q	752	775	775	25	0
2	R	752	775	775	24	0
2	S	752	775	775	18	0
2	T	752	775	775	26	0
2	U	752	775	775	35	1
2	V	752	775	775	16	0
2	W	752	775	775	19	0
2	X	752	775	775	24	0
2	Y	752	775	775	23	0
2	Z	752	775	775	21	0
3	A	27	0	12	3	0
3	B	27	0	12	3	0
3	C	27	0	12	8	0
3	D	27	0	12	4	0
3	E	27	0	12	3	0
3	F	27	0	12	2	0
3	G	27	0	12	6	0
3	H	27	0	12	2	0
3	I	27	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	27	0	12	4	0
3	K	27	0	12	2	0
3	L	27	0	12	3	0
3	M	27	0	12	3	0
3	N	27	0	12	5	0
4	A	4	0	0	1	0
4	B	4	0	0	2	0
4	C	4	0	0	2	0
4	D	4	0	0	3	0
4	E	4	0	0	2	0
4	F	4	0	0	2	0
4	G	4	0	0	4	0
4	H	4	0	0	2	0
4	I	4	0	0	2	0
4	J	4	0	0	3	0
4	K	4	0	0	0	0
4	L	4	0	0	2	0
4	M	4	0	0	1	0
4	N	4	0	0	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	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	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	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	66038	68273	68568	1587	2

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 12.

The worst 5 of 1587 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:L:31:MET:O	1:L:455:ILE:CD1	1.69	1.40
1:L:95:LEU:HD21	1:L:451:PRO:CG	1.59	1.29
1:L:31:MET:C	1:L:455:ILE:HD13	1.60	1.27
1:L:95:LEU:CD2	1:L:451:PRO:HG3	1.69	1.21
1:L:31:MET:SD	1:L:454:THR:HG22	1.83	1.18

All (2) 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:J:352:GLU:OE2	2:U:8:LYS:HZ2[2_555]	1.48	0.12
1:J:316:HIS:NE2	1:F:269:VAL:O[2_555]	2.17	0.03

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	526/549 (96%)	491 (93%)	34 (6%)	1 (0%)	43 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	526/549 (96%)	490 (93%)	35 (7%)	1 (0%)	43	72
1	C	526/549 (96%)	490 (93%)	35 (7%)	1 (0%)	43	72
1	D	526/549 (96%)	491 (93%)	33 (6%)	2 (0%)	30	60
1	E	526/549 (96%)	488 (93%)	36 (7%)	2 (0%)	30	60
1	F	526/549 (96%)	490 (93%)	35 (7%)	1 (0%)	43	72
1	G	526/549 (96%)	489 (93%)	35 (7%)	2 (0%)	30	60
1	H	526/549 (96%)	488 (93%)	36 (7%)	2 (0%)	30	60
1	I	526/549 (96%)	485 (92%)	40 (8%)	1 (0%)	43	72
1	J	526/549 (96%)	489 (93%)	36 (7%)	1 (0%)	43	72
1	K	526/549 (96%)	492 (94%)	33 (6%)	1 (0%)	43	72
1	L	526/549 (96%)	495 (94%)	29 (6%)	2 (0%)	30	60
1	M	526/549 (96%)	489 (93%)	34 (6%)	3 (1%)	21	52
1	N	526/549 (96%)	488 (93%)	37 (7%)	1 (0%)	43	72
2	1	98/102 (96%)	82 (84%)	16 (16%)	0	100	100
2	2	98/102 (96%)	80 (82%)	18 (18%)	0	100	100
2	O	98/102 (96%)	82 (84%)	16 (16%)	0	100	100
2	P	98/102 (96%)	79 (81%)	19 (19%)	0	100	100
2	Q	98/102 (96%)	80 (82%)	18 (18%)	0	100	100
2	R	98/102 (96%)	80 (82%)	18 (18%)	0	100	100
2	S	98/102 (96%)	80 (82%)	18 (18%)	0	100	100
2	T	98/102 (96%)	80 (82%)	18 (18%)	0	100	100
2	U	98/102 (96%)	82 (84%)	16 (16%)	0	100	100
2	V	98/102 (96%)	81 (83%)	17 (17%)	0	100	100
2	W	98/102 (96%)	80 (82%)	18 (18%)	0	100	100
2	X	98/102 (96%)	82 (84%)	16 (16%)	0	100	100
2	Y	98/102 (96%)	80 (82%)	18 (18%)	0	100	100
2	Z	98/102 (96%)	81 (83%)	17 (17%)	0	100	100
All	All	8736/9114 (96%)	7984 (91%)	731 (8%)	21 (0%)	43	72

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	269	VAL

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Mol	Chain	Res	Type
1	I	269	VAL
1	H	269	VAL
1	N	269	VAL
1	M	269	VAL

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	426/437 (98%)	425 (100%)	1 (0%)	87	86
1	B	426/437 (98%)	425 (100%)	1 (0%)	87	86
1	C	426/437 (98%)	425 (100%)	1 (0%)	87	86
1	D	426/437 (98%)	424 (100%)	2 (0%)	81	80
1	E	426/437 (98%)	424 (100%)	2 (0%)	81	80
1	F	426/437 (98%)	424 (100%)	2 (0%)	81	80
1	G	426/437 (98%)	425 (100%)	1 (0%)	87	86
1	H	426/437 (98%)	426 (100%)	0	100	100
1	I	426/437 (98%)	425 (100%)	1 (0%)	87	86
1	J	426/437 (98%)	425 (100%)	1 (0%)	87	86
1	K	426/437 (98%)	425 (100%)	1 (0%)	87	86
1	L	426/437 (98%)	425 (100%)	1 (0%)	87	86
1	M	426/437 (98%)	425 (100%)	1 (0%)	87	86
1	N	426/437 (98%)	425 (100%)	1 (0%)	87	86
2	1	80/82 (98%)	80 (100%)	0	100	100
2	2	80/82 (98%)	80 (100%)	0	100	100
2	O	80/82 (98%)	80 (100%)	0	100	100
2	P	80/82 (98%)	80 (100%)	0	100	100
2	Q	80/82 (98%)	80 (100%)	0	100	100
2	R	80/82 (98%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	80/82 (98%)	80 (100%)	0	100	100
2	T	80/82 (98%)	80 (100%)	0	100	100
2	U	80/82 (98%)	80 (100%)	0	100	100
2	V	80/82 (98%)	80 (100%)	0	100	100
2	W	80/82 (98%)	80 (100%)	0	100	100
2	X	80/82 (98%)	80 (100%)	0	100	100
2	Y	80/82 (98%)	80 (100%)	0	100	100
2	Z	80/82 (98%)	80 (100%)	0	100	100
All	All	7084/7266 (98%)	7068 (100%)	16 (0%)	87	86

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	321	VAL
1	C	308	LEU
1	F	321	VAL
1	D	308	LEU
1	F	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	42	GLN
1	E	231	GLN
1	F	68	ASN
1	F	367	ASN
1	D	231	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 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	L	601	6	28,29,29	1.40	5 (17%)	43,45,45	2.17	10 (23%)
4	BEF	G	602	3	0,3,3	-	-	-		
4	BEF	D	602	-	0,3,3	-	-	-		
4	BEF	N	602	3	0,3,3	-	-	-		
3	ADP	K	601	5,6	28,29,29	1.43	3 (10%)	43,45,45	1.85	10 (23%)
4	BEF	F	602	3	0,3,3	-	-	-		
4	BEF	H	602	3	0,3,3	-	-	-		
4	BEF	I	602	-	0,3,3	-	-	-		
3	ADP	H	601	5,6,4	28,29,29	1.35	3 (10%)	43,45,45	2.03	12 (27%)
3	ADP	F	601	6,4	28,29,29	1.40	4 (14%)	43,45,45	2.10	11 (25%)
3	ADP	D	601	5,6	28,29,29	1.37	4 (14%)	43,45,45	1.91	10 (23%)
3	ADP	J	601	5,6	28,29,29	1.41	4 (14%)	43,45,45	1.91	8 (18%)
4	BEF	C	602	-	0,3,3	-	-	-		
3	ADP	I	601	6	28,29,29	1.43	3 (10%)	43,45,45	2.05	9 (20%)
3	ADP	G	601	5,6,4	28,29,29	1.39	4 (14%)	43,45,45	2.10	11 (25%)
4	BEF	A	602	3	0,3,3	-	-	-		
3	ADP	E	601	5,6	28,29,29	1.41	4 (14%)	43,45,45	1.86	12 (27%)
4	BEF	B	602	3	0,3,3	-	-	-		
3	ADP	A	601	5,6,4	28,29,29	1.37	4 (14%)	43,45,45	1.94	13 (30%)
4	BEF	K	602	-	0,3,3	-	-	-		
4	BEF	M	602	-	0,3,3	-	-	-		
3	ADP	N	601	5,6,4	28,29,29	1.34	4 (14%)	43,45,45	1.89	10 (23%)
4	BEF	J	602	-	0,3,3	-	-	-		
3	ADP	B	601	5,6,4	28,29,29	1.33	3 (10%)	43,45,45	1.96	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BEF	L	602	-	0,3,3	-	-	-	-	-
3	ADP	M	601	5,6	28,29,29	1.39	4 (14%)	43,45,45	2.02	9 (20%)
3	ADP	C	601	6	28,29,29	1.47	6 (21%)	43,45,45	2.32	17 (39%)
4	BEF	E	602	-	0,3,3	-	-	-	-	-

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	L	601	6	-	0/16/32/32	0/3/3/3
3	ADP	D	601	5,6	-	4/16/32/32	0/3/3/3
3	ADP	J	601	5,6	-	3/16/32/32	0/3/3/3
3	ADP	N	601	5,6,4	-	0/16/32/32	0/3/3/3
3	ADP	B	601	5,6,4	-	0/16/32/32	0/3/3/3
3	ADP	A	601	5,6,4	-	3/16/32/32	0/3/3/3
3	ADP	I	601	6	-	2/16/32/32	0/3/3/3
3	ADP	M	601	5,6	-	3/16/32/32	0/3/3/3
3	ADP	K	601	5,6	-	9/16/32/32	0/3/3/3
3	ADP	C	601	6	-	6/16/32/32	0/3/3/3
3	ADP	G	601	5,6,4	-	2/16/32/32	0/3/3/3
3	ADP	H	601	5,6,4	-	0/16/32/32	0/3/3/3
3	ADP	E	601	5,6	-	9/16/32/32	0/3/3/3
3	ADP	F	601	6,4	-	2/16/32/32	0/3/3/3

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	601	ADP	C5-C4	5.04	1.48	1.39
3	I	601	ADP	C5-C4	5.00	1.48	1.39
3	E	601	ADP	C5-C4	4.86	1.47	1.39
3	J	601	ADP	C5-C4	4.83	1.47	1.39
3	F	601	ADP	C5-C4	4.82	1.47	1.39

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	601	ADP	C5-C4-N3	-6.97	117.11	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	601	ADP	C5-C4-N3	-6.48	117.80	126.72
3	C	601	ADP	C5-C4-N3	-6.31	118.03	126.72
3	G	601	ADP	C5-C4-N3	-6.29	118.06	126.72
3	J	601	ADP	C5-C4-N3	-6.27	118.08	126.72

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	601	ADP	PA-O3A-PB-O2B
3	E	601	ADP	C5'-O5'-PA-O1A
3	E	601	ADP	C5'-O5'-PA-O2A
3	E	601	ADP	O4'-C4'-C5'-O5'
3	D	601	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

27 monomers are involved in 64 short contacts:

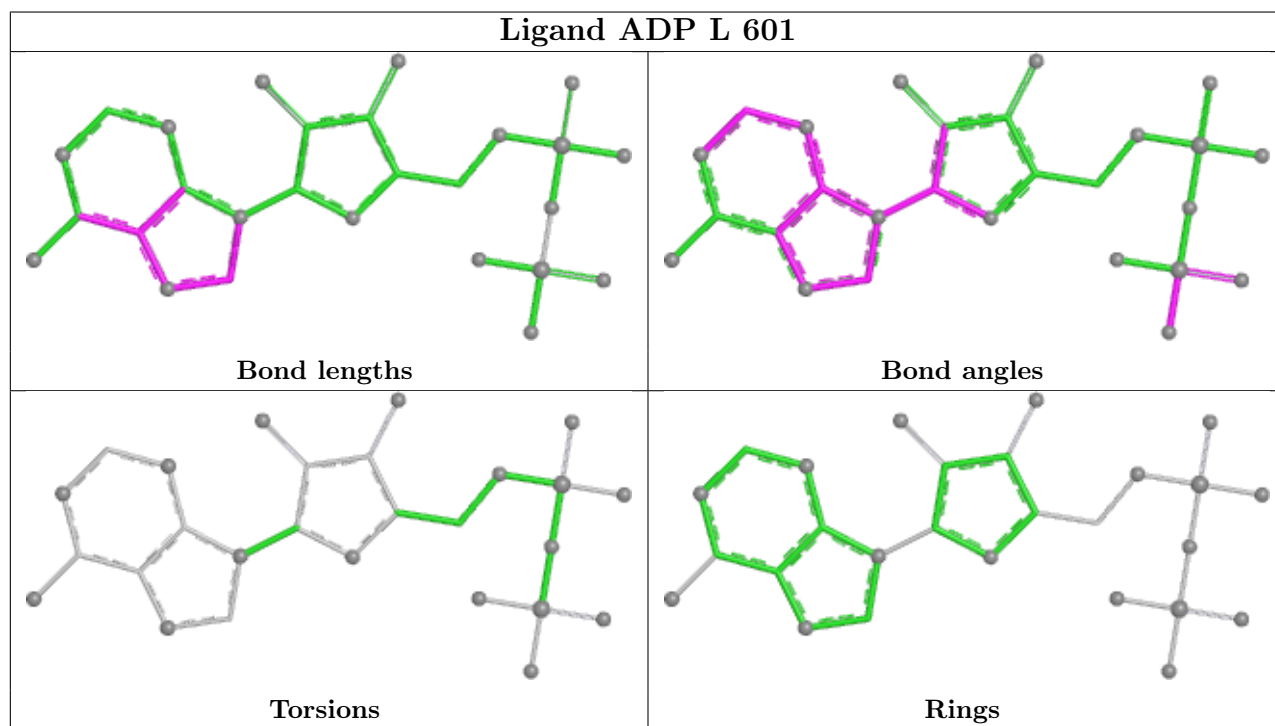
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	601	ADP	3	0
4	G	602	BEF	4	0
4	D	602	BEF	3	0
4	N	602	BEF	2	0
3	K	601	ADP	2	0
4	F	602	BEF	2	0
4	H	602	BEF	2	0
4	I	602	BEF	2	0
3	H	601	ADP	2	0
3	F	601	ADP	2	0
3	D	601	ADP	4	0
3	J	601	ADP	4	0
4	C	602	BEF	2	0
3	I	601	ADP	5	0
3	G	601	ADP	6	0
4	A	602	BEF	1	0
3	E	601	ADP	3	0
4	B	602	BEF	2	0
3	A	601	ADP	3	0
4	M	602	BEF	1	0
3	N	601	ADP	5	0
4	J	602	BEF	3	0

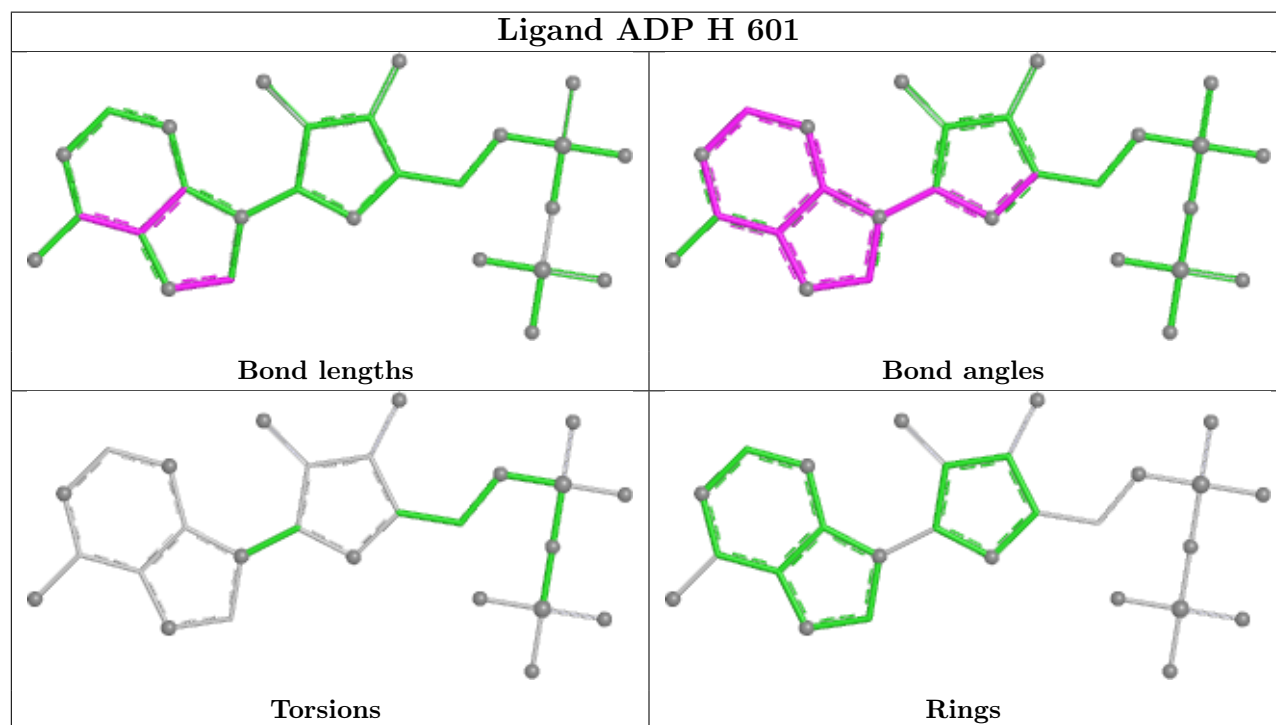
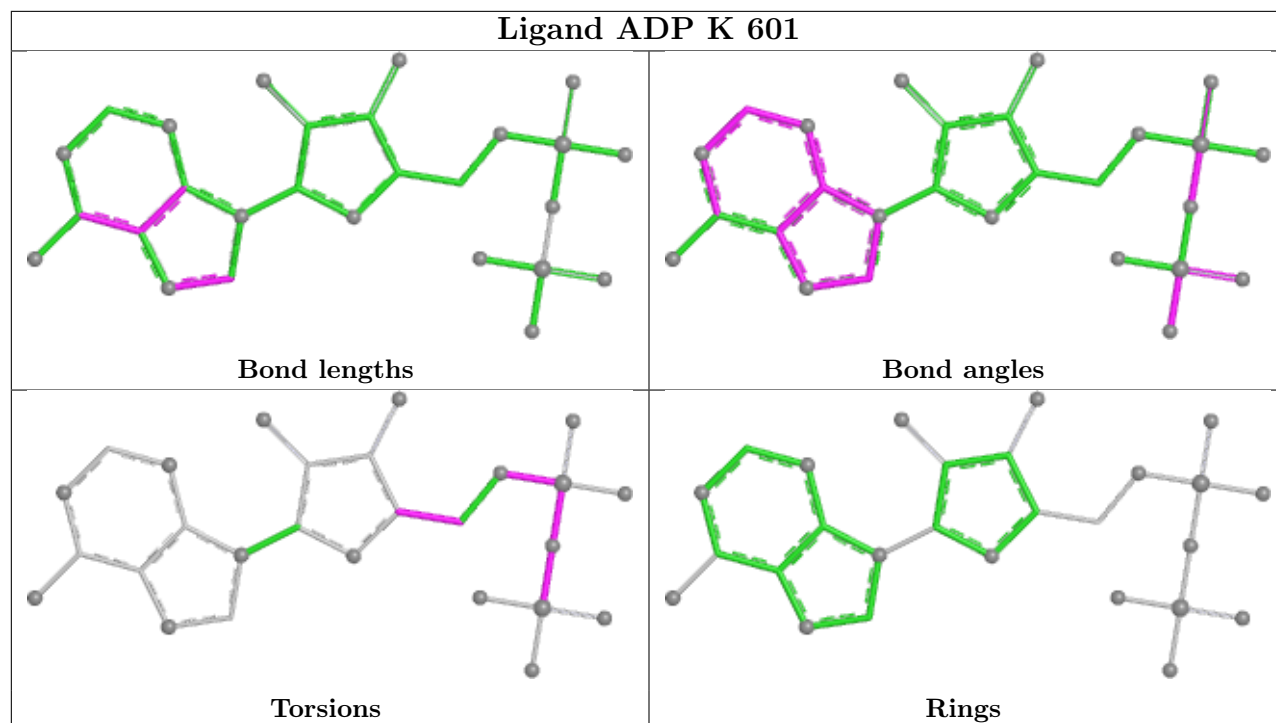
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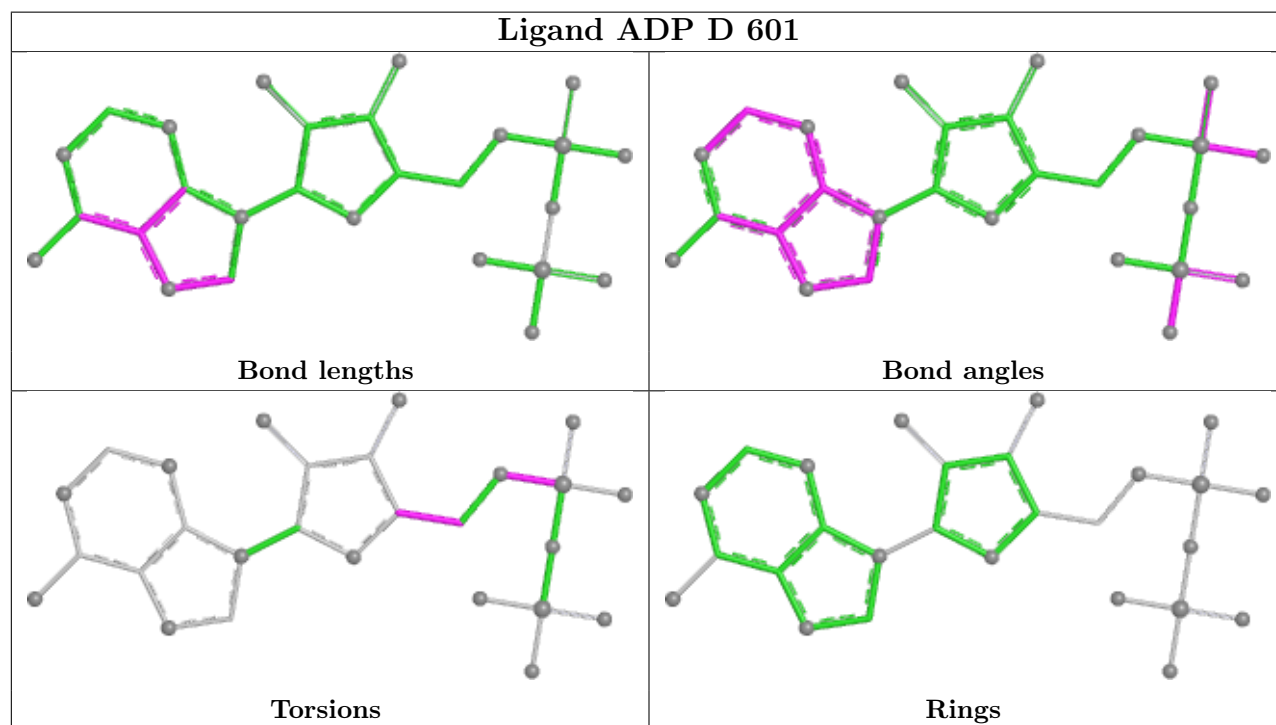
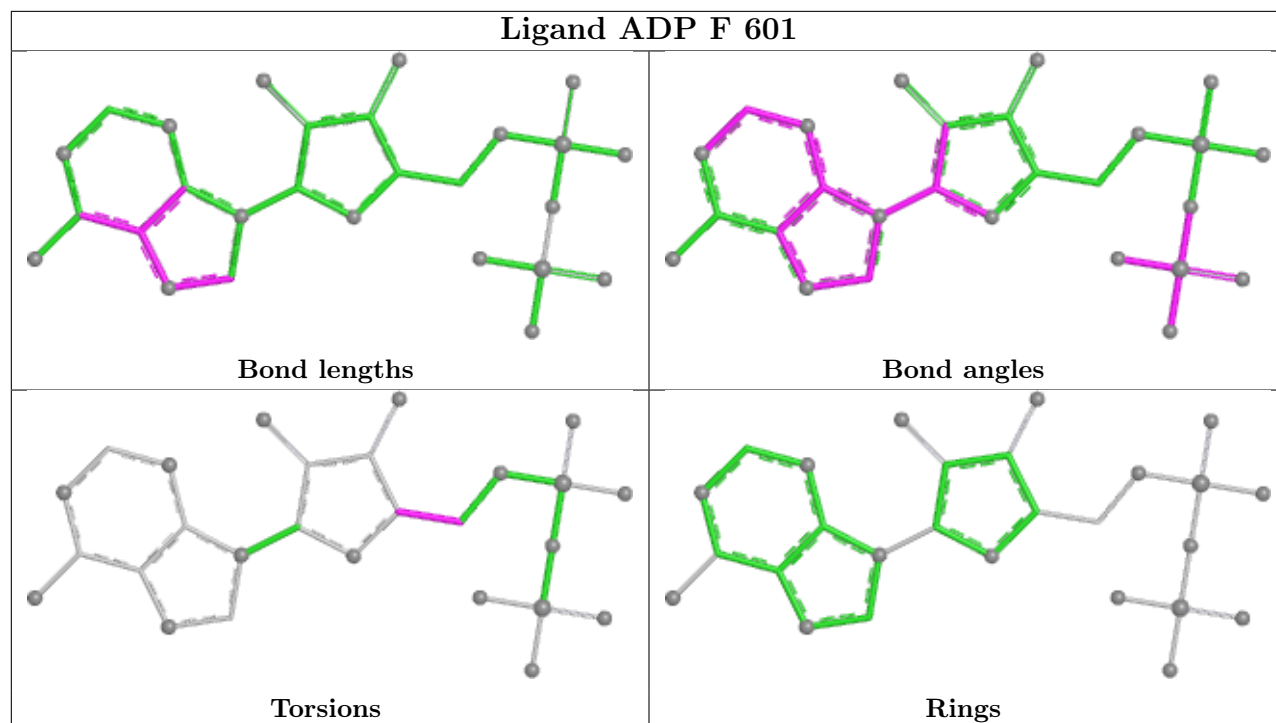
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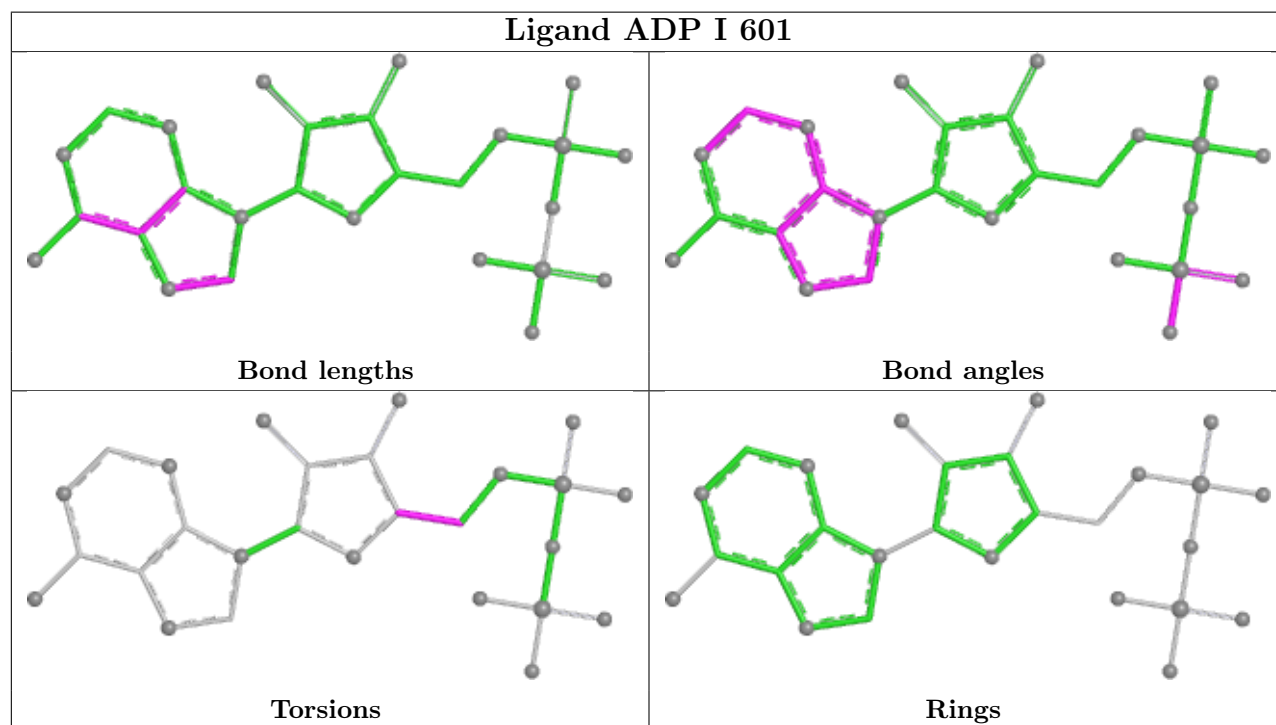
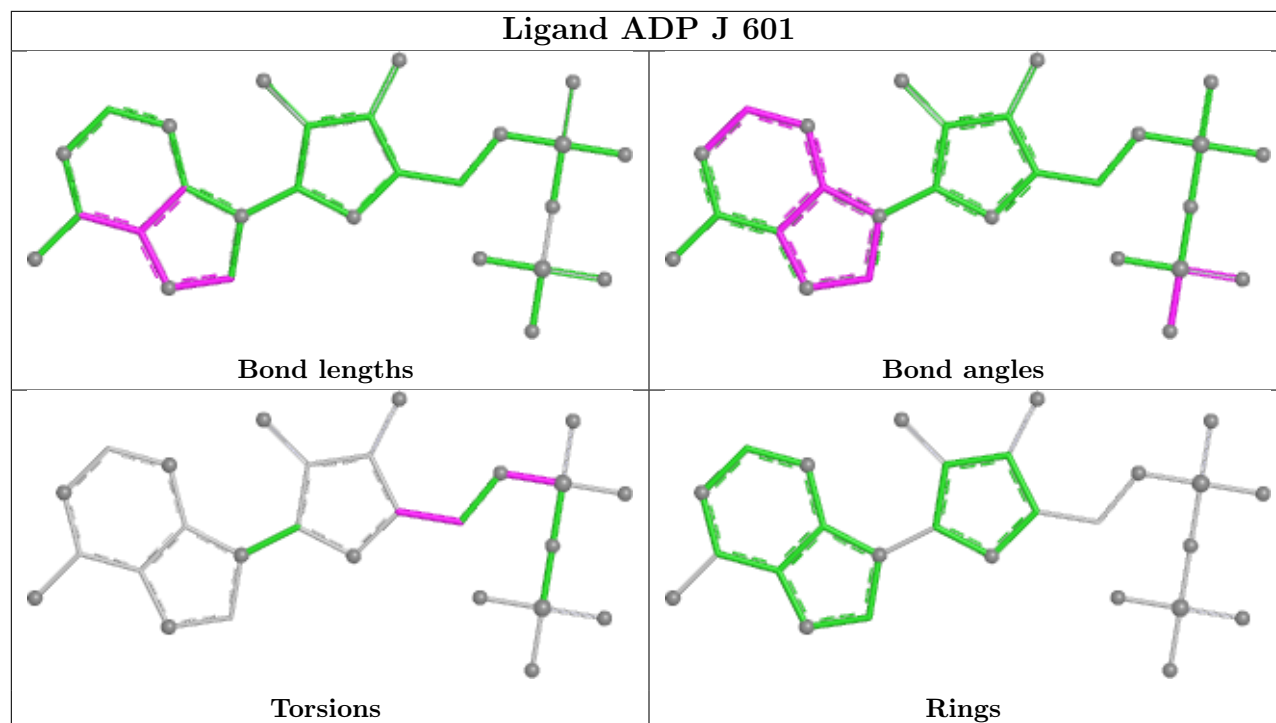
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	ADP	3	0
4	L	602	BEF	2	0
3	M	601	ADP	3	0
3	C	601	ADP	8	0
4	E	602	BEF	2	0

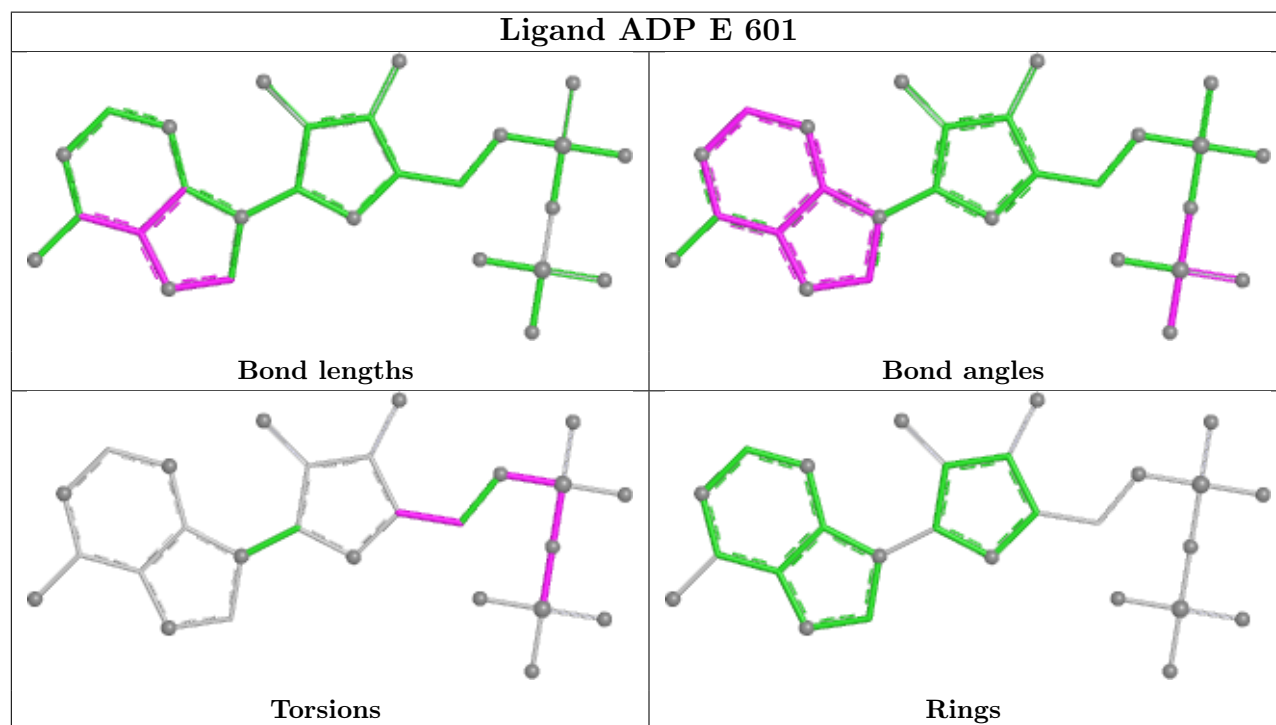
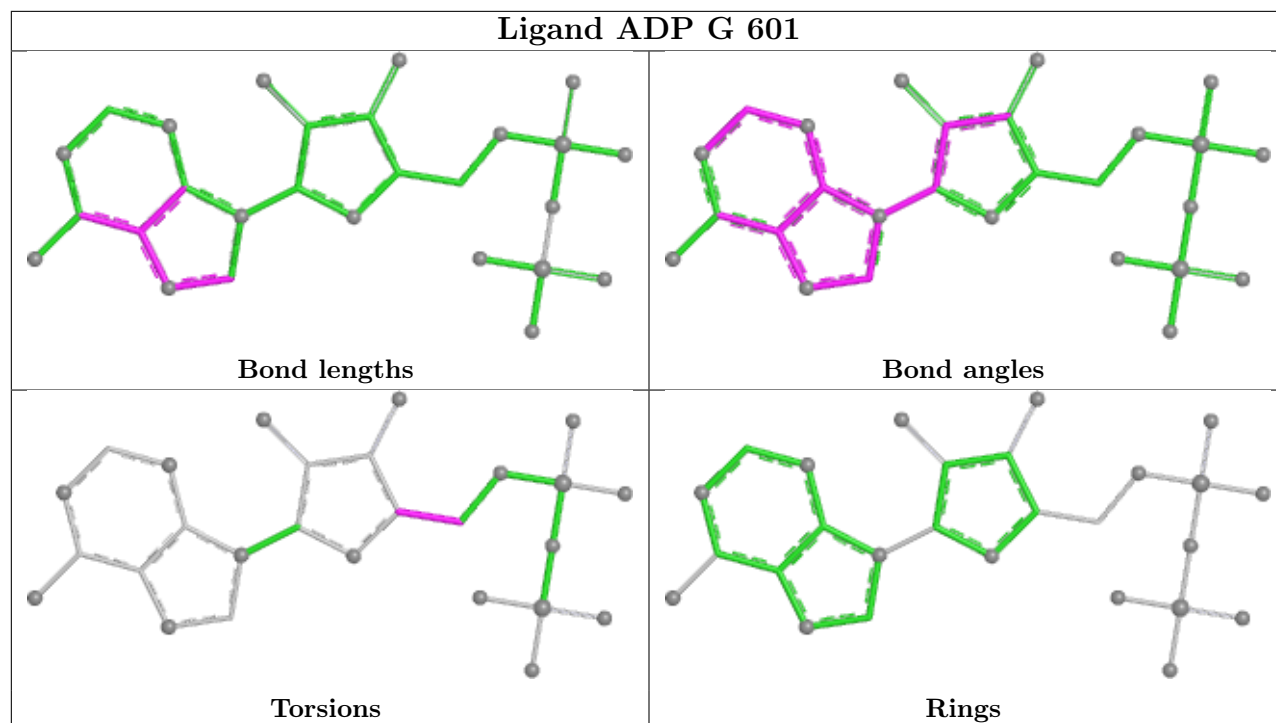
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

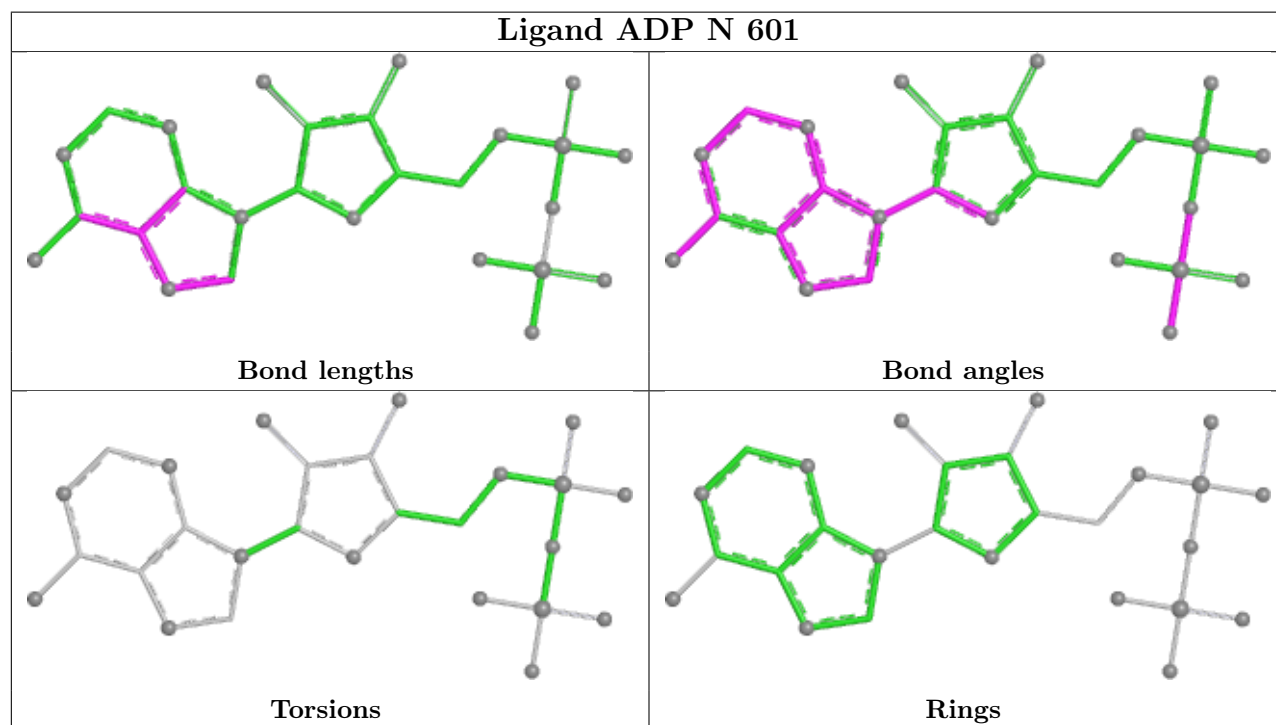
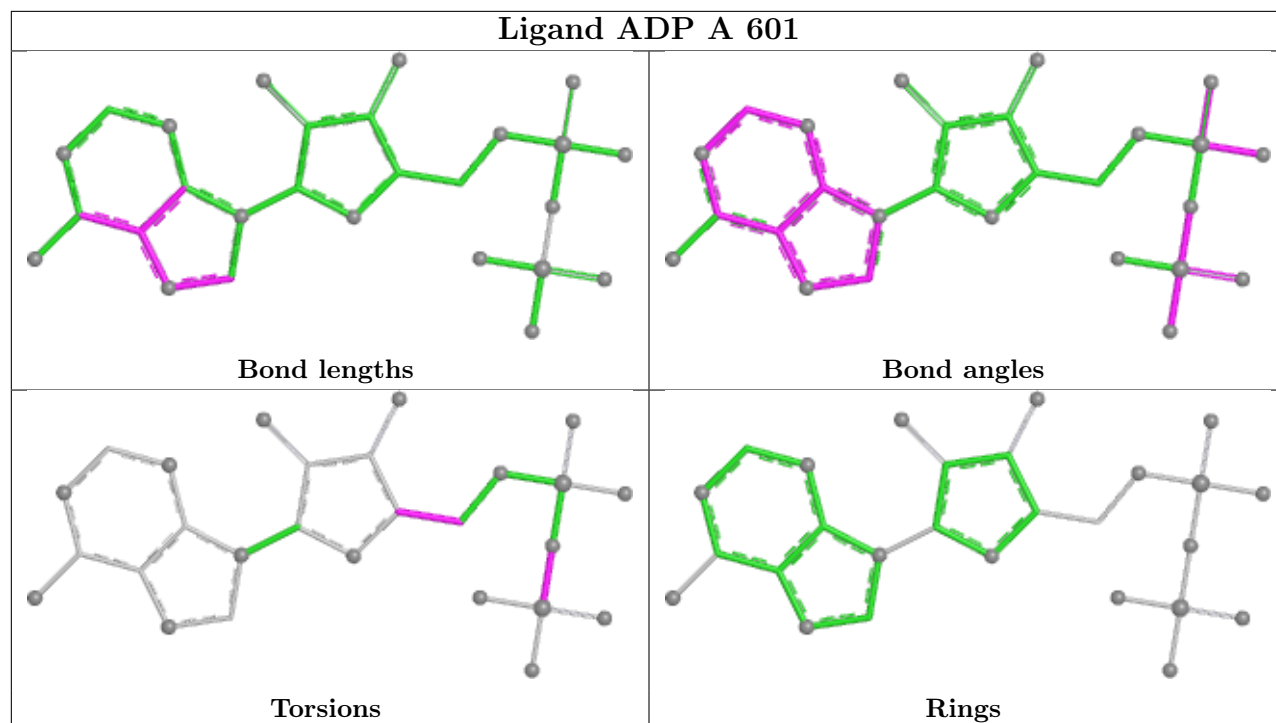


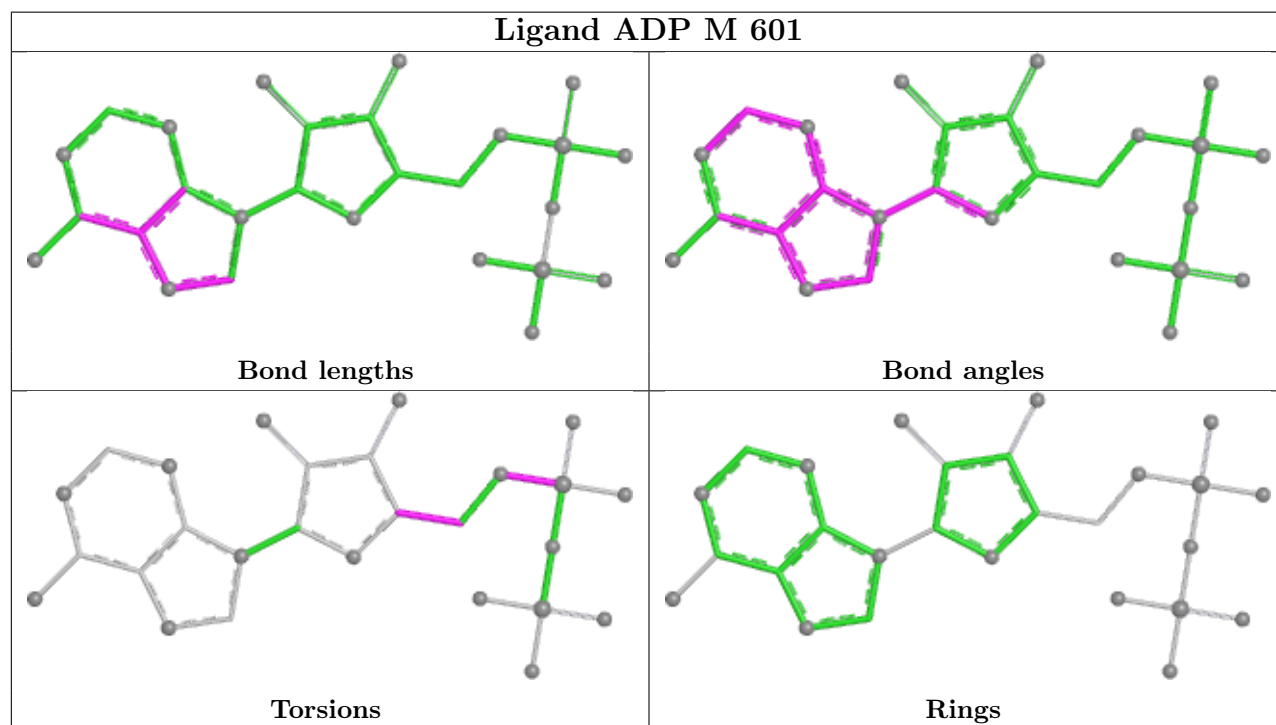
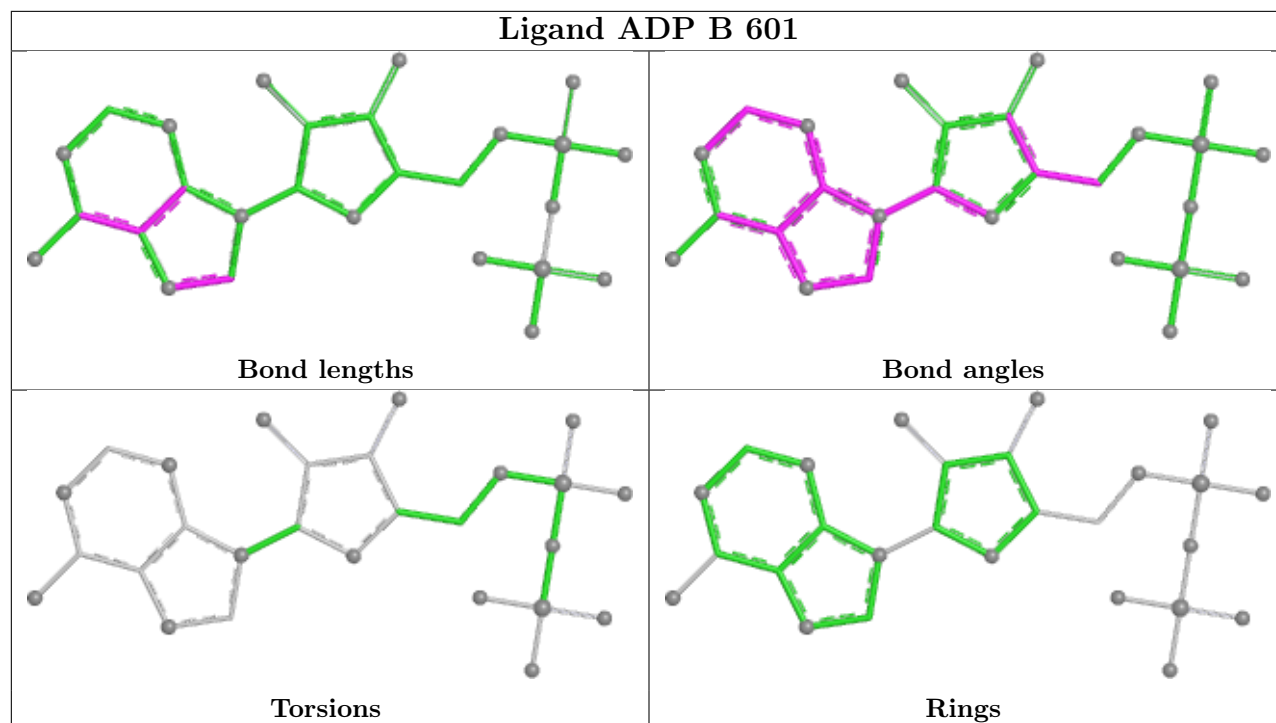


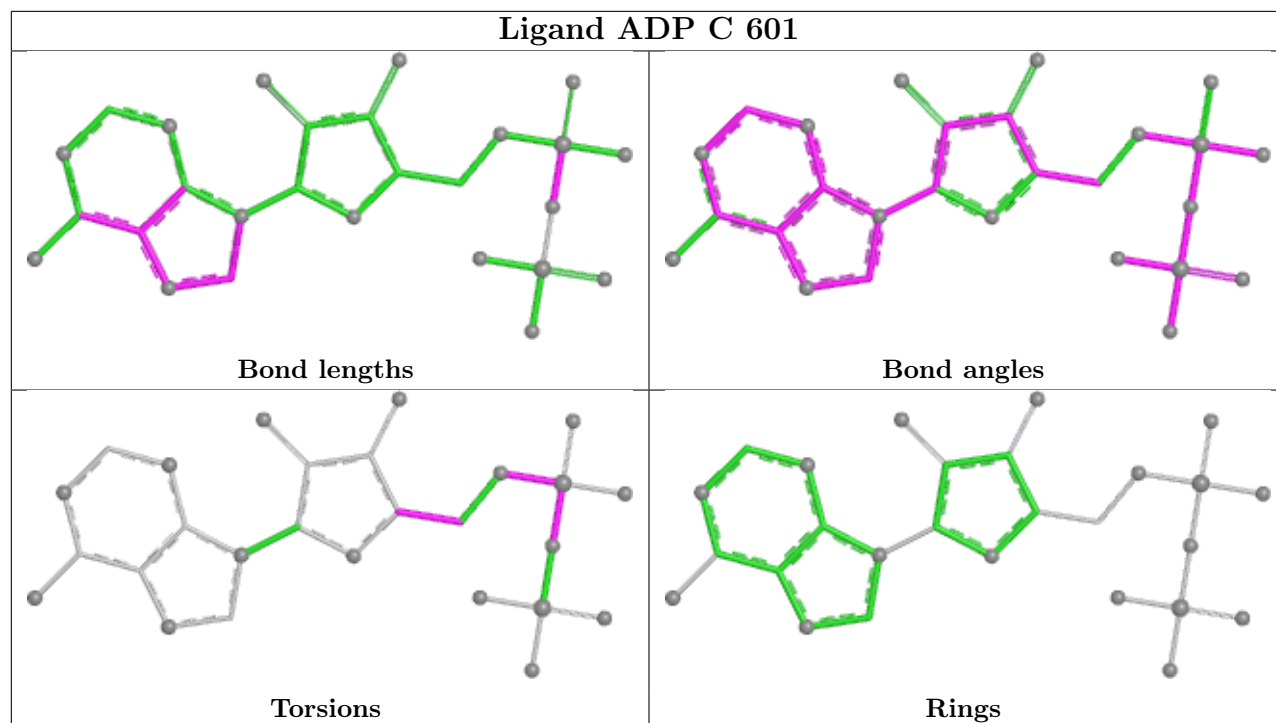












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	528/549 (96%)	-0.29	1 (0%) 91 80	94, 154, 214, 249	0
1	B	528/549 (96%)	-0.31	1 (0%) 91 80	106, 157, 238, 283	0
1	C	528/549 (96%)	-0.32	1 (0%) 91 80	100, 144, 187, 249	0
1	D	528/549 (96%)	-0.40	1 (0%) 91 80	107, 151, 196, 218	0
1	E	528/549 (96%)	-0.37	1 (0%) 91 80	101, 154, 188, 224	0
1	F	528/549 (96%)	-0.32	1 (0%) 91 80	103, 153, 188, 219	0
1	G	528/549 (96%)	-0.34	2 (0%) 88 72	102, 149, 198, 216	0
1	H	528/549 (96%)	-0.28	3 (0%) 85 66	109, 160, 226, 247	0
1	I	528/549 (96%)	-0.30	2 (0%) 88 72	98, 151, 191, 221	0
1	J	528/549 (96%)	-0.31	1 (0%) 91 80	102, 160, 204, 222	0
1	K	528/549 (96%)	-0.36	2 (0%) 88 72	97, 151, 193, 214	0
1	L	528/549 (96%)	-0.29	2 (0%) 88 72	30, 155, 199, 221	0
1	M	528/549 (96%)	-0.36	3 (0%) 85 66	102, 151, 212, 240	0
1	N	528/549 (96%)	-0.33	2 (0%) 88 72	97, 161, 218, 245	0
2	1	100/102 (98%)	-0.44	0 100 100	147, 182, 214, 228	0
2	2	100/102 (98%)	-0.40	0 100 100	153, 181, 222, 241	0
2	O	100/102 (98%)	-0.36	0 100 100	142, 177, 207, 223	0
2	P	100/102 (98%)	-0.41	0 100 100	117, 163, 216, 232	0
2	Q	100/102 (98%)	-0.41	0 100 100	123, 154, 229, 252	0
2	R	100/102 (98%)	-0.39	0 100 100	130, 171, 202, 228	0
2	S	100/102 (98%)	-0.43	0 100 100	144, 185, 235, 258	0
2	T	100/102 (98%)	-0.30	0 100 100	148, 178, 265, 295	0
2	U	100/102 (98%)	-0.30	0 100 100	138, 171, 214, 228	0
2	V	100/102 (98%)	-0.39	0 100 100	138, 176, 232, 245	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	100/102 (98%)	-0.35	0 100 100	140, 176, 222, 235	0
2	X	100/102 (98%)	-0.38	0 100 100	145, 175, 243, 261	0
2	Y	100/102 (98%)	-0.38	0 100 100	146, 173, 208, 228	0
2	Z	100/102 (98%)	-0.46	0 100 100	157, 184, 230, 247	0
All	All	8792/9114 (96%)	-0.34	23 (0%) 90 76	30, 158, 212, 295	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	516	THR	3.0
1	I	323	GLU	2.8
1	H	416	GLY	2.7
1	L	456	ALA	2.7
1	J	323	GLU	2.6

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
5	MG	G	603	1/1	0.72	0.19	92,92,92,92	0
5	MG	B	603	1/1	0.73	0.22	100,100,100,100	0
6	K	C	604	1/1	0.75	0.20	143,143,143,143	0
5	MG	F	603	1/1	0.76	0.14	101,101,101,101	0
5	MG	C	603	1/1	0.80	0.19	89,89,89,89	0
6	K	E	604	1/1	0.84	0.07	155,155,155,155	0
5	MG	M	603	1/1	0.84	0.17	96,96,96,96	0

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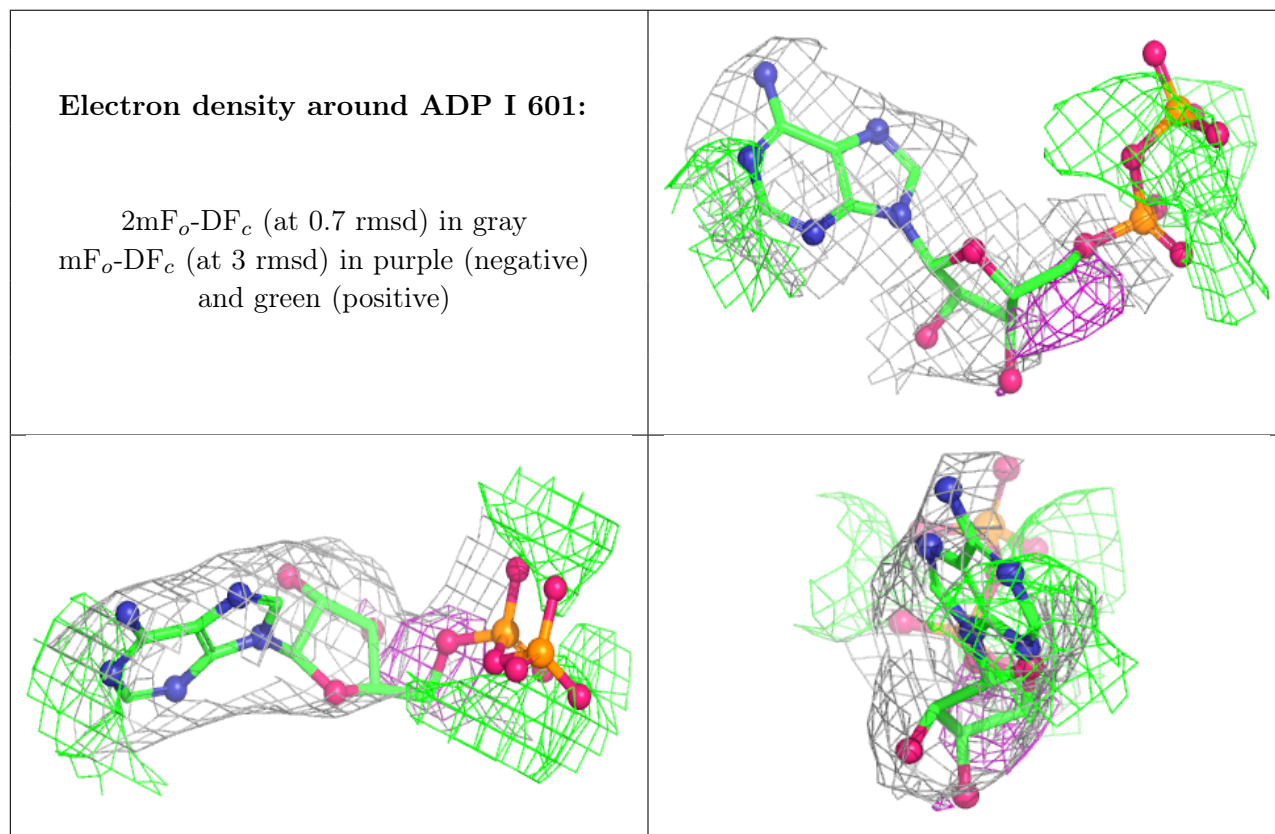
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	K	K	604	1/1	0.86	0.08	125,125,125,125	0
6	K	F	604	1/1	0.86	0.06	109,109,109,109	0
5	MG	N	603	1/1	0.86	0.18	113,113,113,113	0
5	MG	J	603	1/1	0.86	0.15	126,126,126,126	0
6	K	D	604	1/1	0.87	0.07	146,146,146,146	0
6	K	J	604	1/1	0.88	0.09	175,175,175,175	0
5	MG	L	603	1/1	0.88	0.17	96,96,96,96	0
5	MG	I	603	1/1	0.90	0.06	88,88,88,88	0
3	ADP	I	601	27/27	0.90	0.11	80,98,130,150	0
5	MG	E	603	1/1	0.91	0.18	81,81,81,81	0
5	MG	H	603	1/1	0.91	0.15	108,108,108,108	0
3	ADP	H	601	27/27	0.91	0.09	94,107,127,155	0
5	MG	A	603	1/1	0.92	0.11	91,91,91,91	0
3	ADP	E	601	27/27	0.92	0.10	94,113,134,148	0
3	ADP	A	601	27/27	0.92	0.10	93,104,133,145	0
6	K	G	604	1/1	0.92	0.06	89,89,89,89	0
4	BEF	K	602	4/4	0.92	0.10	98,98,99,101	0
5	MG	D	603	1/1	0.92	0.16	100,100,100,100	0
4	BEF	A	602	4/4	0.92	0.12	90,92,97,118	0
3	ADP	J	601	27/27	0.92	0.10	102,117,140,171	0
3	ADP	B	601	27/27	0.93	0.11	106,130,146,162	0
3	ADP	L	601	27/27	0.93	0.11	99,111,138,158	0
4	BEF	N	602	4/4	0.93	0.11	112,114,127,132	0
6	K	I	604	1/1	0.93	0.06	99,99,99,99	0
3	ADP	G	601	27/27	0.93	0.09	68,80,133,147	0
4	BEF	D	602	4/4	0.93	0.07	97,97,100,102	0
4	BEF	B	602	4/4	0.93	0.10	107,117,121,127	0
3	ADP	M	601	27/27	0.93	0.09	89,94,126,146	0
3	ADP	D	601	27/27	0.93	0.09	99,110,128,151	0
3	ADP	C	601	27/27	0.93	0.09	84,98,105,185	0
3	ADP	F	601	27/27	0.94	0.09	102,110,128,155	0
3	ADP	K	601	27/27	0.94	0.08	103,118,133,149	0
6	K	M	604	1/1	0.95	0.05	110,110,110,110	0
6	K	L	604	1/1	0.95	0.07	115,115,115,115	0
5	MG	K	603	1/1	0.95	0.09	96,96,96,96	0
4	BEF	L	602	4/4	0.95	0.09	103,105,108,114	0
4	BEF	H	602	4/4	0.95	0.11	114,124,133,134	0
4	BEF	G	602	4/4	0.95	0.06	70,76,92,93	0
3	ADP	N	601	27/27	0.95	0.08	118,124,137,159	0
6	K	H	604	1/1	0.95	0.04	132,132,132,132	0
4	BEF	C	602	4/4	0.96	0.06	88,88,89,89	0
4	BEF	F	602	4/4	0.96	0.06	105,108,112,118	0

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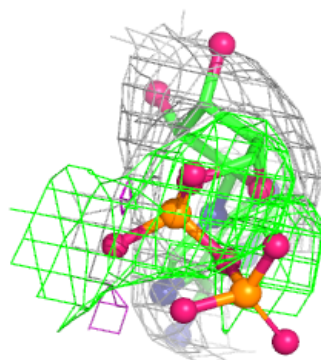
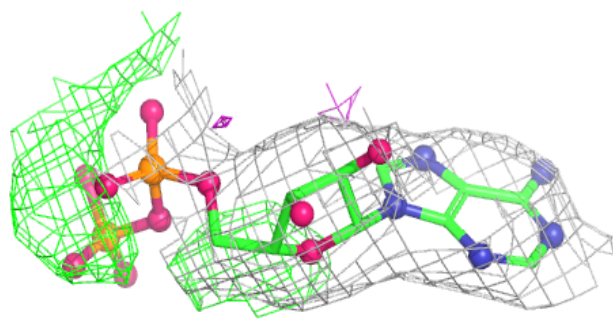
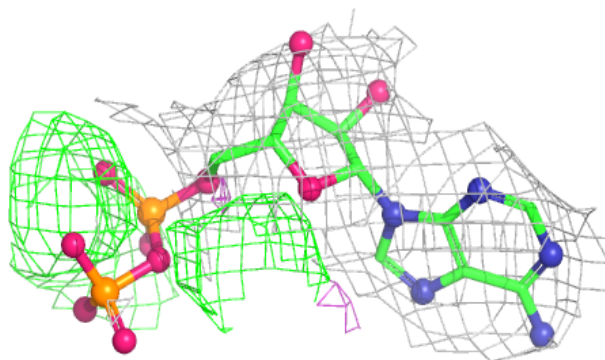
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BEF	E	602	4/4	0.96	0.10	83,85,85,93	0
4	BEF	M	602	4/4	0.96	0.08	94,96,97,104	0
6	K	A	604	1/1	0.96	0.09	151,151,151,151	0
4	BEF	I	602	4/4	0.97	0.06	76,77,98,100	0
4	BEF	J	602	4/4	0.97	0.07	101,102,118,121	0
6	K	B	604	1/1	0.97	0.04	130,130,130,130	0
6	K	N	604	1/1	0.97	0.10	141,141,141,141	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.

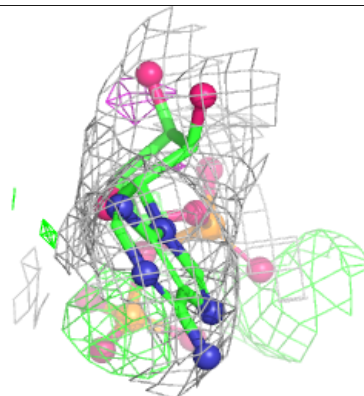
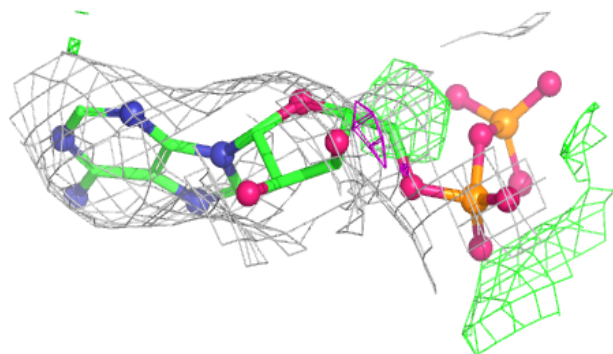
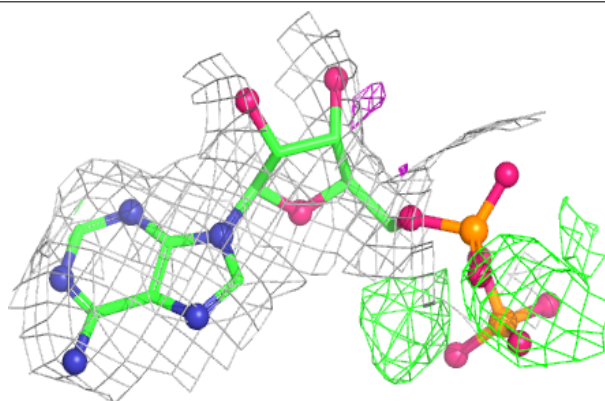


Electron density around ADP H 601:

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

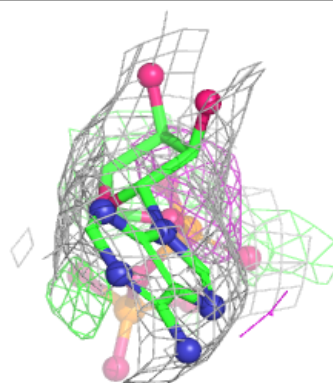
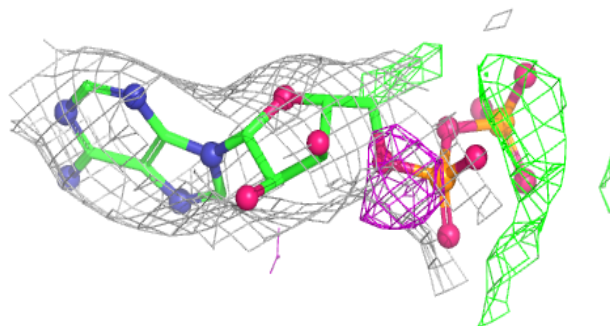
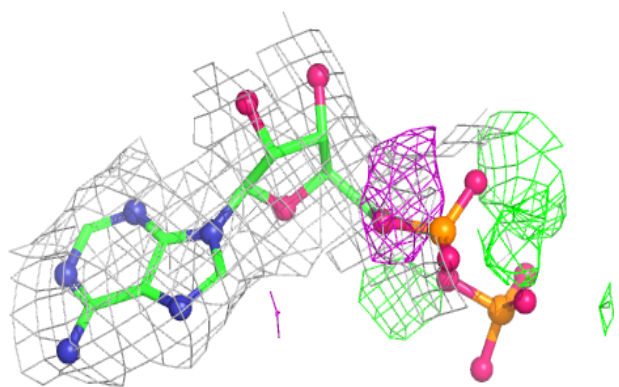
**Electron density around ADP E 601:**

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

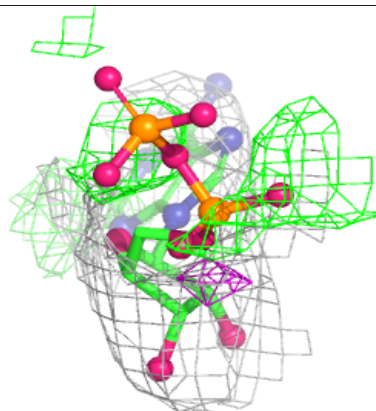
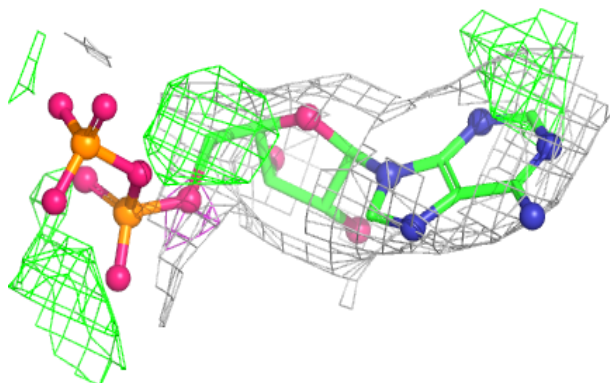
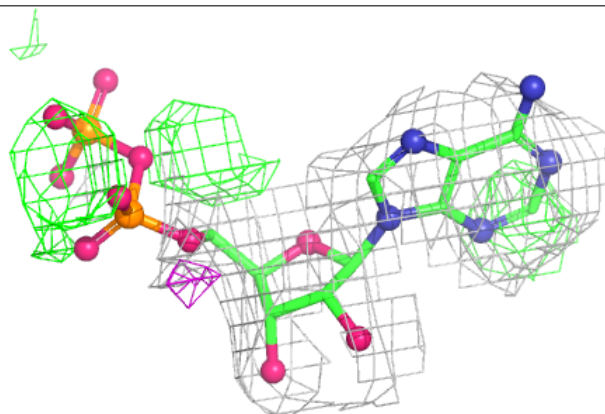


Electron density around ADP A 601:

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

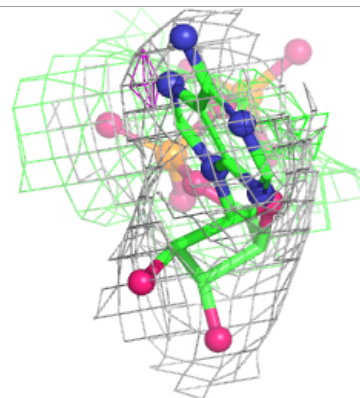
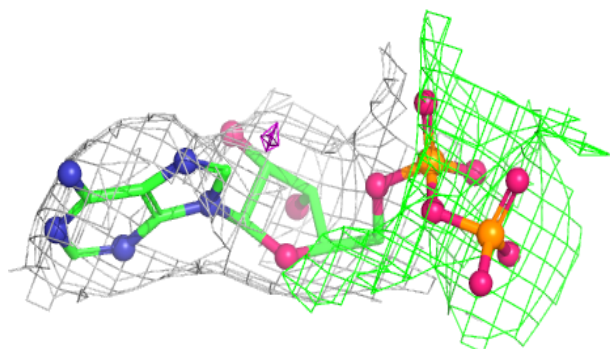
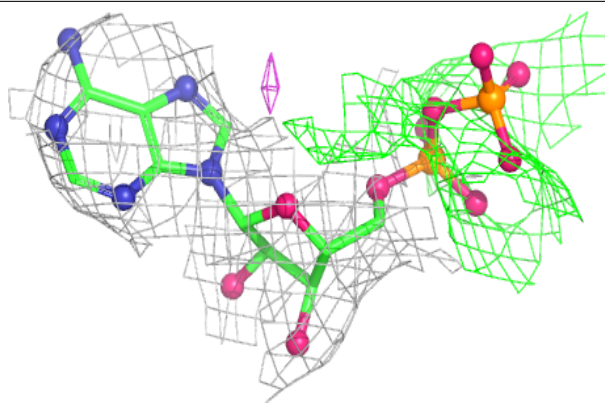
**Electron density around ADP J 601:**

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and green (positive)

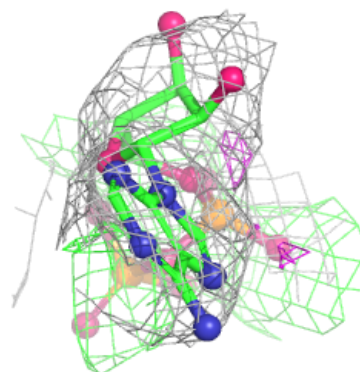
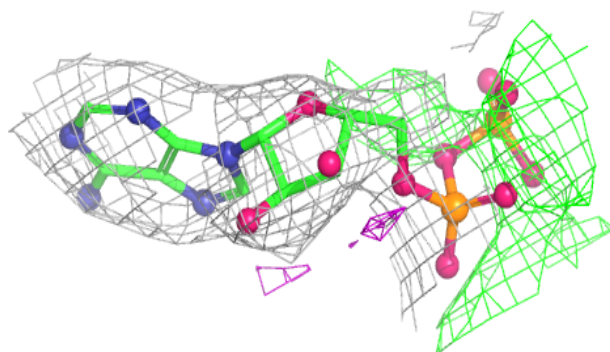
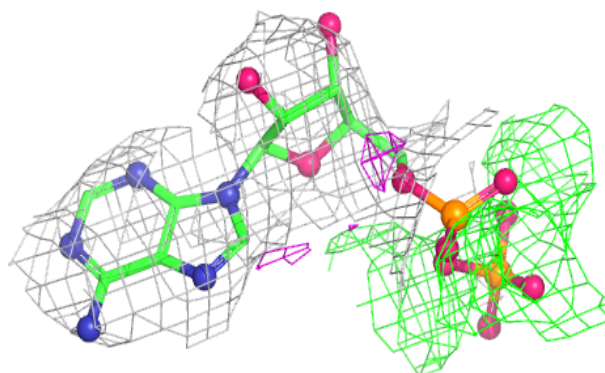


Electron density around ADP B 601:

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and green (positive)

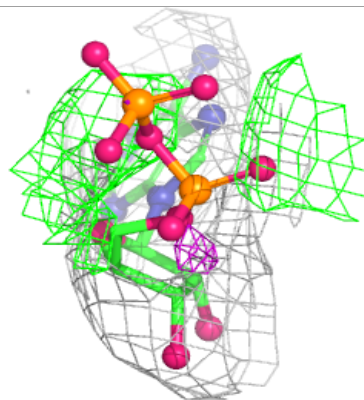
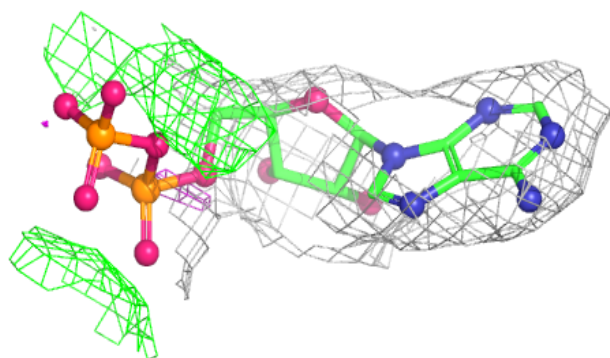
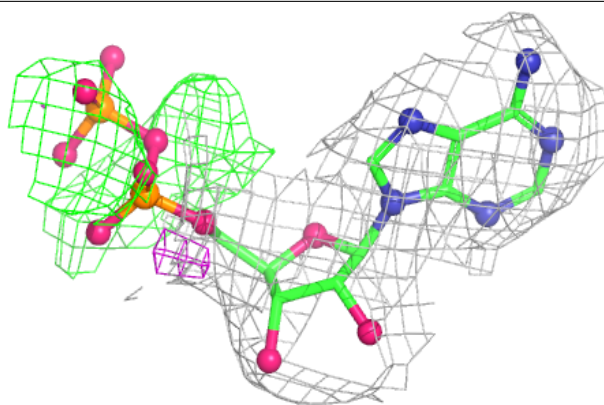
**Electron density around ADP L 601:**

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and green (positive)

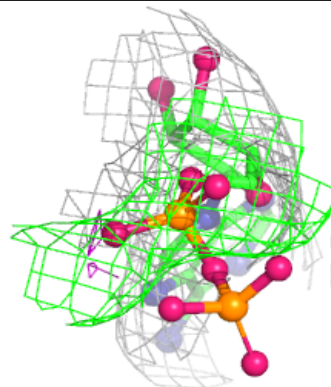
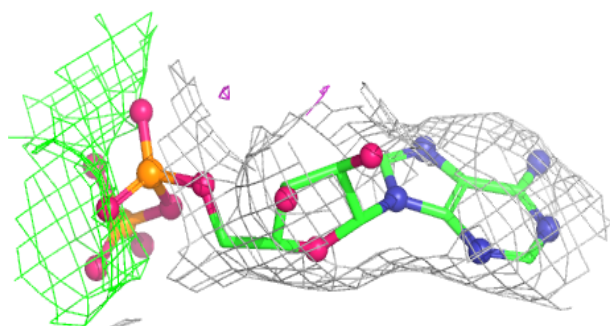
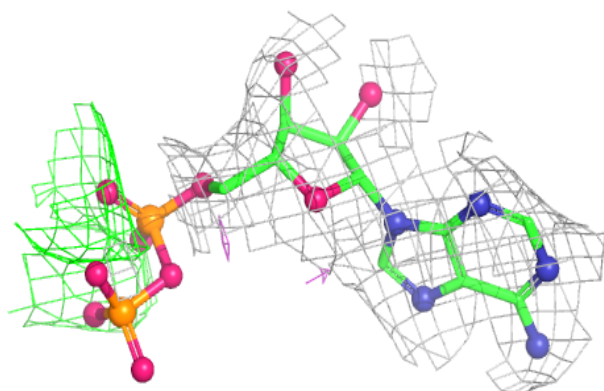


Electron density around ADP G 601:

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and green (positive)

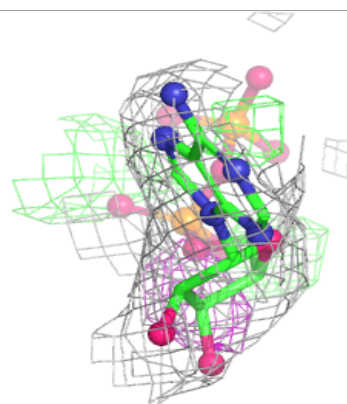
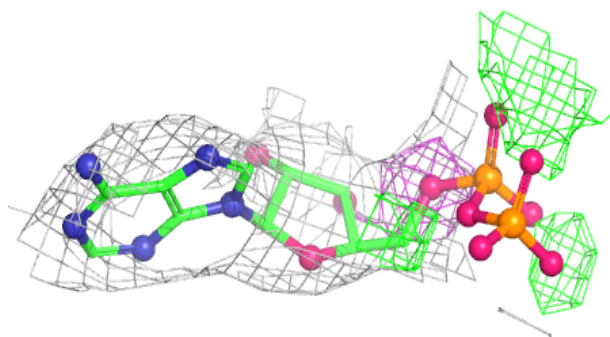
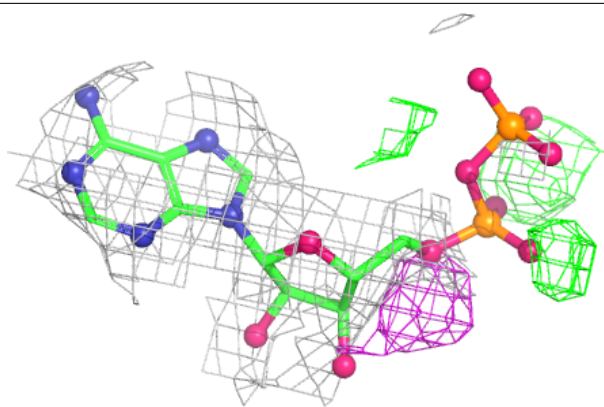
**Electron density around ADP M 601:**

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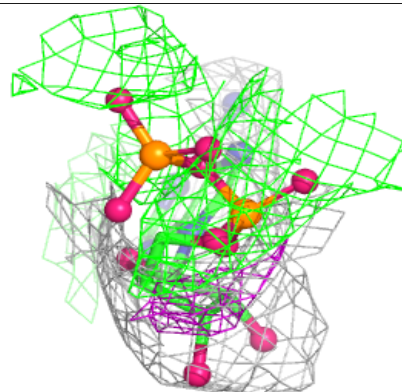
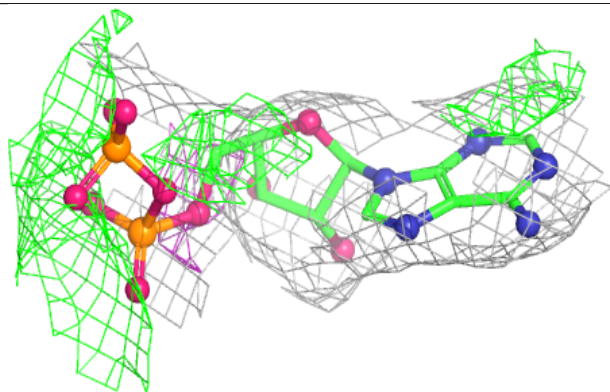
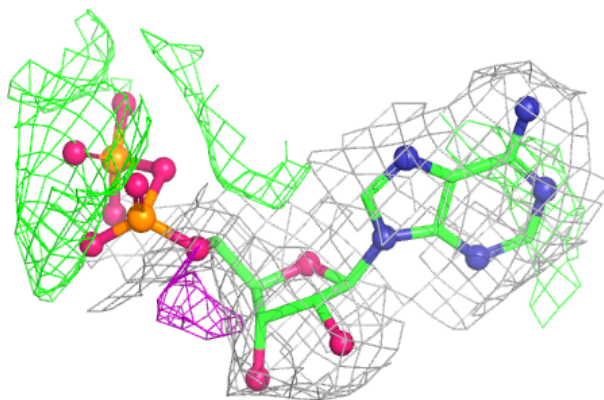


Electron density around ADP D 601:

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

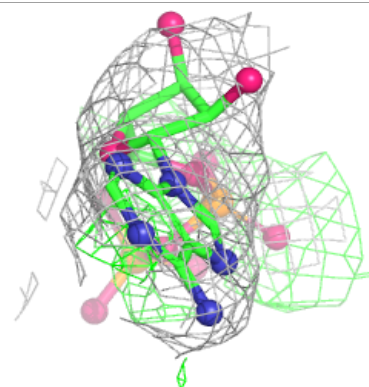
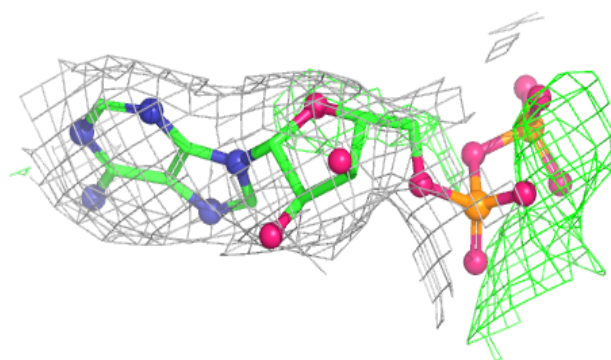
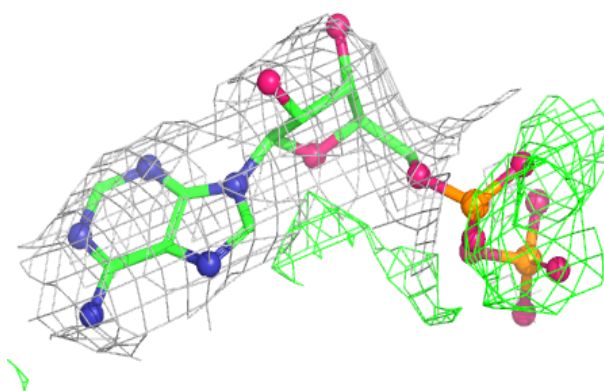
**Electron density around ADP C 601:**

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

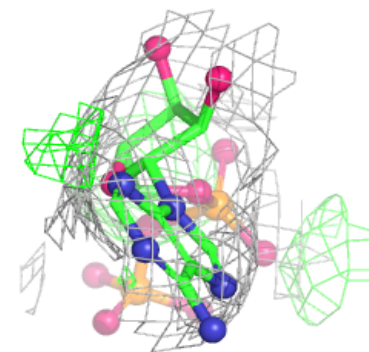
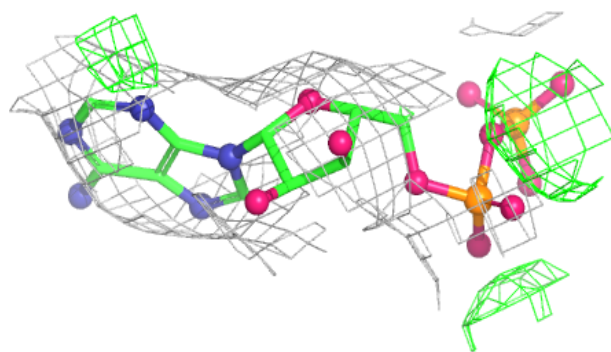
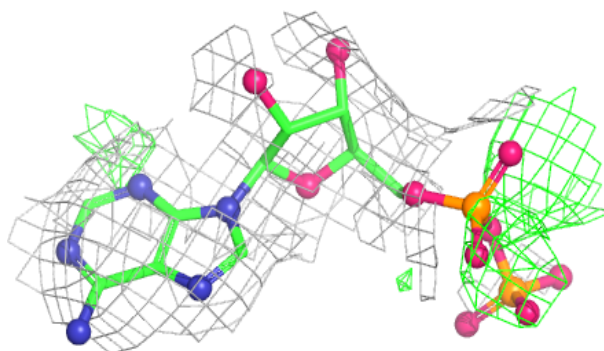


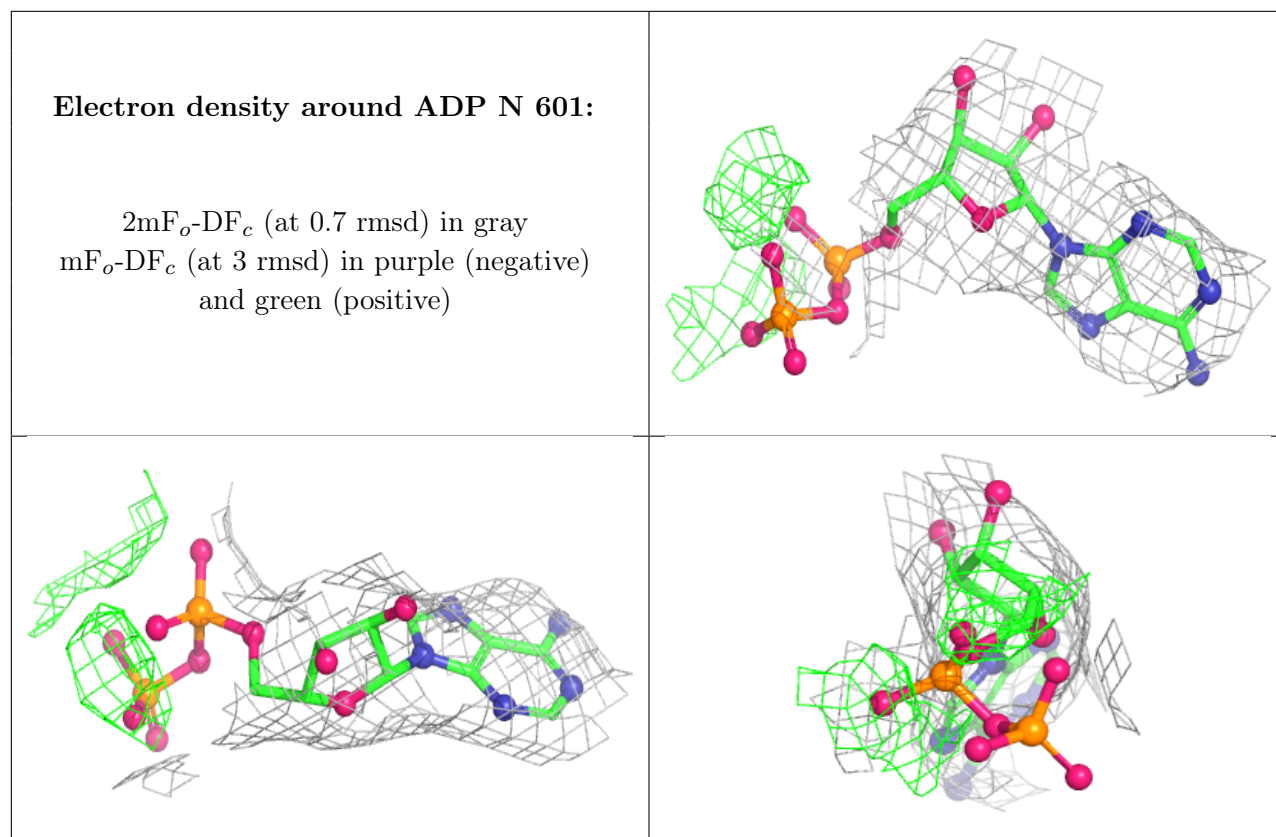
Electron density around ADP F 601:

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

**Electron density around ADP K 601:**

$2mF_o-DF_c$ (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.