



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 01:56 AM UTC

PDB ID : 8FWI / pdb_00008fwi
EMDB ID : EMD-29505
Title : Structure of dodecameric KaiC-RS-S413E/S414E solved by cryo-EM
Authors : Padua, R.A.P.; Grant, T.; Pitsawong, W.; Hoemberger, M.S.; Otten, R.; Bradshaw, N.; Grigorieff, N.; Kern, D.
Deposited on : 2023-01-22
Resolution : 2.90 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

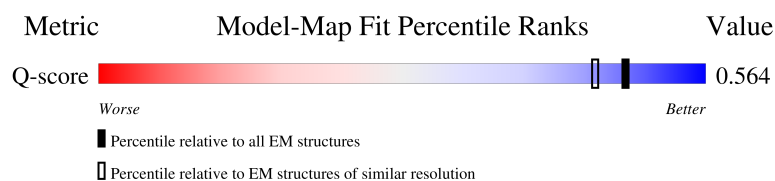
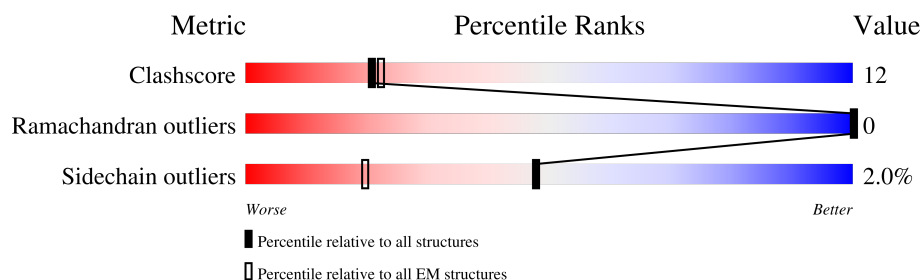
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



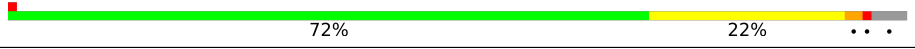
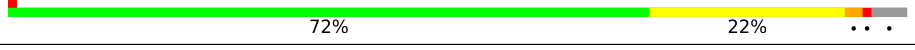
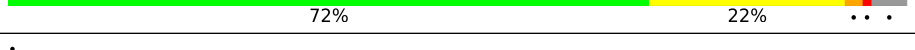
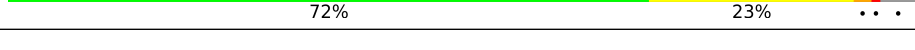
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	568	
1	B	568	
1	C	568	
1	D	568	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	568	
1	F	568	
1	G	568	
1	H	568	
1	I	568	
1	J	568	
1	K	568	
1	L	568	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 103188 atoms, of which 51324 are hydrogens and 0 are deuteriums.

In the tables below, 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 Circadian clock protein KaiC.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	B	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	C	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	D	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	E	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	F	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	G	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	H	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	I	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	J	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	K	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		
1	L	548	Total	C	H	N	O	S	0	0
			8511	2665	4255	773	802	16		

There are 48 discrepancies between the modelled and reference sequences:

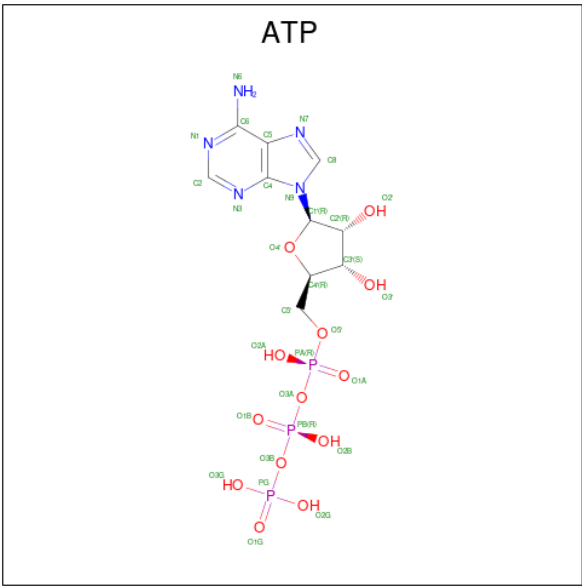
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B9KWX8
A	0	ALA	-	expression tag	UNP B9KWX8
A	413	GLU	SER	engineered mutation	UNP B9KWX8
A	414	GLU	SER	engineered mutation	UNP B9KWX8
B	-1	GLY	-	expression tag	UNP B9KWX8
B	0	ALA	-	expression tag	UNP B9KWX8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	413	GLU	SER	engineered mutation	UNP B9KWX8
B	414	GLU	SER	engineered mutation	UNP B9KWX8
C	-1	GLY	-	expression tag	UNP B9KWX8
C	0	ALA	-	expression tag	UNP B9KWX8
C	413	GLU	SER	engineered mutation	UNP B9KWX8
C	414	GLU	SER	engineered mutation	UNP B9KWX8
D	-1	GLY	-	expression tag	UNP B9KWX8
D	0	ALA	-	expression tag	UNP B9KWX8
D	413	GLU	SER	engineered mutation	UNP B9KWX8
D	414	GLU	SER	engineered mutation	UNP B9KWX8
E	-1	GLY	-	expression tag	UNP B9KWX8
E	0	ALA	-	expression tag	UNP B9KWX8
E	413	GLU	SER	engineered mutation	UNP B9KWX8
E	414	GLU	SER	engineered mutation	UNP B9KWX8
F	-1	GLY	-	expression tag	UNP B9KWX8
F	0	ALA	-	expression tag	UNP B9KWX8
F	413	GLU	SER	engineered mutation	UNP B9KWX8
F	414	GLU	SER	engineered mutation	UNP B9KWX8
G	-1	GLY	-	expression tag	UNP B9KWX8
G	0	ALA	-	expression tag	UNP B9KWX8
G	413	GLU	SER	engineered mutation	UNP B9KWX8
G	414	GLU	SER	engineered mutation	UNP B9KWX8
H	-1	GLY	-	expression tag	UNP B9KWX8
H	0	ALA	-	expression tag	UNP B9KWX8
H	413	GLU	SER	engineered mutation	UNP B9KWX8
H	414	GLU	SER	engineered mutation	UNP B9KWX8
I	-1	GLY	-	expression tag	UNP B9KWX8
I	0	ALA	-	expression tag	UNP B9KWX8
I	413	GLU	SER	engineered mutation	UNP B9KWX8
I	414	GLU	SER	engineered mutation	UNP B9KWX8
J	-1	GLY	-	expression tag	UNP B9KWX8
J	0	ALA	-	expression tag	UNP B9KWX8
J	413	GLU	SER	engineered mutation	UNP B9KWX8
J	414	GLU	SER	engineered mutation	UNP B9KWX8
K	-1	GLY	-	expression tag	UNP B9KWX8
K	0	ALA	-	expression tag	UNP B9KWX8
K	413	GLU	SER	engineered mutation	UNP B9KWX8
K	414	GLU	SER	engineered mutation	UNP B9KWX8
L	-1	GLY	-	expression tag	UNP B9KWX8
L	0	ALA	-	expression tag	UNP B9KWX8
L	413	GLU	SER	engineered mutation	UNP B9KWX8
L	414	GLU	SER	engineered mutation	UNP B9KWX8

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	B	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	C	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	D	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	E	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	F	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	G	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	H	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	I	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	J	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	K	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
2	L	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	B	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	C	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	D	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	E	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	F	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	G	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	H	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	I	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	J	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	K	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
3	L	1	Total 38	C 10	H 11	N 5	O 10	P 2	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total 2	Mg 2	0
4	B	2	Total 2	Mg 2	0
4	C	2	Total 2	Mg 2	0
4	D	2	Total 2	Mg 2	0
4	E	2	Total 2	Mg 2	0
4	F	2	Total 2	Mg 2	0
4	G	2	Total 2	Mg 2	0
4	H	2	Total 2	Mg 2	0
4	I	2	Total 2	Mg 2	0
4	J	2	Total 2	Mg 2	0
4	K	2	Total 2	Mg 2	0
4	L	2	Total 2	Mg 2	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	5	Total 5	O 5	0
5	B	6	Total 6	O 6	0
5	C	6	Total 6	O 6	0
5	D	6	Total 6	O 6	0
5	E	6	Total 6	O 6	0
5	F	6	Total 6	O 6	0
5	G	6	Total 6	O 6	0
5	H	6	Total 6	O 6	0

Continued on next page...

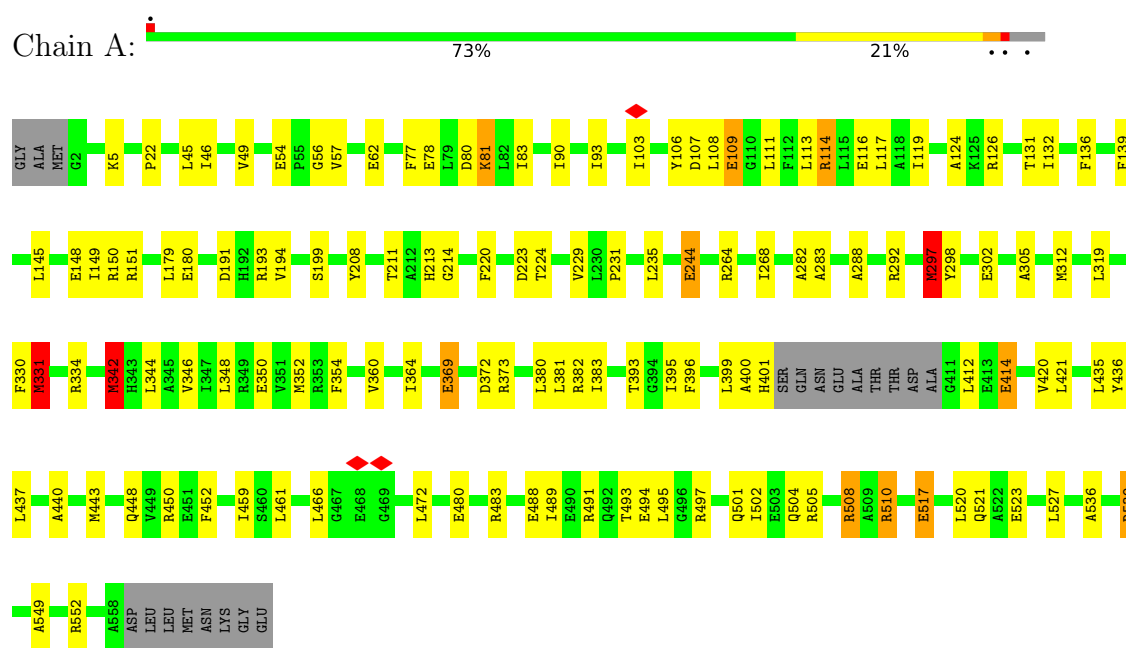
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
5	I	5	Total 5	O 5	0
5	J	6	Total 6	O 6	0
5	K	7	Total 7	O 7	0
5	L	7	Total 7	O 7	0

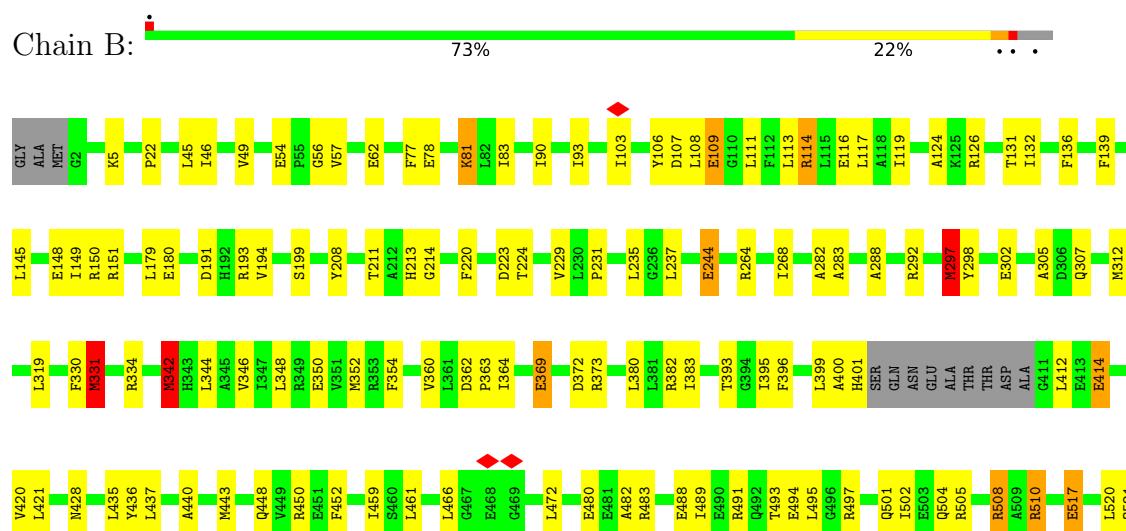
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Circadian clock protein KaiC

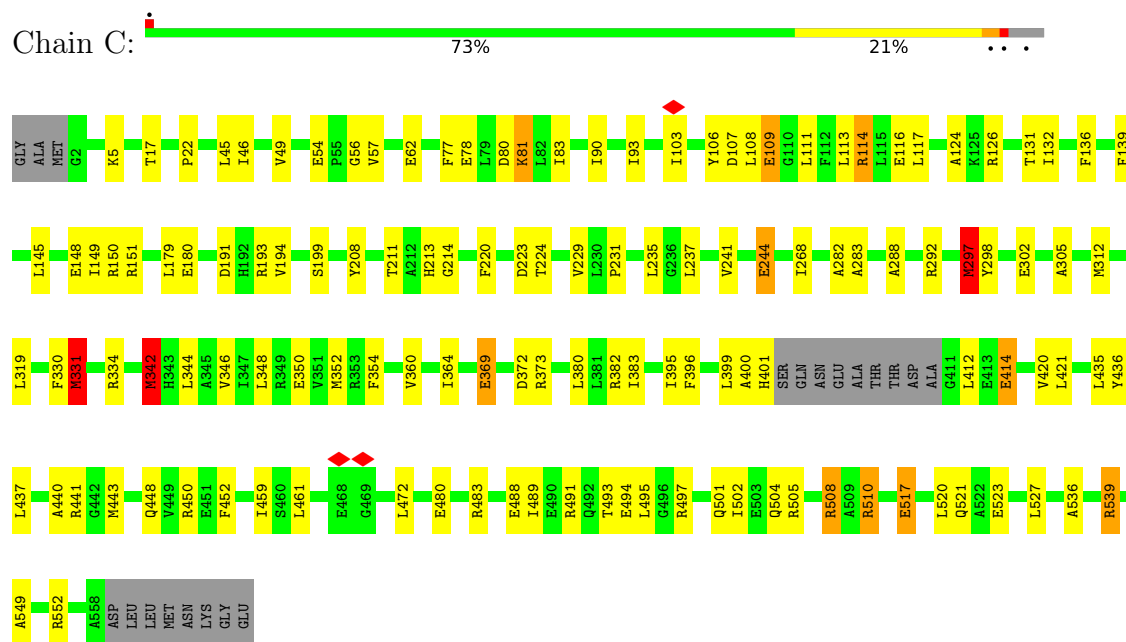


• Molecule 1: Circadian clock protein KaiC

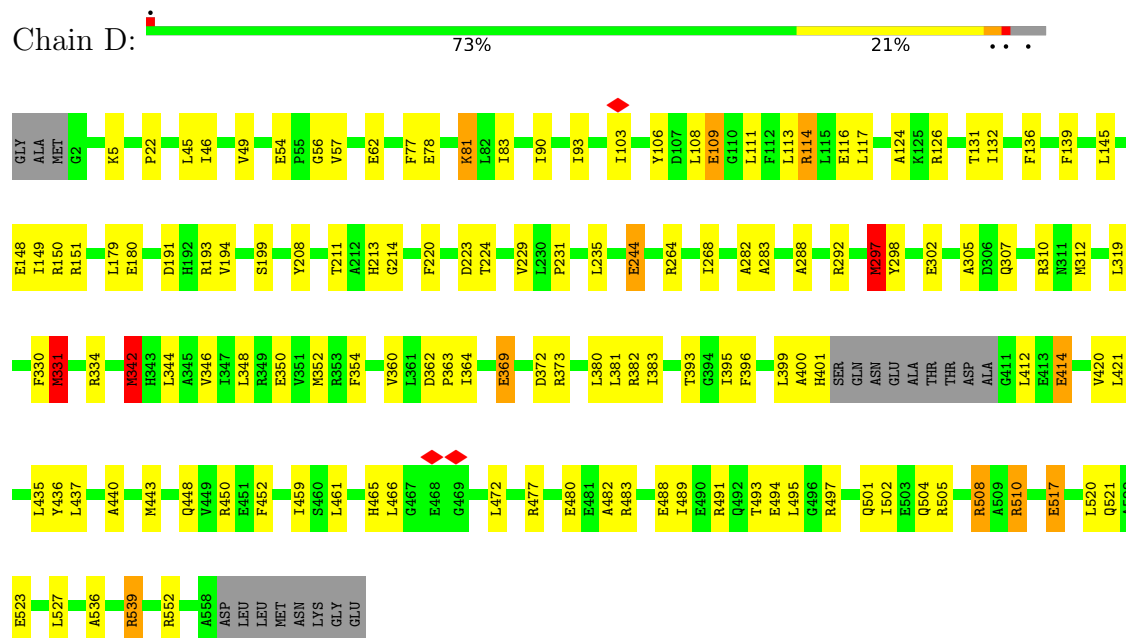




• Molecule 1: Circadian clock protein KaiC

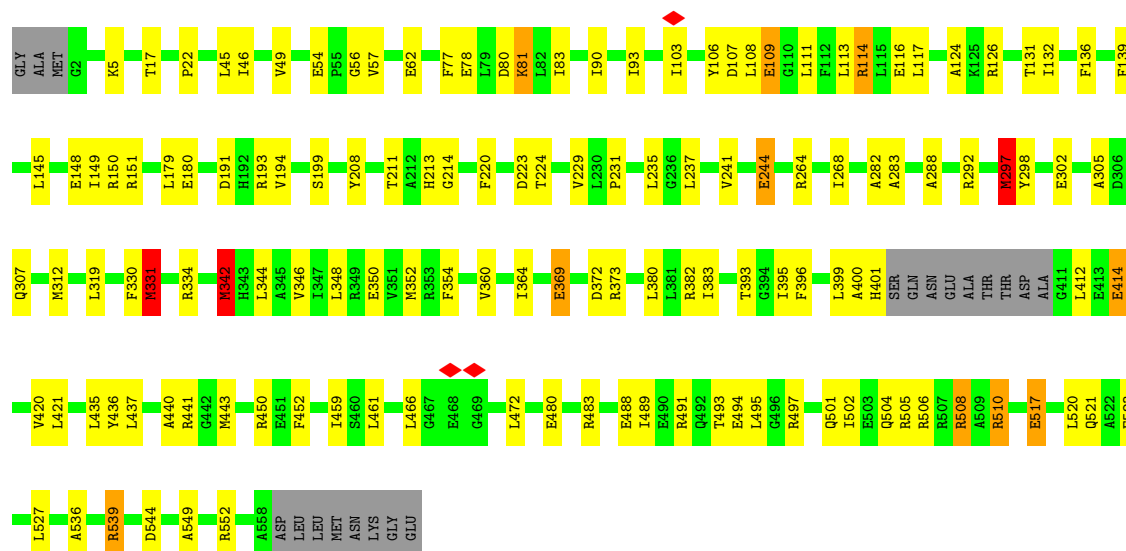


• Molecule 1: Circadian clock protein KaiC



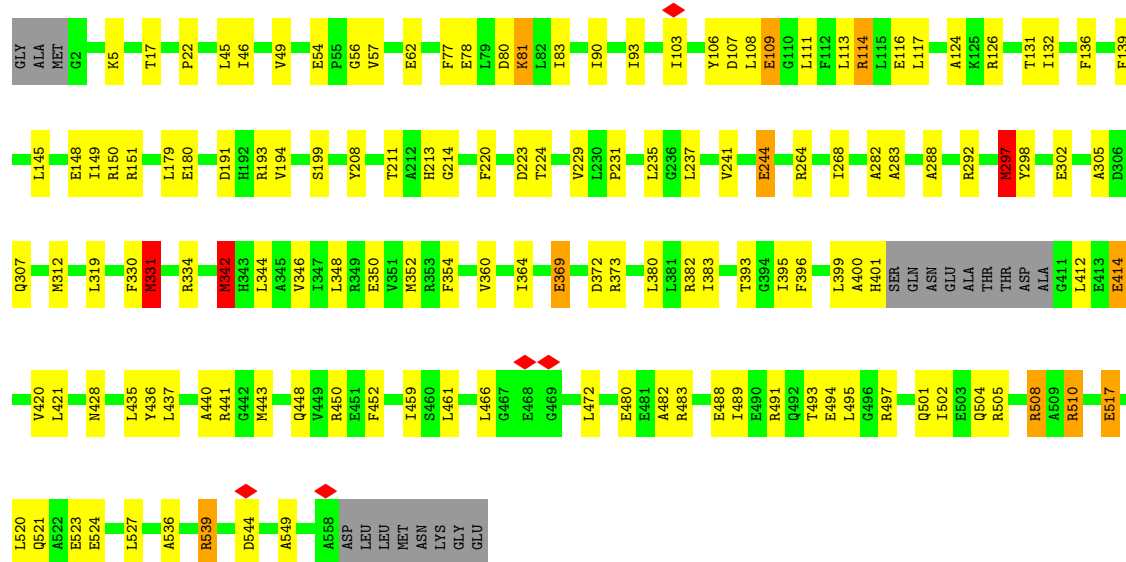
• Molecule 1: Circadian clock protein KaiC





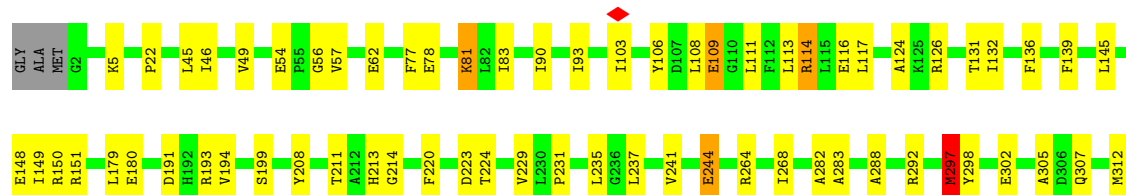
• Molecule 1: Circadian clock protein KaiC

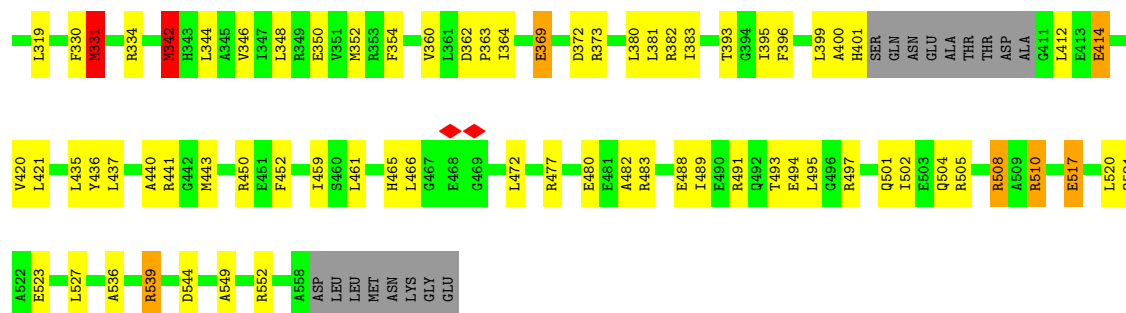
Chain F: 72% 22%



• Molecule 1: Circadian clock protein KaiC

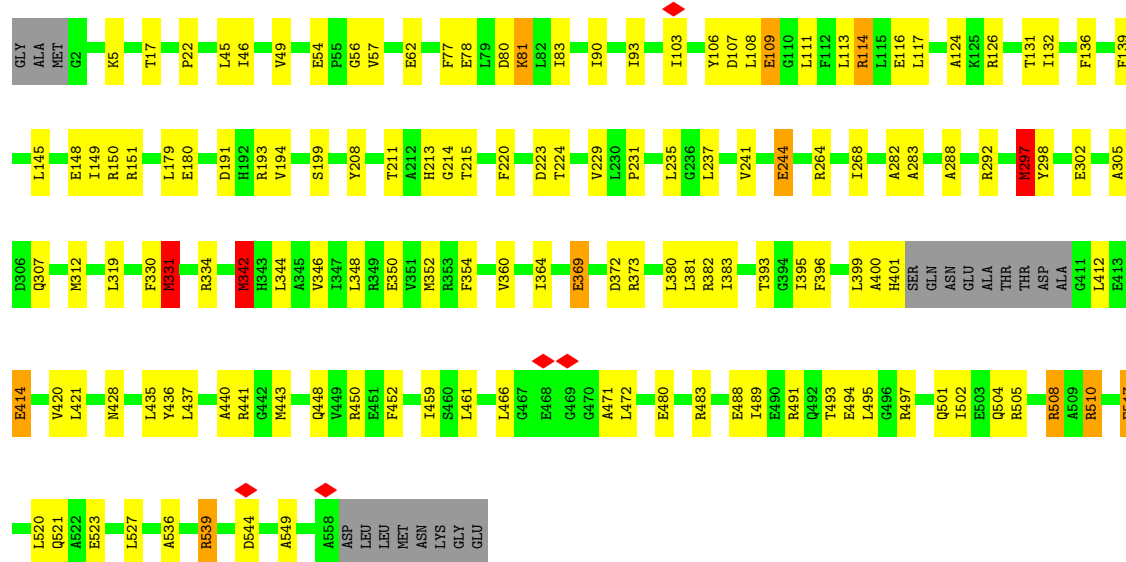
Chain G: 72% 22%





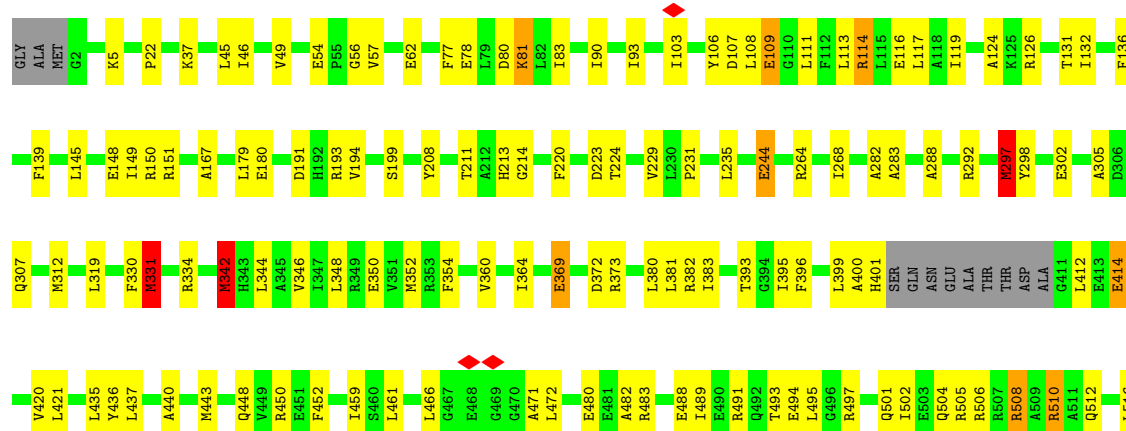
• Molecule 1: Circadian clock protein KaiC

Chain H: 72% 22%



• Molecule 1: Circadian clock protein KaiC

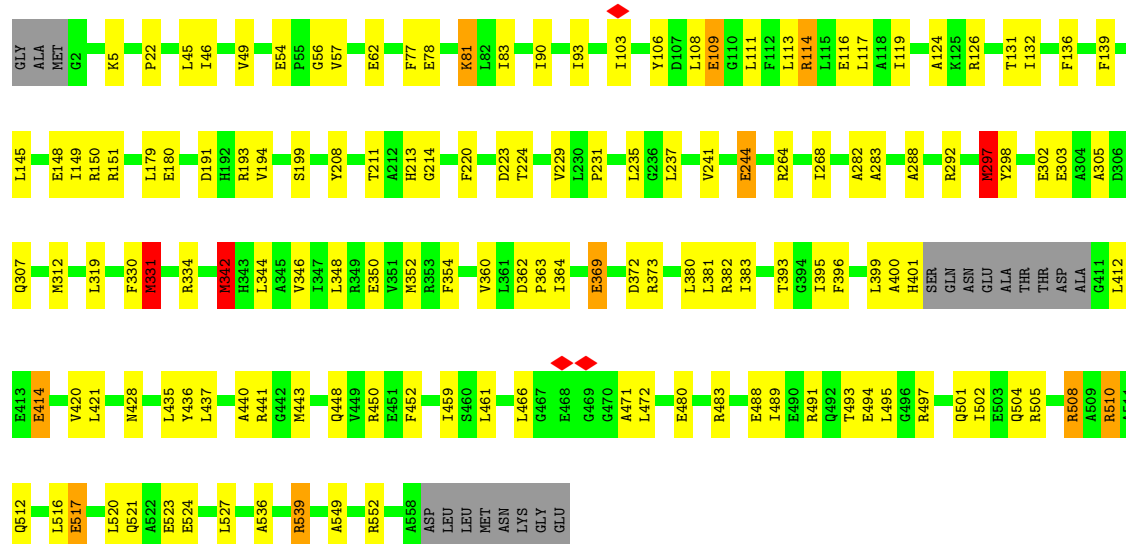
Chain I: 72% 22%





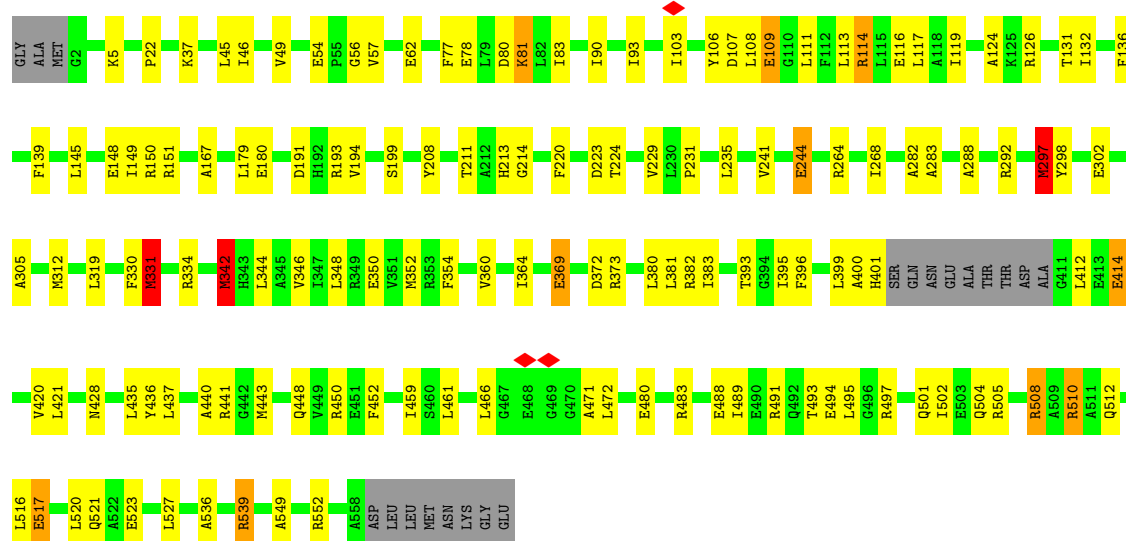
• Molecule 1: Circadian clock protein KaiC

Chain J: 71% 23%



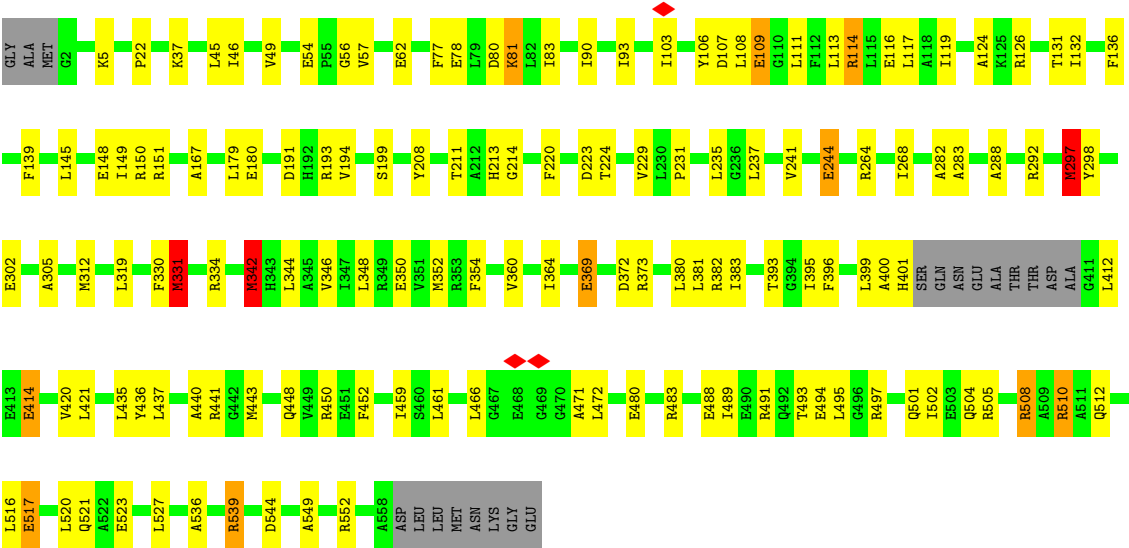
• Molecule 1: Circadian clock protein KaiC

Chain K: 72% 22%



• Molecule 1: Circadian clock protein KaiC

Chain L: 72% 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	320000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.134	Depositor
Minimum map value	-0.477	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	378, 378, 378	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, 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	0.31	0/4321	0.59	11/5824 (0.2%)
1	B	0.31	0/4321	0.59	11/5824 (0.2%)
1	C	0.31	0/4321	0.59	11/5824 (0.2%)
1	D	0.31	0/4321	0.59	11/5824 (0.2%)
1	E	0.31	0/4321	0.59	11/5824 (0.2%)
1	F	0.31	0/4321	0.59	11/5824 (0.2%)
1	G	0.31	0/4321	0.59	11/5824 (0.2%)
1	H	0.31	0/4321	0.59	11/5824 (0.2%)
1	I	0.31	0/4321	0.59	11/5824 (0.2%)
1	J	0.31	0/4321	0.59	11/5824 (0.2%)
1	K	0.31	0/4321	0.59	11/5824 (0.2%)
1	L	0.31	0/4321	0.59	11/5824 (0.2%)
All	All	0.31	0/51852	0.59	132/69888 (0.2%)

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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3
1	J	0	3
1	K	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	3
All	All	0	36

There are no bond length outliers.

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	510	ARG	CB-CG-CD	9.56	133.29	111.30
1	H	510	ARG	CB-CG-CD	9.55	133.27	111.30
1	F	510	ARG	CB-CG-CD	9.55	133.26	111.30
1	B	510	ARG	CB-CG-CD	9.54	133.25	111.30
1	G	510	ARG	CB-CG-CD	9.54	133.24	111.30

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ARG	Sidechain
1	A	508	ARG	Sidechain
1	A	539	ARG	Sidechain
1	B	114	ARG	Sidechain
1	B	508	ARG	Sidechain

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	4256	4255	4256	109	0
1	B	4256	4255	4256	111	0
1	C	4256	4255	4256	108	0
1	D	4256	4255	4256	112	0
1	E	4256	4255	4256	115	0
1	F	4256	4255	4256	121	0
1	G	4256	4255	4256	114	0
1	H	4256	4255	4256	116	0
1	I	4256	4255	4256	119	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	4256	4255	4256	122	0
1	K	4256	4255	4256	114	0
1	L	4256	4255	4256	118	0
2	A	31	11	12	0	0
2	B	31	11	12	1	0
2	C	31	11	12	0	0
2	D	31	11	12	1	0
2	E	31	11	12	1	0
2	F	31	11	12	1	0
2	G	31	11	12	1	0
2	H	31	11	12	1	0
2	I	31	11	12	1	0
2	J	31	11	12	1	0
2	K	31	11	12	0	0
2	L	31	11	12	0	0
3	A	27	11	11	0	0
3	B	27	11	11	0	0
3	C	27	11	11	0	0
3	D	27	11	11	0	0
3	E	27	11	11	0	0
3	F	27	11	11	0	0
3	G	27	11	11	0	0
3	H	27	11	11	0	0
3	I	27	11	11	0	0
3	J	27	11	11	0	0
3	K	27	11	11	0	0
3	L	27	11	11	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	5	0	0	0	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	6	0	0	0	0
5	E	6	0	0	0	0
5	F	6	0	0	0	0
5	G	6	0	0	0	0
5	H	6	0	0	0	0
5	I	5	0	0	0	0
5	J	6	0	0	0	0
5	K	7	0	0	0	0
5	L	7	0	0	0	0
All	All	51864	51324	51348	1234	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 1234 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:E:466:LEU:HD21	1:F:549:ALA:HA	1.55	0.87
1:E:466:LEU:CD2	1:F:549:ALA:HA	2.05	0.86
1:I:466:LEU:HD21	1:J:549:ALA:HA	1.62	0.79
1:G:466:LEU:HD21	1:H:549:ALA:HA	1.64	0.79
1:K:549:ALA:HA	1:L:466:LEU:HD21	1.65	0.78

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
1	B	544/568 (96%)	534 (98%)	10 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
1	D	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
1	E	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
1	F	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
1	G	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
1	H	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
1	I	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
1	J	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
1	K	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
1	L	544/568 (96%)	534 (98%)	10 (2%)	0	100	100
All	All	6528/6816 (96%)	6408 (98%)	120 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	442/457 (97%)	433 (98%)	9 (2%)	48	78
1	B	442/457 (97%)	433 (98%)	9 (2%)	48	78
1	C	442/457 (97%)	433 (98%)	9 (2%)	48	78
1	D	442/457 (97%)	433 (98%)	9 (2%)	48	78
1	E	442/457 (97%)	433 (98%)	9 (2%)	48	78
1	F	442/457 (97%)	433 (98%)	9 (2%)	48	78
1	G	442/457 (97%)	433 (98%)	9 (2%)	48	78
1	H	442/457 (97%)	433 (98%)	9 (2%)	48	78
1	I	442/457 (97%)	433 (98%)	9 (2%)	48	78
1	J	442/457 (97%)	433 (98%)	9 (2%)	48	78
1	K	442/457 (97%)	433 (98%)	9 (2%)	48	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	442/457 (97%)	433 (98%)	9 (2%)	48 78
All	All	5304/5484 (97%)	5196 (98%)	108 (2%)	48 78

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	297	MET
1	H	517	GLU
1	L	109	GLU
1	G	342	MET
1	H	244	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	432	ASN
1	K	432	ASN
1	L	197	GLN
1	J	432	ASN
1	E	512	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 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	$\# Z > 2$
2	ATP	F	601	4	32,33,33	3.57	15 (46%)	48,52,52	2.06	15 (31%)
2	ATP	I	601	4	32,33,33	3.57	15 (46%)	48,52,52	2.06	15 (31%)
3	ADP	L	602	4	28,29,29	3.03	10 (35%)	43,45,45	2.71	12 (27%)
3	ADP	H	602	4	28,29,29	3.03	10 (35%)	43,45,45	2.70	12 (27%)
3	ADP	J	602	4	28,29,29	3.02	10 (35%)	43,45,45	2.71	11 (25%)
2	ATP	K	601	4	32,33,33	3.56	15 (46%)	48,52,52	2.06	15 (31%)
3	ADP	C	602	4	28,29,29	3.03	10 (35%)	43,45,45	2.70	12 (27%)
3	ADP	B	602	4	28,29,29	3.02	10 (35%)	43,45,45	2.70	11 (25%)
2	ATP	G	601	4	32,33,33	3.58	15 (46%)	48,52,52	2.06	15 (31%)
2	ATP	J	601	4	32,33,33	3.56	15 (46%)	48,52,52	2.06	15 (31%)
3	ADP	E	602	4	28,29,29	3.03	11 (39%)	43,45,45	2.71	11 (25%)
2	ATP	L	601	4	32,33,33	3.57	15 (46%)	48,52,52	2.06	15 (31%)
3	ADP	A	602	4	28,29,29	3.03	10 (35%)	43,45,45	2.71	12 (27%)
2	ATP	E	601	4	32,33,33	3.56	15 (46%)	48,52,52	2.07	15 (31%)
2	ATP	C	601	4	32,33,33	3.56	15 (46%)	48,52,52	2.06	15 (31%)
3	ADP	F	602	4	28,29,29	3.03	10 (35%)	43,45,45	2.71	12 (27%)
2	ATP	B	601	4	32,33,33	3.56	15 (46%)	48,52,52	2.06	15 (31%)
2	ATP	H	601	4	32,33,33	3.57	15 (46%)	48,52,52	2.06	15 (31%)
3	ADP	D	602	4	28,29,29	3.03	10 (35%)	43,45,45	2.71	12 (27%)
2	ATP	A	601	4	32,33,33	3.56	15 (46%)	48,52,52	2.06	15 (31%)
3	ADP	I	602	4	28,29,29	3.02	10 (35%)	43,45,45	2.71	11 (25%)
2	ATP	D	601	4	32,33,33	3.56	15 (46%)	48,52,52	2.06	15 (31%)
3	ADP	K	602	4	28,29,29	3.03	10 (35%)	43,45,45	2.70	12 (27%)
3	ADP	G	602	4	28,29,29	3.02	10 (35%)	43,45,45	2.71	12 (27%)

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
2	ATP	F	601	4	-	6/22/38/38	0/3/3/3
2	ATP	I	601	4	-	6/22/38/38	0/3/3/3
3	ADP	L	602	4	-	0/16/32/32	0/3/3/3
3	ADP	H	602	4	-	0/16/32/32	0/3/3/3
3	ADP	J	602	4	-	0/16/32/32	0/3/3/3
2	ATP	K	601	4	-	6/22/38/38	0/3/3/3
3	ADP	C	602	4	-	0/16/32/32	0/3/3/3
3	ADP	B	602	4	-	0/16/32/32	0/3/3/3
2	ATP	G	601	4	-	5/22/38/38	0/3/3/3
2	ATP	J	601	4	-	6/22/38/38	0/3/3/3
3	ADP	E	602	4	-	0/16/32/32	0/3/3/3
2	ATP	L	601	4	-	6/22/38/38	0/3/3/3
3	ADP	A	602	4	-	0/16/32/32	0/3/3/3
2	ATP	E	601	4	-	6/22/38/38	0/3/3/3
2	ATP	C	601	4	-	6/22/38/38	0/3/3/3
3	ADP	F	602	4	-	0/16/32/32	0/3/3/3
2	ATP	B	601	4	-	6/22/38/38	0/3/3/3
2	ATP	H	601	4	-	5/22/38/38	0/3/3/3
3	ADP	D	602	4	-	0/16/32/32	0/3/3/3
2	ATP	A	601	4	-	6/22/38/38	0/3/3/3
3	ADP	I	602	4	-	0/16/32/32	0/3/3/3
2	ATP	D	601	4	-	6/22/38/38	0/3/3/3
3	ADP	K	602	4	-	0/16/32/32	0/3/3/3
3	ADP	G	602	4	-	0/16/32/32	0/3/3/3

The worst 5 of 301 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	ATP	C2'-C3'	-10.64	1.24	1.53
2	I	601	ATP	C2'-C3'	-10.63	1.24	1.53
2	J	601	ATP	C2'-C3'	-10.62	1.24	1.53
2	H	601	ATP	C2'-C3'	-10.62	1.24	1.53
2	F	601	ATP	C2'-C3'	-10.61	1.24	1.53

The worst 5 of 320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	602	ADP	C1'-N9-C8	-8.67	107.85	127.09
3	D	602	ADP	C1'-N9-C8	-8.67	107.86	127.09
3	J	602	ADP	C1'-N9-C8	-8.67	107.86	127.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	602	ADP	C1'-N9-C8	-8.67	107.86	127.09
3	F	602	ADP	C1'-N9-C8	-8.66	107.87	127.09

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	PB-O3B-PG-O3G
2	A	601	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	PB-O3B-PG-O3G
2	B	601	ATP	C5'-O5'-PA-O1A
2	C	601	ATP	PB-O3B-PG-O3G

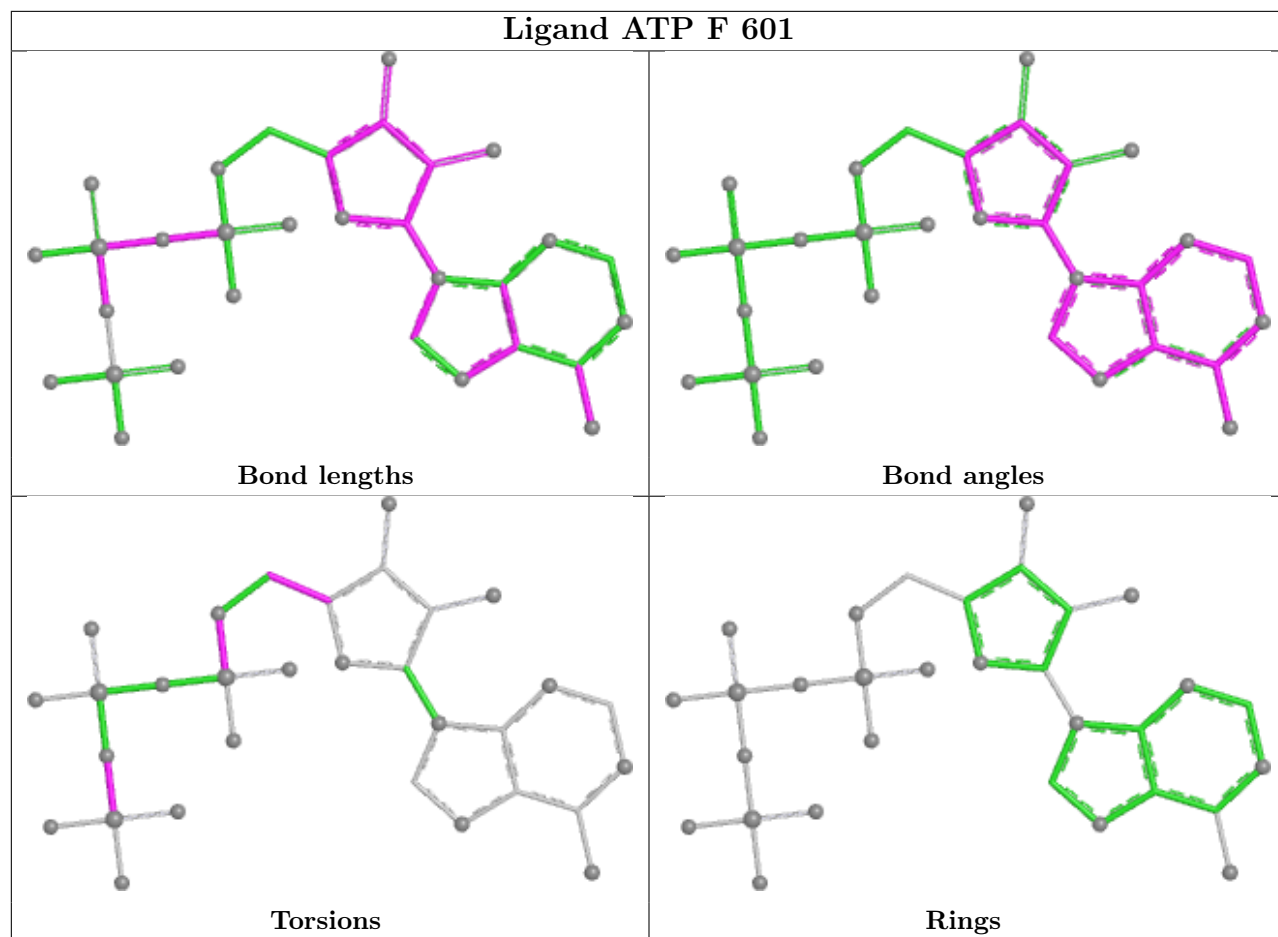
There are no ring outliers.

8 monomers are involved in 8 short contacts:

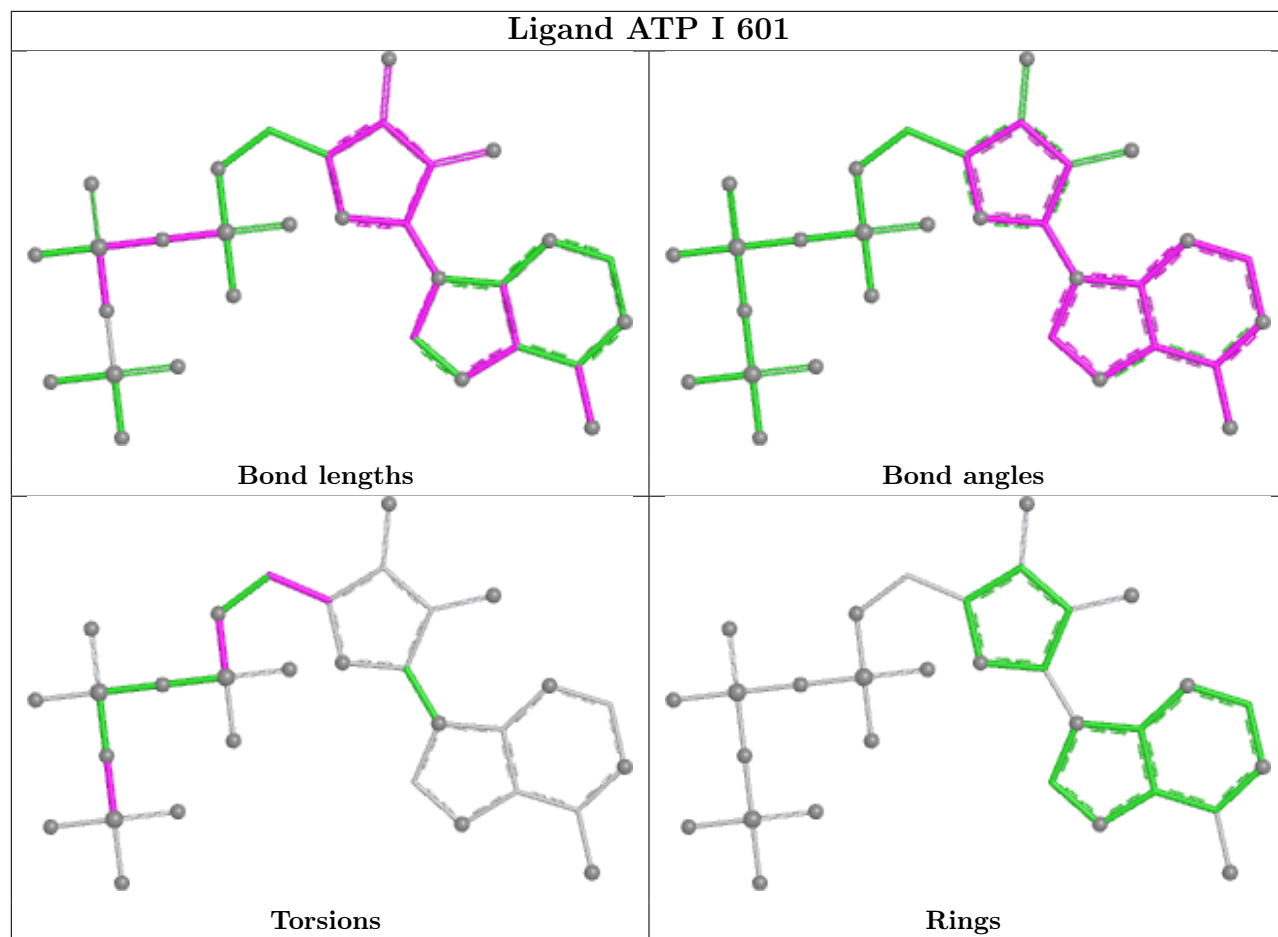
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	ATP	1	0
2	I	601	ATP	1	0
2	G	601	ATP	1	0
2	J	601	ATP	1	0
2	E	601	ATP	1	0
2	B	601	ATP	1	0
2	H	601	ATP	1	0
2	D	601	ATP	1	0

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.

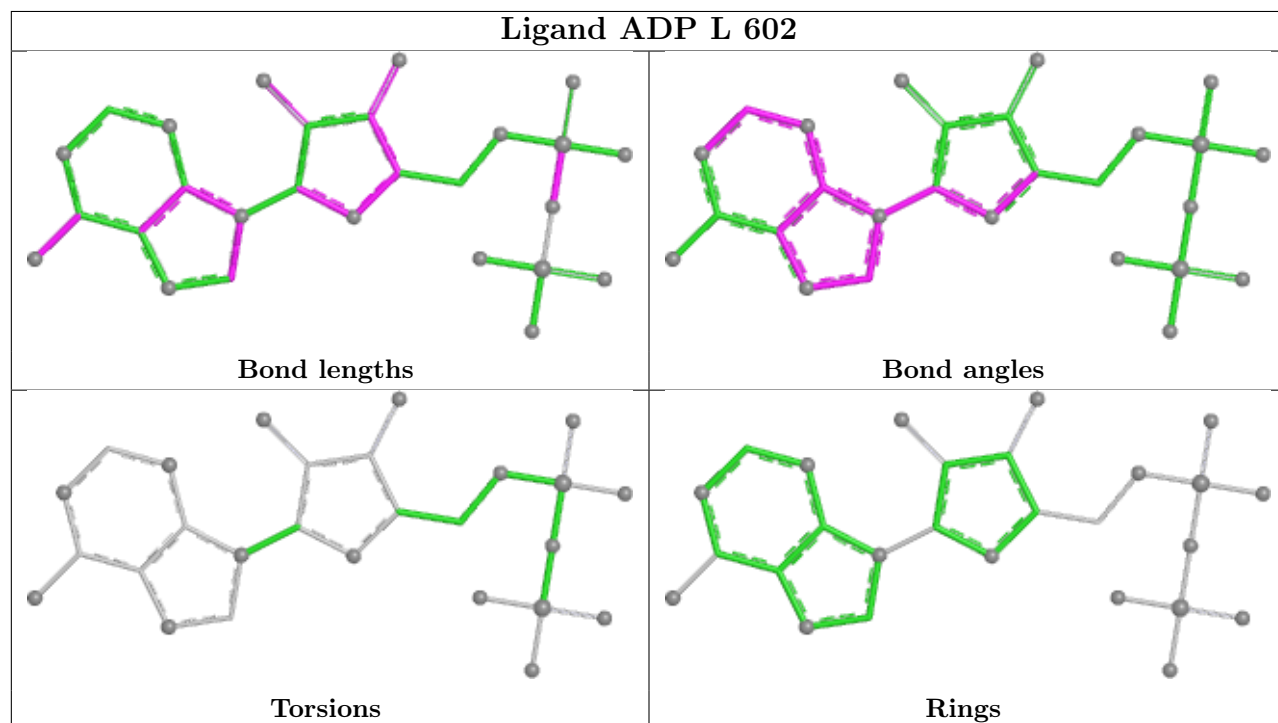
Ligand ATP F 601

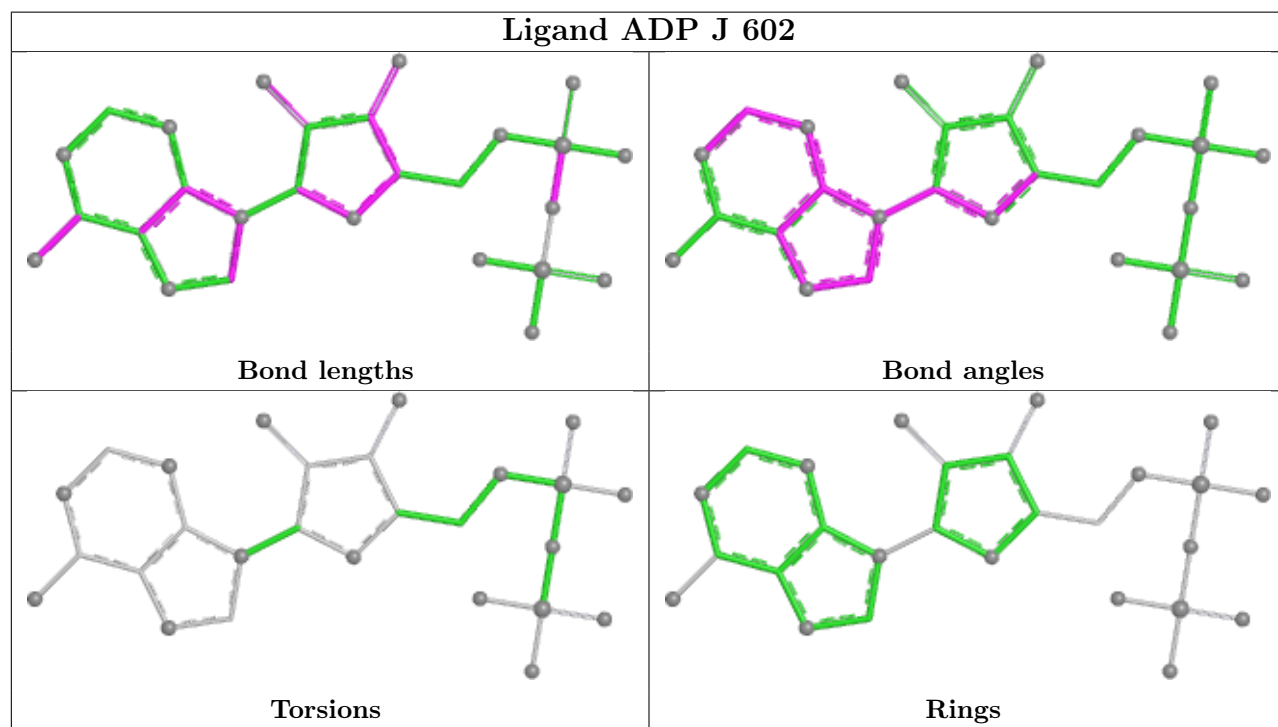
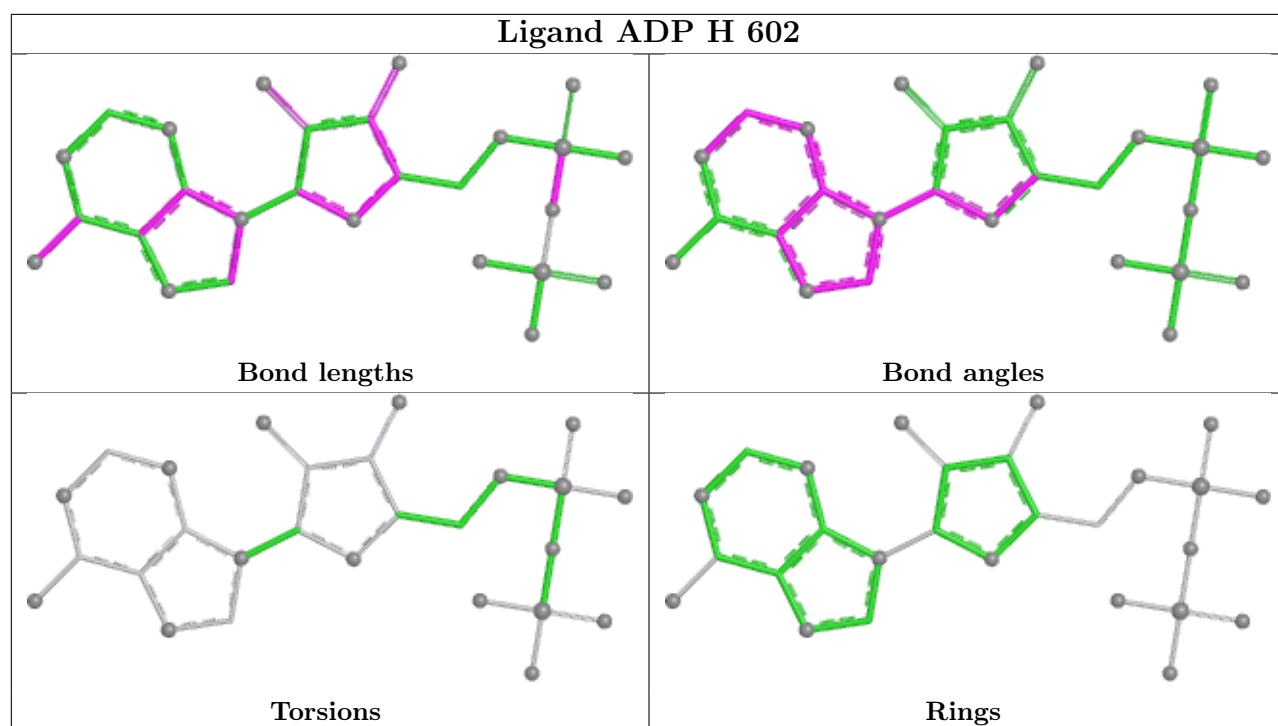


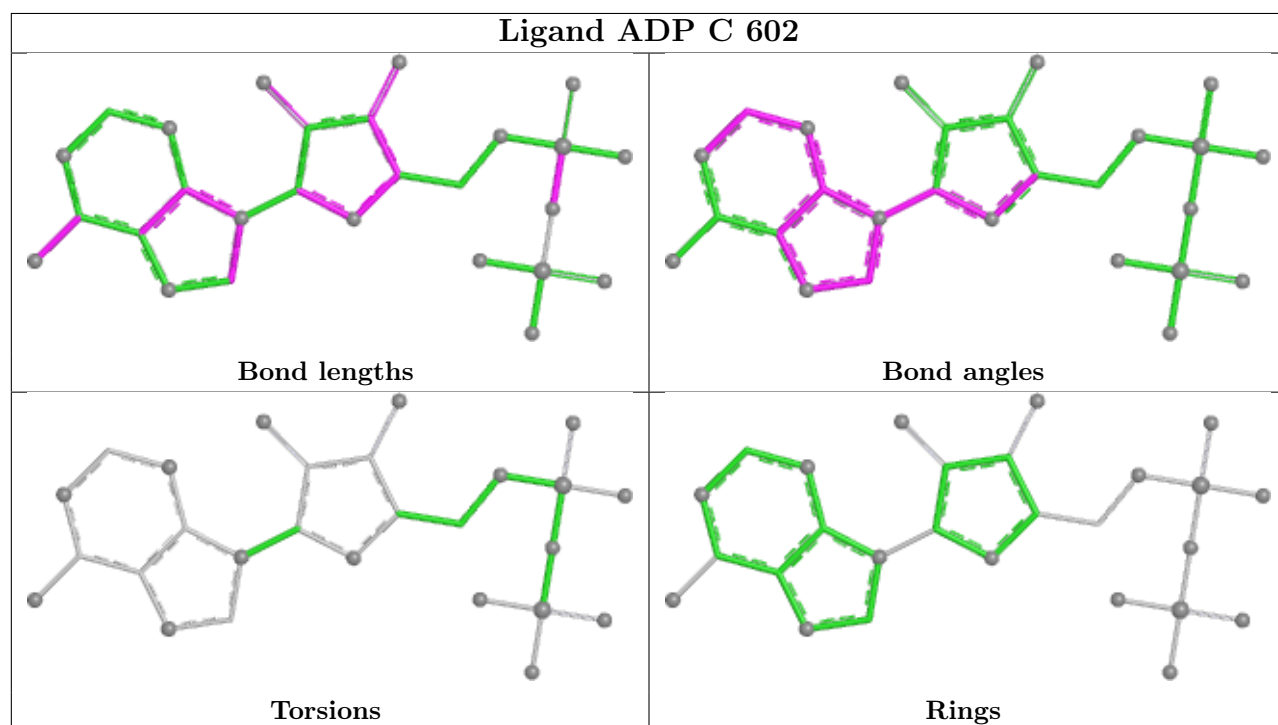
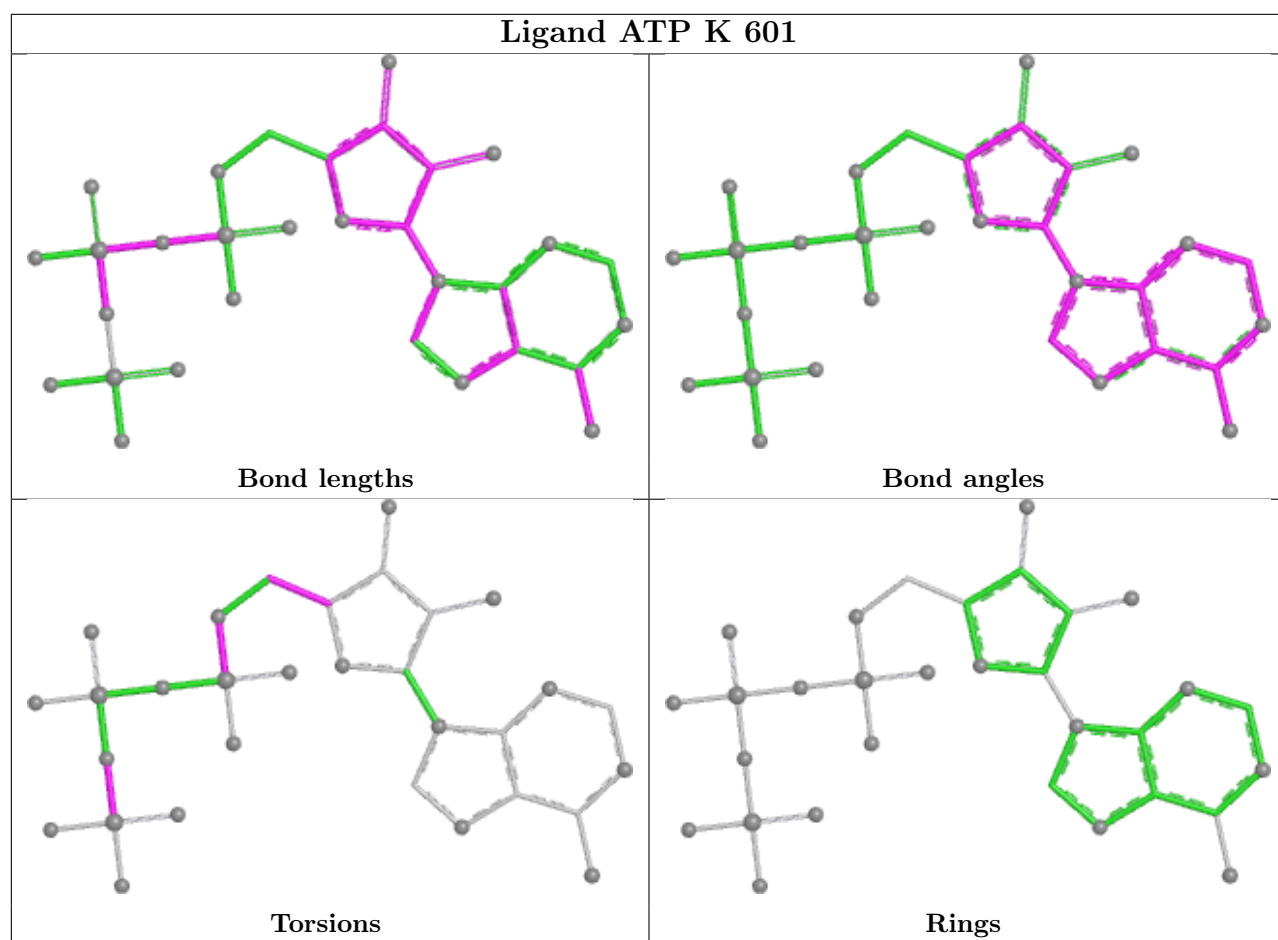
Ligand ATP I 601

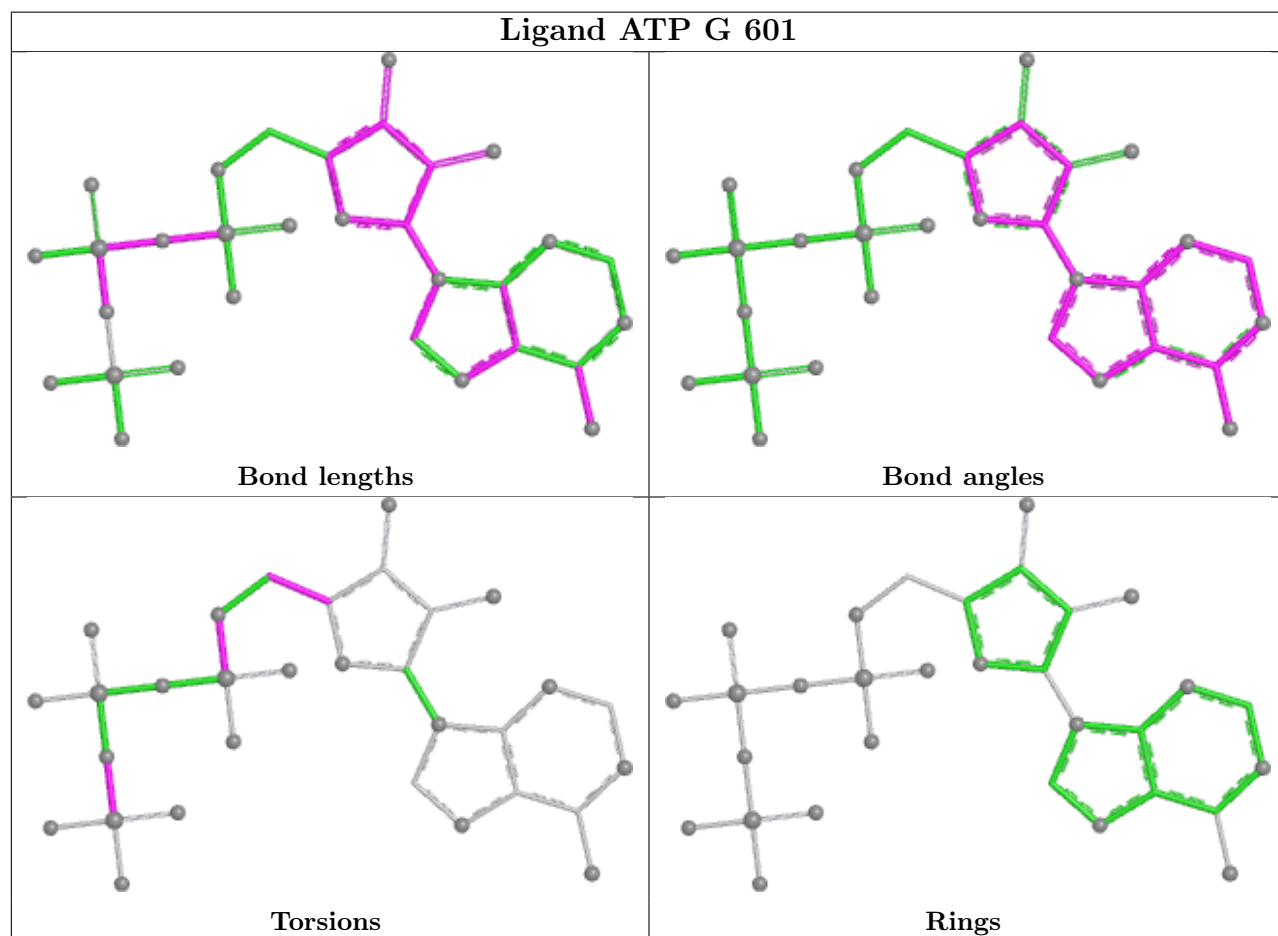
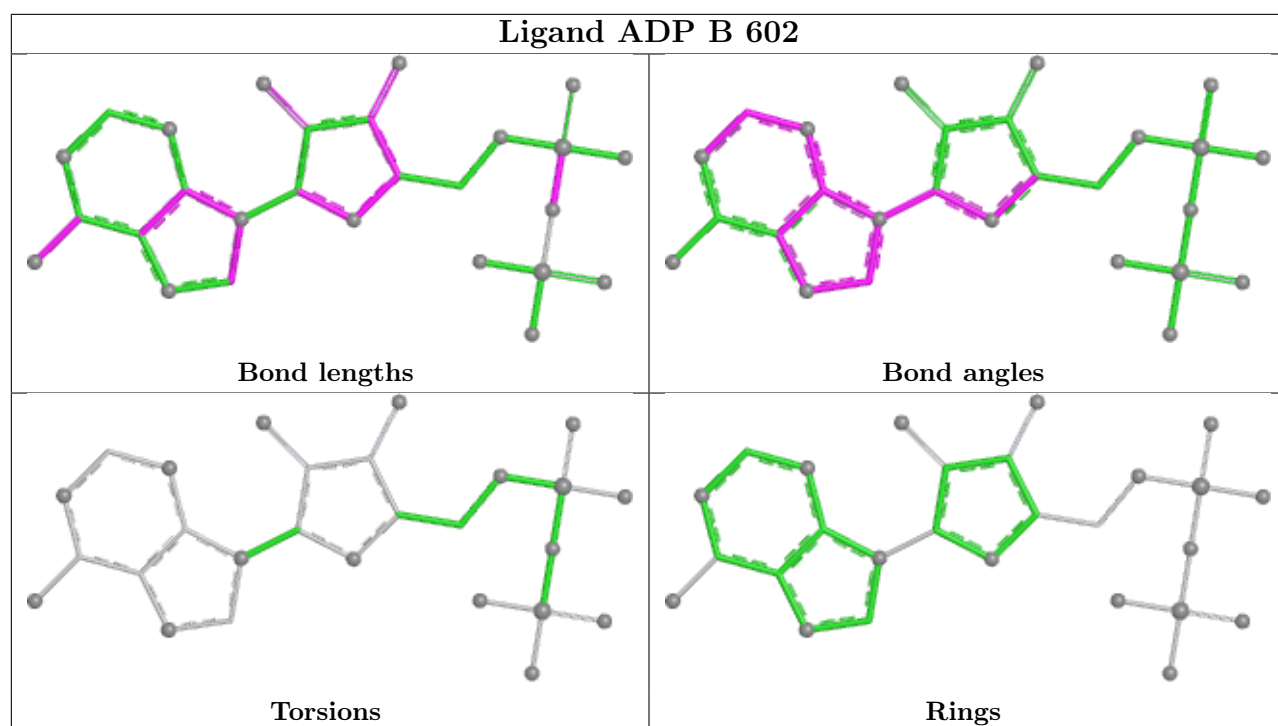


Ligand ADP L 602

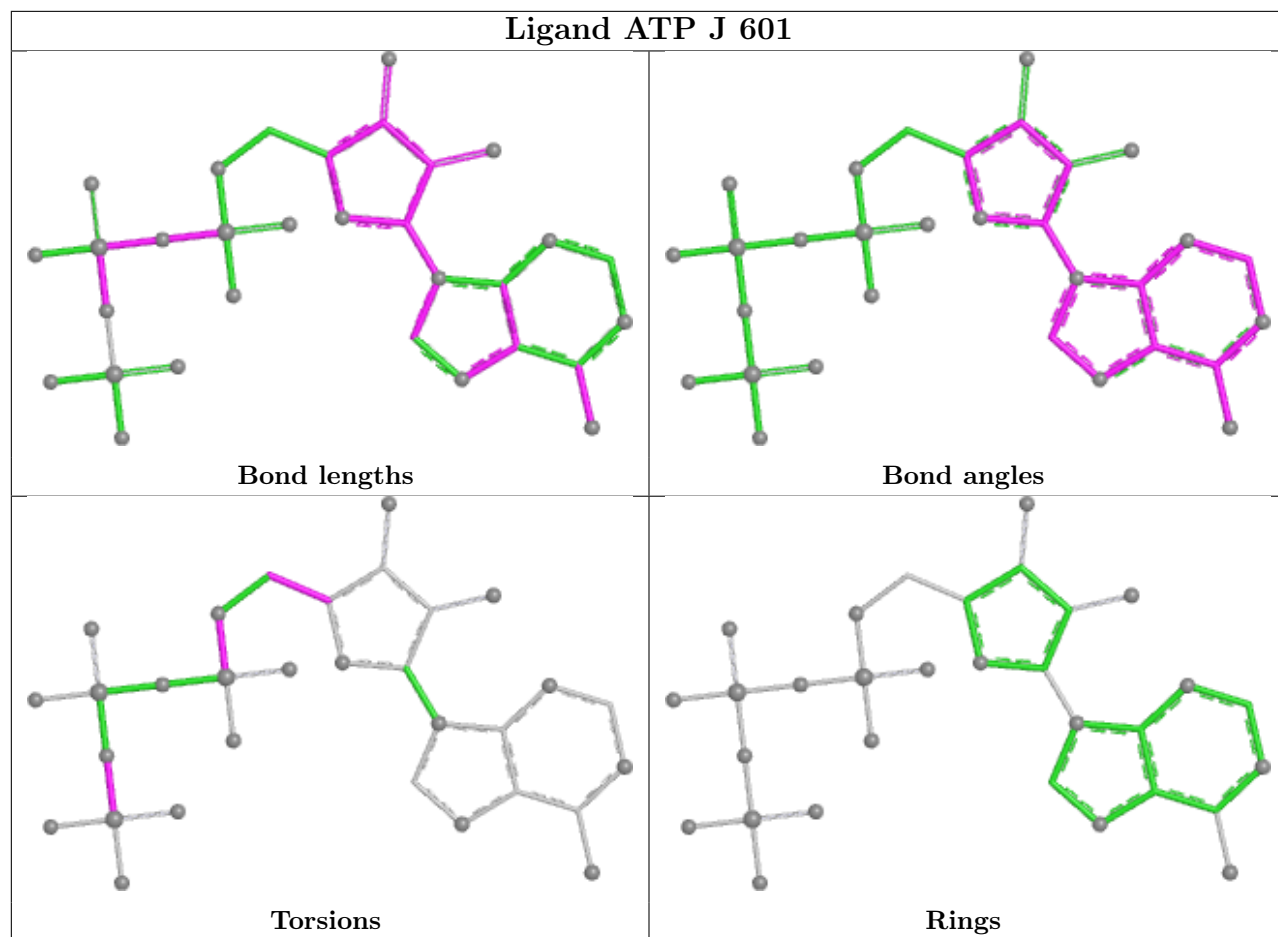




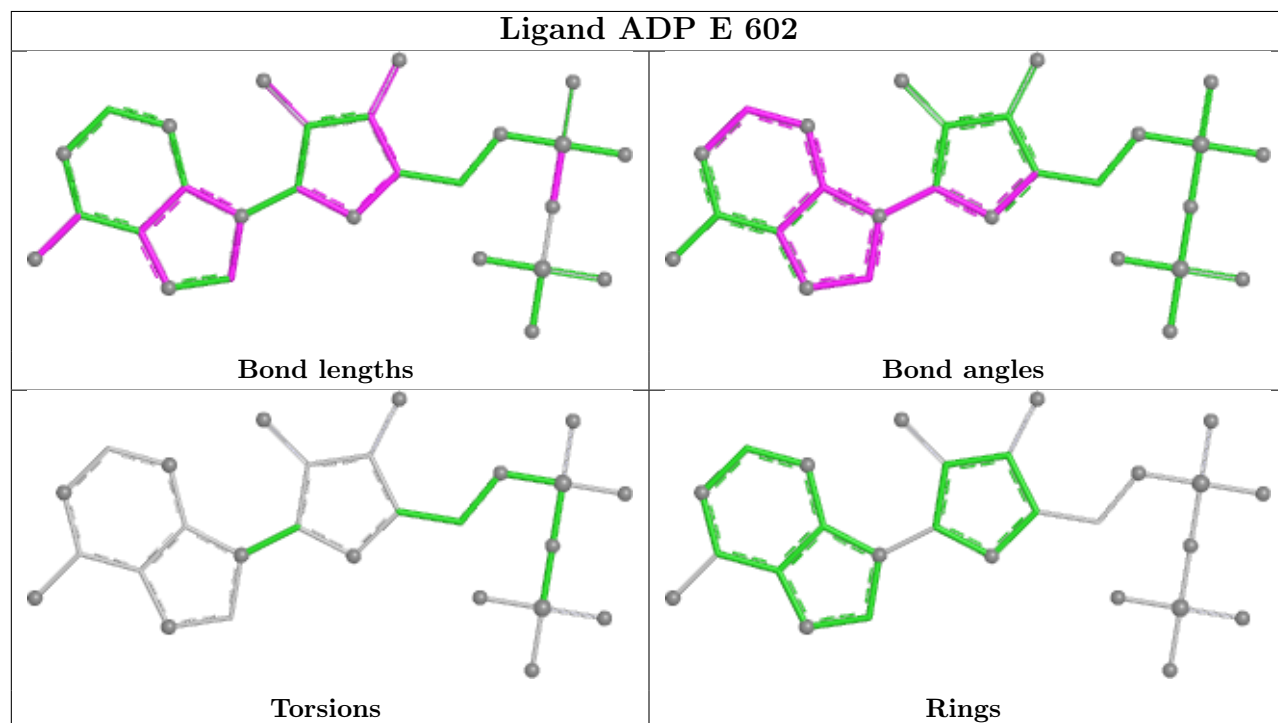




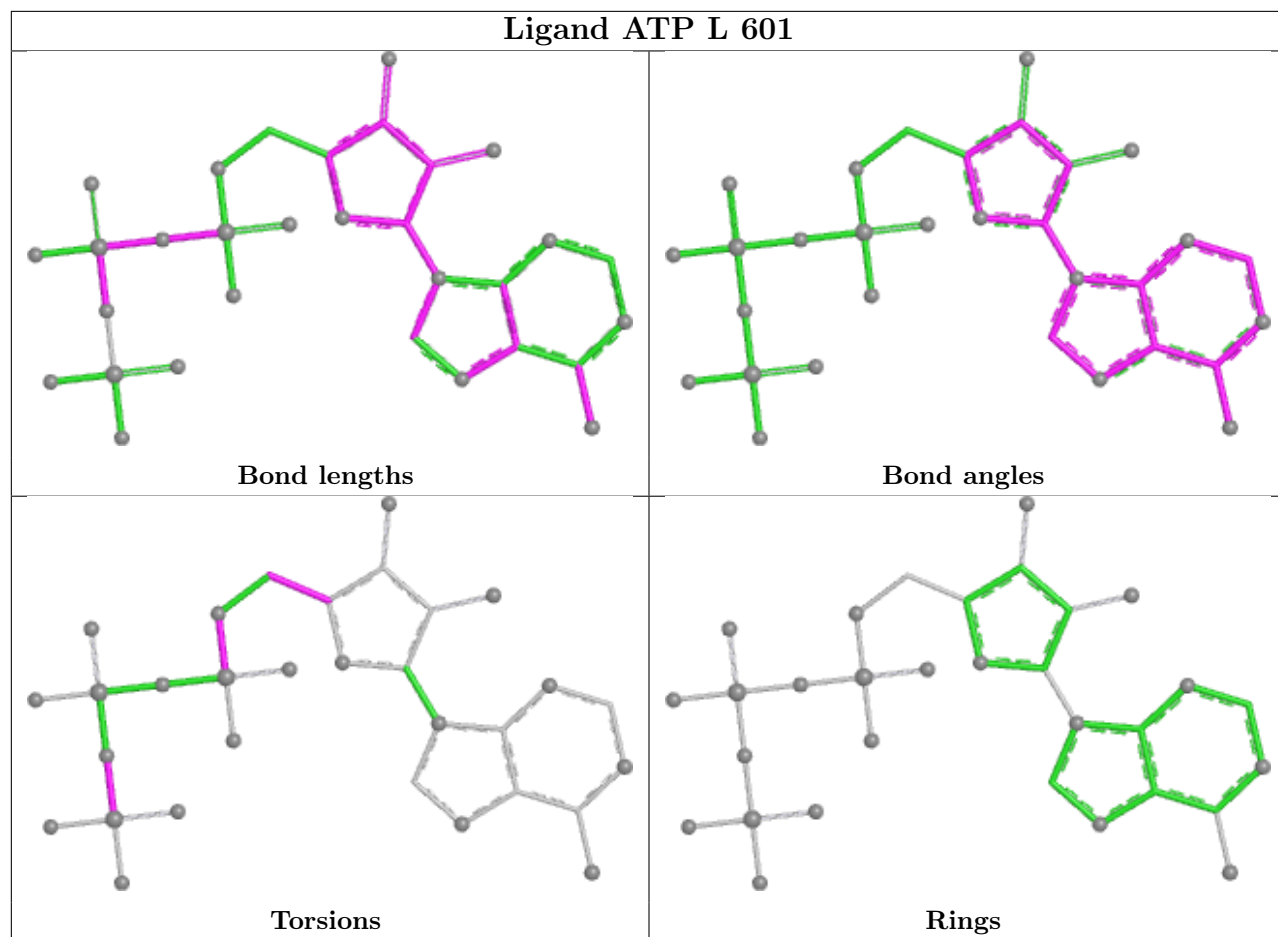
Ligand ATP J 601



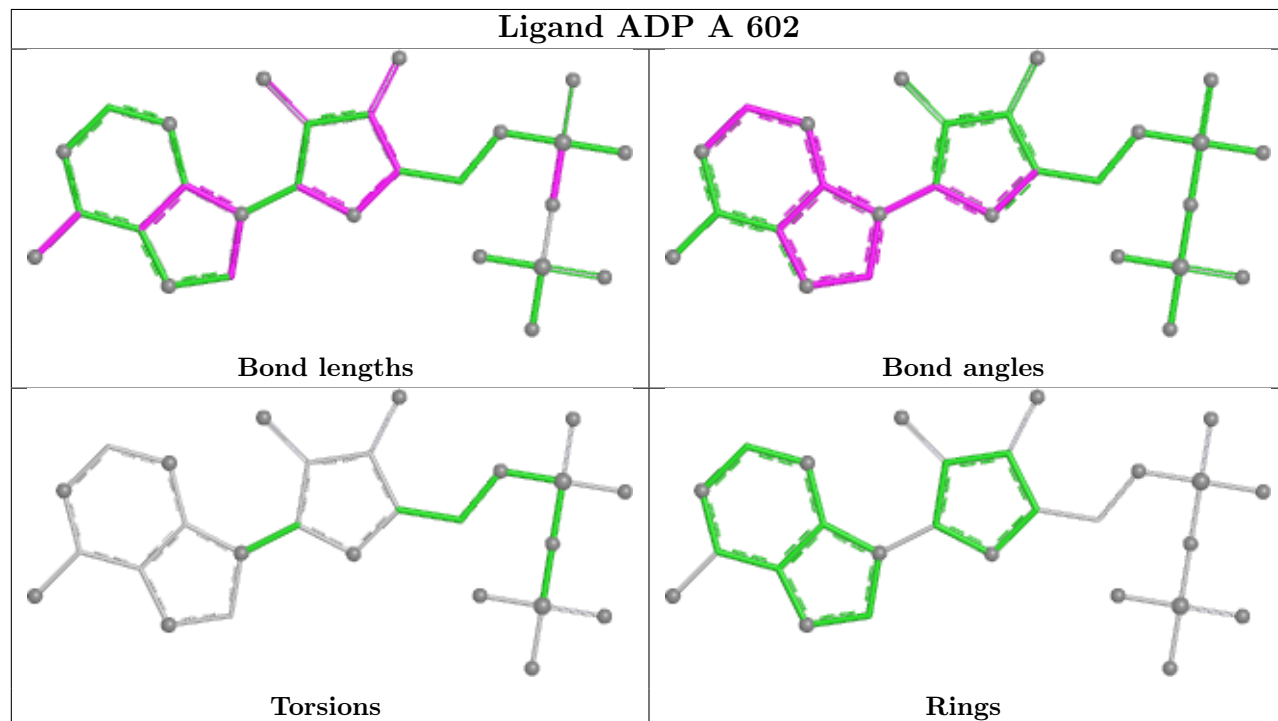
Ligand ADP E 602



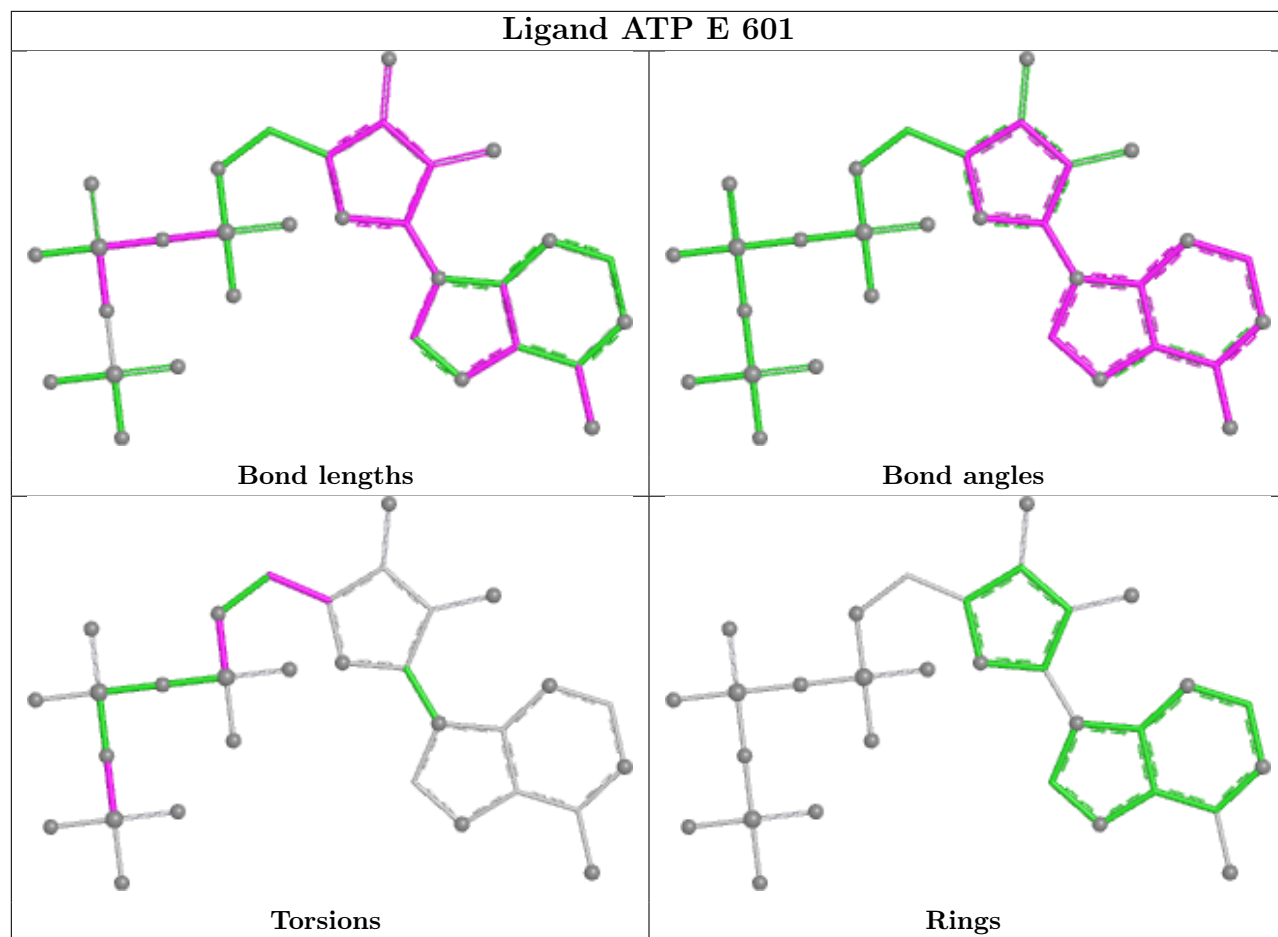
Ligand ATP L 601



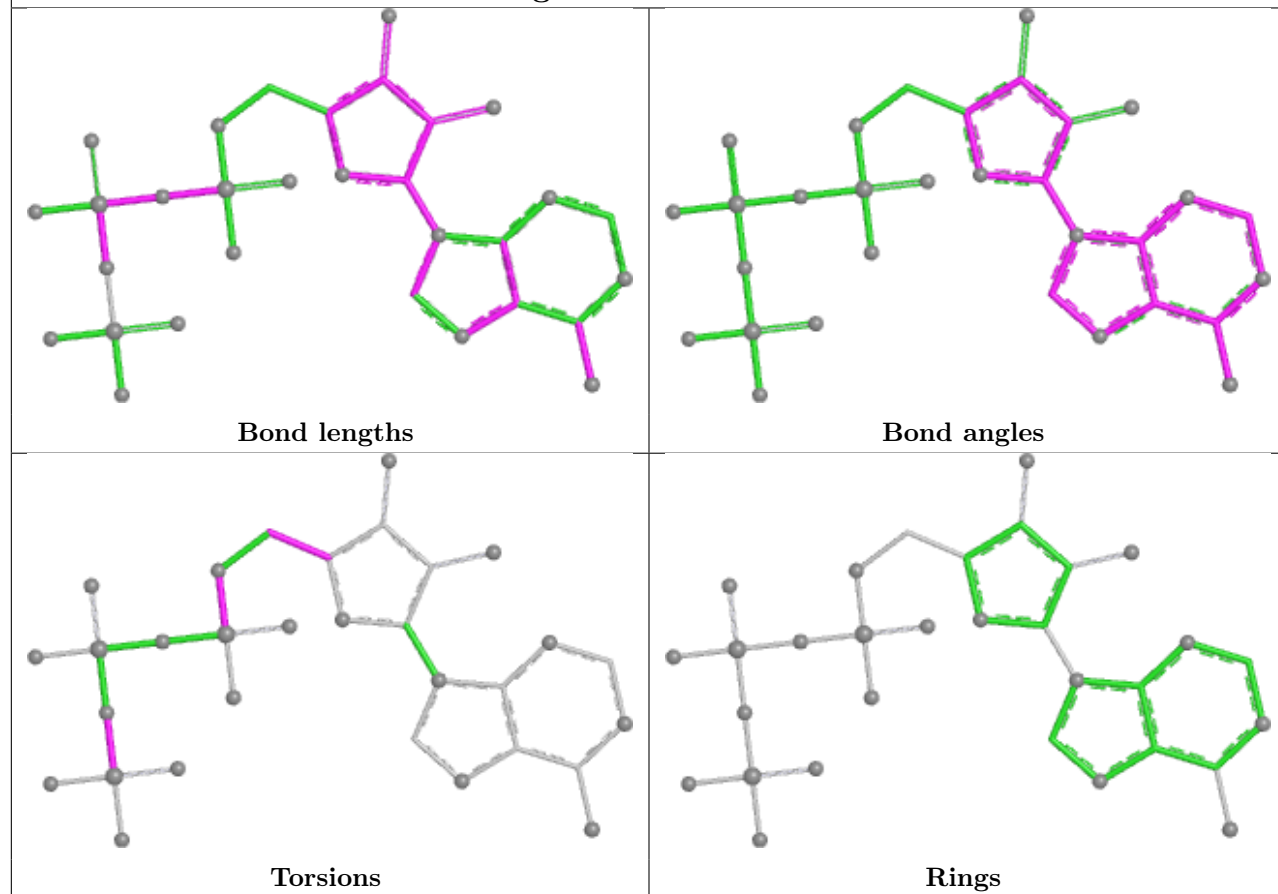
Ligand ADP A 602



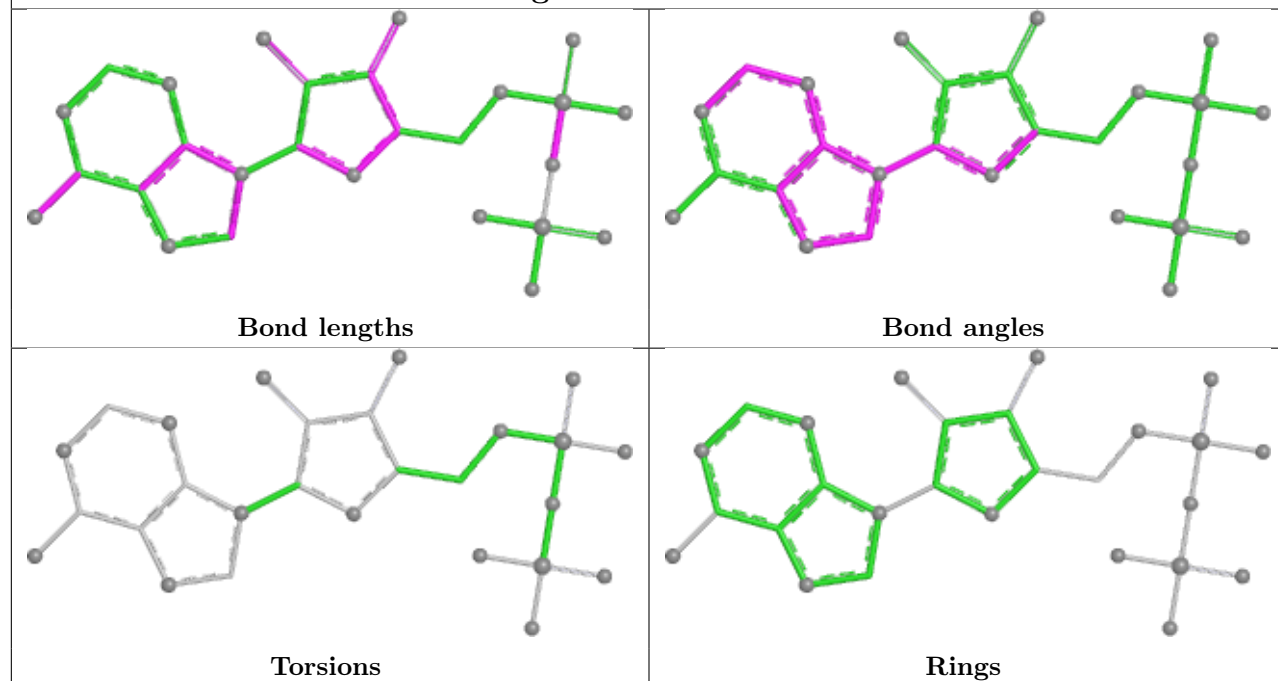
Ligand ATP E 601

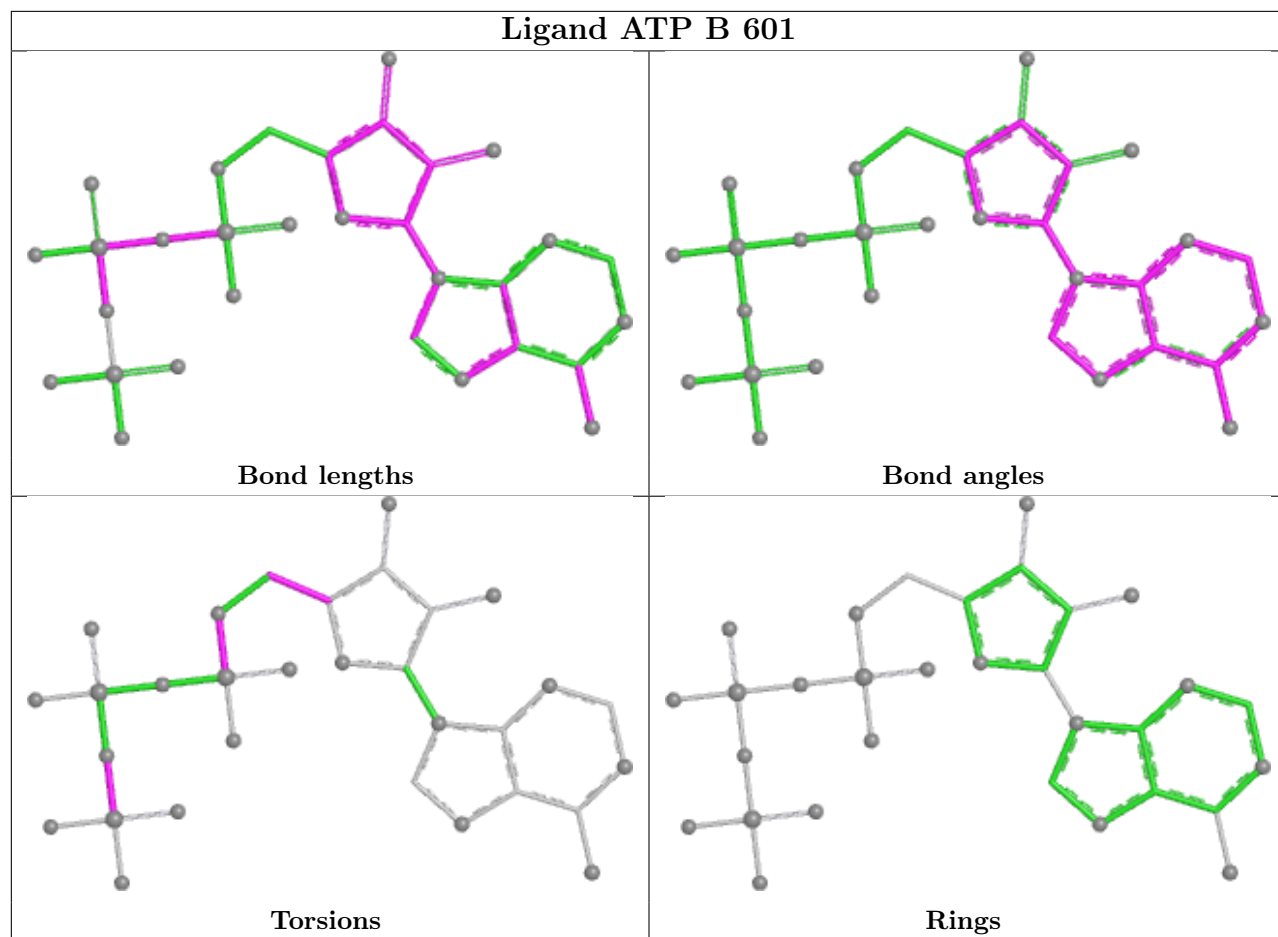


Ligand ATP C 601

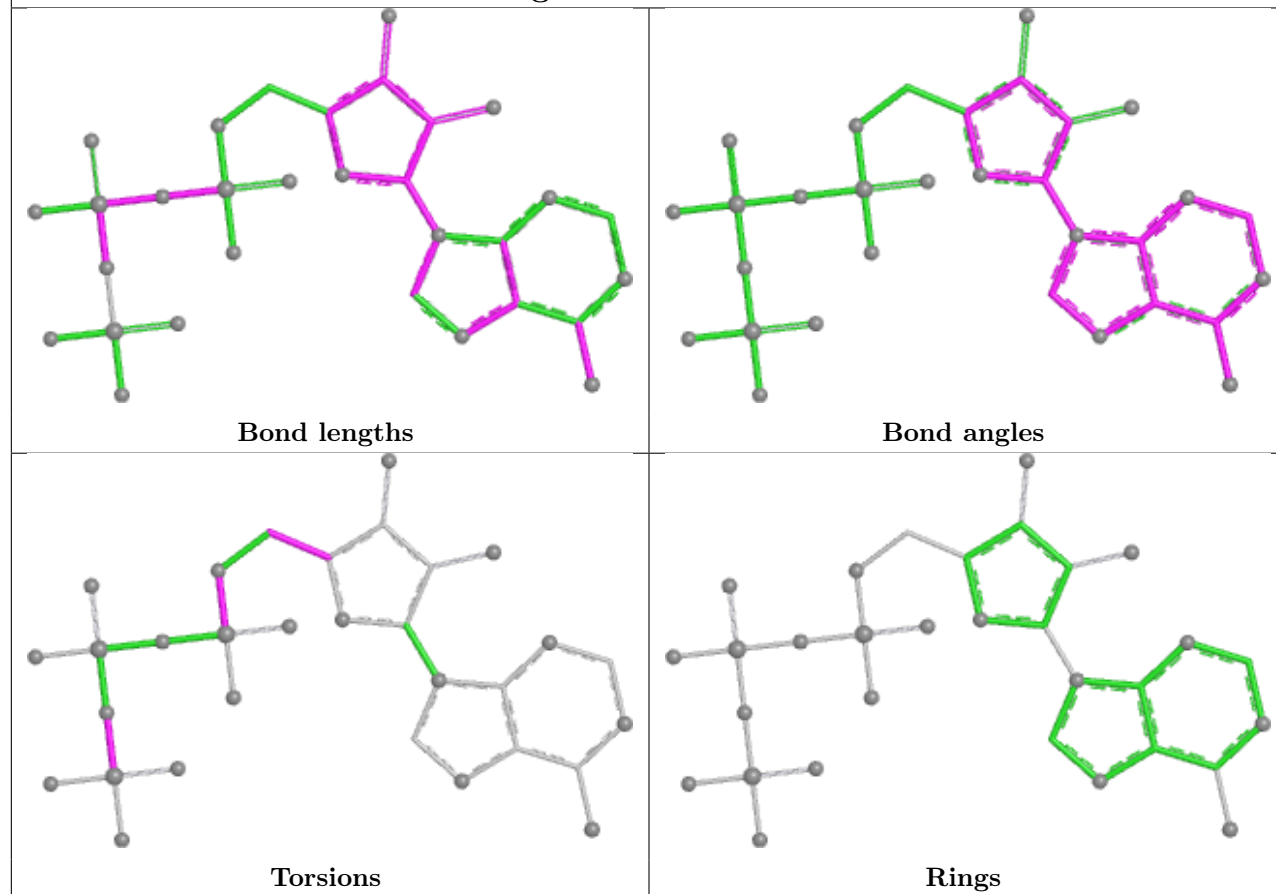


Ligand ADP F 602

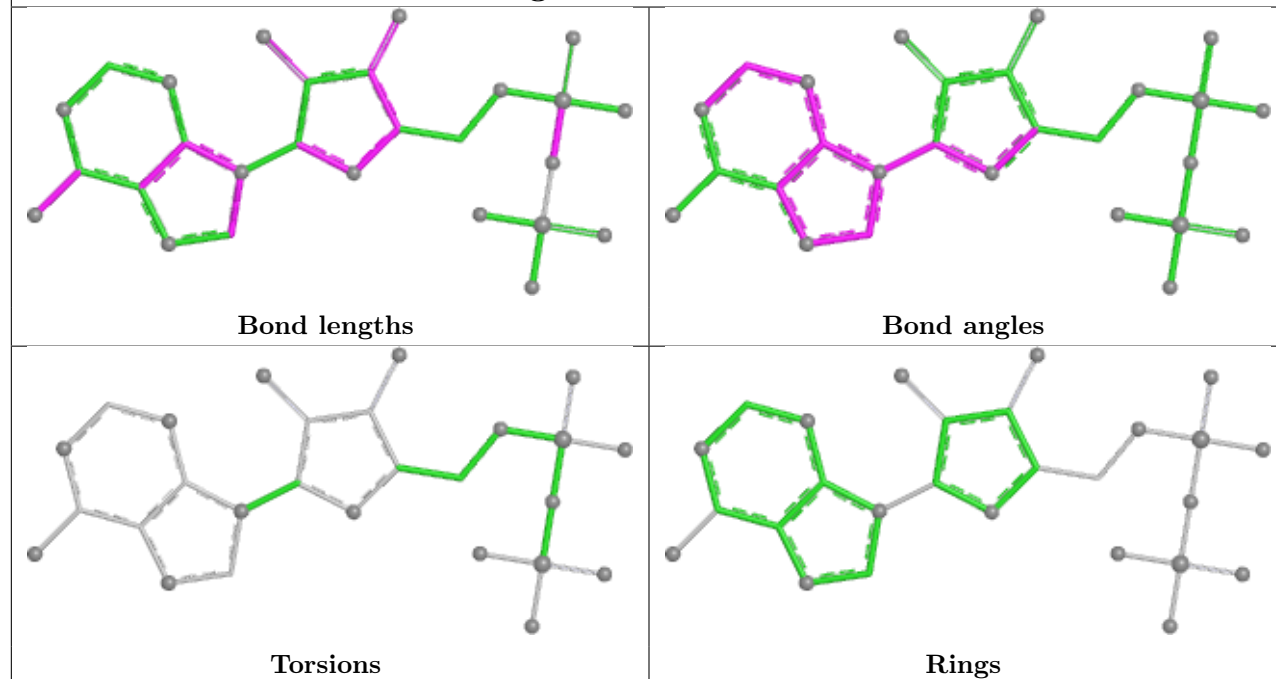




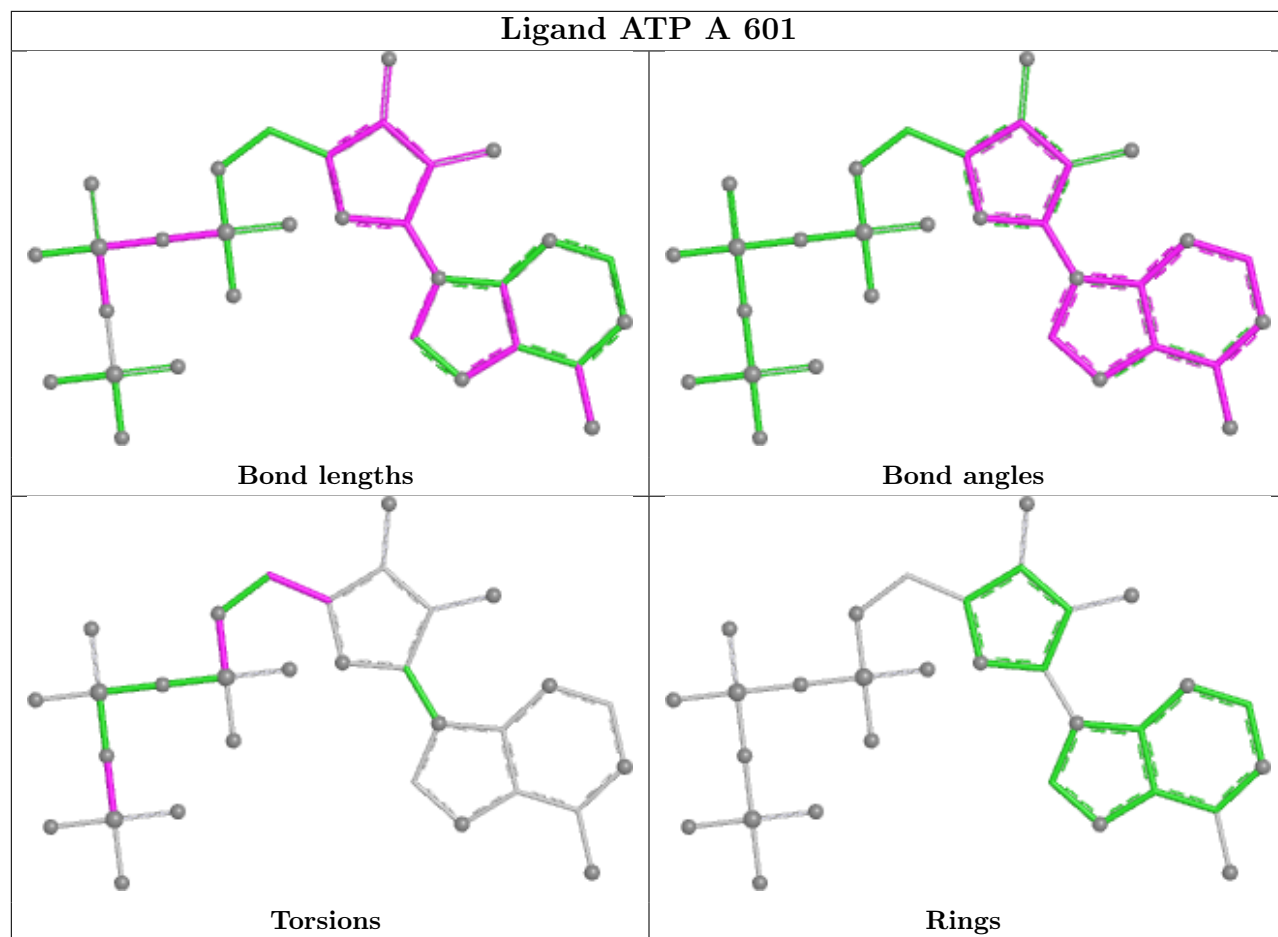
Ligand ATP H 601



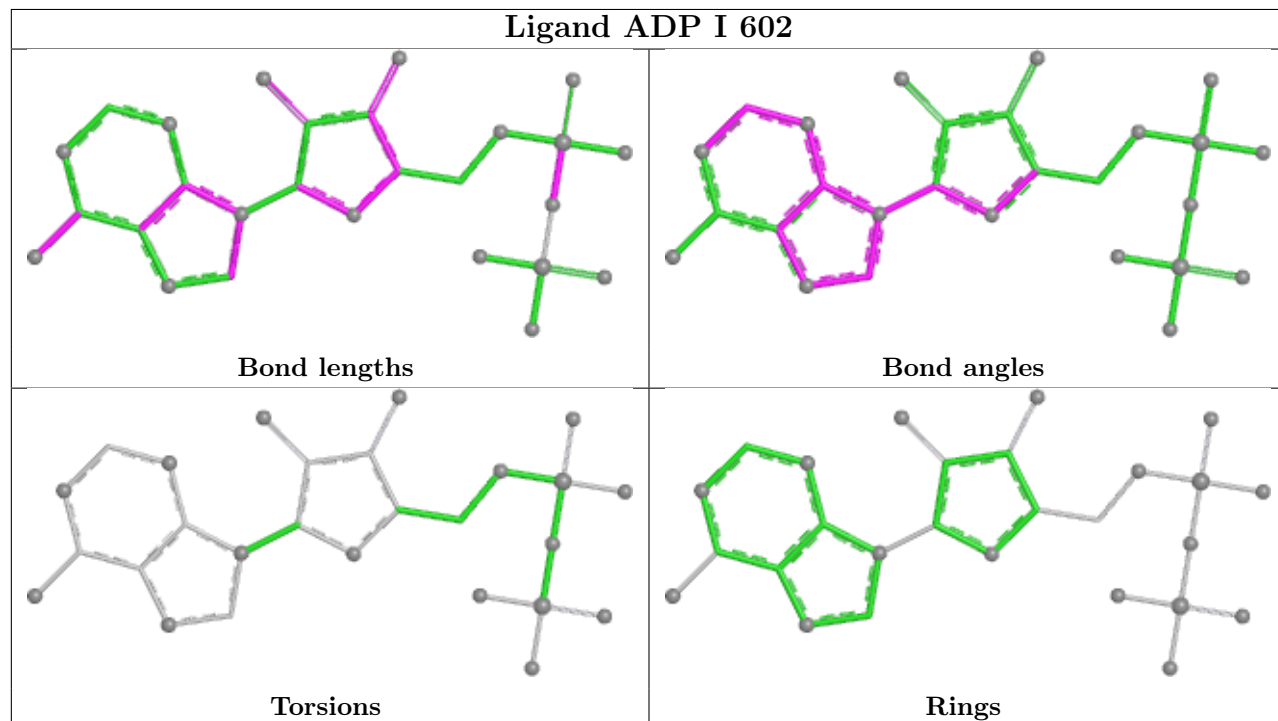
Ligand ADP D 602

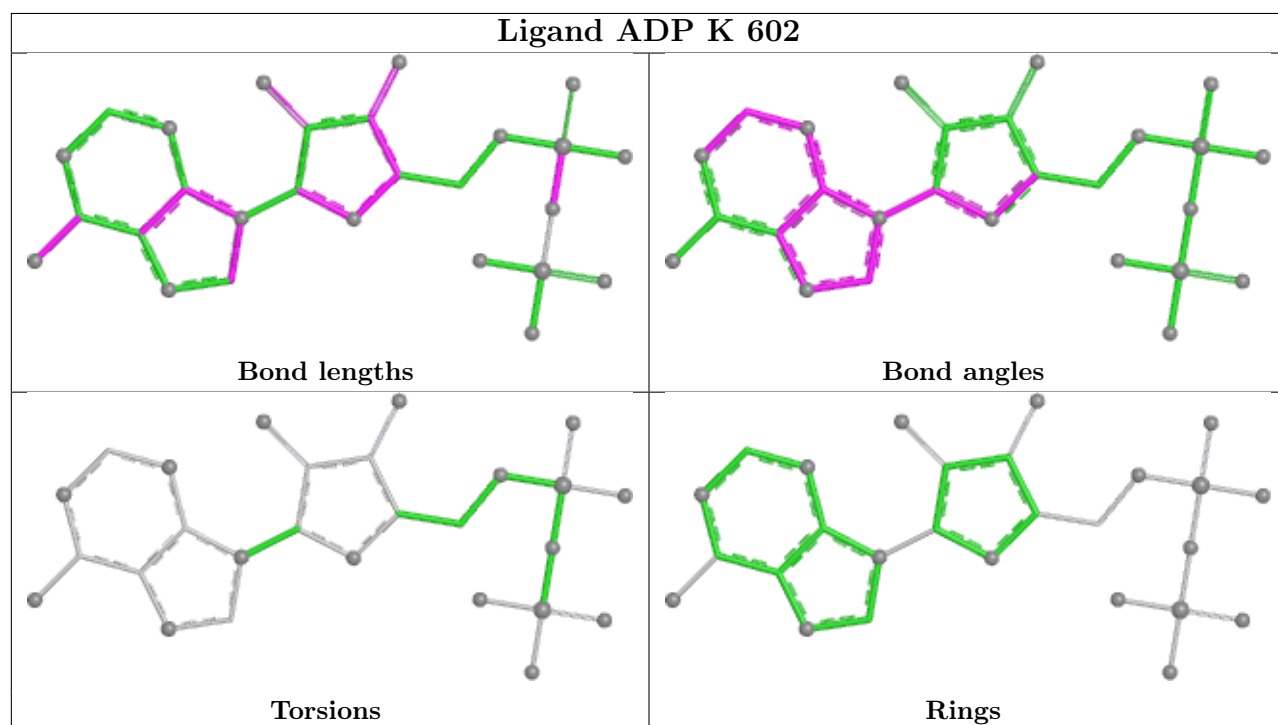
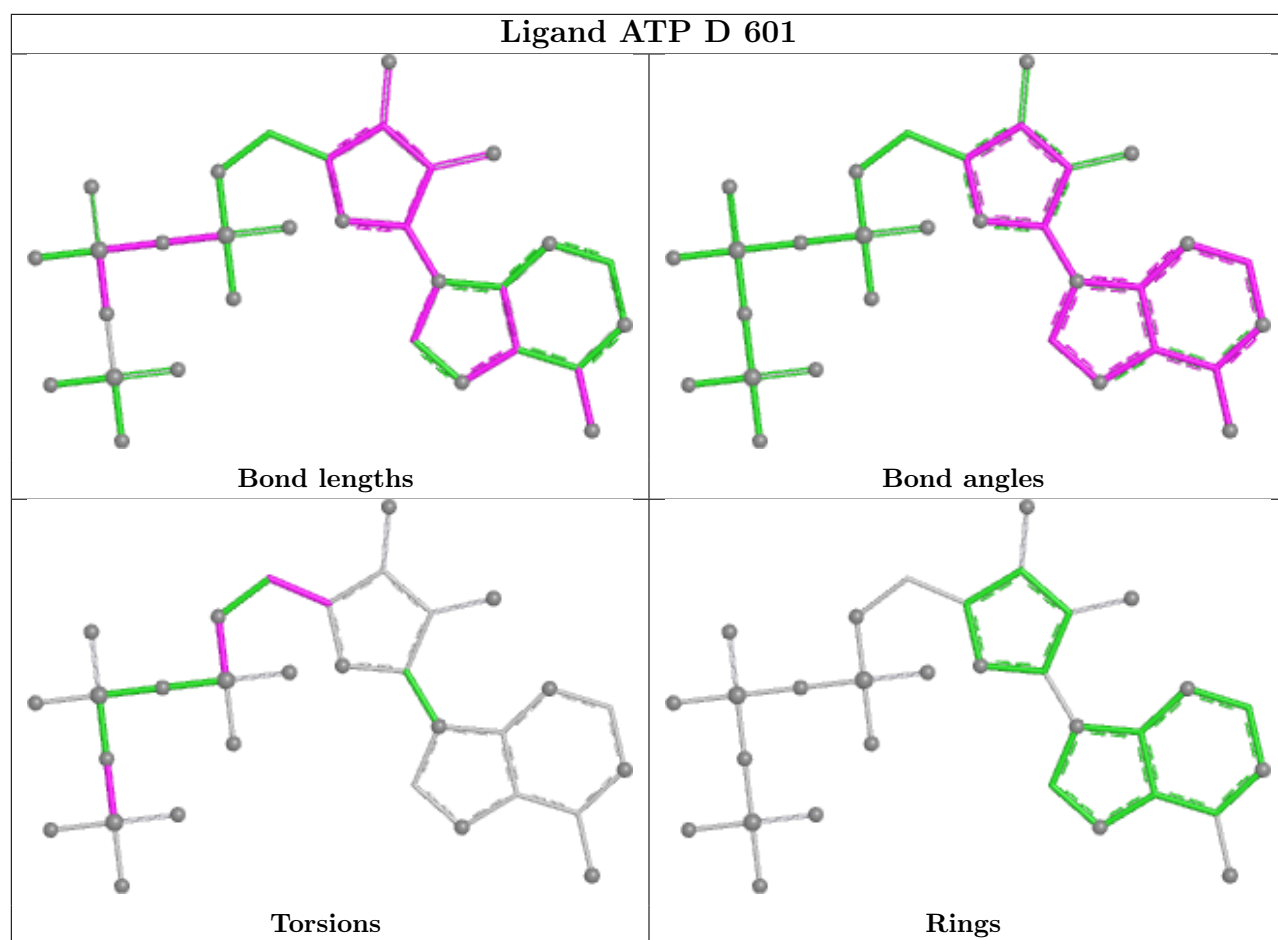


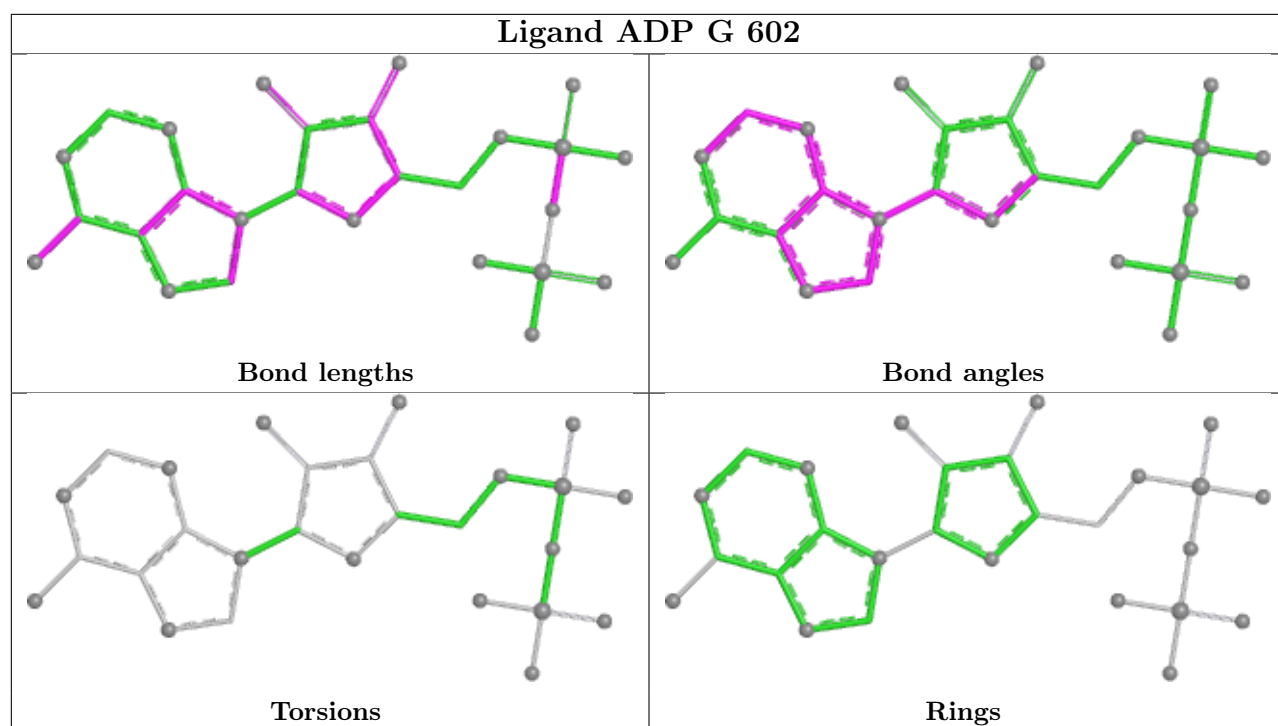
Ligand ATP A 601



Ligand ADP I 602







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.

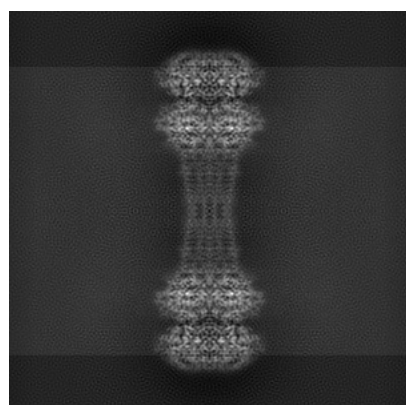
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29505. These allow visual inspection of the internal detail of the map and identification of artifacts.

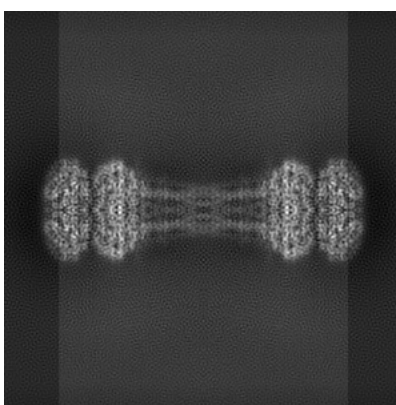
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

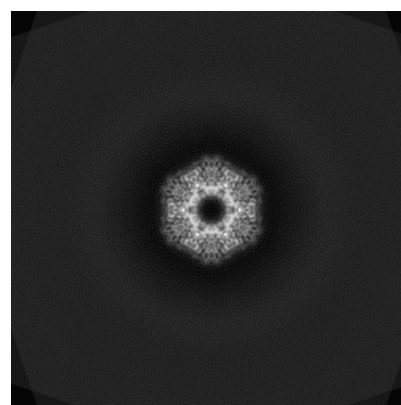
6.1.1 Primary map



X



Y

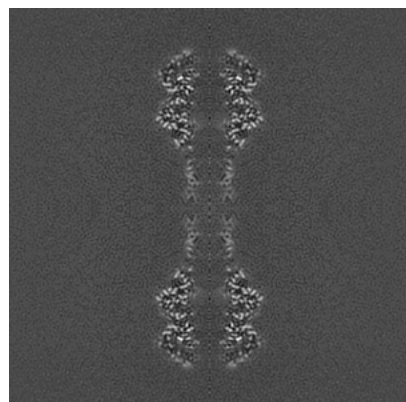


Z

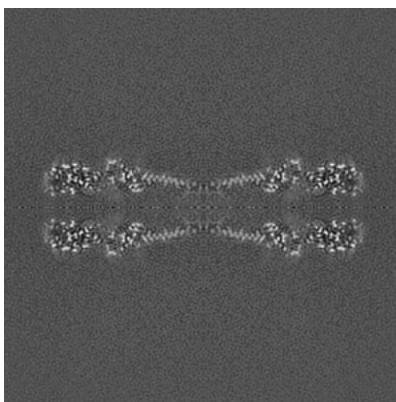
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

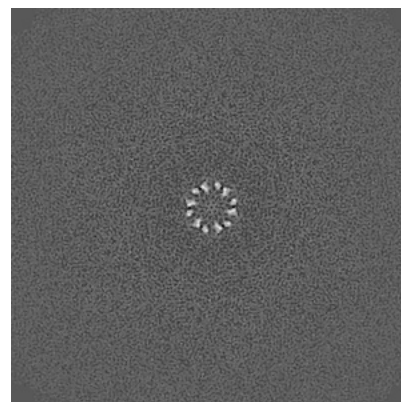
6.2.1 Primary map



X Index: 189



Y Index: 189

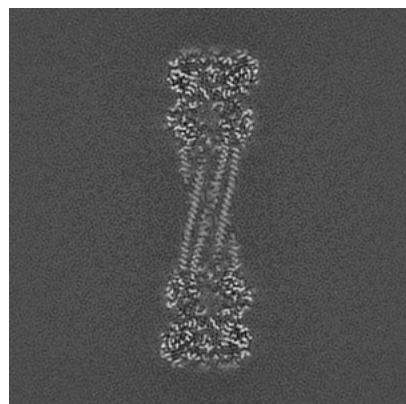


Z Index: 189

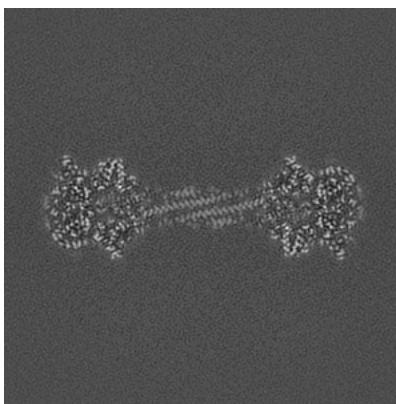
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

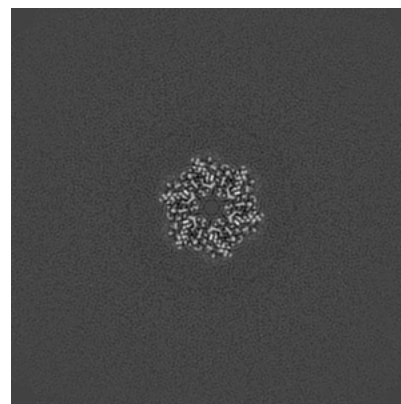
6.3.1 Primary map



X Index: 174



Y Index: 208

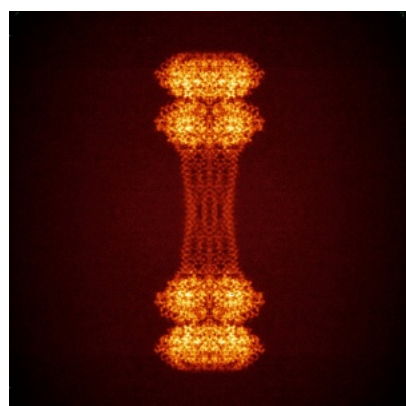


Z Index: 311

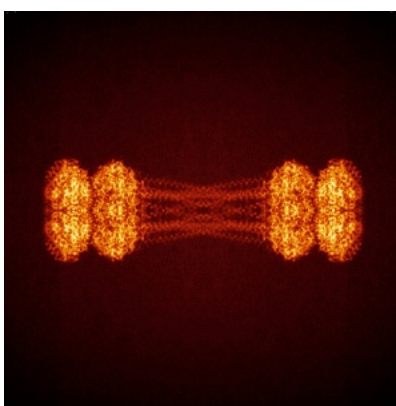
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

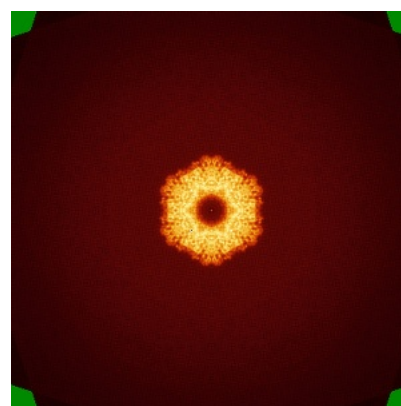
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

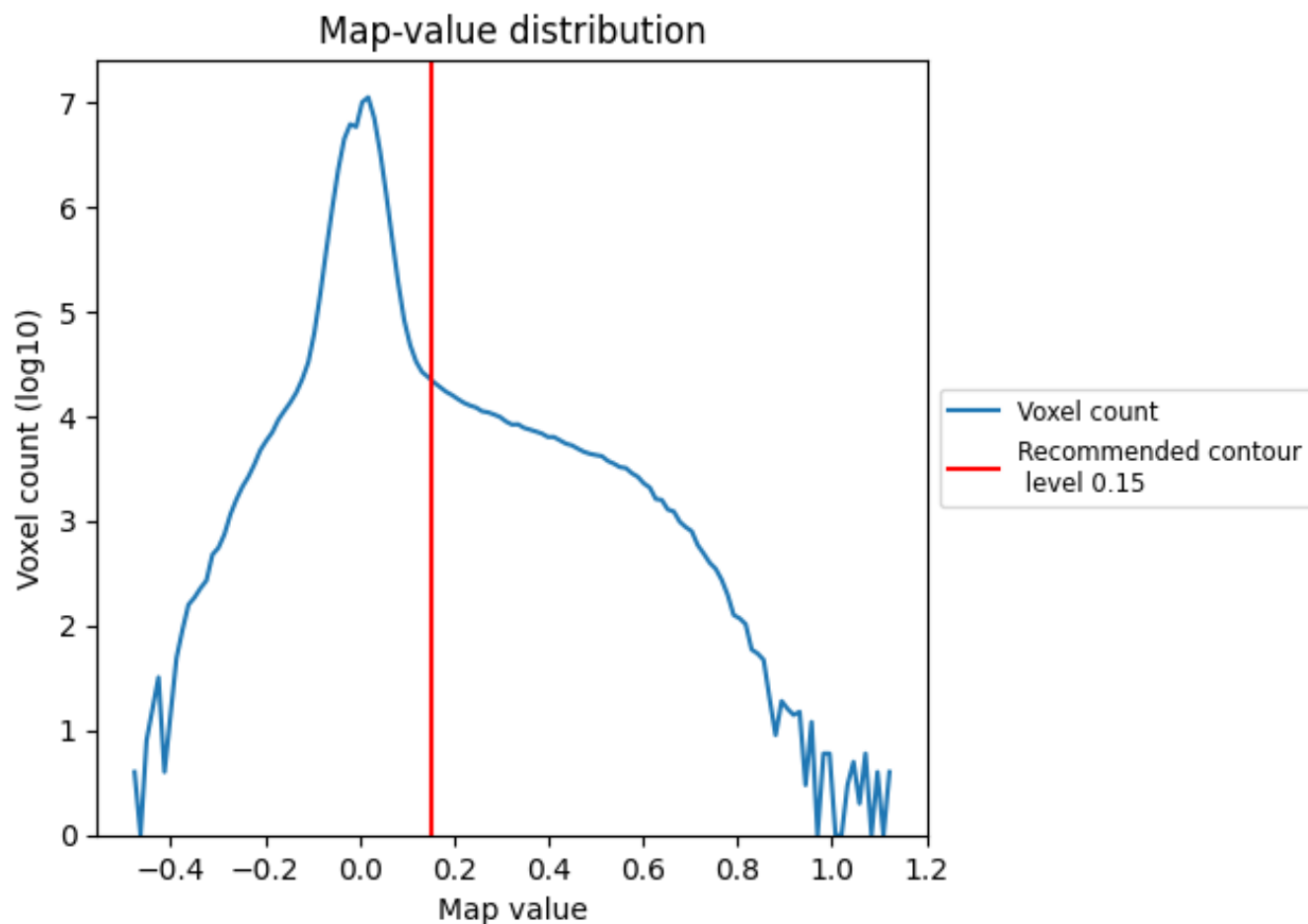
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

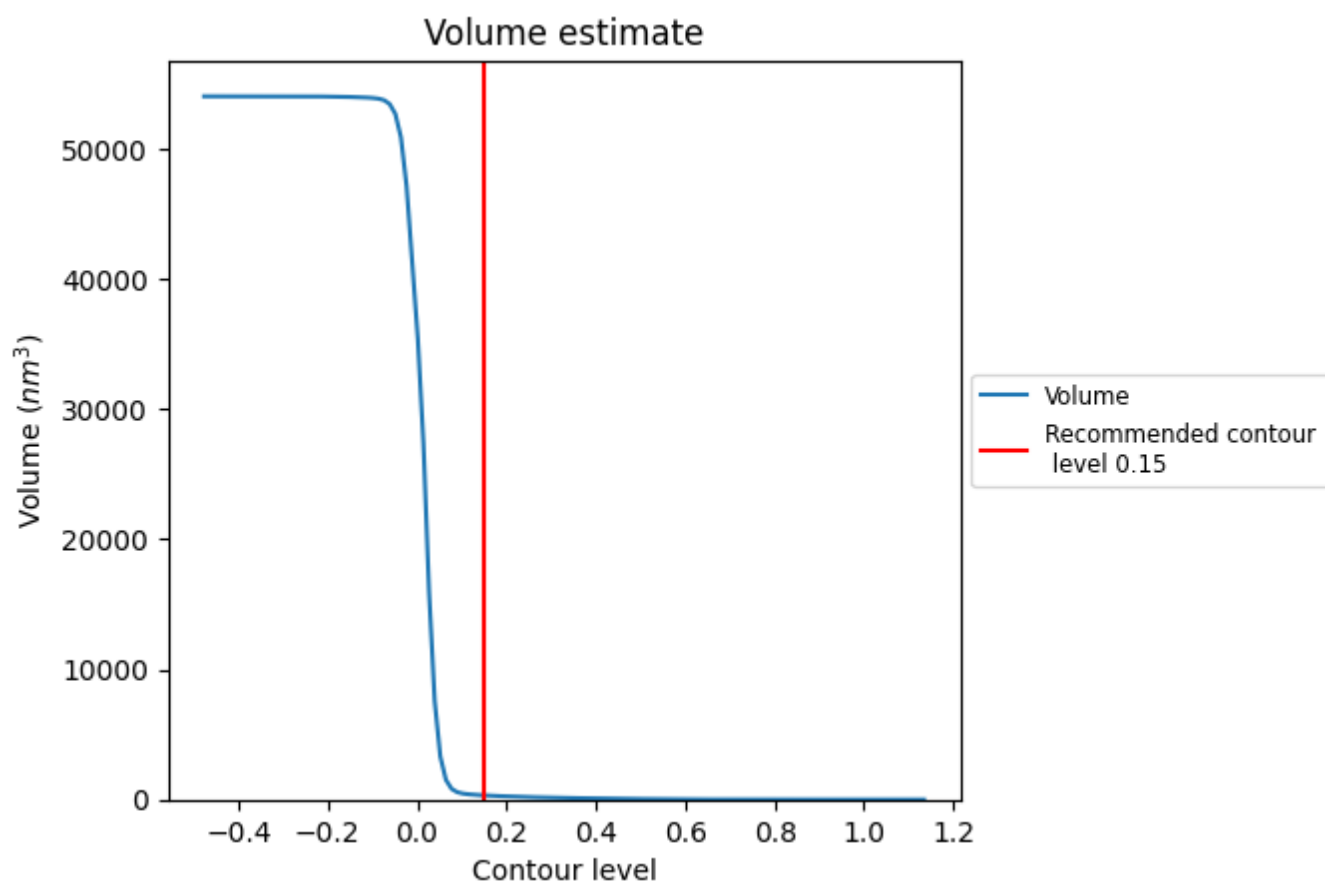
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

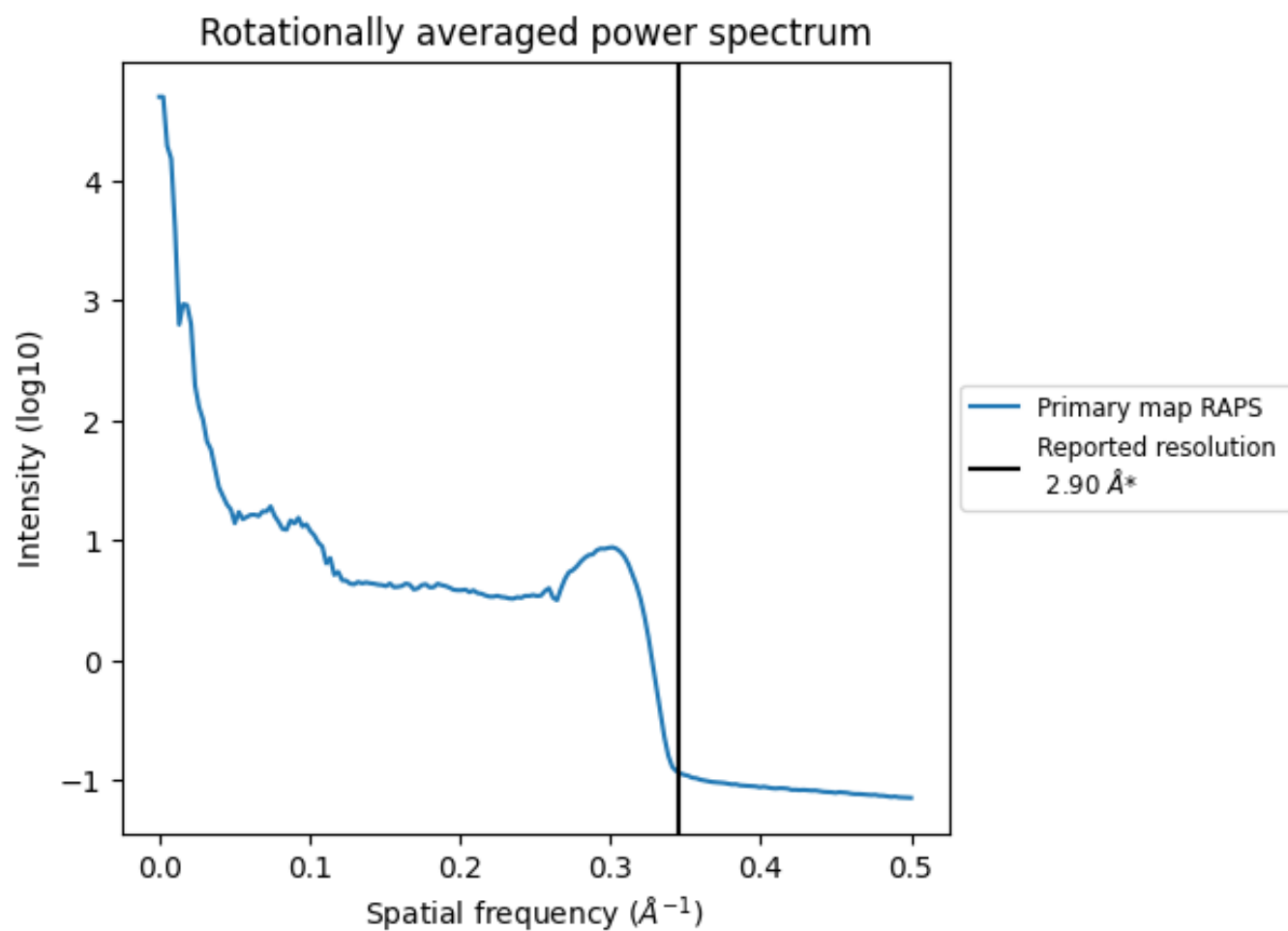
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 322 nm³; this corresponds to an approximate mass of 291 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

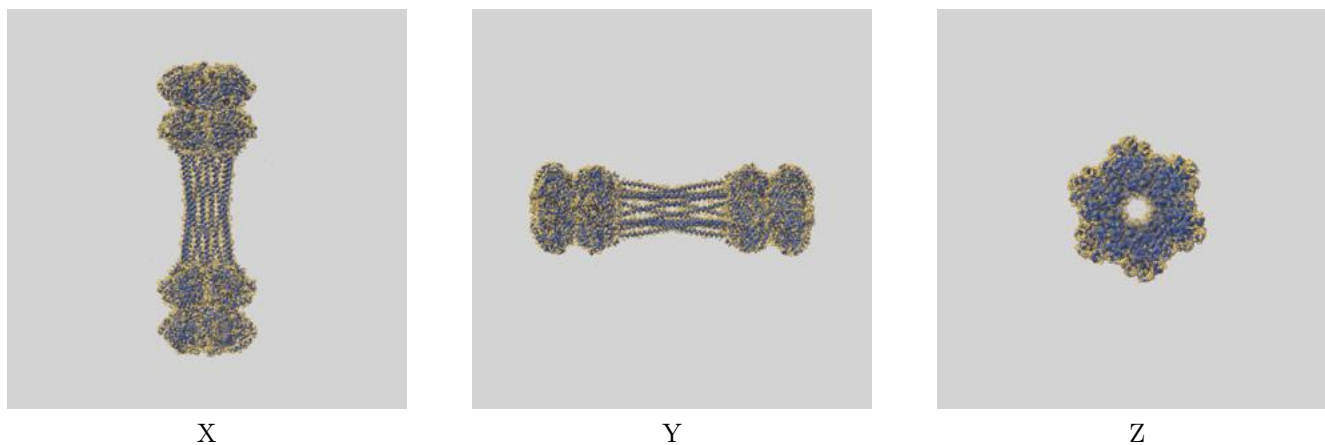
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

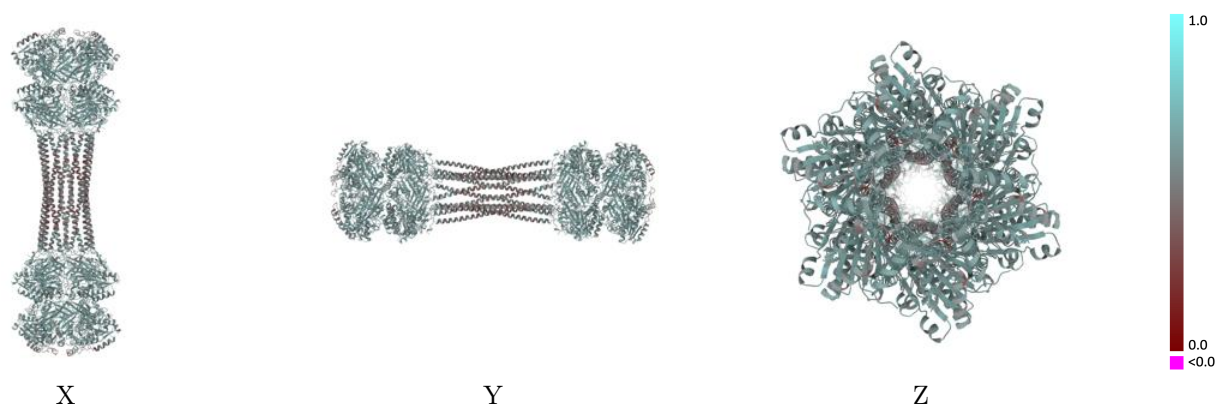
This section contains information regarding the fit between EMDB map EMD-29505 and PDB model 8FWI. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



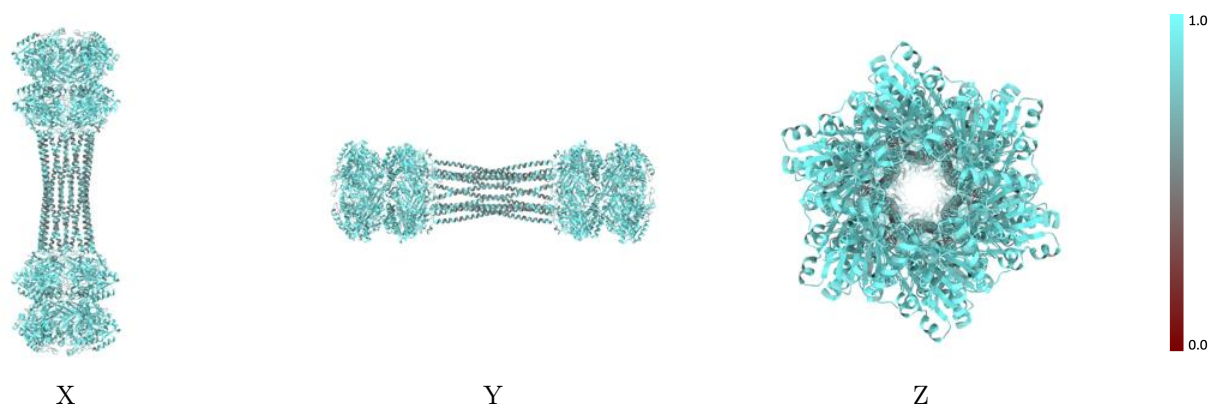
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



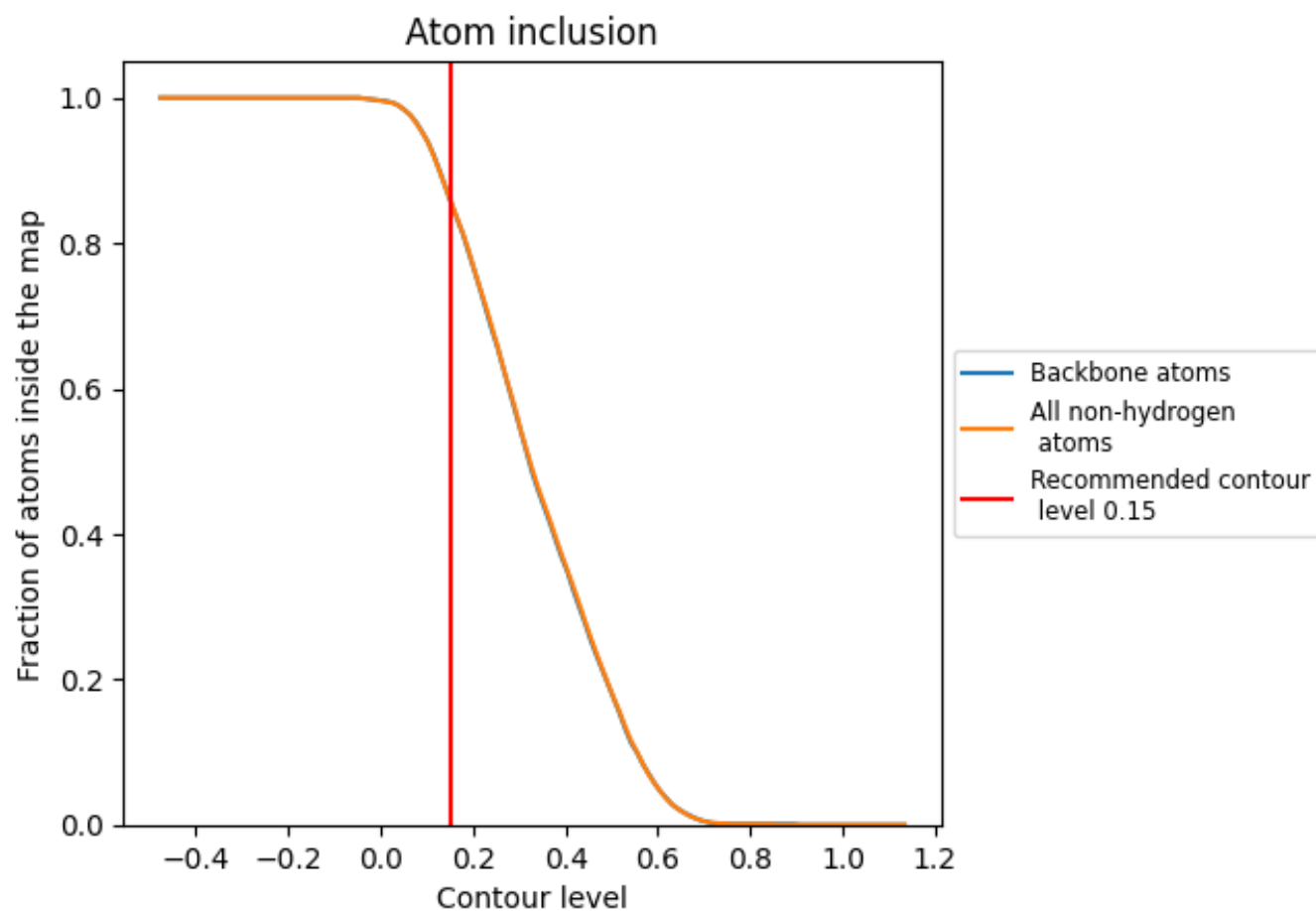
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8600	0.5640
A	0.8660	0.5640
B	0.8660	0.5640
C	0.8700	0.5650
D	0.8670	0.5600
E	0.8670	0.5650
F	0.8680	0.5630
G	0.8680	0.5670
H	0.8700	0.5640
I	0.8670	0.5640
J	0.8670	0.5640
K	0.8680	0.5650
L	0.8700	0.5680

