



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:25 PM UTC

PDB ID : 4IJM / pdb_00004ijm
Title : Crystal structure of circadian clock protein KaiC A422V mutant
Authors : Egli, M.; Pattanayek, R.
Deposited on : 2012-12-21
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

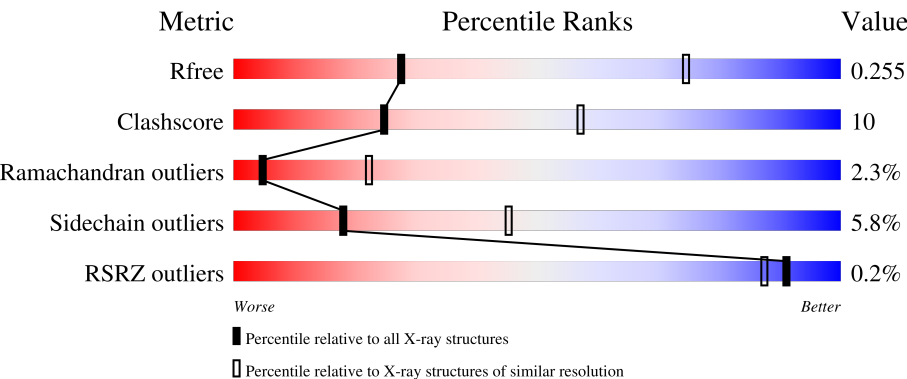
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	512	% 72% 23% ..
1	B	512	71% 23% ..
1	C	512	66% 26% • 5%
1	D	512	69% 22% • 5%
1	E	512	69% 24% ..

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Mol	Chain	Length	Quality of chain
1	F	512	72% 23% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24219 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3991	2511	701	763	1	15			
1	B	489	Total	C	N	O	P	S	0	0	0
			3861	2433	676	736	1	15			
1	C	488	Total	C	N	O	P	S	0	0	0
			3852	2427	674	735	1	15			
1	D	485	Total	C	N	O	P	S	0	0	0
			3828	2413	671	728	1	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3884	2447	679	742	1	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3987	2509	701	761	1	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	VAL	ALA	engineered mutation	UNP Q79PF4
A	520	HIS	-	expression tag	UNP Q79PF4
A	521	HIS	-	expression tag	UNP Q79PF4
A	522	HIS	-	expression tag	UNP Q79PF4
A	523	HIS	-	expression tag	UNP Q79PF4
A	524	HIS	-	expression tag	UNP Q79PF4
A	525	HIS	-	expression tag	UNP Q79PF4
B	422	VAL	ALA	engineered mutation	UNP Q79PF4
B	520	HIS	-	expression tag	UNP Q79PF4
B	521	HIS	-	expression tag	UNP Q79PF4
B	522	HIS	-	expression tag	UNP Q79PF4
B	523	HIS	-	expression tag	UNP Q79PF4
B	524	HIS	-	expression tag	UNP Q79PF4
B	525	HIS	-	expression tag	UNP Q79PF4
C	422	VAL	ALA	engineered mutation	UNP Q79PF4
C	520	HIS	-	expression tag	UNP Q79PF4
C	521	HIS	-	expression tag	UNP Q79PF4

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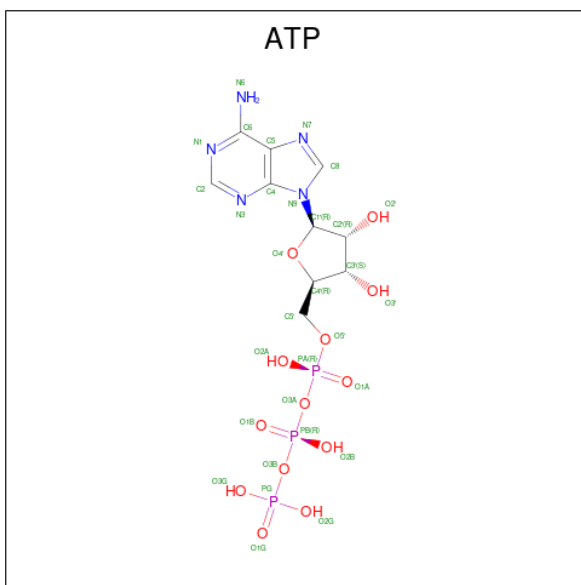
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Chain	Residue	Modelled	Actual	Comment	Reference
C	522	HIS	-	expression tag	UNP Q79PF4
C	523	HIS	-	expression tag	UNP Q79PF4
C	524	HIS	-	expression tag	UNP Q79PF4
C	525	HIS	-	expression tag	UNP Q79PF4
D	422	VAL	ALA	engineered mutation	UNP Q79PF4
D	520	HIS	-	expression tag	UNP Q79PF4
D	521	HIS	-	expression tag	UNP Q79PF4
D	522	HIS	-	expression tag	UNP Q79PF4
D	523	HIS	-	expression tag	UNP Q79PF4
D	524	HIS	-	expression tag	UNP Q79PF4
D	525	HIS	-	expression tag	UNP Q79PF4
E	422	VAL	ALA	engineered mutation	UNP Q79PF4
E	520	HIS	-	expression tag	UNP Q79PF4
E	521	HIS	-	expression tag	UNP Q79PF4
E	522	HIS	-	expression tag	UNP Q79PF4
E	523	HIS	-	expression tag	UNP Q79PF4
E	524	HIS	-	expression tag	UNP Q79PF4
E	525	HIS	-	expression tag	UNP Q79PF4
F	422	VAL	ALA	engineered mutation	UNP Q79PF4
F	520	HIS	-	expression tag	UNP Q79PF4
F	521	HIS	-	expression tag	UNP Q79PF4
F	522	HIS	-	expression tag	UNP Q79PF4
F	523	HIS	-	expression tag	UNP Q79PF4
F	524	HIS	-	expression tag	UNP Q79PF4
F	525	HIS	-	expression tag	UNP Q79PF4

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	2	Total Mg 2 2	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	F	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	53	Total	O	0	0
			53	53		
5	C	83	Total	O	0	0
			83	83		
5	D	66	Total	O	0	0
			66	66		

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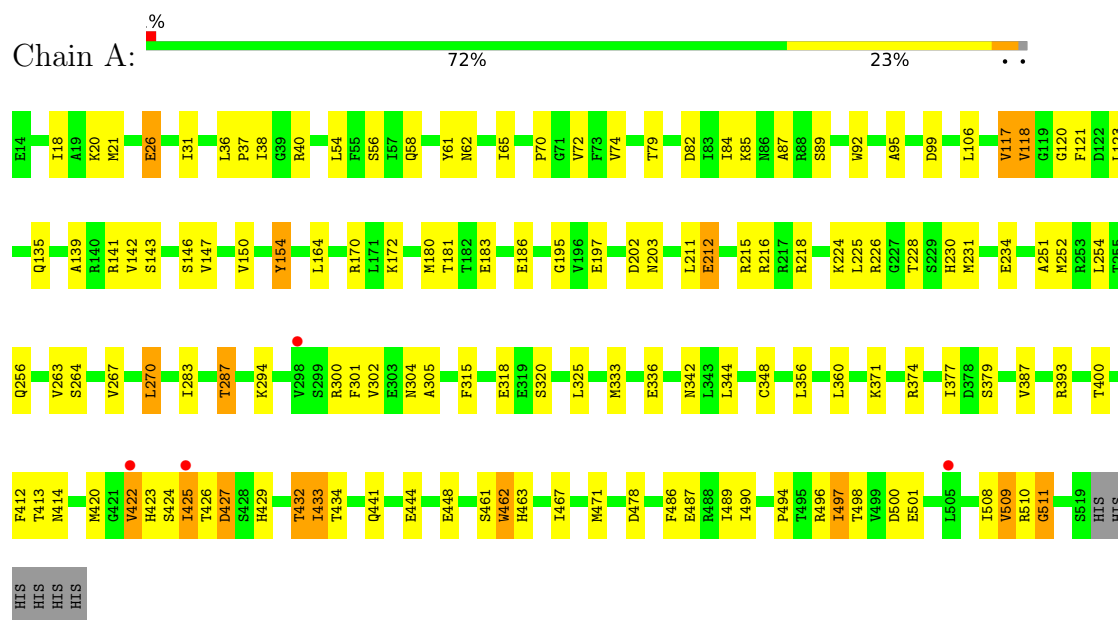
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	54	Total	O	0	0
			54	54		
5	F	67	Total	O	0	0
			67	67		

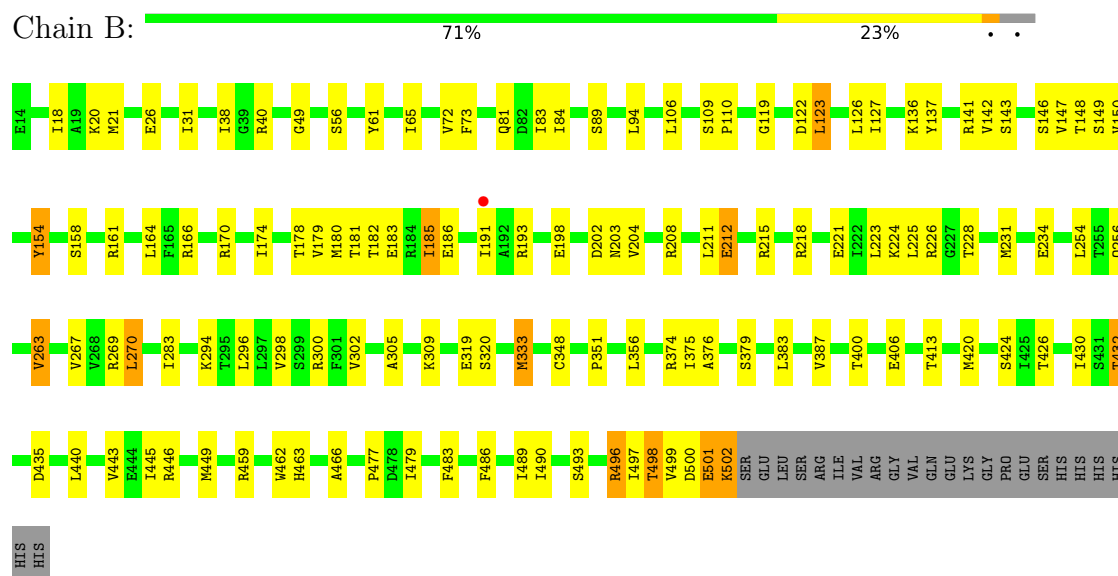
3 Residue-property plots

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: Circadian clock protein kinase KaiC

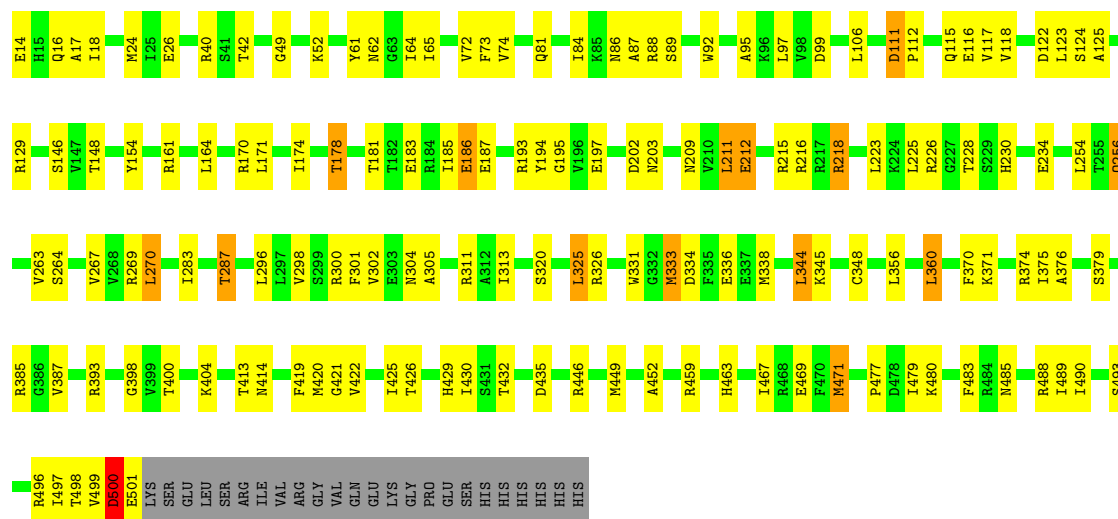


- Molecule 1: Circadian clock protein kinase KaiC



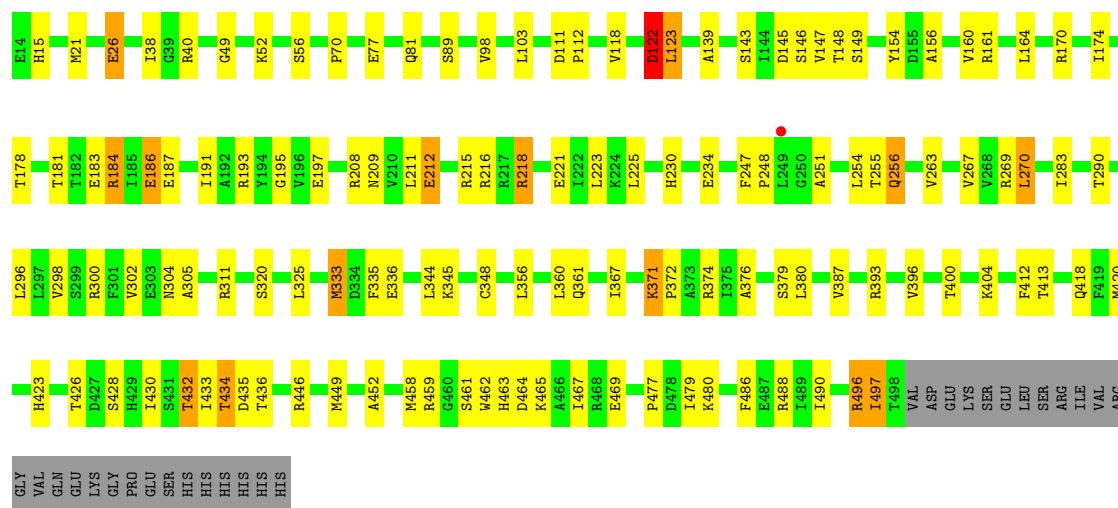
- Molecule 1: Circadian clock protein kinase KaiC

Chain C:  66% 26% 5%



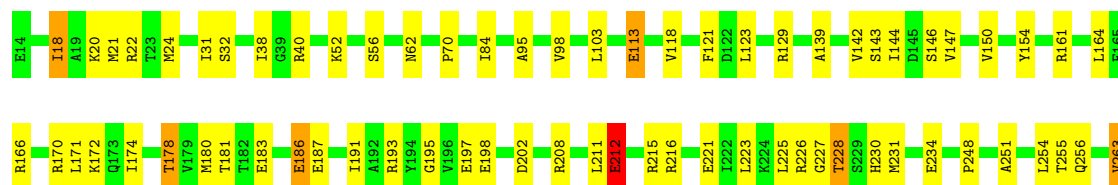
- Molecule 1: Circadian clock protein kinase KaiC

Chain D:  69% 22% 5%



- Molecule 1: Circadian clock protein kinase KaiC

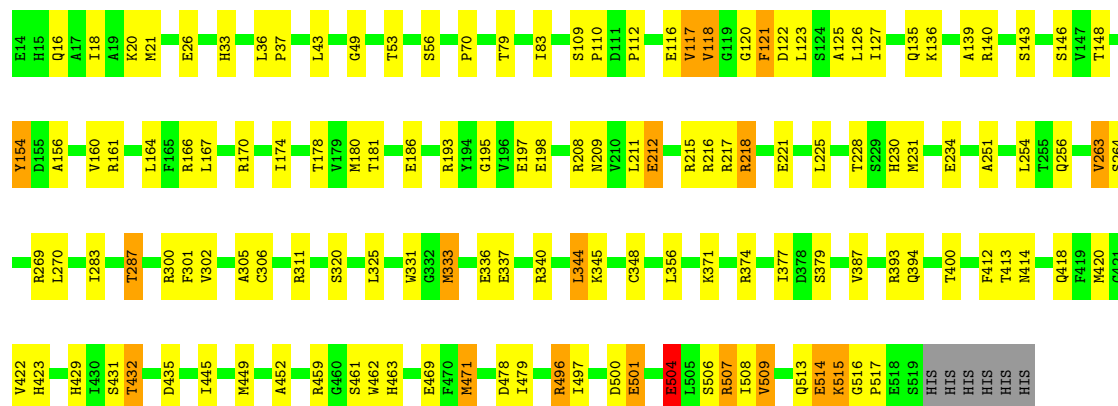
Chain E:  69% 24% 5%





- Molecule 1: Circadian clock protein kinase KaiC

Chain F: 72% 23% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.36Å 134.47Å 203.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.35 29.96 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.96-3.35) 94.8 (29.96-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 3.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168), CNS	Depositor
R, R_{free}	0.217 , 0.261 0.216 , 0.255	Depositor DCC
R_{free} test set	2665 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24219	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4, ATP, TPO

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	0.34	3/4045 (0.1%)	0.74	3/5448 (0.1%)
1	B	0.32	1/3914 (0.0%)	0.73	2/5273 (0.0%)
1	C	0.27	0/3905	0.71	0/5262
1	D	0.28	0/3881	0.72	2/5229 (0.0%)
1	E	0.28	0/3937	0.72	2/5304 (0.0%)
1	F	0.27	0/4041	0.72	0/5443
All	All	0.29	4/23723 (0.0%)	0.72	9/31959 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	MET	C-O	-7.41	1.14	1.23
1	A	252	MET	CA-C	-6.02	1.45	1.52
1	A	252	MET	CA-CB	-5.61	1.44	1.53
1	B	158	SER	C-O	-5.06	1.17	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ALA	CA-C-N	-8.65	109.05	121.42
1	A	251	ALA	C-N-CA	-8.65	109.05	121.42
1	B	158	SER	CA-CB-OG	6.53	124.16	111.10
1	D	118	VAL	N-CA-C	-6.52	107.51	113.71
1	A	252	MET	CA-CB-CG	-5.48	103.14	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3991	0	3988	75	0
1	B	3861	0	3855	87	0
1	C	3852	0	3842	101	0
1	D	3828	0	3823	83	0
1	E	3884	0	3877	88	0
1	F	3987	0	3983	76	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	93	0	36	6	0
3	B	62	0	24	2	0
3	C	62	0	24	3	0
3	D	62	0	24	1	0
3	E	62	0	24	1	0
3	F	31	0	12	1	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	1	0
5	A	74	0	0	8	0
5	B	53	0	0	5	0
5	C	83	0	0	5	0
5	D	66	0	0	2	0
5	E	54	0	0	9	0
5	F	67	0	0	3	0
All	All	24219	0	23512	464	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 10.

The worst 5 of 464 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:503:SER:HB3	1:E:504:GLU:HB2	1.29	1.12
1:B:499:VAL:C	1:B:501:GLU:HA	1.76	1.10
1:D:379:SER:H	1:D:413:THR:HB	1.41	0.83
1:F:379:SER:H	1:F:413:THR:HB	1.41	0.82
1:E:379:SER:H	1:E:413:THR:HB	1.43	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	503/512 (98%)	448 (89%)	39 (8%)	16 (3%)	3	17
1	B	486/512 (95%)	449 (92%)	28 (6%)	9 (2%)	6	25
1	C	485/512 (95%)	442 (91%)	31 (6%)	12 (2%)	4	20
1	D	482/512 (94%)	448 (93%)	27 (6%)	7 (2%)	8	29
1	E	489/512 (96%)	442 (90%)	37 (8%)	10 (2%)	6	24
1	F	503/512 (98%)	452 (90%)	37 (7%)	14 (3%)	4	19
All	All	2948/3072 (96%)	2681 (91%)	199 (7%)	68 (2%)	5	22

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ILE
1	C	17	ALA
1	C	117	VAL
1	E	463	HIS
1	F	154	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/438 (99%)	408 (94%)	24 (6%)	19	46
1	B	417/438 (95%)	396 (95%)	21 (5%)	22	49
1	C	416/438 (95%)	394 (95%)	22 (5%)	20	48
1	D	413/438 (94%)	388 (94%)	25 (6%)	17	44
1	E	420/438 (96%)	396 (94%)	24 (6%)	18	46
1	F	431/438 (98%)	400 (93%)	31 (7%)	13	39
All	All	2529/2628 (96%)	2382 (94%)	147 (6%)	18	45

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	499	VAL
1	F	504	GLU
1	F	83	ILE
1	F	218	ARG
1	C	111	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	454	ASN
1	D	342	ASN
1	D	203	ASN
1	E	342	ASN
1	B	153	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	TPO	E	432	1	8,10,11	1.10	0	10,14,16	2.07	2 (20%)
1	TPO	A	432	1	8,10,11	1.64	1 (12%)	10,14,16	2.11	2 (20%)
1	TPO	B	432	1	8,10,11	1.65	1 (12%)	10,14,16	2.00	2 (20%)
1	TPO	F	432	1	8,10,11	1.11	0	10,14,16	2.11	2 (20%)
1	TPO	C	432	1	8,10,11	1.63	1 (12%)	10,14,16	2.14	2 (20%)
1	TPO	D	432	1	8,10,11	1.13	0	10,14,16	2.19	2 (20%)

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
1	TPO	E	432	1	-	0/9/11/13	-
1	TPO	A	432	1	-	3/9/11/13	-
1	TPO	B	432	1	-	3/9/11/13	-
1	TPO	F	432	1	-	1/9/11/13	-
1	TPO	C	432	1	-	2/9/11/13	-
1	TPO	D	432	1	-	4/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	432	TPO	P-O1P	3.53	1.61	1.50
1	A	432	TPO	P-O1P	3.50	1.61	1.50
1	C	432	TPO	P-O1P	3.47	1.61	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	432	TPO	P-OG1-CB	-6.02	106.98	123.33
1	D	432	TPO	P-OG1-CB	-5.95	107.15	123.33
1	F	432	TPO	P-OG1-CB	-5.88	107.36	123.33
1	A	432	TPO	P-OG1-CB	-5.84	107.45	123.33
1	E	432	TPO	P-OG1-CB	-5.74	107.73	123.33

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	432	TPO	N-CA-CB-OG1
1	A	432	TPO	O-C-CA-CB
1	B	432	TPO	N-CA-CB-CG2
1	B	432	TPO	N-CA-CB-OG1
1	D	432	TPO	N-CA-CB-CG2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	432	TPO	2	0
1	B	432	TPO	1	0
1	F	432	TPO	1	0
1	D	432	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 7 are monoatomic - leaving 20 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	ATP	E	603	-	32,33,33	1.41	5 (15%)	48,52,52	1.77	10 (20%)
3	ATP	C	602	2	32,33,33	1.42	4 (12%)	48,52,52	1.78	9 (18%)
3	ATP	C	603	-	32,33,33	1.42	4 (12%)	48,52,52	1.77	10 (20%)
4	PO4	B	605	-	4,4,4	0.98	0	6,6,6	0.46	0
3	ATP	E	602	2	32,33,33	1.41	4 (12%)	48,52,52	1.76	9 (18%)
4	PO4	E	604	-	4,4,4	0.97	0	6,6,6	0.48	0
4	PO4	B	604	-	4,4,4	0.96	0	6,6,6	0.46	0
4	PO4	F	604	-	4,4,4	0.98	0	6,6,6	0.46	0
3	ATP	D	603	-	32,33,33	1.41	4 (12%)	48,52,52	1.76	9 (18%)
3	ATP	D	602	2	32,33,33	1.45	5 (15%)	48,52,52	1.76	9 (18%)
3	ATP	B	602	2	32,33,33	1.46	7 (21%)	48,52,52	1.73	9 (18%)
4	PO4	C	604	-	4,4,4	0.98	0	6,6,6	0.47	0
4	PO4	E	605	-	4,4,4	0.97	0	6,6,6	0.46	0
3	ATP	F	602	2	32,33,33	1.43	5 (15%)	48,52,52	1.78	9 (18%)
4	PO4	F	603	-	4,4,4	0.98	0	6,6,6	0.44	0
3	ATP	A	803	-	32,33,33	1.43	5 (15%)	48,52,52	1.75	9 (18%)
3	ATP	A	802	2	32,33,33	1.47	7 (21%)	48,52,52	1.74	9 (18%)
3	ATP	A	804	-	32,33,33	1.42	4 (12%)	48,52,52	1.77	11 (22%)
4	PO4	D	604	-	4,4,4	0.98	0	6,6,6	0.48	0
3	ATP	B	603	-	32,33,33	1.41	5 (15%)	48,52,52	1.77	11 (22%)

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	ATP	E	603	-	-	3/22/38/38	0/3/3/3
3	ATP	A	803	-	-	4/22/38/38	0/3/3/3
3	ATP	E	602	2	-	2/22/38/38	0/3/3/3
3	ATP	C	602	2	-	4/22/38/38	0/3/3/3
3	ATP	A	802	2	-	2/22/38/38	0/3/3/3
3	ATP	F	602	2	-	5/22/38/38	0/3/3/3
3	ATP	A	804	-	-	5/22/38/38	0/3/3/3
3	ATP	C	603	-	-	5/22/38/38	0/3/3/3
3	ATP	D	603	-	-	4/22/38/38	0/3/3/3
3	ATP	D	602	2	-	8/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	603	-	-	3/22/38/38	0/3/3/3
3	ATP	B	602	2	-	7/22/38/38	0/3/3/3

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	ATP	C5-C4	4.84	1.47	1.39
3	D	603	ATP	C5-C4	4.83	1.47	1.39
3	C	602	ATP	C5-C4	4.82	1.47	1.39
3	D	602	ATP	C5-C4	4.81	1.47	1.39
3	A	803	ATP	C5-C4	4.80	1.47	1.39

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	ATP	C5-C4-N3	-6.01	118.44	126.72
3	D	603	ATP	C5-C4-N3	-5.98	118.48	126.72
3	F	602	ATP	C5-C4-N3	-5.97	118.49	126.72
3	E	602	ATP	C5-C4-N3	-5.96	118.51	126.72
3	C	603	ATP	C5-C4-N3	-5.93	118.55	126.72

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	ATP	C5'-O5'-PA-O1A
3	A	803	ATP	C5'-O5'-PA-O2A
3	A	803	ATP	C5'-O5'-PA-O3A
3	A	804	ATP	C5'-O5'-PA-O1A
3	A	804	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

10 monomers are involved in 15 short contacts:

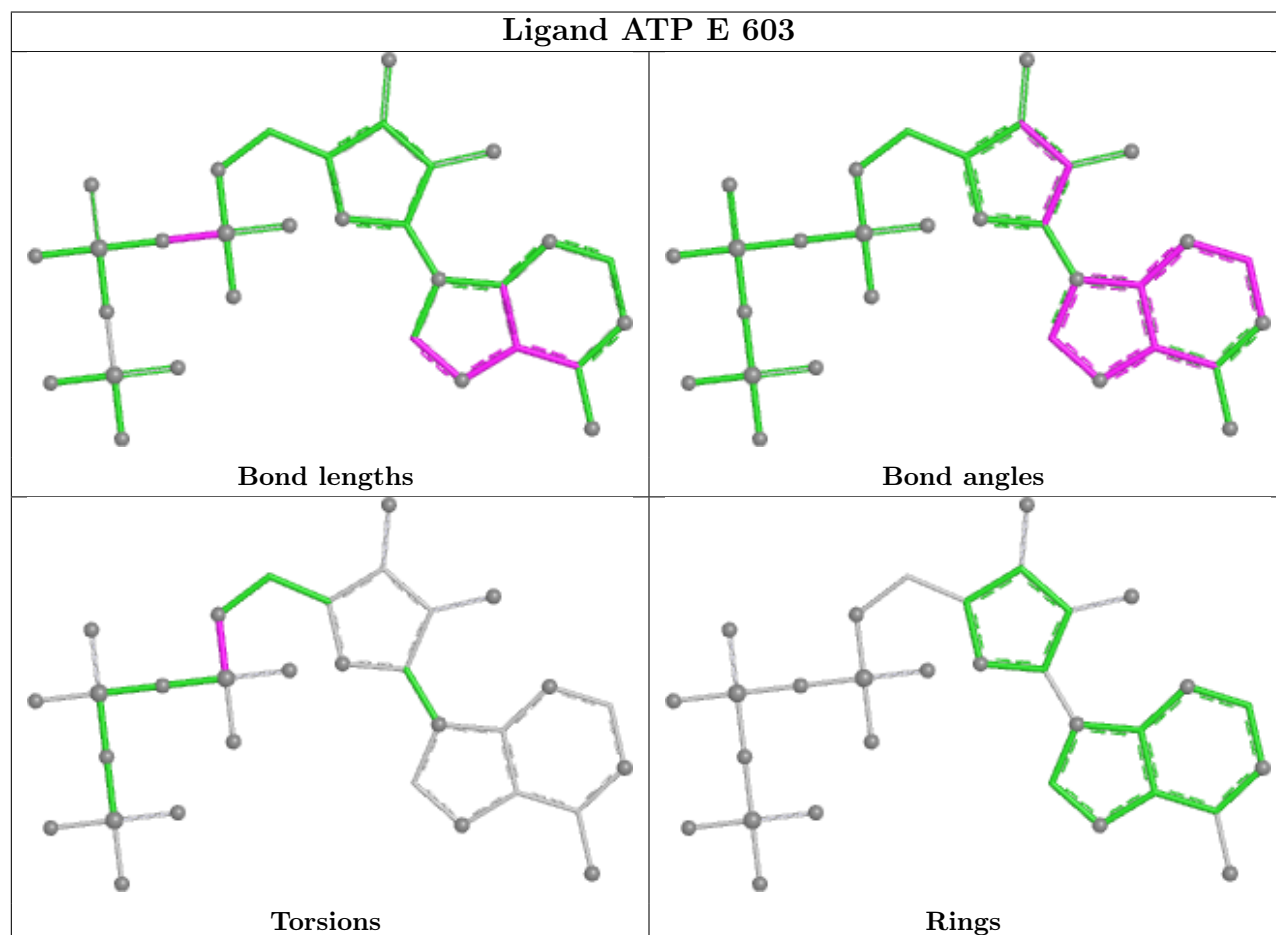
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	ATP	1	0
3	C	603	ATP	2	0
3	E	602	ATP	1	0
4	F	604	PO4	1	0
3	D	603	ATP	1	0

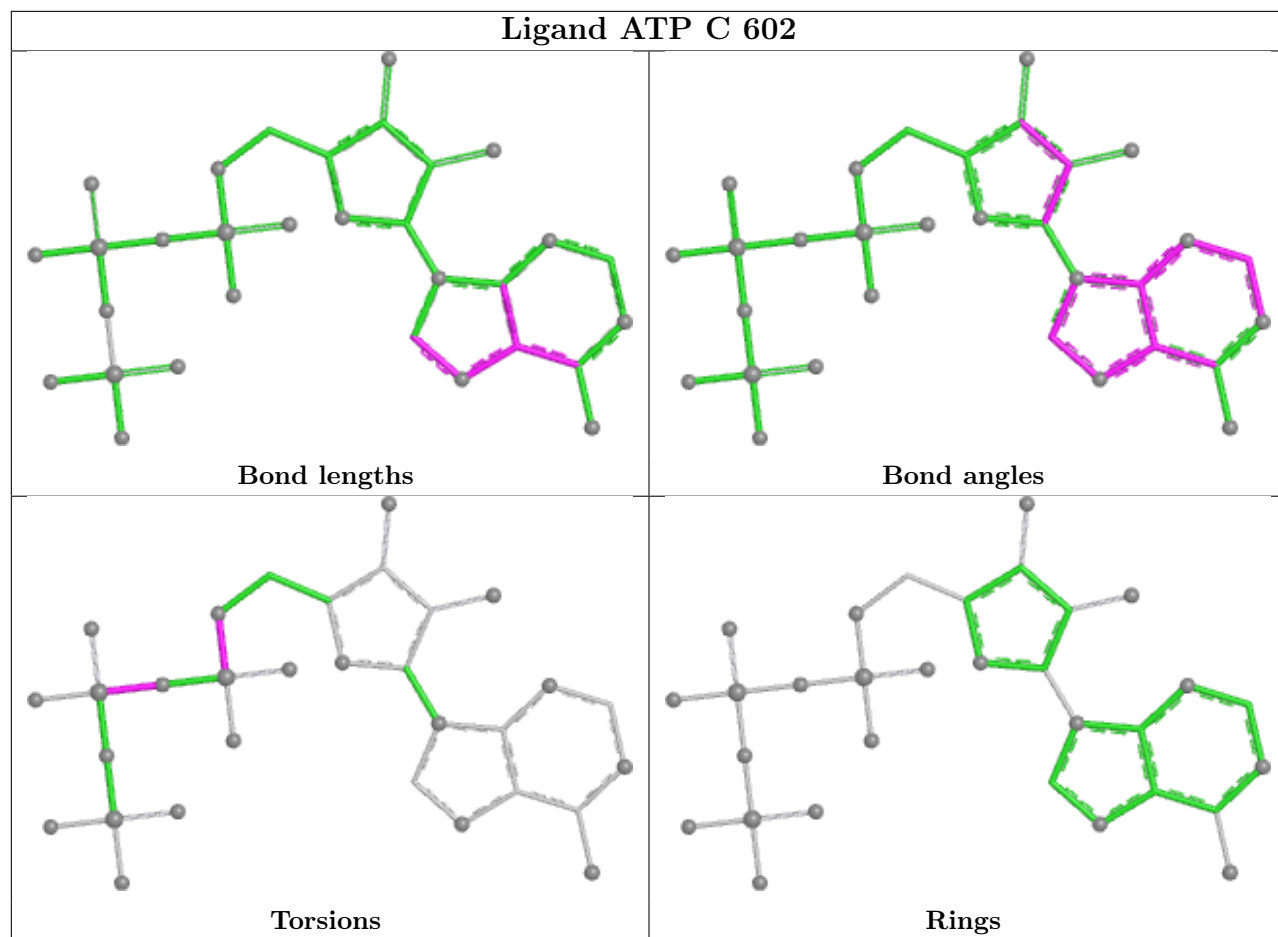
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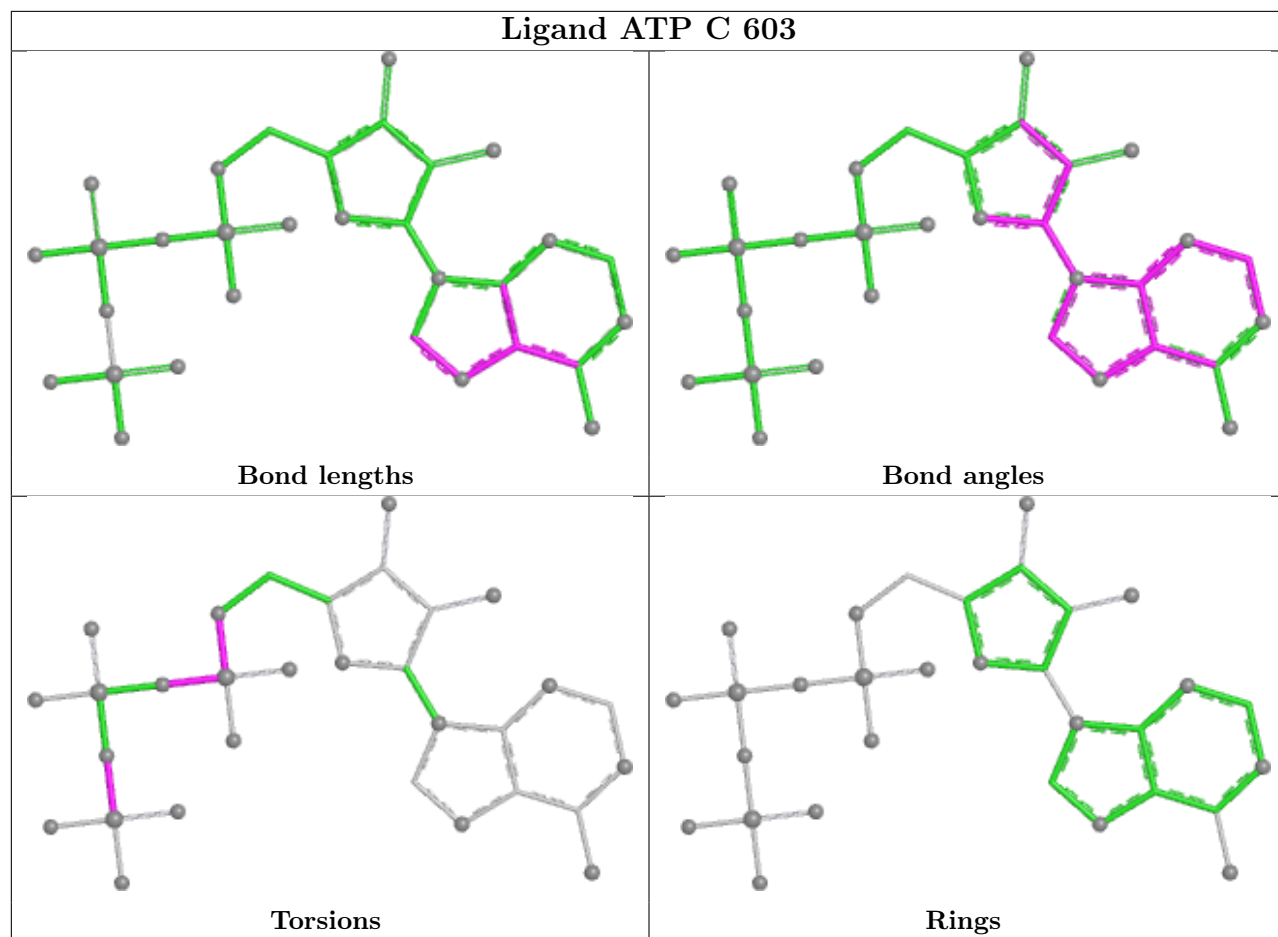
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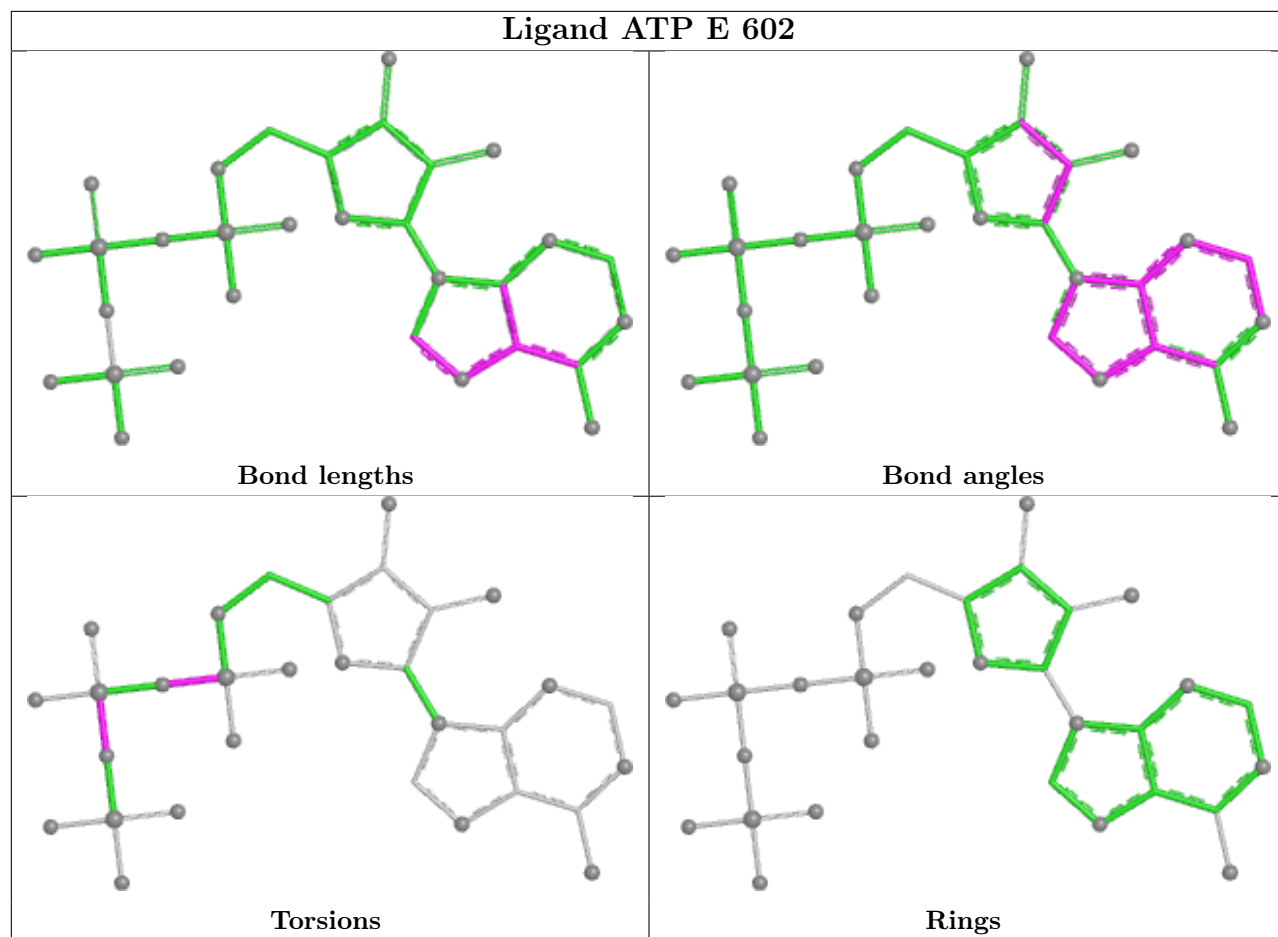
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	602	ATP	1	0
3	A	803	ATP	3	0
3	A	802	ATP	2	0
3	A	804	ATP	1	0
3	B	603	ATP	2	0

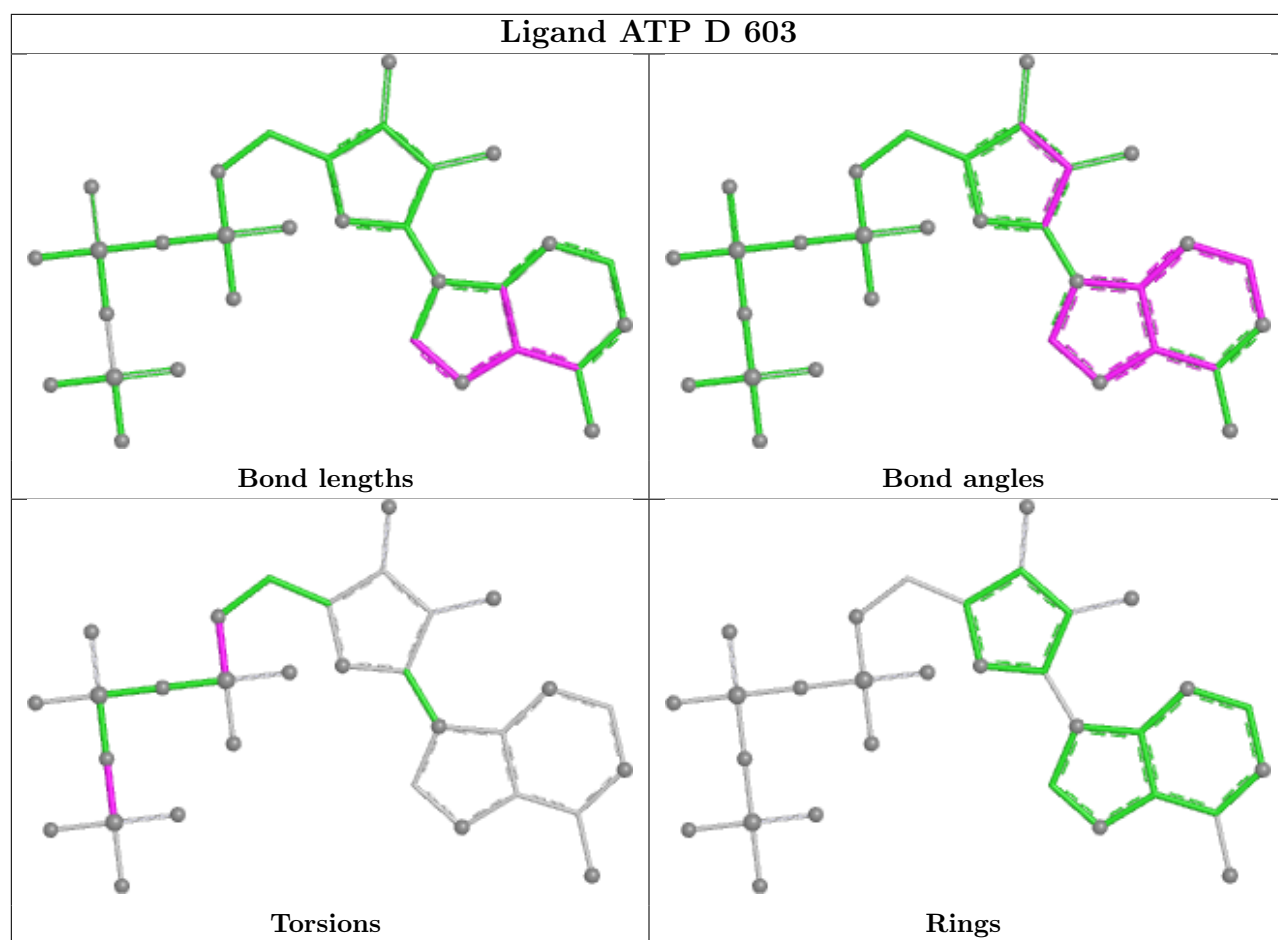
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

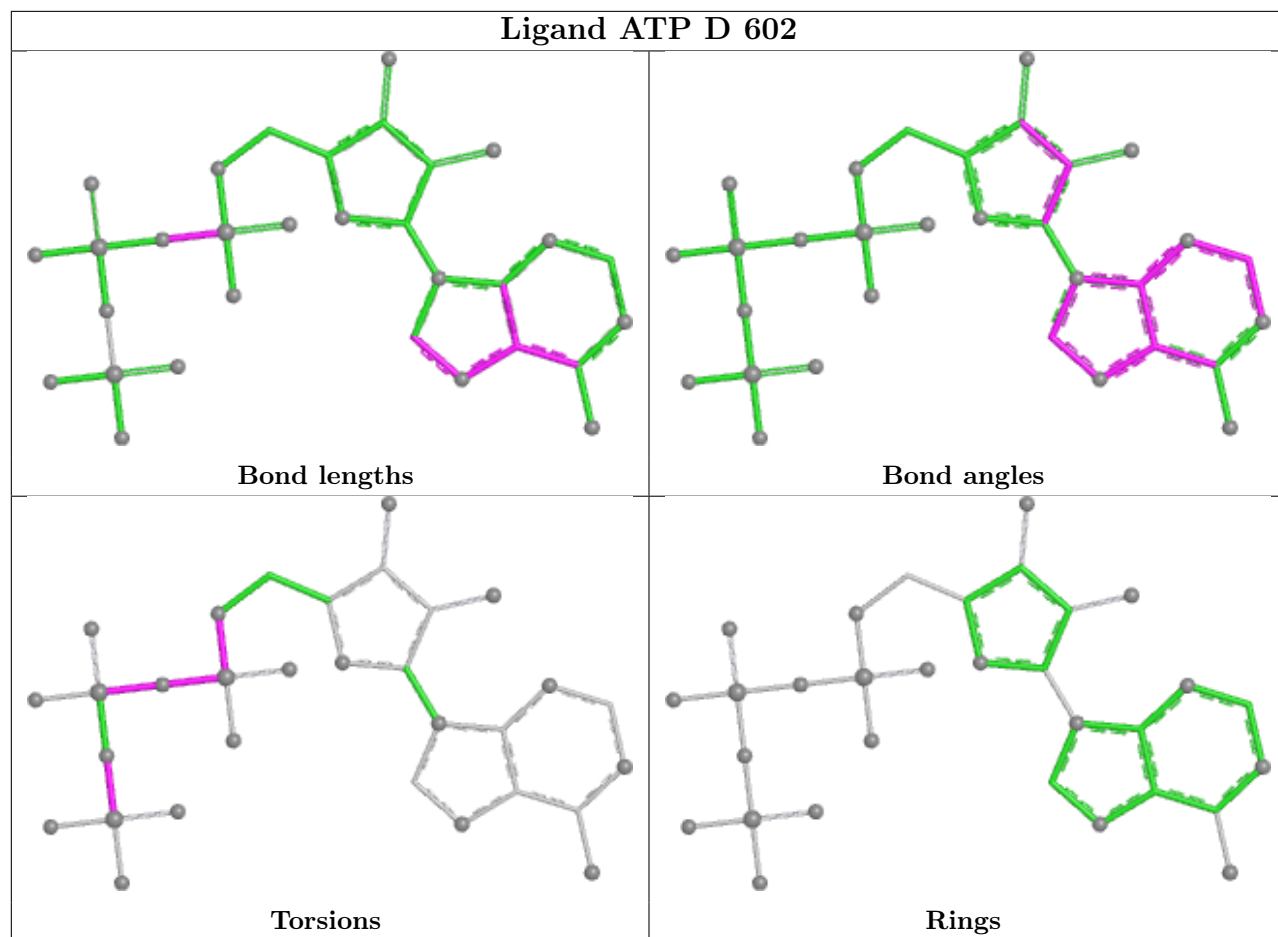


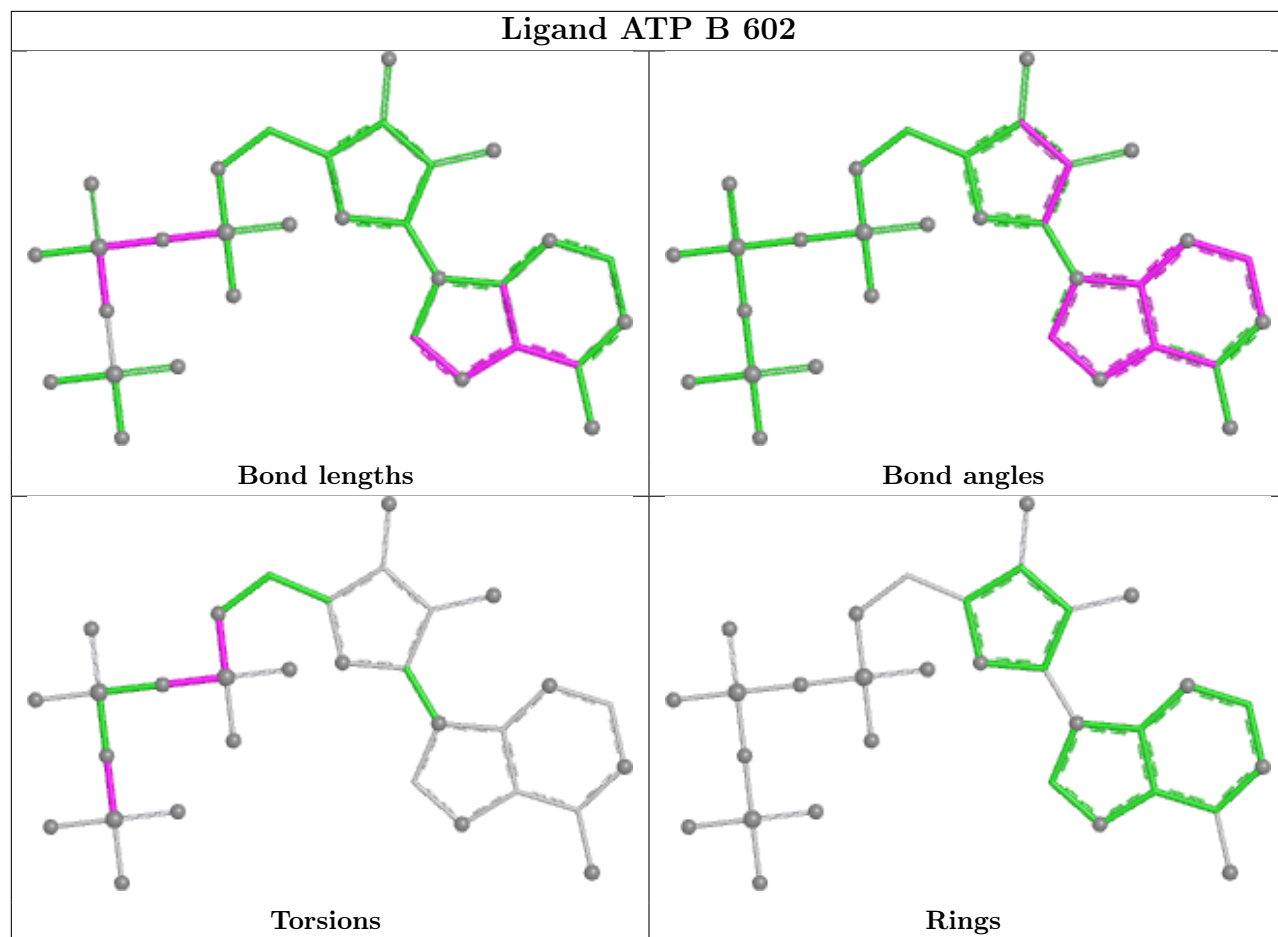


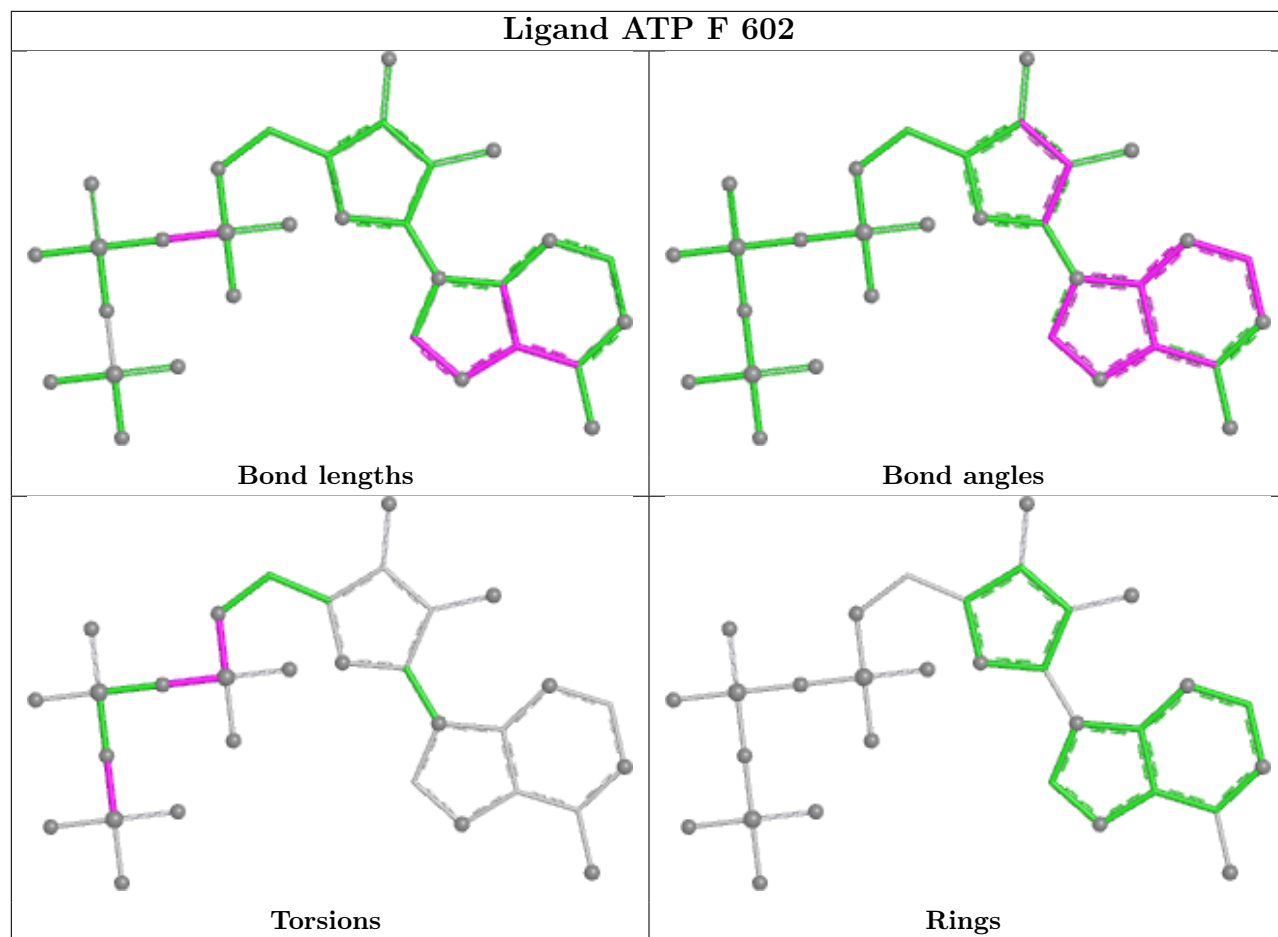


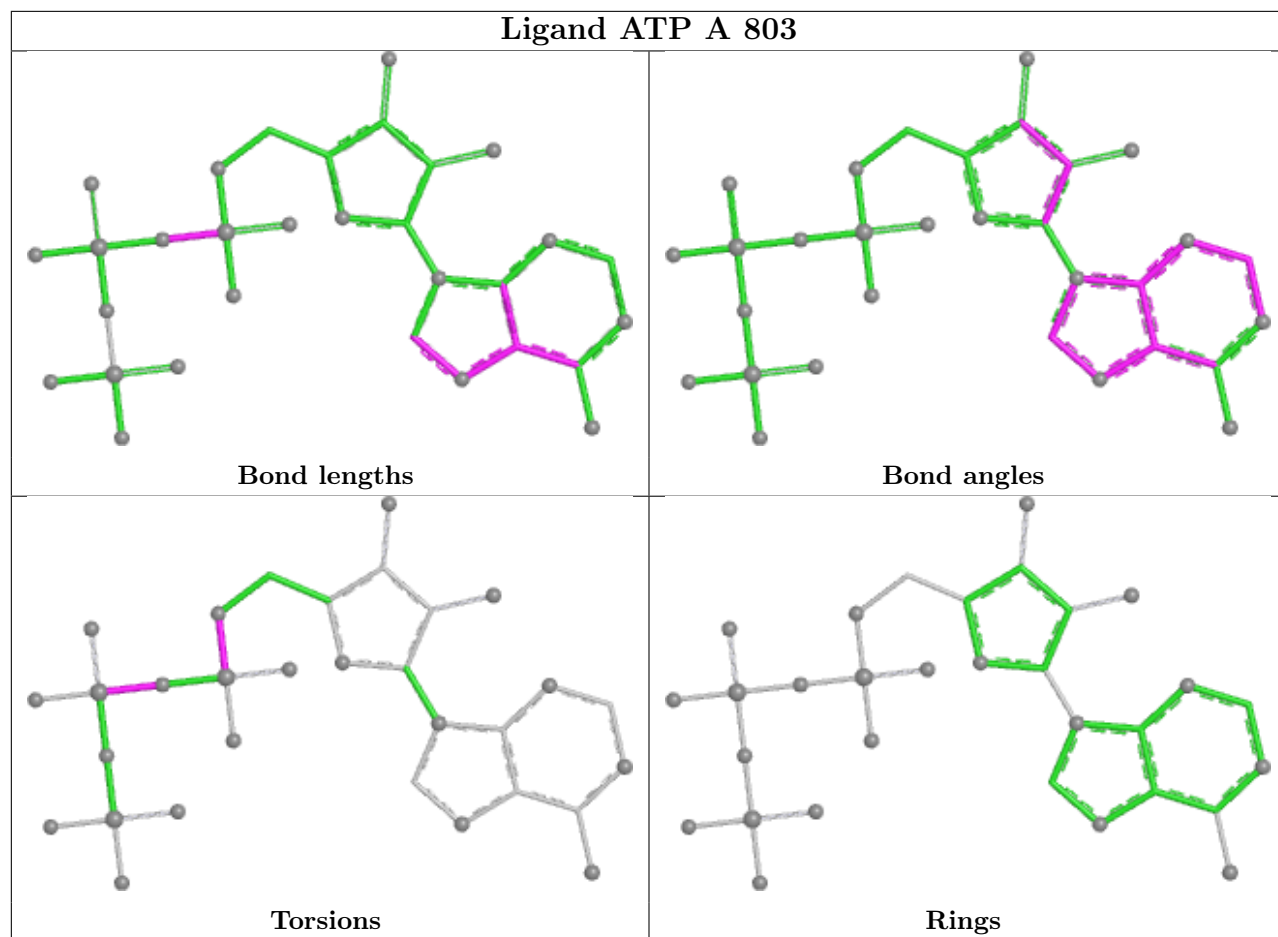


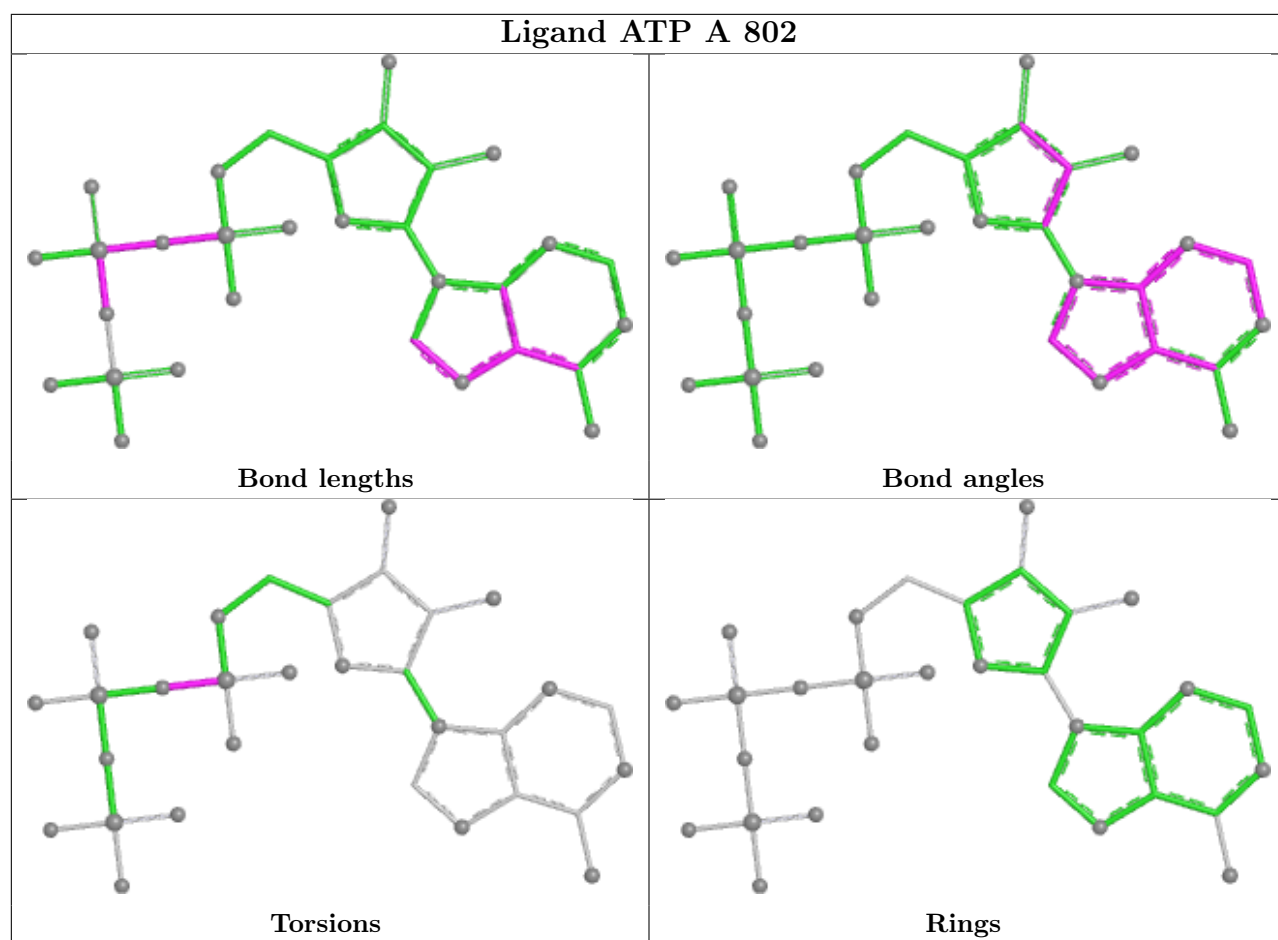


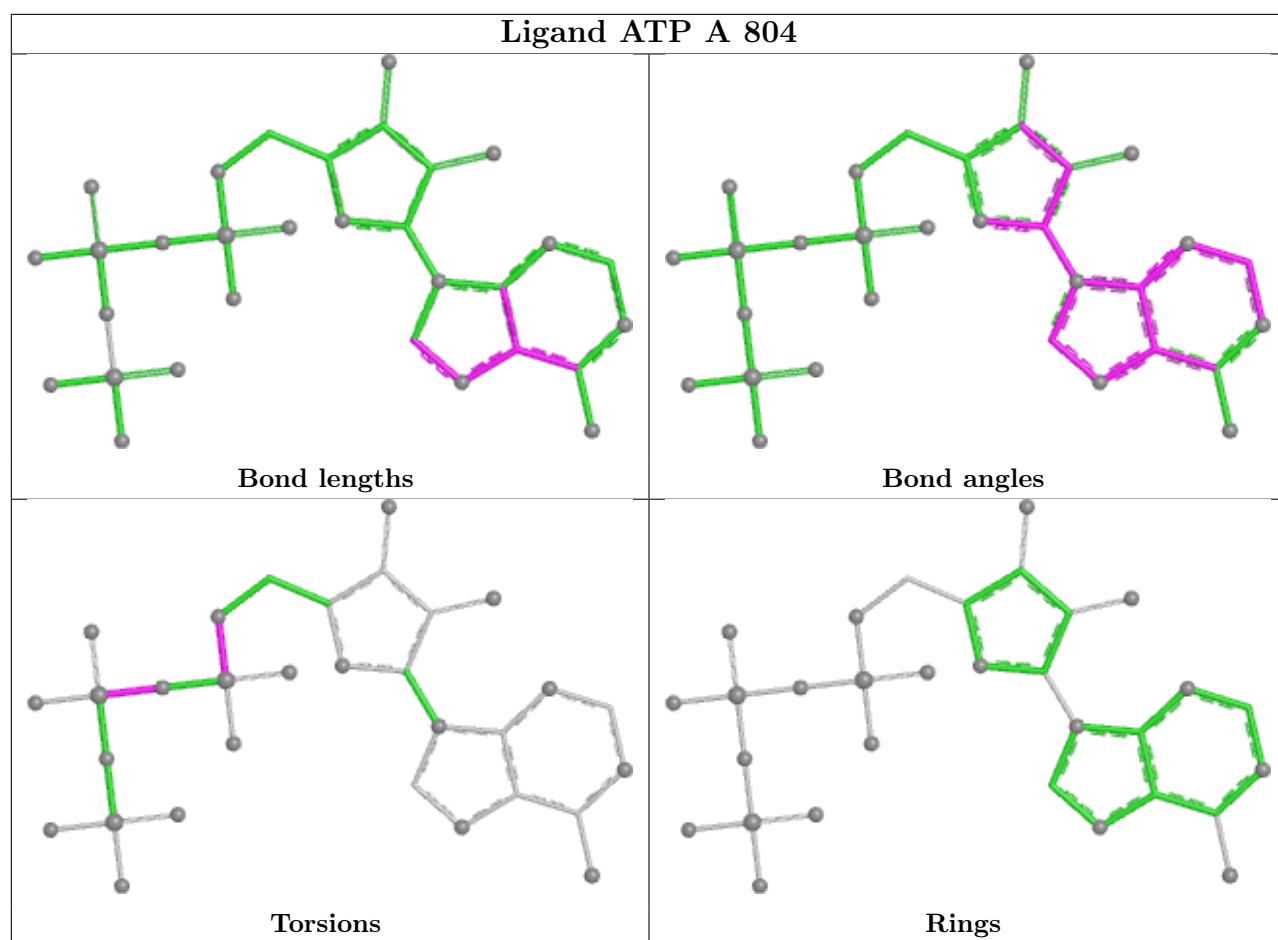


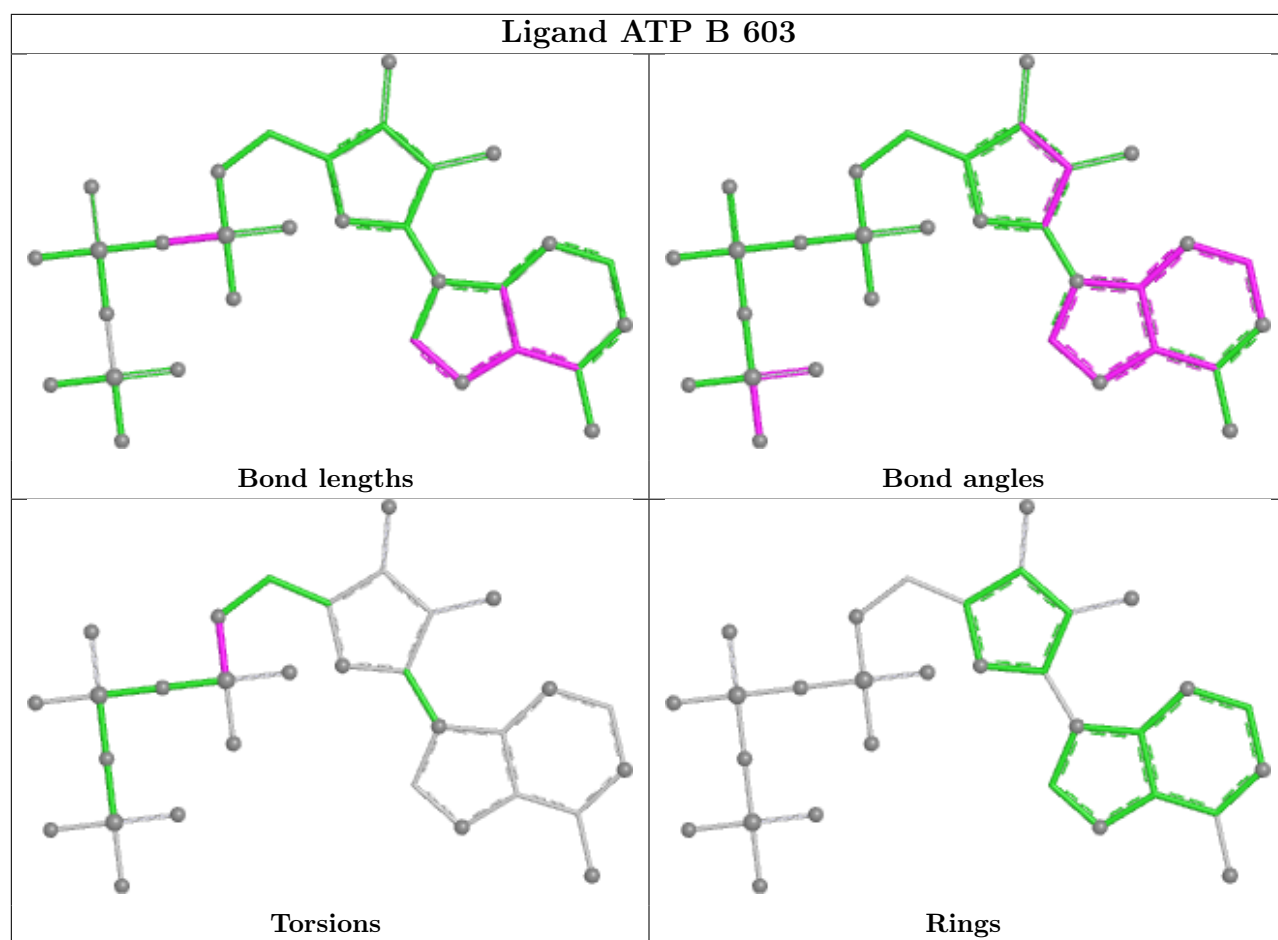












5.7 Other polymers [i](#)

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	505/512 (98%)	-0.23	4 (0%) 82 71	27, 84, 140, 180	0
1	B	488/512 (95%)	-0.19	1 (0%) 91 87	38, 84, 134, 171	0
1	C	487/512 (95%)	-0.33	0 100 100	29, 67, 120, 176	0
1	D	484/512 (94%)	-0.47	1 (0%) 91 87	13, 50, 114, 144	0
1	E	491/512 (95%)	-0.46	1 (0%) 91 87	8, 54, 120, 167	0
1	F	505/512 (98%)	-0.42	0 100 100	8, 66, 136, 181	0
All	All	2960/3072 (96%)	-0.35	7 (0%) 91 87	8, 69, 130, 181	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	422	VAL	3.1
1	D	249	LEU	2.6
1	B	191	ILE	2.5
1	A	298	VAL	2.3
1	A	425	ILE	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	A	432	11/12	0.63	0.09	83,90,112,116	0
1	TPO	B	432	11/12	0.83	0.08	68,87,103,106	0
1	TPO	F	432	11/12	0.85	0.10	46,73,98,100	0
1	TPO	D	432	11/12	0.86	0.10	38,55,98,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPO	C	432	11/12	0.86	0.09	45,57,76,83	0
1	TPO	E	432	11/12	0.89	0.09	33,45,78,90	0

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($\text{\AA}^2$)	Q<0.9
4	PO4	B	604	5/5	0.31	0.16	126,129,146,151	0
2	MG	F	601	1/1	0.70	0.09	85,85,85,85	0
4	PO4	F	604	5/5	0.73	0.23	77,78,106,143	0
4	PO4	E	605	5/5	0.79	0.24	55,64,81,115	0
4	PO4	E	604	5/5	0.80	0.07	112,123,141,148	0
4	PO4	D	604	5/5	0.83	0.30	71,83,87,111	0
4	PO4	B	605	5/5	0.83	0.30	81,94,105,120	0
4	PO4	F	603	5/5	0.86	0.25	62,66,103,119	0
3	ATP	F	602	31/31	0.86	0.09	66,101,113,120	0
3	ATP	B	603	31/31	0.87	0.09	55,80,104,117	0
3	ATP	B	602	31/31	0.89	0.08	52,66,86,93	0
2	MG	C	601	1/1	0.89	0.09	43,43,43,43	0
4	PO4	C	604	5/5	0.89	0.15	43,74,89,107	0
3	ATP	A	803	31/31	0.89	0.10	34,64,97,99	0
3	ATP	E	602	31/31	0.90	0.09	38,79,94,95	0
3	ATP	A	802	31/31	0.91	0.08	58,82,97,100	0
2	MG	B	601	1/1	0.92	0.06	63,63,63,63	0
3	ATP	C	603	31/31	0.92	0.09	22,50,78,105	0
3	ATP	D	602	31/31	0.94	0.07	32,54,66,77	0
2	MG	B	606	1/1	0.94	0.07	69,69,69,69	0
3	ATP	E	603	31/31	0.94	0.08	7,18,53,72	0
3	ATP	D	603	31/31	0.95	0.09	3,17,54,88	0
3	ATP	A	804	31/31	0.95	0.07	8,37,63,78	0
3	ATP	C	602	31/31	0.95	0.07	23,46,74,82	0
2	MG	E	601	1/1	0.96	0.04	59,59,59,59	0
2	MG	D	601	1/1	0.96	0.06	55,55,55,55	0

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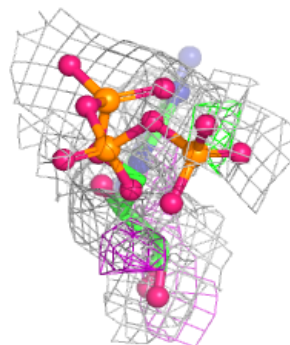
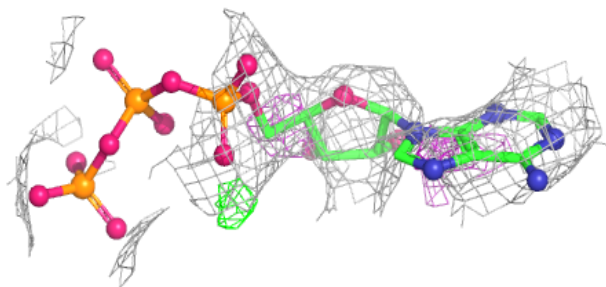
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	801	1/1	0.98	0.04	82,82,82,82	0

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.

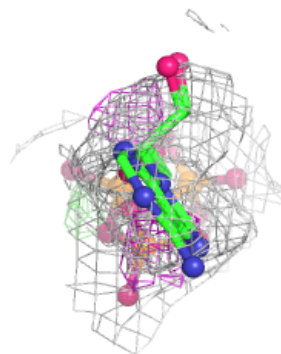
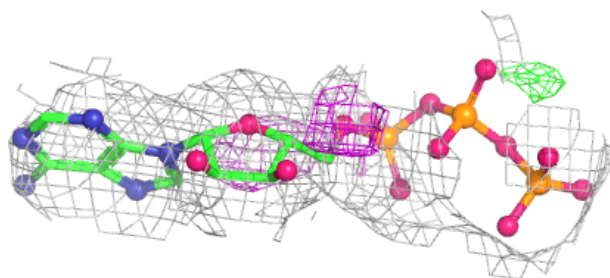
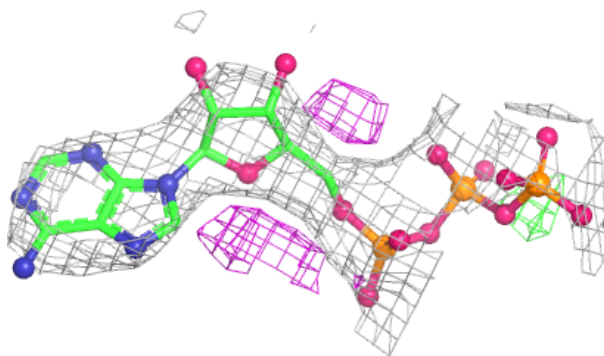
Electron density around ATP F 602:

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

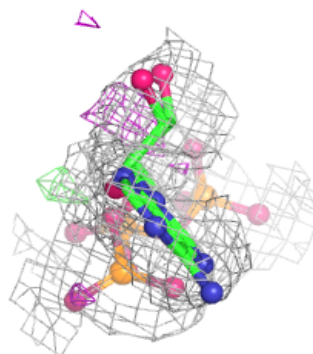
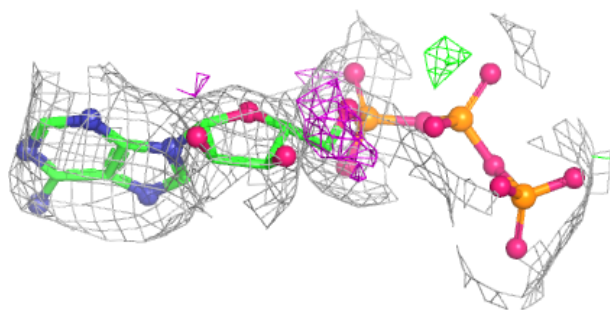
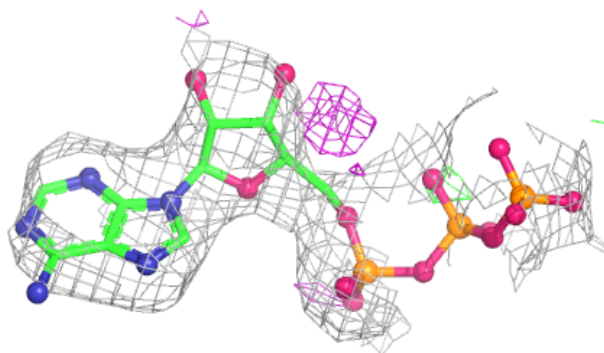


Electron density around ATP B 603:

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

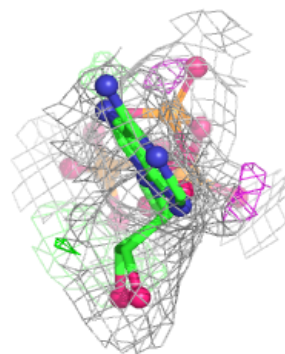
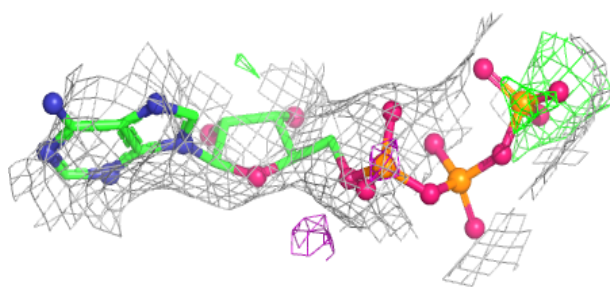
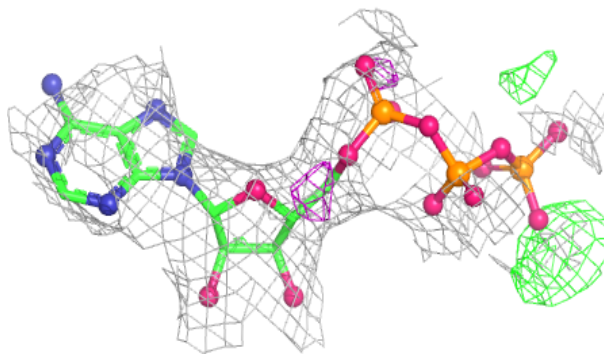
**Electron density around ATP B 602:**

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and green (positive)

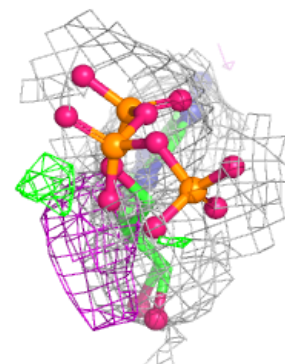
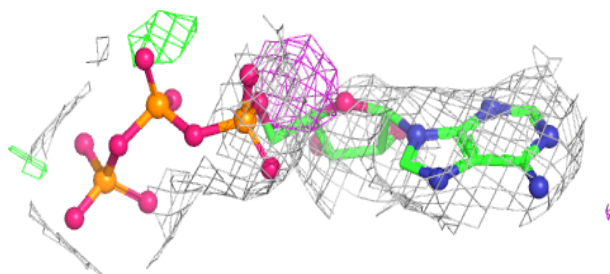
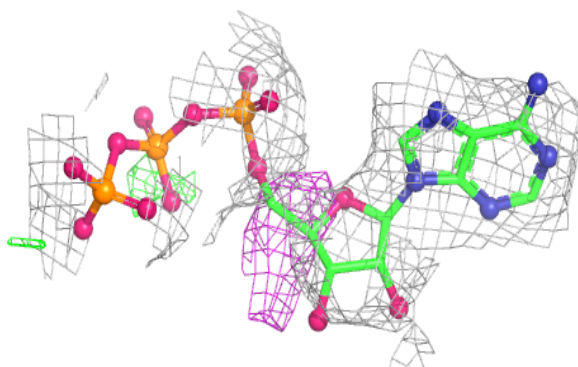


Electron density around ATP A 803:

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

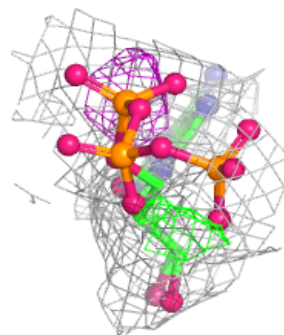
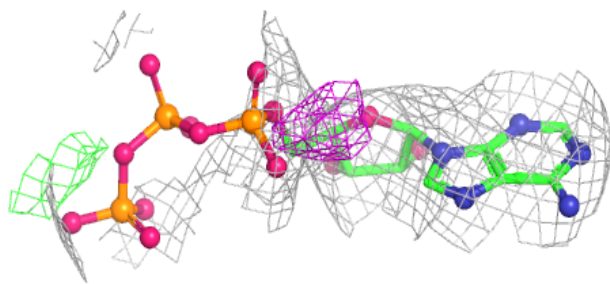
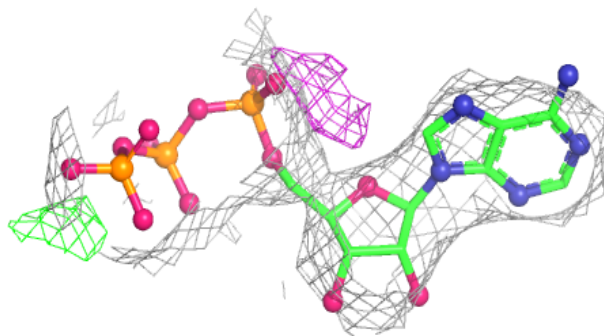
**Electron density around ATP E 602:**

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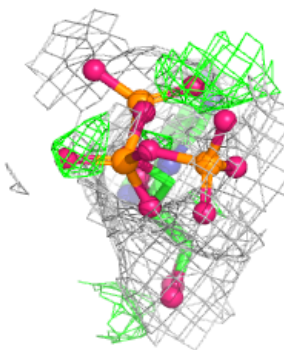
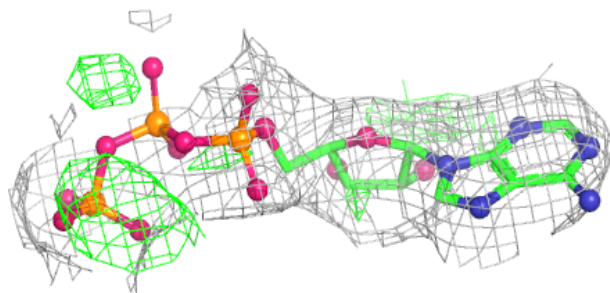
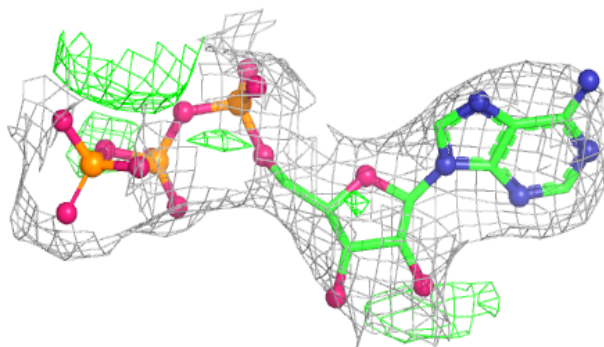


Electron density around ATP A 802:

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and green (positive)

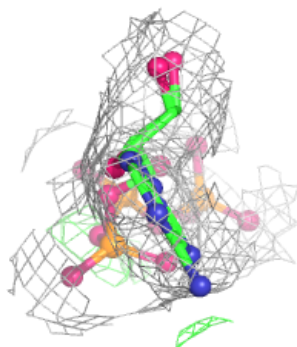
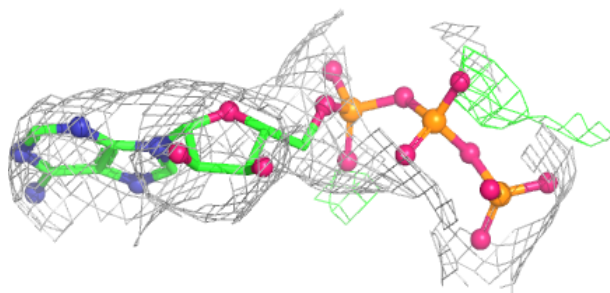
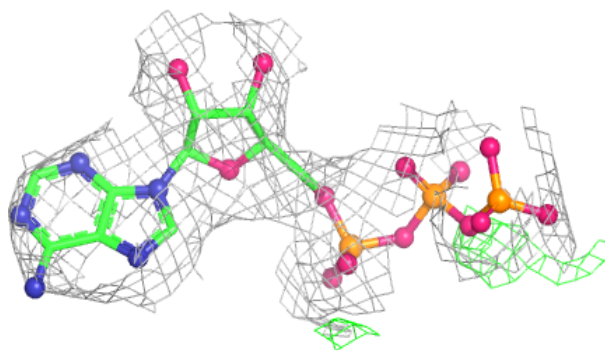
**Electron density around ATP C 603:**

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

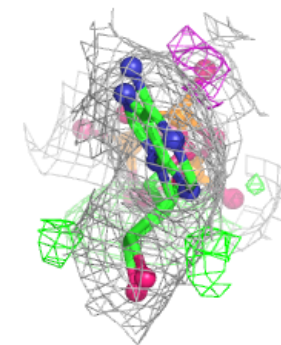
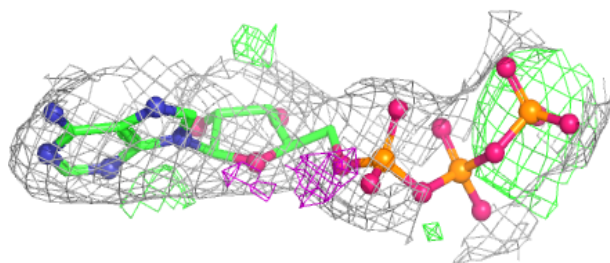
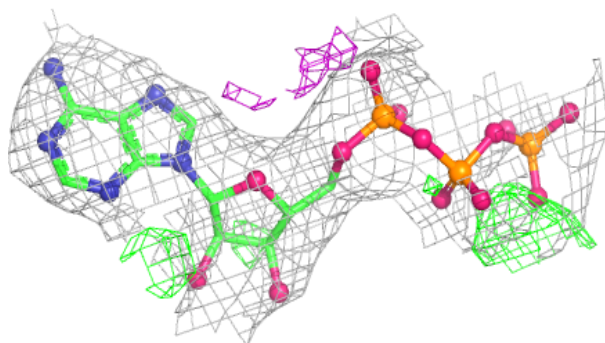


Electron density around ATP D 602:

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

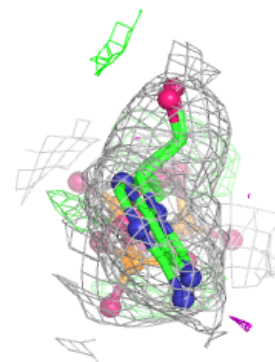
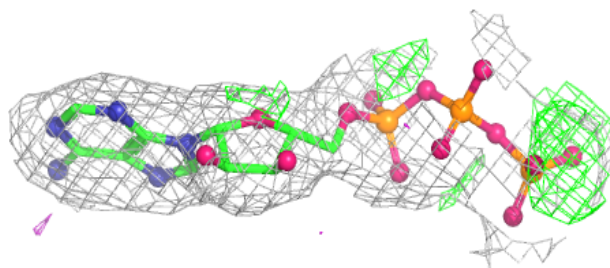
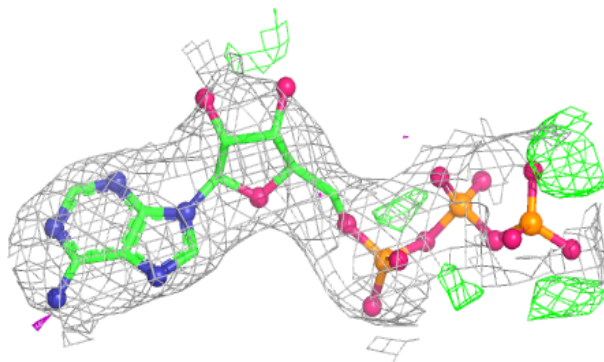
**Electron density around ATP E 603:**

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

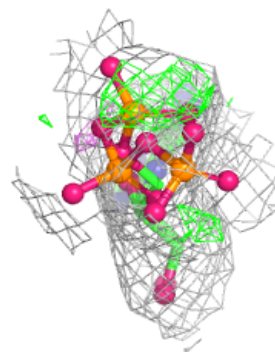
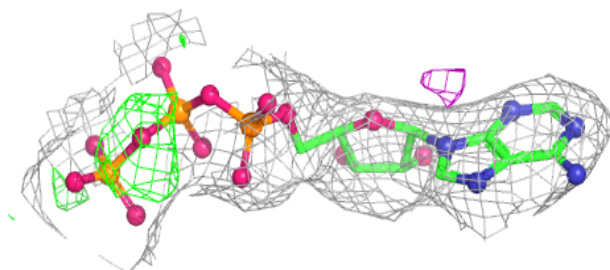
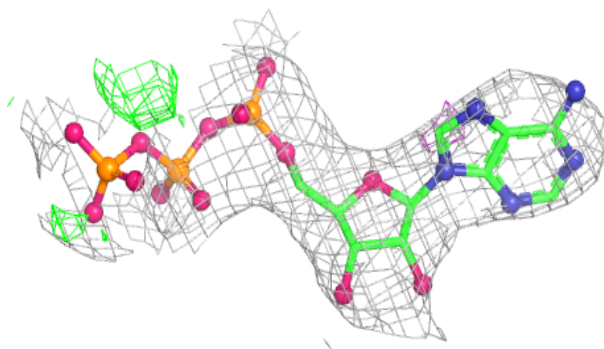


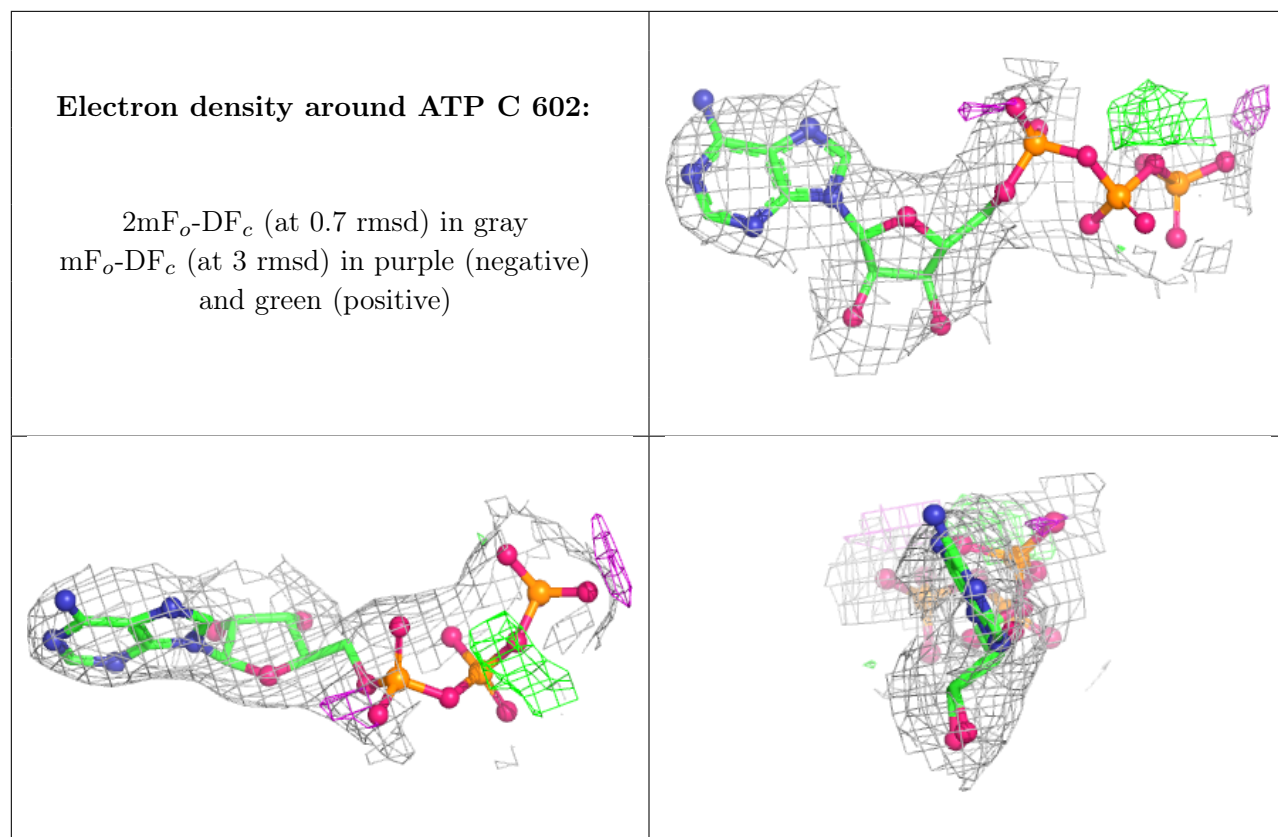
Electron density around ATP D 603:

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

**Electron density around ATP A 804:**

$2mF_o-DF_c$ (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.