



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 05:43 PM EDT

PDB ID : 3H0R / pdb_00003h0r
Title : Structure of trna-dependent amidotransferase gatcab from aquifex aeolicus
Authors : Wu, J.; Bu, W.; Sheppard, K.; Kitabatake, M.; Soll, D.; Smith, J.L.
Deposited on : 2009-04-10
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

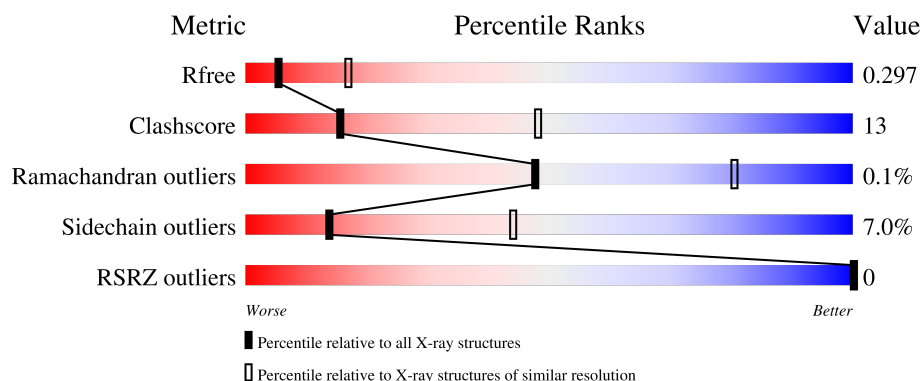
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



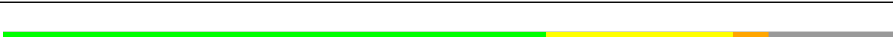
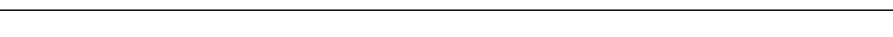
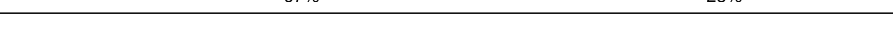
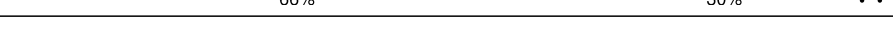
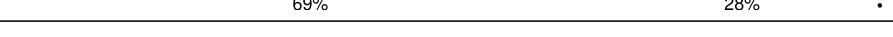
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	478	71% 25% .
1	D	478	72% 24% .
1	G	478	76% 22% .
1	J	478	72% 25% ..
1	M	478	76% 21% .

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Mol	Chain	Length	Quality of chain
1	P	478	
1	S	478	
1	V	478	
2	B	478	
2	E	478	
2	H	478	
2	K	478	
2	N	478	
2	Q	478	
2	T	478	
2	W	478	
3	C	94	
3	F	94	
3	I	94	
3	L	94	
3	O	94	
3	R	94	
3	U	94	
3	X	94	

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	ASN	D	902	-	-	X	-
4	ASN	S	907	-	-	X	-
4	ASN	V	908	-	-	X	-
9	ASP	H	482	-	-	X	-
9	ASP	N	482	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 63243 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	D	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	G	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	J	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	M	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	P	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	S	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	V	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	E	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	H	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	K	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	N	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	Q	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

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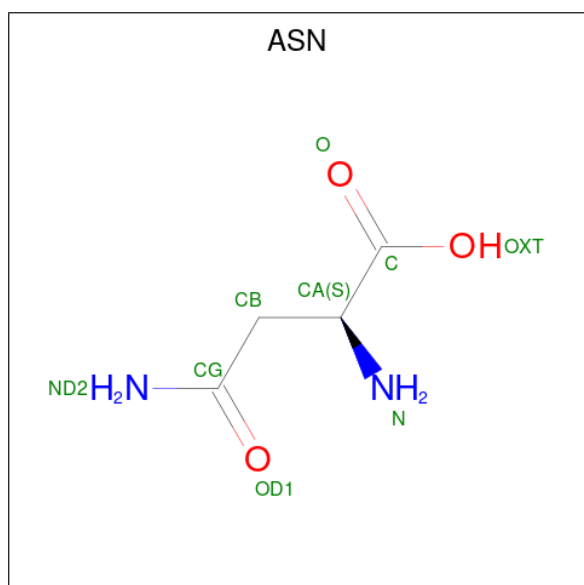
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	W	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	F	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	I	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	L	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	O	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	R	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	U	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	X	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			

- Molecule 4 is ASPARAGINE (CCD ID: ASN) (formula: C₄H₈N₂O₃).

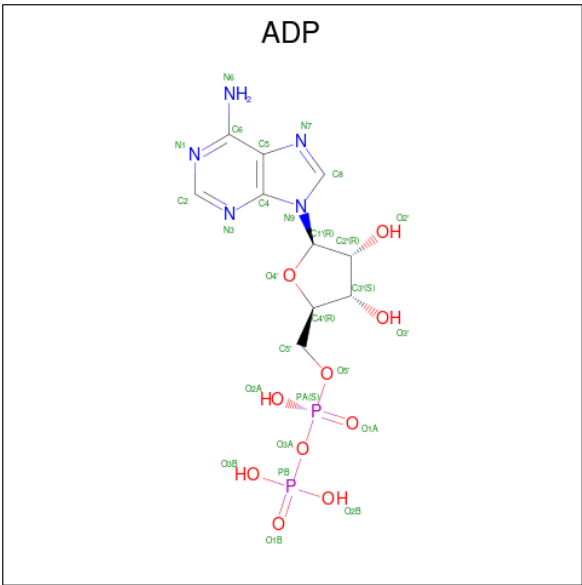


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	D	1	Total	C	N	O	0	0
			8	4	1	3		
4	G	1	Total	C	N	O	0	0
			8	4	1	3		
4	J	1	Total	C	N	O	0	0
			8	4	1	3		
4	M	1	Total	C	N	O	0	0
			8	4	1	3		
4	P	1	Total	C	N	O	0	0
			8	4	1	3		
4	S	1	Total	C	N	O	0	0
			8	4	1	3		
4	V	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		
5	H	1	Total	Zn	0	0
			1	1		
5	K	1	Total	Zn	0	0
			1	1		
5	N	1	Total	Zn	0	0
			1	1		
5	Q	1	Total	Zn	0	0
			1	1		
5	T	1	Total	Zn	0	0
			1	1		
5	W	1	Total	Zn	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

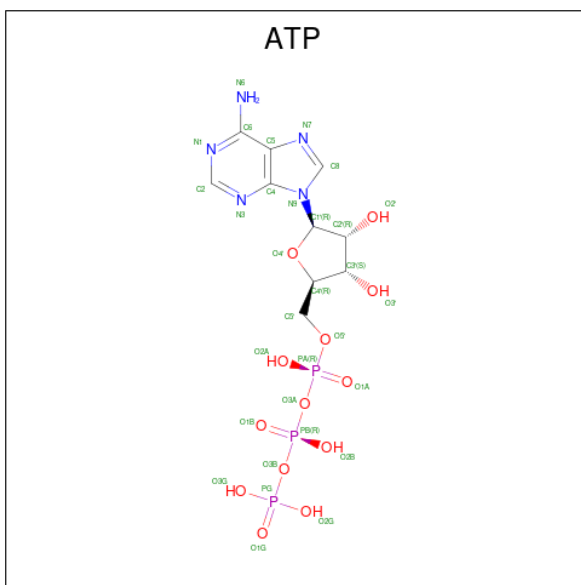


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	T	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

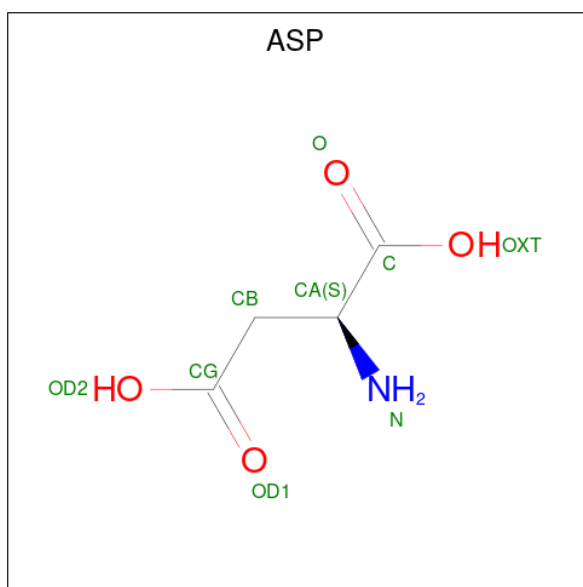
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Mn	0	0
			2	2		
7	E	2	Total	Mn	0	0
			2	2		
7	H	2	Total	Mn	0	0
			2	2		
7	K	2	Total	Mn	0	0
			2	2		
7	N	2	Total	Mn	0	0
			2	2		
7	Q	2	Total	Mn	0	0
			2	2		
7	T	2	Total	Mn	0	0
			2	2		
7	W	2	Total	Mn	0	0
			2	2		

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
8	H	1	Total 31	C 10	N 5	O 13	P 3	0	0
8	K	1	Total 31	C 10	N 5	O 13	P 3	0	0
8	N	1	Total 31	C 10	N 5	O 13	P 3	0	0
8	Q	1	Total 31	C 10	N 5	O 13	P 3	0	0
8	W	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 9 is ASPARTIC ACID (CCD ID: ASP) (formula: $\text{C}_4\text{H}_7\text{NO}_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			9	4	1	4		
9	N	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			1	1		
10	B	4	Total	O	0	0
			4	4		
10	E	3	Total	O	0	0
			3	3		
10	G	2	Total	O	0	0
			2	2		
10	H	3	Total	O	0	0
			3	3		
10	J	2	Total	O	0	0
			2	2		
10	K	5	Total	O	0	0
			5	5		
10	M	3	Total	O	0	0
			3	3		
10	N	5	Total	O	0	0
			5	5		
10	P	2	Total	O	0	0
			2	2		

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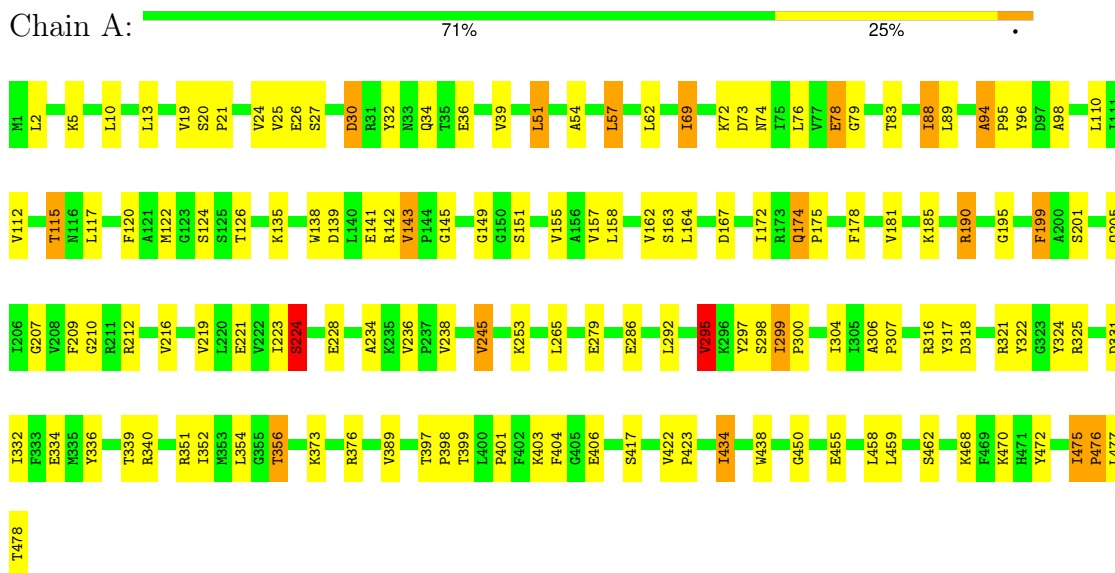
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	Q	7	Total 7	O 7	0	0
10	T	5	Total 5	O 5	0	0
10	V	1	Total 1	O 1	0	0
10	W	6	Total 6	O 6	0	0

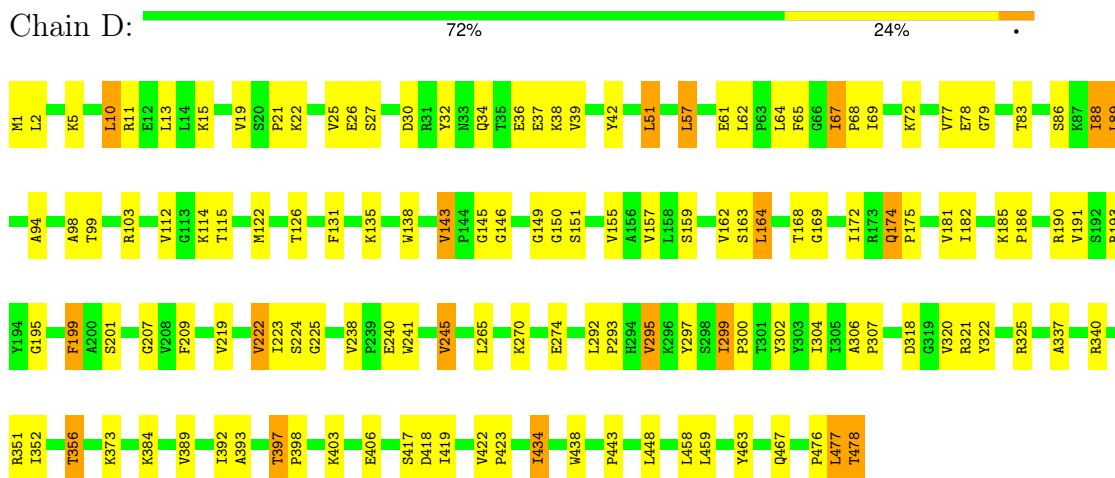
3 Residue-property plots

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: Glutamyl-tRNA(Gln) amidotransferase subunit A

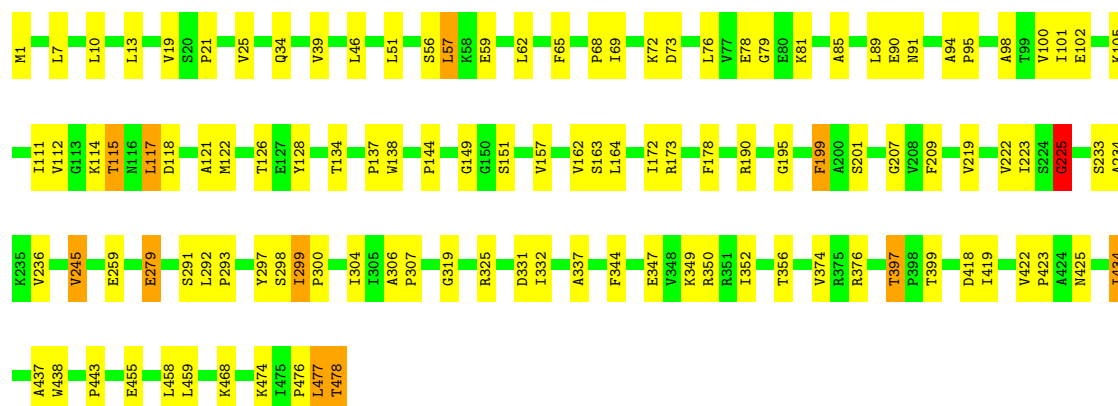


- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



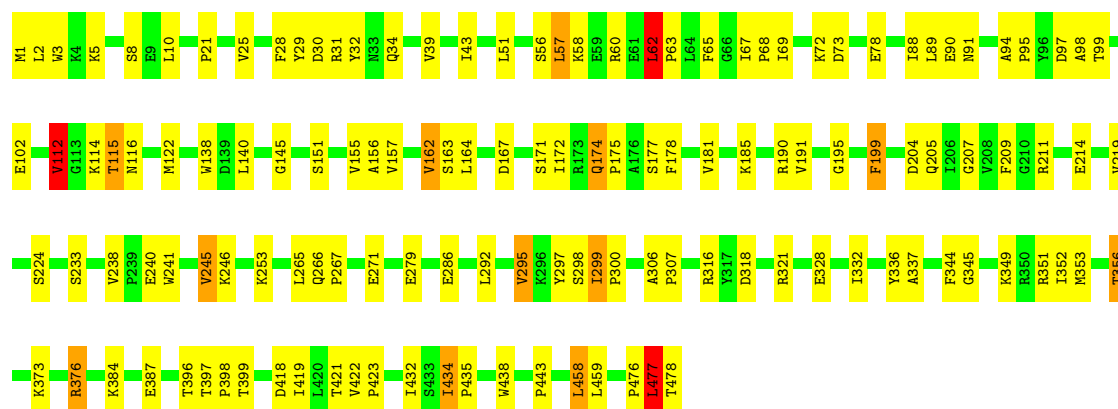
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain G:  76% 22% .



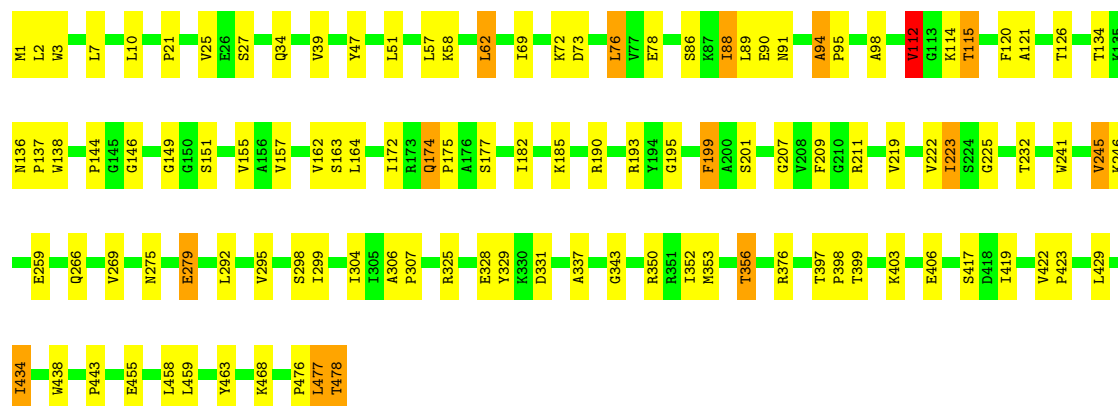
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain J:  72% 25% ..



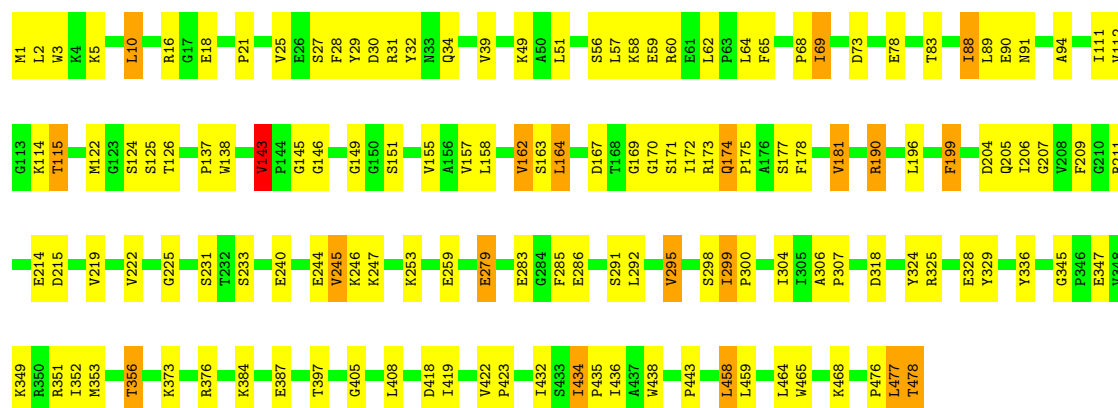
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain M:  76% 21% .



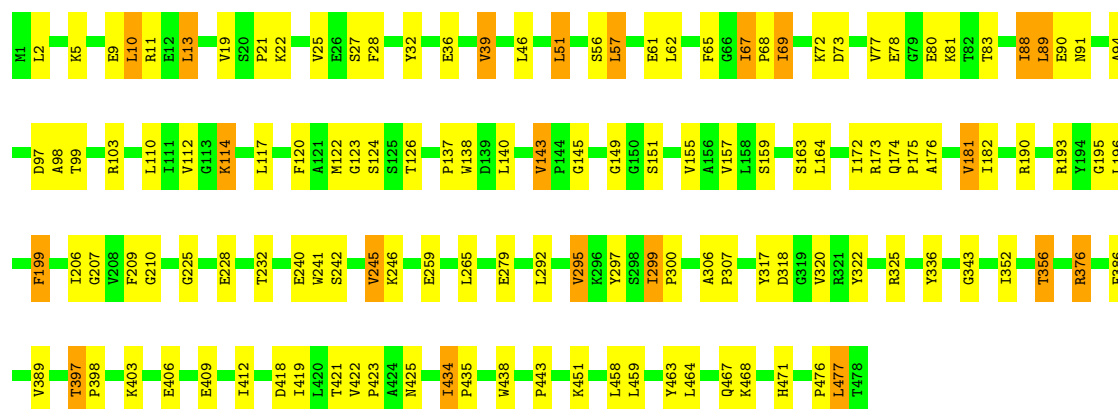
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain P:  70% 26%



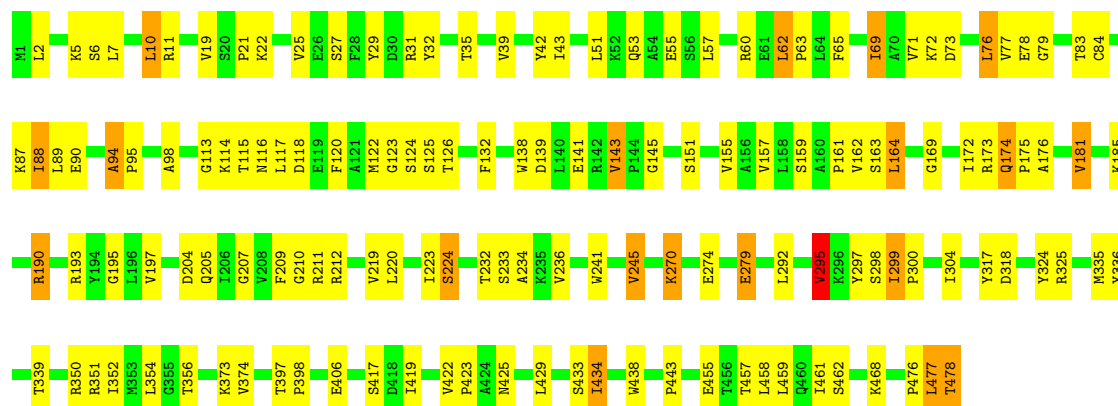
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain S:  72% 24%



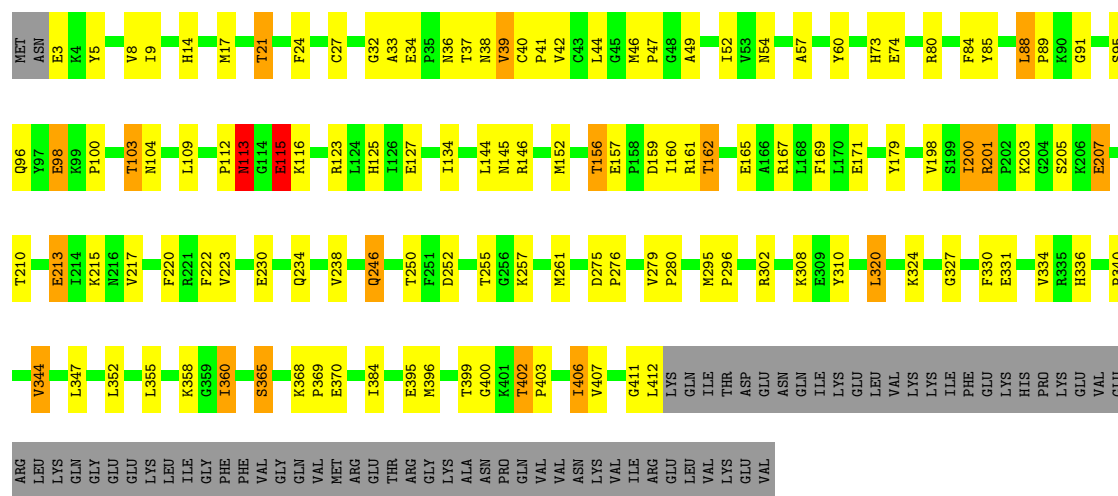
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain V:  70% 26%



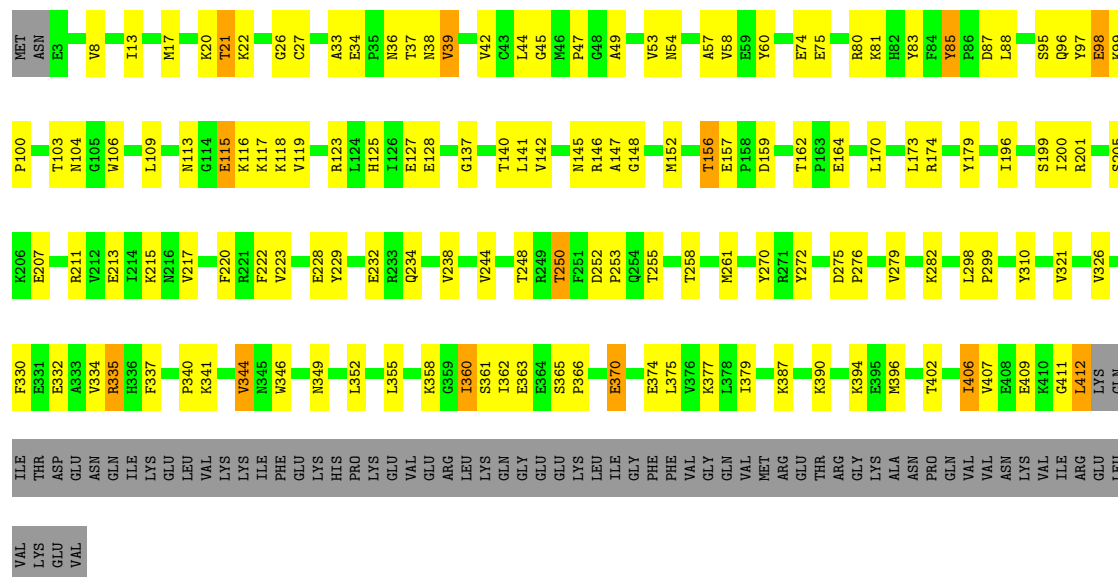
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain B: 



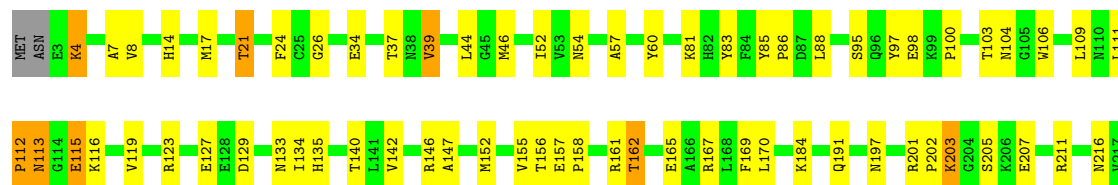
- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

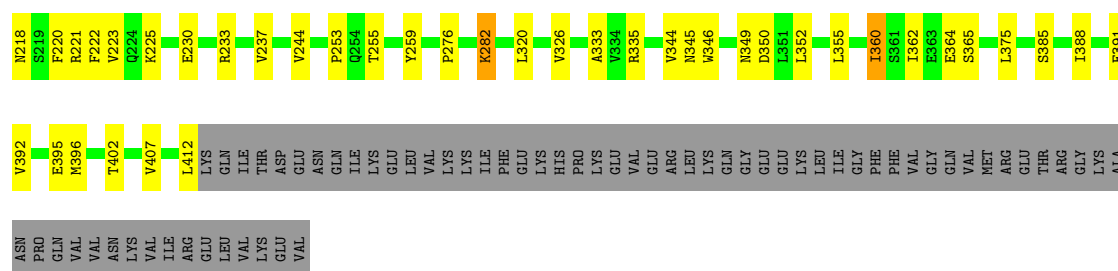
Chain E: 



- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

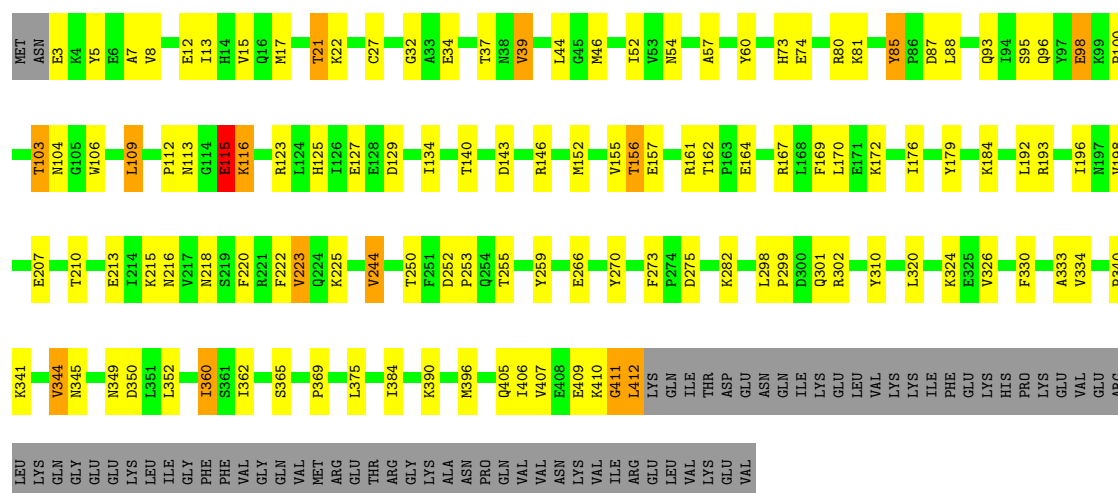
Chain H: 





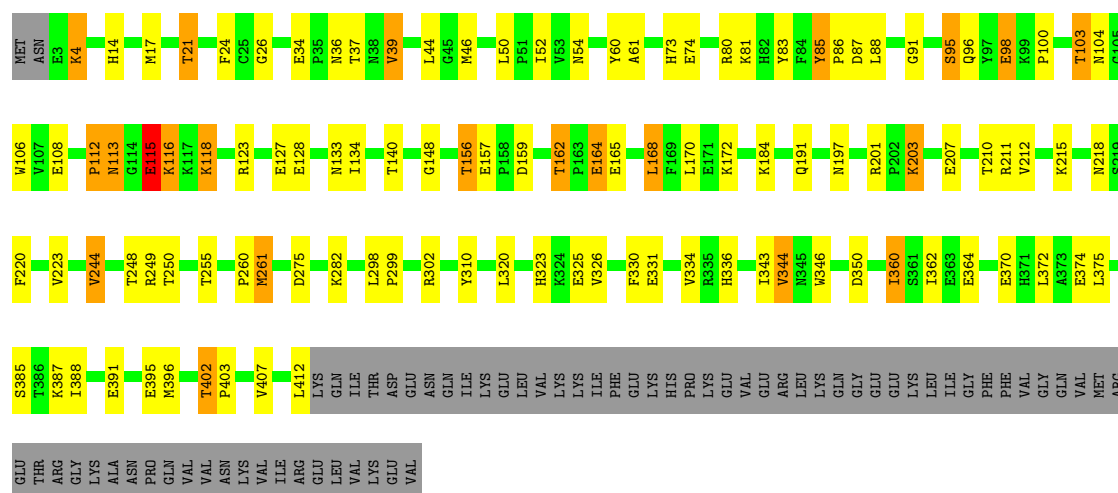
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain K: 60% 22% 14%



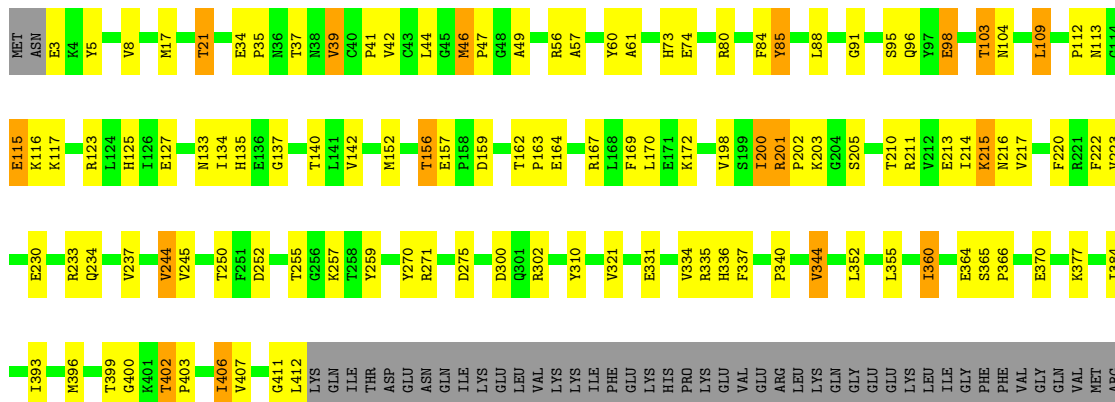
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain N: 63% 19% 14%



• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain Q: 61% 21% 14%



GLU
THR
ARG
GLY
LYS
ALA
ASN
PRO
GLN
VAL
VAL
ASN
LYS
VAL
TLE
ARG
GLU
LEU
VAL
LYS
GLU
VAL

- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain C:  71% 26%

MET V2 R15 L16 I23 Q27 S31 D32 I33 I37 D38 L43 E46 P50 Y51 I52 F55 E56 P59 M60 E62 D63 E64 R61 E62 D63 D70 D71 R71 E72 K73 M76 G84 V92 GLU VAL

- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain F:  66% 29%

MET V2 D3 R4 V7 L8 A14 E17 Q27 S31 D32 I33 L34 I37 P50 Y51 I52 P59 M60 R61 E62 D63 E64 P65 D70 R71 L75 A78 P79 E80 G84 F85 F86 V87 V88 P89 R90 V91 V92 GLU VAL

- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain I:  67% 28%

MET V2 E5 A14 R15 I33 L34 I37 D38 I33 Q39 L40 T45 E46 E47 I52 F55 E56 R61 E62 D63 E64 P65 K73 M76 P79 F80 R81 F86 V87 V88 P89 R90 V91 V92 GLU VAL

- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain L:  66% 30%

MET V2 D3 V7 A14 E17 S31 D32 I33 L34 I37 E42 T45 E46 M47 I52 F55 E56 T58 R61 E62 D63 P65 R61 R90 R91 V91 V92 GLU VAL

- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain O:  78% 18%

MET V2 R15 F26 L34 D38 E46 I52 Q53 E54 F55 T58 R61 E62 D63 P65 R61 G84 P89 R90 R91 V91 V92 GLU VAL

- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain R:  69% 28%

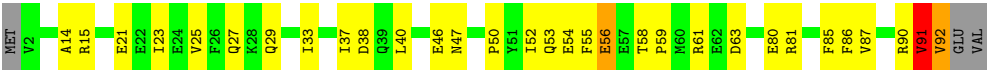
MET V2 R4 V7 L8 A14 I33 L34 I37 T45 E46 M47 P50 Y51 I52 F55 E56 E57 T58 P59 M60 R61 E62 D63 H66 R71 R81 P89 R90 V91 V92 GLU VAL

- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain U:  69% 27%



● Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	127.38Å 130.41Å 153.97Å 89.89° 90.21° 89.95°	Depositor
Resolution (Å)	48.97 – 3.00 48.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.97-3.00) 95.5 (48.97-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.263 , 0.306 0.258 , 0.297	Depositor DCC
R_{free} test set	11760 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.988	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -k,h,l 0.000 for k,-h,l 0.140 for h,-k,-l 0.439 for -h,k,-l 0.145 for -h,-k,l 0.000 for -k,-h,-l 0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	63243	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6768e-04. 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: ADP, ZN, MN, ATP

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	0.74	0/3874	0.96	4/5244 (0.1%)
1	D	0.73	1/3874 (0.0%)	0.95	4/5244 (0.1%)
1	G	0.72	1/3874 (0.0%)	0.94	1/5244 (0.0%)
1	J	0.75	1/3874 (0.0%)	1.00	11/5244 (0.2%)
1	M	0.74	0/3874	0.95	4/5244 (0.1%)
1	P	0.73	0/3874	0.96	6/5244 (0.1%)
1	S	0.72	1/3874 (0.0%)	0.96	3/5244 (0.1%)
1	V	0.77	1/3874 (0.0%)	0.98	4/5244 (0.1%)
2	B	0.69	0/3371	0.99	6/4541 (0.1%)
2	E	0.71	0/3371	0.98	8/4541 (0.2%)
2	H	0.74	0/3371	0.99	3/4541 (0.1%)
2	K	0.74	0/3371	1.01	6/4541 (0.1%)
2	N	0.72	0/3371	1.00	7/4541 (0.2%)
2	Q	0.73	0/3371	0.99	7/4541 (0.2%)
2	T	0.75	0/3371	1.01	7/4541 (0.2%)
2	W	0.71	0/3371	1.00	7/4541 (0.2%)
3	C	0.69	0/778	1.03	1/1050 (0.1%)
3	F	0.71	0/778	1.07	3/1050 (0.3%)
3	I	0.74	0/778	1.03	2/1050 (0.2%)
3	L	0.77	0/778	1.13	4/1050 (0.4%)
3	O	0.77	0/778	1.06	2/1050 (0.2%)
3	R	0.73	0/778	1.09	2/1050 (0.2%)
3	U	0.73	0/778	1.09	2/1050 (0.2%)
3	X	0.69	0/778	1.00	0/1050
All	All	0.73	5/64184 (0.0%)	0.99	104/86680 (0.1%)

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	4
1	D	0	2
1	G	0	3
1	M	0	4
1	P	0	1
1	S	0	1
2	B	0	4
2	E	0	3
2	H	0	2
2	K	0	4
2	N	0	2
2	Q	0	2
2	T	0	2
2	W	0	3
3	I	0	1
3	R	0	1
All	All	0	39

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	299	ILE	CA-CB	9.31	1.59	1.54
1	S	299	ILE	CA-CB	8.81	1.59	1.54
1	G	299	ILE	CA-CB	6.77	1.58	1.54
1	D	299	ILE	CA-CB	6.41	1.57	1.54
1	V	299	ILE	CA-CB	5.72	1.57	1.54

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	85	TYR	CA-C-N	8.90	129.80	119.47
2	N	85	TYR	C-N-CA	8.90	129.80	119.47
2	W	85	TYR	CA-C-N	8.71	129.57	119.47
2	W	85	TYR	C-N-CA	8.71	129.57	119.47
2	H	85	TYR	CA-C-N	8.07	128.84	119.47

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	ILE	Peptide
1	A	224	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	475	ILE	Peptide
1	A	477	LEU	Peptide
2	B	32	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3784	0	3816	113	0
1	D	3784	0	3816	117	0
1	G	3784	0	3816	99	0
1	J	3784	0	3816	108	0
1	M	3784	0	3816	92	0
1	P	3784	0	3816	119	0
1	S	3784	0	3816	104	0
1	V	3784	0	3816	110	0
2	B	3308	0	3354	113	0
2	E	3308	0	3353	122	0
2	H	3308	0	3353	99	0
2	K	3308	0	3353	90	0
2	N	3308	0	3353	88	0
2	Q	3308	0	3353	93	0
2	T	3308	0	3353	101	0
2	W	3308	0	3353	97	0
3	C	764	0	755	21	0
3	F	764	0	755	23	0
3	I	764	0	755	30	0
3	L	764	0	755	24	0
3	O	764	0	755	18	0
3	R	764	0	755	18	0
3	U	764	0	755	18	0
3	X	764	0	755	32	0
4	A	8	0	3	1	0
4	D	8	0	3	5	0
4	G	8	0	3	0	0
4	J	8	0	3	0	0
4	M	8	0	3	1	0
4	P	8	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	8	0	3	4	0
4	V	8	0	3	4	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
5	N	1	0	0	0	0
5	Q	1	0	0	0	0
5	T	1	0	0	0	0
5	W	1	0	0	0	0
6	B	27	0	12	0	0
6	T	27	0	12	2	0
7	B	2	0	0	0	0
7	E	2	0	0	0	0
7	H	2	0	0	0	0
7	K	2	0	0	0	0
7	N	2	0	0	0	0
7	Q	2	0	0	0	0
7	T	2	0	0	0	0
7	W	2	0	0	0	0
8	E	31	0	12	1	0
8	H	31	0	12	5	0
8	K	31	0	12	1	0
8	N	31	0	12	1	0
8	Q	31	0	12	1	0
8	W	31	0	12	1	0
9	H	9	0	3	6	0
9	N	9	0	3	5	0
10	A	1	0	0	0	0
10	B	4	0	0	0	0
10	E	3	0	0	0	0
10	G	2	0	0	1	0
10	H	3	0	0	2	0
10	J	2	0	0	1	0
10	K	5	0	0	0	0
10	M	3	0	0	2	0
10	N	5	0	0	1	0
10	P	2	0	0	1	0
10	Q	7	0	0	0	0
10	T	5	0	0	0	0
10	V	1	0	0	0	0
10	W	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	63243	0	63519	1701	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 13.

The worst 5 of 1701 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:384:ILE:HG22	2:W:412:LEU:CD2	1.62	1.28
1:D:83:THR:HG21	1:D:131:PHE:CZ	1.78	1.19
2:B:280:PRO:HD2	3:C:55:PHE:CZ	1.85	1.12
2:K:115:GLU:HA	2:K:115:GLU:OE2	1.48	1.10
1:V:190:ARG:HH11	1:V:190:ARG:HG3	1.11	1.10

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	476/478 (100%)	455 (96%)	20 (4%)	1 (0%)	43	76
1	D	476/478 (100%)	457 (96%)	19 (4%)	0	100	100
1	G	476/478 (100%)	454 (95%)	21 (4%)	1 (0%)	43	76
1	J	476/478 (100%)	458 (96%)	17 (4%)	1 (0%)	43	76
1	M	476/478 (100%)	454 (95%)	22 (5%)	0	100	100
1	P	476/478 (100%)	455 (96%)	21 (4%)	0	100	100
1	S	476/478 (100%)	458 (96%)	18 (4%)	0	100	100
1	V	476/478 (100%)	458 (96%)	18 (4%)	0	100	100
2	B	408/478 (85%)	388 (95%)	19 (5%)	1 (0%)	43	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	408/478 (85%)	381 (93%)	27 (7%)	0	100	100
2	H	408/478 (85%)	385 (94%)	23 (6%)	0	100	100
2	K	408/478 (85%)	381 (93%)	27 (7%)	0	100	100
2	N	408/478 (85%)	388 (95%)	20 (5%)	0	100	100
2	Q	408/478 (85%)	383 (94%)	24 (6%)	1 (0%)	43	76
2	T	408/478 (85%)	375 (92%)	32 (8%)	1 (0%)	43	76
2	W	408/478 (85%)	388 (95%)	19 (5%)	1 (0%)	43	76
3	C	89/94 (95%)	82 (92%)	7 (8%)	0	100	100
3	F	89/94 (95%)	84 (94%)	5 (6%)	0	100	100
3	I	89/94 (95%)	80 (90%)	8 (9%)	1 (1%)	11	43
3	L	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	O	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	R	89/94 (95%)	82 (92%)	7 (8%)	0	100	100
3	U	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	X	89/94 (95%)	78 (88%)	10 (11%)	1 (1%)	11	43
All	All	7784/8400 (93%)	7379 (95%)	396 (5%)	9 (0%)	48	80

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	56	GLU
2	B	113	ASN
2	T	216	ASN
2	W	216	ASN
1	J	477	LEU

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	406/406 (100%)	378 (93%)	28 (7%)	14	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	406/406 (100%)	374 (92%)	32 (8%)	11	39
1	G	406/406 (100%)	384 (95%)	22 (5%)	20	53
1	J	406/406 (100%)	375 (92%)	31 (8%)	12	41
1	M	406/406 (100%)	382 (94%)	24 (6%)	18	50
1	P	406/406 (100%)	372 (92%)	34 (8%)	10	37
1	S	406/406 (100%)	372 (92%)	34 (8%)	10	37
1	V	406/406 (100%)	376 (93%)	30 (7%)	13	42
2	B	364/427 (85%)	335 (92%)	29 (8%)	11	38
2	E	364/427 (85%)	340 (93%)	24 (7%)	15	46
2	H	364/427 (85%)	344 (94%)	20 (6%)	19	53
2	K	364/427 (85%)	341 (94%)	23 (6%)	16	48
2	N	364/427 (85%)	333 (92%)	31 (8%)	10	36
2	Q	364/427 (85%)	339 (93%)	25 (7%)	14	45
2	T	364/427 (85%)	340 (93%)	24 (7%)	15	46
2	W	364/427 (85%)	338 (93%)	26 (7%)	13	43
3	C	86/89 (97%)	81 (94%)	5 (6%)	18	51
3	F	86/89 (97%)	81 (94%)	5 (6%)	18	51
3	I	86/89 (97%)	80 (93%)	6 (7%)	14	44
3	L	86/89 (97%)	81 (94%)	5 (6%)	18	51
3	O	86/89 (97%)	80 (93%)	6 (7%)	14	44
3	R	86/89 (97%)	81 (94%)	5 (6%)	18	51
3	U	86/89 (97%)	81 (94%)	5 (6%)	18	51
3	X	86/89 (97%)	80 (93%)	6 (7%)	14	44
All	All	6848/7376 (93%)	6368 (93%)	480 (7%)	14	44

5 of 480 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	10	LEU
1	V	417	SER
3	O	38	ASP
1	V	245	VAL
2	W	407	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	T	110	ASN
2	W	216	ASN
2	T	216	ASN
1	V	34	GLN
1	M	53	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 42 ligands modelled in this entry, 24 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ADP	B	479	-	28,29,29	1.46	6 (21%)	43,45,45	2.00	12 (27%)
8	ATP	N	479	-	32,33,33	1.54	7 (21%)	48,52,52	1.73	10 (20%)
4	ASN	J	904	1	6,7,8	1.06	0	3,8,10	2.82	1 (33%)
4	ASN	G	903	1	6,7,8	1.26	1 (16%)	3,8,10	2.36	1 (33%)
9	ASP	H	482	7	7,8,8	1.10	1 (14%)	6,10,10	1.89	1 (16%)
8	ATP	K	479	-	32,33,33	1.45	5 (15%)	48,52,52	1.72	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ADP	T	479	-	28,29,29	1.44	7 (25%)	43,45,45	1.90	10 (23%)
4	ASN	D	902	1	6,7,8	1.24	1 (16%)	3,8,10	2.81	2 (66%)
4	ASN	V	908	1	6,7,8	1.25	1 (16%)	3,8,10	2.69	2 (66%)
8	ATP	W	479	-	32,33,33	1.60	6 (18%)	48,52,52	2.29	17 (35%)
8	ATP	H	479	-	32,33,33	1.66	7 (21%)	48,52,52	1.81	9 (18%)
4	ASN	P	906	1	6,7,8	1.07	1 (16%)	3,8,10	1.92	1 (33%)
4	ASN	S	907	1	6,7,8	1.22	1 (16%)	3,8,10	2.31	1 (33%)
8	ATP	E	479	-	32,33,33	1.50	8 (25%)	48,52,52	1.88	9 (18%)
9	ASP	N	482	-	7,8,8	1.43	1 (14%)	6,10,10	1.25	1 (16%)
8	ATP	Q	479	-	32,33,33	1.44	5 (15%)	48,52,52	1.88	8 (16%)
4	ASN	A	901	1	6,7,8	1.35	1 (16%)	3,8,10	2.43	2 (66%)
4	ASN	M	905	1	6,7,8	1.16	1 (16%)	3,8,10	2.21	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	B	479	-	-	0/16/32/32	0/3/3/3
8	ATP	N	479	-	-	8/22/38/38	0/3/3/3
4	ASN	J	904	1	-	1/7/7/8	-
4	ASN	G	903	1	-	0/7/7/8	-
9	ASP	H	482	7	-	6/8/8/8	-
8	ATP	K	479	-	-	4/22/38/38	0/3/3/3
6	ADP	T	479	-	-	5/16/32/32	0/3/3/3
4	ASN	D	902	1	-	3/7/7/8	-
4	ASN	V	908	1	-	4/7/7/8	-
8	ATP	W	479	-	-	6/22/38/38	0/3/3/3
8	ATP	H	479	-	-	5/22/38/38	0/3/3/3
4	ASN	P	906	1	-	1/7/7/8	-
4	ASN	S	907	1	-	4/7/7/8	-
8	ATP	E	479	-	-	5/22/38/38	0/3/3/3
9	ASP	N	482	-	-	3/8/8/8	-
8	ATP	Q	479	-	-	4/22/38/38	0/3/3/3
4	ASN	A	901	1	-	2/7/7/8	-
4	ASN	M	905	1	-	1/7/7/8	-

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	479	ATP	C5-C4	4.91	1.47	1.39
8	H	479	ATP	C5-C4	4.47	1.47	1.39
8	K	479	ATP	C5-C4	4.36	1.46	1.39
6	T	479	ADP	C5-C4	4.08	1.46	1.39
8	E	479	ATP	C5-C4	4.05	1.46	1.39

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	479	ATP	C5-C4-N3	-6.83	117.31	126.72
8	E	479	ATP	C5-C4-N3	-6.79	117.37	126.72
6	T	479	ADP	C5-C4-N3	-6.21	118.17	126.72
8	H	479	ATP	C5-C4-N3	-5.86	118.65	126.72
8	K	479	ATP	C5-C4-N3	-5.76	118.79	126.72

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	902	ASN	O-C-CA-N
4	S	907	ASN	O-C-CA-N
4	S	907	ASN	C-CA-CB-CG
4	V	908	ASN	O-C-CA-N
4	V	908	ASN	C-CA-CB-CG

There are no ring outliers.

15 monomers are involved in 37 short contacts:

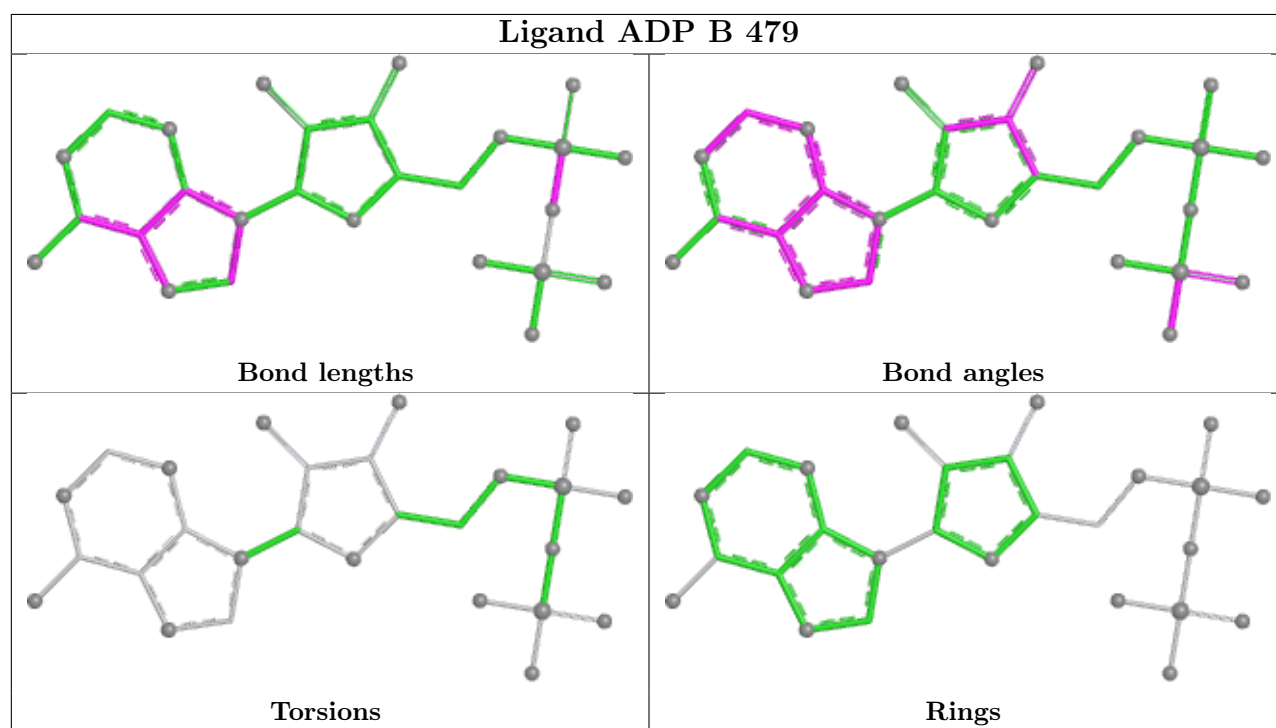
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	479	ATP	1	0
9	H	482	ASP	6	0
8	K	479	ATP	1	0
6	T	479	ADP	2	0
4	D	902	ASN	5	0
4	V	908	ASN	4	0
8	W	479	ATP	1	0
8	H	479	ATP	5	0
4	P	906	ASN	1	0
4	S	907	ASN	4	0
8	E	479	ATP	1	0

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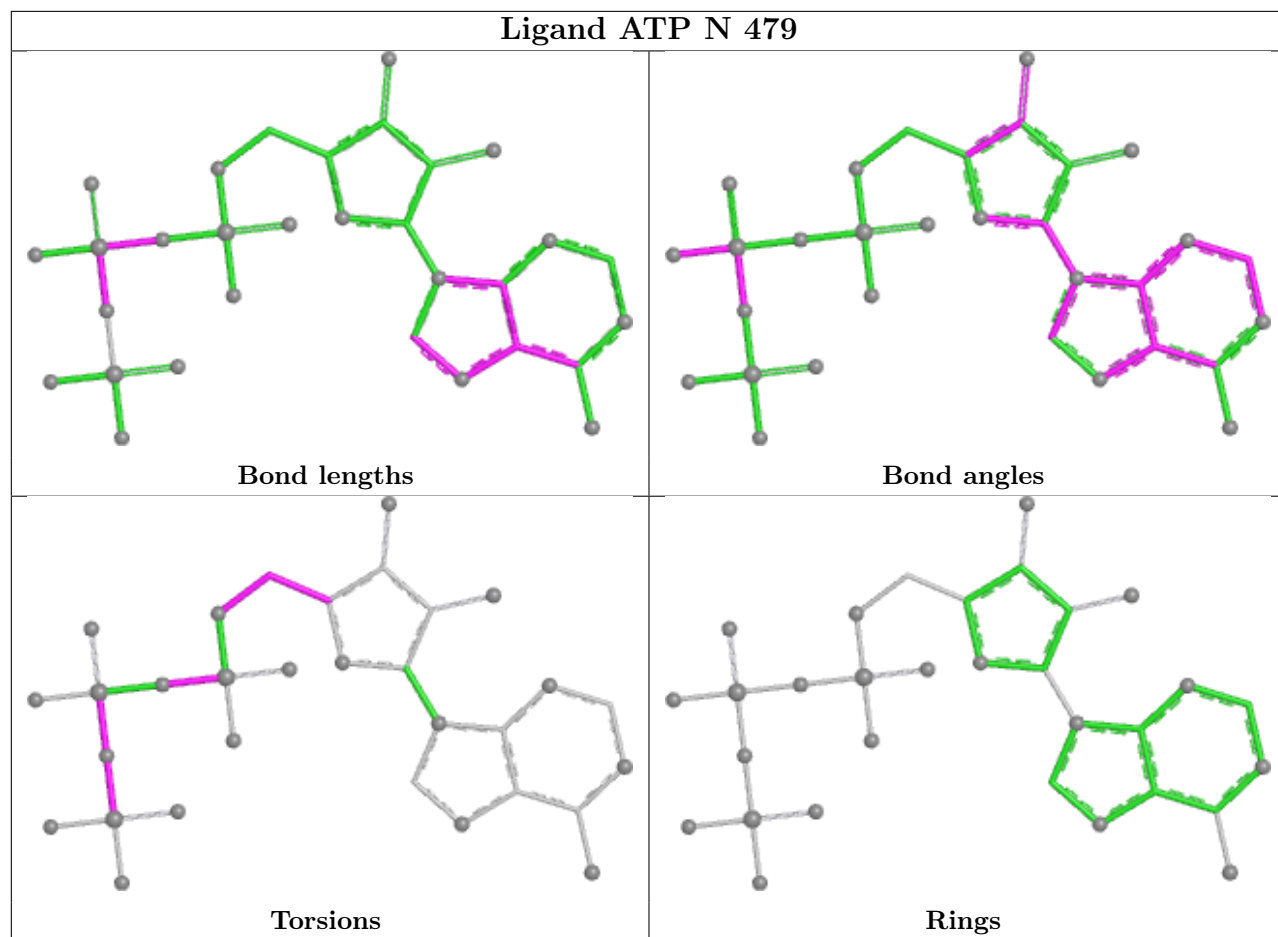
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	482	ASP	5	0
8	Q	479	ATP	1	0
4	A	901	ASN	1	0
4	M	905	ASN	1	0

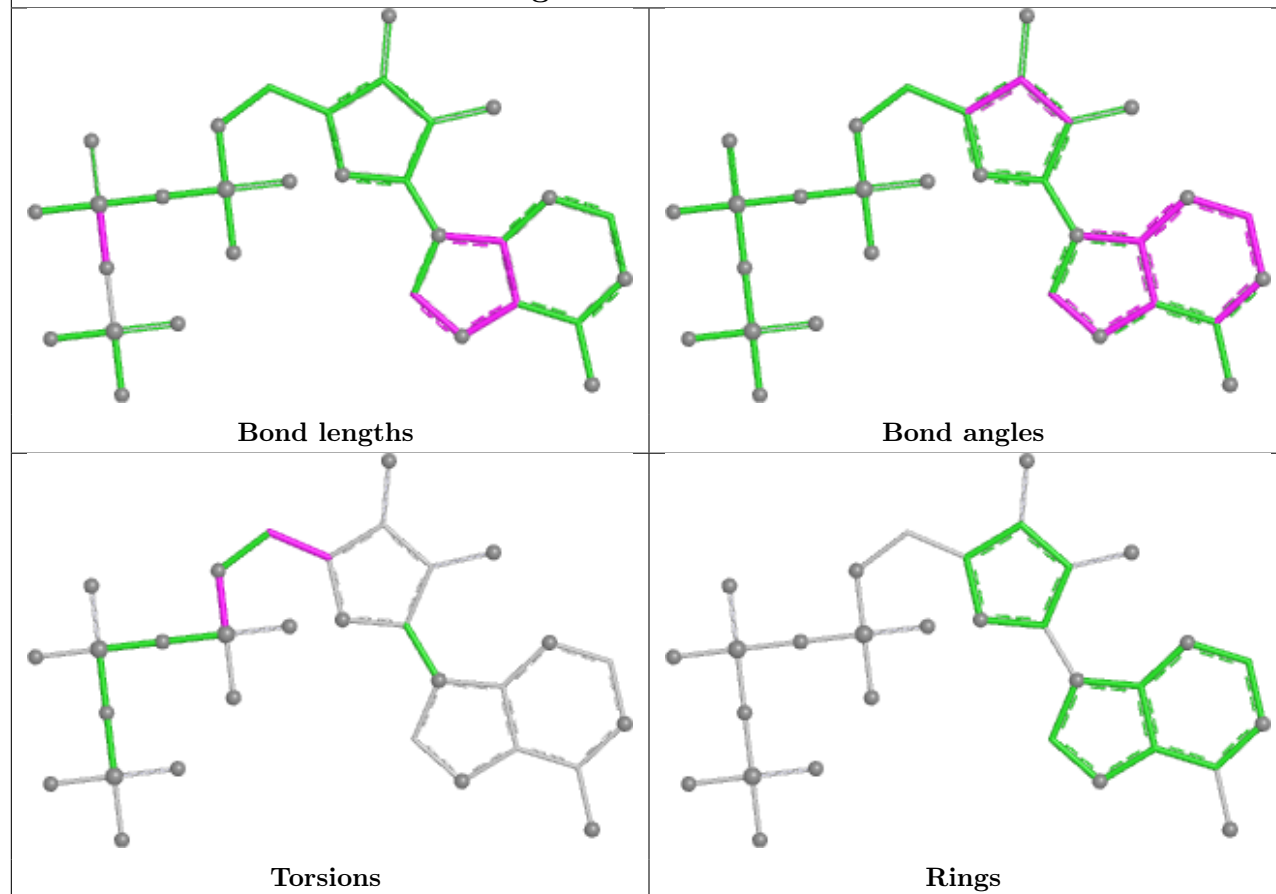
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



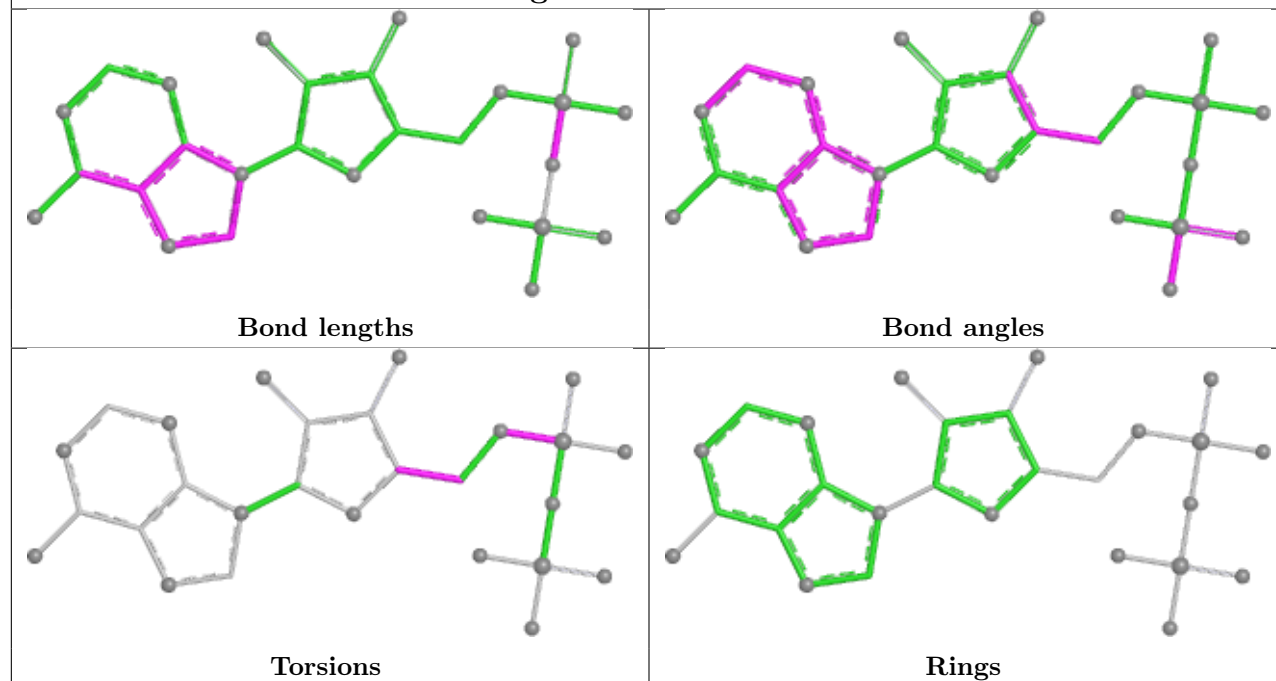
Ligand ATP N 479

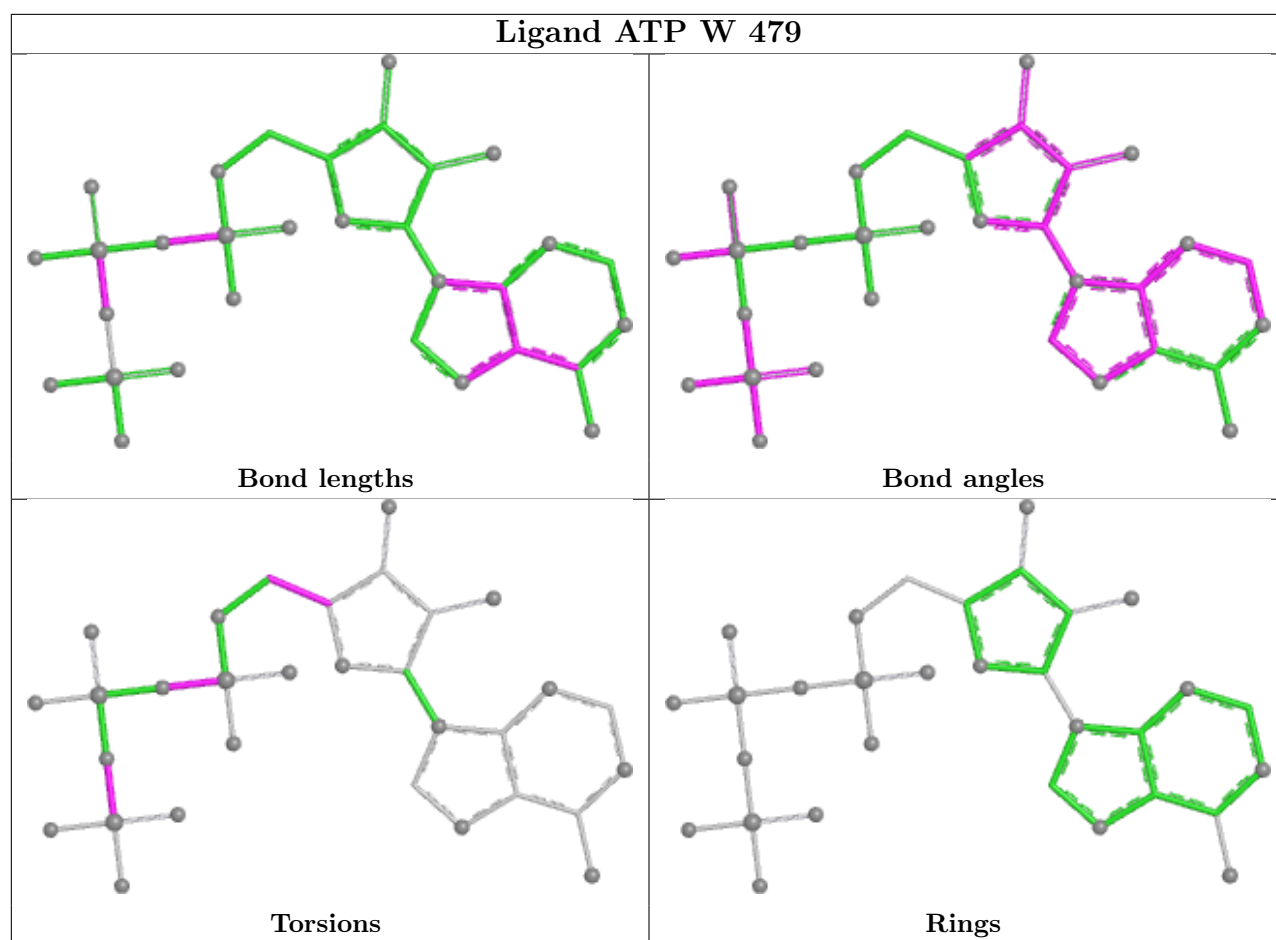


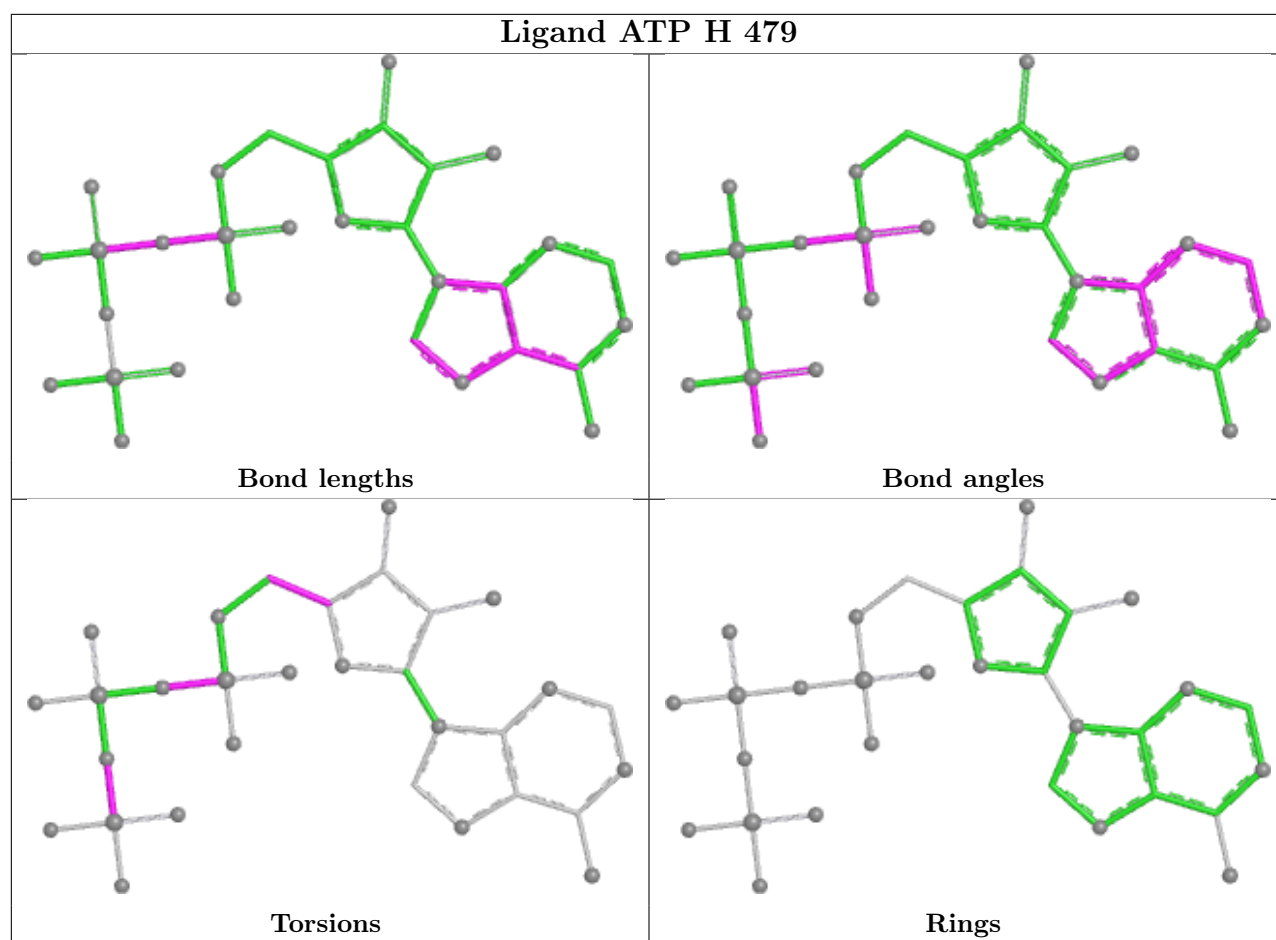
Ligand ATP K 479



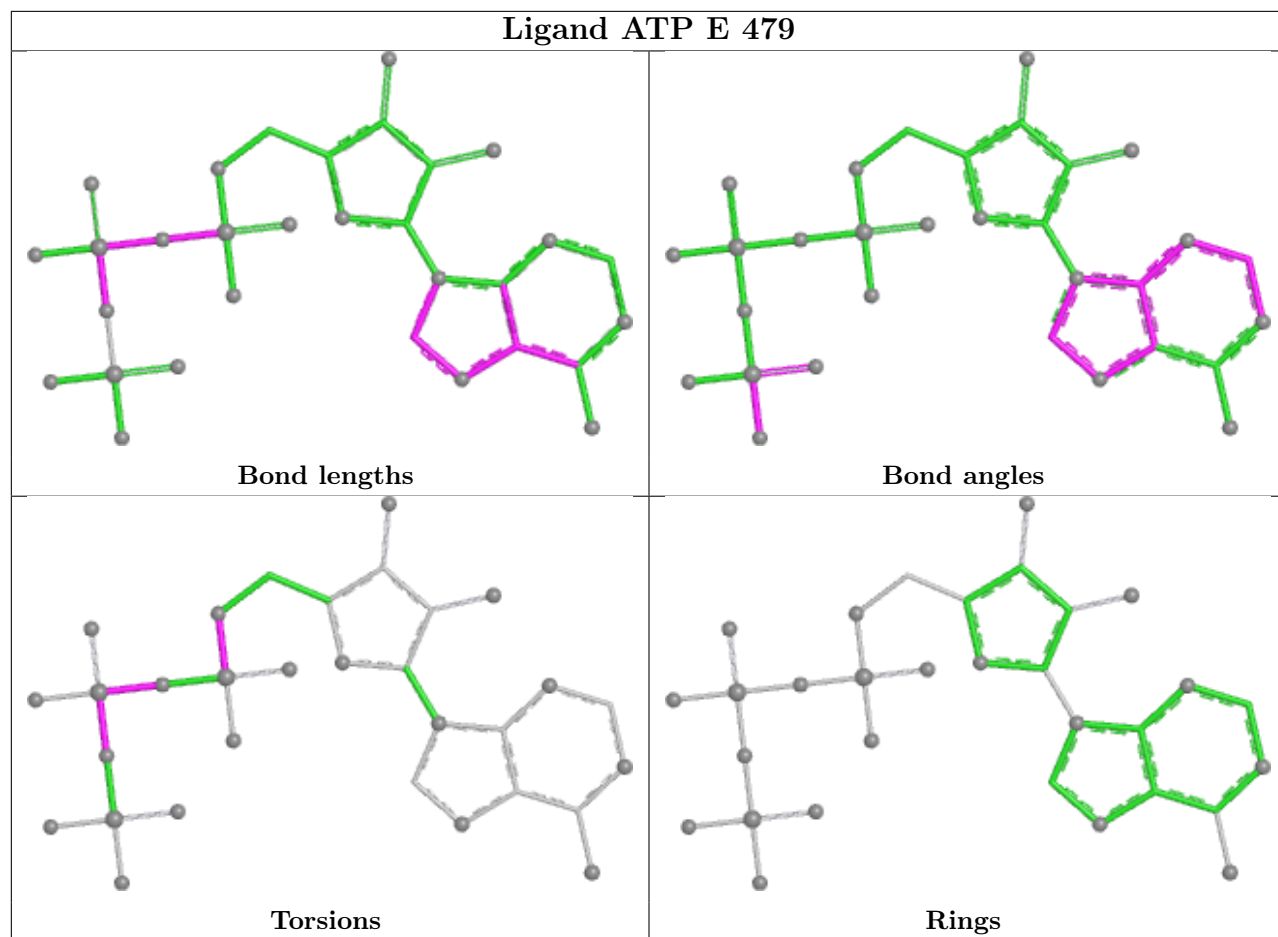
Ligand ADP T 479

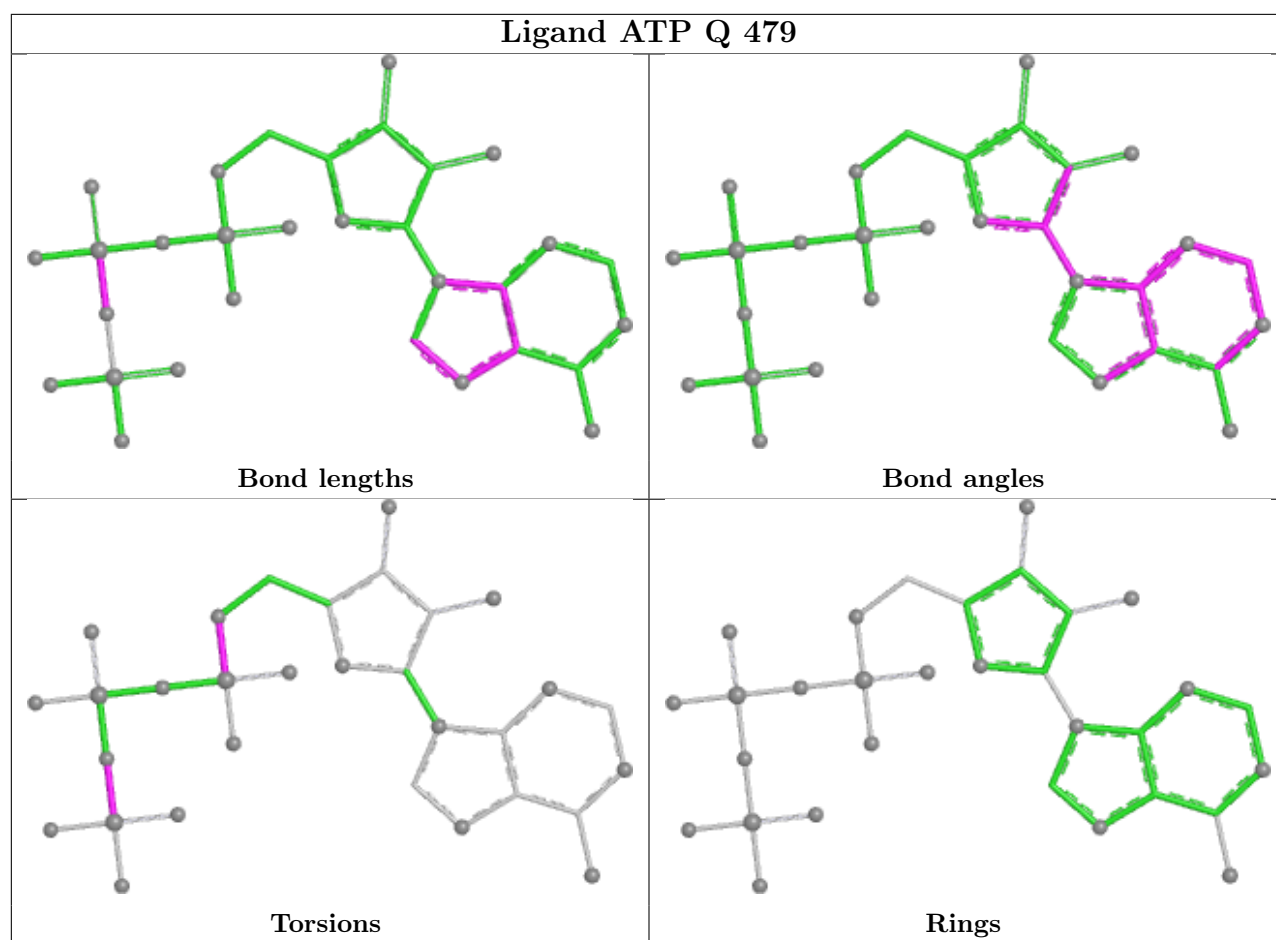






Ligand ATP E 479





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	478/478 (100%)	-1.50	0 100 100	23, 53, 79, 88	0
1	D	478/478 (100%)	-1.52	0 100 100	23, 53, 79, 88	0
1	G	478/478 (100%)	-1.50	0 100 100	23, 53, 78, 88	0
1	J	478/478 (100%)	-1.49	0 100 100	23, 53, 78, 88	0
1	M	478/478 (100%)	-1.52	0 100 100	23, 53, 79, 88	0
1	P	478/478 (100%)	-1.52	0 100 100	23, 53, 78, 88	0
1	S	478/478 (100%)	-1.52	0 100 100	23, 53, 79, 88	0
1	V	478/478 (100%)	-1.52	0 100 100	23, 53, 79, 88	0
2	B	410/478 (85%)	-1.51	0 100 100	31, 63, 93, 112	0
2	E	410/478 (85%)	-1.46	0 100 100	31, 63, 94, 112	0
2	H	410/478 (85%)	-1.50	0 100 100	31, 63, 93, 112	0
2	K	410/478 (85%)	-1.48	0 100 100	31, 63, 93, 112	0
2	N	410/478 (85%)	-1.51	0 100 100	31, 63, 93, 112	0
2	Q	410/478 (85%)	-1.51	0 100 100	31, 63, 93, 112	0
2	T	410/478 (85%)	-1.47	0 100 100	31, 63, 93, 112	0
2	W	410/478 (85%)	-1.49	0 100 100	31, 63, 93, 112	0
3	C	91/94 (96%)	-1.50	0 100 100	25, 60, 72, 76	0
3	F	91/94 (96%)	-1.53	0 100 100	25, 60, 72, 76	0
3	I	91/94 (96%)	-1.54	0 100 100	25, 59, 72, 76	0
3	L	91/94 (96%)	-1.51	0 100 100	25, 59, 71, 76	0
3	O	91/94 (96%)	-1.51	0 100 100	25, 59, 71, 76	0
3	R	91/94 (96%)	-1.54	0 100 100	25, 59, 71, 76	0
3	U	91/94 (96%)	-1.43	0 100 100	25, 60, 72, 76	0
3	X	91/94 (96%)	-1.54	0 100 100	25, 59, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7832/8400 (93%)	-1.50	0 100 100	23, 56, 88, 112	0

There are no RSRZ outliers to report.

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
9	ASP	N	482	9/9	0.97	0.08	71,79,81,82	0
4	ASN	M	905	8/9	0.98	0.13	31,31,32,32	8
4	ASN	S	907	8/9	0.98	0.05	53,53,55,57	0
7	MN	B	481	1/1	0.98	0.10	56,56,56,56	1
7	MN	E	481	1/1	0.98	0.09	85,85,85,85	1
7	MN	N	481	1/1	0.98	0.04	86,86,86,86	1
8	ATP	E	479	31/31	0.98	0.04	34,40,85,85	31
8	ATP	K	479	31/31	0.98	0.06	24,35,57,58	31
9	ASP	H	482	9/9	0.98	0.06	71,79,81,82	0
4	ASN	A	901	8/9	0.98	0.13	31,32,34,35	8
4	ASN	J	904	8/9	0.99	0.03	52,53,54,54	0
4	ASN	D	902	8/9	0.99	0.05	62,62,62,62	0
7	MN	H	481	1/1	0.99	0.03	75,75,75,75	1
7	MN	K	481	1/1	0.99	0.05	63,63,63,63	1
4	ASN	P	906	8/9	0.99	0.12	28,28,29,29	8
7	MN	Q	481	1/1	0.99	0.03	64,64,64,64	1
7	MN	T	481	1/1	0.99	0.04	75,75,75,75	0
7	MN	W	481	1/1	0.99	0.06	82,82,82,82	1
4	ASN	G	903	8/9	0.99	0.07	27,29,30,31	8

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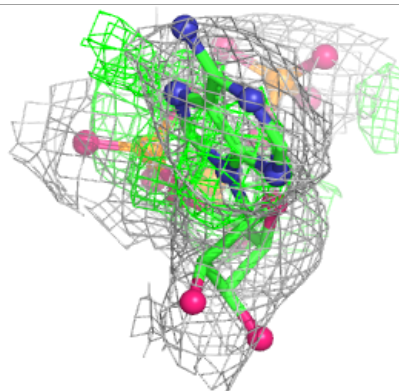
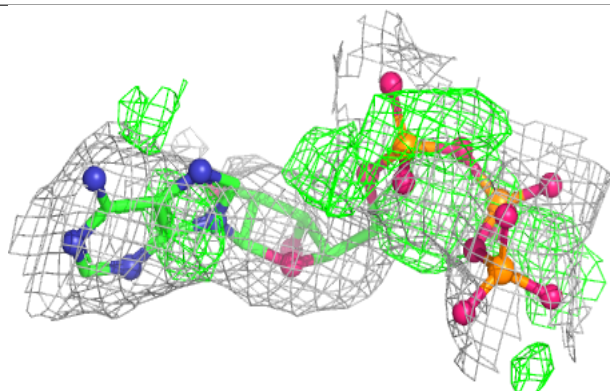
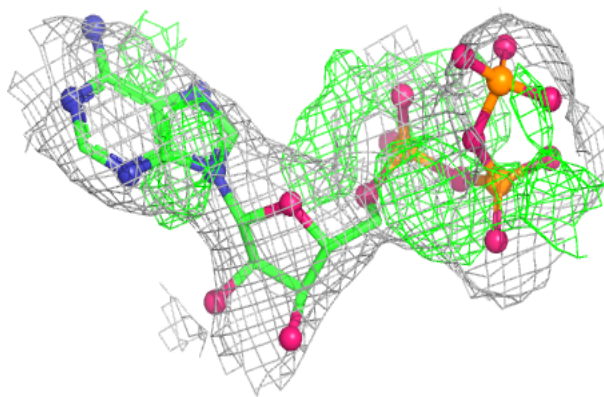
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ATP	H	479	31/31	0.99	0.03	21,28,49,51	31
4	ASN	V	908	8/9	0.99	0.09	28,29,29,30	8
8	ATP	N	479	31/31	0.99	0.04	35,39,66,66	31
8	ATP	Q	479	31/31	0.99	0.04	30,37,49,50	31
8	ATP	W	479	31/31	0.99	0.03	14,21,28,32	31
6	ADP	B	479	27/27	0.99	0.04	70,71,82,82	27
6	ADP	T	479	27/27	0.99	0.05	75,76,87,88	27
7	MN	N	480	1/1	1.00	0.01	49,49,49,49	0
5	ZN	T	907	1/1	1.00	0.01	55,55,55,55	0
7	MN	Q	480	1/1	1.00	0.01	51,51,51,51	0
5	ZN	W	908	1/1	1.00	0.01	55,55,55,55	0
7	MN	T	480	1/1	1.00	0.01	55,55,55,55	0
5	ZN	B	901	1/1	1.00	0.01	57,57,57,57	0
7	MN	W	480	1/1	1.00	0.02	52,52,52,52	0
5	ZN	E	902	1/1	1.00	0.01	59,59,59,59	0
7	MN	B	480	1/1	1.00	0.02	44,44,44,44	0
5	ZN	H	903	1/1	1.00	0.01	53,53,53,53	0
7	MN	E	480	1/1	1.00	0.01	53,53,53,53	0
5	ZN	K	904	1/1	1.00	0.01	50,50,50,50	0
7	MN	H	480	1/1	1.00	0.01	50,50,50,50	0
5	ZN	N	905	1/1	1.00	0.01	53,53,53,53	0
7	MN	K	480	1/1	1.00	0.01	45,45,45,45	0
5	ZN	Q	906	1/1	1.00	0.01	51,51,51,51	0

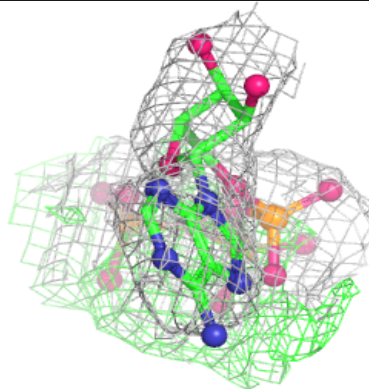
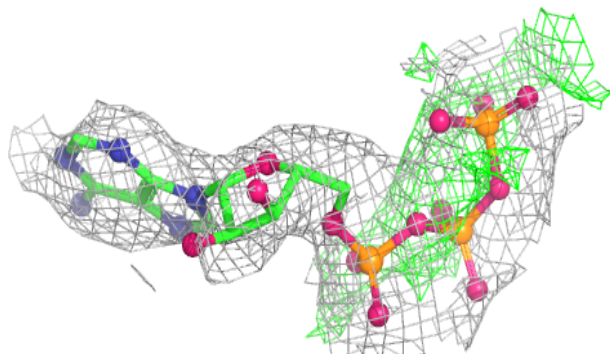
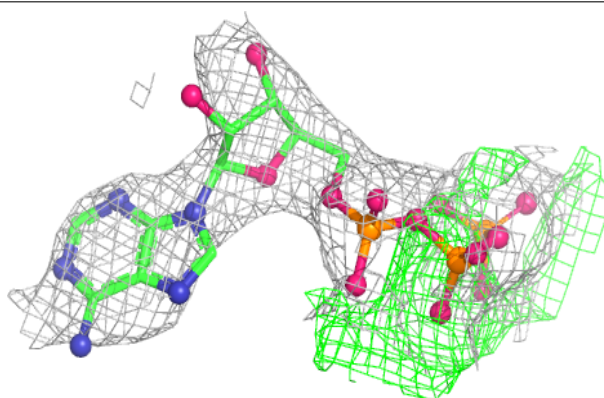
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP E 479:

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

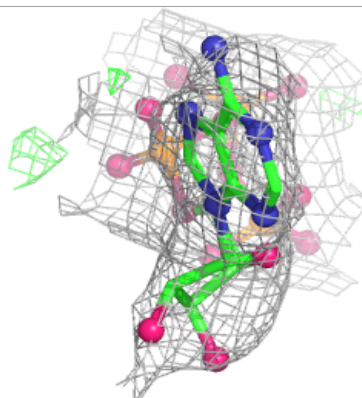
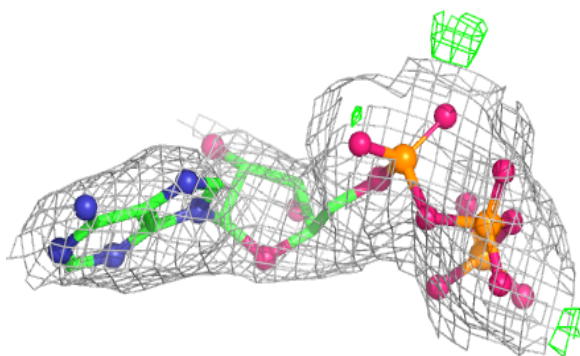
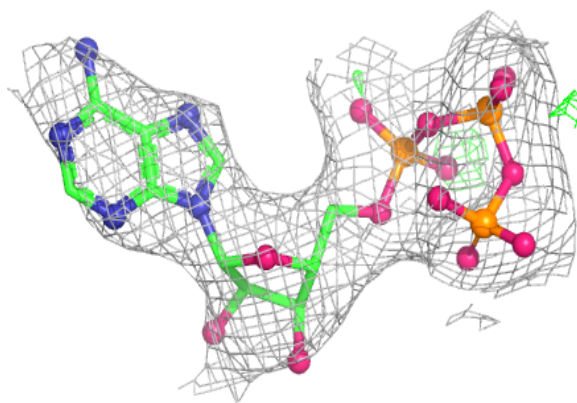
**Electron density around ATP K 479:**

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

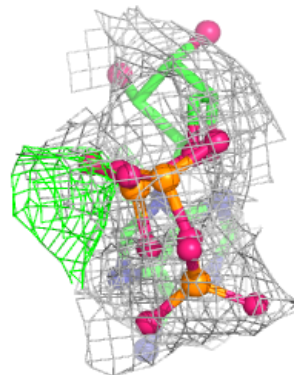
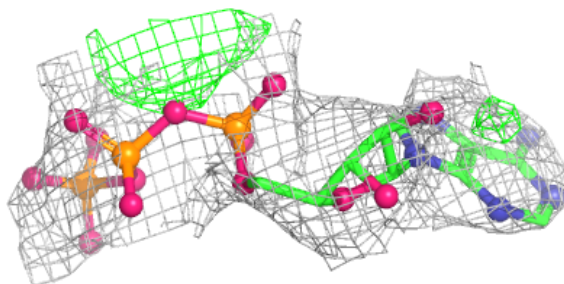
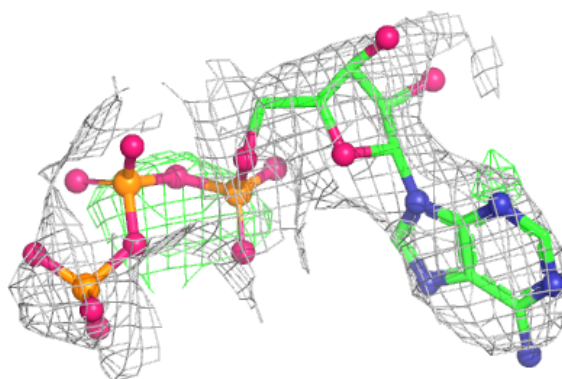


Electron density around ATP H 479:

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

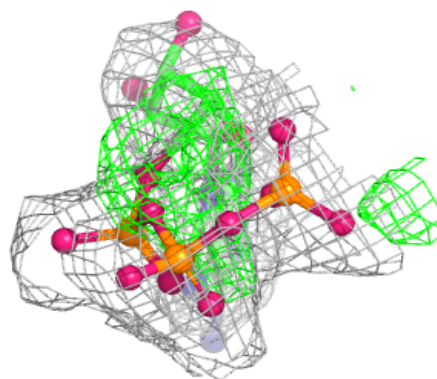
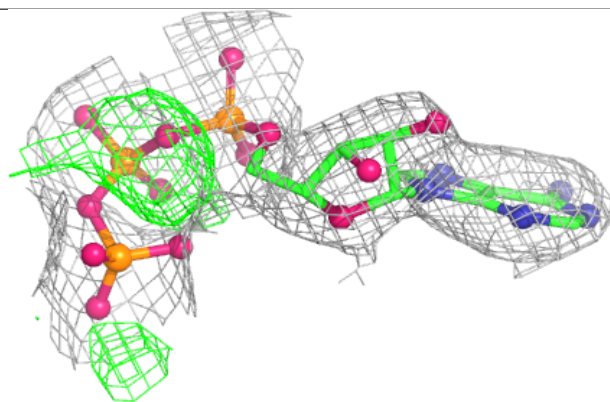
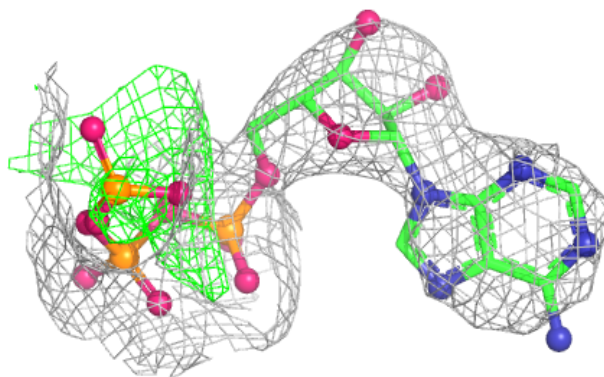
**Electron density around ATP N 479:**

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

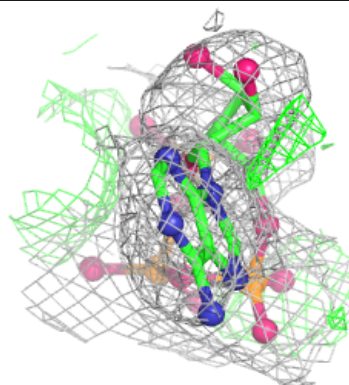
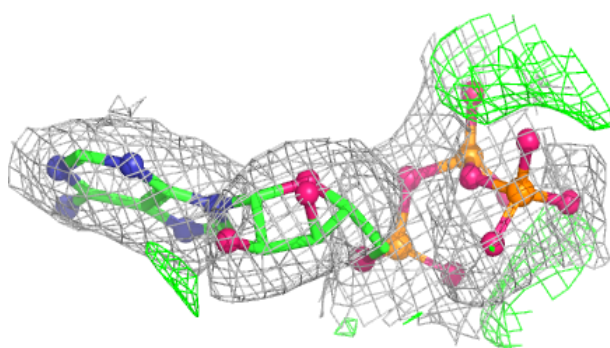
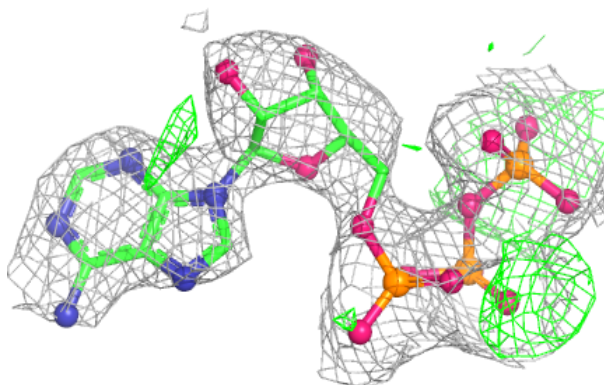


Electron density around ATP Q 479:

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

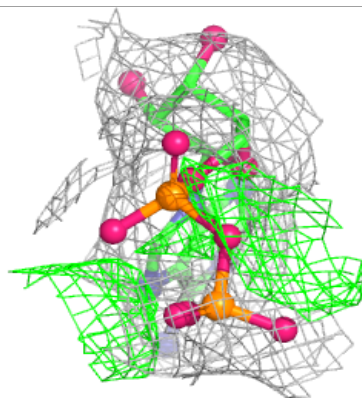
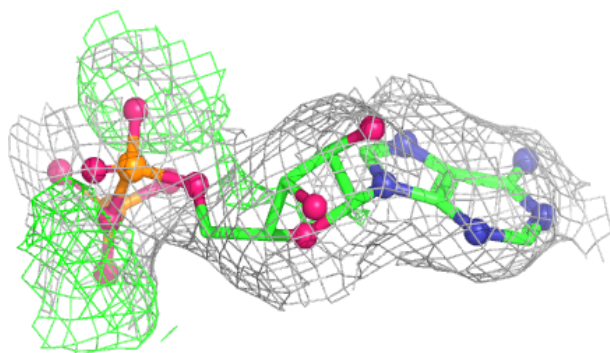
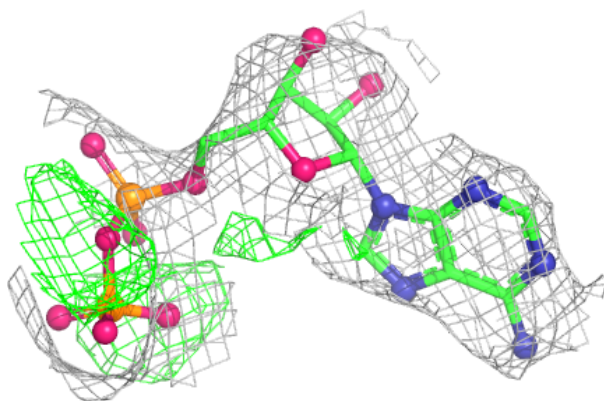
**Electron density around ATP W 479:**

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

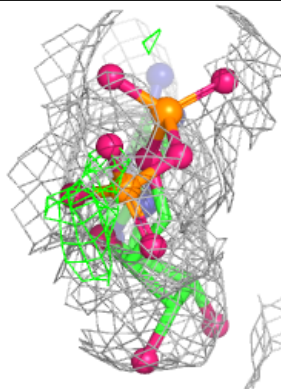
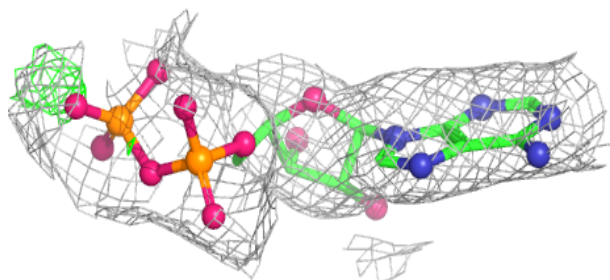
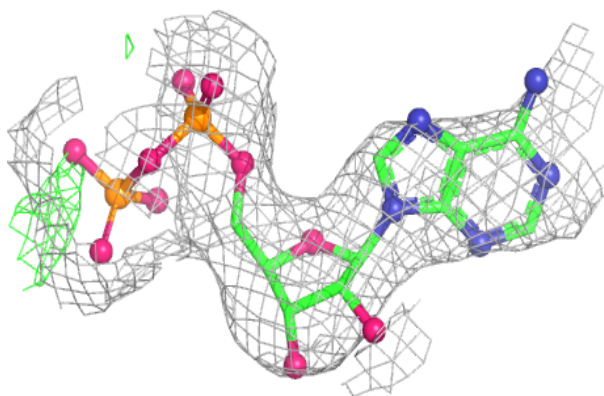


Electron density around ADP B 479:

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

**Electron density around ADP T 479:**

$2mF_o-DF_c$ (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.