



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2022 – 12:29 AM JST

PDB ID : 7V3X  
Title : Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC  
Authors : Furuike, Y.; Akiyama, S.  
Deposited on : 2021-08-11  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

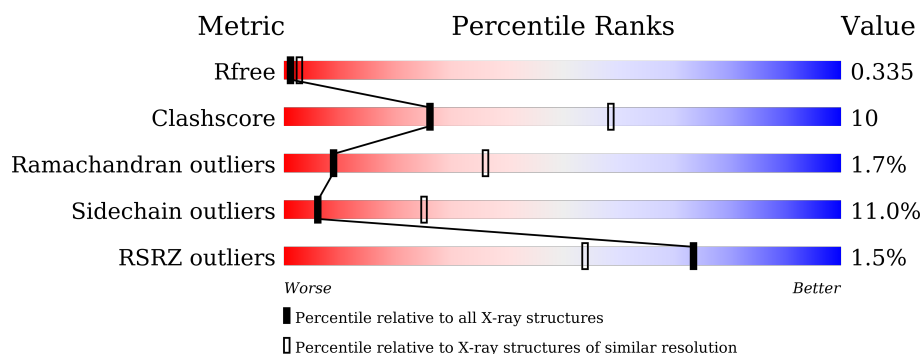
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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





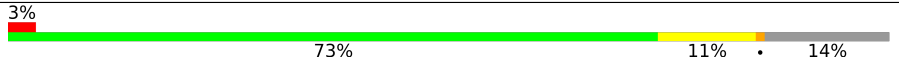
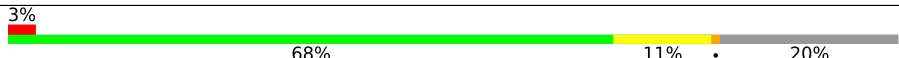
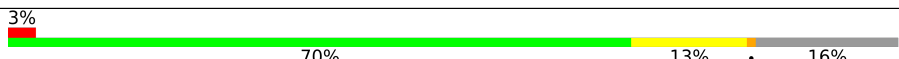
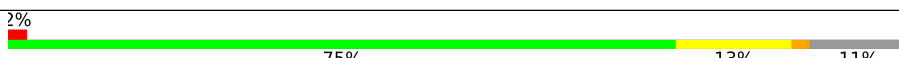
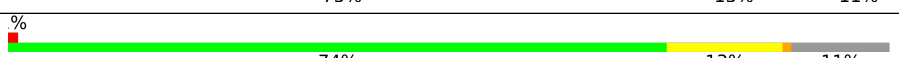
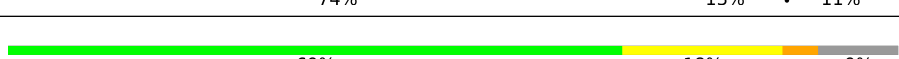
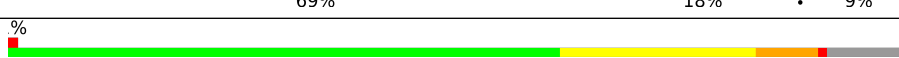
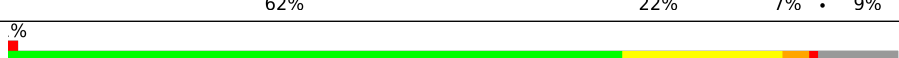








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>64%</div> <div>21%</div> <div>• • 10%</div> </div>
1	B	519	<div> <div>%</div> <div>63%</div> <div>22%</div> <div>5%</div> <div>10%</div> </div>
1	G	519	<div> <div>63%</div> <div>22%</div> <div>• 10%</div> </div>
1	H	519	<div> <div>%</div> <div>63%</div> <div>22%</div> <div>5%</div> <div>10%</div> </div>
1	M	519	<div> <div>3%</div> <div>74%</div> <div>14%</div> <div>• 11%</div> </div>
1	N	519	<div> <div>2%</div> <div>74%</div> <div>12%</div> <div>• 12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	P	519	
1	R	519	
1	S	519	
1	T	519	
1	V	519	
1	W	519	
1	X	519	
2	C	519	
2	D	519	
2	E	519	
2	F	519	
2	I	519	
2	J	519	
2	K	519	
2	L	519	
2	O	519	
2	Q	519	
2	U	519	

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
5	ADP	U	702	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 78739 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	468	Total	C	N	O	P	S	0	0	0
			3506	2208	606	677	1	14			
1	B	469	Total	C	N	O	P	S	0	0	0
			3432	2156	601	662	1	12			
1	G	467	Total	C	N	O	P	S	0	0	0
			3448	2178	590	666	1	13			
1	H	468	Total	C	N	O	P	S	0	0	0
			3476	2183	608	671	1	13			
1	N	455	Total	C	N	O	P	S	0	0	0
			3010	1858	545	594	1	12			
1	R	463	Total	C	N	O	P	S	0	0	0
			3201	1997	572	619	1	12			
1	M	463	Total	C	N	O	P	S	0	0	0
			3123	1935	557	616	1	14			
1	P	456	Total	C	N	O	P	S	0	0	0
			3096	1922	541	620	1	12			
1	T	415	Total	C	N	O	P	S	0	0	0
			2427	1462	473	485	1	6			
1	X	461	Total	C	N	O	P	S	0	0	0
			3074	1907	553	601	1	12			
1	S	444	Total	C	N	O	P	S	0	0	0
			2706	1648	509	541	1	7			
1	V	437	Total	C	N	O	P	S	0	0	0
			2914	1800	522	582	1	9			
1	W	464	Total	C	N	O	P	S	0	0	0
			3126	1926	573	613	1	13			

- Molecule 2 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	470	Total	C	N	O	P	S	0	0	0
			3424	2159	590	661	2	12			

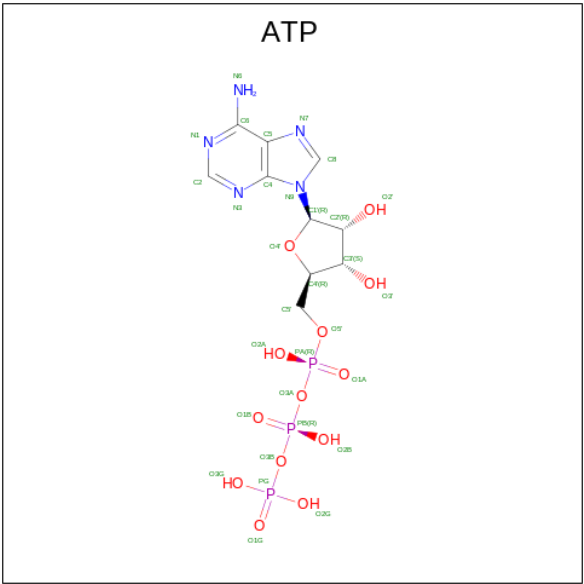
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	F	468	Total 3436	C 2156	N 599	O 666	P 2	S 13	0	0	0
2	C	472	Total 3436	C 2159	N 595	O 666	P 2	S 14	0	0	0
2	D	471	Total 3456	C 2170	N 594	O 676	P 2	S 14	0	0	0
2	K	471	Total 3444	C 2171	N 592	O 666	P 2	S 13	0	0	0
2	L	470	Total 3471	C 2181	N 598	O 676	P 2	S 14	0	0	0
2	I	473	Total 3477	C 2181	N 603	O 678	P 2	S 13	0	0	0
2	J	468	Total 3442	C 2161	N 598	O 668	P 2	S 13	0	0	0
2	O	461	Total 3072	C 1899	N 552	O 607	P 2	S 12	0	0	0
2	Q	466	Total 3303	C 2057	N 583	O 646	P 2	S 15	0	0	0
2	U	430	Total 2635	C 1596	N 500	O 530	P 2	S 7	0	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	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
3	F	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	G	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	H	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	H	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	K	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	K	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	L	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	L	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	N	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	N	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	O	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	O	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	R	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	R	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	M	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	M	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	P	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	P	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	Q	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	T	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	T	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	U	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	X	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	X	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	S	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	S	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	V	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	V	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	W	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

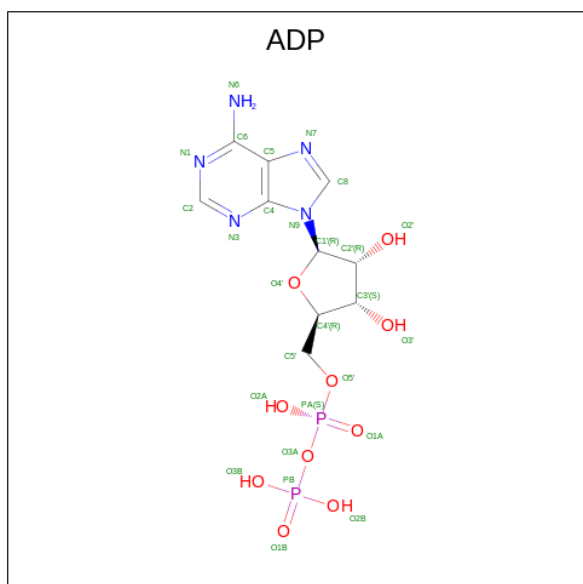
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		
4	G	2	Total	Mg	0	0
			2	2		
4	H	2	Total	Mg	0	0
			2	2		
4	K	2	Total	Mg	0	0
			2	2		
4	L	2	Total	Mg	0	0
			2	2		
4	I	2	Total	Mg	0	0
			2	2		
4	J	2	Total	Mg	0	0
			2	2		
4	N	2	Total	Mg	0	0
			2	2		
4	O	1	Total	Mg	0	0
			1	1		
4	R	2	Total	Mg	0	0
			2	2		
4	M	1	Total	Mg	0	0
			1	1		
4	P	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	1	Total	Mg	0	0
			1	1		
4	T	1	Total	Mg	0	0
			1	1		
4	U	1	Total	Mg	0	0
			1	1		
4	V	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	Q	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	U	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	W	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	9	Total	O	0	0
			9	9		

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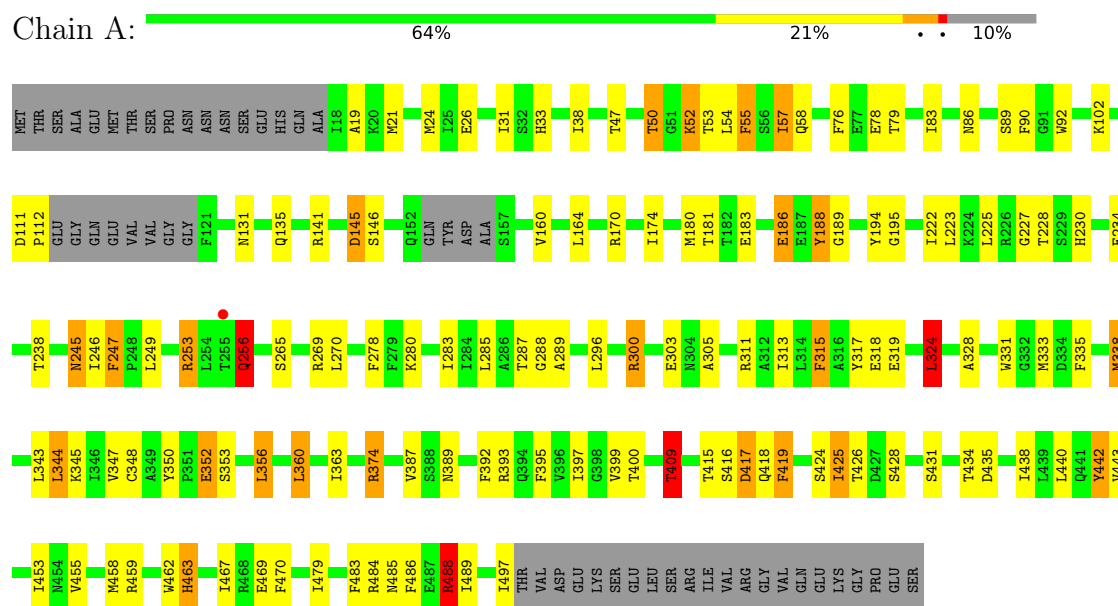
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	4	Total O 4 4	0	0
6	F	6	Total O 6 6	0	0
6	C	7	Total O 7 7	0	0
6	D	4	Total O 4 4	0	0
6	G	4	Total O 4 4	0	0
6	H	4	Total O 4 4	0	0
6	K	3	Total O 3 3	0	0
6	L	6	Total O 6 6	0	0
6	I	5	Total O 5 5	0	0
6	J	4	Total O 4 4	0	0
6	N	2	Total O 2 2	0	0
6	O	5	Total O 5 5	0	0
6	R	2	Total O 2 2	0	0
6	M	1	Total O 1 1	0	0
6	P	4	Total O 4 4	0	0
6	Q	5	Total O 5 5	0	0
6	U	2	Total O 2 2	0	0
6	X	2	Total O 2 2	0	0
6	S	2	Total O 2 2	0	0
6	V	2	Total O 2 2	0	0
6	W	3	Total O 3 3	0	0

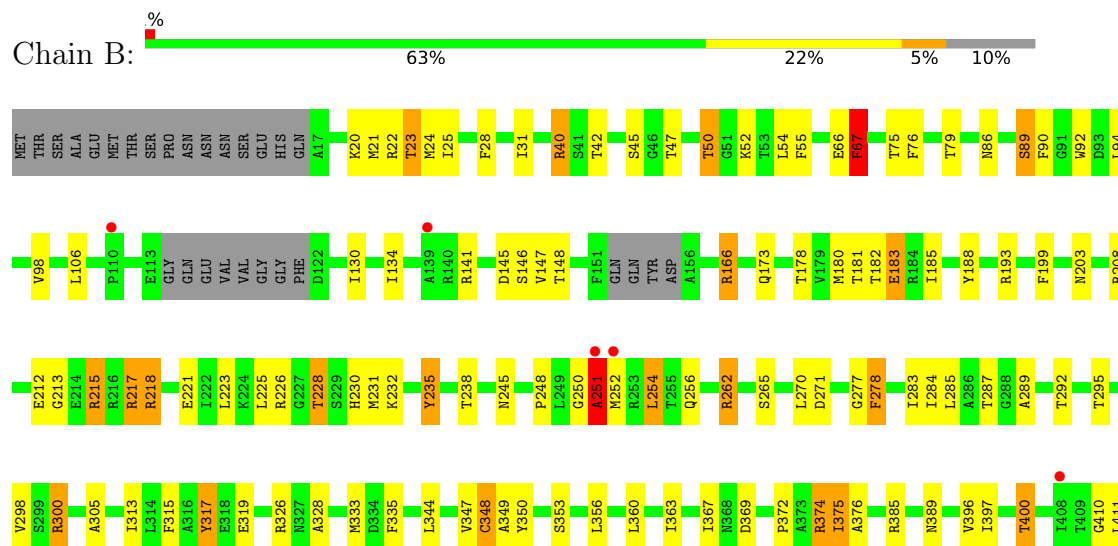
### 3 Residue-property plots

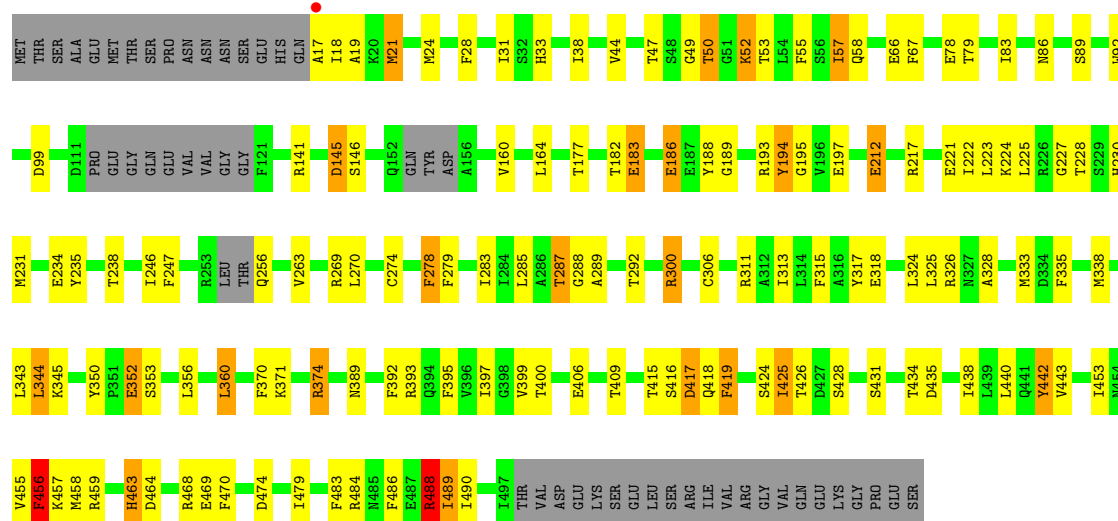
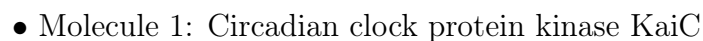
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Circadian clock protein kinase KaiC

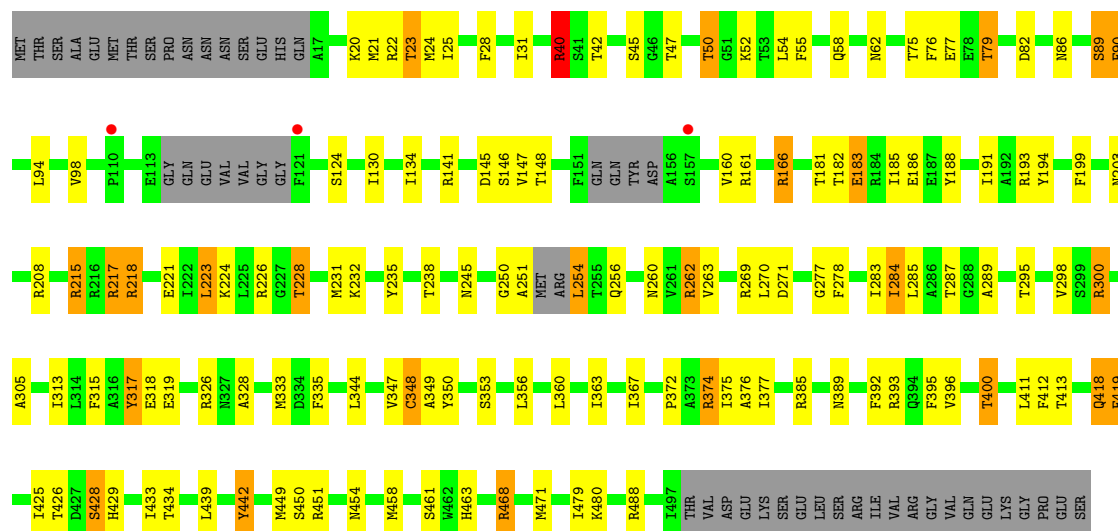


#### • Molecule 1: Circadian clock protein kinase KaiC

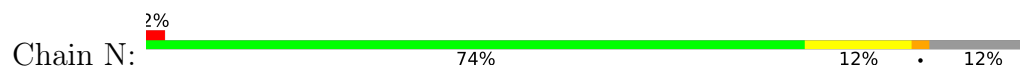




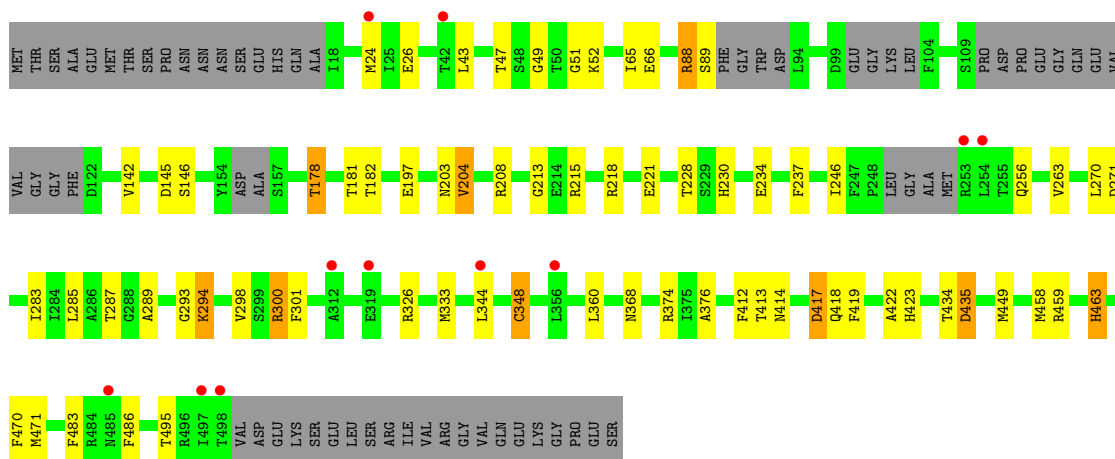
- Molecule 1: Circadian clock protein kinase KaiC



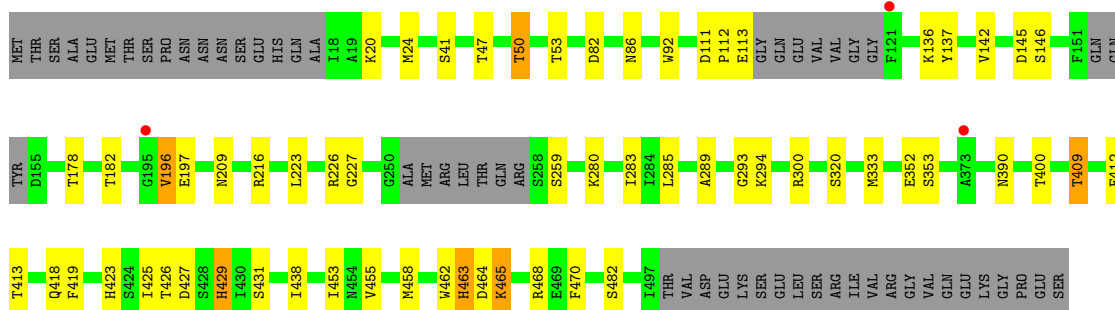
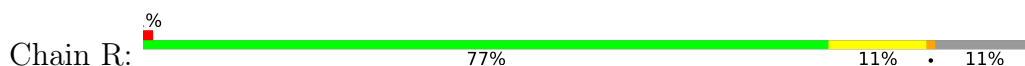
- Molecule 1: Circadian clock protein kinase KaiC



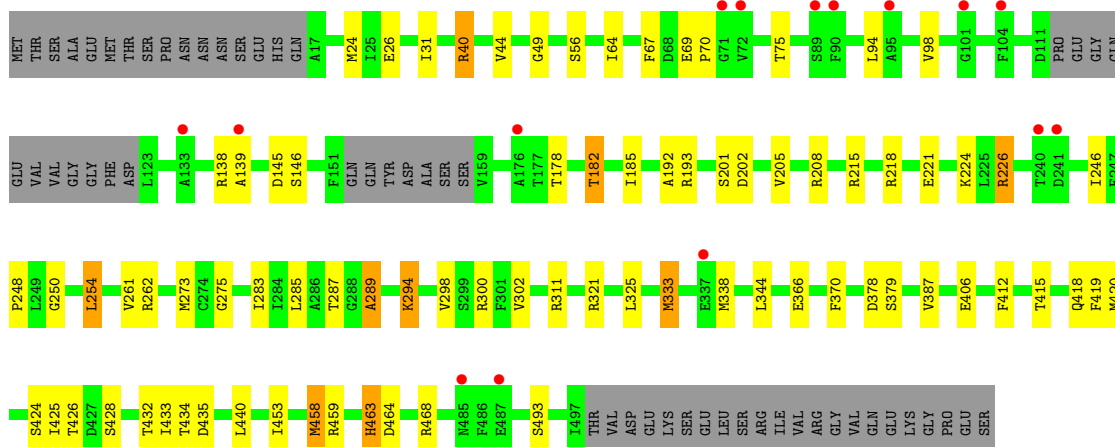
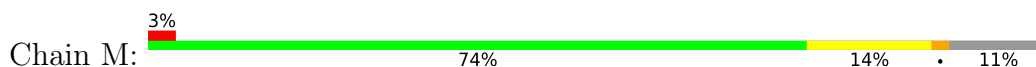




- Molecule 1: Circadian clock protein kinase KaiC

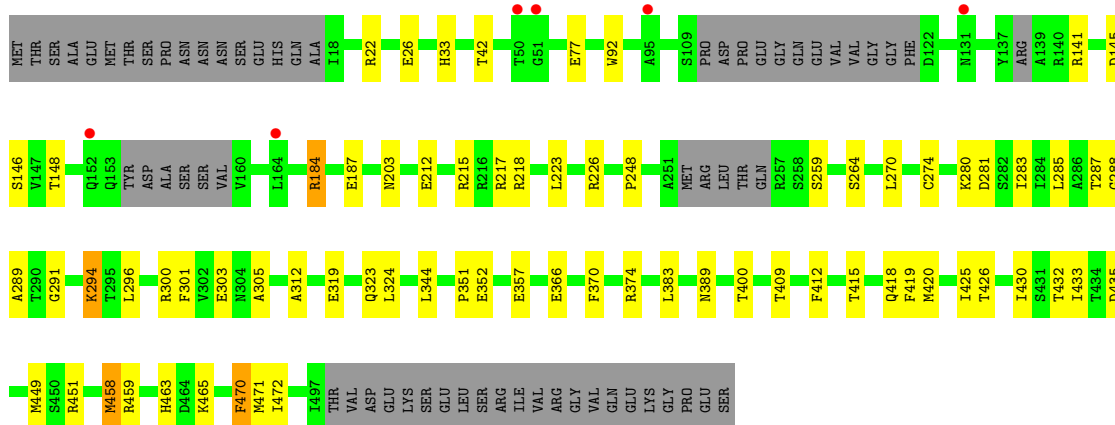


- Molecule 1: Circadian clock protein kinase KaiC

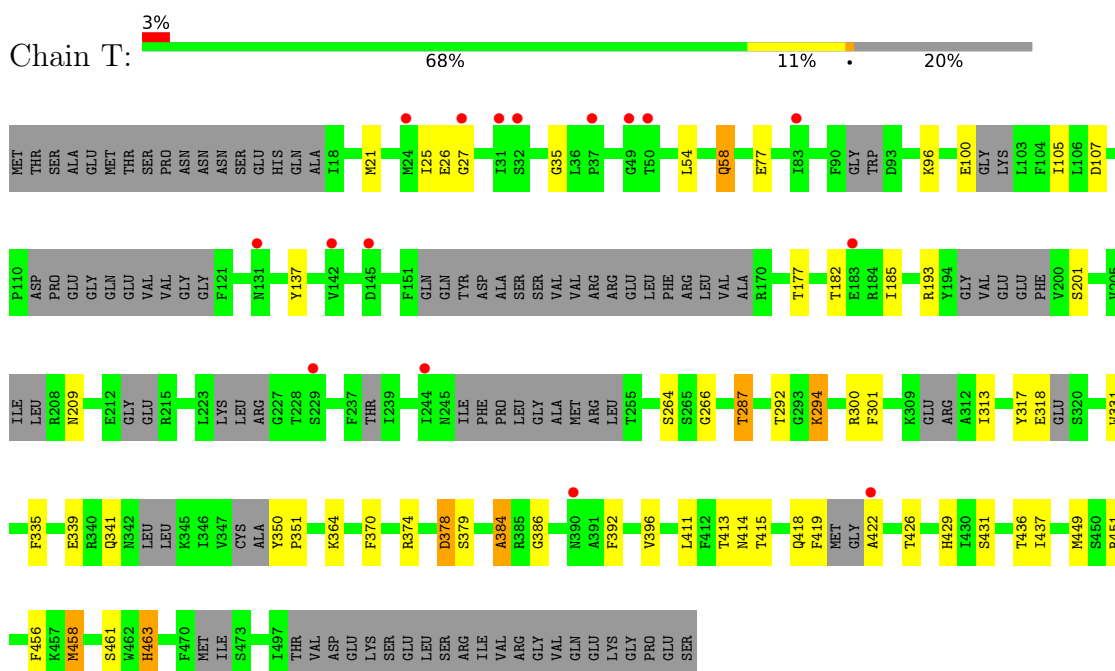


- Molecule 1: Circadian clock protein kinase KaiC

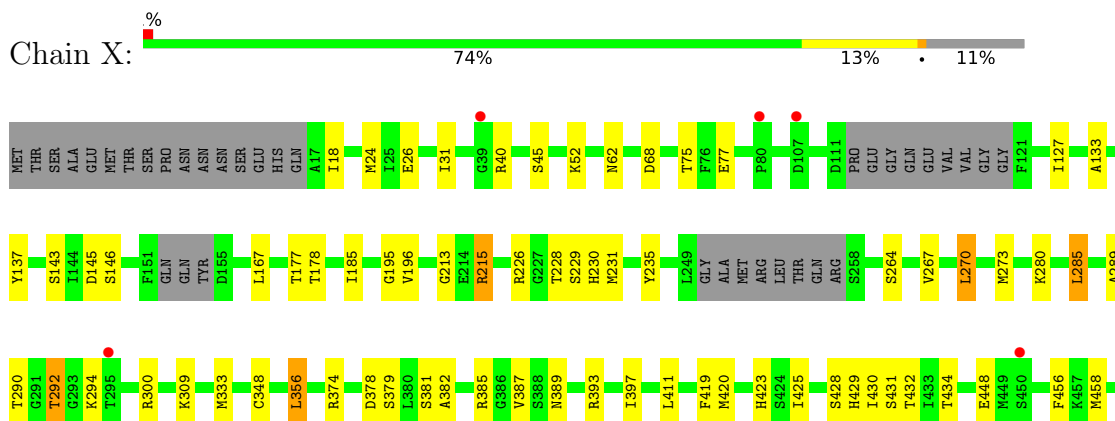


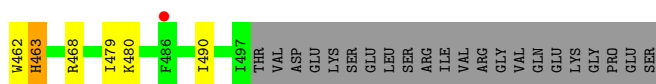


- Molecule 1: Circadian clock protein kinase KaiC

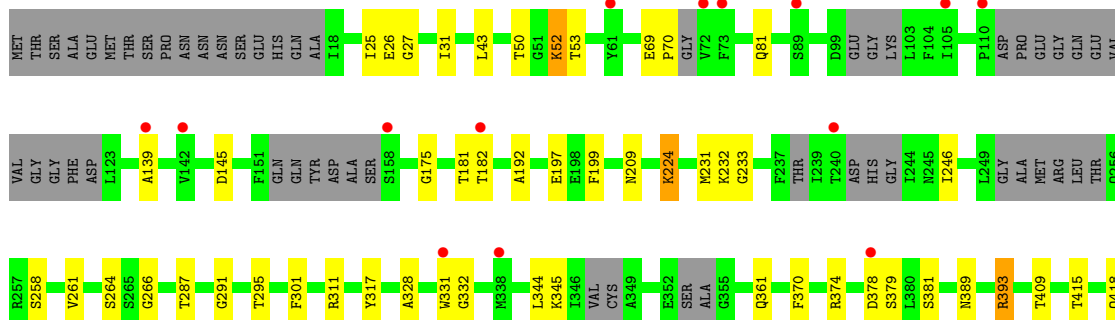
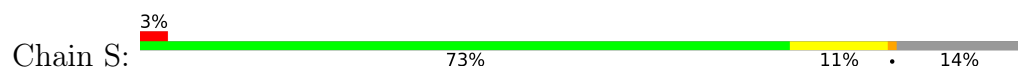


- Molecule 1: Circadian clock protein kinase KaiC

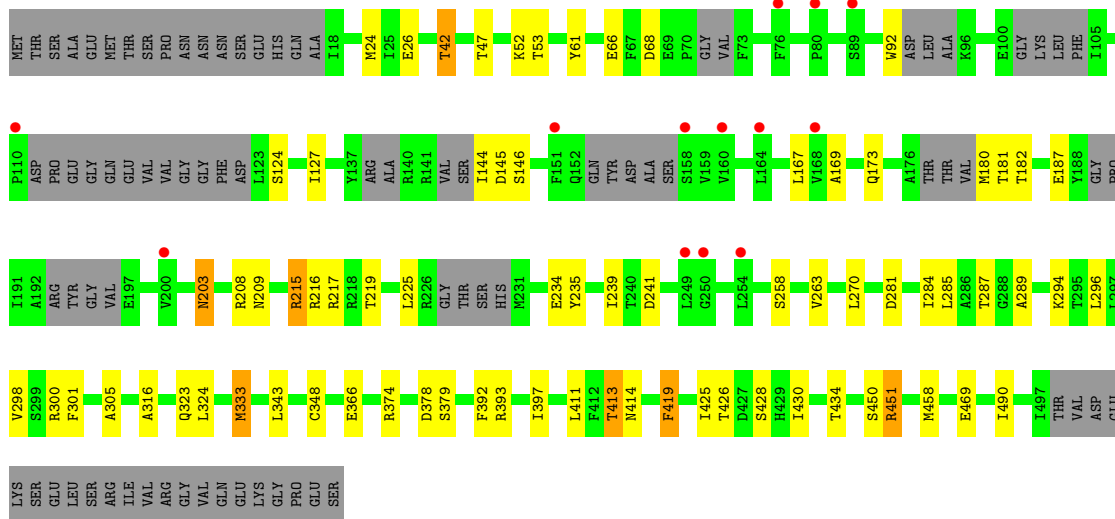




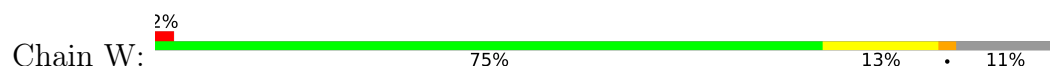
- Molecule 1: Circadian clock protein kinase KaiC

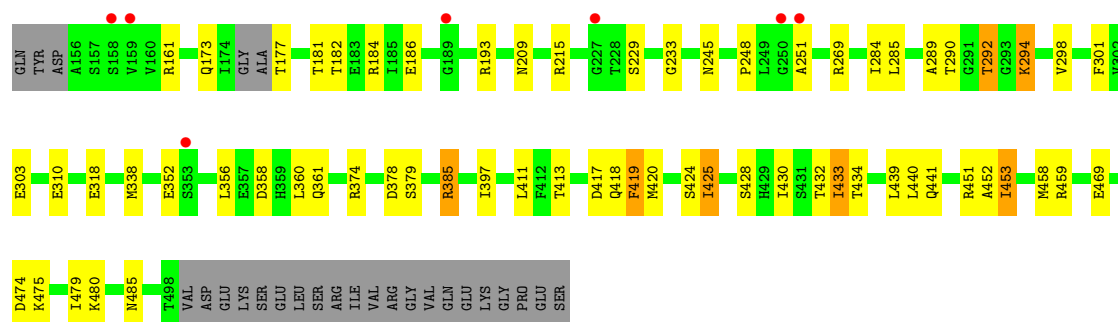


- Molecule 1: Circadian clock protein kinase KaiC

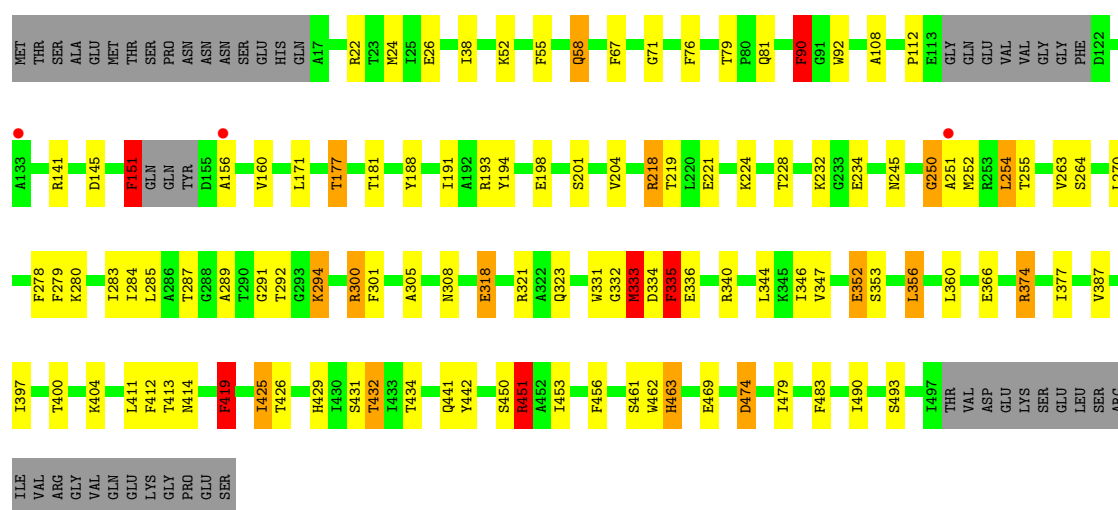


- Molecule 1: Circadian clock protein kinase KaiC

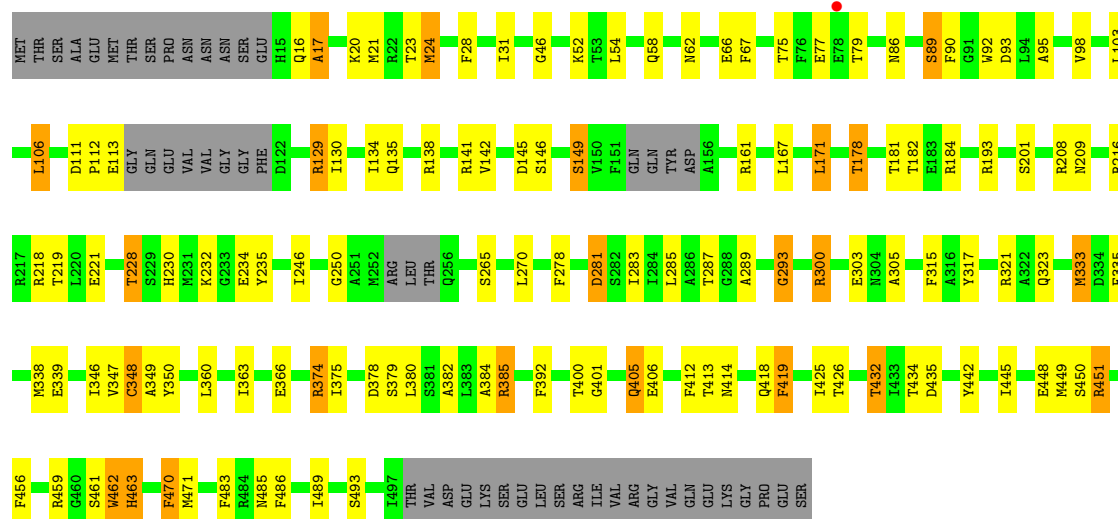




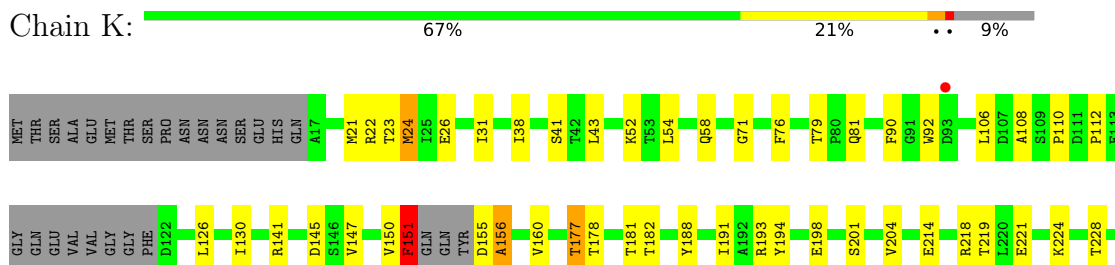
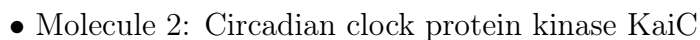
• Molecule 2: Circadian clock protein kinase KaiC

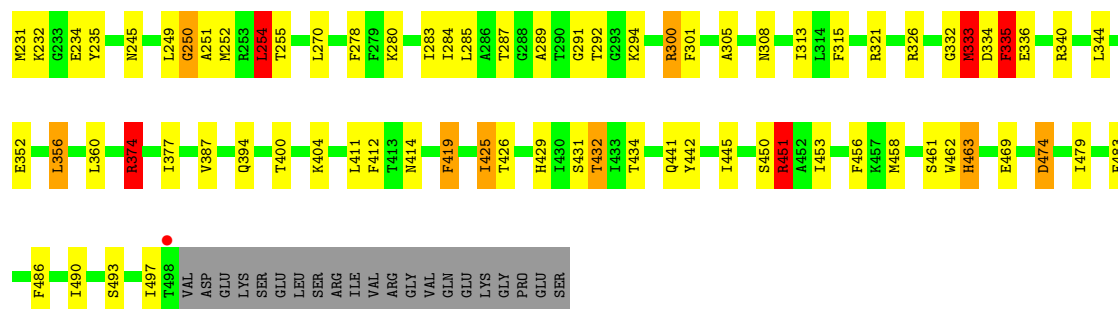


• Molecule 2: Circadian clock protein kinase KaiC



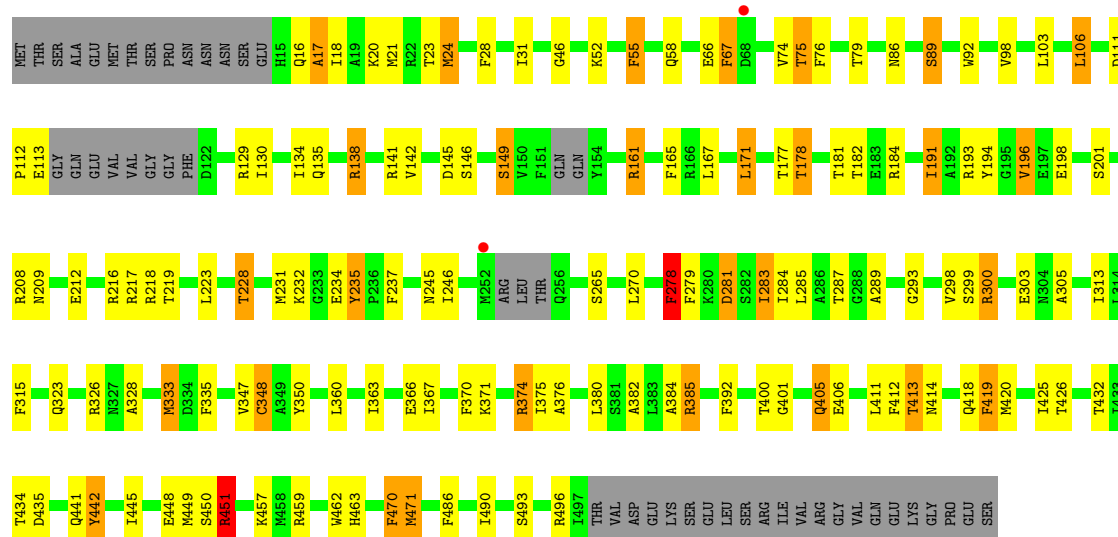
• Molecule 2: Circadian clock protein kinase KaiC





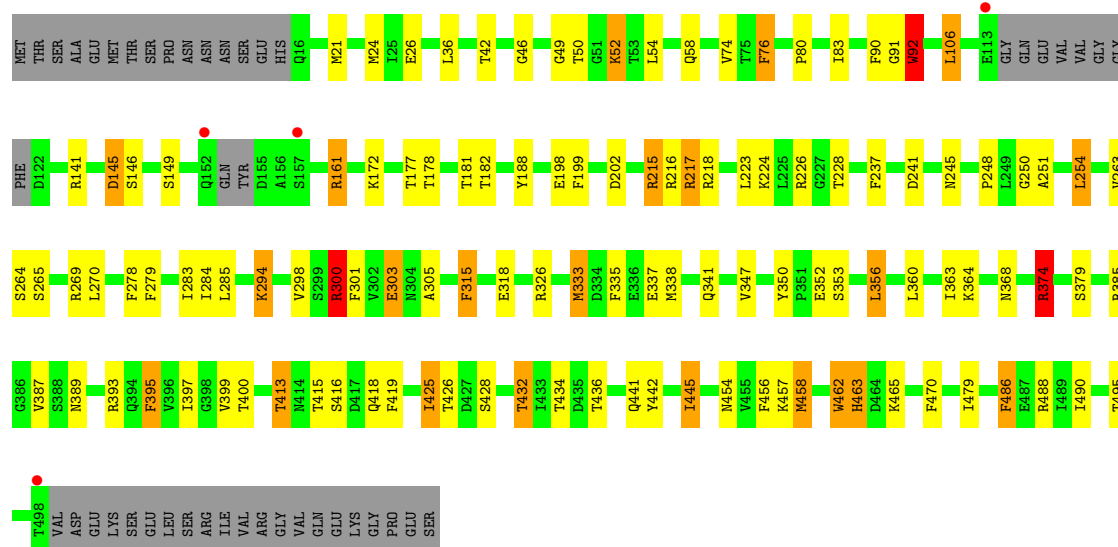
● Molecule 2: Circadian clock protein kinase KaiC

Chain L:  63% 21% 6% 9%

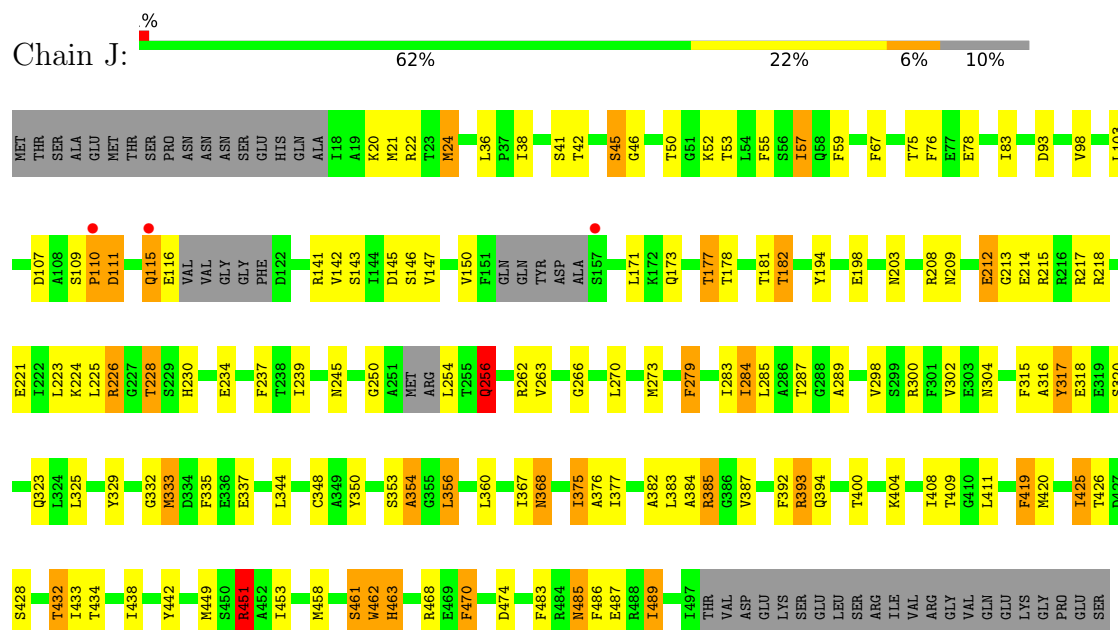


● Molecule 2: Circadian clock protein kinase KaiC

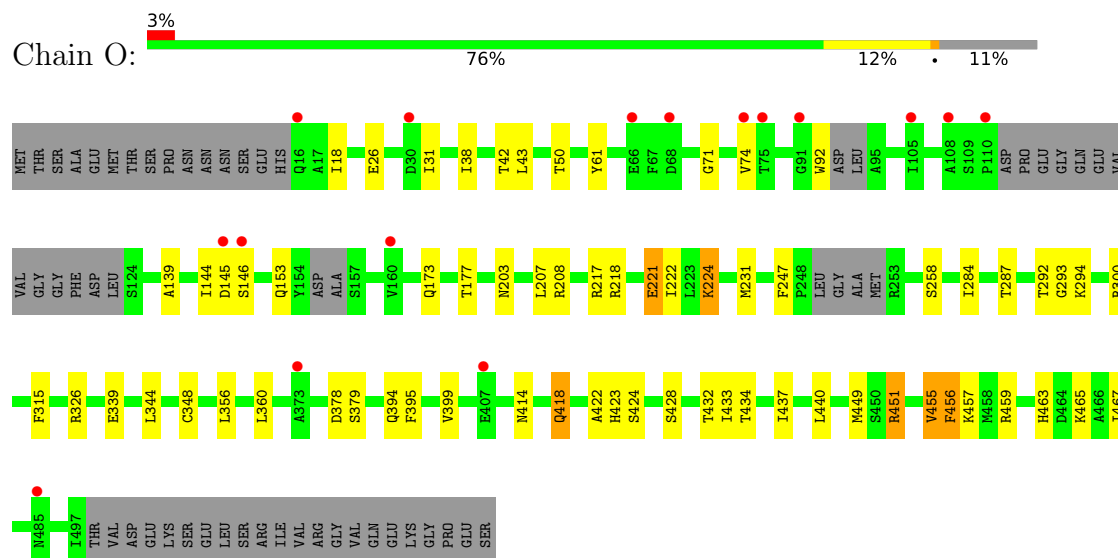
Chain I:  68% 18% 9%



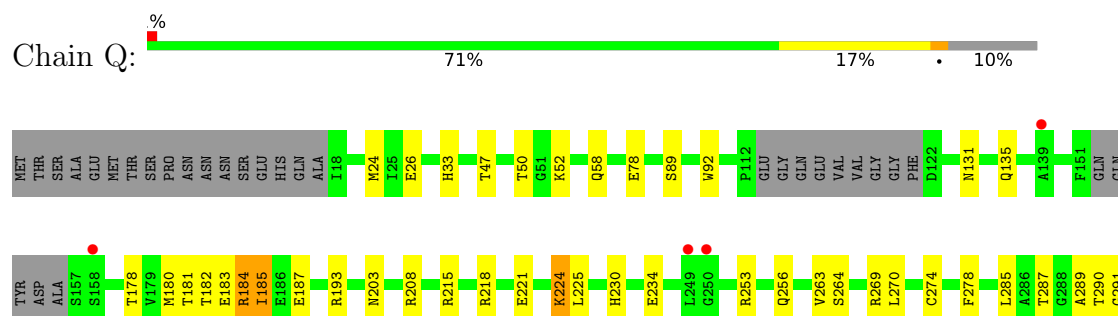
• Molecule 2: Circadian clock protein kinase KaiC

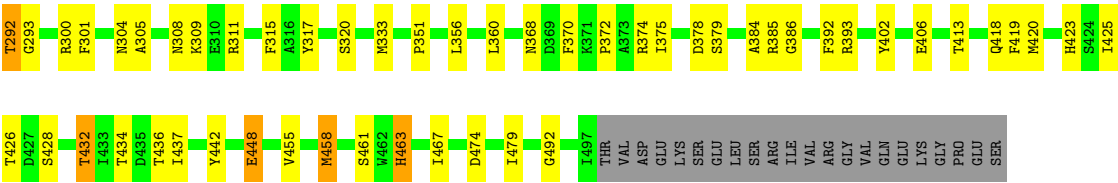


• Molecule 2: Circadian clock protein kinase KaiC

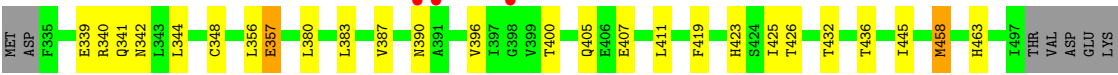
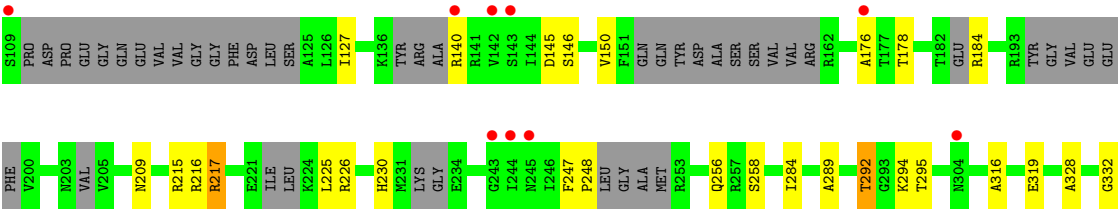
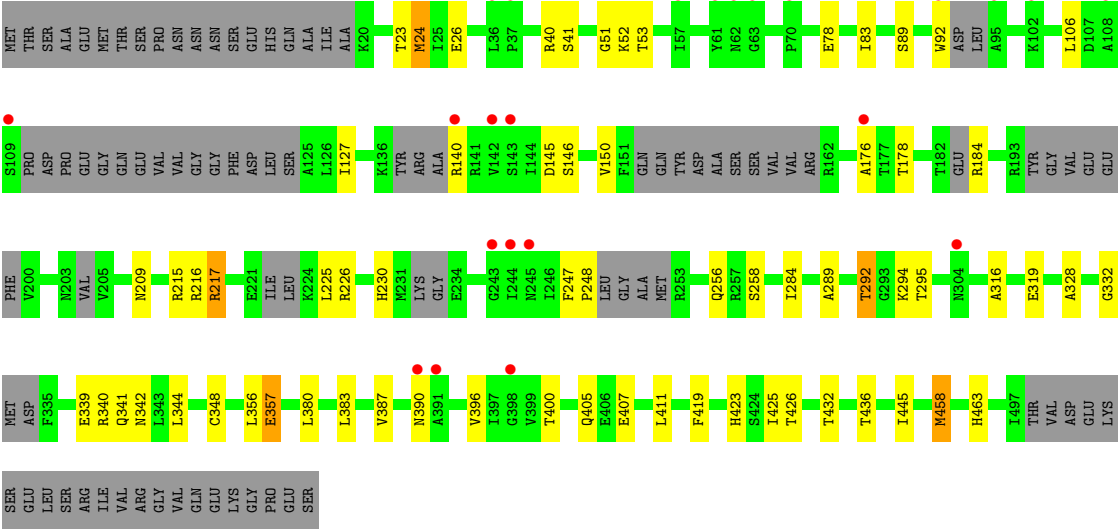


• Molecule 2: Circadian clock protein kinase KaiC





• Molecule 2: Circadian clock protein kinase KaiC





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.49Å 205.80Å 186.18Å 90.00° 115.14° 90.00°	Depositor
Resolution (Å)	49.22 – 3.10 49.17 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.7 (49.22-3.10) 93.7 (49.17-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.275 , 0.340 0.272 , 0.335	Depositor DCC
$R_{free}$ test set	10614 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	78739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	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 74.56 % 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 1.4924e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.78	0/3555	1.03	17/4815 (0.4%)
1	B	0.82	2/3479 (0.1%)	1.50	52/4719 (1.1%)
1	G	0.79	0/3494	1.03	20/4734 (0.4%)
1	H	0.81	1/3523 (0.0%)	1.47	50/4770 (1.0%)
1	M	0.71	0/3164	0.76	0/4307
1	N	0.72	0/3041	0.76	0/4142
1	P	0.71	0/3132	0.76	0/4259
1	R	0.69	0/3243	0.77	0/4406
1	S	0.75	0/2725	0.78	0/3730
1	T	0.77	0/2431	0.78	0/3319
1	V	0.72	0/2936	0.76	0/3993
1	W	0.71	0/3160	0.77	0/4293
1	X	0.71	0/3109	0.77	0/4232
2	C	0.83	4/3473 (0.1%)	1.31	35/4710 (0.7%)
2	D	0.80	1/3491 (0.0%)	1.21	34/4732 (0.7%)
2	E	0.79	2/3460 (0.1%)	1.19	25/4695 (0.5%)
2	F	0.78	0/3471	1.16	26/4699 (0.6%)
2	I	0.82	1/3513 (0.0%)	1.30	32/4758 (0.7%)
2	J	0.80	1/3476 (0.0%)	1.22	29/4709 (0.6%)
2	K	0.79	1/3479 (0.0%)	1.17	20/4720 (0.4%)
2	L	0.77	0/3507	1.18	29/4752 (0.6%)
2	O	0.72	0/3096	0.77	0/4219
2	Q	0.68	0/3338	0.76	0/4529
2	U	0.75	0/2638	0.78	0/3600
All	All	0.76	13/77934 (0.0%)	1.05	369/105842 (0.3%)

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	B	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	374	ARG	CZ-NH2	-7.44	1.23	1.33
2	E	374	ARG	CZ-NH2	-7.19	1.23	1.33
1	B	22	ARG	CZ-NH2	-6.29	1.24	1.33
2	C	92	TRP	CD2-CE3	-5.93	1.31	1.40
1	H	22	ARG	CZ-NH2	-5.86	1.25	1.33
2	C	92	TRP	NE1-CE2	-5.50	1.30	1.37
2	C	215	ARG	CZ-NH2	-5.16	1.26	1.33
2	D	217	ARG	CZ-NH2	-5.15	1.26	1.33
1	B	451	ARG	CZ-NH2	-5.08	1.26	1.33
2	C	161	ARG	CZ-NH2	-5.07	1.26	1.33
2	E	321	ARG	CZ-NH2	-5.06	1.26	1.33
2	J	217	ARG	CZ-NH2	-5.02	1.26	1.33
2	I	442	TYR	CG-CD1	-5.00	1.32	1.39

All (369) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	374	ARG	NE-CZ-NH1	28.43	134.51	120.30
2	K	374	ARG	NE-CZ-NH1	26.64	133.62	120.30
1	B	22	ARG	NE-CZ-NH1	22.32	131.46	120.30
1	B	262	ARG	NE-CZ-NH1	-19.71	110.44	120.30
1	H	488	ARG	NE-CZ-NH2	-19.45	110.57	120.30
1	B	262	ARG	NE-CZ-NH2	18.86	129.73	120.30
1	H	22	ARG	NE-CZ-NH1	18.36	129.48	120.30
2	I	488	ARG	NE-CZ-NH1	-18.11	111.24	120.30
1	B	488	ARG	NE-CZ-NH1	-17.77	111.41	120.30
2	K	451	ARG	NE-CZ-NH1	-17.39	111.61	120.30
2	E	451	ARG	NE-CZ-NH2	-17.37	111.61	120.30
1	H	468	ARG	NE-CZ-NH2	-17.35	111.62	120.30
2	C	300	ARG	NE-CZ-NH2	-17.35	111.63	120.30
1	H	488	ARG	NE-CZ-NH1	17.31	128.96	120.30
1	B	488	ARG	NE-CZ-NH2	17.10	128.85	120.30
1	B	166	ARG	NE-CZ-NH2	17.02	128.81	120.30
2	J	226	ARG	NE-CZ-NH2	-17.01	111.80	120.30
1	H	262	ARG	NE-CZ-NH2	-17.00	111.80	120.30
2	C	374	ARG	NE-CZ-NH1	-16.98	111.81	120.30
1	B	300	ARG	NE-CZ-NH2	-16.97	111.82	120.30
1	B	468	ARG	NE-CZ-NH2	16.95	128.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	488	ARG	NE-CZ-NH2	-16.95	111.83	120.30
2	D	226	ARG	NE-CZ-NH1	-16.81	111.89	120.30
1	H	300	ARG	NE-CZ-NH1	-16.75	111.93	120.30
2	I	300	ARG	NE-CZ-NH1	-16.71	111.95	120.30
2	L	451	ARG	NE-CZ-NH2	-16.66	111.97	120.30
2	K	451	ARG	NE-CZ-NH2	16.47	128.54	120.30
2	I	488	ARG	NE-CZ-NH2	16.45	128.53	120.30
2	I	161	ARG	NE-CZ-NH2	16.45	128.52	120.30
2	C	488	ARG	NE-CZ-NH1	16.42	128.51	120.30
2	I	300	ARG	NE-CZ-NH2	16.41	128.50	120.30
2	F	451	ARG	NE-CZ-NH1	-16.38	112.11	120.30
2	C	374	ARG	NE-CZ-NH2	16.37	128.48	120.30
2	E	451	ARG	NE-CZ-NH1	16.27	128.44	120.30
2	I	374	ARG	NE-CZ-NH1	16.14	128.37	120.30
1	B	300	ARG	NE-CZ-NH1	16.13	128.36	120.30
2	I	374	ARG	NE-CZ-NH2	-16.06	112.27	120.30
1	B	468	ARG	NE-CZ-NH1	-16.00	112.30	120.30
2	J	226	ARG	NE-CZ-NH1	15.99	128.30	120.30
1	H	166	ARG	NE-CZ-NH2	15.99	128.29	120.30
2	C	161	ARG	NE-CZ-NH2	15.97	128.29	120.30
2	J	385	ARG	NE-CZ-NH2	-15.90	112.35	120.30
1	H	468	ARG	NE-CZ-NH1	15.87	128.24	120.30
1	H	300	ARG	NE-CZ-NH2	15.85	128.23	120.30
1	H	326	ARG	NE-CZ-NH1	15.76	128.18	120.30
2	C	300	ARG	NE-CZ-NH1	15.75	128.18	120.30
1	H	326	ARG	NE-CZ-NH2	-15.75	112.42	120.30
2	D	226	ARG	NE-CZ-NH2	15.72	128.16	120.30
2	I	215	ARG	NE-CZ-NH2	15.69	128.15	120.30
1	B	326	ARG	NE-CZ-NH2	15.57	128.09	120.30
2	F	451	ARG	NE-CZ-NH2	15.47	128.03	120.30
2	J	385	ARG	NE-CZ-NH1	15.34	127.97	120.30
1	G	374	ARG	NE-CZ-NH1	15.15	127.88	120.30
1	H	451	ARG	NE-CZ-NH2	15.15	127.87	120.30
2	K	321	ARG	NE-CZ-NH2	15.12	127.86	120.30
2	L	451	ARG	NE-CZ-NH1	15.12	127.86	120.30
2	I	217	ARG	NE-CZ-NH2	15.10	127.85	120.30
2	D	385	ARG	NE-CZ-NH1	-15.09	112.75	120.30
1	H	262	ARG	NE-CZ-NH1	15.06	127.83	120.30
2	D	385	ARG	NE-CZ-NH2	15.02	127.81	120.30
2	J	393	ARG	NE-CZ-NH2	15.01	127.80	120.30
2	L	138	ARG	NE-CZ-NH2	-14.90	112.85	120.30
1	H	217	ARG	NE-CZ-NH1	14.87	127.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	393	ARG	NE-CZ-NH2	-14.73	112.93	120.30
2	J	393	ARG	NE-CZ-NH1	-14.66	112.97	120.30
2	L	374	ARG	NE-CZ-NH1	-14.66	112.97	120.30
1	H	218	ARG	NE-CZ-NH2	14.48	127.54	120.30
2	F	138	ARG	NE-CZ-NH2	14.30	127.45	120.30
2	L	374	ARG	NE-CZ-NH2	14.01	127.30	120.30
2	D	217	ARG	NE-CZ-NH1	13.95	127.28	120.30
2	E	321	ARG	NE-CZ-NH2	13.90	127.25	120.30
2	J	217	ARG	NE-CZ-NH2	13.87	127.24	120.30
2	F	374	ARG	NE-CZ-NH2	-13.81	113.40	120.30
2	D	393	ARG	NE-CZ-NH1	13.69	127.15	120.30
1	B	218	ARG	NE-CZ-NH1	13.69	127.14	120.30
2	C	215	ARG	NE-CZ-NH2	13.47	127.04	120.30
1	B	326	ARG	NE-CZ-NH1	-13.41	113.59	120.30
2	L	138	ARG	NE-CZ-NH1	13.28	126.94	120.30
2	F	138	ARG	NE-CZ-NH1	-13.24	113.68	120.30
1	B	451	ARG	NE-CZ-NH1	13.07	126.83	120.30
2	C	217	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	B	374	ARG	NE-CZ-NH1	-12.96	113.82	120.30
2	L	129	ARG	NE-CZ-NH2	-12.84	113.88	120.30
2	D	217	ARG	NE-CZ-NH2	12.70	126.65	120.30
2	E	321	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	B	451	ARG	NE-CZ-NH2	12.54	126.57	120.30
1	H	374	ARG	NE-CZ-NH2	-12.43	114.08	120.30
2	F	374	ARG	NE-CZ-NH1	12.29	126.44	120.30
2	L	385	ARG	NE-CZ-NH2	-12.21	114.19	120.30
2	J	217	ARG	NE-CZ-NH1	12.20	126.40	120.30
2	C	161	ARG	NH1-CZ-NH2	-12.20	105.98	119.40
2	D	217	ARG	NH1-CZ-NH2	-12.12	106.07	119.40
1	A	374	ARG	NE-CZ-NH2	12.09	126.34	120.30
2	E	321	ARG	NH1-CZ-NH2	-12.06	106.14	119.40
2	I	215	ARG	NH1-CZ-NH2	-11.94	106.26	119.40
1	H	451	ARG	NH1-CZ-NH2	-11.93	106.27	119.40
2	C	215	ARG	NE-CZ-NH1	11.92	126.26	120.30
2	I	161	ARG	NH1-CZ-NH2	-11.90	106.31	119.40
2	J	217	ARG	NH1-CZ-NH2	-11.87	106.35	119.40
2	E	218	ARG	CG-CD-NE	11.84	136.66	111.80
2	K	321	ARG	NH1-CZ-NH2	-11.84	106.38	119.40
1	B	374	ARG	NE-CZ-NH2	11.82	126.21	120.30
2	F	129	ARG	NE-CZ-NH1	-11.81	114.39	120.30
1	B	451	ARG	NH1-CZ-NH2	-11.64	106.59	119.40
2	C	215	ARG	NH1-CZ-NH2	-11.54	106.70	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	129	ARG	NE-CZ-NH2	11.44	126.02	120.30
2	L	385	ARG	NE-CZ-NH1	11.44	126.02	120.30
2	K	218	ARG	CG-CD-NE	11.37	135.67	111.80
2	L	129	ARG	NE-CZ-NH1	11.35	125.98	120.30
2	F	385	ARG	NE-CZ-NH1	-11.22	114.69	120.30
1	H	451	ARG	NE-CZ-NH1	11.10	125.85	120.30
2	E	451	ARG	CD-NE-CZ	11.07	139.10	123.60
1	B	217	ARG	NE-CZ-NH2	11.06	125.83	120.30
2	K	321	ARG	NE-CZ-NH1	10.93	125.76	120.30
1	H	488	ARG	CD-NE-CZ	10.88	138.84	123.60
2	C	161	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	B	262	ARG	CD-NE-CZ	10.81	138.74	123.60
2	C	300	ARG	CD-NE-CZ	10.78	138.70	123.60
2	C	217	ARG	NH1-CZ-NH2	-10.78	107.54	119.40
1	B	166	ARG	CG-CD-NE	10.72	134.32	111.80
1	H	374	ARG	NE-CZ-NH1	10.59	125.59	120.30
2	I	217	ARG	NH1-CZ-NH2	-10.57	107.77	119.40
2	F	385	ARG	NE-CZ-NH2	10.56	125.58	120.30
2	I	419	PHE	CB-CG-CD2	10.55	128.18	120.80
2	C	217	ARG	NE-CZ-NH2	10.54	125.57	120.30
2	C	419	PHE	CB-CG-CD2	10.50	128.15	120.80
2	I	215	ARG	NE-CZ-NH1	10.47	125.53	120.30
2	I	300	ARG	CD-NE-CZ	10.41	138.18	123.60
1	H	468	ARG	CD-NE-CZ	10.38	138.13	123.60
2	L	451	ARG	CD-NE-CZ	10.24	137.94	123.60
1	B	218	ARG	NH1-CZ-NH2	-10.16	108.22	119.40
2	C	488	ARG	CD-NE-CZ	10.16	137.82	123.60
2	I	488	ARG	CD-NE-CZ	10.14	137.79	123.60
1	B	488	ARG	CD-NE-CZ	10.09	137.72	123.60
2	K	451	ARG	CD-NE-CZ	10.06	137.69	123.60
1	H	166	ARG	CG-CD-NE	10.03	132.86	111.80
2	D	226	ARG	CD-NE-CZ	10.03	137.63	123.60
1	B	468	ARG	CD-NE-CZ	10.01	137.61	123.60
1	H	262	ARG	CD-NE-CZ	9.95	137.53	123.60
2	J	385	ARG	CD-NE-CZ	9.91	137.48	123.60
2	C	374	ARG	CD-NE-CZ	9.90	137.46	123.60
1	B	300	ARG	CD-NE-CZ	9.87	137.42	123.60
1	G	374	ARG	NH1-CZ-NH2	-9.78	108.64	119.40
1	H	300	ARG	CD-NE-CZ	9.77	137.28	123.60
1	H	218	ARG	NH1-CZ-NH2	-9.76	108.66	119.40
2	I	161	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	A	374	ARG	NH1-CZ-NH2	-9.70	108.74	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	226	ARG	CD-NE-CZ	9.66	137.12	123.60
1	B	22	ARG	NH1-CZ-NH2	-9.64	108.79	119.40
2	I	374	ARG	CD-NE-CZ	9.63	137.09	123.60
1	H	326	ARG	CD-NE-CZ	9.61	137.05	123.60
1	B	326	ARG	CD-NE-CZ	9.44	136.81	123.60
2	E	451	ARG	CG-CD-NE	-9.43	92.01	111.80
2	F	451	ARG	CD-NE-CZ	9.42	136.78	123.60
2	E	374	ARG	NH1-CZ-NH2	-9.41	109.05	119.40
1	G	419	PHE	CB-CG-CD1	9.25	127.28	120.80
2	J	393	ARG	CD-NE-CZ	9.20	136.48	123.60
1	A	374	ARG	NE-CZ-NH1	9.20	124.90	120.30
2	D	385	ARG	CD-NE-CZ	9.11	136.35	123.60
2	D	393	ARG	CD-NE-CZ	8.94	136.12	123.60
1	H	217	ARG	NH1-CZ-NH2	-8.86	109.66	119.40
1	B	217	ARG	NH1-CZ-NH2	-8.74	109.79	119.40
2	K	335	PHE	CB-CG-CD2	8.72	126.90	120.80
1	H	22	ARG	NH1-CZ-NH2	-8.69	109.84	119.40
2	L	138	ARG	CD-NE-CZ	8.66	135.72	123.60
1	A	419	PHE	CB-CG-CD1	8.65	126.85	120.80
2	C	300	ARG	CG-CD-NE	-8.50	93.95	111.80
2	F	138	ARG	CD-NE-CZ	8.44	135.42	123.60
2	K	374	ARG	NH1-CZ-NH2	-8.38	110.18	119.40
2	L	374	ARG	CD-NE-CZ	8.37	135.31	123.60
1	B	218	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	H	419	PHE	CB-CG-CD1	8.27	126.59	120.80
1	A	409	THR	CA-CB-CG2	8.23	123.93	112.40
2	K	374	ARG	NE-CZ-NH2	-8.22	116.19	120.30
2	I	217	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	217	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	B	326	ARG	CG-CD-NE	7.98	128.56	111.80
2	J	451	ARG	CB-CG-CD	7.96	132.30	111.60
2	I	52	LYS	CG-CD-CE	7.80	135.31	111.90
1	B	166	ARG	NH1-CZ-NH2	-7.79	110.83	119.40
2	F	350	TYR	CB-CG-CD1	7.78	125.67	121.00
2	E	374	ARG	NE-CZ-NH2	-7.74	116.43	120.30
2	C	92	TRP	CD1-CG-CD2	-7.71	100.13	106.30
2	D	451	ARG	CB-CG-CD	7.71	131.63	111.60
2	D	194	TYR	CB-CG-CD1	7.67	125.60	121.00
1	B	188	TYR	CB-CG-CD2	7.57	125.54	121.00
2	J	215	ARG	NE-CZ-NH2	7.57	124.08	120.30
2	F	374	ARG	CD-NE-CZ	7.50	134.10	123.60
1	H	262	ARG	CG-CD-NE	-7.42	96.22	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	52	LYS	CG-CD-CE	7.40	134.09	111.90
2	D	256	GLN	CB-CG-CD	7.27	130.51	111.60
2	C	335	PHE	CB-CG-CD1	7.18	125.82	120.80
1	G	409	THR	CA-CB-CG2	7.13	122.39	112.40
2	J	55	PHE	CB-CG-CD1	7.12	125.79	120.80
2	E	335	PHE	CB-CG-CD2	7.09	125.77	120.80
1	H	166	ARG	NH1-CZ-NH2	-7.04	111.66	119.40
2	K	194	TYR	CB-CG-CD1	7.03	125.22	121.00
2	C	279	PHE	CB-CG-CD2	7.00	125.70	120.80
2	D	350	TYR	CB-CG-CD2	6.99	125.19	121.00
2	J	335	PHE	CB-CG-CD2	6.96	125.67	120.80
1	H	218	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	K	294	LYS	CG-CD-CE	6.95	132.76	111.90
1	B	419	PHE	CB-CG-CD1	6.95	125.66	120.80
2	F	235	TYR	CB-CG-CD2	6.94	125.16	121.00
2	J	256	GLN	CB-CG-CD	6.92	129.60	111.60
2	J	215	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	B	262	ARG	CG-CD-NE	6.87	126.22	111.80
2	E	218	ARG	NE-CZ-NH1	-6.84	116.88	120.30
2	D	215	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	B	374	ARG	CD-NE-CZ	6.80	133.12	123.60
2	C	92	TRP	CE2-CD2-CG	6.78	112.72	107.30
2	E	151	PHE	CB-CG-CD1	6.75	125.53	120.80
2	D	329	TYR	CB-CG-CD2	6.75	125.05	121.00
1	B	40	ARG	CG-CD-NE	6.67	125.81	111.80
1	H	40	ARG	CB-CG-CD	6.59	128.74	111.60
2	E	294	LYS	CG-CD-CE	6.57	131.62	111.90
2	F	129	ARG	CG-CD-NE	6.55	125.56	111.80
2	C	350	TYR	CB-CG-CD2	6.55	124.93	121.00
1	B	317	TYR	CB-CG-CD1	6.54	124.92	121.00
1	A	324	LEU	CD1-CG-CD2	-6.51	90.97	110.50
2	D	188	TYR	CB-CG-CD2	6.48	124.89	121.00
2	L	350	TYR	CB-CG-CD1	6.43	124.86	121.00
2	F	419	PHE	CB-CG-CD2	6.42	125.30	120.80
2	L	28	PHE	CB-CG-CD1	6.42	125.29	120.80
2	J	329	TYR	CB-CG-CD2	6.41	124.84	121.00
1	B	350	TYR	CB-CG-CD1	6.40	124.84	121.00
2	L	385	ARG	CG-CD-NE	6.39	125.23	111.80
1	H	317	TYR	CB-CG-CD1	6.39	124.83	121.00
2	E	419	PHE	CB-CG-CD2	6.37	125.26	120.80
2	L	171	LEU	CD1-CG-CD2	-6.36	91.41	110.50
1	B	40	ARG	CB-CG-CD	6.33	128.05	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	92	TRP	CD1-CG-CD2	-6.33	101.24	106.30
2	F	171	LEU	CD1-CG-CD2	-6.32	91.53	110.50
2	D	55	PHE	CB-CG-CD1	6.30	125.21	120.80
1	H	442	TYR	CB-CG-CD1	6.30	124.78	121.00
2	J	194	TYR	CB-CG-CD1	6.24	124.74	121.00
1	G	374	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	A	76	PHE	CB-CG-CD1	6.21	125.14	120.80
2	D	442	TYR	CB-CG-CD2	6.19	124.71	121.00
1	H	350	TYR	CB-CG-CD1	6.16	124.69	121.00
1	B	215	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	H	374	ARG	CD-NE-CZ	6.13	132.18	123.60
2	D	215	ARG	NE-CZ-NH2	6.10	123.35	120.30
2	I	486	PHE	CB-CG-CD2	6.10	125.07	120.80
2	C	194	TYR	CB-CG-CD2	6.09	124.66	121.00
2	K	188	TYR	CB-CG-CD1	6.08	124.65	121.00
2	L	278	PHE	CB-CG-CD2	6.07	125.05	120.80
1	G	188	TYR	CB-CG-CD1	6.02	124.61	121.00
1	H	235	TYR	CB-CG-CD2	6.01	124.61	121.00
1	H	488	ARG	CG-CD-NE	-6.00	99.21	111.80
2	F	470	PHE	CB-CG-CD1	5.99	124.99	120.80
2	E	218	ARG	NE-CZ-NH2	5.98	123.29	120.30
2	L	235	TYR	CB-CG-CD2	5.95	124.57	121.00
2	L	451	ARG	CG-CD-NE	-5.95	99.31	111.80
1	G	278	PHE	CB-CG-CD2	5.94	124.96	120.80
2	D	76	PHE	CB-CG-CD2	5.92	124.94	120.80
1	H	326	ARG	CG-CD-NE	-5.91	99.39	111.80
2	L	419	PHE	CB-CG-CD2	5.89	124.92	120.80
2	F	385	ARG	CG-CD-NE	5.88	124.15	111.80
2	L	129	ARG	CD-NE-CZ	5.87	131.82	123.60
1	A	188	TYR	CB-CG-CD1	5.87	124.52	121.00
2	C	92	TRP	CD2-CE2-CZ2	5.84	129.31	122.30
2	D	278	PHE	CB-CG-CD1	5.82	124.87	120.80
1	H	350	TYR	CD1-CG-CD2	-5.81	111.51	117.90
2	E	90	PHE	CB-CG-CD2	5.81	124.87	120.80
1	G	324	LEU	CD1-CG-CD2	-5.77	93.18	110.50
2	L	470	PHE	CB-CG-CD1	5.77	124.84	120.80
1	G	212	GLU	CB-CG-CD	5.76	129.75	114.20
1	A	188	TYR	CD1-CG-CD2	-5.76	111.57	117.90
1	B	420	MET	CB-CG-SD	5.75	129.66	112.40
2	F	442	TYR	CB-CG-CD1	5.74	124.44	121.00
2	L	350	TYR	CD1-CG-CD2	-5.74	111.59	117.90
2	D	335	PHE	CB-CG-CD2	5.71	124.80	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	317	TYR	CB-CG-CD1	5.71	124.42	121.00
2	K	278	PHE	CB-CG-CD2	5.71	124.80	120.80
2	I	350	TYR	CB-CG-CD2	5.71	124.42	121.00
2	J	385	ARG	CG-CD-NE	5.70	123.76	111.80
1	H	317	TYR	CD1-CG-CD2	-5.68	111.65	117.90
2	F	350	TYR	CD1-CG-CD2	-5.68	111.65	117.90
1	H	188	TYR	CB-CG-CD2	5.68	124.41	121.00
2	K	419	PHE	CB-CG-CD2	5.67	124.77	120.80
1	B	317	TYR	CD1-CG-CD2	-5.67	111.67	117.90
1	A	317	TYR	CB-CG-CD1	5.64	124.39	121.00
2	E	218	ARG	CD-NE-CZ	5.64	131.50	123.60
1	G	470	PHE	CB-CG-CD2	5.63	124.74	120.80
1	B	76	PHE	CB-CG-CD2	5.63	124.74	120.80
1	B	442	TYR	CB-CG-CD1	5.62	124.37	121.00
2	D	329	TYR	CD1-CG-CD2	-5.61	111.73	117.90
2	D	317	TYR	CD1-CG-CD2	-5.61	111.73	117.90
2	J	76	PHE	CB-CG-CD2	5.59	124.71	120.80
2	C	442	TYR	CB-CG-CD2	5.59	124.35	121.00
2	C	470	PHE	CB-CG-CD2	5.58	124.70	120.80
2	J	329	TYR	CD1-CG-CD2	-5.58	111.76	117.90
2	C	278	PHE	CB-CG-CD1	5.57	124.70	120.80
2	K	188	TYR	CD1-CG-CD2	-5.57	111.78	117.90
1	A	317	TYR	CD1-CG-CD2	-5.56	111.79	117.90
1	B	55	PHE	CB-CG-CD2	5.55	124.69	120.80
1	A	470	PHE	CB-CG-CD2	5.55	124.69	120.80
2	I	237	PHE	CB-CG-CD1	5.55	124.69	120.80
1	A	484	ARG	CG-CD-NE	-5.54	100.16	111.80
1	H	55	PHE	CB-CG-CD2	5.54	124.68	120.80
1	H	418	GLN	CB-CA-C	5.53	121.46	110.40
1	H	40	ARG	CG-CD-NE	5.53	123.40	111.80
2	C	350	TYR	CD1-CG-CD2	-5.52	111.83	117.90
2	E	67	PHE	CB-CG-CD1	5.51	124.66	120.80
2	F	235	TYR	CD1-CG-CD2	-5.51	111.84	117.90
2	I	350	TYR	CD1-CG-CD2	-5.50	111.85	117.90
2	L	235	TYR	CD1-CG-CD2	-5.49	111.87	117.90
2	E	278	PHE	CB-CG-CD1	5.48	124.64	120.80
1	H	218	ARG	CG-CD-NE	5.47	123.29	111.80
2	E	188	TYR	CD1-CG-CD2	-5.46	111.89	117.90
2	D	194	TYR	CD1-CG-CD2	-5.45	111.91	117.90
1	H	76	PHE	CB-CG-CD2	5.44	124.61	120.80
1	G	442	TYR	CB-CG-CD1	5.43	124.26	121.00
1	B	278	PHE	CB-CG-CD2	5.42	124.60	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	385	ARG	CD-NE-CZ	5.42	131.19	123.60
2	I	315	PHE	CB-CG-CD1	5.42	124.60	120.80
2	I	470	PHE	CB-CG-CD2	5.40	124.58	120.80
2	K	151	PHE	CB-CG-CD1	5.40	124.58	120.80
2	C	237	PHE	CB-CG-CD1	5.39	124.58	120.80
2	I	76	PHE	CB-CG-CD2	5.39	124.58	120.80
1	A	488	ARG	CG-CD-NE	5.39	123.11	111.80
1	G	409	THR	OG1-CB-CG2	-5.38	97.62	110.00
2	I	188	TYR	CB-CG-CD1	5.37	124.22	121.00
1	B	350	TYR	CD1-CG-CD2	-5.36	112.00	117.90
2	L	237	PHE	CB-CG-CD2	5.36	124.55	120.80
1	G	317	TYR	CD1-CG-CD2	-5.35	112.01	117.90
1	A	442	TYR	CB-CG-CD1	5.35	124.21	121.00
1	B	67	PHE	CB-CG-CD1	5.34	124.54	120.80
2	D	470	PHE	CB-CG-CD2	5.33	124.53	120.80
2	E	188	TYR	CB-CG-CD1	5.33	124.20	121.00
2	J	317	TYR	CD1-CG-CD2	-5.33	112.04	117.90
1	G	484	ARG	CB-CA-C	-5.31	99.78	110.40
2	F	28	PHE	CB-CG-CD1	5.29	124.50	120.80
2	K	451	ARG	CG-CD-NE	5.28	122.89	111.80
1	B	420	MET	CG-SD-CE	5.26	108.62	100.20
2	K	235	TYR	CD1-CG-CD2	-5.26	112.12	117.90
1	H	442	TYR	CD1-CG-CD2	-5.25	112.12	117.90
2	L	442	TYR	CB-CG-CD1	5.25	124.15	121.00
2	J	470	PHE	CB-CG-CD2	5.23	124.46	120.80
2	I	442	TYR	CD1-CG-CD2	-5.23	112.15	117.90
1	G	188	TYR	CD1-CG-CD2	-5.22	112.16	117.90
2	L	55	PHE	CB-CG-CD1	5.21	124.45	120.80
2	I	279	PHE	CB-CG-CD2	5.20	124.44	120.80
2	I	92	TRP	CH2-CZ2-CE2	-5.17	112.23	117.40
2	D	317	TYR	CB-CG-CD2	5.17	124.10	121.00
2	J	215	ARG	CG-CD-NE	-5.16	100.95	111.80
1	G	442	TYR	CD1-CG-CD2	-5.16	112.23	117.90
1	A	486	PHE	CB-CG-CD2	5.15	124.41	120.80
1	G	456	PHE	CB-CG-CD2	5.15	124.40	120.80
2	E	419	PHE	CD1-CG-CD2	-5.14	111.62	118.30
2	D	279	PHE	CB-CG-CD1	5.13	124.39	120.80
2	J	194	TYR	CD1-CG-CD2	-5.13	112.26	117.90
1	A	338	MET	CB-CG-SD	5.12	127.77	112.40
2	L	385	ARG	CD-NE-CZ	5.12	130.77	123.60
2	C	92	TRP	CH2-CZ2-CE2	-5.12	112.28	117.40
2	C	92	TRP	CE3-CZ3-CH2	5.12	126.83	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	488	ARG	CG-CD-NE	5.12	122.54	111.80
1	B	235	TYR	CB-CG-CD2	5.11	124.07	121.00
2	E	279	PHE	CB-CG-CD2	5.09	124.37	120.80
1	H	188	TYR	CD1-CG-CD2	-5.09	112.30	117.90
2	J	279	PHE	CB-CG-CD1	5.08	124.36	120.80
1	G	486	PHE	CB-CG-CD2	5.08	124.36	120.80
2	F	129	ARG	CD-NE-CZ	5.07	130.70	123.60
2	D	215	ARG	CG-CD-NE	-5.06	101.17	111.80
2	J	317	TYR	CB-CG-CD1	5.05	124.03	121.00
2	D	350	TYR	CD1-CG-CD2	-5.04	112.35	117.90
1	B	188	TYR	CD1-CG-CD2	-5.03	112.36	117.90
2	D	188	TYR	CD1-CG-CD2	-5.01	112.39	117.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	251	ALA	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3506	0	3303	122	0
1	B	3432	0	3166	100	0
1	G	3448	0	3229	125	0
1	H	3476	0	3247	110	0
1	M	3123	0	2557	36	0
1	N	3010	0	2393	33	0
1	P	3096	0	2554	35	0
1	R	3201	0	2747	33	0
1	S	2706	0	1911	32	0
1	T	2427	0	1562	31	0
1	V	2914	0	2335	47	0
1	W	3126	0	2564	50	0
1	X	3074	0	2533	39	0
2	C	3436	0	3139	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3456	0	3185	120	0
2	E	3424	0	3156	88	0
2	F	3436	0	3161	86	0
2	I	3477	0	3211	98	0
2	J	3442	0	3178	117	0
2	K	3444	0	3198	93	0
2	L	3471	0	3211	115	0
2	O	3072	0	2498	24	0
2	Q	3303	0	2875	51	0
2	U	2635	0	1858	42	0
3	A	62	0	24	3	0
3	B	62	0	24	6	0
3	C	62	0	24	6	0
3	D	62	0	24	2	0
3	E	62	0	24	4	0
3	F	62	0	24	3	0
3	G	62	0	24	3	0
3	H	62	0	24	3	0
3	I	62	0	24	6	0
3	J	62	0	24	3	0
3	K	62	0	24	2	0
3	L	62	0	24	6	0
3	M	62	0	24	2	0
3	N	62	0	24	3	0
3	O	62	0	24	1	0
3	P	62	0	24	6	0
3	Q	31	0	12	0	0
3	R	62	0	24	1	0
3	S	62	0	24	2	0
3	T	62	0	24	0	0
3	U	31	0	12	1	0
3	V	62	0	24	3	0
3	W	31	0	12	2	0
3	X	62	0	24	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
4	M	1	0	0	0	0
4	N	2	0	0	0	0
4	O	1	0	0	0	0
4	P	2	0	0	0	0
4	Q	1	0	0	0	0
4	R	2	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
5	Q	27	0	12	0	0
5	U	27	0	12	9	0
5	W	27	0	12	0	0
6	A	6	0	0	0	0
6	B	9	0	0	0	0
6	C	7	0	0	0	0
6	D	4	0	0	0	0
6	E	4	0	0	0	0
6	F	6	0	0	0	0
6	G	4	0	0	0	0
6	H	4	0	0	0	0
6	I	5	0	0	0	0
6	J	4	0	0	0	0
6	K	3	0	0	0	0
6	L	6	0	0	0	0
6	M	1	0	0	0	0
6	N	2	0	0	0	0
6	O	5	0	0	0	0
6	P	4	0	0	0	0
6	Q	5	0	0	0	0
6	R	2	0	0	0	0
6	S	2	0	0	0	0
6	U	2	0	0	0	0
6	V	2	0	0	0	0
6	W	3	0	0	0	0
6	X	2	0	0	0	0
All	All	78739	0	67347	1518	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.

All (1518) 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:V:419:PHE:CD2	1:W:425:ILE:HD13	1.69	1.26
1:G:47:THR:O	1:G:50:THR:OG1	1.61	1.18
2:C:419:PHE:CD1	2:D:425:ILE:HD13	1.85	1.10
1:V:419:PHE:CD2	1:W:425:ILE:CD1	2.35	1.09
2:K:250:GLY:O	2:K:252:MET:N	1.87	1.08
1:A:47:THR:O	1:A:50:THR:OG1	1.72	1.07
2:C:419:PHE:HD1	2:D:425:ILE:HD13	1.14	1.04
1:B:54:LEU:HD13	1:B:90:PHE:HE2	1.13	1.03
1:H:396:VAL:O	1:H:400:THR:OG1	1.75	1.03
1:H:231:MET:HE2	1:H:251:ALA:HB2	1.40	1.02
2:C:121:PHE:O	2:C:125:ALA:HB3	1.59	1.02
1:B:231:MET:HE1	1:B:251:ALA:HB2	1.04	1.02
1:B:231:MET:CE	1:B:251:ALA:HB2	1.89	1.01
1:B:47:THR:O	1:B:50:THR:OG1	1.78	1.00
2:K:425:ILE:HD13	2:J:419:PHE:CD2	1.96	1.00
2:L:347:VAL:HG12	2:L:347:VAL:O	1.55	1.00
2:E:151:PHE:CD2	2:E:160:VAL:HG22	1.97	0.99
1:H:215:ARG:HE	1:H:215:ARG:HA	1.26	0.98
1:H:23:THR:OG1	1:H:25:ILE:HG13	1.62	0.98
1:H:47:THR:O	1:H:50:THR:OG1	1.81	0.97
1:B:396:VAL:O	1:B:400:THR:OG1	1.83	0.97
2:E:250:GLY:O	2:E:252:MET:N	1.97	0.97
1:H:231:MET:CE	1:H:251:ALA:HB2	1.93	0.97
2:K:425:ILE:HD13	2:J:419:PHE:HD2	1.26	0.97
1:B:23:THR:OG1	1:B:25:ILE:HG13	1.64	0.96
1:V:419:PHE:CE2	1:W:425:ILE:CD1	2.47	0.96
2:E:292:THR:HG22	2:E:442:TYR:CE1	2.00	0.96
1:H:419:PHE:CD2	2:I:425:ILE:CD1	2.49	0.96
2:F:285:LEU:HB2	2:F:434:THR:HG21	1.47	0.96
2:K:249:LEU:HD11	2:K:394:GLN:NE2	1.81	0.96
2:U:217:ARG:HG2	2:U:357:GLU:OE1	1.67	0.94
1:B:347:VAL:O	1:B:347:VAL:HG12	1.65	0.94
1:A:280:LYS:O	1:A:409:THR:HB	1.67	0.94
1:B:54:LEU:HD13	1:B:90:PHE:CE2	2.04	0.93
1:H:347:VAL:HG12	1:H:347:VAL:O	1.69	0.93
2:K:425:ILE:CD1	2:J:419:PHE:HD2	1.82	0.92
2:I:301:PHE:O	2:I:374:ARG:NH1	2.04	0.91
1:B:231:MET:HE1	1:B:251:ALA:CB	1.99	0.91
1:G:193:ARG:HD2	1:G:194:TYR:HE1	1.34	0.91
2:L:285:LEU:HB2	2:L:434:THR:HG21	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:328:ALA:HB2	1:H:335:PHE:HE1	1.35	0.90
2:I:92:TRP:HD1	2:I:92:TRP:N	1.70	0.90
1:G:417:ASP:OD2	1:H:429:HIS:CE1	2.25	0.90
2:Q:378:ASP:HA	2:Q:413:THR:OG1	1.70	0.89
2:F:283:ILE:HD12	2:F:400:THR:HG23	1.54	0.89
1:B:215:ARG:HH21	2:C:233:GLY:HA3	1.38	0.89
1:T:317:TYR:HB3	1:T:351:PRO:HD3	1.55	0.88
2:I:92:TRP:N	2:I:92:TRP:CD1	2.36	0.88
1:V:285:LEU:HB2	1:V:434:THR:HG21	1.56	0.87
1:A:313:ILE:CG2	1:A:315:PHE:CE2	2.57	0.87
1:H:283:ILE:HG13	1:H:400:THR:HG22	1.57	0.87
2:D:483:PHE:HB2	2:D:489:ILE:CD1	2.05	0.87
2:I:265:SER:HB3	2:I:278:PHE:CE1	2.10	0.86
2:E:442:TYR:HE2	2:F:456:PHE:CZ	1.92	0.86
2:Q:225:LEU:HD12	2:Q:230:HIS:HB3	1.57	0.84
2:L:278:PHE:CE1	2:L:284:ILE:HG21	2.12	0.84
1:B:278:PHE:CD1	1:B:284:ILE:HD13	2.12	0.84
2:E:151:PHE:HD2	2:E:160:VAL:HG22	1.39	0.84
1:G:490:ILE:HG21	2:L:420:MET:HE2	1.58	0.84
1:W:289:ALA:HB2	1:W:419:PHE:HA	1.59	0.84
1:B:418:GLN:HG3	2:C:423:HIS:HB3	1.60	0.84
2:F:305:ALA:HB2	2:F:374:ARG:HD2	1.59	0.84
2:J:483:PHE:HB2	2:J:489:ILE:HD12	1.60	0.83
1:G:469:GLU:HB2	1:G:483:PHE:HE1	1.41	0.83
2:C:419:PHE:CD1	2:D:425:ILE:CD1	2.61	0.83
2:K:425:ILE:CD1	2:J:419:PHE:CD2	2.59	0.83
1:B:54:LEU:CD1	1:B:90:PHE:HE2	1.91	0.83
2:L:347:VAL:O	2:L:347:VAL:CG1	2.24	0.82
2:J:21:MET:SD	2:J:141:ARG:NE	2.51	0.82
2:E:432:TPO:O2P	2:D:318:GLU:OE2	1.96	0.82
2:E:442:TYR:CE2	2:F:456:PHE:CZ	2.67	0.82
1:V:419:PHE:CE2	1:W:425:ILE:HD13	2.13	0.82
2:E:287:THR:HG21	2:E:425:ILE:O	1.80	0.81
1:H:328:ALA:CB	1:H:335:PHE:CE1	2.63	0.81
1:H:278:PHE:CD1	1:H:284:ILE:HD12	2.14	0.81
2:I:91:GLY:C	2:I:92:TRP:HD1	1.84	0.81
2:U:52:LYS:N	5:U:702:ADP:O1A	2.13	0.81
1:X:285:LEU:HG	1:X:434:THR:HG21	1.62	0.81
1:H:231:MET:HE1	1:H:251:ALA:CB	2.11	0.81
1:N:52:LYS:NZ	3:N:702:ATP:O1B	2.11	0.81
2:I:415:THR:HB	2:J:432:TPO:O1P	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:395:PHE:CE2	2:I:399:VAL:HG21	2.15	0.81
2:E:442:TYR:HE2	2:F:456:PHE:CE2	1.98	0.80
2:C:415:THR:HB	2:D:432:TPO:O1P	1.80	0.80
2:K:425:ILE:HG22	2:K:426:THR:HG23	1.64	0.80
1:B:130:ILE:O	1:B:134:ILE:HG13	1.81	0.80
1:G:469:GLU:HB2	1:G:483:PHE:CE1	2.16	0.80
1:A:328:ALA:CB	1:A:335:PHE:CD1	2.64	0.80
1:H:328:ALA:HB2	1:H:335:PHE:CE1	2.17	0.79
2:I:337:GLU:O	2:I:341:GLN:HG3	1.81	0.79
1:S:389:ASN:O	1:S:393:ARG:HG2	1.82	0.79
2:E:285:LEU:HB2	2:E:434:THR:HG21	1.63	0.79
2:I:278:PHE:CE2	2:I:284:ILE:HG21	2.17	0.79
2:C:301:PHE:O	2:C:374:ARG:NH1	2.16	0.79
2:K:287:THR:HG21	2:K:425:ILE:O	1.83	0.79
2:Q:264:SER:O	2:Q:374:ARG:NH2	2.16	0.79
1:H:419:PHE:CD2	2:I:425:ILE:HD13	2.17	0.78
1:P:472:ILE:HG22	3:P:701:ATP:N3	1.98	0.78
1:A:195:GLY:O	2:F:193:ARG:NH2	2.16	0.78
1:V:419:PHE:CE2	1:W:425:ILE:HD12	2.18	0.78
2:K:292:THR:HG22	2:K:442:TYR:CE1	2.18	0.78
2:K:285:LEU:HB2	2:K:434:THR:HG21	1.63	0.78
2:L:305:ALA:HB2	2:L:374:ARG:HD3	1.64	0.78
1:H:231:MET:CE	1:H:251:ALA:CB	2.62	0.78
2:J:483:PHE:HB2	2:J:489:ILE:CD1	2.14	0.78
2:K:150:VAL:CG1	2:K:151:PHE:CE1	2.67	0.77
2:E:151:PHE:HE2	2:E:160:VAL:HG13	1.49	0.77
2:E:456:PHE:CZ	2:D:419:PHE:HD2	2.02	0.77
1:X:425:ILE:HD11	1:X:456:PHE:CE2	2.19	0.77
1:A:328:ALA:CB	1:A:335:PHE:HD1	1.97	0.77
2:K:334:ASP:O	2:K:336:GLU:N	2.17	0.77
2:L:265:SER:HB3	2:L:278:PHE:CE2	2.18	0.77
2:J:22:ARG:HH12	2:J:24:MET:CE	1.97	0.77
1:T:292:THR:O	1:T:451:ARG:HD3	1.84	0.77
1:T:386:GLY:HA2	2:U:390:ASN:HD21	1.48	0.77
2:E:425:ILE:HG22	2:E:426:THR:HG23	1.67	0.77
2:F:347:VAL:O	2:F:348:CYS:O	2.03	0.77
2:K:432:TPO:O2P	2:J:318:GLU:OE2	2.03	0.76
2:I:265:SER:CB	2:I:278:PHE:HE1	1.98	0.76
2:J:425:ILE:HG22	2:J:426:THR:HG23	1.66	0.76
2:D:54:LEU:HD13	2:D:90:PHE:CE2	2.21	0.76
2:D:289:ALA:HB2	2:D:419:PHE:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:419:PHE:HD1	2:J:420:MET:N	1.83	0.76
1:N:417:ASP:O	2:O:424:SER:HB3	1.85	0.76
1:P:430:ILE:HA	1:P:433:ILE:HD13	1.66	0.76
2:C:248:PRO:HB2	2:C:251:ALA:HB3	1.67	0.76
2:U:51:GLY:CA	5:U:702:ADP:O1A	2.34	0.76
2:E:305:ALA:HB2	2:E:374:ARG:HD2	1.67	0.76
2:F:167:LEU:O	2:F:171:LEU:HD12	1.84	0.76
1:A:419:PHE:CD1	1:B:425:ILE:HD12	2.20	0.76
2:K:250:GLY:C	2:K:252:MET:H	1.90	0.76
2:D:425:ILE:HG22	2:D:426:THR:HG23	1.67	0.76
1:G:247:PHE:CD1	1:G:360:LEU:HD13	2.19	0.76
1:R:423:HIS:CD2	2:Q:418:GLN:NE2	2.55	0.75
2:D:285:LEU:HB2	2:D:434:THR:HG21	1.67	0.75
1:G:488:ARG:HH11	1:G:488:ARG:HG2	1.49	0.75
2:K:150:VAL:CG1	2:K:151:PHE:CD1	2.69	0.75
1:A:488:ARG:HG2	1:A:488:ARG:HH11	1.51	0.75
2:E:234:GLU:HB2	2:D:214:GLU:HG2	1.68	0.75
1:H:215:ARG:HE	1:H:215:ARG:CA	2.00	0.75
2:I:248:PRO:HB2	2:I:251:ALA:HB3	1.69	0.75
2:J:289:ALA:HB2	2:J:419:PHE:HA	1.68	0.75
1:P:435:ASP:HA	1:P:459:ARG:HD2	1.68	0.75
2:U:89:SER:CB	5:U:702:ADP:N6	2.50	0.75
1:A:26:GLU:OE1	1:A:245:ASN:OD1	2.05	0.75
2:D:483:PHE:HB2	2:D:489:ILE:HD12	1.69	0.75
2:I:445:ILE:HD12	2:I:486:PHE:CE2	2.21	0.75
1:H:425:ILE:HG22	1:H:426:THR:HG23	1.69	0.75
2:I:303:GLU:HA	2:I:338:MET:CE	2.16	0.75
2:C:425:ILE:HG22	2:C:426:THR:HG23	1.69	0.74
1:R:280:LYS:O	1:R:409:THR:HB	1.85	0.74
1:R:425:ILE:HG22	1:R:426:THR:HG23	1.67	0.74
2:E:224:LYS:NZ	3:D:702:ATP:O3G	2.19	0.74
1:G:44:VAL:HG21	1:G:55:PHE:CE2	2.22	0.74
2:L:283:ILE:HD12	2:L:400:THR:HG23	1.67	0.74
2:I:425:ILE:HG22	2:I:426:THR:HG23	1.69	0.74
1:B:347:VAL:O	1:B:347:VAL:CG1	2.36	0.74
1:G:195:GLY:O	2:L:193:ARG:NH2	2.20	0.74
1:B:54:LEU:CD1	1:B:90:PHE:CE2	2.69	0.74
1:A:435:ASP:HA	1:A:459:ARG:HD2	1.69	0.74
2:U:289:ALA:HB2	2:U:419:PHE:HA	1.69	0.74
1:B:283:ILE:HG13	1:B:400:THR:HG22	1.70	0.73
2:E:429:HIS:HA	2:E:431:SEP:O1P	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:419:PHE:HE2	1:M:425:ILE:N	1.85	0.73
1:P:301:PHE:O	1:P:374:ARG:NH1	2.21	0.73
2:F:347:VAL:O	2:F:347:VAL:HG12	1.86	0.73
2:D:21:MET:SD	2:D:141:ARG:NE	2.61	0.73
1:B:262:ARG:NH1	1:B:461:SER:OG	2.22	0.73
1:A:313:ILE:HG21	1:A:315:PHE:CE2	2.23	0.73
2:C:54:LEU:HD13	2:C:90:PHE:CE2	2.24	0.73
1:B:425:ILE:HG22	1:B:426:THR:HG23	1.70	0.72
2:L:142:VAL:HB	2:L:178:THR:HG22	1.71	0.72
2:I:265:SER:CB	2:I:278:PHE:CE1	2.72	0.72
1:B:285:LEU:HB2	1:B:434:THR:HG21	1.71	0.72
1:H:215:ARG:HA	1:H:215:ARG:NE	2.04	0.72
1:X:75:THR:HA	1:X:145:ASP:O	1.90	0.71
1:A:315:PHE:CD1	1:A:363:ILE:HG12	2.25	0.71
2:C:283:ILE:HG13	2:C:400:THR:HG23	1.70	0.71
2:Q:378:ASP:HA	2:Q:413:THR:HG1	1.54	0.71
2:D:57:ILE:HD11	2:D:83:ILE:HG23	1.71	0.71
2:D:234:GLU:C	2:D:235:TYR:HD2	1.93	0.71
1:B:348:CYS:HB3	2:C:254:LEU:HB3	1.73	0.71
2:O:455:VAL:O	2:O:456:PHE:HB2	1.91	0.71
2:J:289:ALA:CB	2:J:419:PHE:HA	2.20	0.71
1:W:432:THR:O	1:W:459:ARG:NH2	2.23	0.71
2:K:150:VAL:HG13	2:K:151:PHE:CD1	2.26	0.71
1:G:193:ARG:CD	1:G:194:TYR:HE1	2.04	0.71
2:D:235:TYR:HD2	2:D:235:TYR:N	1.89	0.71
2:I:90:PHE:O	2:I:92:TRP:NE1	2.24	0.70
2:K:54:LEU:HD13	2:K:90:PHE:CE1	2.26	0.70
2:D:289:ALA:CB	2:D:419:PHE:HA	2.22	0.70
1:H:285:LEU:HB2	1:H:434:THR:HG21	1.73	0.70
1:V:305:ALA:HB2	1:V:374:ARG:HD3	1.73	0.70
1:A:313:ILE:CG2	1:A:315:PHE:HE2	2.03	0.70
2:D:142:VAL:HB	2:D:178:THR:HG22	1.73	0.70
1:G:160:VAL:HG21	1:G:194:TYR:CD2	2.26	0.70
1:S:425:ILE:HG22	1:S:426:THR:HG23	1.71	0.70
1:H:208:ARG:NH2	1:H:221:GLU:OE2	2.25	0.69
2:K:429:HIS:HA	2:K:431:SEP:O1P	1.91	0.69
2:L:16:GLN:O	2:L:17:ALA:O	2.10	0.69
1:G:435:ASP:HA	1:G:459:ARG:HD2	1.74	0.69
1:H:419:PHE:HD2	2:I:425:ILE:HD13	1.57	0.69
2:L:66:GLU:C	2:L:67:PHE:HD1	1.95	0.69
2:I:305:ALA:HB2	2:I:374:ARG:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:303:GLU:HA	2:C:338:MET:CE	2.21	0.69
2:J:285:LEU:HB2	2:J:434:THR:HG21	1.74	0.69
1:W:289:ALA:CB	1:W:419:PHE:HA	2.22	0.69
1:A:350:TYR:HE1	1:B:397:ILE:HG23	1.58	0.69
2:D:38:ILE:HA	2:D:177:THR:HG23	1.74	0.69
2:J:57:ILE:HD11	2:J:83:ILE:HG23	1.73	0.69
2:F:347:VAL:O	2:F:347:VAL:CG1	2.40	0.69
2:J:142:VAL:HB	2:J:178:THR:HG22	1.74	0.69
1:T:294:LYS:HE3	1:T:415:THR:HA	1.74	0.69
1:A:313:ILE:HG22	1:A:315:PHE:CE2	2.28	0.69
3:O:702:ATP:O1G	1:P:226:ARG:NH2	2.26	0.69
3:C:702:ATP:O1G	2:D:226:ARG:NH2	2.26	0.69
2:F:16:GLN:O	2:F:17:ALA:O	2.10	0.68
2:Q:315:PHE:CE1	2:Q:375:ILE:HD11	2.28	0.68
2:I:283:ILE:HG13	2:I:400:THR:HG23	1.74	0.68
1:B:215:ARG:HE	1:B:215:ARG:HA	1.58	0.68
2:J:419:PHE:HD1	2:J:419:PHE:C	1.96	0.68
2:C:21:MET:SD	2:C:141:ARG:NE	2.65	0.68
1:G:292:THR:HG22	1:G:442:TYR:CE1	2.29	0.68
1:G:52:LYS:HD3	3:G:702:ATP:O2B	1.94	0.68
2:K:234:GLU:HB2	2:J:214:GLU:HG2	1.76	0.68
1:N:52:LYS:HD2	1:N:181:THR:CG2	2.24	0.68
1:G:483:PHE:HB2	1:G:489:ILE:HD12	1.74	0.68
1:A:315:PHE:CE1	1:A:363:ILE:HG12	2.28	0.68
2:O:418:GLN:HG3	2:O:422:ALA:HA	1.76	0.68
1:R:289:ALA:HB2	1:R:419:PHE:HA	1.76	0.68
2:F:283:ILE:CD1	2:F:400:THR:HG23	2.25	0.67
2:L:75:THR:C	2:L:76:PHE:HD1	1.98	0.67
1:N:417:ASP:O	2:O:424:SER:CB	2.42	0.67
2:F:20:LYS:HE3	2:F:228:THR:HG21	1.77	0.67
1:G:456:PHE:CE2	2:L:442:TYR:CE1	2.83	0.67
2:L:171:LEU:HD13	2:L:178:THR:HG21	1.75	0.67
2:F:425:ILE:HG22	2:F:426:THR:HG23	1.77	0.67
2:D:191:ILE:HD12	2:D:198:GLU:OE2	1.95	0.67
1:N:301:PHE:O	1:N:374:ARG:NH1	2.27	0.67
2:U:419:PHE:CD2	1:V:425:ILE:CD1	2.77	0.67
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.26	0.67
2:F:21:MET:SD	2:F:141:ARG:NE	2.68	0.67
1:N:285:LEU:HD22	1:N:434:THR:HG21	1.77	0.67
2:E:456:PHE:CE1	2:D:419:PHE:HD2	2.13	0.67
2:I:285:LEU:HB2	2:I:434:THR:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:490:ILE:HD11	2:D:449:MET:HE3	1.77	0.66
2:F:321:ARG:NH2	2:F:339:GLU:OE2	2.27	0.66
2:D:251:ALA:O	2:D:253:ARG:N	2.29	0.66
1:N:294:LYS:HB3	1:N:413:THR:HB	1.76	0.66
1:B:305:ALA:HB2	1:B:374:ARG:HD3	1.76	0.66
2:D:235:TYR:N	2:D:235:TYR:CD2	2.61	0.66
2:D:317:TYR:CE1	2:D:383:LEU:HD21	2.30	0.66
2:J:256:GLN:HG3	2:J:404:LYS:HB3	1.77	0.66
1:B:66:GLU:HG2	1:B:67:PHE:HE2	1.60	0.66
2:C:285:LEU:HB2	2:C:434:THR:HG21	1.78	0.66
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.25	0.66
2:L:425:ILE:HG22	2:L:426:THR:HG23	1.78	0.66
1:R:464:ASP:OD2	1:R:468:ARG:NH1	2.29	0.66
1:G:292:THR:CG2	1:G:442:TYR:CE1	2.79	0.66
1:A:285:LEU:HB2	1:A:434:THR:HG21	1.76	0.66
2:K:326:ARG:NH1	2:L:279:PHE:CD2	2.63	0.66
1:A:33:HIS:ND1	1:A:230:HIS:HA	2.10	0.66
1:A:469:GLU:HB2	1:A:483:PHE:CE1	2.31	0.66
1:G:193:ARG:HD2	1:G:194:TYR:CE1	2.25	0.66
1:G:33:HIS:ND1	1:G:230:HIS:HA	2.11	0.65
2:L:287:THR:HG22	2:L:414:ASN:HB3	1.77	0.65
3:C:702:ATP:O2G	2:D:224:LYS:NZ	2.24	0.65
1:G:52:LYS:NZ	3:G:702:ATP:O2G	2.27	0.65
1:V:42:THR:O	1:V:180:MET:CB	2.44	0.65
1:G:224:LYS:NZ	3:L:702:ATP:O3G	2.28	0.65
2:L:20:LYS:HE3	2:L:228:THR:HG21	1.78	0.65
1:B:215:ARG:HA	1:B:215:ARG:NE	2.11	0.65
2:C:303:GLU:HA	2:C:338:MET:HE1	1.79	0.65
2:L:21:MET:SD	2:L:141:ARG:NE	2.70	0.65
1:T:54:LEU:O	1:T:58:GLN:NE2	2.30	0.65
1:V:419:PHE:CG	1:W:425:ILE:CD1	2.79	0.65
2:D:486:PHE:HB2	2:D:489:ILE:HD11	1.80	0.64
1:P:294:LYS:NZ	1:P:415:THR:OG1	2.27	0.64
2:C:31:ILE:HD11	2:C:246:ILE:HG21	1.79	0.64
2:D:317:TYR:CD1	2:D:383:LEU:HD21	2.33	0.64
1:W:385:ARG:NH1	1:W:417:ASP:OD1	2.30	0.64
1:H:160:VAL:HG11	1:H:194:TYR:HD1	1.63	0.64
1:G:456:PHE:HE2	2:L:442:TYR:CE1	2.15	0.64
1:H:348:CYS:HB3	2:I:254:LEU:HB3	1.77	0.64
2:K:490:ILE:HD11	2:J:449:MET:HE3	1.80	0.64
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:289:ALA:CB	1:G:419:PHE:HA	2.28	0.64
2:I:264:SER:O	2:I:374:ARG:NH2	2.25	0.64
2:J:38:ILE:HA	2:J:177:THR:HG23	1.80	0.64
2:E:254:LEU:HD23	2:D:350:TYR:CE2	2.33	0.64
3:I:702:ATP:O2G	2:J:226:ARG:NH2	2.31	0.64
1:N:49:GLY:O	1:N:218:ARG:NH2	2.31	0.64
2:F:54:LEU:HD13	2:F:90:PHE:CE2	2.32	0.64
2:J:22:ARG:HH12	2:J:24:MET:HE3	1.62	0.64
2:L:74:VAL:HG12	2:L:76:PHE:HE1	1.62	0.63
2:U:316:ALA:O	2:U:348:CYS:HA	1.97	0.63
2:K:38:ILE:HA	2:K:177:THR:HG23	1.80	0.63
2:U:51:GLY:HA2	5:U:702:ADP:O1A	1.99	0.63
2:E:469:GLU:HB2	2:E:483:PHE:CZ	2.33	0.63
2:K:469:GLU:HB2	2:K:483:PHE:CZ	2.34	0.63
2:L:142:VAL:HB	2:L:178:THR:CG2	2.28	0.63
1:B:419:PHE:CD1	2:C:425:ILE:CD1	2.81	0.63
1:B:23:THR:HG21	1:B:28:PHE:CD2	2.34	0.63
2:J:21:MET:SD	2:J:141:ARG:CZ	2.87	0.63
2:Q:289:ALA:CB	2:Q:419:PHE:HA	2.29	0.63
1:A:350:TYR:CE1	1:B:397:ILE:HG23	2.33	0.63
2:E:397:ILE:HG23	2:D:350:TYR:CE1	2.33	0.63
2:D:287:THR:HG21	2:D:425:ILE:O	1.99	0.63
2:J:21:MET:HE3	2:J:177:THR:HG21	1.79	0.63
1:V:289:ALA:CB	1:V:419:PHE:HA	2.29	0.63
2:F:171:LEU:HD22	2:F:178:THR:HG21	1.81	0.63
1:V:289:ALA:HB2	1:V:419:PHE:HA	1.80	0.63
1:A:54:LEU:HD13	1:A:90:PHE:CE2	2.33	0.62
2:L:278:PHE:HD1	2:L:284:ILE:HG13	1.63	0.62
1:A:160:VAL:HG11	1:A:194:TYR:HD2	1.63	0.62
2:E:250:GLY:C	2:E:252:MET:H	2.02	0.62
1:G:44:VAL:HG21	1:G:55:PHE:HE2	1.62	0.62
1:G:263:VAL:HG12	1:G:374:ARG:NH2	2.13	0.62
2:K:292:THR:CG2	2:K:442:TYR:CE1	2.82	0.62
1:A:52:LYS:NZ	3:A:702:ATP:O1G	2.27	0.62
2:J:419:PHE:CD1	2:J:420:MET:N	2.65	0.62
2:C:335:PHE:HA	2:C:338:MET:SD	2.40	0.62
1:H:393:ARG:NH1	1:H:428:SER:O	2.31	0.62
2:L:21:MET:HE3	2:L:177:THR:HG21	1.79	0.62
2:J:50:THR:HG22	2:J:209:ASN:HB2	1.82	0.62
2:F:451:ARG:HB3	2:F:470:PHE:CE1	2.34	0.62
2:C:90:PHE:HB2	2:C:92:TRP:CD1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:287:THR:HG23	2:O:414:ASN:HD22	1.64	0.62
1:W:385:ARG:HH12	1:W:417:ASP:CG	2.02	0.62
1:P:291:GLY:O	1:P:451:ARG:NH1	2.32	0.62
2:K:287:THR:HG23	2:K:414:ASN:HD22	1.65	0.62
2:L:278:PHE:CD1	2:L:284:ILE:HG13	2.34	0.62
1:X:31:ILE:HA	1:X:231:MET:HG3	1.82	0.62
1:G:289:ALA:HB2	1:G:419:PHE:HA	1.81	0.62
2:J:419:PHE:C	2:J:419:PHE:CD1	2.72	0.62
1:X:127:ILE:HD11	1:X:167:LEU:HA	1.82	0.62
2:F:287:THR:HG22	2:F:414:ASN:HB3	1.81	0.62
1:H:305:ALA:HB2	1:H:374:ARG:HD2	1.81	0.62
1:X:382:ALA:O	1:X:385:ARG:HG2	2.00	0.62
1:W:397:ILE:CD1	1:W:433:ILE:HD13	2.30	0.62
2:K:441:GLN:HE22	2:K:490:ILE:HD13	1.65	0.61
1:T:294:LYS:HD3	1:T:414:ASN:O	1.99	0.61
1:V:419:PHE:CG	1:W:425:ILE:HD11	2.34	0.61
2:D:234:GLU:C	2:D:235:TYR:CD2	2.73	0.61
3:K:701:ATP:O3G	2:L:457:LYS:NZ	2.33	0.61
2:L:66:GLU:C	2:L:67:PHE:CD1	2.73	0.61
1:A:247:PHE:CD1	1:A:360:LEU:HD13	2.35	0.61
2:D:50:THR:HG22	2:D:209:ASN:HB2	1.83	0.61
2:L:161:ARG:HG3	2:L:196:VAL:CG1	2.30	0.61
2:J:287:THR:HG21	2:J:425:ILE:O	2.00	0.61
1:A:328:ALA:HB1	1:A:335:PHE:CD1	2.35	0.61
1:B:23:THR:HG1	1:B:25:ILE:HG13	1.64	0.61
2:K:155:ASP:O	2:K:156:ALA:O	2.17	0.61
1:G:193:ARG:CD	1:G:194:TYR:CE1	2.83	0.61
2:K:445:ILE:HD12	2:K:486:PHE:CE1	2.36	0.61
2:U:289:ALA:CB	2:U:419:PHE:HA	2.31	0.61
2:C:31:ILE:HG22	2:C:222:ILE:HD12	1.82	0.61
1:G:285:LEU:HB2	1:G:434:THR:HG21	1.82	0.61
1:H:250:GLY:O	1:H:251:ALA:HB2	2.00	0.61
2:K:249:LEU:HD11	2:K:394:GLN:HE21	1.62	0.61
2:L:278:PHE:HE1	2:L:284:ILE:HG21	1.65	0.61
2:L:161:ARG:HD2	2:L:196:VAL:HG11	1.81	0.61
3:P:702:ATP:O2G	2:Q:224:LYS:NZ	2.33	0.61
2:E:441:GLN:HE22	2:E:490:ILE:HD13	1.66	0.60
2:F:89:SER:OG	3:F:702:ATP:N6	2.29	0.60
1:A:483:PHE:HB2	1:A:489:ILE:CD1	2.31	0.60
2:C:356:LEU:HD21	2:C:387:VAL:HG11	1.83	0.60
2:J:110:PRO:O	2:J:111:ASP:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:264:SER:O	1:P:374:ARG:NH2	2.34	0.60
1:A:328:ALA:HB2	1:A:335:PHE:CE1	2.36	0.60
1:B:315:PHE:HE2	1:B:375:ILE:HD11	1.65	0.60
1:A:417:ASP:OD2	1:B:429:HIS:ND1	2.35	0.60
1:H:385:ARG:HD3	2:I:393:ARG:HH21	1.66	0.60
1:H:400:THR:HG21	1:H:433:ILE:CG2	2.31	0.60
1:R:111:ASP:O	1:R:113:GLU:N	2.34	0.60
2:F:289:ALA:HB2	2:F:419:PHE:HA	1.84	0.60
2:F:445:ILE:CD1	2:F:486:PHE:CE1	2.85	0.60
1:A:328:ALA:CB	1:A:335:PHE:CE1	2.85	0.60
1:B:66:GLU:HG2	1:B:67:PHE:CE2	2.37	0.60
1:G:247:PHE:HD1	1:G:360:LEU:HD13	1.66	0.60
1:H:263:VAL:HG12	1:H:374:ARG:NH2	2.17	0.60
2:U:89:SER:CB	5:U:702:ADP:HN61	2.15	0.59
1:A:269:ARG:HB3	1:A:479:ILE:HD12	1.84	0.59
1:A:335:PHE:HD2	1:A:344:LEU:HD11	1.67	0.59
2:E:151:PHE:CE2	2:E:160:VAL:HG13	2.35	0.59
2:U:51:GLY:C	5:U:702:ADP:O1A	2.40	0.59
1:B:278:PHE:CD1	1:B:284:ILE:CD1	2.84	0.59
2:F:445:ILE:HD12	2:F:486:PHE:CE1	2.37	0.59
2:C:121:PHE:C	2:C:122:ASP:O	2.39	0.59
1:H:130:ILE:O	1:H:134:ILE:HG12	2.01	0.59
2:L:445:ILE:HD12	2:L:486:PHE:CE1	2.36	0.59
2:I:294:LYS:HE2	3:I:701:ATP:O1B	2.02	0.59
1:A:350:TYR:CE1	1:B:397:ILE:CG2	2.85	0.59
2:L:21:MET:HE3	2:L:177:THR:CG2	2.32	0.59
2:I:21:MET:HE1	2:I:177:THR:HB	1.83	0.59
2:J:486:PHE:HB2	2:J:489:ILE:HD11	1.84	0.59
2:D:256:GLN:HG2	2:D:404:LYS:HB3	1.85	0.59
1:M:70:PRO:HG3	1:M:138:ARG:O	2.03	0.59
1:A:417:ASP:OD2	1:B:429:HIS:CG	2.56	0.59
2:F:142:VAL:HB	2:F:178:THR:CG2	2.33	0.59
2:C:31:ILE:CD1	2:C:246:ILE:HG21	2.33	0.59
2:D:483:PHE:CB	2:D:489:ILE:CD1	2.81	0.59
1:T:419:PHE:CD2	2:U:423:HIS:O	2.56	0.59
1:G:269:ARG:HB3	1:G:479:ILE:HD12	1.85	0.59
1:G:350:TYR:CE2	1:H:254:LEU:HG	2.38	0.59
2:J:21:MET:HE1	2:J:177:THR:OG1	2.03	0.59
1:N:289:ALA:HB2	1:N:419:PHE:HA	1.85	0.59
1:P:433:ILE:N	1:P:433:ILE:HD12	2.17	0.59
2:Q:434:THR:OG1	2:Q:437:ILE:HD11	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:247:PHE:N	2:U:248:PRO:HD3	2.17	0.59
1:V:425:ILE:HG22	1:V:426:THR:HG23	1.83	0.59
2:K:150:VAL:HG12	2:K:151:PHE:CD1	2.36	0.58
2:F:401:GLY:O	2:F:405:GLN:HG2	2.03	0.58
2:L:21:MET:CE	2:L:177:THR:HG22	2.33	0.58
2:I:335:PHE:HA	2:I:338:MET:SD	2.42	0.58
1:W:397:ILE:HD11	1:W:433:ILE:HD13	1.85	0.58
2:C:121:PHE:O	2:C:125:ALA:CB	2.46	0.58
1:X:423:HIS:O	1:W:418:GLN:HA	2.04	0.58
1:S:291:GLY:O	1:S:451:ARG:NH2	2.36	0.58
1:W:71:GLY:HA2	1:W:141:ARG:O	2.03	0.58
2:I:395:PHE:C	2:I:395:PHE:CD2	2.75	0.58
1:G:490:ILE:HG21	2:L:420:MET:CE	2.30	0.58
2:J:419:PHE:CE1	2:J:420:MET:HB2	2.39	0.58
1:N:294:LYS:HB3	1:N:413:THR:CG2	2.34	0.58
1:R:320:SER:HA	1:M:254:LEU:HD23	1.85	0.58
1:X:230:HIS:NE2	3:W:702:ATP:O2'	2.37	0.58
2:D:115:GLN:O	2:D:117:VAL:N	2.36	0.58
1:G:425:ILE:HG22	1:G:426:THR:HG23	1.86	0.58
2:K:356:LEU:HD22	2:K:387:VAL:HG11	1.84	0.58
2:L:328:ALA:HB2	2:L:335:PHE:CE1	2.37	0.58
1:A:253:ARG:O	1:A:256:GLN:HG2	2.03	0.58
1:H:313:ILE:CG2	1:H:315:PHE:CE1	2.87	0.58
1:X:429:HIS:CG	1:W:385:ARG:NH1	2.71	0.58
1:A:313:ILE:HB	1:A:315:PHE:HE2	1.69	0.58
1:A:425:ILE:HG22	1:A:426:THR:HG23	1.86	0.58
1:G:186:GLU:OE2	1:G:189:GLY:N	2.36	0.58
1:H:23:THR:HG21	1:H:28:PHE:CD2	2.39	0.58
2:J:254:LEU:HA	2:J:256:GLN:OE1	2.04	0.58
1:H:328:ALA:CB	1:H:335:PHE:HE1	2.02	0.57
2:J:22:ARG:NH1	2:J:24:MET:CE	2.66	0.57
2:E:356:LEU:HD22	2:E:387:VAL:HG11	1.85	0.57
2:F:66:GLU:O	2:F:67:PHE:HD1	1.87	0.57
1:H:347:VAL:O	1:H:347:VAL:CG1	2.42	0.57
2:C:377:ILE:HD12	2:C:412:PHE:CE1	2.39	0.57
1:G:44:VAL:HG21	1:G:55:PHE:CD2	2.39	0.57
1:A:289:ALA:CB	1:A:419:PHE:HA	2.34	0.57
1:B:23:THR:OG1	1:B:25:ILE:CG1	2.46	0.57
2:E:441:GLN:NE2	2:E:490:ILE:HD13	2.19	0.57
1:H:313:ILE:HD12	1:H:372:PRO:HG3	1.86	0.57
1:B:313:ILE:HD12	1:B:372:PRO:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:328:ALA:CB	1:H:335:PHE:CD1	2.87	0.57
1:T:386:GLY:CA	2:U:390:ASN:HD21	2.17	0.57
2:U:356:LEU:HD11	2:U:387:VAL:HG21	1.86	0.57
2:F:265:SER:HB3	2:F:278:PHE:CE2	2.39	0.57
2:C:419:PHE:CE1	2:D:425:ILE:CD1	2.87	0.57
2:E:490:ILE:HD11	2:D:449:MET:CE	2.33	0.57
2:I:463:HIS:O	2:I:465:LYS:HE2	2.04	0.57
2:J:21:MET:CE	2:J:177:THR:OG1	2.53	0.57
2:U:419:PHE:CD2	1:V:425:ILE:HD13	2.39	0.57
1:G:419:PHE:CD2	1:H:425:ILE:HD12	2.40	0.57
2:K:441:GLN:NE2	2:K:490:ILE:HD13	2.20	0.57
1:X:273:MET:SD	1:X:468:ARG:HD2	2.45	0.57
1:S:31:ILE:HA	1:S:231:MET:HG3	1.87	0.57
2:D:75:THR:OG1	2:D:78:GLU:O	2.14	0.57
2:J:262:ARG:NH2	2:J:461:SER:HB2	2.20	0.57
2:D:262:ARG:HH22	2:D:461:SER:HB2	1.70	0.56
1:H:23:THR:OG1	1:H:25:ILE:CG1	2.44	0.56
2:E:404:LYS:NZ	2:D:323:GLN:OE1	2.38	0.56
1:H:287:THR:HG21	1:H:425:ILE:O	2.05	0.56
2:I:46:GLY:O	2:I:52:LYS:HE3	2.04	0.56
1:R:431:SEP:HB2	2:Q:290:THR:HG21	1.85	0.56
1:B:90:PHE:HE1	3:B:702:ATP:C5	2.23	0.56
2:E:287:THR:HG23	2:E:414:ASN:HD22	1.71	0.56
2:K:58:GLN:HG3	2:K:92:TRP:CH2	2.40	0.56
2:E:456:PHE:CE1	2:D:419:PHE:CD2	2.94	0.56
2:D:262:ARG:NH2	2:D:461:SER:HB2	2.20	0.56
2:J:20:LYS:HE3	2:J:228:THR:HG21	1.87	0.56
2:J:262:ARG:HH22	2:J:461:SER:HB2	1.71	0.56
1:B:90:PHE:HD2	1:B:92:TRP:CZ3	2.23	0.56
2:F:485:ASN:O	2:F:486:PHE:CD2	2.59	0.56
2:D:42:THR:HA	2:D:203:ASN:HB2	1.87	0.56
2:L:289:ALA:HB2	2:L:419:PHE:HA	1.88	0.56
1:A:305:ALA:HB2	1:A:374:ARG:NE	2.20	0.56
2:K:404:LYS:NZ	2:J:323:GLN:OE1	2.38	0.56
2:I:90:PHE:HE1	3:I:702:ATP:N7	2.03	0.56
1:N:449:MET:HE3	2:O:467:ILE:HD11	1.88	0.56
1:A:54:LEU:HD13	1:A:90:PHE:HE2	1.71	0.56
1:B:441:GLN:HE22	1:B:490:ILE:HD12	1.71	0.56
2:F:142:VAL:HB	2:F:178:THR:HG23	1.87	0.56
1:G:469:GLU:CB	1:G:483:PHE:HE1	2.17	0.56
1:G:193:ARG:HB3	1:G:194:TYR:HD1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:GLU:OE1	1:G:352:GLU:N	2.37	0.56
1:S:52:LYS:HG2	1:S:181:THR:HG23	1.87	0.56
2:C:121:PHE:O	2:C:122:ASP:O	2.24	0.56
2:D:110:PRO:O	2:D:111:ASP:O	2.24	0.56
1:A:289:ALA:HB2	1:A:419:PHE:HA	1.87	0.55
2:C:61:TYR:CE2	2:C:92:TRP:CE3	2.94	0.55
1:G:353:SER:HA	1:H:250:GLY:HA3	1.88	0.55
1:H:183:GLU:HB3	2:I:199:PHE:CE1	2.41	0.55
1:T:335:PHE:O	1:T:339:GLU:CB	2.55	0.55
1:A:435:ASP:CG	2:F:323:GLN:HE22	2.09	0.55
2:F:382:ALA:O	2:F:385:ARG:HG2	2.05	0.55
2:C:379:SER:CB	2:C:413:THR:OG1	2.54	0.55
2:Q:269:ARG:HG2	2:Q:479:ILE:HB	1.87	0.55
1:S:344:LEU:HD13	1:S:345:LYS:N	2.21	0.55
1:G:483:PHE:CB	1:G:489:ILE:CD1	2.84	0.55
1:X:215:ARG:NH2	1:S:233:GLY:HA3	2.22	0.55
2:C:90:PHE:HB2	2:C:92:TRP:NE1	2.21	0.55
2:L:401:GLY:O	2:L:405:GLN:HG2	2.06	0.55
2:U:215:ARG:NH2	1:V:234:GLU:O	2.40	0.55
1:A:247:PHE:CE1	1:A:360:LEU:HD13	2.42	0.55
1:G:247:PHE:CE1	1:G:360:LEU:HD13	2.40	0.55
1:G:435:ASP:CG	2:L:323:GLN:HE22	2.09	0.55
2:K:305:ALA:HB2	2:K:374:ARG:HD2	1.88	0.55
2:E:334:ASP:O	2:E:336:GLU:N	2.40	0.55
2:F:265:SER:CB	2:F:278:PHE:CE2	2.89	0.55
1:G:483:PHE:HB2	1:G:489:ILE:CD1	2.37	0.55
2:K:425:ILE:HD13	2:J:419:PHE:CE2	2.42	0.55
2:K:425:ILE:HD11	2:J:419:PHE:CD2	2.41	0.55
2:J:107:ASP:OD1	2:J:109:SER:OG	2.24	0.55
1:A:443:VAL:HG11	1:A:483:PHE:CE2	2.42	0.55
2:L:21:MET:CE	2:L:177:THR:CG2	2.84	0.55
2:L:21:MET:HE1	2:L:177:THR:HG22	1.87	0.55
2:L:315:PHE:CD2	2:L:363:ILE:HG12	2.41	0.55
2:J:382:ALA:O	2:J:385:ARG:HB2	2.07	0.55
2:U:419:PHE:CG	1:V:425:ILE:CD1	2.90	0.55
1:X:419:PHE:CE2	1:S:425:ILE:CD1	2.90	0.55
1:X:419:PHE:CD2	1:S:425:ILE:HD13	2.42	0.55
1:V:419:PHE:HE2	1:W:424:SER:C	2.10	0.55
1:B:287:THR:HG21	1:B:425:ILE:O	2.06	0.55
2:E:301:PHE:O	2:E:374:ARG:NH2	2.39	0.55
2:I:90:PHE:O	2:I:92:TRP:CD1	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:289:ALA:HB2	1:M:419:PHE:HA	1.89	0.55
1:P:472:ILE:HG22	3:P:701:ATP:C4	2.42	0.55
1:X:429:HIS:CD2	1:W:385:ARG:HH11	2.25	0.55
2:I:298:VAL:HG21	2:I:413:THR:CG2	2.37	0.55
2:I:364:LYS:O	2:I:368:ASN:OD1	2.25	0.55
2:J:52:LYS:NZ	3:J:702:ATP:O3G	2.40	0.55
2:K:356:LEU:CD2	2:K:387:VAL:HG11	2.37	0.55
2:K:490:ILE:HD11	2:J:449:MET:CE	2.37	0.55
1:T:264:SER:O	1:T:374:ARG:NH2	2.38	0.55
1:B:363:ILE:O	1:B:367:ILE:HG13	2.07	0.54
1:G:193:ARG:HB3	1:G:194:TYR:CD1	2.42	0.54
2:J:75:THR:OG1	2:J:78:GLU:O	2.17	0.54
2:E:58:GLN:HG3	2:E:92:TRP:CH2	2.41	0.54
2:D:31:ILE:CD1	2:D:246:ILE:HG21	2.37	0.54
1:G:300:ARG:HG3	1:G:333:MET:HE3	1.89	0.54
1:H:353:SER:HA	2:I:250:GLY:HA3	1.89	0.54
2:I:90:PHE:CE1	3:I:702:ATP:N7	2.75	0.54
2:I:356:LEU:HD21	2:I:387:VAL:HG11	1.89	0.54
1:X:40:ARG:NH1	1:X:226:ARG:O	2.40	0.54
2:C:298:VAL:HG21	2:C:413:THR:CG2	2.37	0.54
2:L:283:ILE:CD1	2:L:400:THR:HG23	2.36	0.54
1:T:384:ALA:HB2	1:T:392:PHE:CD1	2.42	0.54
1:A:186:GLU:OE2	1:A:189:GLY:N	2.40	0.54
1:A:315:PHE:CE1	1:A:363:ILE:HG23	2.42	0.54
2:C:248:PRO:CB	2:C:251:ALA:HB3	2.35	0.54
2:D:20:LYS:HE3	2:D:228:THR:HG21	1.90	0.54
1:H:262:ARG:HH12	1:H:461:SER:CB	2.20	0.54
2:C:419:PHE:CE1	2:D:425:ILE:HD13	2.40	0.54
1:G:417:ASP:OD2	1:H:429:HIS:ND1	2.41	0.54
2:I:265:SER:HB2	2:I:278:PHE:HE1	1.73	0.54
1:A:313:ILE:CB	1:A:315:PHE:HE2	2.21	0.54
1:H:52:LYS:HD2	1:H:181:THR:HG23	1.90	0.54
2:J:316:ALA:O	2:J:348:CYS:HA	2.07	0.54
1:X:419:PHE:CE2	1:S:425:ILE:HD13	2.43	0.54
2:F:432:TPO:HG21	2:F:432:TPO:O3P	2.08	0.54
1:G:328:ALA:HB2	1:G:335:PHE:CE1	2.43	0.54
1:G:440:LEU:HD23	1:G:453:ILE:HD12	1.89	0.54
2:J:24:MET:SD	2:J:67:PHE:HE2	2.30	0.54
1:A:315:PHE:HE1	1:A:363:ILE:HA	1.73	0.54
1:A:353:SER:HA	1:B:250:GLY:HA3	1.90	0.54
2:L:315:PHE:CE2	2:L:363:ILE:HG12	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:392:PHE:O	1:T:396:VAL:HG23	2.08	0.54
2:D:31:ILE:HD11	2:D:246:ILE:HG21	1.90	0.53
1:X:448:GLU:HA	1:S:466:ALA:HA	1.90	0.53
1:A:57:ILE:HD11	1:A:83:ILE:HG23	1.91	0.53
1:H:419:PHE:CD2	2:I:425:ILE:HD12	2.41	0.53
2:K:377:ILE:HD12	2:K:412:PHE:CE2	2.44	0.53
2:O:31:ILE:HG22	2:O:222:ILE:HD12	1.89	0.53
1:P:472:ILE:HG21	3:P:701:ATP:C1'	2.39	0.53
2:D:400:THR:HG21	2:D:433:ILE:HG23	1.90	0.53
2:E:356:LEU:CD2	2:E:387:VAL:HG11	2.38	0.53
2:D:316:ALA:O	2:D:348:CYS:HA	2.08	0.53
1:G:306:CYS:HB2	1:G:338:MET:SD	2.48	0.53
1:G:395:PHE:O	1:G:399:VAL:HG23	2.08	0.53
2:J:42:THR:HA	2:J:203:ASN:HB2	1.90	0.53
1:S:311:ARG:NH1	1:S:370:PHE:O	2.42	0.53
1:B:419:PHE:CD1	2:C:425:ILE:HD13	2.44	0.53
2:C:380:LEU:HD21	2:C:412:PHE:HD1	1.73	0.53
1:P:22:ARG:O	1:P:141:ARG:NH2	2.41	0.53
1:B:231:MET:HE1	1:B:250:GLY:O	2.09	0.53
2:D:462:TRP:O	2:D:463:HIS:CD2	2.62	0.53
3:H:701:ATP:O3G	2:I:457:LYS:NZ	2.41	0.53
1:P:215:ARG:NH2	2:Q:234:GLU:O	2.42	0.53
2:Q:287:THR:HG21	2:Q:425:ILE:O	2.09	0.53
2:E:219:THR:HB	2:E:234:GLU:HB3	1.91	0.53
2:L:74:VAL:CG1	2:L:76:PHE:HE1	2.21	0.53
2:O:433:ILE:HD12	2:O:433:ILE:N	2.23	0.53
1:M:298:VAL:O	1:M:302:VAL:HG23	2.08	0.53
2:C:379:SER:HB3	2:C:413:THR:OG1	2.08	0.53
1:G:194:TYR:CD1	1:G:194:TYR:N	2.77	0.53
1:G:443:VAL:HG11	1:G:483:PHE:CE2	2.44	0.53
2:I:74:VAL:HG12	2:I:76:PHE:HE1	1.74	0.53
1:T:292:THR:HA	1:T:451:ARG:HD3	1.91	0.53
2:I:379:SER:CB	2:I:413:THR:OG1	2.57	0.53
1:A:395:PHE:O	1:A:399:VAL:HG23	2.09	0.53
2:K:219:THR:HB	2:K:234:GLU:HB3	1.91	0.53
1:V:124:SER:HA	1:V:127:ILE:HD13	1.91	0.53
1:A:440:LEU:HD23	1:A:453:ILE:HD12	1.90	0.52
1:B:52:LYS:HD2	1:B:181:THR:HG23	1.91	0.52
2:E:397:ILE:HG23	2:D:350:TYR:HE1	1.74	0.52
2:F:300:ARG:HA	2:F:333:MET:HE1	1.90	0.52
2:C:441:GLN:HE22	2:C:490:ILE:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:TYR:HD1	1:G:194:TYR:N	2.07	0.52
1:H:363:ILE:O	1:H:367:ILE:HG13	2.09	0.52
1:P:289:ALA:HB2	1:P:419:PHE:HA	1.91	0.52
1:A:313:ILE:HG22	1:A:315:PHE:CD2	2.45	0.52
1:B:441:GLN:HE22	1:B:490:ILE:CD1	2.22	0.52
1:A:21:MET:SD	1:A:141:ARG:NE	2.82	0.52
2:I:326:ARG:NH1	2:J:279:PHE:CD1	2.78	0.52
1:A:352:GLU:N	1:A:352:GLU:OE1	2.40	0.52
2:K:291:GLY:O	2:K:451:ARG:NH1	2.42	0.52
1:N:294:LYS:NZ	3:N:701:ATP:O2B	2.29	0.52
1:R:209:ASN:O	1:R:216:ARG:NH1	2.41	0.52
1:P:351:PRO:HB3	1:P:383:LEU:HD23	1.91	0.52
2:Q:289:ALA:HB2	2:Q:419:PHE:HA	1.92	0.52
1:B:90:PHE:HE1	3:B:702:ATP:C6	2.27	0.52
2:E:151:PHE:N	2:E:151:PHE:CD1	2.78	0.52
2:E:331:TRP:HZ2	3:E:701:ATP:H5'2	1.74	0.52
2:E:377:ILE:HD12	2:E:412:PHE:CE2	2.45	0.52
2:K:150:VAL:HG12	2:K:151:PHE:CE1	2.44	0.52
1:R:455:VAL:HG11	1:R:463:HIS:HB2	1.90	0.52
1:P:472:ILE:CG2	3:P:701:ATP:C4	2.93	0.52
1:V:393:ARG:O	1:V:397:ILE:HG12	2.10	0.52
1:A:160:VAL:HG21	1:A:194:TYR:CD2	2.44	0.52
2:F:281:ASP:OD1	2:F:281:ASP:N	2.42	0.52
2:F:485:ASN:O	2:F:486:PHE:HD2	1.92	0.52
2:D:45:SER:HB3	2:D:182:THR:HB	1.90	0.52
2:L:146:SER:OG	2:L:149:SER:OG	2.26	0.52
2:L:298:VAL:HG13	2:L:376:ALA:HB1	1.91	0.52
1:V:298:VAL:HG21	1:V:413:THR:HG21	1.90	0.52
1:A:488:ARG:HH11	1:A:488:ARG:CG	2.21	0.52
3:E:701:ATP:O3G	2:F:459:ARG:NH2	2.36	0.52
1:R:429:HIS:HB3	2:Q:385:ARG:CZ	2.39	0.52
1:W:440:LEU:CD2	1:W:453:ILE:HD12	2.40	0.52
1:G:311:ARG:NH1	1:G:370:PHE:O	2.39	0.52
1:H:90:PHE:CD1	1:H:90:PHE:N	2.76	0.52
2:L:328:ALA:CB	2:L:335:PHE:CE1	2.92	0.52
2:I:215:ARG:HG2	2:I:215:ARG:HH21	1.75	0.52
1:A:55:PHE:CD1	1:A:55:PHE:C	2.83	0.52
2:C:90:PHE:CB	2:C:92:TRP:NE1	2.72	0.52
2:C:463:HIS:O	2:C:465:LYS:HE2	2.10	0.52
2:D:382:ALA:O	2:D:385:ARG:HB2	2.09	0.52
1:H:160:VAL:HG11	1:H:194:TYR:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:254:LEU:HD11	2:J:350:TYR:CE2	2.45	0.52
2:C:294:LYS:HE2	3:C:701:ATP:O1B	2.10	0.52
1:G:287:THR:HG21	1:G:425:ILE:O	2.10	0.52
1:H:269:ARG:HG2	1:H:479:ILE:HB	1.92	0.52
1:H:319:GLU:O	2:I:254:LEU:HG	2.10	0.52
2:L:281:ASP:N	2:L:281:ASP:OD1	2.42	0.52
2:U:217:ARG:HG2	2:U:217:ARG:HH11	1.75	0.52
1:A:419:PHE:CD1	1:B:425:ILE:CD1	2.93	0.51
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.92	0.51
2:C:383:LEU:HD13	2:C:395:PHE:CE1	2.46	0.51
2:Q:225:LEU:HD12	2:Q:230:HIS:CB	2.34	0.51
1:S:50:THR:HG22	1:S:209:ASN:HB2	1.92	0.51
1:A:245:ASN:ND2	1:A:247:PHE:CE2	2.78	0.51
1:A:300:ARG:HG3	1:A:333:MET:HE1	1.91	0.51
2:D:218:ARG:CZ	2:D:239:ILE:HD12	2.41	0.51
1:G:328:ALA:CB	1:G:335:PHE:CD1	2.93	0.51
1:H:20:LYS:HE3	1:H:228:THR:HG21	1.92	0.51
2:K:126:LEU:O	2:K:130:ILE:HG13	2.11	0.51
1:N:283:ILE:HG23	1:N:412:PHE:CE1	2.46	0.51
1:R:423:HIS:NE2	2:Q:418:GLN:NE2	2.57	0.51
1:R:438:ILE:CG2	1:R:453:ILE:HD11	2.41	0.51
2:L:289:ALA:CB	2:L:419:PHE:HA	2.41	0.51
2:I:54:LEU:CD1	2:I:90:PHE:CE2	2.94	0.51
2:J:115:GLN:O	2:J:116:GLU:C	2.48	0.51
2:J:400:THR:HG21	2:J:433:ILE:HG23	1.92	0.51
1:V:215:ARG:HG2	1:V:215:ARG:HH11	1.74	0.51
1:G:89:SER:OG	3:G:702:ATP:N6	2.40	0.51
1:G:455:VAL:HG11	1:G:463:HIS:HB2	1.92	0.51
2:K:147:VAL:O	2:K:150:VAL:HG12	2.10	0.51
2:L:67:PHE:CD1	2:L:67:PHE:N	2.79	0.51
2:L:191:ILE:HB	2:L:198:GLU:HG2	1.92	0.51
2:J:483:PHE:CB	2:J:489:ILE:CD1	2.87	0.51
2:C:415:THR:CB	2:D:432:TPO:O1P	2.56	0.51
2:J:218:ARG:CZ	2:J:239:ILE:HD12	2.41	0.51
1:A:55:PHE:C	1:A:55:PHE:HD1	2.14	0.51
1:H:90:PHE:N	1:H:90:PHE:HD1	2.09	0.51
2:L:347:VAL:O	2:L:348:CYS:O	2.29	0.51
2:Q:289:ALA:HB1	2:Q:419:PHE:HA	1.92	0.51
1:V:284:ILE:HB	1:V:411:LEU:HD12	1.91	0.51
1:A:131:ASN:O	1:A:135:GLN:NE2	2.44	0.51
2:E:490:ILE:HG21	2:D:420:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:ARG:NH1	1:G:371:LYS:O	2.44	0.51
2:K:224:LYS:NZ	3:J:702:ATP:O2G	2.39	0.51
2:K:334:ASP:O	2:K:335:PHE:C	2.50	0.51
3:I:702:ATP:O3G	2:J:224:LYS:NZ	2.40	0.51
2:E:263:VAL:CG1	2:E:374:ARG:HH11	2.24	0.51
2:F:289:ALA:CB	2:F:419:PHE:HA	2.41	0.51
1:H:54:LEU:CD1	1:H:90:PHE:CE2	2.94	0.51
2:L:300:ARG:HA	2:L:333:MET:HE1	1.93	0.51
1:N:294:LYS:HB3	1:N:413:THR:CB	2.40	0.51
1:M:287:THR:HG21	1:M:425:ILE:O	2.09	0.51
2:Q:274:CYS:HG	2:Q:278:PHE:HE2	1.59	0.51
2:U:425:ILE:HD13	2:U:425:ILE:N	2.26	0.51
2:L:66:GLU:HB3	2:L:67:PHE:CE1	2.47	0.50
2:L:161:ARG:HG3	2:L:196:VAL:HG12	1.93	0.50
2:I:395:PHE:C	2:I:395:PHE:HD2	2.14	0.50
1:R:142:VAL:O	1:R:178:THR:HA	2.11	0.50
1:M:294:LYS:NZ	3:M:701:ATP:O1B	2.40	0.50
1:W:303:GLU:HA	1:W:338:MET:HE3	1.94	0.50
1:A:483:PHE:CB	1:A:489:ILE:CD1	2.89	0.50
2:E:461:SER:OG	2:E:462:TRP:N	2.44	0.50
2:I:54:LEU:HD11	2:I:90:PHE:CE2	2.46	0.50
1:M:75:THR:HA	1:M:145:ASP:O	2.11	0.50
2:K:334:ASP:O	2:K:334:ASP:OD1	2.28	0.50
2:I:248:PRO:CB	2:I:251:ALA:HB3	2.41	0.50
1:S:328:ALA:O	1:S:332:GLY:O	2.30	0.50
1:V:215:ARG:HG2	1:V:215:ARG:NH1	2.27	0.50
1:A:483:PHE:CB	1:A:489:ILE:HD13	2.42	0.50
2:D:110:PRO:O	2:D:111:ASP:C	2.50	0.50
2:D:215:ARG:NE	2:D:215:ARG:HA	2.27	0.50
2:K:461:SER:OG	2:K:462:TRP:N	2.44	0.50
1:A:319:GLU:HB3	1:A:324:LEU:HD23	1.93	0.50
2:I:441:GLN:HE22	2:I:490:ILE:HD13	1.76	0.50
1:M:208:ARG:NH2	1:M:221:GLU:OE2	2.44	0.50
1:A:483:PHE:HB2	1:A:489:ILE:HD13	1.93	0.50
2:E:254:LEU:CD2	2:D:350:TYR:CE2	2.95	0.50
2:C:237:PHE:CD2	2:C:244:ILE:HG23	2.46	0.50
2:K:425:ILE:CD1	2:J:419:PHE:CE2	2.94	0.50
2:K:490:ILE:HG21	2:J:420:MET:HE2	1.94	0.50
1:N:142:VAL:O	1:N:178:THR:HA	2.12	0.50
1:V:419:PHE:CD2	1:V:419:PHE:N	2.80	0.50
1:B:183:GLU:HB3	2:C:199:PHE:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:SER:CB	1:B:278:PHE:CE2	2.95	0.50
1:G:160:VAL:HG21	1:G:194:TYR:CE2	2.47	0.50
2:I:415:THR:CB	2:J:432:TPO:O1P	2.57	0.50
2:J:45:SER:HB3	2:J:182:THR:HB	1.93	0.50
2:U:419:PHE:CG	1:V:425:ILE:HD13	2.47	0.50
1:X:24:MET:HB2	1:X:62:ASN:HD22	1.77	0.50
1:A:55:PHE:HD1	1:A:55:PHE:O	1.94	0.50
1:H:449:MET:HG3	2:I:454:ASN:HD21	1.76	0.50
1:W:269:ARG:HG2	1:W:479:ILE:HB	1.94	0.50
1:G:28:PHE:CE1	1:G:222:ILE:HD11	2.46	0.50
1:G:325:LEU:HD23	1:G:335:PHE:HB2	1.94	0.50
1:G:353:SER:HA	1:H:250:GLY:CA	2.42	0.50
2:U:209:ASN:O	2:U:216:ARG:NH1	2.39	0.50
1:A:52:LYS:HD3	3:A:702:ATP:O1B	2.12	0.49
1:B:353:SER:HA	2:C:250:GLY:HA3	1.94	0.49
1:G:483:PHE:HD1	1:G:483:PHE:N	2.10	0.49
1:H:419:PHE:CE2	2:I:425:ILE:HD12	2.46	0.49
1:M:275:GLY:O	2:U:340:ARG:HD3	2.11	0.49
1:V:298:VAL:CG2	1:V:413:THR:HG21	2.41	0.49
1:G:58:GLN:HG3	1:G:92:TRP:CH2	2.47	0.49
1:H:295:THR:HG21	1:H:319:GLU:OE2	2.12	0.49
2:L:305:ALA:HB2	2:L:374:ARG:CD	2.38	0.49
3:N:702:ATP:O3G	2:O:224:LYS:NZ	2.44	0.49
2:U:436:THR:HG23	2:U:458:MET:HG2	1.94	0.49
1:B:185:ILE:HD11	1:B:193:ARG:NH1	2.28	0.49
1:G:456:PHE:HE2	2:L:442:TYR:CZ	2.30	0.49
1:G:488:ARG:HH11	1:G:488:ARG:CG	2.24	0.49
1:H:231:MET:HE2	1:H:250:GLY:O	2.13	0.49
3:H:702:ATP:O1G	2:I:224:LYS:NZ	2.45	0.49
2:K:155:ASP:C	2:K:156:ALA:O	2.50	0.49
2:K:313:ILE:CG2	2:K:315:PHE:CE1	2.95	0.49
2:J:375:ILE:HG12	2:J:408:ILE:CG2	2.42	0.49
1:G:456:PHE:HD2	1:G:456:PHE:O	1.94	0.49
1:B:295:THR:HG21	1:B:319:GLU:OE2	2.13	0.49
1:B:419:PHE:CD1	2:C:423:HIS:O	2.65	0.49
2:D:375:ILE:CG1	2:D:408:ILE:HG21	2.43	0.49
2:J:419:PHE:HE1	2:J:420:MET:HB2	1.78	0.49
1:M:321:ARG:O	1:M:325:LEU:HG	2.12	0.49
2:U:396:VAL:O	2:U:400:THR:HG23	2.12	0.49
2:E:160:VAL:HG21	2:E:194:TYR:CD2	2.48	0.49
2:E:305:ALA:HB2	2:E:374:ARG:CD	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:379:SER:HB3	2:I:413:THR:OG1	2.12	0.49
2:L:67:PHE:HD1	2:L:67:PHE:N	2.10	0.49
1:A:443:VAL:HG11	1:A:483:PHE:HE2	1.77	0.49
1:B:283:ILE:HG13	1:B:400:THR:CG2	2.41	0.49
1:B:319:GLU:O	2:C:254:LEU:HG	2.12	0.49
1:B:353:SER:HA	2:C:250:GLY:CA	2.43	0.49
1:A:58:GLN:HG3	1:A:92:TRP:CH2	2.47	0.49
1:A:417:ASP:OD2	1:B:429:HIS:CE1	2.66	0.49
2:F:46:GLY:O	2:F:52:LYS:HE2	2.13	0.49
2:J:462:TRP:CG	2:J:463:HIS:N	2.81	0.49
1:G:438:ILE:CG2	1:G:453:ILE:HD11	2.43	0.49
1:H:21:MET:SD	1:H:141:ARG:NE	2.86	0.49
2:K:204:VAL:HG23	2:K:224:LYS:HE2	1.95	0.49
1:T:317:TYR:O	1:T:350:TYR:HA	2.13	0.49
1:B:145:ASP:OD1	1:B:181:THR:HG21	2.13	0.48
2:E:308:ASN:N	2:E:308:ASN:HD22	2.11	0.48
2:F:23:THR:O	2:F:24:MET:HB2	2.13	0.48
2:F:300:ARG:HA	2:F:333:MET:CE	2.43	0.48
2:K:474:ASP:OD1	2:K:474:ASP:N	2.46	0.48
2:I:389:ASN:HD21	2:I:428:SER:HA	1.77	0.48
2:J:147:VAL:O	2:J:150:VAL:HG12	2.13	0.48
2:J:384:ALA:HB2	2:J:392:PHE:CZ	2.48	0.48
2:L:52:LYS:HD2	2:L:181:THR:HG23	1.95	0.48
1:W:248:PRO:HB2	1:W:251:ALA:HB3	1.96	0.48
1:A:303:GLU:HA	1:A:338:MET:CE	2.43	0.48
1:A:328:ALA:HB1	1:A:335:PHE:HD1	1.72	0.48
2:E:250:GLY:C	2:E:252:MET:N	2.65	0.48
1:H:54:LEU:HD21	1:H:90:PHE:HE2	1.78	0.48
2:Q:185:ILE:HD11	2:Q:193:ARG:NH1	2.28	0.48
2:U:140:ARG:O	2:U:176:ALA:HB1	2.13	0.48
1:B:67:PHE:N	1:B:67:PHE:CD2	2.81	0.48
2:D:194:TYR:N	2:D:194:TYR:CD2	2.82	0.48
2:K:249:LEU:CD1	2:K:394:GLN:NE2	2.68	0.48
2:L:161:ARG:HD2	2:L:196:VAL:CG1	2.43	0.48
3:A:702:ATP:O2'	1:B:230:HIS:NE2	2.46	0.48
2:E:323:GLN:HE22	2:F:435:ASP:CG	2.17	0.48
2:E:442:TYR:CD2	2:F:456:PHE:CZ	3.02	0.48
1:R:283:ILE:HG13	1:R:400:THR:HG23	1.95	0.48
1:P:449:MET:CE	2:Q:467:ILE:HD11	2.44	0.48
1:T:25:ILE:O	1:T:27:GLY:N	2.47	0.48
3:B:701:ATP:C2	2:C:462:TRP:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:395:PHE:CE2	2:I:399:VAL:CG2	2.92	0.48
2:J:110:PRO:O	2:J:111:ASP:C	2.52	0.48
2:J:485:ASN:OD1	2:J:485:ASN:N	2.47	0.48
1:M:285:LEU:HD21	1:M:426:THR:CG2	2.44	0.48
1:P:305:ALA:HB2	1:P:374:ARG:HD3	1.95	0.48
1:V:219:THR:HA	1:V:235:TYR:O	2.14	0.48
1:A:350:TYR:CE2	1:B:254:LEU:HB2	2.49	0.48
2:C:21:MET:HE1	2:C:177:THR:HB	1.94	0.48
1:H:328:ALA:HB1	1:H:335:PHE:CE1	2.47	0.48
2:I:80:PRO:HA	2:I:83:ILE:HD12	1.95	0.48
1:N:52:LYS:HD2	1:N:181:THR:HG23	1.96	0.48
1:P:451:ARG:HB3	1:P:470:PHE:HE2	1.79	0.48
1:G:393:ARG:O	1:G:397:ILE:HG12	2.13	0.48
2:L:46:GLY:O	2:L:52:LYS:HE2	2.13	0.48
2:L:441:GLN:HE22	2:L:490:ILE:HA	1.79	0.48
2:Q:384:ALA:HB2	2:Q:392:PHE:CZ	2.49	0.48
1:A:353:SER:HA	1:B:250:GLY:CA	2.43	0.48
2:E:264:SER:O	2:E:374:ARG:NH1	2.38	0.48
2:E:334:ASP:O	2:E:335:PHE:C	2.52	0.48
1:P:184:ARG:NH1	1:P:187:GLU:O	2.47	0.48
1:X:356:LEU:HD21	1:X:387:VAL:HG11	1.95	0.48
1:W:397:ILE:HD11	1:W:433:ILE:CD1	2.44	0.48
2:D:283:ILE:HG13	2:D:400:THR:HG23	1.96	0.48
1:H:94:LEU:O	1:H:98:VAL:HG23	2.13	0.48
1:H:250:GLY:O	1:H:251:ALA:CB	2.62	0.48
2:J:225:LEU:HD12	2:J:230:HIS:HB3	1.95	0.48
1:S:393:ARG:NH1	1:S:429:HIS:O	2.46	0.48
1:H:400:THR:HG21	1:H:433:ILE:HG22	1.94	0.47
2:L:328:ALA:HB2	2:L:335:PHE:HE1	1.78	0.47
2:Q:420:MET:HE3	2:Q:492:GLY:HA3	1.96	0.47
1:V:127:ILE:HG13	1:V:167:LEU:HD11	1.96	0.47
1:B:20:LYS:HE3	1:B:228:THR:HG21	1.96	0.47
1:N:449:MET:CE	2:O:467:ILE:HD11	2.43	0.47
1:N:483:PHE:HB3	1:N:486:PHE:HB2	1.96	0.47
1:A:131:ASN:OD1	1:A:135:GLN:NE2	2.47	0.47
1:A:328:ALA:HB2	1:A:335:PHE:CD1	2.49	0.47
1:B:298:VAL:CG2	1:B:413:THR:HG21	2.45	0.47
2:F:66:GLU:C	2:F:67:PHE:CD1	2.87	0.47
2:D:218:ARG:HB3	2:D:237:PHE:CZ	2.48	0.47
1:H:442:TYR:HE1	2:I:456:PHE:CE2	2.32	0.47
2:I:432:TPO:HG21	2:I:432:TPO:O1P	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:52:LYS:HB3	2:Q:181:THR:HG23	1.96	0.47
2:Q:58:GLN:HG2	2:Q:92:TRP:CH2	2.49	0.47
1:V:52:LYS:HB3	1:V:181:THR:HG23	1.96	0.47
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.95	0.47
1:G:483:PHE:N	1:G:483:PHE:CD1	2.82	0.47
1:H:191:ILE:CD1	1:H:223:LEU:HD12	2.45	0.47
2:J:57:ILE:HD11	2:J:83:ILE:CG2	2.42	0.47
2:J:283:ILE:HG13	2:J:400:THR:HG23	1.96	0.47
1:N:287:THR:HG22	1:N:414:ASN:HB3	1.95	0.47
1:R:462:TRP:O	1:R:463:HIS:CD2	2.67	0.47
2:D:54:LEU:HD13	2:D:90:PHE:HE2	1.77	0.47
2:D:273:MET:SD	2:D:468:ARG:HD2	2.54	0.47
1:H:289:ALA:CB	1:H:419:PHE:HA	2.44	0.47
2:K:214:GLU:OE2	2:L:217:ARG:NH1	2.43	0.47
2:L:98:VAL:HA	2:L:103:LEU:O	2.13	0.47
1:N:326:ARG:HD3	2:O:258:SER:OG	2.14	0.47
2:Q:455:VAL:HG11	2:Q:463:HIS:HB2	1.96	0.47
1:A:315:PHE:CD2	1:A:315:PHE:N	2.82	0.47
2:C:294:LYS:HE2	2:C:294:LYS:HB2	1.74	0.47
2:D:384:ALA:HB2	2:D:392:PHE:CZ	2.50	0.47
2:L:74:VAL:HG12	2:L:76:PHE:CE1	2.47	0.47
2:J:461:SER:C	2:J:462:TRP:O	2.52	0.47
1:T:287:THR:HG22	1:T:414:ASN:HD22	1.80	0.47
1:W:301:PHE:CZ	1:W:374:ARG:HD2	2.50	0.47
1:H:300:ARG:HA	1:H:333:MET:HE1	1.97	0.47
1:H:353:SER:HA	2:I:250:GLY:CA	2.44	0.47
1:H:442:TYR:CE1	2:I:456:PHE:CZ	3.03	0.47
2:I:298:VAL:HG21	2:I:413:THR:HG21	1.96	0.47
1:P:285:LEU:HA	1:P:412:PHE:O	2.15	0.47
1:S:287:THR:HG21	1:S:425:ILE:O	2.15	0.47
1:V:419:PHE:CZ	1:W:425:ILE:HD12	2.47	0.47
2:C:80:PRO:HA	2:C:83:ILE:HD12	1.95	0.47
2:C:318:GLU:OE2	2:D:432:TPO:HG21	2.15	0.47
1:G:417:ASP:OD2	1:H:429:HIS:NE2	2.48	0.47
2:K:313:ILE:HG21	2:K:315:PHE:CE1	2.50	0.47
2:O:42:THR:HA	2:O:203:ASN:HB2	1.97	0.47
2:O:437:ILE:HD12	2:O:457:LYS:HD3	1.97	0.47
2:U:89:SER:CB	5:U:702:ADP:HN62	2.25	0.47
1:B:385:ARG:HD3	2:C:393:ARG:HH21	1.80	0.47
2:F:52:LYS:HD2	2:F:181:THR:HG23	1.96	0.47
2:C:202:ASP:OD1	2:C:226:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:GLY:C	2:D:333:MET:HG2	2.35	0.47
1:H:313:ILE:HG22	1:H:315:PHE:CE1	2.50	0.47
1:N:234:GLU:O	1:M:215:ARG:NH2	2.48	0.47
1:R:465:LYS:O	2:Q:448:GLU:HG3	2.14	0.47
1:P:283:ILE:HG13	1:P:400:THR:HG23	1.96	0.47
1:B:45:SER:HA	1:B:182:THR:O	2.15	0.47
2:L:194:TYR:N	2:L:194:TYR:CD2	2.83	0.47
2:J:353:SER:O	2:J:354:ALA:HB2	2.15	0.47
1:R:468:ARG:HA	1:R:482:SER:HA	1.97	0.47
1:T:292:THR:O	1:T:451:ARG:CD	2.61	0.47
2:E:38:ILE:HA	2:E:177:THR:HG23	1.95	0.46
2:E:490:ILE:HG21	2:D:420:MET:CE	2.45	0.46
2:C:49:GLY:O	2:C:218:ARG:NH2	2.48	0.46
2:D:225:LEU:HD12	2:D:230:HIS:HB3	1.96	0.46
2:D:375:ILE:HD12	2:D:375:ILE:HG21	1.48	0.46
2:K:52:LYS:HE2	3:K:702:ATP:O2B	2.15	0.46
2:L:315:PHE:CE2	2:L:363:ILE:HA	2.50	0.46
2:J:462:TRP:CD2	2:J:463:HIS:N	2.84	0.46
1:N:237:PHE:HB3	1:N:246:ILE:HA	1.96	0.46
2:O:292:THR:O	2:O:451:ARG:NH1	2.48	0.46
1:T:96:LYS:O	1:T:100:GLU:N	2.47	0.46
1:V:145:ASP:HA	1:V:146:SER:HA	1.73	0.46
1:W:145:ASP:HA	1:W:146:SER:HA	1.67	0.46
2:E:90:PHE:N	2:E:90:PHE:CD2	2.83	0.46
2:D:198:GLU:H	2:D:198:GLU:HG3	1.53	0.46
2:D:353:SER:O	2:D:354:ALA:HB2	2.15	0.46
1:G:57:ILE:HD11	1:G:83:ILE:HG23	1.97	0.46
1:H:271:ASP:HA	1:H:277:GLY:HA2	1.96	0.46
2:O:31:ILE:HG23	2:O:231:MET:HB2	1.97	0.46
2:O:38:ILE:HA	2:O:177:THR:CG2	2.45	0.46
2:Q:434:THR:OG1	2:Q:437:ILE:CD1	2.64	0.46
1:X:215:ARG:NH2	1:S:232:LYS:O	2.45	0.46
1:S:264:SER:O	1:S:374:ARG:NH2	2.46	0.46
1:A:440:LEU:CD2	1:A:453:ILE:HD12	2.46	0.46
2:L:382:ALA:O	2:L:385:ARG:HG2	2.15	0.46
2:I:202:ASP:OD1	2:I:226:ARG:NH1	2.49	0.46
2:I:318:GLU:OE2	2:J:432:TPO:HG21	2.15	0.46
2:D:266:GLY:HA2	2:D:304:ASN:HD22	1.80	0.46
1:G:425:ILE:HD11	1:G:456:PHE:CD1	2.51	0.46
1:G:435:ASP:OD1	2:L:323:GLN:NE2	2.41	0.46
2:J:218:ARG:HB3	2:J:237:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:295:THR:N	3:S:701:ATP:O1B	2.46	0.46
1:A:315:PHE:N	1:A:315:PHE:HD2	2.14	0.46
2:C:283:ILE:HG23	2:C:412:PHE:CE2	2.50	0.46
1:N:47:THR:O	1:N:52:LYS:NZ	2.48	0.46
1:X:267:VAL:HB	1:X:270:LEU:HB2	1.97	0.46
1:A:467:ILE:HD11	2:F:449:MET:HE2	1.97	0.46
2:C:21:MET:HE3	2:C:177:THR:HG21	1.97	0.46
1:G:227:GLY:O	2:L:89:SER:HB2	2.16	0.46
1:H:393:ARG:NH2	1:H:429:HIS:O	2.47	0.46
2:L:231:MET:HB3	2:L:235:TYR:OH	2.15	0.46
2:I:74:VAL:HG12	2:I:76:PHE:CE1	2.51	0.46
2:O:395:PHE:O	2:O:399:VAL:HG23	2.15	0.46
1:S:331:TRP:CZ2	3:S:701:ATP:C8	3.04	0.46
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.97	0.46
2:E:263:VAL:HG13	2:E:374:ARG:HH11	1.81	0.46
2:F:208:ARG:O	2:F:218:ARG:HA	2.16	0.46
2:L:219:THR:HB	2:L:234:GLU:HB3	1.97	0.46
2:I:445:ILE:HD12	2:I:486:PHE:CZ	2.51	0.46
1:P:285:LEU:HD21	1:P:426:THR:CG2	2.45	0.46
2:Q:131:ASN:O	2:Q:135:GLN:HG2	2.15	0.46
1:X:24:MET:O	1:X:62:ASN:ND2	2.49	0.46
1:B:67:PHE:N	1:B:67:PHE:HD2	2.13	0.46
1:B:94:LEU:O	1:B:98:VAL:HG23	2.15	0.46
2:C:188:TYR:CE1	2:C:208:ARG:HD3	2.50	0.46
2:D:41:SER:HB3	2:D:178:THR:OG1	2.16	0.46
2:L:52:LYS:NZ	3:L:702:ATP:O2G	2.36	0.46
2:J:332:GLY:C	2:J:333:MET:HG2	2.36	0.46
1:M:289:ALA:CB	1:M:419:PHE:HA	2.45	0.46
1:X:490:ILE:CB	1:W:420:MET:CE	2.94	0.46
1:W:284:ILE:HB	1:W:411:LEU:HD12	1.97	0.46
1:A:145:ASP:HB2	1:A:181:THR:HB	1.98	0.46
2:F:283:ILE:HG23	2:F:412:PHE:CE1	2.50	0.46
2:C:300:ARG:HA	2:C:333:MET:HE1	1.97	0.46
1:H:183:GLU:OE2	2:I:161:ARG:NH1	2.49	0.46
2:L:111:ASP:O	2:L:113:GLU:N	2.47	0.46
2:Q:458:MET:HB3	2:Q:461:SER:HB3	1.98	0.46
1:A:344:LEU:HD22	1:A:345:LYS:N	2.30	0.45
1:G:225:LEU:HD12	1:G:230:HIS:HB3	1.97	0.45
1:H:419:PHE:CE2	2:I:425:ILE:CD1	2.99	0.45
2:L:380:LEU:HD12	2:L:412:PHE:HB3	1.99	0.45
1:P:451:ARG:HB3	1:P:470:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASP:OD2	1:A:112:PRO:N	2.49	0.45
2:C:333:MET:H	2:C:333:MET:HG2	1.58	0.45
2:C:436:THR:HG23	2:C:458:MET:HG2	1.98	0.45
2:D:52:LYS:HB3	2:D:181:THR:HG23	1.98	0.45
2:J:142:VAL:O	2:J:178:THR:HA	2.16	0.45
2:J:273:MET:SD	2:J:468:ARG:HD2	2.56	0.45
1:N:43:LEU:HD11	1:N:182:THR:HG23	1.99	0.45
1:T:426:THR:N	1:T:431:SEP:O3P	2.49	0.45
1:B:145:ASP:HA	1:B:146:SER:HA	1.79	0.45
2:D:337:GLU:OE1	2:D:340:ARG:NH1	2.50	0.45
1:G:263:VAL:CG1	1:G:374:ARG:NH2	2.79	0.45
1:H:419:PHE:CD2	2:I:425:ILE:HD11	2.48	0.45
2:L:298:VAL:HG21	2:L:413:THR:HG21	1.98	0.45
1:T:378:ASP:HA	1:T:379:SER:HA	1.62	0.45
2:C:451:ARG:NH2	3:C:701:ATP:O2'	2.49	0.45
2:D:21:MET:SD	2:D:141:ARG:CZ	3.04	0.45
2:D:107:ASP:OD1	2:D:109:SER:OG	2.33	0.45
2:I:49:GLY:O	2:I:218:ARG:NH2	2.50	0.45
2:J:356:LEU:HD21	2:J:387:VAL:HG11	1.98	0.45
2:J:419:PHE:CD1	2:J:420:MET:HB2	2.52	0.45
1:N:230:HIS:NE2	3:M:702:ATP:O2'	2.35	0.45
1:R:419:PHE:HE2	1:M:424:SER:C	2.19	0.45
1:M:49:GLY:O	1:M:218:ARG:NH2	2.49	0.45
1:T:21:MET:CE	1:T:177:THR:CB	2.94	0.45
1:T:418:GLN:CB	1:T:422:ALA:HB2	2.47	0.45
1:W:289:ALA:O	1:W:292:THR:OG1	2.35	0.45
1:A:311:ARG:HA	1:A:343:LEU:O	2.17	0.45
1:A:438:ILE:CG2	1:A:453:ILE:HD11	2.47	0.45
2:E:318:GLU:OE2	2:F:432:TPO:HG21	2.17	0.45
2:C:188:TYR:HE1	2:C:208:ARG:CD	2.29	0.45
1:H:145:ASP:HA	1:H:146:SER:HA	1.79	0.45
1:H:278:PHE:CG	1:H:284:ILE:HD12	2.49	0.45
2:J:212:GLU:OE2	2:J:212:GLU:HA	2.16	0.45
2:J:356:LEU:CD2	2:J:387:VAL:HG11	2.47	0.45
2:J:375:ILE:HG12	2:J:408:ILE:HG21	1.99	0.45
1:R:136:LYS:HD3	1:R:137:TYR:CE2	2.52	0.45
1:P:296:LEU:CD2	1:P:472:ILE:HG12	2.46	0.45
2:E:332:GLY:O	2:E:333:MET:O	2.34	0.45
2:E:335:PHE:HD2	2:E:346:ILE:HD11	1.81	0.45
2:D:188:TYR:HE2	2:D:210:VAL:CG2	2.29	0.45
2:K:490:ILE:HG21	2:J:420:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:367:ILE:HD11	2:J:375:ILE:CD1	2.47	0.45
1:V:169:ALA:O	1:V:173:GLN:N	2.48	0.45
1:B:271:ASP:HA	1:B:277:GLY:HA2	1.99	0.45
3:B:701:ATP:HO2'	2:C:463:HIS:CD2	2.31	0.45
2:E:474:ASP:OD1	2:E:474:ASP:N	2.50	0.45
2:C:31:ILE:HD11	2:C:246:ILE:CG2	2.46	0.45
2:C:303:GLU:HA	2:C:338:MET:HE2	1.97	0.45
1:G:283:ILE:HG13	1:G:400:THR:HG23	1.98	0.45
2:L:285:LEU:HG	2:L:287:THR:HG23	1.99	0.45
1:B:21:MET:SD	1:B:141:ARG:NE	2.90	0.45
2:F:209:ASN:HD21	2:F:216:ARG:HB3	1.82	0.45
2:D:142:VAL:O	2:D:178:THR:HA	2.16	0.45
1:H:313:ILE:HG21	1:H:315:PHE:CE1	2.52	0.45
2:J:289:ALA:HB1	2:J:419:PHE:HA	1.97	0.45
1:M:432:THR:O	1:M:459:ARG:NH2	2.43	0.45
2:U:396:VAL:HG12	2:U:400:THR:HG21	1.97	0.45
1:X:429:HIS:CG	1:W:385:ARG:HH11	2.34	0.45
2:F:98:VAL:HA	2:F:103:LEU:O	2.16	0.45
2:D:462:TRP:CD2	2:D:463:HIS:N	2.81	0.45
2:D:485:ASN:N	2:D:485:ASN:OD1	2.49	0.45
1:G:464:ASP:OD2	1:G:468:ARG:NH2	2.49	0.45
2:L:106:LEU:C	2:L:106:LEU:HD12	2.37	0.45
2:L:300:ARG:HA	2:L:333:MET:CE	2.47	0.45
1:M:31:ILE:CD1	1:M:246:ILE:HG21	2.46	0.45
1:P:472:ILE:HG21	3:P:701:ATP:H1'	1.99	0.45
1:G:44:VAL:HG11	1:G:55:PHE:HD2	1.81	0.45
1:G:86:ASN:OD1	1:H:40:ARG:NH2	2.43	0.45
1:G:490:ILE:HD11	2:L:449:MET:HE3	1.98	0.45
2:L:299:SER:C	2:L:333:MET:HE1	2.37	0.45
2:I:389:ASN:O	2:I:393:ARG:HG3	2.17	0.45
2:U:53:THR:HG23	5:U:702:ADP:O2B	2.16	0.45
1:V:144:ILE:O	1:V:180:MET:N	2.49	0.45
1:B:66:GLU:CG	1:B:67:PHE:CE2	3.00	0.44
1:B:86:ASN:O	1:B:89:SER:HB3	2.17	0.44
2:C:386:GLY:CA	2:D:390:ASN:HD21	2.30	0.44
2:D:375:ILE:HG12	2:D:408:ILE:CG2	2.47	0.44
1:G:21:MET:SD	1:G:141:ARG:NE	2.91	0.44
1:G:53:THR:O	1:G:57:ILE:HG13	2.17	0.44
1:H:54:LEU:HD11	1:H:90:PHE:CE2	2.52	0.44
2:K:453:ILE:HG21	2:K:479:ILE:HG12	1.98	0.44
2:O:71:GLY:HA2	2:O:139:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:LEU:HB2	1:M:434:THR:HG21	1.99	0.44
2:Q:425:ILE:HG22	2:Q:426:THR:HG23	1.98	0.44
1:A:19:ALA:HB1	1:A:38:ILE:HD12	1.99	0.44
1:A:145:ASP:HA	1:A:146:SER:HA	1.68	0.44
2:E:419:PHE:HD2	2:F:456:PHE:CZ	2.36	0.44
2:F:380:LEU:HD12	2:F:412:PHE:HB3	1.99	0.44
2:C:278:PHE:CD2	2:C:284:ILE:HG13	2.53	0.44
2:C:393:ARG:O	2:C:397:ILE:HG12	2.17	0.44
2:D:21:MET:CE	2:D:177:THR:OG1	2.65	0.44
1:H:315:PHE:CE2	1:H:363:ILE:HA	2.51	0.44
2:L:167:LEU:O	2:L:171:LEU:HG	2.17	0.44
2:J:302:VAL:CG1	2:J:344:LEU:HD13	2.47	0.44
1:R:86:ASN:OD1	1:M:40:ARG:NH2	2.48	0.44
1:B:317:TYR:HA	1:B:349:ALA:O	2.18	0.44
2:D:462:TRP:CG	2:D:463:HIS:N	2.84	0.44
1:G:145:ASP:HA	1:G:146:SER:HA	1.69	0.44
1:G:183:GLU:OE2	1:H:161:ARG:NH1	2.50	0.44
1:G:326:ARG:HG3	1:H:260:ASN:HD21	1.83	0.44
1:H:124:SER:HB3	1:H:166:ARG:HH21	1.82	0.44
2:K:145:ASP:HA	2:K:181:THR:HB	1.99	0.44
2:K:300:ARG:HA	2:K:333:MET:HE1	1.99	0.44
2:K:336:GLU:O	2:K:340:ARG:HG3	2.17	0.44
2:I:436:THR:HG23	2:I:458:MET:HG2	1.99	0.44
2:J:36:LEU:HD12	2:J:59:PHE:CE1	2.51	0.44
1:T:287:THR:HA	1:T:414:ASN:O	2.18	0.44
1:T:419:PHE:CD2	2:U:425:ILE:CD1	3.00	0.44
2:U:53:THR:OG1	5:U:702:ADP:O2A	2.34	0.44
2:U:256:GLN:CB	2:U:405:GLN:HA	2.47	0.44
1:S:182:THR:HG21	1:S:192:ALA:HB1	1.98	0.44
1:A:393:ARG:O	1:A:397:ILE:HG12	2.18	0.44
1:A:463:HIS:CD2	3:F:701:ATP:HO2'	2.32	0.44
2:E:453:ILE:HG21	2:E:479:ILE:HG12	1.98	0.44
2:F:106:LEU:HD12	2:F:106:LEU:C	2.37	0.44
2:C:289:ALA:HB2	2:C:419:PHE:HA	1.98	0.44
2:C:298:VAL:HG21	2:C:413:THR:HG21	1.98	0.44
2:D:54:LEU:CD1	2:D:90:PHE:CE2	2.96	0.44
1:G:21:MET:CE	1:G:177:THR:HB	2.48	0.44
1:G:313:ILE:HG21	1:G:315:PHE:CE2	2.52	0.44
2:L:283:ILE:HG23	2:L:412:PHE:CE1	2.52	0.44
2:J:52:LYS:HB3	2:J:181:THR:HG23	1.99	0.44
1:X:273:MET:O	1:X:463:HIS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:145:ASP:OD2	1:W:181:THR:HB	2.17	0.44
1:A:53:THR:O	1:A:57:ILE:HG13	2.17	0.44
1:G:212:GLU:OE1	1:G:217:ARG:HD3	2.18	0.44
1:G:292:THR:HG23	1:G:442:TYR:CE1	2.51	0.44
1:G:425:ILE:HD11	1:G:456:PHE:CE1	2.51	0.44
1:H:42:THR:HA	1:H:203:ASN:HB2	1.99	0.44
1:H:185:ILE:HD11	1:H:193:ARG:NH1	2.32	0.44
2:K:308:ASN:HD22	2:K:308:ASN:N	2.16	0.44
2:L:130:ILE:O	2:L:134:ILE:N	2.50	0.44
2:Q:378:ASP:HA	2:Q:379:SER:HA	1.77	0.44
2:Q:379:SER:HA	2:Q:413:THR:OG1	2.17	0.44
1:W:440:LEU:HD21	1:W:453:ILE:HD12	1.98	0.44
1:H:317:TYR:HA	1:H:349:ALA:O	2.18	0.44
2:I:356:LEU:CD2	2:I:387:VAL:HG11	2.48	0.44
1:N:435:ASP:HA	1:N:459:ARG:HD2	1.99	0.44
1:R:285:LEU:HA	1:R:412:PHE:O	2.18	0.44
2:Q:301:PHE:O	2:Q:374:ARG:NH1	2.50	0.44
1:X:145:ASP:HA	1:X:146:SER:HA	1.65	0.44
2:E:58:GLN:HG3	2:E:92:TRP:HH2	1.81	0.44
2:E:419:PHE:HD1	2:E:419:PHE:H	1.65	0.44
2:C:45:SER:HB3	2:C:182:THR:HB	2.00	0.44
2:D:298:VAL:HG13	2:D:376:ALA:HB1	2.00	0.44
1:G:86:ASN:O	1:G:89:SER:HB3	2.18	0.44
2:K:76:PHE:CD2	2:K:108:ALA:HB3	2.52	0.44
2:L:313:ILE:CG2	2:L:315:PHE:CE1	3.01	0.44
1:R:41:SER:HA	1:R:178:THR:HG23	1.98	0.44
2:Q:368:ASN:ND2	2:Q:402:TYR:OH	2.50	0.44
2:U:217:ARG:HG2	2:U:357:GLU:CD	2.35	0.44
1:V:316:ALA:O	1:V:348:CYS:HA	2.18	0.44
2:F:111:ASP:O	2:F:113:GLU:N	2.50	0.44
2:F:300:ARG:CA	2:F:333:MET:HE1	2.47	0.44
2:C:389:ASN:HD21	2:C:428:SER:HA	1.81	0.44
2:K:463:HIS:CD2	3:J:701:ATP:HO2'	2.35	0.44
2:I:54:LEU:HD21	2:I:90:PHE:HE2	1.83	0.44
2:J:46:GLY:O	2:J:52:LYS:HE2	2.18	0.44
2:J:317:TYR:CE1	2:J:383:LEU:HD11	2.53	0.44
2:Q:311:ARG:NH1	2:Q:370:PHE:O	2.50	0.44
3:X:702:ATP:O3'	1:S:224:LYS:HB2	2.18	0.44
2:E:52:LYS:HB3	2:E:181:THR:HG23	2.00	0.44
2:E:76:PHE:CD2	2:E:108:ALA:HB3	2.53	0.44
2:C:188:TYR:CE1	2:C:208:ARG:CD	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:VAL:HG12	2:D:76:PHE:CE2	2.53	0.44
1:G:490:ILE:HG13	2:L:420:MET:HE1	2.00	0.44
2:L:86:ASN:O	2:L:89:SER:HB3	2.18	0.44
1:P:296:LEU:HD22	1:P:472:ILE:HG12	2.00	0.44
1:S:70:PRO:CG	1:S:139:ALA:HA	2.47	0.44
1:W:73:PHE:O	1:W:106:LEU:N	2.51	0.44
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.89	0.43
2:C:216:ARG:NE	2:D:221:GLU:OE1	2.51	0.43
2:C:318:GLU:OE2	2:C:379:SER:OG	2.29	0.43
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.48	0.43
1:G:457:LYS:NZ	3:L:701:ATP:O1G	2.48	0.43
1:G:463:HIS:NE2	3:L:701:ATP:O2'	2.49	0.43
2:J:284:ILE:HB	2:J:411:LEU:HD12	2.00	0.43
1:X:378:ASP:HA	1:X:379:SER:HA	1.73	0.43
1:H:442:TYR:CE1	2:I:456:PHE:CE2	3.06	0.43
2:K:332:GLY:O	2:K:333:MET:O	2.36	0.43
2:L:347:VAL:O	2:L:348:CYS:C	2.55	0.43
2:I:145:ASP:HA	2:I:181:THR:HB	2.00	0.43
2:I:300:ARG:HD3	2:I:300:ARG:HA	1.78	0.43
2:Q:311:ARG:HB2	2:Q:372:PRO:HA	2.00	0.43
2:C:303:GLU:CA	2:C:338:MET:HE1	2.48	0.43
2:D:36:LEU:HD12	2:D:59:PHE:CE1	2.53	0.43
1:G:44:VAL:CG2	1:G:55:PHE:HE2	2.31	0.43
2:L:486:PHE:CD2	2:L:496:ARG:HA	2.52	0.43
2:I:333:MET:H	2:I:333:MET:HG2	1.55	0.43
1:R:289:ALA:CB	1:R:419:PHE:HA	2.46	0.43
1:P:274:CYS:HB3	1:P:458:MET:SD	2.59	0.43
1:P:288:GLY:O	1:P:415:THR:HA	2.18	0.43
1:W:294:LYS:O	1:W:298:VAL:HG23	2.18	0.43
1:B:262:ARG:NH1	1:B:461:SER:CB	2.81	0.43
2:C:145:ASP:C	2:C:145:ASP:OD1	2.56	0.43
1:G:344:LEU:HD22	1:G:345:LYS:N	2.33	0.43
2:K:284:ILE:HB	2:K:411:LEU:HD12	2.00	0.43
2:L:31:ILE:HD11	2:L:246:ILE:HG21	2.00	0.43
1:M:145:ASP:HA	1:M:146:SER:HA	1.66	0.43
1:P:145:ASP:HA	1:P:146:SER:HA	1.77	0.43
2:Q:291:GLY:O	2:Q:442:TYR:OH	2.30	0.43
2:E:204:VAL:HG23	2:E:224:LYS:HE2	2.00	0.43
2:E:352:GLU:N	2:E:352:GLU:OE1	2.51	0.43
2:F:461:SER:C	2:F:462:TRP:O	2.56	0.43
3:C:702:ATP:HO2'	2:D:230:HIS:HE2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:ARG:HA	1:G:343:LEU:O	2.18	0.43
1:H:298:VAL:CG2	1:H:413:THR:HG21	2.49	0.43
2:L:145:ASP:OD2	2:L:145:ASP:C	2.56	0.43
2:I:445:ILE:CD1	2:I:486:PHE:CE2	2.99	0.43
1:X:292:THR:N	3:X:701:ATP:O2B	2.52	0.43
1:W:397:ILE:CD1	1:W:433:ILE:CD1	2.96	0.43
1:A:86:ASN:OD1	1:B:40:ARG:NH2	2.49	0.43
2:E:397:ILE:CG2	2:D:350:TYR:CE1	3.01	0.43
2:D:21:MET:HE1	2:D:177:THR:OG1	2.18	0.43
1:N:203:ASN:O	1:N:204:VAL:CB	2.67	0.43
1:P:433:ILE:HG22	1:P:433:ILE:O	2.19	0.43
2:U:78:GLU:CB	2:U:83:ILE:HD11	2.49	0.43
1:A:86:ASN:O	1:A:89:SER:HB3	2.19	0.43
1:A:227:GLY:O	2:F:89:SER:HB2	2.19	0.43
1:B:298:VAL:CG2	1:B:413:THR:CG2	2.96	0.43
2:C:432:TPO:O1P	2:C:432:TPO:HG21	2.18	0.43
1:G:164:LEU:HD23	1:G:164:LEU:HA	1.88	0.43
3:H:701:ATP:C2	2:I:462:TRP:HA	2.54	0.43
2:K:52:LYS:HB3	2:K:181:THR:HG23	2.01	0.43
2:K:254:LEU:HB3	2:J:320:SER:HA	2.00	0.43
2:L:23:THR:O	2:L:24:MET:HB2	2.19	0.43
2:L:435:ASP:HA	2:L:459:ARG:HG3	2.01	0.43
1:P:312:ALA:O	1:P:344:LEU:HA	2.18	0.43
1:A:319:GLU:HB3	1:A:324:LEU:CD2	2.49	0.43
1:A:469:GLU:HB2	1:A:483:PHE:HE1	1.83	0.43
1:B:178:THR:HG22	1:B:180:MET:HG3	2.01	0.43
1:H:45:SER:HA	1:H:182:THR:O	2.19	0.43
2:K:31:ILE:HA	2:K:231:MET:SD	2.59	0.43
2:L:384:ALA:HB2	2:L:392:PHE:CZ	2.53	0.43
1:R:53:THR:HB	3:R:702:ATP:PA	2.59	0.43
1:M:70:PRO:CG	1:M:139:ALA:HA	2.49	0.43
2:U:145:ASP:HA	2:U:146:SER:HA	1.68	0.43
1:V:239:ILE:HG21	3:V:702:ATP:O4'	2.19	0.43
1:A:26:GLU:OE1	1:A:245:ASN:CG	2.56	0.43
2:J:298:VAL:HG13	2:J:376:ALA:HB1	2.01	0.43
1:M:94:LEU:O	1:M:98:VAL:HG23	2.19	0.43
1:V:333:MET:O	1:V:333:MET:HG2	2.18	0.43
1:W:298:VAL:HG21	1:W:413:THR:HG21	2.01	0.43
1:A:392:PHE:O	1:A:395:PHE:HB3	2.19	0.43
1:B:376:ALA:HA	1:B:411:LEU:O	2.18	0.43
2:D:284:ILE:HB	2:D:411:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:LEU:CD2	1:H:90:PHE:HE2	2.31	0.43
1:H:289:ALA:HB2	1:H:419:PHE:HA	2.01	0.43
2:K:254:LEU:CD1	2:J:350:TYR:CZ	3.02	0.43
1:N:145:ASP:HA	1:N:146:SER:HA	1.72	0.43
1:H:79:THR:HG23	1:H:82:ASP:OD2	2.18	0.42
2:K:151:PHE:CE2	2:K:160:VAL:HA	2.54	0.42
2:I:21:MET:SD	2:I:141:ARG:NE	2.92	0.42
2:J:451:ARG:HB2	2:J:470:PHE:CE2	2.54	0.42
1:A:31:ILE:HD11	1:A:246:ILE:HG21	2.01	0.42
1:A:247:PHE:N	1:A:247:PHE:CD2	2.87	0.42
2:E:145:ASP:HA	2:E:181:THR:HB	2.00	0.42
2:C:353:SER:HA	2:D:250:GLY:CA	2.49	0.42
1:G:66:GLU:HB3	1:G:67:PHE:CE1	2.54	0.42
1:G:230:HIS:NE2	3:L:702:ATP:O2'	2.46	0.42
1:H:377:ILE:HD12	1:H:412:PHE:CE2	2.54	0.42
2:K:250:GLY:HA2	2:J:353:SER:HB2	2.01	0.42
1:N:88:ARG:O	1:N:89:SER:CB	2.66	0.42
1:R:227:GLY:O	2:Q:89:SER:CB	2.67	0.42
1:M:378:ASP:HA	1:M:379:SER:HA	1.82	0.42
2:Q:305:ALA:HB2	2:Q:374:ARG:HD3	2.00	0.42
1:T:437:ILE:O	1:T:456:PHE:N	2.52	0.42
1:W:298:VAL:HG21	1:W:413:THR:CG2	2.50	0.42
3:E:702:ATP:O2'	2:F:230:HIS:CD2	2.73	0.42
2:F:31:ILE:HD11	2:F:246:ILE:HG21	2.01	0.42
2:F:130:ILE:O	2:F:134:ILE:N	2.52	0.42
2:F:146:SER:OG	2:F:149:SER:OG	2.25	0.42
3:C:701:ATP:H3'	2:D:458:MET:O	2.19	0.42
1:G:483:PHE:HB3	1:G:489:ILE:CD1	2.49	0.42
2:L:313:ILE:HD11	2:L:370:PHE:HB3	2.01	0.42
1:T:436:THR:HG23	1:T:458:MET:HG2	2.01	0.42
1:S:25:ILE:O	1:S:27:GLY:N	2.51	0.42
1:V:301:PHE:O	1:V:374:ARG:NH1	2.51	0.42
1:W:441:GLN:HG3	1:W:452:ALA:HB3	2.02	0.42
1:A:303:GLU:HA	1:A:338:MET:HE3	2.00	0.42
1:A:315:PHE:HD1	1:A:363:ILE:HG12	1.76	0.42
1:B:231:MET:CE	1:B:250:GLY:O	2.66	0.42
1:B:289:ALA:CB	1:B:419:PHE:HA	2.49	0.42
2:E:331:TRP:CZ2	3:E:701:ATP:H5'2	2.54	0.42
2:F:317:TYR:HA	2:F:349:ALA:O	2.20	0.42
2:F:335:PHE:HD2	2:F:346:ILE:HD11	1.84	0.42
2:D:194:TYR:O	2:D:196:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:ILE:HD12	1:G:18:ILE:N	2.34	0.42
2:K:283:ILE:HG13	2:K:400:THR:CG2	2.49	0.42
2:I:318:GLU:OE2	2:I:379:SER:OG	2.31	0.42
1:X:231:MET:HB3	1:X:235:TYR:OH	2.20	0.42
3:V:702:ATP:C2	1:W:229:SER:HA	2.54	0.42
2:E:191:ILE:HB	2:E:198:GLU:HG2	2.02	0.42
2:D:368:ASN:N	2:D:368:ASN:HD22	2.17	0.42
1:G:440:LEU:CD2	1:G:453:ILE:HD12	2.50	0.42
2:J:375:ILE:HD12	2:J:375:ILE:HG21	1.70	0.42
1:N:298:VAL:HG13	1:N:376:ALA:HB1	2.00	0.42
1:M:300:ARG:N	1:M:333:MET:HE1	2.35	0.42
2:U:295:THR:OG1	3:U:701:ATP:O1B	2.38	0.42
1:S:69:GLU:CB	1:S:70:PRO:CD	2.98	0.42
1:S:331:TRP:HA	1:S:474:ASP:O	2.19	0.42
1:W:285:LEU:HB2	1:W:434:THR:HG21	2.00	0.42
1:W:298:VAL:HA	1:W:411:LEU:HD23	2.01	0.42
1:B:300:ARG:HA	1:B:333:MET:HE1	2.00	0.42
2:D:356:LEU:HD21	2:D:387:VAL:HG11	2.01	0.42
2:K:41:SER:HA	2:K:178:THR:OG1	2.19	0.42
2:K:71:GLY:HA2	2:K:141:ARG:O	2.20	0.42
2:K:289:ALA:HB2	2:K:419:PHE:HA	2.01	0.42
2:I:216:ARG:NE	2:J:221:GLU:OE1	2.52	0.42
2:O:145:ASP:HA	2:O:146:SER:HA	1.82	0.42
1:M:202:ASP:HA	1:M:226:ARG:HE	1.84	0.42
1:P:280:LYS:O	1:P:409:THR:OG1	2.23	0.42
2:Q:184:ARG:C	2:Q:185:ILE:HD13	2.40	0.42
2:Q:432:TPO:O3P	2:Q:432:TPO:HG21	2.19	0.42
1:T:21:MET:O	1:T:35:GLY:HA3	2.19	0.42
1:X:264:SER:O	1:X:374:ARG:NH1	2.52	0.42
1:S:389:ASN:C	1:S:393:ARG:HG2	2.39	0.42
1:A:54:LEU:CD1	1:A:90:PHE:CE2	3.01	0.42
1:A:335:PHE:CD2	1:A:344:LEU:HD11	2.50	0.42
1:B:235:TYR:HD1	1:B:248:PRO:HA	1.85	0.42
2:E:291:GLY:O	2:E:451:ARG:NH1	2.53	0.42
2:F:347:VAL:O	2:F:348:CYS:C	2.58	0.42
1:G:289:ALA:HB1	1:G:419:PHE:HA	1.98	0.42
1:H:86:ASN:O	1:H:89:SER:HB3	2.20	0.42
2:K:191:ILE:HB	2:K:198:GLU:HG2	2.02	0.42
2:I:315:PHE:CE1	2:I:363:ILE:HG23	2.53	0.42
2:J:22:ARG:HH12	2:J:24:MET:HE1	1.79	0.42
2:U:289:ALA:O	2:U:292:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:263:VAL:CG1	2:E:374:ARG:NH1	2.83	0.42
2:E:336:GLU:O	2:E:340:ARG:HG3	2.20	0.42
2:F:58:GLN:HG3	2:F:92:TRP:CH2	2.55	0.42
2:F:86:ASN:O	2:F:89:SER:HB3	2.19	0.42
2:D:21:MET:CE	2:D:177:THR:HG21	2.50	0.42
1:G:288:GLY:O	1:G:415:THR:HA	2.19	0.42
1:H:262:ARG:NH1	1:H:461:SER:OG	2.42	0.42
2:K:23:THR:O	2:K:24:MET:HB2	2.18	0.42
2:K:43:LEU:HD11	2:K:182:THR:OG1	2.20	0.42
2:J:98:VAL:HA	2:J:103:LEU:O	2.20	0.42
1:R:196:VAL:HG13	1:R:197:GLU:N	2.35	0.42
1:R:353:SER:HA	1:M:250:GLY:CA	2.49	0.42
1:M:64:ILE:HA	1:M:69:GLU:O	2.20	0.42
1:X:285:LEU:CG	1:X:434:THR:HG21	2.40	0.42
1:X:393:ARG:O	1:X:397:ILE:HG12	2.19	0.42
1:A:288:GLY:O	1:A:415:THR:HA	2.19	0.42
2:E:250:GLY:HA2	2:D:353:SER:CB	2.50	0.42
2:E:300:ARG:HA	2:E:333:MET:HE1	2.01	0.42
2:F:285:LEU:HG	2:F:287:THR:HG23	2.02	0.42
2:D:24:MET:SD	2:D:67:PHE:HE2	2.43	0.42
2:K:301:PHE:CZ	2:K:374:ARG:HG2	2.55	0.42
2:K:334:ASP:O	2:K:334:ASP:CG	2.57	0.42
3:I:701:ATP:HO2'	2:J:463:HIS:CD2	2.38	0.42
2:J:208:ARG:NH2	2:J:221:GLU:OE2	2.53	0.42
1:V:42:THR:HG23	1:V:203:ASN:HB2	2.02	0.42
1:W:397:ILE:HD13	1:W:433:ILE:HD13	2.02	0.42
1:B:292:THR:HG22	1:B:442:TYR:CE2	2.55	0.42
1:B:420:MET:CE	2:C:490:ILE:HG13	2.50	0.42
1:B:453:ILE:HG22	1:B:470:PHE:HD1	1.85	0.42
2:D:171:LEU:HD22	2:D:178:THR:HG21	2.02	0.42
1:G:325:LEU:HD23	1:G:335:PHE:CB	2.49	0.42
1:G:333:MET:H	1:G:333:MET:HG2	1.42	0.42
2:L:31:ILE:CD1	2:L:246:ILE:HG21	2.50	0.42
2:L:161:ARG:HG3	2:L:196:VAL:HG11	2.01	0.42
2:L:300:ARG:N	2:L:333:MET:HE1	2.35	0.42
2:I:58:GLN:HG3	2:I:92:TRP:CH2	2.55	0.42
2:I:106:LEU:HD12	2:I:106:LEU:C	2.40	0.42
1:N:294:LYS:HB3	1:N:413:THR:HG21	2.02	0.42
1:N:300:ARG:HA	1:N:333:MET:HE1	2.00	0.42
1:M:273:MET:O	1:M:464:ASP:N	2.47	0.42
2:E:353:SER:HB2	2:F:250:GLY:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:300:ARG:N	2:F:333:MET:HE1	2.34	0.41
2:D:375:ILE:HG12	2:D:408:ILE:HG21	2.01	0.41
1:H:199:PHE:O	1:H:226:ARG:NH2	2.44	0.41
2:Q:304:ASN:O	2:Q:308:ASN:ND2	2.53	0.41
1:T:301:PHE:O	1:T:374:ARG:NH1	2.53	0.41
1:T:419:PHE:CD2	2:U:425:ILE:HD13	2.55	0.41
1:S:53:THR:HG22	1:S:145:ASP:CB	2.49	0.41
1:S:378:ASP:HA	1:S:379:SER:HA	1.72	0.41
1:V:305:ALA:HB2	1:V:374:ARG:CD	2.46	0.41
1:W:378:ASP:HA	1:W:413:THR:OG1	2.20	0.41
1:A:265:SER:CB	1:A:278:PHE:CE2	3.03	0.41
2:E:151:PHE:CE2	2:E:160:VAL:HA	2.55	0.41
2:F:66:GLU:O	2:F:67:PHE:CD1	2.70	0.41
2:I:300:ARG:HA	2:I:333:MET:HE1	2.01	0.41
2:O:74:VAL:HB	2:O:144:ILE:HA	2.00	0.41
2:Q:203:ASN:CG	2:Q:225:LEU:HD23	2.39	0.41
2:U:24:MET:SD	2:U:24:MET:N	2.93	0.41
1:A:442:TYR:CE2	1:B:456:PHE:CZ	3.08	0.41
2:C:106:LEU:C	2:C:106:LEU:HD12	2.40	0.41
2:D:46:GLY:O	2:D:52:LYS:HE2	2.20	0.41
2:D:462:TRP:O	2:D:463:HIS:HD2	2.02	0.41
1:G:19:ALA:HB1	1:G:38:ILE:HD12	2.02	0.41
2:K:151:PHE:CD2	2:K:160:VAL:HG22	2.55	0.41
2:L:191:ILE:CG2	2:L:198:GLU:HG2	2.50	0.41
2:I:36:LEU:HD22	2:I:42:THR:HG21	2.02	0.41
2:O:208:ARG:NH2	2:O:221:GLU:OE2	2.53	0.41
1:M:182:THR:HG21	1:M:192:ALA:HB1	2.01	0.41
1:B:31:ILE:HA	1:B:231:MET:SD	2.60	0.41
2:E:419:PHE:HD2	2:F:456:PHE:CE1	2.38	0.41
2:F:145:ASP:OD2	2:F:145:ASP:C	2.59	0.41
2:C:495:THR:HG22	2:D:487:GLU:OE2	2.19	0.41
1:G:300:ARG:HG3	1:G:333:MET:CE	2.50	0.41
2:L:208:ARG:O	2:L:218:ARG:HA	2.20	0.41
2:L:451:ARG:HB3	2:L:470:PHE:CE2	2.56	0.41
2:I:495:THR:HG22	2:J:487:GLU:OE2	2.20	0.41
2:Q:285:LEU:HD23	2:Q:437:ILE:HD12	2.02	0.41
1:V:61:TYR:CZ	1:V:92:TRP:CB	3.03	0.41
2:E:254:LEU:HB3	2:D:320:SER:HA	2.01	0.41
2:D:145:ASP:HA	2:D:146:SER:HA	1.79	0.41
1:G:17:ALA:C	1:G:18:ILE:HD12	2.41	0.41
1:H:392:PHE:O	1:H:395:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:21:MET:HB2	2:K:38:ILE:HG12	2.01	0.41
2:K:250:GLY:HA2	2:J:353:SER:CB	2.50	0.41
2:K:289:ALA:CB	2:K:419:PHE:HA	2.51	0.41
2:L:209:ASN:HD21	2:L:216:ARG:HB3	1.85	0.41
2:J:145:ASP:HA	2:J:146:SER:HA	1.79	0.41
1:R:390:ASN:HD21	2:Q:386:GLY:HA2	1.84	0.41
2:Q:208:ARG:NH2	2:Q:221:GLU:OE2	2.53	0.41
2:U:328:ALA:O	2:U:332:GLY:N	2.54	0.41
1:X:133:ALA:O	1:X:137:TYR:HB2	2.20	0.41
1:X:431:SEP:HB2	1:W:290:THR:HG21	2.02	0.41
1:X:490:ILE:CB	1:W:420:MET:HE3	2.50	0.41
2:F:462:TRP:CG	2:F:463:HIS:N	2.89	0.41
1:H:31:ILE:HA	1:H:231:MET:SD	2.60	0.41
2:I:353:SER:HA	2:J:250:GLY:CA	2.50	0.41
2:J:315:PHE:HB2	2:J:377:ILE:HG13	2.02	0.41
1:M:283:ILE:HG23	1:M:412:PHE:CE1	2.56	0.41
1:A:112:PRO:HG2	1:B:173:GLN:HE22	1.85	0.41
1:B:42:THR:HA	1:B:203:ASN:HB2	2.01	0.41
2:F:219:THR:HB	2:F:234:GLU:HB3	2.01	0.41
2:F:335:PHE:CD2	2:F:346:ILE:HD11	2.55	0.41
2:D:289:ALA:HB1	2:D:419:PHE:HA	2.00	0.41
1:H:58:GLN:HE21	1:H:62:ASN:HD21	1.67	0.41
2:L:52:LYS:HE3	3:L:702:ATP:O1B	2.21	0.41
2:J:171:LEU:HD22	2:J:178:THR:HG21	2.03	0.41
2:Q:203:ASN:HB3	2:Q:225:LEU:HD23	2.02	0.41
2:Q:289:ALA:O	2:Q:292:THR:OG1	2.31	0.41
1:V:216:ARG:HG2	1:W:233:GLY:HA2	2.02	0.41
1:V:451:ARG:NH2	3:V:701:ATP:O2'	2.48	0.41
2:E:442:TYR:CE2	2:F:456:PHE:CE2	2.91	0.41
2:F:384:ALA:HB2	2:F:392:PHE:CZ	2.55	0.41
2:F:483:PHE:HB2	2:F:489:ILE:HD11	2.03	0.41
2:C:145:ASP:HA	2:C:146:SER:HA	1.78	0.41
1:H:376:ALA:HA	1:H:411:LEU:O	2.20	0.41
2:L:300:ARG:CA	2:L:333:MET:HE1	2.51	0.41
1:N:418:GLN:HA	2:O:424:SER:HB3	2.03	0.41
2:O:378:ASP:HA	2:O:379:SER:HA	1.86	0.41
2:Q:436:THR:HG23	2:Q:458:MET:HG2	2.03	0.41
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.56	0.41
1:B:328:ALA:HB1	1:B:335:PHE:CE1	2.56	0.41
2:E:284:ILE:HB	2:E:411:LEU:HD12	2.02	0.41
2:F:315:PHE:CE2	2:F:363:ILE:HG23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:LEU:HB2	2:D:434:THR:CG2	2.45	0.41
1:G:31:ILE:HD11	1:G:246:ILE:HG21	2.03	0.41
1:G:328:ALA:HB2	1:G:335:PHE:CD1	2.56	0.41
1:G:392:PHE:O	1:G:395:PHE:HB3	2.21	0.41
2:K:456:PHE:CZ	2:J:442:TYR:CE1	3.09	0.41
2:L:76:PHE:N	2:L:76:PHE:CD1	2.88	0.41
2:L:367:ILE:O	2:L:371:LYS:N	2.53	0.41
2:I:91:GLY:C	2:I:92:TRP:CD1	2.75	0.41
2:I:145:ASP:HA	2:I:146:SER:HA	1.77	0.41
2:J:53:THR:HA	2:J:145:ASP:OD1	2.21	0.41
1:R:426:THR:OG1	1:R:431:SEP:O1P	2.36	0.41
1:M:273:MET:SD	1:M:468:ARG:HD2	2.60	0.41
1:M:458:MET:HB2	1:M:463:HIS:HB3	2.03	0.41
1:P:42:THR:HG23	1:P:203:ASN:HB2	2.03	0.41
2:U:41:SER:HA	2:U:178:THR:O	2.21	0.41
1:X:229:SER:HB3	3:W:702:ATP:C2	2.55	0.41
1:X:289:ALA:O	1:X:292:THR:OG1	2.38	0.41
1:S:317:TYR:N	1:S:378:ASP:O	2.54	0.41
1:B:52:LYS:NZ	3:B:702:ATP:O3G	2.54	0.41
1:B:375:ILE:HG22	1:B:410:GLY:HA2	2.03	0.41
2:F:378:ASP:HA	2:F:379:SER:HA	1.87	0.41
1:G:417:ASP:OD2	1:H:429:HIS:CG	2.74	0.41
2:K:283:ILE:HG21	2:K:400:THR:HG23	2.03	0.41
2:J:368:ASN:HD22	2:J:368:ASN:N	2.19	0.41
1:M:44:VAL:HA	1:M:205:VAL:O	2.21	0.41
1:M:440:LEU:HD21	1:M:453:ILE:HD13	2.03	0.41
1:W:385:ARG:NH2	1:W:417:ASP:OD1	2.53	0.41
1:A:186:GLU:OE2	1:A:188:TYR:N	2.44	0.40
1:A:245:ASN:C	1:A:245:ASN:HD22	2.25	0.40
2:E:283:ILE:HG13	2:E:400:THR:CG2	2.51	0.40
2:F:93:ASP:OD1	2:F:95:ALA:HB3	2.21	0.40
2:L:471:MET:N	2:L:471:MET:SD	2.94	0.40
1:T:429:HIS:HA	1:T:431:SEP:O2P	2.20	0.40
1:A:462:TRP:O	1:A:463:HIS:CD2	2.74	0.40
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.56	0.40
2:E:463:HIS:CD2	3:D:701:ATP:HO2'	2.39	0.40
2:C:145:ASP:HA	2:C:181:THR:HB	2.03	0.40
2:D:57:ILE:CD1	2:D:83:ILE:HG23	2.48	0.40
1:G:274:CYS:HG	1:G:278:PHE:HE2	1.68	0.40
1:G:279:PHE:CD2	2:L:326:ARG:NH1	2.89	0.40
1:R:145:ASP:HA	1:R:146:SER:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:389:ASN:HD21	1:X:428:SER:HA	1.86	0.40
1:V:419:PHE:CZ	1:W:425:ILE:CD1	2.98	0.40
1:B:225:LEU:HD12	1:B:230:HIS:HB3	2.03	0.40
1:G:456:PHE:C	1:G:456:PHE:CD2	2.94	0.40
2:K:110:PRO:HG2	2:L:165:PHE:CE2	2.56	0.40
2:L:58:GLN:HG3	2:L:92:TRP:CH2	2.56	0.40
2:I:269:ARG:HG2	2:I:479:ILE:HB	2.02	0.40
1:P:357:GLU:CD	1:P:357:GLU:H	2.24	0.40
1:X:40:ARG:O	1:X:177:THR:HA	2.21	0.40
1:A:31:ILE:HG22	1:A:222:ILE:HD12	2.02	0.40
1:A:170:ARG:O	1:A:174:ILE:HG12	2.20	0.40
3:B:702:ATP:C2	2:C:229:SER:HB3	2.57	0.40
2:E:289:ALA:CB	2:E:419:PHE:HA	2.51	0.40
2:E:347:VAL:HG21	2:E:366:GLU:HG2	2.04	0.40
2:C:64:ILE:HG21	2:C:97:LEU:HD13	2.03	0.40
1:G:49:GLY:HA3	1:H:224:LYS:HB3	2.03	0.40
1:G:231:MET:HB3	1:G:235:TYR:OH	2.20	0.40
1:H:160:VAL:HG21	1:H:194:TYR:CD1	2.56	0.40
2:K:483:PHE:HB3	2:K:486:PHE:HD1	1.87	0.40
2:L:55:PHE:CD2	2:L:55:PHE:C	2.95	0.40
2:I:393:ARG:O	2:I:397:ILE:HG12	2.21	0.40
2:J:438:ILE:CG2	2:J:453:ILE:HD11	2.51	0.40
1:R:47:THR:O	1:R:50:THR:OG1	2.38	0.40
1:M:261:VAL:HG12	1:M:262:ARG:H	1.87	0.40
1:S:27:GLY:HA3	1:S:246:ILE:HB	2.03	0.40
1:S:418:GLN:HE21	1:S:418:GLN:HB2	1.68	0.40
1:V:287:THR:HA	1:V:414:ASN:O	2.21	0.40
1:V:378:ASP:HA	1:V:379:SER:HA	1.93	0.40
1:V:392:PHE:HE2	1:V:430:ILE:HG12	1.87	0.40
1:W:379:SER:CB	1:W:413:THR:OG1	2.69	0.40
1:A:333:MET:H	1:A:333:MET:HG2	1.43	0.40
1:B:199:PHE:O	1:B:226:ARG:NH2	2.44	0.40
2:E:71:GLY:HA2	2:E:141:ARG:O	2.22	0.40
2:F:24:MET:HB2	2:F:62:ASN:HB3	2.03	0.40
2:F:293:GLY:N	3:F:701:ATP:O1B	2.49	0.40
2:D:299:SER:C	2:D:333:MET:HE1	2.41	0.40
1:G:221:GLU:OE1	2:L:216:ARG:NE	2.52	0.40
2:L:298:VAL:HA	2:L:411:LEU:HD23	2.03	0.40
2:I:385:ARG:HD2	2:J:393:ARG:HD3	2.03	0.40
2:J:266:GLY:HA2	2:J:304:ASN:HD22	1.86	0.40
2:O:61:TYR:CE1	2:O:92:TRP:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:317:TYR:HB3	2:Q:351:PRO:HG3	2.04	0.40
1:T:58:GLN:HE21	1:T:58:GLN:N	2.20	0.40

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	461/519 (89%)	433 (94%)	22 (5%)	6 (1%)	12	42
1	B	462/519 (89%)	431 (93%)	24 (5%)	7 (2%)	10	39
1	G	458/519 (88%)	433 (94%)	23 (5%)	2 (0%)	34	69
1	H	459/519 (88%)	430 (94%)	26 (6%)	3 (1%)	22	57
1	M	456/519 (88%)	410 (90%)	39 (9%)	7 (2%)	10	39
1	N	442/519 (85%)	387 (88%)	43 (10%)	12 (3%)	5	25
1	P	445/519 (86%)	400 (90%)	39 (9%)	6 (1%)	12	42
1	R	454/519 (88%)	414 (91%)	35 (8%)	5 (1%)	14	46
1	S	423/519 (82%)	360 (85%)	55 (13%)	8 (2%)	8	33
1	T	380/519 (73%)	299 (79%)	67 (18%)	14 (4%)	3	19
1	V	412/519 (79%)	359 (87%)	50 (12%)	3 (1%)	22	57
1	W	453/519 (87%)	386 (85%)	57 (13%)	10 (2%)	6	29
1	X	452/519 (87%)	408 (90%)	31 (7%)	13 (3%)	4	24
2	C	464/519 (89%)	428 (92%)	31 (7%)	5 (1%)	14	46
2	D	463/519 (89%)	419 (90%)	34 (7%)	10 (2%)	6	29
2	E	462/519 (89%)	427 (92%)	26 (6%)	9 (2%)	8	33
2	F	458/519 (88%)	432 (94%)	19 (4%)	7 (2%)	10	39
2	I	465/519 (90%)	430 (92%)	33 (7%)	2 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	458/519 (88%)	414 (90%)	36 (8%)	8 (2%)	9	36
2	K	463/519 (89%)	427 (92%)	26 (6%)	10 (2%)	6	29
2	L	460/519 (89%)	431 (94%)	23 (5%)	6 (1%)	12	42
2	O	449/519 (86%)	399 (89%)	40 (9%)	10 (2%)	6	29
2	Q	458/519 (88%)	416 (91%)	38 (8%)	4 (1%)	17	52
2	U	404/519 (78%)	340 (84%)	53 (13%)	11 (3%)	5	25
All	All	10761/12456 (86%)	9713 (90%)	870 (8%)	178 (2%)	9	36

All (178) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ARG
1	A	256	GLN
1	B	252	MET
1	B	254	LEU
1	B	348	CYS
1	B	463	HIS
2	E	156	ALA
2	E	251	ALA
2	E	333	MET
2	E	335	PHE
2	F	17	ALA
2	F	348	CYS
2	C	122	ASP
2	C	198	GLU
2	D	111	ASP
2	D	116	GLU
2	D	333	MET
2	D	354	ALA
2	D	462	TRP
2	D	463	HIS
1	H	463	HIS
2	K	156	ALA
2	K	251	ALA
2	K	333	MET
2	K	335	PHE
2	L	17	ALA
2	L	348	CYS
2	L	462	TRP
2	L	463	HIS

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Mol	Chain	Res	Type
2	I	198	GLU
2	I	463	HIS
2	J	111	ASP
2	J	333	MET
2	J	354	ALA
2	J	462	TRP
1	N	26	GLU
1	N	204	VAL
2	O	455	VAL
2	O	456	PHE
1	R	226	ARG
1	P	463	HIS
2	Q	253	ARG
1	T	26	GLU
1	T	137	TYR
1	T	185	ILE
1	T	313	ILE
1	T	341	GLN
1	T	370	PHE
1	T	463	HIS
2	U	40	ARG
2	U	225	LEU
2	U	226	ARG
2	U	342	ASN
1	X	463	HIS
1	S	26	GLU
1	V	26	GLU
1	W	77	GLU
1	W	485	ASN
1	A	463	HIS
1	B	251	ALA
2	E	250	GLY
2	E	254	LEU
2	E	463	HIS
2	F	462	TRP
2	C	463	HIS
2	D	252	MET
1	G	463	HIS
2	K	250	GLY
2	K	254	LEU
2	K	463	HIS
2	J	463	HIS

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Mol	Chain	Res	Type
1	N	66	GLU
2	O	463	HIS
1	M	338	MET
1	M	370	PHE
1	P	26	GLU
1	P	77	GLU
1	P	370	PHE
2	Q	463	HIS
1	T	107	ASP
1	T	201	SER
1	T	384	ALA
2	U	344	LEU
1	X	185	ILE
1	X	196	VAL
1	X	213	GLY
1	X	309	LYS
1	S	43	LEU
1	S	175	GLY
1	S	197	GLU
1	S	199	PHE
1	S	261	VAL
1	V	66	GLU
1	W	149	SER
1	W	475	LYS
1	W	480	LYS
2	F	463	HIS
2	D	115	GLN
1	H	348	CYS
2	J	115	GLN
1	N	88	ARG
1	N	213	GLY
1	N	422	ALA
2	O	18	ILE
2	O	26	GLU
2	O	153	GLN
2	O	293	GLY
2	O	315	PHE
2	O	459	ARG
1	R	112	PRO
1	R	463	HIS
2	Q	26	GLU
1	T	77	GLU

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Mol	Chain	Res	Type
1	T	105	ILE
1	X	26	GLU
1	X	68	ASP
1	X	195	GLY
1	X	348	CYS
1	X	479	ILE
1	S	422	ALA
1	W	21	MET
1	W	474	ASP
1	A	249	LEU
1	A	348	CYS
1	B	147	VAL
2	K	26	GLU
2	L	112	PRO
1	N	51	GLY
1	N	197	GLU
1	N	463	HIS
1	R	196	VAL
1	M	26	GLU
1	M	67	PHE
1	P	248	PRO
1	P	420	MET
2	U	341	GLN
2	U	407	GLU
1	W	33	HIS
2	E	26	GLU
2	F	112	PRO
2	C	156	ALA
2	C	348	CYS
2	D	213	GLY
2	K	497	ILE
2	J	213	GLY
2	O	348	CYS
1	R	293	GLY
1	M	193	ARG
1	M	289	ALA
1	T	193	ARG
2	U	26	GLU
1	X	77	GLU
1	X	480	LYS
1	W	112	PRO
2	E	112	PRO

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Mol	Chain	Res	Type
2	F	77	GLU
1	G	197	GLU
2	K	112	PRO
1	N	348	CYS
2	Q	293	GLY
1	W	186	GLU
1	N	65	ILE
1	T	266	GLY
2	U	150	VAL
1	X	18	ILE
1	A	347	VAL
2	F	293	GLY
2	J	110	PRO
1	N	293	GLY
2	U	127	ILE
2	U	445	ILE
2	D	110	PRO
2	L	293	GLY
1	M	248	PRO
1	H	147	VAL
1	B	213	GLY
1	S	266	GLY
1	V	490	ILE

### 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	351/443 (79%)	310 (88%)	41 (12%)	5	22
1	B	328/443 (74%)	294 (90%)	34 (10%)	7	27
1	G	338/443 (76%)	299 (88%)	39 (12%)	5	22
1	H	341/443 (77%)	301 (88%)	40 (12%)	5	22
1	M	247/443 (56%)	221 (90%)	26 (10%)	7	26
1	N	222/443 (50%)	198 (89%)	24 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	249/443 (56%)	221 (89%)	28 (11%)	6	24
1	R	270/443 (61%)	250 (93%)	20 (7%)	13	42
1	S	155/443 (35%)	138 (89%)	17 (11%)	6	25
1	T	109/443 (25%)	93 (85%)	16 (15%)	3	13
1	V	221/443 (50%)	188 (85%)	33 (15%)	3	13
1	W	242/443 (55%)	212 (88%)	30 (12%)	4	19
1	X	239/443 (54%)	217 (91%)	22 (9%)	9	33
2	C	323/442 (73%)	293 (91%)	30 (9%)	9	32
2	D	332/442 (75%)	291 (88%)	41 (12%)	4	19
2	E	324/442 (73%)	289 (89%)	35 (11%)	6	25
2	F	327/442 (74%)	294 (90%)	33 (10%)	7	28
2	I	334/442 (76%)	299 (90%)	35 (10%)	7	26
2	J	330/442 (75%)	293 (89%)	37 (11%)	6	24
2	K	330/442 (75%)	300 (91%)	30 (9%)	9	33
2	L	336/442 (76%)	295 (88%)	41 (12%)	5	19
2	O	237/442 (54%)	211 (89%)	26 (11%)	6	25
2	Q	289/442 (65%)	257 (89%)	32 (11%)	6	24
2	U	151/442 (34%)	131 (87%)	20 (13%)	4	17
All	All	6625/10621 (62%)	5895 (89%)	730 (11%)	6	25

All (730) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	50	THR
1	A	52	LYS
1	A	55	PHE
1	A	57	ILE
1	A	78	GLU
1	A	79	THR
1	A	102	LYS
1	A	145	ASP
1	A	180	MET
1	A	183	GLU
1	A	186	GLU
1	A	223	LEU

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Mol	Chain	Res	Type
1	A	228	THR
1	A	234	GLU
1	A	238	THR
1	A	245	ASN
1	A	247	PHE
1	A	256	GLN
1	A	270	LEU
1	A	287	THR
1	A	300	ARG
1	A	315	PHE
1	A	318	GLU
1	A	324	LEU
1	A	344	LEU
1	A	352	GLU
1	A	356	LEU
1	A	360	LEU
1	A	389	ASN
1	A	409	THR
1	A	416	SER
1	A	417	ASP
1	A	418	GLN
1	A	424	SER
1	A	425	ILE
1	A	428	SER
1	A	458	MET
1	A	485	ASN
1	A	488	ARG
1	A	497	ILE
1	B	23	THR
1	B	24	MET
1	B	50	THR
1	B	67	PHE
1	B	75	THR
1	B	79	THR
1	B	89	SER
1	B	106	LEU
1	B	148	THR
1	B	166	ARG
1	B	183	GLU
1	B	212	GLU
1	B	217	ARG
1	B	218	ARG

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Mol	Chain	Res	Type
1	B	223	LEU
1	B	228	THR
1	B	232	LYS
1	B	238	THR
1	B	245	ASN
1	B	256	GLN
1	B	270	LEU
1	B	344	LEU
1	B	356	LEU
1	B	360	LEU
1	B	369	ASP
1	B	375	ILE
1	B	389	ASN
1	B	400	THR
1	B	428	SER
1	B	439	LEU
1	B	450	SER
1	B	454	ASN
1	B	458	MET
1	B	468	ARG
2	E	22	ARG
2	E	24	MET
2	E	55	PHE
2	E	58	GLN
2	E	79	THR
2	E	81	GLN
2	E	90	PHE
2	E	151	PHE
2	E	171	LEU
2	E	177	THR
2	E	193	ARG
2	E	201	SER
2	E	218	ARG
2	E	221	GLU
2	E	228	THR
2	E	232	LYS
2	E	245	ASN
2	E	255	THR
2	E	270	LEU
2	E	280	LYS
2	E	294	LYS
2	E	300	ARG

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Mol	Chain	Res	Type
2	E	318	GLU
2	E	333	MET
2	E	344	LEU
2	E	352	GLU
2	E	356	LEU
2	E	360	LEU
2	E	413	THR
2	E	419	PHE
2	E	425	ILE
2	E	450	SER
2	E	451	ARG
2	E	474	ASP
2	E	493	SER
2	F	24	MET
2	F	75	THR
2	F	79	THR
2	F	89	SER
2	F	106	LEU
2	F	129	ARG
2	F	135	GLN
2	F	149	SER
2	F	161	ARG
2	F	178	THR
2	F	182	THR
2	F	184	ARG
2	F	201	SER
2	F	221	GLU
2	F	228	THR
2	F	232	LYS
2	F	270	LEU
2	F	281	ASP
2	F	300	ARG
2	F	303	GLU
2	F	333	MET
2	F	338	MET
2	F	360	LEU
2	F	366	GLU
2	F	375	ILE
2	F	405	GLN
2	F	406	GLU
2	F	413	THR
2	F	418	GLN

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Mol	Chain	Res	Type
2	F	448	GLU
2	F	450	SER
2	F	471	MET
2	F	493	SER
2	C	21	MET
2	C	24	MET
2	C	50	THR
2	C	52	LYS
2	C	103	LEU
2	C	106	LEU
2	C	149	SER
2	C	172	LYS
2	C	178	THR
2	C	184	ARG
2	C	212	GLU
2	C	228	THR
2	C	241	ASP
2	C	245	ASN
2	C	254	LEU
2	C	263	VAL
2	C	270	LEU
2	C	294	LYS
2	C	300	ARG
2	C	333	MET
2	C	352	GLU
2	C	356	LEU
2	C	360	LEU
2	C	413	THR
2	C	416	SER
2	C	418	GLN
2	C	419	PHE
2	C	425	ILE
2	C	458	MET
2	C	462	TRP
2	D	24	MET
2	D	41	SER
2	D	45	SER
2	D	57	ILE
2	D	85	LYS
2	D	93	ASP
2	D	143	SER
2	D	173	GLN

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Mol	Chain	Res	Type
2	D	177	THR
2	D	182	THR
2	D	198	GLU
2	D	212	GLU
2	D	215	ARG
2	D	223	LEU
2	D	234	GLU
2	D	235	TYR
2	D	245	ASN
2	D	256	GLN
2	D	263	VAL
2	D	270	LEU
2	D	284	ILE
2	D	300	ARG
2	D	325	LEU
2	D	337	GLU
2	D	344	LEU
2	D	356	LEU
2	D	360	LEU
2	D	368	ASN
2	D	375	ILE
2	D	385	ARG
2	D	394	GLN
2	D	409	THR
2	D	414	ASN
2	D	419	PHE
2	D	425	ILE
2	D	428	SER
2	D	458	MET
2	D	461	SER
2	D	474	ASP
2	D	485	ASN
2	D	489	ILE
1	G	21	MET
1	G	24	MET
1	G	50	THR
1	G	52	LYS
1	G	57	ILE
1	G	78	GLU
1	G	79	THR
1	G	99	ASP
1	G	145	ASP

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Mol	Chain	Res	Type
1	G	182	THR
1	G	183	GLU
1	G	186	GLU
1	G	194	TYR
1	G	223	LEU
1	G	228	THR
1	G	234	GLU
1	G	238	THR
1	G	256	GLN
1	G	270	LEU
1	G	287	THR
1	G	300	ARG
1	G	318	GLU
1	G	344	LEU
1	G	352	GLU
1	G	356	LEU
1	G	360	LEU
1	G	389	ASN
1	G	406	GLU
1	G	416	SER
1	G	417	ASP
1	G	418	GLN
1	G	424	SER
1	G	425	ILE
1	G	428	SER
1	G	456	PHE
1	G	458	MET
1	G	474	ASP
1	G	488	ARG
1	G	489	ILE
1	H	23	THR
1	H	24	MET
1	H	40	ARG
1	H	50	THR
1	H	75	THR
1	H	77	GLU
1	H	79	THR
1	H	89	SER
1	H	90	PHE
1	H	148	THR
1	H	183	GLU
1	H	186	GLU

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Mol	Chain	Res	Type
1	H	215	ARG
1	H	217	ARG
1	H	218	ARG
1	H	223	LEU
1	H	228	THR
1	H	232	LYS
1	H	238	THR
1	H	245	ASN
1	H	254	LEU
1	H	256	GLN
1	H	270	LEU
1	H	284	ILE
1	H	318	GLU
1	H	344	LEU
1	H	356	LEU
1	H	360	LEU
1	H	375	ILE
1	H	389	ASN
1	H	400	THR
1	H	418	GLN
1	H	428	SER
1	H	439	LEU
1	H	450	SER
1	H	454	ASN
1	H	458	MET
1	H	468	ARG
1	H	471	MET
1	H	480	LYS
2	K	22	ARG
2	K	24	MET
2	K	79	THR
2	K	81	GLN
2	K	106	LEU
2	K	151	PHE
2	K	177	THR
2	K	193	ARG
2	K	201	SER
2	K	221	GLU
2	K	228	THR
2	K	232	LYS
2	K	245	ASN
2	K	254	LEU

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Mol	Chain	Res	Type
2	K	255	THR
2	K	270	LEU
2	K	280	LYS
2	K	300	ARG
2	K	333	MET
2	K	344	LEU
2	K	352	GLU
2	K	356	LEU
2	K	360	LEU
2	K	374	ARG
2	K	425	ILE
2	K	450	SER
2	K	451	ARG
2	K	458	MET
2	K	474	ASP
2	K	493	SER
2	L	18	ILE
2	L	24	MET
2	L	67	PHE
2	L	75	THR
2	L	79	THR
2	L	89	SER
2	L	106	LEU
2	L	135	GLN
2	L	138	ARG
2	L	149	SER
2	L	161	ARG
2	L	178	THR
2	L	182	THR
2	L	184	ARG
2	L	191	ILE
2	L	196	VAL
2	L	201	SER
2	L	212	GLU
2	L	223	LEU
2	L	228	THR
2	L	232	LYS
2	L	245	ASN
2	L	270	LEU
2	L	278	PHE
2	L	281	ASP
2	L	283	ILE

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Mol	Chain	Res	Type
2	L	300	ARG
2	L	303	GLU
2	L	333	MET
2	L	360	LEU
2	L	366	GLU
2	L	375	ILE
2	L	405	GLN
2	L	406	GLU
2	L	413	THR
2	L	418	GLN
2	L	448	GLU
2	L	450	SER
2	L	451	ARG
2	L	471	MET
2	L	493	SER
2	I	24	MET
2	I	26	GLU
2	I	50	THR
2	I	92	TRP
2	I	106	LEU
2	I	145	ASP
2	I	149	SER
2	I	172	LYS
2	I	178	THR
2	I	182	THR
2	I	217	ARG
2	I	223	LEU
2	I	228	THR
2	I	241	ASP
2	I	245	ASN
2	I	254	LEU
2	I	263	VAL
2	I	270	LEU
2	I	294	LYS
2	I	300	ARG
2	I	303	GLU
2	I	333	MET
2	I	347	VAL
2	I	352	GLU
2	I	356	LEU
2	I	360	LEU
2	I	374	ARG

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Mol	Chain	Res	Type
2	I	395	PHE
2	I	413	THR
2	I	416	SER
2	I	418	GLN
2	I	425	ILE
2	I	445	ILE
2	I	458	MET
2	I	462	TRP
2	J	24	MET
2	J	41	SER
2	J	45	SER
2	J	57	ILE
2	J	93	ASP
2	J	143	SER
2	J	173	GLN
2	J	177	THR
2	J	182	THR
2	J	198	GLU
2	J	212	GLU
2	J	223	LEU
2	J	228	THR
2	J	234	GLU
2	J	245	ASN
2	J	256	GLN
2	J	263	VAL
2	J	270	LEU
2	J	284	ILE
2	J	300	ARG
2	J	325	LEU
2	J	337	GLU
2	J	356	LEU
2	J	360	LEU
2	J	368	ASN
2	J	375	ILE
2	J	394	GLN
2	J	409	THR
2	J	419	PHE
2	J	425	ILE
2	J	428	SER
2	J	451	ARG
2	J	458	MET
2	J	461	SER

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Mol	Chain	Res	Type
2	J	474	ASP
2	J	485	ASN
2	J	489	ILE
1	N	24	MET
1	N	178	THR
1	N	208	ARG
1	N	215	ARG
1	N	221	GLU
1	N	228	THR
1	N	256	GLN
1	N	263	VAL
1	N	270	LEU
1	N	271	ASP
1	N	294	LYS
1	N	300	ARG
1	N	344	LEU
1	N	348	CYS
1	N	360	LEU
1	N	368	ASN
1	N	417	ASP
1	N	423	HIS
1	N	435	ASP
1	N	458	MET
1	N	463	HIS
1	N	470	PHE
1	N	471	MET
1	N	495	THR
2	O	43	LEU
2	O	50	THR
2	O	173	GLN
2	O	207	LEU
2	O	217	ARG
2	O	218	ARG
2	O	221	GLU
2	O	224	LYS
2	O	247	PHE
2	O	284	ILE
2	O	294	LYS
2	O	300	ARG
2	O	326	ARG
2	O	339	GLU
2	O	344	LEU

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Mol	Chain	Res	Type
2	O	356	LEU
2	O	360	LEU
2	O	394	GLN
2	O	418	GLN
2	O	423	HIS
2	O	428	SER
2	O	434	THR
2	O	440	LEU
2	O	449	MET
2	O	451	ARG
2	O	465	LYS
1	R	20	LYS
1	R	24	MET
1	R	50	THR
1	R	82	ASP
1	R	92	TRP
1	R	182	THR
1	R	223	LEU
1	R	259	SER
1	R	294	LYS
1	R	300	ARG
1	R	333	MET
1	R	352	GLU
1	R	409	THR
1	R	413	THR
1	R	418	GLN
1	R	427	ASP
1	R	429	HIS
1	R	458	MET
1	R	465	LYS
1	R	470	PHE
1	M	24	MET
1	M	40	ARG
1	M	56	SER
1	M	178	THR
1	M	182	THR
1	M	185	ILE
1	M	201	SER
1	M	224	LYS
1	M	226	ARG
1	M	254	LEU
1	M	294	LYS

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Mol	Chain	Res	Type
1	M	311	ARG
1	M	333	MET
1	M	344	LEU
1	M	366	GLU
1	M	387	VAL
1	M	406	GLU
1	M	415	THR
1	M	418	GLN
1	M	420	MET
1	M	428	SER
1	M	433	ILE
1	M	435	ASP
1	M	458	MET
1	M	463	HIS
1	M	493	SER
1	P	33	HIS
1	P	92	TRP
1	P	148	THR
1	P	184	ARG
1	P	212	GLU
1	P	217	ARG
1	P	218	ARG
1	P	223	LEU
1	P	259	SER
1	P	270	LEU
1	P	281	ASP
1	P	287	THR
1	P	294	LYS
1	P	300	ARG
1	P	303	GLU
1	P	319	GLU
1	P	323	GLN
1	P	324	LEU
1	P	352	GLU
1	P	366	GLU
1	P	389	ASN
1	P	418	GLN
1	P	425	ILE
1	P	432	THR
1	P	458	MET
1	P	465	LYS
1	P	470	PHE

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Mol	Chain	Res	Type
1	P	471	MET
2	Q	24	MET
2	Q	33	HIS
2	Q	47	THR
2	Q	50	THR
2	Q	78	GLU
2	Q	178	THR
2	Q	180	MET
2	Q	182	THR
2	Q	183	GLU
2	Q	184	ARG
2	Q	185	ILE
2	Q	187	GLU
2	Q	215	ARG
2	Q	218	ARG
2	Q	224	LYS
2	Q	256	GLN
2	Q	263	VAL
2	Q	270	LEU
2	Q	292	THR
2	Q	300	ARG
2	Q	309	LYS
2	Q	320	SER
2	Q	333	MET
2	Q	356	LEU
2	Q	360	LEU
2	Q	393	ARG
2	Q	406	GLU
2	Q	423	HIS
2	Q	428	SER
2	Q	448	GLU
2	Q	458	MET
2	Q	474	ASP
1	T	58	GLN
1	T	182	THR
1	T	209	ASN
1	T	287	THR
1	T	294	LYS
1	T	300	ARG
1	T	318	GLU
1	T	331	TRP
1	T	364	LYS

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Mol	Chain	Res	Type
1	T	378	ASP
1	T	411	LEU
1	T	413	THR
1	T	449	MET
1	T	458	MET
1	T	461	SER
1	T	463	HIS
2	U	23	THR
2	U	24	MET
2	U	92	TRP
2	U	106	LEU
2	U	184	ARG
2	U	217	ARG
2	U	230	HIS
2	U	258	SER
2	U	284	ILE
2	U	292	THR
2	U	294	LYS
2	U	319	GLU
2	U	339	GLU
2	U	357	GLU
2	U	380	LEU
2	U	383	LEU
2	U	411	LEU
2	U	426	THR
2	U	458	MET
2	U	463	HIS
1	X	45	SER
1	X	52	LYS
1	X	143	SER
1	X	178	THR
1	X	215	ARG
1	X	228	THR
1	X	270	LEU
1	X	280	LYS
1	X	285	LEU
1	X	290	THR
1	X	292	THR
1	X	294	LYS
1	X	300	ARG
1	X	333	MET
1	X	356	LEU

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Mol	Chain	Res	Type
1	X	381	SER
1	X	411	LEU
1	X	420	MET
1	X	430	ILE
1	X	432	THR
1	X	458	MET
1	X	462	TRP
1	S	52	LYS
1	S	81	GLN
1	S	224	LYS
1	S	258	SER
1	S	301	PHE
1	S	361	GLN
1	S	381	SER
1	S	393	ARG
1	S	409	THR
1	S	415	THR
1	S	420	MET
1	S	425	ILE
1	S	433	ILE
1	S	435	ASP
1	S	451	ARG
1	S	458	MET
1	S	471	MET
1	V	24	MET
1	V	42	THR
1	V	47	THR
1	V	53	THR
1	V	68	ASP
1	V	182	THR
1	V	187	GLU
1	V	203	ASN
1	V	208	ARG
1	V	209	ASN
1	V	215	ARG
1	V	217	ARG
1	V	225	LEU
1	V	241	ASP
1	V	258	SER
1	V	263	VAL
1	V	270	LEU
1	V	281	ASP

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Mol	Chain	Res	Type
1	V	294	LYS
1	V	296	LEU
1	V	300	ARG
1	V	323	GLN
1	V	324	LEU
1	V	333	MET
1	V	343	LEU
1	V	366	GLU
1	V	413	THR
1	V	419	PHE
1	V	428	SER
1	V	450	SER
1	V	451	ARG
1	V	458	MET
1	V	469	GLU
1	W	33	HIS
1	W	161	ARG
1	W	173	GLN
1	W	177	THR
1	W	182	THR
1	W	184	ARG
1	W	193	ARG
1	W	209	ASN
1	W	215	ARG
1	W	245	ASN
1	W	292	THR
1	W	294	LYS
1	W	310	GLU
1	W	318	GLU
1	W	352	GLU
1	W	356	LEU
1	W	358	ASP
1	W	360	LEU
1	W	361	GLN
1	W	385	ARG
1	W	419	PHE
1	W	425	ILE
1	W	428	SER
1	W	430	ILE
1	W	433	ILE
1	W	439	LEU
1	W	451	ARG

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Mol	Chain	Res	Type
1	W	453	ILE
1	W	458	MET
1	W	469	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	260	ASN
1	A	342	ASN
1	A	389	ASN
1	A	441	GLN
1	B	62	ASN
1	B	173	GLN
1	B	209	ASN
1	B	260	ASN
1	B	368	ASN
1	B	389	ASN
1	B	441	GLN
2	E	308	ASN
2	E	323	GLN
2	E	389	ASN
2	E	414	ASN
2	E	441	GLN
2	F	209	ASN
2	F	389	ASN
2	C	209	ASN
2	C	414	ASN
2	C	418	GLN
2	D	33	HIS
2	D	62	ASN
2	D	209	ASN
2	D	368	ASN
2	D	414	ASN
1	G	389	ASN
1	G	441	GLN
1	H	62	ASN
1	H	209	ASN
1	H	260	ASN
1	H	368	ASN
1	H	389	ASN
1	H	418	GLN

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Mol	Chain	Res	Type
2	K	33	HIS
2	K	209	ASN
2	K	308	ASN
2	K	389	ASN
2	K	414	ASN
2	K	441	GLN
2	L	209	ASN
2	L	389	ASN
2	L	441	GLN
2	I	209	ASN
2	I	418	GLN
2	J	62	ASN
2	J	209	ASN
2	J	368	ASN
2	J	389	ASN
2	J	414	ASN
1	N	209	ASN
1	N	342	ASN
1	N	368	ASN
1	N	414	ASN
1	N	423	HIS
1	N	454	ASN
2	O	327	ASN
2	O	414	ASN
1	R	308	ASN
1	R	418	GLN
1	R	429	HIS
1	R	441	GLN
1	R	454	ASN
1	M	209	ASN
1	P	209	ASN
1	P	323	GLN
1	P	389	ASN
2	Q	256	GLN
2	Q	368	ASN
2	Q	389	ASN
2	Q	418	GLN
1	T	58	GLN
1	T	209	ASN
1	T	389	ASN
1	T	414	ASN
2	U	390	ASN

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Mol	Chain	Res	Type
2	U	441	GLN
1	X	389	ASN
1	X	418	GLN
1	X	429	HIS
1	S	260	ASN
1	S	414	ASN
1	S	418	GLN
1	V	323	GLN
1	V	368	ASN
1	W	341	GLN
1	W	361	GLN
1	W	368	ASN
1	W	389	ASN
1	W	418	GLN
1	W	454	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

35 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	SEP	P	431	1	8,9,10	0.62	0	8,12,14	0.62	0
2	SEP	K	431	2	8,9,10	0.59	0	8,12,14	0.83	0
2	TPO	J	432	2	8,10,11	0.87	1 (12%)	10,14,16	0.86	0
2	SEP	J	431	2	8,9,10	0.68	0	8,12,14	0.57	0
1	SEP	S	431	1	8,9,10	0.61	0	8,12,14	0.61	0
2	TPO	L	432	2	8,10,11	1.50	2 (25%)	10,14,16	0.91	0
1	SEP	M	431	1	8,9,10	0.65	0	8,12,14	0.61	0
2	TPO	O	432	2	8,10,11	0.99	1 (12%)	10,14,16	1.03	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SEP	D	431	2	8,9,10	0.68	0	8,12,14	0.57	0
2	TPO	E	432	2	8,10,11	1.32	1 (12%)	10,14,16	1.09	0
2	TPO	I	432	2	8,10,11	1.41	2 (25%)	10,14,16	0.82	0
1	SEP	T	431	1	8,9,10	0.74	0	8,12,14	0.74	0
1	SEP	V	431	1	8,9,10	0.67	0	8,12,14	0.62	0
2	SEP	U	431	2	8,9,10	0.69	0	8,12,14	0.62	0
2	SEP	C	431	2	8,9,10	0.64	0	8,12,14	0.58	0
1	SEP	A	431	1	8,9,10	1.12	1 (12%)	8,12,14	1.01	0
2	SEP	F	431	2	8,9,10	0.56	0	8,12,14	0.66	0
1	SEP	X	431	1	8,9,10	0.57	0	8,12,14	0.68	0
1	SEP	N	431	1	8,9,10	0.70	0	8,12,14	0.71	0
2	TPO	K	432	2	8,10,11	1.28	1 (12%)	10,14,16	1.14	0
1	SEP	H	431	1	8,9,10	0.62	0	8,12,14	0.58	0
2	SEP	Q	431	2	8,9,10	0.68	0	8,12,14	0.59	0
2	SEP	I	431	2	8,9,10	0.62	0	8,12,14	0.55	0
2	SEP	O	431	2	8,9,10	0.70	0	8,12,14	0.75	0
2	TPO	D	432	2	8,10,11	0.91	1 (12%)	10,14,16	0.88	0
2	TPO	F	432	2	8,10,11	1.53	2 (25%)	10,14,16	0.91	0
1	SEP	R	431	1	8,9,10	0.68	0	8,12,14	0.74	0
2	SEP	E	431	2	8,9,10	0.59	0	8,12,14	0.71	0
2	SEP	L	431	2	8,9,10	0.55	0	8,12,14	0.65	0
1	SEP	B	431	1	8,9,10	0.62	0	8,12,14	0.58	0
1	SEP	G	431	1	8,9,10	1.10	1 (12%)	8,12,14	1.07	1 (12%)
2	TPO	U	432	2	8,10,11	0.97	1 (12%)	10,14,16	1.04	1 (10%)
2	TPO	C	432	2	8,10,11	1.41	2 (25%)	10,14,16	0.78	0
2	TPO	Q	432	2	8,10,11	0.94	1 (12%)	10,14,16	1.08	1 (10%)
1	SEP	W	431	1	8,9,10	0.57	0	8,12,14	0.68	0

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	SEP	P	431	1	-	3/5/8/10	-
2	SEP	K	431	2	-	4/5/8/10	-
2	TPO	J	432	2	-	1/9/11/13	-
2	SEP	J	431	2	-	2/5/8/10	-
1	SEP	S	431	1	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	L	432	2	-	6/9/11/13	-
1	SEP	M	431	1	-	1/5/8/10	-
2	TPO	O	432	2	-	1/9/11/13	-
2	SEP	D	431	2	-	1/5/8/10	-
2	TPO	E	432	2	-	2/9/11/13	-
2	TPO	I	432	2	-	4/9/11/13	-
1	SEP	T	431	1	-	1/5/8/10	-
1	SEP	V	431	1	-	1/5/8/10	-
2	SEP	U	431	2	-	2/5/8/10	-
2	SEP	C	431	2	-	1/5/8/10	-
1	SEP	A	431	1	-	1/5/8/10	-
2	SEP	F	431	2	-	1/5/8/10	-
1	SEP	X	431	1	-	0/5/8/10	-
1	SEP	N	431	1	-	1/5/8/10	-
2	TPO	K	432	2	-	3/9/11/13	-
1	SEP	H	431	1	-	1/5/8/10	-
2	SEP	Q	431	2	-	1/5/8/10	-
2	SEP	I	431	2	-	1/5/8/10	-
2	SEP	O	431	2	-	1/5/8/10	-
2	TPO	D	432	2	-	1/9/11/13	-
2	TPO	F	432	2	-	4/9/11/13	-
1	SEP	R	431	1	-	4/5/8/10	-
2	SEP	E	431	2	-	4/5/8/10	-
2	SEP	L	431	2	-	1/5/8/10	-
1	SEP	B	431	1	-	1/5/8/10	-
1	SEP	G	431	1	-	3/5/8/10	-
2	TPO	U	432	2	-	1/9/11/13	-
2	TPO	C	432	2	-	3/9/11/13	-
2	TPO	Q	432	2	-	4/9/11/13	-
1	SEP	W	431	1	-	0/5/8/10	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	432	TPO	P-O2P	-2.92	1.43	1.54
2	L	432	TPO	P-O2P	-2.88	1.43	1.54
2	E	432	TPO	P-O2P	-2.79	1.44	1.54
2	F	432	TPO	P-OG1	2.64	1.64	1.59
2	L	432	TPO	P-OG1	2.53	1.64	1.59
2	I	432	TPO	P-O2P	-2.49	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	432	TPO	P-O2P	-2.47	1.45	1.54
1	A	431	SEP	P-O2P	-2.46	1.45	1.54
2	K	432	TPO	P-O2P	-2.42	1.45	1.54
2	U	432	TPO	P-OG1	2.15	1.63	1.59
2	C	432	TPO	P-O3P	-2.13	1.46	1.54
2	I	432	TPO	P-O3P	-2.13	1.46	1.54
2	D	432	TPO	P-OG1	2.11	1.63	1.59
2	O	432	TPO	P-OG1	2.11	1.63	1.59
1	G	431	SEP	P-O2P	-2.08	1.46	1.54
2	Q	432	TPO	P-OG1	2.04	1.63	1.59
2	J	432	TPO	P-OG1	2.02	1.63	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	432	TPO	O-C-CA	-2.77	117.52	124.78
2	Q	432	TPO	O-C-CA	-2.72	117.65	124.78
2	O	432	TPO	O-C-CA	-2.61	117.93	124.78
1	G	431	SEP	O3P-P-O2P	2.05	115.47	107.64

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	431	SEP	N-CA-CB-OG
2	E	431	SEP	N-CA-CB-OG
2	E	431	SEP	CB-OG-P-O1P
2	E	431	SEP	CB-OG-P-O2P
2	E	431	SEP	CB-OG-P-O3P
2	F	431	SEP	N-CA-CB-OG
2	F	432	TPO	N-CA-CB-CG2
2	F	432	TPO	N-CA-CB-OG1
2	F	432	TPO	C-CA-CB-CG2
2	F	432	TPO	O-C-CA-CB
2	C	432	TPO	C-CA-CB-CG2
2	D	432	TPO	O-C-CA-CB
1	G	431	SEP	N-CA-CB-OG
1	G	431	SEP	CB-OG-P-O2P
2	K	431	SEP	N-CA-CB-OG
2	K	431	SEP	CB-OG-P-O1P
2	K	431	SEP	CB-OG-P-O2P
2	K	431	SEP	CB-OG-P-O3P

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Mol	Chain	Res	Type	Atoms
2	L	431	SEP	N-CA-CB-OG
2	L	432	TPO	N-CA-CB-CG2
2	L	432	TPO	N-CA-CB-OG1
2	L	432	TPO	C-CA-CB-CG2
2	L	432	TPO	O-C-CA-CB
2	L	432	TPO	CB-OG1-P-O1P
2	I	432	TPO	C-CA-CB-CG2
2	J	432	TPO	O-C-CA-CB
1	N	431	SEP	N-CA-CB-OG
2	O	431	SEP	N-CA-CB-OG
1	R	431	SEP	CB-OG-P-O1P
1	R	431	SEP	CB-OG-P-O2P
1	R	431	SEP	CB-OG-P-O3P
1	P	431	SEP	CB-OG-P-O1P
1	P	431	SEP	CB-OG-P-O3P
2	Q	431	SEP	N-CA-CB-OG
2	Q	432	TPO	N-CA-CB-OG1
2	Q	432	TPO	C-CA-CB-CG2
2	Q	432	TPO	O-C-CA-CB
2	U	431	SEP	CB-OG-P-O2P
2	U	431	SEP	CB-OG-P-O3P
2	U	432	TPO	O-C-CA-CB
1	S	431	SEP	N-CA-CB-OG
1	V	431	SEP	N-CA-CB-OG
2	Q	432	TPO	N-CA-CB-CG2
1	T	431	SEP	CB-OG-P-O3P
1	B	431	SEP	N-CA-CB-OG
2	C	431	SEP	N-CA-CB-OG
2	D	431	SEP	N-CA-CB-OG
1	H	431	SEP	N-CA-CB-OG
2	I	431	SEP	N-CA-CB-OG
2	J	431	SEP	N-CA-CB-OG
1	R	431	SEP	N-CA-CB-OG
1	M	431	SEP	N-CA-CB-OG
2	C	432	TPO	N-CA-CB-CG2
2	I	432	TPO	N-CA-CB-CG2
2	C	432	TPO	CB-OG1-P-O1P
2	I	432	TPO	CB-OG1-P-O1P
2	J	431	SEP	CB-OG-P-O2P
2	O	432	TPO	CB-OG1-P-O1P
2	E	432	TPO	CB-OG1-P-O3P
1	G	431	SEP	CA-CB-OG-P

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Mol	Chain	Res	Type	Atoms
2	K	432	TPO	CB-OG1-P-O2P
2	K	432	TPO	CB-OG1-P-O3P
2	L	432	TPO	CB-OG1-P-O3P
2	I	432	TPO	CB-OG1-P-O3P
1	P	431	SEP	CA-CB-OG-P
2	E	432	TPO	O-C-CA-CB
2	K	432	TPO	O-C-CA-CB

There are no ring outliers.

13 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	431	SEP	1	0
2	J	432	TPO	3	0
2	E	432	TPO	1	0
2	I	432	TPO	1	0
1	T	431	SEP	2	0
1	X	431	SEP	1	0
2	K	432	TPO	1	0
2	D	432	TPO	3	0
2	F	432	TPO	2	0
1	R	431	SEP	2	0
2	E	431	SEP	1	0
2	C	432	TPO	1	0
2	Q	432	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 84 ligands modelled in this entry, 36 are monoatomic - leaving 48 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	D	702	4	26,33,33	0.67	0	31,52,52	0.98	2 (6%)
5	ADP	U	702	-	24,29,29	0.68	0	29,45,45	0.77	1 (3%)
3	ATP	S	702	-	26,33,33	0.66	0	31,52,52	0.85	2 (6%)
3	ATP	K	701	4	26,33,33	0.65	0	31,52,52	1.00	2 (6%)
3	ATP	I	702	4	26,33,33	0.67	0	31,52,52	0.75	1 (3%)
3	ATP	H	701	4	26,33,33	0.67	0	31,52,52	0.86	0
3	ATP	R	702	4	26,33,33	0.66	0	31,52,52	0.89	2 (6%)
3	ATP	G	701	4	26,33,33	0.66	0	31,52,52	1.01	2 (6%)
3	ATP	J	701	4	26,33,33	0.62	0	31,52,52	0.89	2 (6%)
3	ATP	O	701	4	26,33,33	0.66	0	31,52,52	1.02	2 (6%)
3	ATP	T	701	4	26,33,33	0.67	0	31,52,52	1.08	3 (9%)
5	ADP	Q	701	-	24,29,29	0.67	0	29,45,45	0.76	1 (3%)
3	ATP	K	702	4	26,33,33	0.66	0	31,52,52	0.88	2 (6%)
3	ATP	L	702	4	26,33,33	0.65	0	31,52,52	1.06	2 (6%)
3	ATP	V	702	-	26,33,33	0.67	0	31,52,52	0.72	1 (3%)
3	ATP	X	702	-	26,33,33	0.64	0	31,52,52	1.01	2 (6%)
3	ATP	V	701	4	26,33,33	0.65	0	31,52,52	0.85	1 (3%)
3	ATP	U	701	4	26,33,33	0.65	0	31,52,52	0.91	2 (6%)
3	ATP	X	701	-	26,33,33	0.67	0	31,52,52	0.89	2 (6%)
3	ATP	W	702	-	26,33,33	0.66	0	31,52,52	1.01	2 (6%)
3	ATP	A	701	4	26,33,33	0.65	0	31,52,52	0.97	2 (6%)
3	ATP	P	702	4	26,33,33	0.68	0	31,52,52	1.03	2 (6%)
3	ATP	F	701	4	26,33,33	0.64	0	31,52,52	0.94	2 (6%)
3	ATP	N	702	4	26,33,33	0.67	0	31,52,52	1.01	2 (6%)
3	ATP	N	701	4	26,33,33	0.66	0	31,52,52	1.04	2 (6%)
3	ATP	P	701	4	26,33,33	0.65	0	31,52,52	1.00	2 (6%)
3	ATP	J	702	4	26,33,33	0.68	0	31,52,52	1.02	2 (6%)
3	ATP	C	701	4	26,33,33	0.64	0	31,52,52	0.94	2 (6%)
3	ATP	M	702	-	26,33,33	0.66	0	31,52,52	0.99	2 (6%)
3	ATP	T	702	-	26,33,33	0.64	0	31,52,52	0.93	2 (6%)
5	ADP	W	701	-	24,29,29	0.66	0	29,45,45	0.72	1 (3%)
3	ATP	O	702	-	26,33,33	0.66	0	31,52,52	1.03	2 (6%)
3	ATP	G	702	4	26,33,33	0.67	0	31,52,52	1.11	3 (9%)
3	ATP	L	701	4	26,33,33	0.64	0	31,52,52	0.99	2 (6%)
3	ATP	I	701	4	26,33,33	0.64	0	31,52,52	0.90	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	A	702	4	26,33,33	0.67	0	31,52,52	0.84	2 (6%)
3	ATP	D	701	4	26,33,33	0.64	0	31,52,52	0.81	1 (3%)
3	ATP	E	702	4	26,33,33	0.65	0	31,52,52	0.91	2 (6%)
3	ATP	S	701	-	26,33,33	0.66	0	31,52,52	0.79	1 (3%)
3	ATP	R	701	4	26,33,33	0.67	0	31,52,52	0.78	1 (3%)
3	ATP	B	702	4	26,33,33	0.66	0	31,52,52	0.99	2 (6%)
3	ATP	C	702	4	26,33,33	0.67	0	31,52,52	0.95	2 (6%)
3	ATP	H	702	4	26,33,33	0.65	0	31,52,52	0.93	2 (6%)
3	ATP	E	701	4	26,33,33	0.68	0	31,52,52	1.00	2 (6%)
3	ATP	B	701	4	26,33,33	0.67	0	31,52,52	0.79	1 (3%)
3	ATP	M	701	4	26,33,33	0.65	0	31,52,52	0.82	1 (3%)
3	ATP	Q	702	4	26,33,33	0.65	0	31,52,52	1.12	3 (9%)
3	ATP	F	702	4	26,33,33	0.66	0	31,52,52	0.91	2 (6%)

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	D	702	4	-	3/18/38/38	0/3/3/3
5	ADP	U	702	-	-	5/12/32/32	0/3/3/3
3	ATP	S	702	-	-	0/18/38/38	0/3/3/3
3	ATP	K	701	4	-	1/18/38/38	0/3/3/3
3	ATP	I	702	4	-	8/18/38/38	0/3/3/3
3	ATP	H	701	4	-	2/18/38/38	0/3/3/3
3	ATP	R	702	4	-	3/18/38/38	0/3/3/3
3	ATP	G	701	4	-	1/18/38/38	0/3/3/3
3	ATP	J	701	4	-	7/18/38/38	0/3/3/3
3	ATP	O	701	4	-	2/18/38/38	0/3/3/3
3	ATP	T	701	4	-	4/18/38/38	0/3/3/3
5	ADP	Q	701	-	-	3/12/32/32	0/3/3/3
3	ATP	K	702	4	-	1/18/38/38	0/3/3/3
3	ATP	L	702	4	-	4/18/38/38	0/3/3/3
3	ATP	V	702	-	-	5/18/38/38	0/3/3/3
3	ATP	X	702	-	-	6/18/38/38	0/3/3/3
3	ATP	V	701	4	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	U	701	4	-	0/18/38/38	0/3/3/3
3	ATP	X	701	-	-	8/18/38/38	0/3/3/3
3	ATP	W	702	-	-	3/18/38/38	0/3/3/3
3	ATP	A	701	4	-	0/18/38/38	0/3/3/3
3	ATP	P	702	4	-	1/18/38/38	0/3/3/3
3	ATP	F	701	4	-	4/18/38/38	0/3/3/3
3	ATP	N	702	4	-	4/18/38/38	0/3/3/3
3	ATP	N	701	4	-	5/18/38/38	0/3/3/3
3	ATP	P	701	4	-	2/18/38/38	0/3/3/3
3	ATP	J	702	4	-	0/18/38/38	0/3/3/3
3	ATP	C	701	4	-	2/18/38/38	0/3/3/3
3	ATP	M	702	-	-	5/18/38/38	0/3/3/3
3	ATP	T	702	-	-	1/18/38/38	0/3/3/3
5	ADP	W	701	-	-	5/12/32/32	0/3/3/3
3	ATP	O	702	-	-	4/18/38/38	0/3/3/3
3	ATP	G	702	4	-	0/18/38/38	0/3/3/3
3	ATP	L	701	4	-	1/18/38/38	0/3/3/3
3	ATP	I	701	4	-	4/18/38/38	0/3/3/3
3	ATP	A	702	4	-	5/18/38/38	0/3/3/3
3	ATP	D	701	4	-	7/18/38/38	0/3/3/3
3	ATP	E	702	4	-	2/18/38/38	0/3/3/3
3	ATP	S	701	-	-	3/18/38/38	0/3/3/3
3	ATP	R	701	4	-	5/18/38/38	0/3/3/3
3	ATP	B	702	4	-	2/18/38/38	0/3/3/3
3	ATP	C	702	4	-	5/18/38/38	0/3/3/3
3	ATP	H	702	4	-	2/18/38/38	0/3/3/3
3	ATP	E	701	4	-	4/18/38/38	0/3/3/3
3	ATP	B	701	4	-	6/18/38/38	0/3/3/3
3	ATP	M	701	4	-	4/18/38/38	0/3/3/3
3	ATP	Q	702	4	-	3/18/38/38	0/3/3/3
3	ATP	F	702	4	-	7/18/38/38	0/3/3/3

There are no bond length outliers.

All (85) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	702	ATP	C3'-C2'-C1'	3.13	105.70	100.98
3	W	702	ATP	C3'-C2'-C1'	3.12	105.68	100.98
3	G	702	ATP	C3'-C2'-C1'	3.03	105.55	100.98
3	N	701	ATP	C3'-C2'-C1'	3.01	105.52	100.98
3	P	702	ATP	C3'-C2'-C1'	2.99	105.48	100.98
3	K	701	ATP	C3'-C2'-C1'	2.97	105.46	100.98
3	G	701	ATP	C3'-C2'-C1'	2.97	105.45	100.98
3	Q	702	ATP	C3'-C2'-C1'	2.97	105.44	100.98
3	L	702	ATP	C3'-C2'-C1'	2.94	105.41	100.98
3	T	701	ATP	PA-O3A-PB	-2.94	122.75	132.83
3	J	702	ATP	C3'-C2'-C1'	2.94	105.40	100.98
3	X	702	ATP	C3'-C2'-C1'	2.90	105.35	100.98
3	D	702	ATP	C3'-C2'-C1'	2.88	105.32	100.98
3	M	702	ATP	C3'-C2'-C1'	2.86	105.29	100.98
3	E	701	ATP	C3'-C2'-C1'	2.84	105.26	100.98
3	O	701	ATP	C3'-C2'-C1'	2.84	105.25	100.98
3	A	701	ATP	C3'-C2'-C1'	2.82	105.22	100.98
3	N	702	ATP	C3'-C2'-C1'	2.76	105.14	100.98
3	T	701	ATP	C3'-C2'-C1'	2.75	105.12	100.98
3	C	702	ATP	C3'-C2'-C1'	2.72	105.07	100.98
3	B	702	ATP	C3'-C2'-C1'	2.69	105.03	100.98
3	F	701	ATP	C3'-C2'-C1'	2.66	104.98	100.98
3	P	701	ATP	C3'-C2'-C1'	2.65	104.97	100.98
3	R	702	ATP	C3'-C2'-C1'	2.45	104.67	100.98
3	L	701	ATP	C3'-C2'-C1'	2.43	104.64	100.98
3	C	701	ATP	C3'-C2'-C1'	2.41	104.60	100.98
3	F	702	ATP	C3'-C2'-C1'	2.41	104.60	100.98
3	B	702	ATP	C5-C6-N6	2.39	123.98	120.35
3	H	702	ATP	C5-C6-N6	2.38	123.97	120.35
3	J	701	ATP	C3'-C2'-C1'	2.37	104.55	100.98
3	V	701	ATP	C5-C6-N6	2.37	123.95	120.35
3	T	702	ATP	C3'-C2'-C1'	2.35	104.52	100.98
3	K	702	ATP	C5-C6-N6	2.35	123.92	120.35
3	F	702	ATP	C5-C6-N6	2.34	123.91	120.35
3	X	702	ATP	C5-C6-N6	2.34	123.90	120.35
3	L	702	ATP	C5-C6-N6	2.33	123.90	120.35
3	R	702	ATP	C5-C6-N6	2.33	123.89	120.35
3	K	702	ATP	C3'-C2'-C1'	2.32	104.47	100.98
3	U	701	ATP	C3'-C2'-C1'	2.32	104.47	100.98
3	X	701	ATP	C5-C6-N6	2.31	123.86	120.35
3	I	701	ATP	C5-C6-N6	2.31	123.86	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	ATP	C5-C6-N6	2.30	123.85	120.35
3	E	702	ATP	C5-C6-N6	2.29	123.84	120.35
3	G	701	ATP	C5-C6-N6	2.29	123.84	120.35
3	F	701	ATP	C5-C6-N6	2.29	123.84	120.35
3	N	701	ATP	C5-C6-N6	2.28	123.82	120.35
3	M	701	ATP	C5-C6-N6	2.28	123.81	120.35
3	A	702	ATP	C3'-C2'-C1'	2.28	104.41	100.98
3	Q	702	ATP	C5-C6-N6	2.26	123.79	120.35
3	N	702	ATP	C5-C6-N6	2.26	123.78	120.35
3	A	701	ATP	C5-C6-N6	2.25	123.77	120.35
3	L	701	ATP	C5-C6-N6	2.25	123.76	120.35
3	S	702	ATP	C5-C6-N6	2.24	123.76	120.35
3	W	702	ATP	C5-C6-N6	2.24	123.76	120.35
3	U	701	ATP	C5-C6-N6	2.24	123.75	120.35
3	T	702	ATP	C5-C6-N6	2.23	123.75	120.35
3	P	702	ATP	C5-C6-N6	2.23	123.74	120.35
3	P	701	ATP	C5-C6-N6	2.23	123.74	120.35
3	X	701	ATP	C3'-C2'-C1'	2.23	104.33	100.98
3	O	702	ATP	C5-C6-N6	2.23	123.73	120.35
3	O	701	ATP	C5-C6-N6	2.22	123.73	120.35
5	W	701	ADP	C5-C6-N6	2.22	123.73	120.35
3	R	701	ATP	C5-C6-N6	2.22	123.72	120.35
3	G	702	ATP	C5-C6-N6	2.19	123.69	120.35
3	A	702	ATP	C5-C6-N6	2.19	123.69	120.35
3	J	701	ATP	C5-C6-N6	2.19	123.69	120.35
5	U	702	ADP	C5-C6-N6	2.19	123.68	120.35
3	M	702	ATP	C5-C6-N6	2.19	123.68	120.35
3	T	701	ATP	C5-C6-N6	2.19	123.68	120.35
3	V	702	ATP	C5-C6-N6	2.17	123.65	120.35
3	Q	702	ATP	PB-O3B-PG	-2.17	125.39	132.83
3	S	701	ATP	C5-C6-N6	2.16	123.64	120.35
5	Q	701	ADP	C5-C6-N6	2.16	123.63	120.35
3	S	702	ATP	C3'-C2'-C1'	2.16	104.22	100.98
3	C	701	ATP	C5-C6-N6	2.15	123.61	120.35
3	C	702	ATP	C5-C6-N6	2.14	123.60	120.35
3	E	701	ATP	C5-C6-N6	2.14	123.60	120.35
3	D	701	ATP	C5-C6-N6	2.13	123.59	120.35
3	H	702	ATP	C3'-C2'-C1'	2.13	104.18	100.98
3	J	702	ATP	C5-C6-N6	2.12	123.58	120.35
3	D	702	ATP	C5-C6-N6	2.11	123.57	120.35
3	E	702	ATP	C3'-C2'-C1'	2.11	104.15	100.98
3	I	702	ATP	C5-C6-N6	2.10	123.54	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	702	ATP	PA-O3A-PB	-2.07	125.72	132.83
3	K	701	ATP	C5-C6-N6	2.05	123.47	120.35

There are no chirality outliers.

All (161) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	ATP	C5'-O5'-PA-O1A
3	A	702	ATP	C5'-O5'-PA-O2A
3	B	701	ATP	C5'-O5'-PA-O2A
3	B	701	ATP	C5'-O5'-PA-O3A
3	B	701	ATP	C3'-C4'-C5'-O5'
3	E	701	ATP	C5'-O5'-PA-O3A
3	F	702	ATP	C5'-O5'-PA-O1A
3	F	702	ATP	C5'-O5'-PA-O2A
3	F	702	ATP	O4'-C4'-C5'-O5'
3	C	701	ATP	O4'-C4'-C5'-O5'
3	C	701	ATP	C3'-C4'-C5'-O5'
3	C	702	ATP	PB-O3B-PG-O2G
3	D	701	ATP	PB-O3B-PG-O2G
3	D	701	ATP	C5'-O5'-PA-O1A
3	L	702	ATP	C5'-O5'-PA-O3A
3	I	701	ATP	C5'-O5'-PA-O3A
3	I	701	ATP	O4'-C4'-C5'-O5'
3	J	701	ATP	PB-O3B-PG-O2G
3	J	701	ATP	C5'-O5'-PA-O1A
3	N	701	ATP	C5'-O5'-PA-O1A
3	N	701	ATP	C3'-C4'-C5'-O5'
3	N	702	ATP	C5'-O5'-PA-O1A
3	N	702	ATP	C3'-C4'-C5'-O5'
3	R	701	ATP	C5'-O5'-PA-O1A
3	R	701	ATP	C5'-O5'-PA-O2A
3	R	702	ATP	PB-O3B-PG-O2G
3	T	701	ATP	C5'-O5'-PA-O1A
3	T	701	ATP	C5'-O5'-PA-O2A
3	T	701	ATP	C5'-O5'-PA-O3A
3	X	701	ATP	C5'-O5'-PA-O1A
3	X	701	ATP	C5'-O5'-PA-O2A
3	X	701	ATP	C5'-O5'-PA-O3A
3	X	702	ATP	C5'-O5'-PA-O2A
3	X	702	ATP	C5'-O5'-PA-O3A
3	X	702	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	S	701	ATP	C5'-O5'-PA-O1A
3	V	702	ATP	C5'-O5'-PA-O2A
5	Q	701	ADP	C5'-O5'-PA-O1A
5	U	702	ADP	C5'-O5'-PA-O2A
5	U	702	ADP	O4'-C4'-C5'-O5'
5	U	702	ADP	C3'-C4'-C5'-O5'
5	W	701	ADP	C5'-O5'-PA-O1A
3	B	701	ATP	O4'-C4'-C5'-O5'
3	E	701	ATP	O4'-C4'-C5'-O5'
3	E	701	ATP	C3'-C4'-C5'-O5'
3	I	701	ATP	C3'-C4'-C5'-O5'
3	M	702	ATP	O4'-C4'-C5'-O5'
3	M	702	ATP	C3'-C4'-C5'-O5'
3	Q	702	ATP	C3'-C4'-C5'-O5'
3	X	701	ATP	C3'-C4'-C5'-O5'
3	V	702	ATP	O4'-C4'-C5'-O5'
5	W	701	ADP	O4'-C4'-C5'-O5'
5	W	701	ADP	C3'-C4'-C5'-O5'
3	N	701	ATP	O4'-C4'-C5'-O5'
3	N	702	ATP	O4'-C4'-C5'-O5'
3	X	701	ATP	O4'-C4'-C5'-O5'
3	L	702	ATP	O4'-C4'-C5'-O5'
3	Q	702	ATP	O4'-C4'-C5'-O5'
3	V	702	ATP	C3'-C4'-C5'-O5'
3	B	701	ATP	PB-O3A-PA-O1A
3	C	702	ATP	PB-O3A-PA-O1A
3	I	702	ATP	PG-O3B-PB-O1B
3	I	702	ATP	O4'-C4'-C5'-O5'
3	D	701	ATP	C5'-O5'-PA-O3A
3	J	701	ATP	C5'-O5'-PA-O3A
3	R	701	ATP	C5'-O5'-PA-O3A
3	S	701	ATP	C5'-O5'-PA-O3A
3	V	702	ATP	C5'-O5'-PA-O3A
5	U	702	ADP	C5'-O5'-PA-O3A
5	W	701	ADP	C5'-O5'-PA-O3A
3	B	702	ATP	PA-O3A-PB-O2B
3	F	702	ATP	PA-O3A-PB-O1B
3	D	701	ATP	PA-O3A-PB-O2B
3	H	702	ATP	PG-O3B-PB-O1B
3	M	702	ATP	PB-O3A-PA-O1A
3	X	702	ATP	PG-O3B-PB-O1B
3	V	701	ATP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	W	702	ATP	PG-O3B-PB-O1B
3	E	701	ATP	C5'-O5'-PA-O1A
3	D	701	ATP	C5'-O5'-PA-O2A
3	L	702	ATP	C5'-O5'-PA-O1A
3	I	701	ATP	C5'-O5'-PA-O1A
3	I	702	ATP	C5'-O5'-PA-O2A
3	J	701	ATP	C5'-O5'-PA-O2A
3	S	701	ATP	C5'-O5'-PA-O2A
3	V	702	ATP	C5'-O5'-PA-O1A
5	Q	701	ADP	C5'-O5'-PA-O2A
3	R	701	ATP	O4'-C4'-C5'-O5'
3	N	701	ATP	C4'-C5'-O5'-PA
3	N	702	ATP	C4'-C5'-O5'-PA
3	B	701	ATP	PB-O3A-PA-O2A
3	E	702	ATP	PA-O3A-PB-O2B
3	C	702	ATP	PB-O3A-PA-O2A
3	D	701	ATP	PA-O3A-PB-O1B
3	D	702	ATP	PG-O3B-PB-O2B
3	G	701	ATP	PG-O3B-PB-O1B
3	I	702	ATP	PG-O3B-PB-O2B
3	I	702	ATP	PB-O3A-PA-O2A
3	O	702	ATP	PB-O3A-PA-O2A
3	R	701	ATP	PB-O3A-PA-O2A
3	M	701	ATP	PA-O3A-PB-O1B
3	V	701	ATP	PG-O3B-PB-O2B
3	M	702	ATP	C4'-C5'-O5'-PA
3	M	701	ATP	C3'-C4'-C5'-O5'
3	W	702	ATP	O4'-C4'-C5'-O5'
3	F	701	ATP	PB-O3B-PG-O1G
3	X	701	ATP	PB-O3B-PG-O1G
3	P	701	ATP	C3'-C4'-C5'-O5'
3	F	702	ATP	PA-O3A-PB-O2B
3	K	701	ATP	PA-O3A-PB-O1B
3	M	701	ATP	PA-O3A-PB-O2B
3	P	701	ATP	PG-O3B-PB-O1B
5	W	701	ADP	PB-O3A-PA-O1A
3	L	702	ATP	C3'-C4'-C5'-O5'
3	R	702	ATP	O4'-C4'-C5'-O5'
3	X	702	ATP	C3'-C4'-C5'-O5'
3	I	702	ATP	C3'-C4'-C5'-O5'
3	J	701	ATP	C3'-C4'-C5'-O5'
3	M	701	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	A	702	ATP	PB-O3B-PG-O3G
3	F	701	ATP	PB-O3B-PG-O2G
3	F	701	ATP	PB-O3B-PG-O3G
3	D	701	ATP	PB-O3B-PG-O3G
3	D	702	ATP	PB-O3B-PG-O3G
3	O	702	ATP	PB-O3B-PG-O3G
3	X	701	ATP	PB-O3B-PG-O2G
3	X	701	ATP	PB-O3B-PG-O3G
3	A	702	ATP	C5'-O5'-PA-O3A
3	F	702	ATP	C5'-O5'-PA-O3A
3	I	702	ATP	C5'-O5'-PA-O3A
3	N	701	ATP	C5'-O5'-PA-O3A
3	Q	702	ATP	C5'-O5'-PA-O3A
5	Q	701	ADP	C5'-O5'-PA-O3A
3	T	701	ATP	C4'-C5'-O5'-PA
3	F	702	ATP	C3'-C4'-C5'-O5'
3	T	702	ATP	O4'-C4'-C5'-O5'
3	B	702	ATP	PA-O3A-PB-O1B
3	E	702	ATP	PG-O3B-PB-O1B
3	F	701	ATP	PB-O3A-PA-O1A
3	D	702	ATP	PG-O3B-PB-O1B
3	H	701	ATP	PG-O3B-PB-O2B
3	H	702	ATP	PG-O3B-PB-O2B
3	K	702	ATP	PA-O3A-PB-O2B
3	L	701	ATP	PA-O3A-PB-O1B
3	I	702	ATP	PB-O3A-PA-O1A
3	J	701	ATP	PA-O3A-PB-O2B
3	O	701	ATP	PA-O3A-PB-O1B
3	O	701	ATP	PA-O3A-PB-O2B
3	R	702	ATP	PB-O3A-PA-O2A
3	P	702	ATP	PA-O3A-PB-O1B
3	X	702	ATP	PG-O3B-PB-O2B
3	W	702	ATP	PG-O3B-PB-O2B
3	C	702	ATP	C5'-O5'-PA-O1A
3	O	702	ATP	C5'-O5'-PA-O1A
3	M	702	ATP	C5'-O5'-PA-O1A
5	U	702	ADP	C5'-O5'-PA-O1A
3	A	702	ATP	O4'-C4'-C5'-O5'
3	C	702	ATP	O4'-C4'-C5'-O5'
3	H	701	ATP	C3'-C4'-C5'-O5'
3	O	702	ATP	O4'-C4'-C5'-O5'
3	J	701	ATP	PB-O3B-PG-O1G

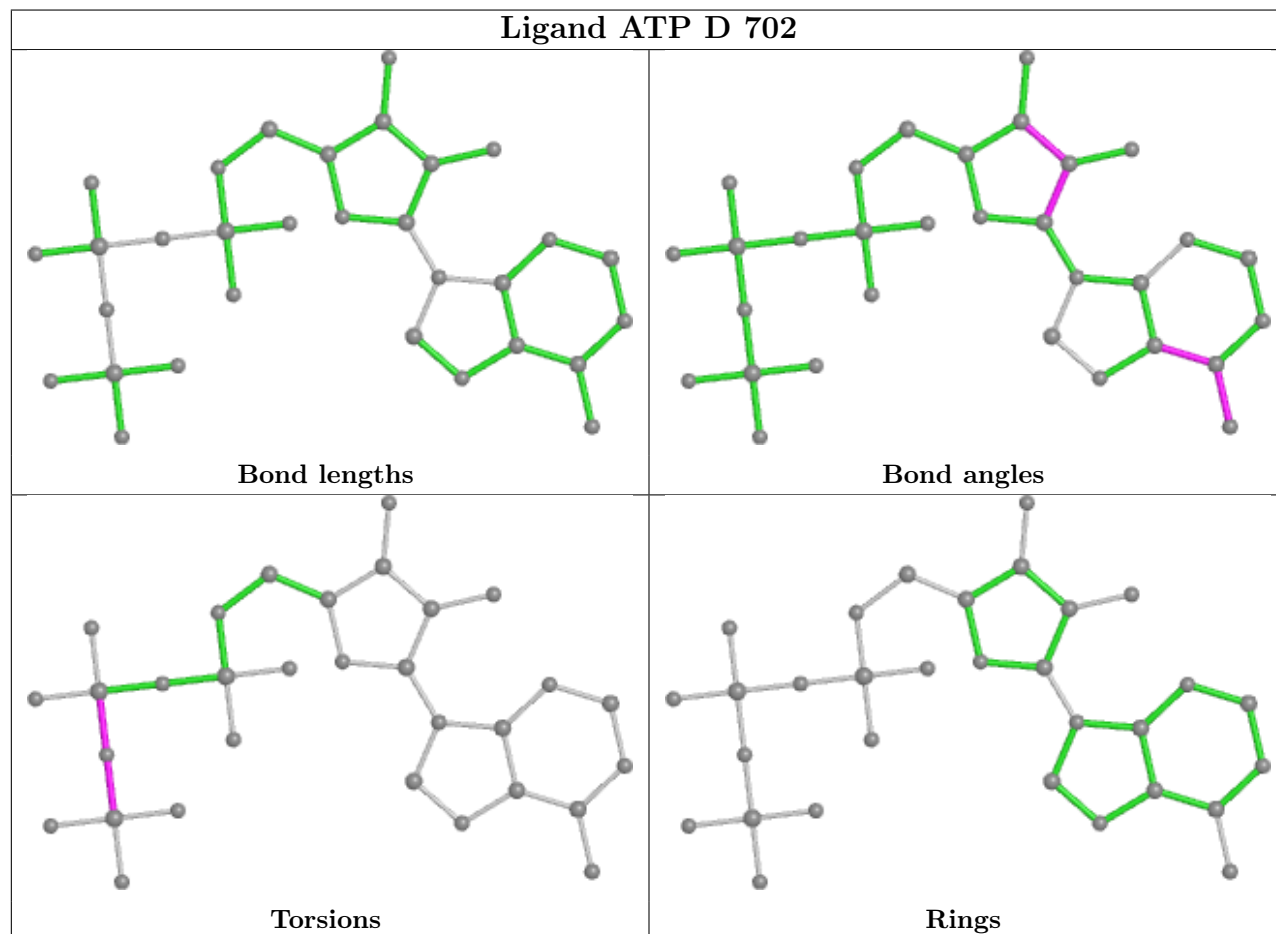
There are no ring outliers.

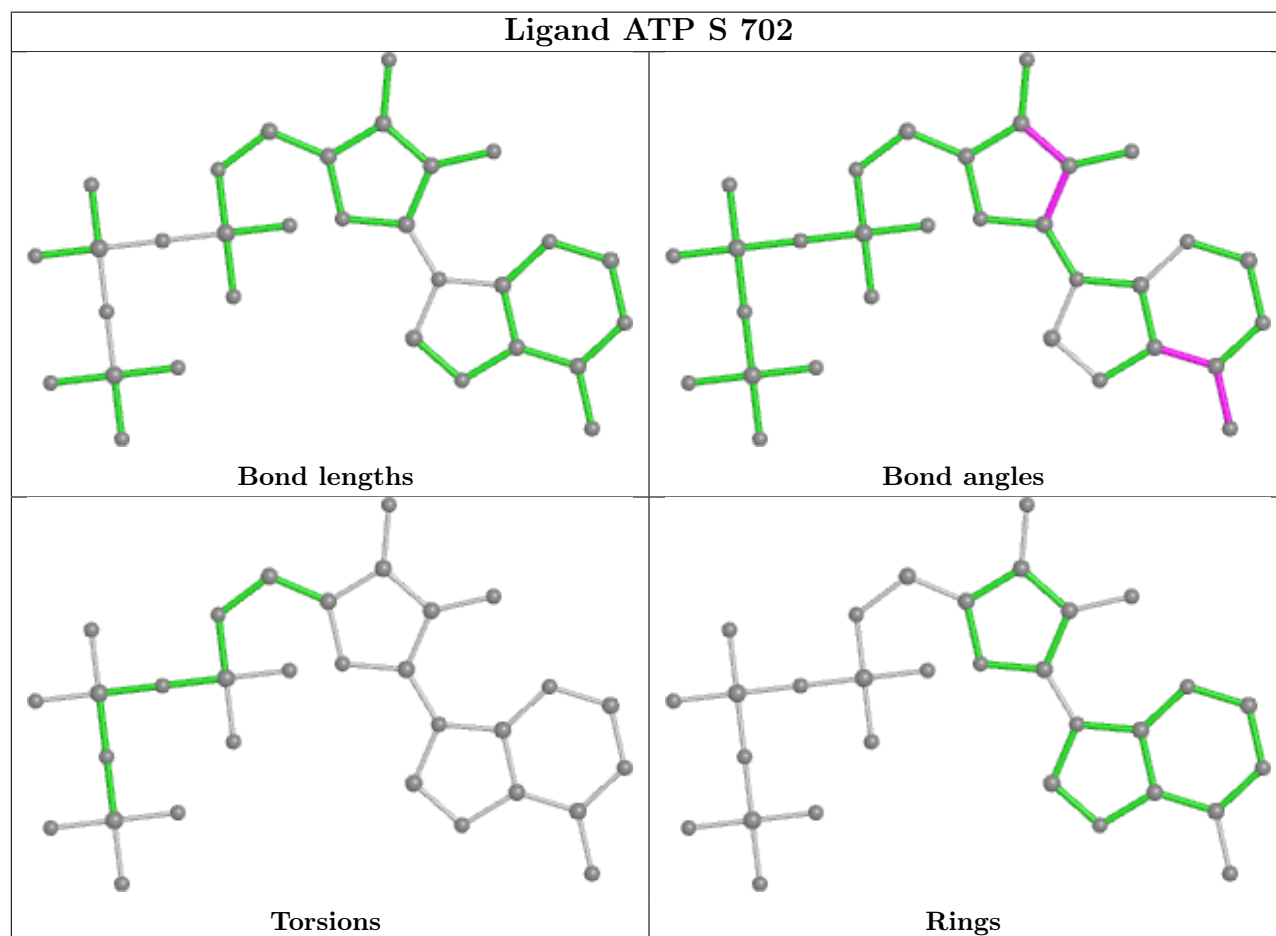
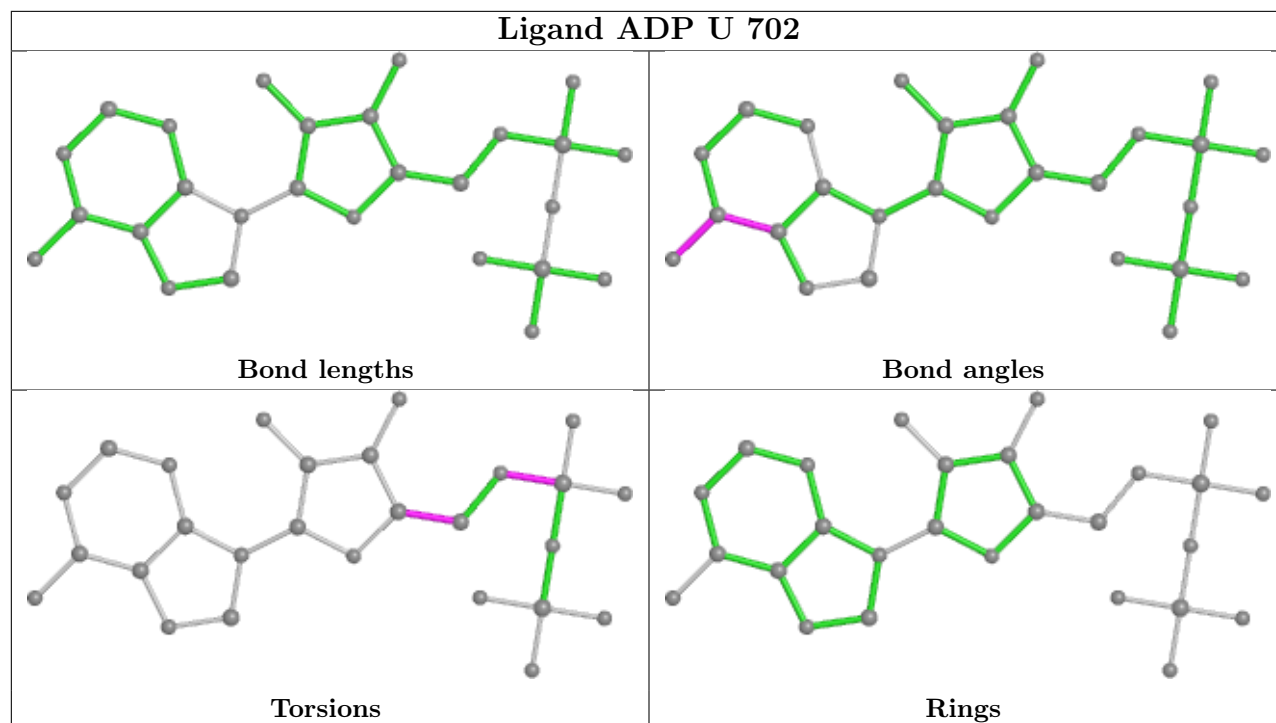
38 monomers are involved in 79 short contacts:

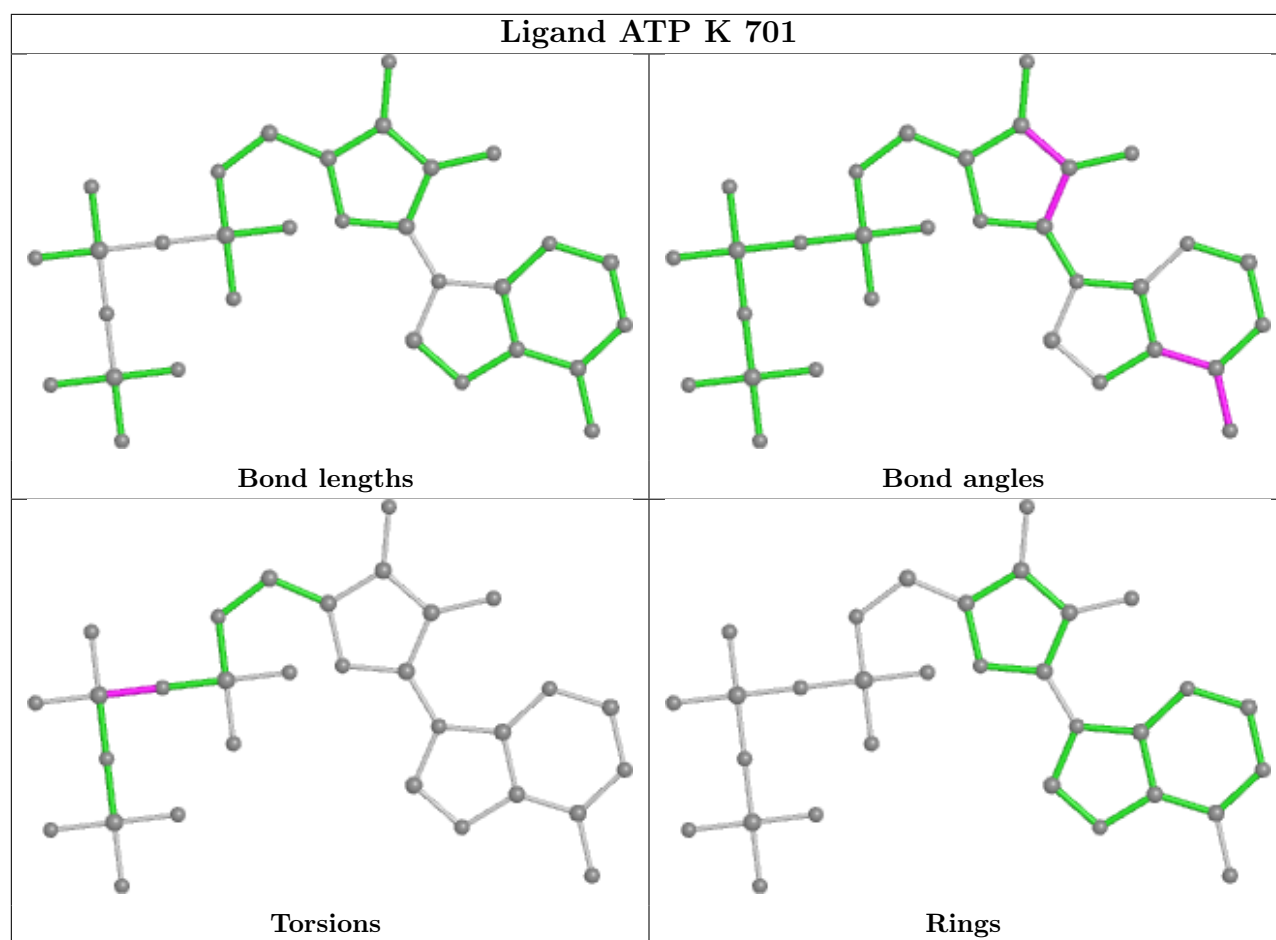
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	702	ATP	1	0
5	U	702	ADP	9	0
3	K	701	ATP	1	0
3	I	702	ATP	4	0
3	H	701	ATP	2	0
3	R	702	ATP	1	0
3	J	701	ATP	1	0
3	K	702	ATP	1	0
3	L	702	ATP	4	0
3	V	702	ATP	2	0
3	X	702	ATP	1	0
3	V	701	ATP	1	0
3	U	701	ATP	1	0
3	X	701	ATP	1	0
3	W	702	ATP	2	0
3	P	702	ATP	1	0
3	F	701	ATP	2	0
3	N	702	ATP	2	0
3	N	701	ATP	1	0
3	P	701	ATP	5	0
3	J	702	ATP	2	0
3	C	701	ATP	3	0
3	M	702	ATP	1	0
3	O	702	ATP	1	0
3	G	702	ATP	3	0
3	L	701	ATP	2	0
3	I	701	ATP	2	0
3	A	702	ATP	3	0
3	D	701	ATP	1	0
3	E	702	ATP	1	0
3	S	701	ATP	2	0
3	B	702	ATP	4	0
3	C	702	ATP	3	0
3	H	702	ATP	1	0
3	E	701	ATP	3	0
3	B	701	ATP	2	0
3	M	701	ATP	1	0
3	F	702	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.

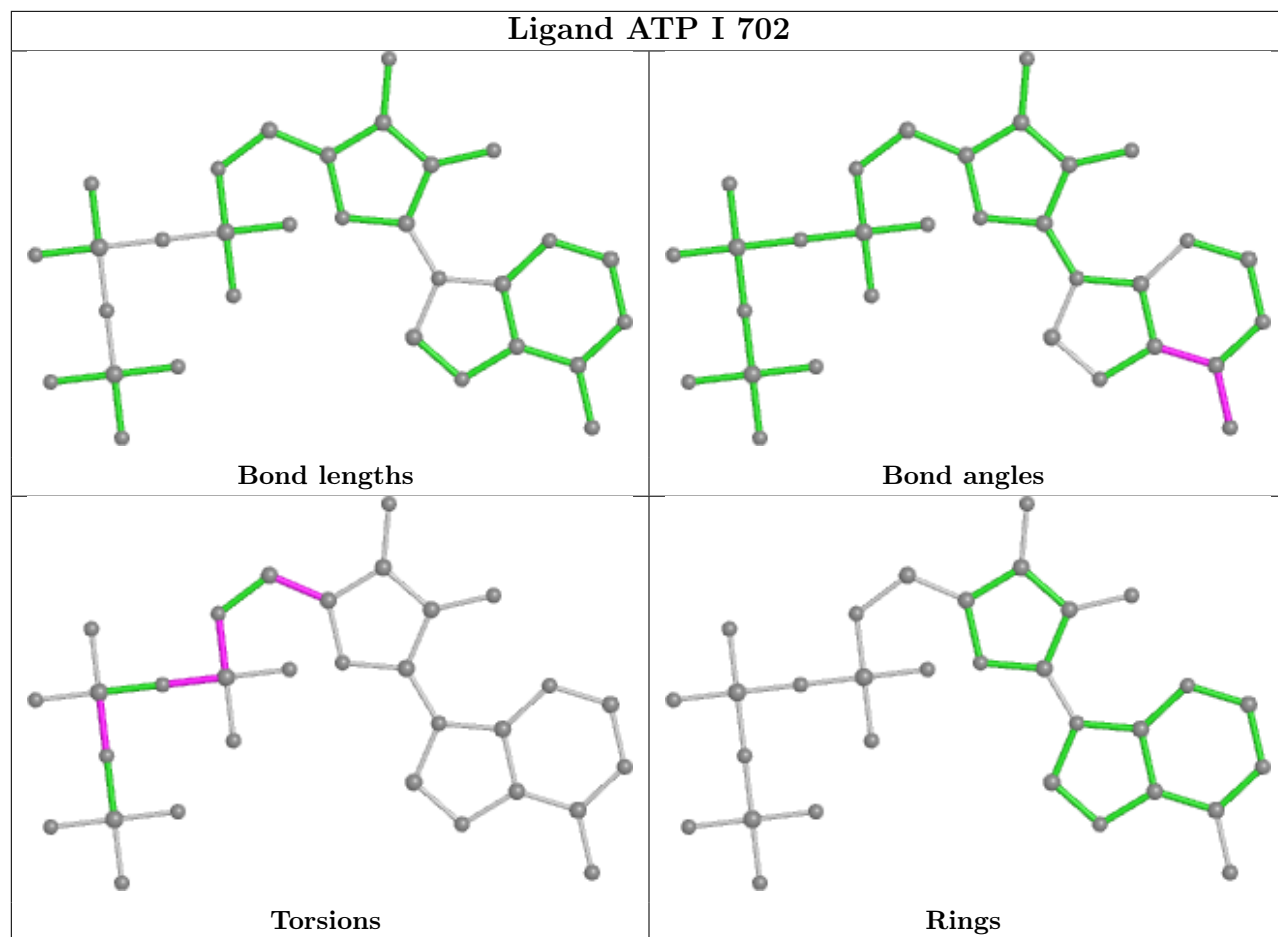


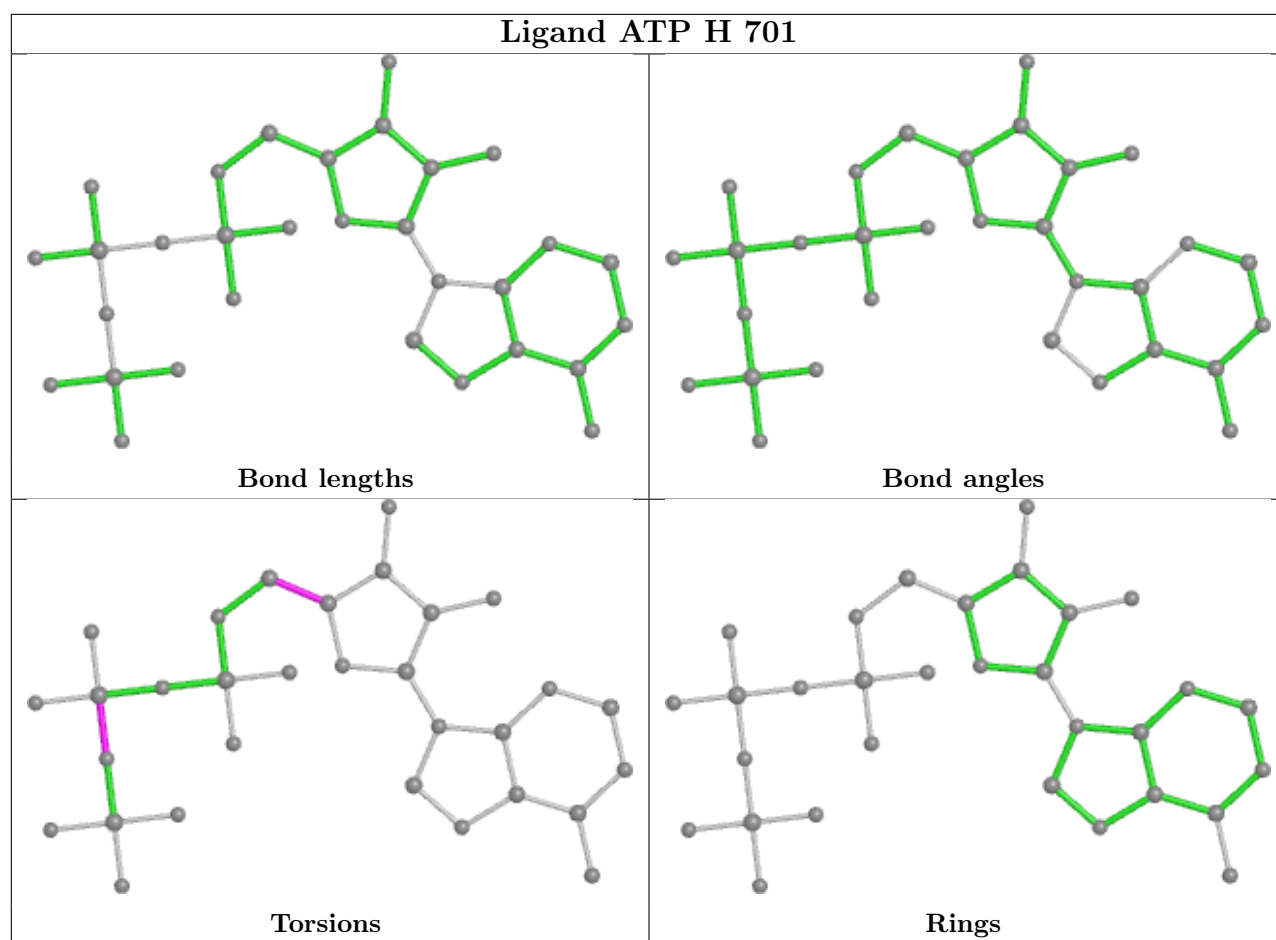


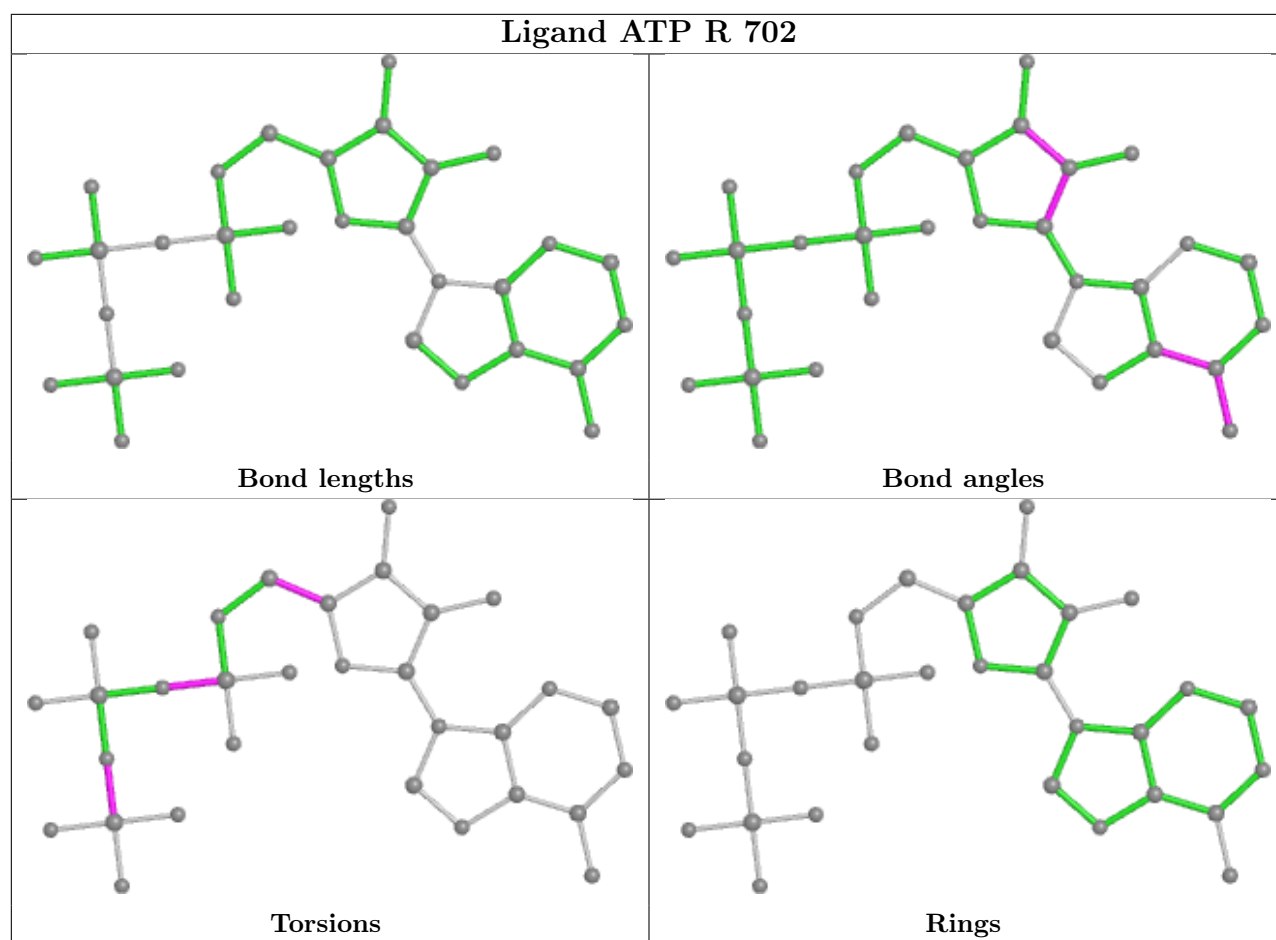


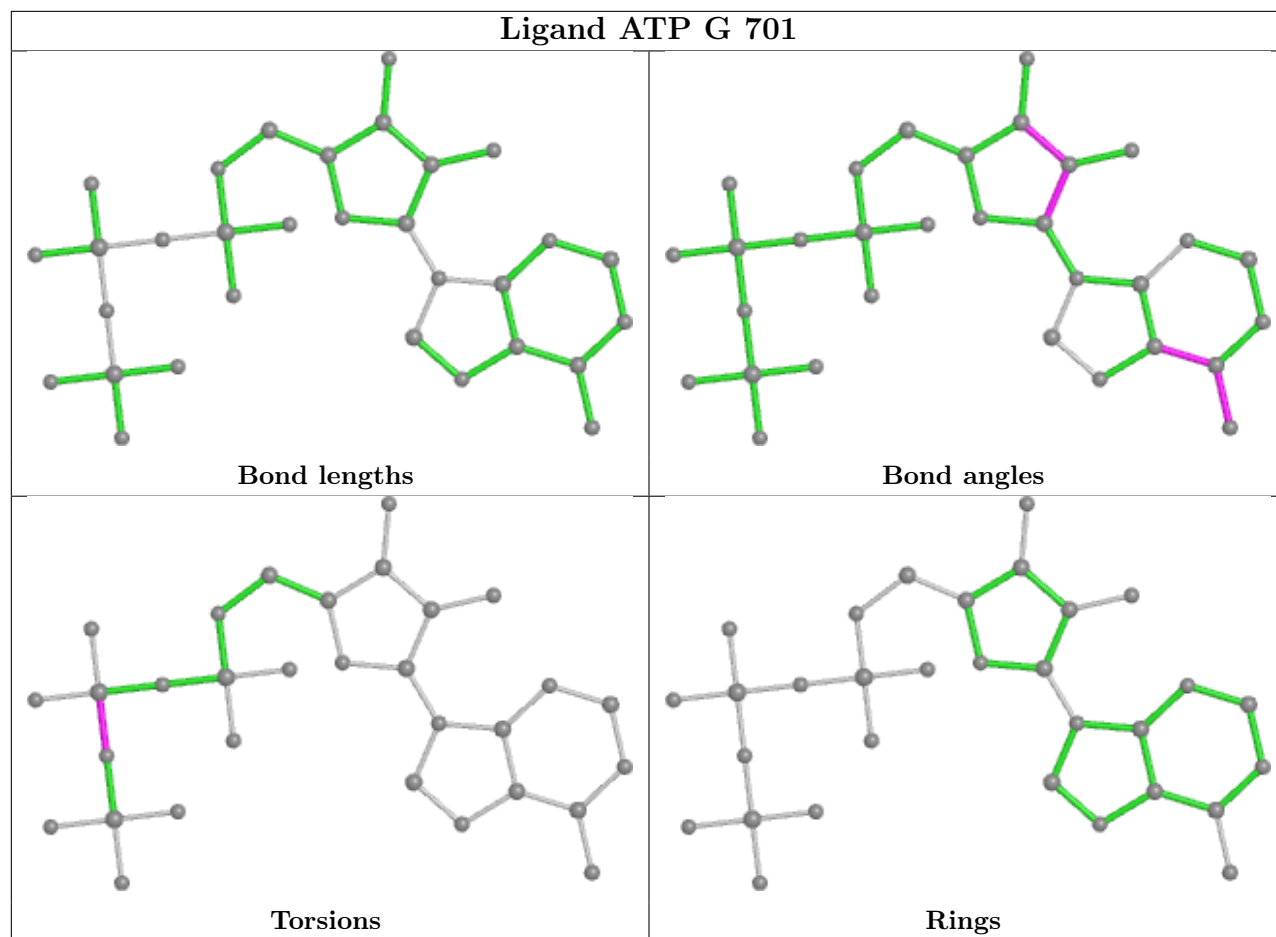


## Ligand ATP I 702

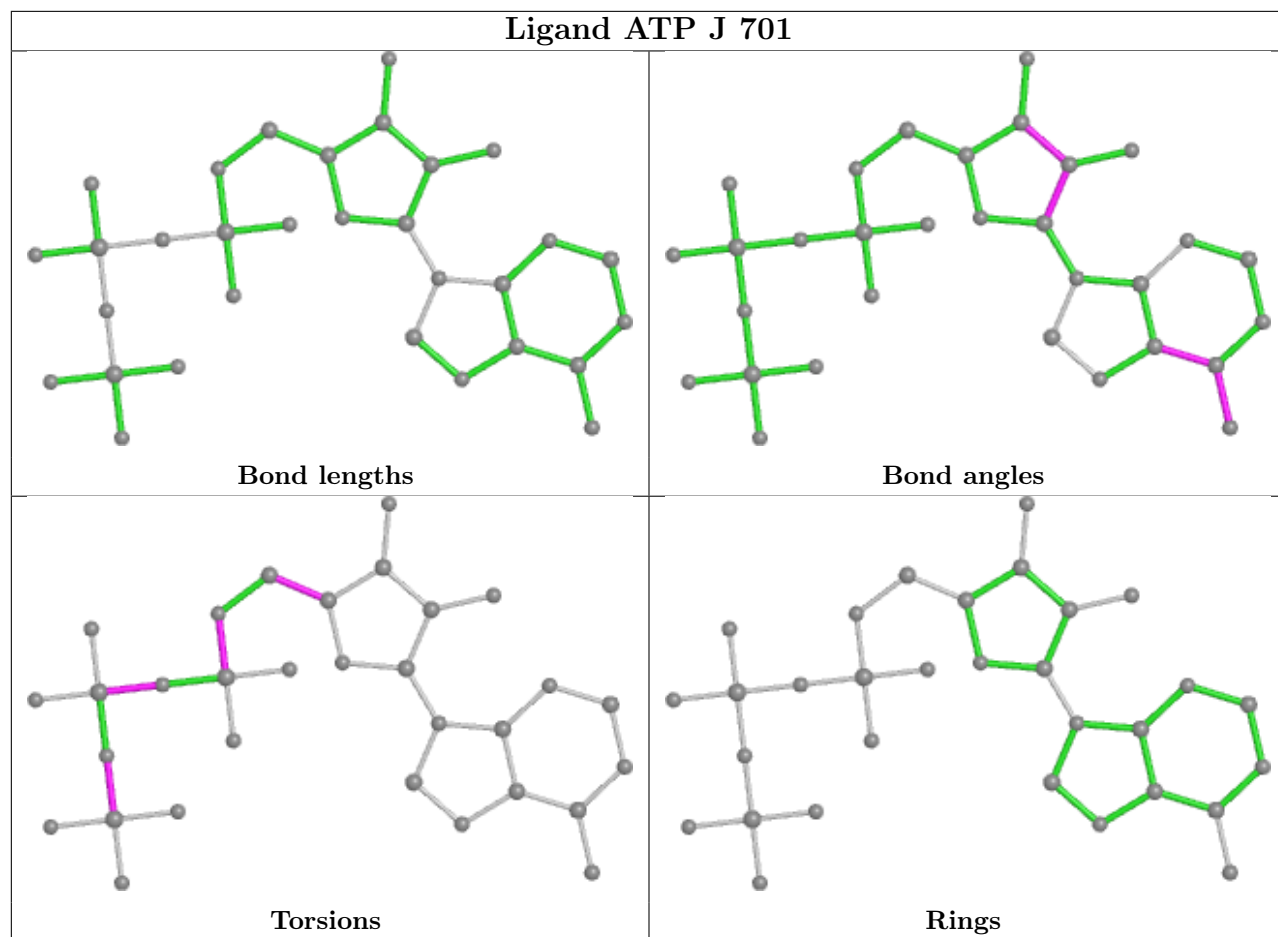


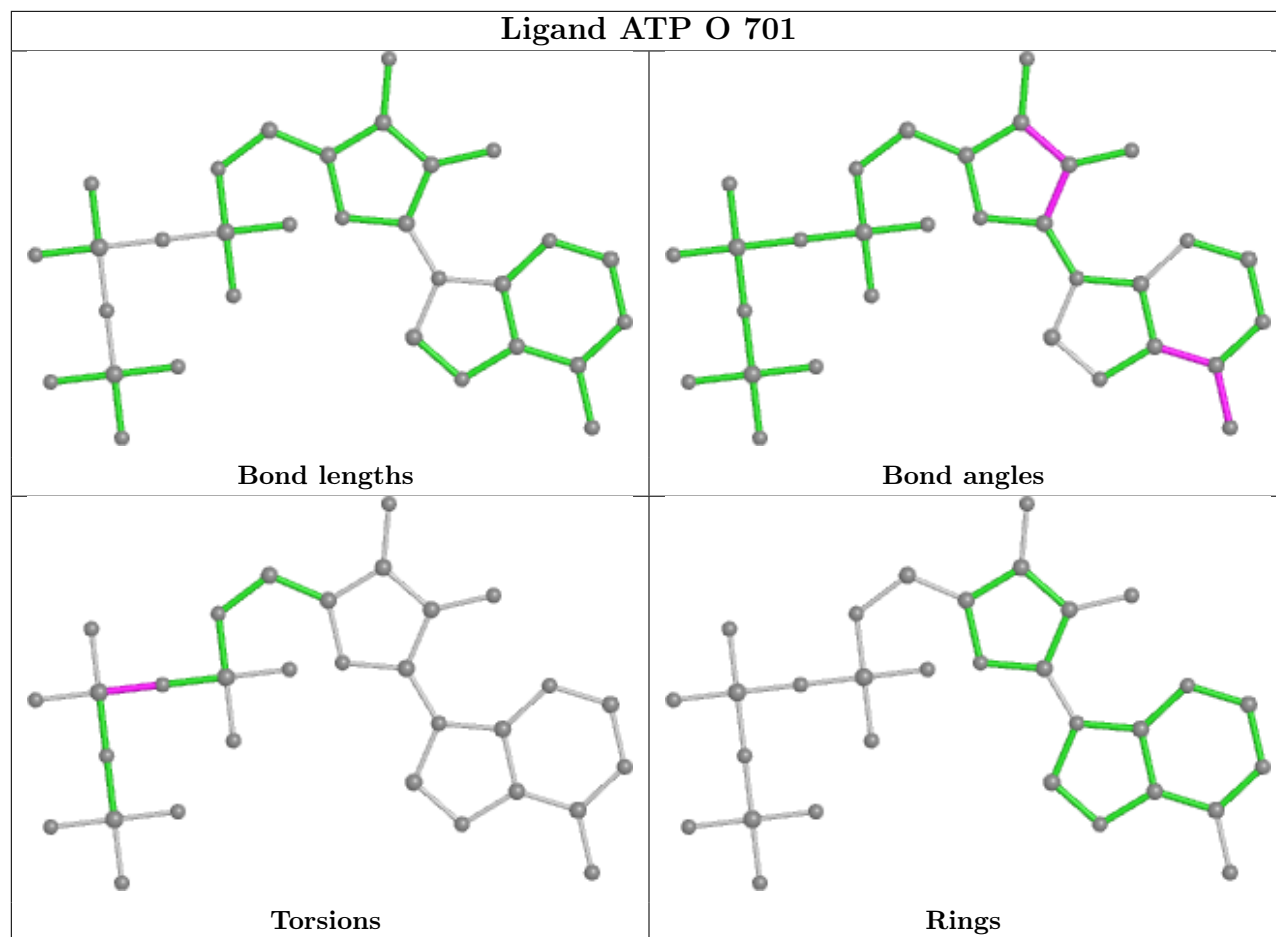




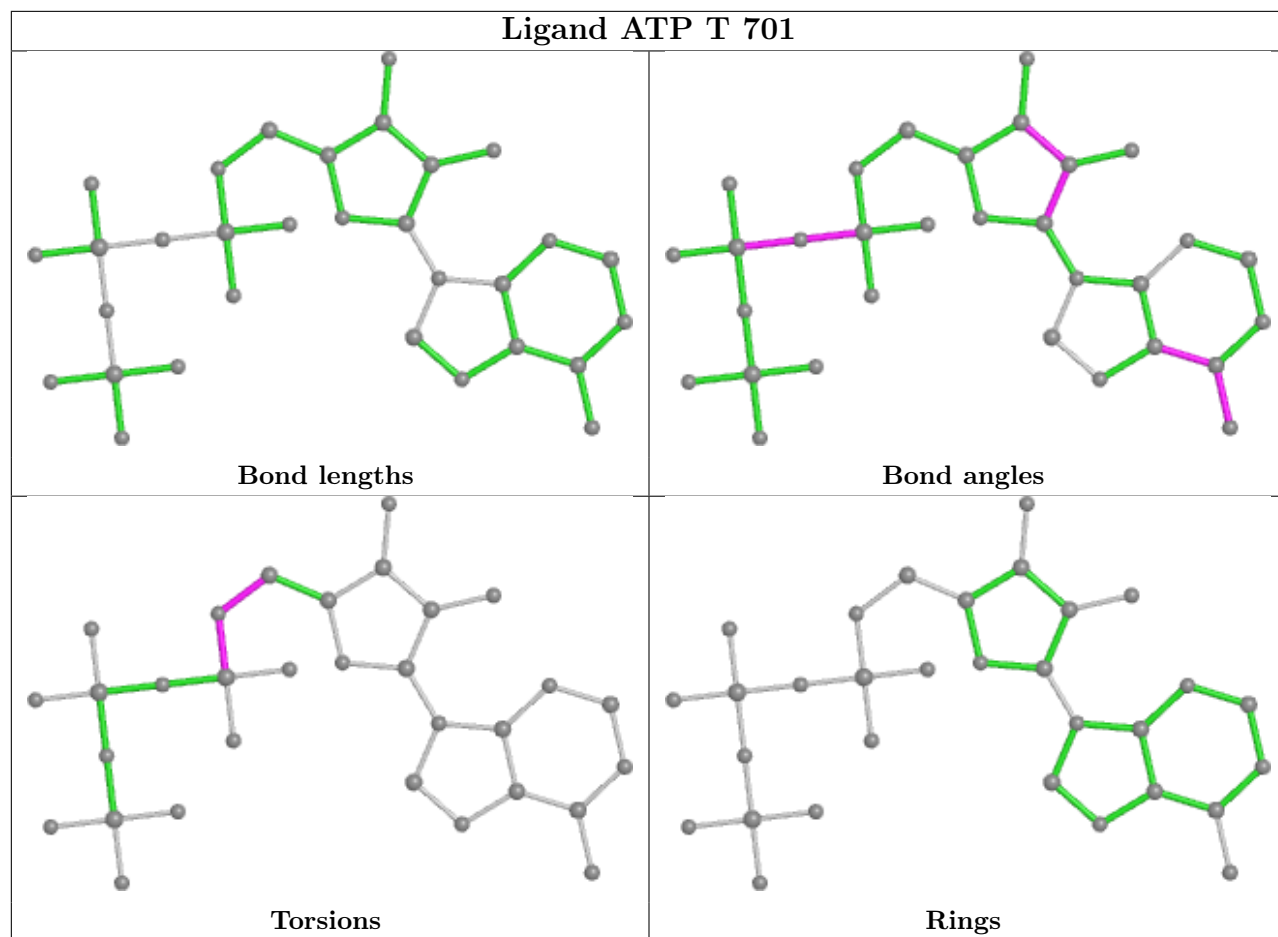


## Ligand ATP J 701

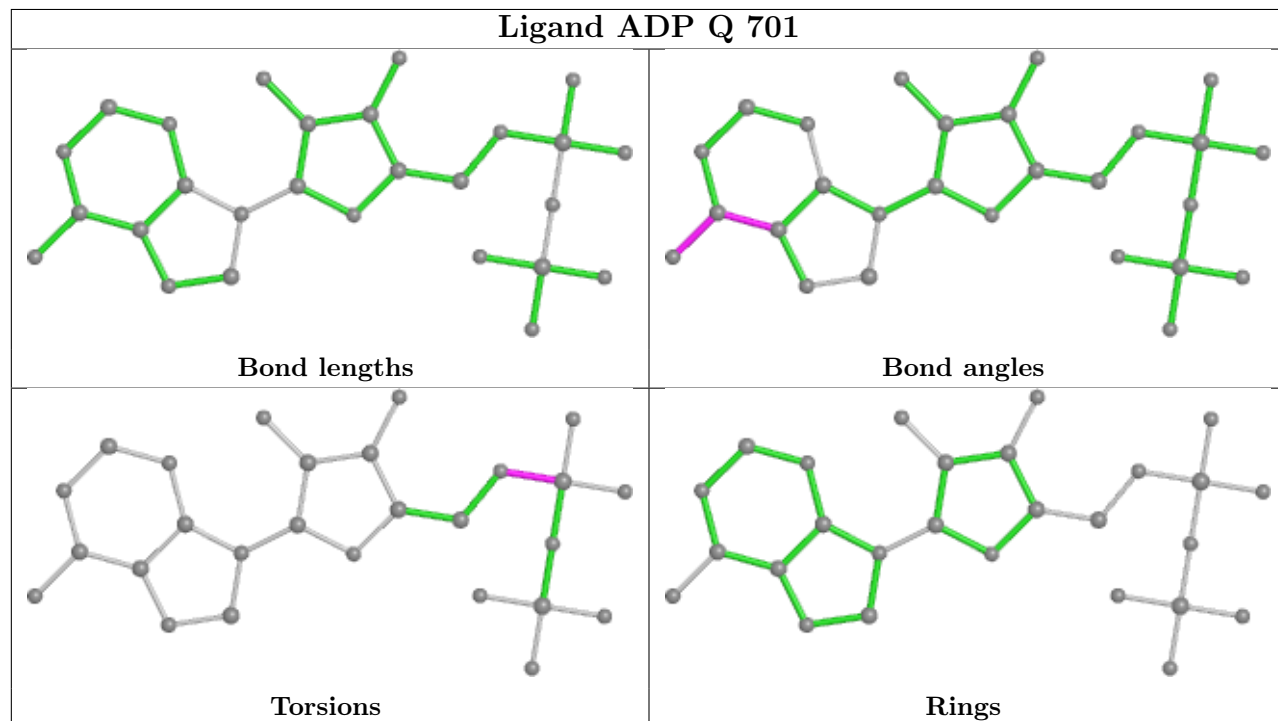


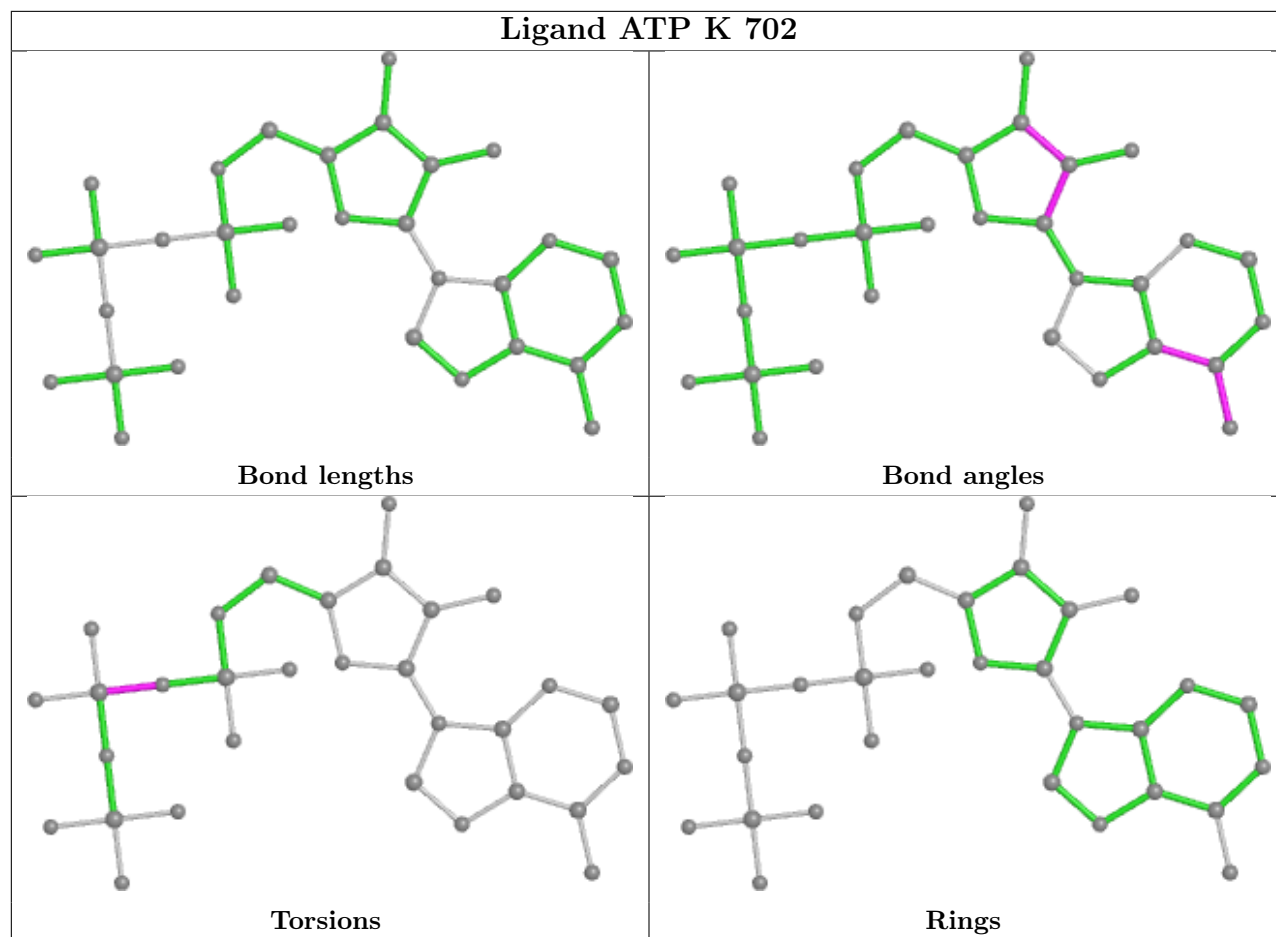


## Ligand ATP T 701

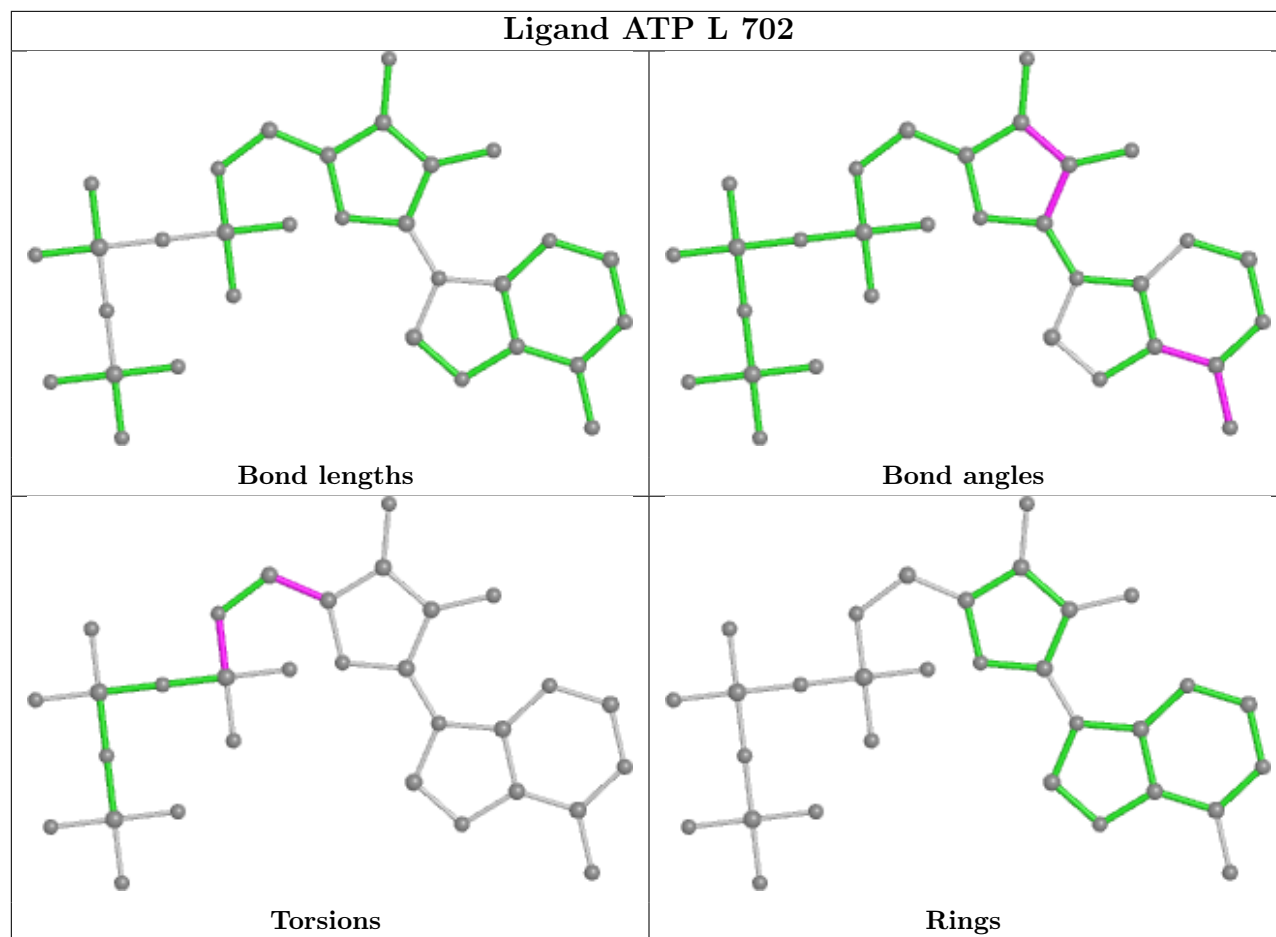


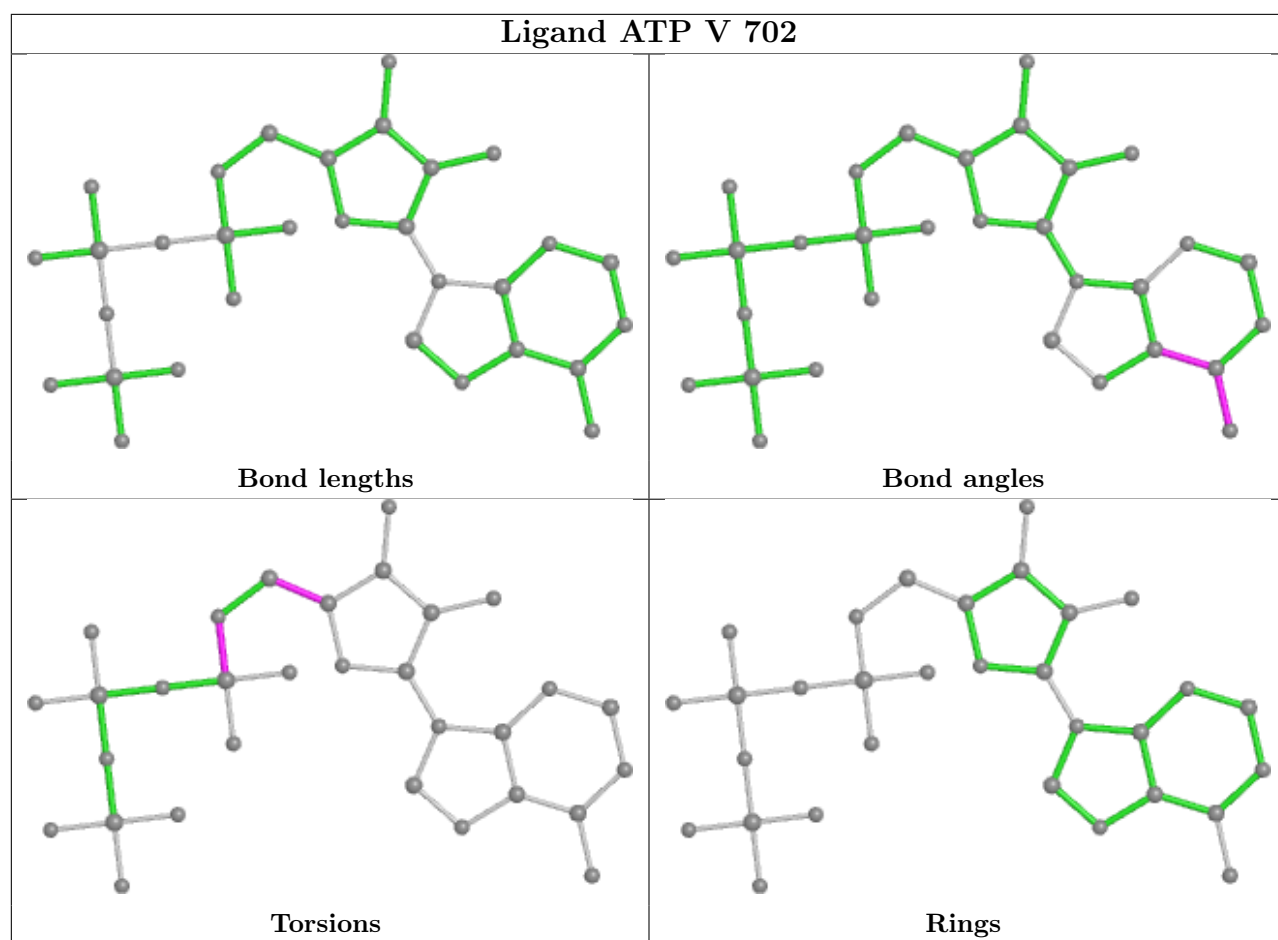
## Ligand ADP Q 701

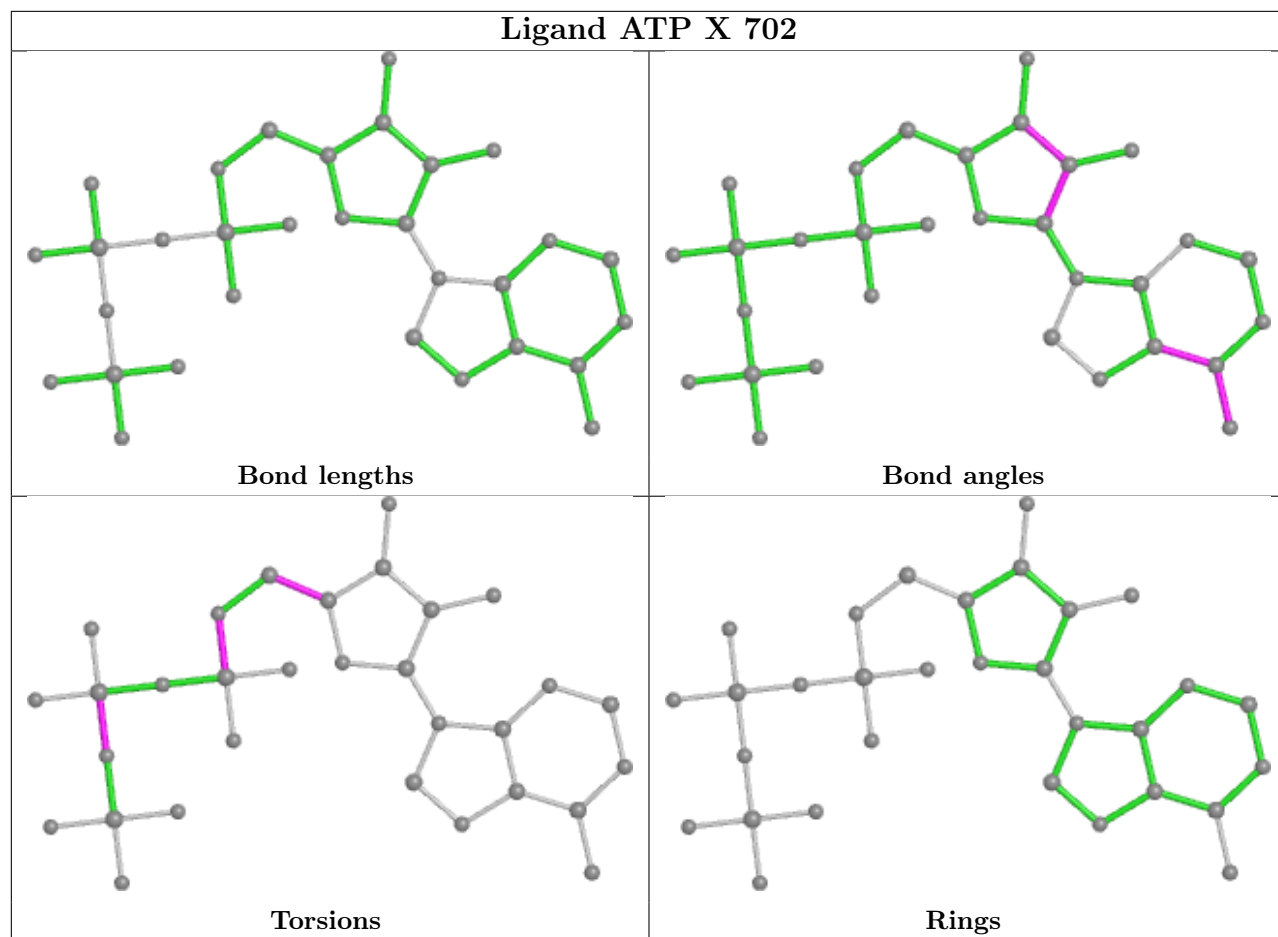


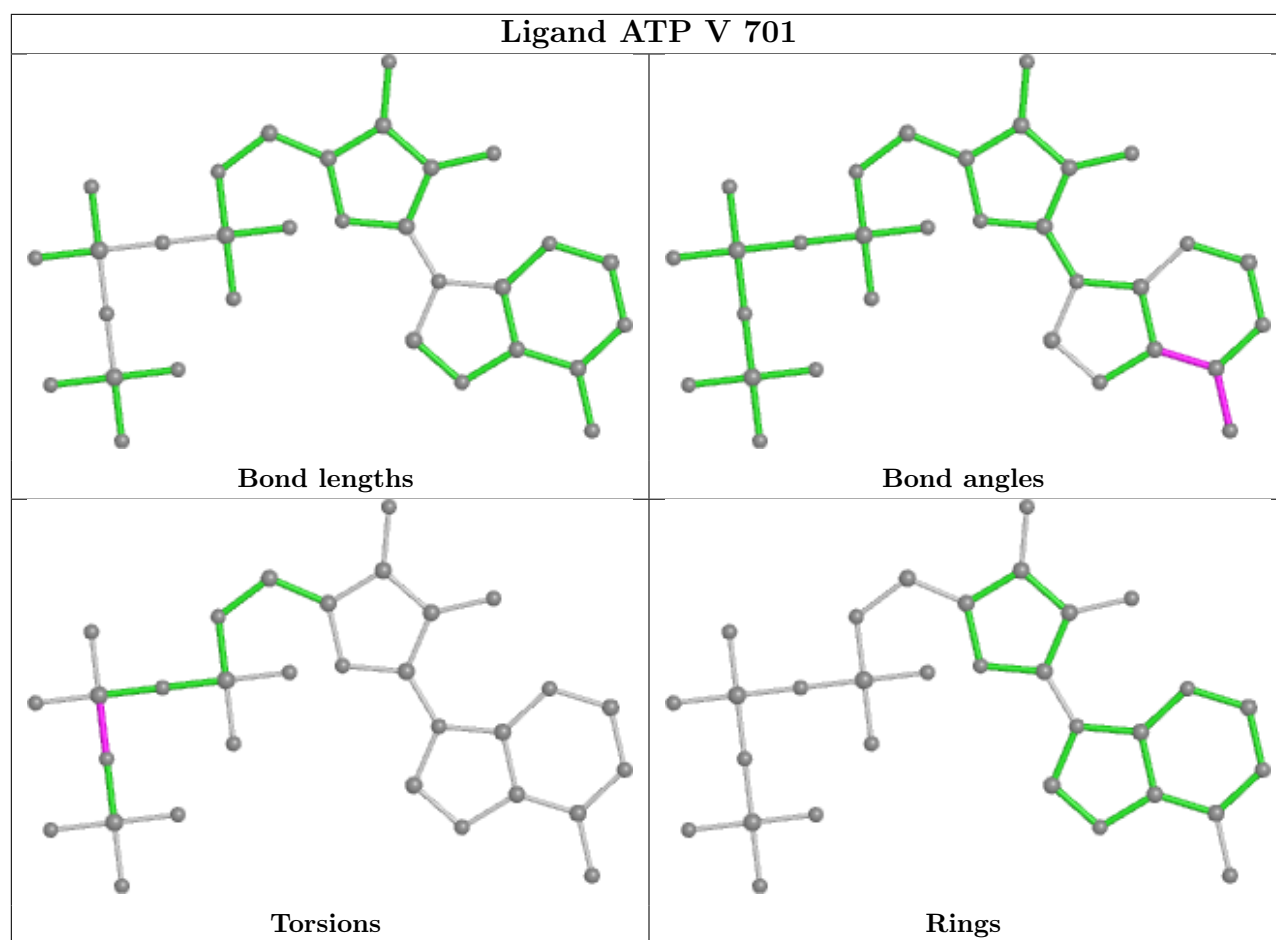


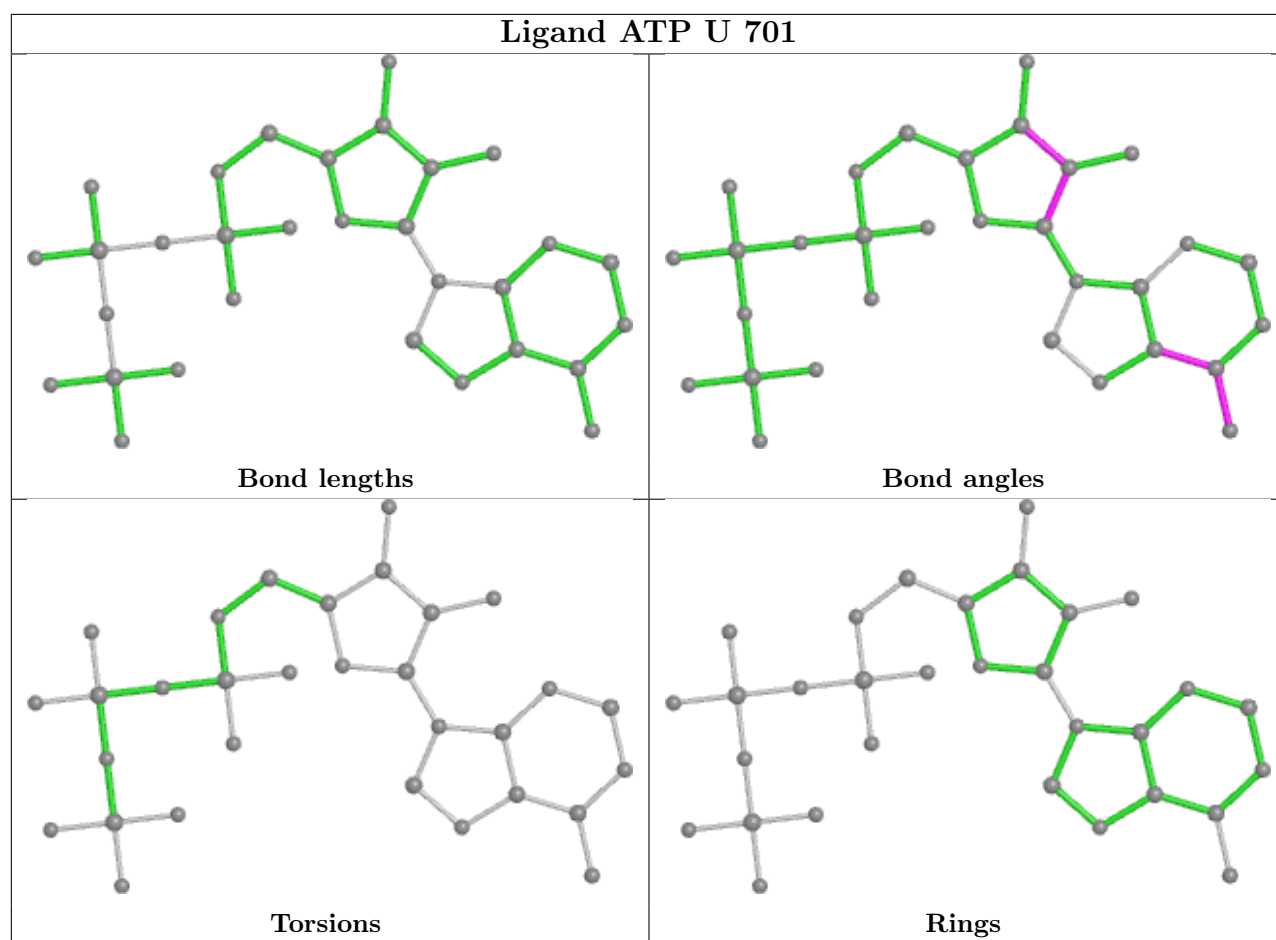


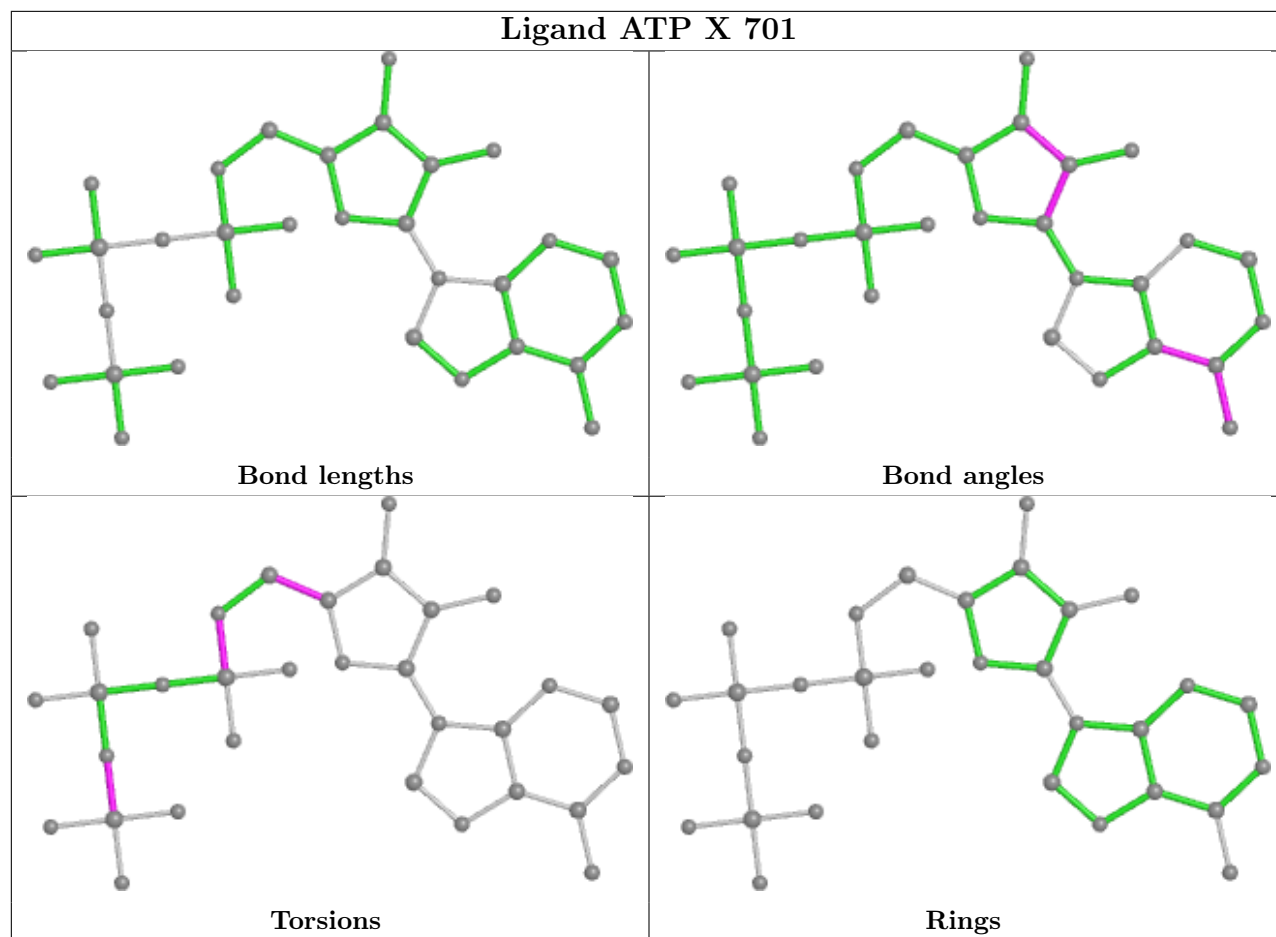


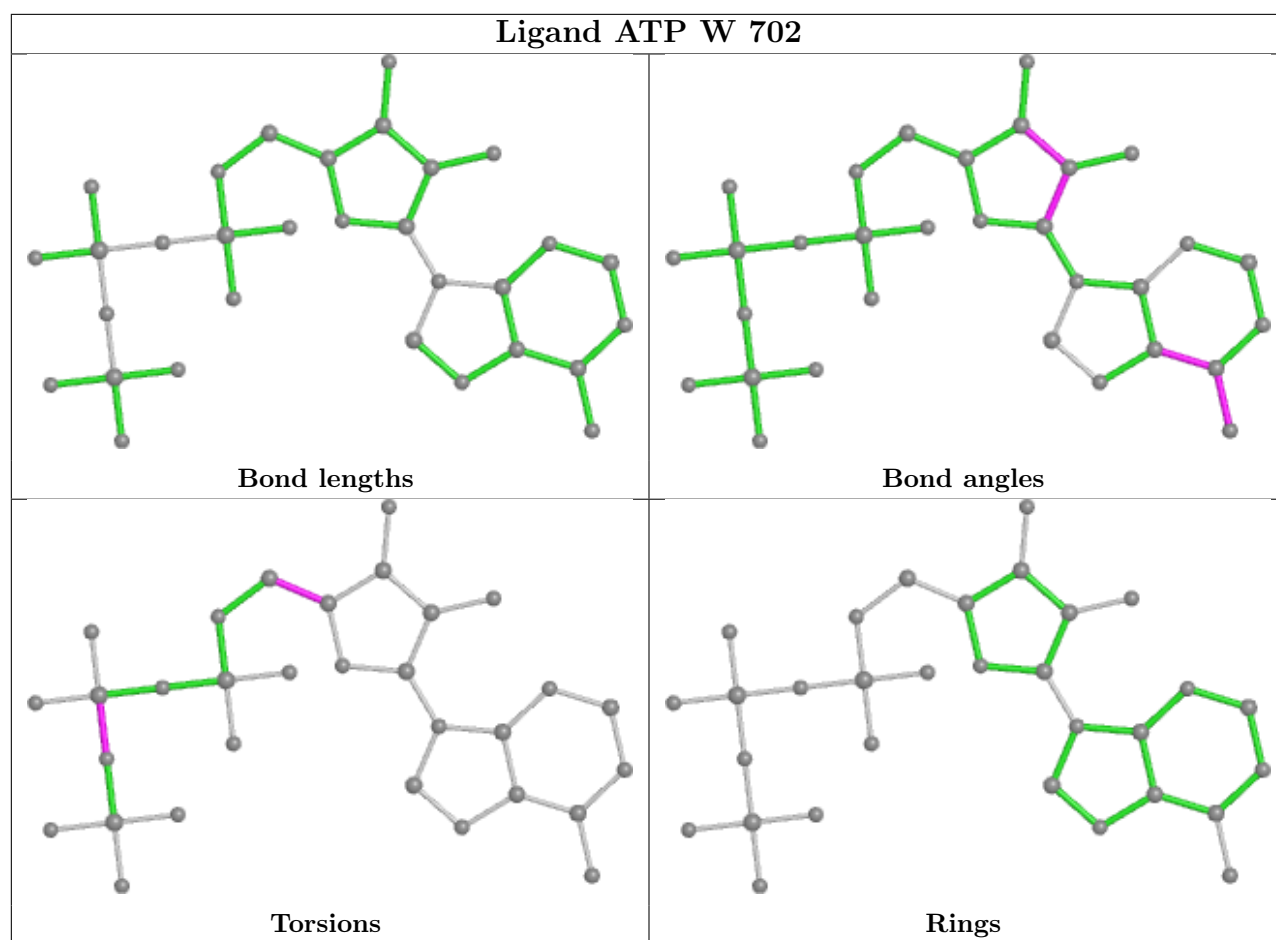


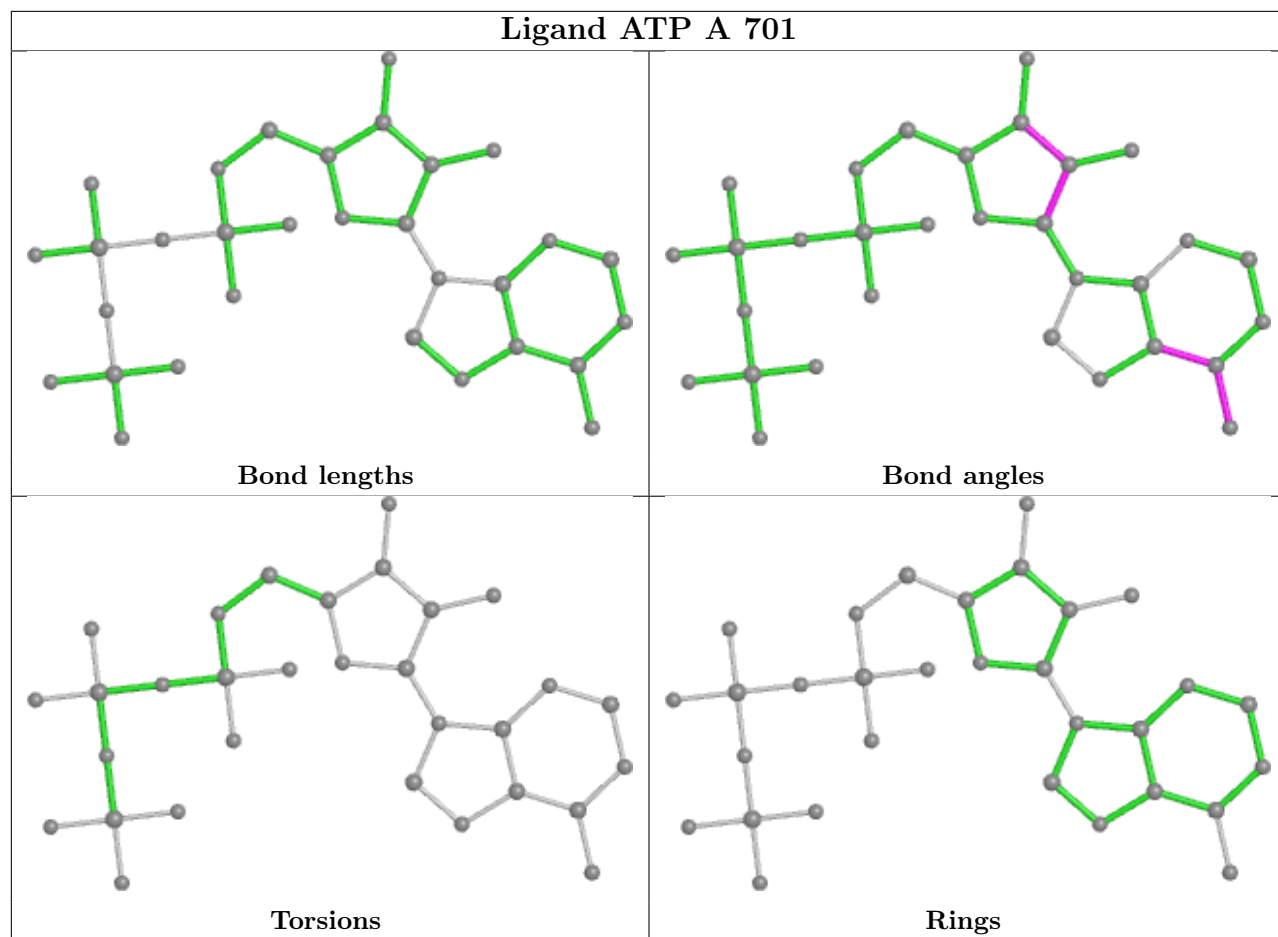




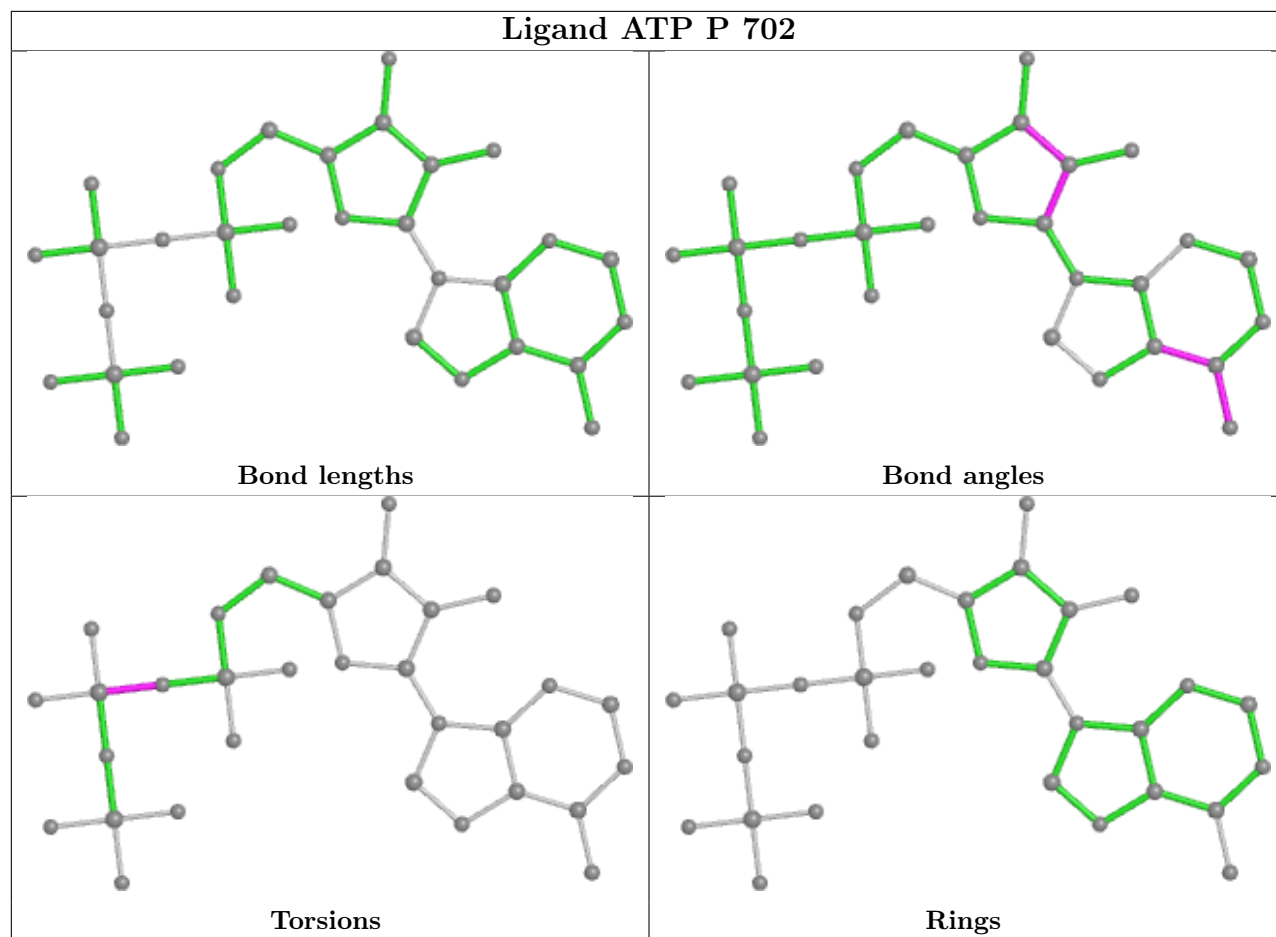


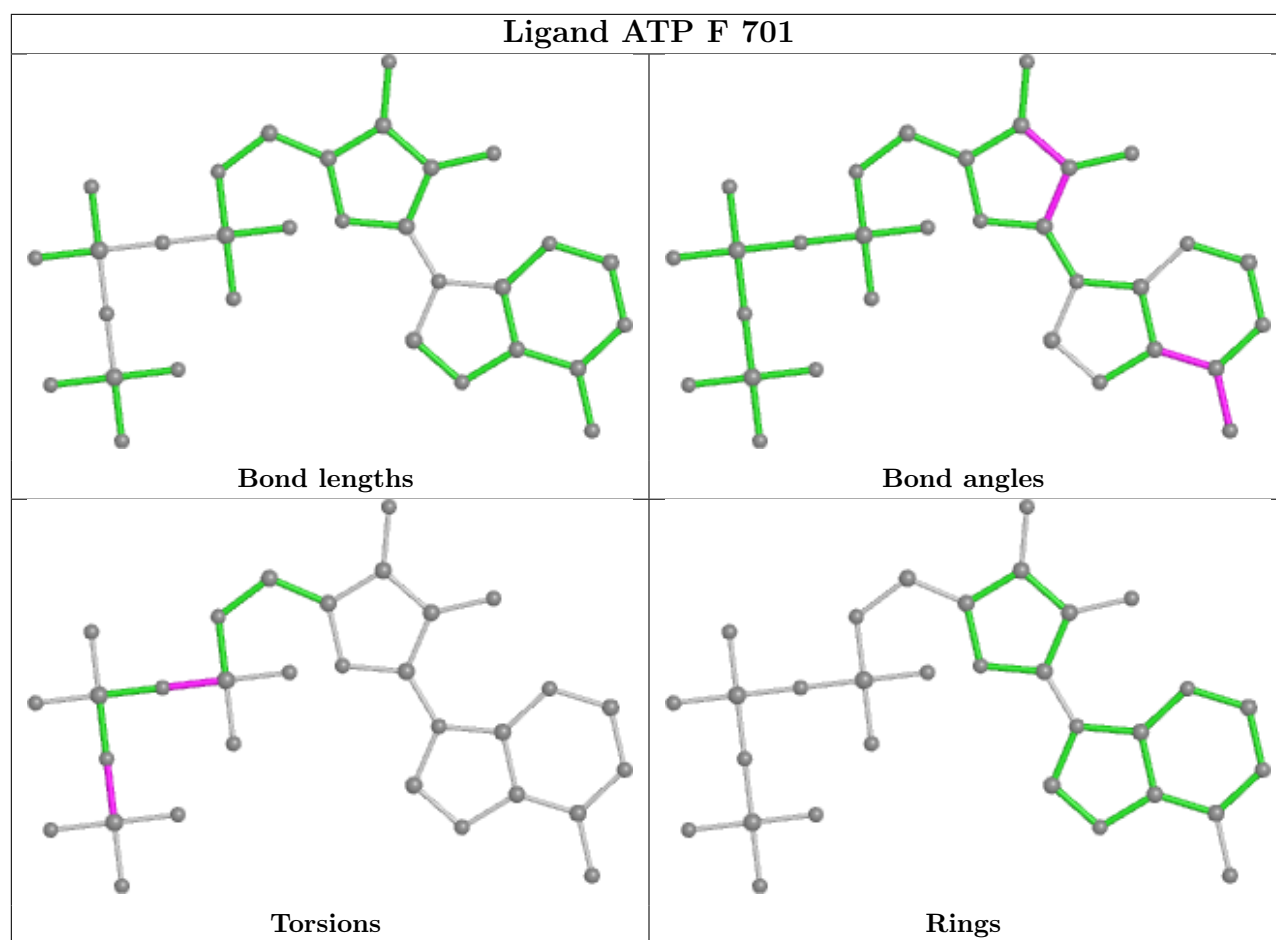


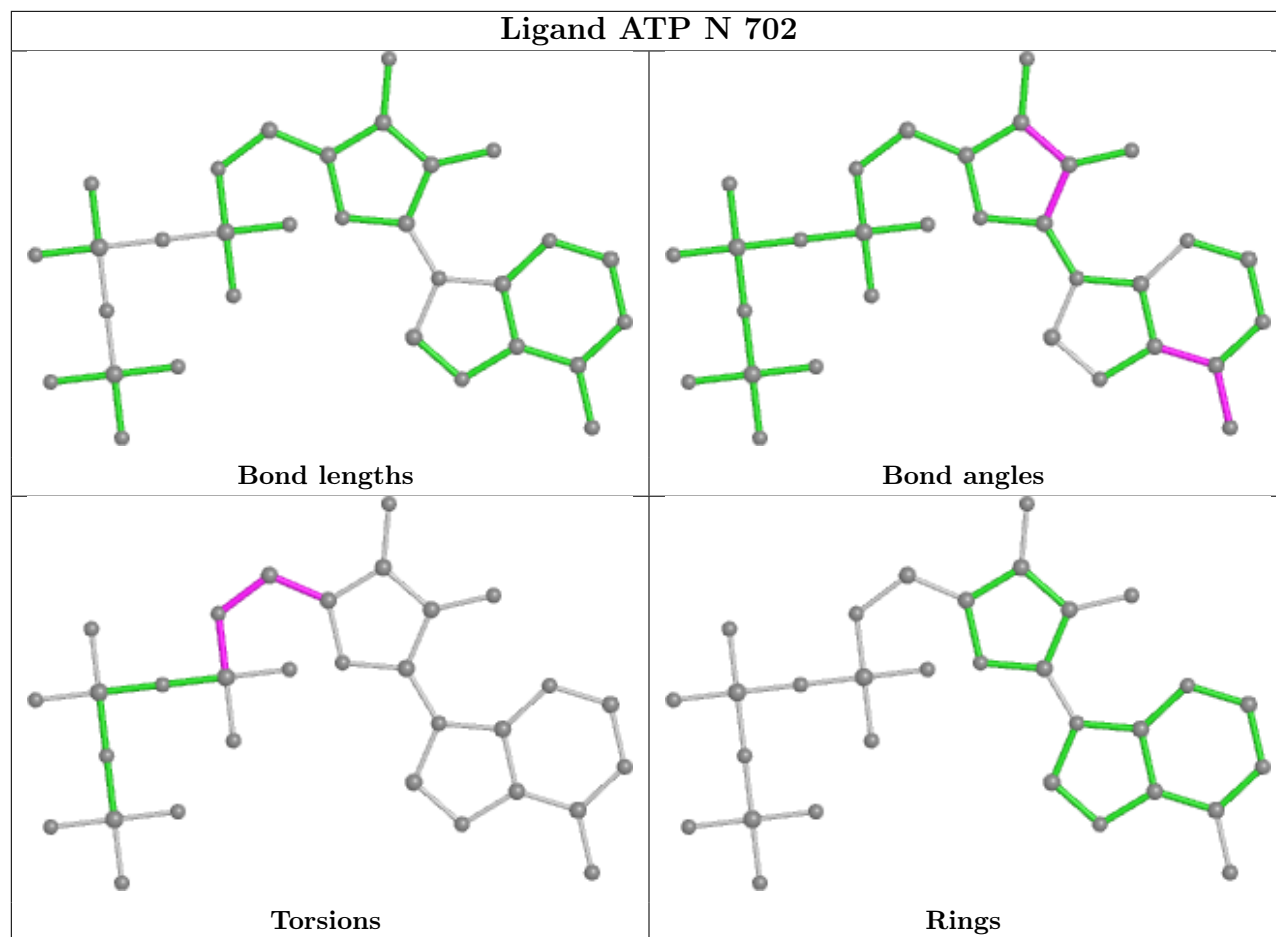


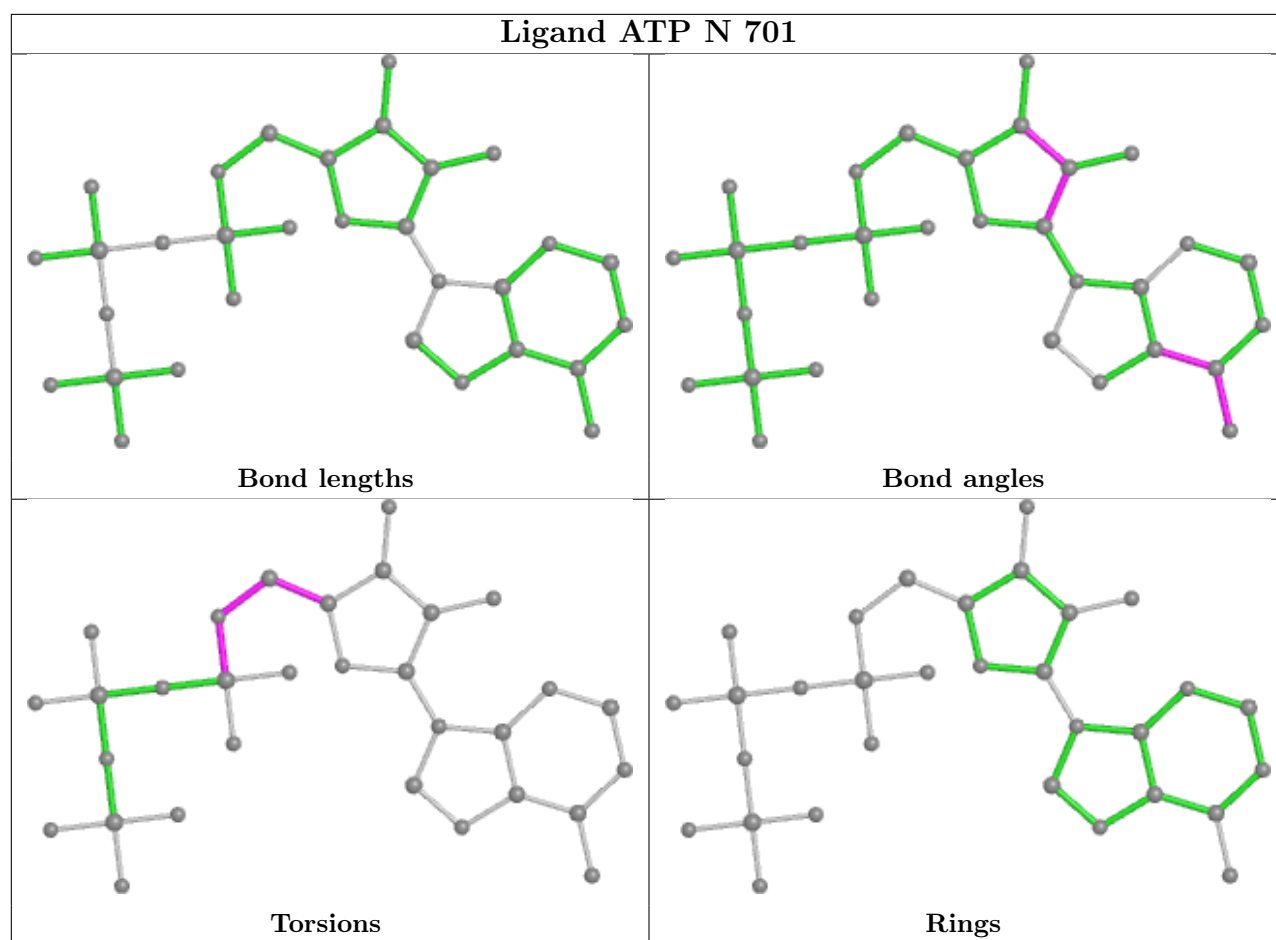


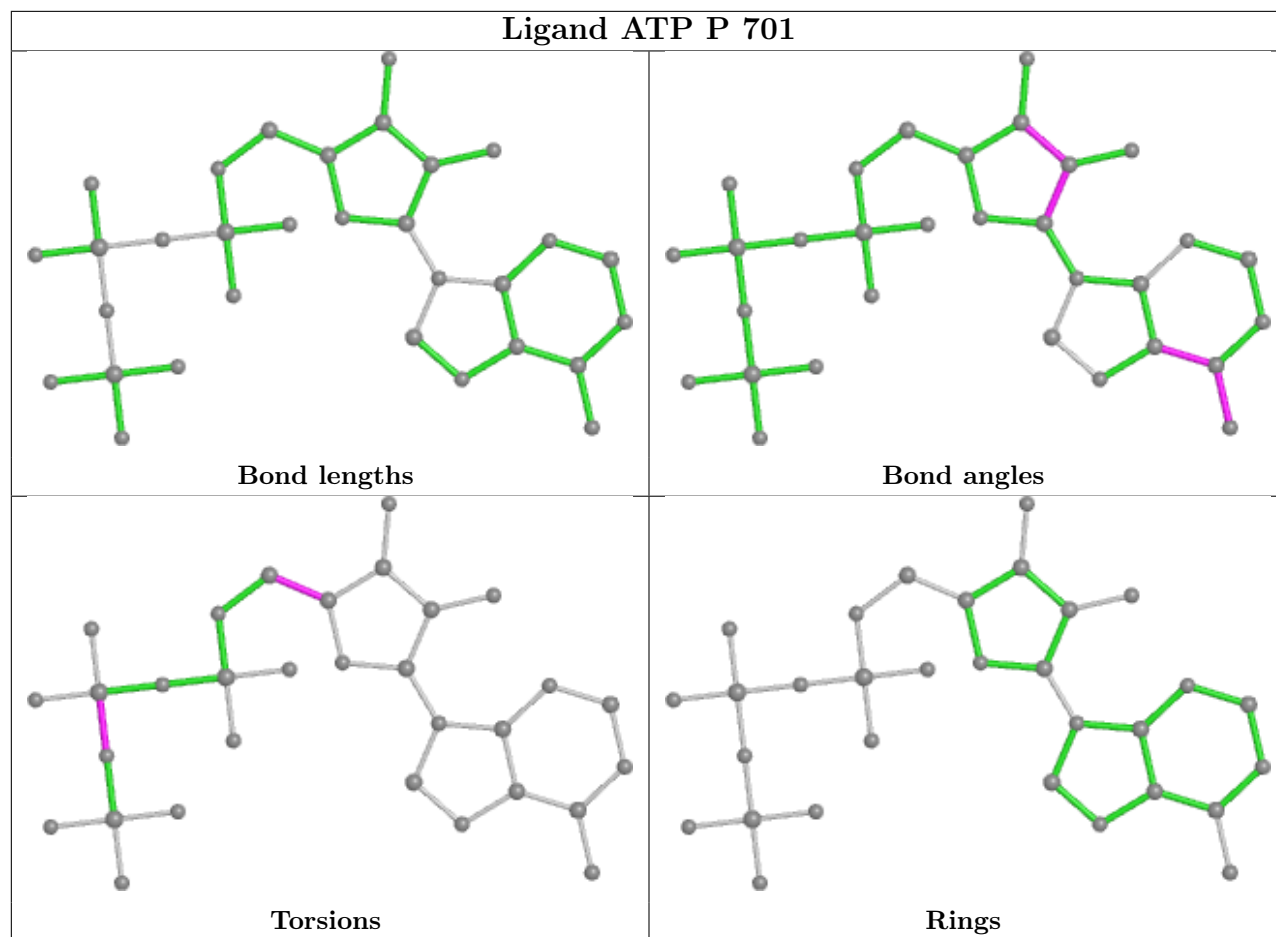




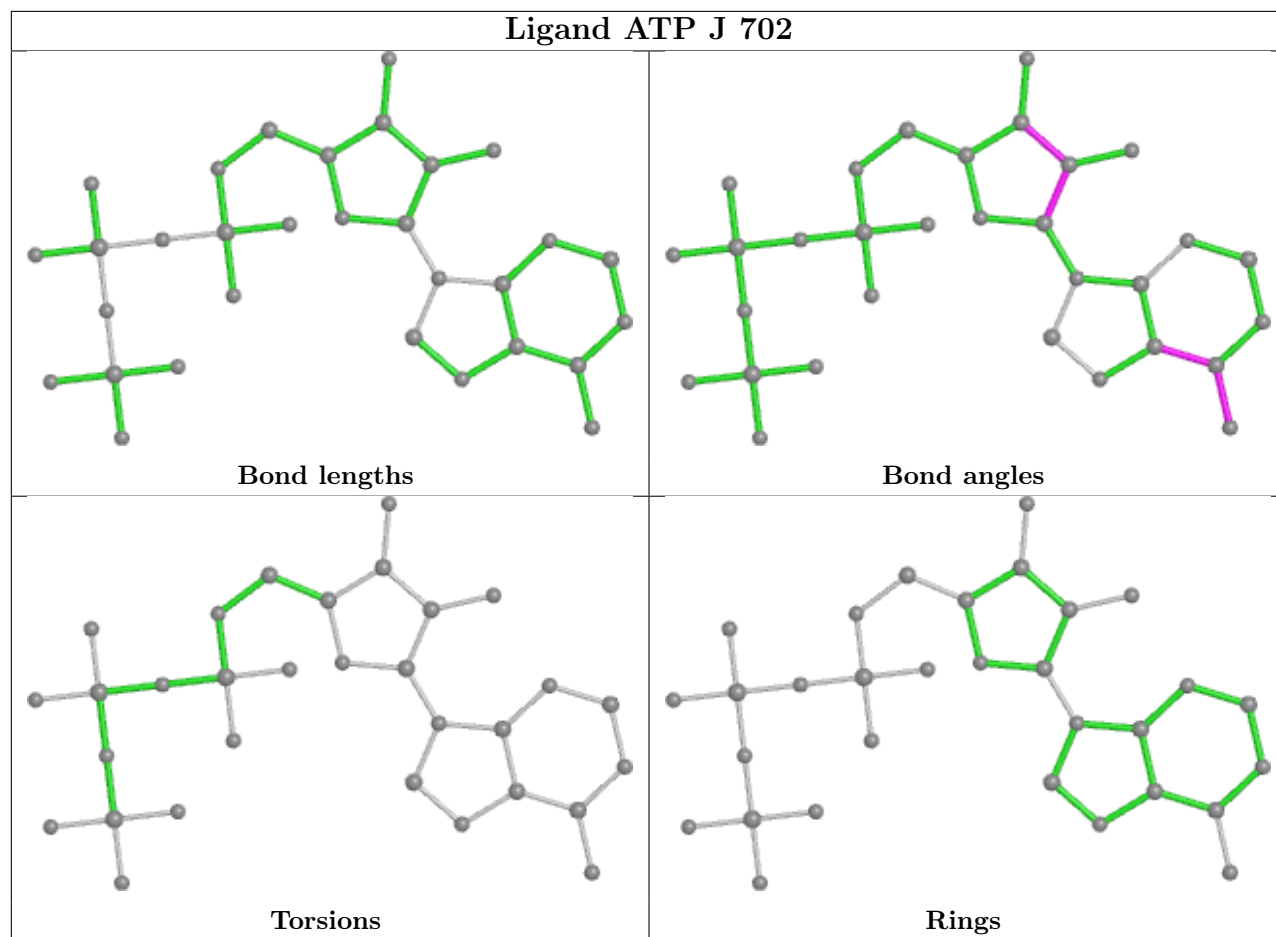


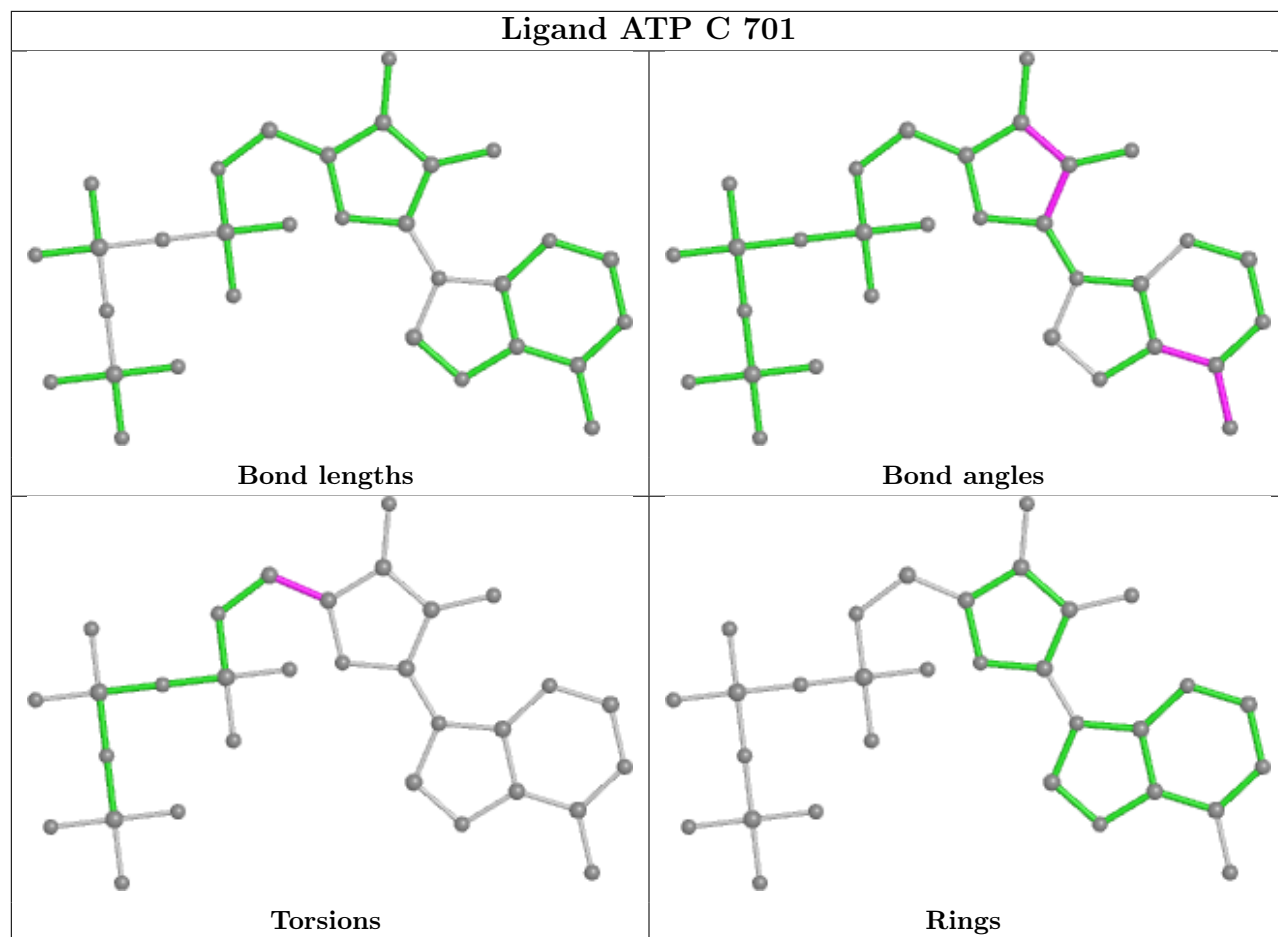


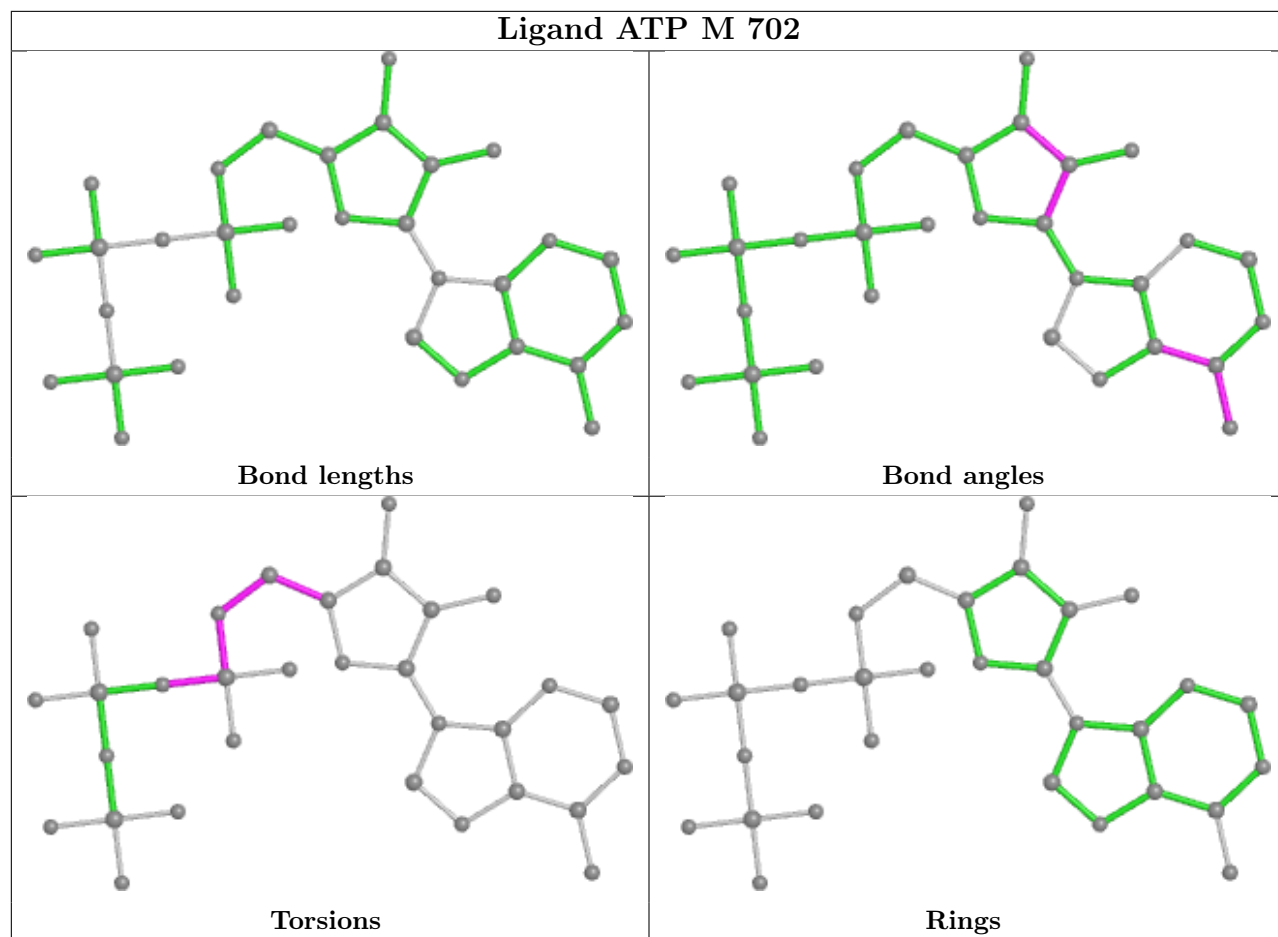




## Ligand ATP J 702

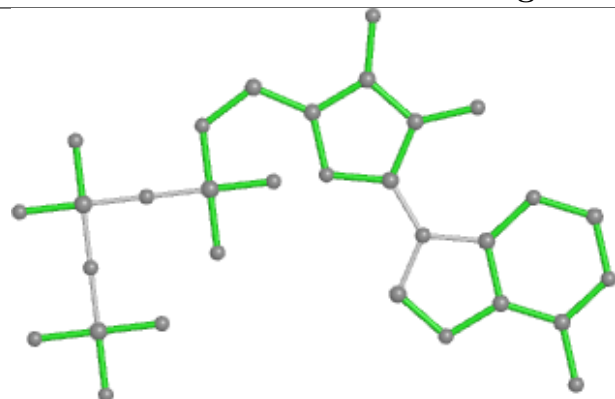




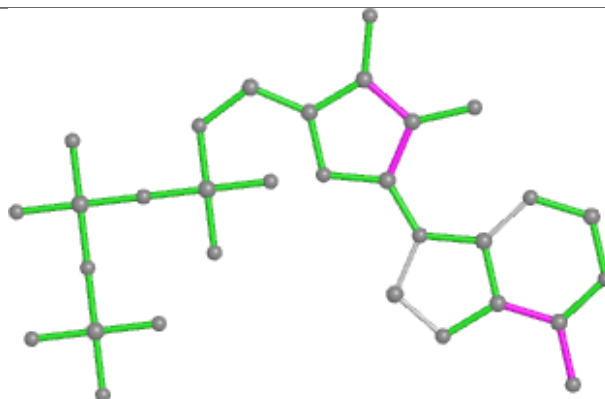




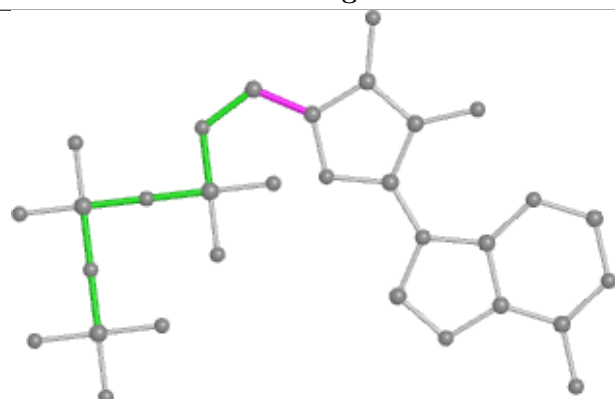
## Ligand ATP T 702



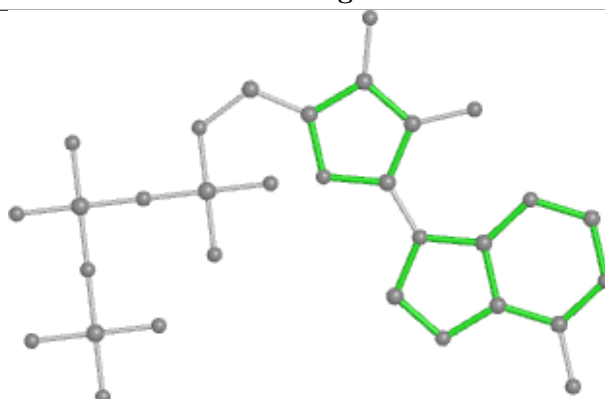
Bond lengths



Bond angles

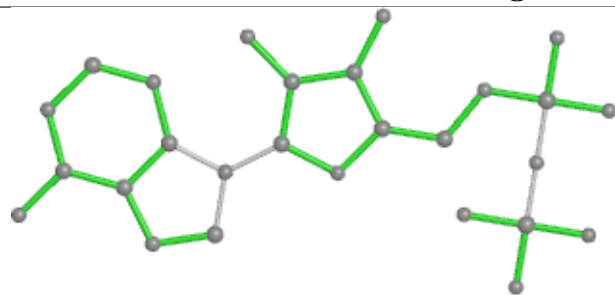


Torsions

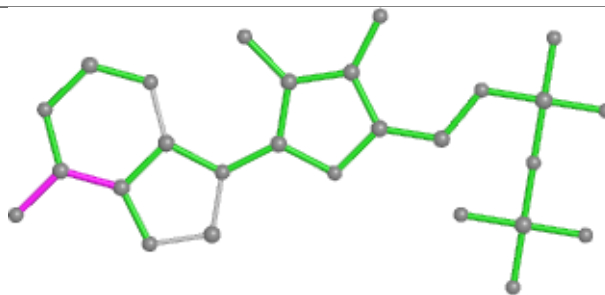


Rings

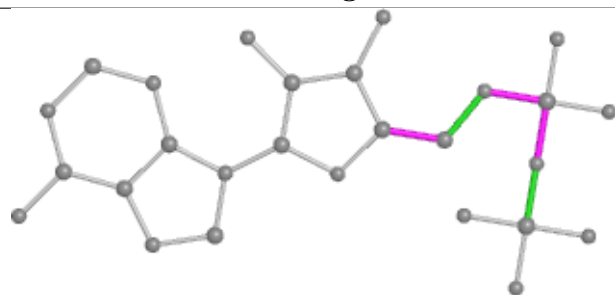
## Ligand ADP W 701



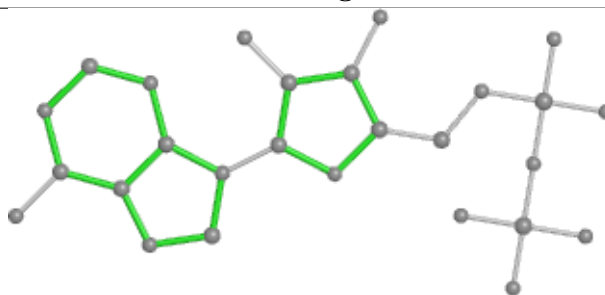
Bond lengths



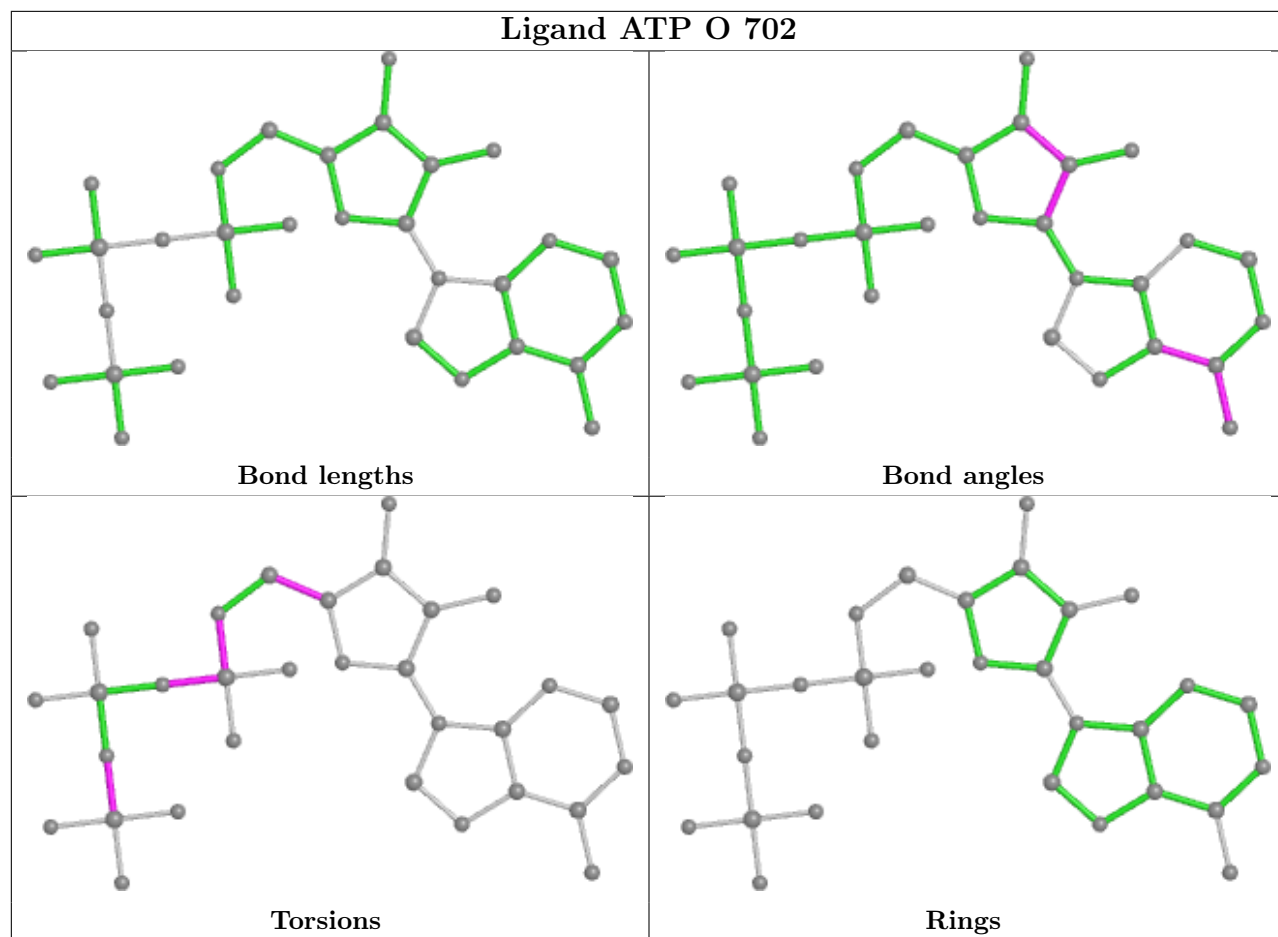
Bond angles

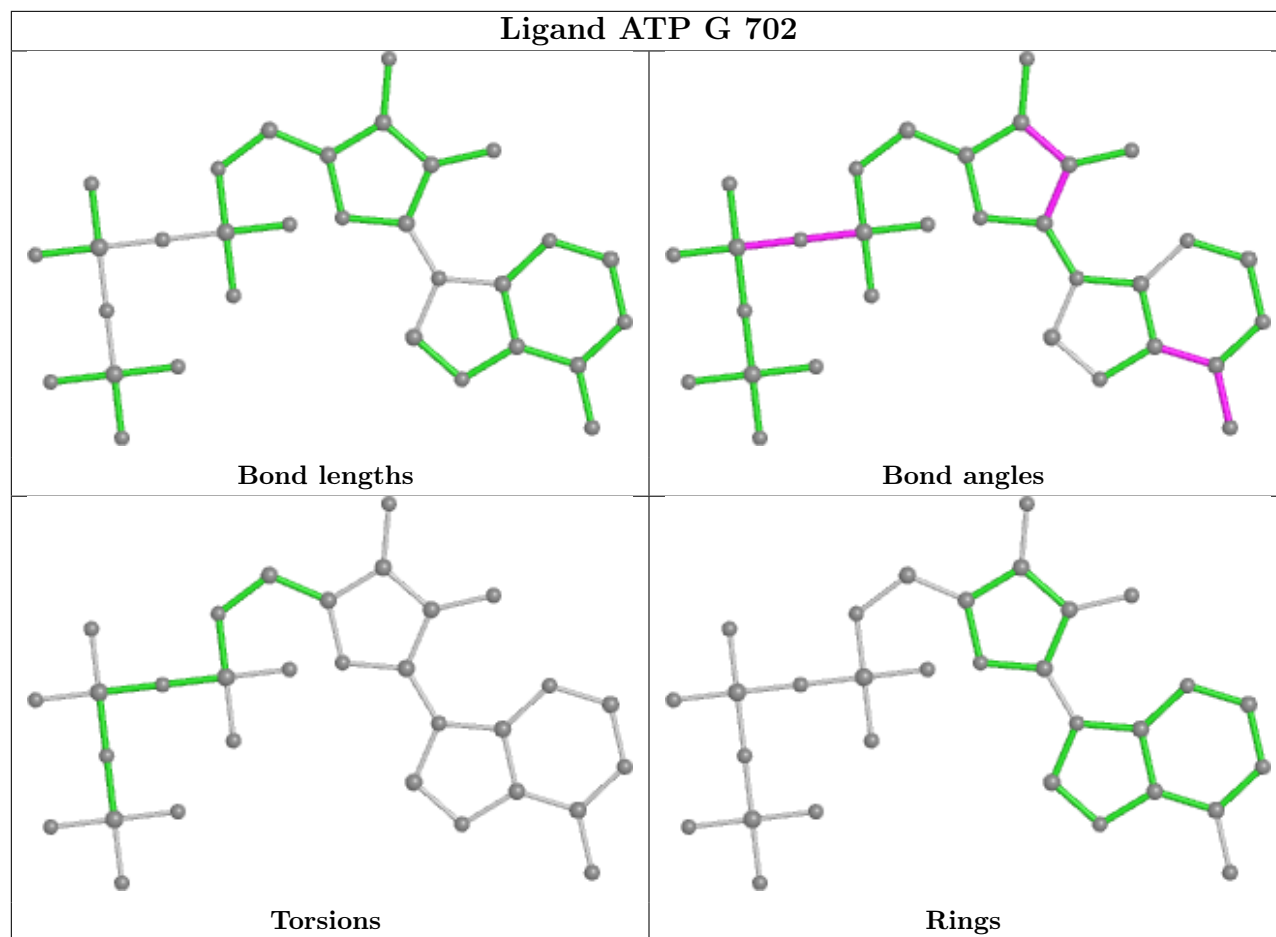


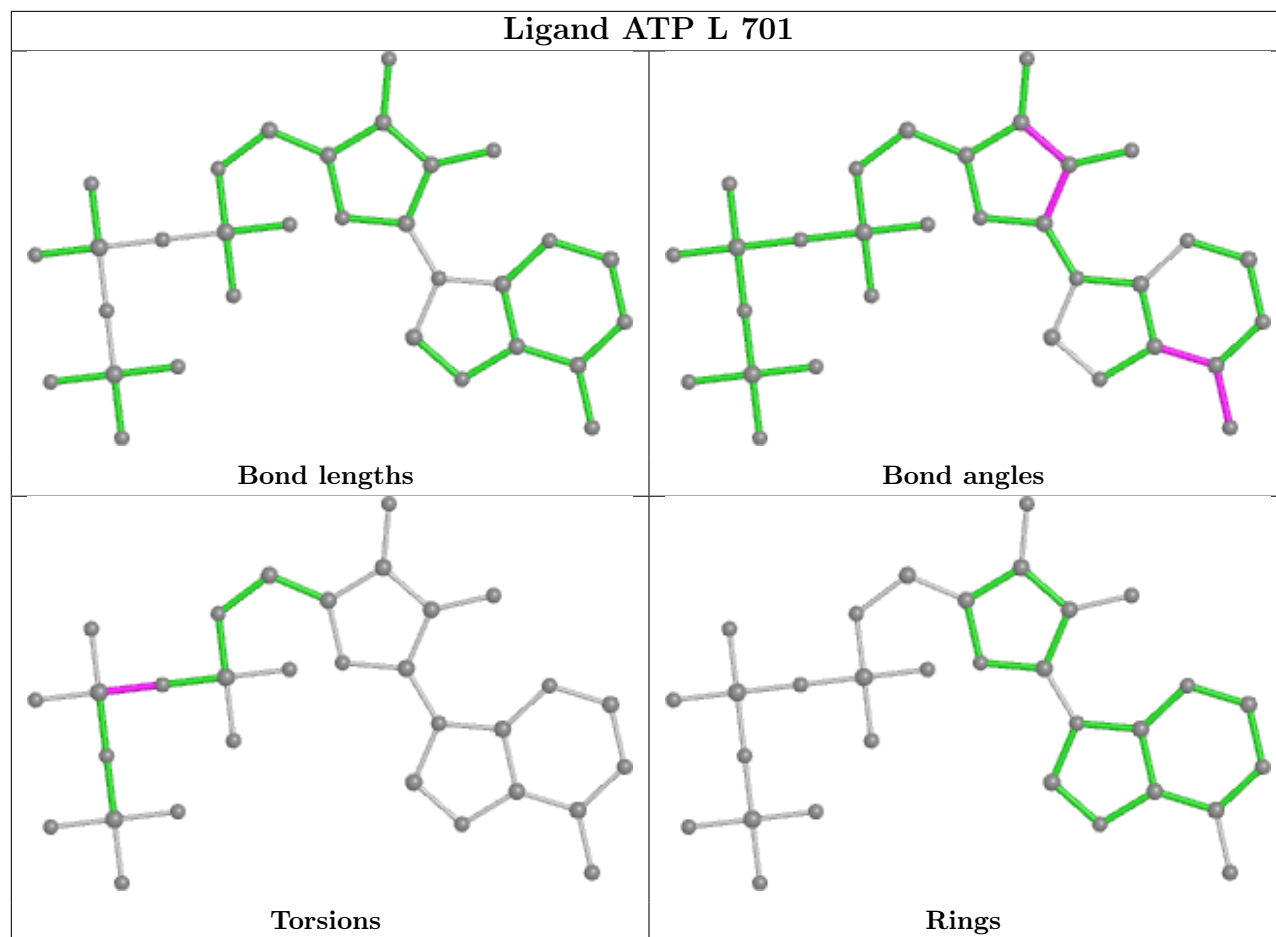
Torsions

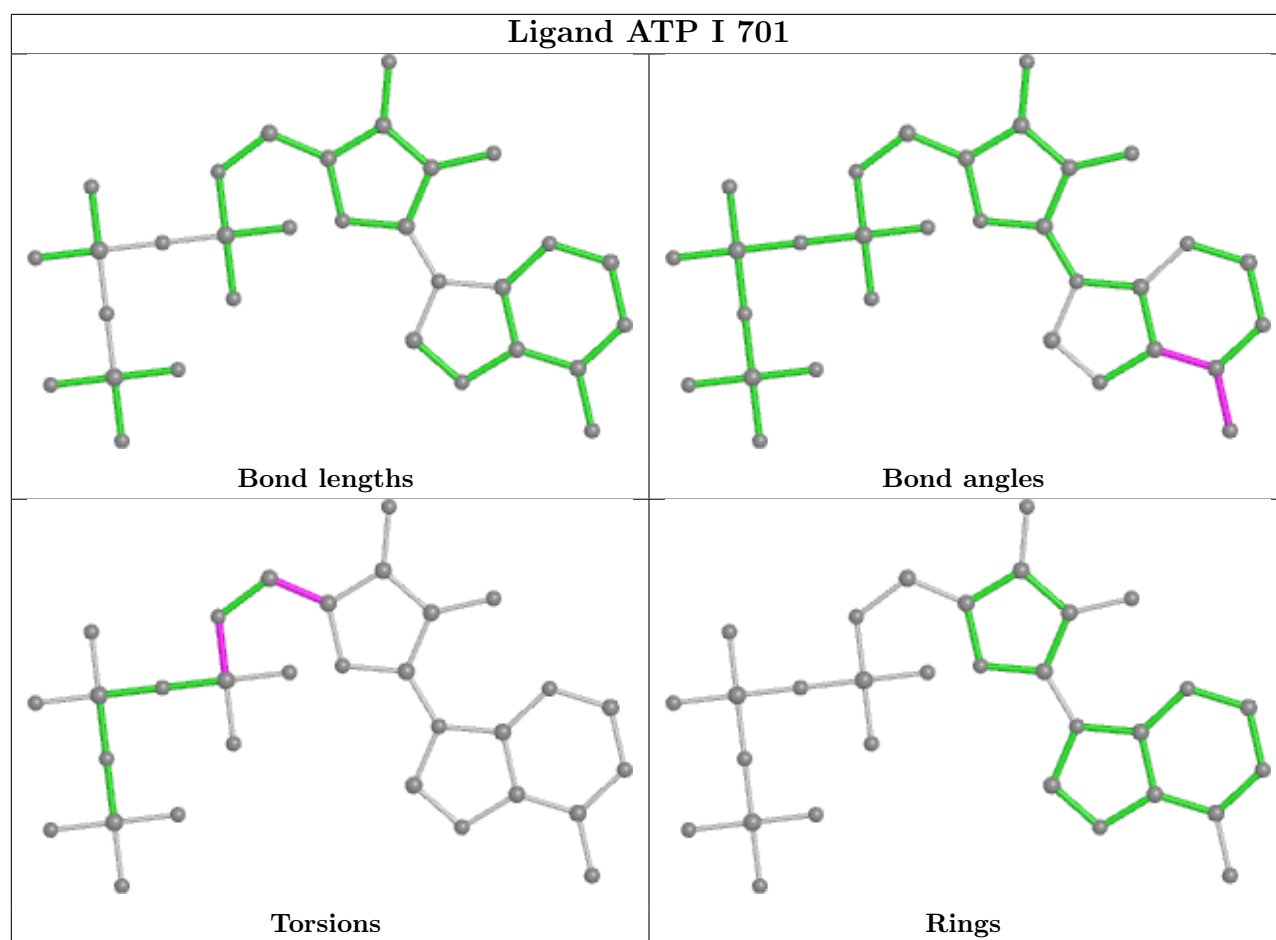


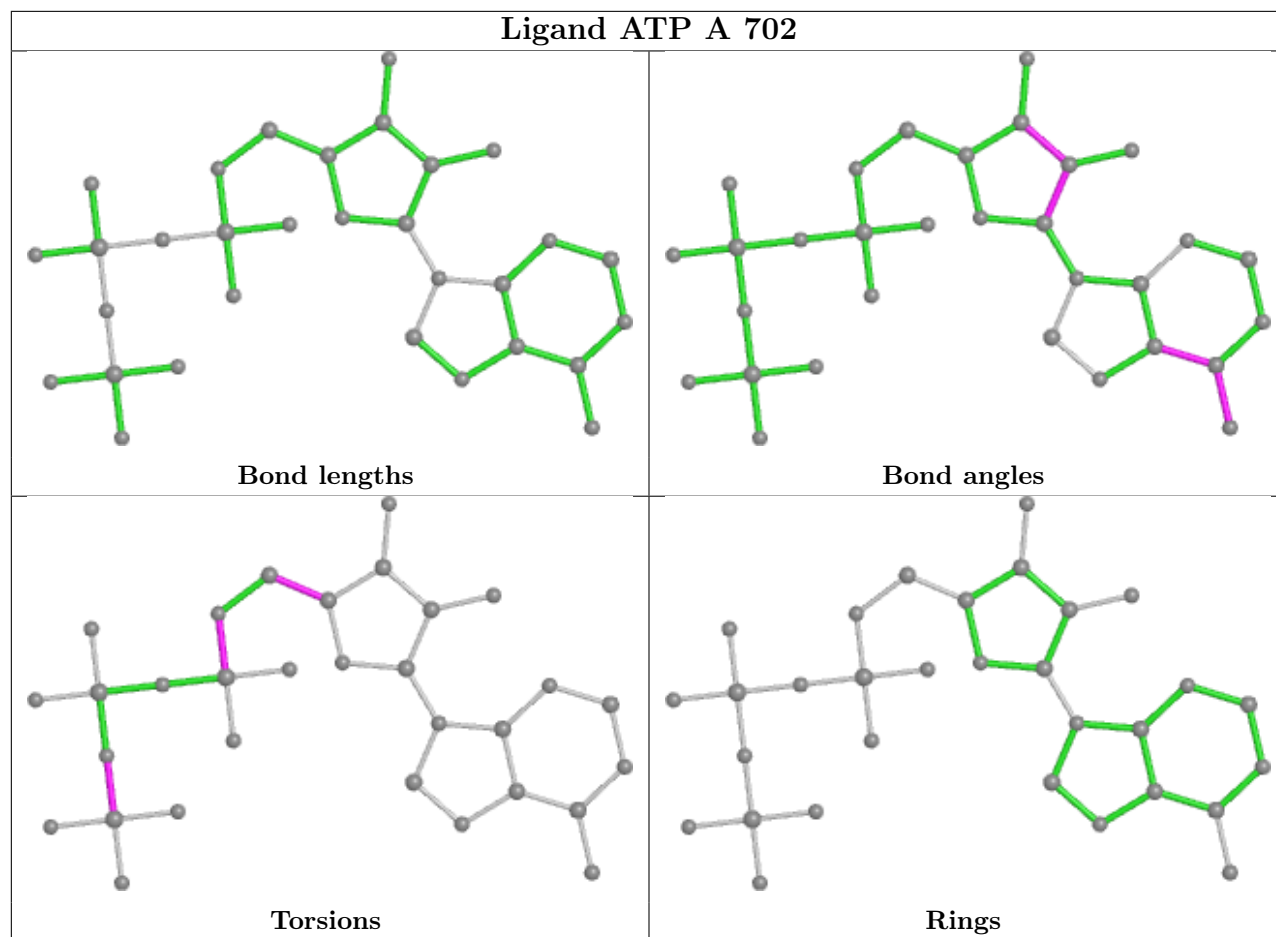
Rings

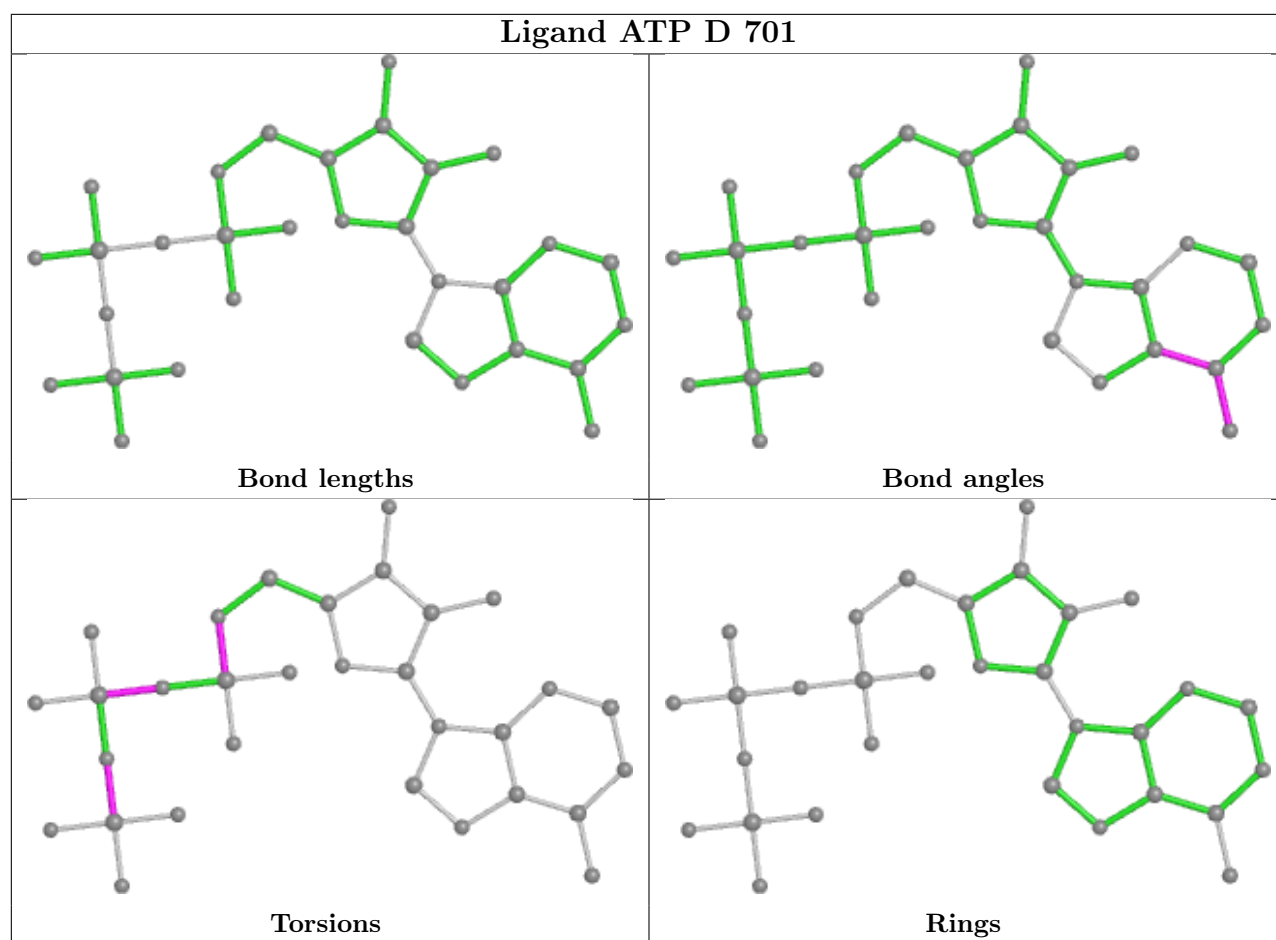


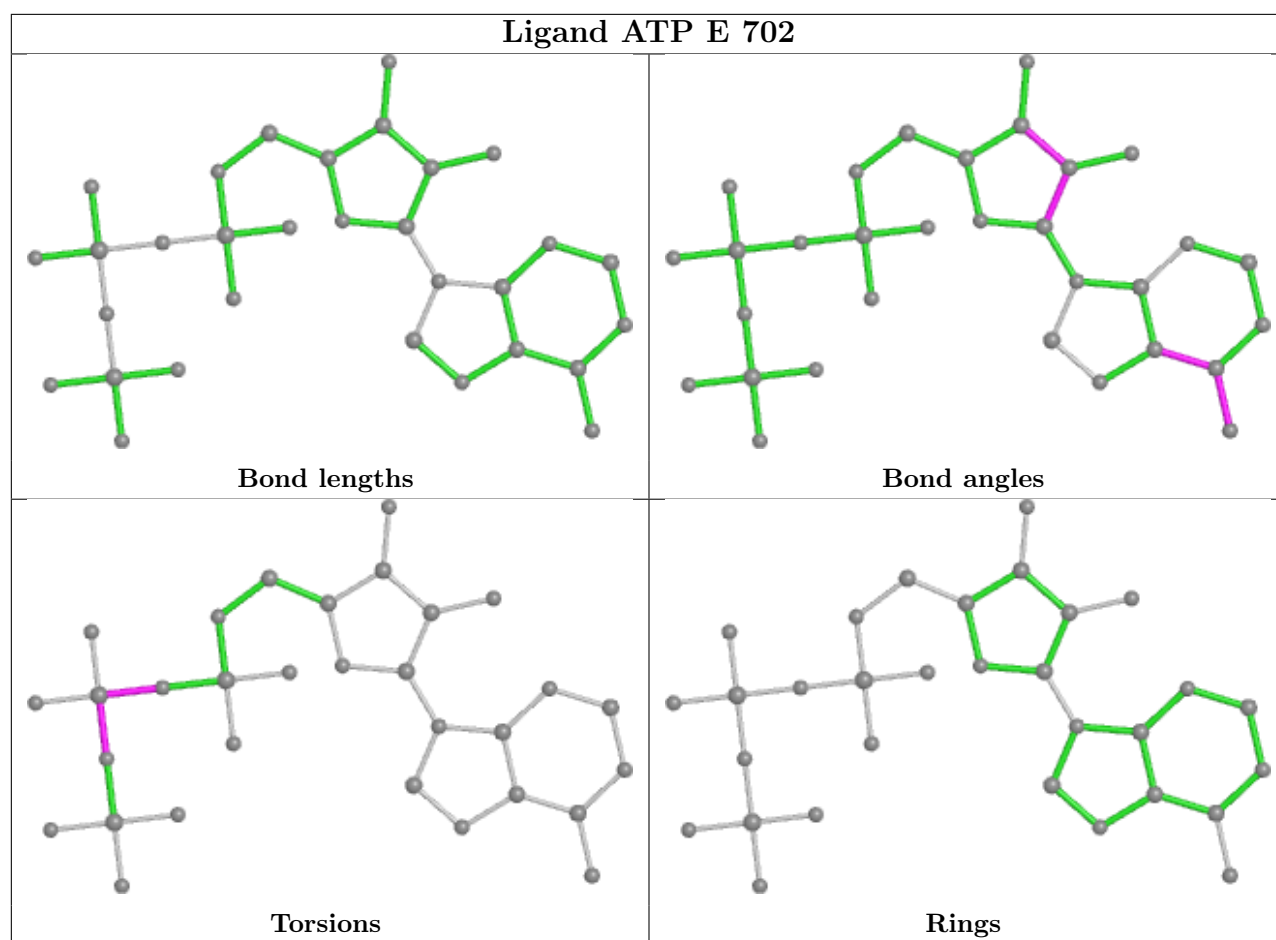




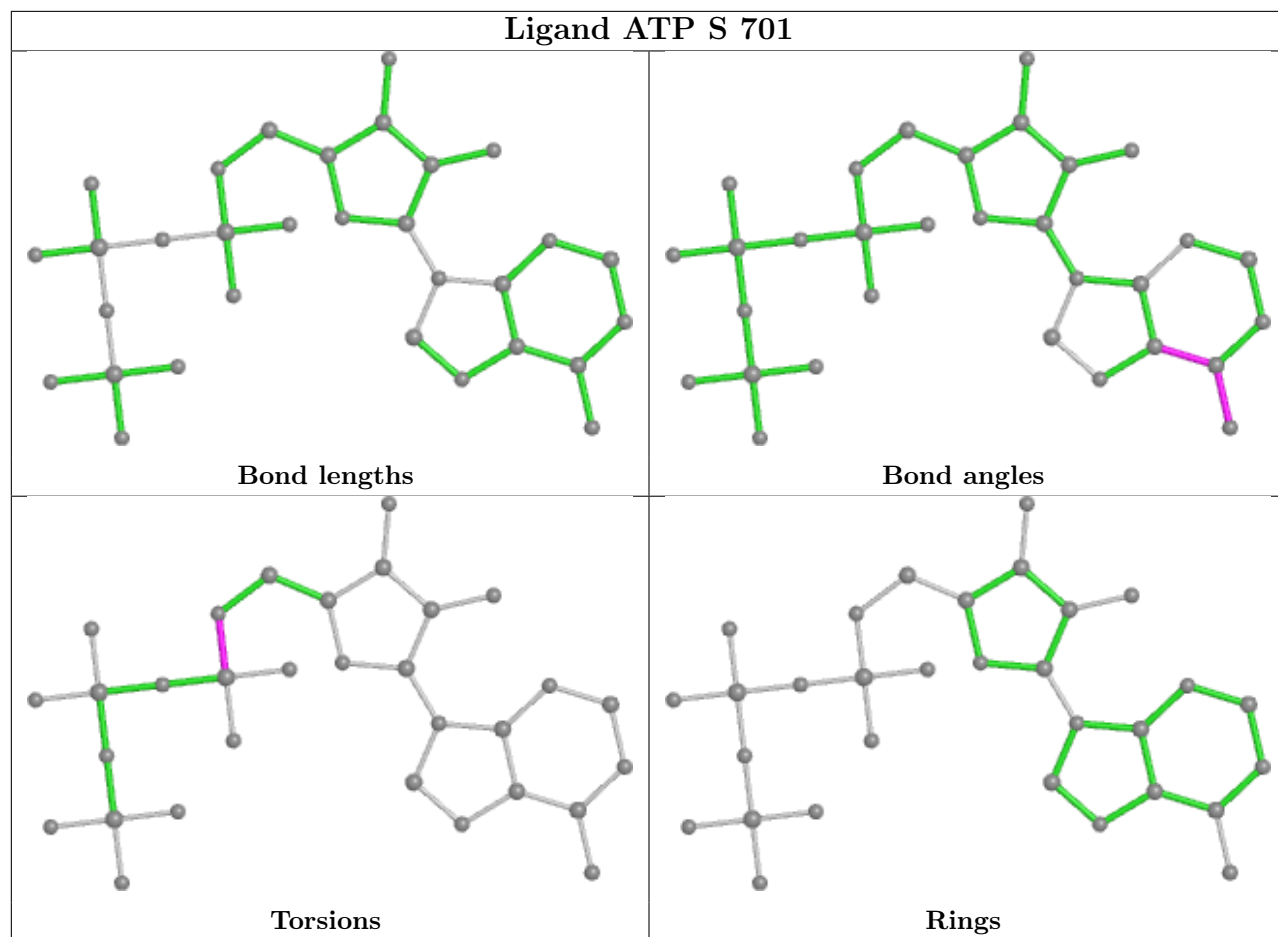


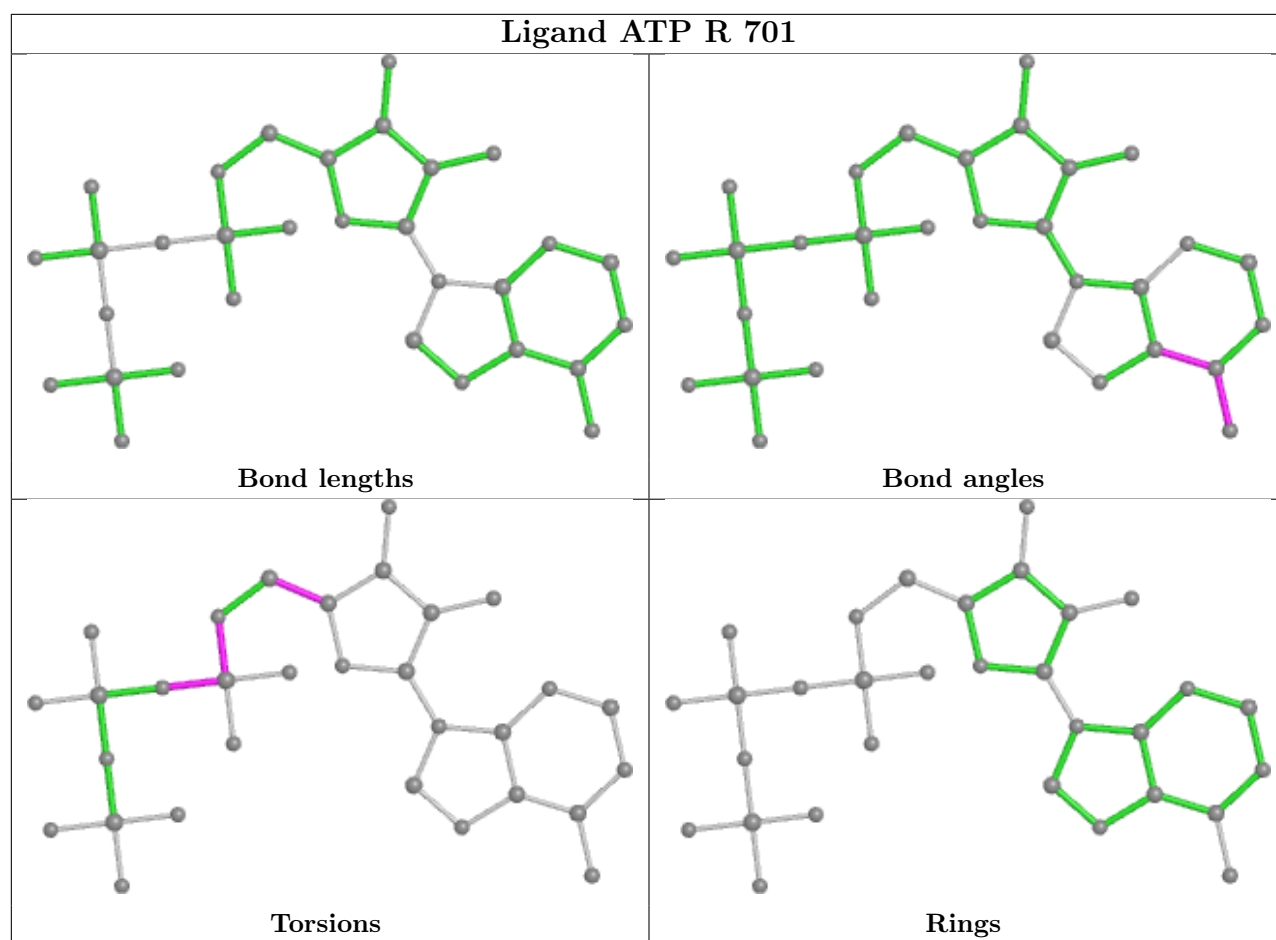




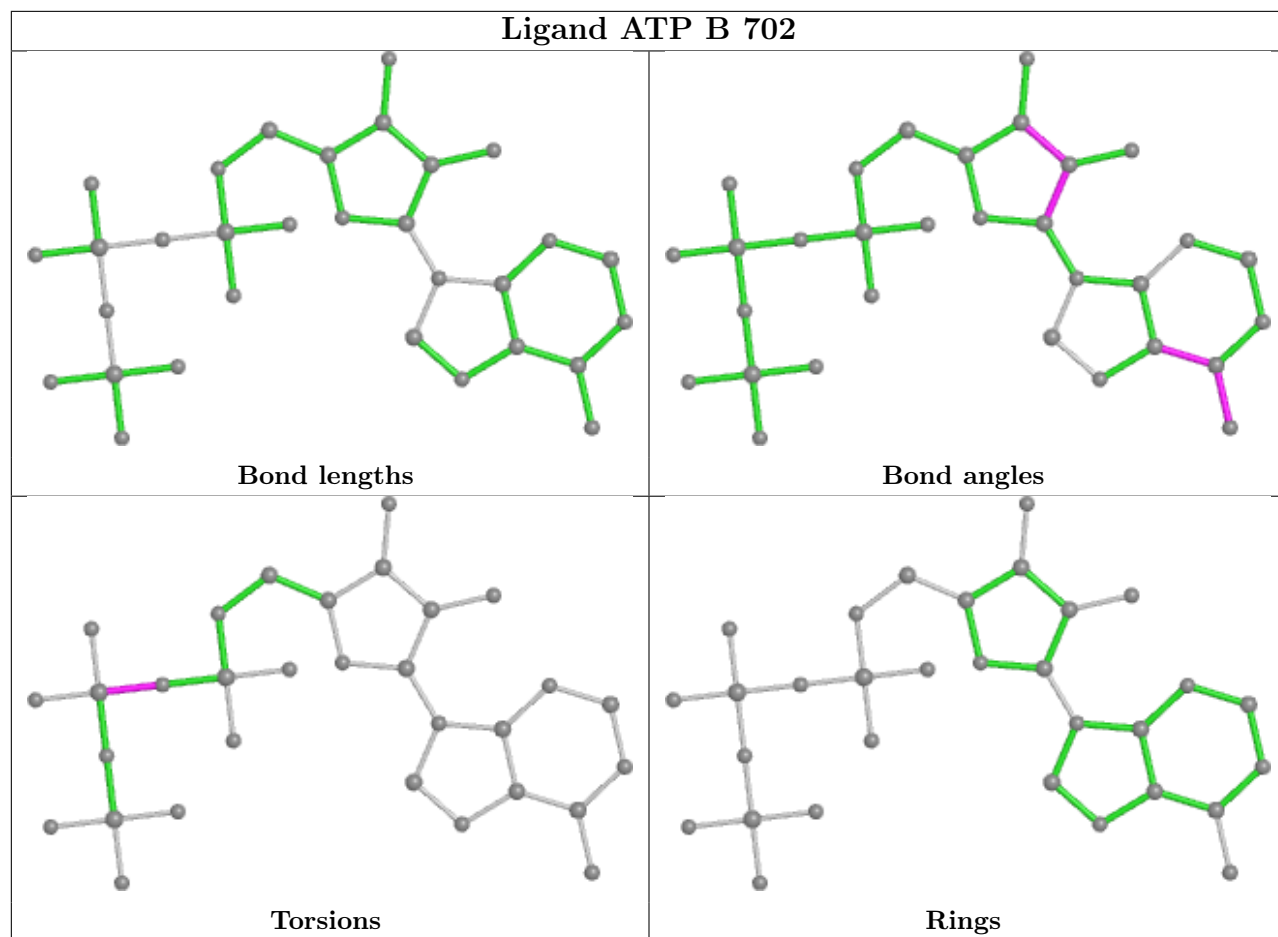


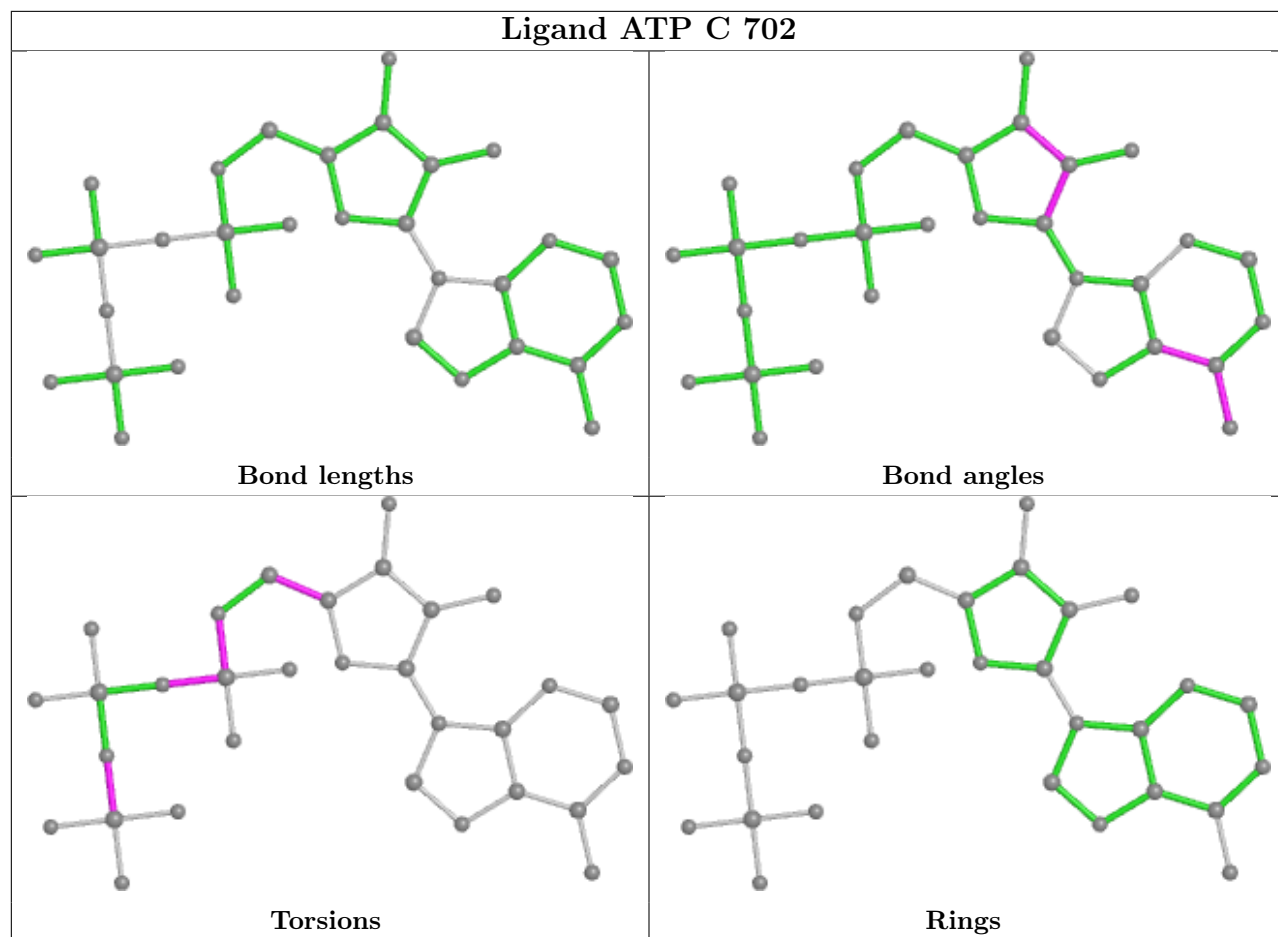


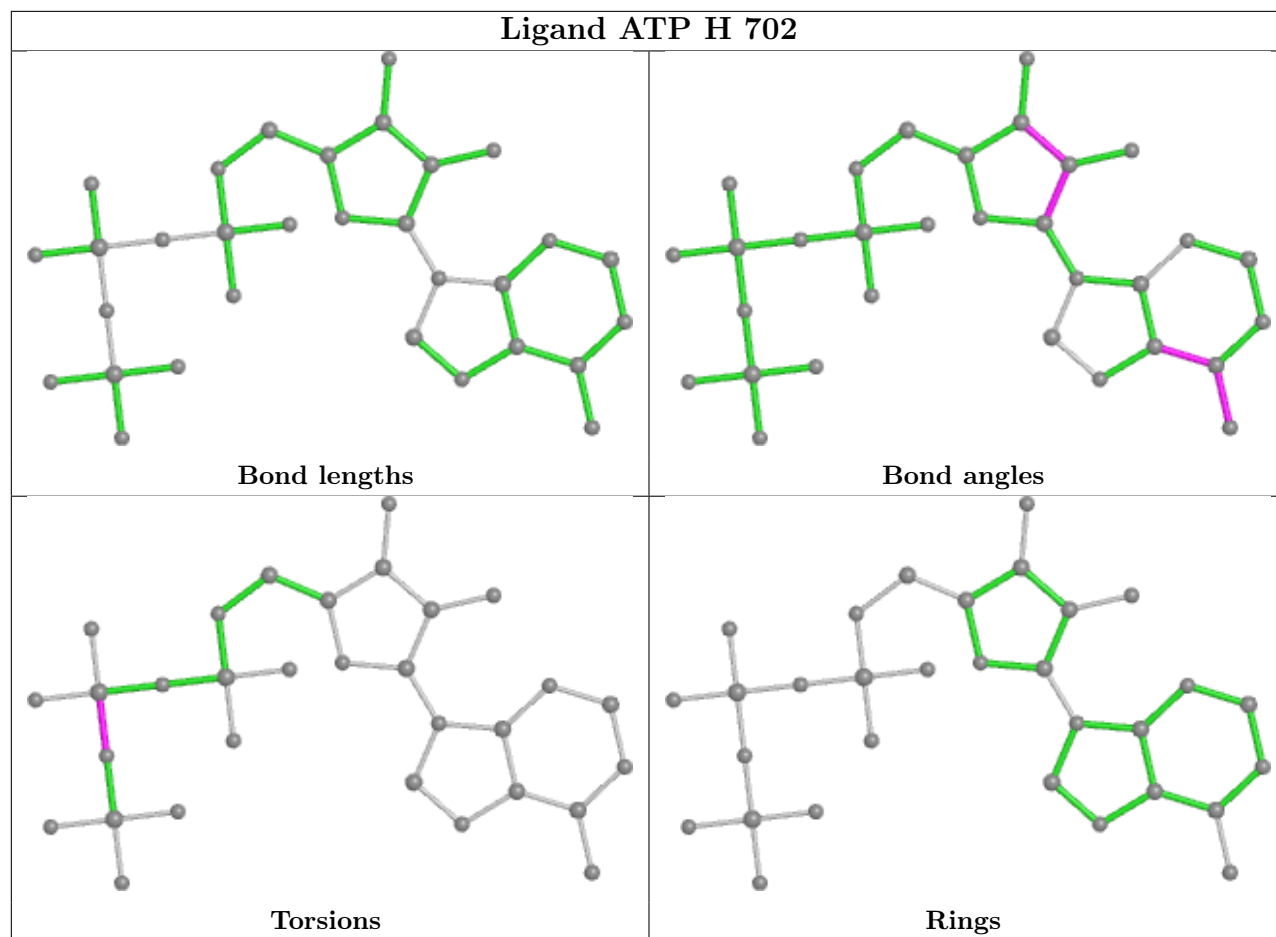




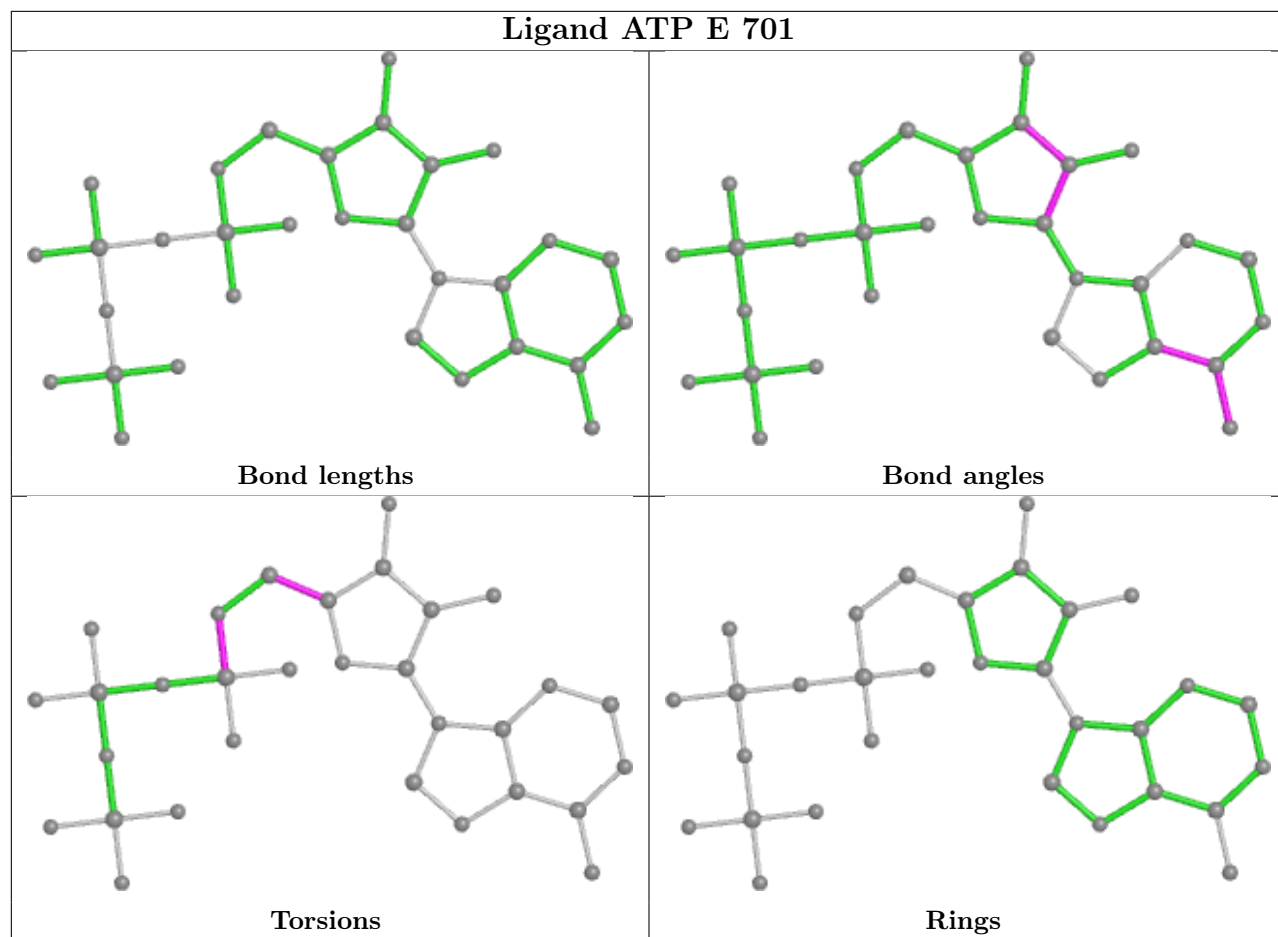
## Ligand ATP B 702

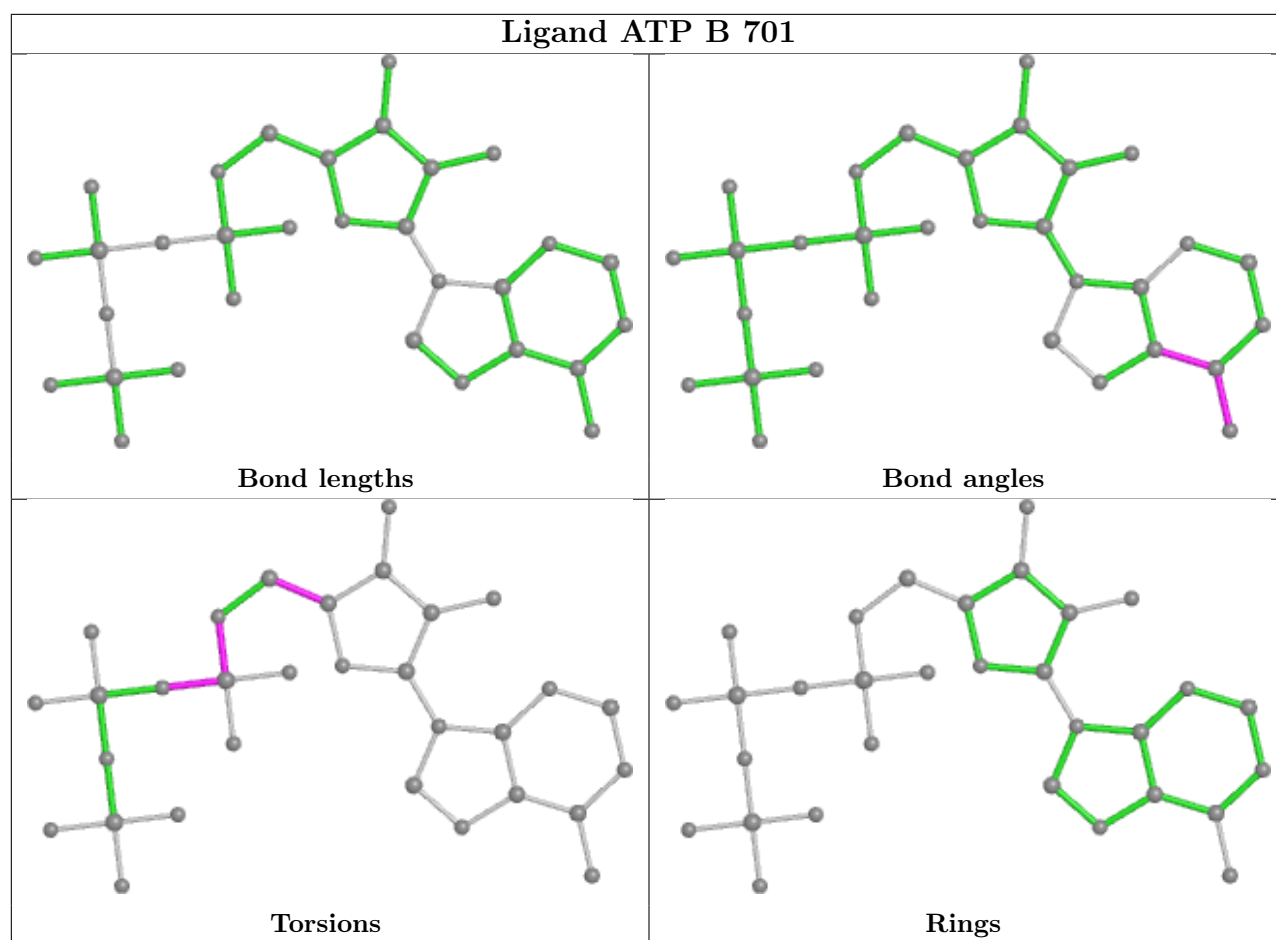


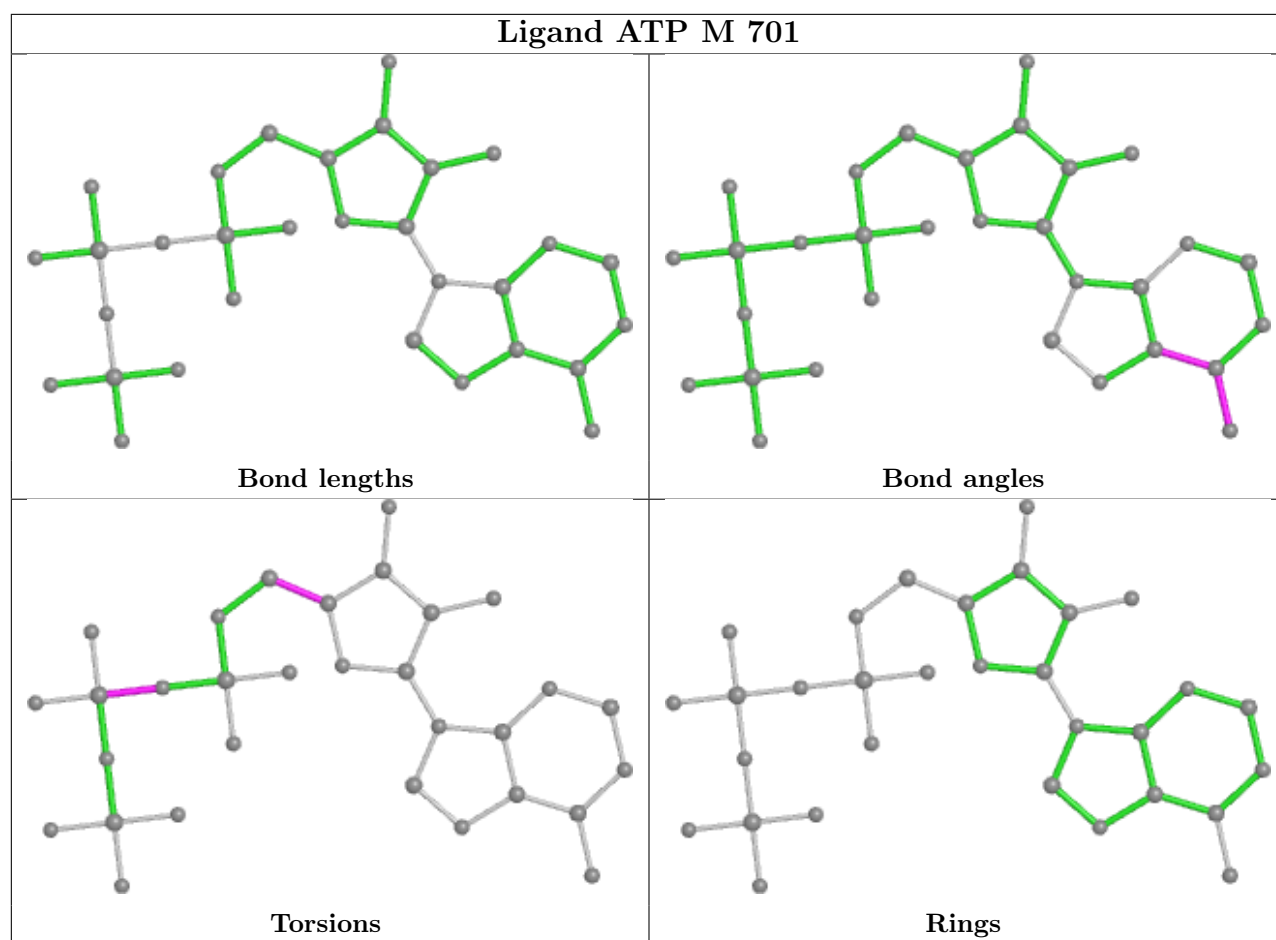




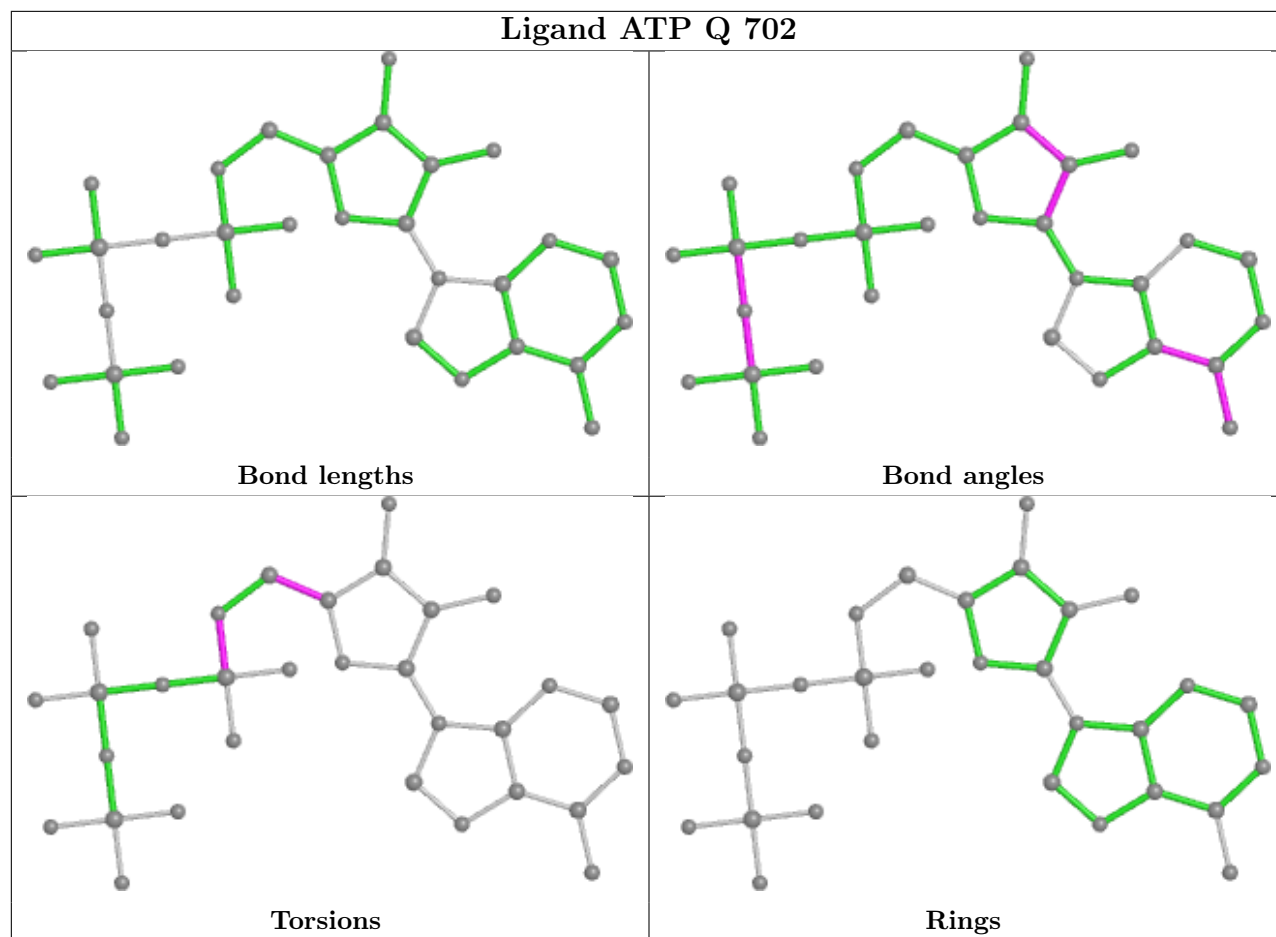
## Ligand ATP E 701

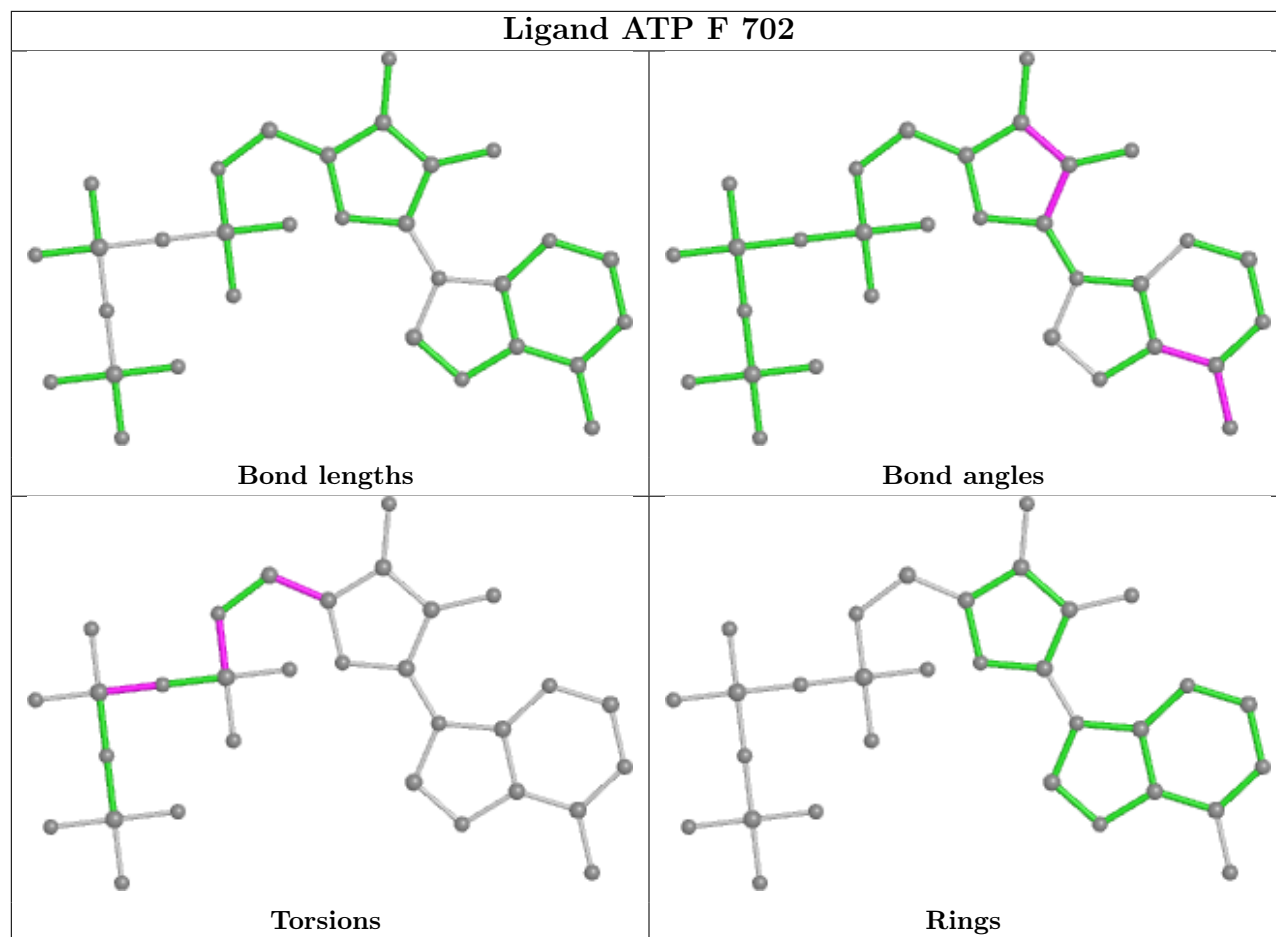












## 5.7 Other polymers [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	467/519 (89%)	-0.31	1 (0%) 95 90	23, 46, 74, 115	0
1	B	468/519 (90%)	-0.29	5 (1%) 80 64	25, 48, 69, 106	0
1	G	466/519 (89%)	-0.38	1 (0%) 95 90	23, 43, 63, 98	0
1	H	467/519 (89%)	-0.28	3 (0%) 89 78	26, 45, 69, 105	0
1	M	462/519 (89%)	0.08	15 (3%) 47 25	43, 68, 102, 130	0
1	N	454/519 (87%)	0.03	11 (2%) 59 37	48, 70, 99, 120	0
1	P	455/519 (87%)	-0.11	6 (1%) 77 59	39, 62, 96, 129	0
1	R	462/519 (89%)	-0.11	3 (0%) 89 78	37, 61, 84, 142	0
1	S	443/519 (85%)	0.19	15 (3%) 45 24	56, 89, 118, 132	0
1	T	414/519 (79%)	0.17	16 (3%) 39 20	57, 96, 121, 131	0
1	V	436/519 (84%)	0.12	13 (2%) 50 27	41, 68, 119, 132	0
1	W	463/519 (89%)	-0.08	9 (1%) 66 46	37, 63, 99, 137	0
1	X	460/519 (88%)	0.00	6 (1%) 77 59	42, 68, 94, 118	0
2	C	470/519 (90%)	-0.30	0 100 100	26, 46, 75, 122	0
2	D	469/519 (90%)	-0.26	5 (1%) 80 64	22, 47, 77, 124	0
2	E	468/519 (90%)	-0.33	3 (0%) 89 78	20, 40, 71, 113	0
2	F	466/519 (89%)	-0.28	1 (0%) 95 90	21, 45, 72, 88	0
2	I	471/519 (90%)	-0.26	4 (0%) 86 72	22, 43, 78, 121	0
2	J	466/519 (89%)	-0.27	3 (0%) 89 78	20, 45, 75, 108	0
2	K	469/519 (90%)	-0.34	2 (0%) 92 84	20, 40, 72, 119	0
2	L	468/519 (90%)	-0.29	2 (0%) 92 84	23, 44, 72, 105	0
2	O	459/519 (88%)	0.14	16 (3%) 44 23	47, 70, 101, 125	0
2	Q	464/519 (89%)	-0.20	4 (0%) 84 69	36, 56, 83, 125	0
2	U	428/519 (82%)	0.22	23 (5%) 25 12	51, 82, 120, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	11015/12456 (88%)	-0.14	167 (1%)	73	54	20, 56, 104, 142	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	76	PHE	5.3
2	Q	250	GLY	5.2
2	U	63	GLY	5.1
2	U	95	ALA	5.0
1	T	183	GLU	4.9
2	K	498	THR	4.7
1	A	255	THR	4.6
2	D	252	MET	4.5
2	I	113	GLU	4.2
2	U	61	TYR	4.1
1	S	453	ILE	4.0
2	U	176	ALA	3.9
1	M	101	GLY	3.9
1	M	90	PHE	3.8
2	J	115	GLN	3.7
1	V	110	PRO	3.6
1	T	37	PRO	3.5
1	V	151	PHE	3.5
2	U	398	GLY	3.4
1	S	182	THR	3.4
1	M	71	GLY	3.4
1	M	241	ASP	3.4
1	S	89	SER	3.4
1	S	139	ALA	3.3
2	U	92	TRP	3.3
2	U	108	ALA	3.3
1	G	17	ALA	3.3
1	T	24	MET	3.2
1	W	159	VAL	3.2
1	V	89	SER	3.2
2	Q	158	SER	3.2
1	W	250	GLY	3.2
2	O	407	GLU	3.1
2	D	117	VAL	3.1
2	U	62	ASN	3.1
2	I	152	GLN	3.1
1	P	51	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	U	37	PRO	3.1
2	U	245	ASN	3.1
1	M	104	PHE	3.1
1	M	176	ALA	3.0
2	D	251	ALA	3.0
1	W	353	SER	3.0
1	H	157	SER	3.0
1	T	27	GLY	2.9
1	B	252	MET	2.9
2	O	16	GLN	2.9
1	S	158	SER	2.9
1	M	89	SER	2.9
1	W	251	ALA	2.9
2	O	110	PRO	2.9
2	O	485	ASN	2.9
2	O	66	GLU	2.9
2	O	74	VAL	2.9
1	X	107	ASP	2.9
2	D	115	GLN	2.9
1	S	61	TYR	2.9
1	N	344	LEU	2.9
1	T	390	ASN	2.8
2	Q	139	ALA	2.8
1	N	254	LEU	2.8
1	P	164	LEU	2.8
1	M	337	GLU	2.8
1	T	49	GLY	2.8
1	S	142	VAL	2.8
2	O	145	ASP	2.8
1	B	139	ALA	2.7
1	X	39	GLY	2.7
1	W	158	SER	2.7
2	O	91	GLY	2.7
1	T	83	ILE	2.7
2	O	30	ASP	2.6
1	M	95	ALA	2.6
1	T	32	SER	2.6
1	S	72	VAL	2.6
1	W	189	GLY	2.6
2	U	391	ALA	2.6
1	V	164	LEU	2.6
1	N	498	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	U	57	ILE	2.6
1	R	195	GLY	2.6
1	N	253	ARG	2.6
1	B	110	PRO	2.6
1	S	110	PRO	2.5
2	Q	249	LEU	2.5
1	N	497	ILE	2.5
1	X	295	THR	2.5
1	W	95	ALA	2.5
1	V	200	VAL	2.5
2	U	70	PRO	2.5
1	X	486	PHE	2.5
1	M	139	ALA	2.5
1	V	250	GLY	2.5
1	V	254	LEU	2.5
1	M	72	VAL	2.5
1	W	227	GLY	2.5
2	J	157	SER	2.5
2	U	143	SER	2.4
1	N	24	MET	2.4
1	T	145	ASP	2.4
2	L	68	ASP	2.4
1	V	158	SER	2.4
1	B	251	ALA	2.4
1	H	110	PRO	2.4
1	X	80	PRO	2.4
2	I	157	SER	2.4
2	E	133	ALA	2.4
2	U	109	SER	2.4
1	M	133	ALA	2.4
2	O	108	ALA	2.4
1	P	152	GLN	2.4
1	V	168	VAL	2.4
1	N	319	GLU	2.4
2	U	142	VAL	2.3
1	S	378	ASP	2.3
2	I	498	THR	2.3
1	N	485	ASN	2.3
1	T	142	VAL	2.3
1	T	422	ALA	2.3
1	P	131	ASN	2.3
1	N	356	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	U	140	ARG	2.2
1	H	121	PHE	2.2
1	S	105	ILE	2.2
1	P	95	ALA	2.2
1	W	115	GLN	2.2
1	T	229	SER	2.2
1	V	249	LEU	2.2
1	M	487	GLU	2.2
2	U	102	LYS	2.2
2	O	68	ASP	2.2
1	S	73	PHE	2.2
2	U	243	GLY	2.2
1	N	312	ALA	2.2
1	X	450	SER	2.2
1	V	160	VAL	2.2
2	O	146	SER	2.1
2	U	244	ILE	2.1
1	P	50	THR	2.1
1	S	331	TRP	2.1
2	E	251	ALA	2.1
2	O	105	ILE	2.1
2	U	36	LEU	2.1
2	K	93	ASP	2.1
1	V	80	PRO	2.1
2	F	78	GLU	2.1
2	L	252	MET	2.1
2	U	390	ASN	2.1
1	T	31	ILE	2.1
1	T	244	ILE	2.1
2	O	160	VAL	2.1
2	O	373	ALA	2.1
1	S	338	MET	2.1
1	M	485	ASN	2.1
1	B	408	ILE	2.1
2	O	75	THR	2.0
1	R	121	PHE	2.0
1	R	373	ALA	2.0
2	E	156	ALA	2.0
1	T	50	THR	2.0
2	U	304	ASN	2.0
1	N	42	THR	2.0
1	M	240	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	T	131	ASN	2.0
1	S	240	THR	2.0
2	J	110	PRO	2.0
2	D	253	ARG	2.0

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	TPO	C	432	11/12	0.86	0.24	52,56,61,61	4
1	SEP	S	431	10/11	0.86	0.21	71,75,82,82	0
1	SEP	T	431	10/11	0.87	0.21	82,84,87,87	0
2	TPO	O	432	11/12	0.87	0.18	71,74,80,80	0
2	TPO	I	432	11/12	0.88	0.25	46,50,54,54	4
2	TPO	U	432	11/12	0.88	0.19	72,76,79,79	4
1	SEP	M	431	10/11	0.88	0.21	65,68,72,72	0
2	SEP	O	431	10/11	0.89	0.26	70,71,71,71	4
2	TPO	L	432	11/12	0.89	0.22	46,51,56,56	4
2	TPO	F	432	11/12	0.89	0.19	41,45,50,50	4
1	SEP	V	431	10/11	0.89	0.22	55,58,61,62	4
2	TPO	J	432	11/12	0.90	0.21	41,44,48,48	4
1	SEP	N	431	10/11	0.90	0.19	65,66,69,70	0
2	SEP	C	431	10/11	0.90	0.20	55,57,62,62	0
2	SEP	U	431	10/11	0.91	0.23	75,78,82,83	0
1	SEP	R	431	10/11	0.91	0.18	58,60,61,61	0
1	SEP	H	431	10/11	0.91	0.21	41,43,46,46	4
2	TPO	K	432	11/12	0.91	0.19	40,43,45,45	4
1	SEP	P	431	10/11	0.92	0.19	52,53,53,54	4
2	SEP	Q	431	10/11	0.93	0.19	53,55,57,58	0
2	TPO	Q	432	11/12	0.93	0.22	58,61,63,64	4
2	SEP	D	431	10/11	0.93	0.20	42,43,44,44	4
2	SEP	I	431	10/11	0.93	0.18	48,50,54,54	0
2	TPO	D	432	11/12	0.93	0.19	40,43,45,45	4
1	SEP	X	431	10/11	0.93	0.16	52,56,60,60	0
2	TPO	E	432	11/12	0.93	0.16	39,42,44,44	4
1	SEP	A	431	10/11	0.93	0.17	46,46,47,47	4
1	SEP	W	431	10/11	0.93	0.18	51,52,53,53	4
2	SEP	K	431	10/11	0.94	0.17	42,43,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SEP	J	431	10/11	0.94	0.15	42,43,44,44	4
2	SEP	L	431	10/11	0.94	0.16	46,46,46,47	4
2	SEP	F	431	10/11	0.95	0.15	41,42,42,42	4
2	SEP	E	431	10/11	0.95	0.17	38,39,41,41	0
1	SEP	B	431	10/11	0.95	0.17	42,43,44,44	4
1	SEP	G	431	10/11	0.95	0.15	48,49,50,51	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	P	704	1/1	0.82	0.16	44,44,44,44	0
3	ATP	S	702	31/31	0.85	0.25	94,95,99,99	0
3	ATP	M	702	31/31	0.88	0.28	76,79,81,81	0
5	ADP	U	702	27/27	0.89	0.18	92,104,112,112	0
3	ATP	T	702	31/31	0.90	0.16	85,88,90,91	0
3	ATP	W	702	31/31	0.91	0.17	71,74,76,77	0
4	MG	G	703	1/1	0.91	0.19	43,43,43,43	0
3	ATP	S	701	31/31	0.91	0.19	77,78,83,83	0
3	ATP	X	701	31/31	0.91	0.22	59,63,70,70	0
4	MG	G	704	1/1	0.92	0.11	48,48,48,48	0
4	MG	F	704	1/1	0.92	0.09	39,39,39,39	0
4	MG	Q	703	1/1	0.92	0.11	51,51,51,51	0
3	ATP	Q	702	31/31	0.92	0.20	59,62,73,73	0
4	MG	H	704	1/1	0.93	0.17	46,46,46,46	0
4	MG	C	704	1/1	0.93	0.10	48,48,48,48	0
3	ATP	O	702	31/31	0.93	0.22	84,98,105,105	0
3	ATP	T	701	31/31	0.93	0.19	69,71,74,75	0
3	ATP	F	702	31/31	0.94	0.20	40,41,44,44	0
4	MG	B	704	1/1	0.94	0.17	58,58,58,58	0
4	MG	E	704	1/1	0.94	0.22	22,22,22,22	0
3	ATP	N	701	31/31	0.94	0.16	56,60,64,64	0
3	ATP	N	702	31/31	0.94	0.18	61,64,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ATP	O	701	31/31	0.94	0.16	60,62,64,65	0
3	ATP	B	701	31/31	0.94	0.15	39,39,40,40	0
3	ATP	X	702	31/31	0.94	0.17	66,70,74,75	0
4	MG	L	704	1/1	0.94	0.09	36,36,36,36	0
4	MG	R	704	1/1	0.94	0.13	44,44,44,44	0
3	ATP	R	701	31/31	0.94	0.17	48,55,59,59	0
3	ATP	M	701	31/31	0.94	0.14	54,56,58,58	0
3	ATP	V	702	31/31	0.94	0.15	83,85,89,90	0
5	ADP	W	701	27/27	0.94	0.17	45,49,52,52	0
3	ATP	K	702	31/31	0.95	0.15	39,42,46,47	0
3	ATP	L	702	31/31	0.95	0.17	38,39,43,43	0
3	ATP	I	702	31/31	0.95	0.14	41,42,45,45	0
3	ATP	P	702	31/31	0.95	0.14	55,56,60,62	0
4	MG	I	704	1/1	0.95	0.14	47,47,47,47	0
4	MG	O	703	1/1	0.95	0.13	38,38,38,38	0
4	MG	R	703	1/1	0.95	0.18	33,33,33,33	0
3	ATP	E	702	31/31	0.95	0.16	43,44,47,48	0
3	ATP	C	702	31/31	0.95	0.14	41,42,46,47	0
3	ATP	D	702	31/31	0.95	0.16	43,46,47,48	0
5	ADP	Q	701	27/27	0.95	0.16	45,49,51,51	0
3	ATP	U	701	31/31	0.95	0.16	60,62,62,62	0
3	ATP	H	701	31/31	0.95	0.16	36,37,38,38	0
3	ATP	J	702	31/31	0.96	0.15	42,45,46,47	0
3	ATP	G	701	31/31	0.96	0.18	37,40,44,45	0
3	ATP	G	702	31/31	0.96	0.14	37,40,42,42	0
3	ATP	F	701	31/31	0.96	0.16	39,40,44,44	0
4	MG	L	703	1/1	0.96	0.05	35,35,35,35	0
3	ATP	H	702	31/31	0.96	0.15	44,46,49,50	0
4	MG	I	703	1/1	0.96	0.07	36,36,36,36	0
3	ATP	K	701	31/31	0.96	0.13	29,31,33,33	0
4	MG	J	704	1/1	0.96	0.15	23,23,23,23	0
3	ATP	R	702	31/31	0.96	0.14	58,59,63,63	0
3	ATP	V	701	31/31	0.96	0.15	44,49,54,55	0
3	ATP	A	701	31/31	0.96	0.15	41,45,50,50	0
4	MG	M	703	1/1	0.96	0.32	27,27,27,27	0
4	MG	P	703	1/1	0.96	0.10	43,43,43,43	0
3	ATP	L	701	31/31	0.96	0.14	37,38,42,42	0
4	MG	A	704	1/1	0.96	0.08	27,27,27,27	0
4	MG	U	703	1/1	0.96	0.18	51,51,51,51	0
3	ATP	P	701	31/31	0.96	0.17	52,56,65,66	0
3	ATP	B	702	31/31	0.96	0.17	44,46,49,50	0
3	ATP	A	702	31/31	0.96	0.17	40,41,45,45	0

*Continued on next page...*

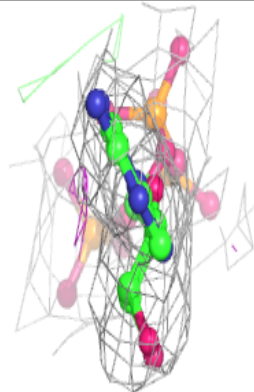
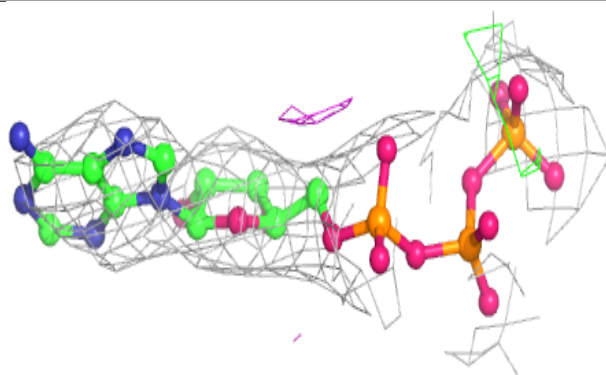
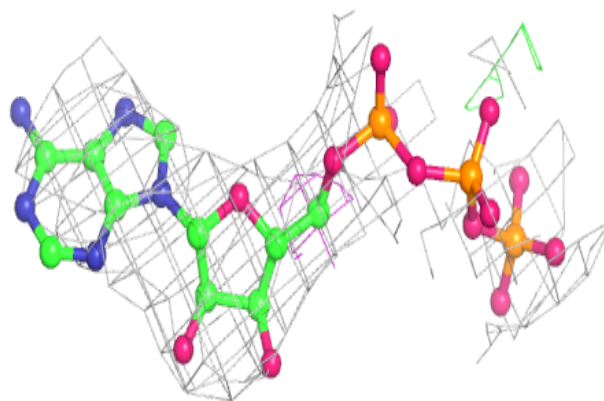
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	J	703	1/1	0.97	0.23	18,18,18,18	0
4	MG	C	703	1/1	0.97	0.13	43,43,43,43	0
4	MG	N	704	1/1	0.97	0.11	47,47,47,47	0
4	MG	A	703	1/1	0.97	0.16	34,34,34,34	0
4	MG	D	703	1/1	0.97	0.11	26,26,26,26	0
4	MG	D	704	1/1	0.97	0.14	41,41,41,41	0
3	ATP	E	701	31/31	0.97	0.13	30,32,35,35	0
4	MG	B	703	1/1	0.97	0.10	31,31,31,31	0
3	ATP	J	701	31/31	0.97	0.14	27,29,31,32	0
4	MG	K	704	1/1	0.97	0.16	20,20,20,20	0
4	MG	E	703	1/1	0.97	0.10	21,21,21,21	0
4	MG	V	703	1/1	0.97	0.07	36,36,36,36	0
3	ATP	C	701	31/31	0.97	0.12	33,34,34,35	0
4	MG	F	703	1/1	0.97	0.11	40,40,40,40	0
3	ATP	I	701	31/31	0.97	0.13	29,30,31,31	0
4	MG	K	703	1/1	0.98	0.11	23,23,23,23	0
4	MG	H	703	1/1	0.98	0.22	25,25,25,25	0
3	ATP	D	701	31/31	0.98	0.14	28,29,30,30	0
4	MG	T	703	1/1	0.99	0.18	50,50,50,50	0
4	MG	N	703	1/1	0.99	0.13	37,37,37,37	0

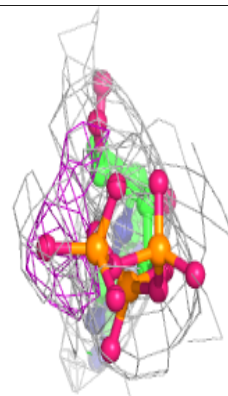
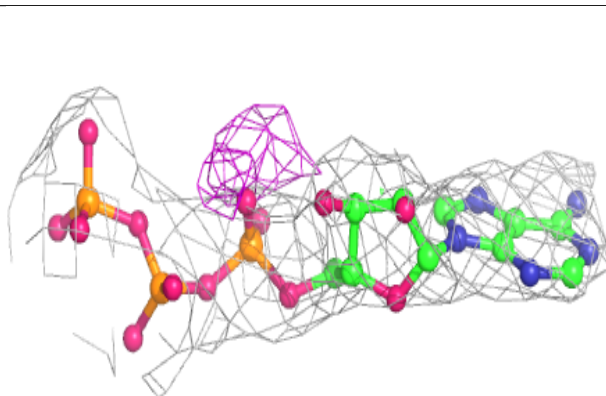
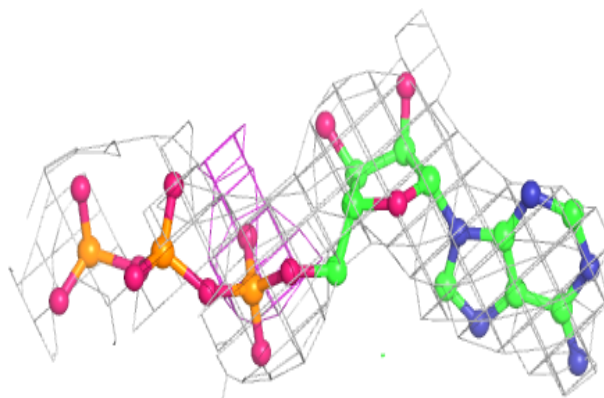
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP S 702:**

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

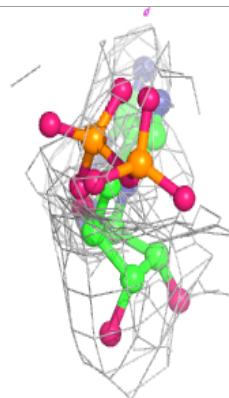
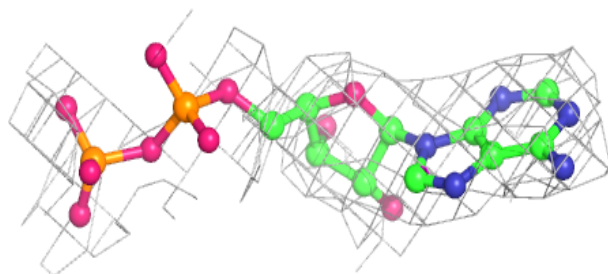
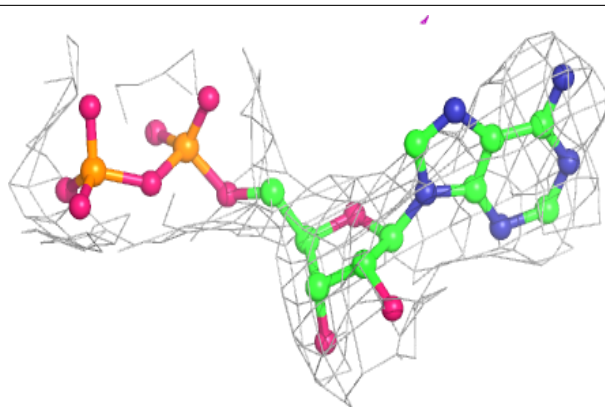
**Electron density around ATP M 702:**

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

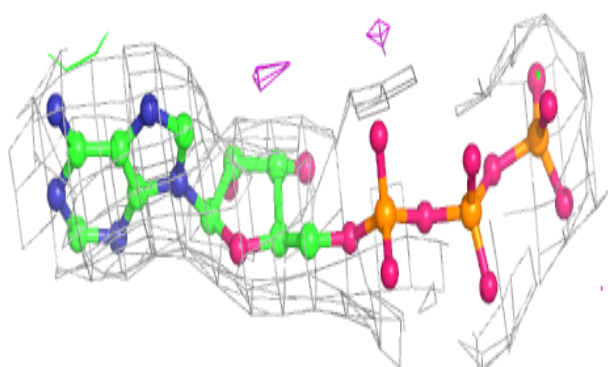
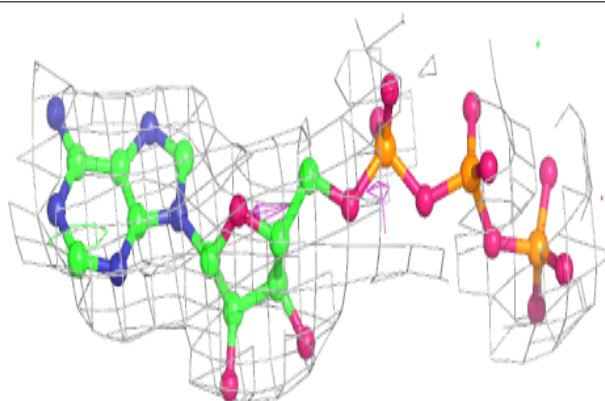


**Electron density around ADP U 702:**

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

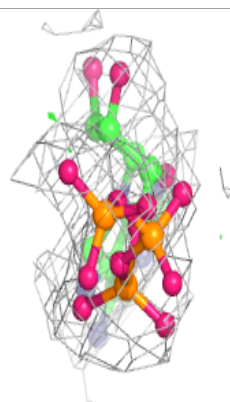
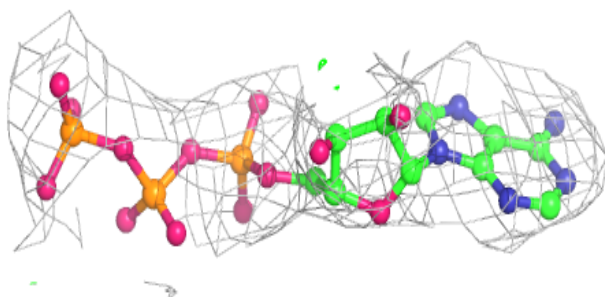
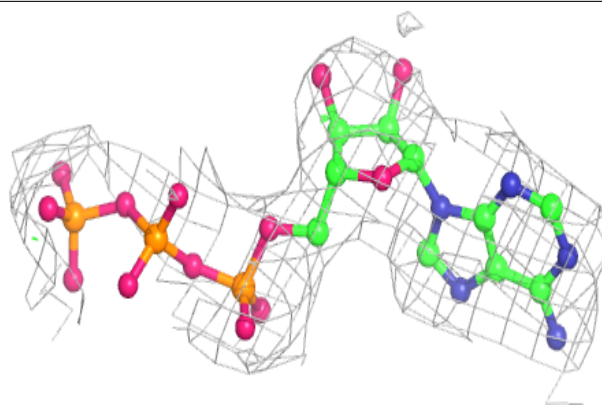
**Electron density around ATP T 702:**

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

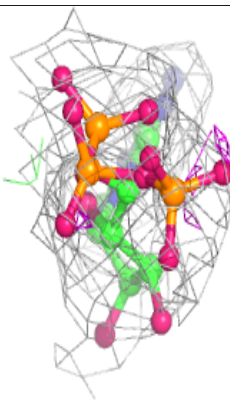
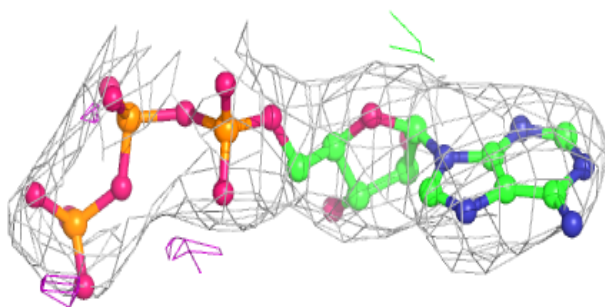
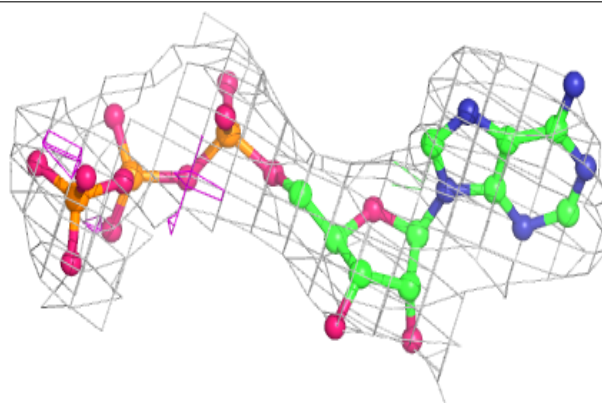


**Electron density around ATP W 702:**

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

**Electron density around ATP S 701:**

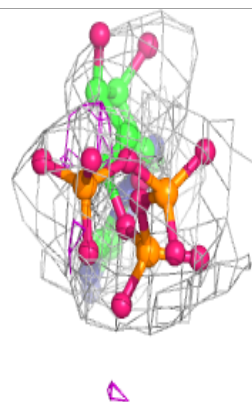
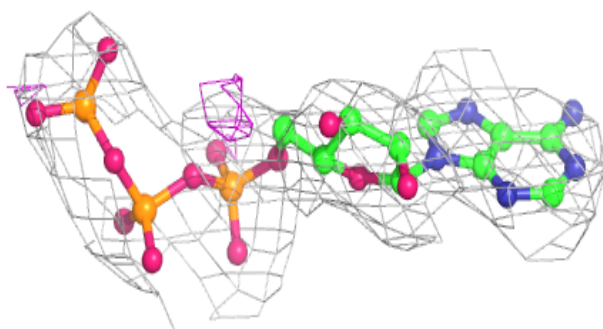
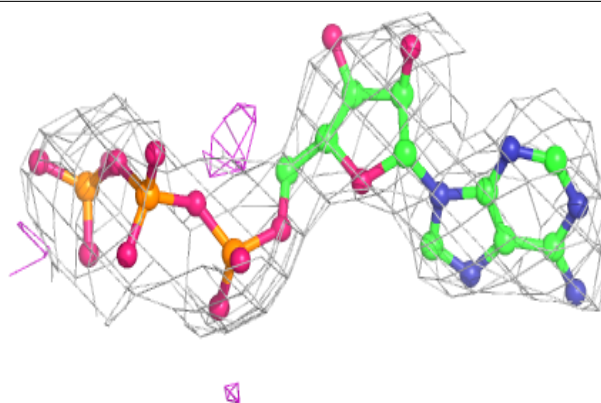
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



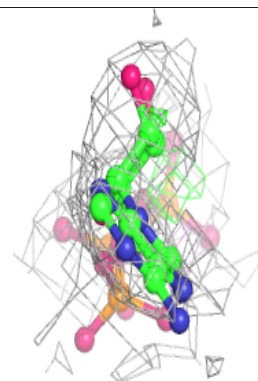
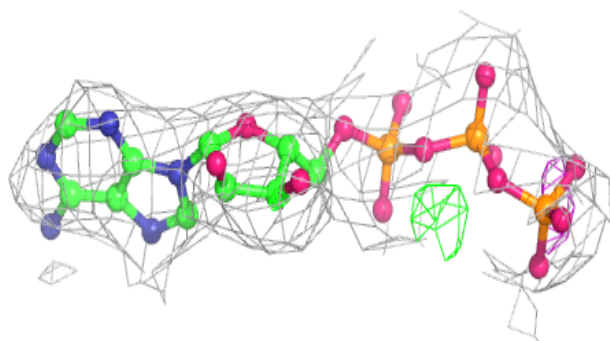
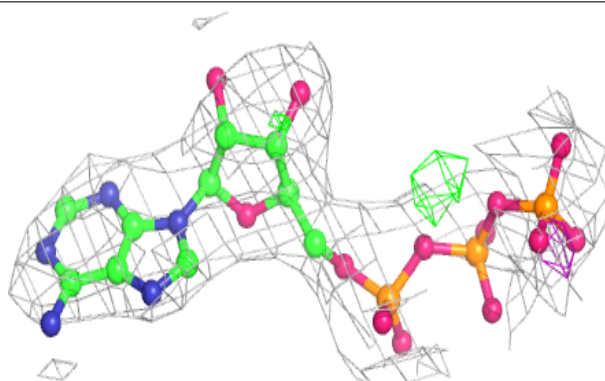


**Electron density around ATP X 701:**

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

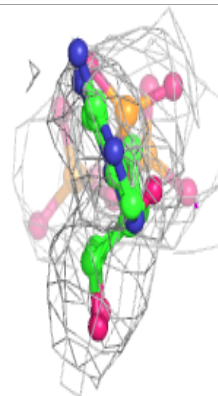
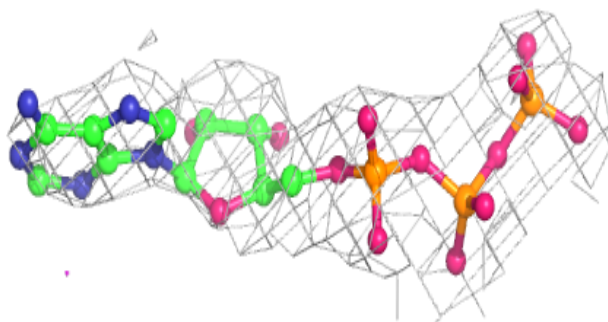
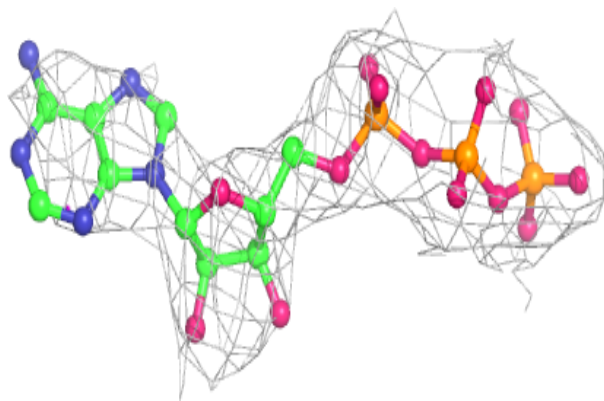
**Electron density around ATP Q 702:**

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

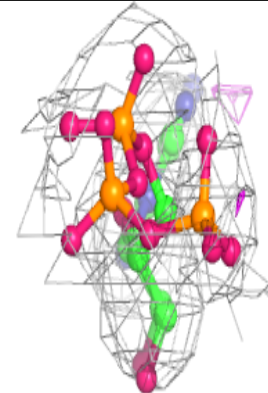
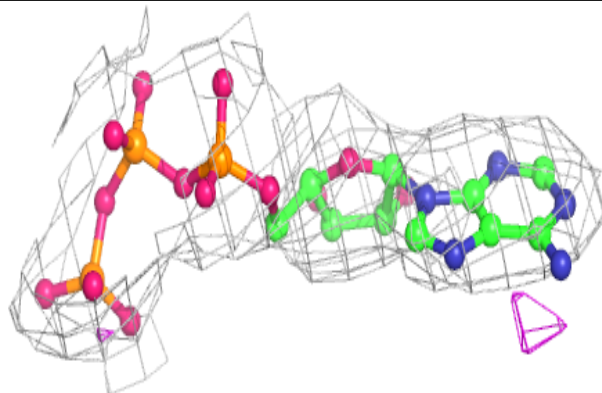
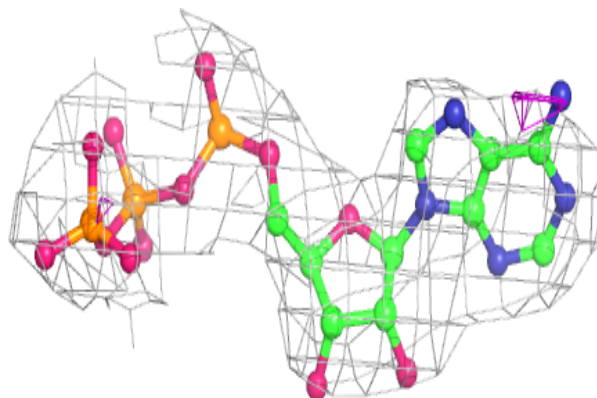


**Electron density around ATP O 702:**

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

**Electron density around ATP T 701:**

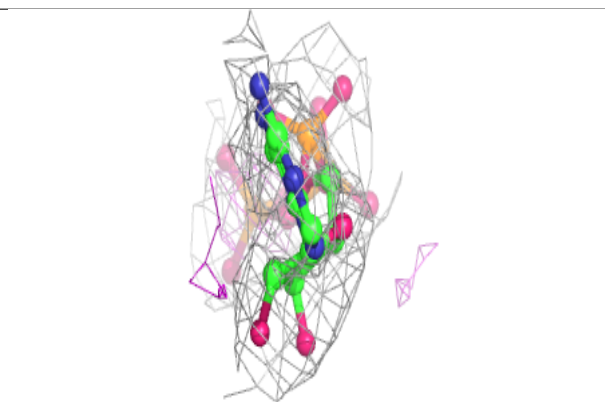
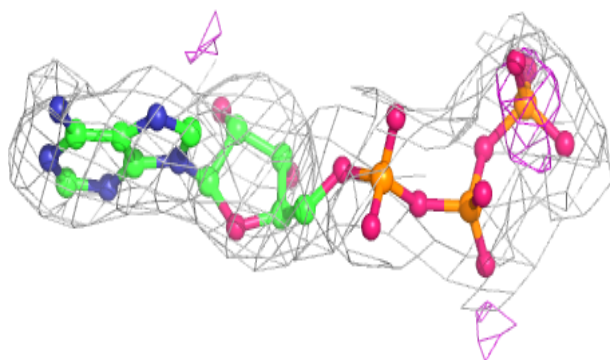
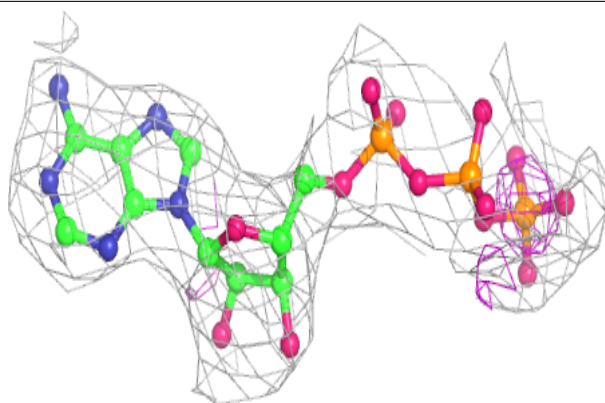
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



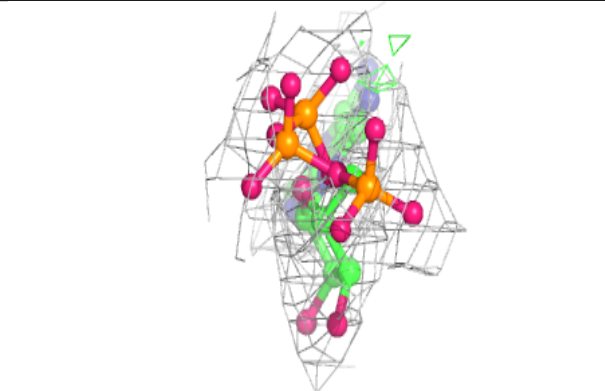
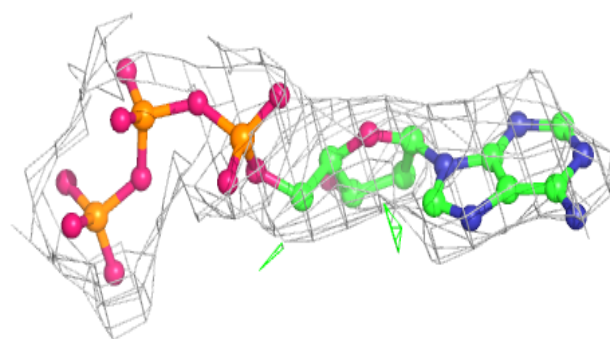
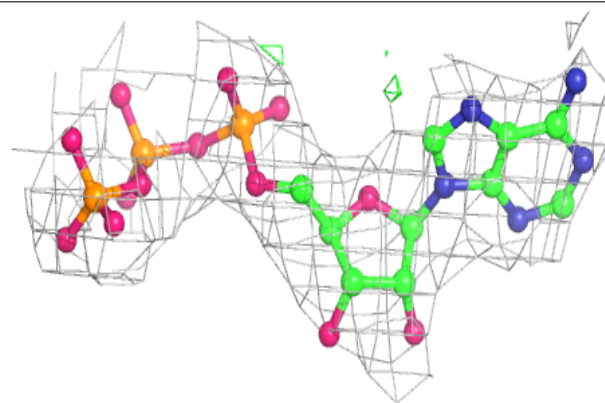


**Electron density around ATP F 702:**

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and green (positive)

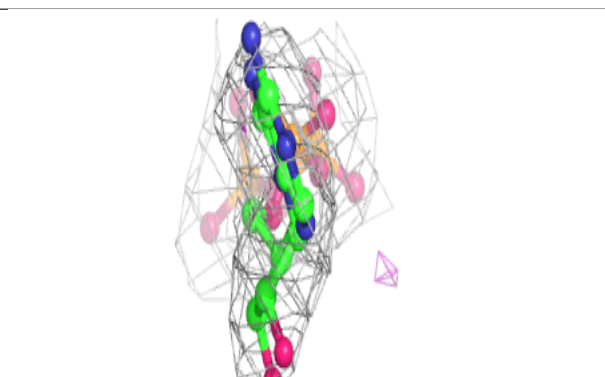
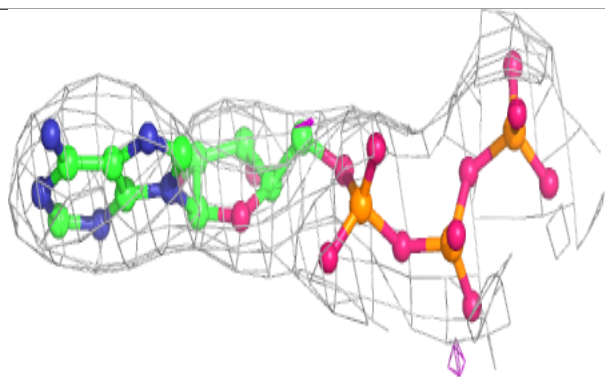
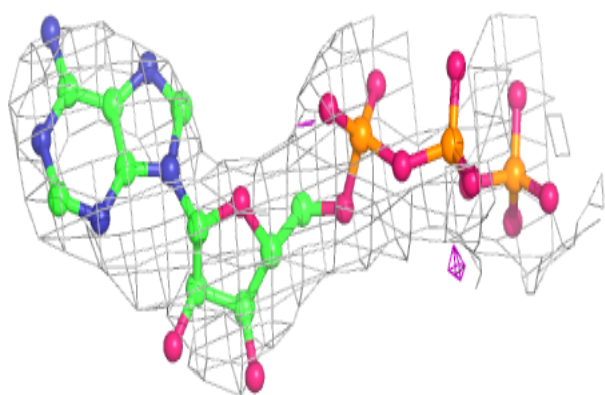
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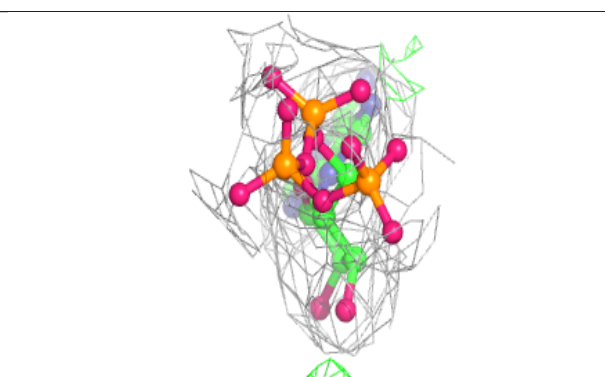
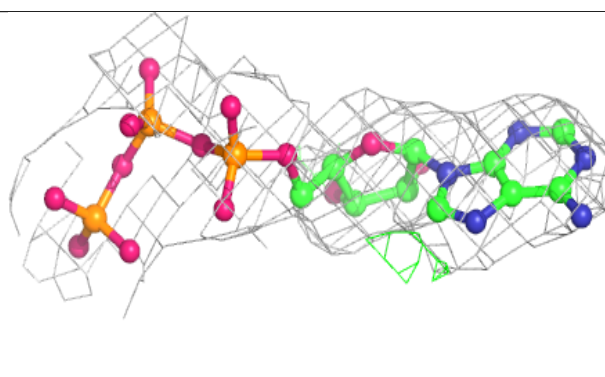
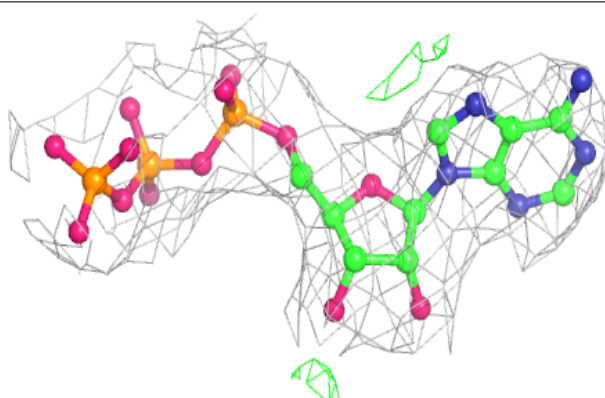


**Electron density around ATP N 702:**

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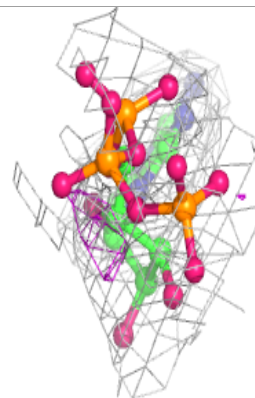
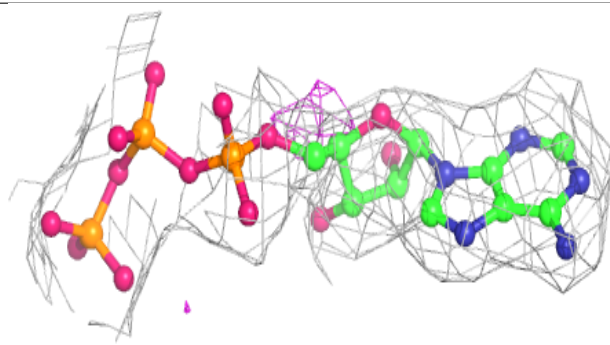
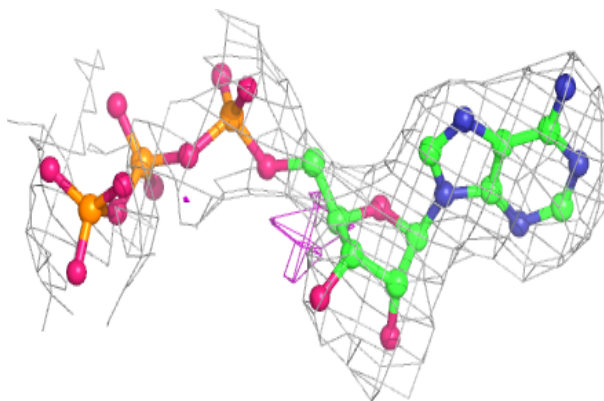
**Electron density around ATP O 701:**

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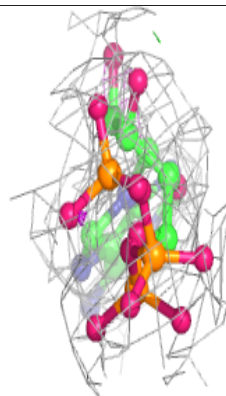
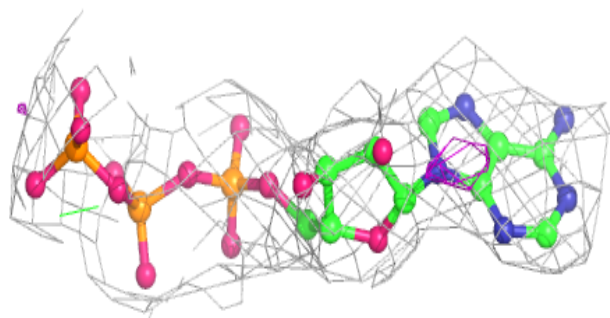
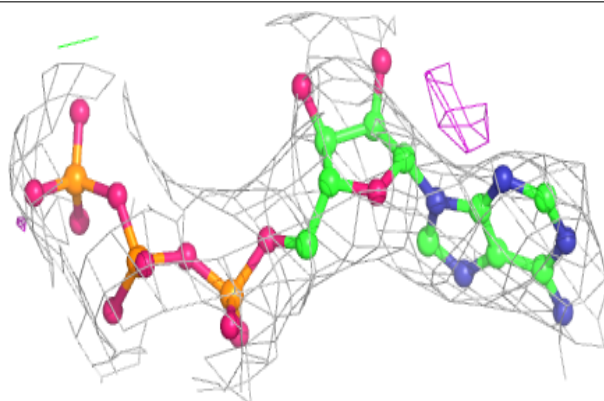


**Electron density around ATP B 701:**

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

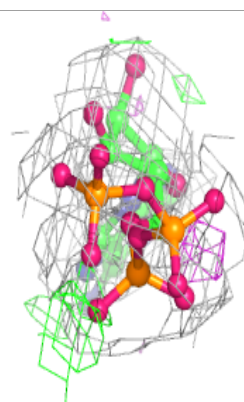
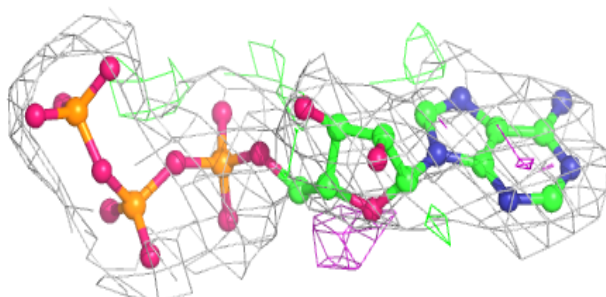
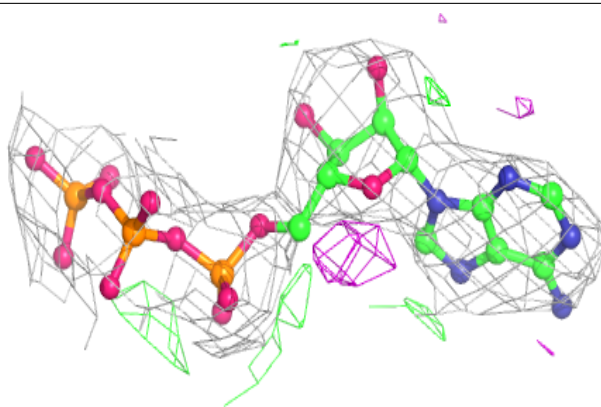
**Electron density around ATP X 702:**

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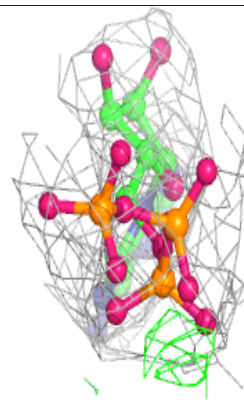
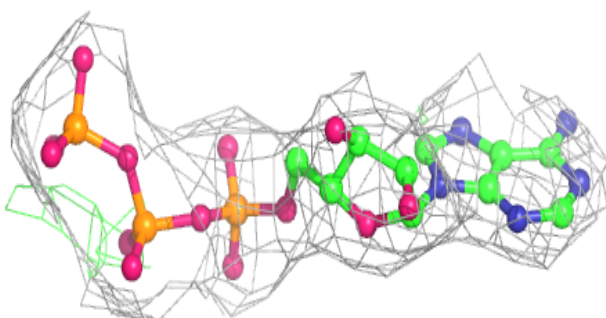
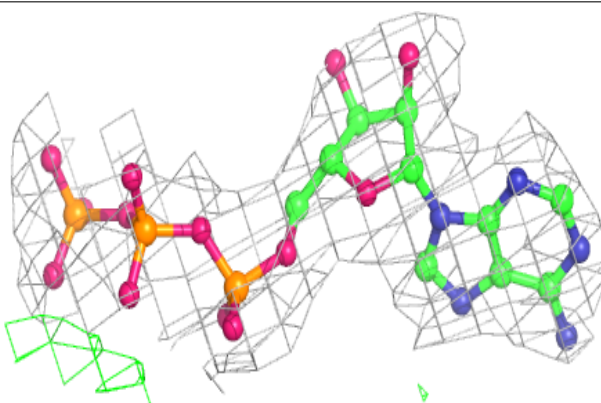


**Electron density around ATP R 701:**

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

**Electron density around ATP M 701:**

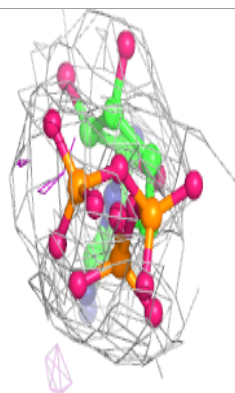
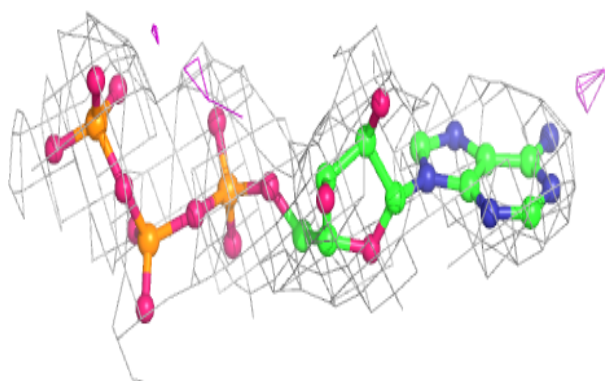
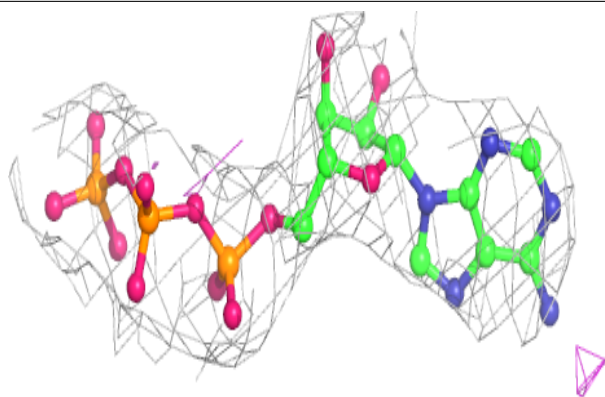
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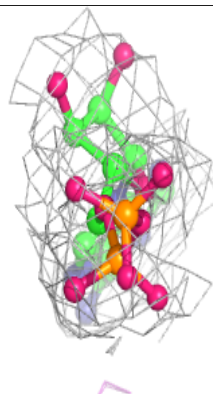
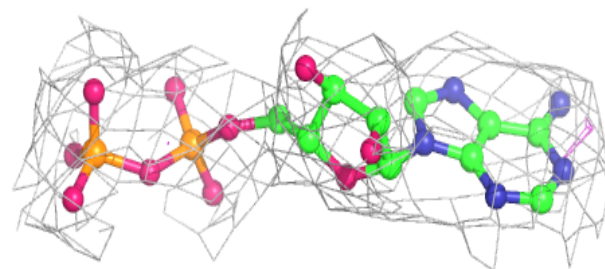
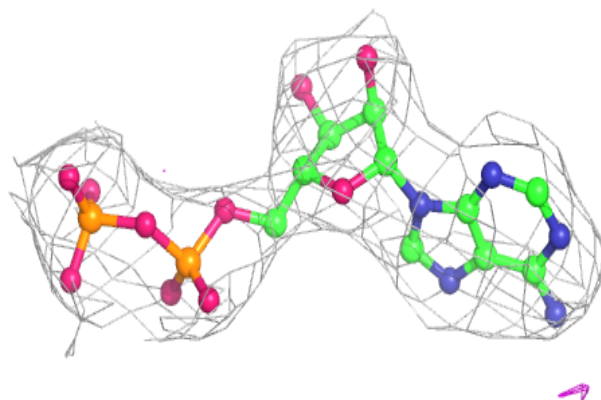


**Electron density around ATP V 702:**

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

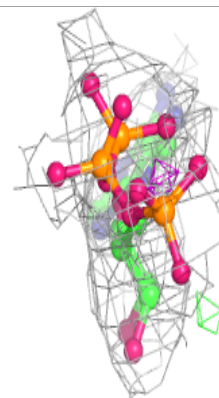
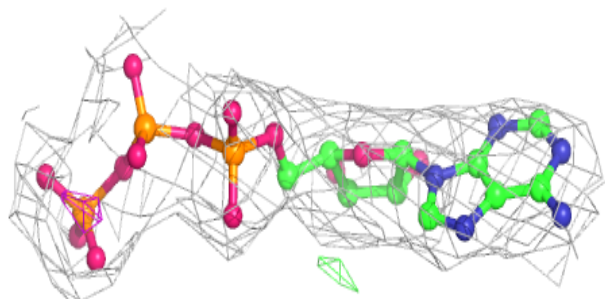
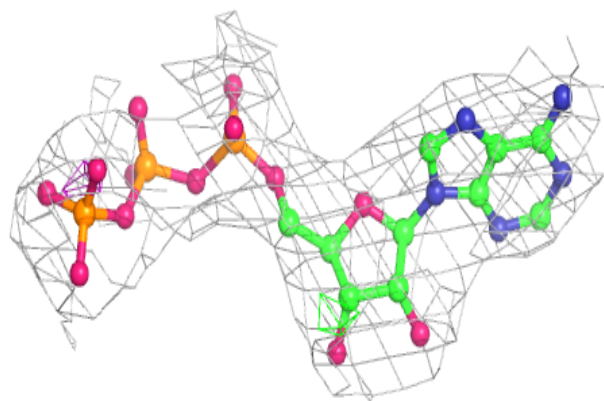
**Electron density around ADP W 701:**

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

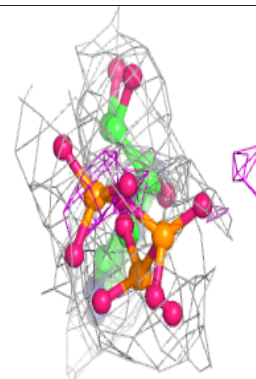
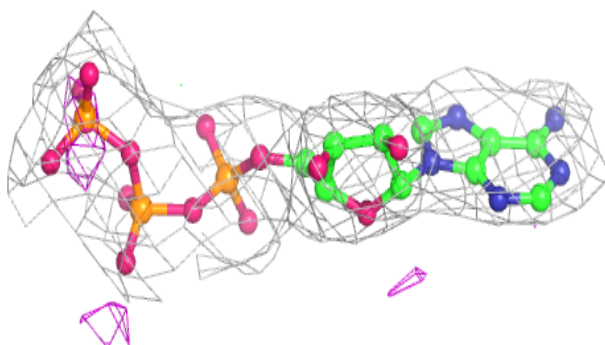
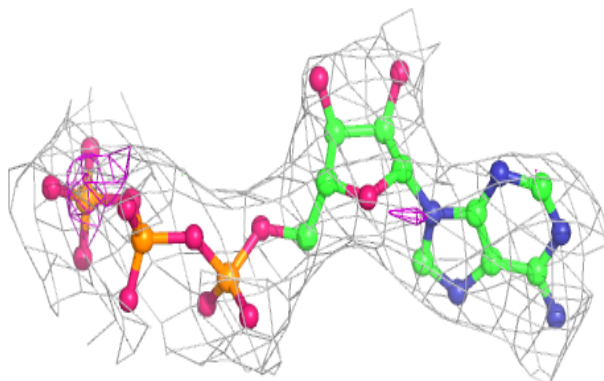


**Electron density around ATP K 702:**

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and green (positive)

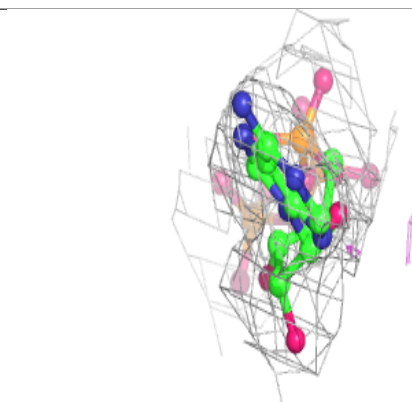
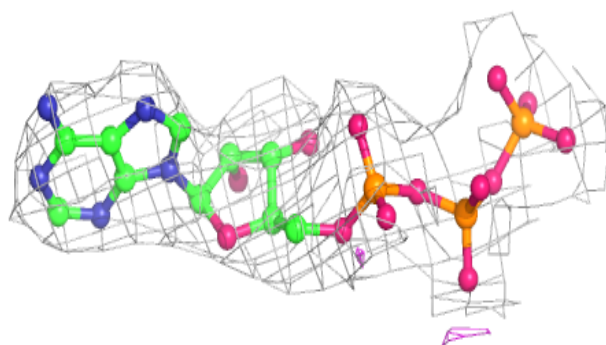
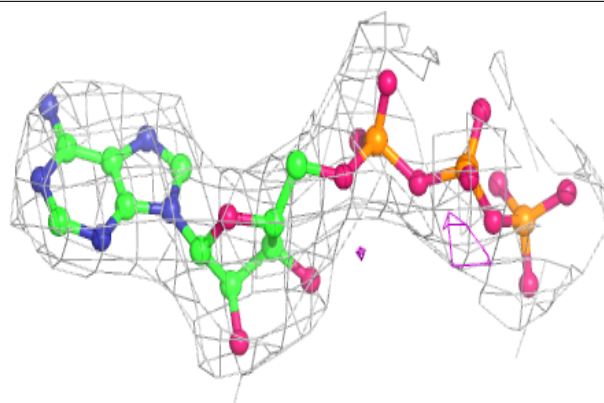
**Electron density around ATP L 702:**

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and green (positive)

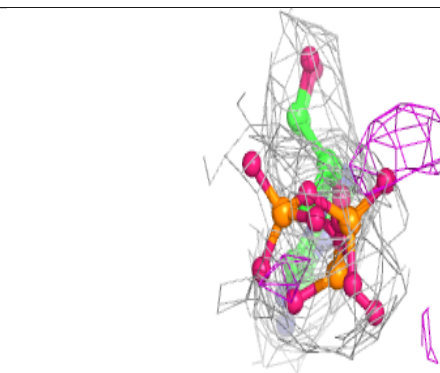
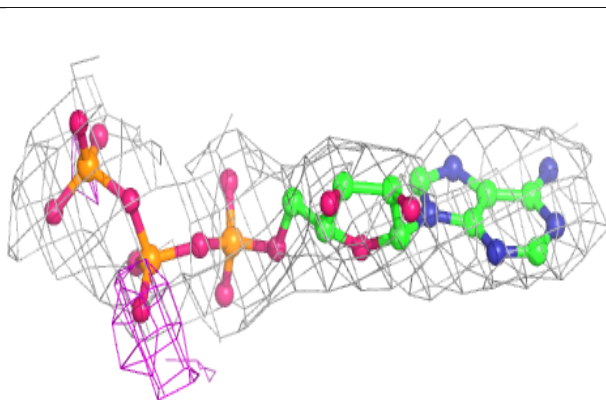
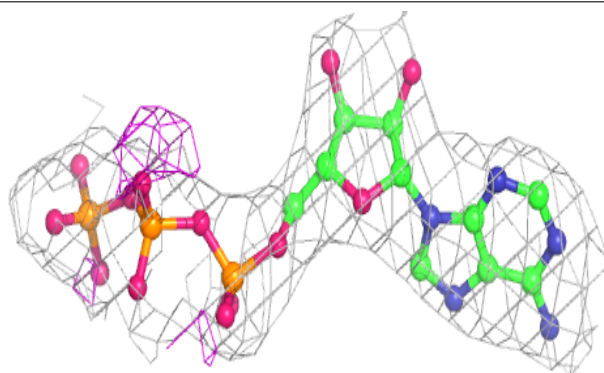


**Electron density around ATP I 702:**

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

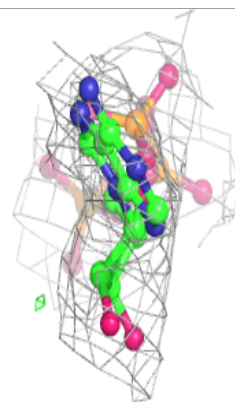
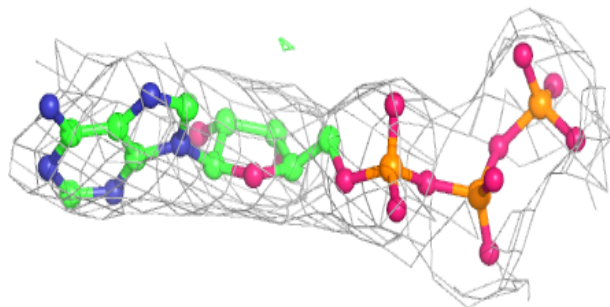
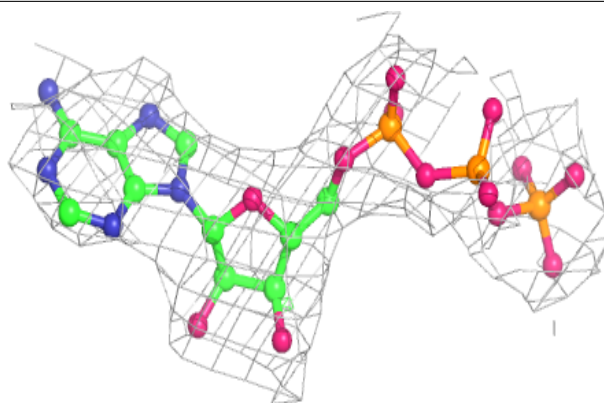
**Electron density around ATP P 702:**

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

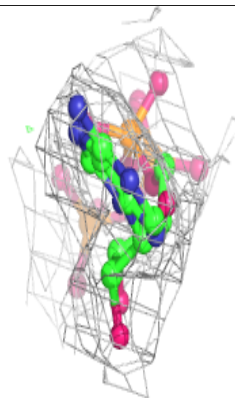
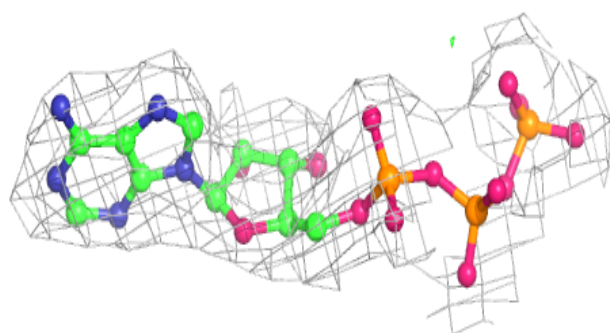
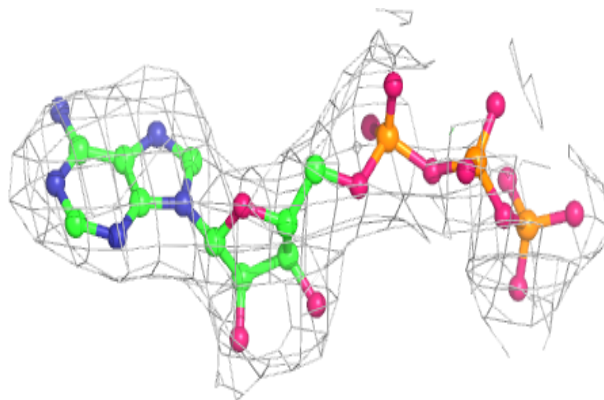


**Electron density around ATP E 702:**

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

**Electron density around ATP C 702:**

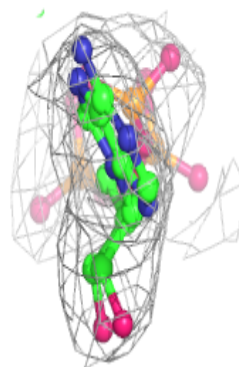
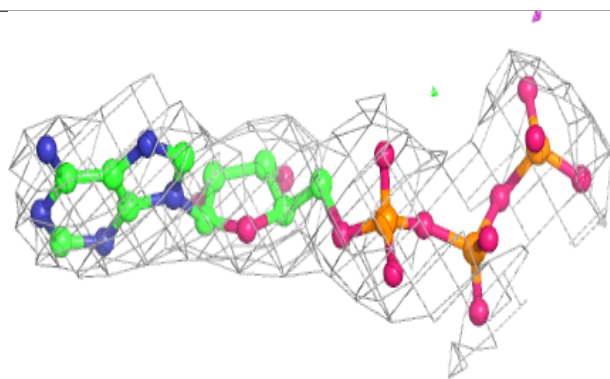
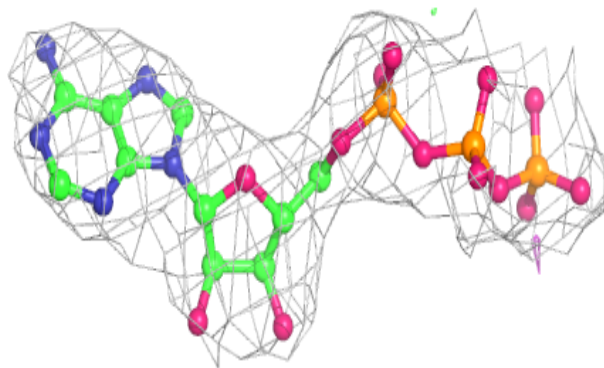
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



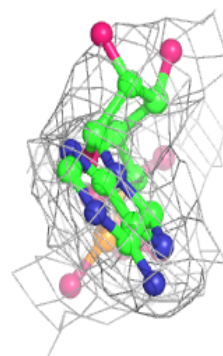
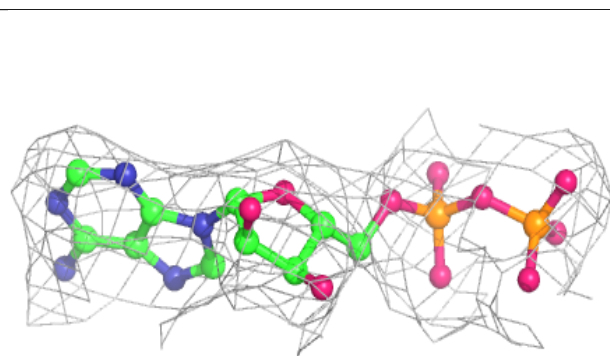
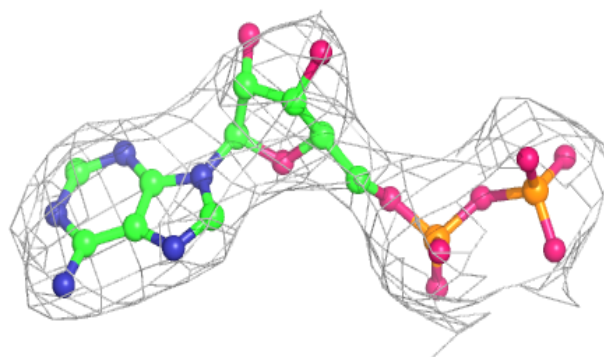


**Electron density around ATP D 702:**

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

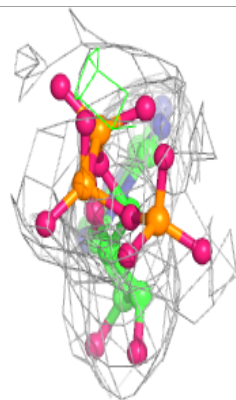
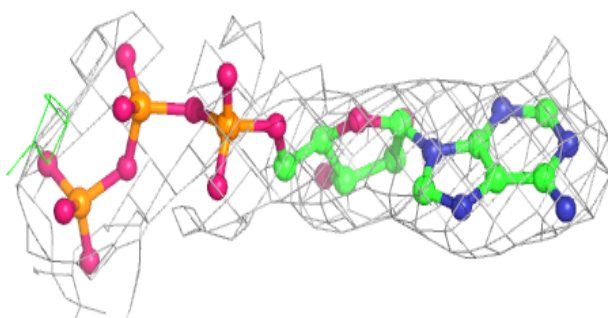
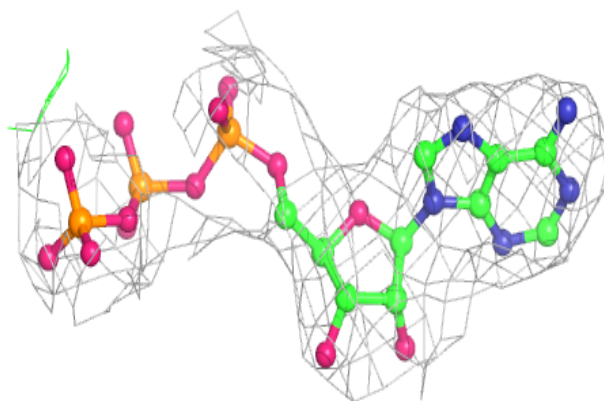
**Electron density around ADP Q 701:**

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

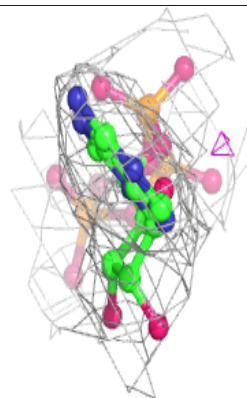
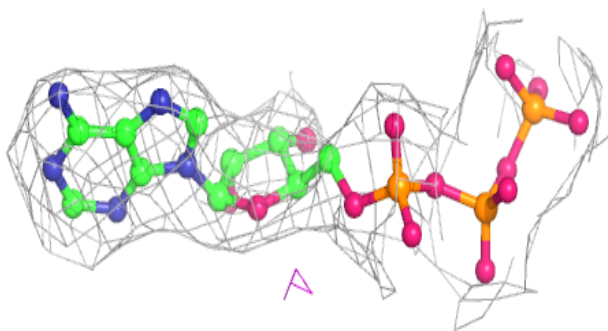
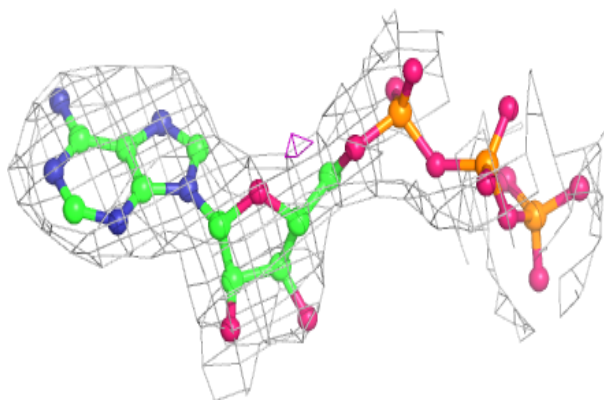


**Electron density around ATP U 701:**

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

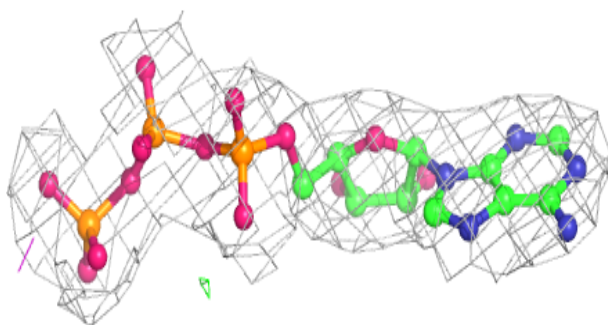
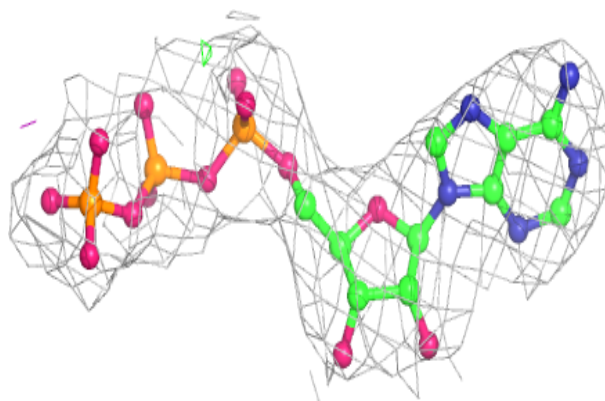
**Electron density around ATP H 701:**

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

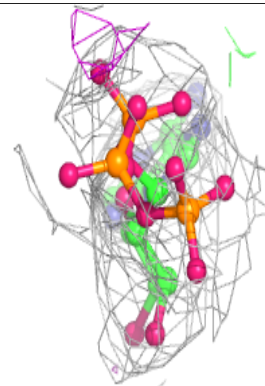
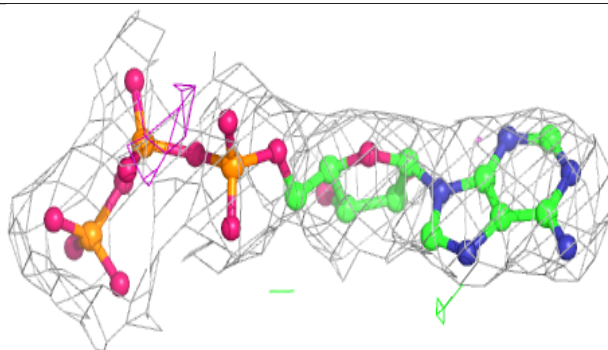
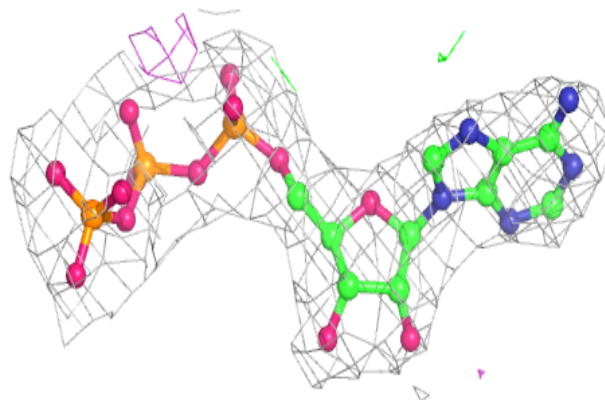


**Electron density around ATP J 702:**

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

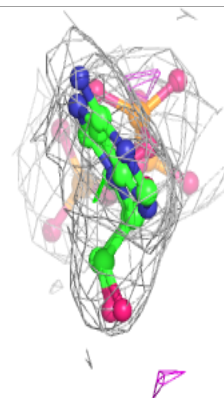
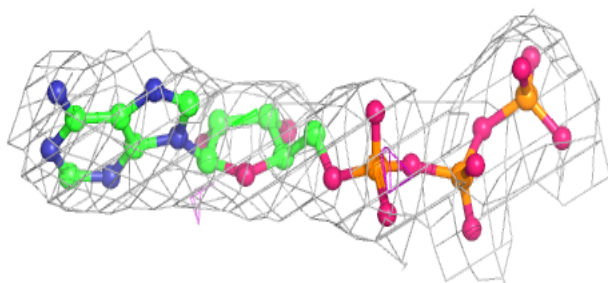
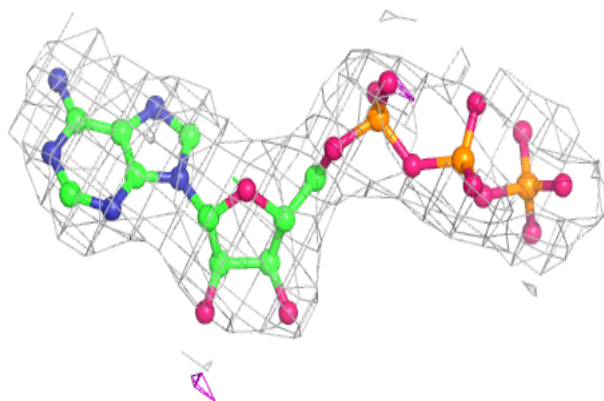
**Electron density around ATP G 701:**

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

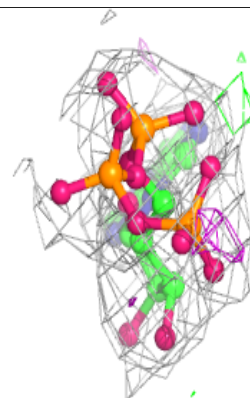
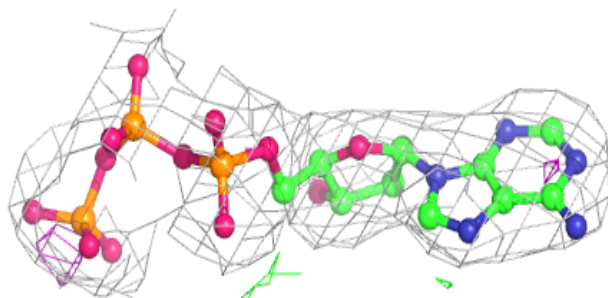
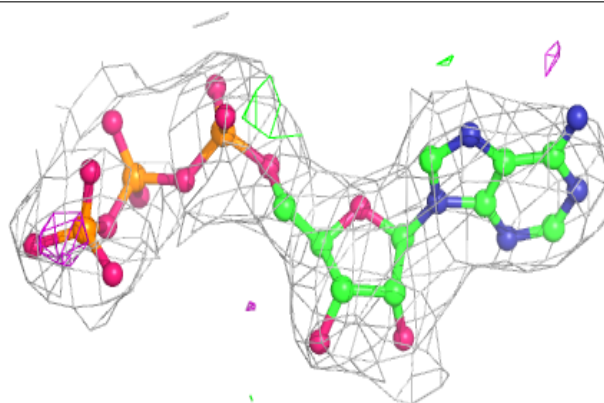


**Electron density around ATP G 702:**

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

**Electron density around ATP F 701:**

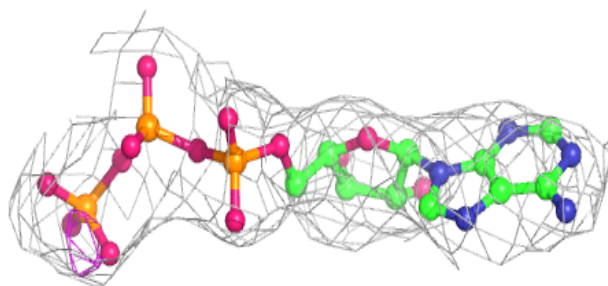
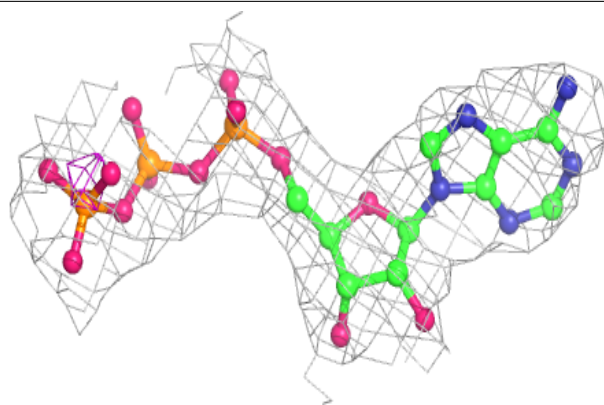
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



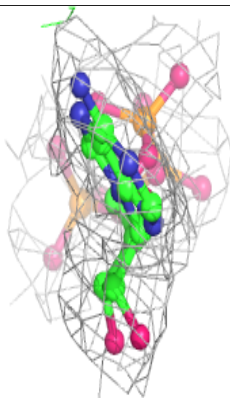
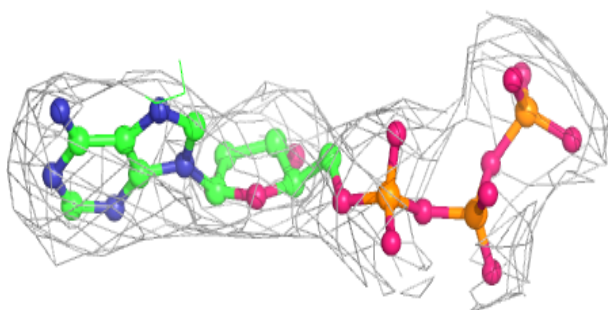
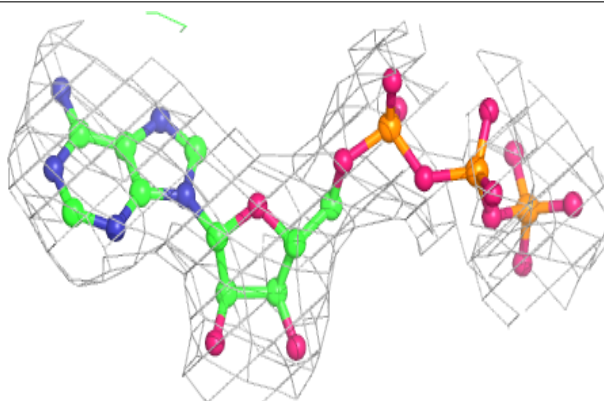


**Electron density around ATP H 702:**

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

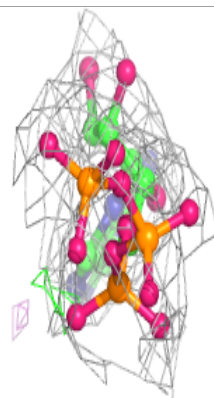
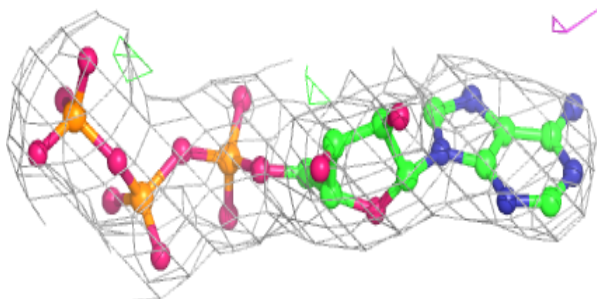
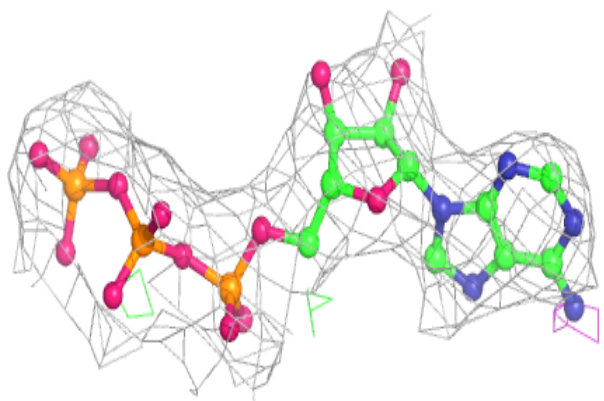
**Electron density around ATP K 701:**

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

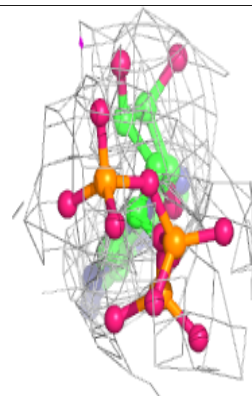
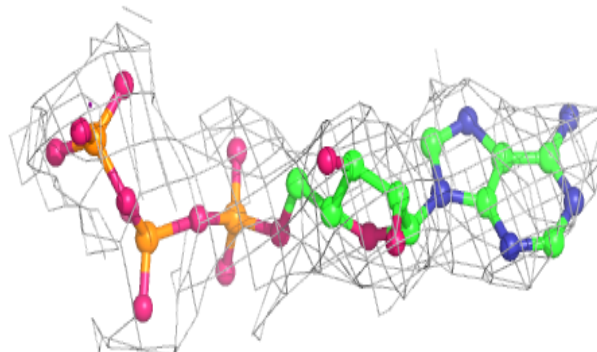
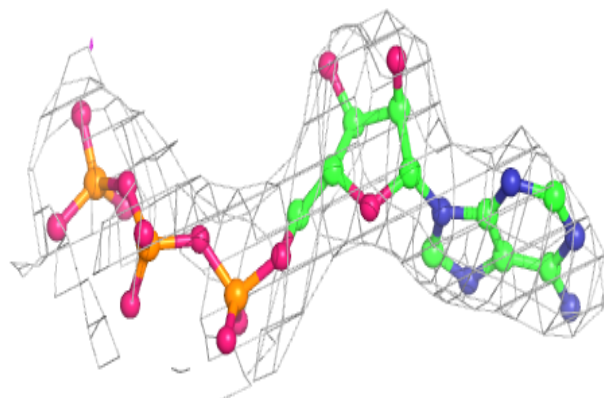


**Electron density around ATP R 702:**

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

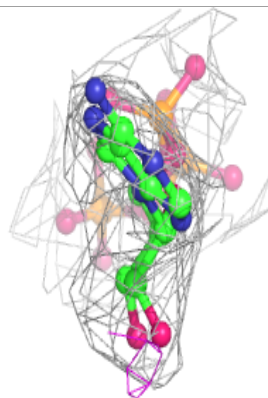
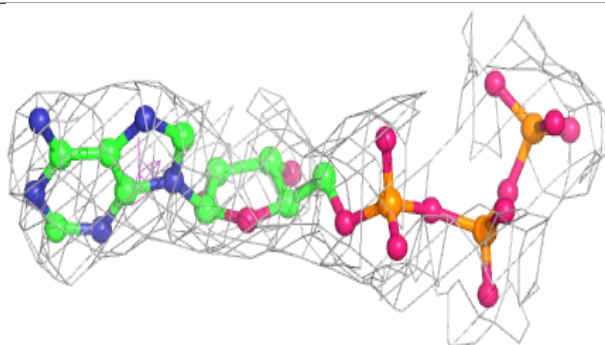
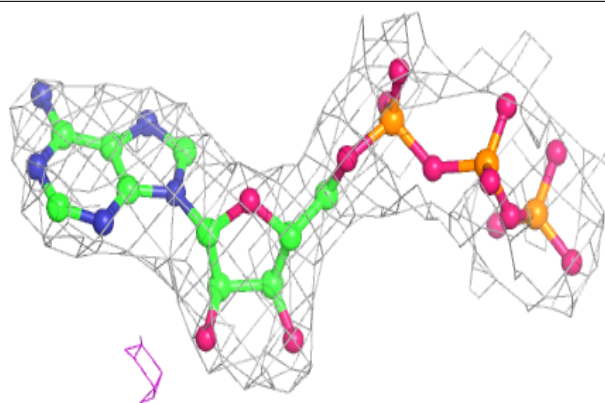
**Electron density around ATP V 701:**

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

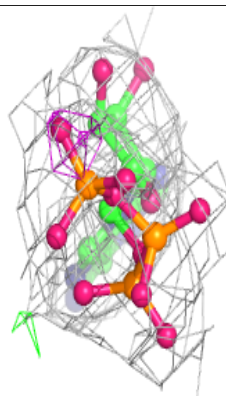
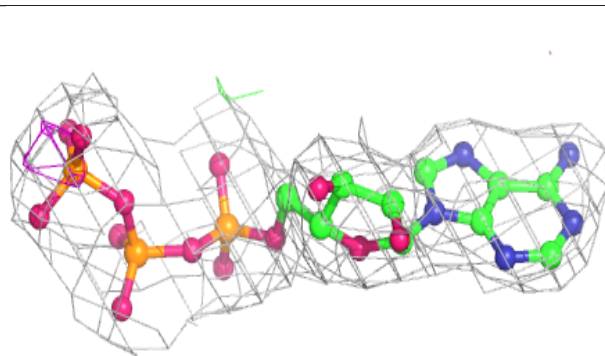
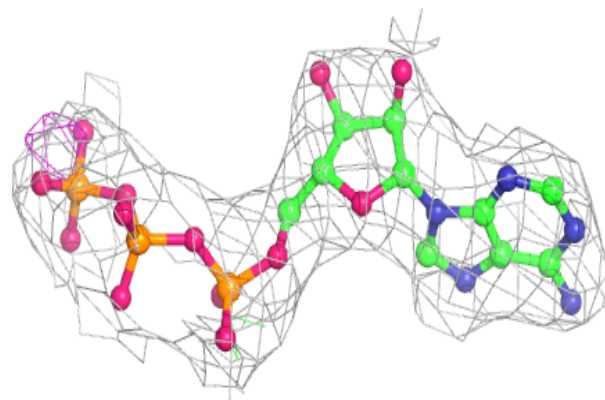


**Electron density around ATP A 701:**

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

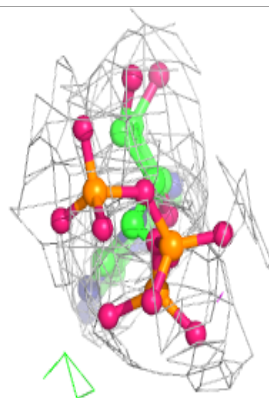
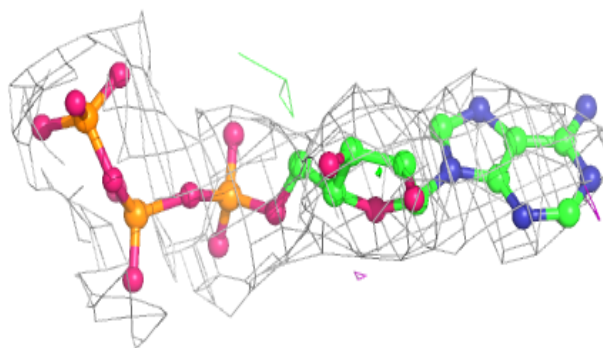
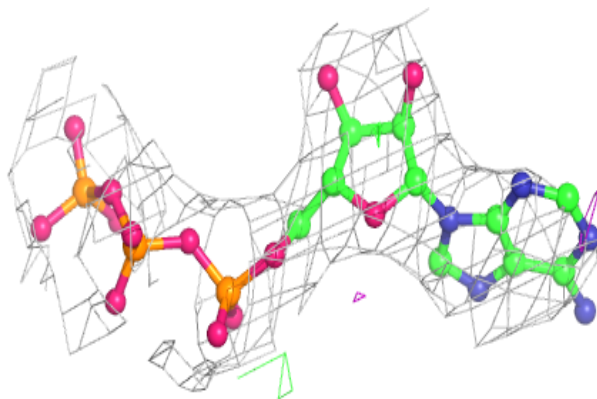
**Electron density around ATP L 701:**

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

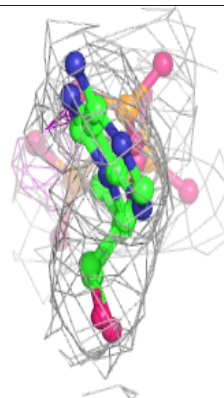
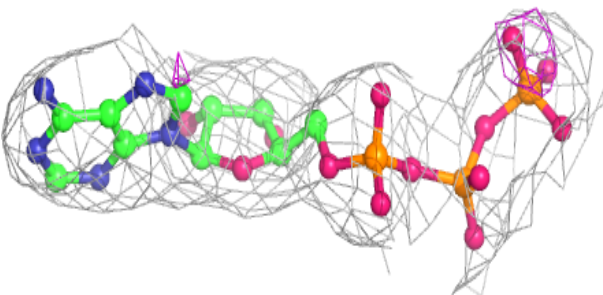
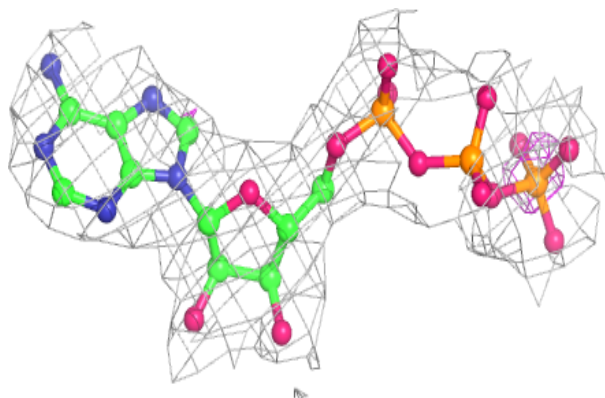


**Electron density around ATP P 701:**

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

**Electron density around ATP B 702:**

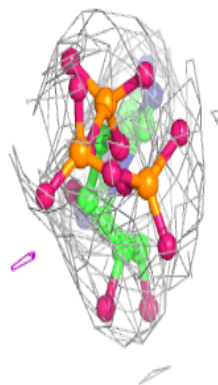
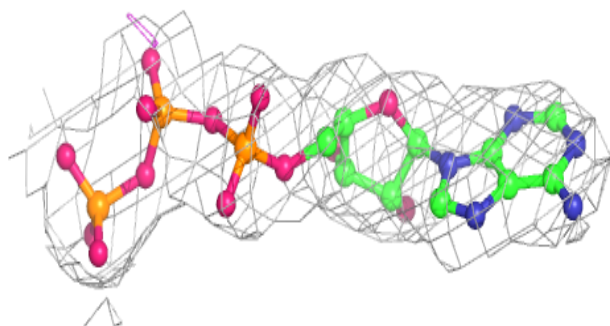
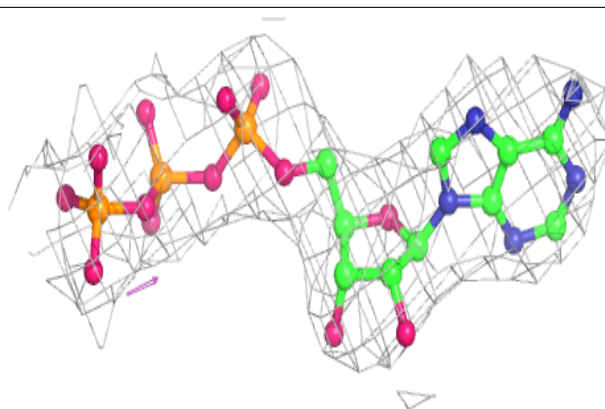
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



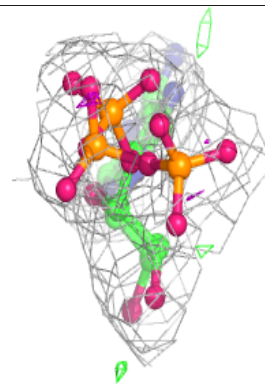
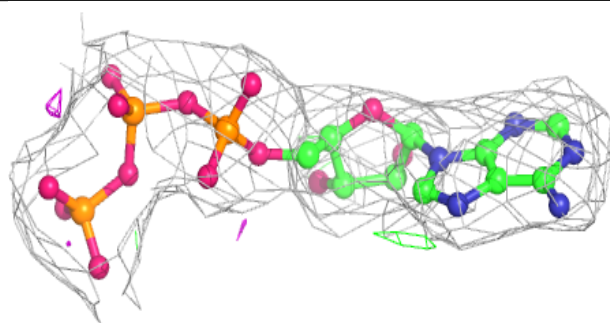
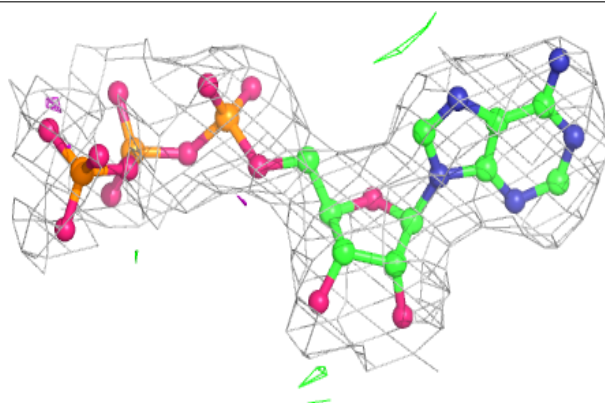


**Electron density around ATP A 702:**

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

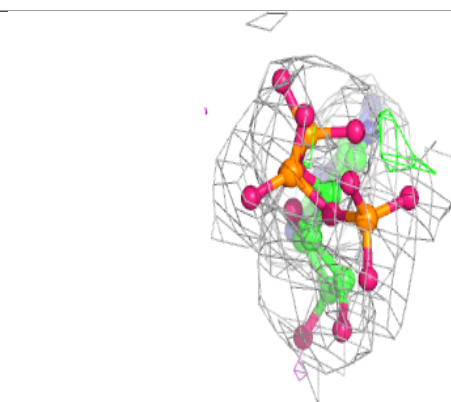
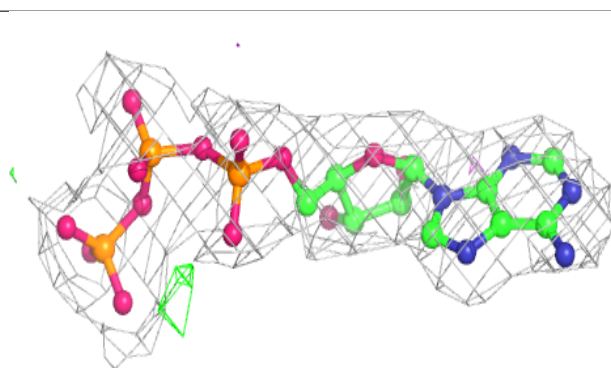
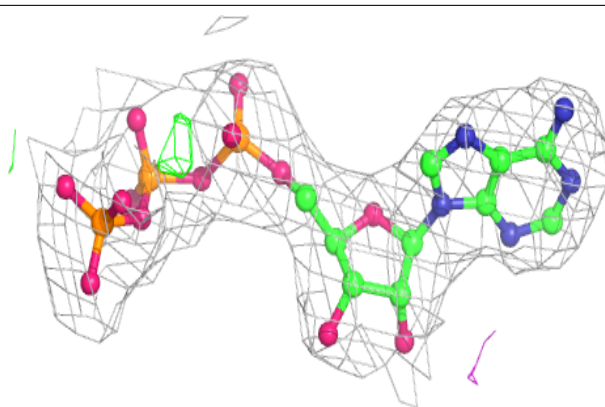
**Electron density around ATP E 701:**

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

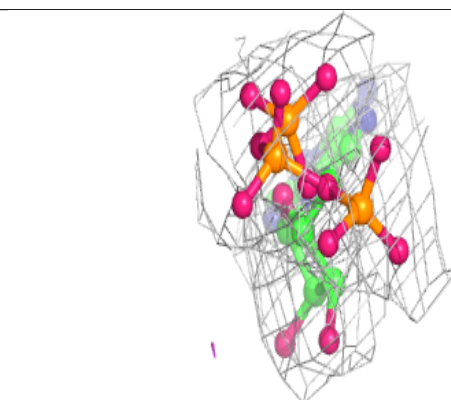
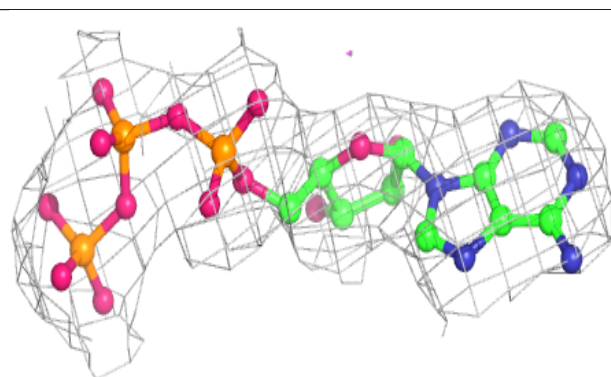
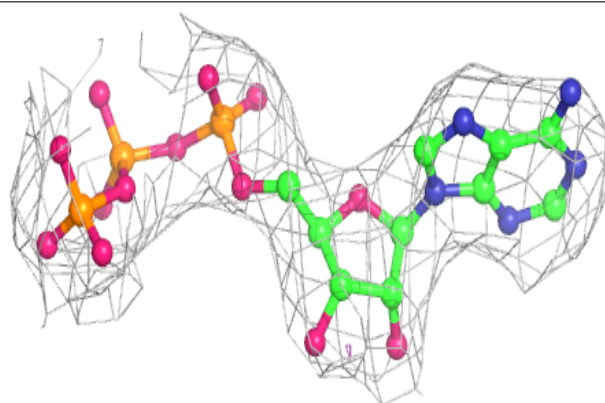


**Electron density around ATP J 701:**

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

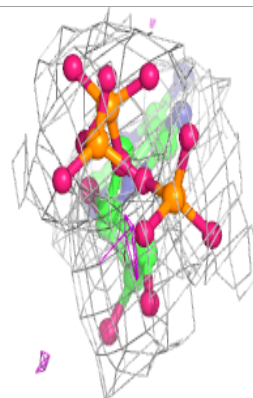
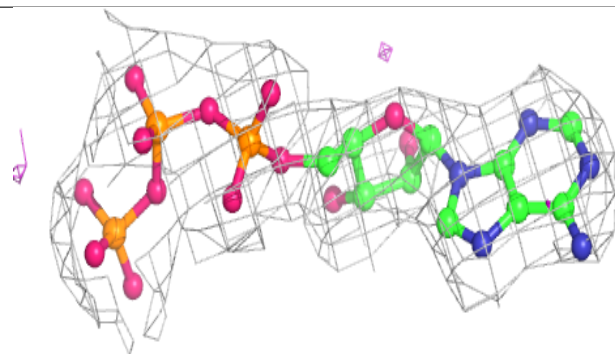
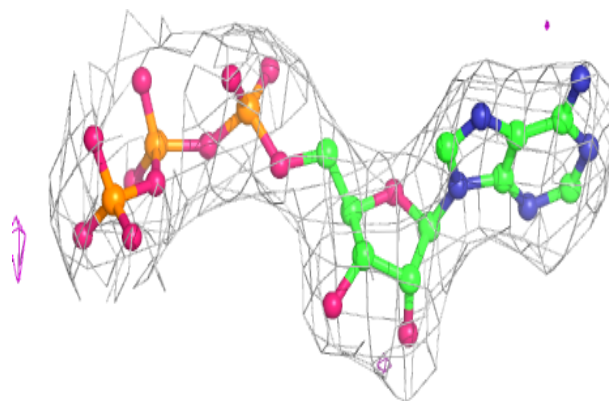
**Electron density around ATP C 701:**

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

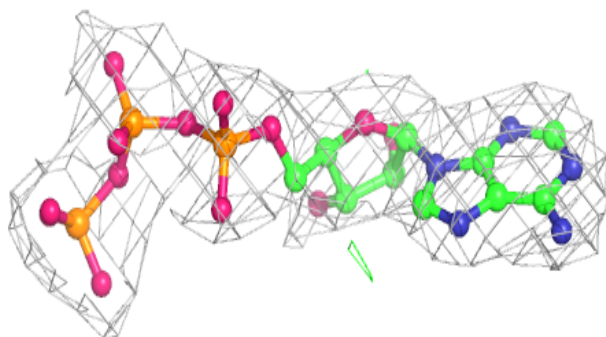
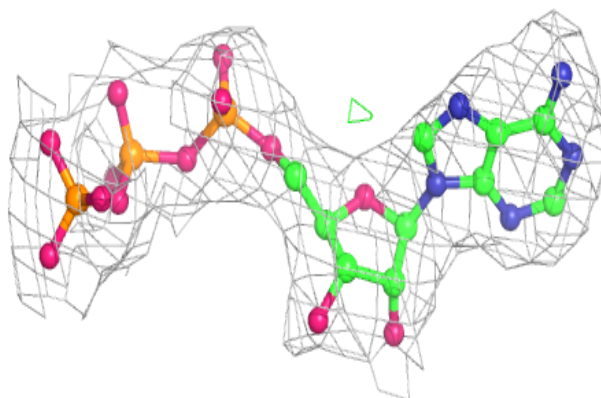


**Electron density around ATP I 701:**

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

**Electron density around ATP D 701:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.