



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:29 AM EDT

PDB ID : 7V3X / pdb_00007v3x
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

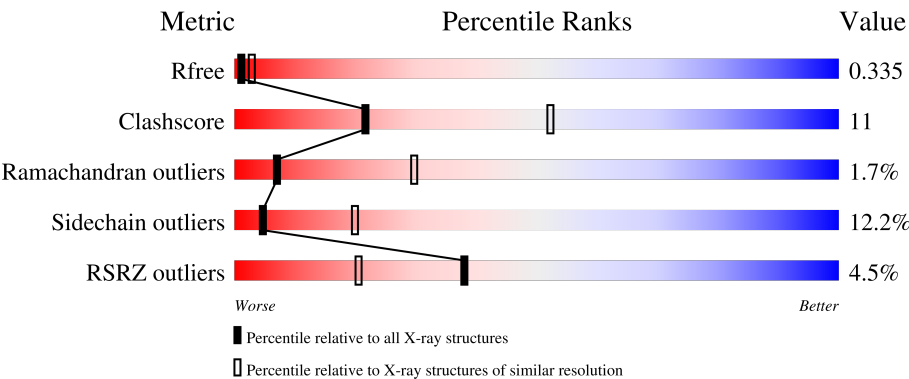
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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.



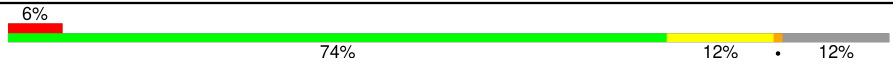
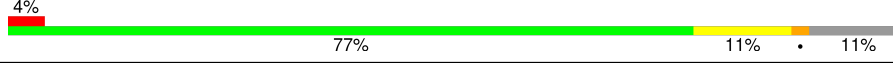
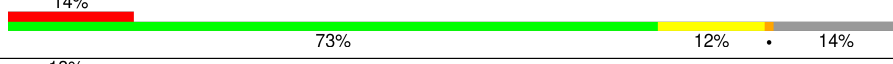
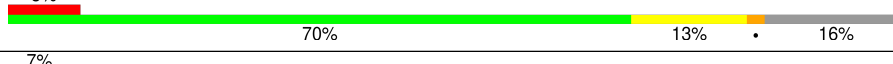
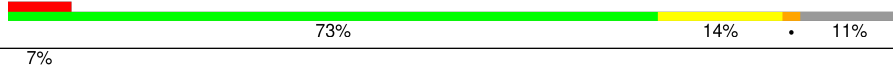
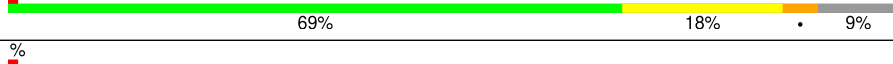
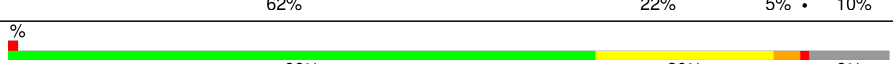
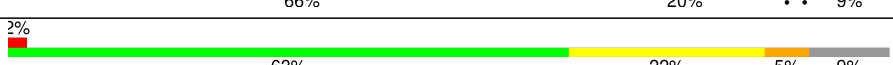
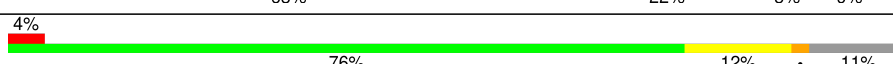
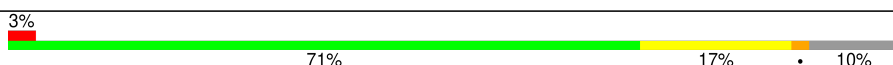
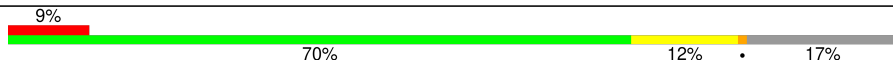
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 ≥ 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	
1	B	519	
1	G	519	
1	H	519	
1	M	519	

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Mol	Chain	Length	Quality of chain
1	N	519	
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.

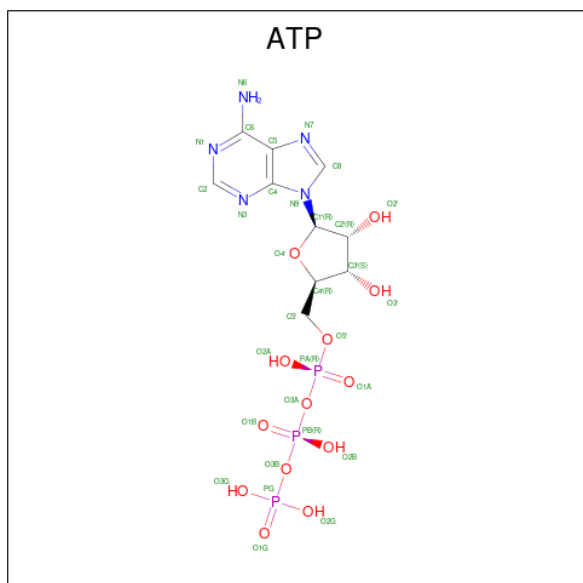
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	470	Total	C	N	O	P	S	0	0	0
			3424	2159	590	661	2	12			

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

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

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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 (CCD ID: MG) (formula: Mg).

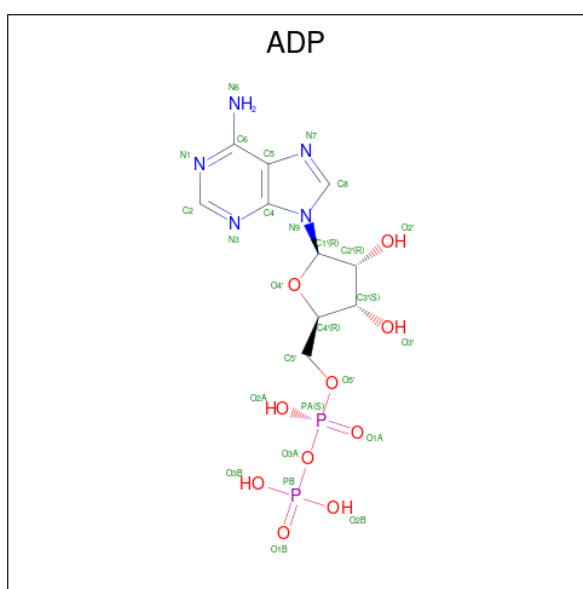
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		
4	G	2	Total	Mg	0	0
			2	2		
4	H	2	Total	Mg	0	0
			2	2		
4	K	2	Total	Mg	0	0
			2	2		
4	L	2	Total	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 (CCD ID: 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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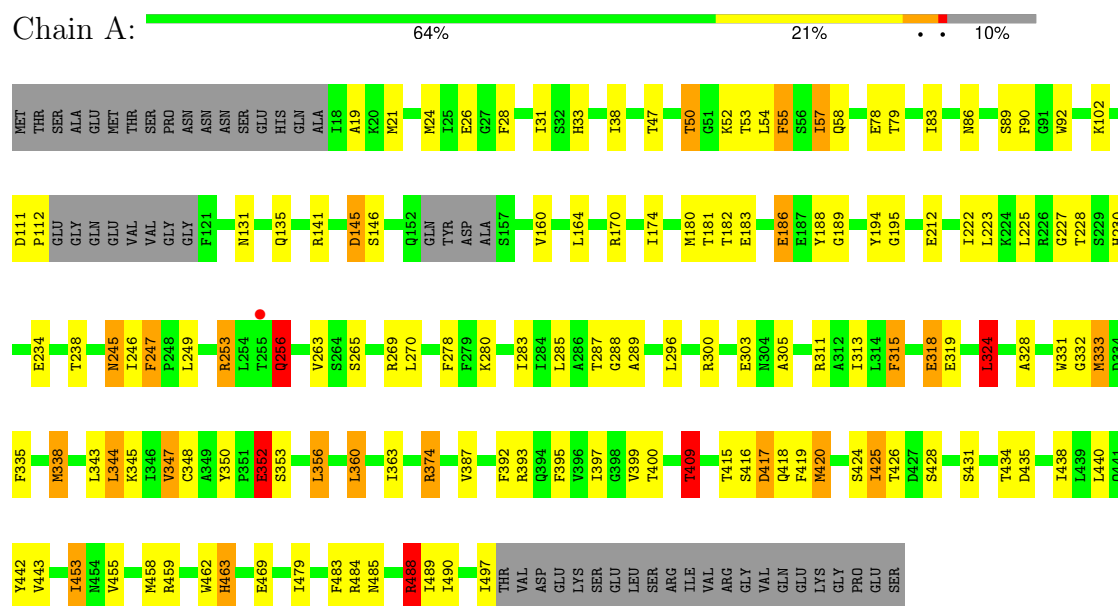
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	4	Total O 4 4	0	0
6	F	6	Total O 6 6	0	0
6	C	7	Total O 7 7	0	0
6	D	4	Total O 4 4	0	0
6	G	4	Total O 4 4	0	0
6	H	4	Total O 4 4	0	0
6	K	3	Total O 3 3	0	0
6	L	6	Total O 6 6	0	0
6	I	5	Total O 5 5	0	0
6	J	4	Total 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

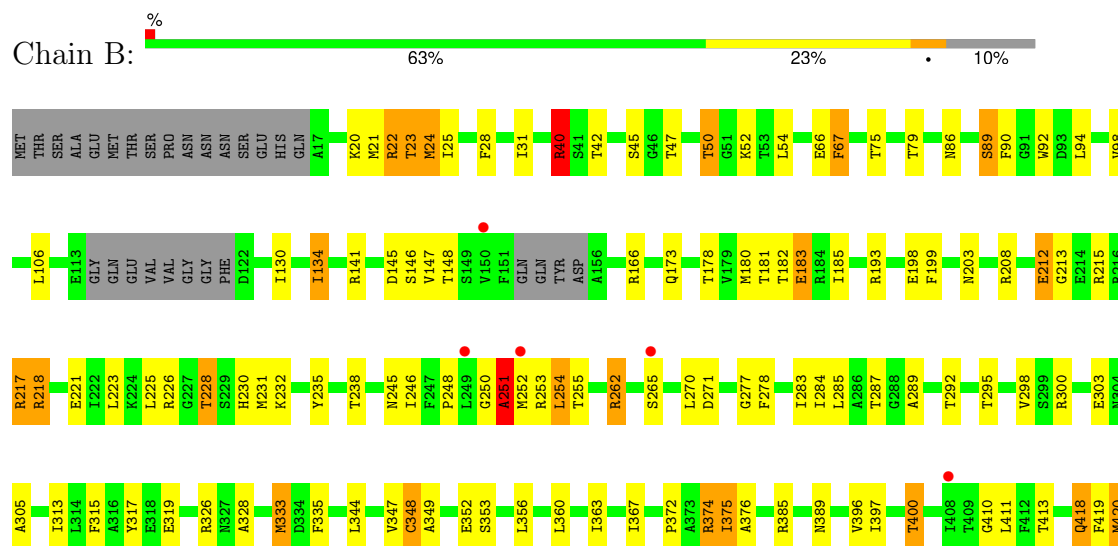
3 Residue-property plots

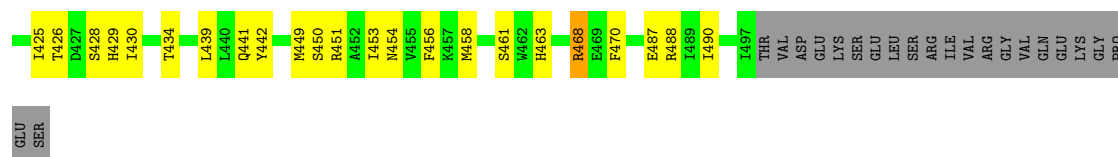
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



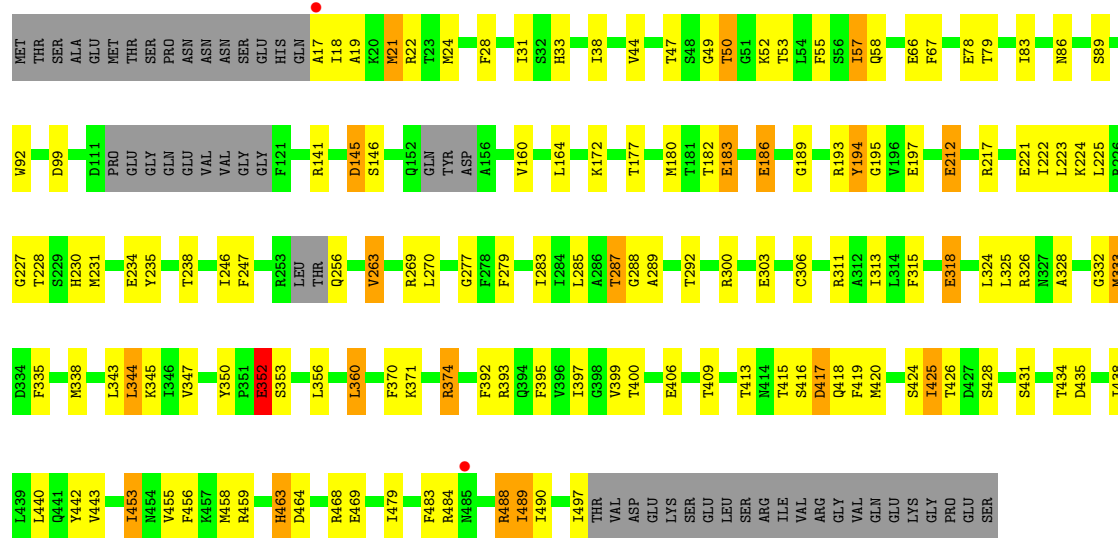
• Molecule 1: Circadian clock protein kinase KaiC





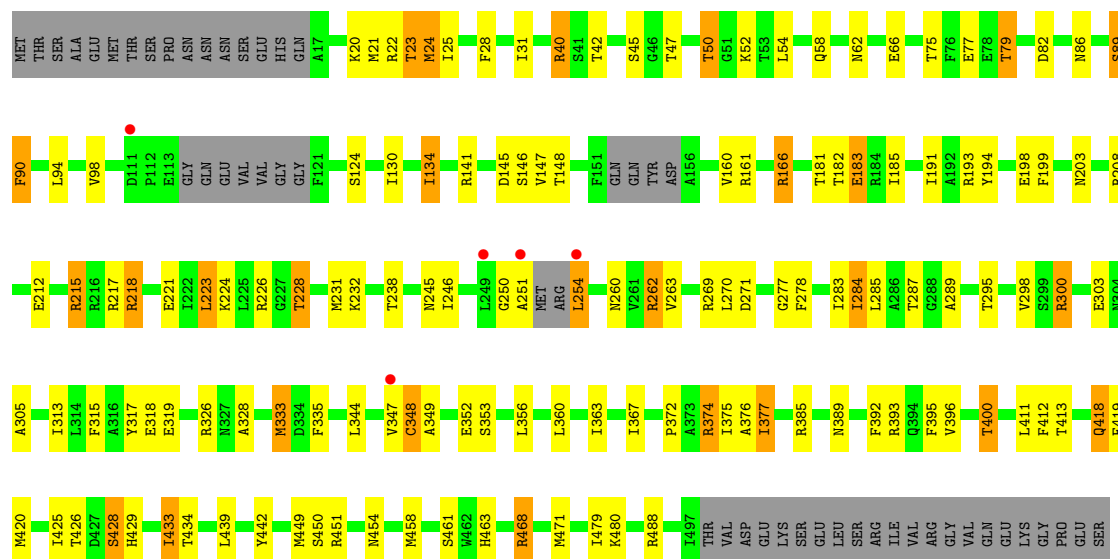
• Molecule 1: Circadian clock protein kinase KaiC

Chain G: 63% 23% 10%



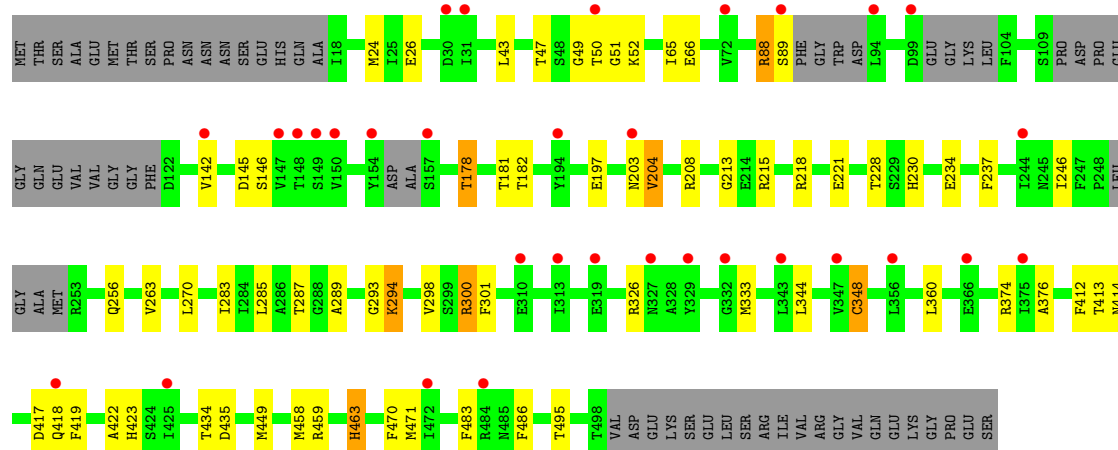
• Molecule 1: Circadian clock protein kinase KaiC

Chain H: 63% 22% 5% 10%

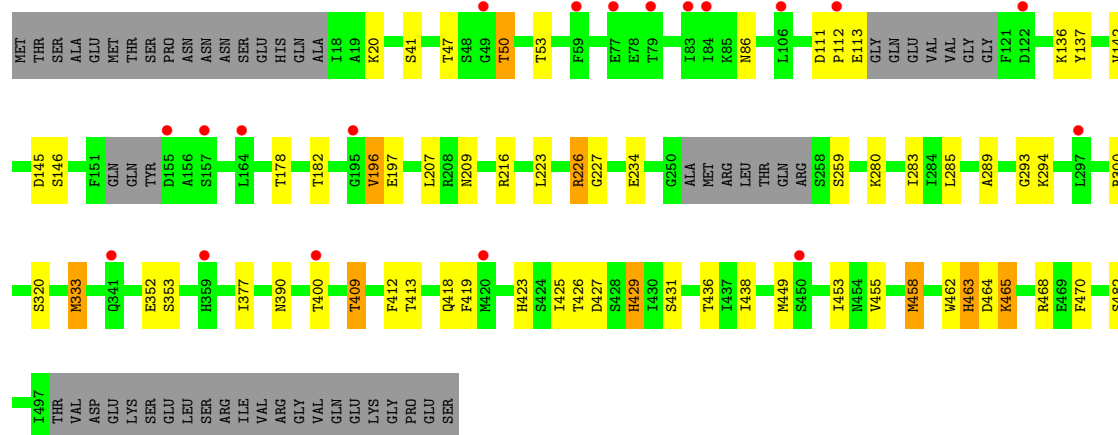
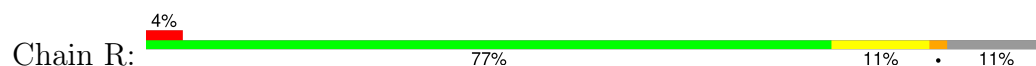


• Molecule 1: Circadian clock protein kinase KaiC

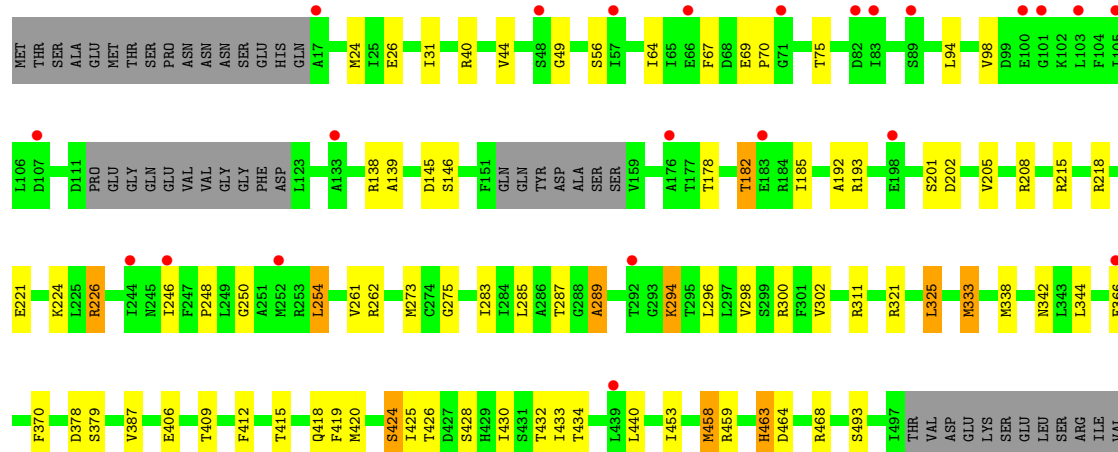
Chain N: 74% 12% 12%



• Molecule 1: Circadian clock protein kinase KaiC



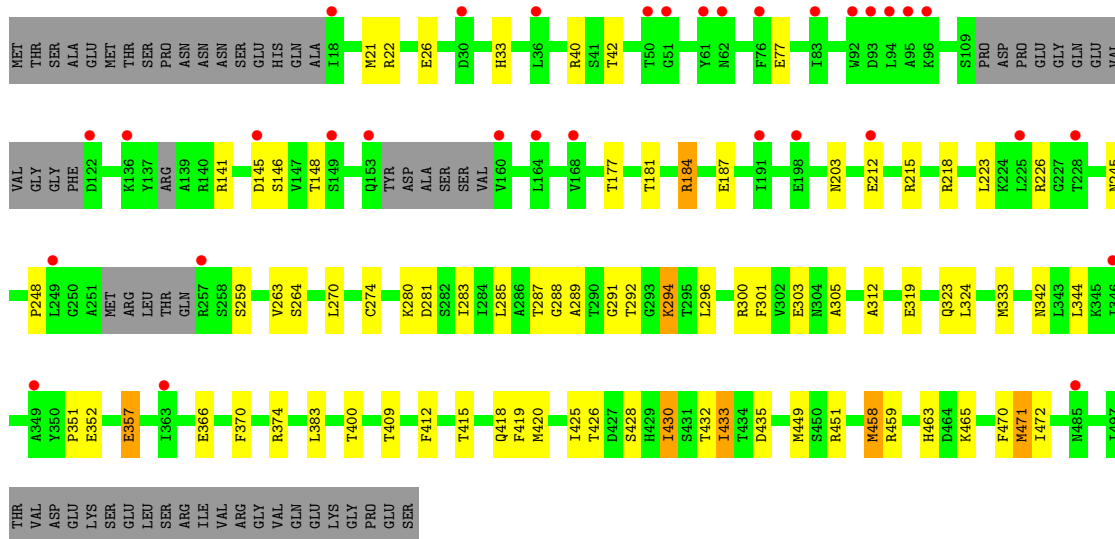
• Molecule 1: Circadian clock protein kinase KaiC



ARG
GLY
VAL
SER
GLN
GLU
LYS
GLY
PRO
GLU
SER

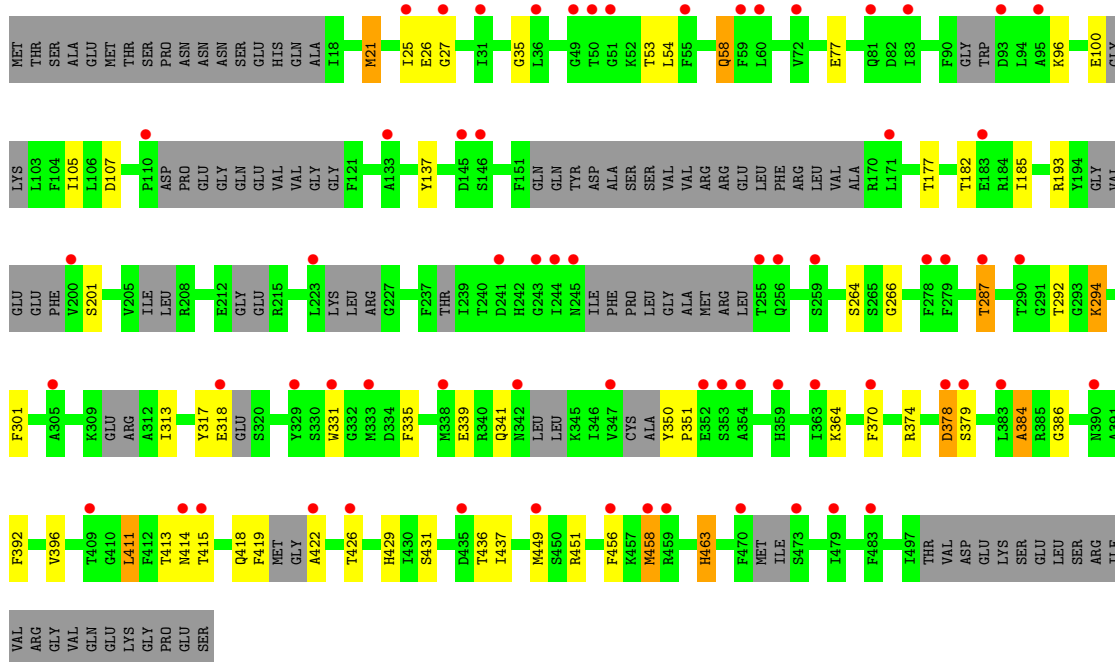
• Molecule 1: Circadian clock protein kinase KaiC

Chain P: 6% 72% 14% 12%



• Molecule 1: Circadian clock protein kinase KaiC

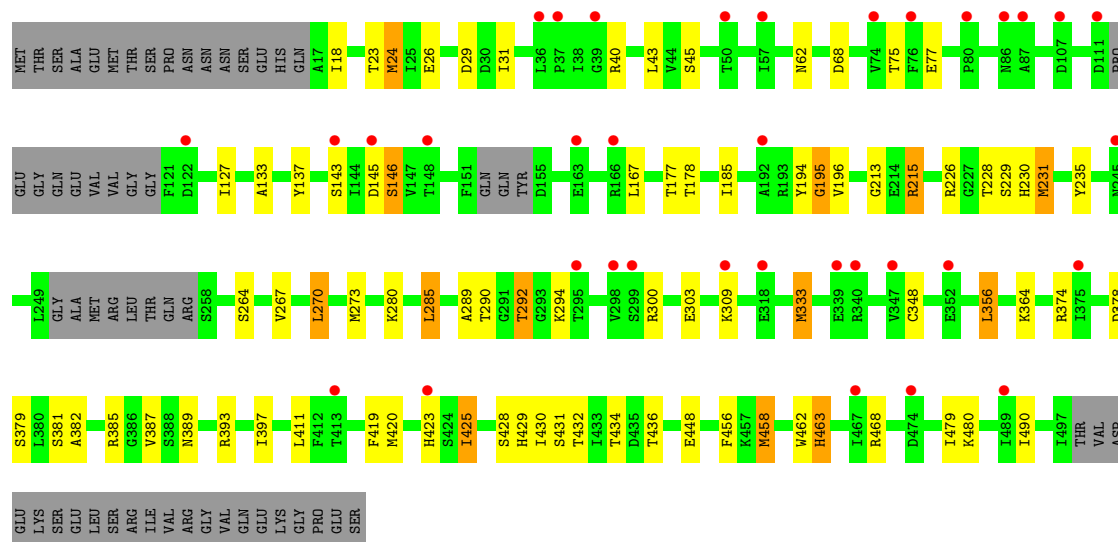
Chain T: 13% 68% 10% 20%



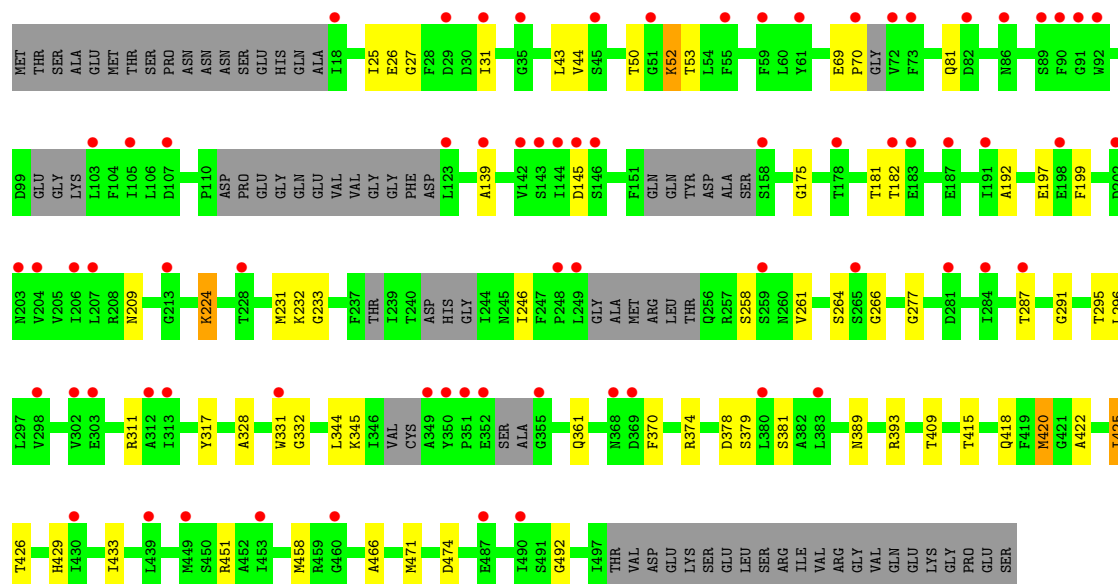
• Molecule 1: Circadian clock protein kinase KaiC

Chain X: 7% 73% 13% 11%

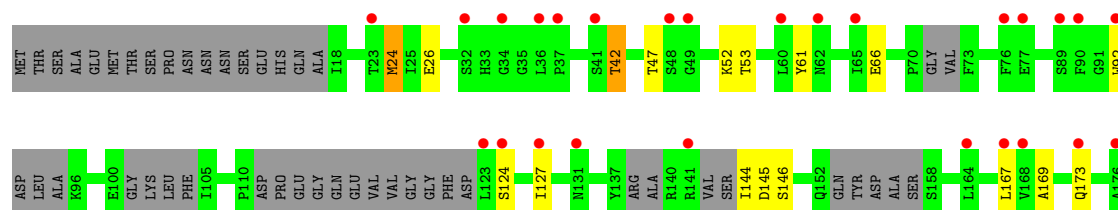


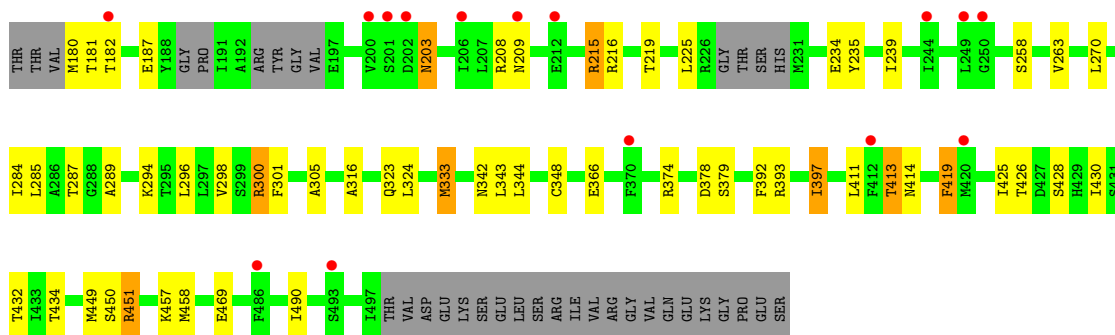


• Molecule 1: Circadian clock protein kinase KaiC

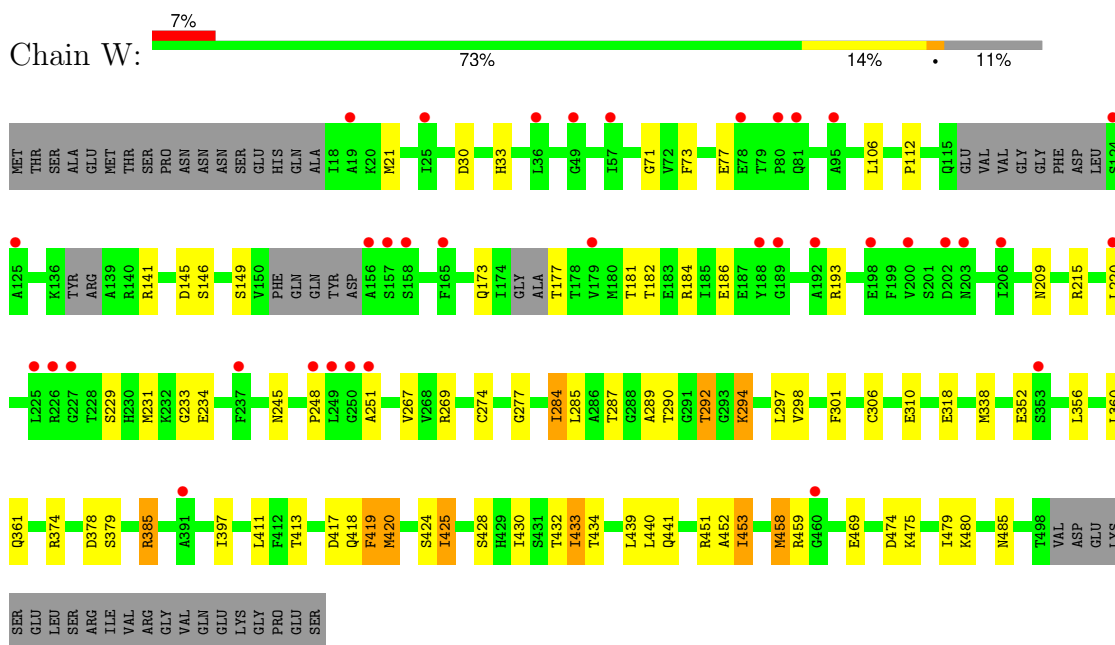


• Molecule 1: Circadian clock protein kinase KaiC

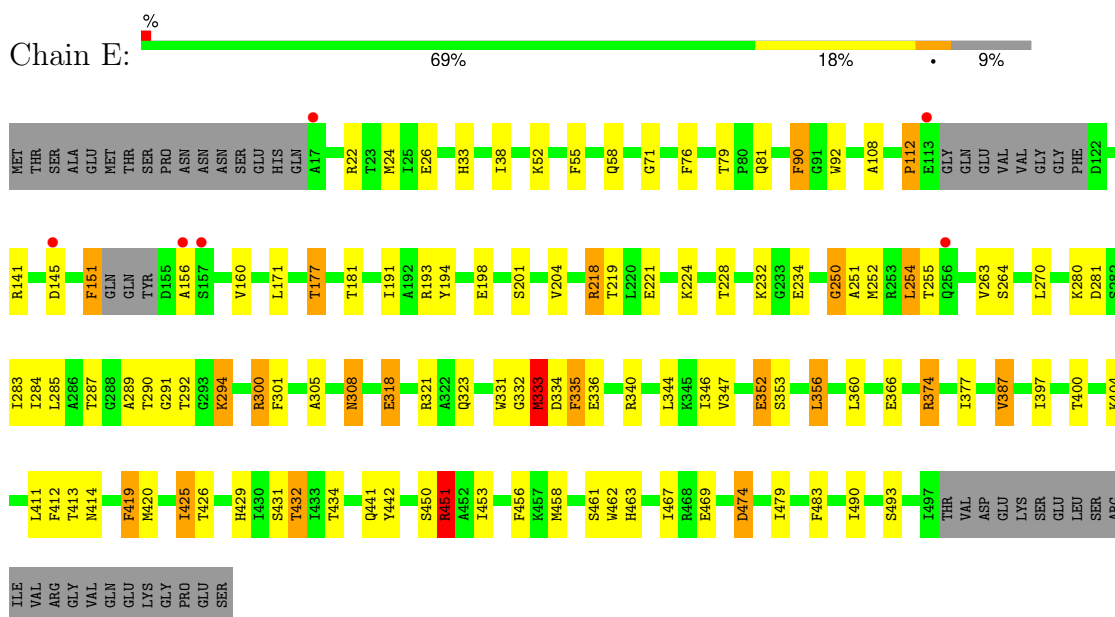




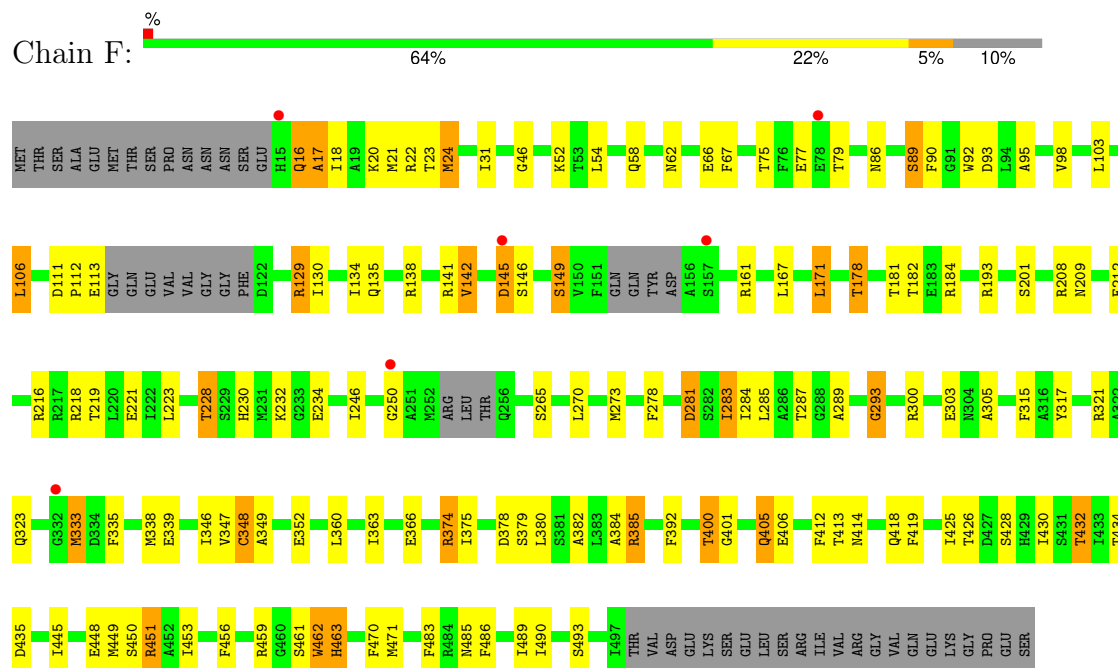
- Molecule 1: Circadian clock protein kinase KaiC



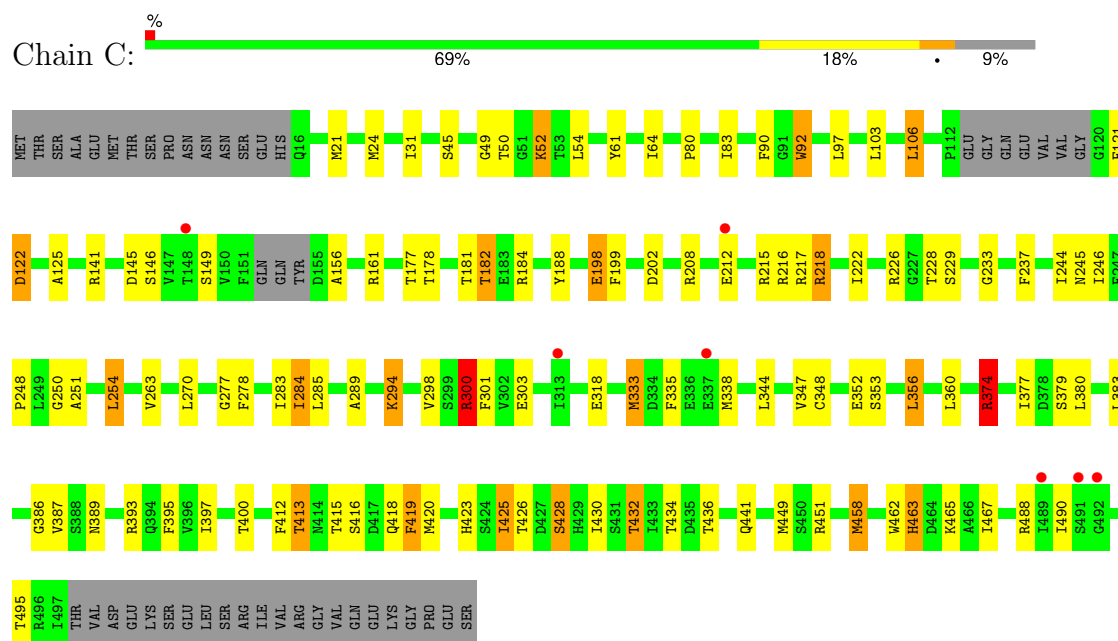
- Molecule 2: Circadian clock protein kinase KaiC



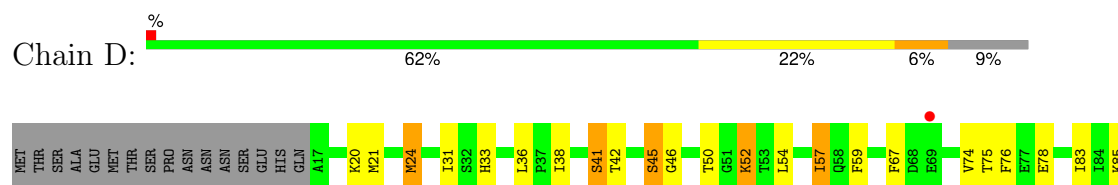
• Molecule 2: Circadian clock protein kinase KaiC

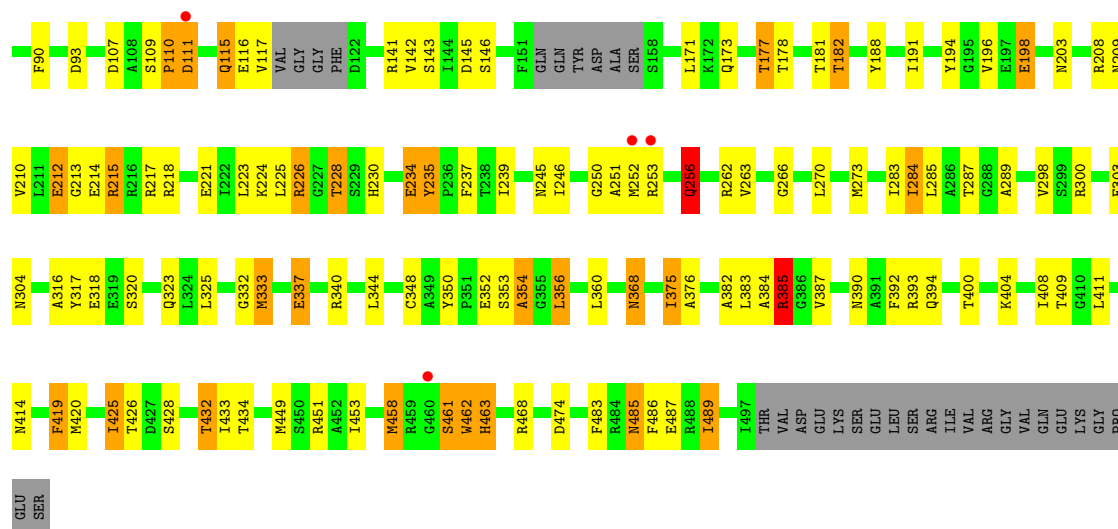


• Molecule 2: Circadian clock protein kinase KaiC

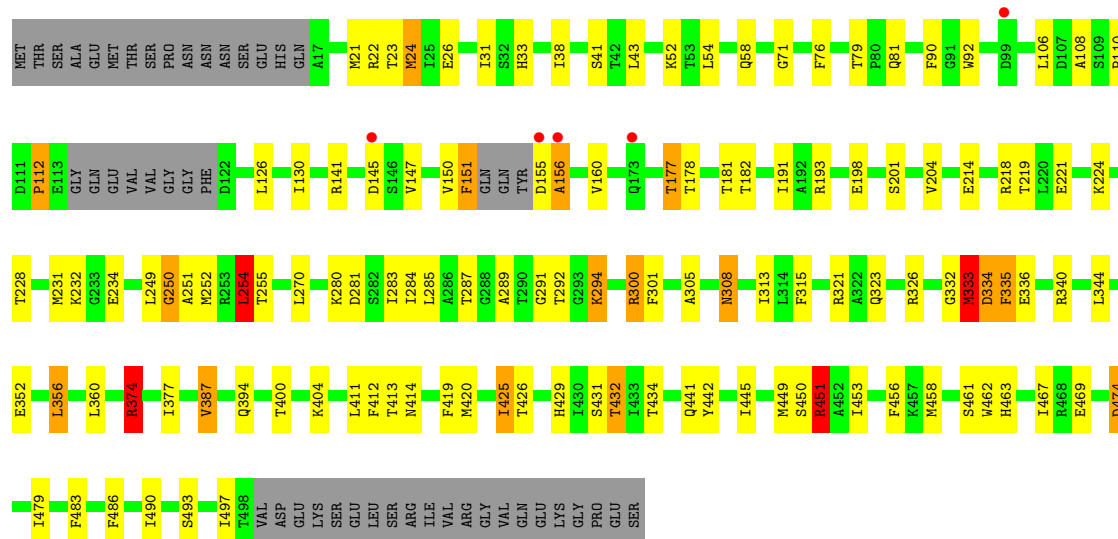


• Molecule 2: Circadian clock protein kinase KaiC

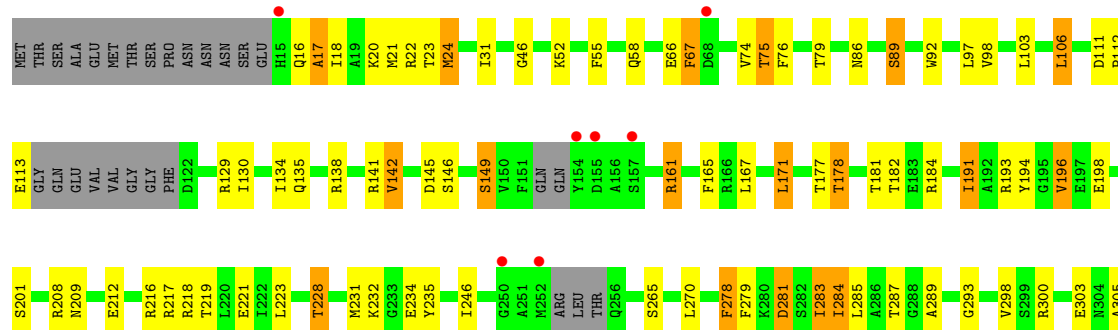


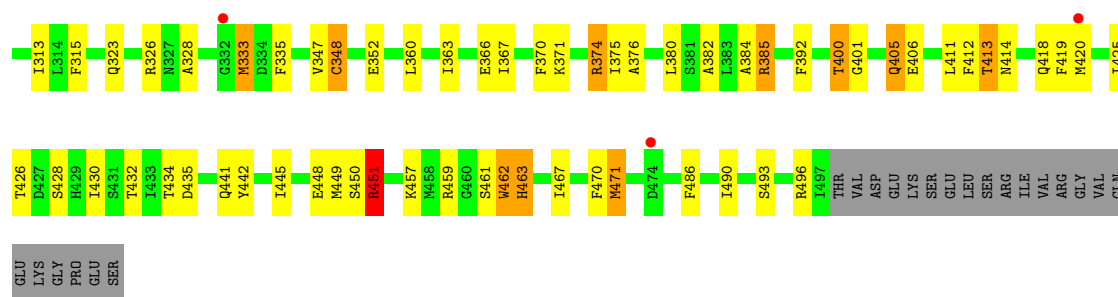


• Molecule 2: Circadian clock protein kinase KaiC

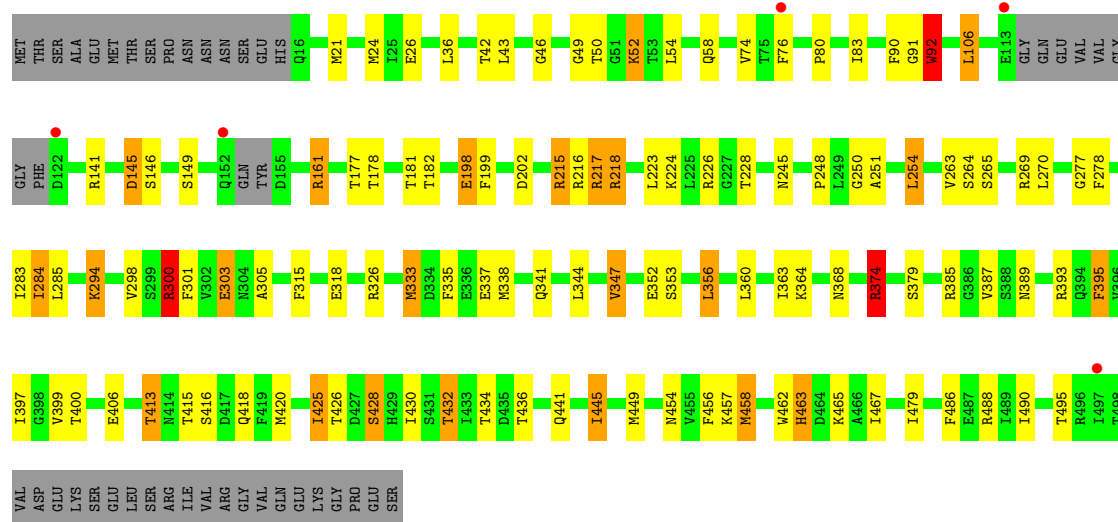


• Molecule 2: Circadian clock protein kinase KaiC

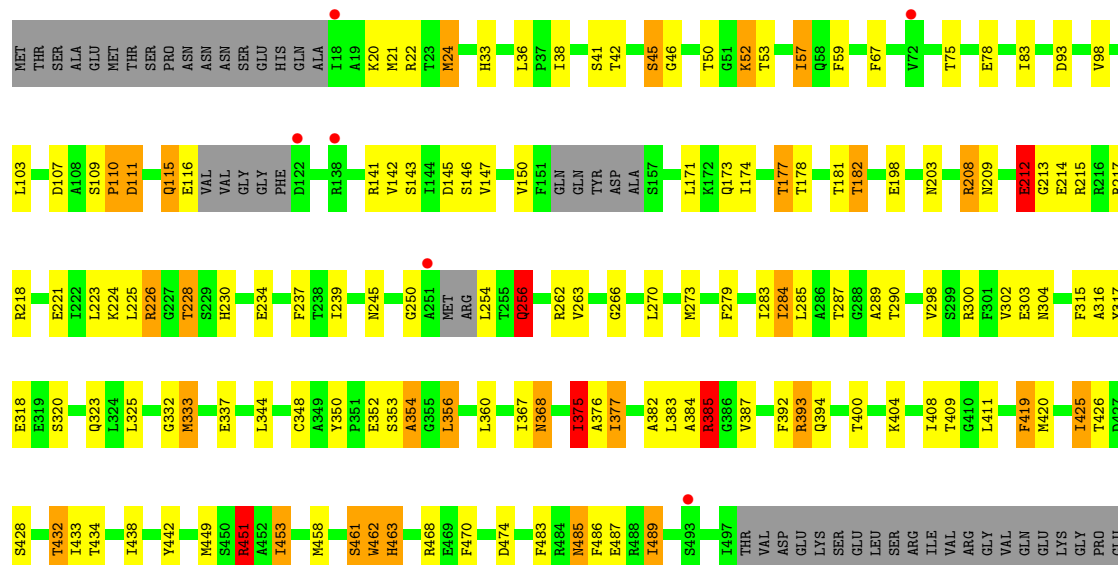




• Molecule 2: Circadian clock protein kinase KaiC

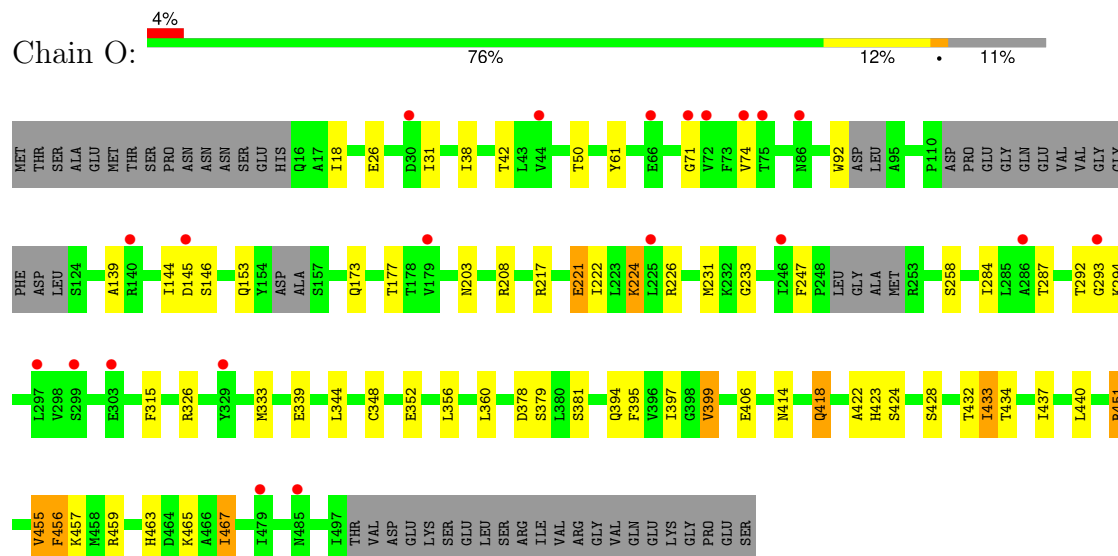


• Molecule 2: Circadian clock protein kinase KaiC

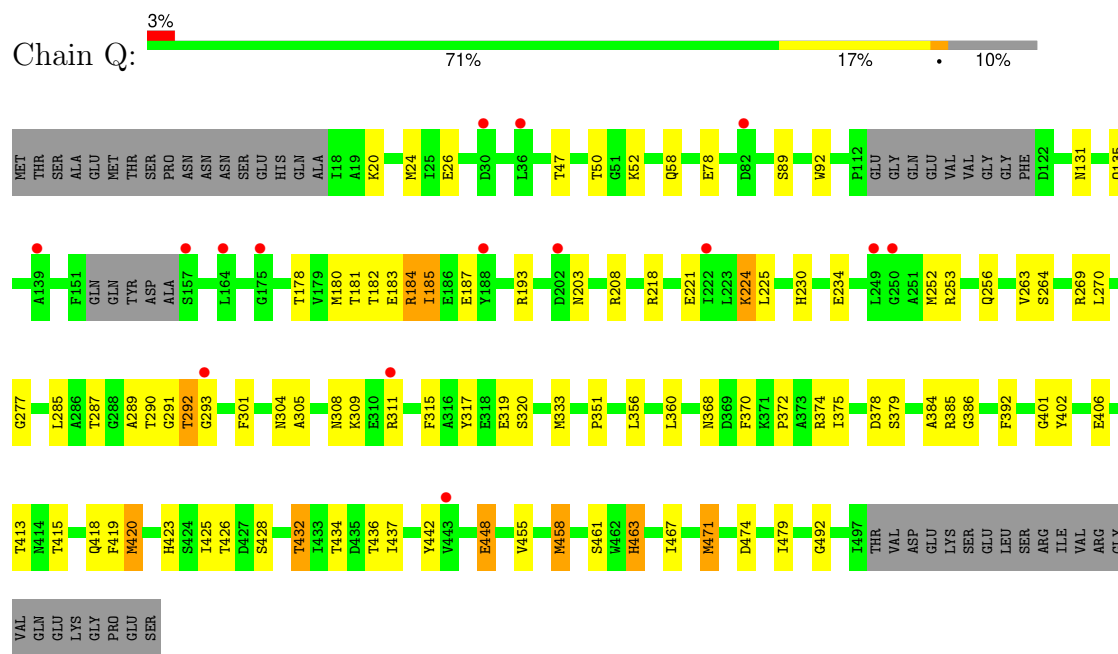


SER

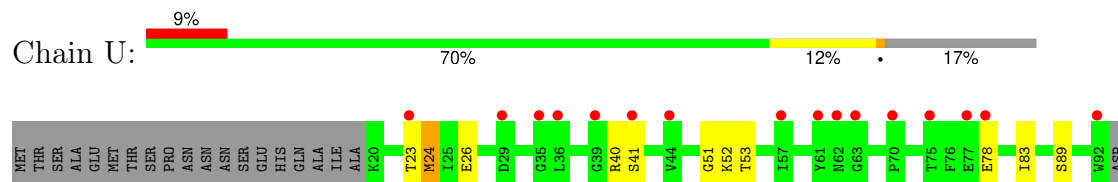
- Molecule 2: Circadian clock protein kinase KaiC

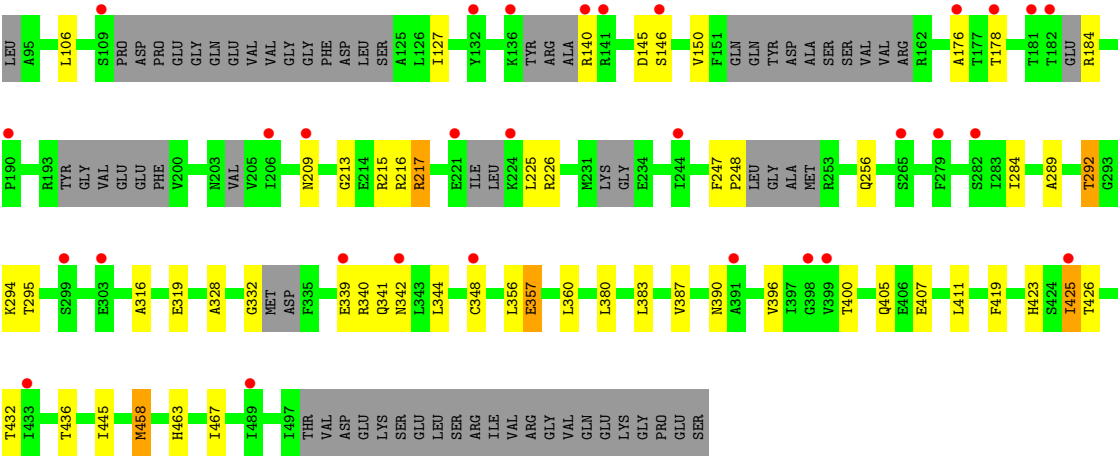


- Molecule 2: Circadian clock protein kinase KaiC



- 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, α , β , γ	185.49Å 205.80Å 186.18Å 90.00° 115.14° 90.00°	Depositor
Resolution (Å)	49.22 – 3.10 49.22 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.7 (49.22-3.10) 94.0 (49.22-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	78739	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.04	1/3555 (0.0%)	1.53	14/4815 (0.3%)
1	B	1.07	2/3479 (0.1%)	1.68	38/4719 (0.8%)
1	G	1.04	2/3494 (0.1%)	1.53	12/4734 (0.3%)
1	H	1.05	3/3523 (0.1%)	1.65	36/4770 (0.8%)
1	M	1.07	0/3164	1.51	0/4307
1	N	1.10	0/3041	1.52	0/4142
1	P	1.08	0/3132	1.49	0/4259
1	R	1.06	0/3243	1.50	0/4406
1	S	1.15	0/2725	1.57	2/3730 (0.1%)
1	T	1.15	0/2431	1.58	0/3319
1	V	1.08	0/2936	1.48	0/3993
1	W	1.07	0/3160	1.49	1/4293 (0.0%)
1	X	1.09	0/3109	1.52	0/4232
2	C	1.09	5/3473 (0.1%)	1.60	21/4710 (0.4%)
2	D	1.06	2/3491 (0.1%)	1.58	16/4732 (0.3%)
2	E	1.06	3/3460 (0.1%)	1.59	14/4695 (0.3%)
2	F	1.04	1/3471 (0.0%)	1.57	17/4699 (0.4%)
2	I	1.08	3/3513 (0.1%)	1.59	18/4758 (0.4%)
2	J	1.06	2/3476 (0.1%)	1.58	20/4709 (0.4%)
2	K	1.06	3/3479 (0.1%)	1.57	12/4720 (0.3%)
2	L	1.04	0/3507	1.56	15/4752 (0.3%)
2	O	1.09	0/3096	1.53	1/4219 (0.0%)
2	Q	1.03	0/3338	1.46	1/4529 (0.0%)
2	U	1.14	0/2638	1.57	1/3600 (0.0%)
All	All	1.07	27/77934 (0.0%)	1.55	239/105842 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	33	HIS	CE1-NE2	-9.47	1.23	1.32
2	D	33	HIS	CE1-NE2	-9.06	1.23	1.32
2	I	347	VAL	C-O	-8.81	1.14	1.24
2	E	33	HIS	CE1-NE2	-8.35	1.24	1.32
2	C	347	VAL	C-O	-8.29	1.14	1.24
2	K	33	HIS	CE1-NE2	-8.18	1.24	1.32
2	K	374	ARG	CZ-NH2	-7.75	1.23	1.33
2	E	374	ARG	CZ-NH2	-7.49	1.23	1.33
1	G	347	VAL	C-O	-7.38	1.16	1.24
1	A	347	VAL	C-O	-6.84	1.16	1.24
1	B	22	ARG	CZ-NH2	-6.60	1.24	1.33
2	C	92	TRP	NE1-CE2	-6.41	1.30	1.37
1	H	22	ARG	CZ-NH2	-6.17	1.25	1.33
2	C	92	TRP	CD2-CE3	-5.49	1.31	1.40
2	C	215	ARG	CZ-NH2	-5.46	1.26	1.33
2	D	217	ARG	CZ-NH2	-5.46	1.26	1.33
1	B	451	ARG	CZ-NH2	-5.38	1.26	1.33
2	C	161	ARG	CZ-NH2	-5.38	1.26	1.33
2	E	321	ARG	CZ-NH2	-5.37	1.26	1.33
2	J	217	ARG	CZ-NH2	-5.32	1.26	1.33
2	I	215	ARG	CZ-NH2	-5.28	1.26	1.33
2	I	161	ARG	CZ-NH2	-5.23	1.26	1.33
2	K	321	ARG	CZ-NH2	-5.23	1.26	1.33
1	G	374	ARG	CZ-NH2	-5.22	1.26	1.33
1	H	451	ARG	CZ-NH2	-5.20	1.26	1.33
1	H	217	ARG	CZ-NH2	-5.12	1.26	1.33
2	F	171	LEU	CG-CD1	-5.01	1.36	1.52

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	374	ARG	NE-CZ-NH1	13.01	134.51	121.50
2	K	374	ARG	NE-CZ-NH1	12.12	133.62	121.50
1	B	262	ARG	NE-CZ-NH2	11.70	129.73	119.20
2	E	218	ARG	CG-CD-NE	11.21	136.66	112.00
1	B	262	ARG	NE-CZ-NH1	-11.06	110.44	121.50
2	K	218	ARG	CG-CD-NE	10.76	135.67	112.00
1	B	488	ARG	NE-CZ-NH2	10.72	128.85	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	ARG	NE-CZ-NH2	10.68	128.81	119.20
1	B	468	ARG	NE-CZ-NH2	10.64	128.77	119.20
2	D	256	GLN	CB-CG-CD	10.53	130.51	112.60
2	E	451	ARG	CD-NE-CZ	10.50	139.10	124.40
2	I	52	LYS	CG-CD-CE	10.44	135.31	111.30
2	K	451	ARG	NE-CZ-NH2	10.37	128.54	119.20
2	I	488	ARG	NE-CZ-NH2	10.36	128.53	119.20
2	I	161	ARG	NE-CZ-NH2	10.36	128.52	119.20
2	I	300	ARG	NE-CZ-NH2	10.34	128.50	119.20
2	C	374	ARG	NE-CZ-NH2	10.31	128.48	119.20
1	H	488	ARG	CD-NE-CZ	10.31	138.84	124.40
2	I	488	ARG	NE-CZ-NH1	-10.26	111.24	121.50
2	C	161	ARG	NH1-CZ-NH2	-10.25	105.98	119.30
1	B	262	ARG	CD-NE-CZ	10.24	138.74	124.40
2	C	300	ARG	CD-NE-CZ	10.21	138.70	124.40
2	D	217	ARG	NH1-CZ-NH2	-10.18	106.07	119.30
1	B	166	ARG	CG-CD-NE	10.15	134.32	112.00
2	E	321	ARG	NH1-CZ-NH2	-10.13	106.14	119.30
1	H	166	ARG	NE-CZ-NH2	10.10	128.29	119.20
2	C	161	ARG	NE-CZ-NH2	10.10	128.29	119.20
1	G	212	GLU	CB-CG-CD	10.09	129.75	112.60
1	B	488	ARG	NE-CZ-NH1	-10.09	111.41	121.50
1	H	300	ARG	NE-CZ-NH2	10.03	128.23	119.20
2	I	215	ARG	NH1-CZ-NH2	-10.03	106.26	119.30
1	H	451	ARG	NH1-CZ-NH2	-10.02	106.27	119.30
2	J	256	GLN	CB-CG-CD	10.00	129.60	112.60
2	I	161	ARG	NH1-CZ-NH2	-9.99	106.31	119.30
2	J	217	ARG	NH1-CZ-NH2	-9.96	106.35	119.30
1	B	22	ARG	NE-CZ-NH1	9.96	131.46	121.50
2	D	226	ARG	NE-CZ-NH2	9.96	128.16	119.20
2	K	321	ARG	NH1-CZ-NH2	-9.94	106.38	119.30
2	I	215	ARG	NE-CZ-NH2	9.94	128.15	119.20
2	C	52	LYS	CG-CD-CE	9.91	134.09	111.30
2	K	451	ARG	NE-CZ-NH1	-9.89	111.61	121.50
1	B	326	ARG	NE-CZ-NH2	9.88	128.09	119.20
2	I	300	ARG	CD-NE-CZ	9.84	138.18	124.40
2	F	451	ARG	NE-CZ-NH2	9.81	128.03	119.20
1	H	468	ARG	CD-NE-CZ	9.81	138.13	124.40
1	B	451	ARG	NH1-CZ-NH2	-9.78	106.59	119.30
2	C	215	ARG	NH1-CZ-NH2	-9.69	106.70	119.30
2	C	374	ARG	NE-CZ-NH1	-9.69	111.81	121.50
2	L	451	ARG	CD-NE-CZ	9.67	137.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	451	ARG	NE-CZ-NH2	9.64	127.87	119.20
2	K	321	ARG	NE-CZ-NH2	9.62	127.86	119.20
2	I	217	ARG	NE-CZ-NH2	9.61	127.85	119.20
2	D	226	ARG	NE-CZ-NH1	-9.61	111.89	121.50
2	C	488	ARG	CD-NE-CZ	9.59	137.82	124.40
1	H	488	ARG	NE-CZ-NH2	-9.59	110.57	119.20
1	H	300	ARG	NE-CZ-NH1	-9.57	111.93	121.50
2	D	385	ARG	NE-CZ-NH2	9.57	127.81	119.20
2	I	488	ARG	CD-NE-CZ	9.57	137.79	124.40
2	J	393	ARG	NE-CZ-NH2	9.56	127.80	119.20
2	I	300	ARG	NE-CZ-NH1	-9.55	111.95	121.50
1	B	488	ARG	CD-NE-CZ	9.52	137.72	124.40
2	K	451	ARG	CD-NE-CZ	9.49	137.69	124.40
1	H	166	ARG	CG-CD-NE	9.48	132.86	112.00
2	D	226	ARG	CD-NE-CZ	9.45	137.63	124.40
1	B	468	ARG	CD-NE-CZ	9.44	137.61	124.40
2	F	451	ARG	NE-CZ-NH1	-9.39	112.11	121.50
1	H	262	ARG	CD-NE-CZ	9.38	137.53	124.40
2	J	385	ARG	CD-NE-CZ	9.34	137.48	124.40
2	C	374	ARG	CD-NE-CZ	9.33	137.46	124.40
2	K	294	LYS	CG-CD-CE	9.33	132.76	111.30
1	B	300	ARG	CD-NE-CZ	9.30	137.42	124.40
1	H	218	ARG	NE-CZ-NH2	9.27	127.54	119.20
1	H	300	ARG	CD-NE-CZ	9.20	137.28	124.40
1	B	468	ARG	NE-CZ-NH1	-9.20	112.30	121.50
2	F	138	ARG	NE-CZ-NH2	9.17	127.45	119.20
2	J	451	ARG	CB-CG-CD	9.13	132.30	111.30
2	E	451	ARG	CG-CD-NE	-9.09	92.01	112.00
2	J	226	ARG	CD-NE-CZ	9.09	137.12	124.40
2	I	374	ARG	CD-NE-CZ	9.06	137.09	124.40
2	C	217	ARG	NH1-CZ-NH2	-9.04	107.54	119.30
1	H	326	ARG	CD-NE-CZ	9.04	137.05	124.40
1	A	324	LEU	CD1-CG-CD2	-9.02	90.97	110.80
2	L	374	ARG	NE-CZ-NH2	9.01	127.30	119.20
2	E	321	ARG	NE-CZ-NH2	8.95	127.25	119.20
2	J	217	ARG	NE-CZ-NH2	8.93	127.24	119.20
2	I	217	ARG	NH1-CZ-NH2	-8.87	107.77	119.30
1	B	326	ARG	CD-NE-CZ	8.87	136.81	124.40
2	F	451	ARG	CD-NE-CZ	8.85	136.78	124.40
2	D	451	ARG	CB-CG-CD	8.84	131.63	111.30
2	E	294	LYS	CG-CD-CE	8.84	131.62	111.30
2	L	171	LEU	CD1-CG-CD2	-8.81	91.41	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	171	LEU	CD1-CG-CD2	-8.76	91.53	110.80
2	D	385	ARG	NE-CZ-NH1	-8.75	112.75	121.50
2	C	215	ARG	NE-CZ-NH2	8.71	127.04	119.20
2	J	393	ARG	CD-NE-CZ	8.63	136.48	124.40
2	D	385	ARG	CD-NE-CZ	8.54	136.35	124.40
2	J	393	ARG	NE-CZ-NH1	-8.53	112.97	121.50
2	L	374	ARG	NE-CZ-NH1	-8.53	112.97	121.50
1	B	218	ARG	NH1-CZ-NH2	-8.52	108.22	119.30
2	E	451	ARG	NE-CZ-NH2	-8.43	111.61	119.20
1	H	468	ARG	NE-CZ-NH2	-8.42	111.62	119.20
2	C	300	ARG	NE-CZ-NH2	-8.41	111.63	119.20
2	D	393	ARG	CD-NE-CZ	8.37	136.12	124.40
1	A	212	GLU	CB-CG-CD	8.32	126.74	112.60
2	D	217	ARG	NE-CZ-NH2	8.28	126.65	119.20
1	B	212	GLU	CB-CG-CD	8.27	126.65	112.60
2	J	226	ARG	NE-CZ-NH2	-8.23	111.80	119.20
1	H	262	ARG	NE-CZ-NH2	-8.22	111.80	119.20
1	B	300	ARG	NE-CZ-NH2	-8.21	111.82	119.20
2	C	300	ARG	CG-CD-NE	-8.21	93.95	112.00
1	G	374	ARG	NH1-CZ-NH2	-8.20	108.64	119.30
2	C	488	ARG	NE-CZ-NH2	-8.19	111.83	119.20
1	B	451	ARG	NE-CZ-NH2	8.19	126.57	119.20
1	H	218	ARG	NH1-CZ-NH2	-8.18	108.66	119.30
1	A	374	ARG	NH1-CZ-NH2	-8.13	108.74	119.30
2	L	138	ARG	CD-NE-CZ	8.09	135.72	124.40
1	B	22	ARG	NH1-CZ-NH2	-8.08	108.79	119.30
2	L	451	ARG	NE-CZ-NH2	-8.04	111.97	119.20
1	G	324	LEU	CD1-CG-CD2	-8.01	93.18	110.80
1	H	22	ARG	NE-CZ-NH1	7.98	129.48	121.50
1	A	374	ARG	NE-CZ-NH2	7.94	126.34	119.20
1	B	326	ARG	NE-CZ-NH1	-7.91	113.59	121.50
1	A	409	THR	CA-CB-CG2	7.90	123.93	110.50
2	E	374	ARG	NH1-CZ-NH2	-7.88	109.05	119.30
2	F	138	ARG	CD-NE-CZ	7.87	135.42	124.40
2	F	138	ARG	NE-CZ-NH1	-7.82	113.68	121.50
2	L	374	ARG	CD-NE-CZ	7.79	135.31	124.40
1	B	374	ARG	NE-CZ-NH2	7.79	126.21	119.20
2	I	374	ARG	NE-CZ-NH2	-7.70	112.27	119.20
1	B	374	ARG	NE-CZ-NH1	-7.68	113.82	121.50
2	J	385	ARG	NE-CZ-NH2	-7.61	112.35	119.20
1	H	40	ARG	CB-CG-CD	7.58	128.74	111.30
2	F	129	ARG	NE-CZ-NH2	7.58	126.02	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	326	ARG	NE-CZ-NH2	-7.53	112.42	119.20
1	B	326	ARG	CG-CD-NE	7.53	128.56	112.00
1	H	488	ARG	NE-CZ-NH1	7.46	128.96	121.50
1	H	217	ARG	NH1-CZ-NH2	-7.42	109.66	119.30
1	B	217	ARG	NE-CZ-NH2	7.37	125.83	119.20
1	B	217	ARG	NH1-CZ-NH2	-7.32	109.79	119.30
1	B	40	ARG	CB-CG-CD	7.28	128.05	111.30
1	H	22	ARG	NH1-CZ-NH2	-7.28	109.84	119.30
1	H	262	ARG	CG-CD-NE	-7.17	96.22	112.00
2	F	129	ARG	NE-CZ-NH1	-7.11	114.39	121.50
2	F	385	ARG	NE-CZ-NH2	7.09	125.58	119.20
2	C	217	ARG	NE-CZ-NH2	7.08	125.57	119.20
2	L	138	ARG	NE-CZ-NH2	-7.05	112.85	119.20
2	K	374	ARG	NH1-CZ-NH2	-7.01	110.18	119.30
2	C	488	ARG	NE-CZ-NH1	7.01	128.51	121.50
1	G	409	THR	CA-CB-CG2	6.99	122.39	110.50
2	D	393	ARG	NE-CZ-NH2	-6.96	112.93	119.20
2	E	451	ARG	NE-CZ-NH1	6.94	128.44	121.50
2	F	374	ARG	CD-NE-CZ	6.93	134.10	124.40
1	H	212	GLU	CB-CG-CD	6.92	124.36	112.60
2	C	92	TRP	CD2-CE2-CZ2	6.91	129.31	122.40
1	H	418	GLN	CB-CA-C	6.87	121.46	110.19
2	I	374	ARG	NE-CZ-NH1	6.87	128.37	121.50
1	B	300	ARG	NE-CZ-NH1	6.86	128.36	121.50
2	F	385	ARG	NE-CZ-NH1	-6.81	114.69	121.50
2	J	226	ARG	NE-CZ-NH1	6.80	128.30	121.50
1	H	468	ARG	NE-CZ-NH1	6.74	128.24	121.50
2	C	300	ARG	NE-CZ-NH1	6.68	128.18	121.50
1	H	326	ARG	NE-CZ-NH1	6.68	128.18	121.50
1	B	166	ARG	NH1-CZ-NH2	-6.51	110.83	119.30
2	J	385	ARG	NE-CZ-NH1	6.47	127.97	121.50
1	B	262	ARG	CG-CD-NE	6.46	126.22	112.00
2	F	374	ARG	NE-CZ-NH2	-6.45	113.40	119.20
1	G	374	ARG	NE-CZ-NH1	6.38	127.88	121.50
2	L	451	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	H	262	ARG	NE-CZ-NH1	6.33	127.83	121.50
1	B	40	ARG	CG-CD-NE	6.28	125.81	112.00
2	J	212	GLU	CB-CG-CD	6.24	123.20	112.60
1	H	217	ARG	NE-CZ-NH1	6.23	127.73	121.50
1	B	374	ARG	CD-NE-CZ	6.22	133.12	124.40
2	D	212	GLU	CB-CG-CD	6.22	123.17	112.60
2	F	129	ARG	CG-CD-NE	6.17	125.56	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	385	ARG	CG-CD-NE	6.01	125.23	112.00
2	L	129	ARG	NE-CZ-NH2	-5.91	113.88	119.20
1	H	166	ARG	NH1-CZ-NH2	-5.88	111.66	119.30
1	B	218	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	G	409	THR	OG1-CB-CG2	-5.84	97.62	109.30
1	H	488	ARG	CG-CD-NE	-5.82	99.21	112.00
2	D	217	ARG	NE-CZ-NH1	5.78	127.28	121.50
2	L	451	ARG	CG-CD-NE	-5.77	99.31	112.00
1	H	326	ARG	CG-CD-NE	-5.73	99.39	112.00
2	I	92	TRP	CD2-CE2-CZ2	5.69	128.09	122.40
1	H	374	ARG	NE-CZ-NH2	-5.68	114.08	119.20
2	K	334	ASP	CB-CA-C	-5.67	101.89	111.02
1	G	484	ARG	CB-CA-C	-5.67	99.78	110.67
1	B	420	MET	CB-CG-SD	5.65	129.66	112.70
2	D	393	ARG	NE-CZ-NH1	5.65	127.15	121.50
1	B	218	ARG	NE-CZ-NH1	5.64	127.14	121.50
2	Q	277	GLY	CA-C-O	-5.60	118.10	122.52
1	G	277	GLY	CA-C-O	-5.59	118.29	122.37
2	L	385	ARG	NE-CZ-NH2	-5.56	114.19	119.20
1	H	374	ARG	CD-NE-CZ	5.55	132.18	124.40
2	J	33	HIS	CB-CG-ND1	5.54	131.02	122.70
1	A	352	GLU	CB-CG-CD	5.54	122.02	112.60
2	F	385	ARG	CG-CD-NE	5.52	124.15	112.00
2	K	112	PRO	CB-CA-C	-5.52	102.45	111.56
1	G	352	GLU	CB-CG-CD	5.47	121.90	112.60
2	D	33	HIS	CB-CG-ND1	5.45	130.87	122.70
2	L	138	ARG	NE-CZ-NH1	5.44	126.94	121.50
2	J	215	ARG	NE-CZ-NH2	5.43	124.08	119.20
2	E	33	HIS	CB-CG-ND1	5.40	130.80	122.70
1	A	484	ARG	CG-CD-NE	-5.38	100.16	112.00
2	E	112	PRO	CB-CA-C	-5.38	102.69	111.56
2	J	375	ILE	CB-CG1-CD1	-5.37	102.52	113.80
2	J	385	ARG	CG-CD-NE	5.35	123.76	112.00
1	B	418	GLN	N-CA-CB	-5.34	101.72	110.42
1	B	451	ARG	NE-CZ-NH1	5.33	126.83	121.50
2	C	217	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	A	318	GLU	CB-CG-CD	5.32	121.64	112.60
1	G	332	GLY	CA-C-N	5.32	128.26	120.71
1	G	332	GLY	C-N-CA	5.32	128.26	120.71
2	L	129	ARG	CD-NE-CZ	5.30	131.82	124.40
1	W	277	GLY	CA-C-O	-5.29	118.34	122.52
2	K	374	ARG	CB-CG-CD	-5.28	99.15	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	318	GLU	CB-CG-CD	5.24	121.50	112.60
1	A	409	THR	OG1-CB-CG2	-5.23	98.84	109.30
2	C	277	GLY	CA-C-O	-5.22	118.40	122.52
2	O	233	GLY	CA-C-O	-5.22	118.63	122.23
2	F	16	GLN	CA-C-N	5.22	131.50	121.54
2	F	16	GLN	C-N-CA	5.22	131.50	121.54
2	I	277	GLY	CA-C-O	-5.20	118.41	122.52
2	U	467	ILE	CA-C-O	-5.20	118.10	122.63
1	H	40	ARG	CG-CD-NE	5.18	123.40	112.00
1	S	44	VAL	CA-C-O	-5.17	118.13	122.63
2	C	300	ARG	CB-CG-CD	5.16	123.17	111.30
1	S	277	GLY	CA-C-O	-5.15	118.74	122.45
1	H	218	ARG	CG-CD-NE	5.13	123.29	112.00
2	E	321	ARG	NE-CZ-NH1	5.11	126.61	121.50
2	J	33	HIS	CG-CD2-NE2	5.09	112.30	107.20
1	A	332	GLY	CA-C-N	5.08	128.31	121.05
1	A	332	GLY	C-N-CA	5.08	128.31	121.05
2	E	218	ARG	CD-NE-CZ	5.07	131.50	124.40
1	A	488	ARG	CG-CD-NE	5.05	123.11	112.00
1	A	484	ARG	N-CA-CB	5.03	118.74	110.39
1	A	338	MET	CB-CG-SD	5.02	127.77	112.70
2	J	215	ARG	CG-CD-NE	-5.02	100.95	112.00

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	125	0
1	B	3432	0	3166	106	0
1	G	3448	0	3229	124	0
1	H	3476	0	3247	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3123	0	2557	37	0
1	N	3010	0	2393	33	0
1	P	3096	0	2554	40	0
1	R	3201	0	2747	36	0
1	S	2706	0	1911	33	0
1	T	2427	0	1562	33	0
1	V	2914	0	2335	49	0
1	W	3126	0	2564	55	0
1	X	3074	0	2533	44	0
2	C	3436	0	3139	96	0
2	D	3456	0	3185	126	0
2	E	3424	0	3156	93	0
2	F	3436	0	3161	87	0
2	I	3477	0	3211	105	0
2	J	3442	0	3178	123	0
2	K	3444	0	3198	97	0
2	L	3471	0	3211	117	0
2	O	3072	0	2499	24	0
2	Q	3303	0	2875	55	0
2	U	2635	0	1858	43	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	1	0
3	E	62	0	24	5	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	5	0
3	J	62	0	24	3	0
3	K	62	0	24	2	0
3	L	62	0	24	5	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	1	0
3	U	31	0	12	1	0
3	V	62	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	67348	1582	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 11.

All (1582) 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
1:H:231:MET:HE1	1:H:251:ALA:CB	1.80	1.11
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:H:231:MET:HE1	1:H:251:ALA:HB2	1.33	1.07
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
2:C:121:PHE:O	2:C:125:ALA:HB3	1.59	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:B:231:MET:HE1	1:B:251:ALA:CB	1.91	0.98
1:G:490:ILE:HG21	2:L:420:MET:HE2	1.45	0.98
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:231:MET:HE1	1:B:251:ALA:HB2	0.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:L:300:ARG:HA	2:L:333:MET:HE1	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:I:91:GLY:C	2:I:92:TRP:HD1	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:300:ARG:HA	2:F:333:MET:HE1	1.58	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
1:G:300:ARG:HG3	1:G:333:MET:HE1	1.60	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: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: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
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:K:250:GLY:C	2:K:252:MET:H	1.90	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:J:22:ARG:HH12	2:J:24:MET:HE3	1.47	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
1:A:300:ARG:HG3	1:A:333:MET:HE1	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:305:ALA:HB2	2:L:374:ARG:HD3	1.64	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
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: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
2:D:234:GLU:C	2:D:235:TYR:HD2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:44:VAL:HG21	1:G:55:PHE:CE2	2.22	0.74
2:L:66:GLU:C	2:L:67:PHE:HD1	1.95	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
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
2:C:303:GLU:HA	2:C:338:MET:HE2	1.69	0.73
2:J:419:PHE:HD1	2:J:419:PHE:C	1.96	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:J:300:ARG:HA	2:J:333:MET:HE1	1.72	0.72
2:L:75:THR:C	2:L:76:PHE:HD1	1.98	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:D:57:ILE:HD11	2:D:83:ILE:HG23	1.71	0.71
2:D:300:ARG:HA	2:D:333:MET:HE1	1.72	0.71
1:B:348:CYS:HB3	2:C:254:LEU:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:224:LYS:NZ	3:D:702:ATP:O3G	2.19	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:Q:378:ASP:HA	2:Q:413:THR:HG1	1.54	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:G:303:GLU:HA	1:G:338:MET:HE1	1.72	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:I:305:ALA:HB2	2:I:374:ARG:HD3	1.73	0.69
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:A:303:GLU:HA	1:A:338:MET:HE1	1.74	0.69
3:C:702:ATP:O2G	2:D:224:LYS:NZ	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ARG:HE	1:B:215:ARG:HA	1.58	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
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
2:E:250:GLY:C	2:E:252:MET:H	2.02	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
2:L:21:MET:HE3	2:L:177:THR:HG21	1.75	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:W:385:ARG:HH12	1:W:417:ASP:CG	2.02	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
1:H:231:MET:CE	1:H:251:ALA:CB	2.62	0.67
2:I:285:LEU:HB2	2:I:434:THR:HG21	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
2:L:66:GLU:C	2:L:67:PHE:CD1	2.73	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:L:462:TRP:CG	2:L:463:HIS:H	2.13	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
2:D:234:GLU:C	2:D:235:TYR:CD2	2.73	0.66
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:419:PHE:C	2:J:419:PHE:CD1	2.72	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
1:V:42:THR:O	1:V:180:MET:CB	2.44	0.65
2:L:21:MET:HE3	2:L:177:THR:CG2	2.26	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: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
2:C:121:PHE:C	2:C:122:ASP:O	2.39	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:U:51:GLY:C	5:U:702:ADP:O1A	2.40	0.64
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.80	0.64
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:L:74:VAL:HG12	2:L:76:PHE:HE1	1.62	0.63
2:J:21:MET:HE1	2:J:177:THR:OG1	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:395:PHE:C	2:I:395:PHE:CD2	2.75	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
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
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:I:21:MET:HE1	2:I:177:THR:HB	1.81	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:J:21:MET:HE3	2:J:177:THR:HG21	1.81	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
2:O:287:THR:HG23	2:O:414:ASN:HD22	1.64	0.62
1:P:291:GLY:O	1:P:451:ARG:NH1	2.32	0.62
1:G:52:LYS:NZ	3:G:702:ATP:O2G	2.27	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
2:D:75:THR:OG1	2:D:78:GLU:O	2.14	0.62
1:G:289:ALA:HB2	1:G:419:PHE:HA	1.81	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
2:C:21:MET:HE1	2:C:177:THR:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:420:MET:HE1	2:F:490:ILE:HG13	1.82	0.61
3:K:701:ATP:O3G	2:L:457:LYS:NZ	2.33	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
2:K:155:ASP:O	2:K:156:ALA:O	2.17	0.61
1:B:23:THR:HG1	1:B:25:ILE:HG13	1.64	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
1:N:294:LYS:NZ	3:N:701:ATP:O2B	2.29	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
2:Q:420:MET:HE3	2:Q:492:GLY:HA3	1.80	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:J:462:TRP:CG	2:J:463:HIS:H	2.18	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
1:A:490:ILE:HD11	2:F:449:MET:HE3	1.81	0.60
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
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:X:490:ILE:CB	1:W:420:MET:HE1	2.32	0.60
1:A:417:ASP:OD2	1:B:429:HIS:ND1	2.35	0.60
1:A:435:ASP:CG	2:F:323:GLN:HE22	2.09	0.60
1:H:385:ARG:HD3	2:I:393:ARG:HH21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:435:ASP:CG	2:L:323:GLN:HE22	2.09	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
1:S:420:MET:HE3	1:S:492:GLY:HA3	1.83	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
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:K:467:ILE:HD11	2:J:449:MET:HE2	1.83	0.59
1:V:419:PHE:HE2	1:W:424:SER:C	2.10	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
2:J:75:THR:OG1	2:J:78:GLU:O	2.17	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:490:ILE:HD11	2:D:449:MET:CE	2.33	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:467:ILE:HD11	2:D:449:MET:HE2	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:231:MET:HE2	1:H:251:ALA:HB2	1.85	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: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
1:B:449:MET:HE2	2:C:467:ILE:HD11	1.87	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:A:55:PHE:CD1	1:A:55:PHE:C	2.83	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
2:J:115:GLN:O	2:J:116:GLU:C	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PHE:C	1:A:55:PHE:HD1	2.14	0.55
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
2:K:334:ASP:O	2:K:335:PHE:C	2.50	0.55
1:T:335:PHE:O	1:T:339:GLU:CB	2.55	0.55
1:X:24:MET:HE2	1:X:24:MET:HA	1.87	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
1:G:490:ILE:HD11	2:L:449:MET:HE3	1.88	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:H:449:MET:HE2	2:I:467:ILE:HD11	1.88	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
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:I:395:PHE:C	2:I:395:PHE:HD2	2.14	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:D:110:PRO:O	2:D:111:ASP:C	2.50	0.55
2:L:21:MET:CE	2:L:177:THR:CG2	2.84	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: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:L:300:ARG:CA	2:L:333:MET:HE1	2.34	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: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: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:K:155:ASP:C	2:K:156:ALA:O	2.50	0.54
1:P:21:MET:HE1	1:P:177:THR:HB	1.89	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:H:231:MET:HE1	1:H:251:ALA:HB3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:MET:HE1	2:D:177:THR:OG1	2.08	0.54
2:L:315:PHE:CE2	2:L:363:ILE:HG12	2.43	0.54
1:T:392:PHE:O	1:T:396:VAL:HG23	2.08	0.54
2:F:300:ARG:CA	2:F:333:MET:HE1	2.34	0.53
2:D:31:ILE:HD11	2:D:246:ILE:HG21	1.90	0.53
2:K:420:MET:HE1	2:L:490:ILE:HG13	1.89	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
1:R:436:THR:OG1	1:R:458:MET:HE3	2.08	0.53
2:E:250:GLY:C	2:E:252:MET:N	2.65	0.53
2:E:356:LEU:CD2	2:E:387:VAL:HG11	2.38	0.53
2:C:300:ARG:HA	2:C:333:MET:HE1	1.91	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:22:ARG:NH1	1:B:24:MET:HE1	2.23	0.53
2:D:462:TRP:O	2:D:463:HIS:CD2	2.62	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:E:323:GLN:HE22	2:F:435:ASP:CG	2.17	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
2:J:110:PRO:O	2:J:111:ASP:C	2.52	0.53
1:T:292:THR:HA	1:T:451:ARG:HD3	1.91	0.53
1:V:24:MET:HE3	1:V:24:MET:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:441:GLN:HE22	2:C:490:ILE:HD13	1.74	0.52
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:E:300:ARG:HA	2:E:333:MET:HE1	1.92	0.52
2:K:291:GLY:O	2:K:451:ARG:NH1	2.42	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:F:66:GLU:C	2:F:67:PHE:CD1	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:461:SER:C	2:J:462:TRP:O	2.52	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
2:K:254:LEU:HD11	2:J:350:TYR:CE2	2.45	0.52
1:W:306:CYS:SG	1:W:338:MET:HE3	2.49	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:N:300:ARG:HA	1:N:333:MET:HE1	1.91	0.51
1:R:300:ARG:HA	1:R:333:MET:HE1	1.92	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
2:D:218:ARG:CZ	2:D:239:ILE:HD12	2.41	0.51
2:D:332:GLY:C	2:D:333:MET:HG2	2.35	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:K:300:ARG:HA	2:K:333:MET:HE1	1.93	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: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
2:E:334:ASP:O	2:E:335:PHE:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:I:702:ATP:O3G	2:J:224:LYS:NZ	2.40	0.51
1:P:300:ARG:HD3	1:P:333:MET:HE1	1.93	0.51
2:F:462:TRP:CG	2:F:463:HIS:H	2.29	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
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
1:M:300:ARG:CA	1:M:333:MET:HE1	2.41	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
1:R:142:VAL:O	1:R:178:THR:HA	2.11	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
2:J:332:GLY:C	2:J:333:MET:HG2	2.36	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: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
2:J:290:THR:OG1	3:J:701:ATP:O1G	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:142:VAL:O	1:N:178:THR:HA	2.12	0.50
1:R:419:PHE:HE2	1:M:424:SER:C	2.19	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
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:L:106:LEU:C	2:L:106:LEU:HD12	2.37	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
2:E:490:ILE:HG21	2:D:420:MET:HE2	1.94	0.49
2:F:106:LEU:HD12	2:F:106:LEU:C	2.37	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
3:H:702:ATP:O1G	2:I:224:LYS:NZ	2.45	0.49
2:K:313:ILE:CG2	2:K:315:PHE:CE1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:375:ILE:HG12	2:J:408:ILE:CG2	2.42	0.49
2:U:217:ARG:HG2	2:U:357:GLU:CD	2.35	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
2:I:303:GLU:HB2	2:I:333:MET:HE3	1.94	0.49
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
2:J:300:ARG:CA	2:J:333:MET:HE1	2.42	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
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
2:L:21:MET:HE1	2:L:177:THR:HG22	1.93	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: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:D:300:ARG:CA	2:D:333:MET:HE1	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:303:GLU:OE1	1:H:333:MET:HE3	2.13	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:442:TYR:CD2	2:F:456:PHE:CZ	3.02	0.48
1:N:449:MET:CE	2:O:467:ILE:HD11	2.43	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
2:D:462:TRP:CG	2:D:463:HIS:H	2.30	0.48
2:L:347:VAL:O	2:L:348:CYS:C	2.55	0.48
2:I:395:PHE:CE2	2:I:399:VAL:CG2	2.92	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:F:273:MET:HE1	2:F:453:ILE:HG23	1.96	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
2:I:300:ARG:HA	2:I:333:MET:HE1	1.96	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:145:ASP:OD2	2:L:145:ASP:C	2.56	0.48
2:L:441:GLN:HE22	2:L:490:ILE:HA	1.79	0.48
1:N:449:MET:HE3	2:O:467:ILE:HD11	1.96	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
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
1:B:303:GLU:OE1	1:B:333:MET:HE3	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:225:LEU:HD12	2:J:230:HIS:HB3	1.95	0.48
2:Q:289:ALA:O	2:Q:292:THR:OG1	2.31	0.48
1:S:393:ARG:NH1	1:S:429:HIS:O	2.46	0.48
1:W:274:CYS:HB3	1:W:458:MET:HE3	1.95	0.48
1:A:26:GLU:OE1	1:A:245:ASN:CG	2.56	0.47
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
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
2:J:462:TRP:CG	2:J:463:HIS:N	2.81	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: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
3:H:701:ATP:O3G	2:I:457:LYS:NZ	2.41	0.47
2:I:432:TPO:HG21	2:I:432:TPO:O1P	2.14	0.47
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
2:C:145:ASP:C	2:C:145:ASP:OD1	2.56	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:I:106:LEU:HD12	2:I:106:LEU:C	2.40	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:K:490:ILE:HG21	2:J:420:MET:HE2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:74:VAL:HG12	2:L:76:PHE:CE1	2.47	0.47
1:T:287:THR:HG22	1:T:414:ASN:HD22	1.80	0.47
1:X:23:THR:OG1	1:X:29:ASP:OD1	2.33	0.47
1:W:301:PHE:CZ	1:W:374:ARG:HD2	2.50	0.47
2:C:106:LEU:C	2:C:106:LEU:HD12	2.40	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:K:490:ILE:HD11	2:J:449:MET:HE3	1.97	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
2:Q:203:ASN:CG	2:Q:225:LEU:HD23	2.39	0.47
1:X:436:THR:HG23	1:X:458:MET:HE3	1.95	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:K:449:MET:HE3	2:L:467:ILE:HD11	1.97	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:Q:184:ARG:C	2:Q:185:ILE:HD13	2.40	0.47
2:U:89:SER:CB	5:U:702:ADP:HN62	2.25	0.47
1:S:389:ASN:C	1:S:393:ARG:HG2	2.39	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:F:347:VAL:O	2:F:348:CYS:C	2.58	0.47
2:C:202:ASP:OD1	2:C:226:ARG:NH1	2.48	0.47
1:H:313:ILE:HG22	1:H:315:PHE:CE1	2.50	0.47
2:K:334:ASP:O	2:K:334:ASP:CG	2.57	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
1:G:230:HIS:NE2	3:L:702:ATP:O2'	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:P:300:ARG:CD	1:P:333:MET:HE1	2.44	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:F:145:ASP:OD2	2:F:145:ASP:C	2.59	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
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:E:490:ILE:HD11	2:D:449:MET:HE3	1.98	0.46
2:F:23:THR:O	2:F:24:MET:HB2	2.13	0.46
2:F:461:SER:C	2:F:462:TRP:O	2.56	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:G:17:ALA:C	1:G:18:ILE:HD12	2.41	0.46
1:G:227:GLY:O	2:L:89:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:289:ALA:CB	1:M:419:PHE:HA	2.45	0.46
1:P:471:MET:HE2	1:P:471:MET:HB2	1.86	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
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
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
2:Q:420:MET:HE2	2:Q:420:MET:HB3	1.83	0.45
1:T:426:THR:N	1:T:431:SEP:O3P	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:L:55:PHE:C	2:L:55:PHE:CD2	2.95	0.45
2:I:91:GLY:C	2:I:92:TRP:CD1	2.75	0.45
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
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
1:G:283:ILE:HG13	1:G:400:THR:HG23	1.98	0.45
1:G:456:PHE:C	1:G:456:PHE:CD2	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:285:LEU:HG	2:L:287:THR:HG23	1.99	0.45
2:J:303:GLU:HB2	2:J:333:MET:HE3	1.98	0.45
1:W:231:MET:HE1	1:W:251:ALA:HB2	1.97	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
1:M:31:ILE:CD1	1:M:246:ILE:HG21	2.46	0.45
1:P:357:GLU:CD	1:P:357:GLU:H	2.24	0.45
1:P:472:ILE:HG21	3:P:701:ATP:H1'	1.99	0.45
1:A:420:MET:HE1	1:B:490:ILE:CG1	2.47	0.45
1:B:347:VAL:O	1:B:348:CYS:C	2.59	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:318:GLU:CD	2:D:432:TPO:HG21	2.43	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:A:245:ASN:C	1:A:245:ASN:HD22	2.25	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: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:28:PHE:CD1	1:A:28:PHE:C	2.95	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:55:PHE:C	2:E:55:PHE:HD1	2.26	0.44
2:E:453:ILE:HG21	2:E:479:ILE:HG12	1.98	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
1:H:300:ARG:HA	1:H:333:MET:HE1	1.98	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
2:Q:471:MET:HE3	2:Q:471:MET:HB3	1.88	0.44
1:X:273:MET:O	1:X:463:HIS:HA	2.17	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:253:ARG:C	1:B:255:THR:H	2.24	0.44
1:G:490:ILE:HG21	2:L:420:MET:CE	2.30	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
1:B:231:MET:CE	1:B:250:GLY:O	2.66	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:C:318:GLU:OE2	2:C:379:SER:OG	2.29	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
2:L:461:SER:C	2:L:462:TRP:O	2.59	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
1:V:316:ALA:O	1:V:348:CYS:HA	2.18	0.44
2:E:55:PHE:C	2:E:55:PHE:CD1	2.96	0.44
2:F:111:ASP:O	2:F:113:GLU:N	2.50	0.44
2:C:318:GLU:CD	2:D:432:TPO:CG2	2.91	0.44
2:C:389:ASN:HD21	2:C:428:SER:HA	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:TYR:CE1	2:C:208:ARG:CD	3.01	0.44
2:D:74:VAL:HG12	2:D:76:PHE:CE2	2.53	0.44
2:L:86:ASN:O	2:L:89:SER:HB3	2.18	0.44
2:I:303:GLU:CB	2:I:333:MET:HE3	2.47	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:D:356:LEU:CD2	2:D:387:VAL:HG11	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:I:145:ASP:HA	2:I:181:THR:HB	2.00	0.43
2:I:300:ARG:HA	2:I:300:ARG:HD3	1.78	0.43
1:M:300:ARG:HA	1:M:333:MET:HE1	1.99	0.43
2:Q:311:ARG:HB2	2:Q:372:PRO:HA	2.00	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
1:H:420:MET:HE1	2:I:490:ILE:HG13	1.99	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:30:ASP:O	1:W:231:MET:HE3	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
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
3:C:702:ATP:HO2'	2:D:230:HIS:HE2	1.65	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:445:ILE:CD1	2:I:486:PHE:CE2	2.99	0.43
1:X:194:TYR:O	1:X:195:GLY:C	2.61	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
3:B:701:ATP:O2'	2:C:463:HIS:NE2	2.46	0.43
2:E:332:GLY:C	2:E:333:MET:HG2	2.42	0.43
2:E:397:ILE:CG2	2:D:350:TYR:CE1	3.01	0.43
1:G:456:PHE:HD2	1:G:456:PHE:C	2.26	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:V:300:ARG:HD2	1:V:333:MET:HE1	2.01	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:K:332:GLY:C	2:K:333:MET:HG2	2.43	0.43
2:L:384:ALA:HB2	2:L:392:PHE:CZ	2.53	0.43
2:I:90:PHE:C	2:I:92:TRP:CD1	2.96	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
2:I:318:GLU:CD	2:J:432:TPO:CG2	2.92	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
2:U:213:GLY:C	2:U:215:ARG:H	2.27	0.43
1:V:333:MET:O	1:V:333:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:318:GLU:CD	2:J:432:TPO:HG21	2.44	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
2:D:303:GLU:HB2	2:D:333:MET:HE3	1.99	0.42
1:G:66:GLU:HB3	1:G:67:PHE:CE1	2.54	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:75:THR:C	2:L:76:PHE:CD1	2.88	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:315:PHE:HD1	1:A:363:ILE:HG12	1.76	0.42
1:B:289:ALA:CB	1:B:419:PHE:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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: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:C:21:MET:HE3	2:C:177:THR:HG21	2.01	0.42
2:C:303:GLU:CB	2:C:333:MET:HE3	2.49	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: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
1:B:449:MET:HE1	2:C:490:ILE:HG13	2.02	0.42
2:E:250:GLY:HA2	2:D:353:SER:CB	2.50	0.42
2:F:285:LEU:HG	2:F:287:THR:HG23	2.02	0.42
2:C:121:PHE:O	2:C:122:ASP:C	2.63	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:J:208:ARG:NH2	2:J:221:GLU:OE2	2.53	0.42
1:T:53:THR:OG1	3:T:702:ATP:O2B	2.36	0.42
1:T:411:LEU:C	1:T:411:LEU:HD12	2.44	0.42
1:V:42:THR:HG23	1:V:203:ASN:HB2	2.02	0.42
1:W:385:ARG:NH1	1:W:417:ASP:CG	2.74	0.42
1:W:397:ILE:HD13	1:W:433:ILE:HD13	2.02	0.42
1:B:253:ARG:C	1:B:255:THR:N	2.78	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:I:58:GLN:HG3	2:I:92:TRP:CH2	2.55	0.42
1:N:294:LYS:HB3	1:N:413:THR:HG21	2.02	0.42
1:M:273:MET:O	1:M:464:ASP:N	2.47	0.42
1:X:333:MET:HE2	1:X:333:MET:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:353:SER:HB2	2:F:250:GLY:O	2.19	0.41
2:C:419:PHE:C	2:C:419:PHE:CD2	2.97	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:K:323:GLN:HE22	2:L:435:ASP:CG	2.27	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:O:74:VAL:HB	2:O:144:ILE:HA	2.00	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:E:290:THR:OG1	3:E:701:ATP:O2G	2.26	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:C:495:THR:HG22	2:D:487:GLU:OE2	2.19	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:H:392:PHE:O	1:H:395:PHE:HB3	2.21	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:W:231:MET:HE1	1:W:251:ALA:CB	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:M:294:LYS:NZ	3:M:701:ATP:O1B	2.40	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
1:R:50:THR:HG21	1:R:207:LEU:C	2.46	0.41
2:Q:203:ASN:HB3	2:Q:225:LEU:HD23	2.02	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:392:PHE:O	1:G:395:PHE:HB3	2.21	0.41
1:H:24:MET:HE2	1:H:66:GLU:HG2	2.02	0.41
2:K:456:PHE:CZ	2:J:442:TYR:CE1	3.09	0.41
2:L:76:PHE:CD1	2:L:76:PHE:N	2.88	0.41
2:L:367:ILE:O	2:L:371:LYS:N	2.53	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
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: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: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
1:P:449:MET:HE3	2:Q:467:ILE:HD11	2.03	0.40
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
2:C:121:PHE:C	2:C:125:ALA:HB3	2.38	0.40
1:G:352:GLU:N	1:G:352:GLU:CD	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Q:252:MET:HE2	2:Q:401:GLY:HA3	2.03	0.40
2:Q:252:MET:HE3	2:Q:252:MET:HB3	1.91	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: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:A:352:GLU:N	1:A:352:GLU:CD	2.79	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
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
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	9	35
1	B	462/519 (89%)	431 (93%)	24 (5%)	7 (2%)	8	32
1	G	458/519 (88%)	433 (94%)	23 (5%)	2 (0%)	30	61
1	H	459/519 (88%)	430 (94%)	26 (6%)	3 (1%)	18	49
1	M	456/519 (88%)	410 (90%)	39 (9%)	7 (2%)	8	32
1	N	442/519 (85%)	387 (88%)	43 (10%)	12 (3%)	4	20
1	P	445/519 (86%)	400 (90%)	39 (9%)	6 (1%)	9	35
1	R	454/519 (88%)	414 (91%)	35 (8%)	5 (1%)	11	39
1	S	423/519 (82%)	360 (85%)	55 (13%)	8 (2%)	6	27
1	T	380/519 (73%)	299 (79%)	67 (18%)	14 (4%)	2	15
1	V	412/519 (79%)	359 (87%)	50 (12%)	3 (1%)	18	49
1	W	453/519 (87%)	386 (85%)	57 (13%)	10 (2%)	5	24
1	X	452/519 (87%)	408 (90%)	31 (7%)	13 (3%)	3	19
2	C	464/519 (89%)	428 (92%)	31 (7%)	5 (1%)	11	39
2	D	463/519 (89%)	419 (90%)	34 (7%)	10 (2%)	5	24
2	E	462/519 (89%)	427 (92%)	26 (6%)	9 (2%)	6	27
2	F	458/519 (88%)	432 (94%)	19 (4%)	7 (2%)	8	32
2	I	465/519 (90%)	430 (92%)	33 (7%)	2 (0%)	30	61
2	J	458/519 (88%)	414 (90%)	36 (8%)	8 (2%)	7	30
2	K	463/519 (89%)	427 (92%)	26 (6%)	10 (2%)	5	24
2	L	460/519 (89%)	431 (94%)	23 (5%)	6 (1%)	9	35
2	O	449/519 (86%)	399 (89%)	40 (9%)	10 (2%)	5	24
2	Q	458/519 (88%)	416 (91%)	38 (8%)	4 (1%)	14	44
2	U	404/519 (78%)	340 (84%)	53 (13%)	11 (3%)	4	20
All	All	10761/12456 (86%)	9713 (90%)	870 (8%)	178 (2%)	7	30

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	351/443 (79%)	308 (88%)	43 (12%)	4	20
1	B	328/443 (74%)	289 (88%)	39 (12%)	5	21
1	G	338/443 (76%)	295 (87%)	43 (13%)	4	18
1	H	341/443 (77%)	298 (87%)	43 (13%)	4	19
1	M	247/443 (56%)	217 (88%)	30 (12%)	5	20
1	N	222/443 (50%)	201 (90%)	21 (10%)	8	30
1	P	249/443 (56%)	216 (87%)	33 (13%)	4	17
1	R	270/443 (61%)	250 (93%)	20 (7%)	13	40
1	S	155/443 (35%)	141 (91%)	14 (9%)	9	33
1	T	109/443 (25%)	95 (87%)	14 (13%)	4	18
1	V	221/443 (50%)	186 (84%)	35 (16%)	2	12
1	W	242/443 (55%)	208 (86%)	34 (14%)	3	15
1	X	239/443 (54%)	211 (88%)	28 (12%)	5	22
2	C	323/442 (73%)	287 (89%)	36 (11%)	6	24
2	D	332/442 (75%)	287 (86%)	45 (14%)	3	16
2	E	324/442 (73%)	288 (89%)	36 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	327/442 (74%)	283 (86%)	44 (14%)	4	16
2	I	334/442 (76%)	292 (87%)	42 (13%)	4	19
2	J	330/442 (75%)	287 (87%)	43 (13%)	4	18
2	K	330/442 (75%)	296 (90%)	34 (10%)	7	27
2	L	336/442 (76%)	289 (86%)	47 (14%)	3	15
2	O	237/442 (54%)	207 (87%)	30 (13%)	4	18
2	Q	289/442 (65%)	256 (89%)	33 (11%)	5	23
2	U	151/442 (34%)	132 (87%)	19 (13%)	4	19
All	All	6625/10621 (62%)	5819 (88%)	806 (12%)	5	20

All (806) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	50	THR
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	182	THR
1	A	183	GLU
1	A	186	GLU
1	A	223	LEU
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	263	VAL
1	A	270	LEU
1	A	287	THR
1	A	315	PHE
1	A	318	GLU
1	A	324	LEU
1	A	333	MET

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Mol	Chain	Res	Type
1	A	344	LEU
1	A	352	GLU
1	A	356	LEU
1	A	360	LEU
1	A	409	THR
1	A	416	SER
1	A	417	ASP
1	A	418	GLN
1	A	420	MET
1	A	424	SER
1	A	425	ILE
1	A	428	SER
1	A	453	ILE
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	40	ARG
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	134	ILE
1	B	148	THR
1	B	183	GLU
1	B	198	GLU
1	B	212	GLU
1	B	217	ARG
1	B	218	ARG
1	B	223	LEU
1	B	228	THR
1	B	232	LYS
1	B	238	THR
1	B	245	ASN
1	B	246	ILE
1	B	270	LEU
1	B	333	MET
1	B	344	LEU

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Mol	Chain	Res	Type
1	B	352	GLU
1	B	356	LEU
1	B	360	LEU
1	B	375	ILE
1	B	389	ASN
1	B	400	THR
1	B	428	SER
1	B	430	ILE
1	B	439	LEU
1	B	450	SER
1	B	454	ASN
1	B	458	MET
1	B	468	ARG
1	B	487	GLU
2	E	22	ARG
2	E	24	MET
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	255	THR
2	E	270	LEU
2	E	280	LYS
2	E	281	ASP
2	E	294	LYS
2	E	300	ARG
2	E	308	ASN
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	387	VAL

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Mol	Chain	Res	Type
2	E	413	THR
2	E	419	PHE
2	E	425	ILE
2	E	450	SER
2	E	451	ARG
2	E	458	MET
2	E	474	ASP
2	E	493	SER
2	F	18	ILE
2	F	22	ARG
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	142	VAL
2	F	145	ASP
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	212	GLU
2	F	221	GLU
2	F	223	LEU
2	F	228	THR
2	F	232	LYS
2	F	270	LEU
2	F	281	ASP
2	F	283	ILE
2	F	284	ILE
2	F	303	GLU
2	F	333	MET
2	F	338	MET
2	F	352	GLU
2	F	360	LEU
2	F	366	GLU
2	F	375	ILE
2	F	400	THR

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Mol	Chain	Res	Type
2	F	405	GLN
2	F	406	GLU
2	F	413	THR
2	F	418	GLN
2	F	428	SER
2	F	430	ILE
2	F	448	GLU
2	F	450	SER
2	F	471	MET
2	F	493	SER
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	178	THR
2	C	182	THR
2	C	184	ARG
2	C	198	GLU
2	C	212	GLU
2	C	218	ARG
2	C	228	THR
2	C	245	ASN
2	C	254	LEU
2	C	263	VAL
2	C	270	LEU
2	C	284	ILE
2	C	294	LYS
2	C	300	ARG
2	C	333	MET
2	C	344	LEU
2	C	352	GLU
2	C	356	LEU
2	C	360	LEU
2	C	374	ARG
2	C	413	THR
2	C	416	SER
2	C	418	GLN
2	C	419	PHE
2	C	420	MET
2	C	425	ILE

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Mol	Chain	Res	Type
2	C	428	SER
2	C	430	ILE
2	C	449	MET
2	C	458	MET
2	D	24	MET
2	D	41	SER
2	D	45	SER
2	D	52	LYS
2	D	57	ILE
2	D	85	LYS
2	D	93	ASP
2	D	143	SER
2	D	173	GLN
2	D	177	THR
2	D	182	THR
2	D	198	GLU
2	D	208	ARG
2	D	212	GLU
2	D	215	ARG
2	D	223	LEU
2	D	228	THR
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	325	LEU
2	D	337	GLU
2	D	344	LEU
2	D	352	GLU
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

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Mol	Chain	Res	Type
2	D	428	SER
2	D	453	ILE
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	22	ARG
1	G	24	MET
1	G	50	THR
1	G	57	ILE
1	G	78	GLU
1	G	79	THR
1	G	99	ASP
1	G	145	ASP
1	G	172	LYS
1	G	180	MET
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	263	VAL
1	G	270	LEU
1	G	287	THR
1	G	318	GLU
1	G	333	MET
1	G	344	LEU
1	G	352	GLU
1	G	356	LEU
1	G	360	LEU
1	G	406	GLU
1	G	413	THR
1	G	416	SER
1	G	417	ASP
1	G	418	GLN
1	G	420	MET

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Mol	Chain	Res	Type
1	G	424	SER
1	G	425	ILE
1	G	428	SER
1	G	453	ILE
1	G	458	MET
1	G	488	ARG
1	G	489	ILE
1	G	497	ILE
1	H	23	THR
1	H	24	MET
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	134	ILE
1	H	148	THR
1	H	183	GLU
1	H	198	GLU
1	H	215	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	246	ILE
1	H	254	LEU
1	H	270	LEU
1	H	284	ILE
1	H	318	GLU
1	H	333	MET
1	H	344	LEU
1	H	352	GLU
1	H	356	LEU
1	H	360	LEU
1	H	375	ILE
1	H	377	ILE
1	H	389	ASN
1	H	400	THR
1	H	418	GLN

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Mol	Chain	Res	Type
1	H	428	SER
1	H	433	ILE
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	254	LEU
2	K	255	THR
2	K	270	LEU
2	K	280	LYS
2	K	281	ASP
2	K	294	LYS
2	K	300	ARG
2	K	308	ASN
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	387	VAL
2	K	413	THR
2	K	425	ILE
2	K	450	SER
2	K	451	ARG
2	K	458	MET
2	K	474	ASP

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Mol	Chain	Res	Type
2	K	493	SER
2	L	18	ILE
2	L	22	ARG
2	L	24	MET
2	L	67	PHE
2	L	75	THR
2	L	79	THR
2	L	89	SER
2	L	97	LEU
2	L	106	LEU
2	L	135	GLN
2	L	142	VAL
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	221	GLU
2	L	223	LEU
2	L	228	THR
2	L	232	LYS
2	L	270	LEU
2	L	278	PHE
2	L	281	ASP
2	L	283	ILE
2	L	284	ILE
2	L	303	GLU
2	L	333	MET
2	L	352	GLU
2	L	360	LEU
2	L	366	GLU
2	L	375	ILE
2	L	400	THR
2	L	405	GLN
2	L	406	GLU
2	L	413	THR
2	L	418	GLN
2	L	428	SER

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Mol	Chain	Res	Type
2	L	430	ILE
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	43	LEU
2	I	50	THR
2	I	92	TRP
2	I	106	LEU
2	I	145	ASP
2	I	149	SER
2	I	178	THR
2	I	182	THR
2	I	198	GLU
2	I	217	ARG
2	I	218	ARG
2	I	223	LEU
2	I	228	THR
2	I	245	ASN
2	I	254	LEU
2	I	263	VAL
2	I	270	LEU
2	I	284	ILE
2	I	294	LYS
2	I	300	ARG
2	I	303	GLU
2	I	333	MET
2	I	344	LEU
2	I	347	VAL
2	I	352	GLU
2	I	356	LEU
2	I	360	LEU
2	I	374	ARG
2	I	395	PHE
2	I	406	GLU
2	I	413	THR
2	I	416	SER
2	I	418	GLN
2	I	420	MET

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Mol	Chain	Res	Type
2	I	425	ILE
2	I	428	SER
2	I	430	ILE
2	I	445	ILE
2	I	449	MET
2	I	458	MET
2	J	24	MET
2	J	41	SER
2	J	45	SER
2	J	52	LYS
2	J	57	ILE
2	J	93	ASP
2	J	143	SER
2	J	173	GLN
2	J	174	ILE
2	J	177	THR
2	J	182	THR
2	J	198	GLU
2	J	208	ARG
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	325	LEU
2	J	337	GLU
2	J	352	GLU
2	J	356	LEU
2	J	360	LEU
2	J	368	ASN
2	J	375	ILE
2	J	377	ILE
2	J	385	ARG
2	J	394	GLN
2	J	409	THR
2	J	419	PHE
2	J	425	ILE
2	J	428	SER

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Mol	Chain	Res	Type
2	J	451	ARG
2	J	453	ILE
2	J	458	MET
2	J	461	SER
2	J	474	ASP
2	J	485	ASN
2	J	489	ILE
1	N	24	MET
1	N	50	THR
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	294	LYS
1	N	300	ARG
1	N	344	LEU
1	N	348	CYS
1	N	360	LEU
1	N	423	HIS
1	N	458	MET
1	N	463	HIS
1	N	470	PHE
1	N	471	MET
1	N	495	THR
2	O	50	THR
2	O	173	GLN
2	O	217	ARG
2	O	221	GLU
2	O	224	LYS
2	O	226	ARG
2	O	247	PHE
2	O	284	ILE
2	O	294	LYS
2	O	326	ARG
2	O	333	MET
2	O	339	GLU
2	O	344	LEU
2	O	352	GLU

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Mol	Chain	Res	Type
2	O	356	LEU
2	O	360	LEU
2	O	381	SER
2	O	394	GLN
2	O	397	ILE
2	O	399	VAL
2	O	406	GLU
2	O	418	GLN
2	O	423	HIS
2	O	428	SER
2	O	433	ILE
2	O	434	THR
2	O	440	LEU
2	O	451	ARG
2	O	465	LYS
2	O	467	ILE
1	R	20	LYS
1	R	50	THR
1	R	182	THR
1	R	223	LEU
1	R	226	ARG
1	R	234	GLU
1	R	259	SER
1	R	294	LYS
1	R	333	MET
1	R	352	GLU
1	R	377	ILE
1	R	409	THR
1	R	413	THR
1	R	418	GLN
1	R	427	ASP
1	R	429	HIS
1	R	449	MET
1	R	458	MET
1	R	465	LYS
1	R	470	PHE
1	M	24	MET
1	M	56	SER
1	M	178	THR
1	M	182	THR
1	M	185	ILE
1	M	201	SER

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Mol	Chain	Res	Type
1	M	224	LYS
1	M	226	ARG
1	M	254	LEU
1	M	294	LYS
1	M	296	LEU
1	M	311	ARG
1	M	325	LEU
1	M	333	MET
1	M	342	ASN
1	M	344	LEU
1	M	366	GLU
1	M	387	VAL
1	M	406	GLU
1	M	409	THR
1	M	415	THR
1	M	418	GLN
1	M	420	MET
1	M	424	SER
1	M	428	SER
1	M	430	ILE
1	M	433	ILE
1	M	458	MET
1	M	463	HIS
1	M	493	SER
1	P	33	HIS
1	P	40	ARG
1	P	148	THR
1	P	181	THR
1	P	184	ARG
1	P	212	GLU
1	P	218	ARG
1	P	223	LEU
1	P	245	ASN
1	P	259	SER
1	P	263	VAL
1	P	270	LEU
1	P	281	ASP
1	P	287	THR
1	P	292	THR
1	P	294	LYS
1	P	303	GLU
1	P	319	GLU

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Mol	Chain	Res	Type
1	P	323	GLN
1	P	324	LEU
1	P	342	ASN
1	P	352	GLU
1	P	357	GLU
1	P	366	GLU
1	P	418	GLN
1	P	425	ILE
1	P	428	SER
1	P	430	ILE
1	P	432	THR
1	P	433	ILE
1	P	458	MET
1	P	465	LYS
1	P	471	MET
2	Q	20	LYS
2	Q	24	MET
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	218	ARG
2	Q	224	LYS
2	Q	256	GLN
2	Q	263	VAL
2	Q	270	LEU
2	Q	292	THR
2	Q	309	LYS
2	Q	319	GLU
2	Q	320	SER
2	Q	333	MET
2	Q	356	LEU
2	Q	360	LEU
2	Q	406	GLU
2	Q	415	THR
2	Q	420	MET

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Mol	Chain	Res	Type
2	Q	423	HIS
2	Q	428	SER
2	Q	448	GLU
2	Q	458	MET
2	Q	471	MET
2	Q	474	ASP
1	T	21	MET
1	T	58	GLN
1	T	182	THR
1	T	287	THR
1	T	294	LYS
1	T	318	GLU
1	T	331	TRP
1	T	364	LYS
1	T	378	ASP
1	T	411	LEU
1	T	413	THR
1	T	449	MET
1	T	458	MET
1	T	463	HIS
2	U	23	THR
2	U	24	MET
2	U	106	LEU
2	U	184	ARG
2	U	217	ARG
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	360	LEU
2	U	380	LEU
2	U	383	LEU
2	U	411	LEU
2	U	425	ILE
2	U	426	THR
2	U	458	MET
2	U	463	HIS
1	X	24	MET
1	X	43	LEU
1	X	45	SER

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Mol	Chain	Res	Type
1	X	143	SER
1	X	146	SER
1	X	178	THR
1	X	215	ARG
1	X	228	THR
1	X	231	MET
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	303	GLU
1	X	333	MET
1	X	356	LEU
1	X	364	LYS
1	X	381	SER
1	X	411	LEU
1	X	420	MET
1	X	425	ILE
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	296	LEU
1	S	361	GLN
1	S	381	SER
1	S	409	THR
1	S	415	THR
1	S	420	MET
1	S	425	ILE
1	S	433	ILE
1	S	458	MET
1	S	471	MET
1	V	24	MET
1	V	42	THR
1	V	47	THR

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Mol	Chain	Res	Type
1	V	53	THR
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	225	LEU
1	V	258	SER
1	V	263	VAL
1	V	270	LEU
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	342	ASN
1	V	343	LEU
1	V	344	LEU
1	V	366	GLU
1	V	397	ILE
1	V	413	THR
1	V	419	PHE
1	V	428	SER
1	V	432	THR
1	V	449	MET
1	V	450	SER
1	V	451	ARG
1	V	457	LYS
1	V	458	MET
1	V	469	GLU
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	220	LEU
1	W	234	GLU
1	W	245	ASN

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Mol	Chain	Res	Type
1	W	267	VAL
1	W	284	ILE
1	W	287	THR
1	W	292	THR
1	W	294	LYS
1	W	297	LEU
1	W	310	GLU
1	W	318	GLU
1	W	352	GLU
1	W	356	LEU
1	W	360	LEU
1	W	361	GLN
1	W	385	ARG
1	W	419	PHE
1	W	420	MET
1	W	425	ILE
1	W	428	SER
1	W	430	ILE
1	W	433	ILE
1	W	439	LEU
1	W	451	ARG
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 (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	245	ASN
1	A	260	ASN
1	A	341	GLN
1	A	342	ASN
1	A	389	ASN
1	A	441	GLN
1	A	454	ASN
1	B	62	ASN
1	B	173	GLN
1	B	209	ASN
1	B	260	ASN
1	B	342	ASN
1	B	368	ASN

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Mol	Chain	Res	Type
1	B	389	ASN
1	B	441	GLN
2	E	62	ASN
2	E	256	GLN
2	E	308	ASN
2	E	323	GLN
2	E	414	ASN
2	E	429	HIS
2	E	441	GLN
2	F	209	ASN
2	F	389	ASN
2	F	429	HIS
2	F	454	ASN
2	C	209	ASN
2	C	389	ASN
2	C	394	GLN
2	D	33	HIS
2	D	368	ASN
2	D	414	ASN
2	D	418	GLN
2	D	441	GLN
1	G	341	GLN
1	G	389	ASN
1	G	441	GLN
1	G	454	ASN
1	H	62	ASN
1	H	209	ASN
1	H	260	ASN
1	H	342	ASN
1	H	368	ASN
1	H	389	ASN
1	H	429	HIS
1	H	441	GLN
2	K	33	HIS
2	K	62	ASN
2	K	209	ASN
2	K	256	GLN
2	K	308	ASN
2	K	323	GLN
2	K	414	ASN
2	K	429	HIS
2	K	441	GLN

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Mol	Chain	Res	Type
2	L	209	ASN
2	L	389	ASN
2	L	418	GLN
2	L	429	HIS
2	L	441	GLN
2	L	454	ASN
2	I	209	ASN
2	I	260	ASN
2	I	389	ASN
2	I	394	GLN
2	I	441	GLN
2	J	368	ASN
2	J	389	ASN
2	J	414	ASN
2	J	418	GLN
2	J	441	GLN
1	N	209	ASN
1	N	256	GLN
1	N	368	ASN
1	N	414	ASN
1	N	423	HIS
1	N	429	HIS
1	N	454	ASN
1	N	463	HIS
2	O	86	ASN
2	O	342	ASN
2	O	389	ASN
2	O	405	GLN
2	O	414	ASN
2	O	418	GLN
2	O	423	HIS
1	R	418	GLN
1	R	429	HIS
1	R	441	GLN
1	R	454	ASN
1	M	209	ASN
1	M	308	ASN
1	M	359	HIS
1	M	441	GLN
1	P	323	GLN
1	P	342	ASN
1	P	418	GLN

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Mol	Chain	Res	Type
1	P	429	HIS
1	P	454	ASN
2	Q	256	GLN
2	Q	368	ASN
2	Q	405	GLN
2	Q	418	GLN
2	Q	423	HIS
1	T	58	GLN
1	T	414	ASN
1	T	429	HIS
2	U	390	ASN
2	U	441	GLN
2	U	454	ASN
1	X	342	ASN
1	X	389	ASN
1	X	418	GLN
1	X	429	HIS
1	X	441	GLN
1	S	209	ASN
1	S	260	ASN
1	S	414	ASN
1	S	418	GLN
1	S	463	HIS
1	V	368	ASN
1	W	256	GLN
1	W	341	GLN
1	W	389	ASN
1	W	418	GLN

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	H	431	1	8,9,10	0.64	0	7,12,14	0.58	0
1	SEP	V	431	1	8,9,10	0.70	0	7,12,14	0.64	0
1	SEP	M	431	1	8,9,10	0.67	0	7,12,14	0.61	0
2	TPO	O	432	2	8,10,11	1.02	1 (12%)	10,14,16	1.05	1 (10%)
2	TPO	U	432	2	8,10,11	1.00	1 (12%)	10,14,16	1.06	1 (10%)
2	TPO	J	432	2	8,10,11	0.89	1 (12%)	10,14,16	0.88	0
2	TPO	K	432	2	8,10,11	1.31	1 (12%)	10,14,16	1.17	0
1	SEP	N	431	1	8,9,10	0.72	0	7,12,14	0.74	0
2	SEP	I	431	2	8,9,10	0.64	0	7,12,14	0.55	0
2	TPO	C	432	2	8,10,11	1.45	2 (25%)	10,14,16	0.80	0
2	SEP	E	431	2	8,9,10	0.60	0	7,12,14	0.73	0
1	SEP	R	431	1	8,9,10	0.70	0	7,12,14	0.77	0
1	SEP	G	431	1	8,9,10	1.13	1 (12%)	7,12,14	1.15	1 (14%)
2	SEP	D	431	2	8,9,10	0.70	0	7,12,14	0.55	0
2	TPO	Q	432	2	8,10,11	0.97	1 (12%)	10,14,16	1.11	1 (10%)
1	SEP	T	431	1	8,9,10	0.76	0	7,12,14	0.78	0
2	SEP	Q	431	2	8,9,10	0.70	0	7,12,14	0.61	0
1	SEP	A	431	1	8,9,10	1.15	1 (12%)	7,12,14	1.09	0
2	SEP	F	431	2	8,9,10	0.57	0	7,12,14	0.69	0
1	SEP	B	431	1	8,9,10	0.64	0	7,12,14	0.59	0
2	SEP	L	431	2	8,9,10	0.57	0	7,12,14	0.68	0
2	TPO	L	432	2	8,10,11	1.55	2 (25%)	10,14,16	0.95	0
2	SEP	K	431	2	8,9,10	0.60	0	7,12,14	0.87	0
2	SEP	U	431	2	8,9,10	0.72	0	7,12,14	0.63	0
2	SEP	C	431	2	8,9,10	0.65	0	7,12,14	0.58	0
2	SEP	J	431	2	8,9,10	0.70	0	7,12,14	0.54	0
1	SEP	X	431	1	8,9,10	0.59	0	7,12,14	0.71	0
2	TPO	I	432	2	8,10,11	1.45	2 (25%)	10,14,16	0.83	0
1	SEP	P	431	1	8,9,10	0.64	0	7,12,14	0.61	0
2	TPO	E	432	2	8,10,11	1.35	1 (12%)	10,14,16	1.12	0
1	SEP	S	431	1	8,9,10	0.62	0	7,12,14	0.63	0
2	TPO	D	432	2	8,10,11	0.93	1 (12%)	10,14,16	0.90	0
1	SEP	W	431	1	8,9,10	0.58	0	7,12,14	0.71	0
2	TPO	F	432	2	8,10,11	1.58	2 (25%)	10,14,16	0.95	0
2	SEP	O	431	2	8,9,10	0.72	0	7,12,14	0.79	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	H	431	1	-	1/6/8/10	-
1	SEP	V	431	1	-	2/6/8/10	-
1	SEP	M	431	1	-	1/6/8/10	-
2	TPO	O	432	2	-	1/9/11/13	-
2	TPO	U	432	2	-	1/9/11/13	-
2	TPO	J	432	2	-	2/9/11/13	-
2	TPO	K	432	2	-	3/9/11/13	-
1	SEP	N	431	1	-	2/6/8/10	-
2	SEP	I	431	2	-	1/6/8/10	-
2	TPO	C	432	2	-	2/9/11/13	-
2	SEP	E	431	2	-	5/6/8/10	-
1	SEP	R	431	1	-	4/6/8/10	-
1	SEP	G	431	1	-	3/6/8/10	-
2	SEP	D	431	2	-	1/6/8/10	-
2	TPO	Q	432	2	-	4/9/11/13	-
1	SEP	T	431	1	-	1/6/8/10	-
2	SEP	Q	431	2	-	1/6/8/10	-
1	SEP	A	431	1	-	1/6/8/10	-
2	SEP	F	431	2	-	1/6/8/10	-
1	SEP	B	431	1	-	1/6/8/10	-
2	SEP	L	431	2	-	1/6/8/10	-
2	TPO	L	432	2	-	6/9/11/13	-
2	SEP	K	431	2	-	5/6/8/10	-
2	SEP	U	431	2	-	2/6/8/10	-
2	SEP	C	431	2	-	1/6/8/10	-
2	SEP	J	431	2	-	2/6/8/10	-
1	SEP	X	431	1	-	0/6/8/10	-
2	TPO	I	432	2	-	3/9/11/13	-
1	SEP	P	431	1	-	3/6/8/10	-
2	TPO	E	432	2	-	1/9/11/13	-
1	SEP	S	431	1	-	1/6/8/10	-
2	TPO	D	432	2	-	2/9/11/13	-
1	SEP	W	431	1	-	0/6/8/10	-
2	TPO	F	432	2	-	4/9/11/13	-
2	SEP	O	431	2	-	1/6/8/10	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	432	TPO	P-O2P	-3.02	1.43	1.54
2	L	432	TPO	P-O2P	-2.98	1.43	1.54
2	E	432	TPO	P-O2P	-2.88	1.44	1.54
2	F	432	TPO	P-OG1	2.72	1.64	1.59
2	L	432	TPO	P-OG1	2.61	1.64	1.59
2	I	432	TPO	P-O2P	-2.58	1.45	1.54
2	C	432	TPO	P-O2P	-2.56	1.45	1.54
1	A	431	SEP	P-O2P	-2.54	1.45	1.54
2	K	432	TPO	P-O2P	-2.50	1.45	1.54
2	C	432	TPO	P-O3P	-2.20	1.46	1.54
2	U	432	TPO	P-OG1	2.20	1.63	1.59
2	I	432	TPO	P-O3P	-2.20	1.46	1.54
2	D	432	TPO	P-OG1	2.15	1.63	1.59
2	O	432	TPO	P-OG1	2.15	1.63	1.59
1	G	431	SEP	P-O2P	-2.14	1.46	1.54
2	Q	432	TPO	P-OG1	2.07	1.63	1.59
2	J	432	TPO	P-OG1	2.05	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	-2.82	117.52	124.77
2	Q	432	TPO	O-C-CA	-2.77	117.65	124.77
2	O	432	TPO	O-C-CA	-2.66	117.93	124.77
1	G	431	SEP	O3P-P-O2P	2.04	115.47	107.80

There are no chirality outliers.

All (70) 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	C-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

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Mol	Chain	Res	Type	Atoms
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	C-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
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	I	432	TPO	C-CA-CB-CG2
2	J	432	TPO	O-C-CA-CB
1	N	431	SEP	N-CA-CB-OG
1	N	431	SEP	C-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

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Mol	Chain	Res	Type	Atoms
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	K	432	TPO	CB-OG1-P-O1P
2	J	431	SEP	CB-OG-P-O2P
1	G	431	SEP	CA-CB-OG-P
1	P	431	SEP	CA-CB-OG-P
2	K	432	TPO	CB-OG1-P-O2P
2	L	432	TPO	CB-OG1-P-O3P
2	I	432	TPO	CB-OG1-P-O3P
2	O	432	TPO	CB-OG1-P-O2P
2	E	432	TPO	O-C-CA-CB
2	K	432	TPO	O-C-CA-CB
1	V	431	SEP	C-CA-CB-OG
2	D	432	TPO	CB-OG1-P-O1P
2	L	432	TPO	CB-OG1-P-O1P
2	J	432	TPO	CB-OG1-P-O1P

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	432	TPO	5	0
2	K	432	TPO	1	0
2	C	432	TPO	1	0
2	E	431	SEP	1	0
1	R	431	SEP	2	0
2	Q	432	TPO	1	0
1	T	431	SEP	2	0
2	K	431	SEP	1	0
1	X	431	SEP	1	0
2	I	432	TPO	1	0
2	E	432	TPO	1	0
2	D	432	TPO	5	0
2	F	432	TPO	2	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
5	ADP	W	701	-	28,29,29	0.46	0	43,45,45	0.46	0
3	ATP	D	701	4	32,33,33	0.57	0	48,52,52	0.60	0
3	ATP	H	701	4	32,33,33	0.51	0	48,52,52	0.65	0
3	ATP	V	701	4	32,33,33	0.48	0	48,52,52	0.58	0
3	ATP	M	701	4	32,33,33	0.53	0	48,52,52	0.59	0
3	ATP	F	702	4	32,33,33	0.52	0	48,52,52	0.67	0
3	ATP	C	701	4	32,33,33	0.51	0	48,52,52	0.66	0
3	ATP	A	702	4	32,33,33	0.53	0	48,52,52	0.63	0
3	ATP	I	702	4	32,33,33	0.49	0	48,52,52	0.55	0
3	ATP	X	702	-	32,33,33	0.51	0	48,52,52	0.73	1 (2%)
3	ATP	K	701	4	32,33,33	0.49	0	48,52,52	0.71	1 (2%)
3	ATP	J	702	4	32,33,33	0.53	0	48,52,52	0.71	1 (2%)
3	ATP	V	702	-	32,33,33	0.57	0	48,52,52	0.55	0
3	ATP	G	701	4	32,33,33	0.54	0	48,52,52	0.72	1 (2%)
3	ATP	Q	702	4	32,33,33	0.51	0	48,52,52	0.74	1 (2%)
3	ATP	S	701	-	32,33,33	0.54	0	48,52,52	0.58	0
3	ATP	G	702	4	32,33,33	0.53	0	48,52,52	0.76	1 (2%)
3	ATP	B	702	4	32,33,33	0.50	0	48,52,52	0.70	0
3	ATP	A	701	4	32,33,33	0.59	0	48,52,52	0.71	0
3	ATP	D	702	4	32,33,33	0.49	0	48,52,52	0.66	1 (2%)
3	ATP	S	702	-	32,33,33	0.55	0	48,52,52	0.60	0
3	ATP	N	701	4	32,33,33	0.51	0	48,52,52	0.72	1 (2%)
3	ATP	M	702	-	32,33,33	0.58	0	48,52,52	0.70	1 (2%)
3	ATP	T	702	-	32,33,33	0.51	0	48,52,52	0.58	0
3	ATP	R	701	4	32,33,33	0.61	0	48,52,52	0.59	0
3	ATP	B	701	4	32,33,33	0.51	0	48,52,52	0.62	0
3	ATP	L	701	4	32,33,33	0.48	0	48,52,52	0.72	0
3	ATP	O	701	4	32,33,33	0.58	0	48,52,52	0.70	1 (2%)
5	ADP	Q	701	-	28,29,29	0.43	0	43,45,45	0.48	0
3	ATP	K	702	4	32,33,33	0.53	0	48,52,52	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	H	702	4	32,33,33	0.50	0	48,52,52	0.64	0
3	ATP	T	701	4	32,33,33	0.54	0	48,52,52	0.70	0
3	ATP	C	702	4	32,33,33	0.51	0	48,52,52	0.66	0
3	ATP	U	701	4	32,33,33	0.55	0	48,52,52	0.64	0
3	ATP	P	701	4	32,33,33	0.52	0	48,52,52	0.68	0
3	ATP	P	702	4	32,33,33	0.54	0	48,52,52	0.69	1 (2%)
3	ATP	N	702	4	32,33,33	0.50	0	48,52,52	0.78	0
3	ATP	R	702	4	32,33,33	0.59	0	48,52,52	0.64	0
3	ATP	F	701	4	32,33,33	0.51	0	48,52,52	0.67	0
3	ATP	J	701	4	32,33,33	0.54	0	48,52,52	0.66	0
3	ATP	L	702	4	32,33,33	0.48	0	48,52,52	0.74	1 (2%)
3	ATP	E	702	4	32,33,33	0.49	0	48,52,52	0.61	0
3	ATP	X	701	-	32,33,33	0.55	0	48,52,52	0.60	0
3	ATP	W	702	-	32,33,33	0.58	0	48,52,52	0.70	1 (2%)
5	ADP	U	702	-	28,29,29	0.47	0	43,45,45	0.50	0
3	ATP	E	701	4	32,33,33	0.50	0	48,52,52	0.70	1 (2%)
3	ATP	I	701	4	32,33,33	0.47	0	48,52,52	0.65	0
3	ATP	O	702	-	32,33,33	0.54	0	48,52,52	0.72	1 (2%)

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
5	ADP	W	701	-	-	6/16/32/32	0/3/3/3
3	ATP	D	701	4	-	8/22/38/38	0/3/3/3
3	ATP	H	701	4	-	2/22/38/38	0/3/3/3
3	ATP	V	701	4	-	2/22/38/38	0/3/3/3
3	ATP	M	701	4	-	4/22/38/38	0/3/3/3
3	ATP	F	702	4	-	7/22/38/38	0/3/3/3
3	ATP	C	701	4	-	2/22/38/38	0/3/3/3
3	ATP	A	702	4	-	4/22/38/38	0/3/3/3
3	ATP	I	702	4	-	7/22/38/38	0/3/3/3
3	ATP	X	702	-	-	6/22/38/38	0/3/3/3
3	ATP	K	701	4	-	1/22/38/38	0/3/3/3
3	ATP	J	702	4	-	1/22/38/38	0/3/3/3
3	ATP	V	702	-	-	6/22/38/38	0/3/3/3
3	ATP	G	701	4	-	1/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	Q	702	4	-	2/22/38/38	0/3/3/3
3	ATP	S	701	-	-	3/22/38/38	0/3/3/3
3	ATP	G	702	4	-	1/22/38/38	0/3/3/3
3	ATP	B	702	4	-	2/22/38/38	0/3/3/3
3	ATP	A	701	4	-	1/22/38/38	0/3/3/3
3	ATP	D	702	4	-	4/22/38/38	0/3/3/3
3	ATP	S	702	-	-	0/22/38/38	0/3/3/3
3	ATP	N	701	4	-	4/22/38/38	0/3/3/3
3	ATP	M	702	-	-	5/22/38/38	0/3/3/3
3	ATP	T	702	-	-	0/22/38/38	0/3/3/3
3	ATP	R	701	4	-	5/22/38/38	0/3/3/3
3	ATP	B	701	4	-	6/22/38/38	0/3/3/3
3	ATP	L	701	4	-	2/22/38/38	0/3/3/3
3	ATP	O	701	4	-	2/22/38/38	0/3/3/3
5	ADP	Q	701	-	-	3/16/32/32	0/3/3/3
3	ATP	K	702	4	-	1/22/38/38	0/3/3/3
3	ATP	H	702	4	-	2/22/38/38	0/3/3/3
3	ATP	T	701	4	-	4/22/38/38	0/3/3/3
3	ATP	C	702	4	-	4/22/38/38	0/3/3/3
3	ATP	U	701	4	-	1/22/38/38	0/3/3/3
3	ATP	P	701	4	-	3/22/38/38	0/3/3/3
3	ATP	P	702	4	-	2/22/38/38	0/3/3/3
3	ATP	N	702	4	-	5/22/38/38	0/3/3/3
3	ATP	R	702	4	-	4/22/38/38	0/3/3/3
3	ATP	F	701	4	-	4/22/38/38	0/3/3/3
3	ATP	J	701	4	-	7/22/38/38	0/3/3/3
3	ATP	L	702	4	-	4/22/38/38	0/3/3/3
3	ATP	E	702	4	-	2/22/38/38	0/3/3/3
3	ATP	X	701	-	-	8/22/38/38	0/3/3/3
3	ATP	W	702	-	-	3/22/38/38	0/3/3/3
5	ADP	U	702	-	-	4/16/32/32	0/3/3/3
3	ATP	E	701	4	-	5/22/38/38	0/3/3/3
3	ATP	I	701	4	-	5/22/38/38	0/3/3/3
3	ATP	O	702	-	-	3/22/38/38	0/3/3/3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	702	ATP	C3'-C2'-C1'	2.24	105.70	101.46
3	W	702	ATP	C3'-C2'-C1'	2.23	105.68	101.46
3	G	702	ATP	C3'-C2'-C1'	2.16	105.55	101.46
3	N	701	ATP	C3'-C2'-C1'	2.14	105.52	101.46
3	P	702	ATP	C3'-C2'-C1'	2.12	105.48	101.46
3	K	701	ATP	C3'-C2'-C1'	2.11	105.46	101.46
3	G	701	ATP	C3'-C2'-C1'	2.11	105.45	101.46
3	Q	702	ATP	C3'-C2'-C1'	2.10	105.44	101.46
3	L	702	ATP	C3'-C2'-C1'	2.09	105.41	101.46
3	J	702	ATP	C3'-C2'-C1'	2.08	105.40	101.46
3	X	702	ATP	C3'-C2'-C1'	2.05	105.35	101.46
3	D	702	ATP	C3'-C2'-C1'	2.04	105.32	101.46
3	M	702	ATP	C3'-C2'-C1'	2.02	105.29	101.46
3	E	701	ATP	C3'-C2'-C1'	2.01	105.26	101.46
3	O	701	ATP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (168) 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	A	702	ATP	C5'-O5'-PA-O3A
3	B	701	ATP	C5'-O5'-PA-O2A
3	B	701	ATP	C5'-O5'-PA-O3A
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	C5'-O5'-PA-O3A
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	D	701	ATP	C5'-O5'-PA-O3A
3	L	702	ATP	C5'-O5'-PA-O3A
3	I	701	ATP	C5'-O5'-PA-O3A
3	I	702	ATP	C5'-O5'-PA-O2A
3	J	701	ATP	PB-O3B-PG-O2G
3	J	701	ATP	C5'-O5'-PA-O1A
3	J	701	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
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	R	701	ATP	C5'-O5'-PA-O1A
3	R	701	ATP	C5'-O5'-PA-O2A
3	R	701	ATP	C5'-O5'-PA-O3A
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	S	701	ATP	C5'-O5'-PA-O1A
3	S	701	ATP	C5'-O5'-PA-O3A
3	V	702	ATP	C5'-O5'-PA-O2A
3	V	702	ATP	C5'-O5'-PA-O3A
5	Q	701	ADP	C5'-O5'-PA-O1A
5	Q	701	ADP	C5'-O5'-PA-O3A
5	U	702	ADP	C5'-O5'-PA-O2A
5	U	702	ADP	O4'-C4'-C5'-O5'
5	W	701	ADP	C5'-O5'-PA-O1A
5	W	701	ADP	C5'-O5'-PA-O3A
3	B	701	ATP	O4'-C4'-C5'-O5'
3	B	701	ATP	C3'-C4'-C5'-O5'
3	N	702	ATP	C3'-C4'-C5'-O5'
3	X	701	ATP	C3'-C4'-C5'-O5'
5	U	702	ADP	C3'-C4'-C5'-O5'
5	W	701	ADP	O4'-C4'-C5'-O5'
3	N	701	ATP	O4'-C4'-C5'-O5'
3	N	702	ATP	O4'-C4'-C5'-O5'
3	M	702	ATP	O4'-C4'-C5'-O5'
3	Q	702	ATP	C3'-C4'-C5'-O5'
3	X	701	ATP	O4'-C4'-C5'-O5'
3	V	702	ATP	O4'-C4'-C5'-O5'
5	W	701	ADP	C3'-C4'-C5'-O5'
3	E	701	ATP	C3'-C4'-C5'-O5'
3	M	702	ATP	C3'-C4'-C5'-O5'
3	E	701	ATP	O4'-C4'-C5'-O5'
3	F	702	ATP	O4'-C4'-C5'-O5'

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

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Mol	Chain	Res	Type	Atoms
3	I	702	ATP	O4'-C4'-C5'-O5'
3	N	701	ATP	C4'-C5'-O5'-PA
3	N	702	ATP	C4'-C5'-O5'-PA
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	R	701	ATP	O4'-C4'-C5'-O5'
3	X	702	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	M	702	ATP	C4'-C5'-O5'-PA
3	J	701	ATP	C3'-C4'-C5'-O5'
3	M	701	ATP	O4'-C4'-C5'-O5'
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	F	702	ATP	C3'-C4'-C5'-O5'
3	L	702	ATP	C3'-C4'-C5'-O5'
3	W	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

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Mol	Chain	Res	Type	Atoms
3	W	702	ATP	PG-O3B-PB-O2B
3	H	701	ATP	C3'-C4'-C5'-O5'
3	T	701	ATP	C4'-C5'-O5'-PA
3	J	701	ATP	PB-O3B-PG-O1G
3	I	702	ATP	C3'-C4'-C5'-O5'
3	A	701	ATP	PG-O3B-PB-O2B
3	E	701	ATP	PB-O3A-PA-O2A
3	D	701	ATP	PG-O3B-PB-O1B
3	D	702	ATP	PA-O3A-PB-O1B
3	G	702	ATP	PA-O3A-PB-O2B
3	L	701	ATP	PA-O3A-PB-O2B
3	I	701	ATP	PB-O3A-PA-O2A
3	J	702	ATP	PA-O3A-PB-O2B
3	N	702	ATP	PB-O3A-PA-O2A
3	R	702	ATP	PG-O3B-PB-O2B
3	P	701	ATP	PG-O3B-PB-O2B
3	P	702	ATP	PA-O3A-PB-O2B
3	U	701	ATP	PA-O3A-PB-O2B
3	V	702	ATP	PA-O3A-PB-O2B
5	W	701	ADP	PB-O3A-PA-O2A
3	R	702	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

38 monomers are involved in 78 short contacts:

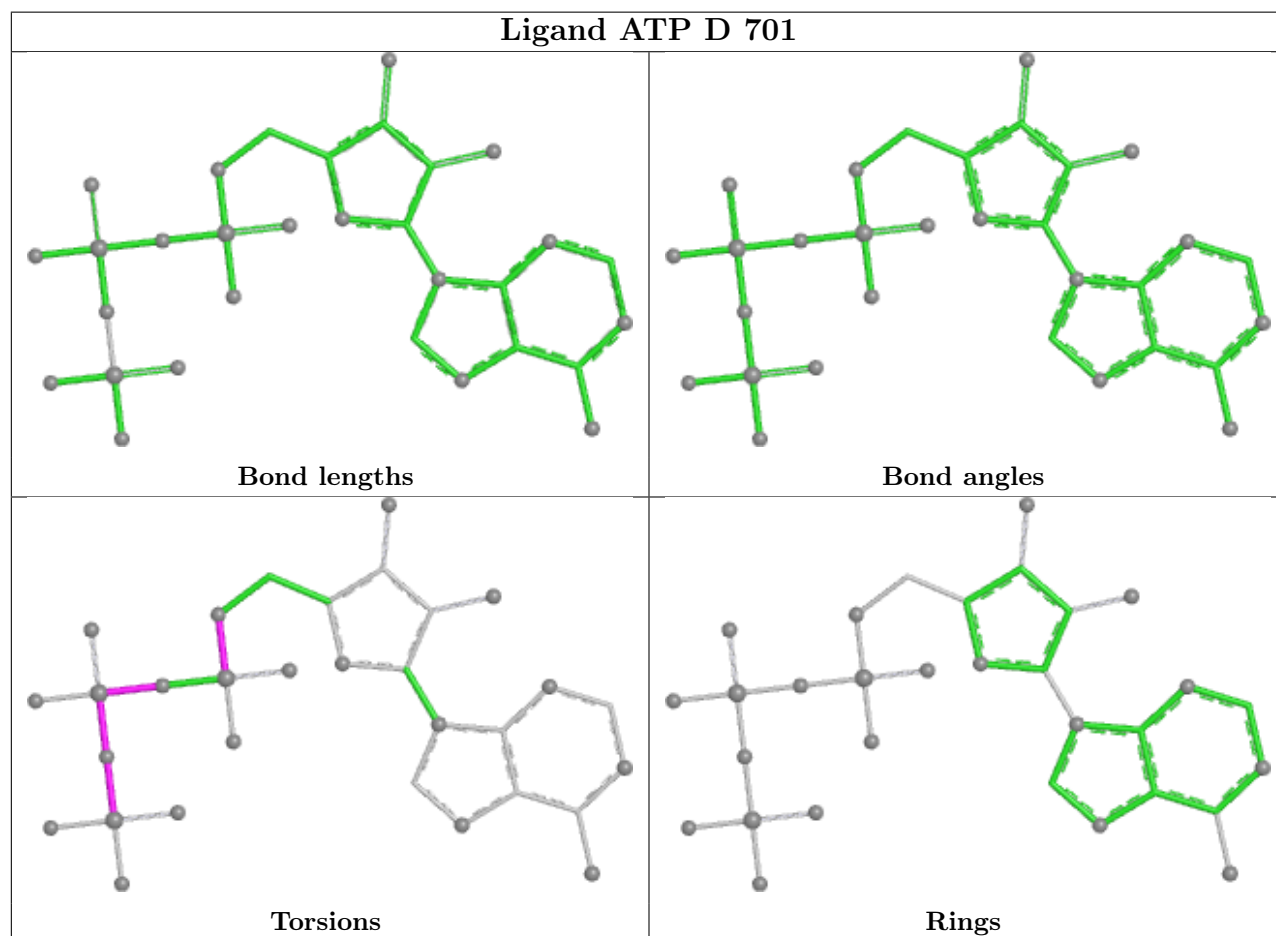
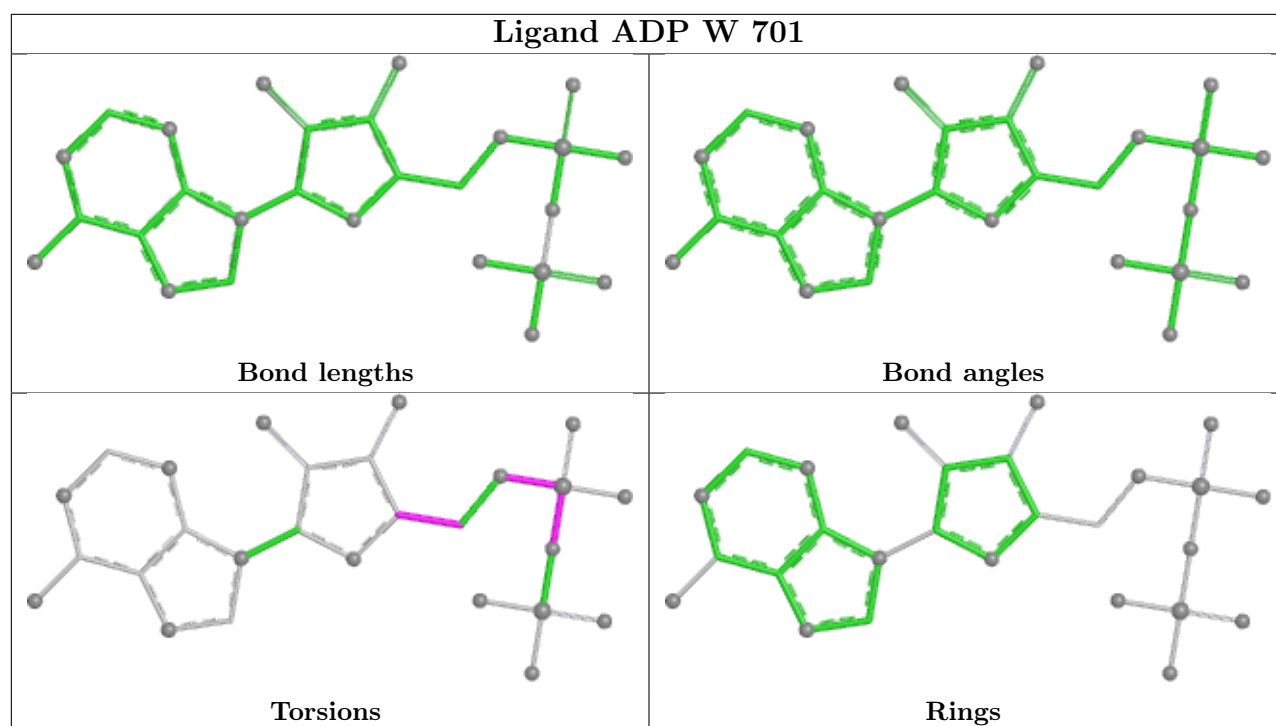
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	701	ATP	2	0
3	V	701	ATP	1	0
3	M	701	ATP	1	0
3	F	702	ATP	1	0
3	C	701	ATP	3	0
3	A	702	ATP	3	0
3	I	702	ATP	4	0
3	X	702	ATP	1	0
3	K	701	ATP	1	0
3	J	702	ATP	2	0
3	V	702	ATP	2	0
3	S	701	ATP	2	0
3	G	702	ATP	3	0
3	B	702	ATP	4	0
3	D	702	ATP	1	0
3	N	701	ATP	1	0

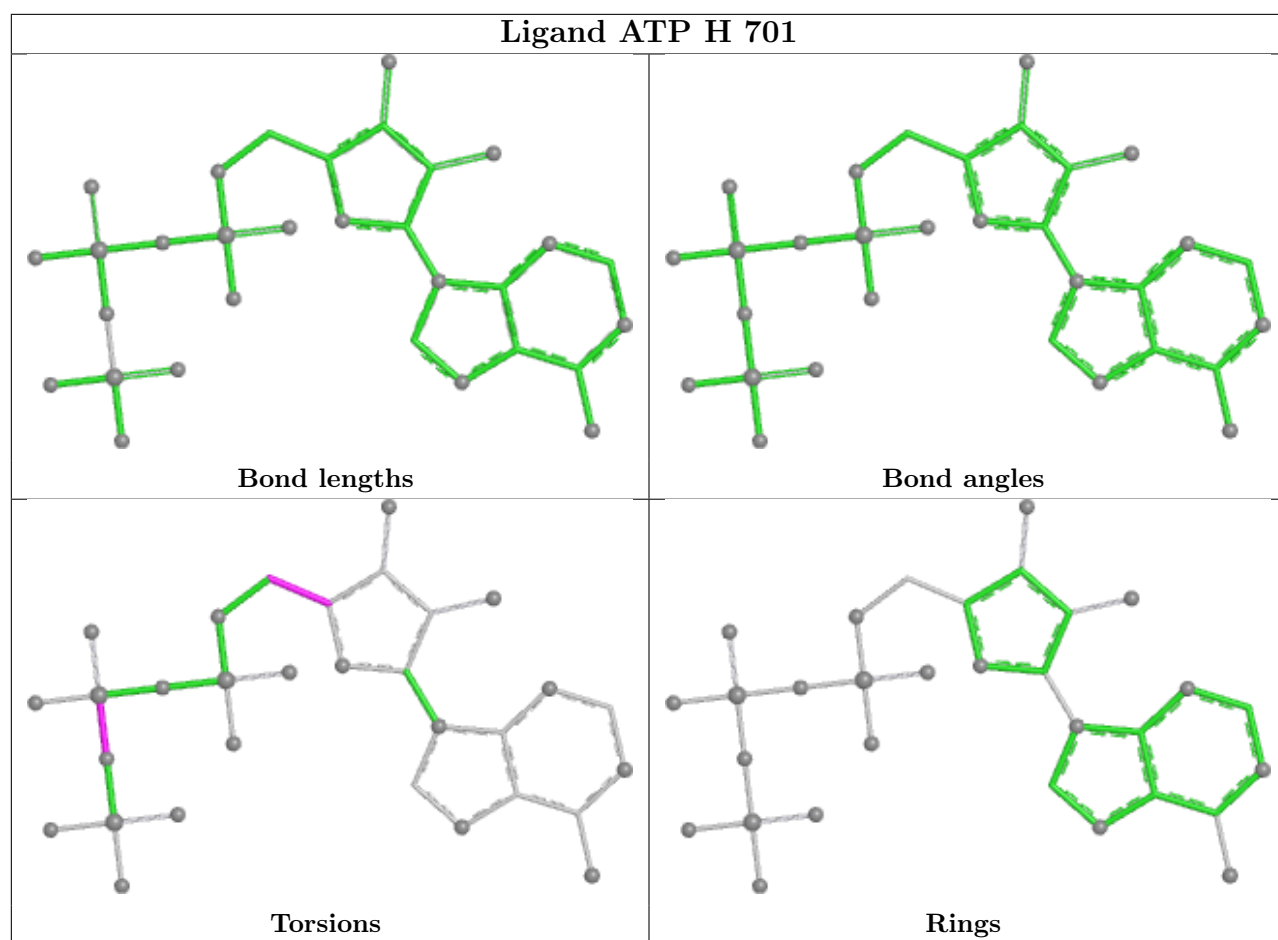
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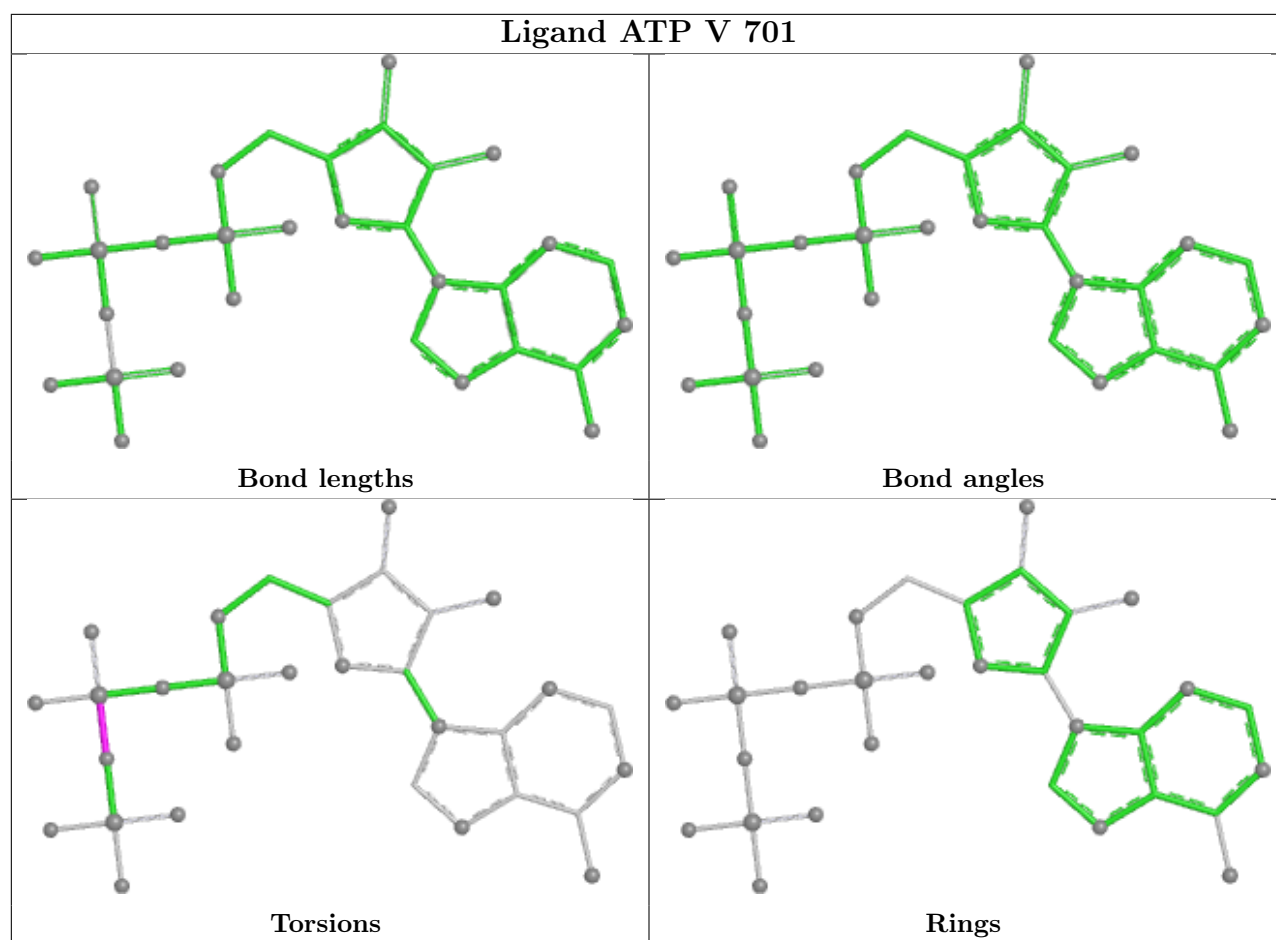
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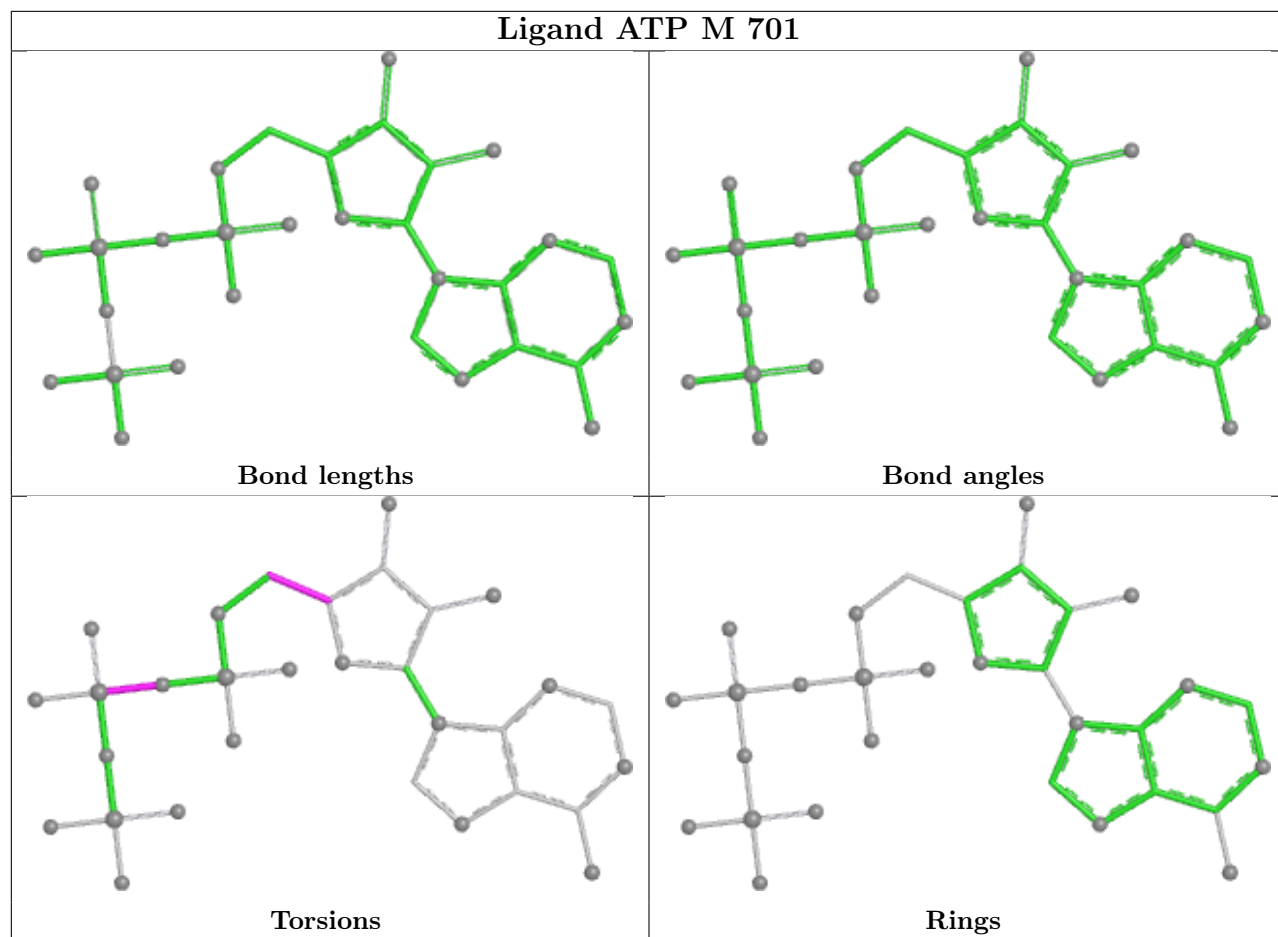
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	702	ATP	1	0
3	T	702	ATP	1	0
3	B	701	ATP	2	0
3	L	701	ATP	1	0
3	K	702	ATP	1	0
3	H	702	ATP	1	0
3	C	702	ATP	3	0
3	U	701	ATP	1	0
3	P	701	ATP	5	0
3	P	702	ATP	1	0
3	N	702	ATP	2	0
3	R	702	ATP	1	0
3	F	701	ATP	2	0
3	J	701	ATP	1	0
3	L	702	ATP	4	0
3	E	702	ATP	1	0
3	X	701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

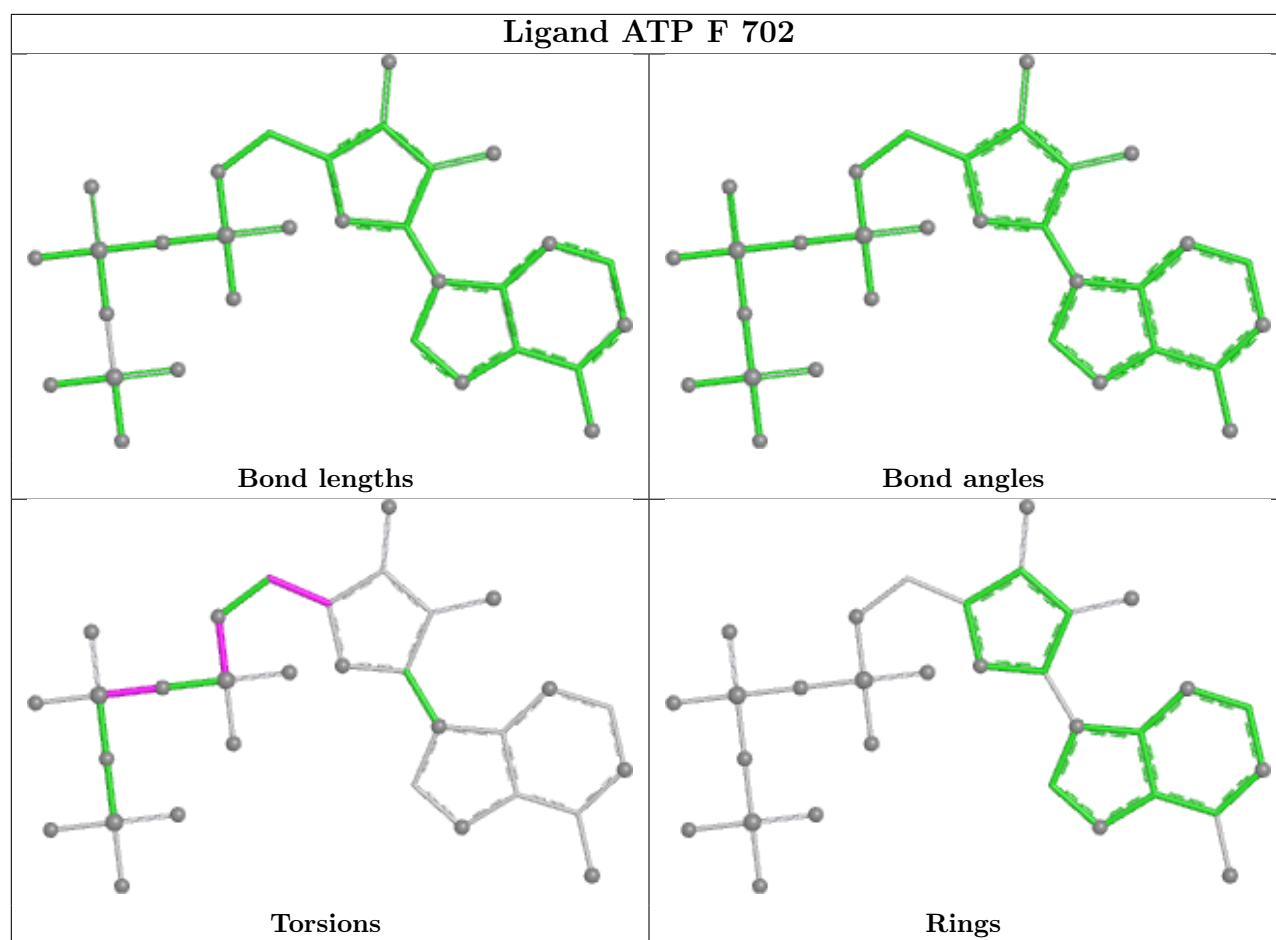
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

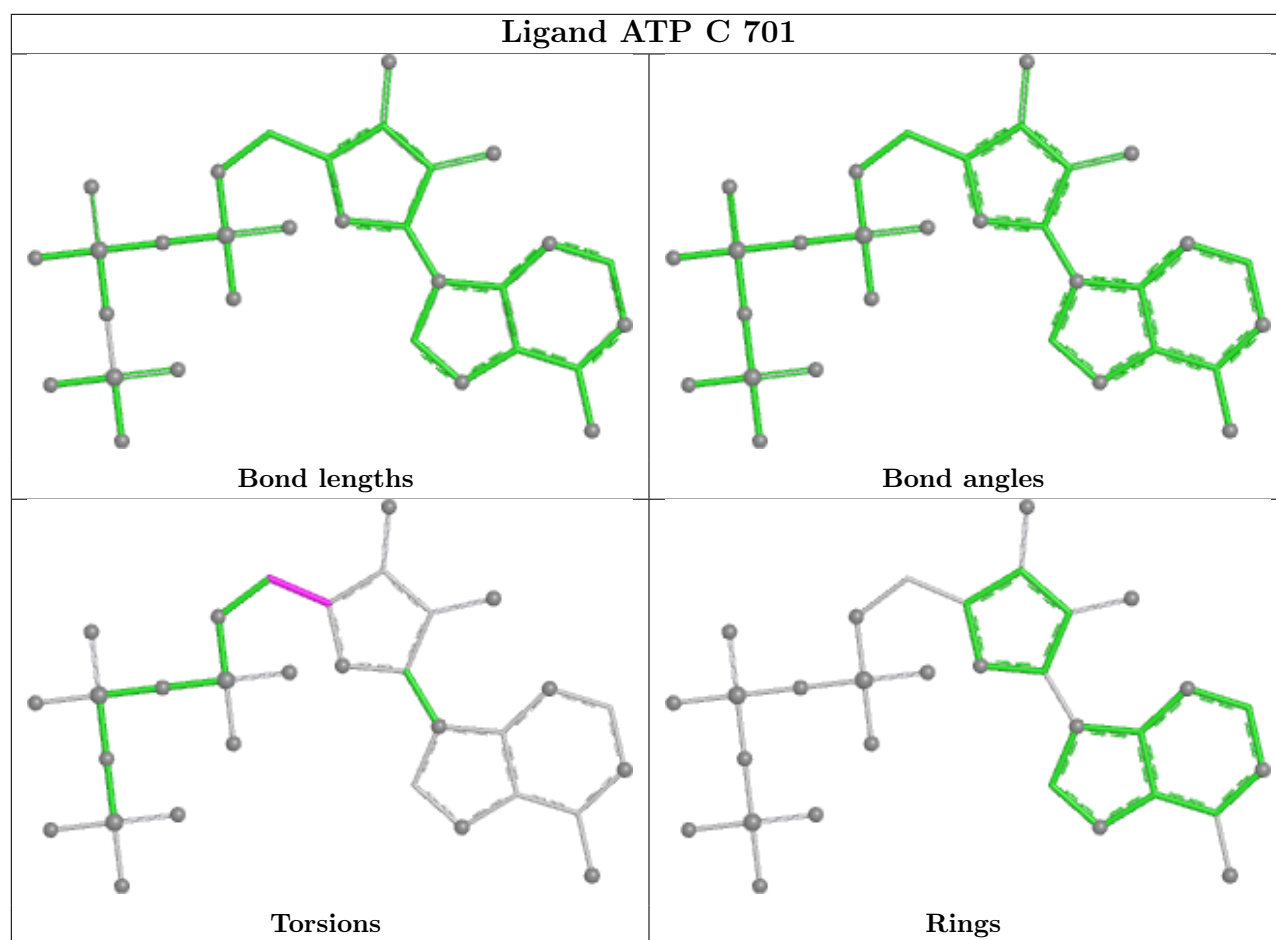


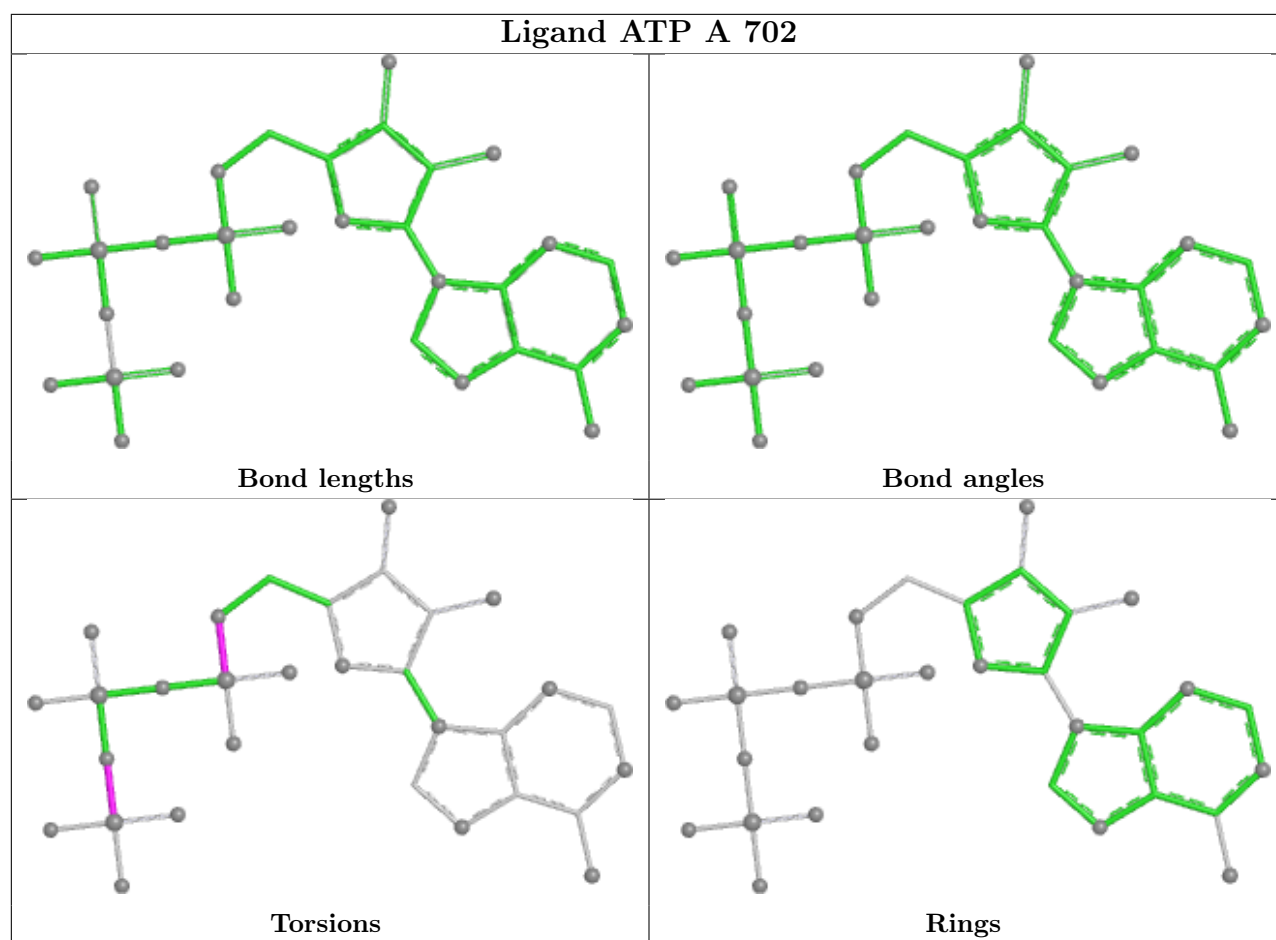




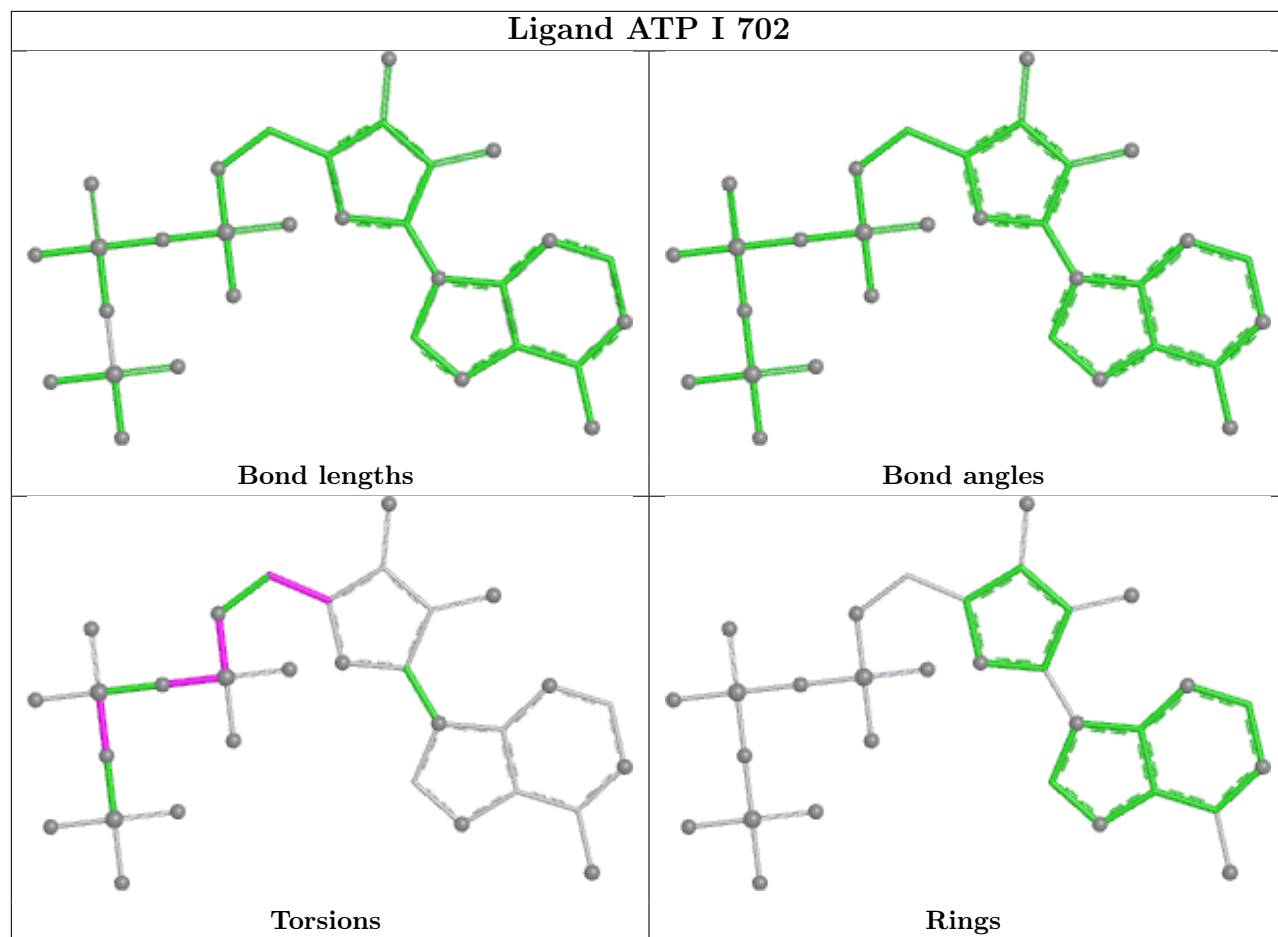


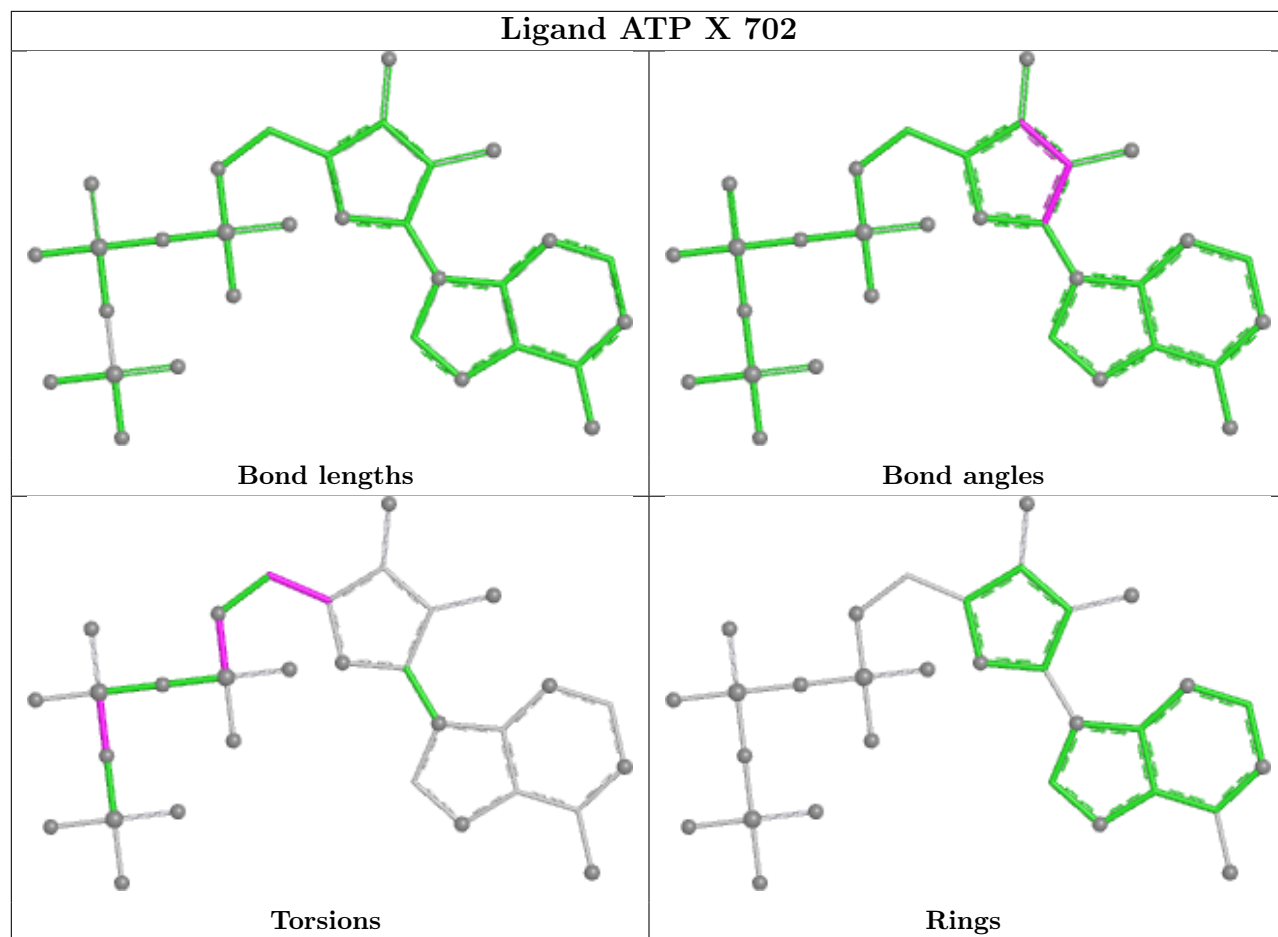


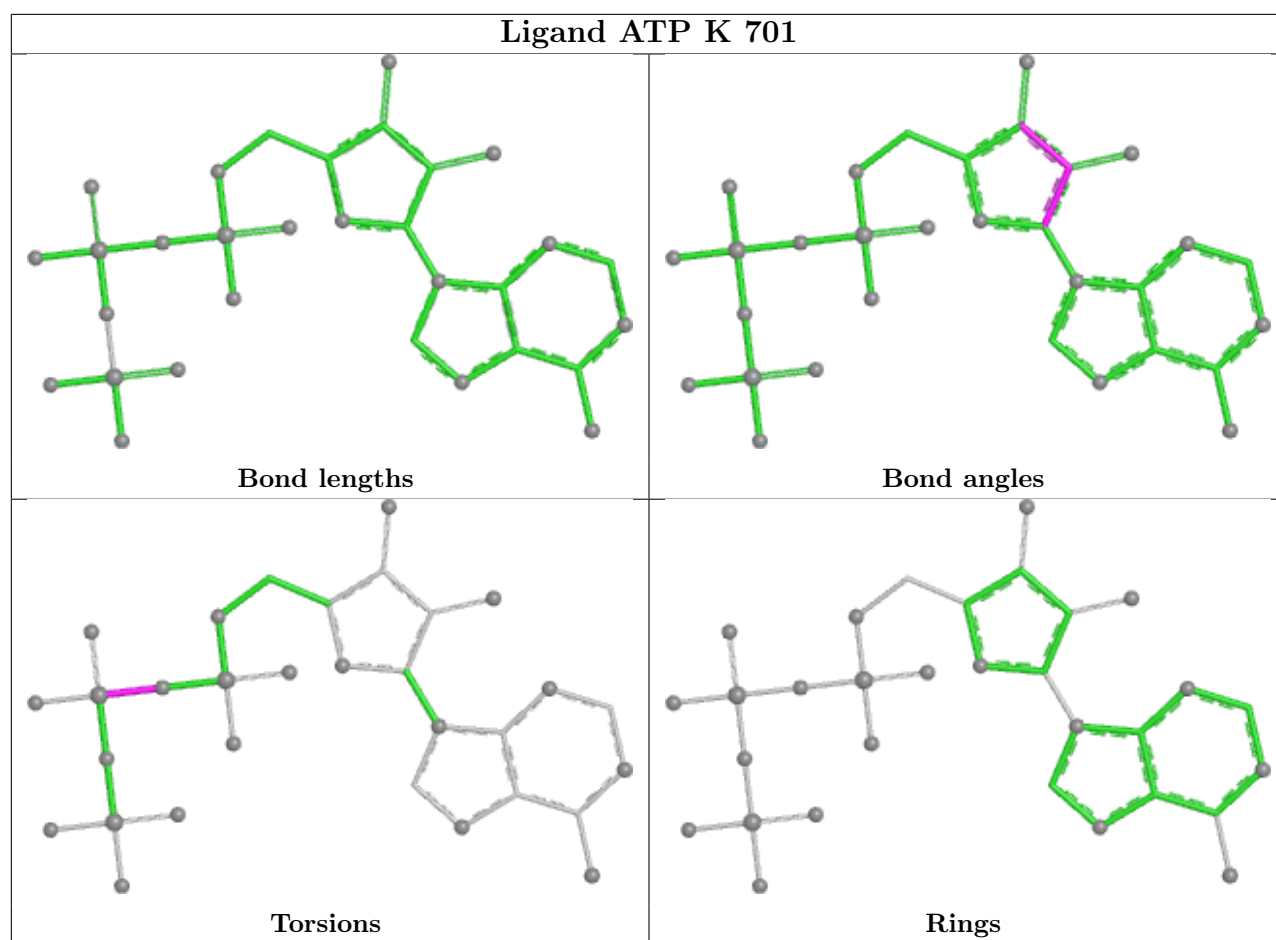




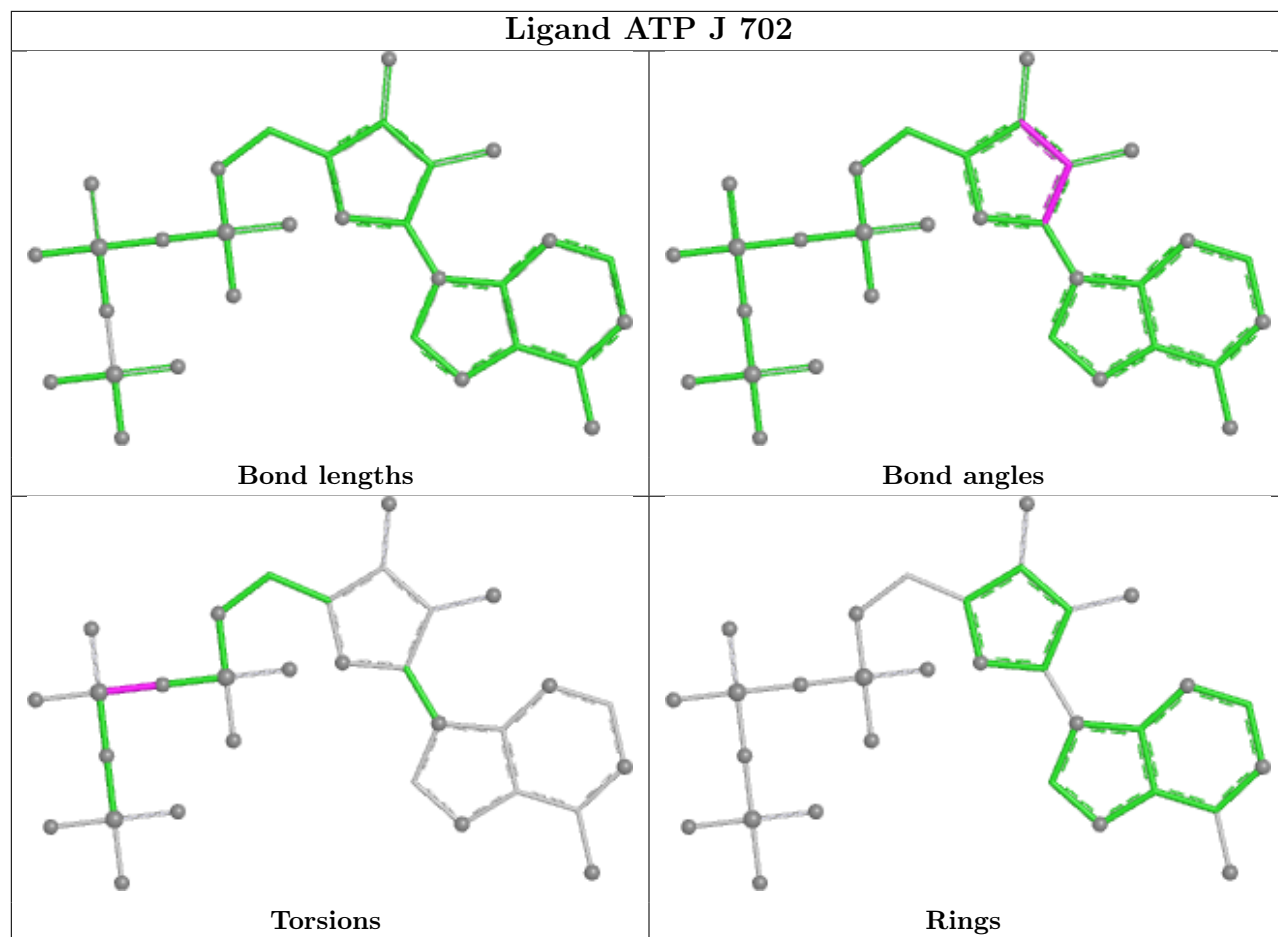
Ligand ATP I 702

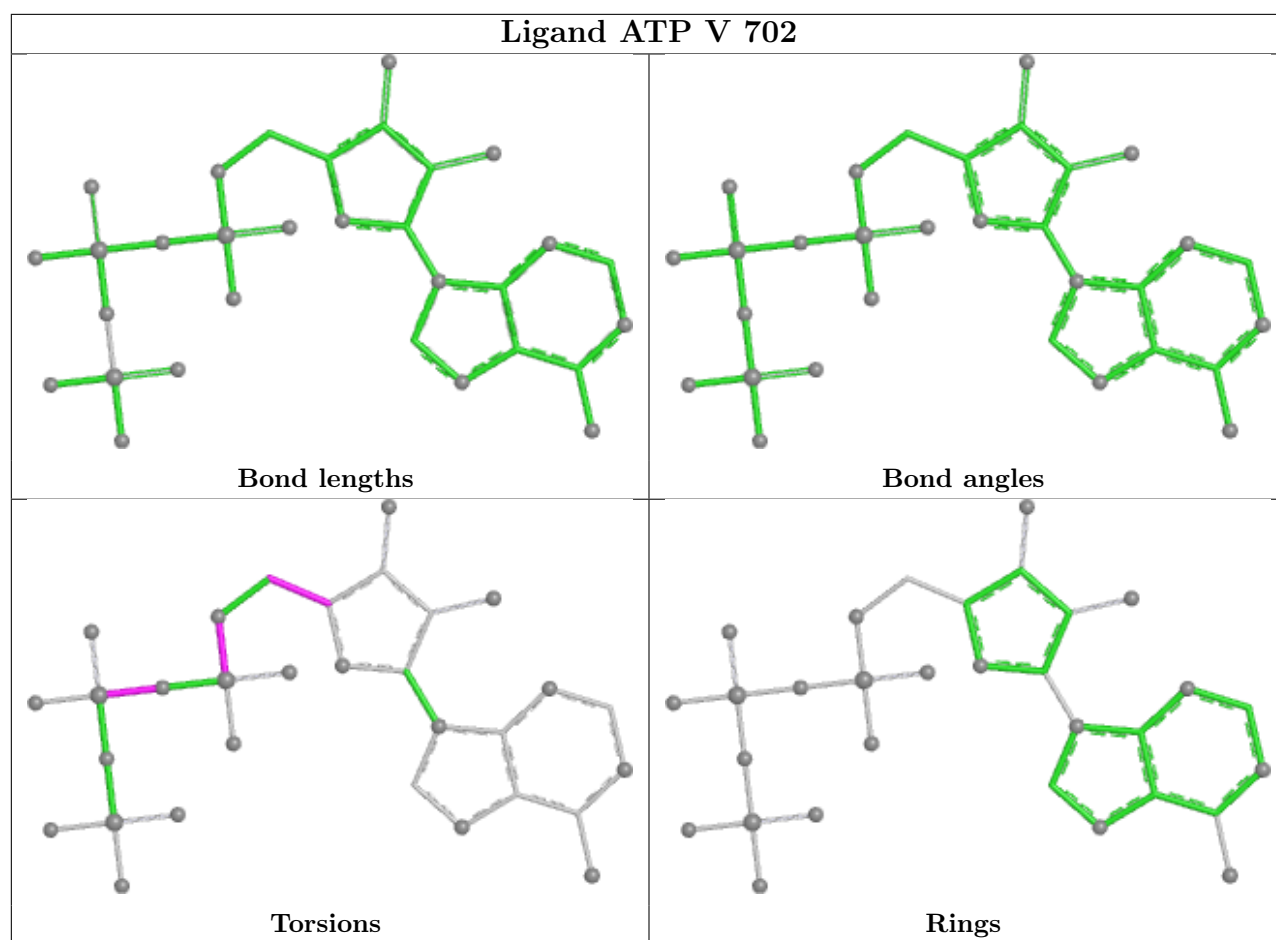


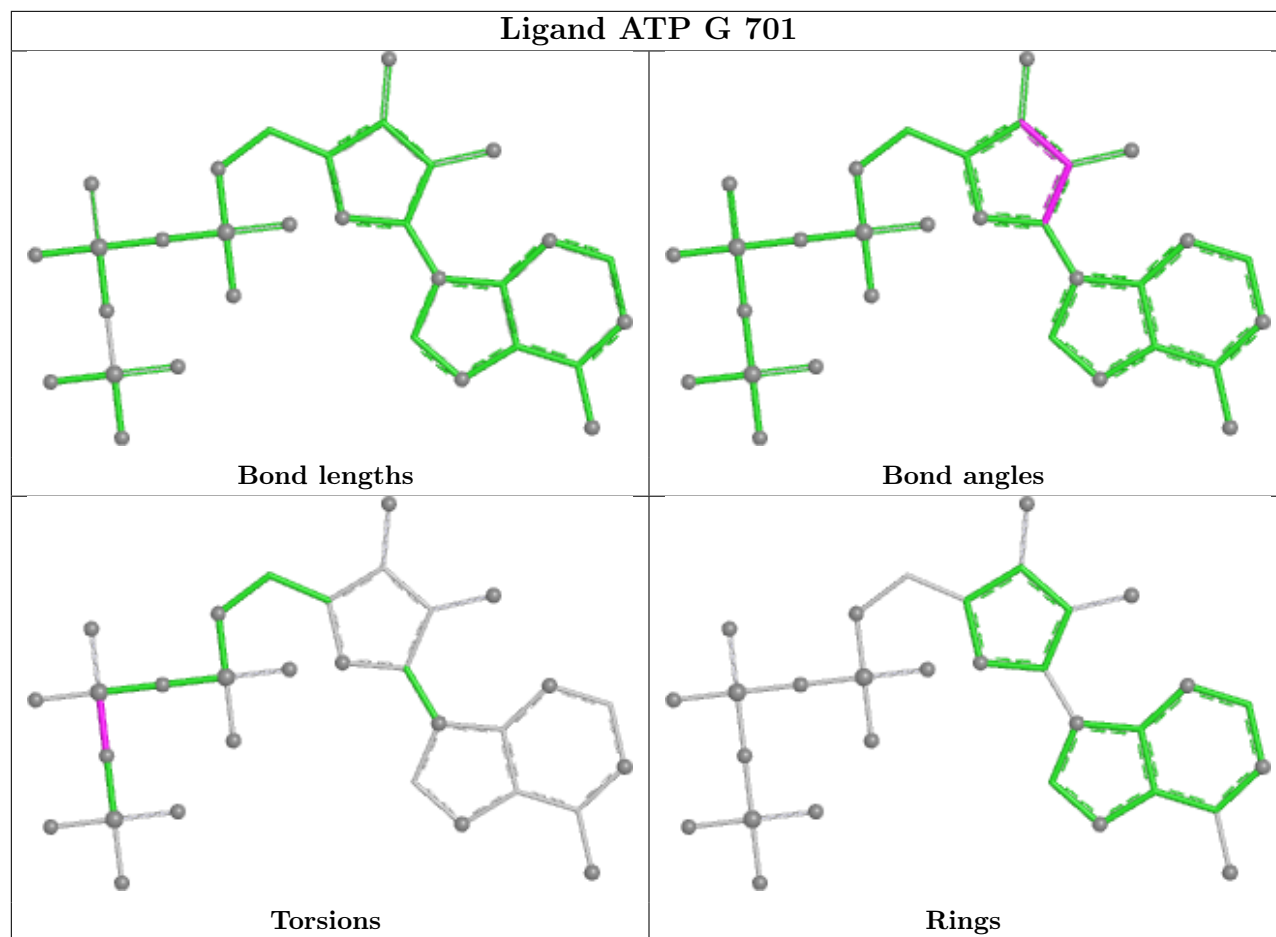


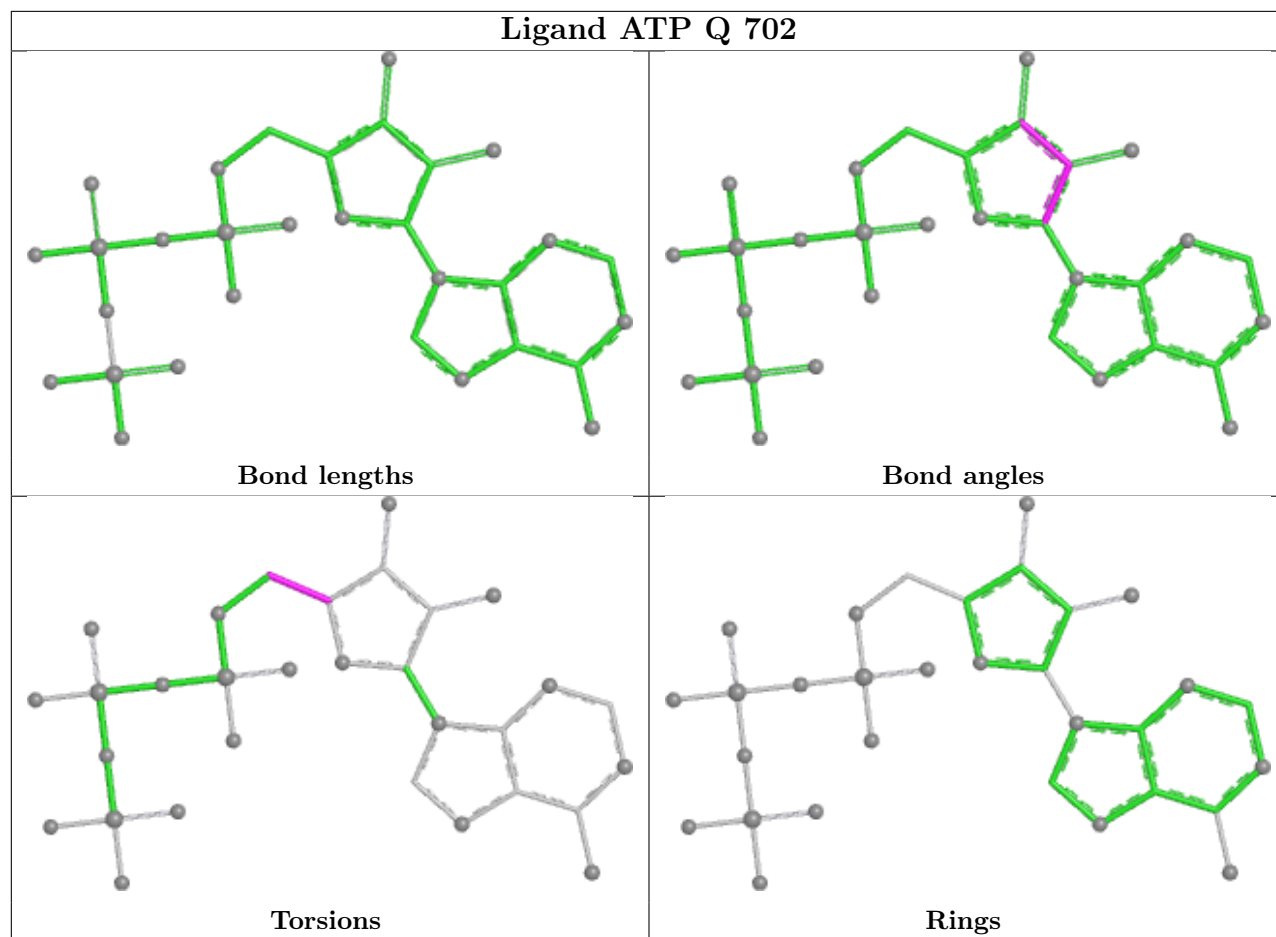


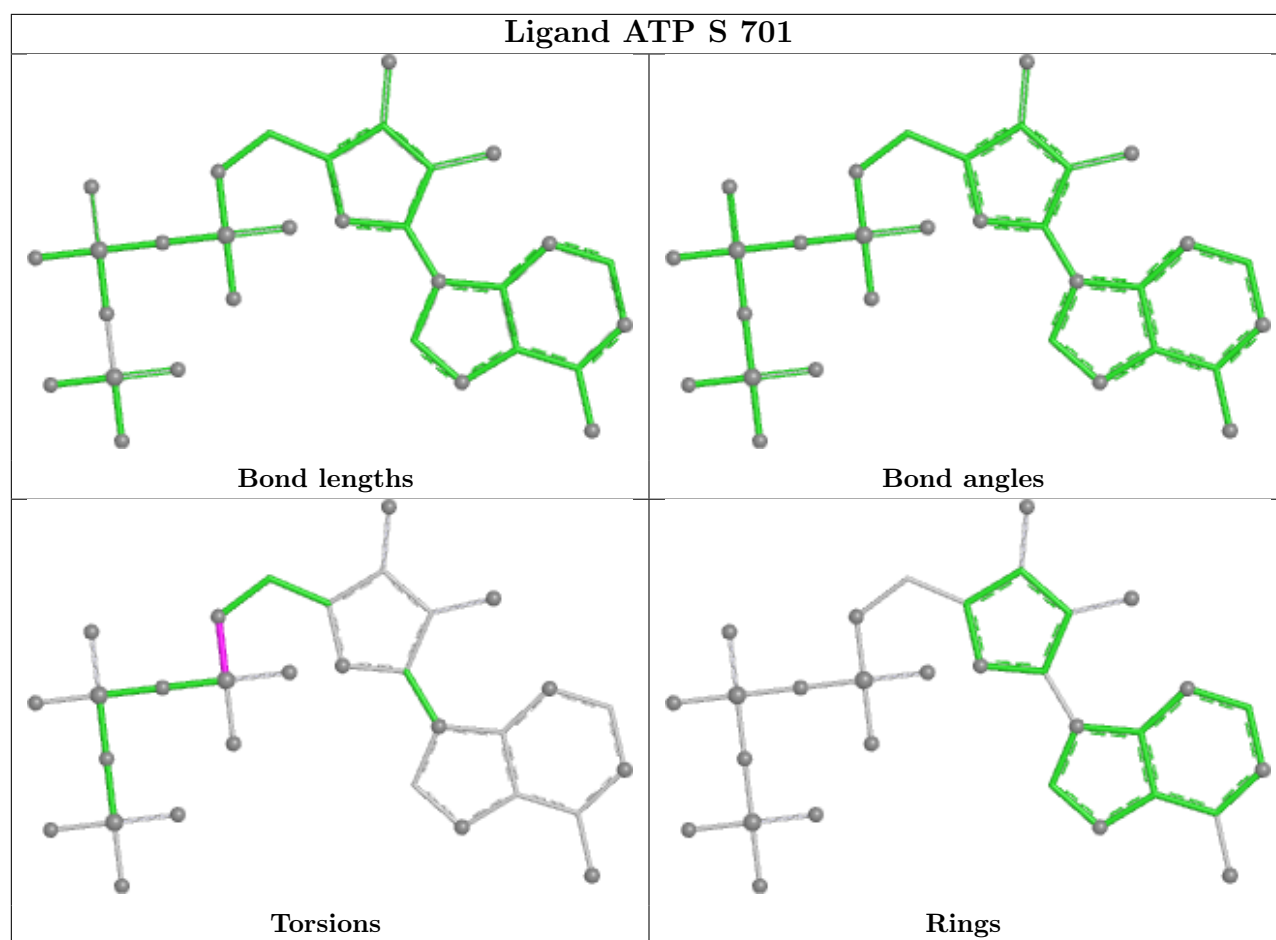
Ligand ATP J 702

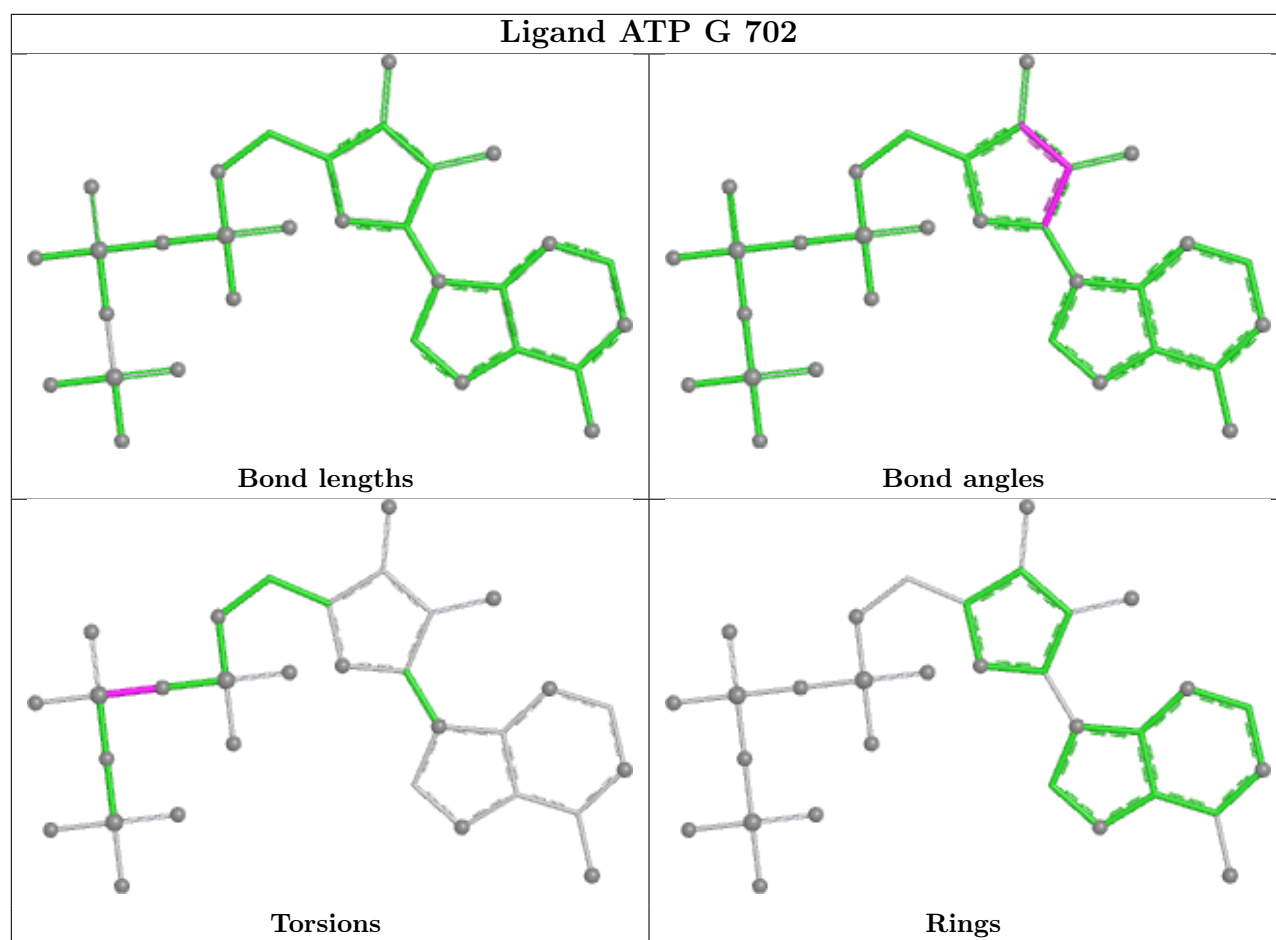


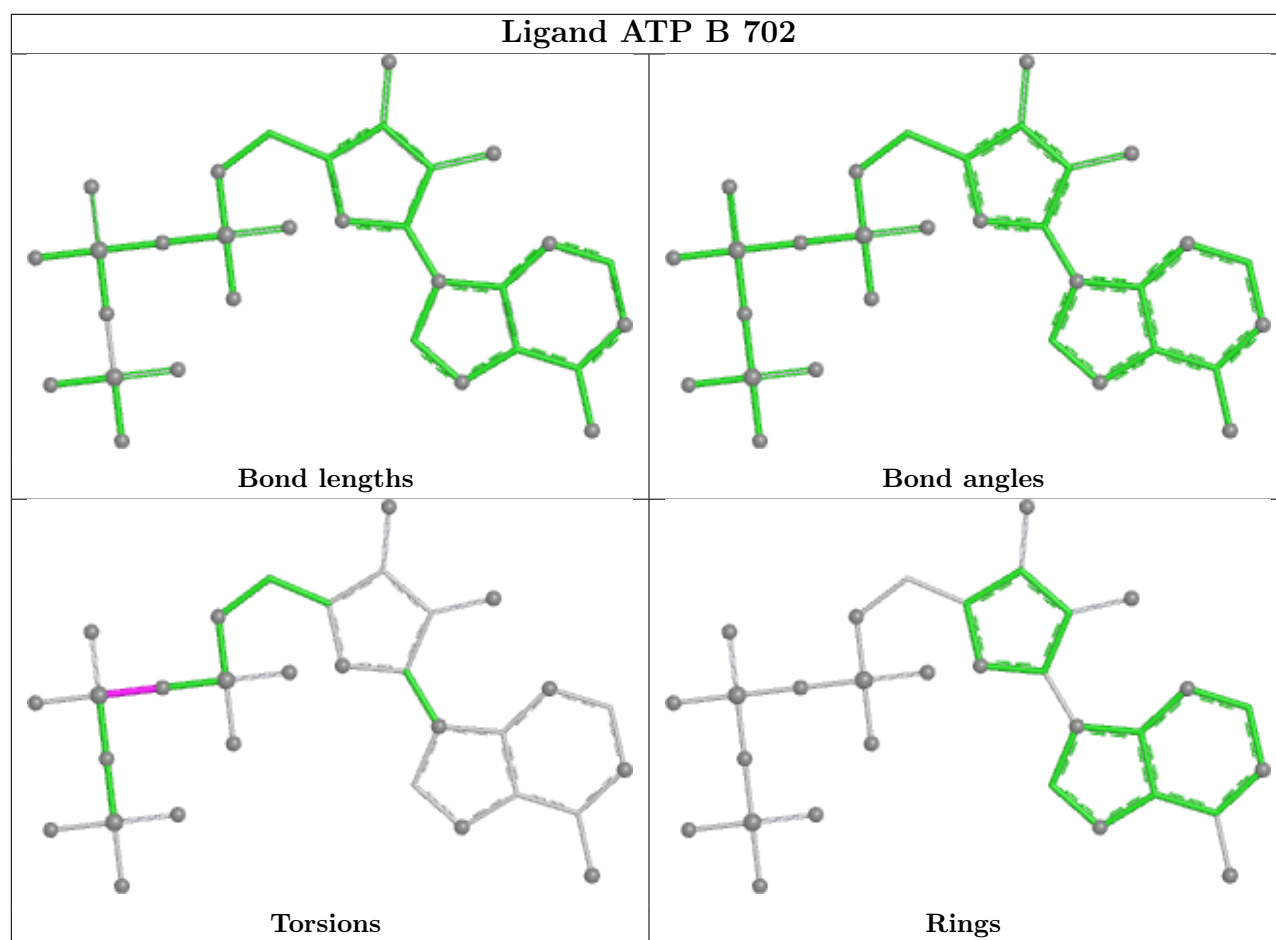


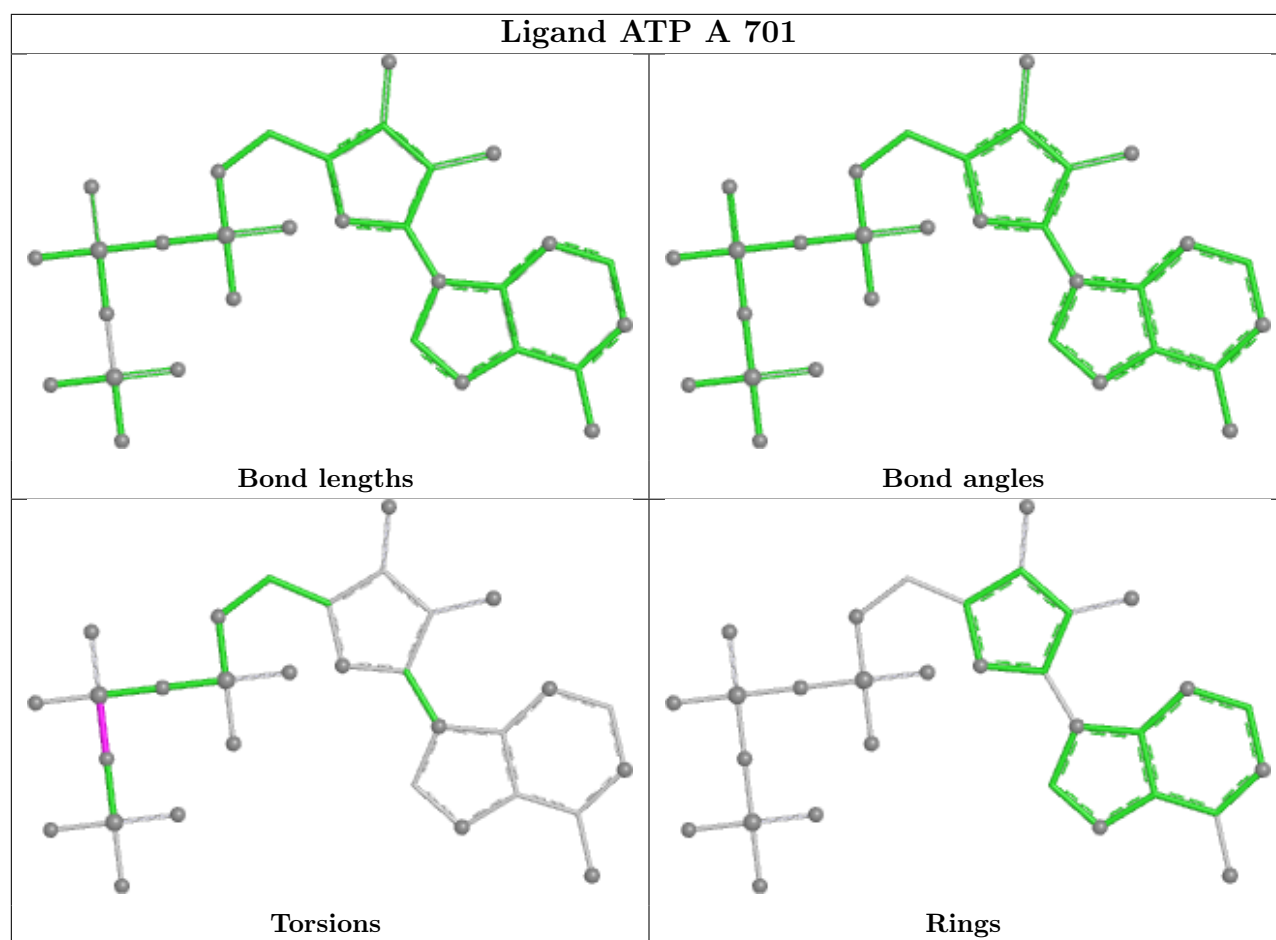


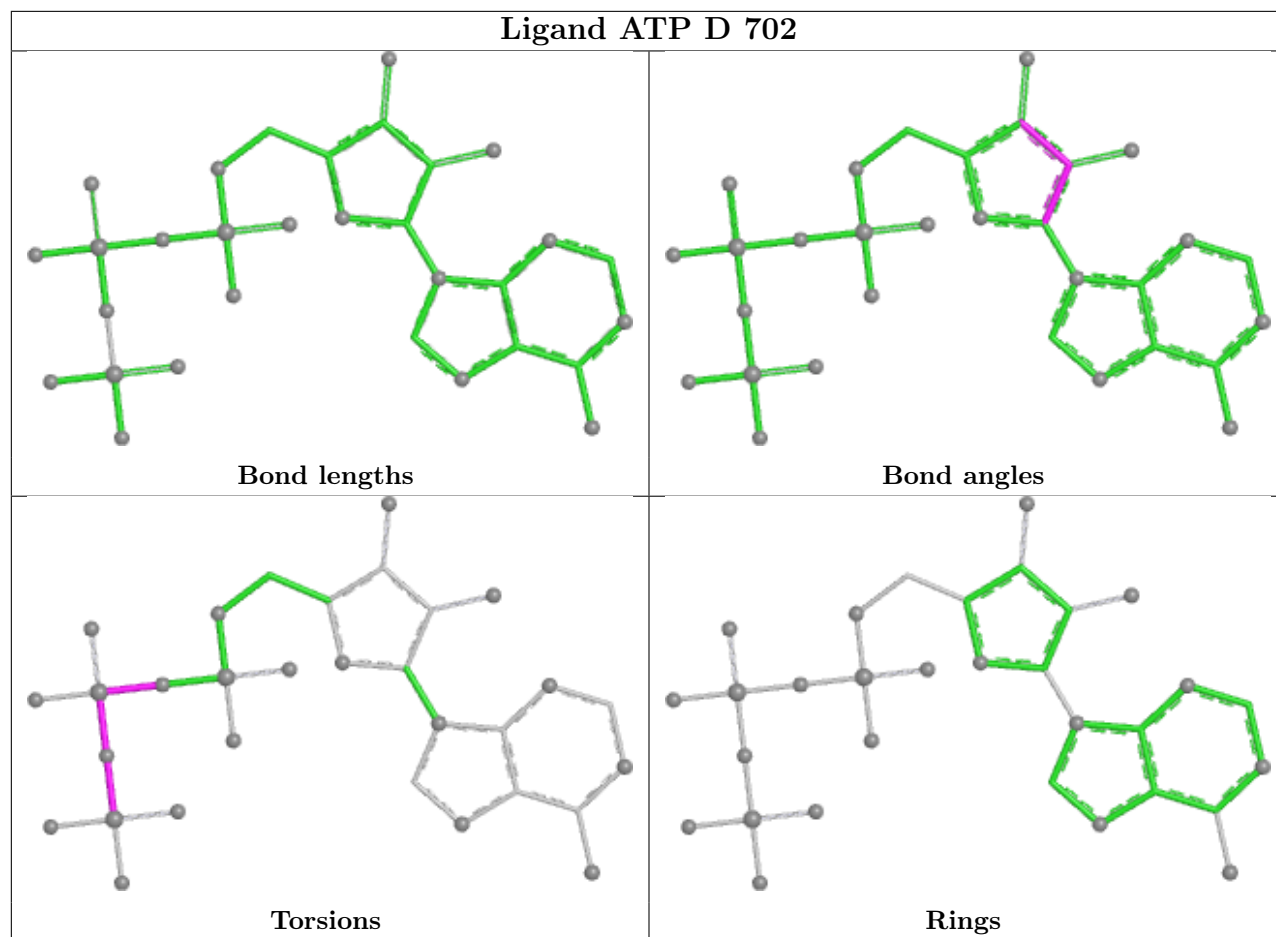


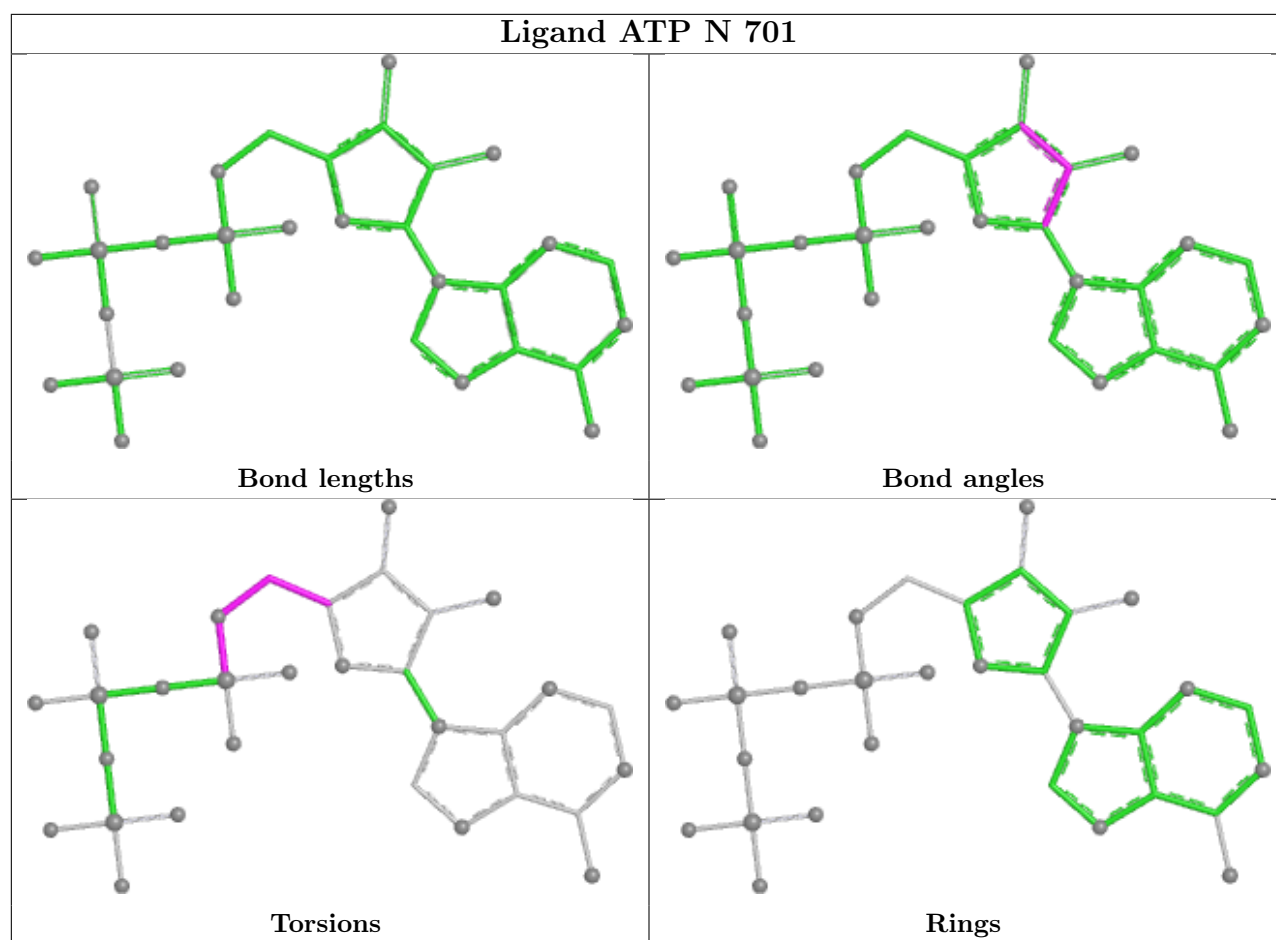


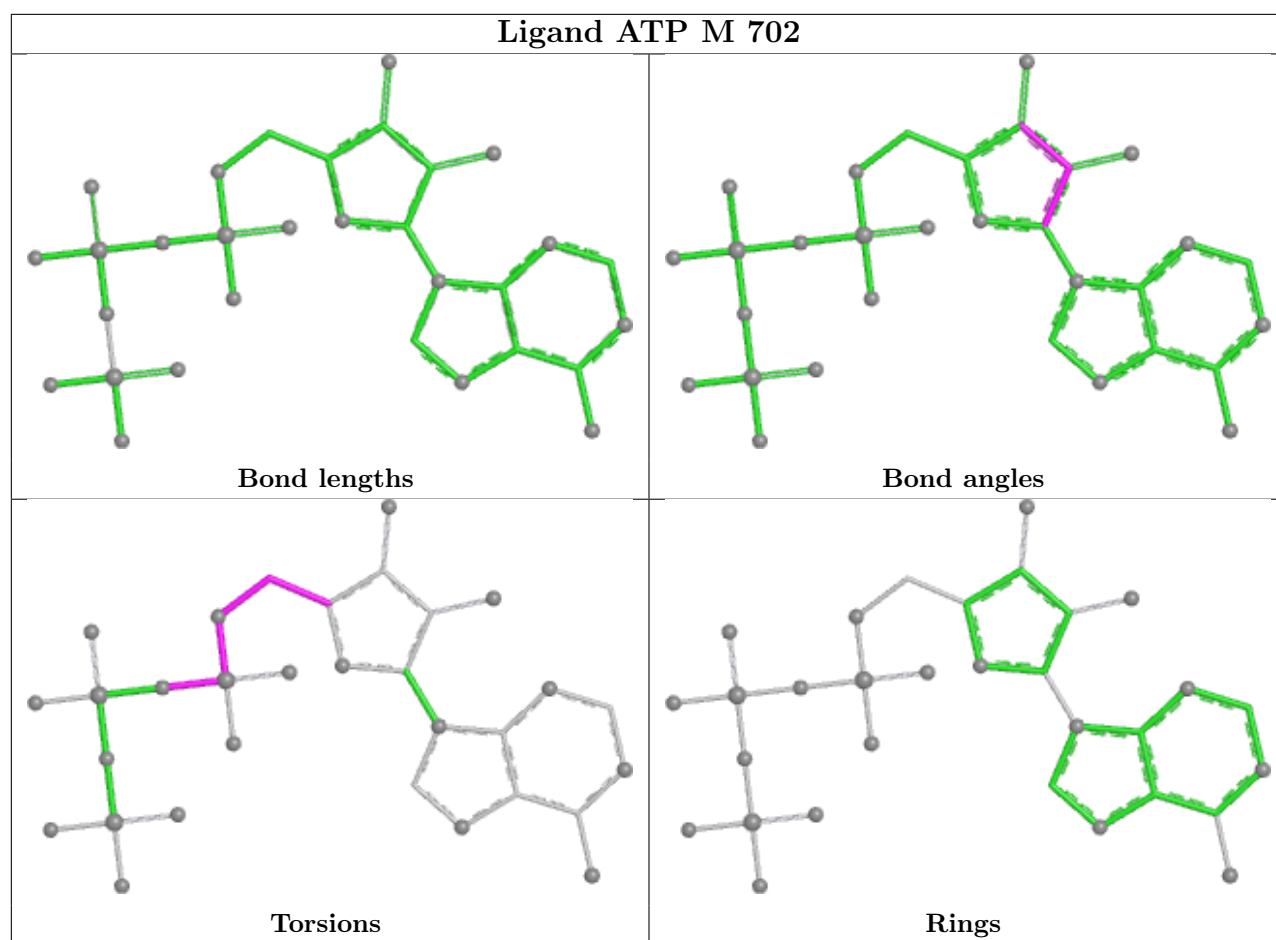


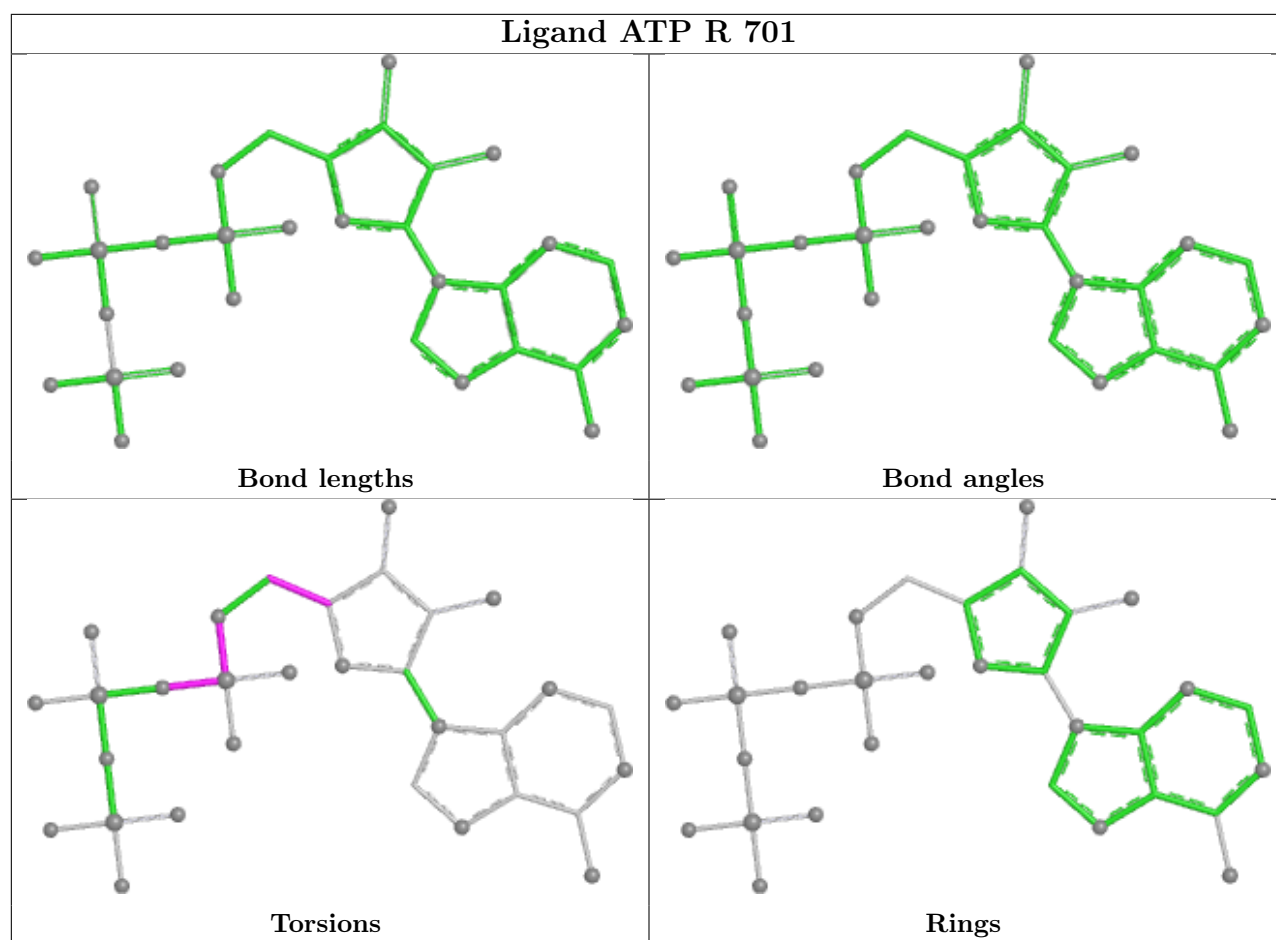


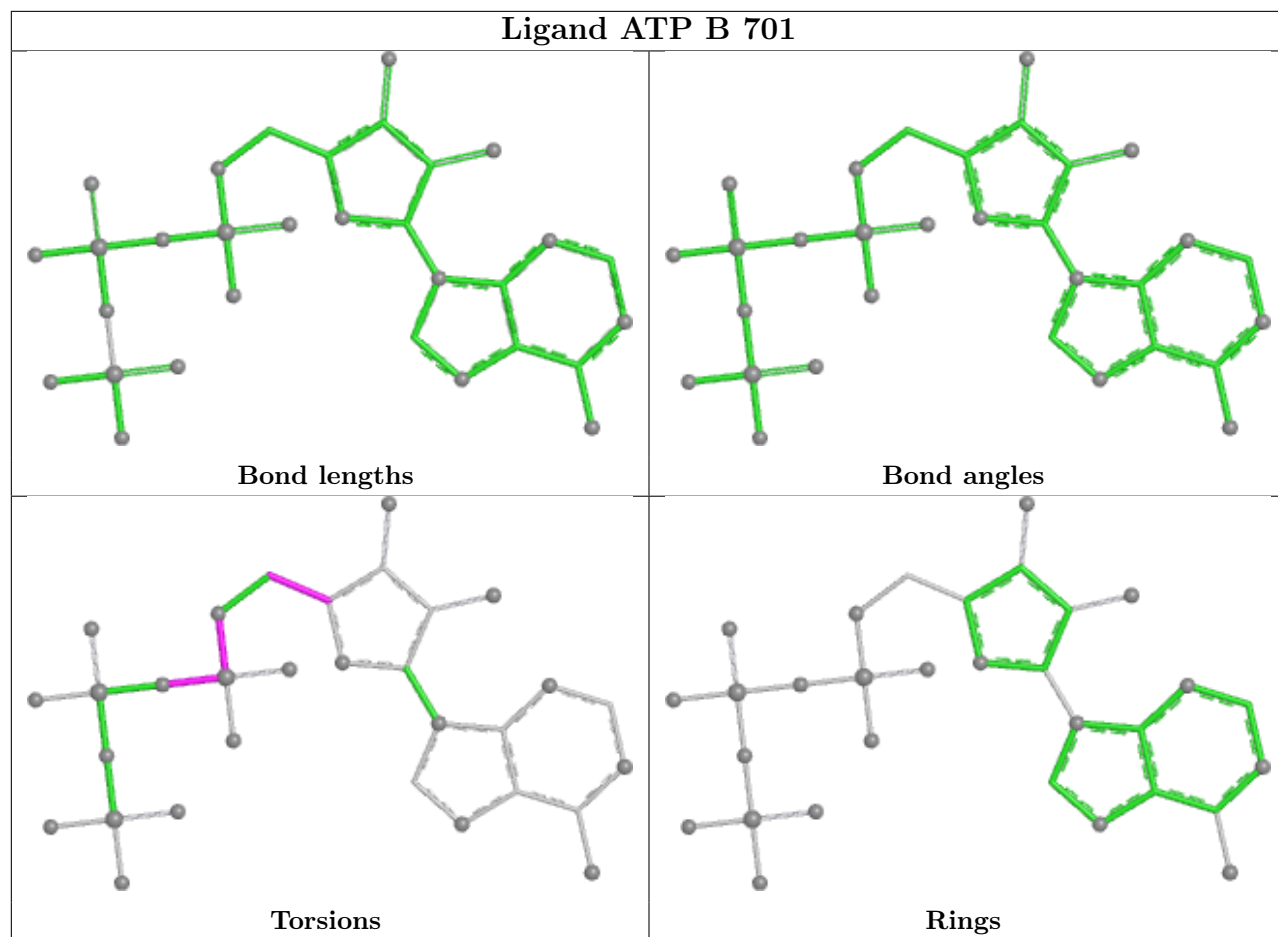


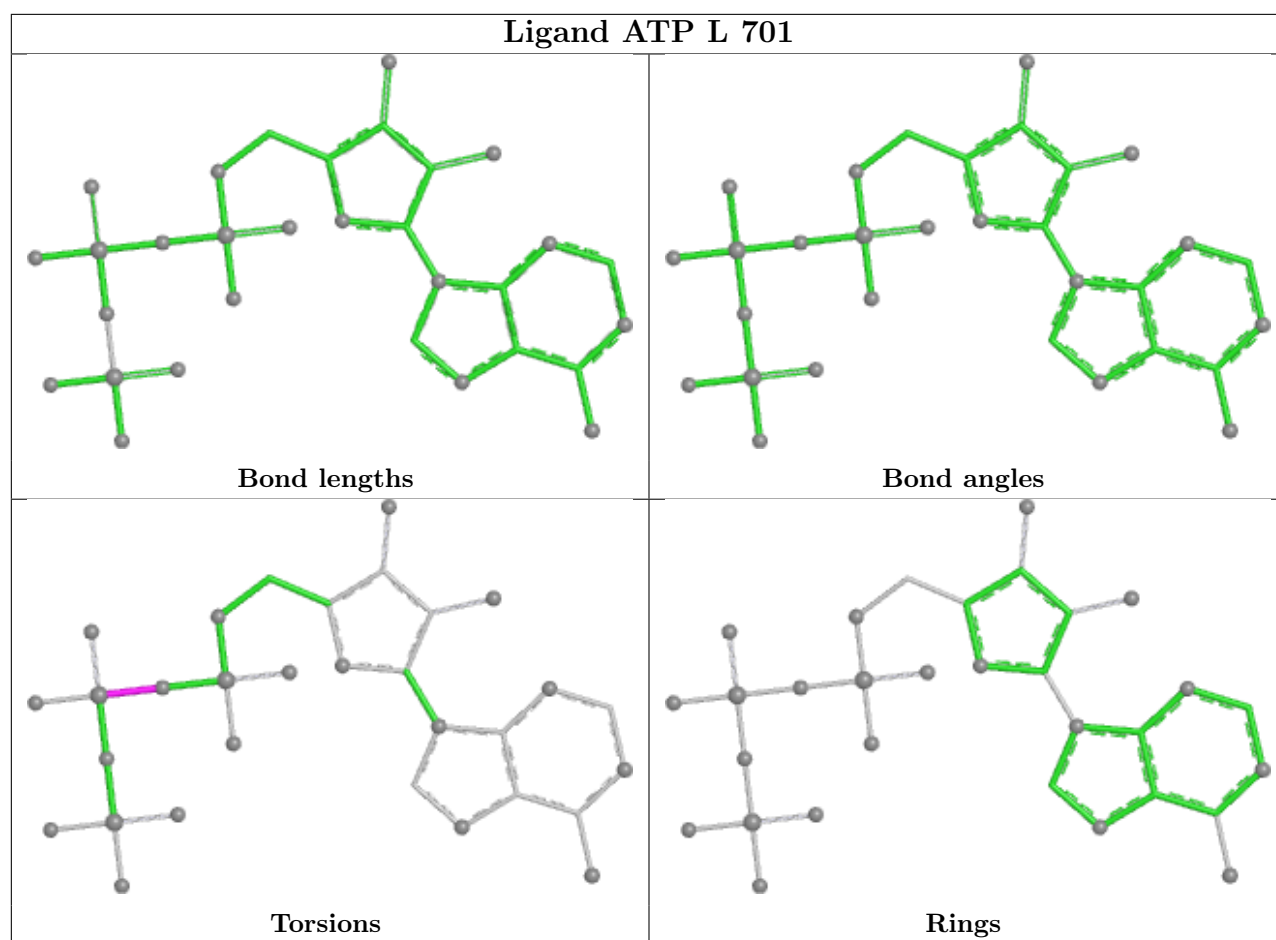




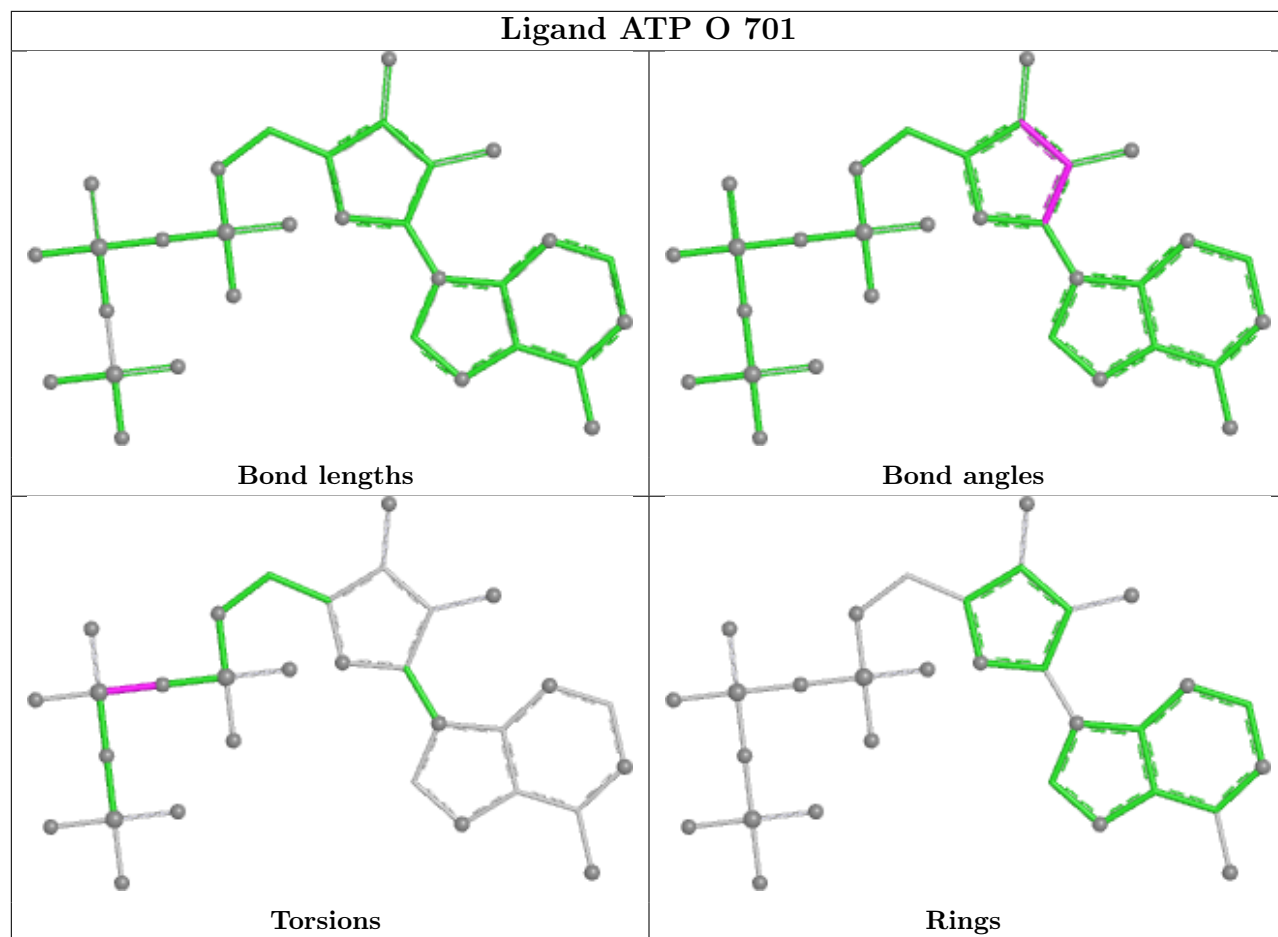




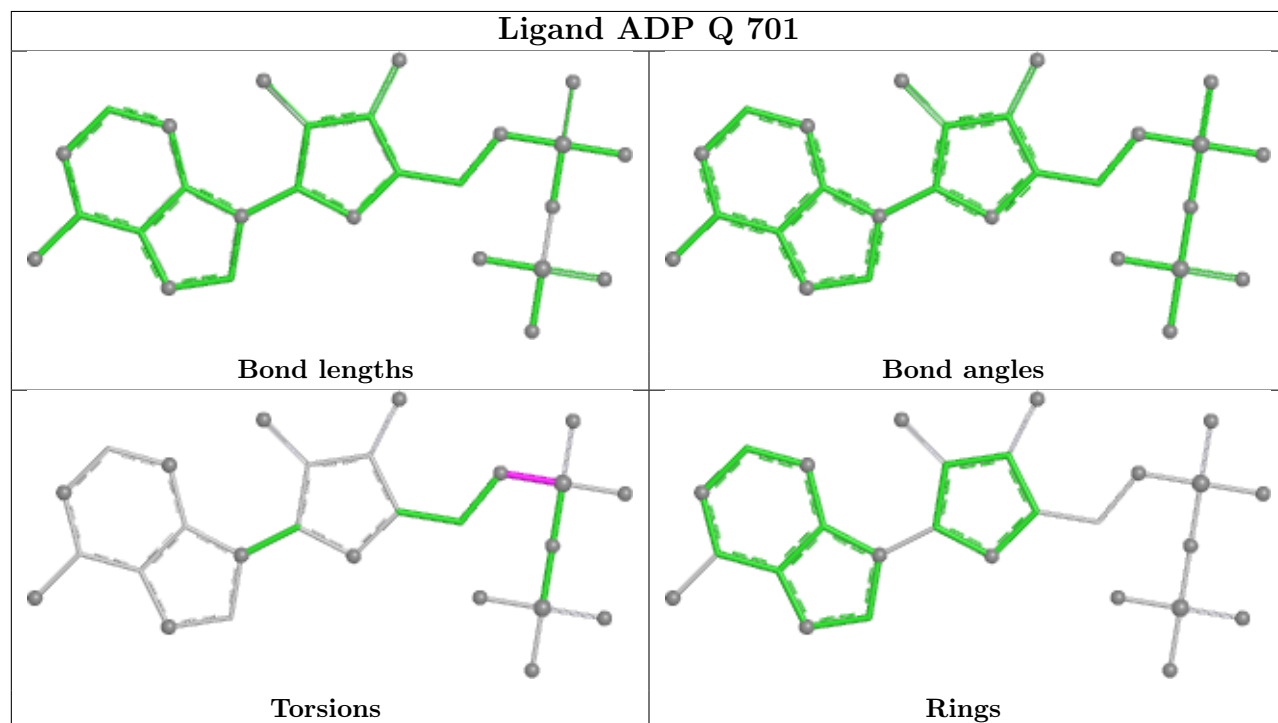


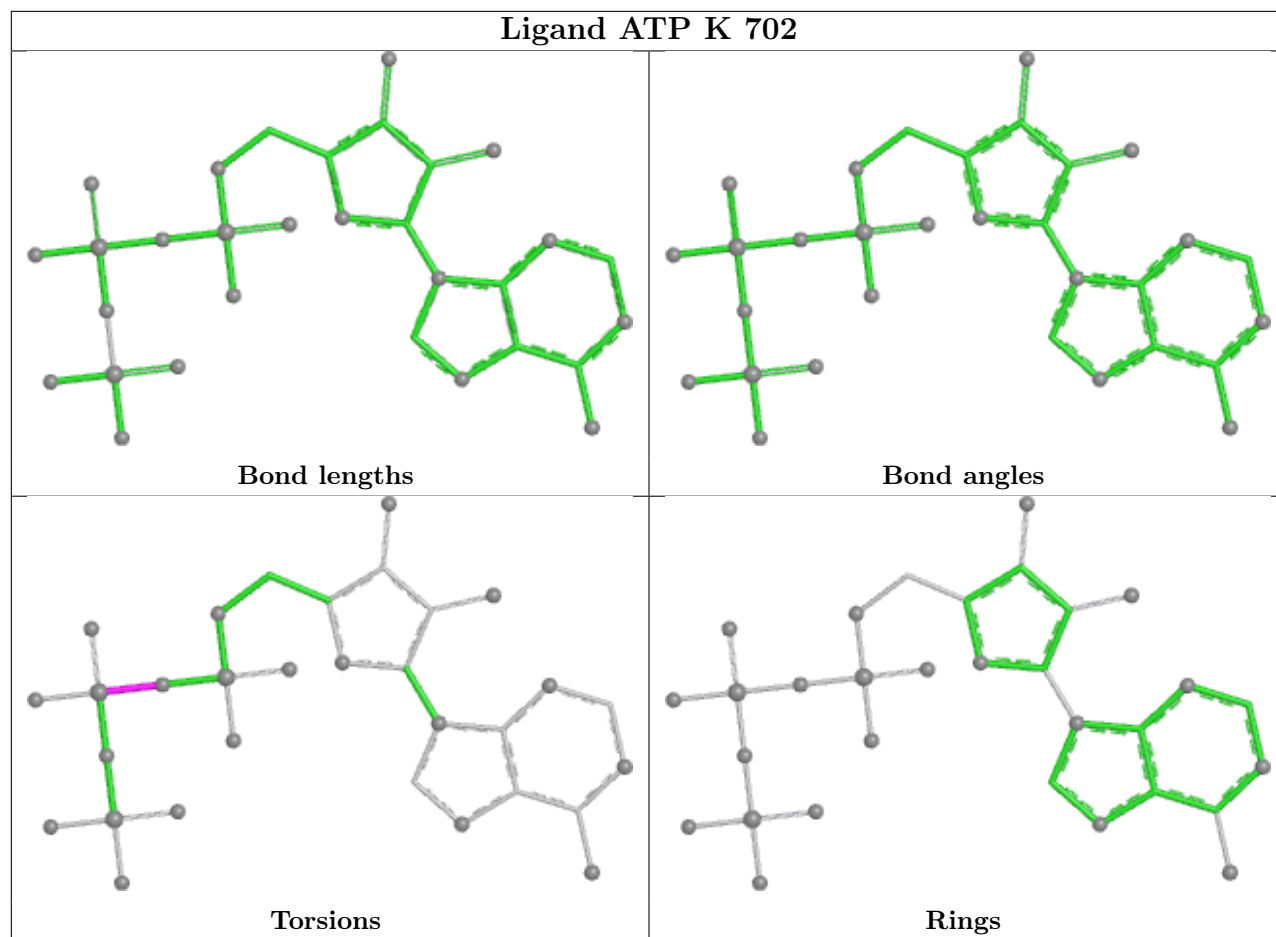


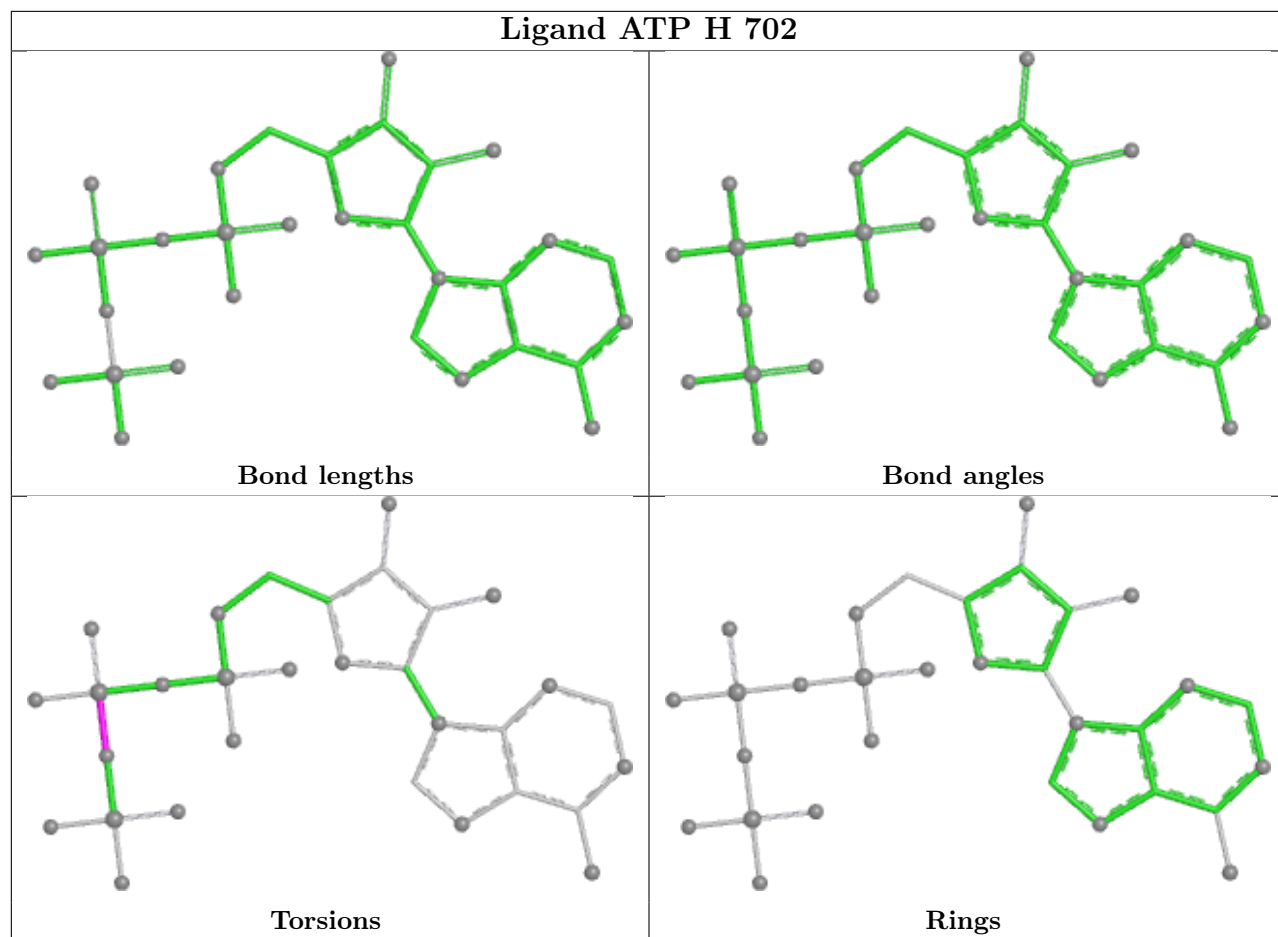
Ligand ATP O 701

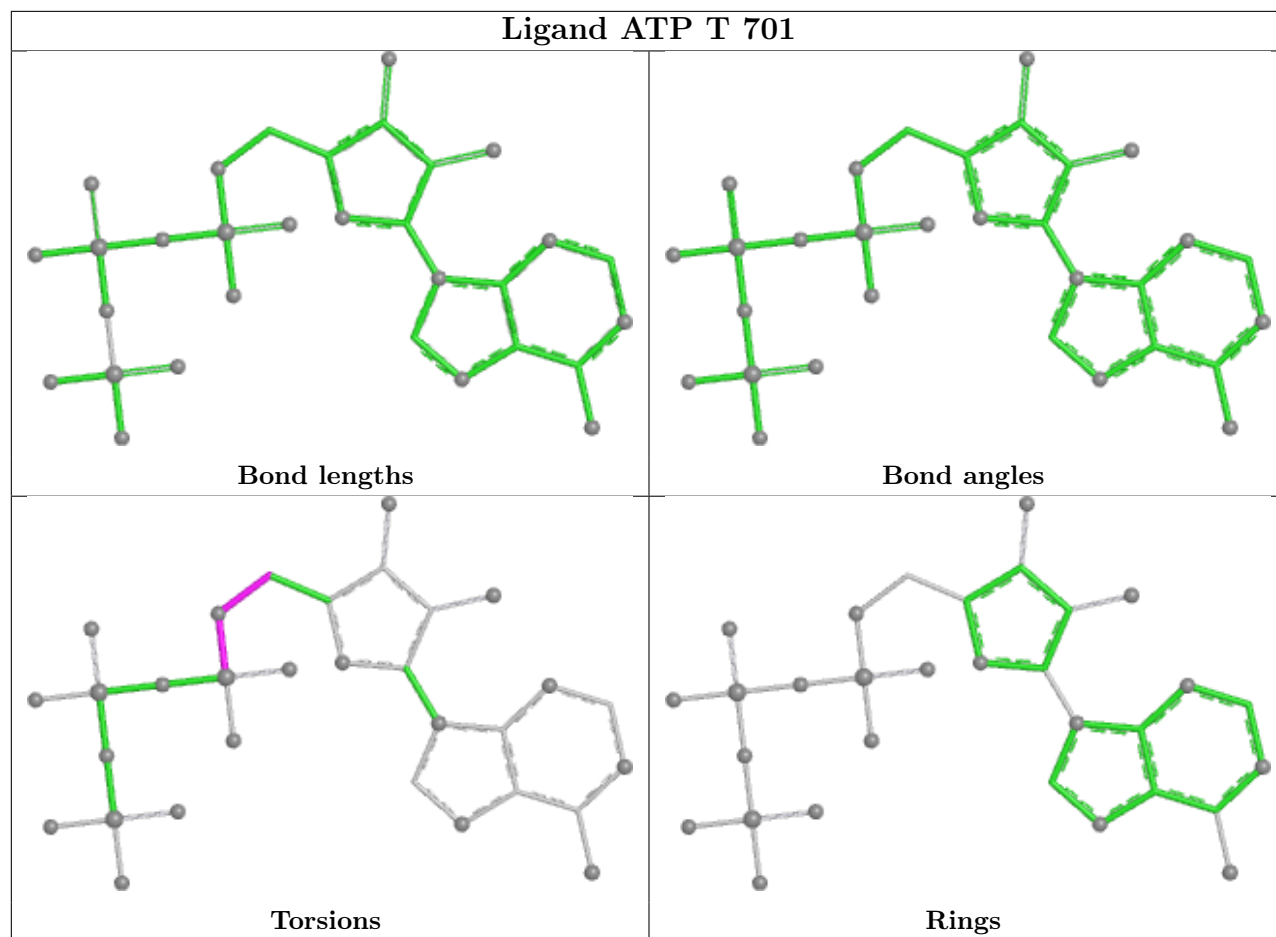


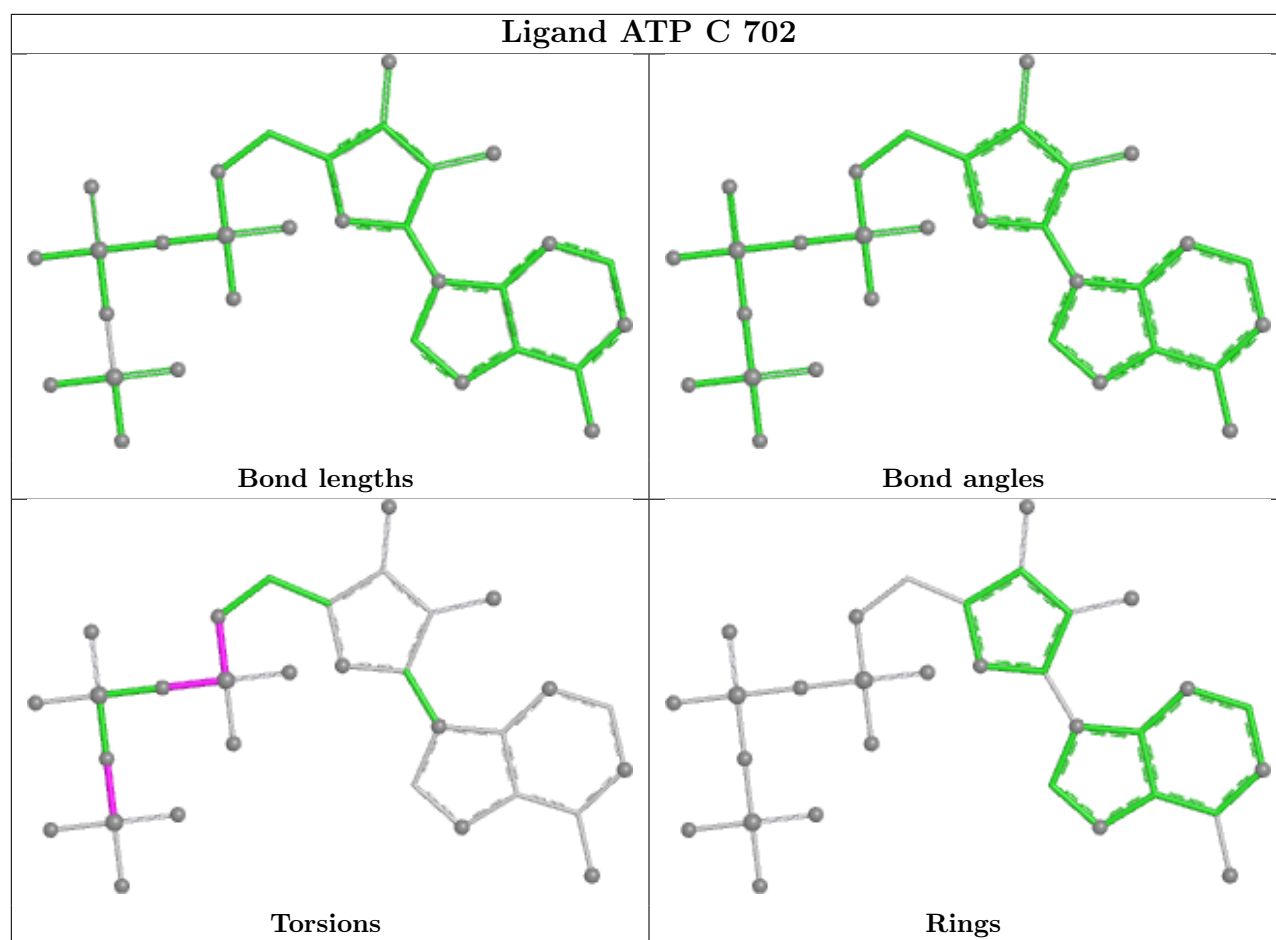
Ligand ADP Q 701

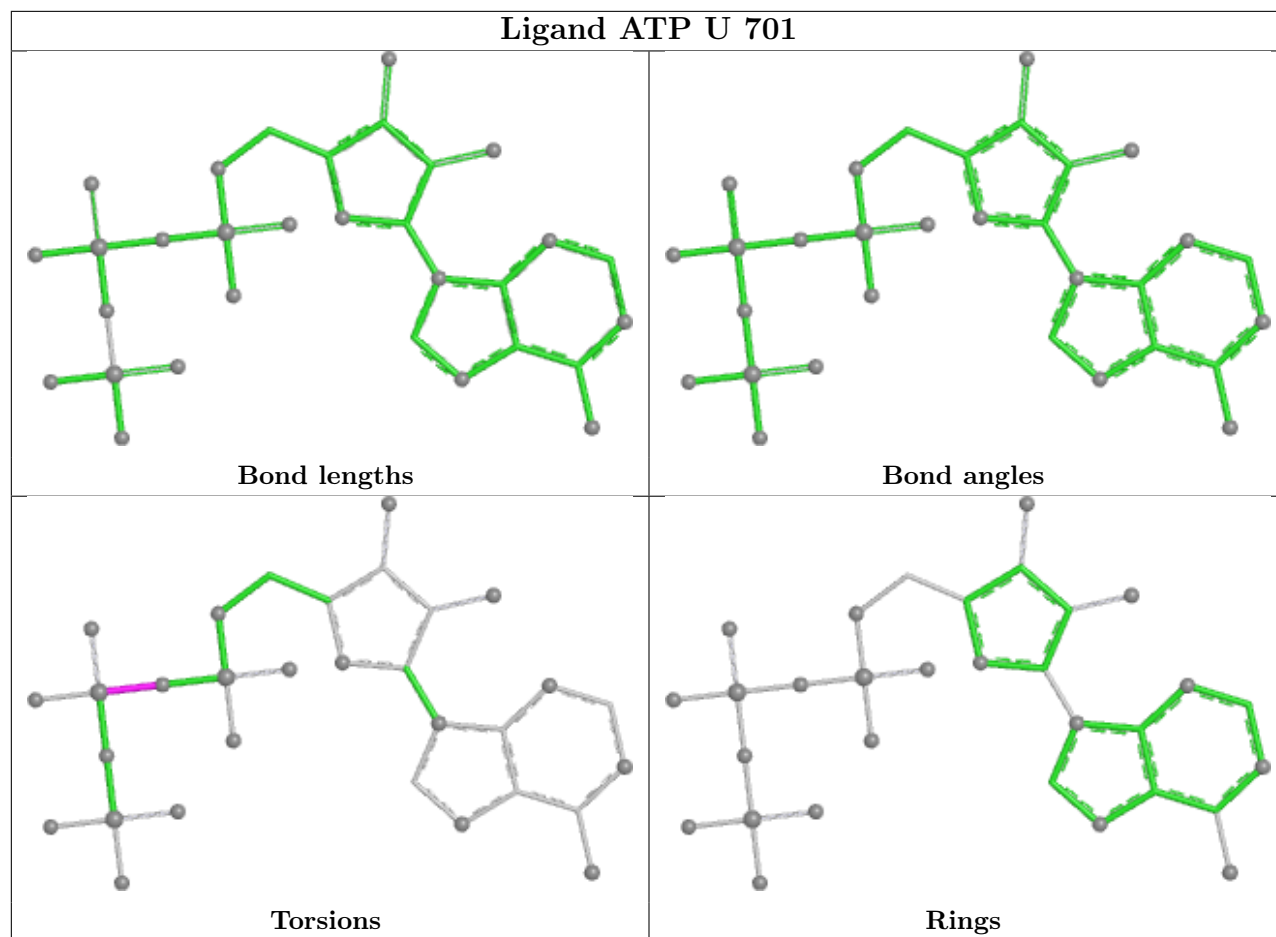


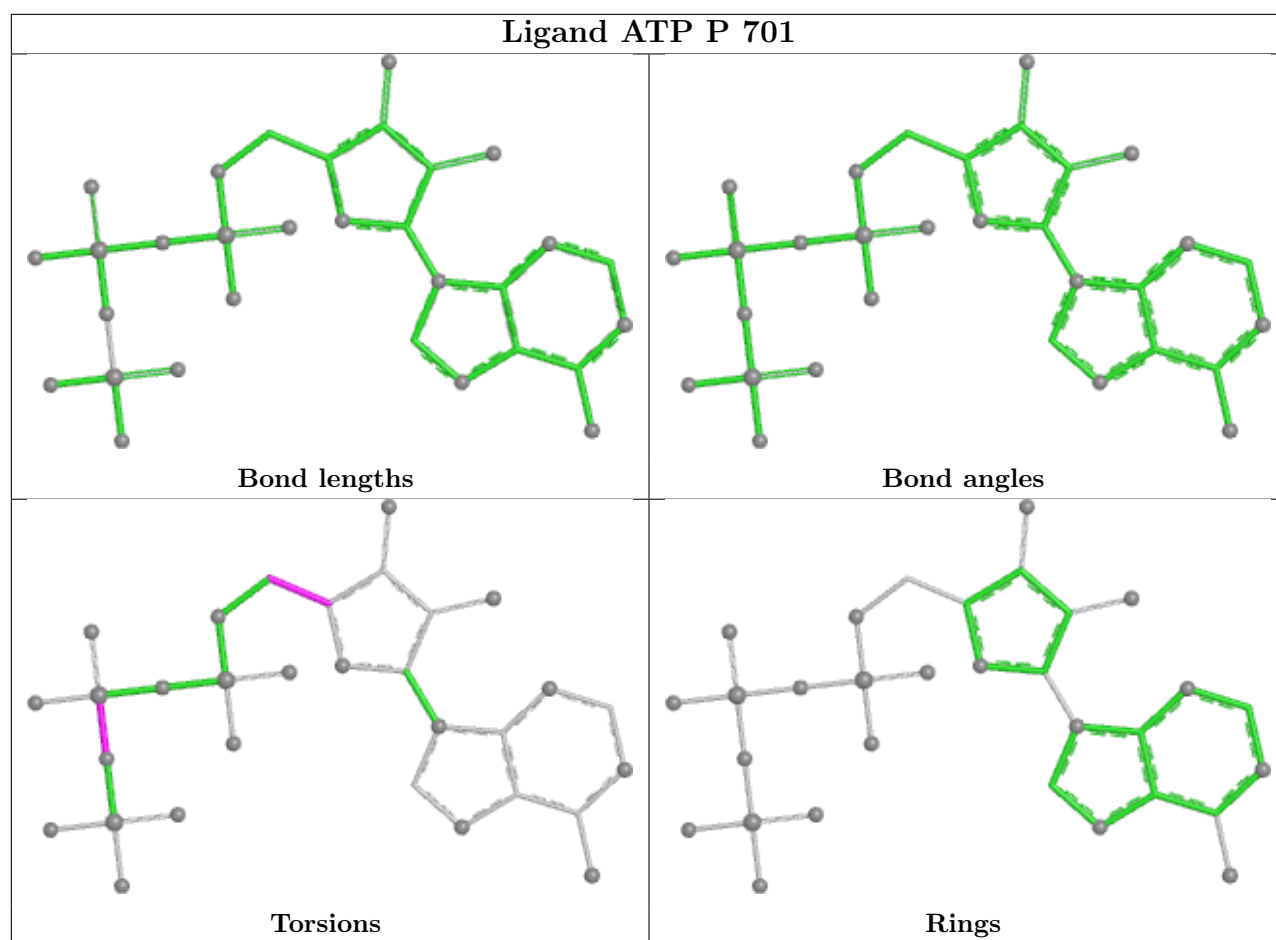


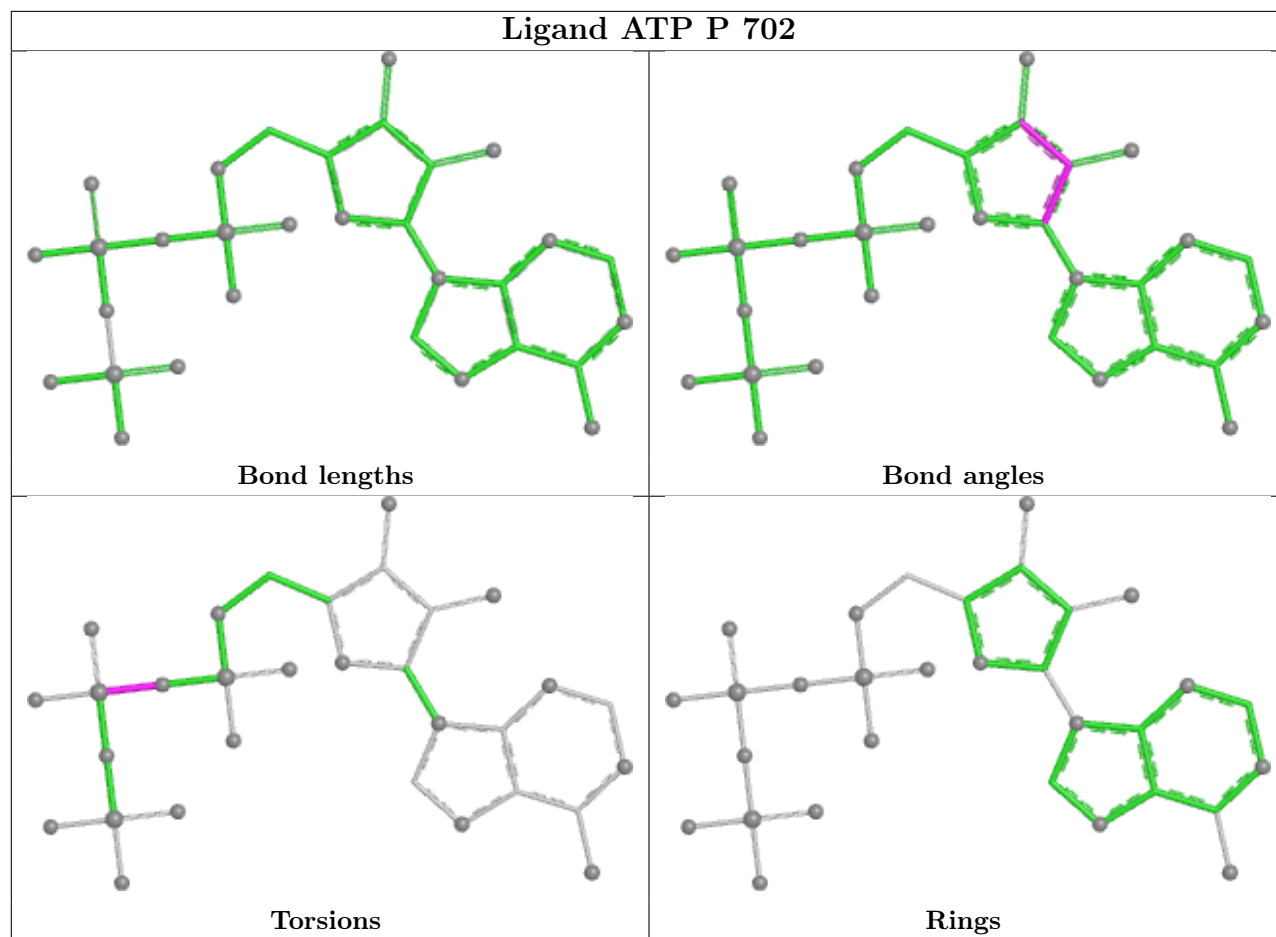


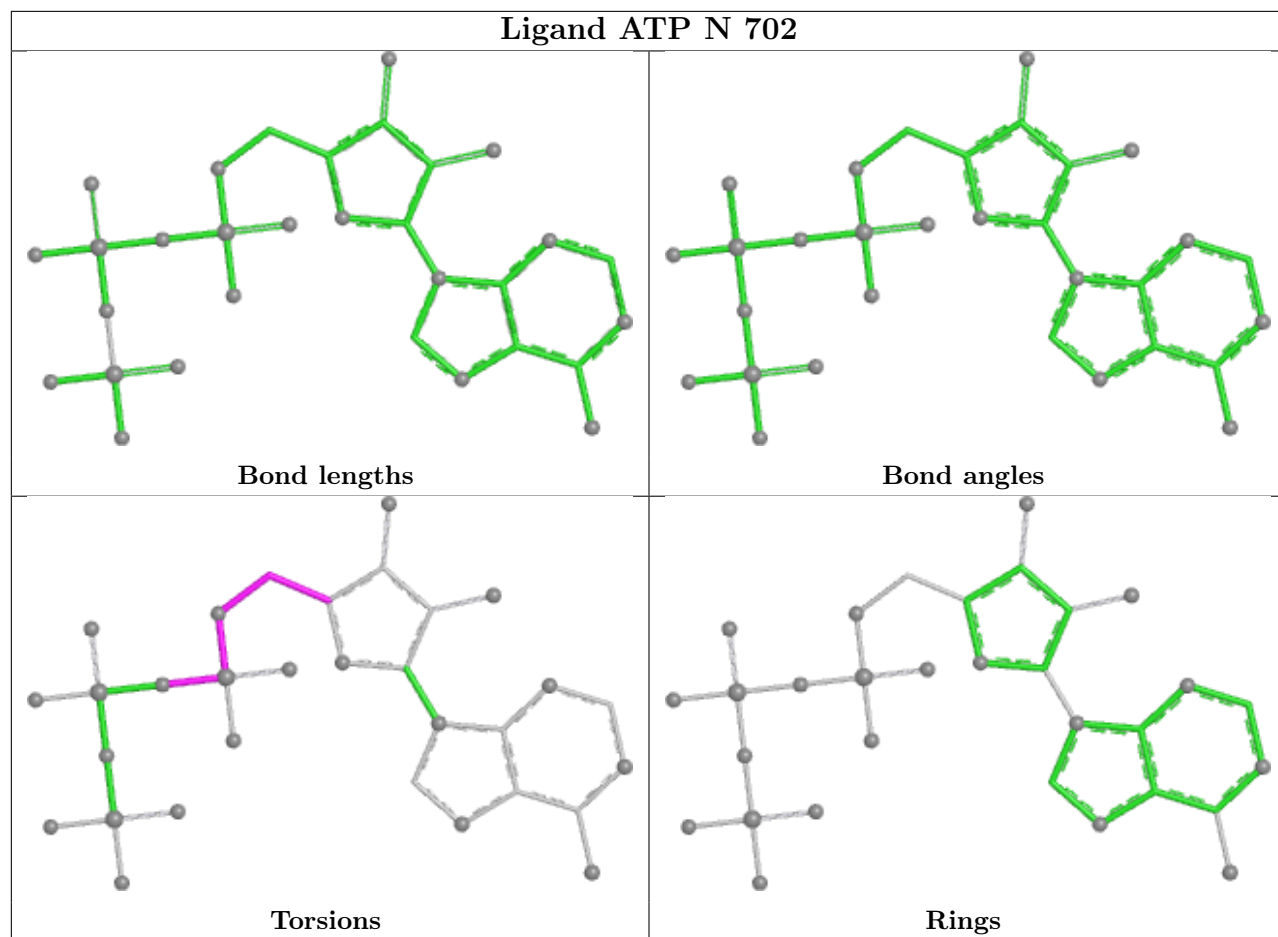


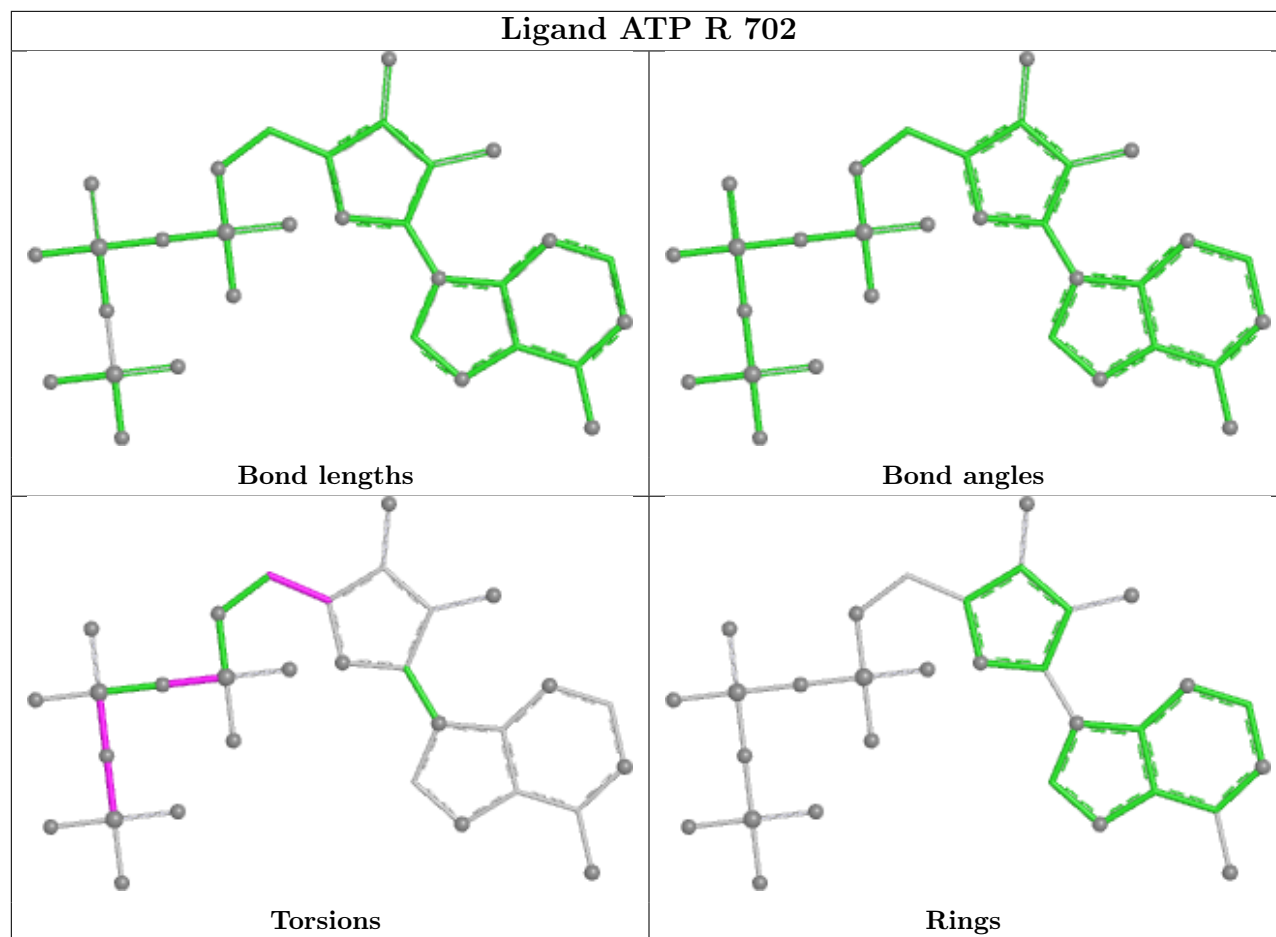


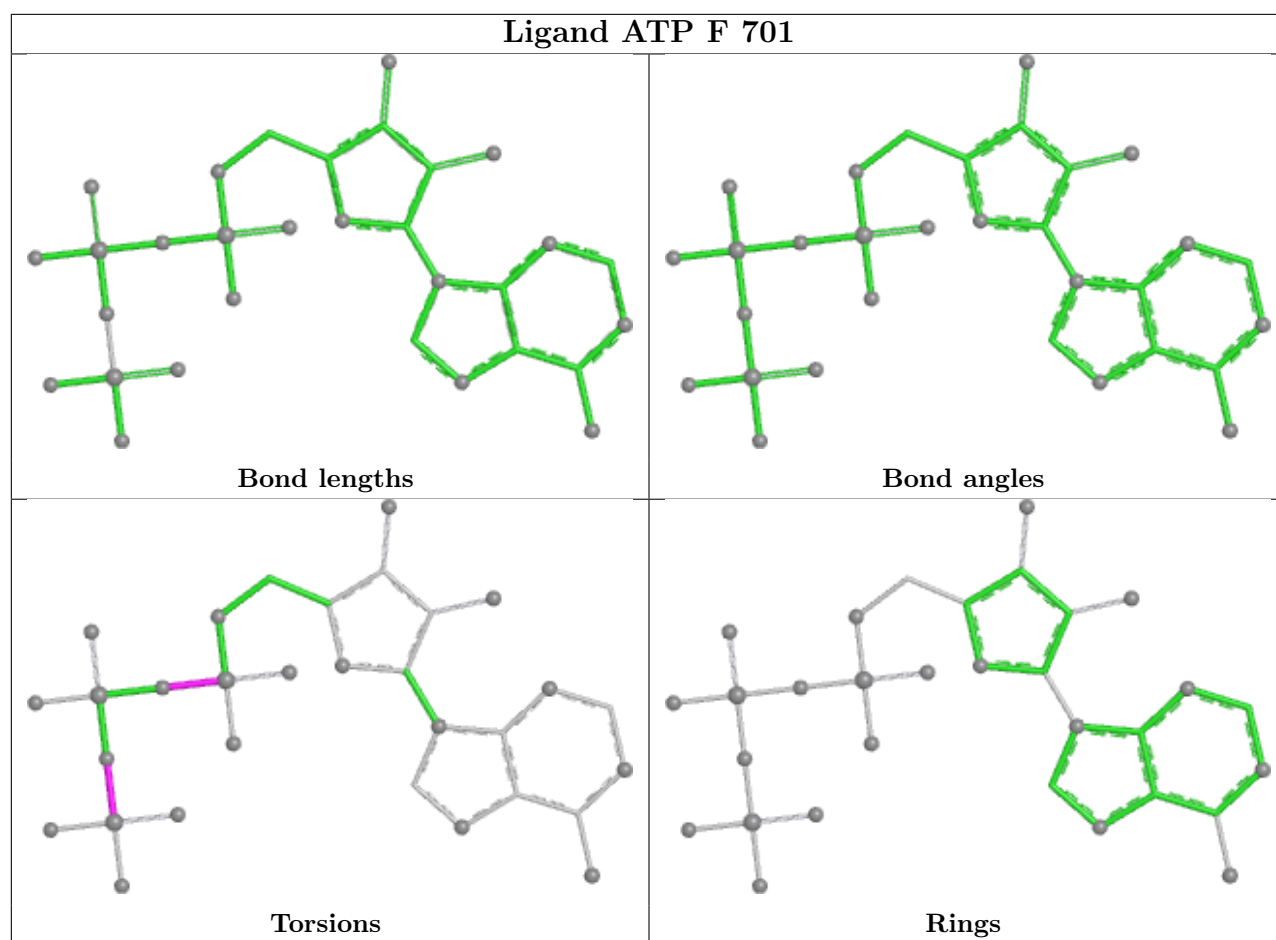


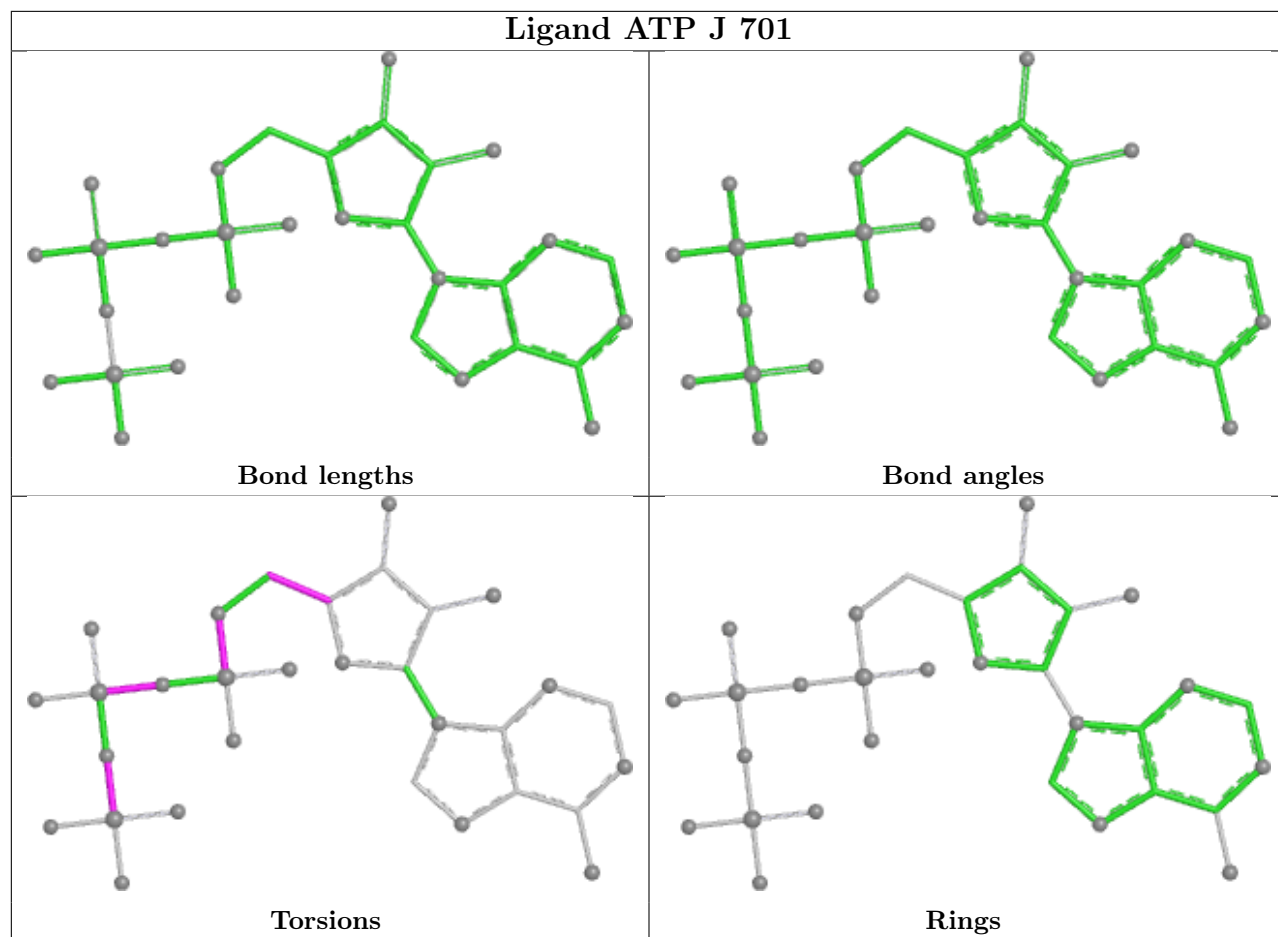




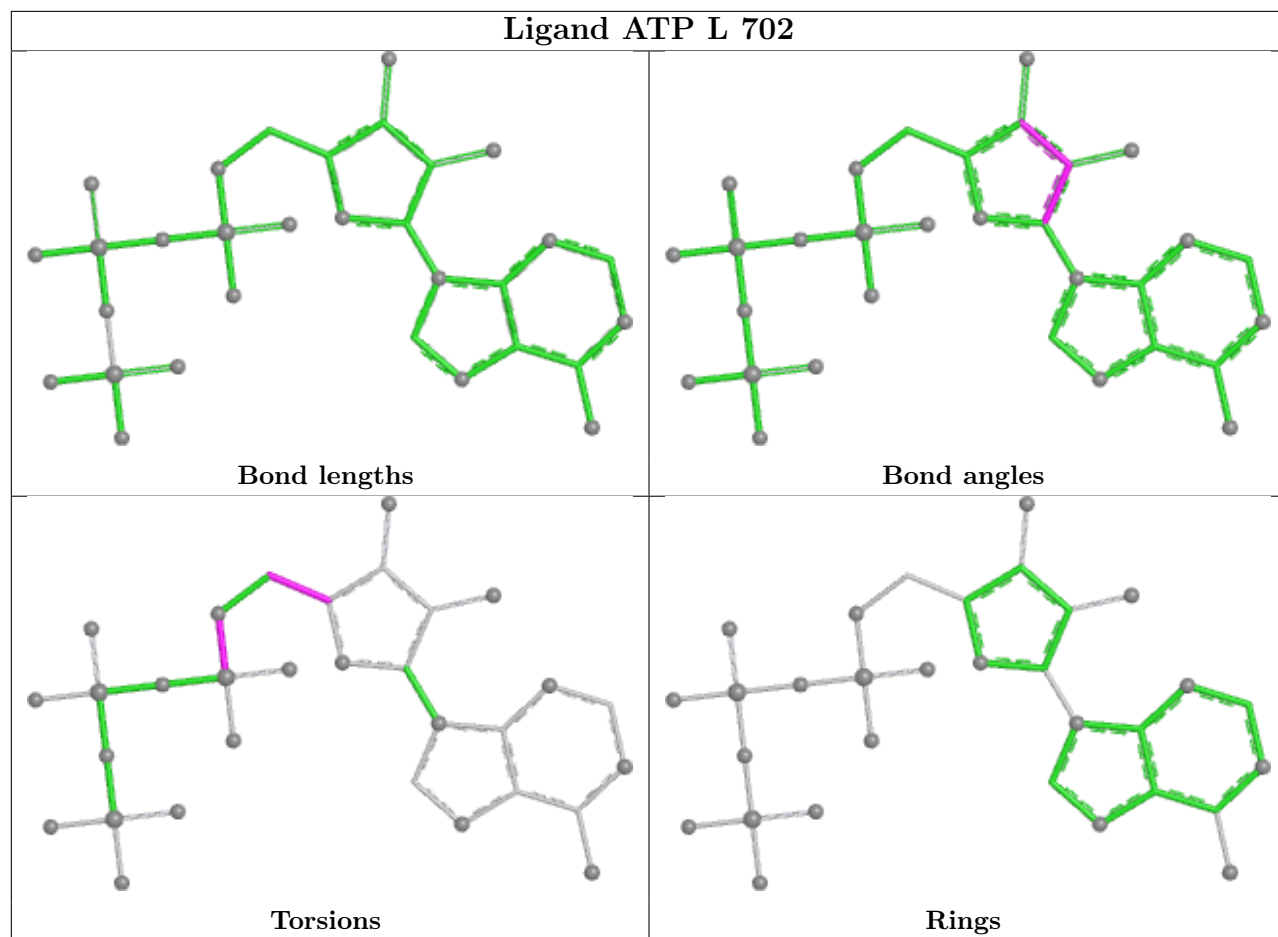


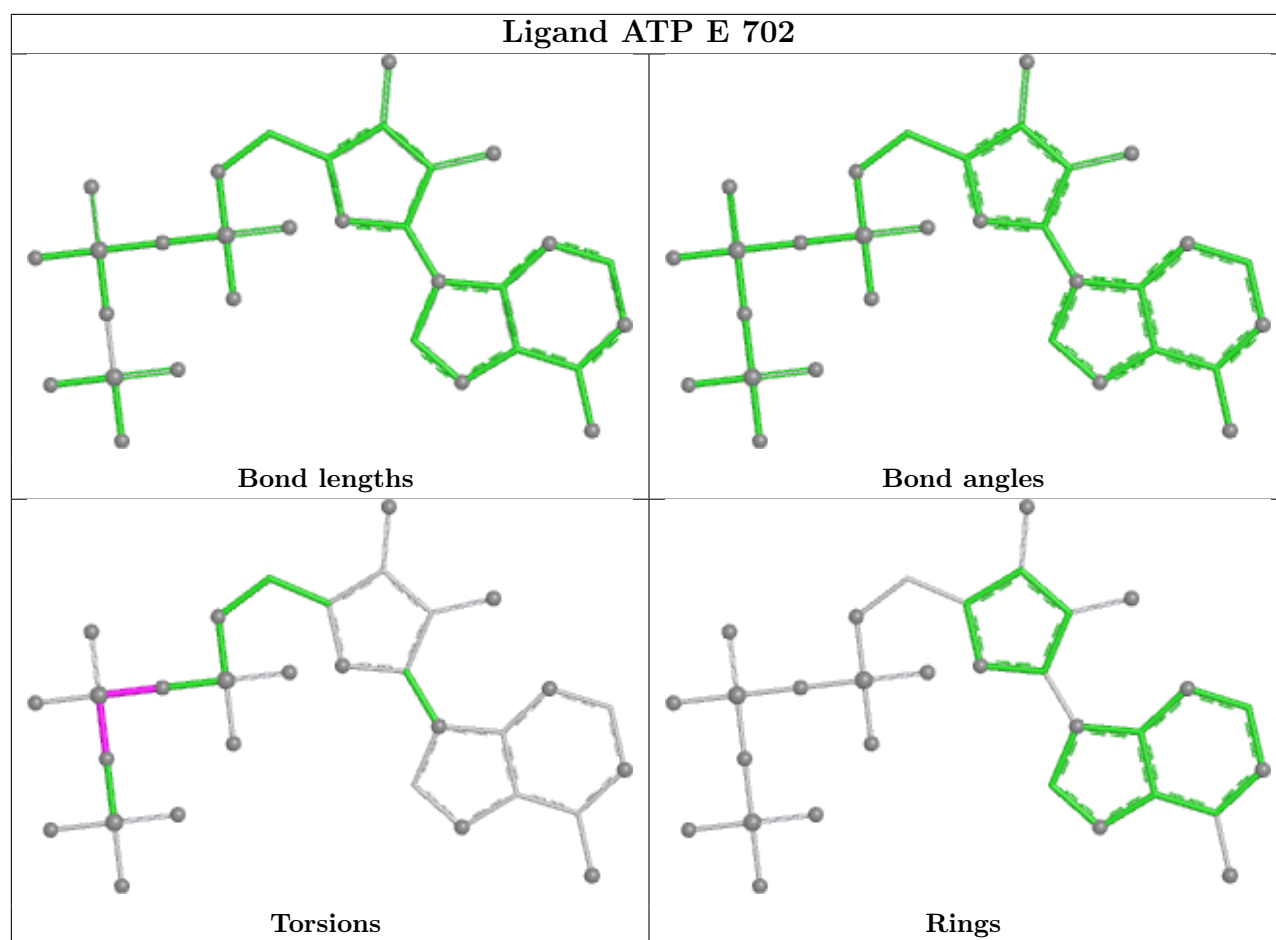


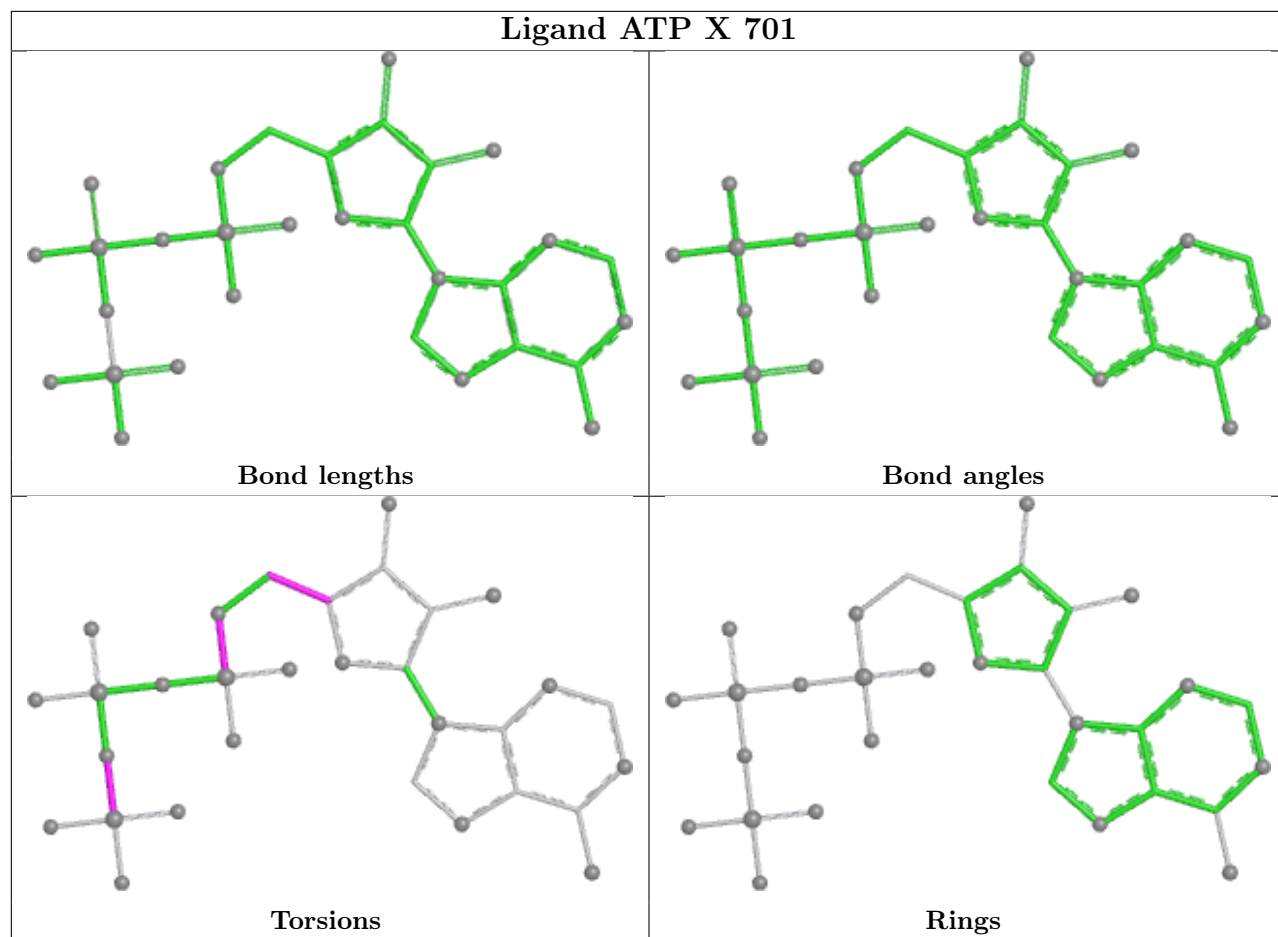


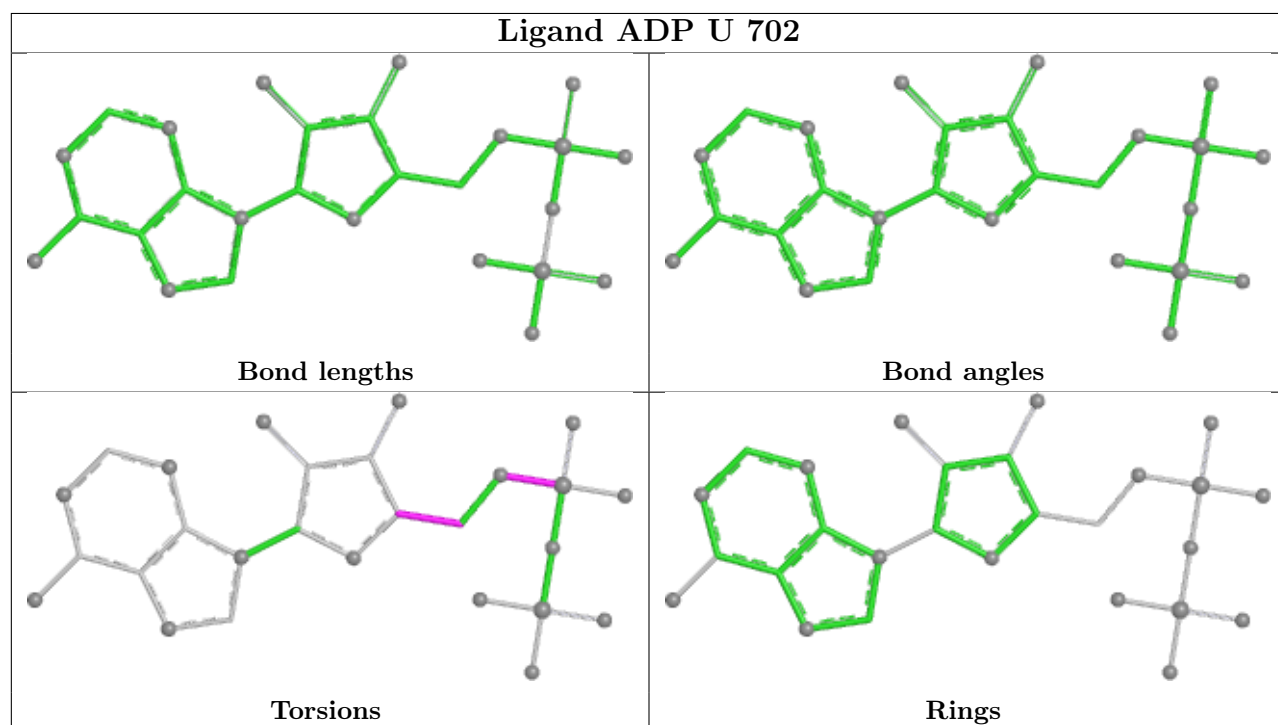
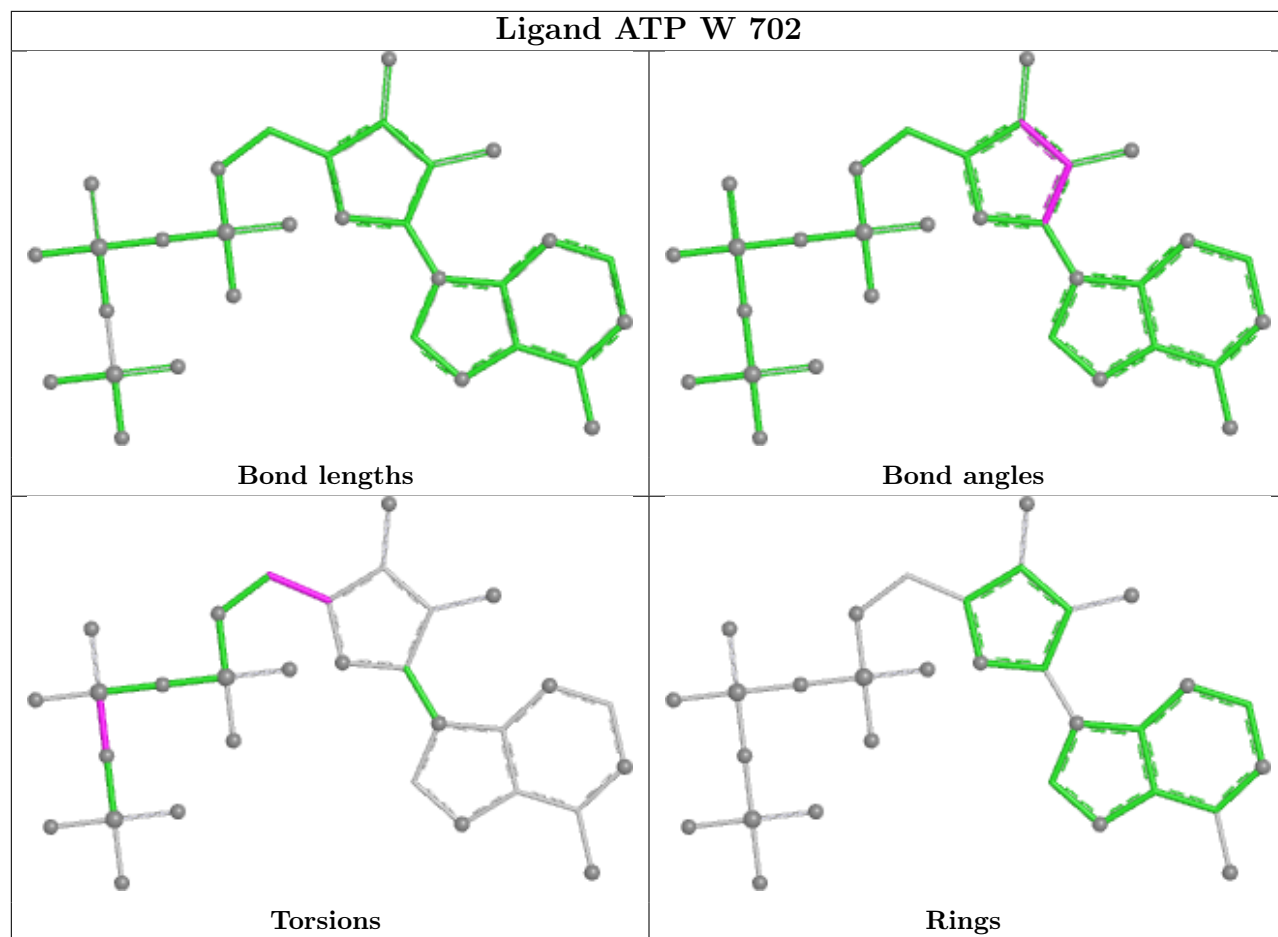


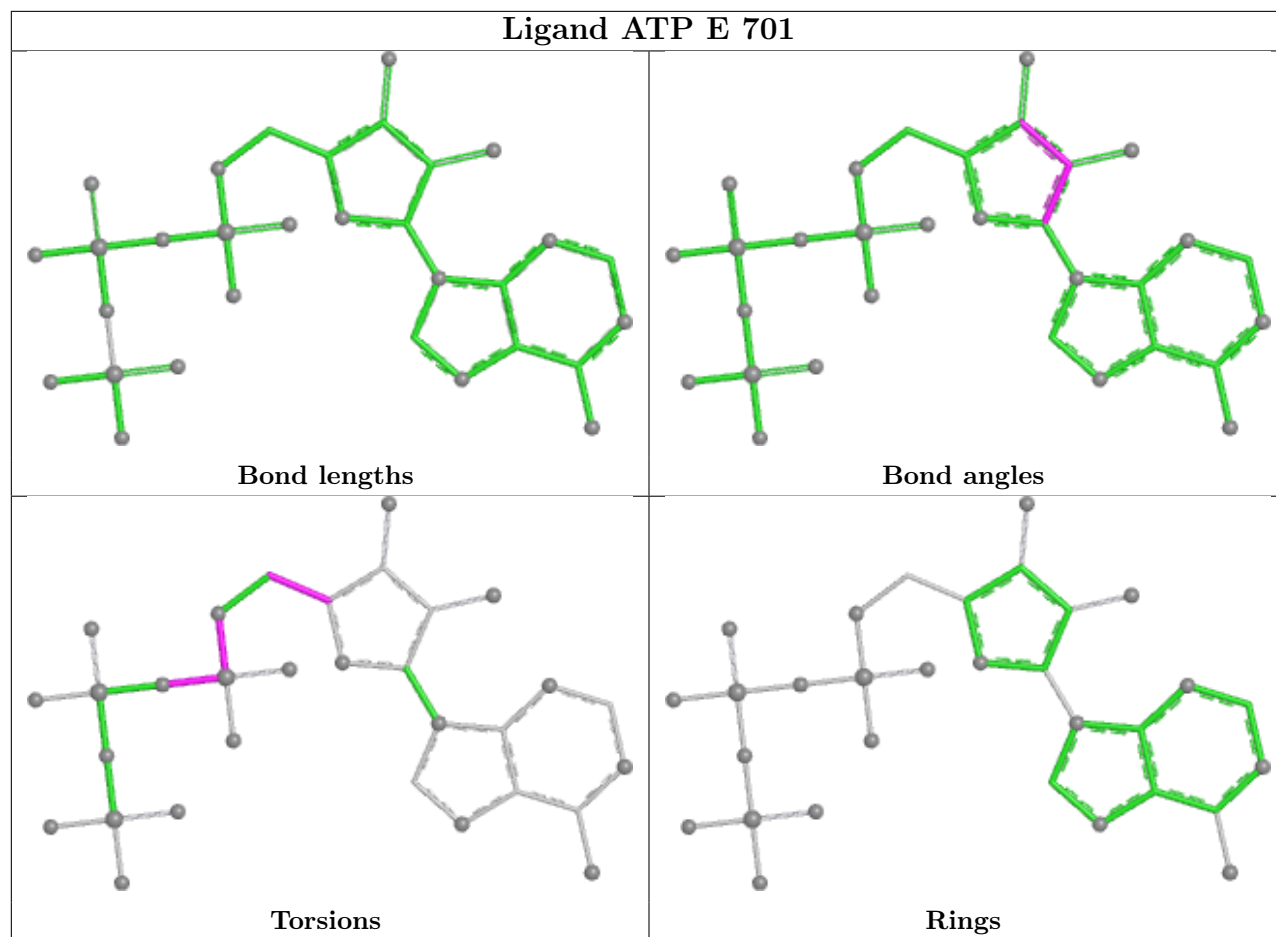
Ligand ATP L 702



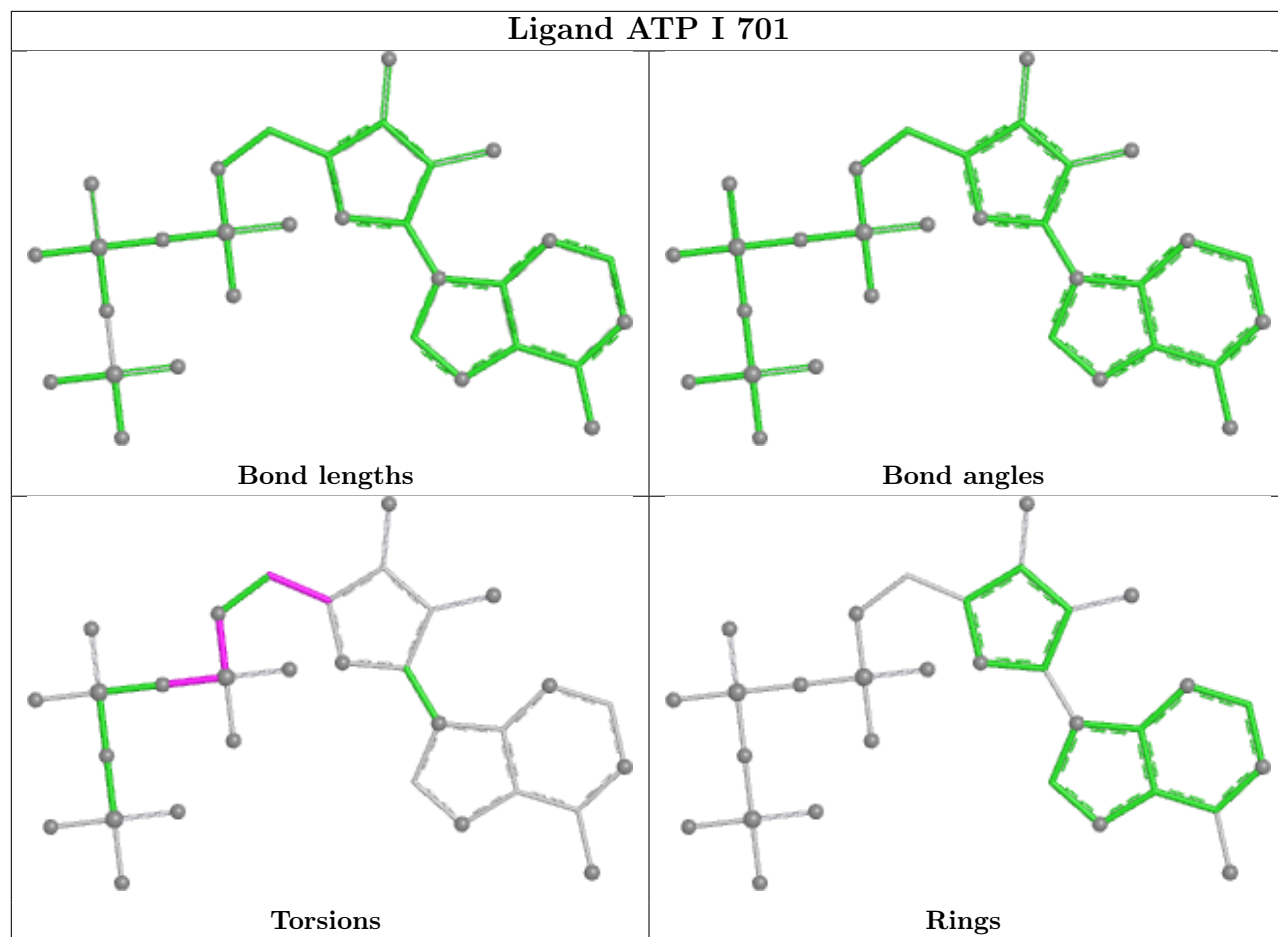


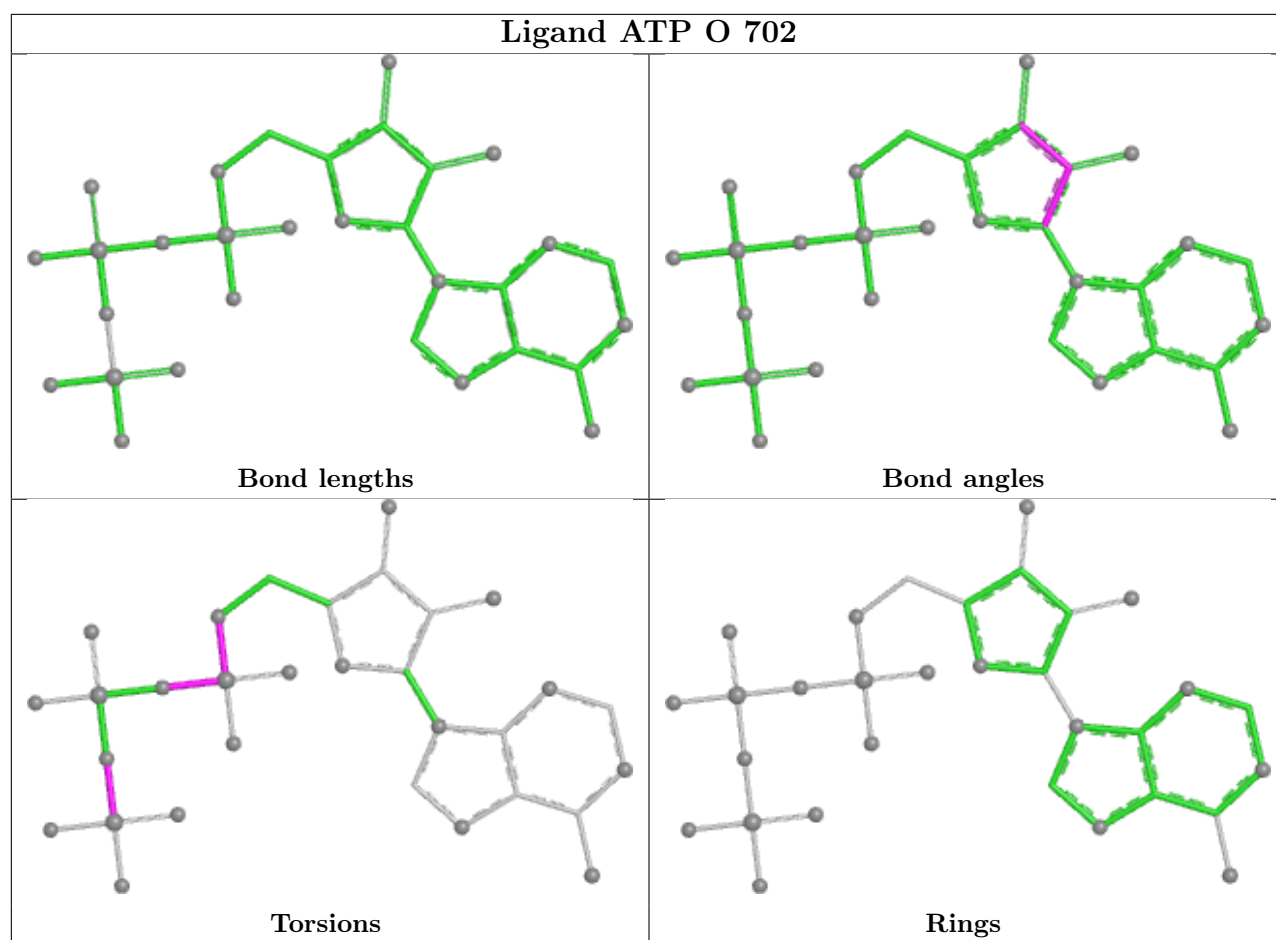






Ligand ATP I 701





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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	467/519 (89%)	0.17	1 (0%) 91 83	23, 46, 74, 115	0
1	B	468/519 (90%)	0.17	5 (1%) 78 59	25, 48, 69, 106	0
1	G	466/519 (89%)	0.09	2 (0%) 88 76	23, 43, 63, 98	0
1	H	467/519 (89%)	0.15	5 (1%) 78 59	26, 45, 69, 105	0
1	M	462/519 (89%)	0.71	23 (4%) 34 18	43, 68, 102, 130	0
1	N	454/519 (87%)	0.72	32 (7%) 22 12	48, 70, 99, 120	0
1	P	455/519 (87%)	0.64	33 (7%) 21 11	39, 62, 96, 129	0
1	R	462/519 (89%)	0.54	19 (4%) 41 23	37, 61, 84, 142	0
1	S	443/519 (85%)	1.14	71 (16%) 5 2	56, 89, 118, 132	0
1	T	414/519 (79%)	1.20	66 (15%) 5 2	57, 96, 121, 131	0
1	V	436/519 (84%)	0.79	41 (9%) 14 8	41, 68, 119, 132	0
1	W	463/519 (89%)	0.64	36 (7%) 19 10	37, 63, 99, 137	0
1	X	460/519 (88%)	0.73	35 (7%) 20 11	42, 68, 94, 118	0
2	C	470/519 (90%)	0.15	7 (1%) 72 52	26, 46, 75, 122	0
2	D	469/519 (90%)	0.15	5 (1%) 78 59	22, 47, 77, 124	0
2	E	468/519 (90%)	0.04	6 (1%) 75 56	20, 40, 71, 113	0
2	F	466/519 (89%)	0.13	6 (1%) 75 56	21, 45, 72, 88	0
2	I	471/519 (90%)	0.16	5 (1%) 78 59	22, 43, 78, 121	0
2	J	466/519 (89%)	0.16	6 (1%) 75 56	20, 45, 75, 108	0
2	K	469/519 (90%)	0.06	5 (1%) 78 59	20, 40, 72, 119	0
2	L	468/519 (90%)	0.11	10 (2%) 63 42	23, 44, 72, 105	0
2	O	459/519 (88%)	0.70	21 (4%) 37 20	47, 70, 101, 125	0
2	Q	464/519 (89%)	0.43	15 (3%) 50 30	36, 56, 83, 125	0
2	U	428/519 (82%)	0.98	46 (10%) 11 6	51, 82, 120, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	11015/12456 (88%)	0.44	501 (4%) 38 20	20, 56, 104, 142	0

All (501) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	51	GLY	6.0
1	T	456	PHE	5.8
1	P	51	GLY	5.7
2	Q	250	GLY	4.8
1	R	195	GLY	4.7
1	T	183	GLU	4.7
1	W	188	TYR	4.5
1	S	453	ILE	4.5
1	S	103	LEU	4.4
1	T	244	ILE	4.4
1	X	295	THR	4.3
1	X	39	GLY	4.3
1	S	350	TYR	4.2
1	R	122	ASP	4.2
1	P	249	LEU	4.2
1	T	470	PHE	4.1
1	N	347	VAL	4.1
1	P	164	LEU	4.0
2	U	398	GLY	4.0
1	T	83	ILE	4.0
2	U	146	SER	4.0
1	S	352	GLU	3.9
1	S	105	ILE	3.9
1	P	50	THR	3.9
1	T	390	ASN	3.8
2	O	30	ASP	3.8
2	U	140	ARG	3.8
1	W	36	LEU	3.8
1	V	124	SER	3.7
1	W	226	ARG	3.7
1	S	70	PRO	3.7
2	Q	249	LEU	3.7
1	T	49	GLY	3.7
1	S	281	ASP	3.7
1	T	331	TRP	3.7
1	T	483	PHE	3.6
1	T	51	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	T	383	LEU	3.6
1	V	62	ASN	3.6
2	U	35	GLY	3.6
1	S	349	ALA	3.6
1	T	60	LEU	3.6
1	W	157	SER	3.5
1	T	435	ASP	3.5
1	T	146	SER	3.5
2	U	265	SER	3.5
1	P	225	LEU	3.4
1	G	17	ALA	3.4
2	L	420	MET	3.4
1	W	353	SER	3.4
1	S	61	TYR	3.4
2	O	293	GLY	3.4
2	D	252	MET	3.4
1	S	146	SER	3.4
1	N	30	ASP	3.4
1	W	81	GLN	3.4
1	S	55	PHE	3.3
1	X	347	VAL	3.3
2	U	109	SER	3.3
1	T	414	ASN	3.3
1	X	87	ALA	3.3
1	V	76	PHE	3.3
1	S	313	ILE	3.3
1	R	164	LEU	3.3
2	O	74	VAL	3.3
1	T	342	ASN	3.3
1	T	458	MET	3.3
1	N	149	SER	3.2
1	V	41	SER	3.2
2	O	303	GLU	3.2
2	Q	293	GLY	3.2
2	Q	139	ALA	3.2
1	N	319	GLU	3.2
1	S	249	LEU	3.2
1	X	299	SER	3.2
1	S	302	VAL	3.2
1	X	107	ASP	3.2
1	X	166	ARG	3.2
1	P	191	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	X	122	ASP	3.1
1	W	220	LEU	3.1
1	R	341	GLN	3.1
1	T	287	THR	3.1
1	V	201	SER	3.1
1	S	73	PHE	3.1
2	U	57	ILE	3.1
1	S	45	SER	3.1
1	X	36	LEU	3.1
1	S	182	THR	3.1
1	P	198	GLU	3.1
1	X	318	GLU	3.1
2	F	250	GLY	3.0
2	L	68	ASP	3.0
2	Q	175	GLY	3.0
1	W	192	ALA	3.0
2	I	113	GLU	3.0
1	M	439	LEU	3.0
2	C	491	SER	3.0
1	S	145	ASP	3.0
1	P	160	VAL	3.0
2	U	342	ASN	3.0
1	V	206	ILE	3.0
1	W	158	SER	3.0
1	W	250	GLY	3.0
1	P	153	GLN	3.0
1	V	141	ARG	2.9
2	U	391	ALA	2.9
2	Q	188	TYR	2.9
1	W	189	GLY	2.9
1	N	356	LEU	2.9
1	V	36	LEU	2.9
2	I	122	ASP	2.9
1	P	36	LEU	2.9
2	U	182	THR	2.9
1	S	158	SER	2.9
1	R	359	HIS	2.9
1	X	111	ASP	2.9
1	P	62	ASN	2.9
2	U	181	THR	2.9
2	O	479	ILE	2.9
1	T	378	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	S	380	LEU	2.9
2	U	244	ILE	2.9
2	O	286	ALA	2.8
1	T	255	THR	2.8
1	S	287	THR	2.8
1	W	227	GLY	2.8
1	V	65	ILE	2.8
1	S	369	ASP	2.8
1	V	48	SER	2.8
2	D	253	ARG	2.8
1	T	409	THR	2.8
1	V	249	LEU	2.8
1	R	420	MET	2.8
1	X	74	VAL	2.8
1	W	57	ILE	2.8
1	P	95	ALA	2.8
1	T	95	ALA	2.8
1	W	391	ALA	2.8
1	M	89	SER	2.8
2	U	206	ILE	2.8
1	H	111	ASP	2.7
2	K	145	ASP	2.7
2	L	250	GLY	2.7
1	T	459	ARG	2.7
1	V	127	ILE	2.7
1	T	347	VAL	2.7
1	N	425	ILE	2.7
1	N	310	GLU	2.7
1	N	157	SER	2.7
1	R	450	SER	2.7
1	N	154	TYR	2.7
1	V	60	LEU	2.7
1	N	313	ILE	2.7
1	M	83	ILE	2.7
1	V	90	PHE	2.7
1	W	165	PHE	2.7
2	F	78	GLU	2.7
2	U	75	THR	2.7
1	S	331	TRP	2.7
1	S	202	ASP	2.7
1	P	363	ILE	2.7
1	T	279	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	T	415	THR	2.7
1	M	176	ALA	2.7
1	W	179	VAL	2.7
1	M	105	ILE	2.6
2	C	313	ILE	2.6
2	U	433	ILE	2.6
1	S	355	GLY	2.6
1	N	72	VAL	2.6
1	T	36	LEU	2.6
2	Q	82	ASP	2.6
1	X	340	ARG	2.6
1	M	100	GLU	2.6
1	X	352	GLU	2.6
1	X	298	VAL	2.6
1	S	439	LEU	2.6
1	P	93	ASP	2.6
1	S	368	ASN	2.6
2	I	152	GLN	2.6
1	T	27	GLY	2.6
2	U	63	GLY	2.6
1	A	255	THR	2.6
2	U	41	SER	2.6
2	U	299	SER	2.6
1	N	366	GLU	2.6
2	O	66	GLU	2.6
2	U	36	LEU	2.6
1	N	147	VAL	2.6
1	P	83	ILE	2.6
1	P	346	ILE	2.6
1	P	61	TYR	2.6
1	M	48	SER	2.6
2	Q	157	SER	2.6
1	S	82	ASP	2.6
1	S	107	ASP	2.6
1	W	202	ASP	2.6
1	S	123	LEU	2.6
1	M	198	GLU	2.6
1	H	249	LEU	2.5
1	P	168	VAL	2.5
2	Q	202	ASP	2.5
1	W	95	ALA	2.5
1	N	31	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	148	THR	2.5
1	S	31	ILE	2.5
2	U	348	CYS	2.5
1	V	49	GLY	2.5
1	W	460	GLY	2.5
2	U	176	ALA	2.5
1	S	490	ILE	2.5
1	S	92	TRP	2.5
1	T	329	TYR	2.5
1	W	49	GLY	2.5
1	V	89	SER	2.5
2	U	282	SER	2.5
1	T	72	VAL	2.5
1	T	200	VAL	2.5
1	S	183	GLU	2.5
1	N	375	ILE	2.5
1	V	209	ASN	2.5
1	W	25	ILE	2.5
1	S	178	THR	2.5
1	V	167	LEU	2.5
1	M	71	GLY	2.5
1	T	379	SER	2.5
1	T	473	SER	2.5
1	T	318	GLU	2.5
1	T	245	ASN	2.5
1	V	486	PHE	2.5
1	T	426	THR	2.5
1	S	91	GLY	2.5
1	S	204	VAL	2.5
1	T	256	GLN	2.5
2	U	489	ILE	2.4
1	T	333	MET	2.4
2	C	212	GLU	2.4
1	N	99	ASP	2.4
1	S	203	ASN	2.4
2	U	29	ASP	2.4
2	U	178	THR	2.4
1	T	359	HIS	2.4
1	S	298	VAL	2.4
2	O	71	GLY	2.4
2	U	425	ILE	2.4
2	O	225	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	485	ASN	2.4
1	P	228	THR	2.4
2	Q	30	ASP	2.4
1	S	248	PRO	2.4
2	U	39	GLY	2.4
1	M	57	ILE	2.4
1	T	25	ILE	2.4
1	X	163	GLU	2.4
1	S	303	GLU	2.4
1	V	77	GLU	2.4
1	W	78	GLU	2.4
2	U	221	GLU	2.4
2	J	493	SER	2.4
1	R	112	PRO	2.4
1	R	400	THR	2.4
1	X	413	THR	2.4
1	N	142	VAL	2.4
1	R	155	ASP	2.4
1	X	192	ALA	2.4
2	U	339	GLU	2.4
1	N	89	SER	2.4
1	V	23	THR	2.4
1	S	460	GLY	2.4
1	V	202	ASP	2.4
2	L	155	ASP	2.4
1	N	472	ILE	2.4
2	E	156	ALA	2.4
1	P	136	LYS	2.4
1	W	237	PHE	2.4
1	M	366	GLU	2.4
2	U	303	GLU	2.4
1	T	353	SER	2.4
2	J	72	VAL	2.4
1	N	332	GLY	2.3
1	M	292	THR	2.3
1	S	213	GLY	2.3
1	H	251	ALA	2.3
1	T	31	ILE	2.3
1	S	312	ALA	2.3
1	H	254	LEU	2.3
1	R	59	PHE	2.3
1	S	72	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	R	79	THR	2.3
2	U	23	THR	2.3
1	W	19	ALA	2.3
1	W	251	ALA	2.3
2	L	15	HIS	2.3
2	O	329	TYR	2.3
1	M	107	ASP	2.3
1	T	241	ASP	2.3
1	X	474	ASP	2.3
2	K	155	ASP	2.3
1	S	383	LEU	2.3
2	E	256	GLN	2.3
1	V	168	VAL	2.3
1	P	257	ARG	2.3
1	R	83	ILE	2.3
1	M	246	ILE	2.3
1	S	206	ILE	2.3
1	V	244	ILE	2.3
1	T	422	ALA	2.3
1	S	139	ALA	2.3
2	E	17	ALA	2.3
1	X	423	HIS	2.3
1	S	86	ASN	2.3
1	P	145	ASP	2.3
2	F	145	ASP	2.3
2	L	474	ASP	2.3
2	O	145	ASP	2.3
1	V	212	GLU	2.3
2	J	138	ARG	2.3
1	W	249	LEU	2.3
1	N	418	GLN	2.3
2	E	145	ASP	2.3
2	K	173	GLN	2.3
2	J	122	ASP	2.3
1	P	212	GLU	2.3
1	T	352	GLU	2.3
1	X	339	GLU	2.3
2	Q	443	VAL	2.3
1	T	479	ILE	2.3
1	M	133	ALA	2.3
1	V	92	TRP	2.3
2	O	297	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	V	32	SER	2.3
2	U	141	ARG	2.3
1	M	82	ASP	2.3
1	S	198	GLU	2.2
1	T	363	ILE	2.2
1	R	49	GLY	2.2
1	M	17	ALA	2.2
1	V	34	GLY	2.2
1	T	50	THR	2.2
1	S	265	SER	2.2
2	L	154	TYR	2.2
1	X	86	ASN	2.2
1	M	66	GLU	2.2
1	M	252	MET	2.2
1	T	243	GLY	2.2
1	V	250	GLY	2.2
2	L	332	GLY	2.2
1	S	59	PHE	2.2
1	N	329	TYR	2.2
2	O	140	ARG	2.2
2	U	61	TYR	2.2
2	F	157	SER	2.2
1	S	142	VAL	2.2
1	M	103	LEU	2.2
1	V	420	MET	2.2
2	L	252	MET	2.2
1	P	92	TRP	2.2
1	V	370	PHE	2.2
1	T	290	THR	2.2
1	X	148	THR	2.2
1	V	200	VAL	2.2
2	E	157	SER	2.2
2	C	489	ILE	2.2
1	X	245	ASN	2.2
2	U	62	ASN	2.2
1	B	249	LEU	2.2
1	T	338	MET	2.2
1	X	80	PRO	2.2
1	V	176	ALA	2.2
1	N	484	ARG	2.2
2	U	279	PHE	2.2
1	X	50	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	44	VAL	2.2
2	O	72	VAL	2.2
2	U	44	VAL	2.2
1	X	375	ILE	2.2
1	V	493	SER	2.2
1	S	187	GLU	2.2
2	E	113	GLU	2.2
2	D	69	GLU	2.2
2	U	78	GLU	2.2
1	X	37	PRO	2.2
2	U	70	PRO	2.2
1	P	76	PHE	2.2
1	T	93	ASP	2.2
2	I	76	PHE	2.2
2	F	15	HIS	2.2
1	H	347	VAL	2.1
1	N	150	VAL	2.1
1	N	94	LEU	2.1
1	T	81	GLN	2.1
1	S	207	LEU	2.1
1	W	225	LEU	2.1
1	B	252	MET	2.1
1	P	149	SER	2.1
1	T	449	MET	2.1
1	W	156	ALA	2.1
2	U	77	GLU	2.1
2	C	492	GLY	2.1
1	V	131	ASN	2.1
1	W	203	ASN	2.1
1	T	59	PHE	2.1
1	P	122	ASP	2.1
1	W	200	VAL	2.1
2	U	92	TRP	2.1
1	V	182	THR	2.1
2	C	148	THR	2.1
1	W	125	ALA	2.1
1	R	157	SER	2.1
1	W	124	SER	2.1
2	U	190	PRO	2.1
1	P	485	ASN	2.1
1	V	412	PHE	2.1
1	S	29	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	228	THR	2.1
1	S	430	ILE	2.1
1	N	194	TYR	2.1
2	K	156	ALA	2.1
1	T	110	PRO	2.1
1	S	351	PRO	2.1
1	V	37	PRO	2.1
2	F	332	GLY	2.1
1	B	265	SER	2.1
1	T	55	PHE	2.1
1	T	278	PHE	2.1
1	S	90	PHE	2.1
1	S	259	SER	2.1
1	N	343	LEU	2.1
1	X	145	ASP	2.1
1	X	309	LYS	2.1
1	X	489	ILE	2.1
1	S	18	ILE	2.1
1	S	144	ILE	2.1
1	S	284	ILE	2.1
1	V	164	LEU	2.1
2	D	111	ASP	2.1
2	O	246	ILE	2.1
2	Q	36	LEU	2.1
2	Q	311	ARG	2.1
2	U	132	TYR	2.1
1	R	77	GLU	2.1
1	M	183	GLU	2.1
1	X	76	PHE	2.1
1	W	198	GLU	2.1
1	X	143	SER	2.1
1	S	143	SER	2.1
2	L	157	SER	2.1
2	O	299	SER	2.1
1	R	84	ILE	2.1
1	T	223	LEU	2.1
1	X	57	ILE	2.1
2	Q	222	ILE	2.1
1	P	30	ASP	2.1
1	T	145	ASP	2.1
2	K	99	ASP	2.1
1	N	50	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	O	75	THR	2.1
1	P	349	ALA	2.1
1	T	133	ALA	2.1
1	T	354	ALA	2.1
1	M	101	GLY	2.1
1	S	35	GLY	2.1
1	V	173	GLN	2.1
1	T	370	PHE	2.1
2	C	337	GLU	2.1
1	B	150	VAL	2.0
1	P	96	LYS	2.0
2	O	179	VAL	2.0
2	U	399	VAL	2.0
1	R	297	LEU	2.0
1	X	467	ILE	2.0
2	D	460	GLY	2.0
1	S	487	GLU	2.0
2	U	224	LYS	2.0
1	V	123	LEU	2.0
2	Q	164	LEU	2.0
1	P	18	ILE	2.0
1	T	259	SER	2.0
1	S	89	SER	2.0
2	I	497	ILE	2.0
1	N	203	ASN	2.0
1	N	327	ASN	2.0
1	S	449	MET	2.0
2	O	86	ASN	2.0
2	O	485	ASN	2.0
2	U	209	ASN	2.0
1	T	305	ALA	2.0
2	J	251	ALA	2.0
1	W	80	PRO	2.0
1	W	248	PRO	2.0
2	U	136	LYS	2.0
1	R	106	LEU	2.0
1	P	94	LEU	2.0
1	T	171	LEU	2.0
1	B	408	ILE	2.0
1	N	244	ILE	2.0
1	M	244	ILE	2.0
1	S	191	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	W	206	ILE	2.0
2	J	18	ILE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TPO	U	432	11/12	0.72	0.16	72,76,79,79	4
1	SEP	S	431	10/11	0.76	0.17	71,75,82,82	0
2	TPO	Q	432	11/12	0.78	0.19	58,61,63,64	4
2	TPO	L	432	11/12	0.80	0.17	46,51,56,56	4
2	SEP	U	431	10/11	0.80	0.17	75,78,82,83	0
2	TPO	O	432	11/12	0.80	0.14	71,74,80,80	0
1	SEP	M	431	10/11	0.80	0.15	65,68,72,72	0
1	SEP	T	431	10/11	0.81	0.18	82,84,87,87	0
2	TPO	C	432	11/12	0.81	0.16	52,56,61,61	4
2	TPO	F	432	11/12	0.81	0.15	41,45,50,50	4
2	TPO	I	432	11/12	0.81	0.17	46,50,54,54	4
1	SEP	V	431	10/11	0.81	0.16	55,58,61,62	4
2	SEP	C	431	10/11	0.86	0.16	55,57,62,62	0
1	SEP	R	431	10/11	0.86	0.13	58,60,61,61	0
1	SEP	N	431	10/11	0.86	0.15	65,66,69,70	0
1	SEP	W	431	10/11	0.86	0.11	51,52,53,53	4
1	SEP	H	431	10/11	0.87	0.14	41,43,46,46	4
2	SEP	Q	431	10/11	0.88	0.13	53,55,57,58	0
2	TPO	J	432	11/12	0.88	0.14	41,44,48,48	4
1	SEP	X	431	10/11	0.89	0.10	52,56,60,60	0
2	SEP	O	431	10/11	0.89	0.15	70,71,71,71	4
2	TPO	D	432	11/12	0.89	0.13	40,43,45,45	4
2	SEP	K	431	10/11	0.89	0.14	42,43,45,46	0
1	SEP	A	431	10/11	0.90	0.12	46,46,47,47	4
2	SEP	I	431	10/11	0.91	0.12	48,50,54,54	0
2	TPO	K	432	11/12	0.91	0.10	40,43,45,45	4
1	SEP	P	431	10/11	0.91	0.12	52,53,53,54	4
1	SEP	B	431	10/11	0.91	0.10	42,43,44,44	4
1	SEP	G	431	10/11	0.92	0.11	48,49,50,51	0
2	SEP	J	431	10/11	0.92	0.10	42,43,44,44	4
2	SEP	D	431	10/11	0.92	0.10	42,43,44,44	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SEP	L	431	10/11	0.93	0.11	46,46,46,47	4
2	TPO	E	432	11/12	0.93	0.09	39,42,44,44	4
2	SEP	E	431	10/11	0.93	0.12	38,39,41,41	0
2	SEP	F	431	10/11	0.94	0.10	41,42,42,42	4

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	S	701	31/31	0.81	0.13	77,78,83,83	0
5	ADP	U	702	27/27	0.82	0.12	92,104,112,112	0
3	ATP	S	702	31/31	0.83	0.11	94,95,99,99	0
3	ATP	M	702	31/31	0.83	0.13	76,79,81,81	0
3	ATP	T	702	31/31	0.85	0.11	85,88,90,91	0
4	MG	B	704	1/1	0.86	0.07	58,58,58,58	0
4	MG	C	704	1/1	0.86	0.09	48,48,48,48	0
3	ATP	X	701	31/31	0.86	0.13	59,63,70,70	0
4	MG	U	703	1/1	0.87	0.09	51,51,51,51	0
3	ATP	R	701	31/31	0.88	0.12	48,55,59,59	0
3	ATP	O	701	31/31	0.88	0.12	60,62,64,65	0
4	MG	R	704	1/1	0.88	0.12	44,44,44,44	0
4	MG	P	704	1/1	0.88	0.06	44,44,44,44	0
3	ATP	V	702	31/31	0.88	0.10	83,85,89,90	0
3	ATP	W	702	31/31	0.88	0.10	71,74,76,77	0
3	ATP	P	702	31/31	0.89	0.10	55,56,60,62	0
4	MG	H	704	1/1	0.89	0.06	46,46,46,46	0
3	ATP	O	702	31/31	0.89	0.10	84,98,105,105	0
3	ATP	X	702	31/31	0.90	0.10	66,70,74,75	0
3	ATP	N	701	31/31	0.90	0.10	56,60,64,64	0
3	ATP	Q	702	31/31	0.90	0.10	59,62,73,73	0
3	ATP	R	702	31/31	0.91	0.09	58,59,63,63	0
3	ATP	T	701	31/31	0.91	0.11	69,71,74,75	0
4	MG	G	703	1/1	0.91	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	M	701	31/31	0.91	0.09	54,56,58,58	0
5	ADP	W	701	27/27	0.91	0.09	45,49,52,52	0
3	ATP	U	701	31/31	0.92	0.09	60,62,62,62	0
4	MG	Q	703	1/1	0.92	0.06	51,51,51,51	0
4	MG	I	704	1/1	0.92	0.10	47,47,47,47	0
5	ADP	Q	701	27/27	0.92	0.09	45,49,51,51	0
3	ATP	N	702	31/31	0.92	0.10	61,64,69,70	0
4	MG	M	703	1/1	0.92	0.18	27,27,27,27	0
3	ATP	B	701	31/31	0.93	0.09	39,39,40,40	0
3	ATP	F	702	31/31	0.93	0.10	40,41,44,44	0
4	MG	E	704	1/1	0.93	0.08	22,22,22,22	0
4	MG	F	704	1/1	0.93	0.07	39,39,39,39	0
3	ATP	F	701	31/31	0.94	0.08	39,40,44,44	0
4	MG	R	703	1/1	0.94	0.16	33,33,33,33	0
3	ATP	L	702	31/31	0.95	0.08	38,39,43,43	0
4	MG	D	704	1/1	0.95	0.08	41,41,41,41	0
3	ATP	I	702	31/31	0.95	0.07	41,42,45,45	0
4	MG	H	703	1/1	0.95	0.13	25,25,25,25	0
3	ATP	J	702	31/31	0.95	0.08	42,45,46,47	0
4	MG	K	704	1/1	0.95	0.04	20,20,20,20	0
3	ATP	E	702	31/31	0.95	0.08	43,44,47,48	0
3	ATP	A	702	31/31	0.95	0.09	40,41,45,45	0
3	ATP	B	702	31/31	0.95	0.09	44,46,49,50	0
3	ATP	C	702	31/31	0.95	0.08	41,42,46,47	0
4	MG	P	703	1/1	0.95	0.06	43,43,43,43	0
3	ATP	D	702	31/31	0.95	0.08	43,46,47,48	0
3	ATP	G	701	31/31	0.95	0.08	37,40,44,45	0
3	ATP	H	702	31/31	0.95	0.08	44,46,49,50	0
3	ATP	K	702	31/31	0.95	0.08	39,42,46,47	0
3	ATP	P	701	31/31	0.95	0.10	52,56,65,66	0
3	ATP	L	701	31/31	0.95	0.07	37,38,42,42	0
3	ATP	I	701	31/31	0.96	0.07	29,30,31,31	0
3	ATP	H	701	31/31	0.96	0.07	36,37,38,38	0
3	ATP	J	701	31/31	0.96	0.07	27,29,31,32	0
3	ATP	E	701	31/31	0.96	0.07	30,32,35,35	0
3	ATP	K	701	31/31	0.96	0.07	29,31,33,33	0
3	ATP	A	701	31/31	0.96	0.07	41,45,50,50	0
3	ATP	V	701	31/31	0.96	0.09	44,49,54,55	0
3	ATP	C	701	31/31	0.96	0.07	33,34,34,35	0
3	ATP	G	702	31/31	0.96	0.07	37,40,42,42	0
4	MG	A	703	1/1	0.96	0.07	34,34,34,34	0
4	MG	C	703	1/1	0.97	0.05	43,43,43,43	0

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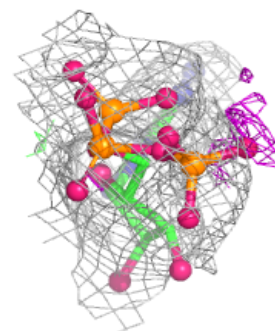
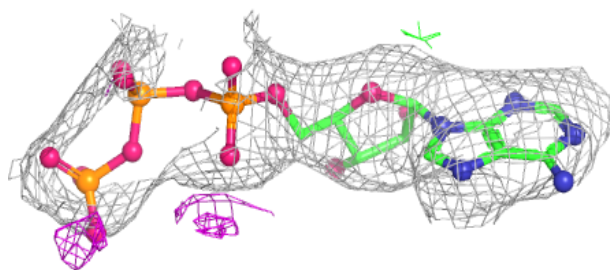
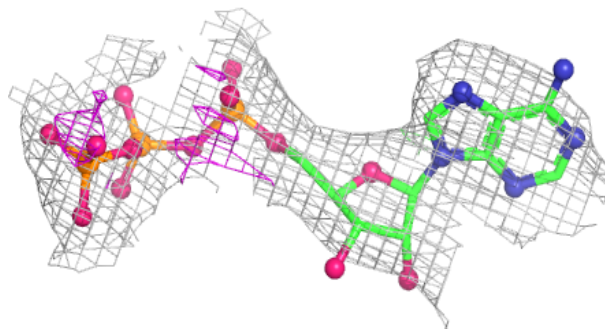
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	704	1/1	0.97	0.04	27,27,27,27	0
4	MG	K	703	1/1	0.97	0.04	23,23,23,23	0
4	MG	F	703	1/1	0.97	0.05	40,40,40,40	0
4	MG	L	703	1/1	0.97	0.04	35,35,35,35	0
3	ATP	D	701	31/31	0.97	0.07	28,29,30,30	0
4	MG	V	703	1/1	0.97	0.04	36,36,36,36	0
4	MG	J	703	1/1	0.97	0.10	18,18,18,18	0
4	MG	J	704	1/1	0.97	0.04	23,23,23,23	0
4	MG	G	704	1/1	0.97	0.04	48,48,48,48	0
4	MG	T	703	1/1	0.98	0.07	50,50,50,50	0
4	MG	D	703	1/1	0.98	0.04	26,26,26,26	0
4	MG	L	704	1/1	0.98	0.04	36,36,36,36	0
4	MG	N	704	1/1	0.98	0.03	47,47,47,47	0
4	MG	O	703	1/1	0.98	0.05	38,38,38,38	0
4	MG	E	703	1/1	0.98	0.04	21,21,21,21	0
4	MG	I	703	1/1	0.99	0.02	36,36,36,36	0
4	MG	B	703	1/1	0.99	0.03	31,31,31,31	0
4	MG	N	703	1/1	1.00	0.02	37,37,37,37	0

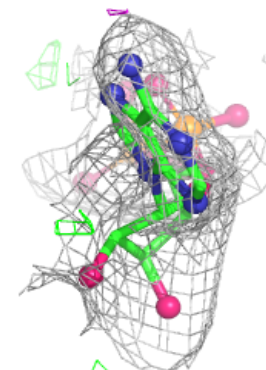
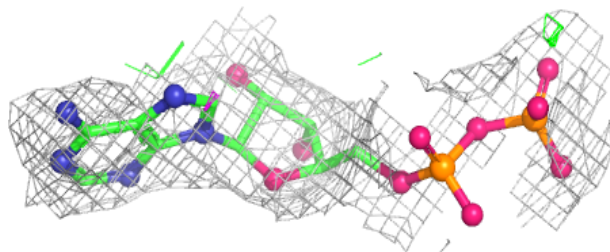
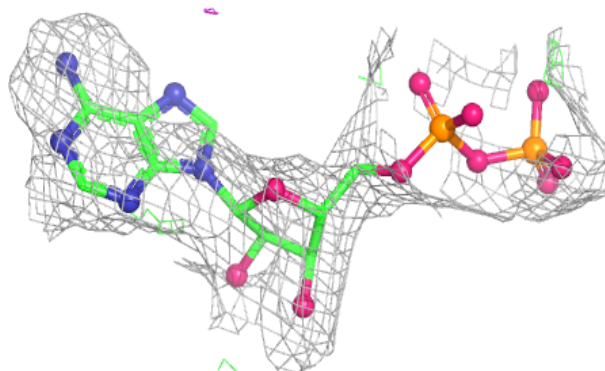
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP S 701:

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

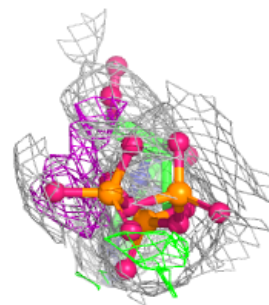
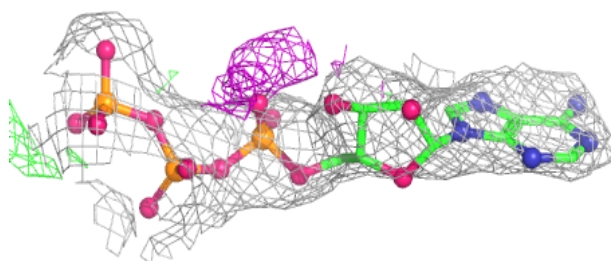
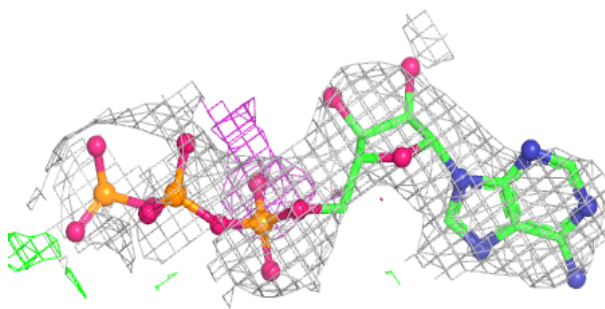
**Electron density around ADP U 702:**

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

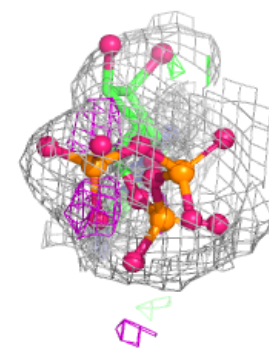
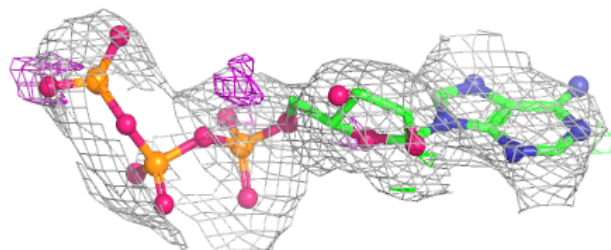
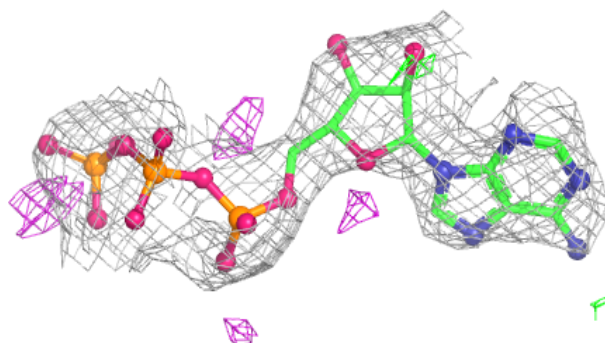


Electron density around ATP M 702:

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

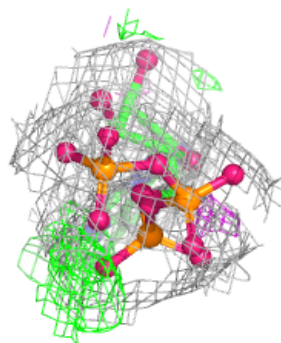
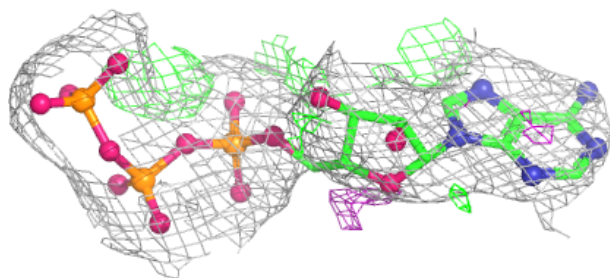
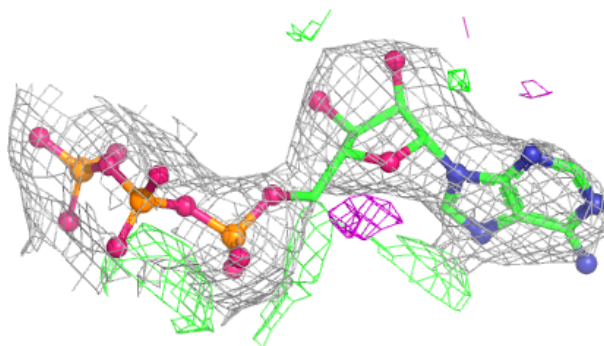
**Electron density around ATP X 701:**

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and green (positive)

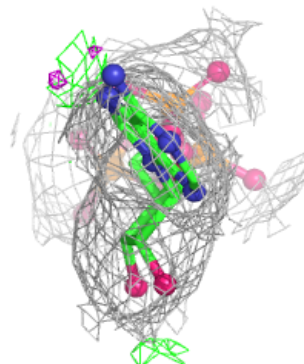
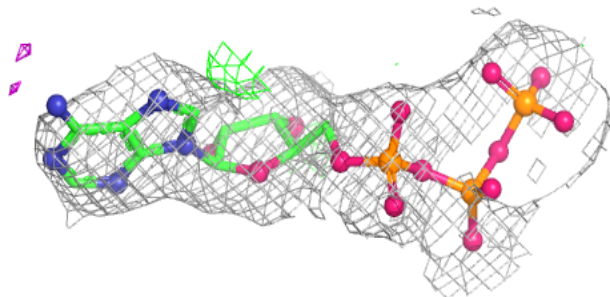
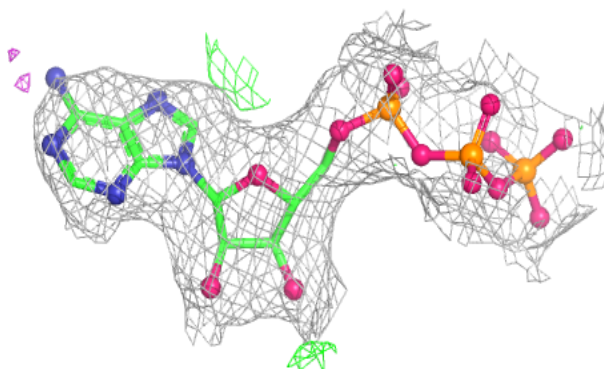


Electron density around ATP R 701:

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

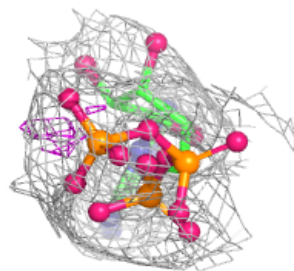
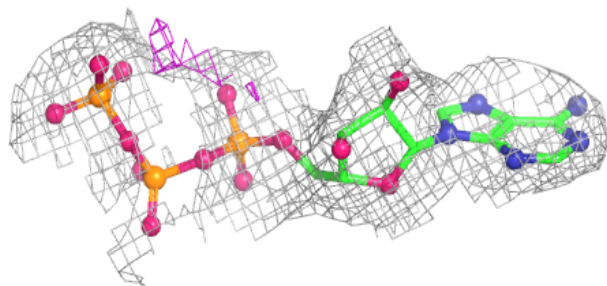
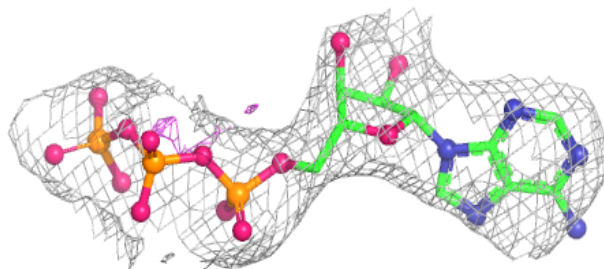
**Electron density around ATP O 701:**

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

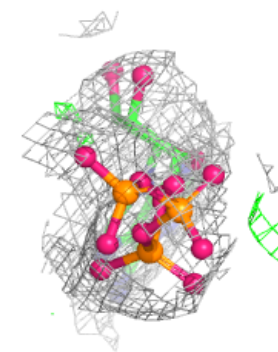
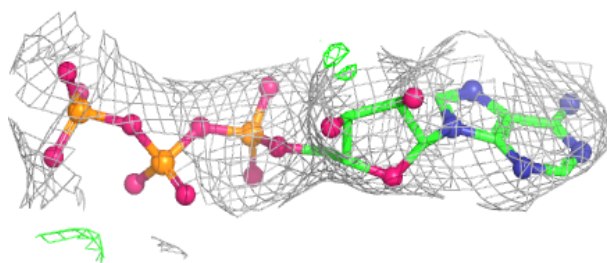
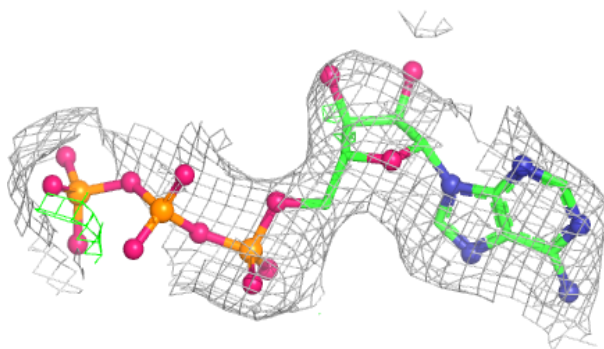


Electron density around ATP V 702:

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

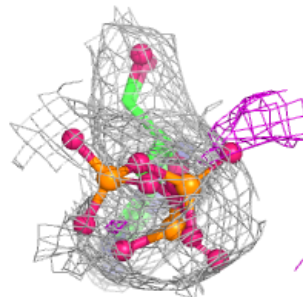
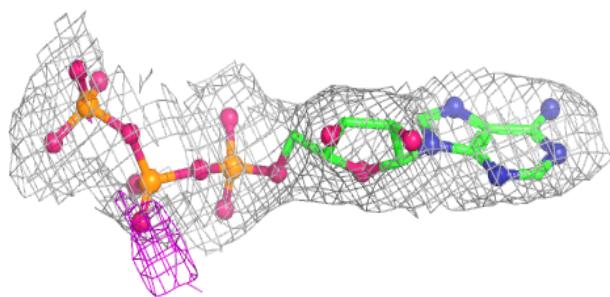
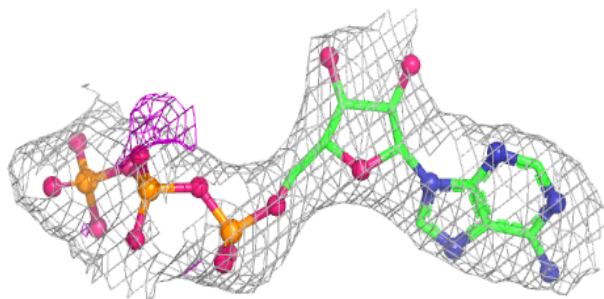
**Electron density around ATP W 702:**

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

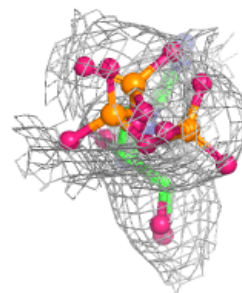
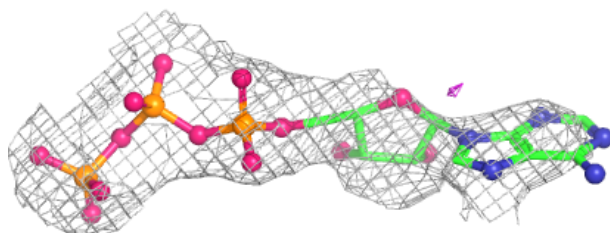
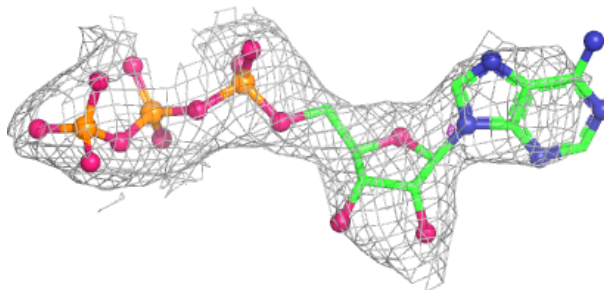


Electron density around ATP P 702:

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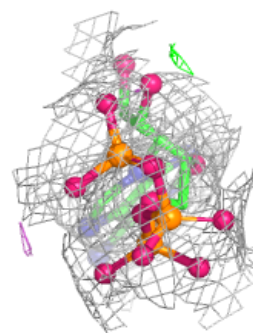
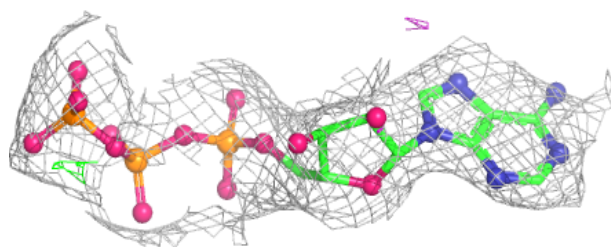
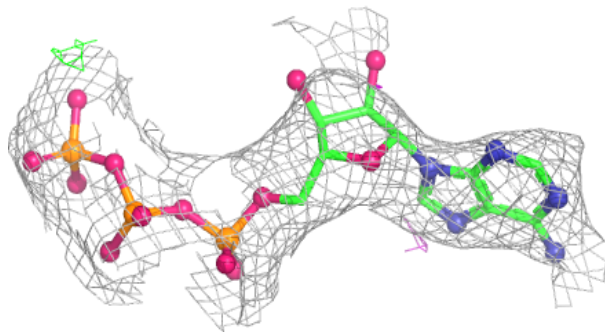
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and green (positive)

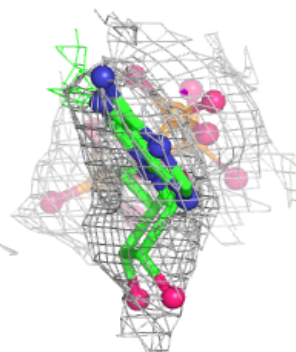
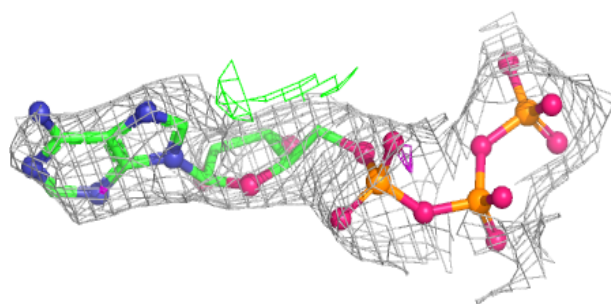
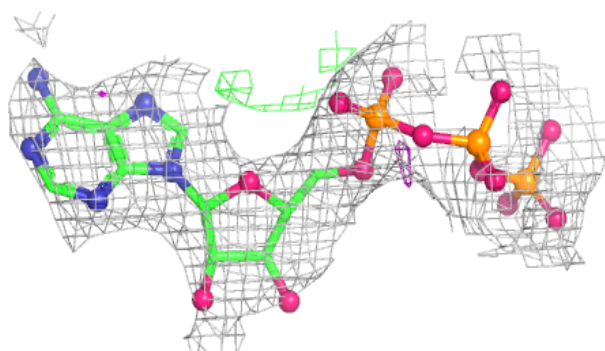


Electron density around ATP X 702:

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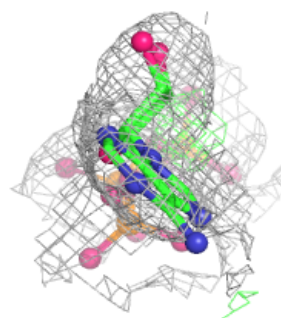
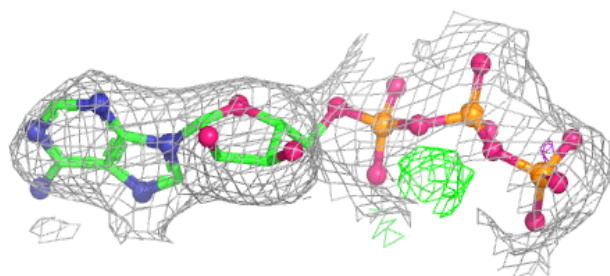
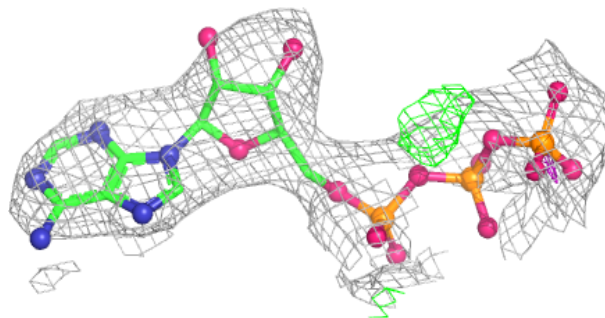
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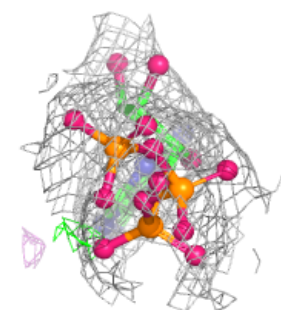
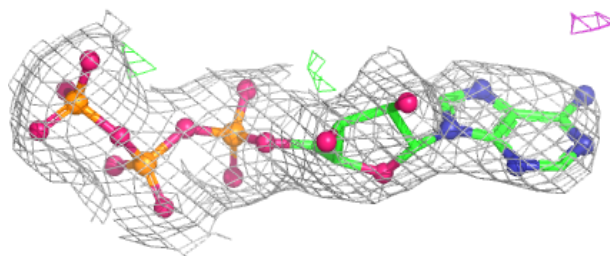
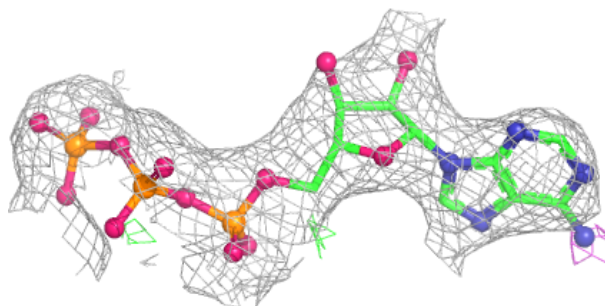


Electron density around ATP Q 702:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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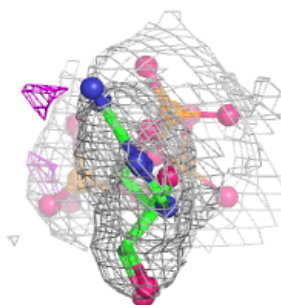
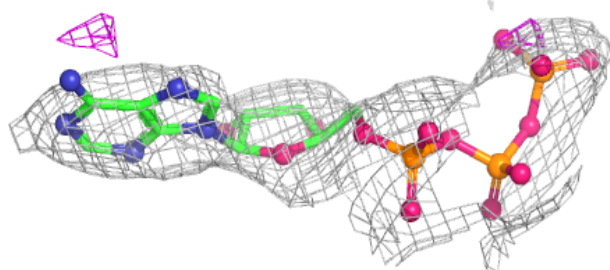
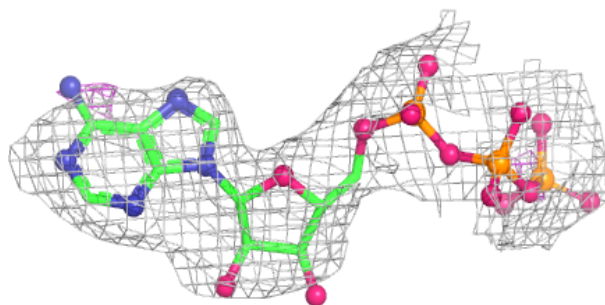
**Electron density around ATP R 702:**

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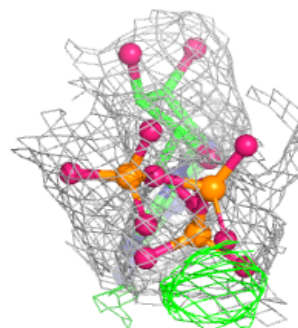
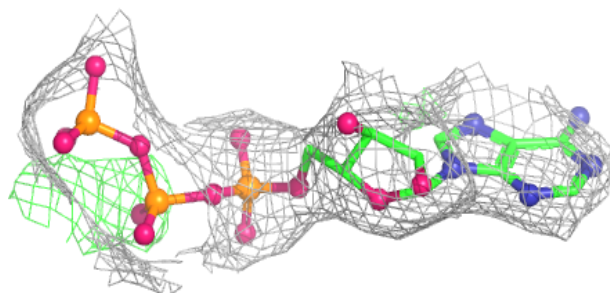
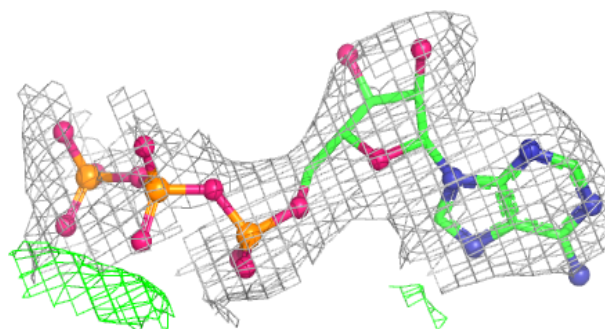


Electron density around ATP T 701:

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and green (positive)

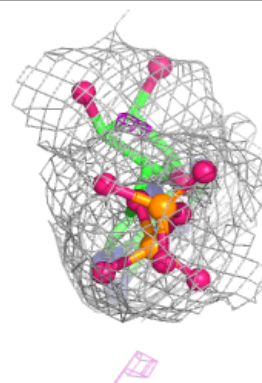
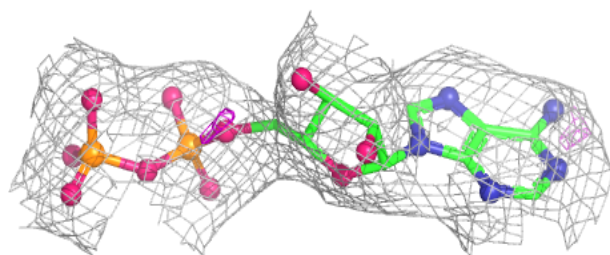
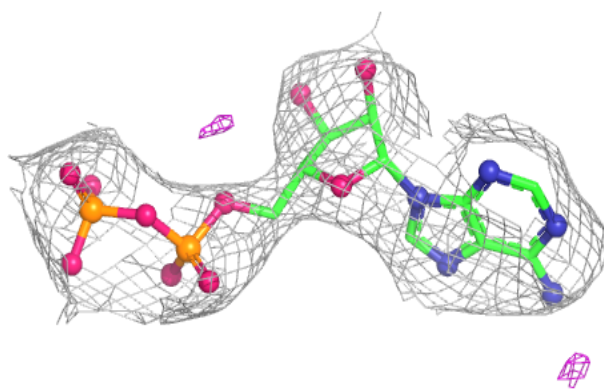
**Electron density around ATP M 701:**

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and green (positive)

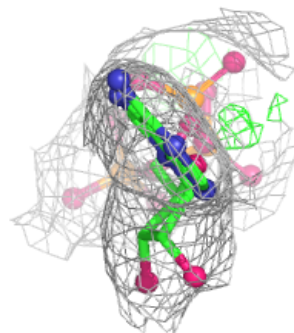
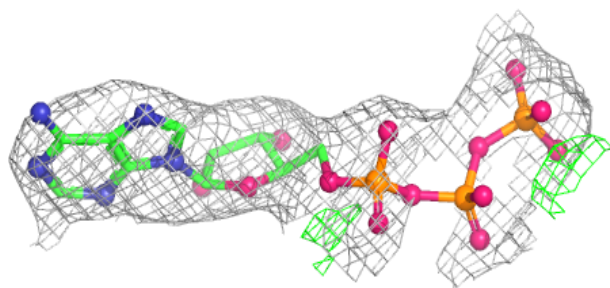
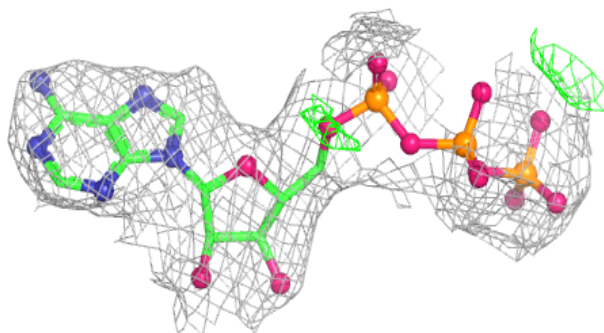


Electron density around ADP W 701:

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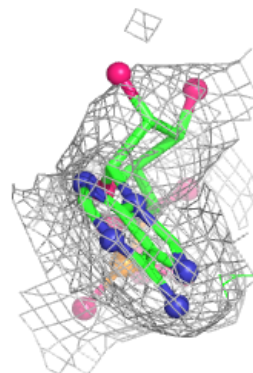
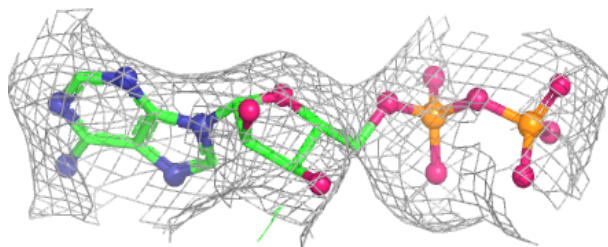
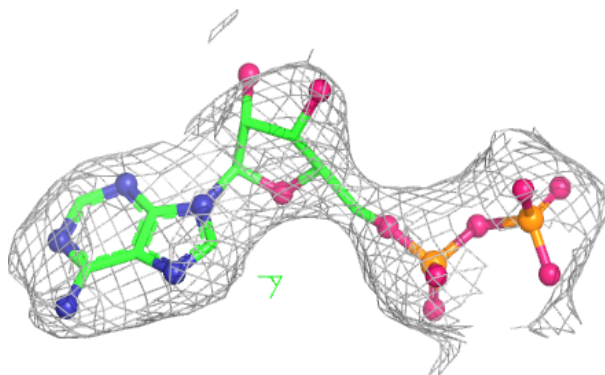
**Electron density around ATP U 701:**

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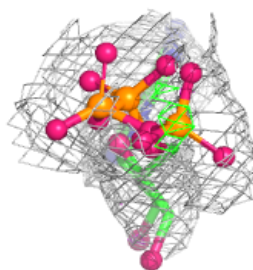
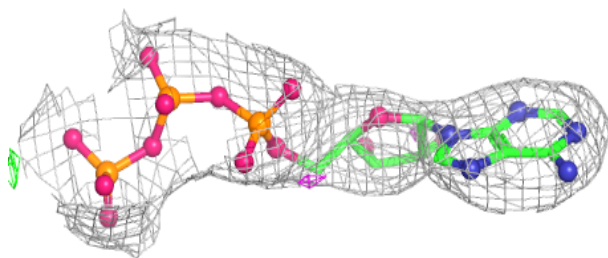
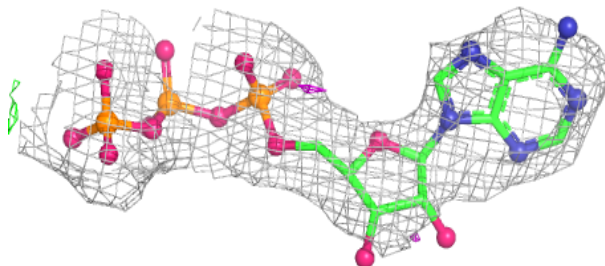


Electron density around ADP Q 701:

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

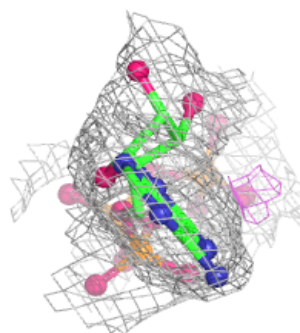
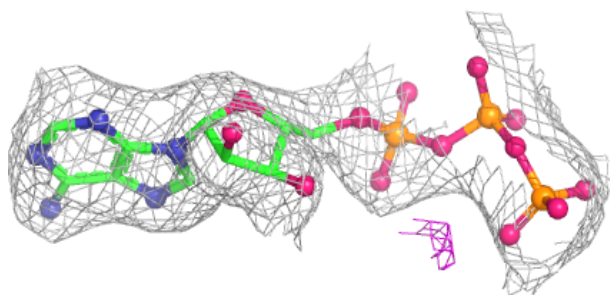
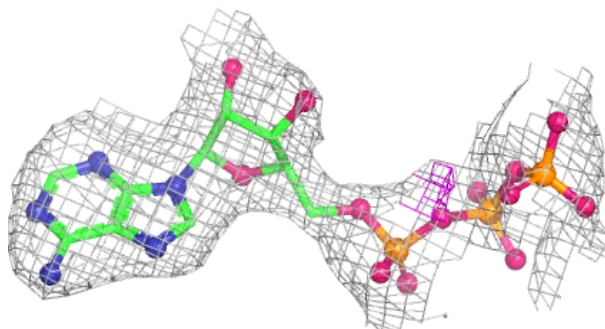
**Electron density around ATP N 702:**

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

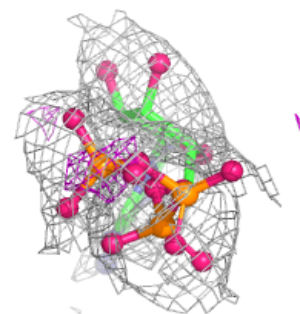
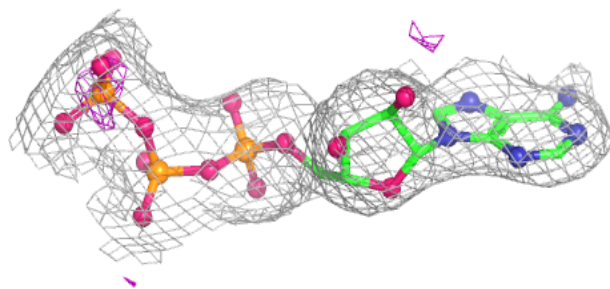
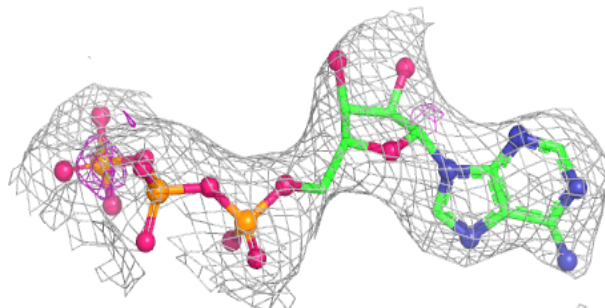


Electron density around ATP B 701:

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

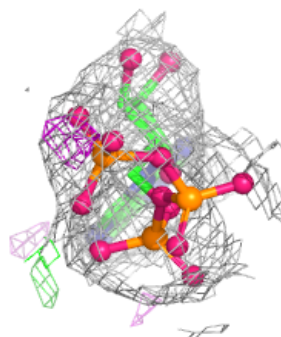
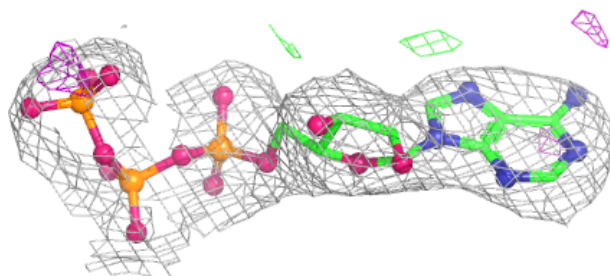
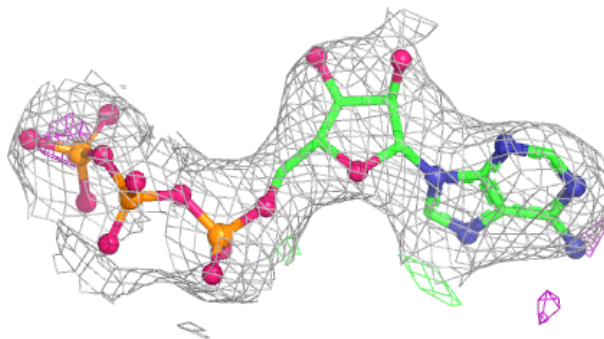
**Electron density around ATP F 702:**

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

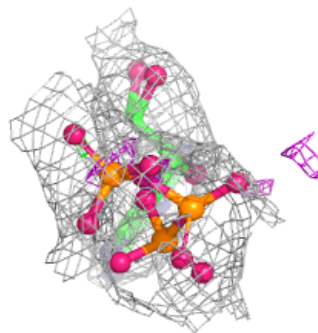
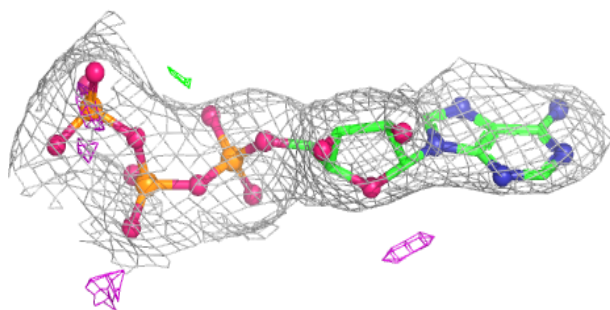
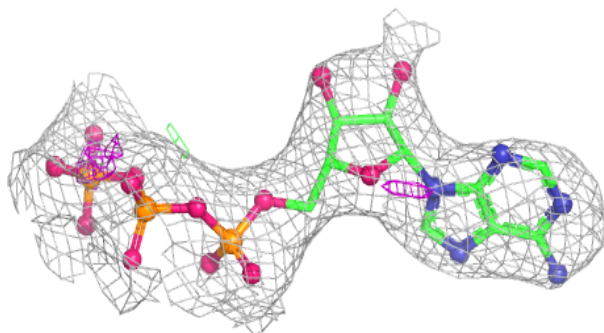


Electron density around ATP F 701:

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

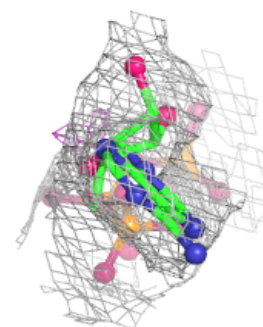
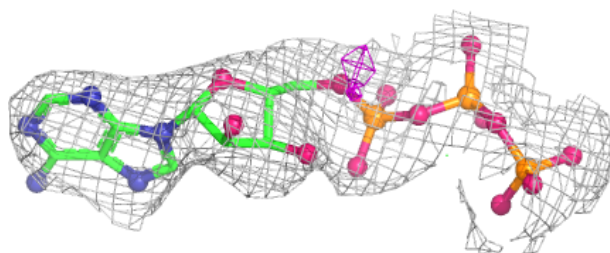
**Electron density around ATP L 702:**

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

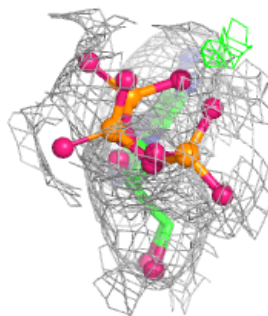
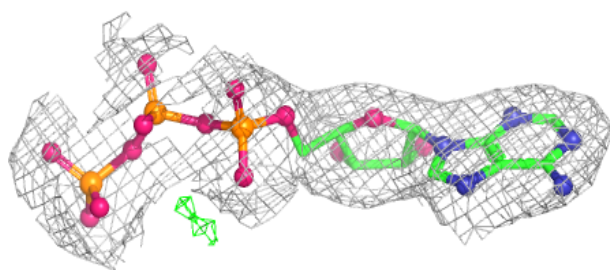
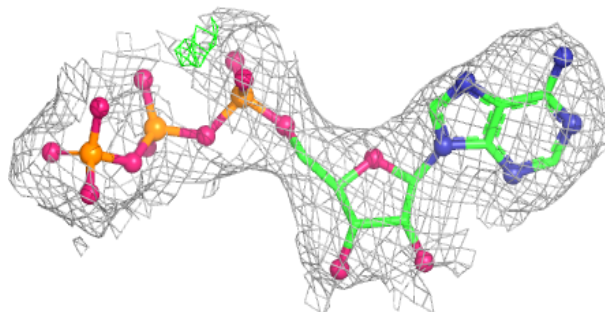


Electron density around ATP I 702:

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

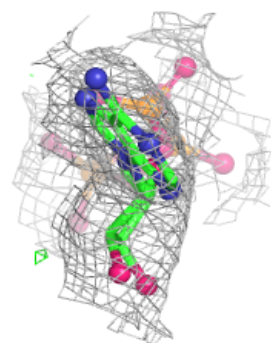
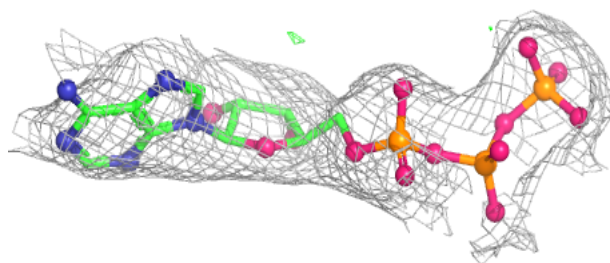
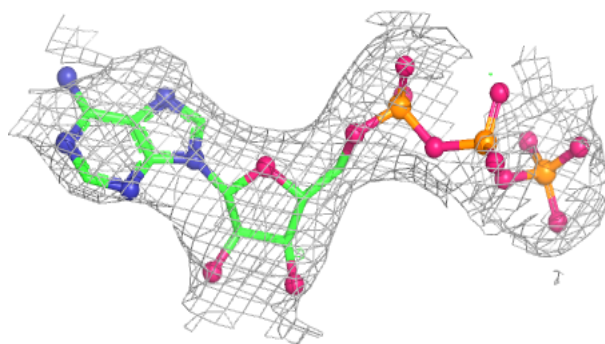
**Electron density around ATP J 702:**

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

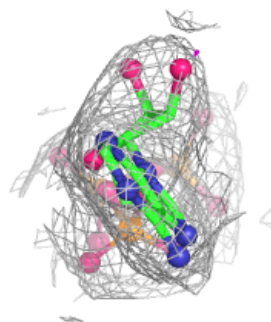
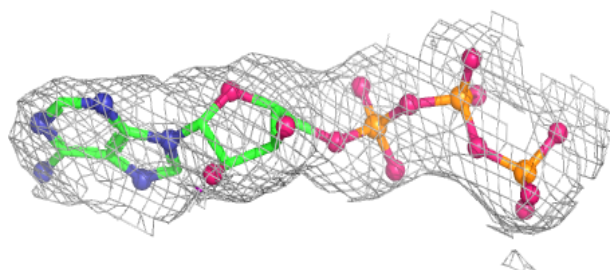
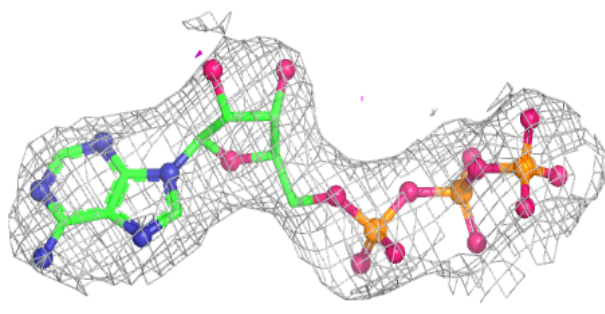


Electron density around ATP E 702:

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

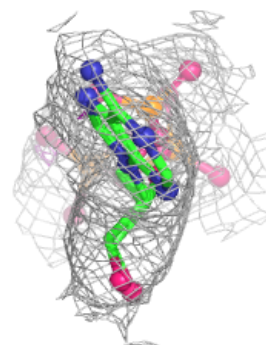
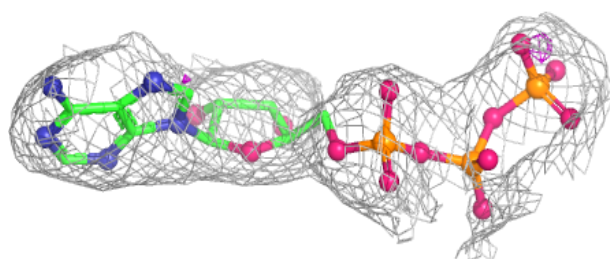
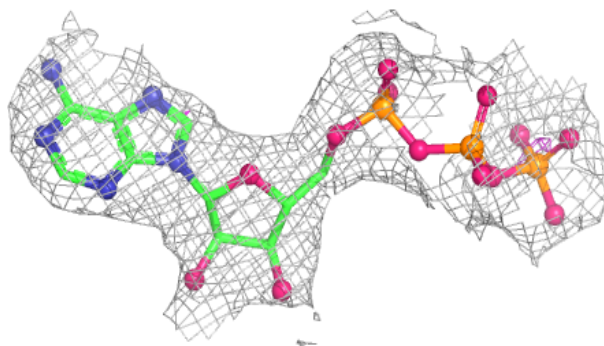
**Electron density around ATP A 702:**

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

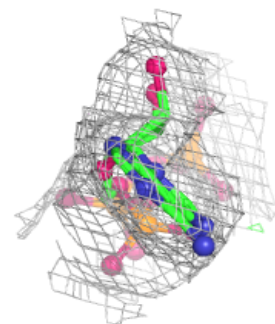
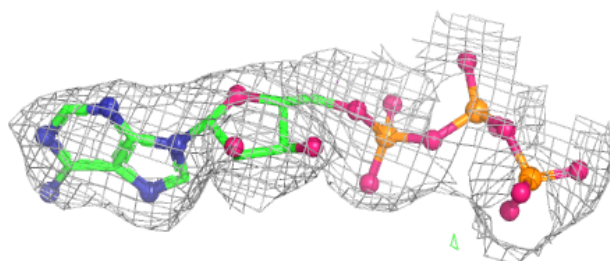
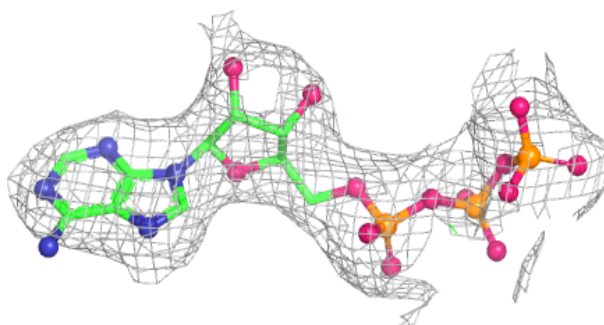


Electron density around ATP B 702:

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

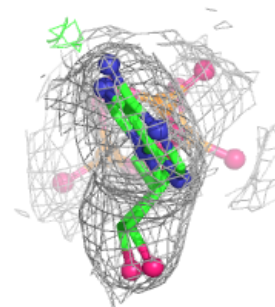
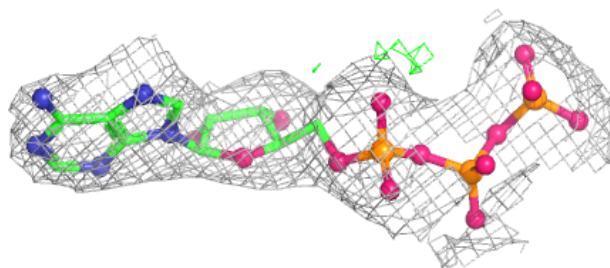
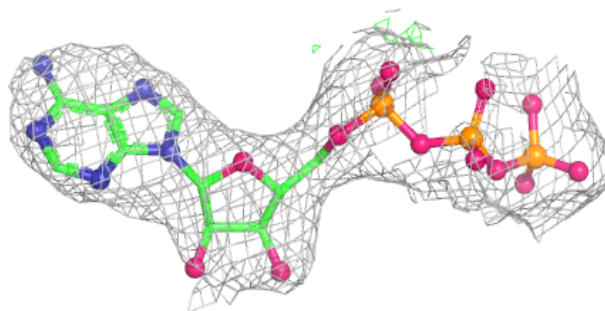
**Electron density around ATP C 702:**

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

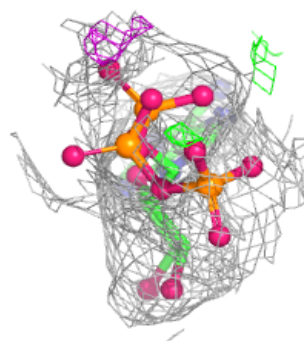
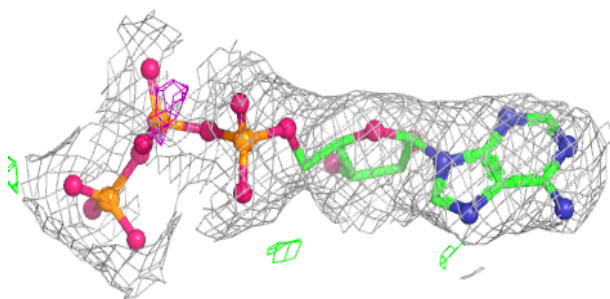
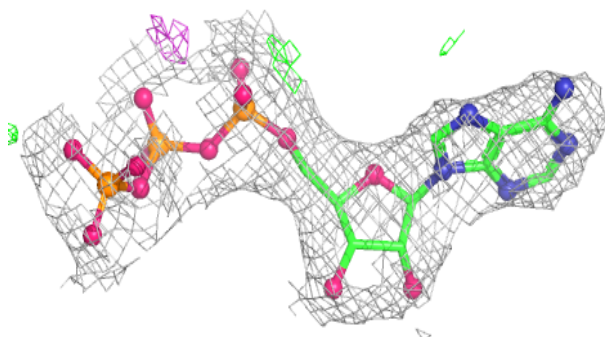


Electron density around ATP D 702:

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

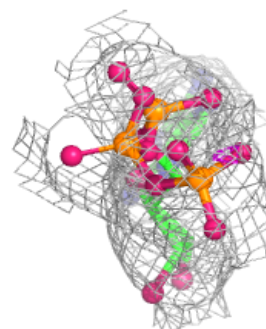
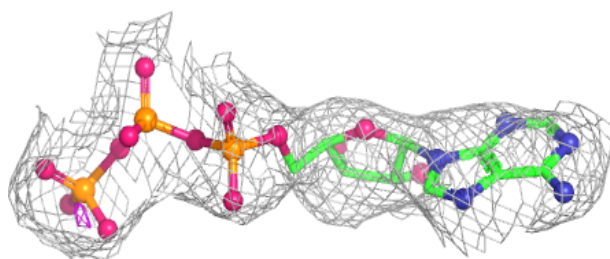
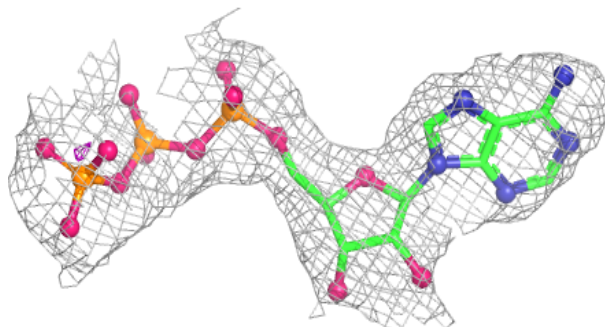
**Electron density around ATP G 701:**

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

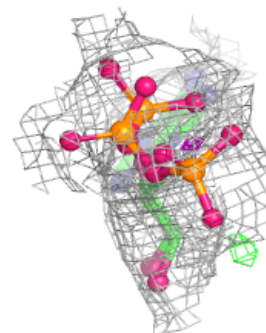
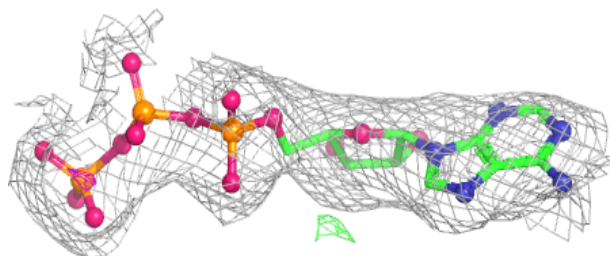
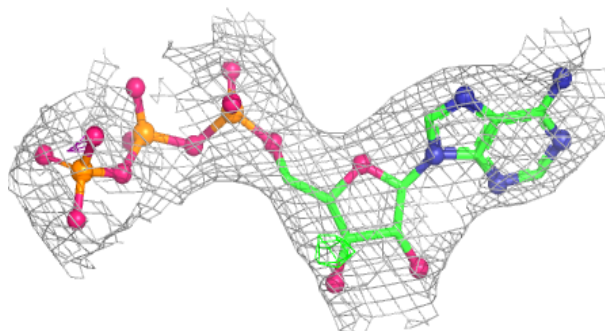


Electron density around ATP H 702:

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

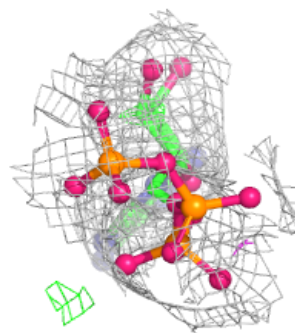
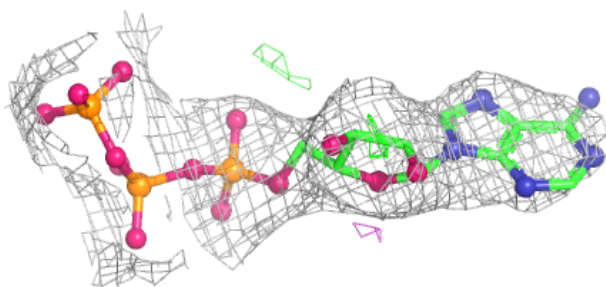
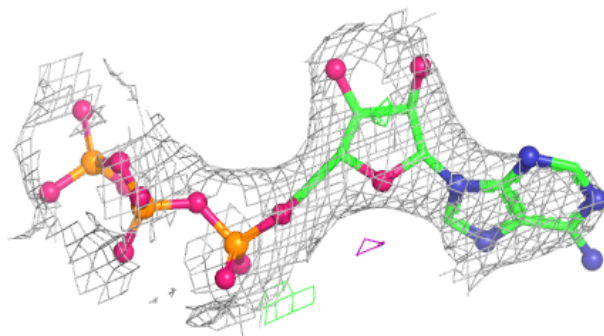
**Electron density around ATP K 702:**

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

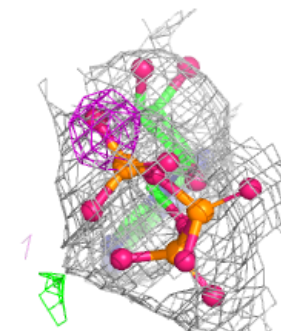
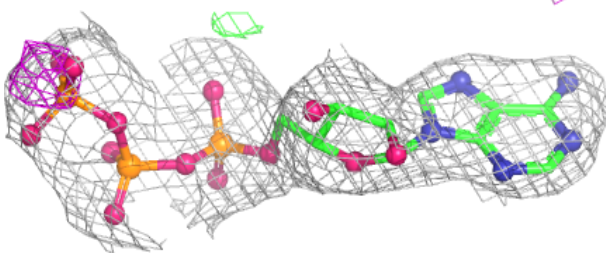
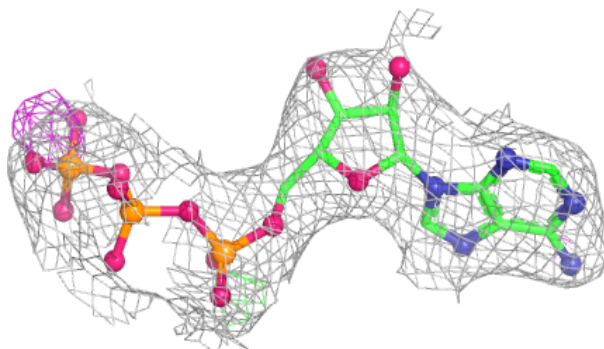


Electron density around ATP P 701:

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

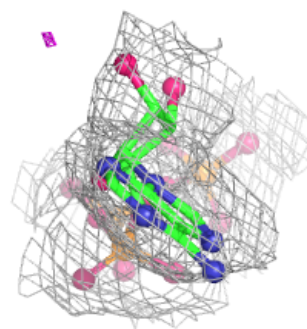
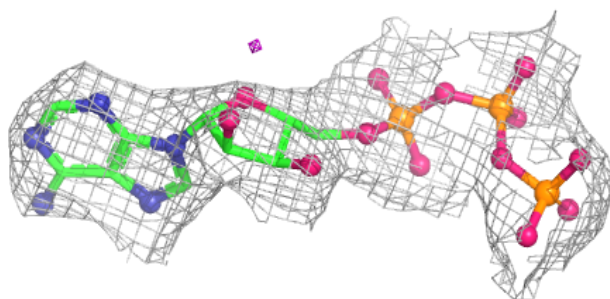
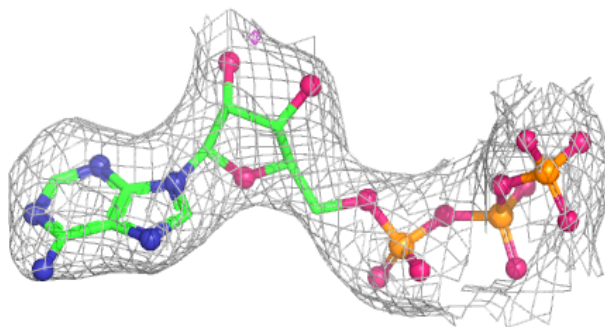
**Electron density around ATP L 701:**

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

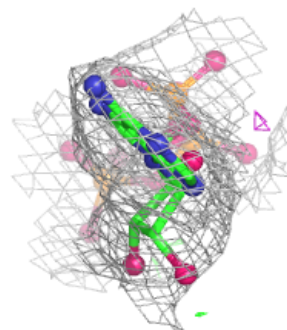
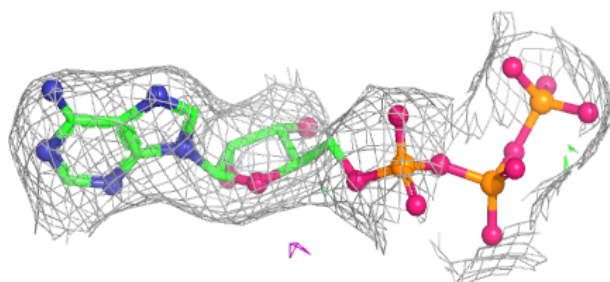
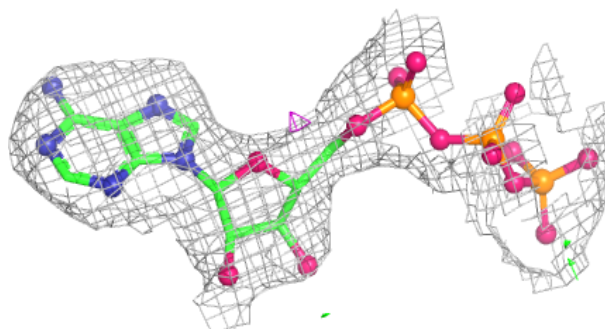


Electron density around ATP I 701:

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

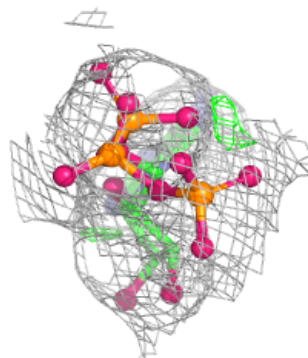
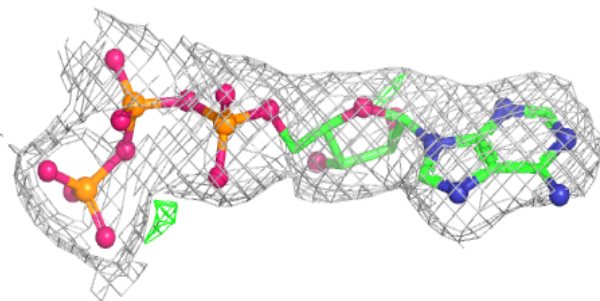
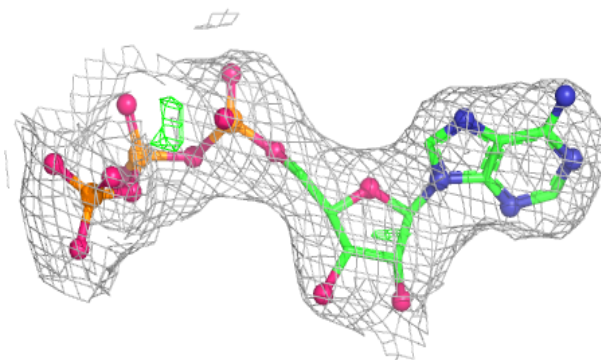
**Electron density around ATP H 701:**

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

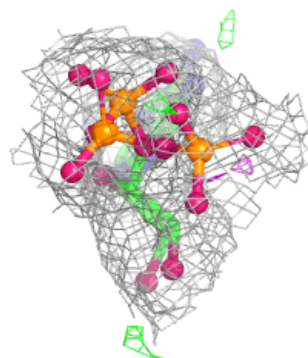
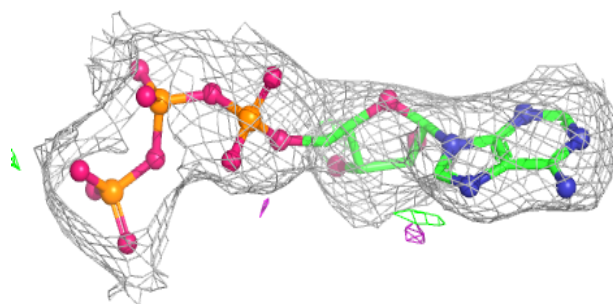
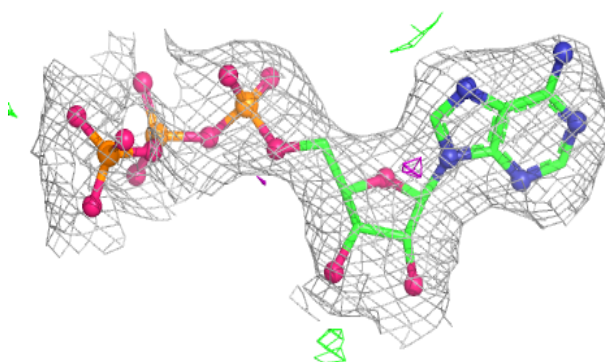


Electron density around ATP J 701:

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

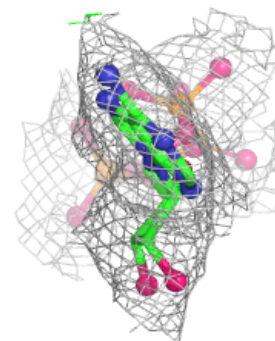
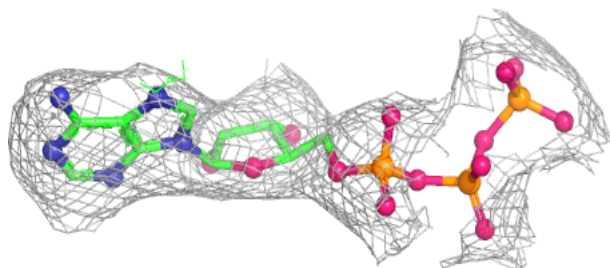
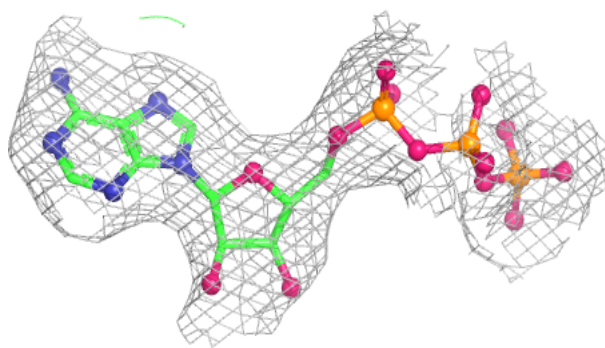
**Electron density around ATP E 701:**

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

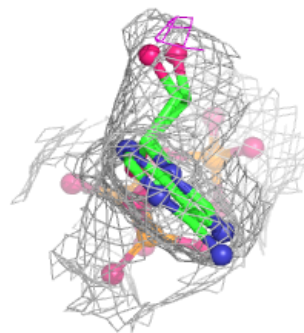
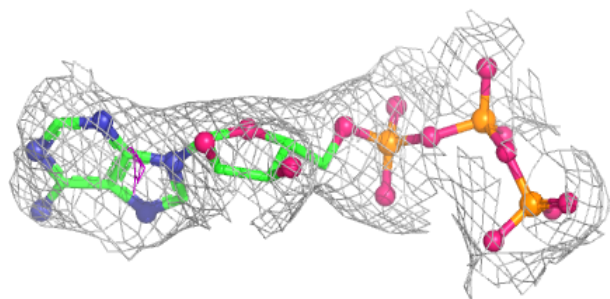
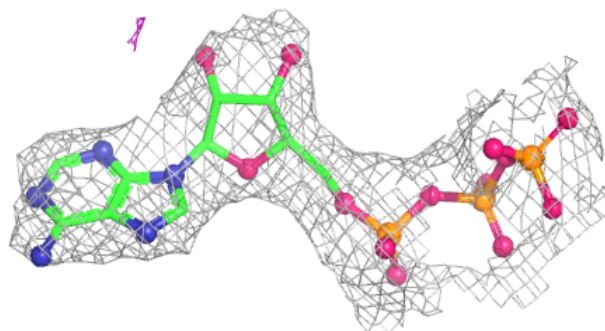


Electron density around ATP K 701:

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

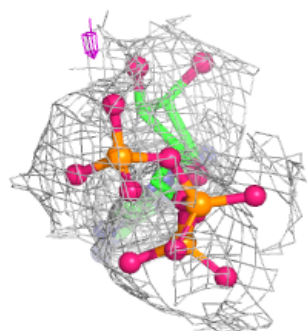
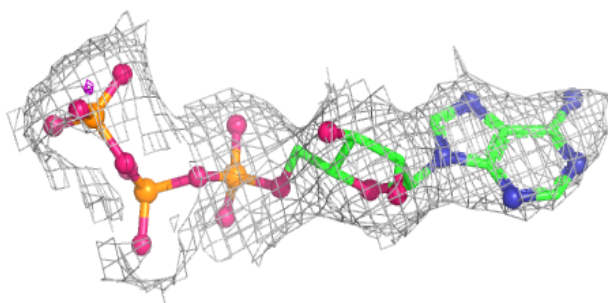
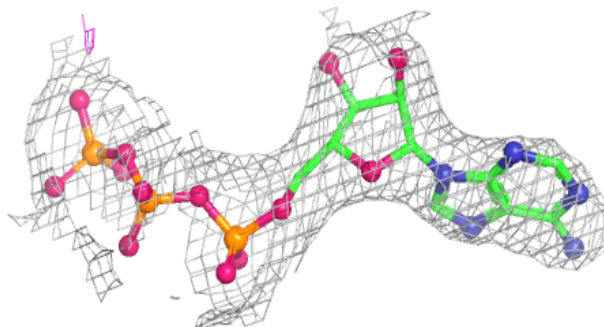
**Electron density around ATP A 701:**

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

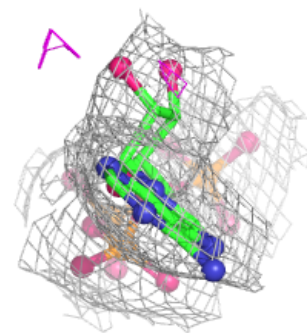
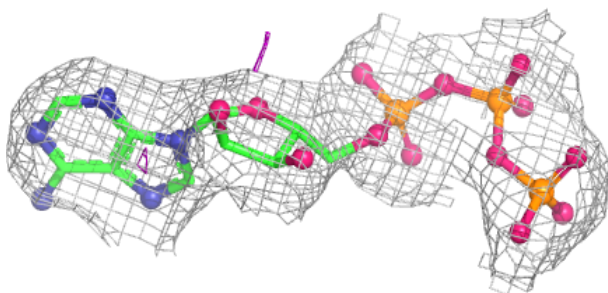
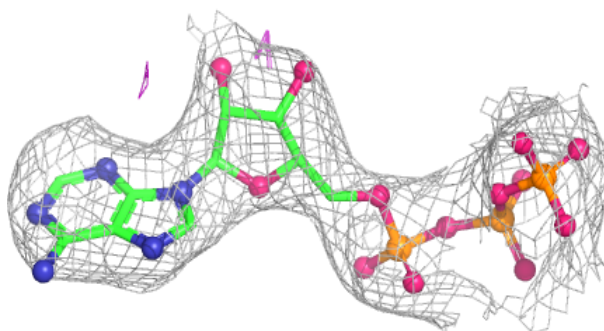


Electron density around ATP V 701:

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

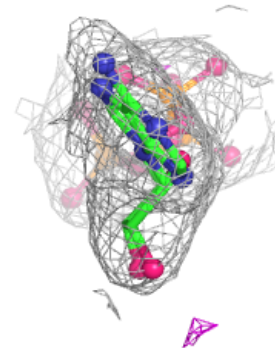
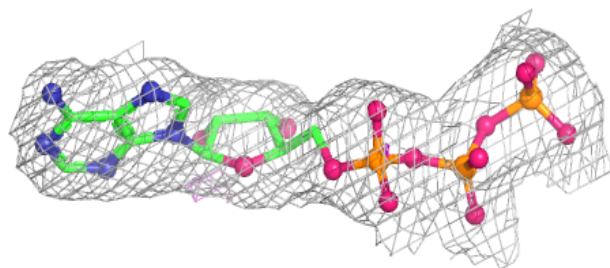
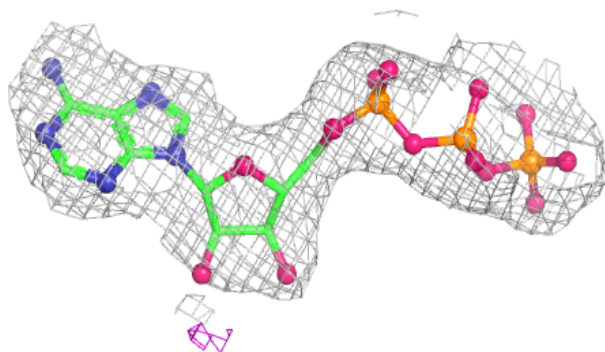
**Electron density around ATP C 701:**

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

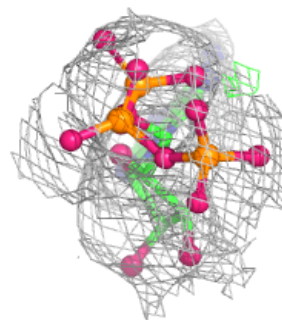
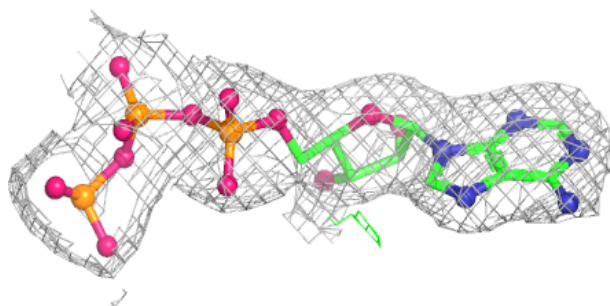
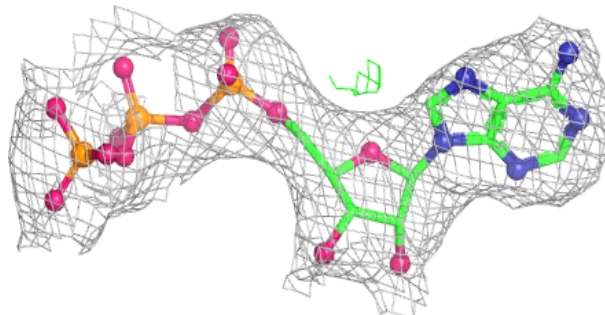


Electron density around ATP G 702:

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

**Electron density around ATP 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 [i](#)

There are no such residues in this entry.