



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2025 – 12:15 AM JST

PDB ID : 9KQ7 / pdb_00009kq7
Title : The structure of the YcfA from Erwinia amylovora bound with ATP
Authors : Zhang, L.; Dou, C.; Zheng, Y.H.; Zhu, X.F.; Cheng, W.
Deposited on : 2024-11-25
Resolution : 2.84 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

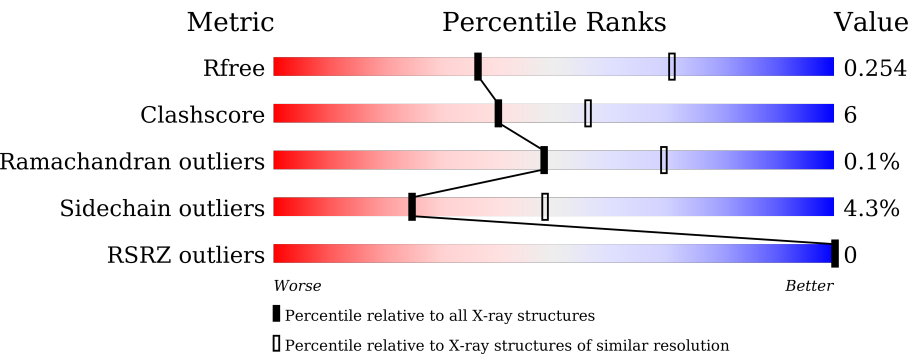
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	164625	1367 (2.86-2.82)
Clashscore	180529	1455 (2.86-2.82)
Ramachandran outliers	177936	1422 (2.86-2.82)
Sidechain outliers	177891	1423 (2.86-2.82)
RSRZ outliers	164620	1368 (2.86-2.82)

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	234	<div><div></div><div></div><div></div><div></div><div></div></div> <div>75%15%• 6%</div>
1	B	234	<div><div></div><div></div><div></div><div></div><div></div></div> <div>76%16%• 8%</div>
1	C	234	<div><div></div><div></div><div></div><div></div><div></div></div> <div>78%13%• 6%</div>
1	D	234	<div><div></div><div></div><div></div><div></div><div></div></div> <div>75%16%•• 6%</div>
1	E	234	<div><div></div><div></div><div></div><div></div><div></div></div> <div>75%16%• 6%</div>
1	F	234	<div><div></div><div></div><div></div><div></div><div></div></div> <div>79%13%• 6%</div>

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Mol	Chain	Length	Quality of chain
1	G	234	 79%11% • 7%
1	H	234	 74%17% • 6%
1	I	234	 79%15% • 6%
1	J	234	 71%21% • 6%
1	K	234	 77%14% • 7%
1	L	234	 69%22% • 7%
1	M	234	 75%16% • 7%
1	N	234	 76%15% • 7%

2 Entry composition

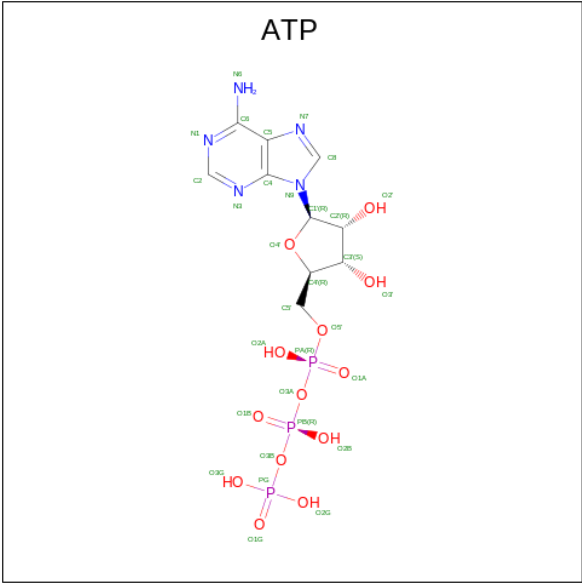
There are 3 unique types of molecules in this entry. The entry contains 24784 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Asparagine synthetase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	216	Total	C	N	O	S	0	0	0
			1703	1084	293	316	10			
1	E	220	Total	C	N	O	S	0	0	0
			1731	1101	298	322	10			
1	G	218	Total	C	N	O	S	0	0	0
			1718	1093	296	319	10			
1	I	221	Total	C	N	O	S	0	0	0
			1738	1106	299	323	10			
1	J	219	Total	C	N	O	S	0	0	0
			1725	1098	297	320	10			
1	L	218	Total	C	N	O	S	0	0	0
			1718	1093	296	319	10			
1	M	218	Total	C	N	O	S	0	0	0
			1716	1092	295	319	10			
1	A	219	Total	C	N	O	S	0	0	0
			1725	1098	297	320	10			
1	C	220	Total	C	N	O	S	0	0	0
			1731	1101	298	322	10			
1	D	219	Total	C	N	O	S	0	0	0
			1725	1098	297	320	10			
1	F	221	Total	C	N	O	S	0	0	0
			1738	1106	299	323	10			
1	H	219	Total	C	N	O	S	0	0	0
			1725	1098	297	320	10			
1	K	218	Total	C	N	O	S	0	0	0
			1718	1093	296	319	10			
1	N	218	Total	C	N	O	S	0	0	0
			1716	1092	295	319	10			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

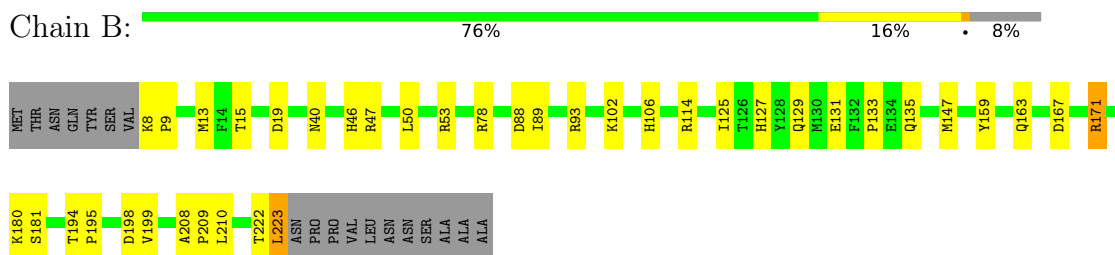
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	19	Total O 19 19	0	0
3	E	11	Total O 11 11	0	0
3	G	9	Total O 9 9	0	0
3	I	15	Total O 15 15	0	0
3	J	8	Total O 8 8	0	0
3	L	10	Total O 10 10	0	0
3	M	8	Total O 8 8	0	0
3	A	20	Total O 20 20	0	0
3	C	29	Total O 29 29	0	0
3	D	30	Total O 30 30	0	0
3	F	20	Total O 20 20	0	0
3	H	9	Total O 9 9	0	0
3	K	12	Total O 12 12	0	0
3	N	23	Total O 23 23	0	0

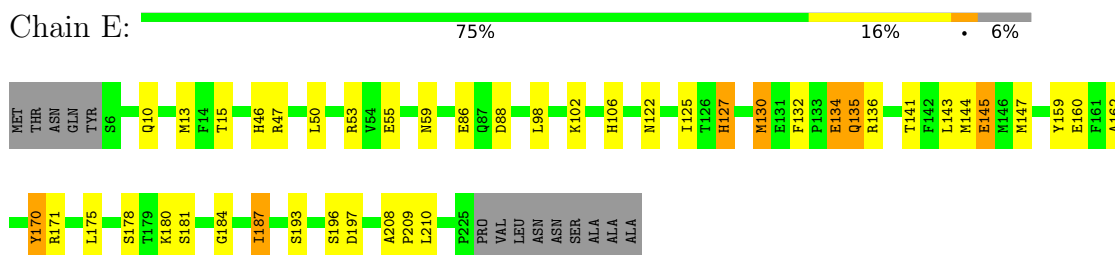
3 Residue-property plots

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.

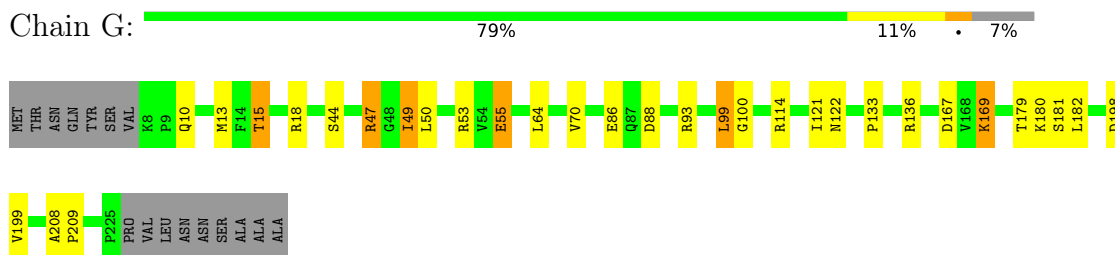
- Molecule 1: Asparagine synthetase domain-containing protein



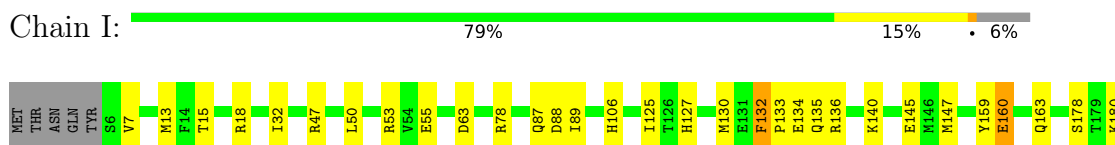
- Molecule 1: Asparagine synthetase domain-containing protein

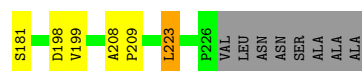


- Molecule 1: Asparagine synthetase domain-containing protein



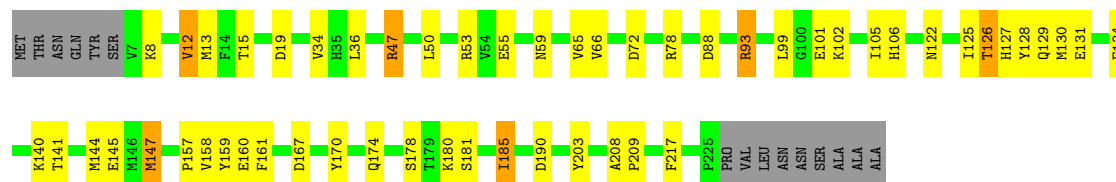
- Molecule 1: Asparagine synthetase domain-containing protein





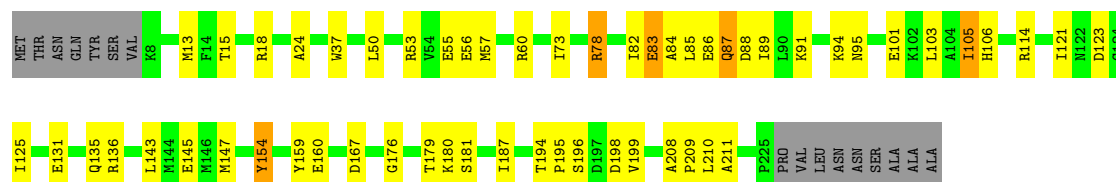
- Molecule 1: Asparagine synthetase domain-containing protein

Chain J: 71% 21% 6%



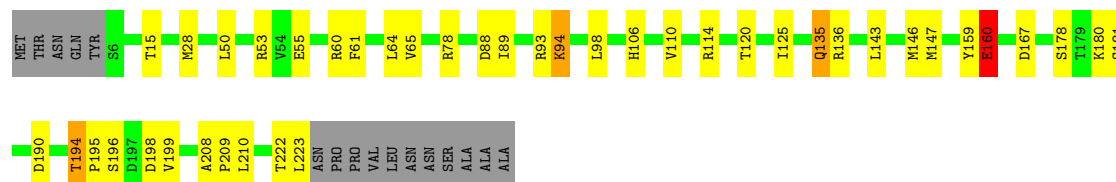
- Molecule 1: Asparagine synthetase domain-containing protein

Chain L: 69% 22% 7%



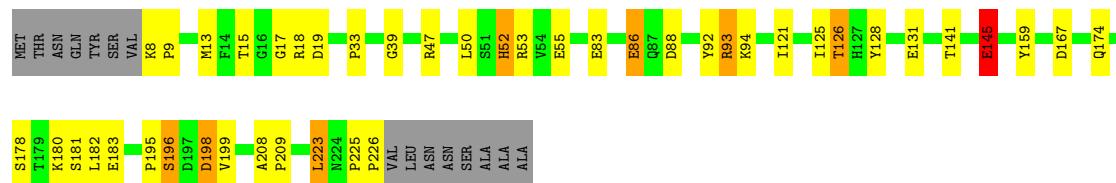
- Molecule 1: Asparagine synthetase domain-containing protein

Chain M: 75% 16% 7%



- Molecule 1: Asparagine synthetase domain-containing protein

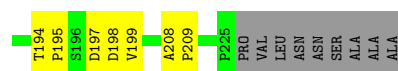
Chain A: 75% 15% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

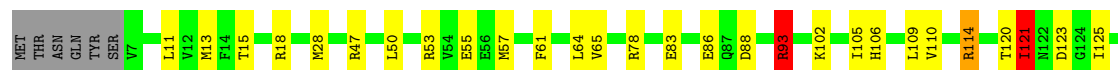
Chain C: 78% 13% 6%





- Molecule 1: Asparagine synthetase domain-containing protein

Chain D: 75% 16% 6%



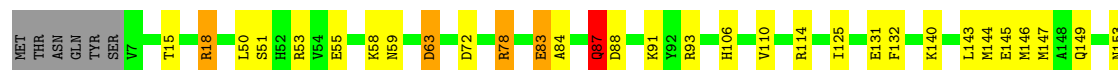
- Molecule 1: Asparagine synthetase domain-containing protein

Chain F: 79% 13% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain H: 74% 17% 6%



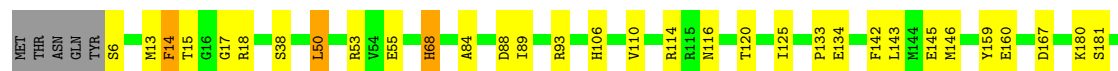
- Molecule 1: Asparagine synthetase domain-containing protein

Chain K: 77% 14% 7%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain N: 76% 15% 7%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.71Å 134.33Å 235.96Å 90.00° 98.43° 90.00°	Depositor
Resolution (Å)	33.34 – 2.84 33.34 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.34-2.84) 99.7 (33.34-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.210 , 0.252 0.218 , 0.254	Depositor DCC
R_{free} test set	5003 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.217 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24784	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.86	0/1760	1.30	10/2382 (0.4%)
1	B	0.88	1/1736 (0.1%)	1.32	10/2347 (0.4%)
1	C	0.97	1/1765 (0.1%)	1.36	9/2388 (0.4%)
1	D	0.99	0/1759	1.38	13/2380 (0.5%)
1	E	0.86	1/1765 (0.1%)	1.35	11/2388 (0.5%)
1	F	0.83	0/1773	1.29	11/2400 (0.5%)
1	G	0.77	0/1752	1.28	11/2370 (0.5%)
1	H	0.87	0/1759	1.38	18/2380 (0.8%)
1	I	0.87	0/1773	1.34	9/2400 (0.4%)
1	J	0.84	0/1759	1.33	10/2380 (0.4%)
1	K	0.86	0/1752	1.38	13/2370 (0.5%)
1	L	0.76	0/1752	1.29	14/2370 (0.6%)
1	M	0.79	0/1749	1.25	7/2365 (0.3%)
1	N	0.93	0/1749	1.38	16/2365 (0.7%)
All	All	0.87	3/24603 (0.0%)	1.33	162/33285 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	4
1	D	0	2
1	E	0	2
1	F	0	3
1	G	0	2
1	H	0	3
1	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	2
1	K	0	2
1	L	0	3
1	M	0	2
1	N	0	2
All	All	0	34

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	127	HIS	CE1-NE2	-5.62	1.26	1.32
1	C	106	HIS	CD2-NE2	5.22	1.43	1.37
1	B	223	LEU	C-O	5.10	1.33	1.23

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	198	ASP	CA-CB-CG	11.21	123.81	112.60
1	D	198	ASP	CA-CB-CG	10.34	122.94	112.60
1	H	59	ASN	CA-CB-CG	-9.98	102.62	112.60
1	H	83	GLU	CB-CG-CD	8.78	127.52	112.60
1	N	145	GLU	CB-CG-CD	8.60	127.23	112.60
1	M	190	ASP	CA-CB-CG	8.31	120.91	112.60
1	A	145	GLU	CB-CG-CD	8.10	126.37	112.60
1	J	59	ASN	CA-CB-CG	-8.04	104.56	112.60
1	I	160	GLU	CB-CG-CD	7.85	125.95	112.60
1	G	169	LYS	CG-CD-CE	7.84	129.33	111.30
1	B	222	THR	CA-C-N	7.75	135.66	121.70
1	B	222	THR	C-N-CA	7.75	135.66	121.70
1	N	68	HIS	CB-CG-CD2	-7.74	121.14	131.20
1	K	63	ASP	CA-CB-CG	7.70	120.30	112.60
1	F	160	GLU	CB-CG-CD	7.58	125.48	112.60
1	A	198	ASP	CA-CB-CG	7.44	120.04	112.60
1	N	68	HIS	CB-CG-ND1	7.35	133.73	122.70
1	L	198	ASP	CA-CB-CG	7.35	119.95	112.60
1	B	198	ASP	CA-CB-CG	7.24	119.84	112.60
1	C	198	ASP	CA-CB-CG	7.22	119.82	112.60
1	N	88	ASP	CA-CB-CG	7.21	119.81	112.60
1	I	87	GLN	CB-CG-CD	-7.09	100.54	112.60
1	B	88	ASP	CA-CB-CG	7.07	119.67	112.60
1	J	167	ASP	CA-CB-CG	7.01	119.61	112.60
1	L	194	THR	CA-CB-OG1	-6.97	99.14	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	94	LYS	CG-CD-CE	6.86	127.08	111.30
1	N	134	GLU	CB-CG-CD	6.83	124.20	112.60
1	M	94	LYS	CB-CG-CD	6.71	126.73	111.30
1	K	194	THR	CA-CB-OG1	-6.71	99.54	109.60
1	C	88	ASP	CA-CB-CG	6.69	119.29	112.60
1	L	105	ILE	CA-CB-CG1	6.68	121.76	110.40
1	J	88	ASP	CA-CB-CG	6.67	119.28	112.60
1	E	88	ASP	CA-CB-CG	6.65	119.25	112.60
1	F	198	ASP	CA-CB-CG	6.64	119.24	112.60
1	H	198	ASP	CA-CB-CG	6.62	119.22	112.60
1	D	88	ASP	CA-CB-CG	6.59	119.19	112.60
1	F	190	ASP	CA-CB-CG	6.56	119.16	112.60
1	G	93	ARG	CB-CG-CD	6.51	126.28	111.30
1	G	88	ASP	CA-CB-CG	6.47	119.07	112.60
1	G	198	ASP	CA-CB-CG	6.41	119.01	112.60
1	L	167	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	174	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	K	88	ASP	CA-CB-CG	6.34	118.94	112.60
1	H	167	ASP	CA-CB-CG	6.34	118.94	112.60
1	K	127	HIS	CA-CB-CG	6.34	120.14	113.80
1	D	83	GLU	CB-CG-CD	-6.32	101.85	112.60
1	F	88	ASP	CA-CB-CG	6.28	118.88	112.60
1	E	55	GLU	CB-CG-CD	6.27	123.26	112.60
1	D	93	ARG	CB-CG-CD	6.26	125.71	111.30
1	A	183	GLU	N-CA-CB	-6.25	101.50	111.62
1	L	160	GLU	CB-CG-CD	6.24	123.20	112.60
1	K	169	LYS	CG-CD-CE	6.22	125.62	111.30
1	D	121	ILE	N-CA-CB	-6.21	100.58	111.39
1	A	88	ASP	CA-CB-CG	6.16	118.76	112.60
1	E	130	MET	CB-CA-C	-6.16	109.46	116.54
1	C	47	ARG	N-CA-CB	-6.16	101.38	110.49
1	E	134	GLU	CB-CG-CD	6.11	122.99	112.60
1	G	167	ASP	CA-CB-CG	6.09	118.69	112.60
1	D	167	ASP	CA-CB-CG	6.09	118.69	112.60
1	J	174	GLN	OE1-CD-NE2	-6.09	116.51	122.60
1	M	167	ASP	CA-CB-CG	6.04	118.64	112.60
1	M	88	ASP	CA-CB-CG	6.02	118.62	112.60
1	D	121	ILE	CA-CB-CG2	6.02	120.74	110.50
1	C	197	ASP	CA-CB-CG	6.01	118.61	112.60
1	H	190	ASP	CA-CB-CG	5.98	118.58	112.60
1	I	88	ASP	CA-CB-CG	5.97	118.58	112.60
1	J	190	ASP	CA-CB-CG	5.97	118.57	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	145	GLU	CB-CG-CD	5.95	122.72	112.60
1	K	190	ASP	CA-CB-CG	5.95	118.55	112.60
1	H	206	GLU	N-CA-C	-5.91	105.90	113.23
1	L	91	LYS	CG-CD-CE	5.86	124.78	111.30
1	N	160	GLU	N-CA-CB	5.85	118.82	110.16
1	K	101	GLU	CB-CG-CD	5.80	122.47	112.60
1	I	198	ASP	CA-CB-CG	5.80	118.40	112.60
1	L	87	GLN	CA-CB-CG	5.80	125.69	114.10
1	C	7	VAL	N-CA-CB	5.79	120.78	111.23
1	I	140	LYS	CB-CG-CD	5.79	124.62	111.30
1	B	19	ASP	CA-CB-CG	5.78	118.38	112.60
1	F	63	ASP	CA-CB-CG	5.78	118.38	112.60
1	H	170	TYR	CB-CA-C	5.76	122.12	110.38
1	J	47	ARG	N-CA-CB	-5.75	101.98	110.49
1	L	18	ARG	CB-CA-C	-5.72	101.66	110.81
1	G	99	LEU	N-CA-C	-5.71	103.87	111.24
1	I	55	GLU	CB-CA-C	5.70	119.91	110.90
1	E	160	GLU	CB-CG-CD	5.69	122.28	112.60
1	L	88	ASP	CA-CB-CG	5.68	118.28	112.60
1	I	223	LEU	N-CA-C	-5.64	106.22	114.39
1	E	59	ASN	CA-CB-CG	-5.62	106.98	112.60
1	E	135	GLN	N-CA-CB	5.60	119.06	110.61
1	N	55	GLU	CB-CA-C	5.58	119.72	110.90
1	H	132	PHE	CA-CB-CG	5.58	119.38	113.80
1	H	149	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	M	160	GLU	N-CA-CB	5.55	118.37	110.16
1	J	55	GLU	CB-CA-C	5.54	119.66	110.90
1	N	160	GLU	CB-CG-CD	5.54	122.02	112.60
1	H	224	ASN	OD1-CG-ND2	5.51	128.11	122.60
1	D	55	GLU	CB-CA-C	5.50	119.60	110.90
1	G	18	ARG	CB-CA-C	-5.50	102.01	110.81
1	E	170	TYR	CB-CA-C	5.50	121.60	110.38
1	C	160	GLU	CB-CG-CD	5.49	121.94	112.60
1	H	18	ARG	CB-CA-C	-5.49	101.68	110.79
1	A	83	GLU	CB-CG-CD	-5.49	103.28	112.60
1	E	197	ASP	CA-CB-CG	5.46	118.06	112.60
1	J	93	ARG	CB-CG-CD	5.46	123.85	111.30
1	F	102	LYS	CB-CG-CD	5.42	123.77	111.30
1	L	18	ARG	CG-CD-NE	-5.42	100.08	112.00
1	D	18	ARG	CB-CA-C	-5.41	102.15	110.81
1	E	187	ILE	N-CA-C	-5.41	105.97	113.00
1	B	46	HIS	CB-CG-CD2	-5.40	124.19	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	GLN	CB-CG-CD	5.39	121.76	112.60
1	N	14	PHE	N-CA-CB	-5.39	102.24	110.65
1	H	58	LYS	CG-CD-CE	5.39	123.69	111.30
1	N	222	THR	CA-CB-OG1	-5.38	101.52	109.60
1	G	55	GLU	CB-CA-C	5.34	119.34	110.90
1	J	170	TYR	CB-CA-C	5.34	121.28	110.38
1	B	194	THR	CA-CB-OG1	-5.34	101.60	109.60
1	K	170	TYR	CB-CA-C	5.34	121.14	109.99
1	N	167	ASP	CA-CB-CG	5.33	117.93	112.60
1	K	18	ARG	CB-CA-C	-5.33	102.28	110.81
1	D	114	ARG	CB-CG-CD	5.29	123.47	111.30
1	E	145	GLU	N-CA-CB	5.29	117.67	110.01
1	K	132	PHE	N-CA-CB	-5.27	100.50	109.57
1	N	221	GLU	CB-CG-CD	5.26	121.55	112.60
1	F	140	LYS	CG-CD-CE	-5.25	99.22	111.30
1	A	167	ASP	CA-CB-CG	5.25	117.85	112.60
1	N	55	GLU	CG-CD-OE2	-5.25	106.33	118.40
1	I	132	PHE	CB-CA-C	5.24	116.97	109.26
1	H	63	ASP	CA-CB-CG	5.22	117.82	112.60
1	L	179	THR	CA-CB-OG1	-5.22	101.77	109.60
1	L	179	THR	OG1-CB-CG2	5.22	119.73	109.30
1	J	65	VAL	N-CA-CB	5.20	117.11	112.06
1	H	87	GLN	CA-CB-CG	5.20	124.49	114.10
1	I	55	GLU	CG-CD-OE1	-5.19	106.47	118.40
1	H	153	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	K	102	LYS	CA-CB-CG	-5.18	103.74	114.10
1	C	93	ARG	CB-CA-C	5.18	119.69	111.51
1	M	55	GLU	CB-CA-C	5.17	119.06	110.90
1	D	18	ARG	CG-CD-NE	-5.15	100.67	112.00
1	F	146	MET	CG-SD-CE	-5.13	89.61	100.90
1	H	55	GLU	CB-CA-C	5.13	119.58	110.85
1	N	55	GLU	CB-CG-CD	5.13	121.33	112.60
1	F	14	PHE	N-CA-CB	-5.13	102.65	110.65
1	A	52	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	N	190	ASP	CA-CB-CG	5.09	117.69	112.60
1	G	18	ARG	CG-CD-NE	-5.08	100.83	112.00
1	D	174	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	C	55	GLU	CB-CA-C	5.06	119.45	110.85
1	F	167	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	86	GLU	CG-CD-OE2	-5.05	106.79	118.40
1	G	86	GLU	CB-CG-CD	-5.04	104.03	112.60
1	B	102	LYS	CB-CG-CD	5.04	122.90	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	93	ARG	CG-CD-NE	-5.04	100.91	112.00
1	H	88	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	47	ARG	CB-CA-C	-5.04	101.66	110.17
1	B	222	THR	CA-CB-CG2	5.03	119.06	110.50
1	F	46	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	N	116	ASN	OD1-CG-ND2	5.03	127.63	122.60
1	B	167	ASP	CA-CB-CG	5.03	117.63	112.60
1	L	194	THR	OG1-CB-CG2	-5.02	99.26	109.30
1	D	170	TYR	CB-CA-C	5.02	120.61	110.38
1	H	72	ASP	CA-CB-CG	5.01	117.61	112.60
1	K	55	GLU	CB-CA-C	5.00	119.36	110.85

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ARG	Sidechain
1	A	93	ARG	Sidechain
1	B	114	ARG	Sidechain
1	B	171	ARG	Sidechain
1	C	136	ARG	Sidechain
1	C	18	ARG	Sidechain
1	C	47	ARG	Sidechain
1	C	78	ARG	Sidechain
1	D	136	ARG	Sidechain
1	D	78	ARG	Sidechain
1	E	136	ARG	Sidechain
1	E	47	ARG	Sidechain
1	F	114	ARG	Sidechain
1	F	60	ARG	Sidechain
1	F	78	ARG	Sidechain
1	G	114	ARG	Sidechain
1	G	47	ARG	Sidechain
1	H	18	ARG	Sidechain
1	H	78	ARG	Sidechain
1	H	93	ARG	Sidechain
1	I	136	ARG	Sidechain
1	I	18	ARG	Sidechain
1	I	78	ARG	Sidechain
1	J	47	ARG	Sidechain
1	J	78	ARG	Sidechain
1	K	78	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	K	93	ARG	Sidechain
1	L	114	ARG	Sidechain
1	L	60	ARG	Sidechain
1	L	78	ARG	Sidechain
1	M	60	ARG	Sidechain
1	M	78	ARG	Sidechain
1	N	18	ARG	Sidechain
1	N	93	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1725	0	1719	27	0
1	B	1703	0	1699	21	0
1	C	1731	0	1726	18	0
1	D	1725	0	1721	31	0
1	E	1731	0	1726	28	3
1	F	1738	0	1733	14	0
1	G	1718	0	1712	20	0
1	H	1725	0	1721	16	0
1	I	1738	0	1733	21	0
1	J	1725	0	1721	32	0
1	K	1718	0	1712	12	0
1	L	1718	0	1712	39	3
1	M	1716	0	1713	24	0
1	N	1716	0	1713	15	0
2	A	31	0	12	4	0
2	B	31	0	12	3	0
2	C	31	0	12	1	0
2	D	31	0	12	1	0
2	E	31	0	12	4	0
2	F	31	0	12	1	0
2	G	31	0	12	1	0
2	H	31	0	12	2	0
2	I	31	0	12	4	0
2	J	31	0	12	2	0
2	K	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	31	0	12	0	0
2	M	31	0	12	0	0
2	N	31	0	12	3	0
3	A	20	0	0	0	0
3	B	19	0	0	2	0
3	C	29	0	0	0	0
3	D	30	0	0	1	0
3	E	11	0	0	1	0
3	F	20	0	0	1	0
3	G	9	0	0	0	0
3	H	9	0	0	1	0
3	I	15	0	0	1	0
3	J	8	0	0	1	0
3	K	12	0	0	0	0
3	L	10	0	0	1	0
3	M	8	0	0	1	0
3	N	23	0	0	1	0
All	All	24784	0	24229	316	3

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 6.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:MET:HE1	1:E:159:TYR:OH	1.43	1.17
1:L:103:LEU:HD21	1:L:211:ALA:HB2	1.33	1.07
1:A:19:ASP:OD2	1:A:126:THR:HG21	1.54	1.07
1:L:103:LEU:CD2	1:L:211:ALA:HB2	1.86	1.05
1:E:130:MET:CE	1:E:159:TYR:OH	2.12	0.97
1:L:103:LEU:HD21	1:L:211:ALA:CB	2.01	0.91
1:G:13:MET:HE2	1:G:121:ILE:CG2	2.05	0.86
1:L:106:HIS:HE2	1:L:154:TYR:HE2	1.24	0.85
1:M:28:MET:HE1	1:M:65:VAL:HG23	1.60	0.82
1:M:28:MET:HE3	1:M:64:LEU:C	2.04	0.82
1:G:13:MET:HE2	1:G:121:ILE:HG21	1.60	0.82
1:L:176:GLY:HA2	3:L:402:HOH:O	1.78	0.81
1:J:19:ASP:OD2	1:J:126:THR:HG21	1.80	0.81
1:M:160:GLU:HB2	3:M:405:HOH:O	1.80	0.81
1:D:28:MET:HE3	1:D:64:LEU:C	2.06	0.80
1:A:19:ASP:OD2	1:A:126:THR:CG2	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:MET:HE1	1:D:65:VAL:HG23	1.68	0.76
1:A:8:LYS:HB3	1:A:9:PRO:HD3	1.68	0.76
1:G:49:ILE:CD1	1:G:182:LEU:HD22	2.16	0.76
1:N:84:ALA:HB3	3:N:404:HOH:O	1.86	0.75
1:D:93:ARG:CB	1:D:93:ARG:HH11	2.00	0.75
1:D:106:HIS:HB3	1:D:146:MET:CE	2.18	0.74
1:B:127:HIS:CD2	1:B:163:GLN:HE22	2.05	0.74
1:I:125:ILE:HG22	1:I:159:TYR:CD1	2.23	0.74
1:L:103:LEU:CD2	1:L:211:ALA:CB	2.64	0.72
1:B:127:HIS:HD2	1:B:163:GLN:HE22	1.36	0.72
1:M:28:MET:HE1	1:M:65:VAL:CG2	2.18	0.72
1:F:125:ILE:HG22	1:F:159:TYR:CD1	2.24	0.72
1:M:196:SER:OG	1:M:199:VAL:HG13	1.90	0.72
1:I:125:ILE:HG22	1:I:159:TYR:HD1	1.54	0.71
1:B:223:LEU:HD22	1:E:171:ARG:HH11	1.54	0.70
1:A:125:ILE:HG22	1:A:159:TYR:HD1	1.57	0.70
1:M:196:SER:HG	1:M:199:VAL:HG13	1.56	0.70
1:C:13:MET:HE3	1:C:105:ILE:CG2	2.22	0.69
1:F:125:ILE:HG22	1:F:159:TYR:HD1	1.56	0.69
1:B:125:ILE:HG22	1:B:159:TYR:HD1	1.58	0.69
1:L:125:ILE:HG22	1:L:159:TYR:HD1	1.58	0.69
1:M:125:ILE:HG22	1:M:159:TYR:HD1	1.58	0.69
1:E:141:THR:O	1:E:145:GLU:HG2	1.93	0.69
1:M:125:ILE:HG23	1:M:135:GLN:HG3	1.75	0.69
1:N:125:ILE:HG22	1:N:159:TYR:HD1	1.57	0.68
1:C:13:MET:HE3	1:C:105:ILE:HG21	1.75	0.68
1:L:94:LYS:HZ3	1:L:195:PRO:HA	1.59	0.68
1:E:130:MET:HE1	1:E:159:TYR:CZ	2.30	0.67
1:J:125:ILE:HG22	1:J:159:TYR:HD1	1.59	0.67
1:D:28:MET:HE1	1:D:65:VAL:CG2	2.24	0.67
1:N:125:ILE:HG22	1:N:159:TYR:CD1	2.30	0.67
1:D:93:ARG:HH11	1:D:93:ARG:HB3	1.58	0.67
1:D:125:ILE:HG22	1:D:159:TYR:HD1	1.60	0.67
1:I:7:VAL:HG11	1:I:32:ILE:HD13	1.77	0.66
1:J:93:ARG:HH11	1:J:93:ARG:HB3	1.60	0.66
1:L:73:ILE:CD1	1:L:105:ILE:HD13	2.25	0.66
1:A:125:ILE:HG22	1:A:159:TYR:CD1	2.31	0.66
1:B:127:HIS:HD2	1:B:163:GLN:NE2	1.94	0.65
1:K:125:ILE:HG22	1:K:159:TYR:HD1	1.60	0.65
1:B:125:ILE:HG22	1:B:159:TYR:CD1	2.31	0.65
1:L:125:ILE:HG22	1:L:159:TYR:CD1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:125:ILE:HG22	1:M:159:TYR:CD1	2.31	0.65
1:C:130:MET:HE2	1:C:159:TYR:CZ	2.32	0.65
1:E:13:MET:HE1	1:E:102:LYS:NZ	2.12	0.64
1:L:196:SER:OG	1:L:199:VAL:HG13	1.96	0.64
1:D:125:ILE:HG22	1:D:159:TYR:CD1	2.32	0.64
1:J:125:ILE:HG22	1:J:159:TYR:CD1	2.32	0.64
1:J:141:THR:HA	1:J:144:MET:HE2	1.79	0.64
1:G:133:PRO:HA	1:G:136:ARG:HD2	1.79	0.64
1:E:125:ILE:HG22	1:E:159:TYR:HD1	1.63	0.64
1:G:49:ILE:HD11	1:G:182:LEU:HD22	1.79	0.64
1:H:125:ILE:HG22	1:H:159:TYR:HD1	1.63	0.64
1:D:11:LEU:HD22	1:D:121:ILE:HG12	1.80	0.63
1:D:93:ARG:HB3	1:D:93:ARG:NH1	2.13	0.63
1:J:93:ARG:HB3	1:J:93:ARG:NH1	2.14	0.63
1:L:154:TYR:CD1	1:L:154:TYR:C	2.76	0.63
1:F:141:THR:HA	1:F:144:MET:HE2	1.79	0.63
1:M:195:PRO:HB2	1:M:199:VAL:CG2	2.28	0.63
1:G:49:ILE:HD13	1:G:182:LEU:HD22	1.80	0.63
1:L:195:PRO:HB2	1:L:199:VAL:CG2	2.28	0.63
1:A:196:SER:O	1:A:199:VAL:HG22	1.98	0.63
1:D:170:TYR:HB2	3:D:420:HOH:O	1.98	0.63
1:J:13:MET:HE1	1:J:102:LYS:HZ2	1.63	0.62
1:M:196:SER:O	1:M:199:VAL:HG22	1.99	0.62
1:L:154:TYR:HD1	1:L:154:TYR:O	1.82	0.62
1:K:125:ILE:HG22	1:K:159:TYR:CD1	2.34	0.62
1:I:127:HIS:CE1	1:I:130:MET:HE1	2.35	0.62
1:I:7:VAL:HG11	1:I:32:ILE:CD1	2.29	0.62
1:M:28:MET:HE2	1:M:61:PHE:HB3	1.81	0.62
1:H:125:ILE:HG22	1:H:159:TYR:CD1	2.34	0.62
1:E:130:MET:C	1:E:132:PHE:H	2.08	0.61
1:G:13:MET:CE	1:G:121:ILE:CG2	2.77	0.61
1:L:196:SER:O	1:L:199:VAL:HG22	1.99	0.61
1:D:109:LEU:HD13	1:D:121:ILE:HD13	1.82	0.61
2:E:301:ATP:H5'1	2:E:301:ATP:H8	1.66	0.61
1:J:19:ASP:OD2	1:J:126:THR:CG2	2.48	0.61
1:L:196:SER:HG	1:L:199:VAL:HG13	1.65	0.61
1:A:15:THR:OG1	2:A:301:ATP:O2G	2.17	0.61
1:D:93:ARG:HH11	1:D:93:ARG:CG	2.13	0.61
1:A:93:ARG:O	1:A:94:LYS:HD2	2.02	0.60
1:L:94:LYS:NZ	1:L:195:PRO:HA	2.17	0.60
1:D:53:ARG:NH2	1:D:180:LYS:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:ILE:HG22	1:E:159:TYR:CD1	2.37	0.59
1:D:106:HIS:HB3	1:D:146:MET:HE3	1.85	0.59
1:E:53:ARG:NH2	1:E:180:LYS:O	2.36	0.59
1:I:127:HIS:CD2	1:I:163:GLN:HE22	2.21	0.59
1:E:10:GLN:HE21	1:E:122:ASN:HD21	1.50	0.59
1:N:208:ALA:HB3	1:N:209:PRO:HD3	1.85	0.59
1:F:125:ILE:CG2	1:F:159:TYR:CD1	2.86	0.58
1:E:130:MET:O	1:E:132:PHE:N	2.33	0.58
1:K:130:MET:O	1:K:131:GLU:C	2.44	0.58
1:E:175:LEU:HA	3:E:404:HOH:O	2.04	0.58
1:I:15:THR:OG1	2:I:301:ATP:O1G	2.21	0.58
1:C:127:HIS:CG	1:C:130:MET:HE3	2.39	0.58
1:K:53:ARG:NH2	1:K:180:LYS:O	2.37	0.58
1:F:53:ARG:NH2	1:F:180:LYS:O	2.38	0.57
1:A:225:PRO:HB2	1:A:226:PRO:HD2	1.86	0.57
1:J:208:ALA:HB3	1:J:209:PRO:HD3	1.87	0.57
1:L:106:HIS:NE2	1:L:154:TYR:HE2	2.00	0.57
1:E:127:HIS:ND1	1:E:130:MET:HE2	2.20	0.56
1:C:127:HIS:HA	1:C:130:MET:HE3	1.86	0.56
1:N:15:THR:OG1	2:N:301:ATP:O3G	2.20	0.56
1:L:53:ARG:NH2	1:L:180:LYS:O	2.37	0.56
1:M:53:ARG:NH2	1:M:180:LYS:O	2.38	0.56
1:C:13:MET:CE	1:C:105:ILE:HG21	2.34	0.56
1:C:18:ARG:HE	1:C:169:LYS:HE2	1.70	0.56
1:I:13:MET:HB3	2:I:301:ATP:N3	2.21	0.56
1:F:125:ILE:CG2	1:F:159:TYR:HD1	2.19	0.56
1:G:53:ARG:NH2	1:G:180:LYS:O	2.39	0.56
1:L:82:ILE:O	1:L:83:GLU:C	2.49	0.56
1:A:126:THR:OG1	1:A:128:TYR:CD2	2.57	0.56
1:J:53:ARG:NH2	1:J:180:LYS:O	2.38	0.56
1:G:13:MET:CE	1:G:121:ILE:HG22	2.36	0.55
1:G:169:LYS:HG2	1:G:179:THR:OG1	2.06	0.55
1:B:53:ARG:NH2	1:B:180:LYS:O	2.39	0.55
1:L:125:ILE:HG12	1:L:135:GLN:HG2	1.87	0.55
1:A:53:ARG:NH2	1:A:180:LYS:O	2.39	0.55
1:A:141:THR:O	1:A:145:GLU:HG2	2.06	0.55
1:H:53:ARG:NH2	1:H:180:LYS:O	2.39	0.55
1:C:53:ARG:NH2	1:C:180:LYS:O	2.39	0.54
1:M:93:ARG:O	1:M:94:LYS:HD2	2.07	0.54
1:D:28:MET:HE2	1:D:61:PHE:HB3	1.89	0.54
1:I:53:ARG:NH2	1:I:180:LYS:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:TYR:C	1:L:154:TYR:HD1	2.16	0.54
1:D:208:ALA:HB3	1:D:209:PRO:HD3	1.88	0.54
1:E:208:ALA:HB3	1:E:209:PRO:HD3	1.90	0.54
2:H:301:ATP:H5'1	2:H:301:ATP:H8	1.73	0.53
1:A:223:LEU:HD22	1:C:26:TYR:CE2	2.44	0.53
1:N:53:ARG:NH2	1:N:180:LYS:O	2.41	0.53
1:D:185:ILE:HG12	1:D:185:ILE:O	2.08	0.53
1:B:13:MET:HB3	2:B:301:ATP:N3	2.23	0.53
1:I:127:HIS:CD2	1:I:163:GLN:NE2	2.77	0.52
1:J:12:VAL:HG23	1:J:36:LEU:HD23	1.90	0.52
1:A:52:HIS:O	1:A:55:GLU:HG2	2.09	0.52
1:I:145:GLU:HB3	3:I:409:HOH:O	2.09	0.52
1:A:196:SER:HB3	1:A:199:VAL:HG13	1.92	0.52
1:K:208:ALA:HB3	1:K:209:PRO:HD3	1.90	0.52
1:B:208:ALA:HB3	1:B:209:PRO:HD3	1.92	0.52
1:B:223:LEU:HD22	1:E:171:ARG:NH1	2.21	0.52
1:B:40:ASN:CG	3:B:405:HOH:O	2.52	0.51
1:G:44:SER:HB2	1:G:47:ARG:HD2	1.93	0.51
1:J:12:VAL:HG12	1:J:122:ASN:HB2	1.91	0.51
1:L:208:ALA:HB3	1:L:209:PRO:HD3	1.92	0.51
1:I:208:ALA:HB3	1:I:209:PRO:HD3	1.93	0.51
1:B:8:LYS:HB3	1:B:9:PRO:HD3	1.93	0.51
1:E:15:THR:HB	2:E:301:ATP:O2G	2.11	0.51
1:A:39:GLY:O	2:A:301:ATP:N6	2.34	0.50
1:H:106:HIS:HB3	1:H:147:MET:HE3	1.93	0.50
1:D:106:HIS:HB3	1:D:146:MET:HE1	1.91	0.50
1:M:28:MET:HE2	1:M:64:LEU:HB2	1.93	0.50
1:C:208:ALA:HB3	1:C:209:PRO:HD3	1.92	0.50
1:F:140:LYS:NZ	3:F:401:HOH:O	2.34	0.50
1:M:136:ARG:NH1	1:M:194:THR:HG22	2.27	0.50
1:L:106:HIS:CE1	1:L:143:LEU:HD13	2.47	0.50
1:J:12:VAL:CG2	1:J:36:LEU:HD23	2.42	0.49
1:G:208:ALA:HB3	1:G:209:PRO:HD3	1.94	0.49
1:H:84:ALA:HB1	1:H:87:GLN:HE21	1.77	0.49
1:J:126:THR:OG1	1:J:128:TYR:CD2	2.61	0.49
1:E:13:MET:HB3	2:E:301:ATP:N3	2.28	0.49
1:H:208:ALA:HB3	1:H:209:PRO:HD3	1.94	0.49
1:M:208:ALA:HB3	1:M:209:PRO:HD3	1.95	0.49
1:D:28:MET:HE2	1:D:64:LEU:HB2	1.95	0.49
1:F:106:HIS:HB3	1:F:147:MET:HE3	1.95	0.49
1:J:106:HIS:O	1:J:147:MET:HE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:MET:HE1	1:D:102:LYS:HZ1	1.79	0.48
1:G:15:THR:HB	2:G:301:ATP:O2G	2.14	0.48
1:H:106:HIS:CE1	1:H:143:LEU:HD13	2.48	0.48
1:J:161:PHE:CD1	1:J:161:PHE:N	2.73	0.48
1:I:127:HIS:ND1	1:I:130:MET:CE	2.77	0.48
1:K:13:MET:HE2	1:K:121:ILE:HD12	1.95	0.47
1:I:125:ILE:HD13	1:I:135:GLN:HA	1.95	0.47
1:L:82:ILE:O	1:L:85:LEU:N	2.48	0.47
1:D:53:ARG:O	1:D:57:MET:HG3	2.13	0.47
1:L:106:HIS:HB3	1:L:147:MET:HE3	1.97	0.47
1:B:135:GLN:NE2	2:B:301:ATP:O1B	2.45	0.47
1:J:72:ASP:HB3	3:J:401:HOH:O	2.15	0.47
1:J:140:LYS:O	1:J:144:MET:HB2	2.14	0.47
1:B:106:HIS:HB3	1:B:147:MET:HE3	1.96	0.47
1:E:10:GLN:NE2	1:E:122:ASN:HD21	2.13	0.47
1:E:13:MET:CE	1:E:102:LYS:HZ3	2.28	0.47
1:G:10:GLN:HE21	1:G:122:ASN:HD21	1.62	0.47
1:I:127:HIS:CE1	1:I:130:MET:CE	2.97	0.47
1:J:157:PRO:O	1:J:161:PHE:CE1	2.67	0.47
1:D:106:HIS:CB	1:D:146:MET:HE1	2.45	0.47
1:M:106:HIS:HB3	1:M:147:MET:HE3	1.96	0.47
1:C:13:MET:HB3	2:C:301:ATP:N3	2.30	0.47
1:N:13:MET:HB3	2:N:301:ATP:N3	2.31	0.46
1:M:28:MET:HE3	1:M:65:VAL:N	2.30	0.46
1:C:15:THR:O	1:C:50:LEU:HD13	2.16	0.46
1:C:110:VAL:O	1:C:114:ARG:HG3	2.15	0.46
1:K:144:MET:HE2	1:K:144:MET:HB3	1.78	0.46
1:J:101:GLU:O	1:J:105:ILE:HG13	2.16	0.46
1:M:106:HIS:CE1	1:M:143:LEU:HD13	2.50	0.46
1:K:133:PRO:HA	1:K:136:ARG:HG3	1.96	0.46
1:B:171:ARG:NH1	1:J:217:PHE:HB2	2.31	0.46
1:E:46:HIS:O	1:E:184:GLY:HA2	2.15	0.46
1:A:13:MET:HB3	2:A:301:ATP:N3	2.31	0.46
1:E:143:LEU:O	1:E:147:MET:HG2	2.15	0.46
1:M:110:VAL:O	1:M:114:ARG:HG3	2.16	0.46
1:G:10:GLN:NE2	1:G:122:ASN:HD21	2.13	0.46
1:N:38:SER:OG	1:N:68:HIS:HE1	1.98	0.46
1:N:106:HIS:CE1	1:N:143:LEU:HD13	2.51	0.45
1:N:133:PRO:HG3	1:N:195:PRO:HG3	1.97	0.45
1:F:15:THR:O	1:F:50:LEU:HD13	2.16	0.45
1:N:14:PHE:CE2	1:N:50:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:VAL:HG13	1:G:70:VAL:O	2.16	0.45
1:J:129:GLN:NE2	2:J:301:ATP:O1B	2.42	0.45
1:A:208:ALA:HB3	1:A:209:PRO:HD3	1.98	0.45
1:C:106:HIS:HB3	1:C:147:MET:HE3	1.96	0.45
1:L:131:GLU:O	1:L:136:ARG:NH1	2.50	0.45
1:L:24:ALA:HB3	1:L:57:MET:HE1	1.98	0.45
1:L:82:ILE:O	1:L:84:ALA:N	2.49	0.45
1:D:110:VAL:O	1:D:114:ARG:HG3	2.17	0.45
1:H:110:VAL:O	1:H:114:ARG:HG3	2.16	0.45
1:N:110:VAL:O	1:N:114:ARG:HG3	2.16	0.45
1:D:106:HIS:CE1	1:D:143:LEU:HD13	2.52	0.45
1:L:73:ILE:HD13	1:L:105:ILE:HD13	1.97	0.45
1:A:225:PRO:HB2	1:A:226:PRO:CD	2.47	0.45
1:L:53:ARG:O	1:L:57:MET:HG3	2.17	0.45
2:D:301:ATP:H5'1	2:D:301:ATP:H8	1.82	0.45
1:N:142:PHE:HE2	1:N:205:ARG:HG2	1.81	0.45
1:I:15:THR:O	1:I:50:LEU:HD13	2.17	0.44
1:N:106:HIS:HB3	1:N:146:MET:HE2	1.98	0.44
1:K:15:THR:O	1:K:50:LEU:HD13	2.17	0.44
1:L:106:HIS:NE2	1:L:154:TYR:CE2	2.75	0.44
1:A:15:THR:O	1:A:50:LEU:HD13	2.17	0.44
1:C:18:ARG:NE	1:C:169:LYS:HE2	2.32	0.44
1:B:125:ILE:HD13	1:B:135:GLN:HA	1.98	0.44
1:J:127:HIS:O	1:J:130:MET:HG3	2.17	0.44
1:A:195:PRO:HB2	1:A:199:VAL:CG2	2.47	0.44
1:H:51:SER:HB2	3:H:401:HOH:O	2.18	0.44
1:E:106:HIS:CE1	1:E:143:LEU:HD13	2.51	0.44
1:A:8:LYS:HG3	1:A:33:PRO:HD2	2.00	0.44
1:A:225:PRO:CB	1:A:226:PRO:CD	2.95	0.44
1:C:136:ARG:NH1	1:C:195:PRO:O	2.35	0.44
1:F:103:LEU:HD11	1:F:146:MET:HE1	2.00	0.44
1:K:129:GLN:O	1:K:130:MET:C	2.60	0.44
1:J:13:MET:HE1	1:J:102:LYS:NZ	2.31	0.44
1:J:15:THR:O	1:J:50:LEU:HD13	2.17	0.43
1:J:185:ILE:HG12	1:J:185:ILE:O	2.17	0.43
1:F:208:ALA:HB3	1:F:209:PRO:HD3	2.00	0.43
1:H:15:THR:OG1	2:H:301:ATP:O3G	2.24	0.43
1:H:140:LYS:O	1:H:144:MET:HG3	2.17	0.43
1:I:223:LEU:HD11	1:J:158:VAL:HG12	2.01	0.43
1:C:13:MET:HE3	1:C:105:ILE:HG22	1.98	0.43
1:F:225:PRO:HB3	1:F:226:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:THR:O	1:E:50:LEU:HD13	2.18	0.43
1:A:92:TYR:O	1:A:94:LYS:HG2	2.18	0.43
1:G:15:THR:O	1:G:50:LEU:HD13	2.18	0.43
1:G:99:LEU:O	1:G:100:GLY:C	2.62	0.43
1:D:28:MET:HE2	1:D:64:LEU:CB	2.49	0.43
1:J:34:VAL:O	1:J:66:VAL:HG22	2.18	0.43
1:J:141:THR:O	1:J:145:GLU:HG3	2.18	0.43
1:M:15:THR:O	1:M:50:LEU:HD13	2.19	0.43
1:E:130:MET:C	1:E:132:PHE:N	2.71	0.43
1:D:109:LEU:HD13	1:D:121:ILE:CD1	2.48	0.43
1:H:91:LYS:NZ	1:H:206:GLU:OE1	2.51	0.43
1:M:106:HIS:HB3	1:M:146:MET:HE2	2.00	0.43
1:I:106:HIS:HB3	1:I:147:MET:HE3	2.00	0.43
1:L:15:THR:O	1:L:50:LEU:HD13	2.19	0.42
1:L:101:GLU:O	1:L:105:ILE:HG12	2.18	0.42
1:K:185:ILE:O	1:K:185:ILE:HG12	2.19	0.42
1:I:134:GLU:HG2	1:I:135:GLN:HG3	2.00	0.42
1:D:28:MET:CE	1:D:64:LEU:CB	2.98	0.42
2:I:301:ATP:O2G	2:I:301:ATP:O3'	2.37	0.42
1:B:78:ARG:NH1	1:E:170:TYR:CD1	2.88	0.42
1:G:180:LYS:HA	1:G:180:LYS:HD3	1.93	0.42
1:I:132:PHE:HA	1:I:133:PRO:HD3	1.96	0.42
1:J:99:LEU:HD23	1:J:203:TYR:CD2	2.54	0.42
1:L:13:MET:HE2	1:L:121:ILE:HD12	2.02	0.42
1:D:57:MET:HE2	1:D:57:MET:HB3	1.92	0.42
1:L:55:GLU:O	1:L:56:GLU:C	2.63	0.41
1:F:17:GLY:HA3	2:F:301:ATP:O1G	2.20	0.41
1:A:13:MET:HE2	1:A:121:ILE:HD12	2.01	0.41
1:B:15:THR:O	1:B:50:LEU:HD13	2.21	0.41
1:L:37:TRP:CZ3	1:L:105:ILE:HG23	2.55	0.41
1:G:49:ILE:HD13	1:G:182:LEU:CD2	2.47	0.41
1:L:123:ASP:OD2	1:L:154:TYR:OH	2.32	0.41
1:A:17:GLY:HA3	2:A:301:ATP:O2G	2.20	0.41
1:B:133:PRO:HG3	1:B:195:PRO:HG3	2.02	0.41
1:J:93:ARG:HH11	1:J:93:ARG:CB	2.29	0.41
1:C:123:ASP:OD1	1:C:125:ILE:HG12	2.19	0.41
1:H:144:MET:HE2	1:H:144:MET:HB3	1.90	0.41
1:H:145:GLU:O	1:H:146:MET:C	2.62	0.41
1:B:15:THR:OG1	2:B:301:ATP:O2G	2.37	0.41
1:I:135:GLN:NE2	2:I:301:ATP:O2A	2.53	0.41
1:L:125:ILE:HD13	1:L:135:GLN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:223:LEU:HD12	1:M:223:LEU:HA	1.85	0.41
1:H:15:THR:O	1:H:50:LEU:HD13	2.21	0.41
1:E:134:GLU:OE1	2:E:301:ATP:H5'2	2.21	0.41
1:B:129:GLN:HG2	3:B:407:HOH:O	2.20	0.41
1:E:141:THR:HA	1:E:144:MET:HE3	2.03	0.41
1:A:52:HIS:HD2	1:A:182:LEU:HD13	1.86	0.40
1:D:123:ASP:OD2	1:D:154:TYR:OH	2.29	0.40
1:N:17:GLY:HA3	2:N:301:ATP:O3G	2.20	0.40
1:K:13:MET:HB3	2:K:301:ATP:N3	2.36	0.40
1:J:13:MET:HE2	2:J:301:ATP:H1'	2.03	0.40
1:D:15:THR:O	1:D:50:LEU:HD13	2.21	0.40
1:F:225:PRO:O	1:F:226:PRO:C	2.64	0.40
1:H:78:ARG:NH1	1:H:83:GLU:HG3	2.37	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:SER:OG	1:L:86:GLU:OE1[2_455]	2.09	0.11
1:E:86:GLU:OE2	1:L:95:ASN:N[2_455]	2.16	0.04
1:E:187:ILE:CG1	1:L:78:ARG:CG[2_455]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/234 (93%)	214 (99%)	3 (1%)	0	100	100
1	B	214/234 (92%)	213 (100%)	1 (0%)	0	100	100
1	C	218/234 (93%)	216 (99%)	1 (0%)	1 (0%)	25	44
1	D	217/234 (93%)	216 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	218/234 (93%)	211 (97%)	6 (3%)	1 (0%)	25	44
1	F	219/234 (94%)	218 (100%)	1 (0%)	0	100	100
1	G	216/234 (92%)	212 (98%)	4 (2%)	0	100	100
1	H	217/234 (93%)	216 (100%)	1 (0%)	0	100	100
1	I	219/234 (94%)	218 (100%)	1 (0%)	0	100	100
1	J	217/234 (93%)	216 (100%)	1 (0%)	0	100	100
1	K	216/234 (92%)	212 (98%)	3 (1%)	1 (0%)	25	44
1	L	216/234 (92%)	212 (98%)	3 (1%)	1 (0%)	25	44
1	M	216/234 (92%)	214 (99%)	2 (1%)	0	100	100
1	N	216/234 (92%)	214 (99%)	2 (1%)	0	100	100
All	All	3036/3276 (93%)	3002 (99%)	30 (1%)	4 (0%)	48	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	VAL
1	E	162	ALA
1	L	83	GLU
1	K	131	GLU

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	188/200 (94%)	179 (95%)	9 (5%)	21	43
1	B	185/200 (92%)	178 (96%)	7 (4%)	28	53
1	C	189/200 (94%)	183 (97%)	6 (3%)	34	59
1	D	188/200 (94%)	177 (94%)	11 (6%)	16	33
1	E	189/200 (94%)	183 (97%)	6 (3%)	34	59
1	F	190/200 (95%)	182 (96%)	8 (4%)	25	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	187/200 (94%)	181 (97%)	6 (3%)	34	59
1	H	188/200 (94%)	181 (96%)	7 (4%)	29	54
1	I	190/200 (95%)	183 (96%)	7 (4%)	29	54
1	J	188/200 (94%)	178 (95%)	10 (5%)	19	38
1	K	187/200 (94%)	176 (94%)	11 (6%)	16	33
1	L	187/200 (94%)	181 (97%)	6 (3%)	34	59
1	M	187/200 (94%)	176 (94%)	11 (6%)	16	33
1	N	187/200 (94%)	180 (96%)	7 (4%)	29	54
All	All	2630/2800 (94%)	2518 (96%)	112 (4%)	25	48

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	ARG
1	B	89	ILE
1	B	93	ARG
1	B	131	GLU
1	B	181	SER
1	B	199	VAL
1	B	210	LEU
1	E	98	LEU
1	E	135	GLN
1	E	178	SER
1	E	181	SER
1	E	196	SER
1	E	210	LEU
1	G	15	THR
1	G	49	ILE
1	G	55	GLU
1	G	64	LEU
1	G	181	SER
1	G	199	VAL
1	I	47	ARG
1	I	63	ASP
1	I	89	ILE
1	I	160	GLU
1	I	178	SER
1	I	181	SER
1	I	199	VAL

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Mol	Chain	Res	Type
1	J	8	LYS
1	J	12	VAL
1	J	126	THR
1	J	131	GLU
1	J	134	GLU
1	J	147	MET
1	J	160	GLU
1	J	178	SER
1	J	181	SER
1	J	185	ILE
1	L	87	GLN
1	L	89	ILE
1	L	154	TYR
1	L	181	SER
1	L	187	ILE
1	L	210	LEU
1	M	89	ILE
1	M	98	LEU
1	M	120	THR
1	M	135	GLN
1	M	160	GLU
1	M	178	SER
1	M	181	SER
1	M	194	THR
1	M	198	ASP
1	M	210	LEU
1	M	222	THR
1	A	86	GLU
1	A	126	THR
1	A	131	GLU
1	A	145	GLU
1	A	178	SER
1	A	181	SER
1	A	196	SER
1	A	198	ASP
1	A	223	LEU
1	C	89	ILE
1	C	160	GLU
1	C	178	SER
1	C	181	SER
1	C	194	THR
1	C	199	VAL

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Mol	Chain	Res	Type
1	D	47	ARG
1	D	86	GLU
1	D	93	ARG
1	D	105	ILE
1	D	120	THR
1	D	121	ILE
1	D	178	SER
1	D	181	SER
1	D	185	ILE
1	D	209	PRO
1	D	210	LEU
1	F	47	ARG
1	F	63	ASP
1	F	125	ILE
1	F	131	GLU
1	F	181	SER
1	F	198	ASP
1	F	199	VAL
1	F	210	LEU
1	H	63	ASP
1	H	87	GLN
1	H	131	GLU
1	H	178	SER
1	H	181	SER
1	H	194	THR
1	H	199	VAL
1	K	49	ILE
1	K	63	ASP
1	K	89	ILE
1	K	102	LYS
1	K	169	LYS
1	K	178	SER
1	K	181	SER
1	K	185	ILE
1	K	198	ASP
1	K	199	VAL
1	K	201	LEU
1	N	6	SER
1	N	50	LEU
1	N	89	ILE
1	N	120	THR
1	N	181	SER

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Mol	Chain	Res	Type
1	N	199	VAL
1	N	222	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	127	HIS
1	B	149	GLN
1	B	163	GLN
1	E	10	GLN
1	E	106	HIS
1	E	108	HIS
1	E	135	GLN
1	E	163	GLN
1	E	216	ASN
1	G	10	GLN
1	G	108	HIS
1	G	129	GLN
1	I	108	HIS
1	I	129	GLN
1	I	163	GLN
1	I	224	ASN
1	J	106	HIS
1	J	108	HIS
1	L	108	HIS
1	M	59	ASN
1	M	106	HIS
1	M	108	HIS
1	A	52	HIS
1	A	108	HIS
1	D	106	HIS
1	D	153	ASN
1	F	108	HIS
1	H	59	ASN
1	H	87	GLN
1	H	106	HIS
1	H	108	HIS
1	H	129	GLN
1	H	153	ASN
1	H	155	GLN
1	K	52	HIS
1	K	108	HIS

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Mol	Chain	Res	Type
1	K	135	GLN
1	K	153	ASN
1	K	155	GLN
1	N	68	HIS
1	N	106	HIS
1	N	108	HIS
1	N	155	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands 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	$\# Z > 2$
2	ATP	K	301	-	26,33,33	0.73	0	31,52,52	0.84	1 (3%)
2	ATP	L	301	-	26,33,33	0.76	0	31,52,52	0.75	1 (3%)
2	ATP	M	301	-	26,33,33	0.75	0	31,52,52	0.79	1 (3%)
2	ATP	H	301	-	26,33,33	0.75	0	31,52,52	0.76	1 (3%)
2	ATP	B	301	-	26,33,33	0.76	0	31,52,52	0.76	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	C	301	-	26,33,33	0.78	0	31,52,52	0.79	1 (3%)
2	ATP	J	301	-	26,33,33	0.75	0	31,52,52	0.86	2 (6%)
2	ATP	D	301	-	26,33,33	0.75	0	31,52,52	0.85	1 (3%)
2	ATP	N	301	-	26,33,33	0.78	0	31,52,52	0.76	1 (3%)
2	ATP	A	301	-	26,33,33	0.77	0	31,52,52	0.75	1 (3%)
2	ATP	I	301	-	26,33,33	0.75	0	31,52,52	0.76	1 (3%)
2	ATP	F	301	-	26,33,33	0.76	0	31,52,52	0.77	1 (3%)
2	ATP	G	301	-	26,33,33	0.73	0	31,52,52	0.78	1 (3%)
2	ATP	E	301	-	26,33,33	0.73	0	31,52,52	0.76	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	K	301	-	-	1/18/38/38	0/3/3/3
2	ATP	L	301	-	-	0/18/38/38	0/3/3/3
2	ATP	M	301	-	-	3/18/38/38	0/3/3/3
2	ATP	H	301	-	-	5/18/38/38	0/3/3/3
2	ATP	B	301	-	-	7/18/38/38	0/3/3/3
2	ATP	C	301	-	-	0/18/38/38	0/3/3/3
2	ATP	J	301	-	-	0/18/38/38	0/3/3/3
2	ATP	D	301	-	-	5/18/38/38	0/3/3/3
2	ATP	N	301	-	-	0/18/38/38	0/3/3/3
2	ATP	A	301	-	-	1/18/38/38	0/3/3/3
2	ATP	I	301	-	-	5/18/38/38	0/3/3/3
2	ATP	F	301	-	-	0/18/38/38	0/3/3/3
2	ATP	G	301	-	-	4/18/38/38	0/3/3/3
2	ATP	E	301	-	-	3/18/38/38	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(°)
2	G	301	ATP	C5-C6-N6	2.41	124.01	120.35
2	C	301	ATP	C5-C6-N6	2.36	123.94	120.35
2	K	301	ATP	C5-C6-N6	2.35	123.92	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	ATP	C5-C6-N6	2.35	123.92	120.35
2	F	301	ATP	C5-C6-N6	2.34	123.90	120.35
2	J	301	ATP	C5-C6-N6	2.33	123.89	120.35
2	E	301	ATP	C5-C6-N6	2.31	123.87	120.35
2	M	301	ATP	C5-C6-N6	2.29	123.83	120.35
2	I	301	ATP	C5-C6-N6	2.26	123.78	120.35
2	L	301	ATP	C5-C6-N6	2.21	123.72	120.35
2	H	301	ATP	C5-C6-N6	2.21	123.72	120.35
2	N	301	ATP	C5-C6-N6	2.17	123.65	120.35
2	B	301	ATP	C5-C6-N6	2.17	123.64	120.35
2	J	301	ATP	PB-O3B-PG	-2.11	125.59	132.83
2	A	301	ATP	C5-C6-N6	2.05	123.46	120.35

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	ATP	O4'-C4'-C5'-O5'
2	H	301	ATP	PB-O3B-PG-O2G
2	H	301	ATP	PB-O3B-PG-O3G
2	G	301	ATP	O4'-C4'-C5'-O5'
2	I	301	ATP	O4'-C4'-C5'-O5'
2	M	301	ATP	O4'-C4'-C5'-O5'
2	H	301	ATP	O4'-C4'-C5'-O5'
2	B	301	ATP	O4'-C4'-C5'-O5'
2	B	301	ATP	C3'-C4'-C5'-O5'
2	I	301	ATP	C3'-C4'-C5'-O5'
2	I	301	ATP	PB-O3B-PG-O1G
2	B	301	ATP	PG-O3B-PB-O1B
2	I	301	ATP	PB-O3A-PA-O1A
2	B	301	ATP	PB-O3A-PA-O5'
2	E	301	ATP	PB-O3A-PA-O5'
2	G	301	ATP	PB-O3A-PA-O5'
2	I	301	ATP	PB-O3A-PA-O5'
2	M	301	ATP	PB-O3A-PA-O5'
2	D	301	ATP	PB-O3A-PA-O5'
2	H	301	ATP	PB-O3A-PA-O5'
2	E	301	ATP	O4'-C4'-C5'-O5'
2	B	301	ATP	C5'-O5'-PA-O2A
2	G	301	ATP	C3'-C4'-C5'-O5'
2	B	301	ATP	PG-O3B-PB-O2B
2	D	301	ATP	PA-O3A-PB-O1B

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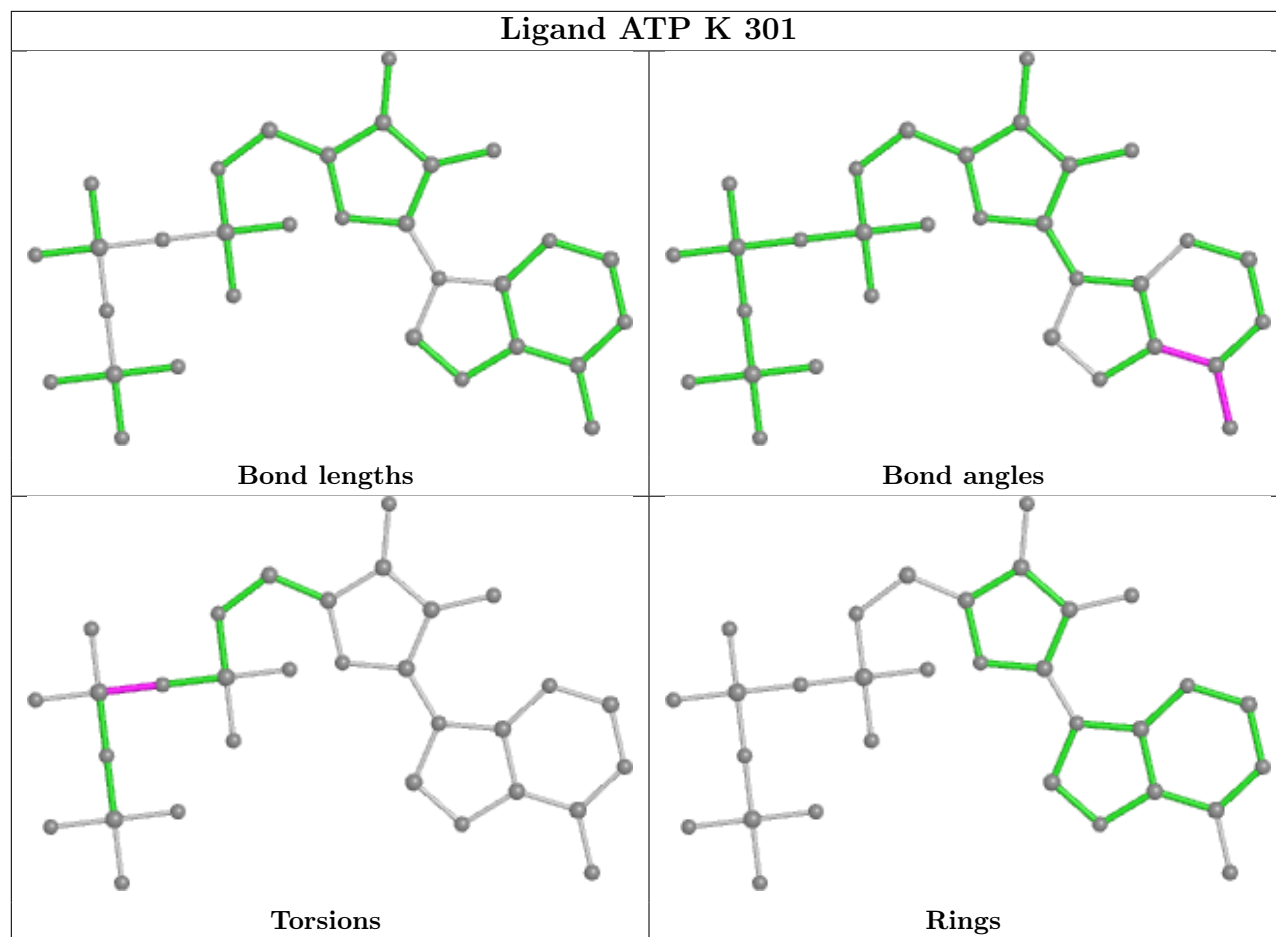
Mol	Chain	Res	Type	Atoms
2	K	301	ATP	PA-O3A-PB-O2B
2	D	301	ATP	C3'-C4'-C5'-O5'
2	M	301	ATP	PG-O3B-PB-O2B
2	B	301	ATP	C5'-O5'-PA-O3A
2	D	301	ATP	C5'-O5'-PA-O3A
2	E	301	ATP	C4'-C5'-O5'-PA
2	A	301	ATP	PG-O3B-PB-O2B
2	G	301	ATP	C5'-O5'-PA-O1A
2	H	301	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

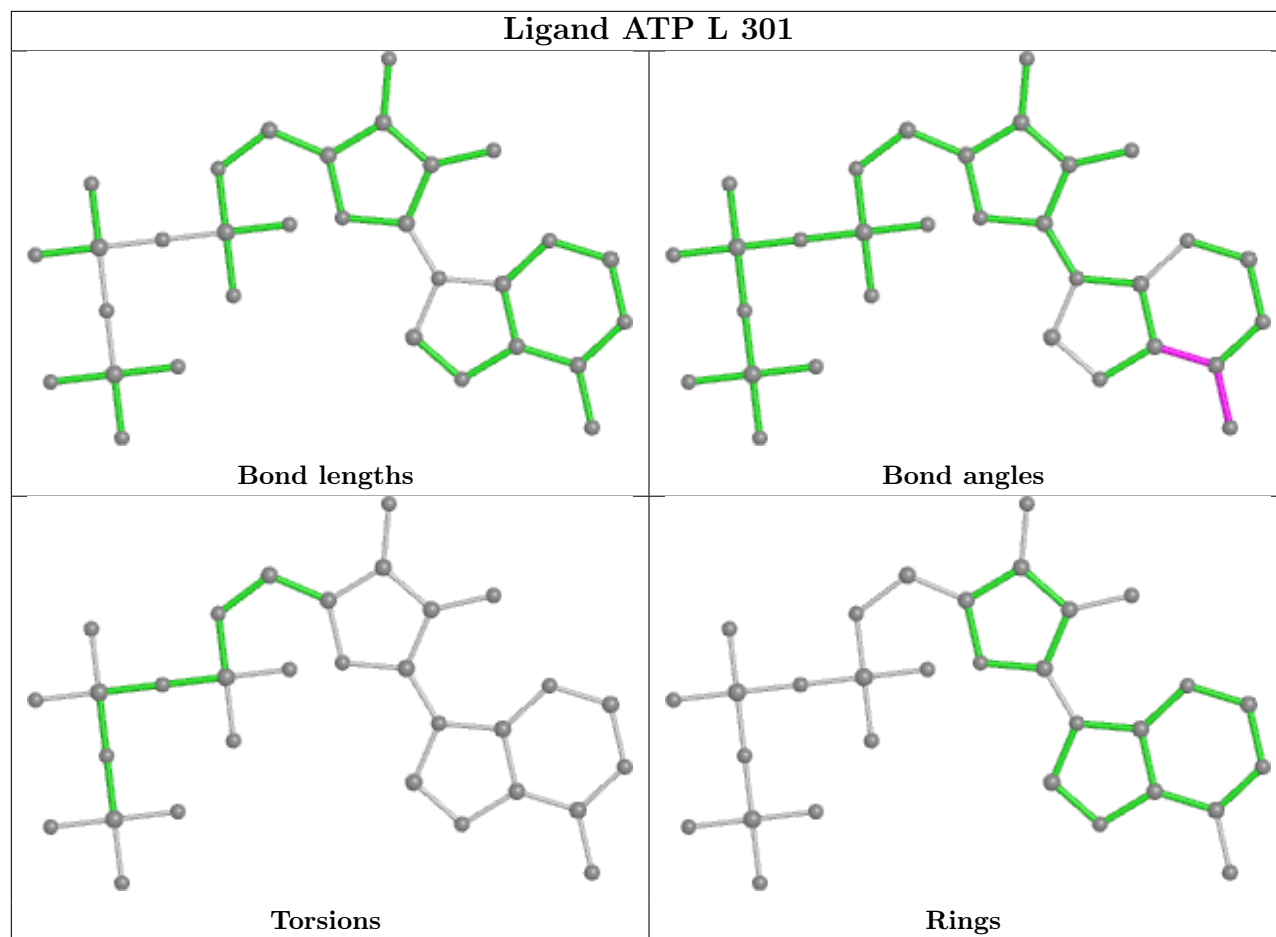
12 monomers are involved in 27 short contacts:

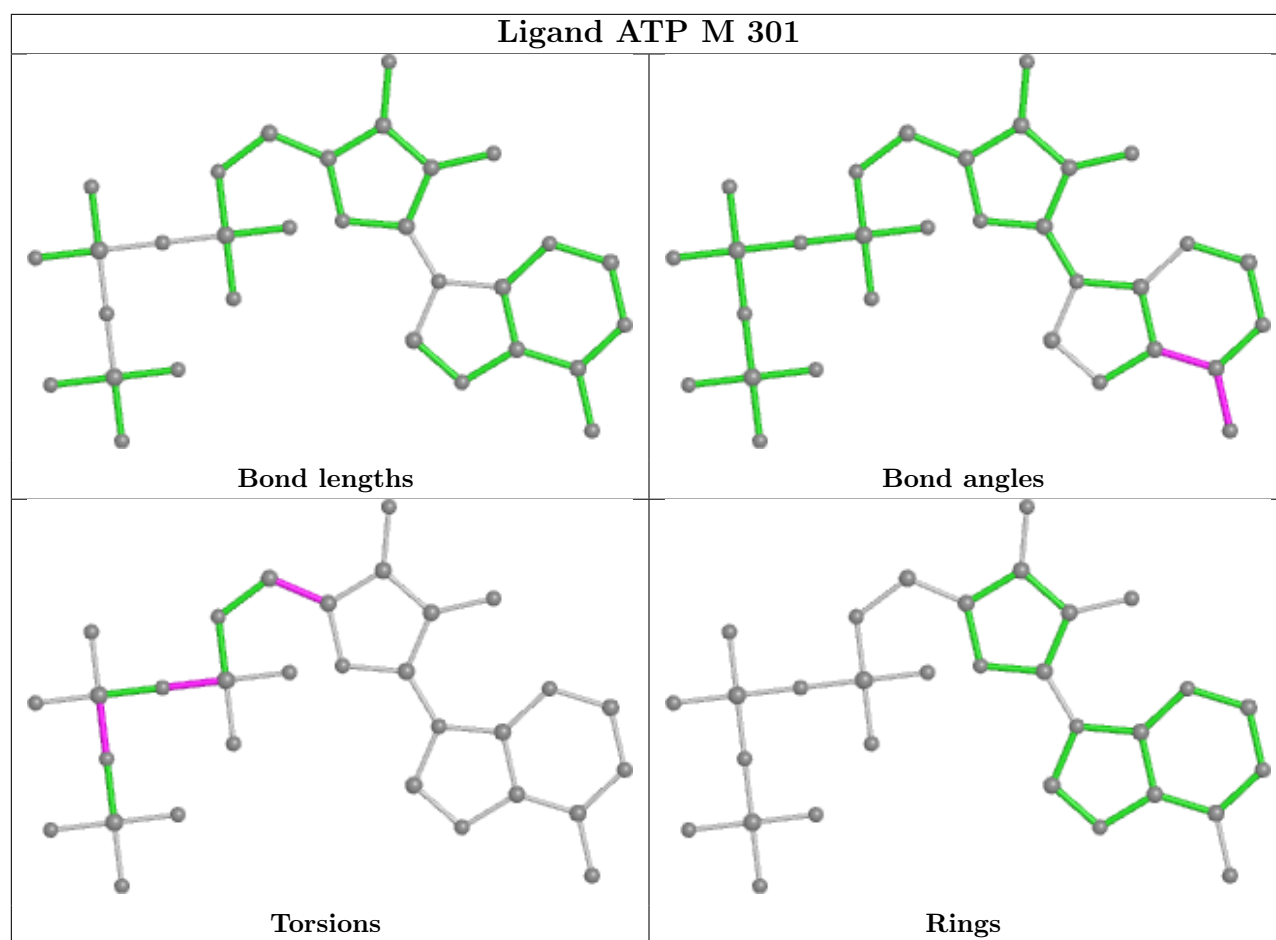
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	301	ATP	1	0
2	H	301	ATP	2	0
2	B	301	ATP	3	0
2	C	301	ATP	1	0
2	J	301	ATP	2	0
2	D	301	ATP	1	0
2	N	301	ATP	3	0
2	A	301	ATP	4	0
2	I	301	ATP	4	0
2	F	301	ATP	1	0
2	G	301	ATP	1	0
2	E	301	ATP	4	0

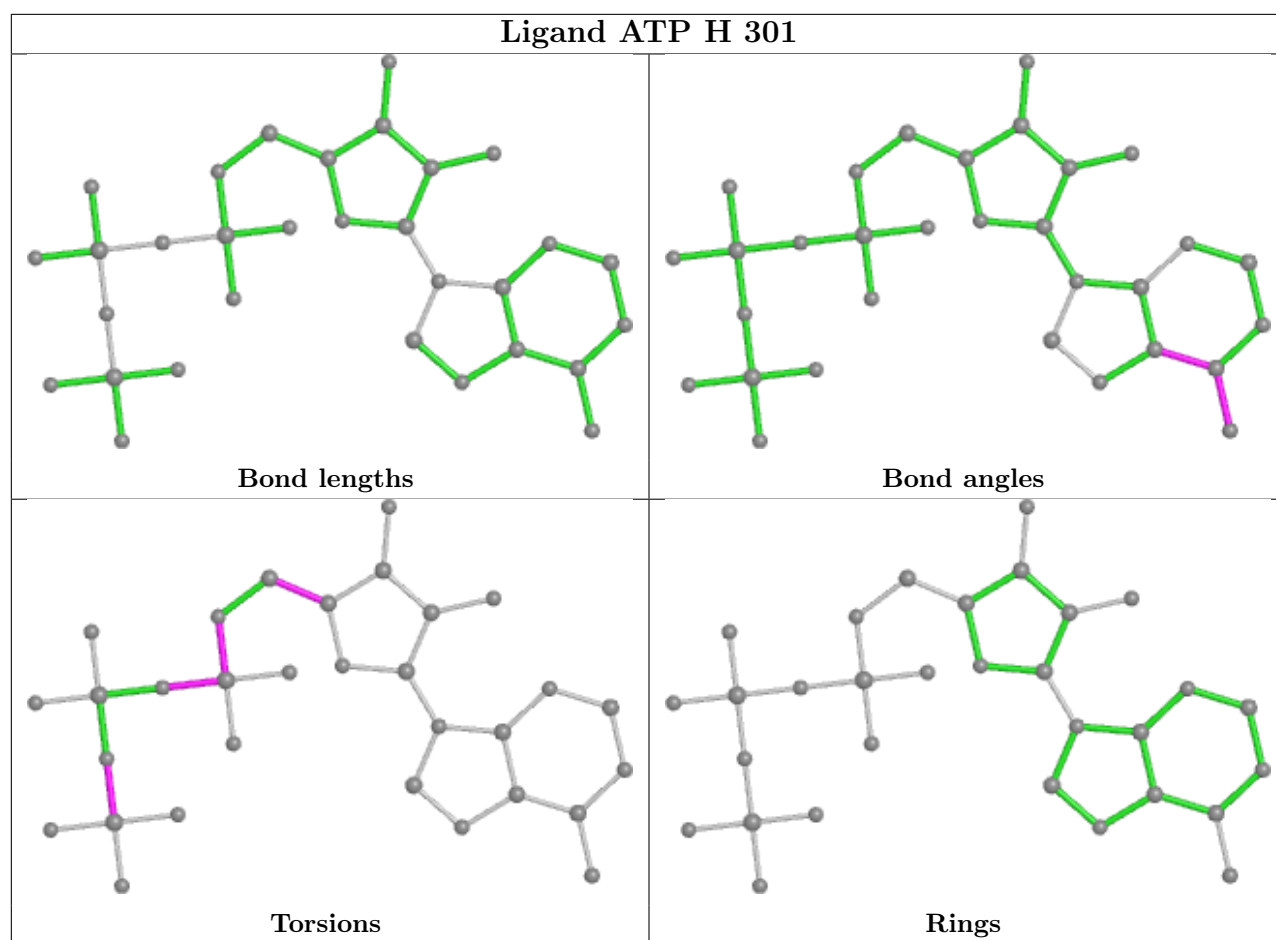
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



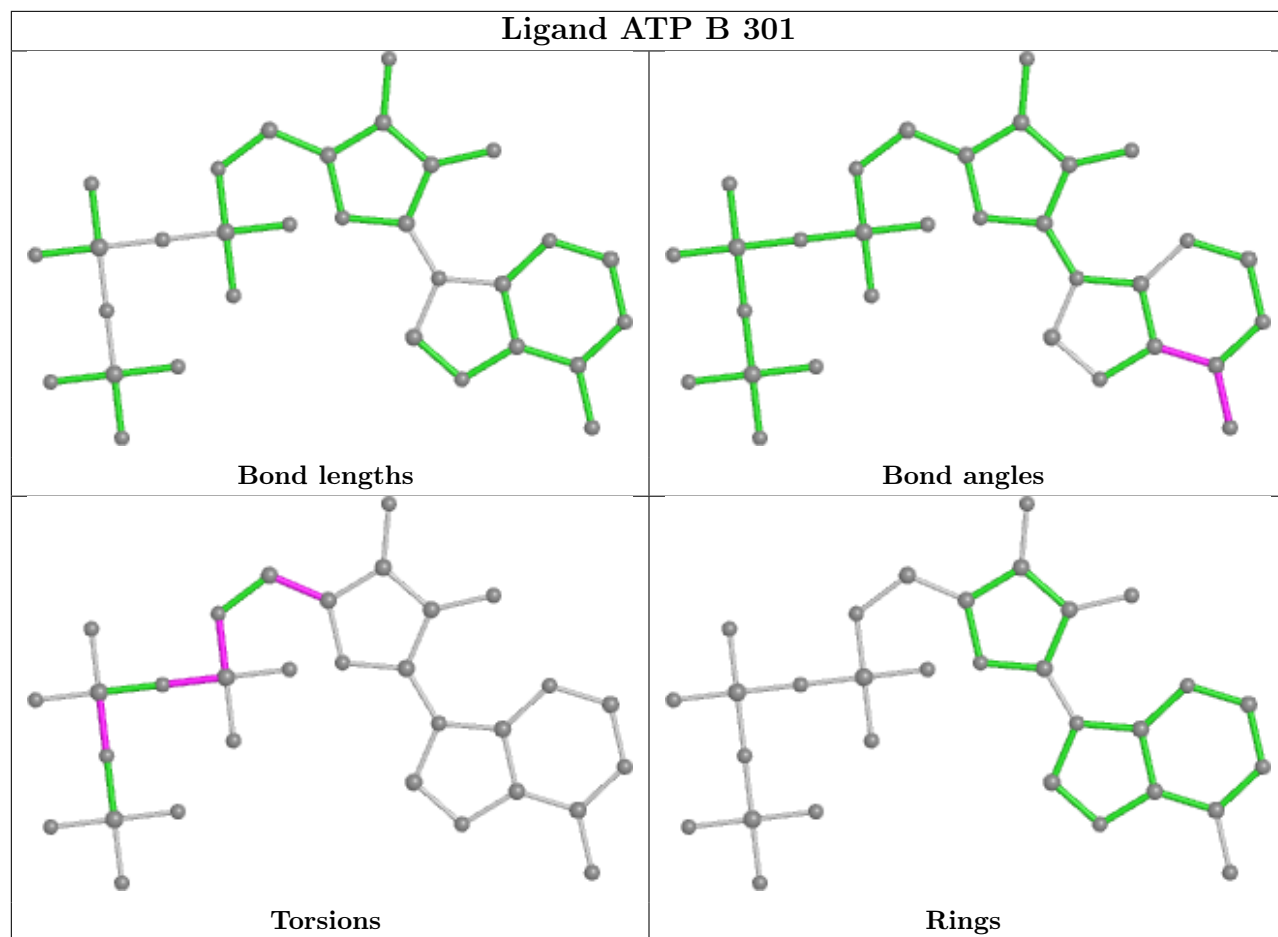
Ligand ATP L 301

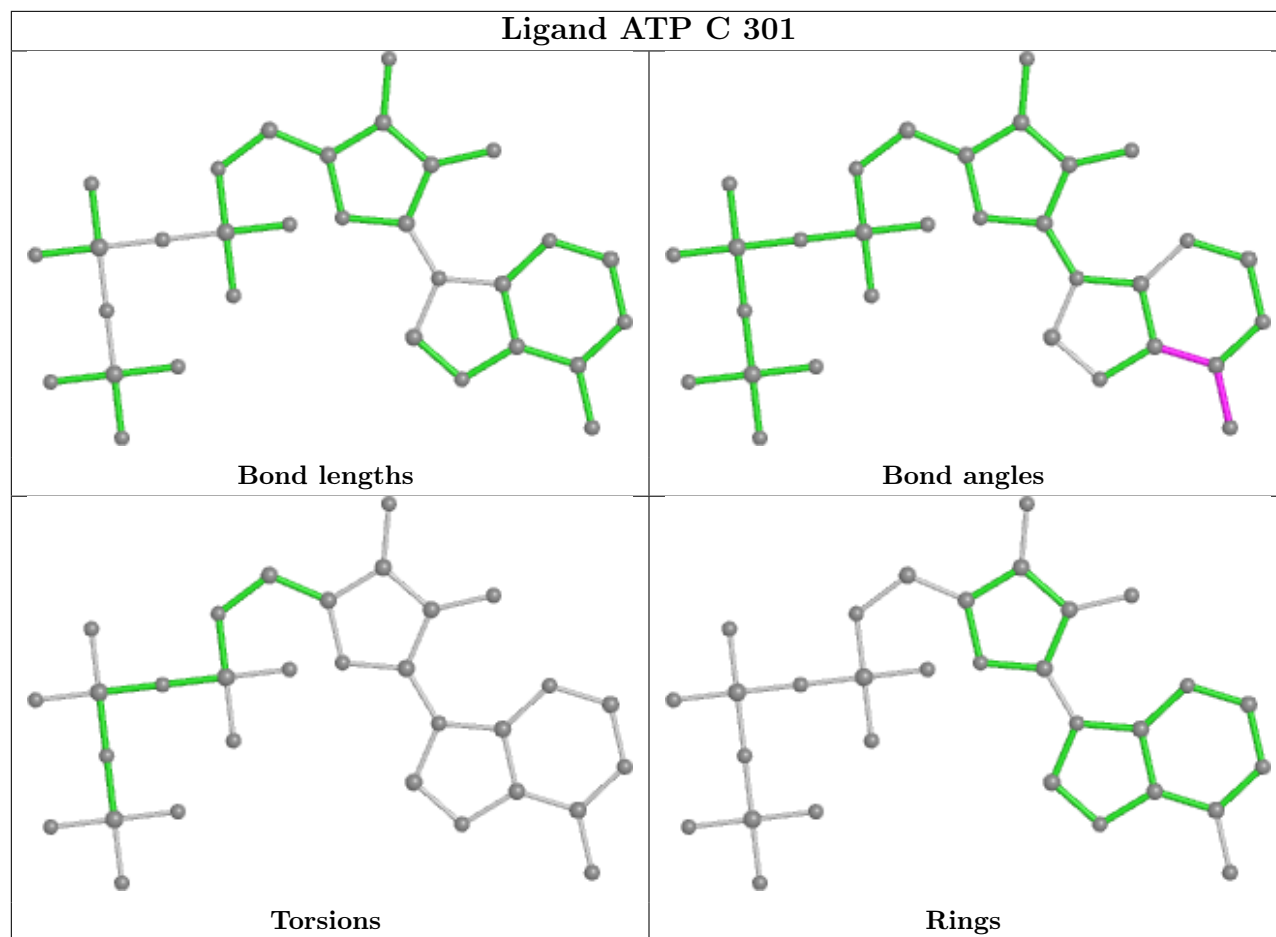




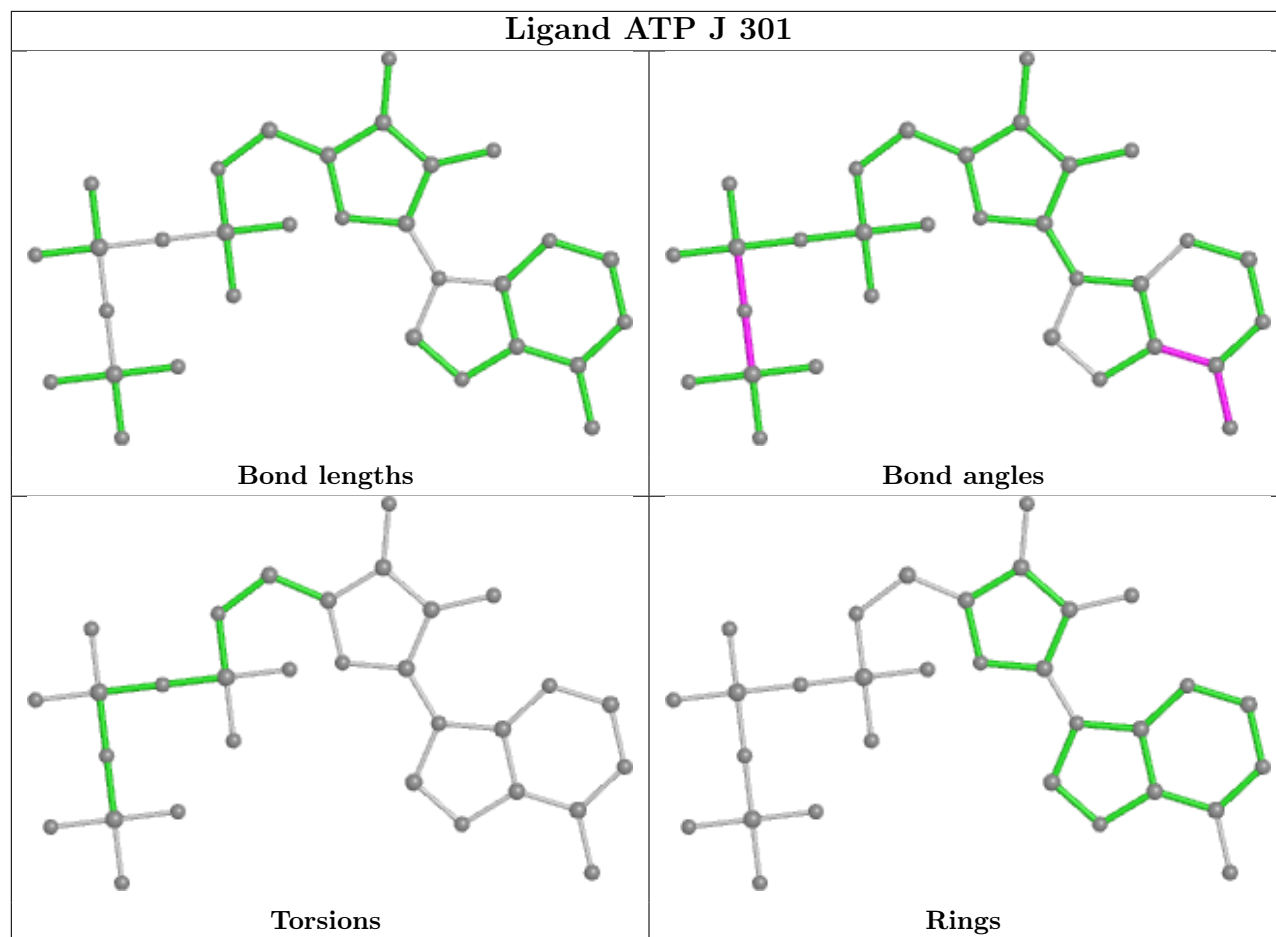


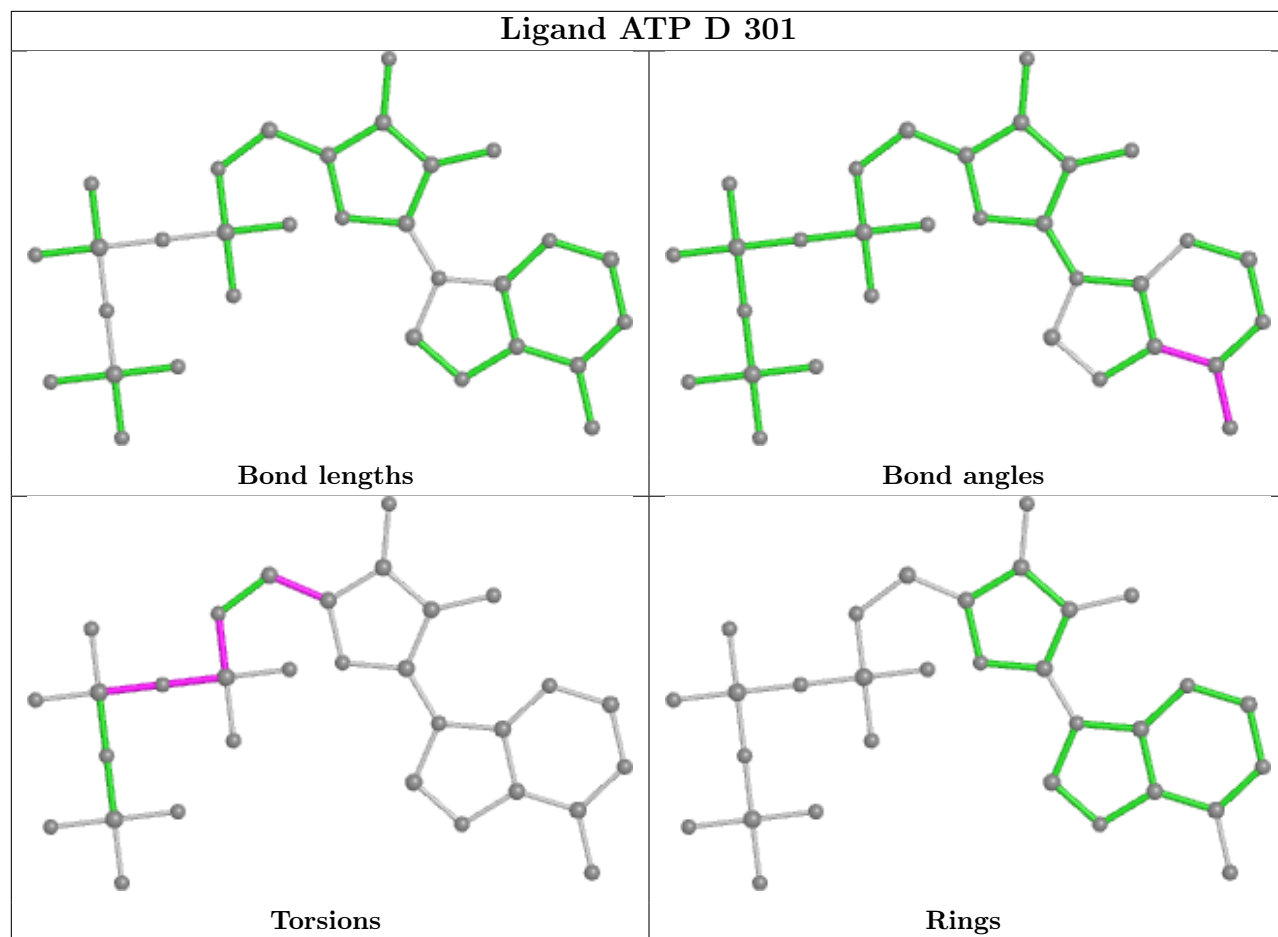
Ligand ATP B 301

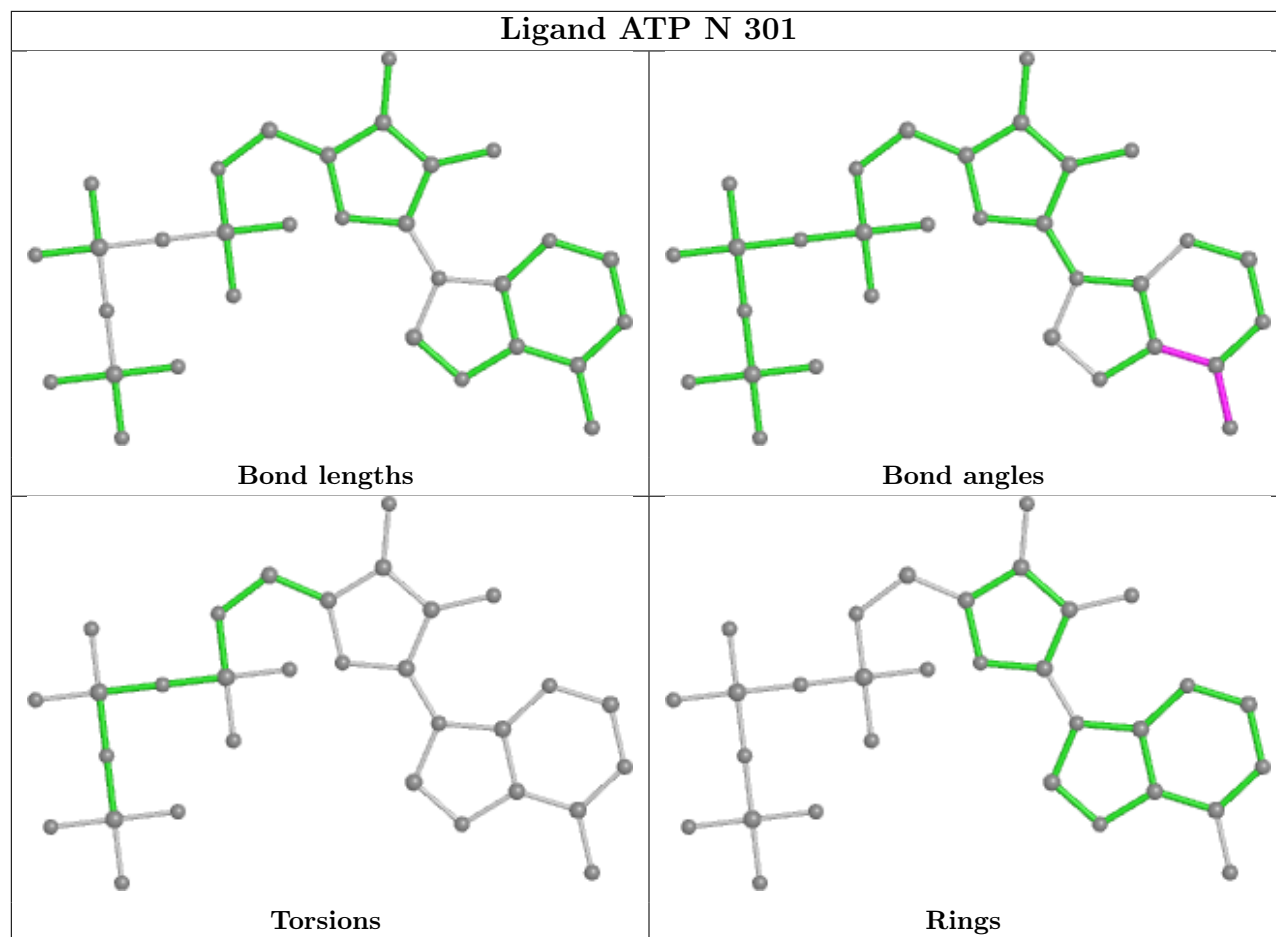


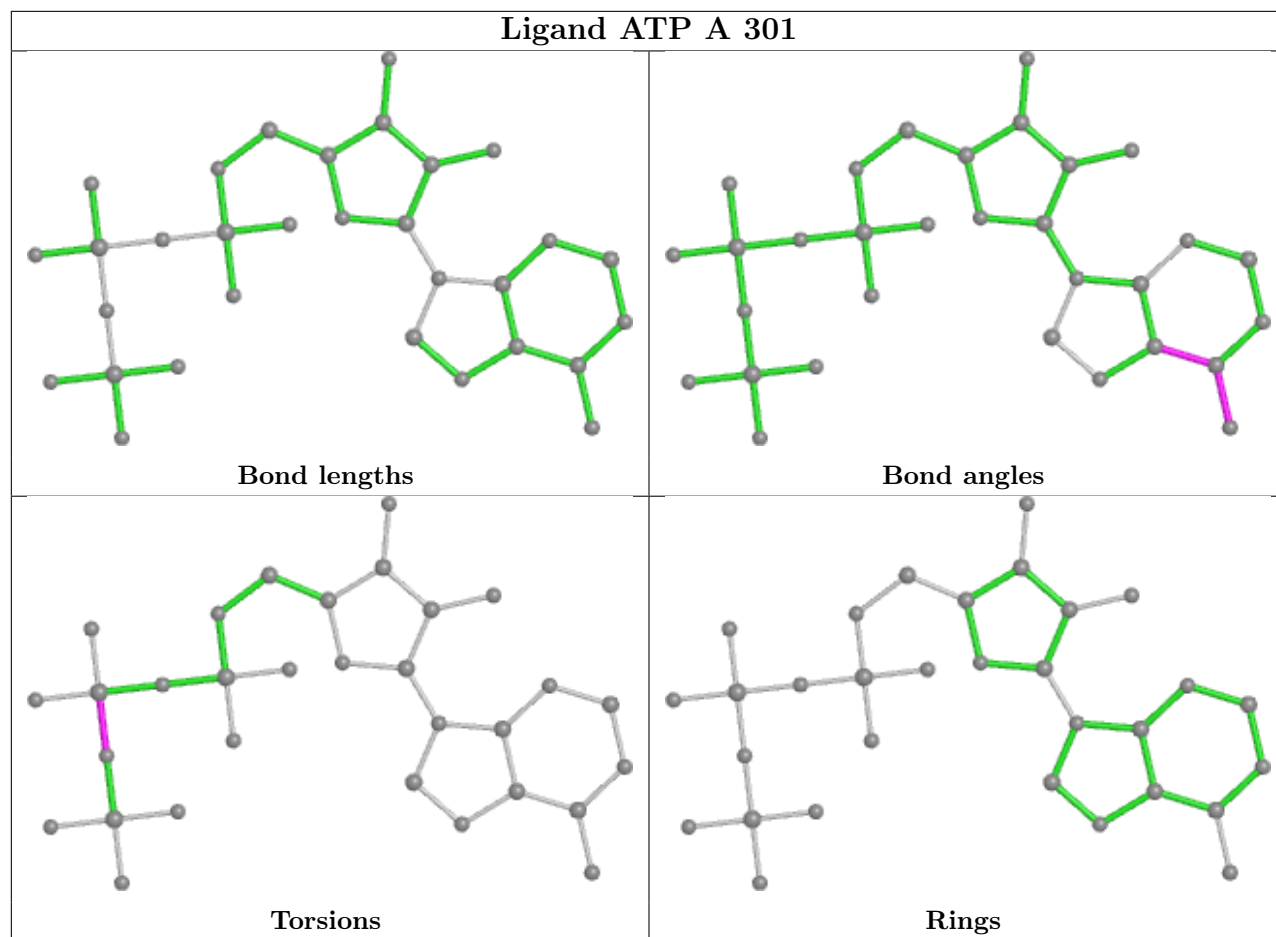


Ligand ATP J 301

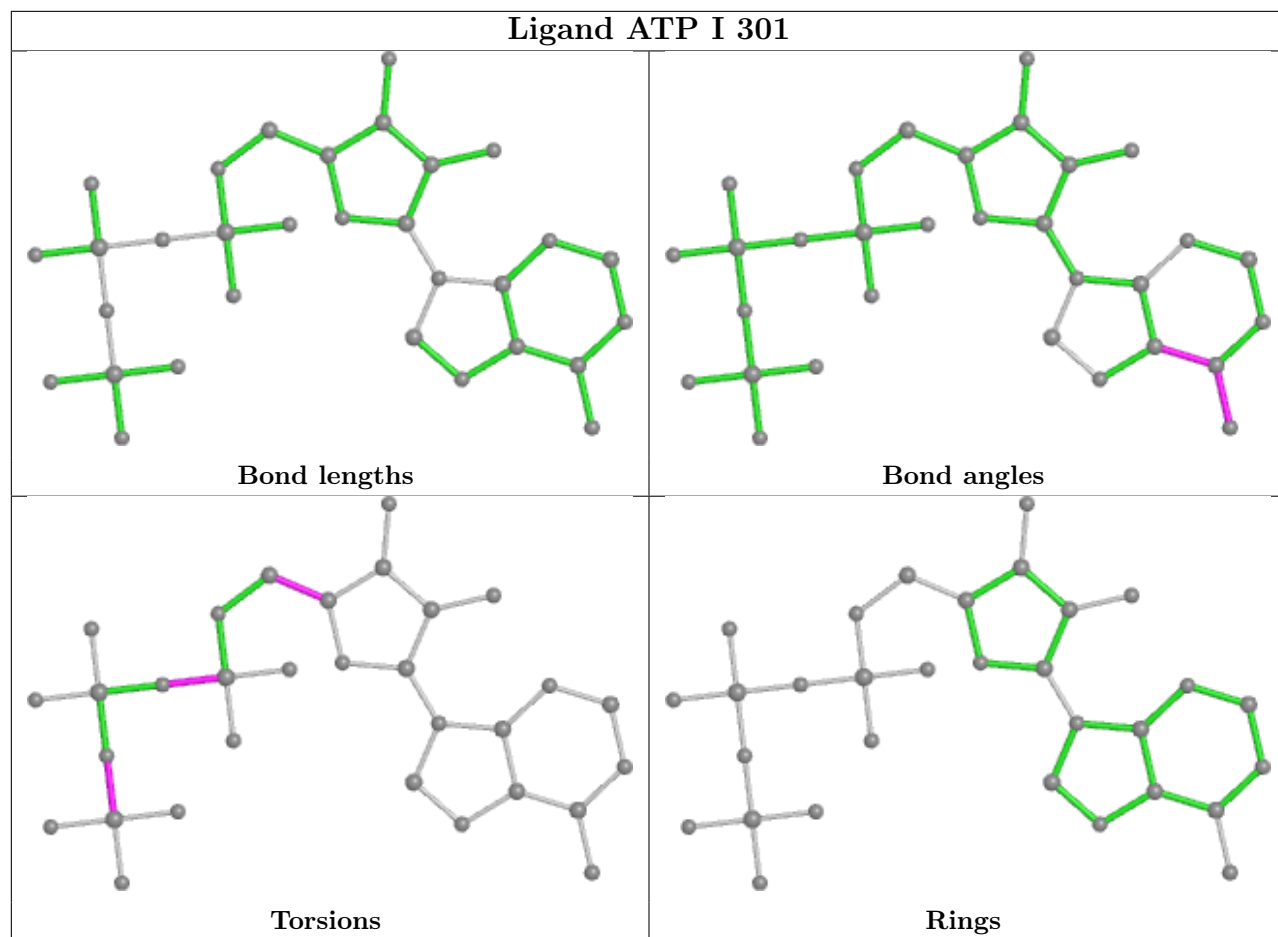




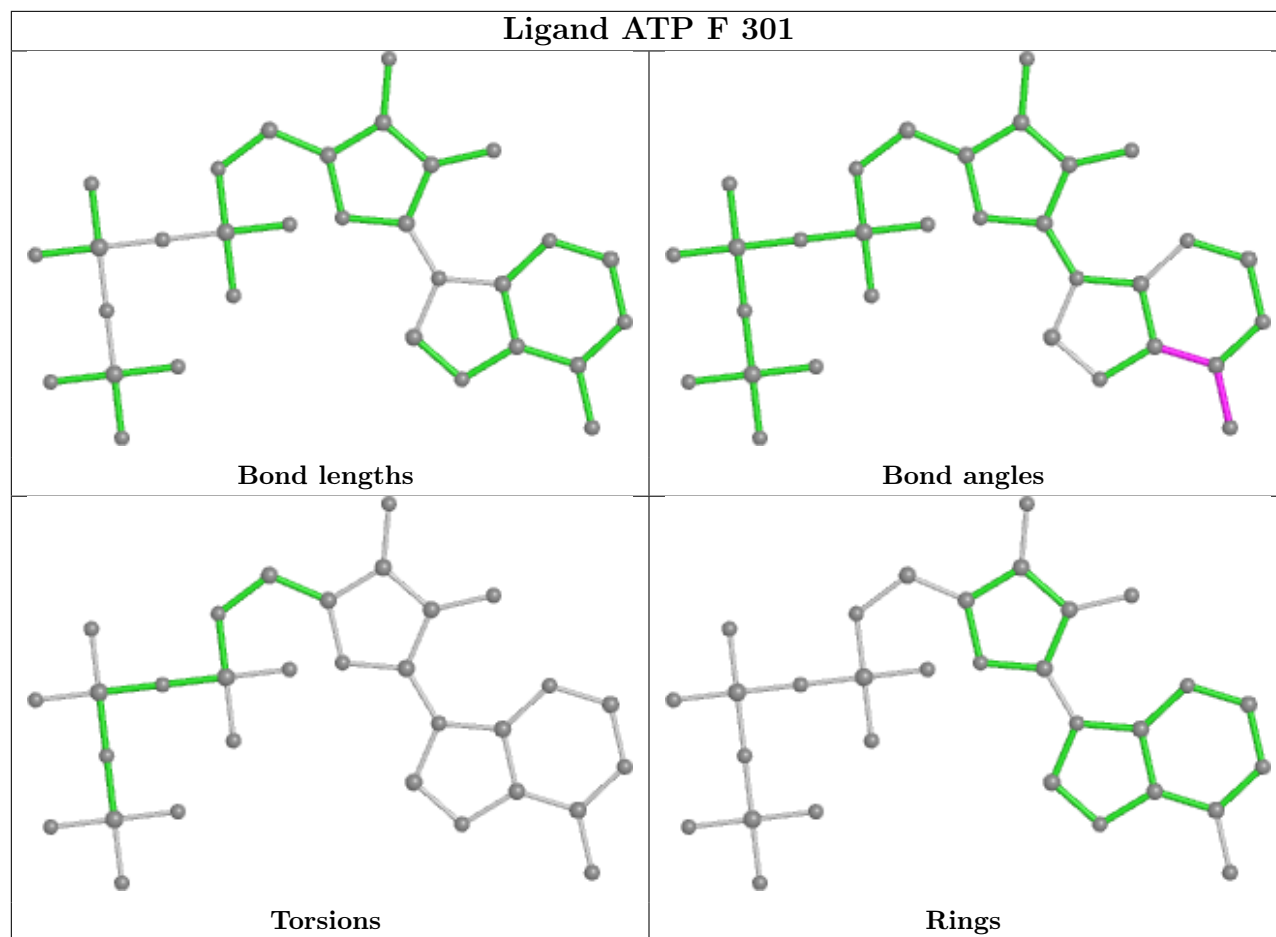


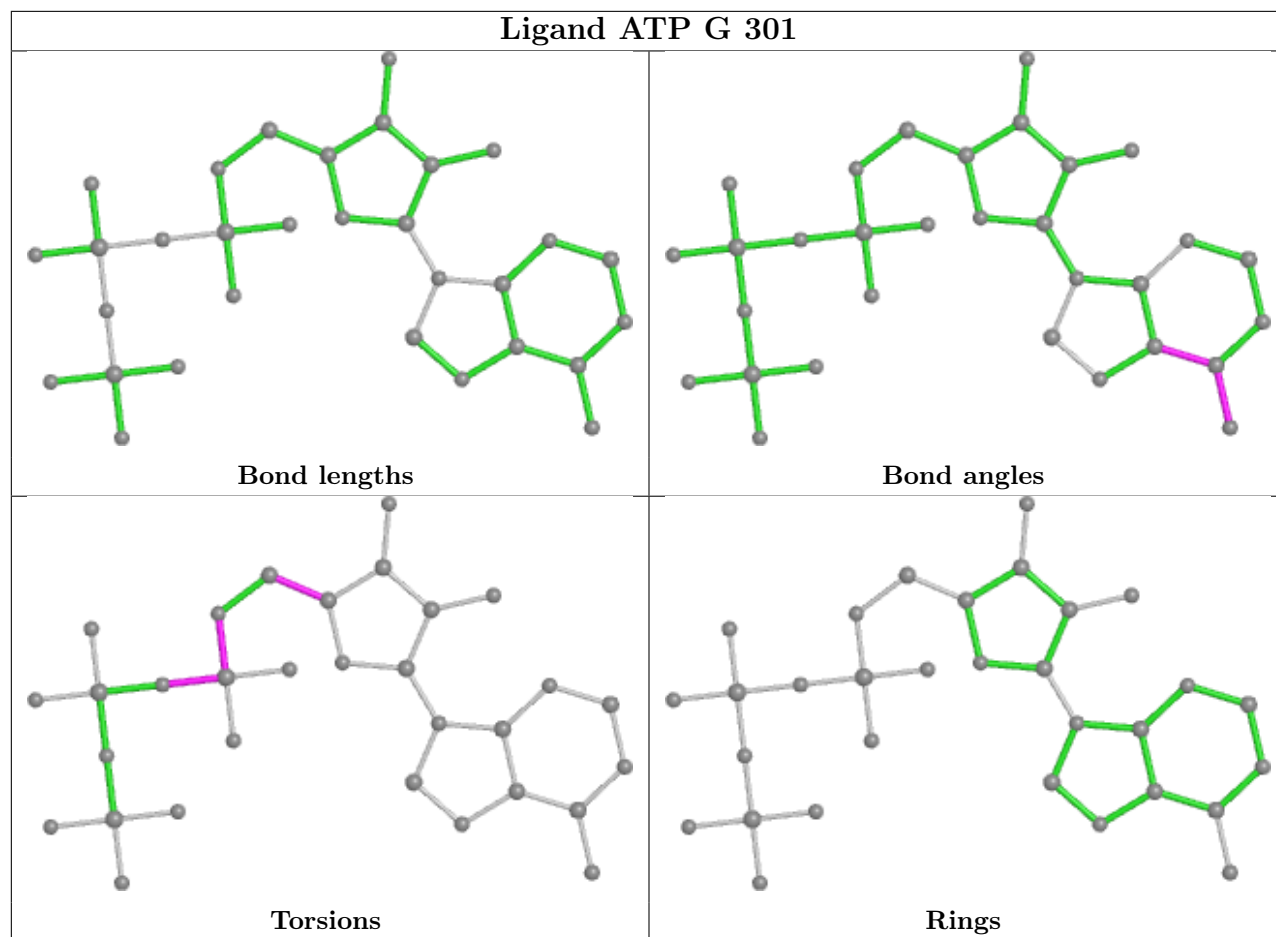


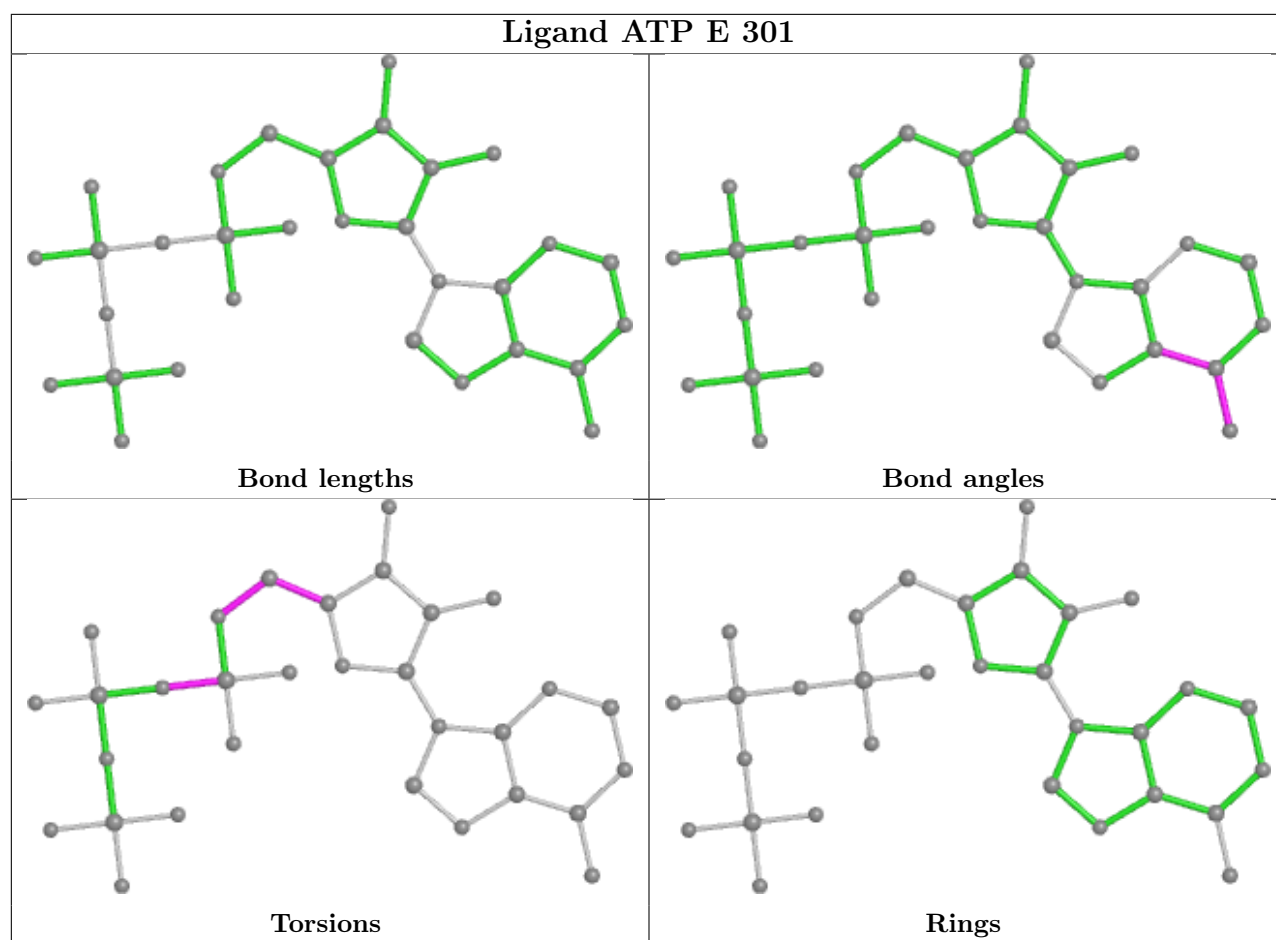
Ligand ATP I 301



Ligand ATP F 301







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/234 (93%)	-1.70	0 100 100	42, 63, 96, 122	0
1	B	216/234 (92%)	-1.35	0 100 100	43, 61, 86, 105	0
1	C	220/234 (94%)	-1.64	0 100 100	32, 49, 72, 83	0
1	D	219/234 (93%)	-1.64	0 100 100	28, 50, 95, 134	0
1	E	220/234 (94%)	-1.44	0 100 100	54, 81, 130, 177	0
1	F	221/234 (94%)	-1.71	0 100 100	40, 61, 88, 114	0
1	G	218/234 (93%)	-1.58	0 100 100	60, 84, 107, 124	0
1	H	219/234 (93%)	-1.74	0 100 100	42, 58, 87, 119	0
1	I	221/234 (94%)	-1.48	0 100 100	38, 61, 87, 113	0
1	J	219/234 (93%)	-1.41	0 100 100	42, 67, 116, 157	0
1	K	218/234 (93%)	-1.62	0 100 100	43, 63, 104, 134	0
1	L	218/234 (93%)	-1.55	0 100 100	60, 87, 119, 150	0
1	M	218/234 (93%)	-1.63	0 100 100	56, 79, 105, 145	0
1	N	218/234 (93%)	-1.63	0 100 100	33, 49, 72, 96	0
All	All	3064/3276 (93%)	-1.58	0 100 100	28, 66, 106, 177	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

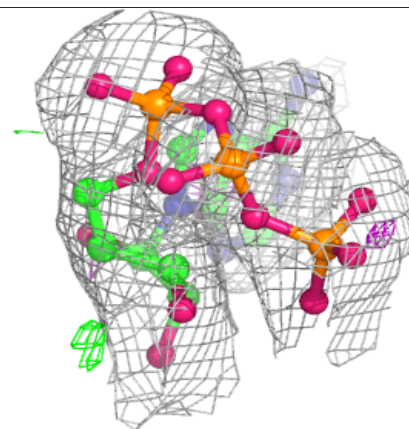
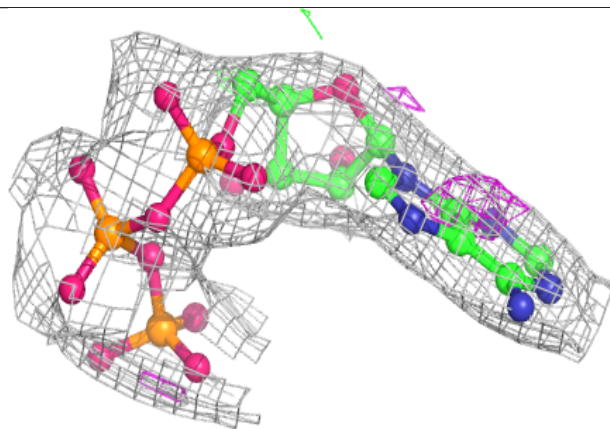
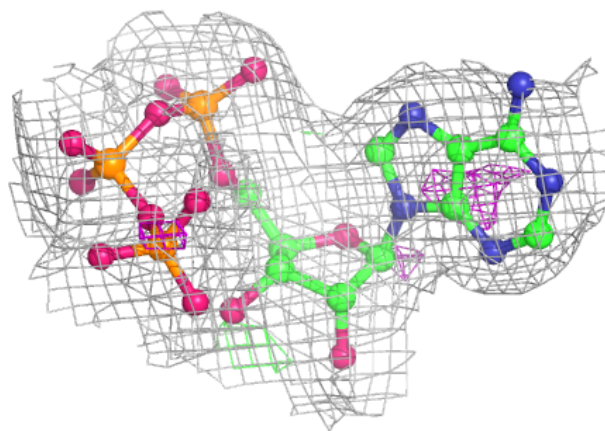
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ATP	B	301	31/31	0.99	0.04	49,65,91,109	0
2	ATP	E	301	31/31	0.99	0.03	63,79,120,135	0
2	ATP	G	301	31/31	0.99	0.03	72,96,110,123	0
2	ATP	I	301	31/31	0.99	0.04	59,79,104,109	0
2	ATP	J	301	31/31	0.99	0.04	52,75,102,137	0
2	ATP	L	301	31/31	0.99	0.03	75,101,124,141	0
2	ATP	M	301	31/31	0.99	0.04	75,95,115,123	0
2	ATP	A	301	31/31	0.99	0.03	49,74,93,97	0
2	ATP	C	301	31/31	0.99	0.04	36,58,73,80	0
2	ATP	D	301	31/31	0.99	0.03	48,58,91,94	0
2	ATP	F	301	31/31	0.99	0.03	52,71,90,109	0
2	ATP	H	301	31/31	0.99	0.03	48,67,101,106	0
2	ATP	K	301	31/31	0.99	0.03	55,69,119,132	0
2	ATP	N	301	31/31	0.99	0.04	44,59,73,80	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.

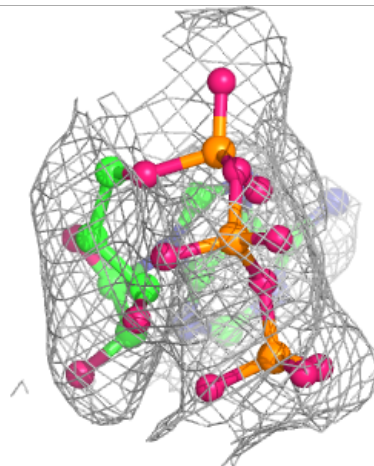
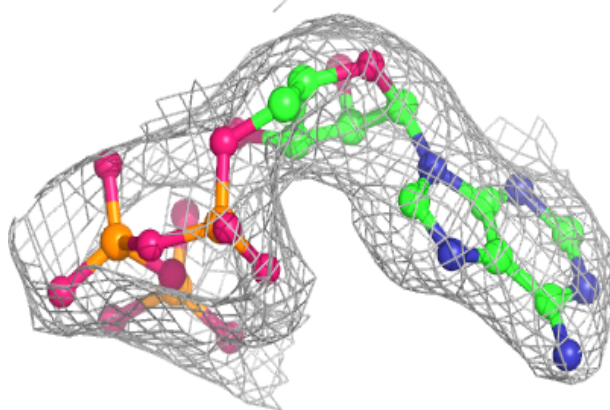
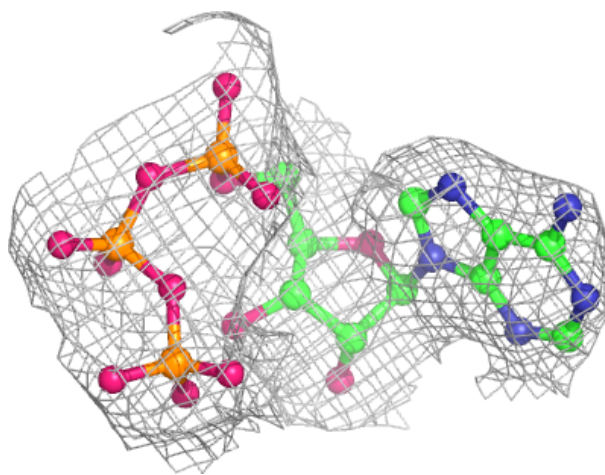
Electron density around ATP B 301:

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



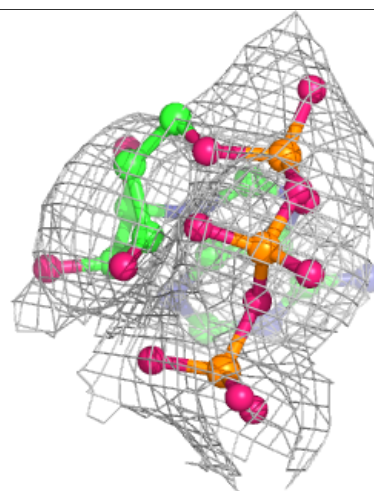
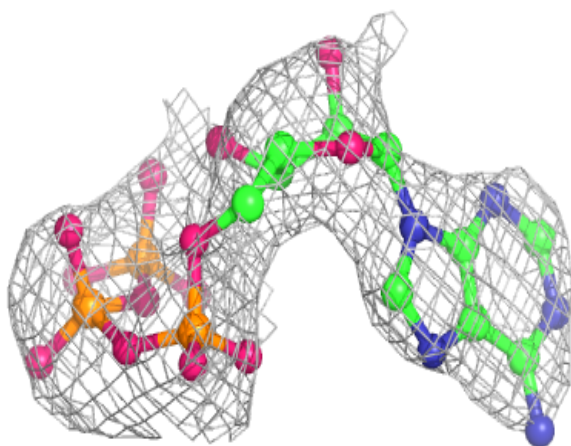
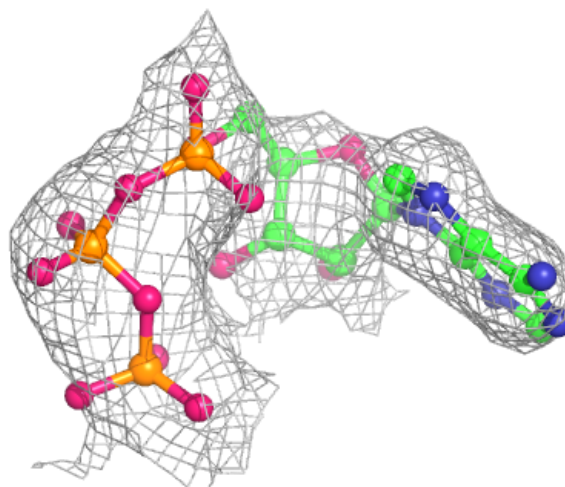
Electron density around ATP E 301:

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



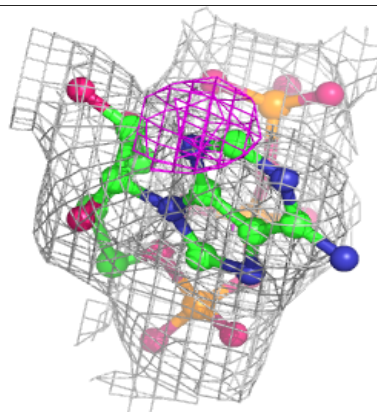
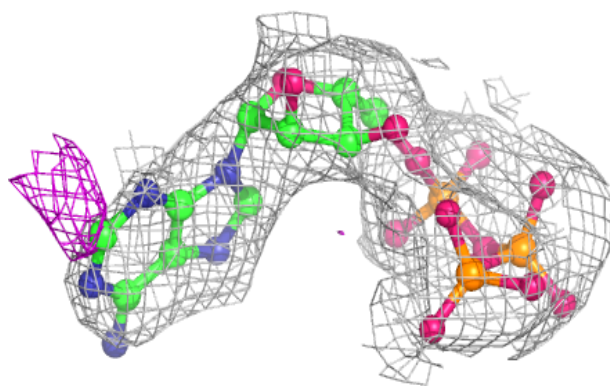
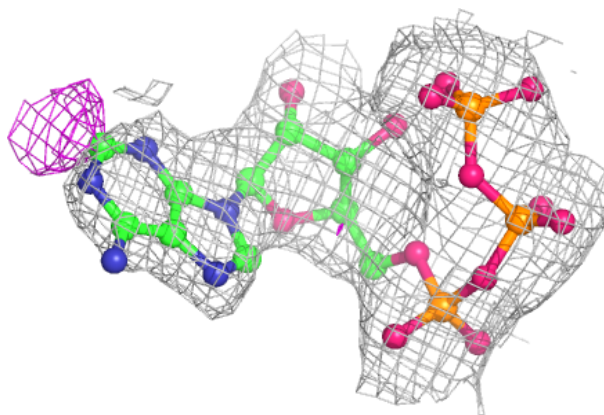
Electron density around ATP G 301:

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



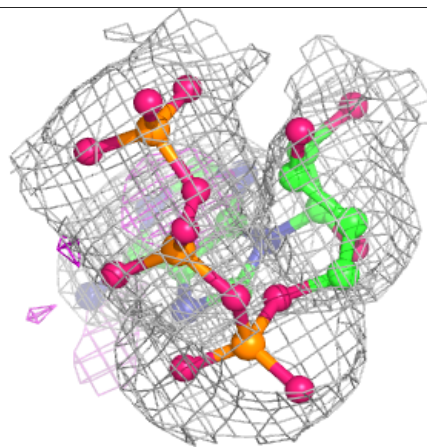
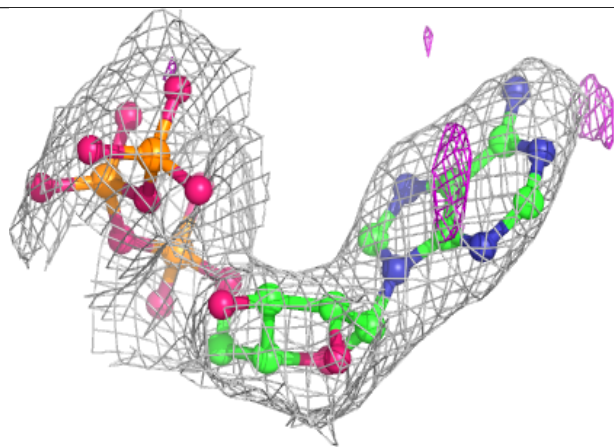
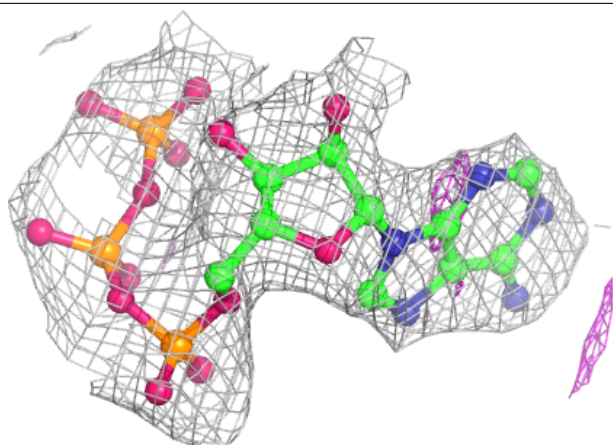
Electron density around ATP I 301:

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



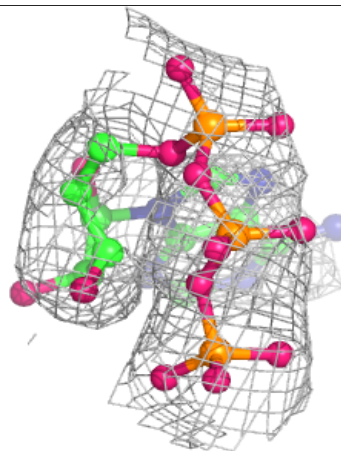
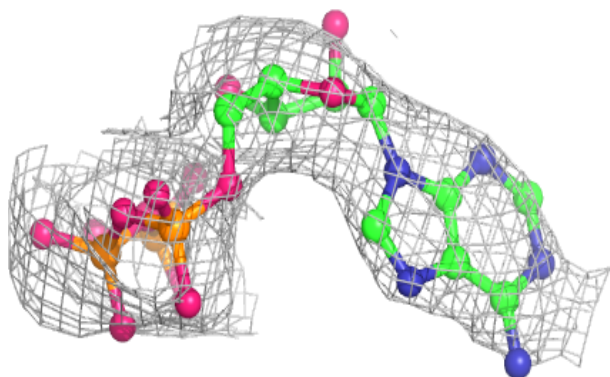
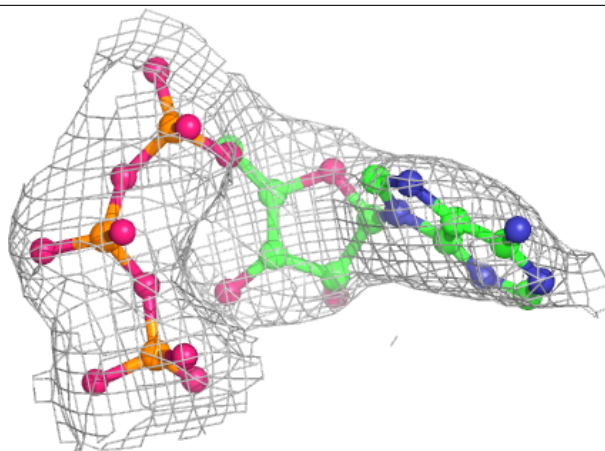
Electron density around ATP J 301:

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

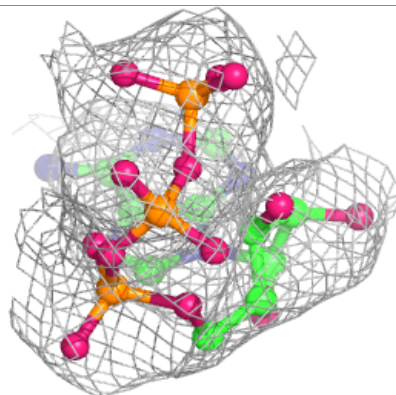
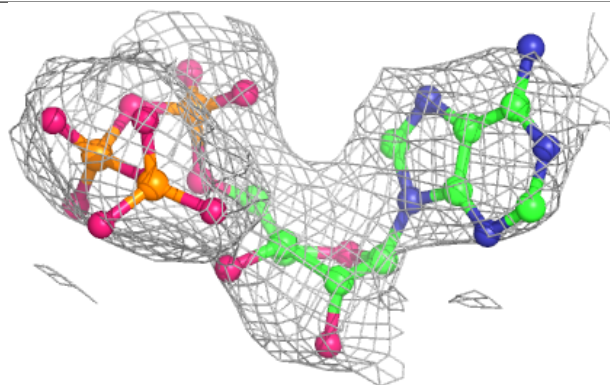
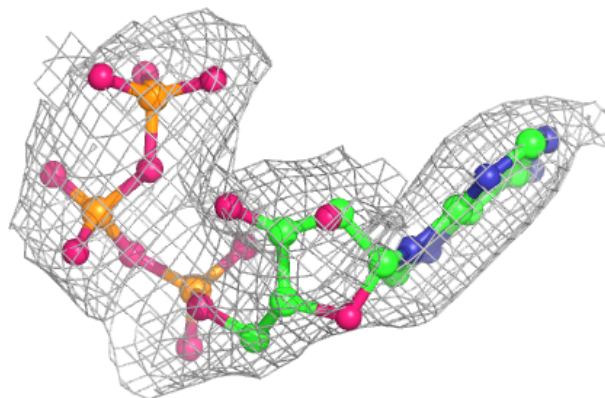


Electron density around ATP L 301:

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

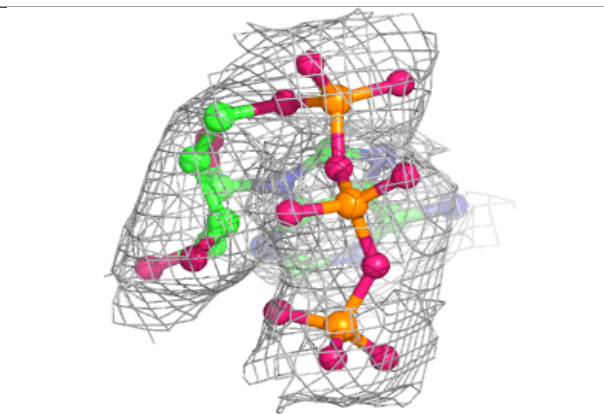
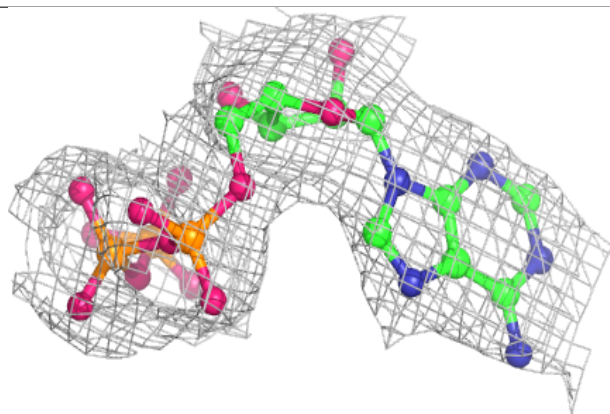
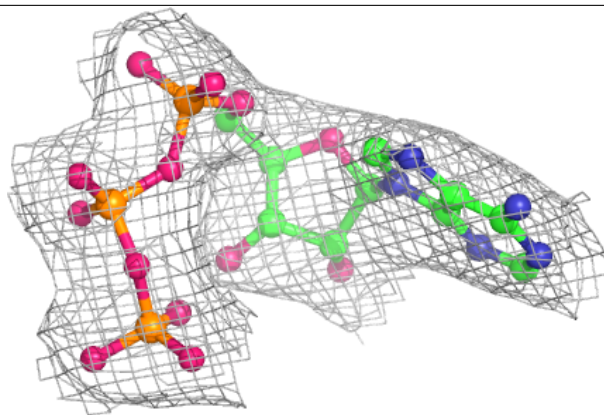
**Electron density around ATP M 301:**

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

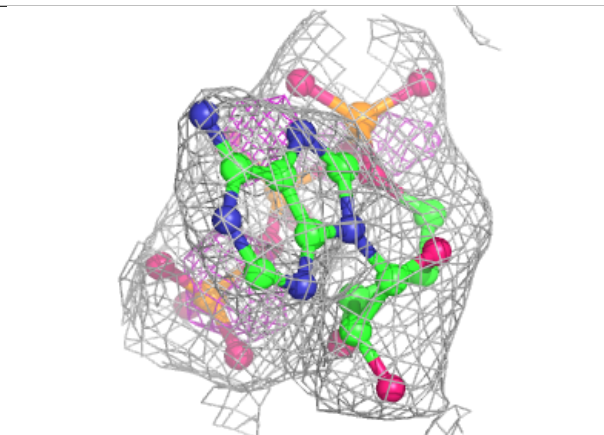
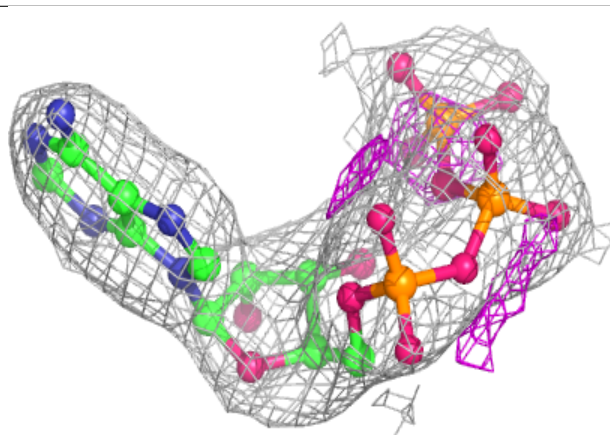
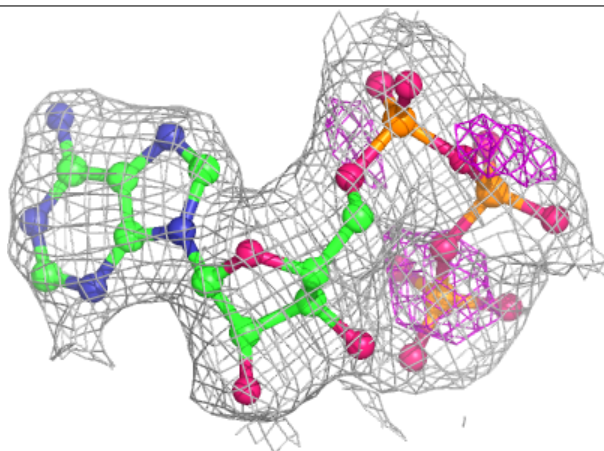


Electron density around ATP A 301:

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

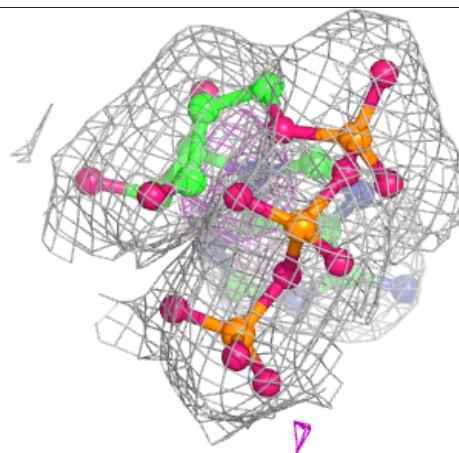
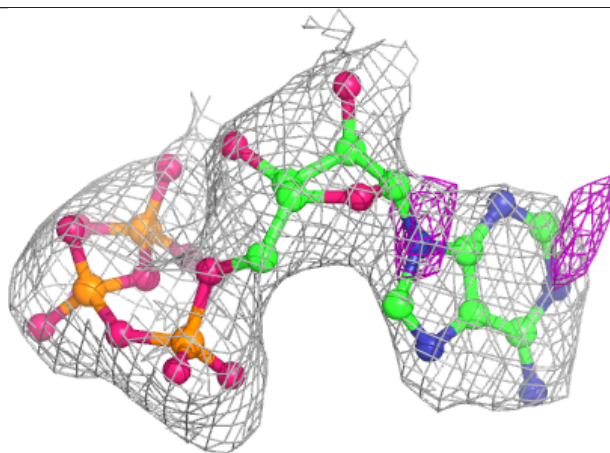
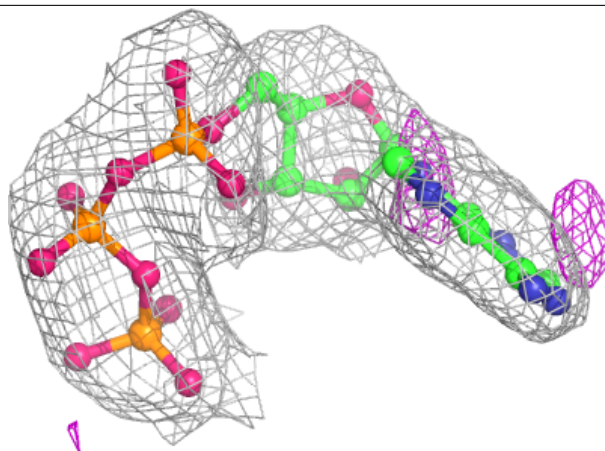
**Electron density around ATP C 301:**

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



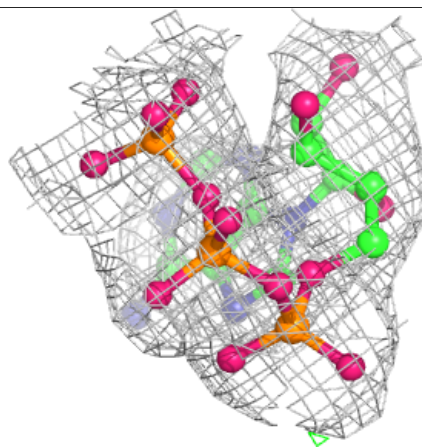
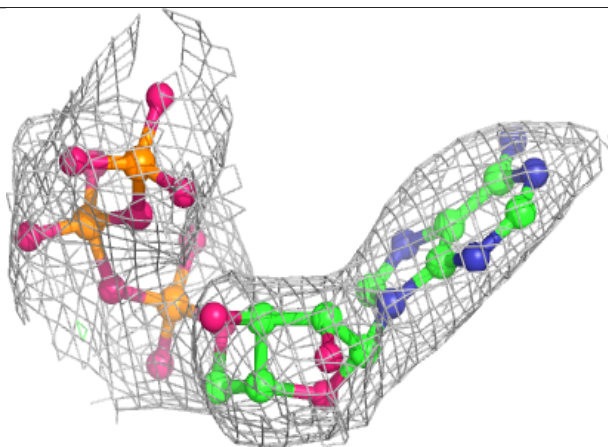
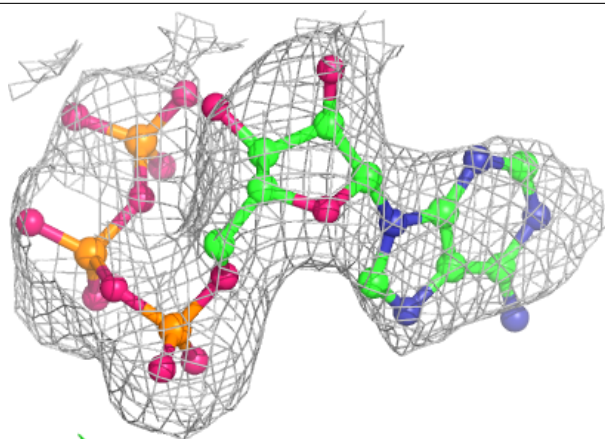
Electron density around ATP D 301:

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



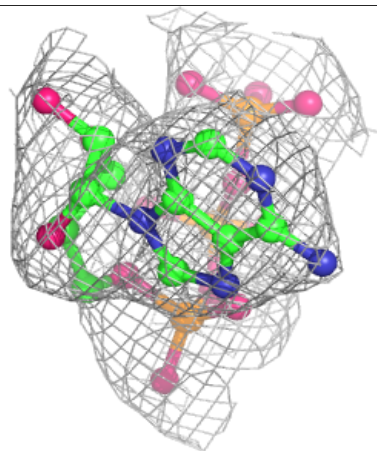
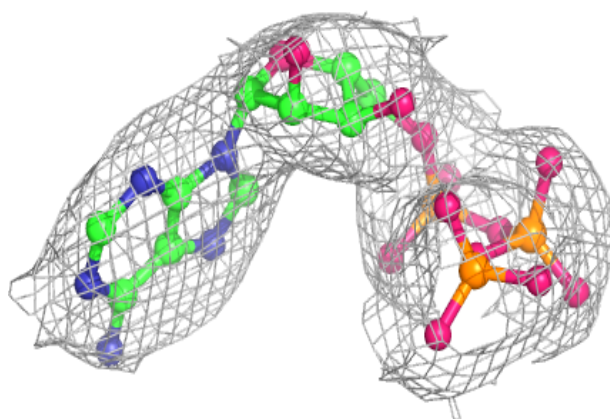
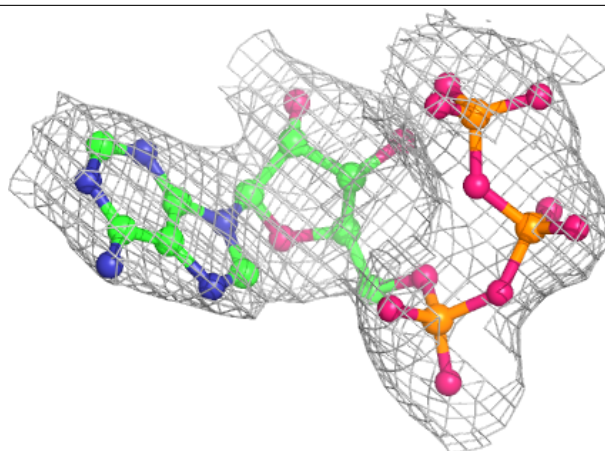
Electron density around ATP F 301:

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



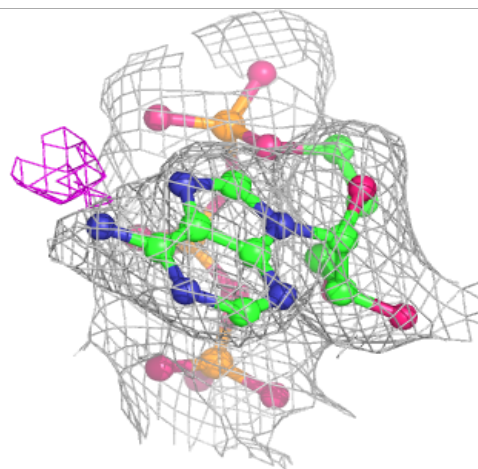
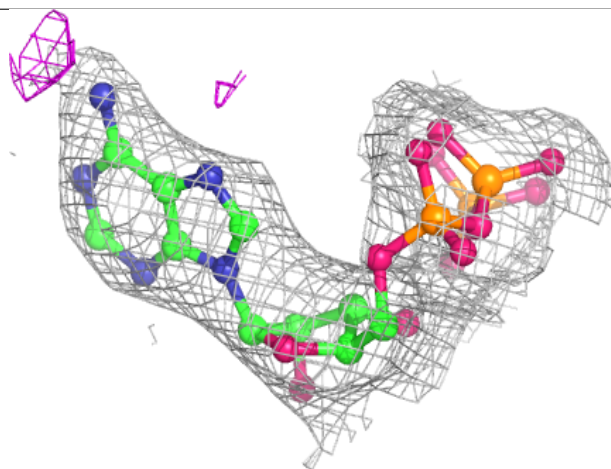
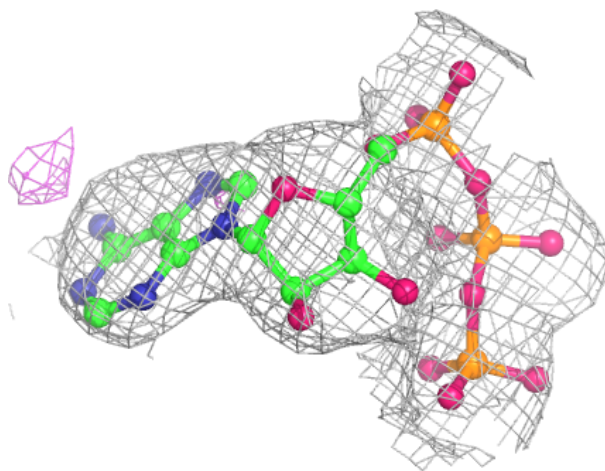
Electron density around ATP H 301:

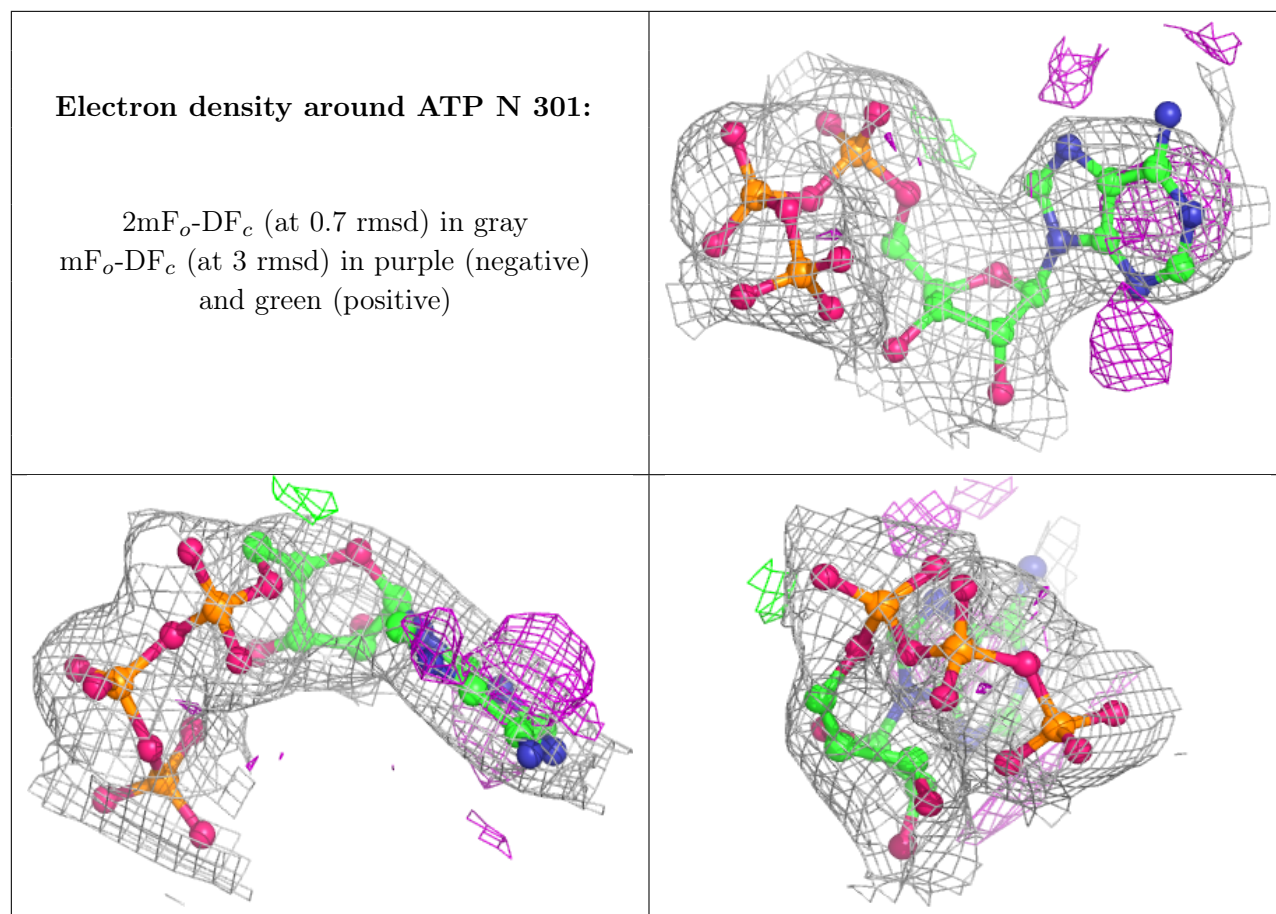
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP K 301:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.