



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:55 pm BST

PDB ID : 6RKE
Title : Molybdenum storage protein - P212121, ADP, molybdate
Authors : Ermler, U.; Bruenle, S.
Deposited on : 2019-04-30
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

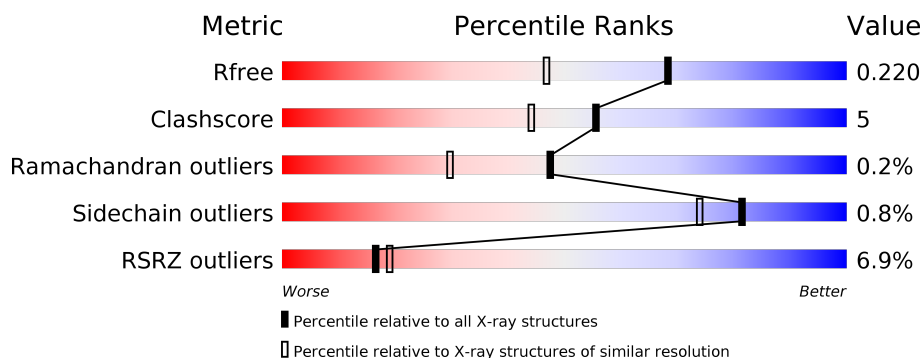
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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	B	269	<div> <div>7%</div> <div> <div></div> <div>88%</div> <div>12%</div> </div> </div>
1	D	269	<div> <div>9%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
1	F	269	<div> <div>8%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
1	H	269	<div> <div>10%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> </div>
1	J	269	<div> <div>11%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
1	L	269	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	A	275	
2	C	275	
2	E	275	
2	G	275	
2	I	275	
2	K	275	

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	8M0	J	302	-	-	-	X
5	8M0	L	303	-	-	X	-
6	MOO	B	304[A]	-	-	X	-
6	MOO	D	303[A]	-	-	X	-
6	MOO	F	304[A]	-	-	X	-
6	MOO	H	304[A]	-	-	X	-
6	MOO	J	304[A]	-	-	X	-
6	MOO	L	304[A]	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26584 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.

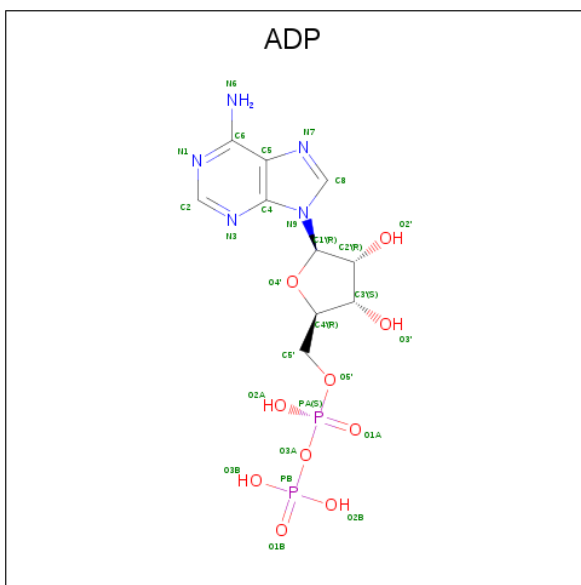
- Molecule 1 is a protein called Molybdenum storage protein subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	268	Total 1997	C 1268	N 348	O 373	S 8	0	5	0
1	D	268	Total 1997	C 1269	N 349	O 371	S 8	0	4	0
1	F	269	Total 1996	C 1267	N 348	O 373	S 8	0	4	0
1	H	268	Total 1987	C 1260	N 347	O 372	S 8	0	3	0
1	J	267	Total 1994	C 1269	N 346	O 371	S 8	0	6	0
1	L	267	Total 1992	C 1266	N 346	O 372	S 8	0	6	0

- Molecule 2 is a protein called Molybdenum storage protein subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	272	Total 2048	C 1292	N 386	O 367	S 3	0	2	0
2	C	271	Total 2043	C 1289	N 385	O 366	S 3	0	2	0
2	E	272	Total 2050	C 1293	N 386	O 368	S 3	0	2	0
2	G	272	Total 2053	C 1295	N 386	O 369	S 3	0	3	0
2	I	272	Total 2050	C 1293	N 386	O 368	S 3	0	2	0
2	K	272	Total 2062	C 1301	N 387	O 371	S 3	0	5	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 36	Mo 8	O 28	0	0
5	A	1	Total 34	Mo 8	O 26	0	0
5	C	1	Total 36	Mo 8	O 28	0	0
5	C	1	Total 34	Mo 8	O 26	0	0
5	F	1	Total 36	Mo 8	O 28	0	0

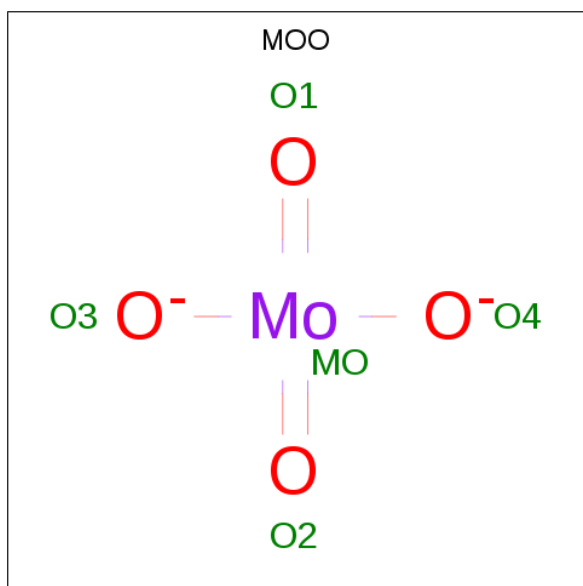


WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	Mo	O	0	0
			34	8	26		
5	H	1	Total	Mo	O	0	0
			36	8	28		
5	G	1	Total	Mo	O	0	0
			34	8	26		
5	J	1	Total	Mo	O	0	0
			36	8	28		
5	I	1	Total	Mo	O	0	0
			34	8	26		
5	L	1	Total	Mo	O	0	0
			36	8	28		
5	K	1	Total	Mo	O	0	0
			34	8	26		

- Molecule 6 is MOLYBDATE ION (three-letter code: MOO) (formula: MoO_4) (labeled as "Ligand of Interest" by author).



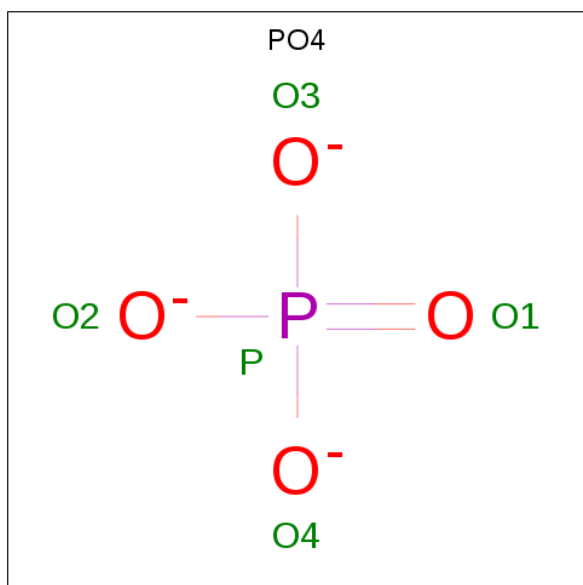
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Mo	O	0	1
			5	1	4		
6	D	1	Total	Mo	O	0	1
			5	1	4		
6	F	1	Total	Mo	O	0	1
			5	1	4		
6	H	1	Total	Mo	O	0	1
			5	1	4		

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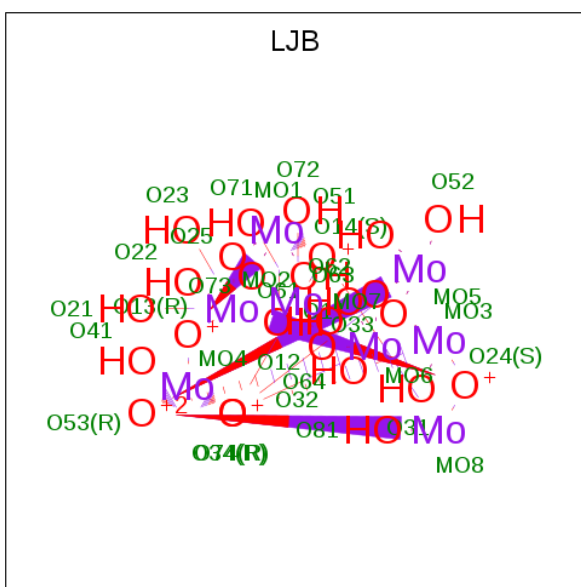
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	J	1	Total	Mo	O	0	1
			5	1	4		
6	L	1	Total	Mo	O	0	1
			5	1	4		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



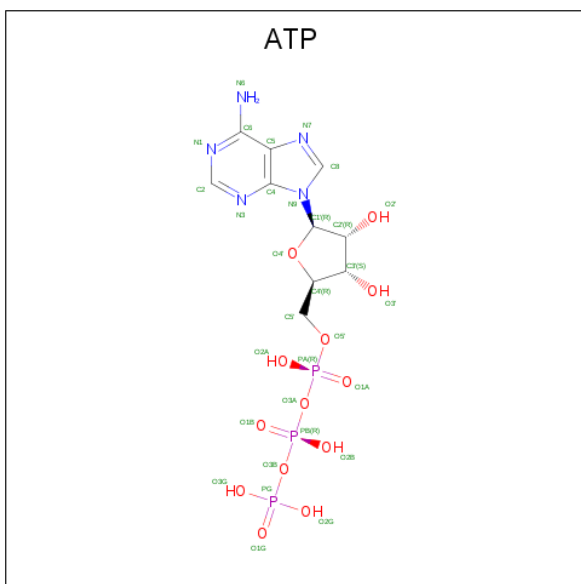
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	1
			5	4	1		
7	D	1	Total	O	P	0	1
			5	4	1		
7	F	1	Total	O	P	0	1
			5	4	1		
7	H	1	Total	O	P	0	1
			5	4	1		
7	J	1	Total	O	P	0	1
			5	4	1		
7	L	1	Total	O	P	0	1
			5	4	1		

- Molecule 8 is MO(8)-O(26) Cluster (three-letter code: LJB) (formula: H₁₅Mo₈O₂₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 34	Mo 8	O 26	26	0
8	L	1	Total 34	Mo 8	O 26	26	0

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



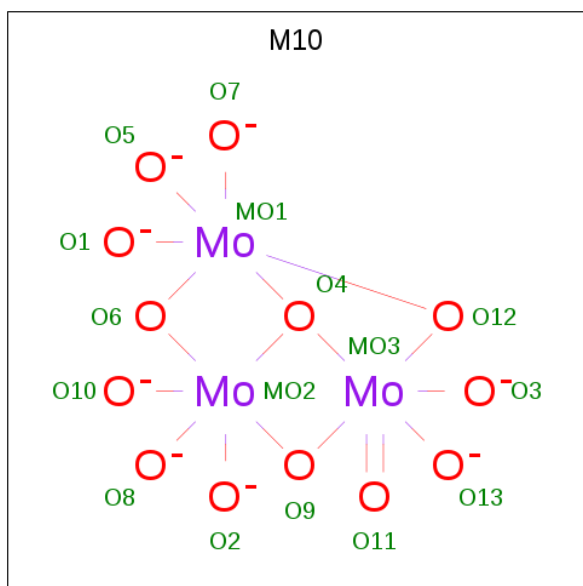
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 31	C 10	N 5	O 13	P 3	0	0

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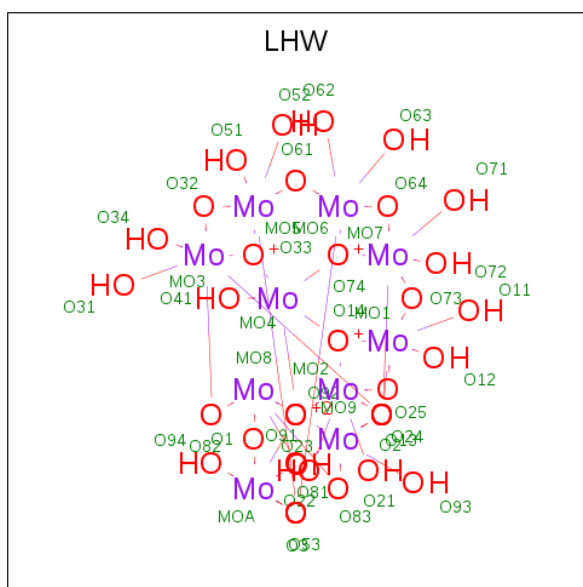
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
9	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
9	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
9	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
9	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 10 is (mu3-oxo)-tris(mu2-oxo)-nonakisoxo-trimolybdenum (VI) (three-letter code: M10) (formula: Mo_3O_{13}).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	Mo	O	0	0
			13	3	10		
10	G	1	Total	Mo	O	0	0
			13	3	10		

- Molecule 11 is MO(10)-O(35) Cluster (three-letter code: LHW) (formula: $\text{H}_{16}\text{Mo}_{10}\text{O}_{35}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total 45	Mo 10	O 35	35	0
11	K	1	Total 45	Mo 10	O 35	34	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	119	Total O 119 119	0	2
12	A	162	Total O 162 162	0	0
12	D	97	Total O 97 97	0	2
12	C	130	Total O 130 130	0	0
12	F	98	Total O 98 98	0	1
12	E	135	Total O 135 135	0	0
12	H	54	Total O 54 54	0	2
12	G	118	Total O 118 118	0	0
12	J	76	Total O 76 76	0	0
12	I	97	Total O 97 97	0	0

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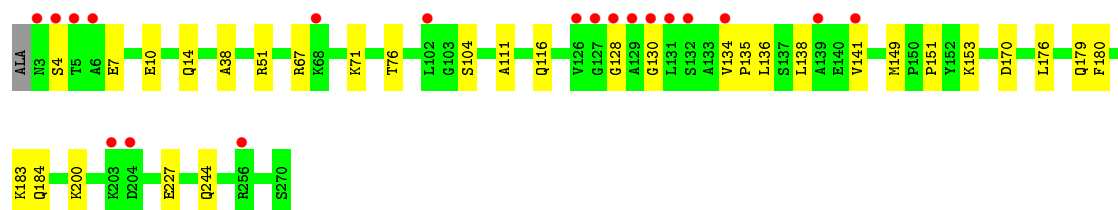
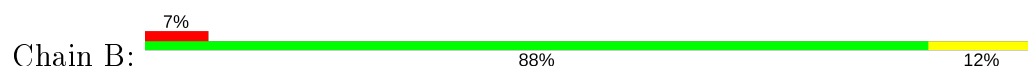
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	87	Total 87	O 87	0	1
12	K	118	Total 118	O 118	0	0

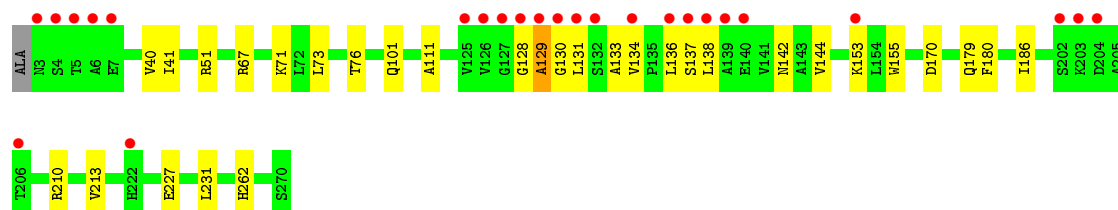
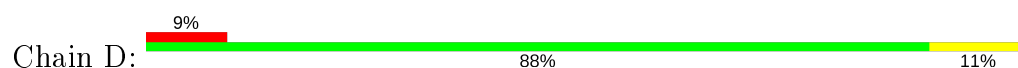
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

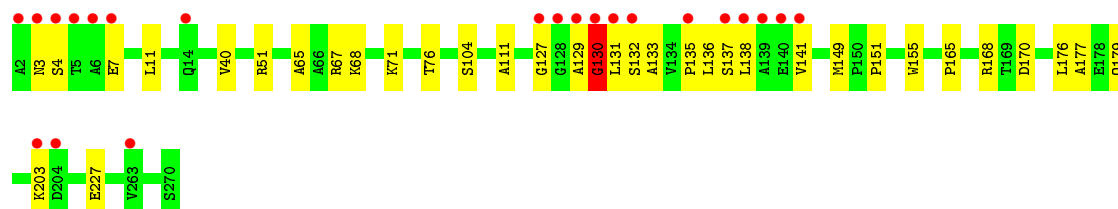
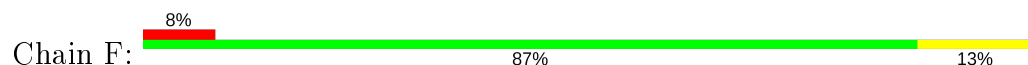
- Molecule 1: Molybdenum storage protein subunit beta



- Molecule 1: Molybdenum storage protein subunit beta

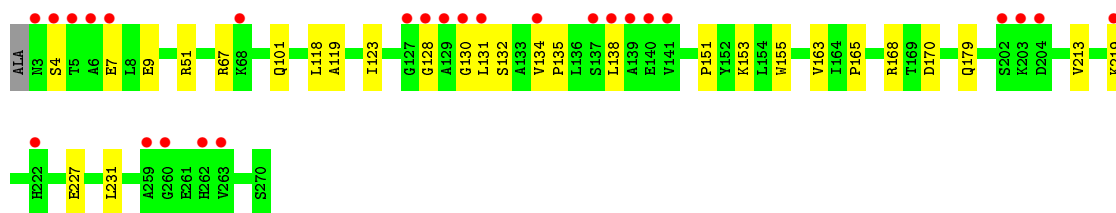


- Molecule 1: Molybdenum storage protein subunit beta

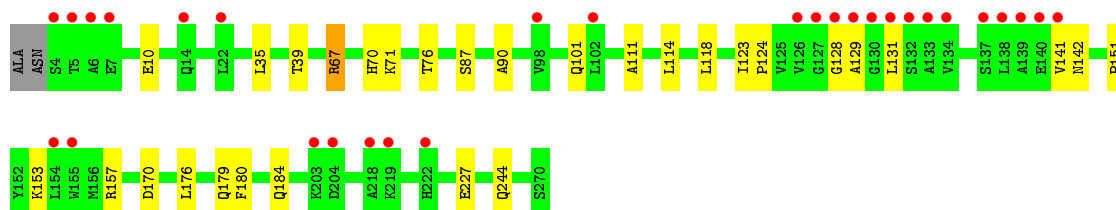
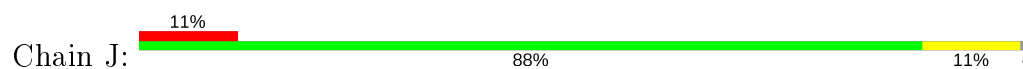


- Molecule 1: Molybdenum storage protein subunit beta

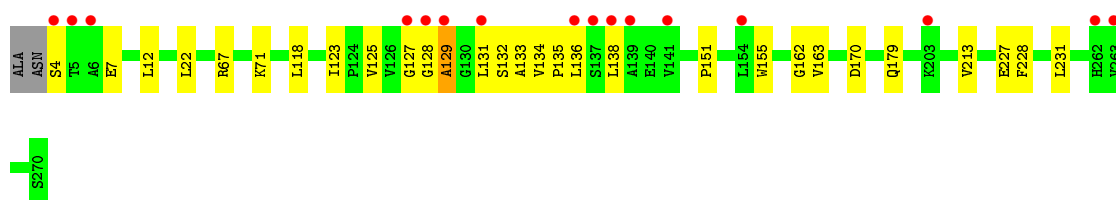
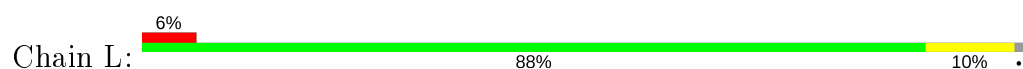




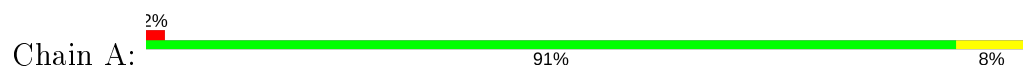
- Molecule 1: Molybdenum storage protein subunit beta



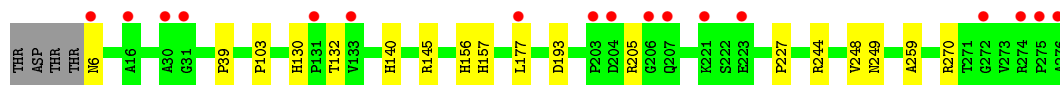
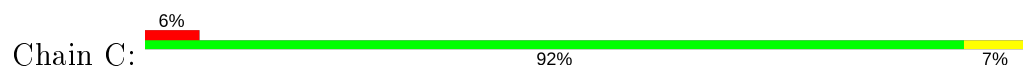
- Molecule 1: Molybdenum storage protein subunit beta



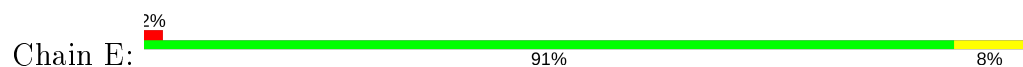
- Molecule 2: Molybdenum storage protein subunit alpha



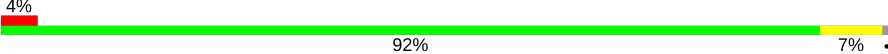
- Molecule 2: Molybdenum storage protein subunit alpha



- Molecule 2: Molybdenum storage protein subunit alpha




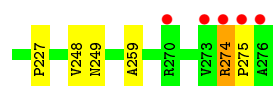
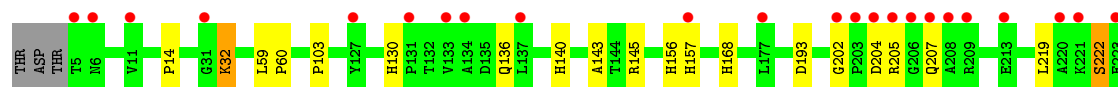
- Molecule 2: Molybdenum storage protein subunit alpha

Chain G: 

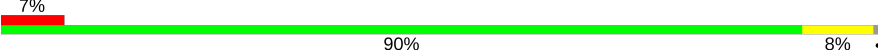


- Molecule 2: Molybdenum storage protein subunit alpha

Chain I: 



- Molecule 2: Molybdenum storage protein subunit alpha

Chain K: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.06Å 148.86Å 183.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 1.70 49.49 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.49-1.70) 97.7 (49.49-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.194 , 0.214 0.200 , 0.220	Depositor DCC
R_{free} test set	18910 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26584	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, PO4, LJB, LHW, M10, MOO, ATP, 8M0

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	B	0.27	0/2048	0.46	0/2782
1	D	0.26	0/2045	0.44	0/2777
1	F	0.30	0/2044	0.51	0/2777
1	H	0.31	0/2031	0.47	0/2759
1	J	0.28	0/2048	0.45	0/2782
1	L	0.29	0/2046	0.49	1/2779 (0.0%)
2	A	0.25	0/2097	0.45	0/2857
2	C	0.31	0/2092	0.47	0/2850
2	E	0.25	0/2099	0.42	0/2860
2	G	0.30	1/2105 (0.0%)	0.50	1/2868 (0.0%)
2	I	0.28	0/2099	0.50	1/2860 (0.0%)
2	K	0.26	0/2120	0.45	0/2888
All	All	0.28	1/24874 (0.0%)	0.47	3/33839 (0.0%)

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	F	0	2
2	K	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	67	LYS	CE-NZ	5.75	1.63	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	67	LYS	CD-CE-NZ	-12.52	82.90	111.70
1	L	128	GLY	C-N-CA	6.69	138.43	121.70
2	I	274	ARG	CB-CG-CD	5.28	125.32	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	130	GLY	Mainchain,Peptide
2	K	274	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1997	0	2058	23	0
1	D	1997	0	2061	21	0
1	F	1996	0	2055	36	0
1	H	1987	0	2043	22	0
1	J	1994	0	2063	26	0
1	L	1992	0	2057	25	0
2	A	2048	0	2105	17	0
2	C	2043	0	2103	19	0
2	E	2050	0	2110	18	0
2	G	2053	0	2115	16	0
2	I	2050	0	2110	19	0
2	K	2062	0	2128	25	0
3	B	27	0	12	2	0
3	D	27	0	12	0	0
3	F	27	0	12	0	0
3	H	27	0	12	0	0
3	J	27	0	12	0	0
3	L	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	34	0	0	1	0
5	B	36	0	0	4	0
5	C	70	0	0	4	0
5	E	34	0	0	1	0
5	F	36	0	0	6	0
5	G	34	0	0	1	0
5	H	36	0	0	2	0
5	I	34	0	0	1	0
5	J	36	0	0	3	0
5	K	34	0	0	2	0
5	L	36	0	0	7	0
6	B	5	0	0	4	0
6	D	5	0	0	4	0
6	F	5	0	0	4	0
6	H	5	0	0	4	0
6	J	5	0	0	4	0
6	L	5	0	0	4	0
7	B	5	0	0	0	0
7	D	5	0	0	0	0
7	F	5	0	0	0	0
7	H	5	0	0	0	0
7	J	5	0	0	0	0
7	L	5	0	0	0	0
8	B	34	0	0	0	0
8	L	34	0	0	0	0
9	A	31	0	12	1	0
9	C	31	0	12	1	0
9	E	31	0	12	2	0
9	G	31	0	12	2	0
9	I	31	0	12	2	0
9	K	31	0	12	1	0
10	A	13	0	0	3	0
10	G	13	0	0	3	0
11	C	45	0	0	0	0
11	K	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	162	0	0	1	0
12	B	119	0	0	1	0
12	C	130	0	0	0	0
12	D	97	0	0	1	0
12	E	135	0	0	0	0
12	F	98	0	0	0	0
12	G	118	0	0	4	0
12	H	54	0	0	0	0
12	I	97	0	0	0	0
12	J	76	0	0	3	0
12	K	118	0	0	3	0
12	L	87	0	0	0	0
All	All	26584	0	25152	258	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 5.

All (258) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:204:ASP:HB3	2:I:207:GLN:HE21	1.12	1.08
2:I:202:GLY:O	2:I:205:ARG:HG2	1.67	0.95
2:G:219:LEU:O	2:G:222:SER:OG	1.93	0.86
1:H:131:LEU:HD11	1:L:125:VAL:O	1.75	0.85
2:K:21:GLN:O	12:K:401:HOH:O	1.95	0.85
2:I:202:GLY:O	2:I:205:ARG:CG	2.25	0.84
1:H:101:GLN:HG2	1:H:153:LYS:HD2	1.59	0.84
2:I:204:ASP:HB3	2:I:207:GLN:NE2	1.92	0.81
1:L:179:GLN:HG2	2:K:157:HIS:HB3	1.65	0.78
1:H:179:GLN:HG2	2:G:157:HIS:HB3	1.67	0.77
1:F:179:GLN:HG2	2:E:157:HIS:HB3	1.66	0.76
1:H:131:LEU:CD1	1:L:125:VAL:O	2.33	0.76
1:F:130:GLY:O	1:F:131:LEU:HG	1.86	0.75
1:J:179:GLN:HG2	2:I:157:HIS:HB3	1.67	0.75
1:J:129:ALA:HA	5:J:302:8M0:O22	1.87	0.74
1:J:35:LEU:HD11	1:J:131:LEU:HD11	1.69	0.74
1:D:73:LEU:HD21	1:D:136:LEU:HD11	1.69	0.74
1:L:129:ALA:HB2	5:L:303:8M0:O22	1.89	0.73
1:F:130:GLY:HA2	2:E:157:HIS:NE2	2.07	0.70
2:C:39:PRO:HG3	12:G:406:HOH:O	1.94	0.68
1:B:179:GLN:HG2	2:A:157:HIS:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:LEU:HD13	1:J:180:PHE:CE1	2.29	0.67
1:D:179:GLN:HG2	2:C:157:HIS:HB3	1.78	0.66
2:K:274:ARG:HG3	2:K:274:ARG:HH21	1.61	0.66
1:F:71:LYS:NZ	1:F:136:LEU:O	2.25	0.64
1:J:131:LEU:HD13	1:J:180:PHE:CZ	2.33	0.64
6:B:304[A]:MOO:MO	6:B:304[A]:MOO:O1	1.70	0.63
6:B:304[A]:MOO:MO	6:B:304[A]:MOO:O3	1.70	0.63
1:B:51:ARG:NH1	2:A:6:ASN:O	2.32	0.63
6:D:303[A]:MOO:O1	6:D:303[A]:MOO:MO	1.70	0.63
6:J:304[A]:MOO:O3	6:J:304[A]:MOO:MO	1.70	0.62
6:L:304[A]:MOO:O1	6:L:304[A]:MOO:MO	1.70	0.62
6:L:304[A]:MOO:MO	6:L:304[A]:MOO:O3	1.70	0.62
6:J:304[A]:MOO:O1	6:J:304[A]:MOO:MO	1.70	0.62
6:F:304[A]:MOO:MO	6:F:304[A]:MOO:O1	1.70	0.62
6:H:304[A]:MOO:O3	6:H:304[A]:MOO:MO	1.70	0.62
6:D:303[A]:MOO:O3	6:D:303[A]:MOO:MO	1.70	0.62
6:H:304[A]:MOO:MO	6:H:304[A]:MOO:O4	1.71	0.62
2:K:33:ARG:HH12	2:K:274:ARG:HH12	1.46	0.62
6:J:304[A]:MOO:MO	6:J:304[A]:MOO:O4	1.72	0.61
1:J:244:GLN:NE2	12:J:401:HOH:O	2.23	0.61
1:B:104[B]:SER:HA	1:B:149:MET:HG3	1.83	0.61
6:H:304[A]:MOO:O1	6:H:304[A]:MOO:MO	1.70	0.61
5:L:303:8M0:MO2	5:L:303:8M0:O8	1.70	0.61
1:B:104[A]:SER:HA	1:B:149:MET:HG3	1.83	0.61
6:F:304[A]:MOO:MO	6:F:304[A]:MOO:O2	1.72	0.61
6:D:303[A]:MOO:O2	6:D:303[A]:MOO:MO	1.72	0.61
6:F:304[A]:MOO:O3	6:F:304[A]:MOO:MO	1.70	0.61
10:G:304:M10:O2	10:G:304:M10:MO2	1.72	0.61
6:F:304[A]:MOO:O4	6:F:304[A]:MOO:MO	1.71	0.61
10:G:304:M10:O1	10:G:304:M10:MO1	1.72	0.61
10:A:304:M10:MO1	10:A:304:M10:O1	1.72	0.61
2:C:39:PRO:CG	12:G:406:HOH:O	2.47	0.61
5:J:302:8M0:O22	5:J:302:8M0:MO8	1.72	0.61
1:F:130:GLY:C	1:F:131:LEU:HG	2.22	0.60
5:L:303:8M0:MO2	5:L:303:8M0:O6	1.72	0.60
10:G:304:M10:MO3	10:G:304:M10:O3	1.72	0.60
6:B:304[A]:MOO:O2	6:B:304[A]:MOO:MO	1.72	0.60
1:F:129:ALA:O	1:F:131:LEU:HB2	2.01	0.60
2:I:130:HIS:HB2	5:I:303:8M0:O21	2.02	0.60
1:B:176:LEU:HD11	5:B:303:8M0:O13	2.01	0.60
6:L:304[A]:MOO:O4	6:L:304[A]:MOO:MO	1.72	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:304[A]:MOO:MO	6:L:304[A]:MOO:O2	1.72	0.60
1:F:176:LEU:HD11	5:F:303:8M0:O13	2.02	0.60
1:L:151:PRO:HB3	5:L:303:8M0:O4	2.02	0.60
6:D:303[A]:MOO:O4	6:D:303[A]:MOO:MO	1.72	0.59
6:B:304[A]:MOO:MO	6:B:304[A]:MOO:O4	1.72	0.59
6:H:304[A]:MOO:O2	6:H:304[A]:MOO:MO	1.72	0.59
10:A:304:M10:MO2	10:A:304:M10:O2	1.72	0.59
10:A:304:M10:O13	10:A:304:M10:MO3	1.72	0.59
1:B:151:PRO:HB3	5:B:303:8M0:O4	2.03	0.59
12:D:409:HOH:O	1:F:131:LEU:CD2	2.50	0.59
6:J:304[A]:MOO:MO	6:J:304[A]:MOO:O2	1.72	0.59
1:F:129:ALA:HA	5:F:303:8M0:O22	2.02	0.58
2:C:244:ARG:HH21	2:C:270:ARG:HH12	1.51	0.58
1:F:127:GLY:HA2	5:F:303:8M0:O17	2.04	0.57
1:H:151:PRO:HB3	5:H:303:8M0:O4	2.04	0.57
1:B:71:LYS:HG2	1:B:136:LEU:HD22	1.86	0.57
1:F:129:ALA:O	1:F:131:LEU:N	2.37	0.57
2:K:130:HIS:HB2	5:K:303:8M0:O21	2.05	0.56
1:D:210:ARG:NH2	1:D:262:HIS:CE1	2.73	0.56
1:J:71:LYS:NZ	1:J:142:ASN:OD1	2.39	0.56
1:D:138:LEU:HD13	1:F:138:LEU:HD21	1.88	0.56
1:F:65:ALA:O	1:F:68:LYS:HE2	2.07	0.55
5:B:303:8M0:O15	2:A:157:HIS:HD2	1.89	0.55
1:H:138:LEU:HD11	1:L:138:LEU:HD13	1.87	0.55
1:F:130:GLY:CA	2:E:157:HIS:NE2	2.68	0.55
1:H:119:ALA:CB	1:J:131:LEU:HD23	2.36	0.55
1:F:130:GLY:N	2:E:157:HIS:NE2	2.54	0.55
5:L:303:8M0:O24	2:K:156:HIS:ND1	2.26	0.55
2:A:103:PRO:HB3	2:A:156:HIS:HD2	1.72	0.55
2:C:130:HIS:HB2	5:C:304:8M0:O21	2.08	0.54
1:L:4:SER:OG	1:L:7:GLU:CB	2.55	0.54
2:I:227:PRO:HD3	9:I:301:ATP:C6	2.43	0.54
2:E:46:ILE:HD12	2:E:61:LEU:HD21	1.89	0.54
1:F:151:PRO:HB3	5:F:303:8M0:O4	2.07	0.54
2:G:67:LYS:NZ	12:G:406:HOH:O	2.41	0.54
5:B:303:8M0:O13	2:A:157:HIS:HB2	2.09	0.53
1:B:130:GLY:HA3	1:B:180:PHE:CE2	2.43	0.53
1:H:119:ALA:HB1	1:J:131:LEU:HD23	1.91	0.53
2:A:130:HIS:HB2	5:A:303:8M0:O21	2.09	0.53
1:D:101:GLN:HG2	1:D:153[B]:LYS:HD2	1.89	0.53
1:D:129:ALA:HA	1:D:144:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:ARG:NH1	2:E:6:ASN:O	2.37	0.53
1:D:40:VAL:HG22	1:D:73:LEU:HB2	1.91	0.53
1:F:127:GLY:HA3	5:F:303:8M0:O18	2.09	0.53
1:B:135:PRO:HG3	1:D:134:VAL:HG21	1.91	0.52
1:B:116:GLN:HG2	1:D:131:LEU:HD21	1.91	0.52
1:J:101:GLN:OE1	1:J:153:LYS:HE3	2.09	0.52
1:J:151:PRO:HB3	5:J:302:8M0:O4	2.10	0.52
2:G:130:HIS:HB2	5:G:303:8M0:O21	2.09	0.52
1:F:133:ALA:O	1:F:137:SER:HB3	2.11	0.51
1:J:124:PRO:HB3	1:L:133:ALA:HB3	1.93	0.51
2:K:227:PRO:HD3	9:K:301:ATP:C6	2.46	0.51
1:D:170:ASP:HB2	1:D:227:GLU:CD	2.31	0.51
2:C:157:HIS:HD2	5:C:301:8M0:O15	1.94	0.51
2:C:244:ARG:HH21	2:C:270:ARG:NH1	2.09	0.51
1:F:4:SER:OG	1:F:7:GLU:HB2	2.10	0.51
1:D:51:ARG:NH1	2:C:6:ASN:O	2.39	0.51
2:I:136:GLN:O	2:I:140:HIS:ND1	2.39	0.51
1:L:132:SER:O	1:L:135:PRO:HD2	2.10	0.51
1:F:104[B]:SER:HA	1:F:149:MET:HG3	1.94	0.50
2:G:227:PRO:HD3	9:G:301:ATP:C6	2.45	0.50
2:E:130:HIS:HB2	5:E:303:8M0:O21	2.11	0.50
5:L:303:8M0:O1	2:K:156:HIS:CE1	2.65	0.50
1:F:135:PRO:HB3	1:F:141:VAL:HG11	1.93	0.50
1:F:104[A]:SER:HA	1:F:149:MET:HG3	1.94	0.50
1:J:87:SER:HB3	2:I:14:PRO:HG2	1.92	0.50
1:H:132:SER:C	1:H:135:PRO:HD2	2.33	0.49
2:A:136:GLN:NE2	12:A:405:HOH:O	2.45	0.49
1:D:210:ARG:NH2	1:D:262:HIS:HE1	2.10	0.49
2:A:227:PRO:HD3	9:A:301:ATP:C6	2.48	0.49
2:A:213:GLU:HG3	2:A:268:LEU:HB2	1.95	0.48
1:B:138:LEU:HD13	1:D:138:LEU:HD21	1.96	0.48
2:E:227:PRO:HD3	9:E:301:ATP:C6	2.49	0.48
1:F:7:GLU:O	1:F:11:LEU:HG	2.13	0.48
1:F:203:LYS:H	1:F:203:LYS:CD	2.27	0.48
1:L:127:GLY:HA2	5:L:303:8M0:O17	2.13	0.48
2:K:274:ARG:HB2	2:K:275:PRO:HD3	1.95	0.48
2:C:157:HIS:HB2	5:C:301:8M0:O13	2.14	0.47
2:A:145[B]:ARG:HH12	2:I:145[B]:ARG:HH12	1.62	0.47
1:B:135:PRO:HB3	1:B:141:VAL:HG11	1.95	0.47
5:F:303:8M0:O24	2:E:156:HIS:ND1	2.43	0.47
1:H:9:GLU:OE2	2:K:9:LYS:NZ	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:SER:HB3	1:H:7:GLU:HB3	1.95	0.47
2:E:145[B]:ARG:HH12	2:K:145[B]:ARG:HH12	1.63	0.47
1:J:70:HIS:HD2	12:J:410:HOH:O	1.97	0.47
1:L:170:ASP:HB2	1:L:227:GLU:CD	2.34	0.47
1:B:104[A]:SER:OG	1:B:153:LYS:HE3	2.14	0.47
2:I:103:PRO:HB3	2:I:156:HIS:HD2	1.80	0.47
2:C:156:HIS:ND1	5:C:301:8M0:O24	2.47	0.47
1:B:183:LYS:O	1:B:184:GLN:HG3	2.15	0.46
2:E:248:VAL:HG11	2:E:259:ALA:HB2	1.98	0.46
1:H:213:VAL:HG13	1:H:231:LEU:HB3	1.97	0.46
2:C:103:PRO:HB3	2:C:156:HIS:HD2	1.80	0.46
1:F:155:TRP:NE1	2:E:177:LEU:HG	2.30	0.46
2:C:227:PRO:HD3	9:C:302:ATP:C6	2.49	0.46
1:D:213:VAL:HG13	1:D:231:LEU:HB3	1.98	0.46
1:F:170:ASP:HB2	1:F:227:GLU:CD	2.35	0.46
1:F:203:LYS:HD2	1:F:203:LYS:N	2.30	0.46
2:I:193:ASP:HA	2:I:249:ASN:HB2	1.96	0.46
2:A:86:HIS:HB2	2:E:11:VAL:HG22	1.97	0.46
2:C:270:ARG:HE	2:C:270:ARG:HB2	1.60	0.46
1:B:38:ALA:HA	1:B:71:LYS:HB3	1.97	0.46
1:F:76:THR:HG21	1:F:111:ALA:HA	1.98	0.46
1:L:163:VAL:HG22	2:K:30:ALA:HB1	1.98	0.45
2:C:193:ASP:HA	2:C:249:ASN:HB2	1.98	0.45
1:J:170:ASP:HB2	1:J:227:GLU:CD	2.37	0.45
1:L:71:LYS:HE3	1:L:136:LEU:O	2.15	0.45
1:D:71:LYS:NZ	1:D:142:ASN:OD1	2.50	0.45
2:K:274:ARG:NH2	2:K:274:ARG:HG3	2.29	0.45
2:K:33:ARG:NH1	2:K:274:ARG:HH12	2.13	0.45
1:L:131:LEU:HD23	1:L:131:LEU:N	2.31	0.45
2:K:178:ALA:HB1	2:K:242:ILE:HD11	1.99	0.45
1:L:118:LEU:HB3	1:L:123:ILE:HB	1.99	0.45
1:L:228:PHE:HE2	12:K:401:HOH:O	1.99	0.45
2:E:136:GLN:O	2:E:140:HIS:ND1	2.40	0.45
2:A:193:ASP:HA	2:A:249:ASN:HB2	1.99	0.45
1:F:165:PRO:O	1:F:168:ARG:NH1	2.45	0.45
2:A:248:VAL:HG11	2:A:259:ALA:HB2	1.99	0.44
1:H:170:ASP:HB2	1:H:227:GLU:CD	2.37	0.44
2:K:130:HIS:N	5:K:303:8M0:O12	2.42	0.44
1:B:138:LEU:HD21	1:F:138:LEU:HD13	1.98	0.44
1:J:128:GLY:HA3	1:J:131:LEU:O	2.18	0.44
2:A:139:ILE:HD13	2:C:140:HIS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:143:ALA:HB1	2:K:143:ALA:HB2	2.00	0.44
2:K:193:ASP:HA	2:K:249:ASN:HB2	1.99	0.44
1:D:130:GLY:HA3	1:D:180:PHE:CE2	2.52	0.44
1:J:70:HIS:CD2	12:J:410:HOH:O	2.70	0.44
1:D:133:ALA:O	1:D:137:SER:HB3	2.18	0.43
2:E:215:SER:OG	2:E:218:ASP:HB2	2.18	0.43
1:J:124:PRO:HG3	1:L:134:VAL:HG23	1.99	0.43
1:L:4:SER:OG	1:L:7:GLU:HB3	2.17	0.43
2:G:193:ASP:HA	2:G:249:ASN:HB2	2.00	0.43
2:G:238:THR:O	2:G:240:ARG:NH1	2.49	0.43
1:D:41:ILE:HG22	1:D:186:ILE:HB	2.01	0.43
2:E:193:ASP:HA	2:E:249:ASN:HB2	1.99	0.43
1:H:134:VAL:O	1:H:138:LEU:HD22	2.18	0.43
2:I:143:ALA:HB2	2:K:143:ALA:HB1	2.01	0.43
1:B:10:GLU:O	1:B:14[B]:GLN:HG2	2.19	0.43
2:I:207:GLN:H	2:I:207:GLN:HG2	1.61	0.43
1:J:76:THR:HG21	1:J:111:ALA:HA	2.00	0.43
2:C:145[B]:ARG:HH12	2:G:145[B]:ARG:HH12	1.67	0.42
2:C:132:THR:HG23	2:C:140:HIS:CE1	2.54	0.42
2:G:248:VAL:HG11	2:G:259:ALA:HB2	2.01	0.42
9:G:301:ATP:H2'	9:G:301:ATP:N3	2.34	0.42
9:I:301:ATP:N3	9:I:301:ATP:H2'	2.34	0.42
1:J:76:THR:HG22	1:J:114[B]:LEU:HD12	2.00	0.42
2:A:209:ARG:HH21	2:A:209:ARG:HG2	1.83	0.42
1:B:170:ASP:HB2	1:B:227:GLU:CD	2.39	0.42
2:I:59:LEU:HB2	2:I:60:PRO:HD3	2.01	0.42
2:G:209:ARG:HD3	2:G:209:ARG:HA	1.92	0.42
1:H:128:GLY:C	1:H:130:GLY:H	2.22	0.42
2:K:136[B]:GLN:NE2	12:K:404:HOH:O	2.33	0.42
1:B:244:GLN:NE2	12:B:409:HOH:O	2.52	0.42
1:J:157:ARG:HD2	2:I:168:HIS:NE2	2.35	0.42
1:J:176:LEU:HD12	1:J:176:LEU:HA	1.90	0.42
1:B:134:VAL:HB	1:B:135:PRO:HD3	2.01	0.42
2:K:248:VAL:HG11	2:K:259:ALA:HB2	2.00	0.42
2:G:67:LYS:CE	12:G:406:HOH:O	2.67	0.42
1:H:163:VAL:HG22	2:G:30:ALA:HB1	2.01	0.42
1:L:162:GLY:O	2:K:240:ARG:NH2	2.50	0.42
1:J:90:ALA:O	2:I:32:LYS:HE3	2.19	0.42
1:D:155:TRP:NE1	2:C:177:LEU:HG	2.34	0.42
1:F:129:ALA:O	1:F:131:LEU:CB	2.66	0.41
9:E:301:ATP:N3	9:E:301:ATP:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:TRP:NE1	2:K:177:LEU:HG	2.35	0.41
1:H:165:PRO:O	1:H:168:ARG:NH1	2.43	0.41
1:B:76:THR:HG21	1:B:111:ALA:HA	2.02	0.41
2:G:67:LYS:HB3	2:G:67:LYS:HE3	1.82	0.41
1:H:51:ARG:NH1	2:G:6:ASN:O	2.46	0.41
1:J:118:LEU:HB3	1:J:123:ILE:HB	2.02	0.41
1:H:155:TRP:NE1	2:G:177:LEU:HG	2.36	0.41
1:J:67:ARG:HD3	1:J:141:VAL:O	2.20	0.41
2:E:59:LEU:HB2	2:E:60:PRO:HD3	2.02	0.41
1:F:176:LEU:HA	1:F:176:LEU:HD12	1.69	0.41
1:H:118:LEU:HB3	1:H:123:ILE:HB	2.02	0.41
1:L:12:LEU:HD23	1:L:22:LEU:HD11	2.03	0.41
1:B:130:GLY:HA3	1:B:180:PHE:CD2	2.56	0.41
1:H:128:GLY:N	5:H:303:8M0:O18	2.53	0.41
1:J:39:THR:HG23	1:J:184:GLN:HB3	2.01	0.41
2:E:145[B]:ARG:NH1	2:K:145[B]:ARG:HH12	2.17	0.41
1:L:213:VAL:HG13	1:L:231:LEU:HB3	2.02	0.41
1:D:130:GLY:HA3	1:D:180:PHE:CZ	2.55	0.40
2:I:219:LEU:O	2:I:222:SER:HB3	2.20	0.40
3:B:301:ADP:H8	2:A:19:THR:HG21	1.85	0.40
1:B:200:LYS:NZ	3:B:301:ADP:O3'	2.53	0.40
1:L:118:LEU:HD22	1:L:123:ILE:HD12	2.03	0.40
1:L:4:SER:OG	1:L:7:GLU:HB2	2.21	0.40
1:D:76:THR:HG21	1:D:111:ALA:HA	2.03	0.40
1:F:203:LYS:HD2	1:F:203:LYS:H	1.85	0.40
2:A:63:GLU:O	2:A:67:LYS:HG3	2.22	0.40
2:C:248:VAL:HG11	2:C:259:ALA:HB2	2.02	0.40
2:I:248:VAL:HG11	2:I:259:ALA:HB2	2.04	0.40
1:H:131:LEU:HD21	1:L:125:VAL:H	1.87	0.40
1:F:203:LYS:N	1:F:203:LYS:CD	2.84	0.40
1:F:40:VAL:HB	1:F:177:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	271/269 (101%)	257 (95%)	12 (4%)	2 (1%)	22	8
1	D	270/269 (100%)	256 (95%)	12 (4%)	2 (1%)	22	8
1	F	271/269 (101%)	256 (94%)	13 (5%)	2 (1%)	22	8
1	H	269/269 (100%)	258 (96%)	11 (4%)	0	100	100
1	J	271/269 (101%)	259 (96%)	12 (4%)	0	100	100
1	L	271/269 (101%)	261 (96%)	9 (3%)	1 (0%)	34	18
2	A	272/275 (99%)	265 (97%)	7 (3%)	0	100	100
2	C	271/275 (98%)	263 (97%)	8 (3%)	0	100	100
2	E	272/275 (99%)	264 (97%)	8 (3%)	0	100	100
2	G	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	I	272/275 (99%)	262 (96%)	10 (4%)	0	100	100
2	K	275/275 (100%)	266 (97%)	8 (3%)	1 (0%)	34	18
All	All	3258/3264 (100%)	3131 (96%)	119 (4%)	8 (0%)	47	30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	SER
1	F	130	GLY
2	K	274	ARG
1	D	128	GLY
1	F	132	SER
1	L	129	ALA
1	B	128	GLY
1	D	129	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	210/205 (102%)	208 (99%)	2 (1%)	76	67
1	D	209/205 (102%)	208 (100%)	1 (0%)	88	83
1	F	209/205 (102%)	207 (99%)	2 (1%)	76	67
1	H	208/205 (102%)	206 (99%)	2 (1%)	76	67
1	J	210/205 (102%)	208 (99%)	2 (1%)	76	67
1	L	210/205 (102%)	209 (100%)	1 (0%)	88	83
2	A	213/215 (99%)	212 (100%)	1 (0%)	88	83
2	C	213/215 (99%)	212 (100%)	1 (0%)	88	83
2	E	214/215 (100%)	213 (100%)	1 (0%)	88	83
2	G	215/215 (100%)	213 (99%)	2 (1%)	78	70
2	I	214/215 (100%)	210 (98%)	4 (2%)	57	41
2	K	217/215 (101%)	215 (99%)	2 (1%)	78	70
All	All	2542/2520 (101%)	2521 (99%)	21 (1%)	81	74

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	GLU
1	B	67	ARG
2	A	274	ARG
1	D	67	ARG
2	C	205	ARG
1	F	3	ASN
1	F	67	ARG
2	E	205	ARG
1	H	67	ARG
1	H	219	LYS
2	G	23	ARG
2	G	205	ARG
1	J	10	GLU
1	J	67	ARG
2	I	32	LYS
2	I	222	SER
2	I	274	ARG
2	I	275	PRO
1	L	67	ARG
2	K	32	LYS
2	K	207	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	ASN
1	B	184	GLN
2	A	157	HIS
1	D	3	ASN
1	D	184	GLN
1	D	262	HIS
2	C	157	HIS
2	C	207	GLN
1	F	14	GLN
1	F	238	GLN
2	E	18	GLN
1	H	21	GLN
1	J	70	HIS
1	J	184	GLN
2	I	207	GLN
2	K	6	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 12 are monoatomic - leaving 42 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	8M0	L	303	-	22,48,48	7.79	11 (50%)	-		
3	ADP	D	301	4	24,29,29	0.99	2 (8%)	29,45,45	1.47	5 (17%)
6	MOO	D	303[A]	-	2,4,4	1.28	0	-		
9	ATP	E	301	4	26,33,33	0.92	2 (7%)	31,52,52	1.63	6 (19%)
5	8M0	K	303	-	14,46,48	8.36	9 (64%)	-		
3	ADP	J	301	4	24,29,29	0.97	2 (8%)	29,45,45	1.49	5 (17%)
3	ADP	F	301	4	24,29,29	0.97	2 (8%)	29,45,45	1.54	5 (17%)
6	MOO	L	304[A]	-	2,4,4	1.24	0	-		
10	M10	G	304	-	1,15,18	164.77	1 (100%)	-		
8	LJB	B	306	-	26,44,44	8.21	4 (15%)	-		
5	8M0	C	301	-	22,48,48	8.08	12 (54%)	-		
3	ADP	B	301	4	24,29,29	1.00	2 (8%)	29,45,45	1.52	5 (17%)
9	ATP	A	301	4	26,33,33	0.91	2 (7%)	31,52,52	1.62	5 (16%)
5	8M0	B	303	-	22,48,48	8.12	12 (54%)	-		
7	PO4	J	305[B]	-	4,4,4	0.87	0	6,6,6	0.47	0
11	LHW	C	305	-	24,59,59	1.19	2 (8%)	-		
9	ATP	G	301	4	26,33,33	0.91	2 (7%)	31,52,52	1.66	6 (19%)
5	8M0	F	303	-	22,48,48	8.20	12 (54%)	-		
5	8M0	E	303	-	14,46,48	8.28	9 (64%)	-		
5	8M0	J	302	-	22,48,48	8.07	12 (54%)	-		
6	MOO	H	304[A]	-	2,4,4	1.27	0	-		
5	8M0	A	303	-	14,46,48	8.32	9 (64%)	-		
9	ATP	C	302	4	26,33,33	0.91	2 (7%)	31,52,52	1.58	6 (19%)
10	M10	A	304	-	3,15,18	6.97	3 (100%)	-		
11	LHW	K	304	-	24,59,59	1.07	2 (8%)	-		
5	8M0	G	303	-	14,46,48	8.25	9 (64%)	-		
5	8M0	C	304	-	14,46,48	7.98	9 (64%)	-		
7	PO4	H	305[B]	4	4,4,4	0.93	0	6,6,6	0.43	0
5	8M0	H	303	-	22,48,48	8.20	12 (54%)	-		
8	LJB	L	306	-	26,44,44	7.55	4 (15%)	-		
7	PO4	L	305[B]	4	4,4,4	0.94	0	6,6,6	0.45	0
5	8M0	I	303	-	14,46,48	8.37	9 (64%)	-		
3	ADP	L	301	4	24,29,29	0.97	2 (8%)	29,45,45	1.50	5 (17%)
7	PO4	D	304[B]	4	4,4,4	0.93	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MOO	J	304[A]	-	2,4,4	1.23	0	-		
7	PO4	F	305[B]	4	4,4,4	0.92	0	6,6,6	0.42	0
3	ADP	H	301	4	24,29,29	1.00	2 (8%)	29,45,45	1.54	5 (17%)
9	ATP	K	301	4	26,33,33	0.93	2 (7%)	31,52,52	1.62	5 (16%)
6	MOO	F	304[A]	-	2,4,4	1.32	0	-		
6	MOO	B	304[A]	-	2,4,4	1.28	0	-		
7	PO4	B	305[B]	4	4,4,4	0.93	0	6,6,6	0.46	0
9	ATP	I	301	4	26,33,33	0.95	2 (7%)	31,52,52	1.64	6 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	301	4	-	3/12/32/32	0/3/3/3
9	ATP	G	301	4	-	2/18/38/38	0/3/3/3
3	ADP	B	301	4	-	2/12/32/32	0/3/3/3
9	ATP	E	301	4	-	0/18/38/38	0/3/3/3
9	ATP	A	301	4	-	0/18/38/38	0/3/3/3
3	ADP	L	301	4	-	2/12/32/32	0/3/3/3
3	ADP	J	301	4	-	3/12/32/32	0/3/3/3
3	ADP	H	301	4	-	3/12/32/32	0/3/3/3
9	ATP	K	301	4	-	0/18/38/38	0/3/3/3
3	ADP	F	301	4	-	3/12/32/32	0/3/3/3
9	ATP	I	301	4	-	0/18/38/38	0/3/3/3
9	ATP	C	302	4	-	3/18/38/38	0/3/3/3
10	M10	G	304	-	-	-	0/3/3/3
10	M10	A	304	-	-	-	0/3/3/3

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	304	M10	O11-MO3	164.77	4.06	1.69
8	B	306	LJB	O24-MO8	30.05	2.24	1.80
8	B	306	LJB	O14-MO8	28.81	2.22	1.80
8	L	306	LJB	O14-MO8	27.82	2.20	1.80
8	L	306	LJB	O24-MO8	26.28	2.18	1.80
5	J	302	8M0	O7-MO4	18.93	1.92	1.74
5	H	303	8M0	O7-MO4	18.39	1.92	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	303	8M0	O7-MO4	18.27	1.92	1.74
5	B	303	8M0	O7-MO4	18.19	1.92	1.74
5	C	301	8M0	O7-MO4	17.57	1.91	1.74
5	L	303	8M0	O7-MO4	17.47	1.91	1.74
5	L	303	8M0	O20-MO8	16.94	1.90	1.74
5	K	303	8M0	O7-MO4	16.93	1.90	1.74
5	F	303	8M0	O20-MO8	16.75	1.90	1.74
5	H	303	8M0	O20-MO8	16.74	1.90	1.74
5	E	303	8M0	O7-MO4	16.70	1.90	1.74
5	C	301	8M0	O20-MO8	16.54	1.90	1.74
5	I	303	8M0	O7-MO4	16.46	1.90	1.74
5	I	303	8M0	O20-MO8	16.42	1.90	1.74
5	B	303	8M0	O20-MO8	16.35	1.90	1.74
5	A	303	8M0	O7-MO4	16.31	1.90	1.74
5	G	303	8M0	O7-MO4	16.30	1.90	1.74
5	A	303	8M0	O20-MO8	16.26	1.90	1.74
5	C	304	8M0	O20-MO8	15.91	1.89	1.74
5	K	303	8M0	O20-MO8	15.80	1.89	1.74
5	B	303	8M0	O9-MO3	15.68	1.90	1.71
5	J	302	8M0	O9-MO3	15.64	1.90	1.71
5	F	303	8M0	O9-MO3	15.63	1.90	1.71
5	C	301	8M0	O9-MO3	15.63	1.90	1.71
5	H	303	8M0	O9-MO3	15.61	1.90	1.71
5	G	303	8M0	O20-MO8	15.60	1.89	1.74
5	E	303	8M0	O20-MO8	15.54	1.89	1.74
5	J	302	8M0	O20-MO8	15.13	1.89	1.74
5	L	303	8M0	O9-MO3	14.07	1.88	1.71
5	C	304	8M0	O7-MO4	14.04	1.88	1.74
5	F	303	8M0	O10-MO3	12.86	1.87	1.71
5	B	303	8M0	O10-MO3	12.75	1.87	1.71
5	C	301	8M0	O10-MO3	12.70	1.87	1.71
5	H	303	8M0	O10-MO3	12.69	1.87	1.71
5	J	302	8M0	O10-MO3	12.65	1.87	1.71
5	C	304	8M0	O23-MO7	11.52	1.88	1.68
5	L	303	8M0	O10-MO3	11.47	1.85	1.71
10	A	304	M10	O4-MO3	11.39	2.37	2.00
5	K	303	8M0	O23-MO7	11.37	1.88	1.68
5	B	303	8M0	O23-MO7	11.37	1.88	1.68
5	E	303	8M0	O23-MO7	11.34	1.88	1.68
5	F	303	8M0	O23-MO7	11.33	1.88	1.68
5	C	301	8M0	O23-MO7	11.31	1.88	1.68
5	H	303	8M0	O23-MO7	11.29	1.88	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	303	8M0	O23-MO7	11.27	1.88	1.68
5	G	303	8M0	O23-MO7	11.25	1.88	1.68
5	I	303	8M0	O23-MO7	11.24	1.88	1.68
5	J	302	8M0	O23-MO7	11.23	1.88	1.68
5	I	303	8M0	O9-MO3	10.83	1.91	1.67
5	G	303	8M0	O9-MO3	10.77	1.90	1.67
5	C	304	8M0	O9-MO3	10.74	1.90	1.67
5	A	303	8M0	O9-MO3	10.73	1.90	1.67
5	E	303	8M0	O9-MO3	10.70	1.90	1.67
5	K	303	8M0	O9-MO3	10.66	1.90	1.67
5	K	303	8M0	O1-MO1	10.42	1.86	1.68
5	C	301	8M0	O1-MO1	10.41	1.86	1.68
5	H	303	8M0	O1-MO1	10.33	1.86	1.68
5	F	303	8M0	O1-MO1	10.32	1.86	1.68
5	B	303	8M0	O1-MO1	10.31	1.86	1.68
5	J	302	8M0	O1-MO1	10.30	1.86	1.68
5	G	303	8M0	O1-MO1	10.27	1.86	1.68
5	L	303	8M0	O23-MO7	10.22	1.86	1.68
5	A	303	8M0	O1-MO1	10.21	1.86	1.68
5	I	303	8M0	O1-MO1	10.17	1.86	1.68
5	E	303	8M0	O1-MO1	10.16	1.86	1.68
5	C	304	8M0	O1-MO1	10.14	1.86	1.68
5	L	303	8M0	O1-MO1	10.04	1.86	1.68
5	L	303	8M0	O18-MO6	9.02	1.84	1.68
5	C	301	8M0	O28-MO5	8.40	1.81	1.71
5	B	303	8M0	O28-MO5	8.35	1.81	1.71
5	H	303	8M0	O28-MO5	8.34	1.81	1.71
5	F	303	8M0	O28-MO5	8.32	1.81	1.71
5	J	302	8M0	O28-MO5	8.29	1.81	1.71
5	L	303	8M0	O28-MO5	7.80	1.81	1.71
5	H	303	8M0	O18-MO6	7.09	1.80	1.68
5	B	303	8M0	O18-MO6	7.03	1.80	1.68
5	G	303	8M0	O18-MO6	7.03	1.80	1.68
5	E	303	8M0	O18-MO6	7.01	1.80	1.68
5	J	302	8M0	O18-MO6	7.01	1.80	1.68
5	C	301	8M0	O18-MO6	6.99	1.80	1.68
5	I	303	8M0	O18-MO6	6.98	1.80	1.68
5	C	304	8M0	O18-MO6	6.93	1.80	1.68
5	K	303	8M0	O18-MO6	6.91	1.80	1.68
5	A	303	8M0	O18-MO6	6.90	1.80	1.68
5	F	303	8M0	O26-MO4	6.55	2.22	1.88
5	F	303	8M0	O18-MO6	6.55	1.79	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	303	8M0	O26-MO4	6.13	2.20	1.88
5	B	303	8M0	O26-MO4	6.05	2.19	1.88
5	C	301	8M0	O26-MO4	6.04	2.19	1.88
5	J	302	8M0	O26-MO4	5.63	2.17	1.88
5	L	303	8M0	O26-MO4	5.53	2.16	1.88
5	F	303	8M0	O25-MO8	5.22	2.15	1.88
5	H	303	8M0	O25-MO8	5.11	2.14	1.88
5	C	301	8M0	O25-MO8	5.09	2.14	1.88
5	B	303	8M0	O25-MO8	5.09	2.14	1.88
5	J	302	8M0	O25-MO8	4.98	2.14	1.88
5	L	303	8M0	O25-MO8	4.84	2.13	1.88
5	H	303	8M0	O13-MO5	4.73	1.77	1.71
5	F	303	8M0	O13-MO5	4.69	1.77	1.71
11	C	305	LHW	O92-MOA	-4.66	1.86	2.26
5	J	302	8M0	O13-MO5	4.65	1.77	1.71
5	G	303	8M0	O13-MO5	4.51	1.77	1.67
5	I	303	8M0	O13-MO5	4.51	1.77	1.67
5	K	303	8M0	O13-MO5	4.50	1.77	1.67
5	A	303	8M0	O13-MO5	4.49	1.77	1.67
5	E	303	8M0	O13-MO5	4.48	1.77	1.67
5	C	304	8M0	O13-MO5	4.46	1.77	1.67
11	K	304	LHW	O92-MOA	-4.15	1.91	2.26
5	C	301	8M0	O13-MO5	3.93	1.76	1.71
5	G	303	8M0	O8-MO2	3.60	1.74	1.68
5	I	303	8M0	O8-MO2	3.59	1.74	1.68
5	K	303	8M0	O8-MO2	3.55	1.74	1.68
5	E	303	8M0	O8-MO2	3.55	1.74	1.68
5	B	303	8M0	O13-MO5	3.54	1.75	1.71
5	A	303	8M0	O8-MO2	3.54	1.74	1.68
5	C	304	8M0	O8-MO2	3.51	1.74	1.68
5	J	302	8M0	O8-MO2	3.47	1.74	1.68
5	F	303	8M0	O8-MO2	3.46	1.74	1.68
5	H	303	8M0	O8-MO2	3.45	1.74	1.68
5	B	303	8M0	O8-MO2	3.43	1.74	1.68
5	C	301	8M0	O8-MO2	3.37	1.74	1.68
5	L	303	8M0	O13-MO5	3.12	1.75	1.71
5	G	303	8M0	O3-MO3	3.09	2.01	1.89
5	C	304	8M0	O3-MO3	3.08	2.01	1.89
5	I	303	8M0	O3-MO3	3.03	2.00	1.89
5	A	303	8M0	O3-MO3	3.00	2.00	1.89
3	B	301	ADP	O4'-C1'	2.96	1.45	1.41
5	E	303	8M0	O3-MO3	2.95	2.00	1.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	304	M10	O12-MO3	2.89	2.03	1.92
8	B	306	LJB	O53-MO5	-2.89	2.01	2.26
3	H	301	ADP	O4'-C1'	2.88	1.45	1.41
5	K	303	8M0	O3-MO3	2.87	2.00	1.89
3	D	301	ADP	O4'-C1'	2.84	1.45	1.41
8	L	306	LJB	O53-MO5	-2.79	2.02	2.26
10	A	304	M10	O9-MO3	2.77	2.03	1.92
3	L	301	ADP	O4'-C1'	2.77	1.44	1.41
3	J	301	ADP	O4'-C1'	2.75	1.44	1.41
3	F	301	ADP	O4'-C1'	2.69	1.44	1.41
11	C	305	LHW	O92-MO8	-2.66	2.03	2.26
9	I	301	ATP	O4'-C1'	2.63	1.44	1.41
8	L	306	LJB	O53-MO6	-2.59	2.04	2.26
9	E	301	ATP	O4'-C1'	2.57	1.44	1.41
9	G	301	ATP	O4'-C1'	2.47	1.44	1.41
9	K	301	ATP	O4'-C1'	2.46	1.44	1.41
8	B	306	LJB	O53-MO6	-2.45	2.05	2.26
9	A	301	ATP	O4'-C1'	2.34	1.44	1.41
9	C	302	ATP	O4'-C1'	2.29	1.44	1.41
3	B	301	ADP	C5-C4	2.28	1.47	1.40
11	K	304	LHW	O92-MO8	-2.27	2.07	2.26
3	L	301	ADP	C5-C4	2.27	1.46	1.40
9	I	301	ATP	C5-C4	2.24	1.46	1.40
9	K	301	ATP	C5-C4	2.24	1.46	1.40
3	H	301	ADP	C5-C4	2.24	1.46	1.40
3	F	301	ADP	C5-C4	2.24	1.46	1.40
9	C	302	ATP	C5-C4	2.24	1.46	1.40
3	J	301	ADP	C5-C4	2.22	1.46	1.40
3	D	301	ADP	C5-C4	2.21	1.46	1.40
9	A	301	ATP	C5-C4	2.20	1.46	1.40
9	E	301	ATP	C5-C4	2.20	1.46	1.40
9	G	301	ATP	C5-C4	2.16	1.46	1.40

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	301	ATP	C3'-C2'-C1'	4.67	108.01	100.98
9	C	302	ATP	C3'-C2'-C1'	4.59	107.89	100.98
9	G	301	ATP	C3'-C2'-C1'	4.59	107.89	100.98
9	K	301	ATP	C3'-C2'-C1'	4.53	107.80	100.98
9	I	301	ATP	C3'-C2'-C1'	4.51	107.76	100.98
9	E	301	ATP	C3'-C2'-C1'	4.45	107.67	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	ADP	C3'-C2'-C1'	4.10	107.14	100.98
9	E	301	ATP	N3-C2-N1	-4.08	122.30	128.68
9	I	301	ATP	N3-C2-N1	-4.05	122.34	128.68
9	G	301	ATP	N3-C2-N1	-4.04	122.36	128.68
3	F	301	ADP	C3'-C2'-C1'	3.95	106.93	100.98
3	F	301	ADP	N3-C2-N1	-3.95	122.50	128.68
9	K	301	ATP	N3-C2-N1	-3.95	122.50	128.68
3	J	301	ADP	N3-C2-N1	-3.94	122.51	128.68
3	H	301	ADP	N3-C2-N1	-3.91	122.56	128.68
9	C	302	ATP	N3-C2-N1	-3.91	122.57	128.68
3	D	301	ADP	N3-C2-N1	-3.88	122.61	128.68
3	B	301	ADP	N3-C2-N1	-3.88	122.62	128.68
3	L	301	ADP	N3-C2-N1	-3.87	122.63	128.68
3	J	301	ADP	C3'-C2'-C1'	3.86	106.79	100.98
3	L	301	ADP	C3'-C2'-C1'	3.86	106.78	100.98
9	A	301	ATP	N3-C2-N1	-3.82	122.70	128.68
3	D	301	ADP	C3'-C2'-C1'	3.67	106.51	100.98
3	H	301	ADP	C3'-C2'-C1'	3.64	106.46	100.98
3	H	301	ADP	PA-O3A-PB	-2.91	122.84	132.83
9	I	301	ATP	PA-O3A-PB	-2.87	122.99	132.83
9	G	301	ATP	PA-O3A-PB	-2.74	123.41	132.83
9	K	301	ATP	PA-O3A-PB	-2.70	123.56	132.83
9	E	301	ATP	PA-O3A-PB	-2.65	123.72	132.83
9	I	301	ATP	C4-C5-N7	-2.57	106.72	109.40
9	E	301	ATP	PB-O3B-PG	-2.52	124.17	132.83
9	G	301	ATP	C4-C5-N7	-2.52	106.77	109.40
9	G	301	ATP	PB-O3B-PG	-2.51	124.20	132.83
3	F	301	ADP	PA-O3A-PB	-2.51	124.22	132.83
9	I	301	ATP	PB-O3B-PG	-2.50	124.24	132.83
9	E	301	ATP	C4-C5-N7	-2.46	106.83	109.40
9	K	301	ATP	C4-C5-N7	-2.44	106.86	109.40
3	L	301	ADP	PA-O3A-PB	-2.43	124.47	132.83
9	A	301	ATP	C4-C5-N7	-2.43	106.86	109.40
3	J	301	ADP	PA-O3A-PB	-2.42	124.51	132.83
3	D	301	ADP	PA-O3A-PB	-2.41	124.56	132.83
9	A	301	ATP	PA-O3A-PB	-2.39	124.62	132.83
9	C	302	ATP	C4-C5-N7	-2.35	106.95	109.40
9	K	301	ATP	PB-O3B-PG	-2.34	124.79	132.83
9	A	301	ATP	PB-O3B-PG	-2.33	124.85	132.83
3	H	301	ADP	C4-C5-N7	-2.31	106.99	109.40
3	D	301	ADP	C4-C5-N7	-2.30	107.00	109.40
3	J	301	ADP	C4-C5-N7	-2.28	107.03	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	ADP	C4-C5-N7	-2.22	107.08	109.40
3	B	301	ADP	C4-C5-N7	-2.18	107.12	109.40
3	F	301	ADP	C2-N1-C6	2.16	122.45	118.75
3	L	301	ADP	C4-C5-N7	-2.13	107.17	109.40
9	C	302	ATP	PA-O3A-PB	-2.12	125.54	132.83
3	L	301	ADP	C2-N1-C6	2.12	122.38	118.75
9	E	301	ATP	C2-N1-C6	2.10	122.35	118.75
3	B	301	ADP	C2-N1-C6	2.09	122.34	118.75
9	G	301	ATP	C2-N1-C6	2.07	122.30	118.75
9	I	301	ATP	C2-N1-C6	2.07	122.30	118.75
3	J	301	ADP	C2-N1-C6	2.04	122.25	118.75
9	C	302	ATP	PB-O3B-PG	-2.04	125.84	132.83
9	C	302	ATP	C2-N1-C6	2.02	122.21	118.75
3	D	301	ADP	C2-N1-C6	2.01	122.19	118.75
3	B	301	ADP	PA-O3A-PB	-2.01	125.93	132.83
3	H	301	ADP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	301	ADP	C4'-C5'-O5'-PA
3	J	301	ADP	PB-O3A-PA-O1A
3	F	301	ADP	PB-O3A-PA-O2A
3	B	301	ADP	PB-O3A-PA-O2A
3	L	301	ADP	PB-O3A-PA-O2A
3	J	301	ADP	C4'-C5'-O5'-PA
3	F	301	ADP	C4'-C5'-O5'-PA
3	B	301	ADP	C4'-C5'-O5'-PA
3	H	301	ADP	C4'-C5'-O5'-PA
3	L	301	ADP	C4'-C5'-O5'-PA
3	H	301	ADP	PB-O3A-PA-O2A
3	F	301	ADP	PB-O3A-PA-O1A
3	D	301	ADP	PA-O3A-PB-O2B
9	C	302	ATP	C3'-C4'-C5'-O5'
3	D	301	ADP	PB-O3A-PA-O2A
3	J	301	ADP	PB-O3A-PA-O2A
3	H	301	ADP	PB-O3A-PA-O1A
9	G	301	ATP	PA-O3A-PB-O2B
9	G	301	ATP	PB-O3A-PA-O1A
9	C	302	ATP	PA-O3A-PB-O2B
9	C	302	ATP	PB-O3A-PA-O1A

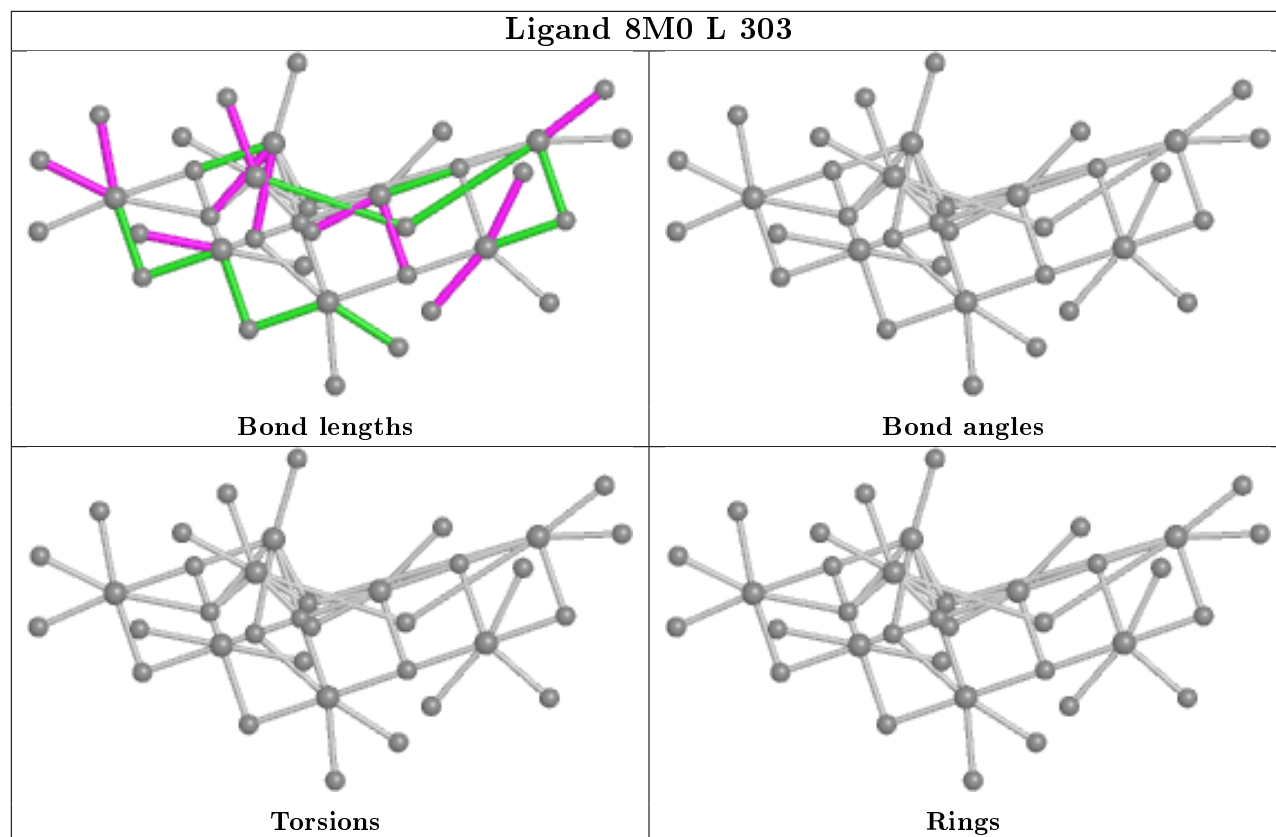
There are no ring outliers.

27 monomers are involved in 73 short contacts:

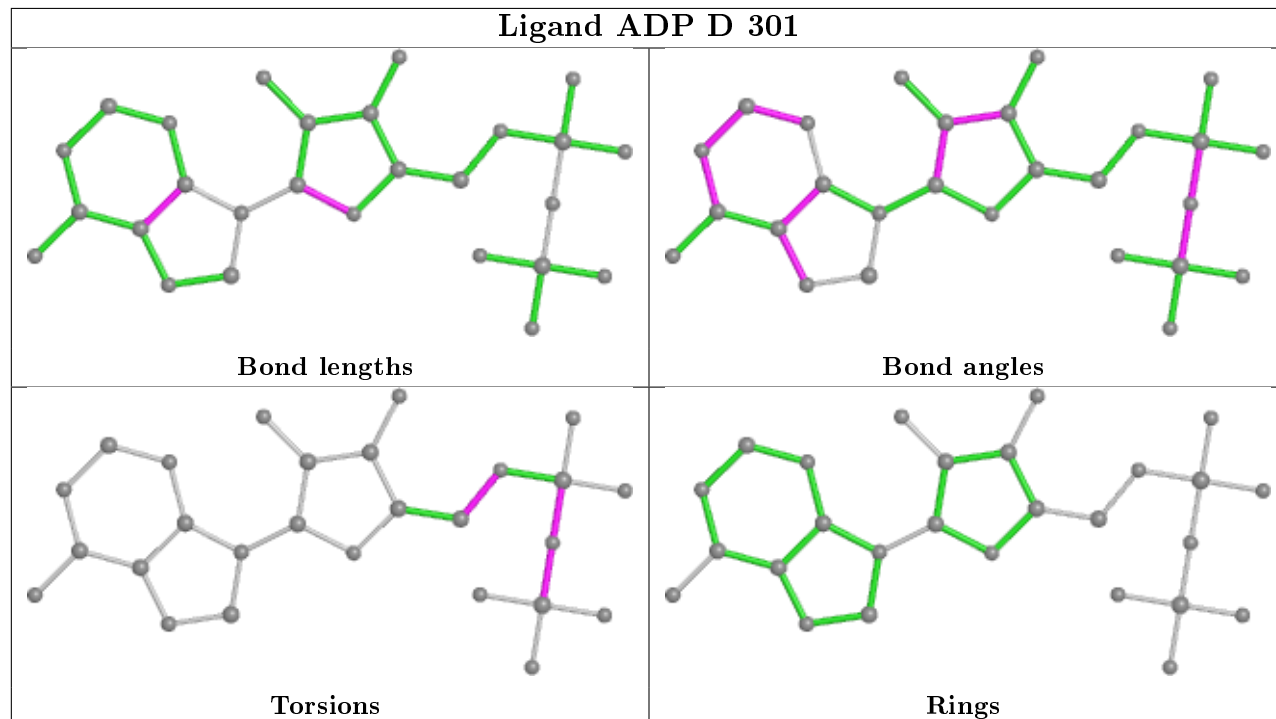
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	303	8M0	7	0
6	D	303[A]	MOO	4	0
9	E	301	ATP	2	0
5	K	303	8M0	2	0
6	L	304[A]	MOO	4	0
10	G	304	M10	3	0
5	C	301	8M0	3	0
3	B	301	ADP	2	0
9	A	301	ATP	1	0
5	B	303	8M0	4	0
9	G	301	ATP	2	0
5	F	303	8M0	6	0
5	E	303	8M0	1	0
5	J	302	8M0	3	0
6	H	304[A]	MOO	4	0
5	A	303	8M0	1	0
9	C	302	ATP	1	0
10	A	304	M10	3	0
5	G	303	8M0	1	0
5	C	304	8M0	1	0
5	H	303	8M0	2	0
5	I	303	8M0	1	0
6	J	304[A]	MOO	4	0
9	K	301	ATP	1	0
6	F	304[A]	MOO	4	0
6	B	304[A]	MOO	4	0
9	I	301	ATP	2	0

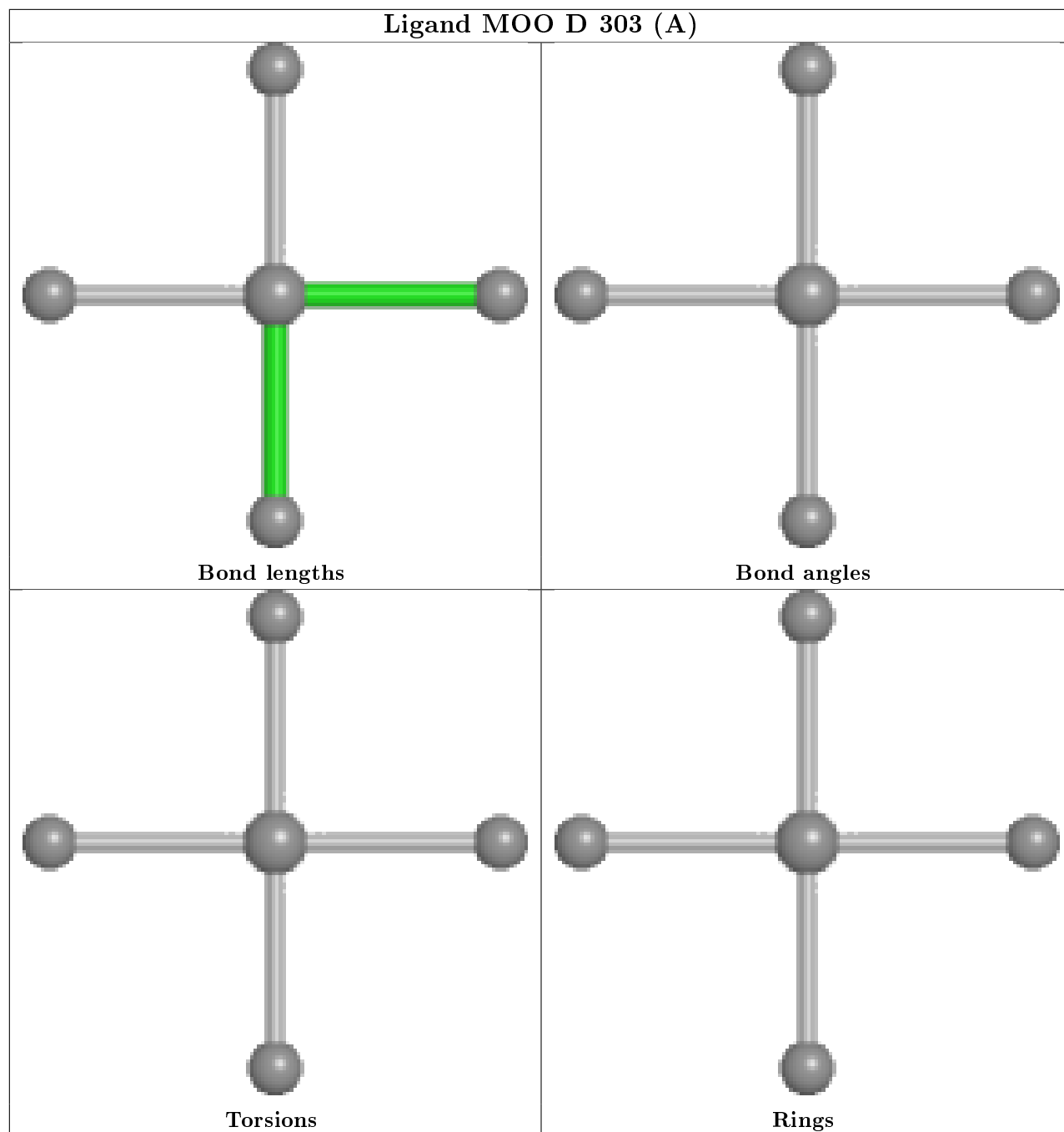
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 8M0 L 303

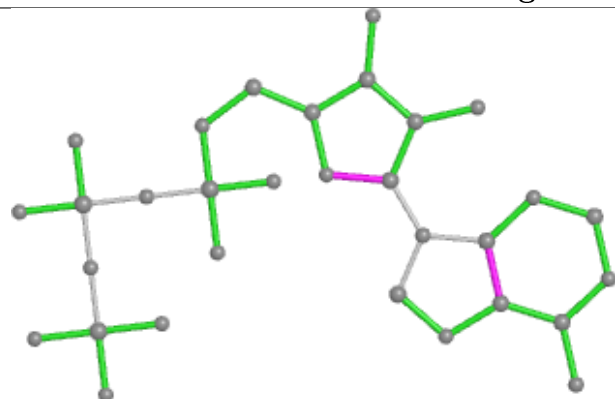


Ligand ADP D 301

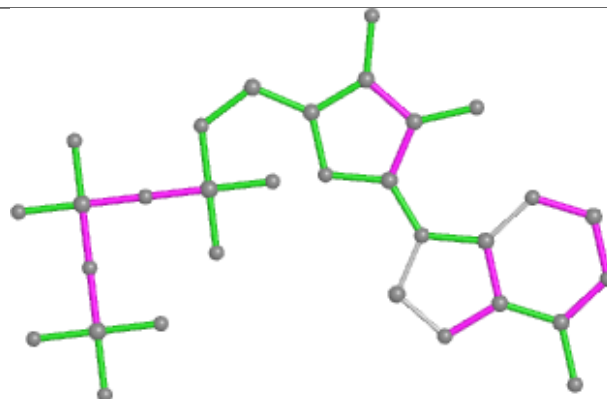




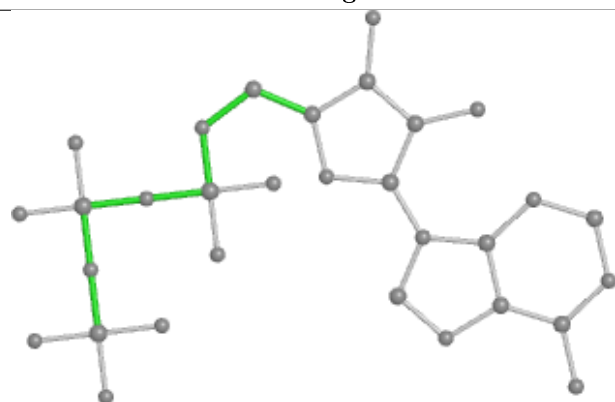
Ligand ATP E 301



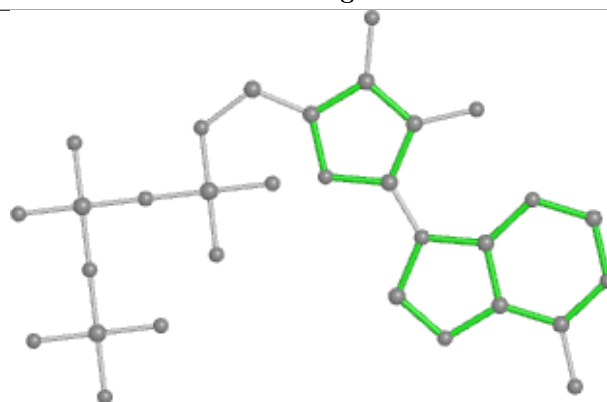
Bond lengths



Bond angles

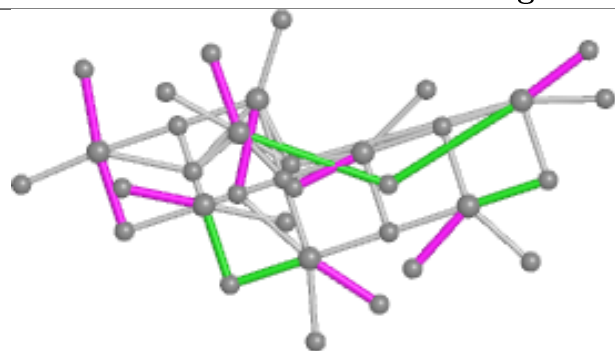


Torsions

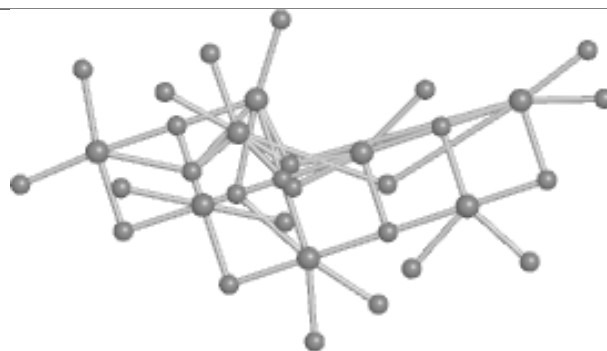


Rings

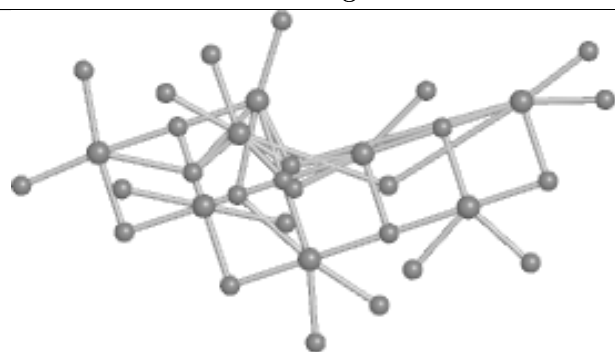
Ligand 8M0 K 303



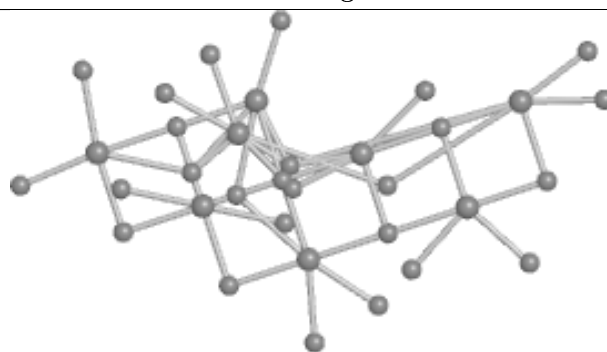
Bond lengths



Bond angles

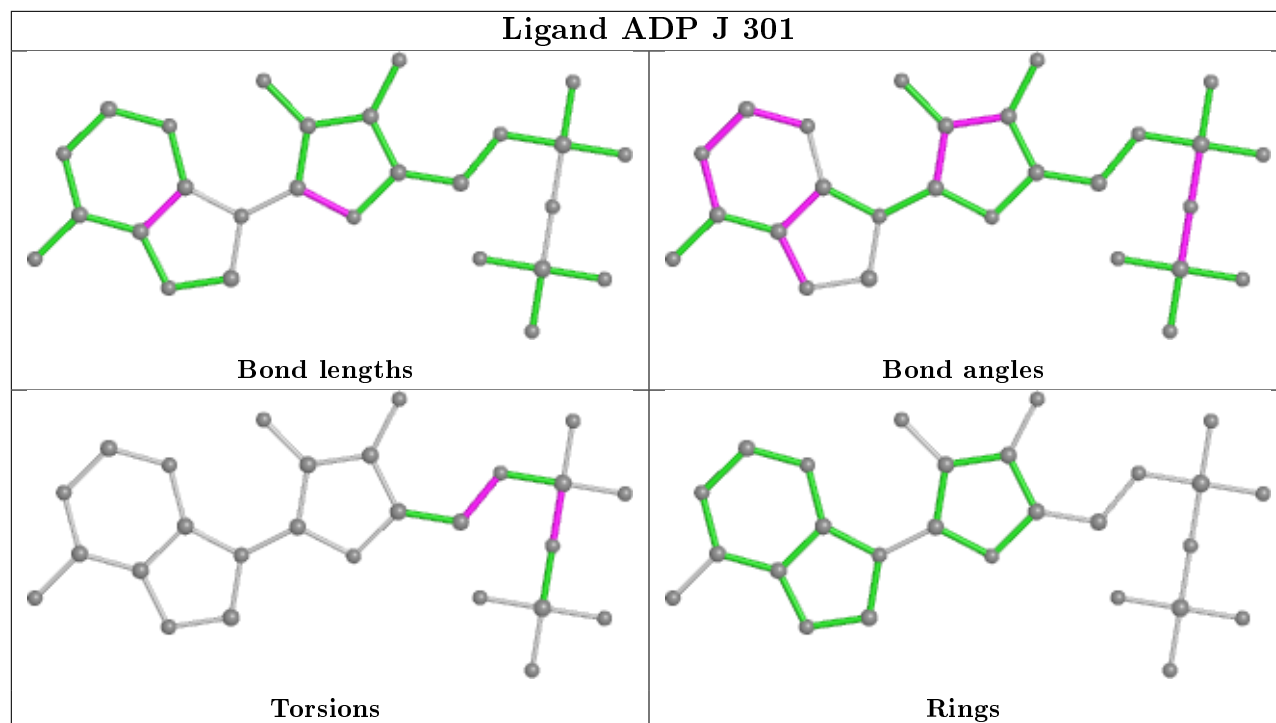


Torsions

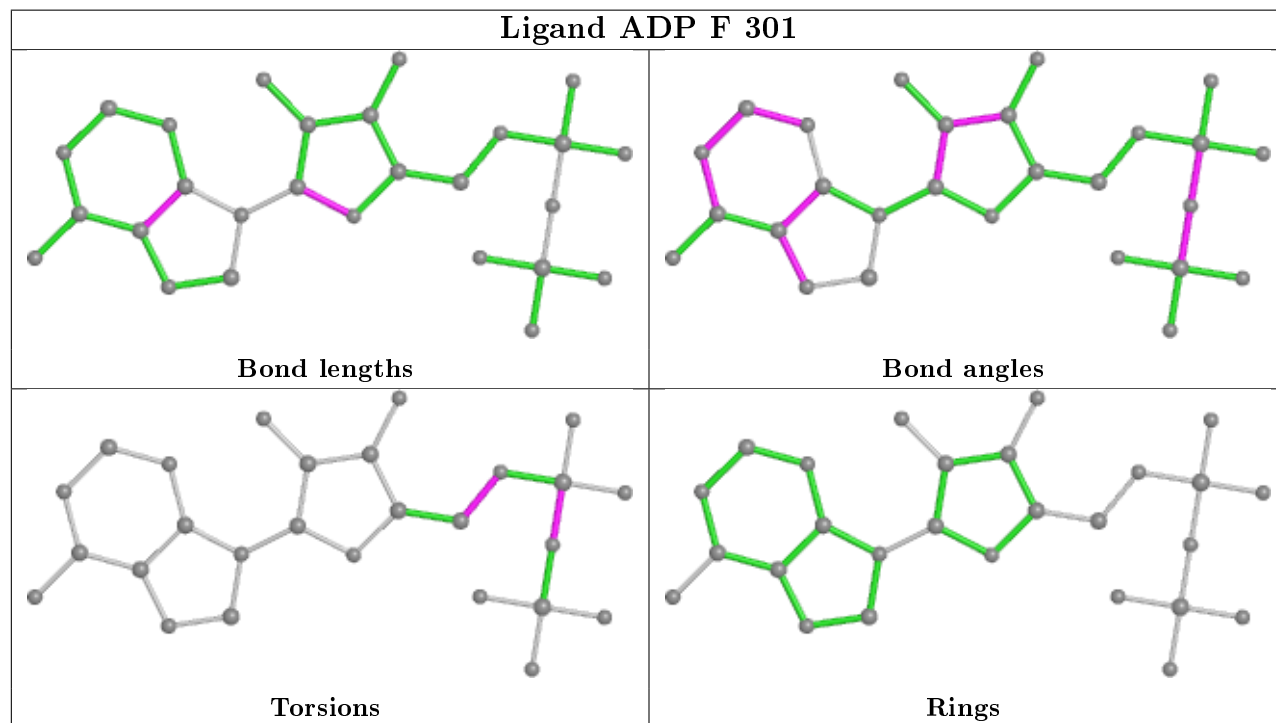


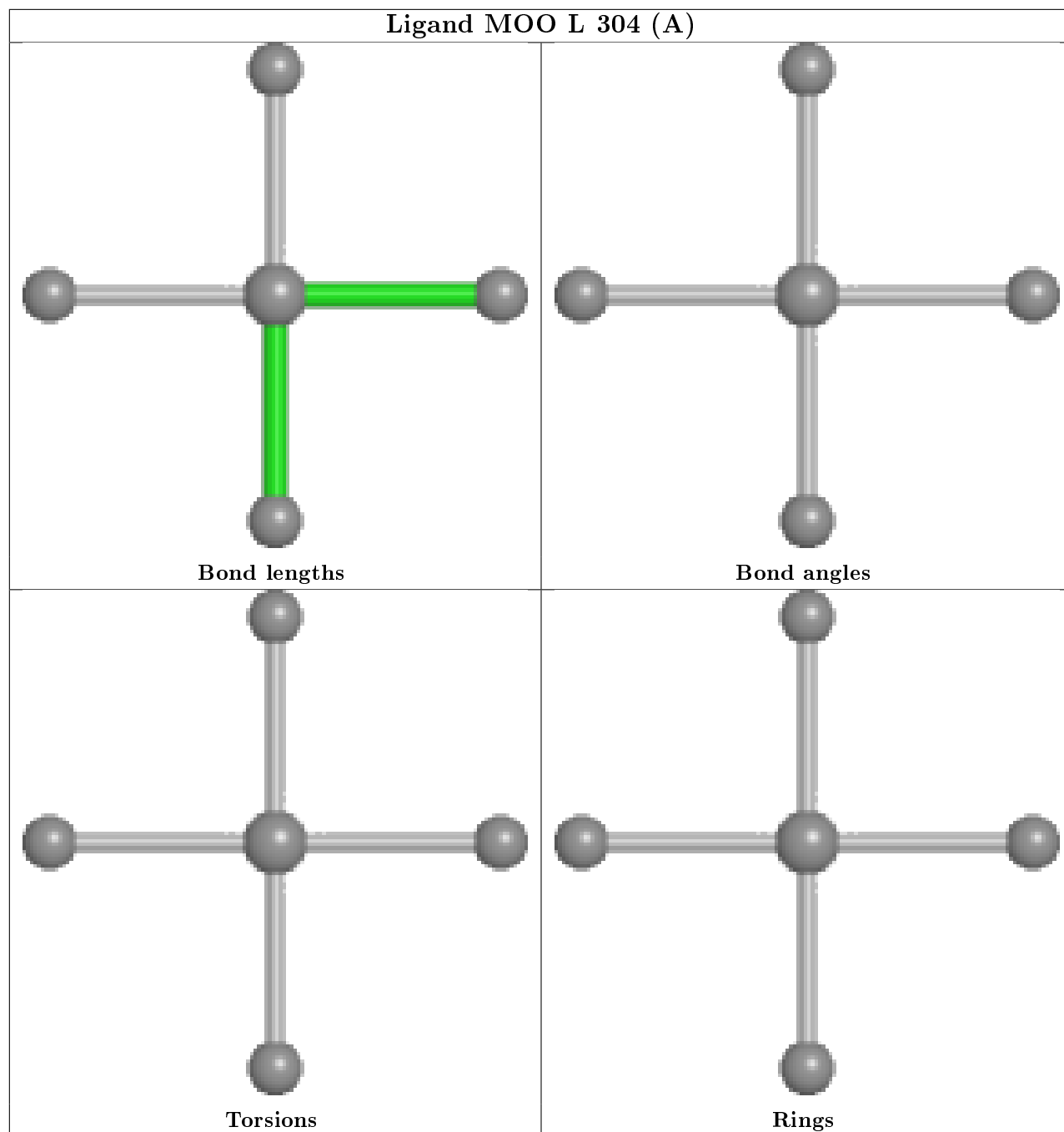
Rings

Ligand ADP J 301

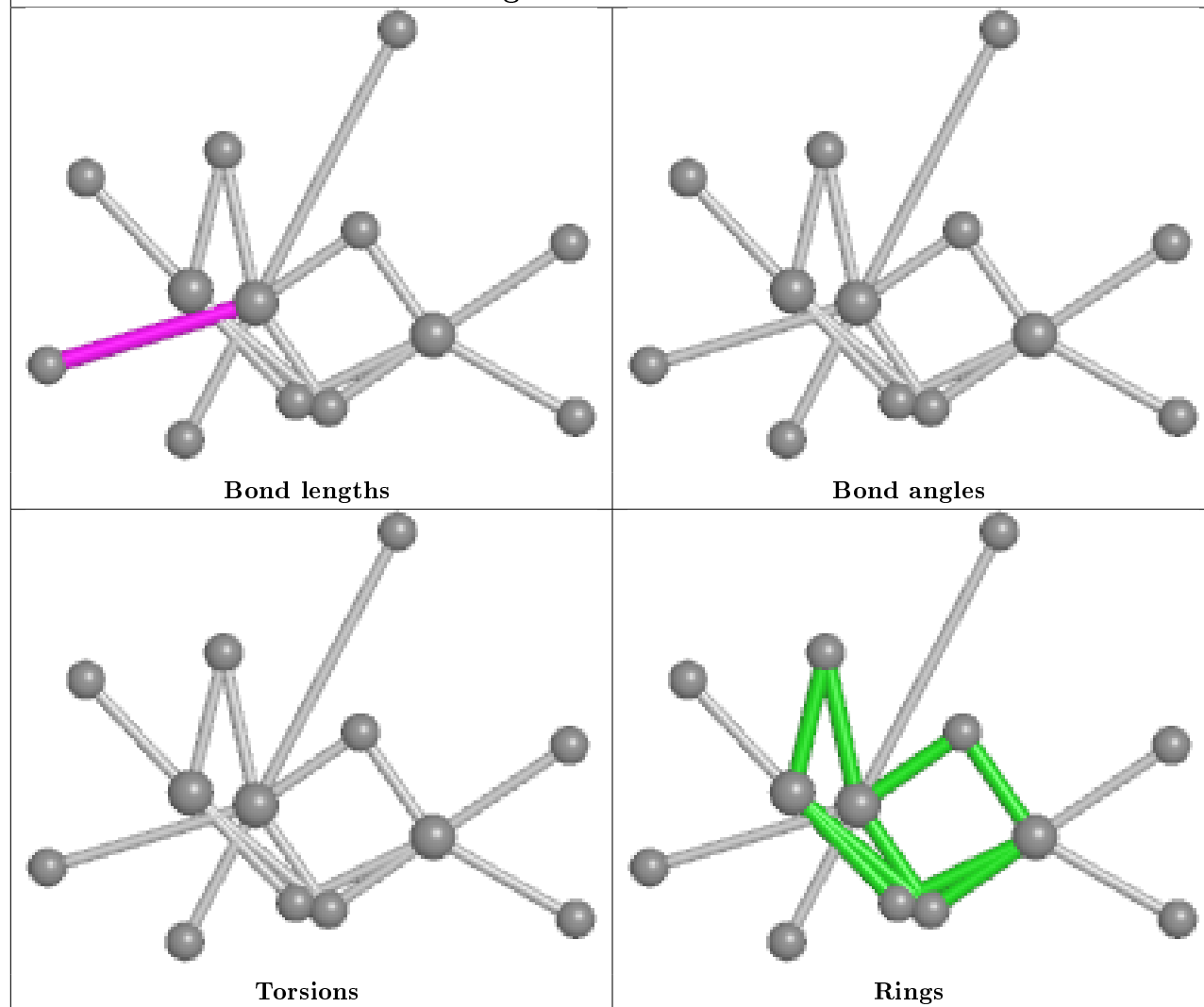


Ligand ADP F 301

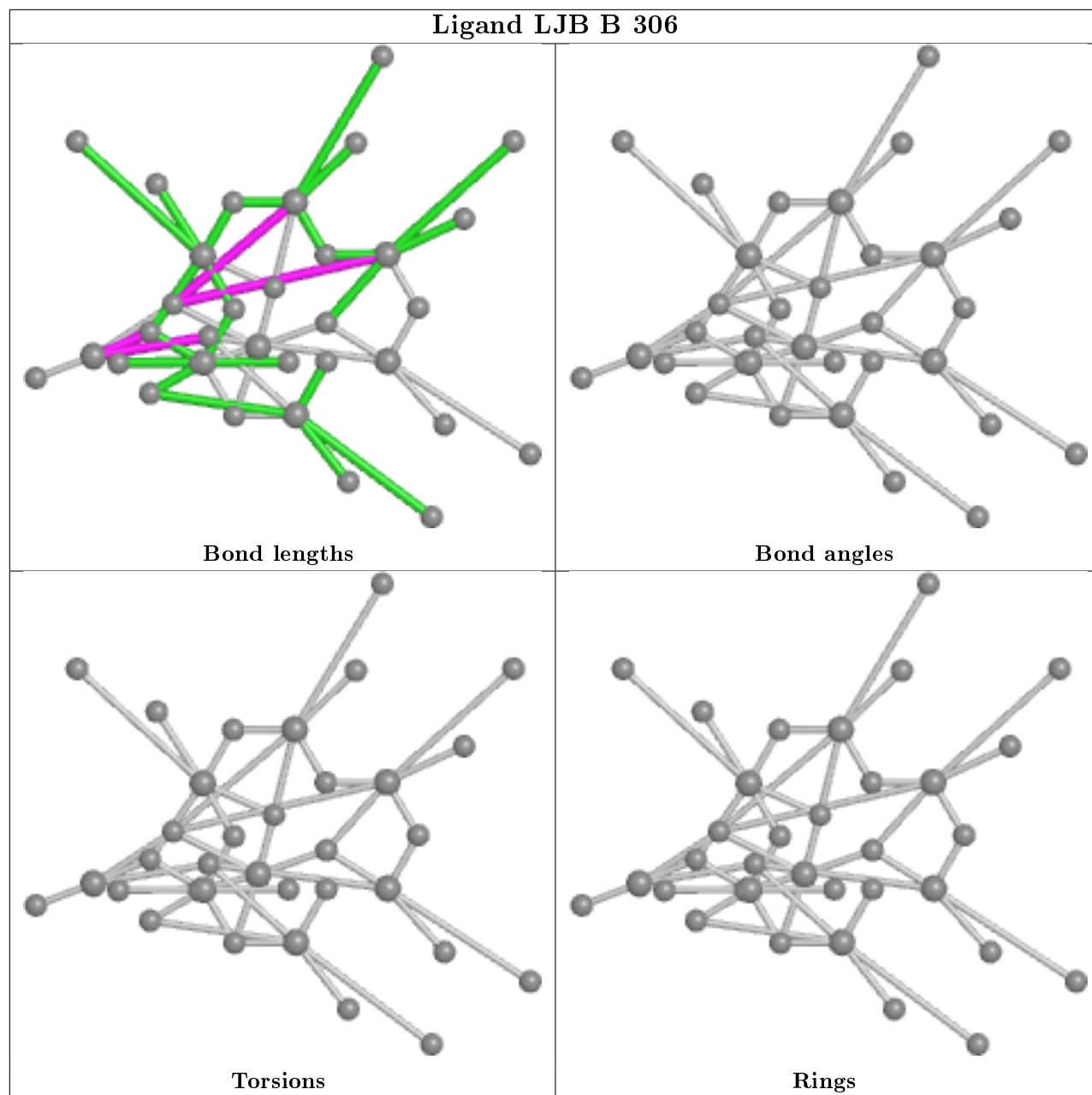




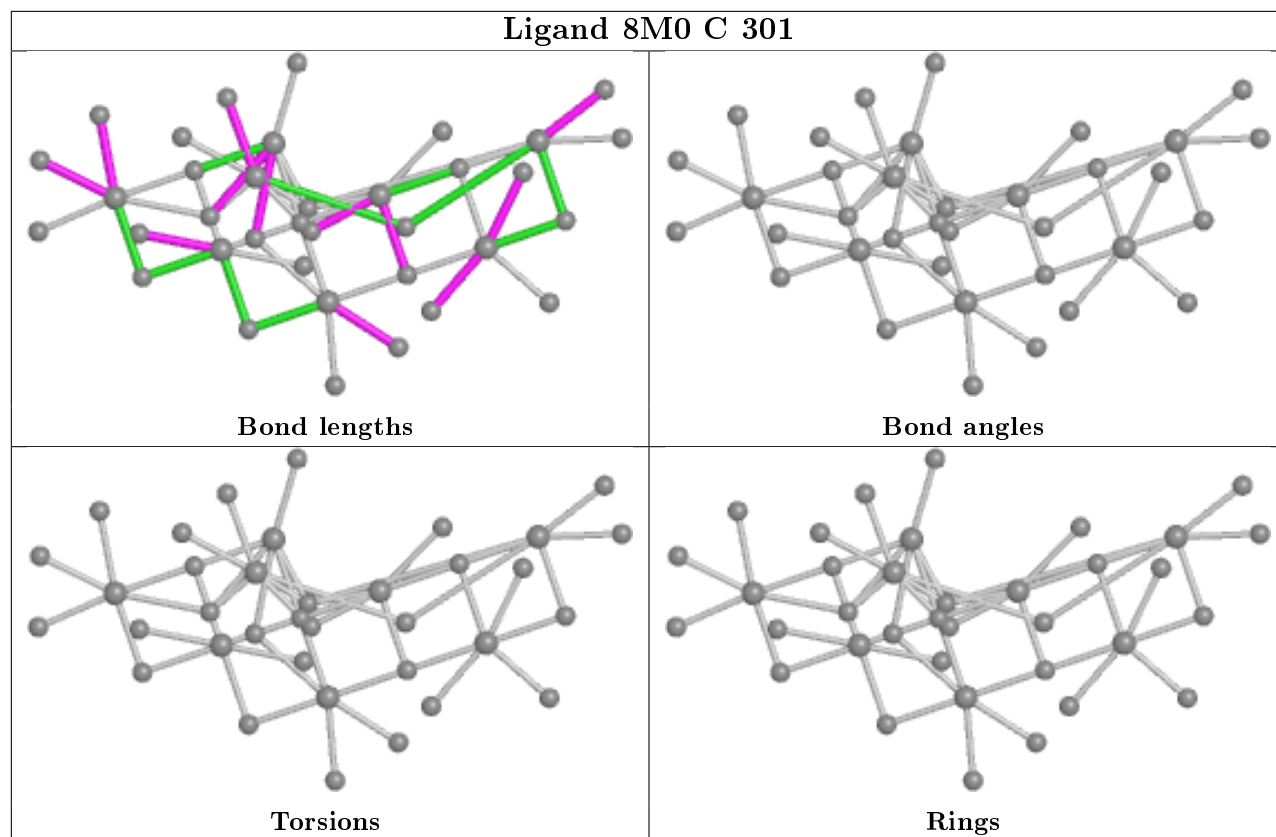
Ligand M10 G 304



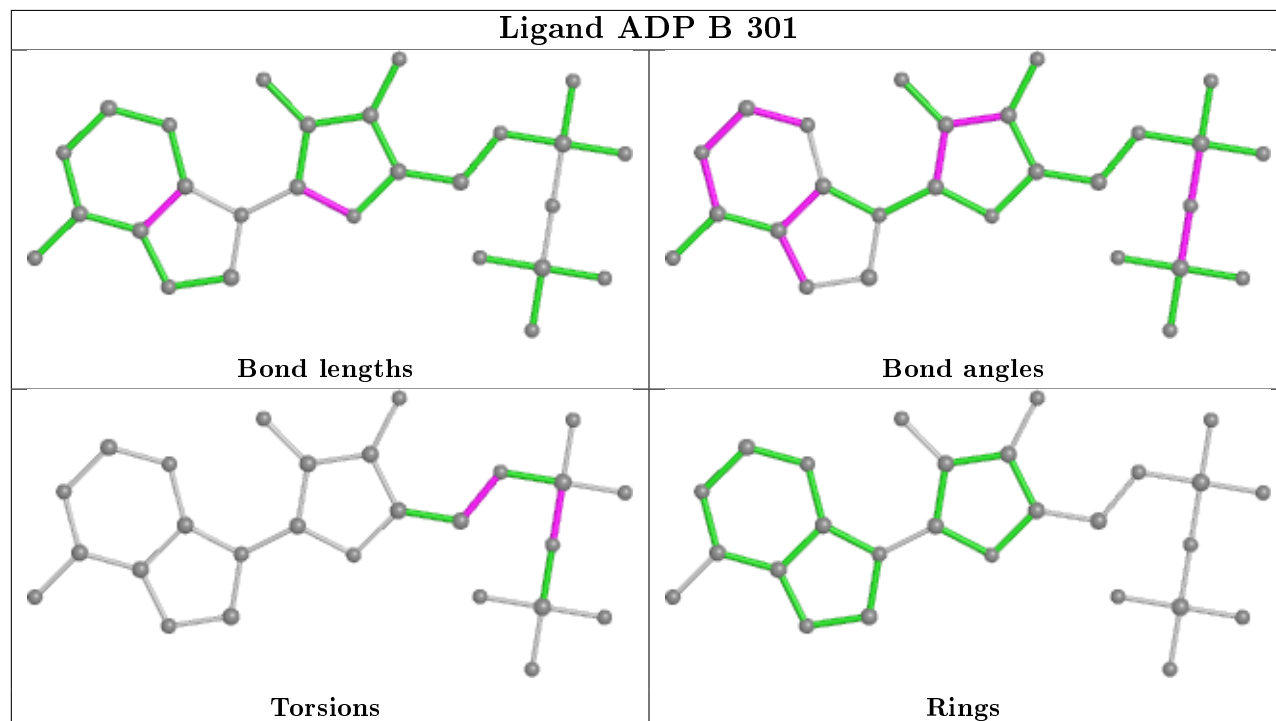
Ligand LJB B 306



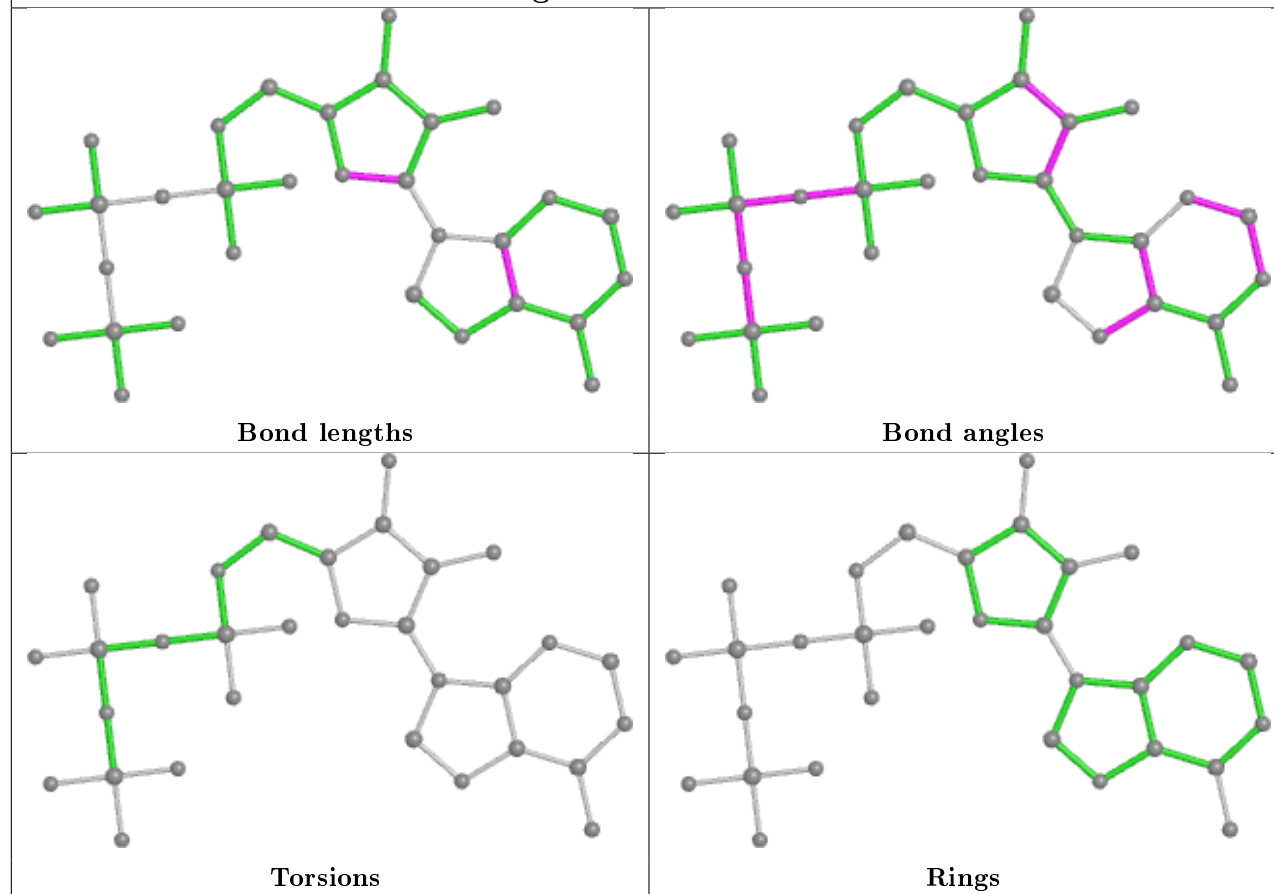
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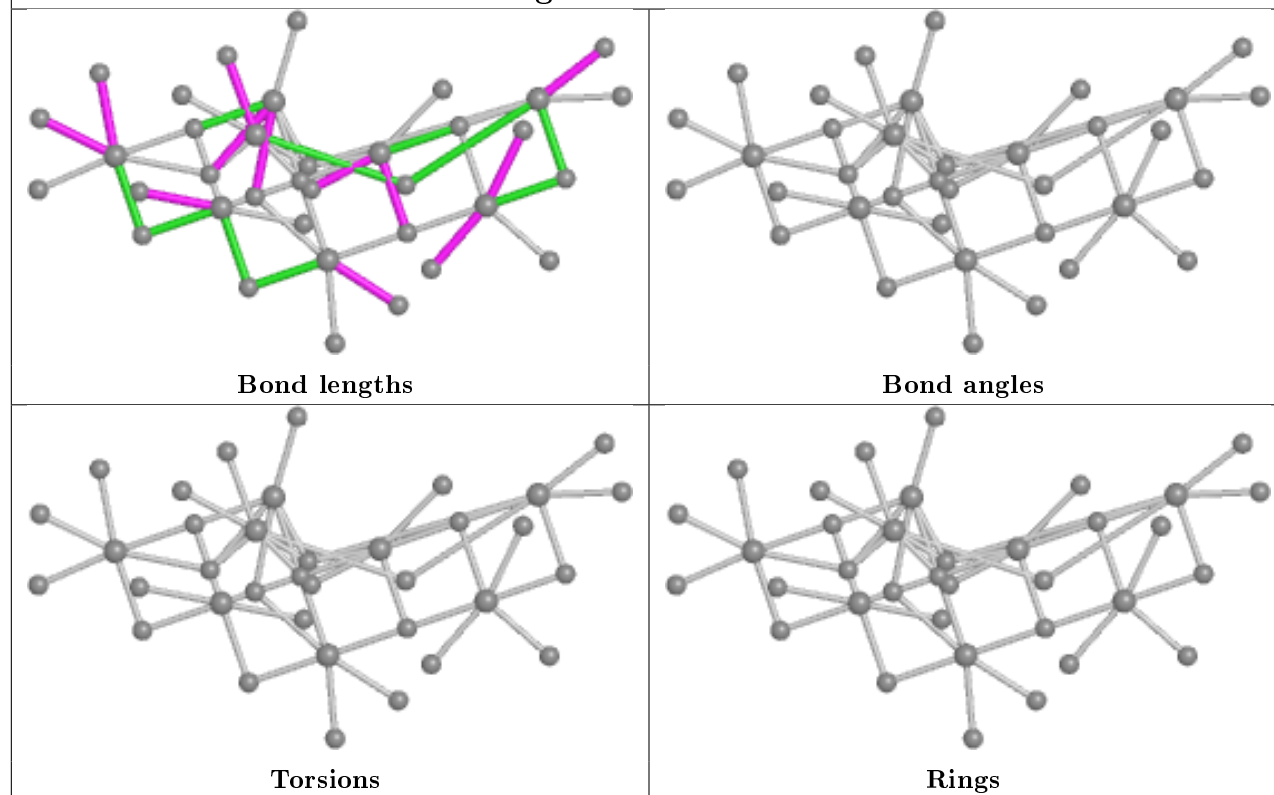
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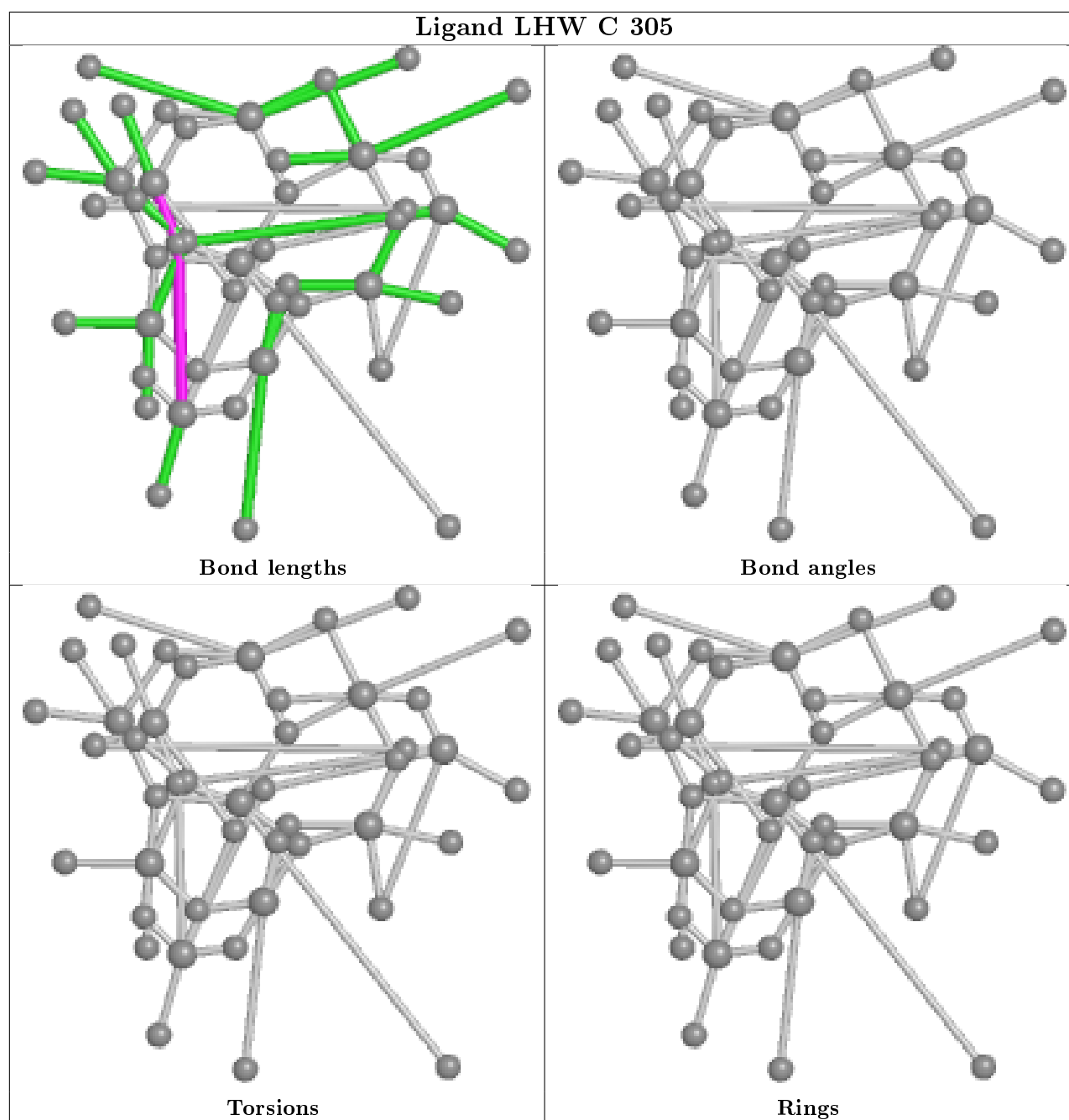


Ligand ATP A 301

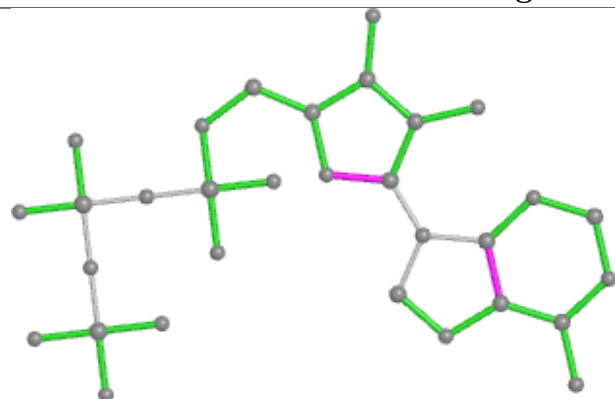


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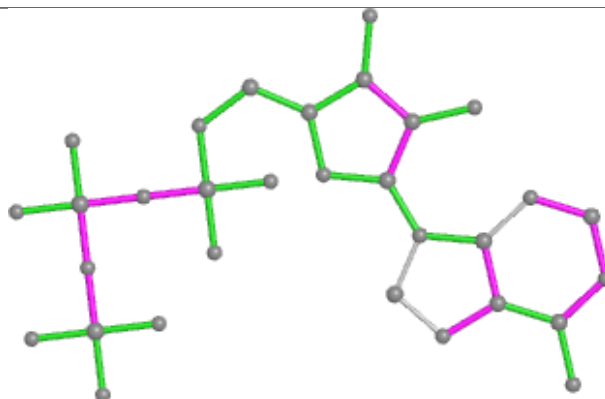




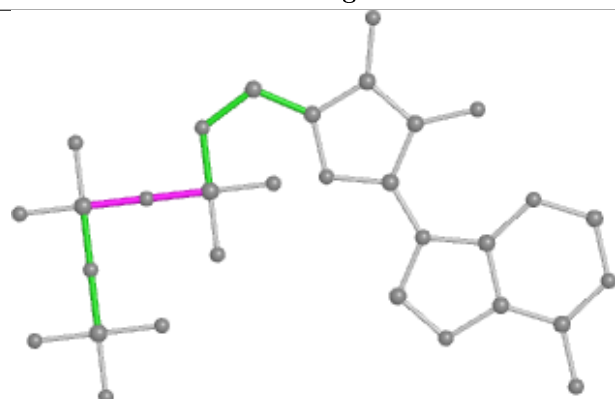
Ligand ATP G 301



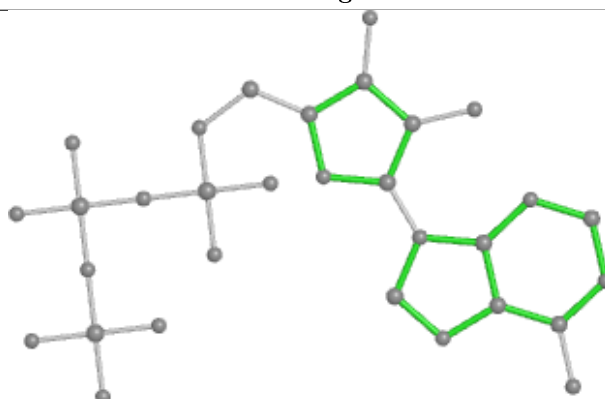
Bond lengths



Bond angles

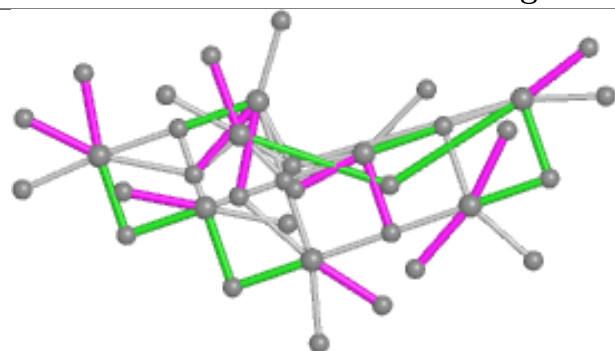


Torsions

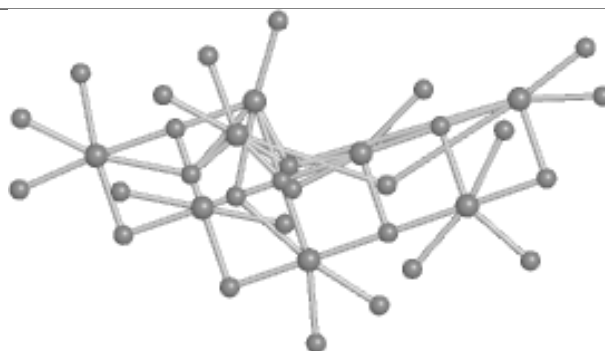


Rings

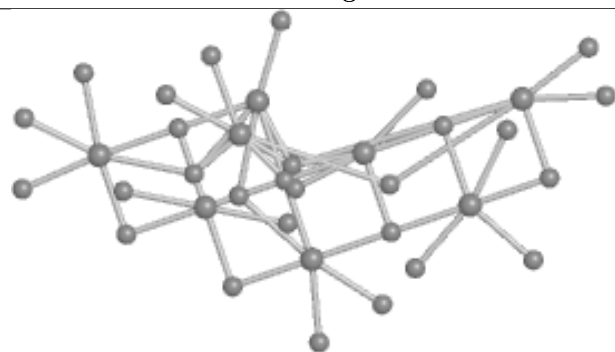
Ligand 8M0 F 303



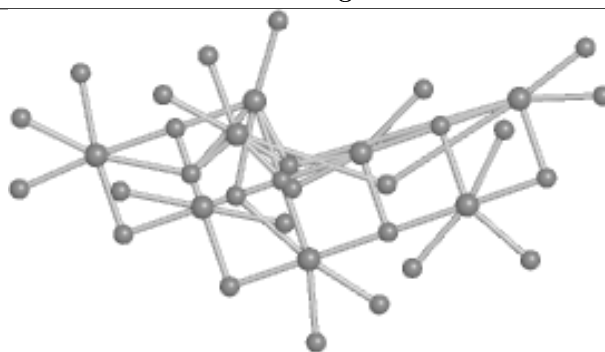
Bond lengths



Bond angles

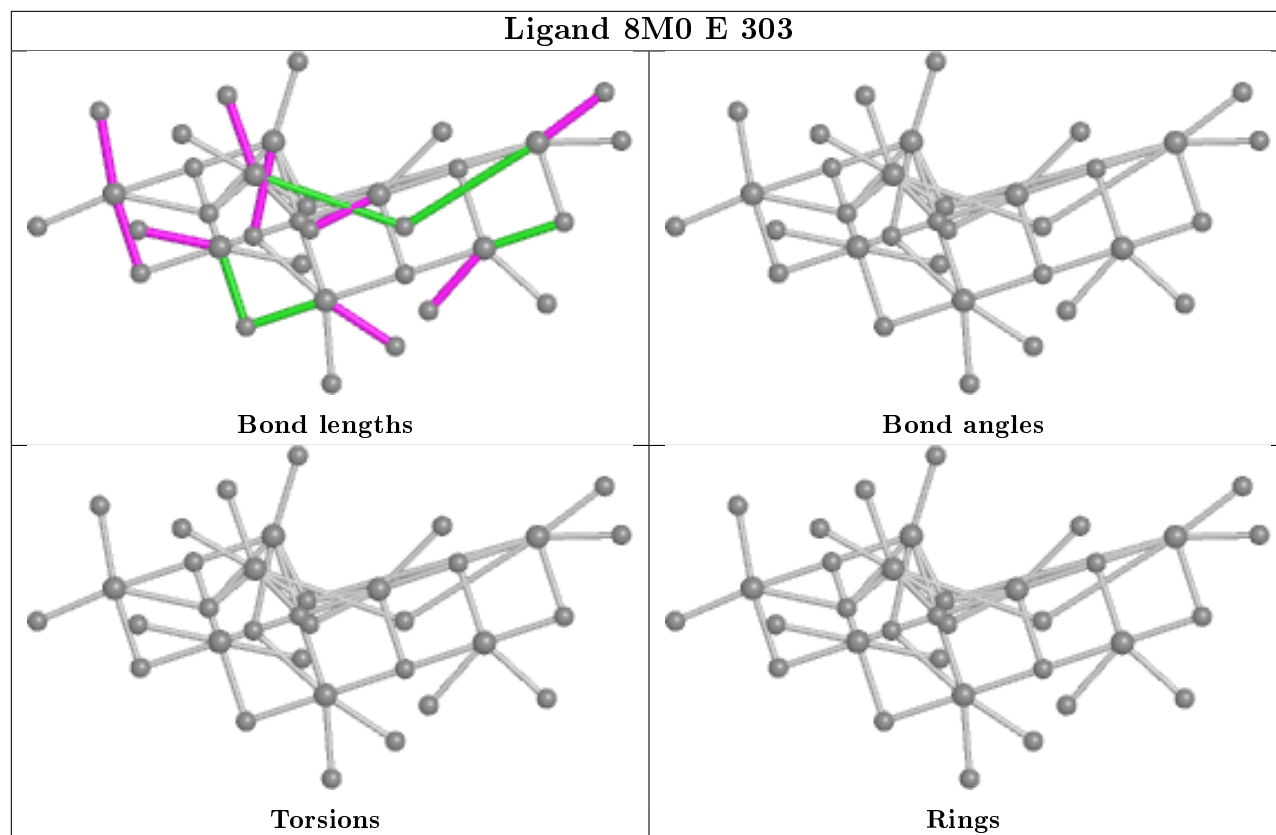


Torsions

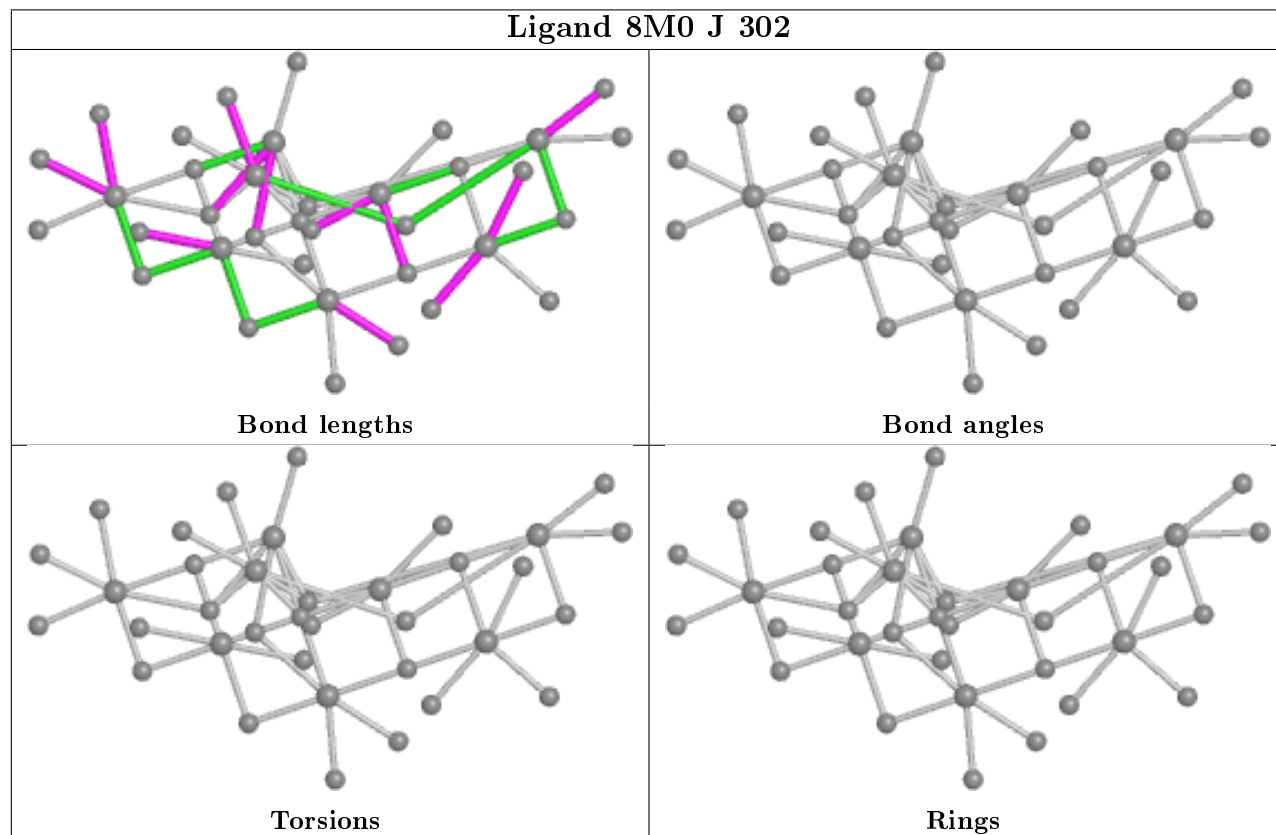


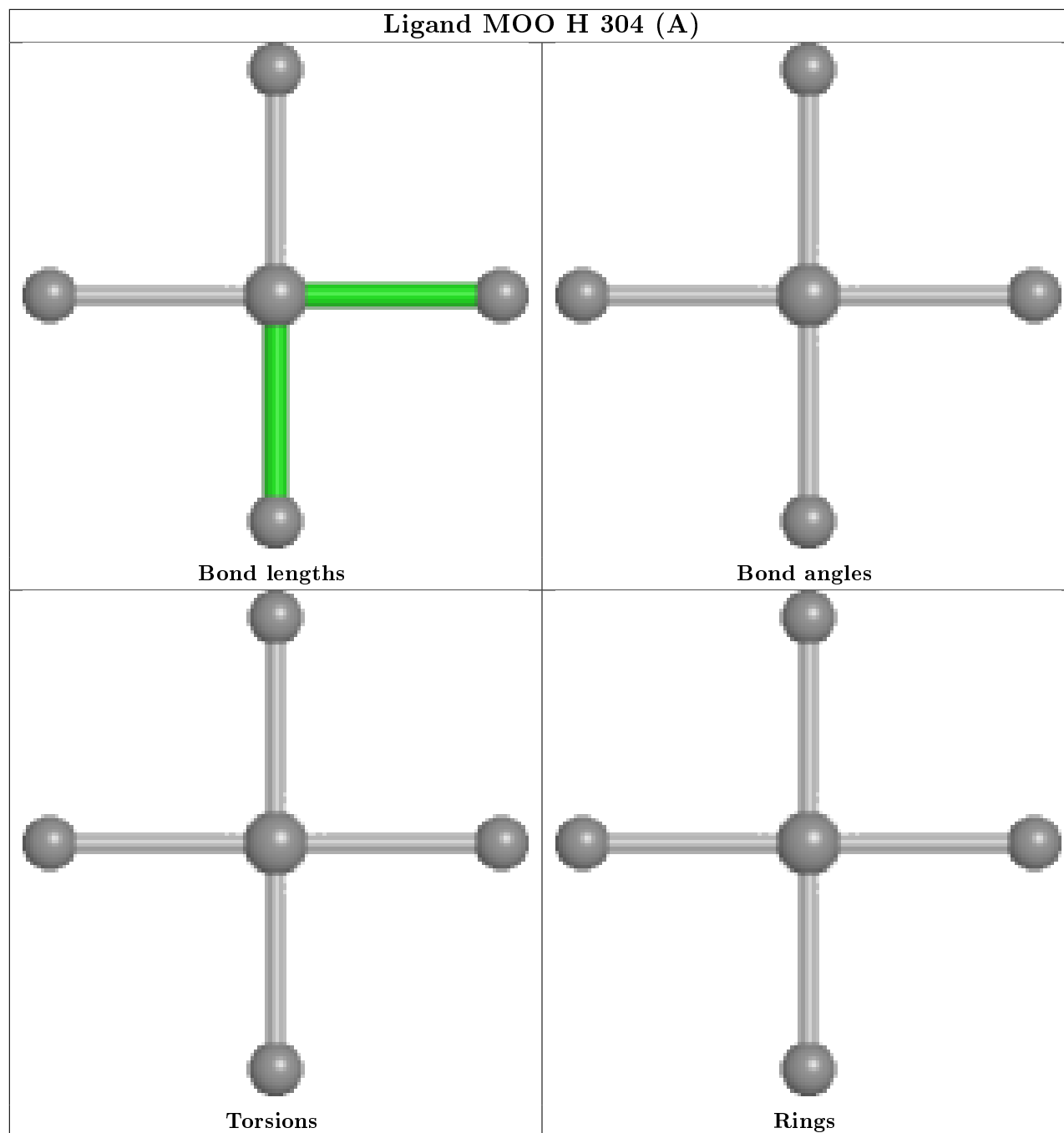
Rings

Ligand 8M0 E 303

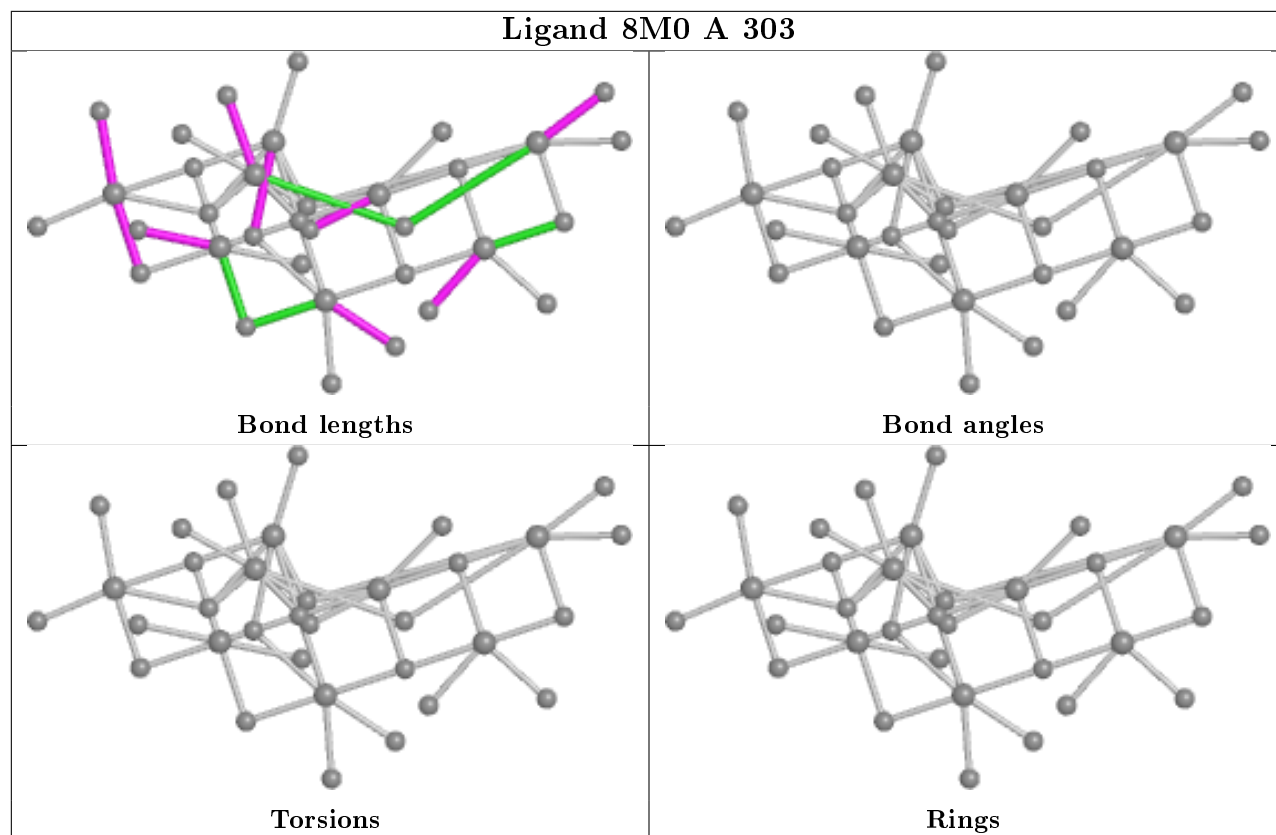


Ligand 8M0 J 302

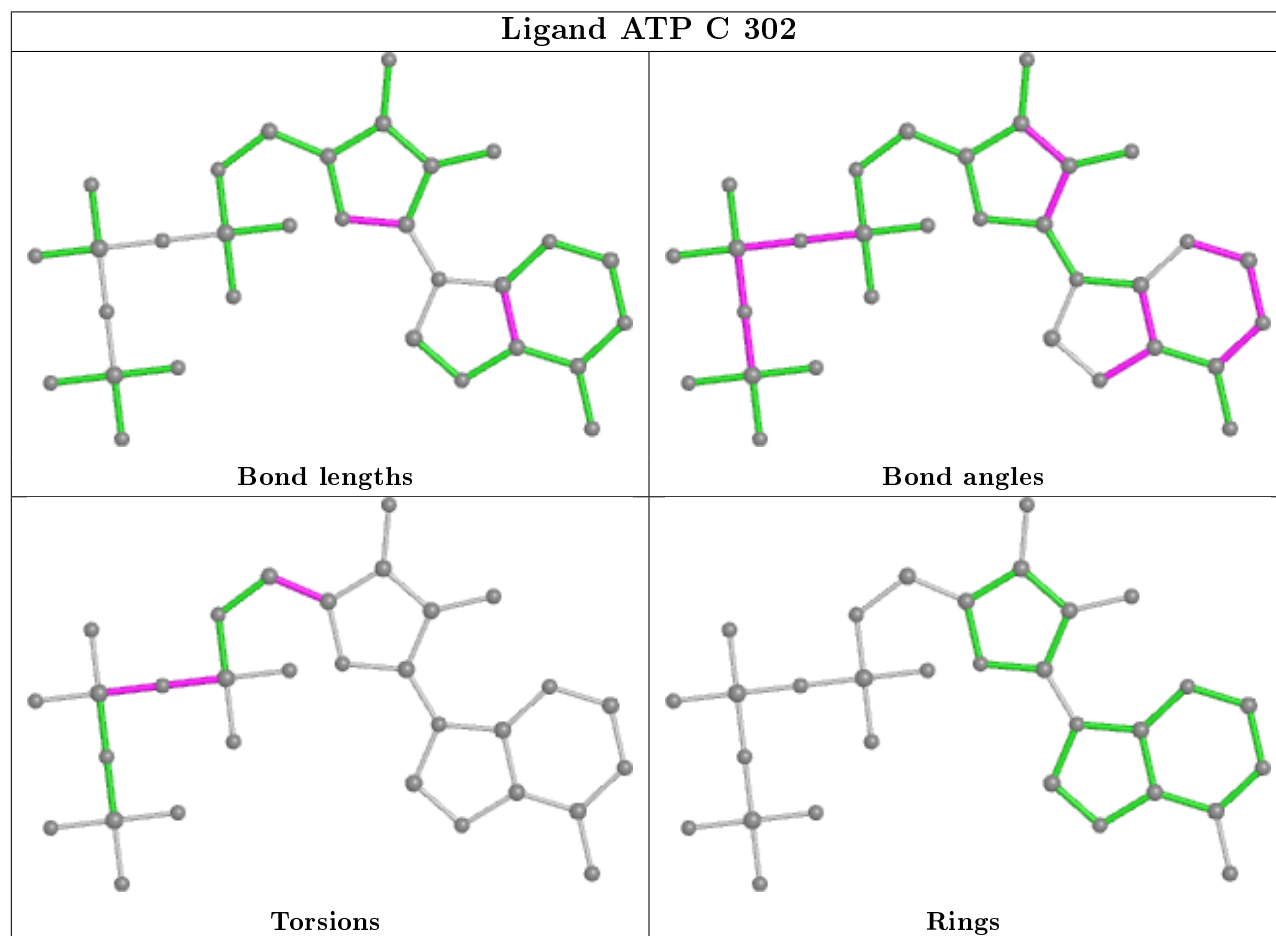


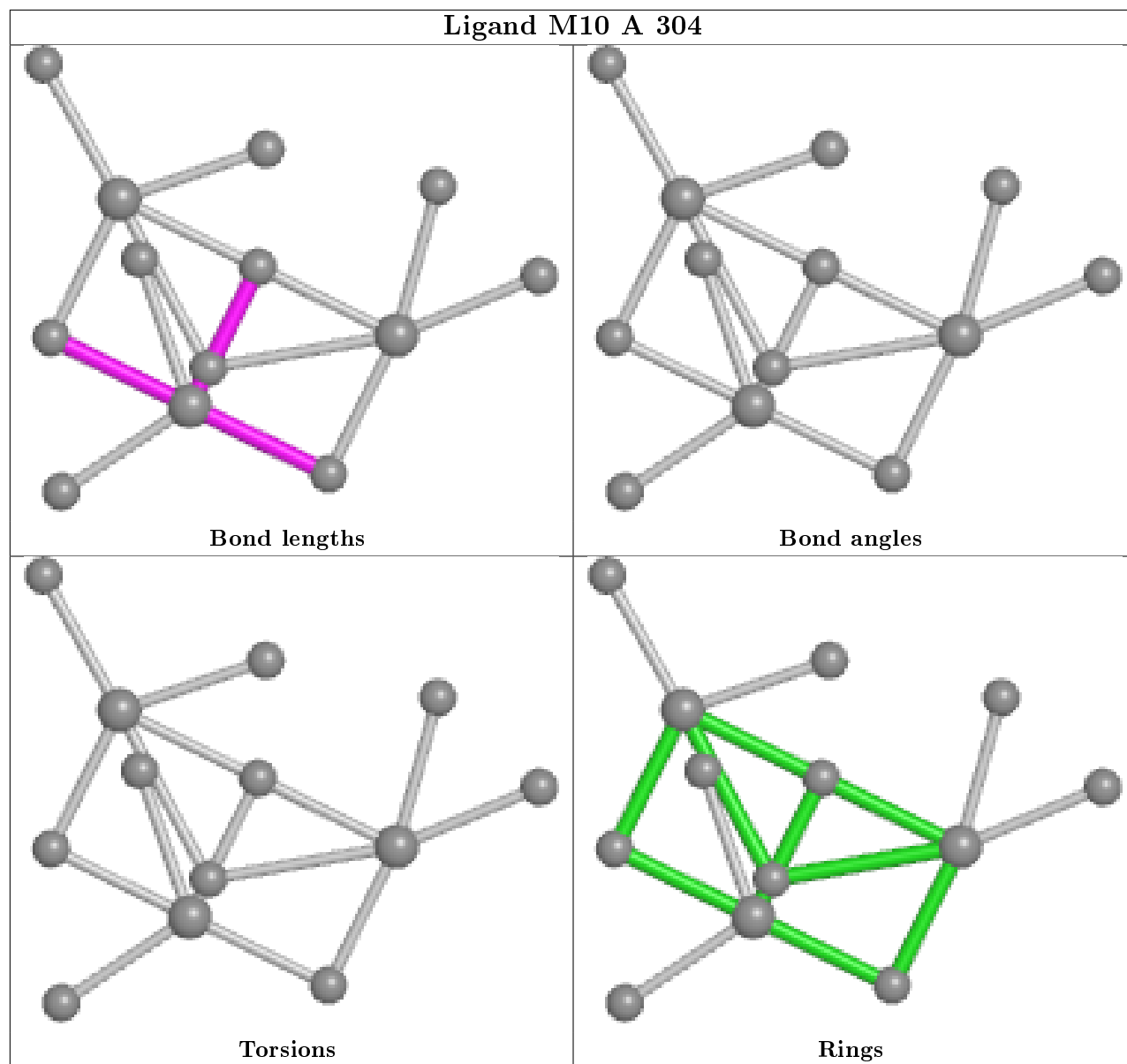


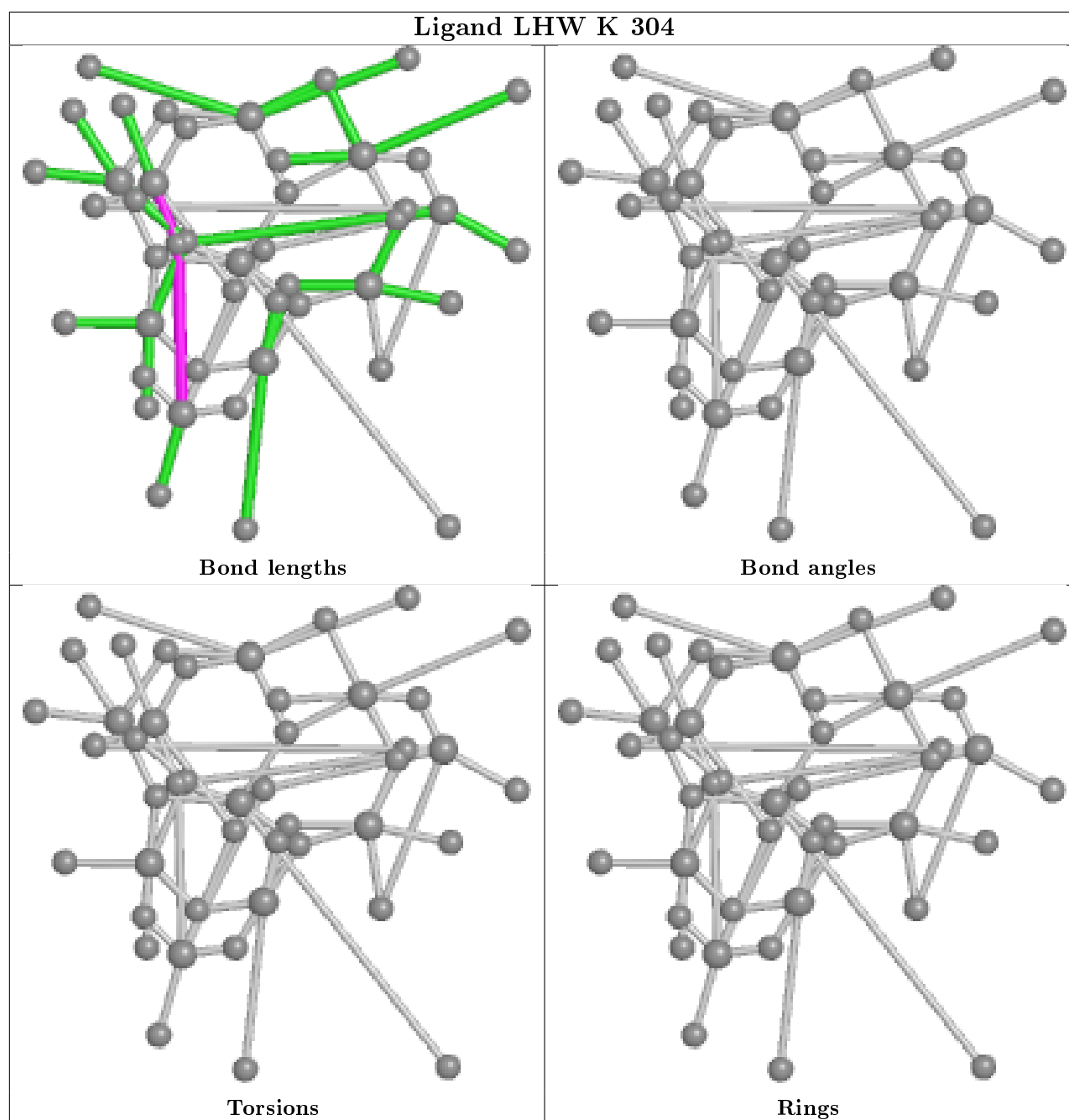
Ligand 8M0 A 303



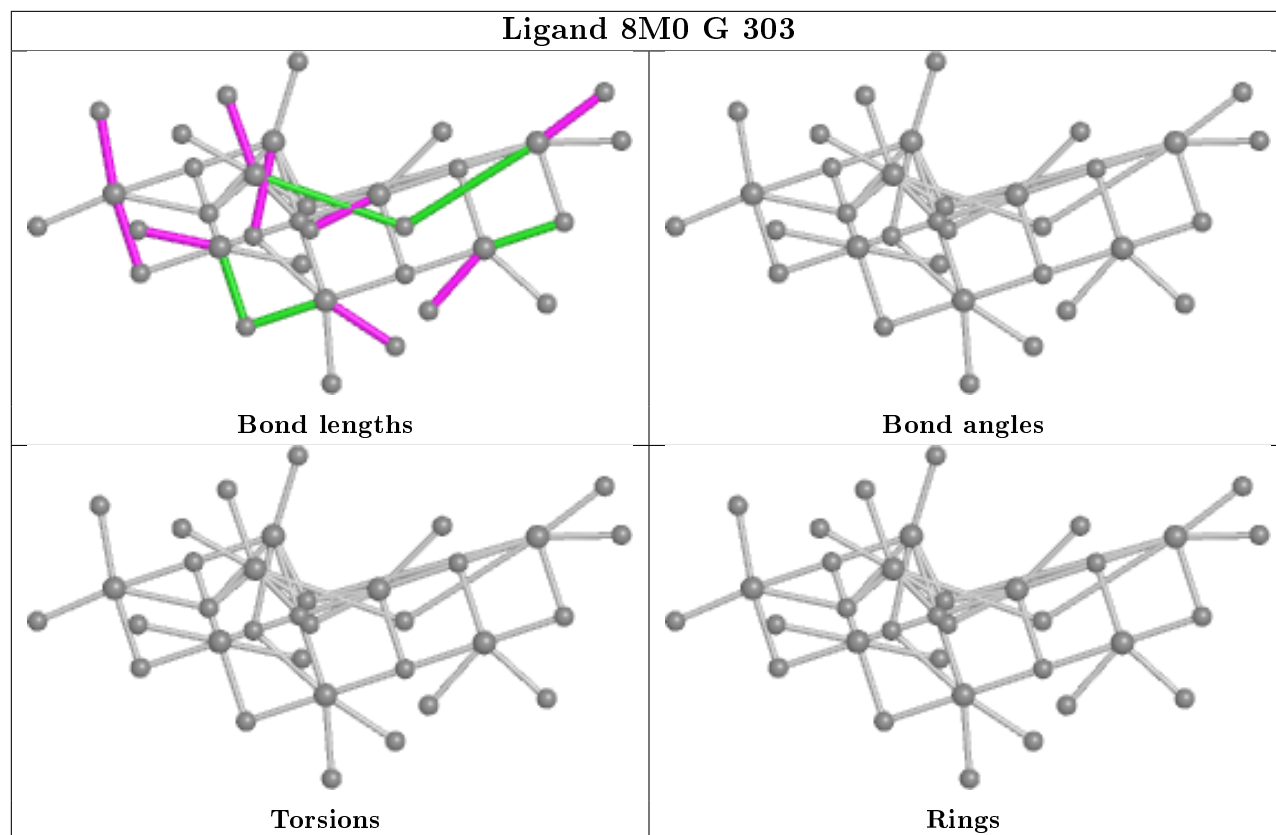
Ligand ATP C 302



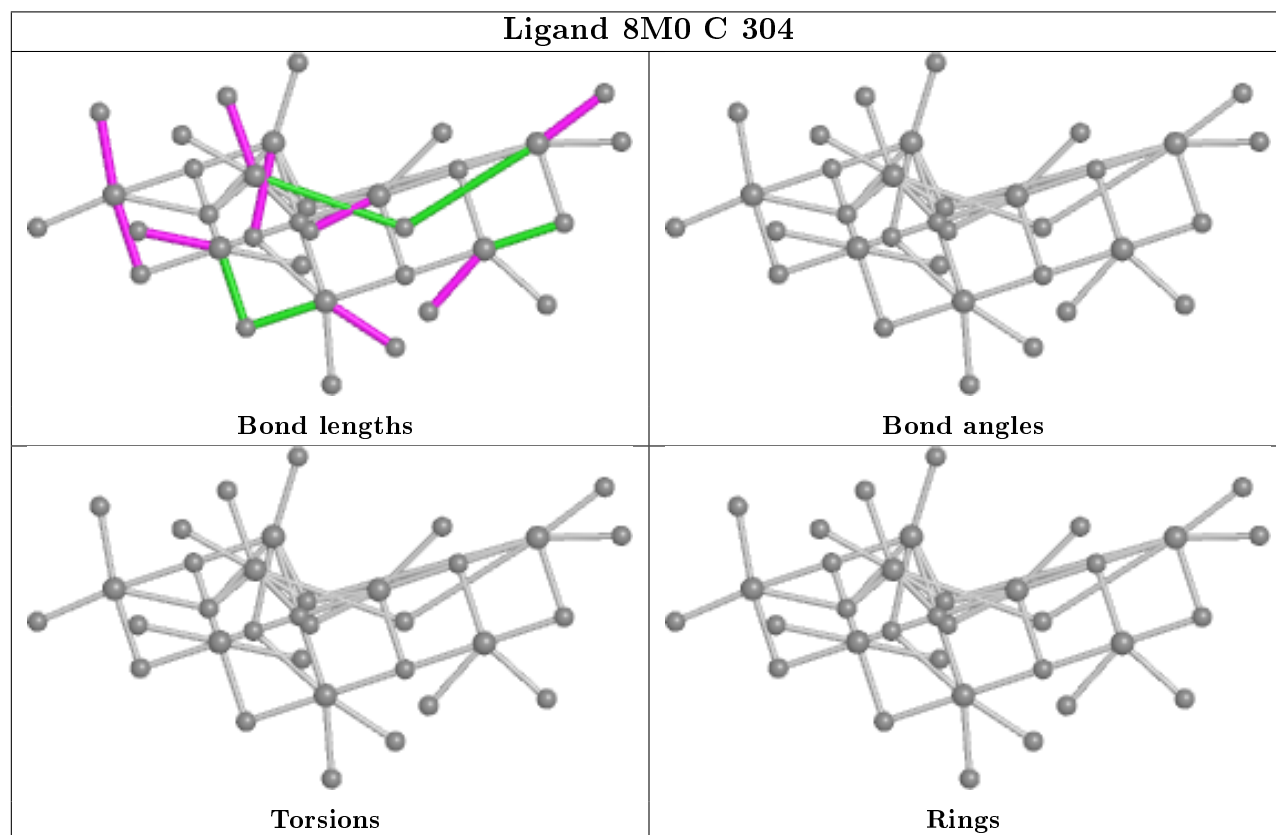


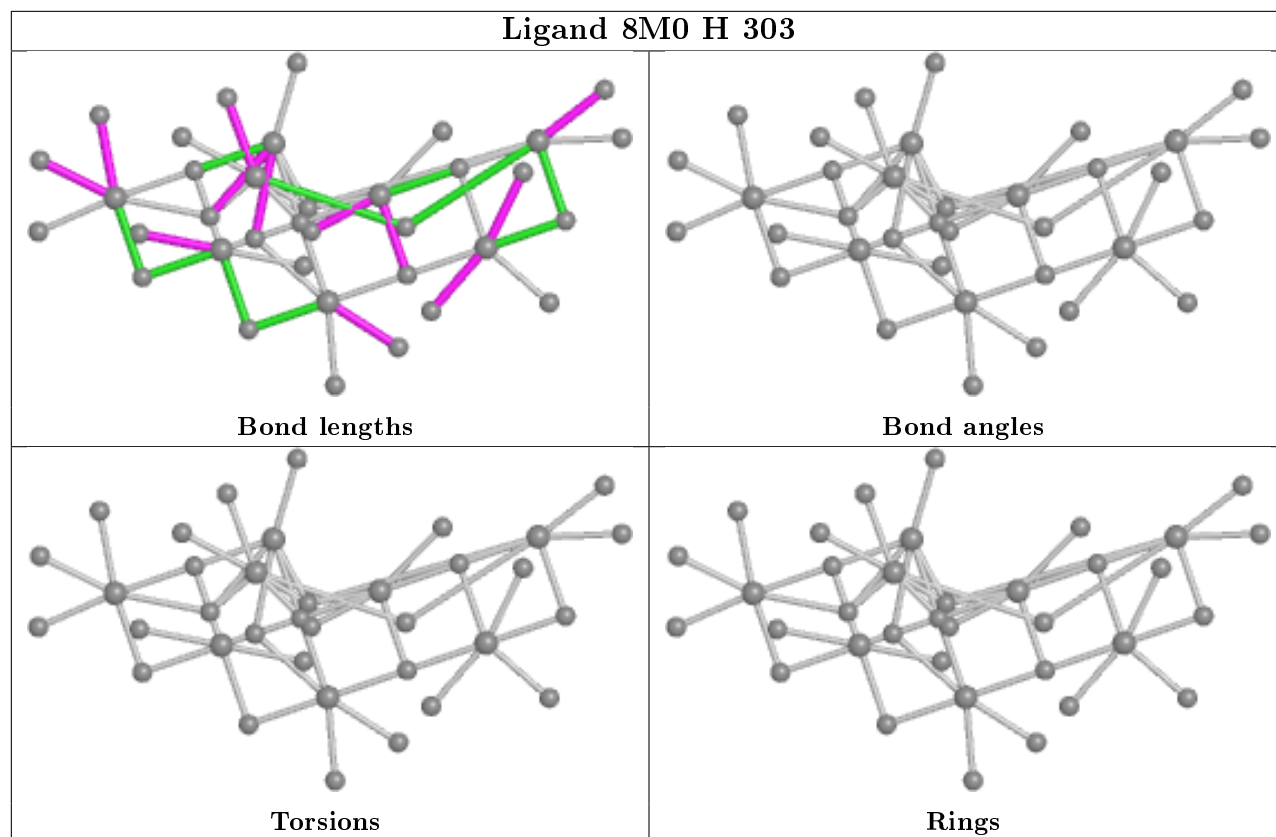


Ligand 8M0 G 303

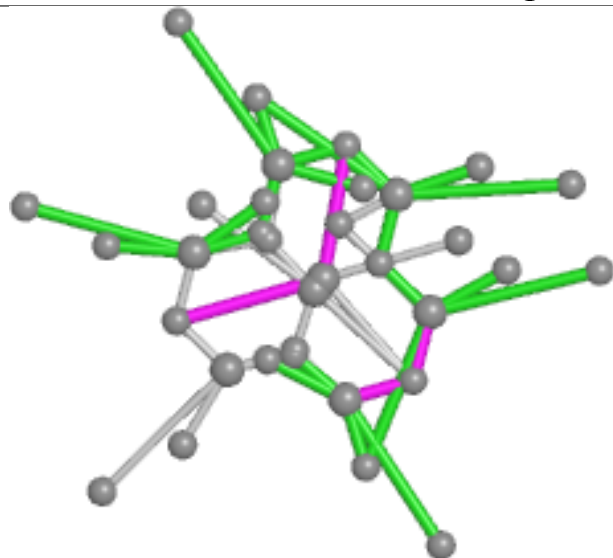


Ligand 8M0 C 304

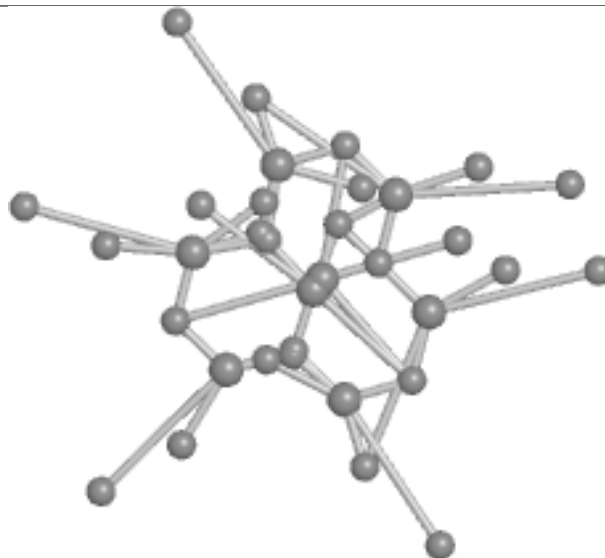




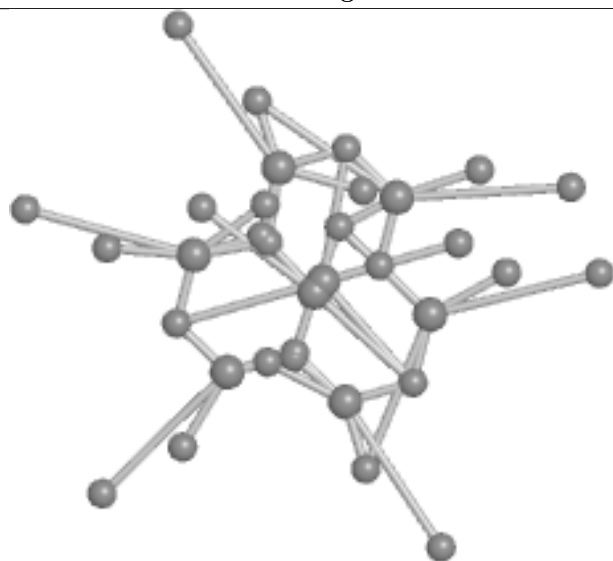
Ligand LJB L 306



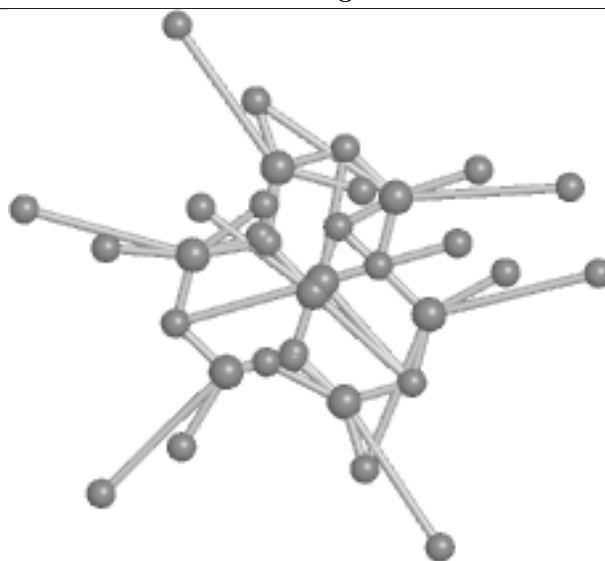
Bond lengths



Bond angles

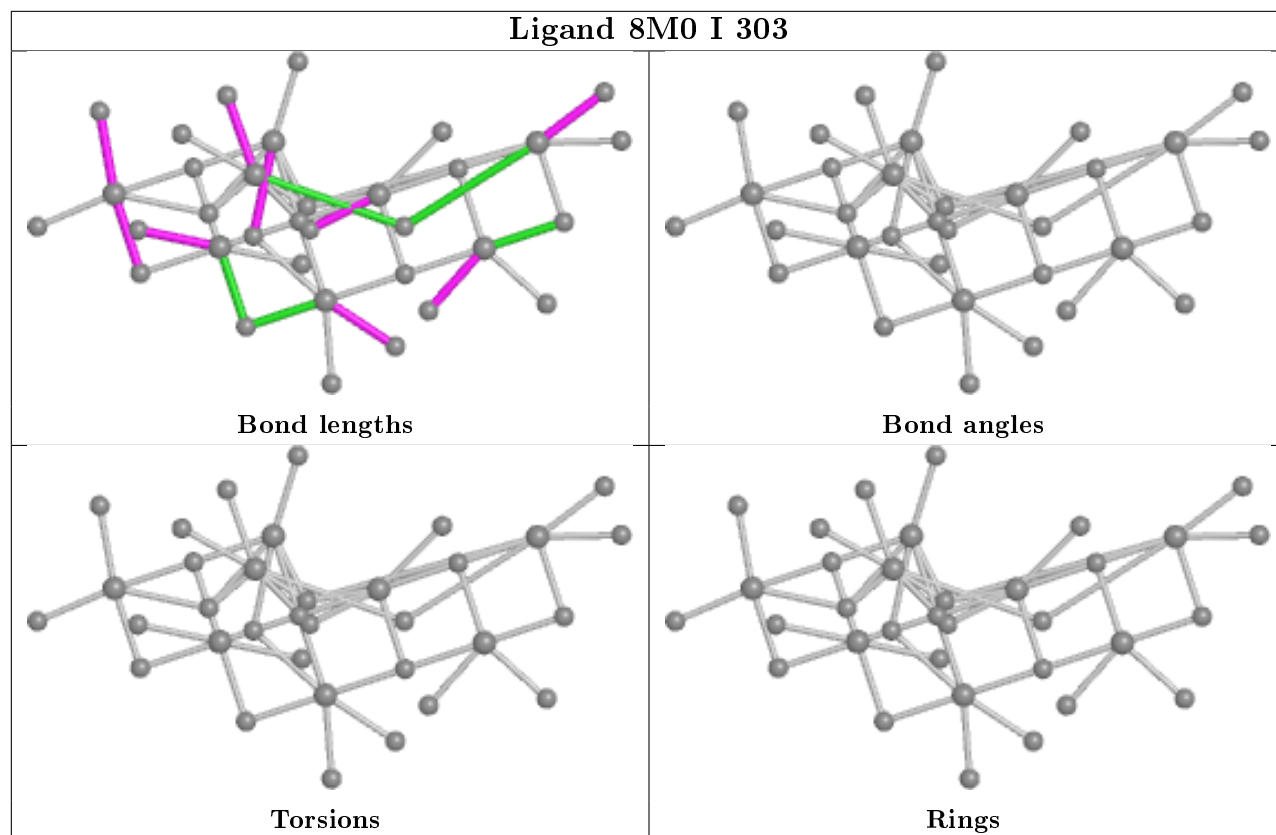


Torsions

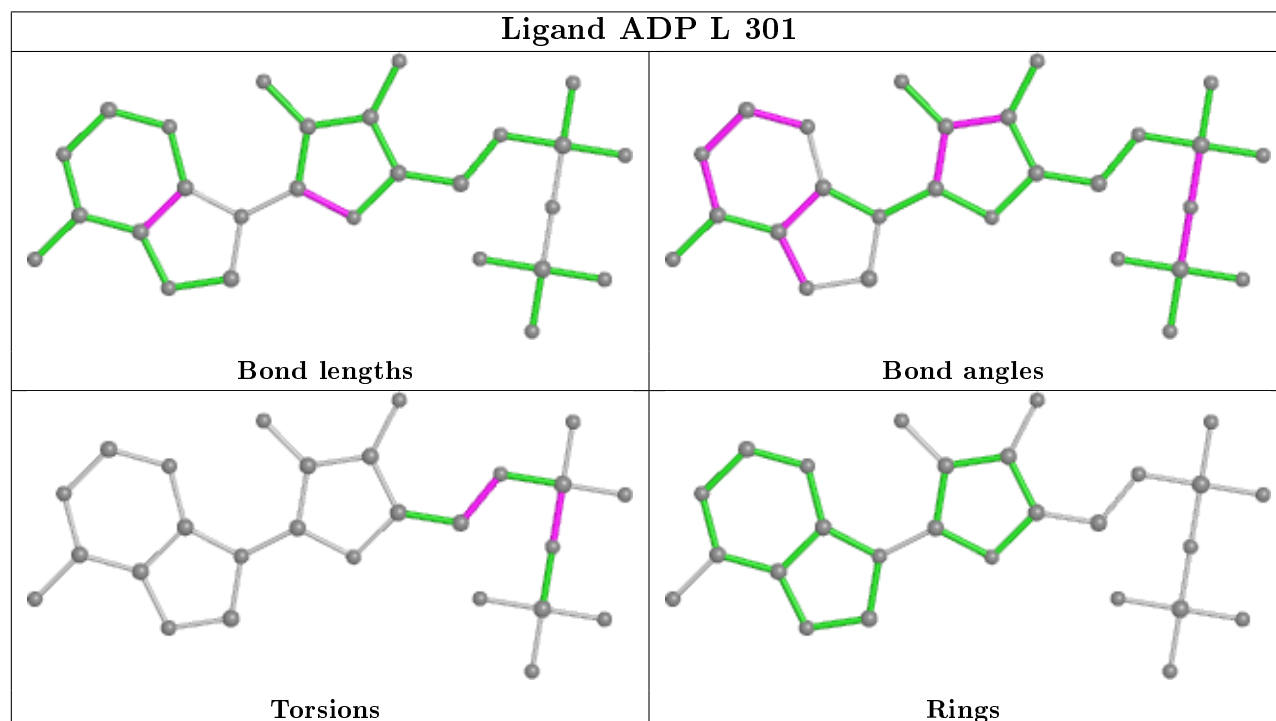


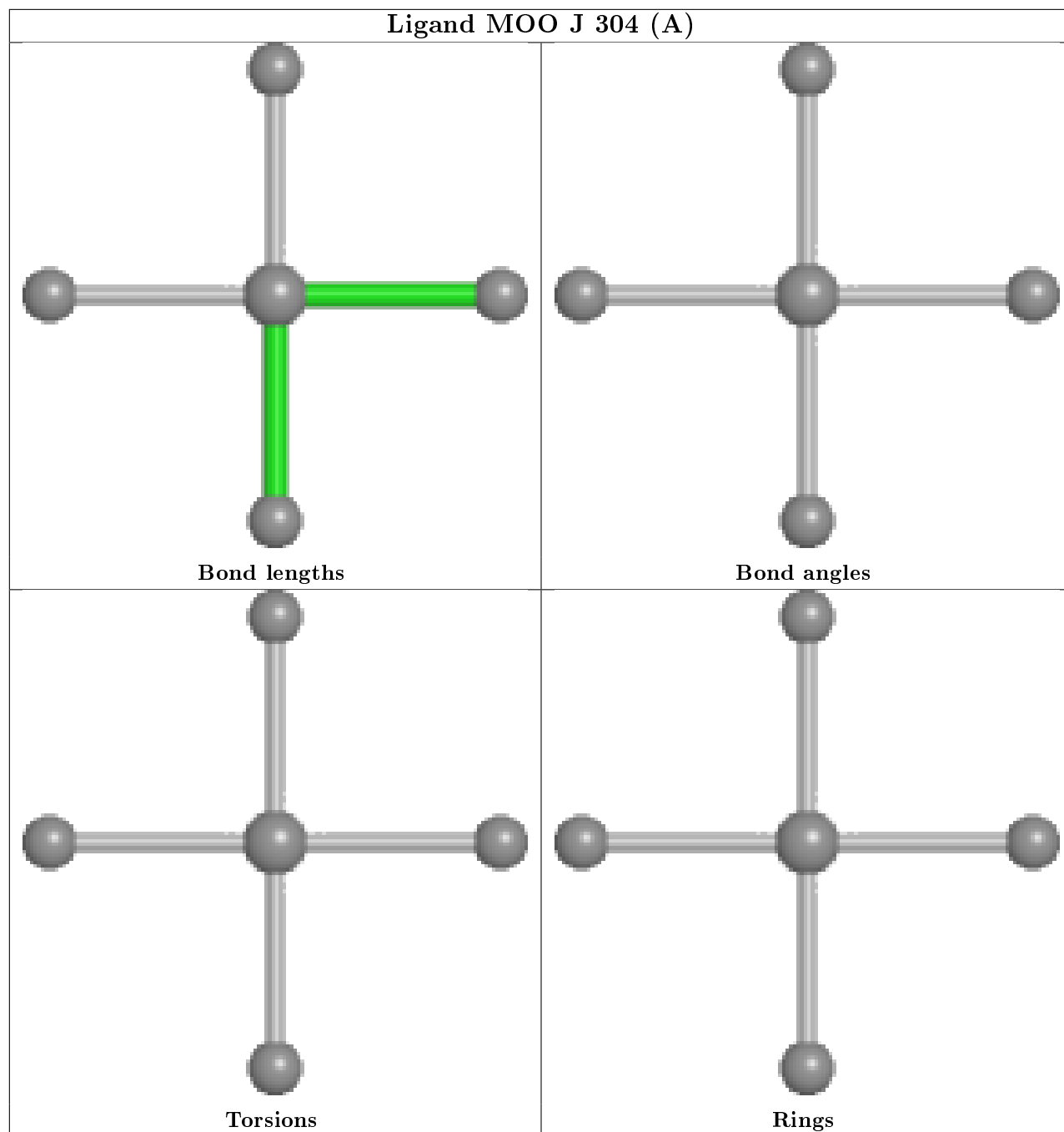
Rings

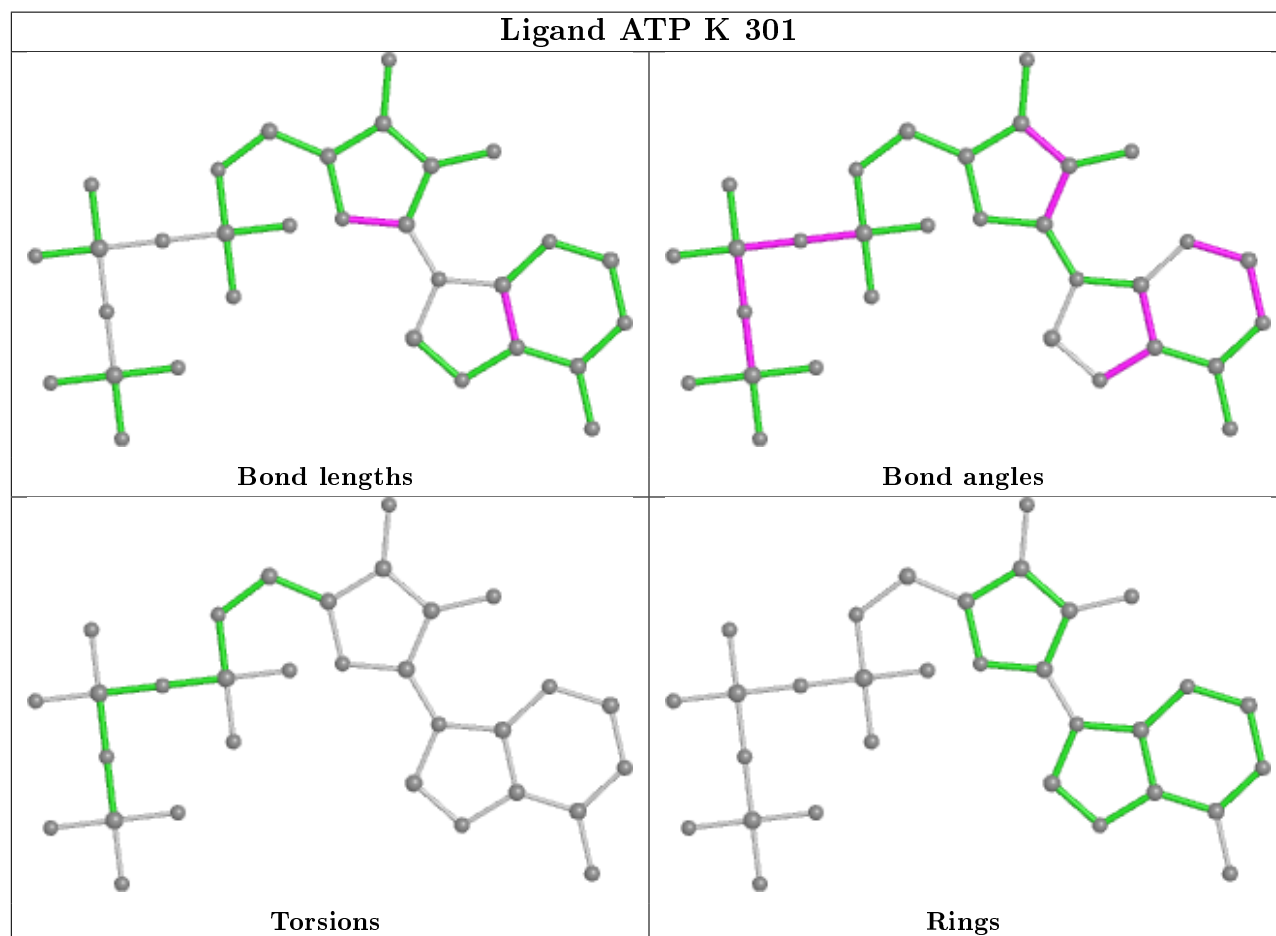
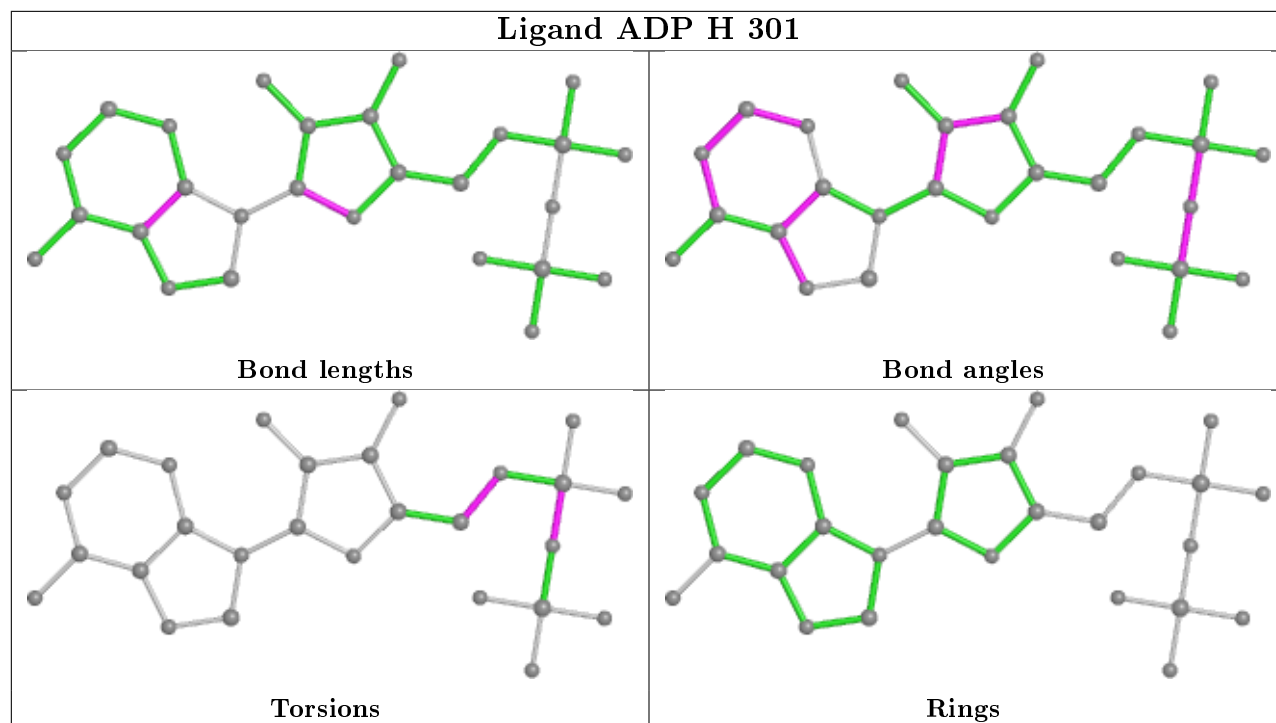
Ligand 8M0 I 303

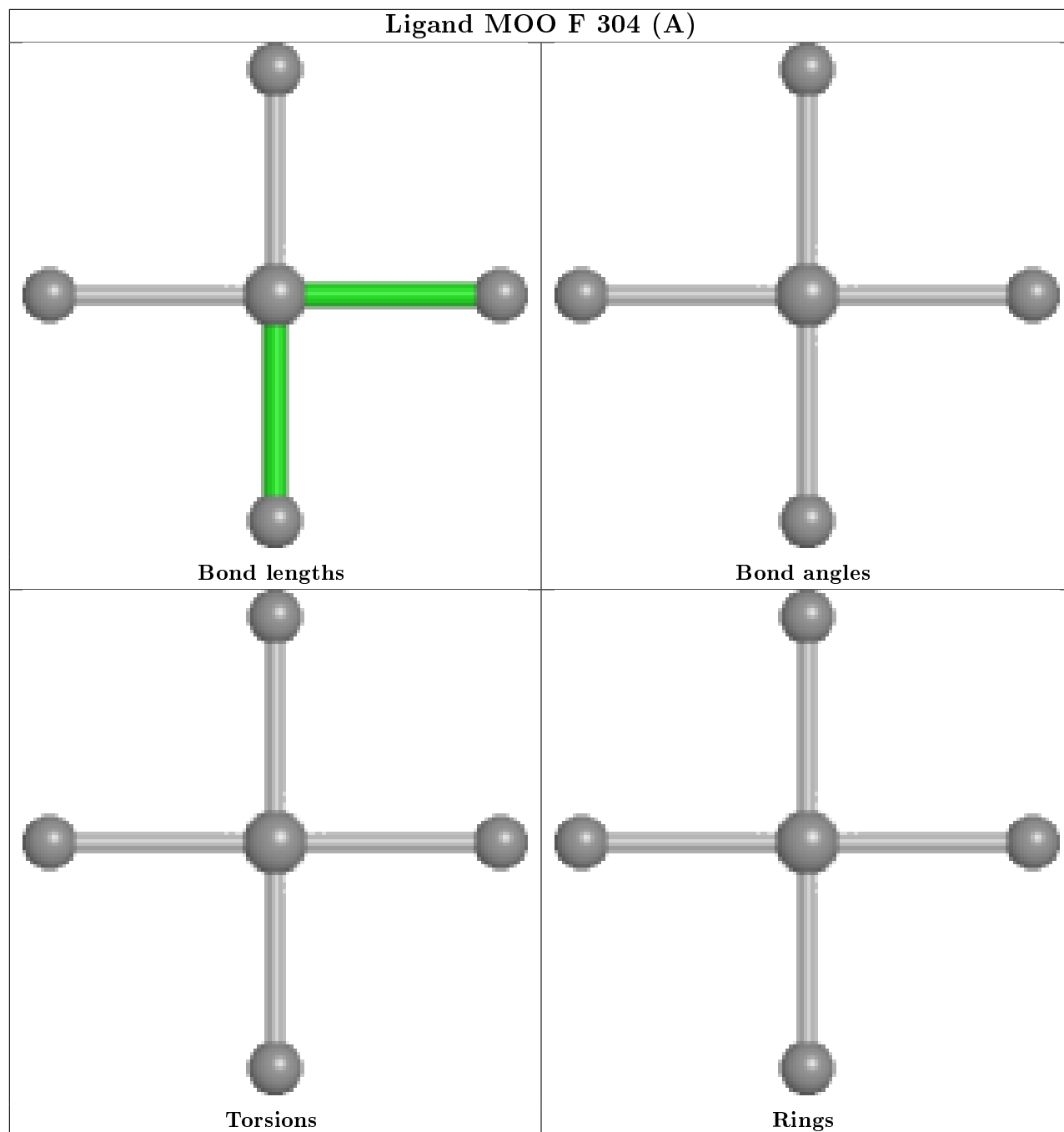


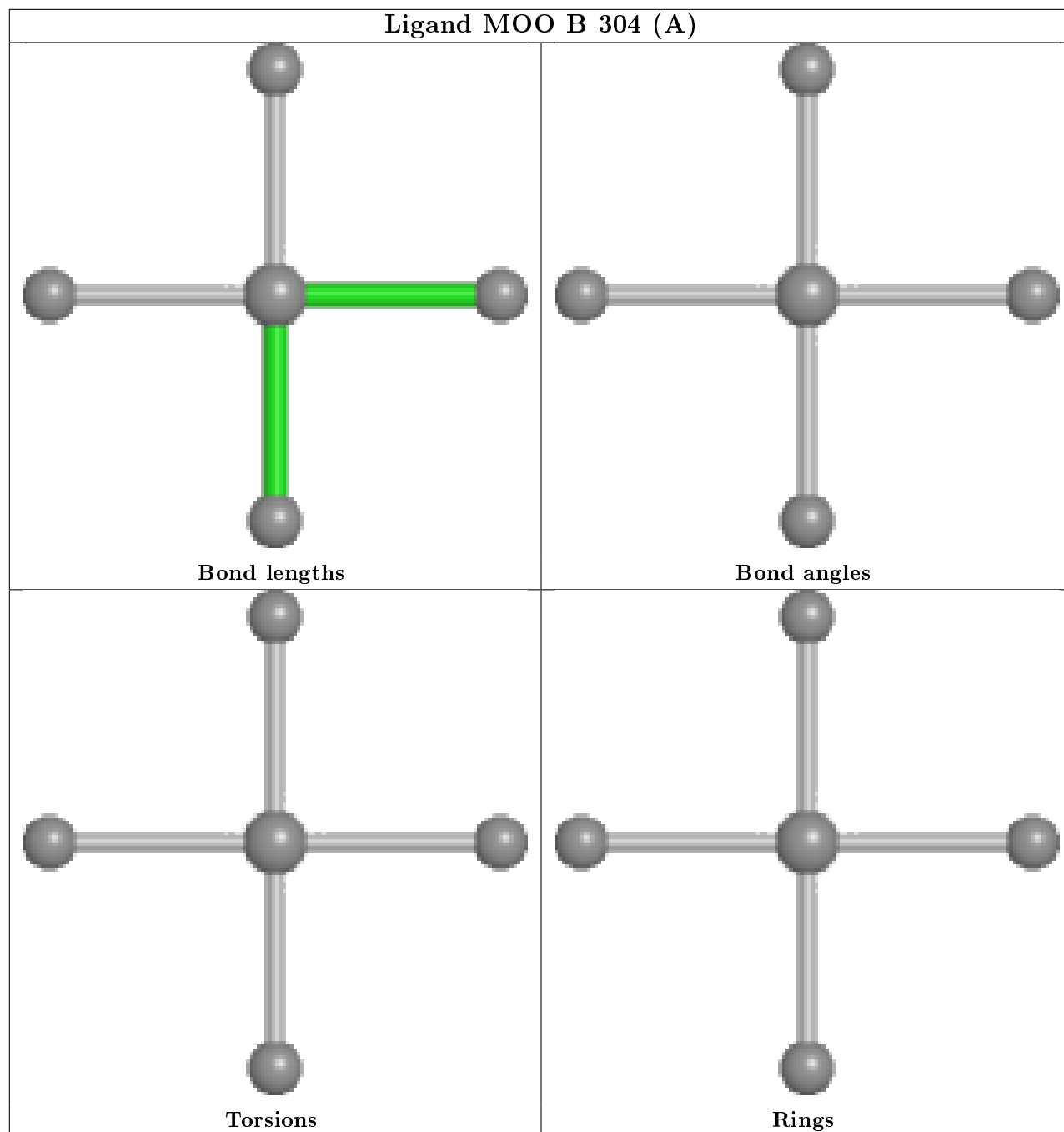
Ligand ADP L 301

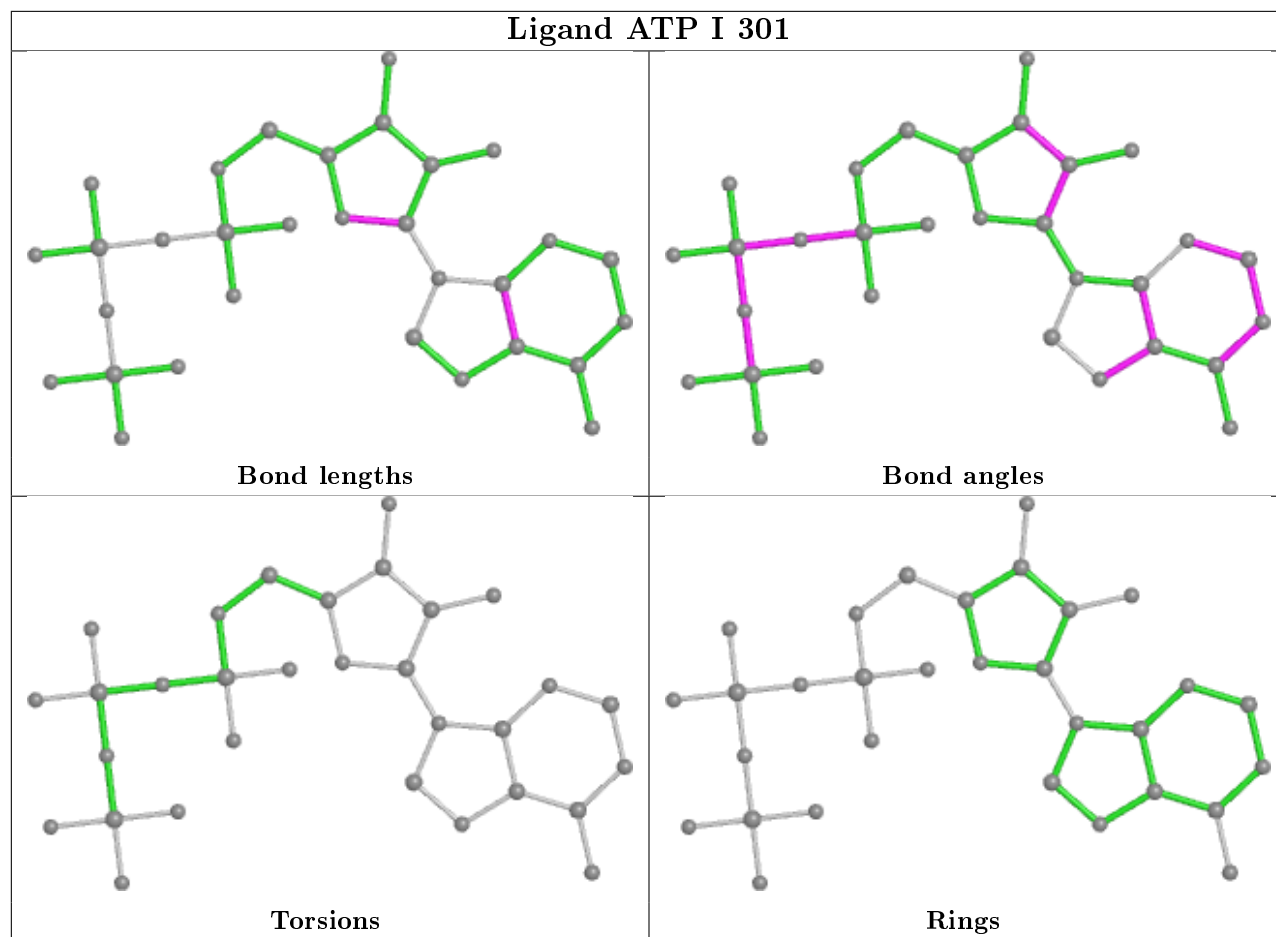












5.7 Other polymers [i](#)

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

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	B	268/269 (99%)	0.62	19 (7%) 16 18	14, 22, 45, 75	0
1	D	268/269 (99%)	0.65	25 (9%) 8 9	17, 23, 44, 72	0
1	F	269/269 (100%)	0.63	22 (8%) 11 13	15, 24, 49, 85	0
1	H	268/269 (99%)	0.78	26 (9%) 7 8	20, 31, 50, 79	0
1	J	267/269 (99%)	0.71	29 (10%) 5 6	18, 28, 53, 83	0
1	L	267/269 (99%)	0.36	16 (5%) 21 24	17, 24, 48, 66	0
2	A	272/275 (98%)	0.30	5 (1%) 68 72	13, 19, 35, 79	0
2	C	271/275 (98%)	0.51	17 (6%) 20 22	14, 19, 43, 63	0
2	E	272/275 (98%)	0.28	6 (2%) 62 66	15, 21, 43, 65	0
2	G	272/275 (98%)	0.43	11 (4%) 38 42	17, 23, 44, 89	0
2	I	272/275 (98%)	0.76	28 (10%) 6 7	17, 25, 51, 95	0
2	K	272/275 (98%)	0.52	20 (7%) 14 16	15, 22, 49, 74	0
All	All	3238/3264 (99%)	0.55	224 (6%) 16 19	13, 23, 48, 95	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	276	ALA	25.1
1	F	131	LEU	15.8
1	B	130	GLY	15.3
1	D	128	GLY	15.3
1	J	130	GLY	14.7
1	B	129	ALA	14.5
1	J	131	LEU	13.4
1	B	128	GLY	12.4
1	D	130	GLY	12.1
2	K	5	THR	12.1
1	F	129	ALA	12.0

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Mol	Chain	Res	Type	RSRZ
1	H	129	ALA	11.1
1	D	131	LEU	10.4
1	H	131	LEU	10.1
1	F	130	GLY	9.5
1	B	131	LEU	9.2
2	G	276	ALA	9.1
1	F	4	SER	8.8
1	D	129	ALA	8.7
2	G	275	PRO	8.4
1	J	129	ALA	8.4
1	J	4	SER	8.4
2	A	276	ALA	8.3
1	D	3	ASN	8.2
1	H	4	SER	8.2
1	H	3	ASN	8.1
2	I	275	PRO	8.0
1	H	128	GLY	8.0
1	J	5	THR	7.8
1	D	139	ALA	7.7
1	F	2	ALA	7.6
1	L	4	SER	7.6
1	B	3	ASN	7.3
1	L	128	GLY	7.1
1	D	127	GLY	7.0
2	G	5	THR	6.7
1	L	127	GLY	6.7
1	B	4	SER	6.7
2	K	276	ALA	6.5
1	F	3	ASN	6.5
1	L	129	ALA	6.3
2	A	274	ARG	6.2
1	B	127	GLY	6.1
1	F	128	GLY	6.0
2	E	5	THR	5.8
2	K	274	ARG	5.6
2	I	5	THR	5.6
1	H	6	ALA	5.6
2	I	205	ARG	5.4
2	I	206	GLY	5.2
1	L	131	LEU	5.0
2	K	275	PRO	4.9
2	I	203	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	138	LEU	4.7
1	H	5	THR	4.7
2	I	274	ARG	4.6
2	I	207	GLN	4.6
2	A	5	THR	4.6
1	J	204	ASP	4.5
2	I	273	VAL	4.4
2	C	275	PRO	4.4
2	I	6	ASN	4.4
2	A	275	PRO	4.3
1	L	138	LEU	4.3
1	B	204	ASP	4.3
1	H	127	GLY	4.3
1	L	5	THR	4.3
1	H	222	HIS	4.2
2	K	205	ARG	4.2
1	F	203	LYS	4.2
1	D	203	LYS	4.2
2	C	206	GLY	4.1
2	C	274	ARG	4.0
1	H	138	LEU	4.0
1	J	128	GLY	4.0
2	G	274	ARG	4.0
1	H	139	ALA	4.0
2	K	204	ASP	4.0
1	F	138	LEU	3.9
2	C	207	GLN	3.9
2	C	272	GLY	3.8
1	J	154	LEU	3.8
2	K	6	ASN	3.8
1	L	262	HIS	3.7
2	K	207	GLN	3.7
1	D	204	ASP	3.7
1	H	130	GLY	3.7
1	F	5	THR	3.6
1	H	204	ASP	3.6
2	C	221	LYS	3.5
1	F	7	GLU	3.5
2	I	221	LYS	3.5
1	B	139	ALA	3.5
2	K	273	VAL	3.4
1	D	132	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	262	HIS	3.4
1	L	6	ALA	3.4
2	C	203	PRO	3.3
1	H	140	GLU	3.3
1	J	127	GLY	3.3
1	F	132	SER	3.3
1	J	6	ALA	3.3
2	G	273	VAL	3.3
2	C	204	ASP	3.2
2	E	205	ARG	3.2
1	J	7	GLU	3.2
1	J	139	ALA	3.2
1	D	206	THR	3.2
1	D	138	LEU	3.2
1	D	153[A]	LYS	3.1
1	H	203	LYS	3.1
2	K	133	VAL	3.1
1	B	203	LYS	3.1
1	H	68	LYS	3.1
1	D	4	SER	3.1
1	H	137[A]	SER	3.0
2	G	6	ASN	3.0
1	J	133	ALA	3.0
1	D	5	THR	3.0
1	B	132	SER	3.0
1	F	263	VAL	3.0
1	L	263	VAL	3.0
1	F	139	ALA	2.9
2	I	137	LEU	2.9
1	H	7	GLU	2.9
1	H	141	VAL	2.9
1	F	127	GLY	2.9
1	L	154	LEU	2.9
1	J	14[A]	GLN	2.9
2	I	208	ALA	2.9
1	B	134	VAL	2.8
2	G	204	ASP	2.8
1	L	139	ALA	2.8
2	C	6	ASN	2.8
2	E	6	ASN	2.8
1	D	202	SER	2.8
2	I	133	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	141	VAL	2.8
2	K	33	ARG	2.8
2	C	223	GLU	2.8
1	B	256	ARG	2.7
1	F	137	SER	2.7
2	I	202	GLY	2.7
2	K	32	LYS	2.7
1	J	98	VAL	2.7
1	H	263	VAL	2.7
2	G	203	PRO	2.7
1	J	137	SER	2.6
1	B	6	ALA	2.6
1	L	203	LYS	2.6
1	J	132	SER	2.6
2	I	31	GLY	2.6
2	K	177	LEU	2.6
1	D	7	GLU	2.5
1	J	134	VAL	2.5
1	D	126	VAL	2.5
1	B	141	VAL	2.5
2	E	133	VAL	2.5
2	G	137	LEU	2.5
1	H	259	ALA	2.5
2	K	209	ARG	2.5
2	I	204	ASP	2.5
1	J	155	TRP	2.5
2	I	209	ARG	2.4
2	C	133	VAL	2.4
1	J	102	LEU	2.4
1	D	222	HIS	2.4
1	D	125	VAL	2.4
1	D	6	ALA	2.4
2	I	134	ALA	2.4
2	I	177	LEU	2.4
2	I	220	ALA	2.4
2	C	177	LEU	2.4
1	D	140	GLU	2.4
2	K	222	SER	2.4
1	B	126	VAL	2.3
1	F	14	GLN	2.4
2	I	131	PRO	2.3
1	F	6	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	131	PRO	2.3
1	D	137	SER	2.3
2	I	11	VAL	2.3
1	B	5	THR	2.3
1	H	202	SER	2.3
2	K	30	ALA	2.3
2	I	223	GLU	2.3
1	J	203	LYS	2.3
1	J	126	VAL	2.2
2	A	133	VAL	2.2
1	L	136	LEU	2.2
2	C	31	GLY	2.2
1	H	219	LYS	2.2
1	J	222	HIS	2.2
2	C	30	ALA	2.2
1	H	134	VAL	2.2
1	J	141	VAL	2.2
1	B	102	LEU	2.2
2	E	276	ALA	2.2
1	F	135	PRO	2.1
2	E	131	PRO	2.1
2	G	221	LYS	2.1
1	D	136	LEU	2.1
1	F	140	GLU	2.1
2	I	157	HIS	2.1
1	B	68	LYS	2.1
1	J	219	LYS	2.1
1	F	204	ASP	2.1
2	I	270	ARG	2.1
1	J	22	LEU	2.1
2	I	213	GLU	2.1
2	C	276	ALA	2.1
2	G	205	ARG	2.1
1	L	137[A]	SER	2.1
1	D	134	VAL	2.1
1	J	218	ALA	2.1
1	J	140	GLU	2.1
1	H	260	GLY	2.0
2	K	272	GLY	2.0
1	F	141	VAL	2.0
2	K	270	ARG	2.0
2	K	136[A]	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	16	ALA	2.0
2	I	127	TYR	2.0
2	K	128	VAL	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	8M0	J	302	36/36	0.72	0.42	72,77,81,82	36
5	8M0	H	303	36/36	0.81	0.34	56,61,66,67	36
5	8M0	L	303	36/36	0.88	0.23	41,44,50,52	36
5	8M0	F	303	36/36	0.89	0.23	27,37,41,44	36
5	8M0	C	301	36/36	0.90	0.23	27,36,44,46	36
8	LJB	L	306	34/34	0.90	0.06	57,64,74,99	34
8	LJB	B	306	34/34	0.90	0.06	47,60,63,68	34
11	LHW	C	305	45/45	0.91	0.08	40,57,62,63	45
3	ADP	H	301	27/27	0.92	0.13	25,29,34,35	0
5	8M0	B	303	36/36	0.93	0.22	25,34,38,39	36
11	LHW	K	304	45/45	0.93	0.09	48,61,66,70	44
3	ADP	J	301	27/27	0.93	0.11	19,25,28,33	0
7	PO4	B	305[B]	5/5	0.93	0.11	15,16,18,27	5
7	PO4	F	305[B]	5/5	0.94	0.12	16,18,20,27	5
9	ATP	G	301	31/31	0.94	0.10	17,22,27,28	0
7	PO4	H	305[B]	5/5	0.94	0.11	26,26,28,31	5
3	ADP	L	301	27/27	0.95	0.10	18,21,26,29	0
3	ADP	B	301	27/27	0.95	0.10	14,18,21,22	0
3	ADP	F	301	27/27	0.95	0.10	15,20,24,25	0
7	PO4	L	305[B]	5/5	0.95	0.13	20,20,22,25	5

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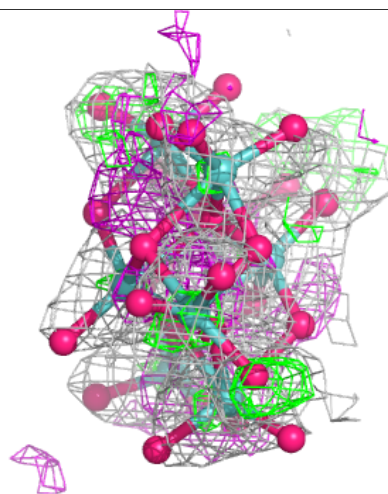
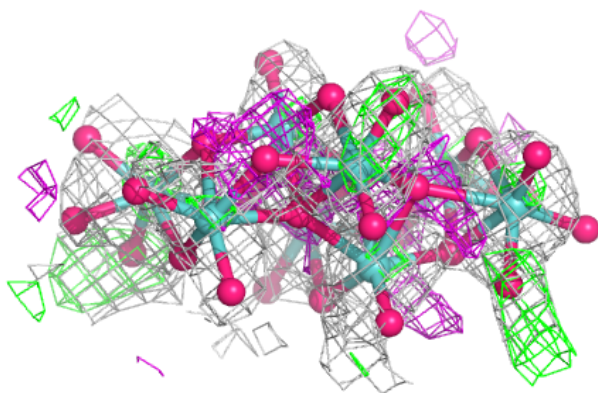
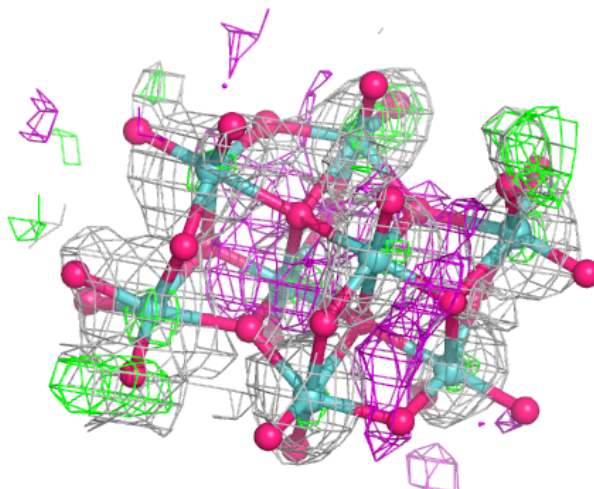
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	ATP	I	301	31/31	0.95	0.11	20,26,32,39	0
9	ATP	C	302	31/31	0.96	0.10	15,17,23,25	0
4	MG	J	303	1/1	0.96	0.17	12,12,12,12	1
9	ATP	A	301	31/31	0.96	0.09	13,17,19,19	0
9	ATP	K	301	31/31	0.96	0.11	16,21,26,28	0
3	ADP	D	301	27/27	0.96	0.10	18,23,28,33	0
9	ATP	E	301	31/31	0.96	0.10	14,21,25,31	0
4	MG	G	302	1/1	0.96	0.05	19,19,19,19	0
4	MG	C	303	1/1	0.97	0.05	14,14,14,14	0
7	PO4	D	304[B]	5/5	0.97	0.14	21,22,24,33	5
4	MG	L	302	1/1	0.97	0.07	21,21,21,21	0
5	8M0	C	304	34/36	0.97	0.13	18,25,30,37	0
4	MG	D	302	1/1	0.97	0.06	21,21,21,21	0
4	MG	I	302	1/1	0.97	0.06	19,19,19,19	0
6	MOO	B	304[A]	5/5	0.97	0.11	14,18,23,27	5
4	MG	H	302	1/1	0.97	0.08	24,24,24,24	0
5	8M0	K	303	34/36	0.97	0.16	22,29,34,41	0
7	PO4	J	305[B]	5/5	0.98	0.09	22,26,29,30	5
5	8M0	G	303	34/36	0.98	0.14	23,29,35,36	0
6	MOO	J	304[A]	5/5	0.98	0.09	21,24,25,29	5
5	8M0	E	303	34/36	0.98	0.13	18,26,30,37	0
4	MG	K	302	1/1	0.98	0.05	19,19,19,19	0
4	MG	E	302	1/1	0.98	0.06	19,19,19,19	0
6	MOO	H	304[A]	5/5	0.98	0.09	25,27,30,31	5
5	8M0	A	303	34/36	0.98	0.12	15,26,31,40	0
4	MG	F	302	1/1	0.98	0.05	17,17,17,17	0
5	8M0	I	303	34/36	0.98	0.12	23,31,37,41	0
6	MOO	D	303[A]	5/5	0.99	0.08	17,19,23,24	5
6	MOO	L	304[A]	5/5	0.99	0.07	18,19,22,22	5
6	MOO	F	304[A]	5/5	0.99	0.10	14,18,20,20	5
10	M10	G	304	13/16	0.99	0.08	16,22,24,27	0
4	MG	B	302	1/1	0.99	0.05	16,16,16,16	0
4	MG	A	302	1/1	0.99	0.05	15,15,15,15	0
10	M10	A	304	13/16	0.99	0.09	16,18,23,23	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.

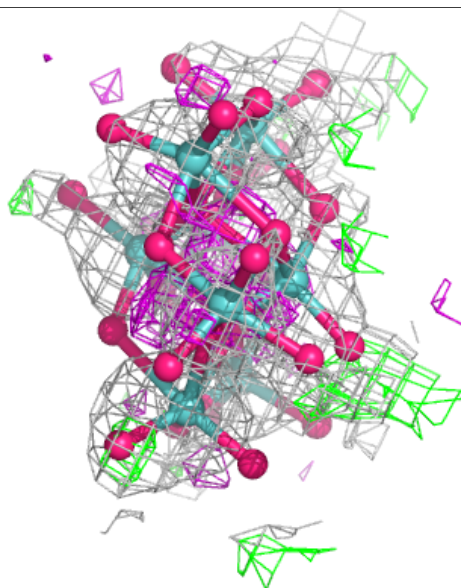
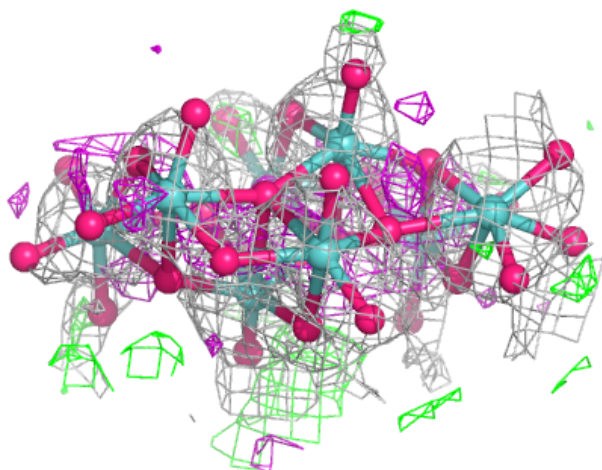
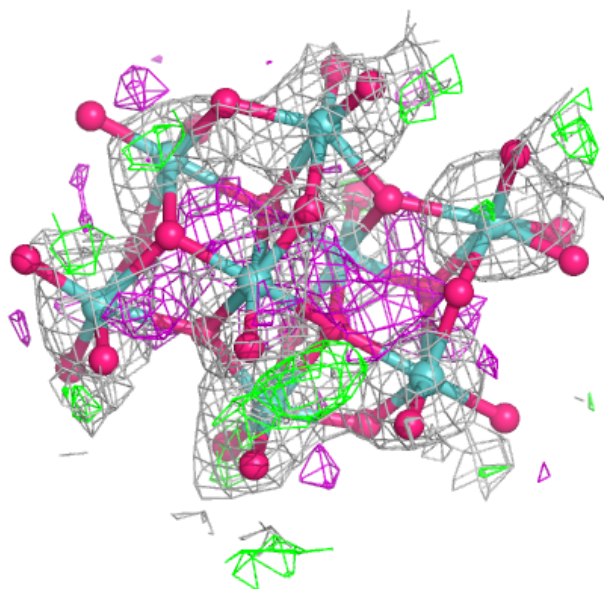
Electron density around 8M0 J 302:

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



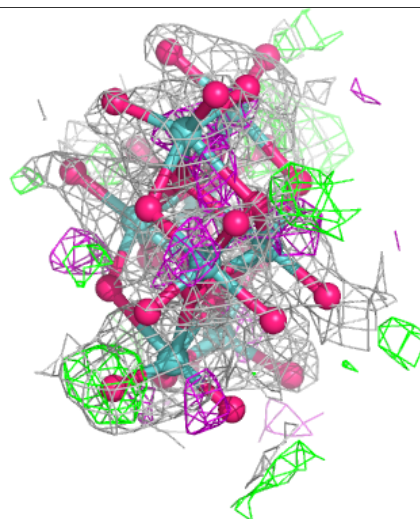
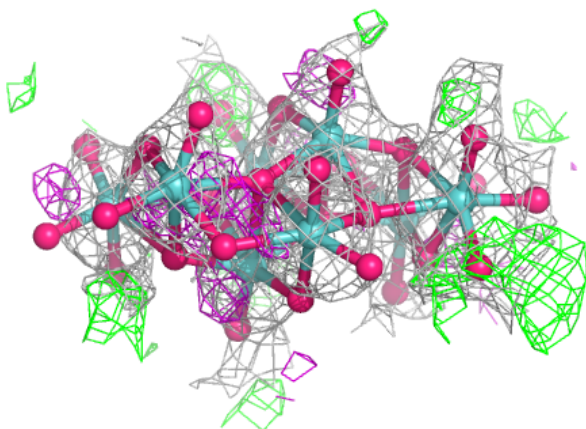
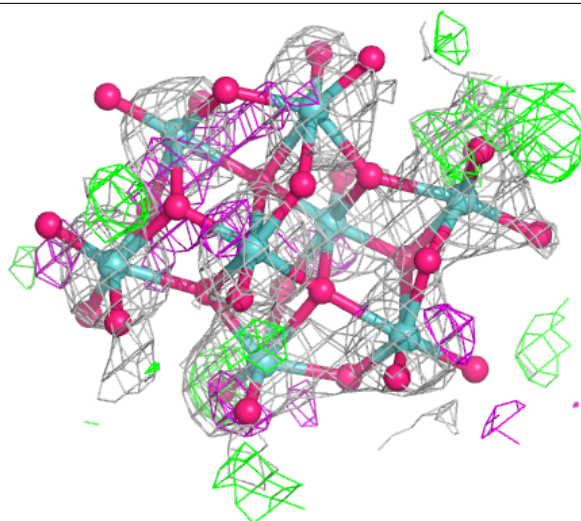
Electron density around 8M0 H 303:

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



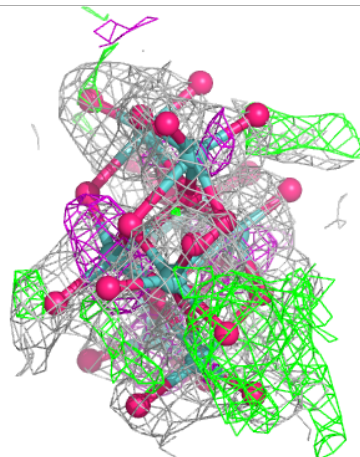
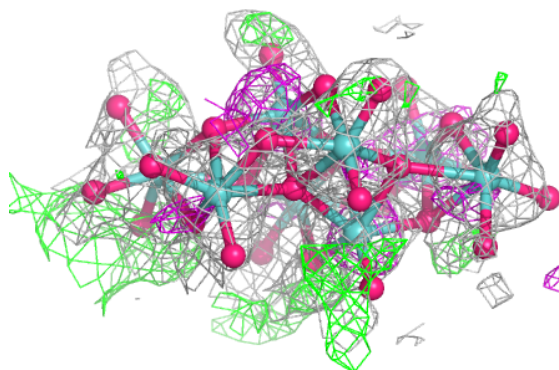
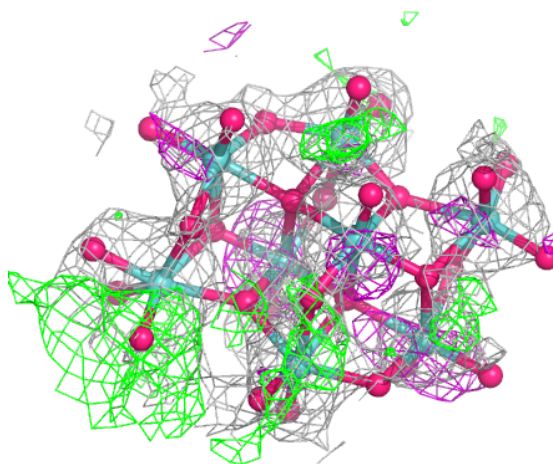
Electron density around 8M0 L 303:

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



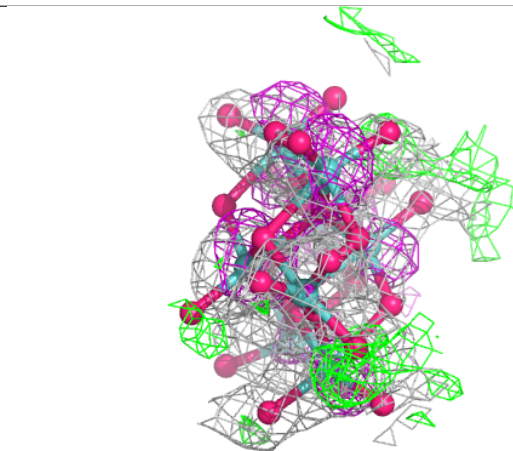
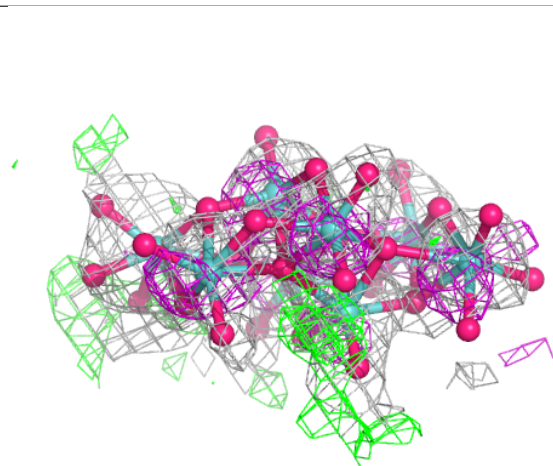
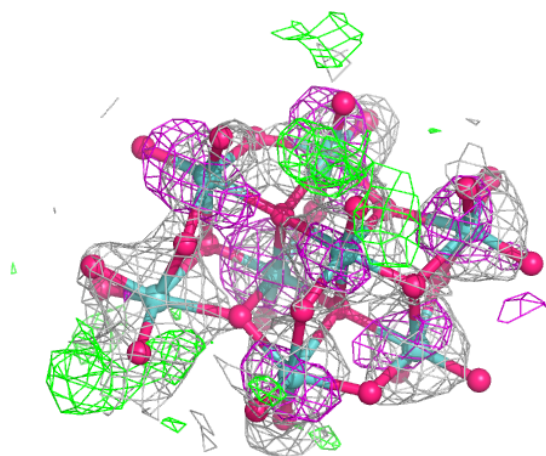
Electron density around 8M0 F 303:

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



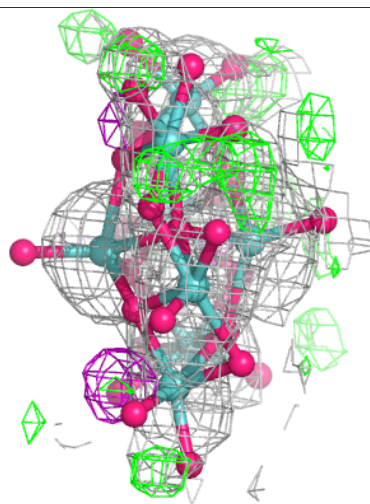
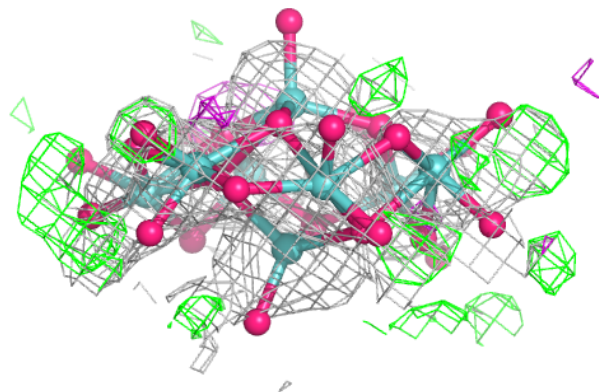
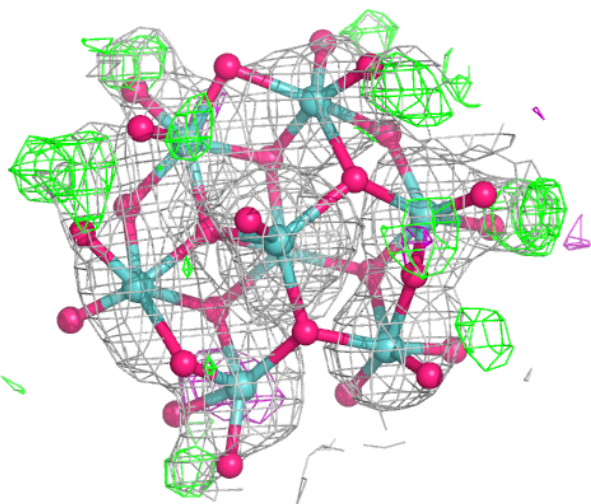
Electron density around 8M0 C 301:

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



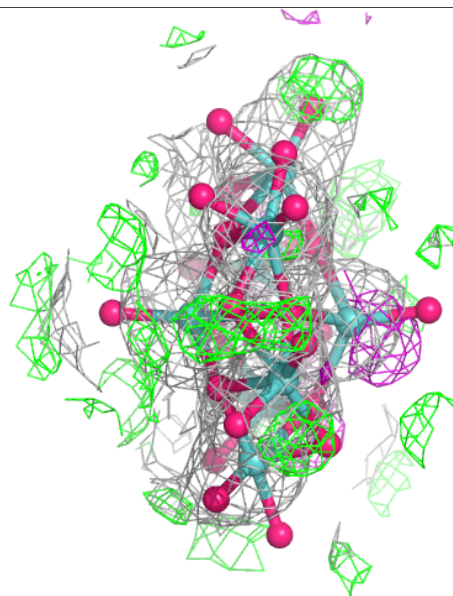
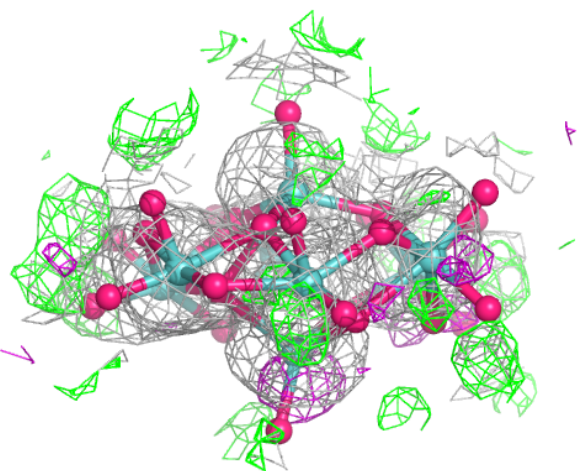
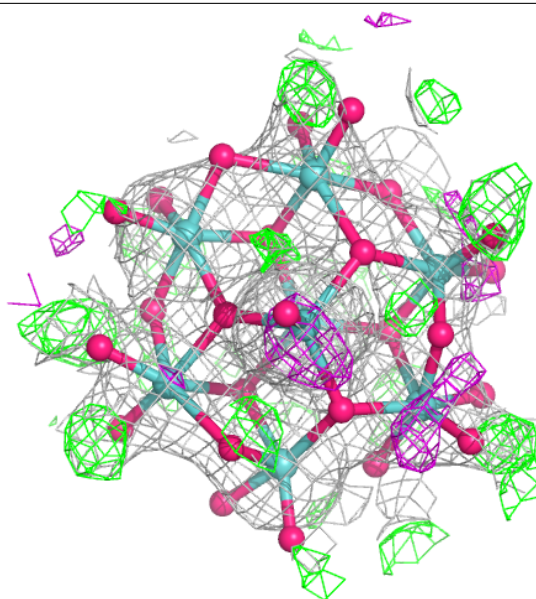
Electron density around LJB L 306:

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



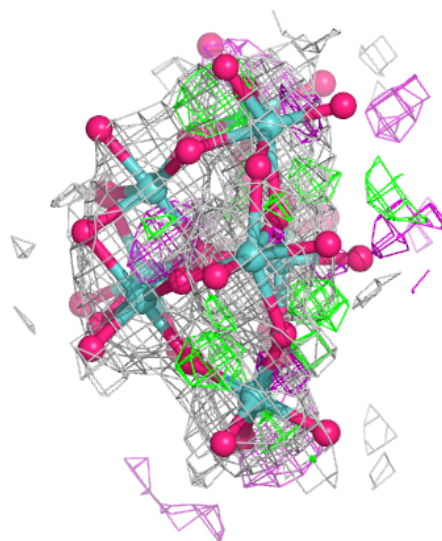
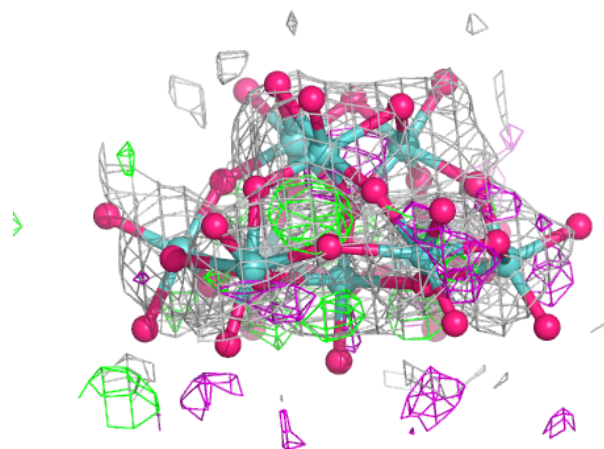
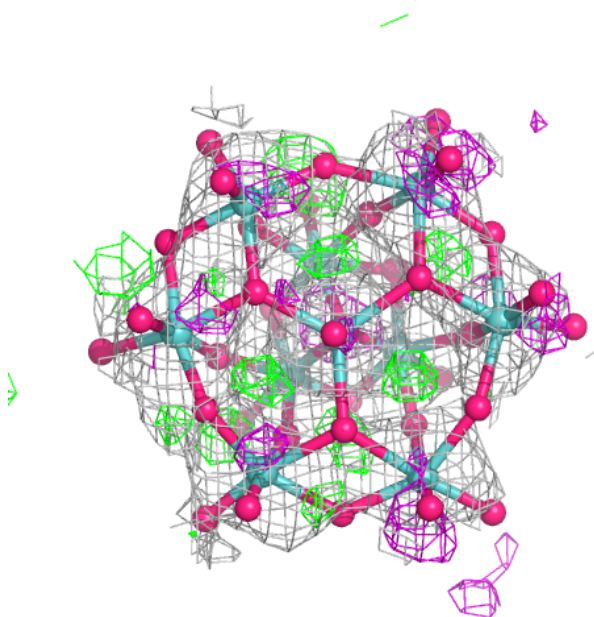
Electron density around LJB B 306:

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



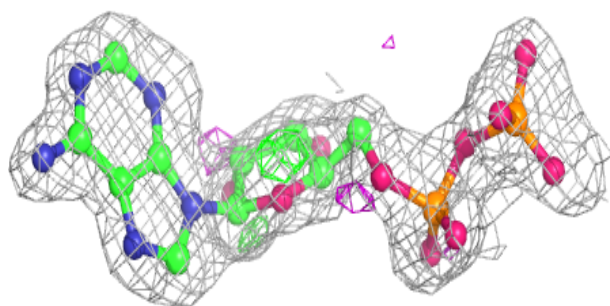
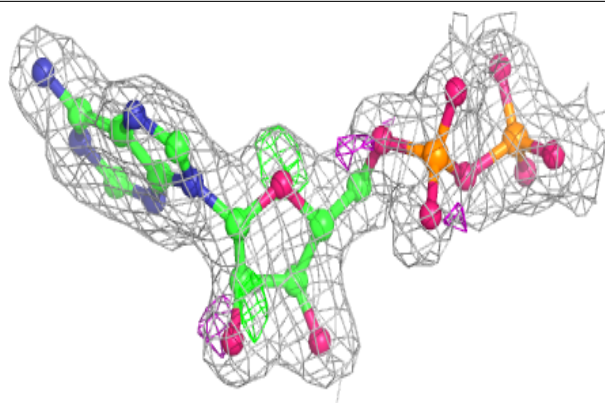
Electron density around LHW C 305:

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



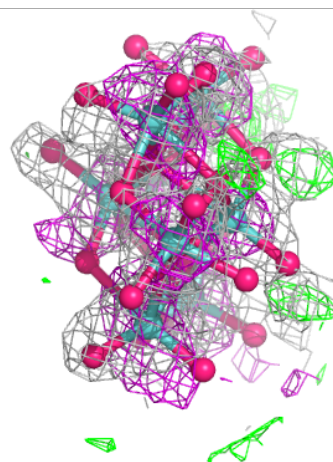
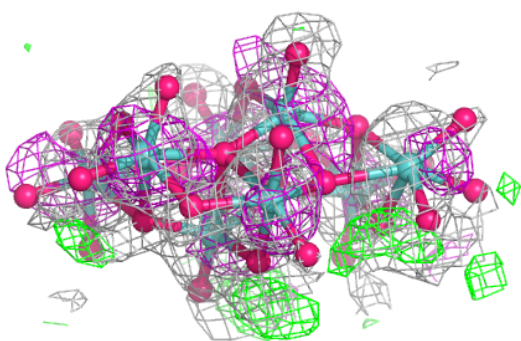
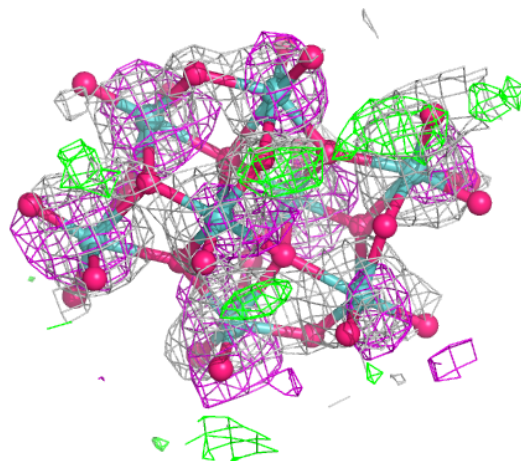
Electron density around ADP H 301:

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



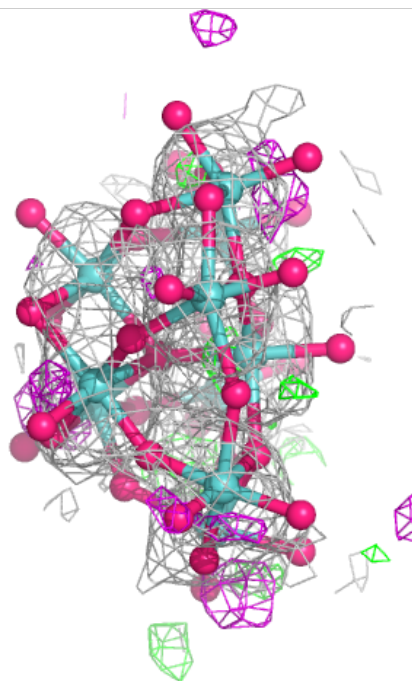
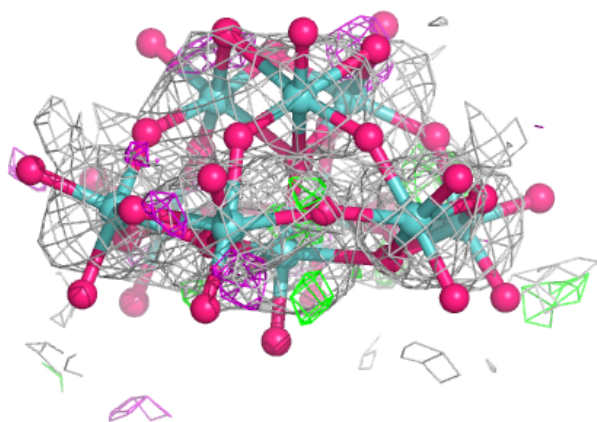
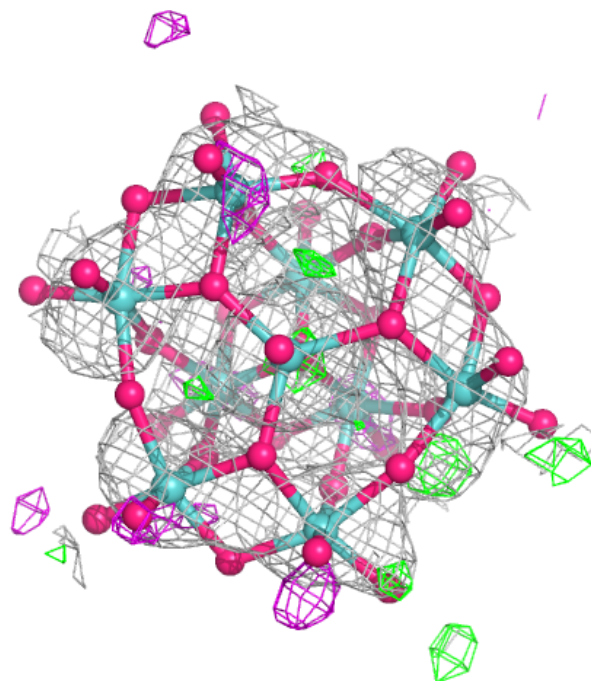
Electron density around 8M0 B 303:

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



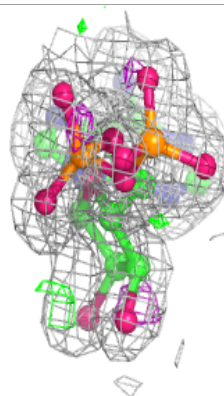
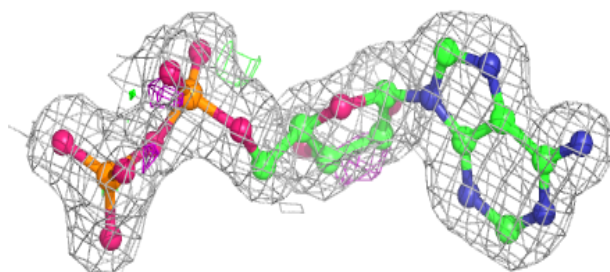
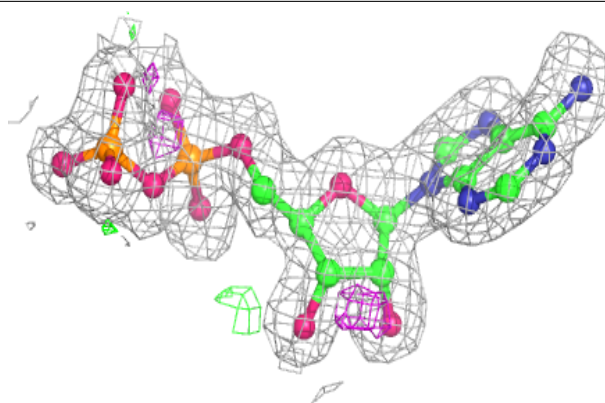
Electron density around LHW K 304:

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

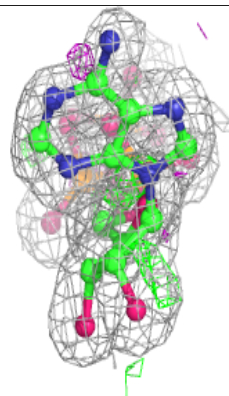
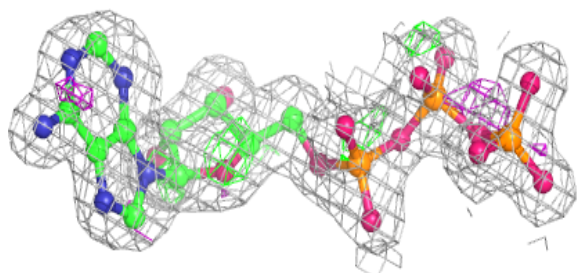
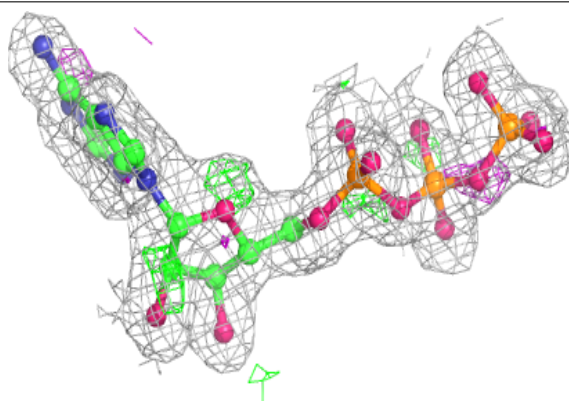


Electron density around ADP J 301:

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

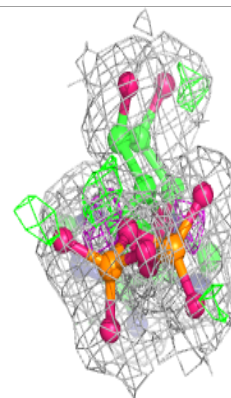
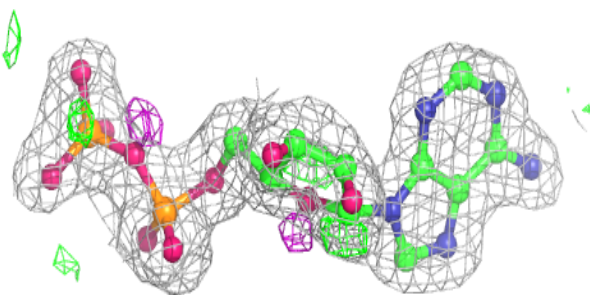
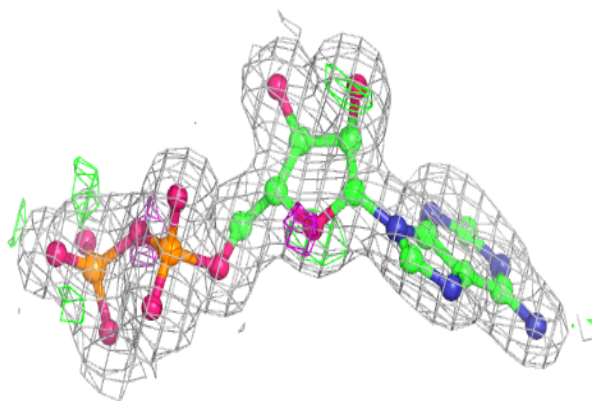
**Electron density around ATP G 301:**

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

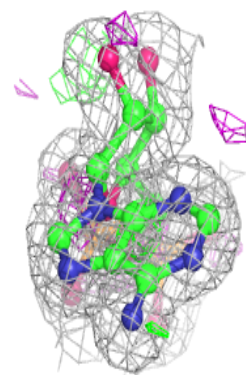
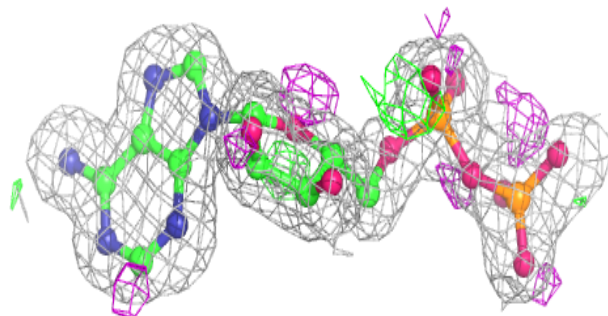
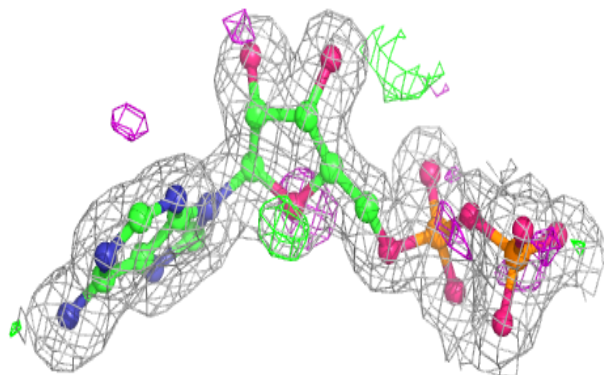


Electron density around ADP L 301:

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

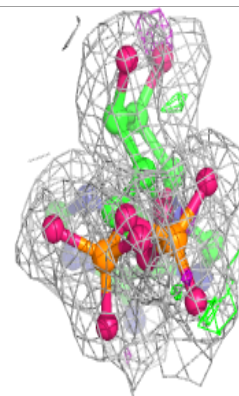
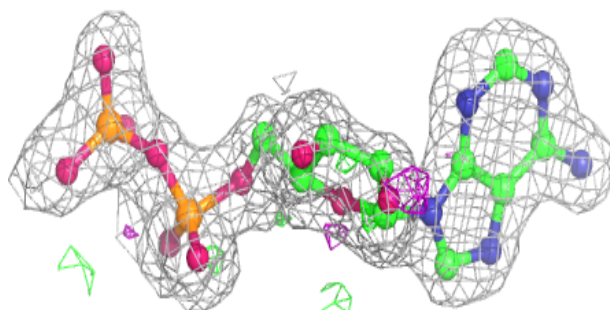
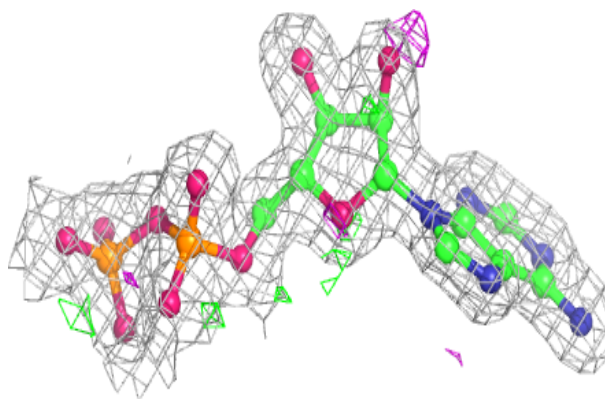
**Electron density around ADP B 301:**

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

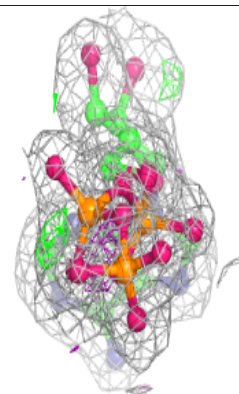
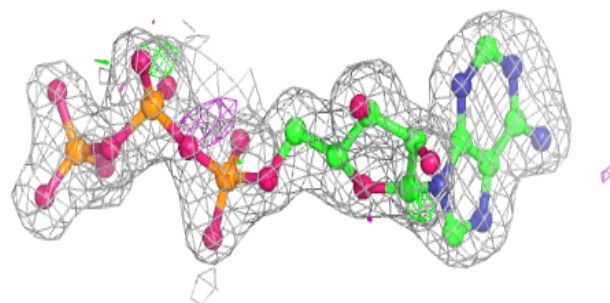
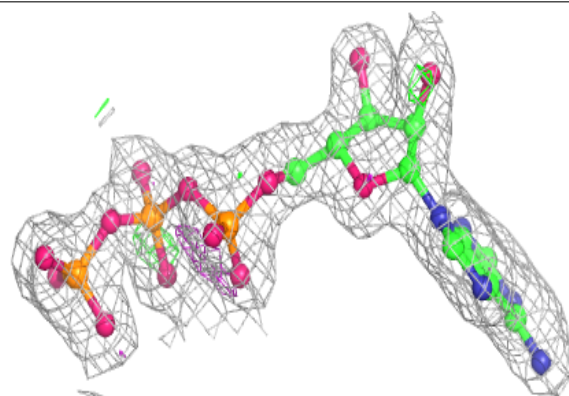


Electron density around ADP F 301:

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

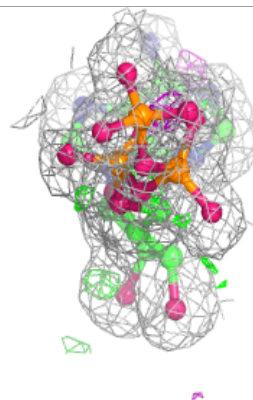
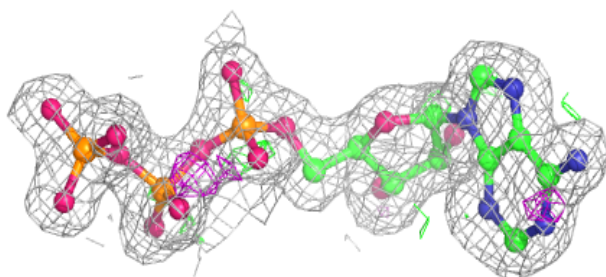
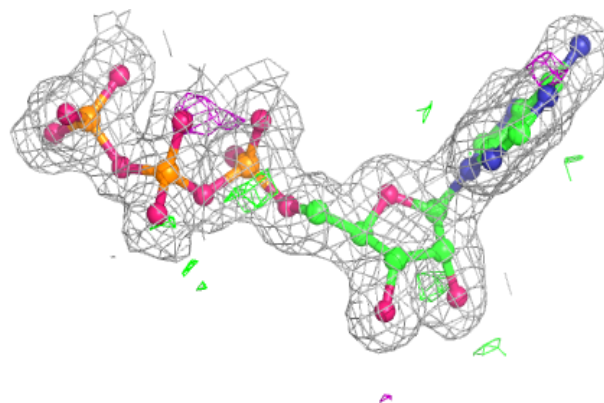
**Electron density around ATP I 301:**

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

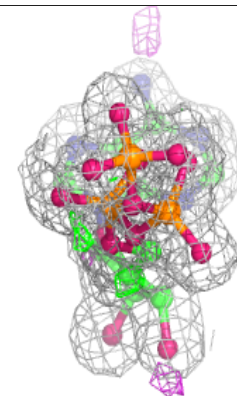
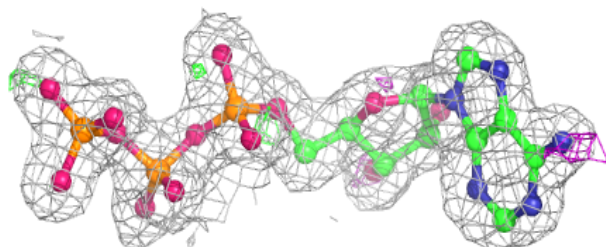
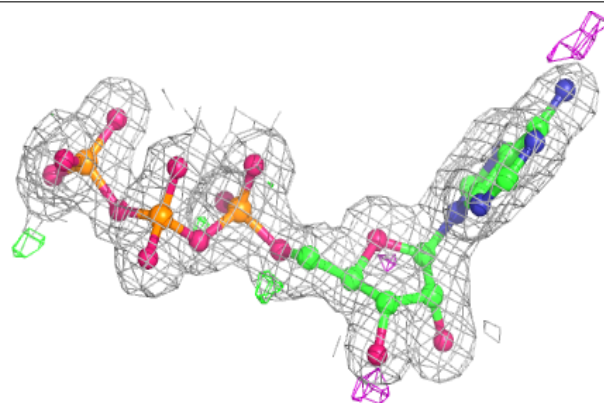


Electron density around ATP C 302:

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

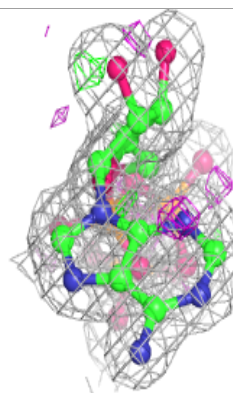
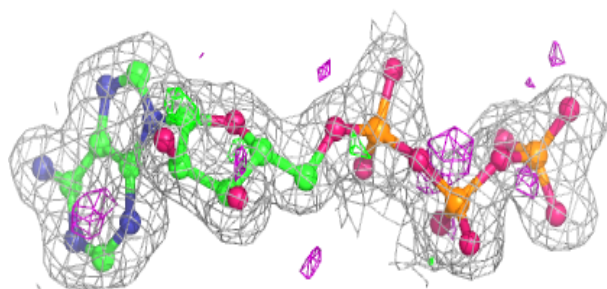
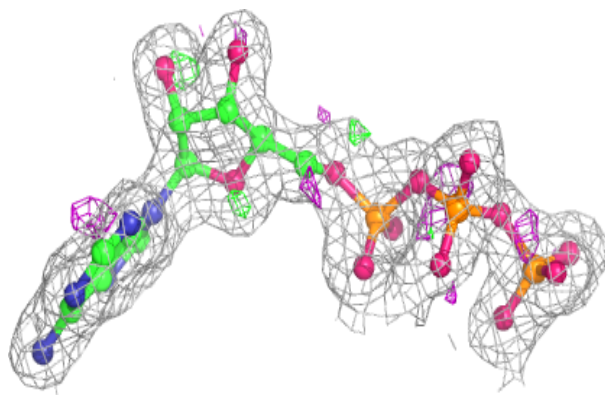
**Electron density around ATP A 301:**

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and green (positive)

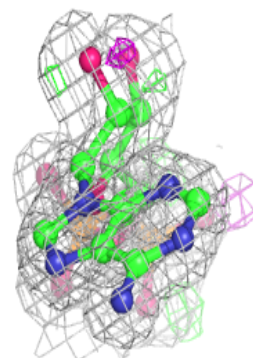
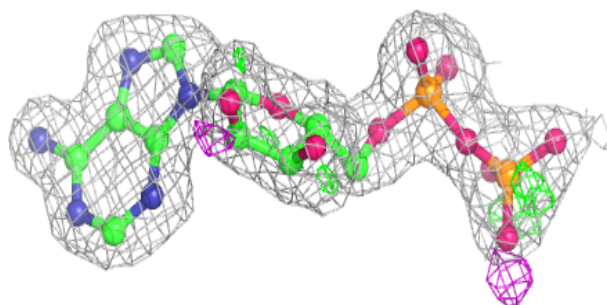
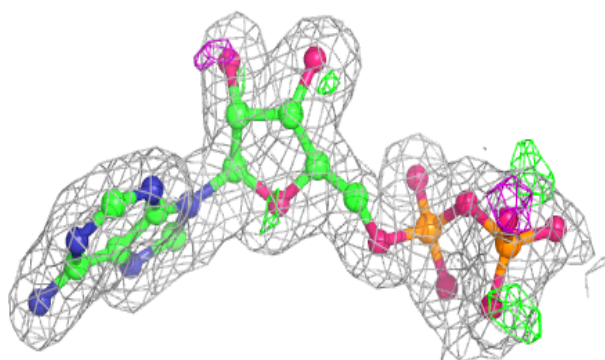


Electron density around ATP K 301:

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

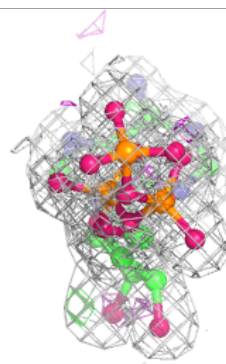
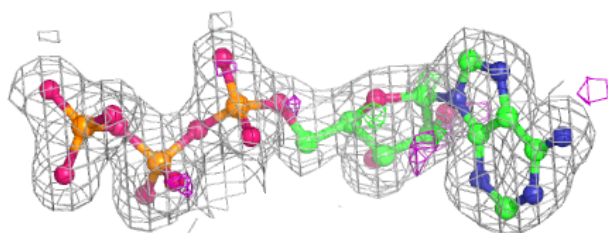
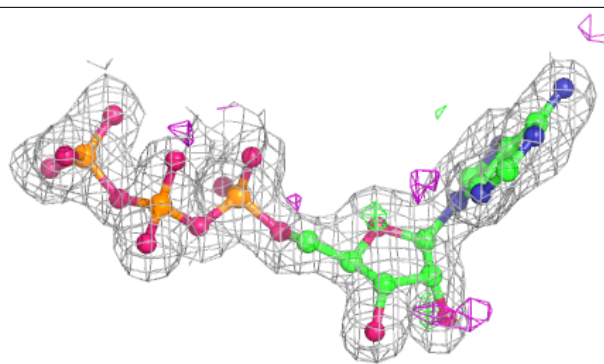
**Electron density around ADP D 301:**

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

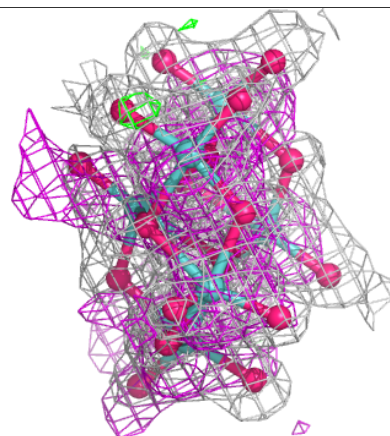
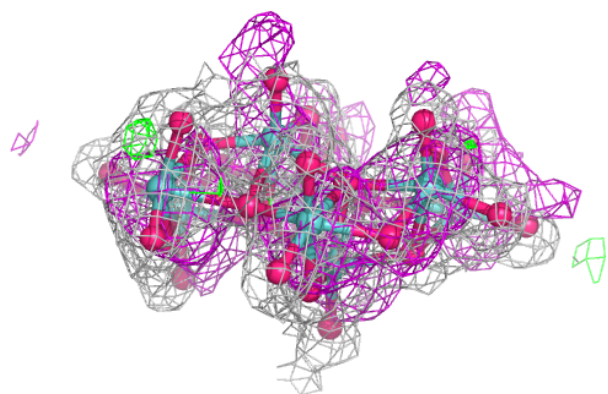
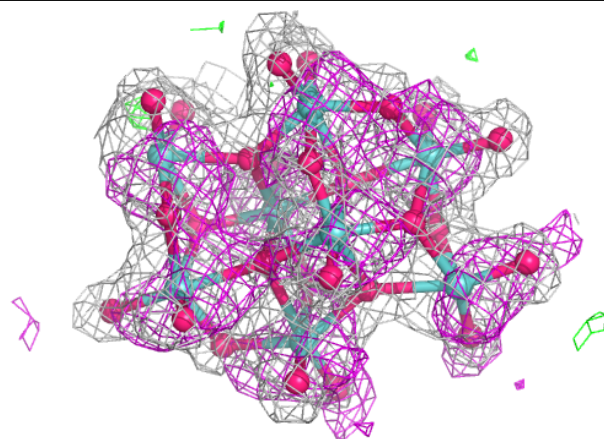


Electron density around ATP E 301:

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

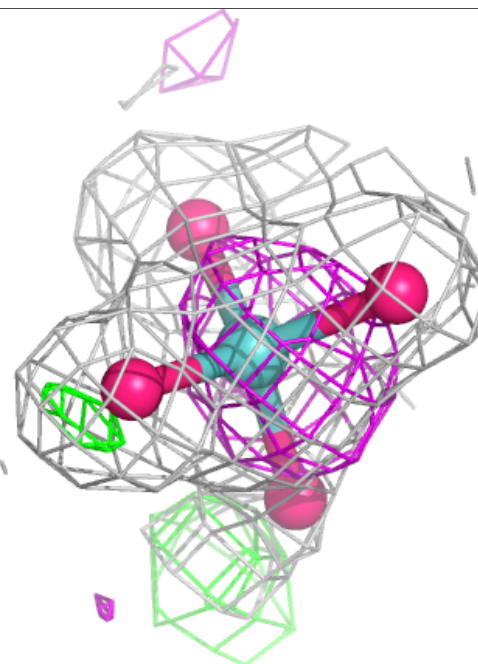
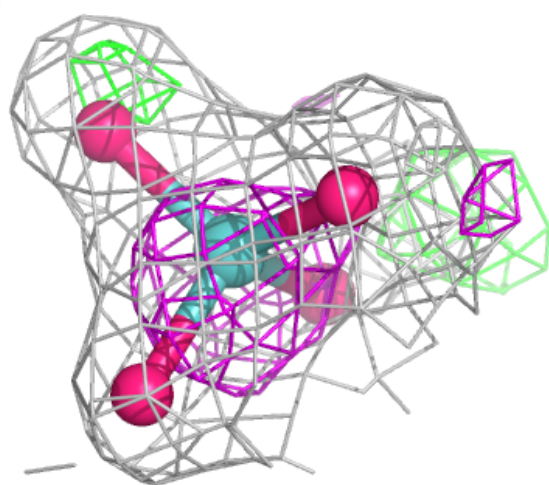
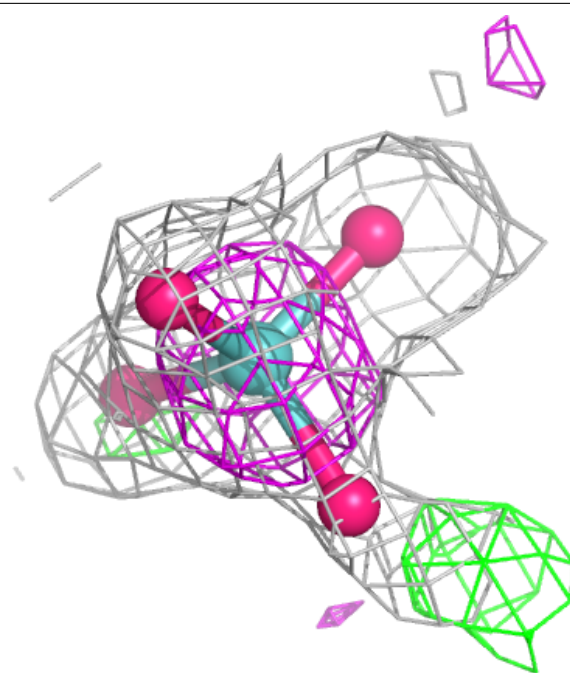
**Electron density around 8M0 C 304:**

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



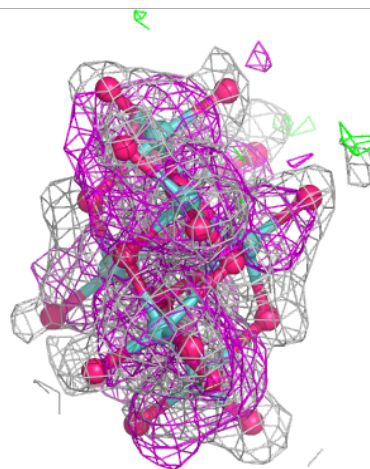
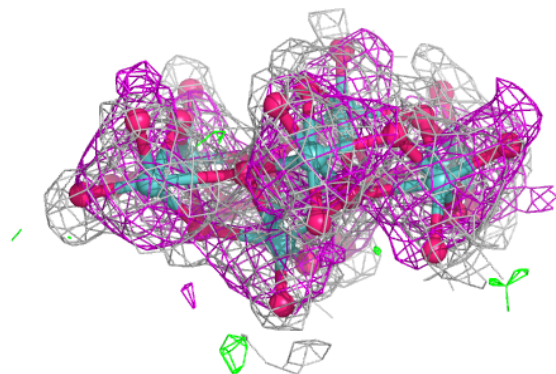
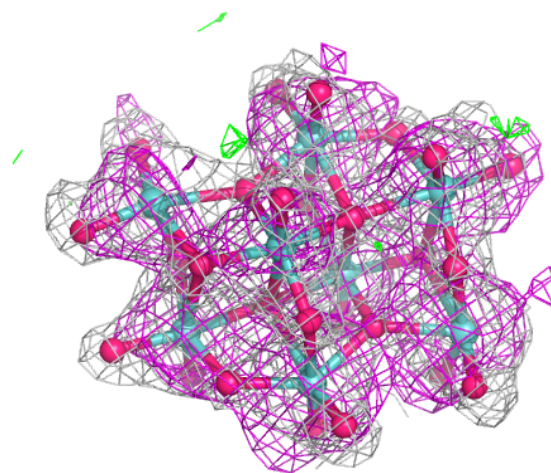
Electron density around MOO B 304 (A):

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



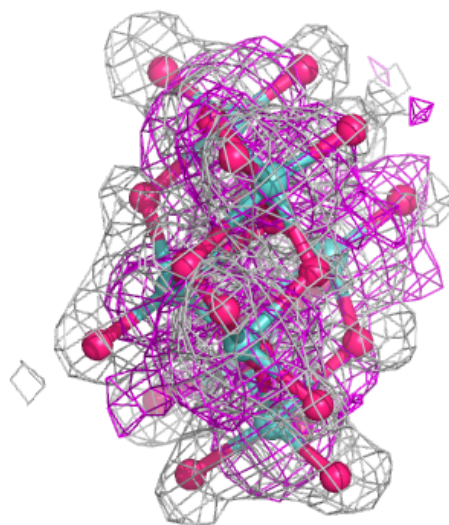
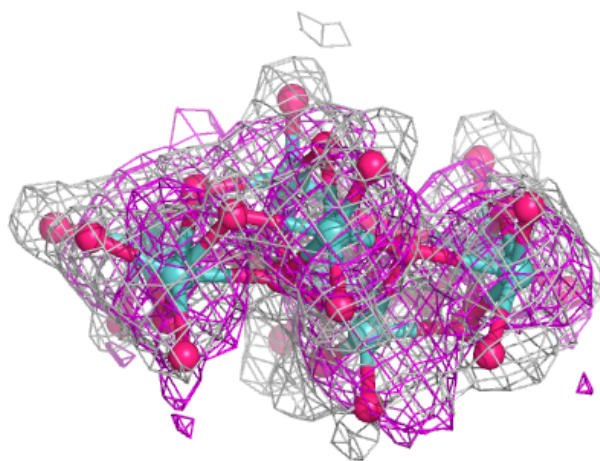
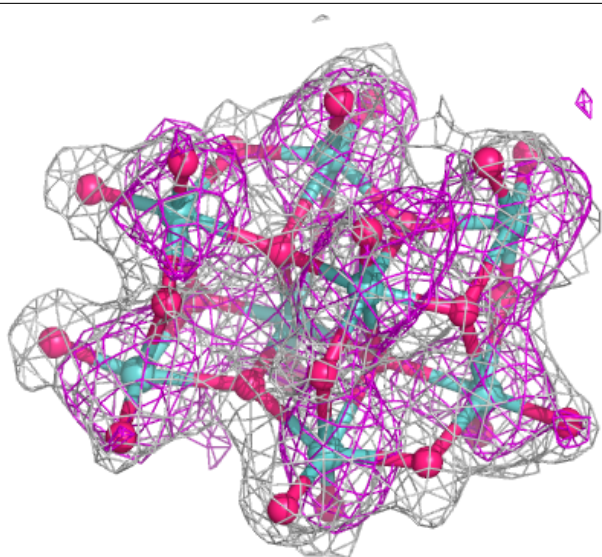
Electron density around 8M0 K 303:

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



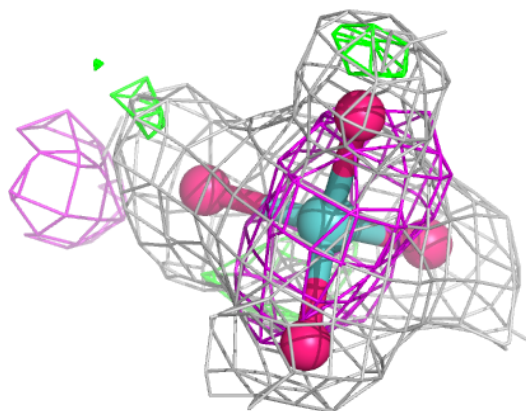
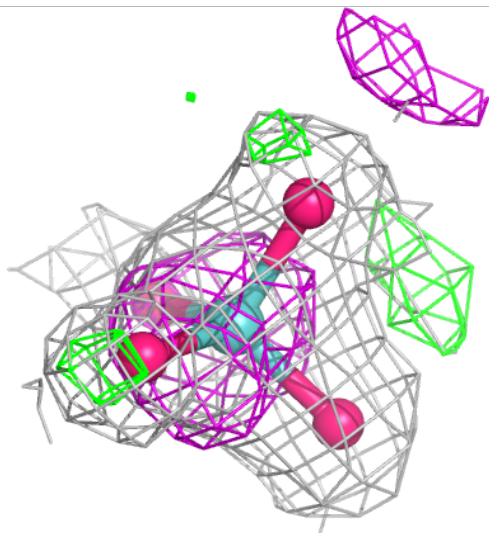
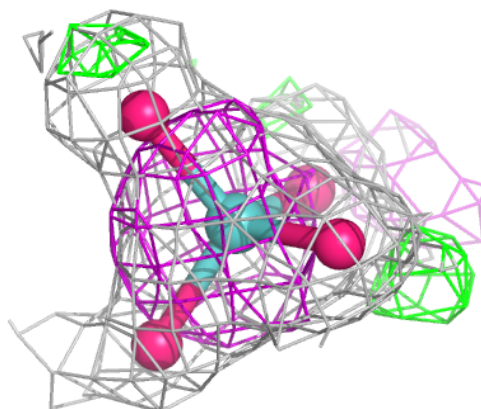
Electron density around 8M0 G 303:

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



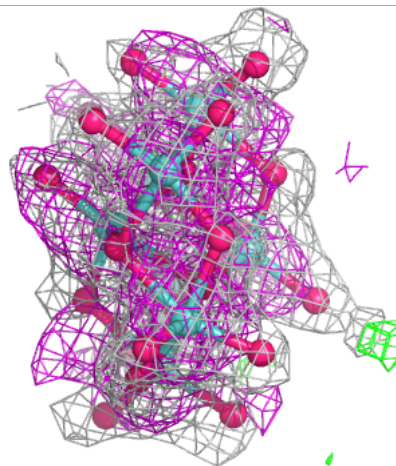
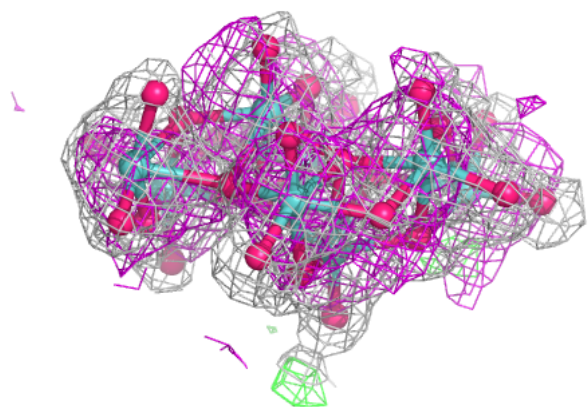
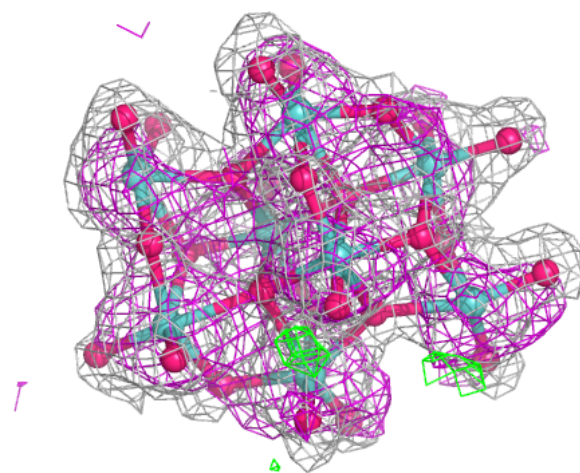
Electron density around MOO J 304 (A):

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



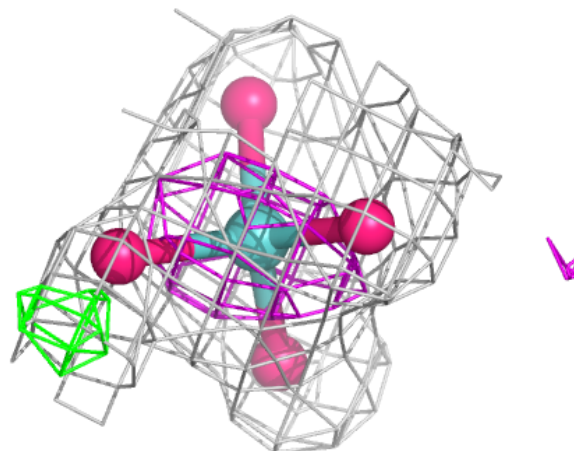
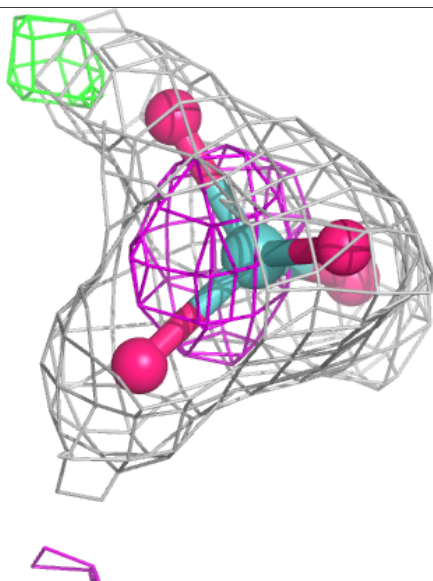
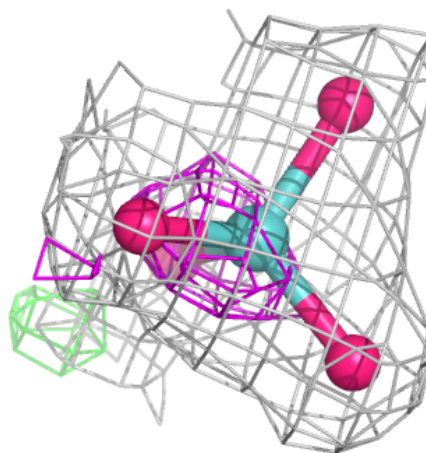
Electron density around 8M0 E 303:

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



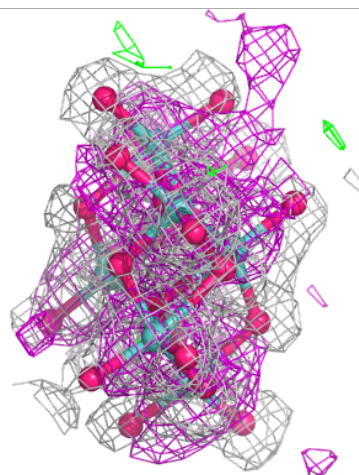
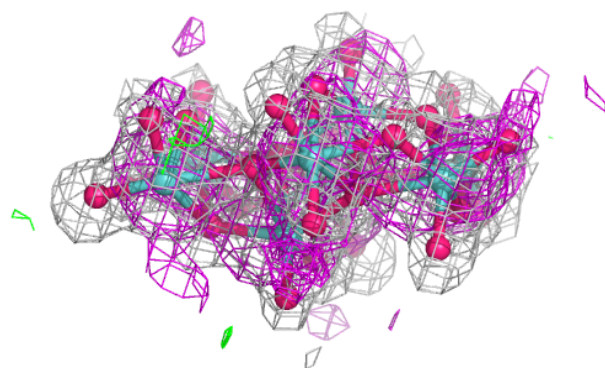
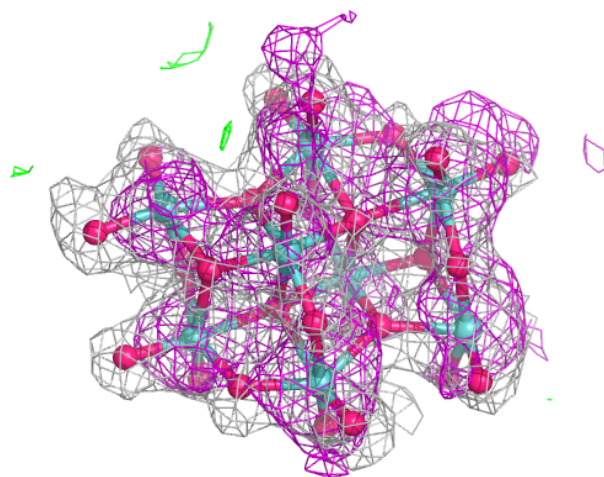
Electron density around MOO H 304 (A):

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



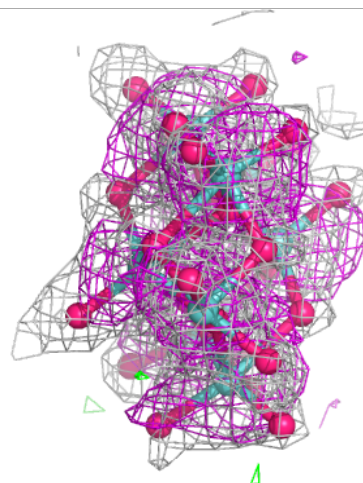
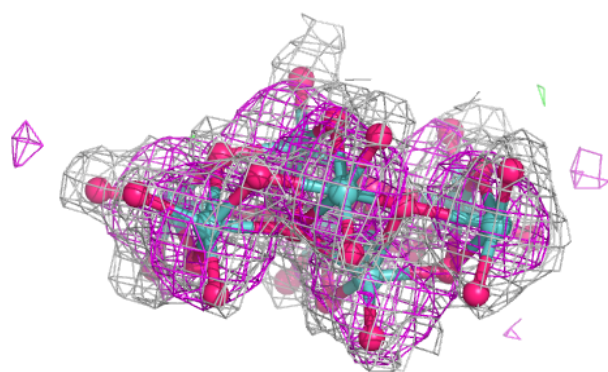
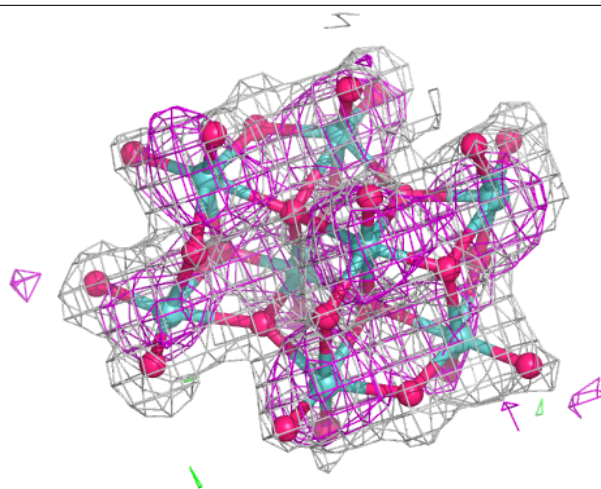
Electron density around 8M0 A 303:

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



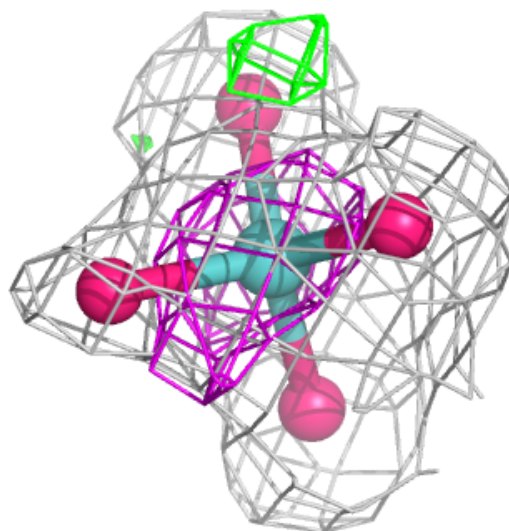
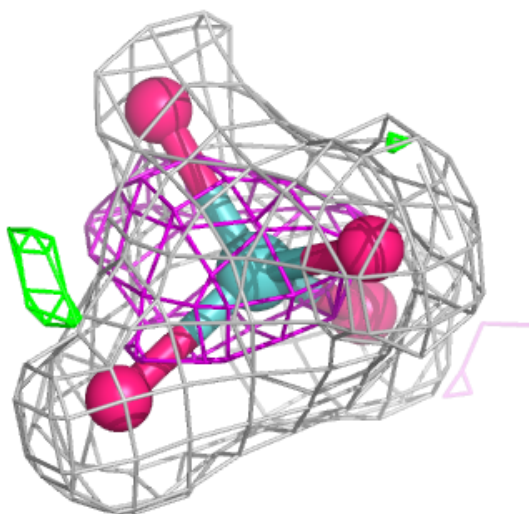
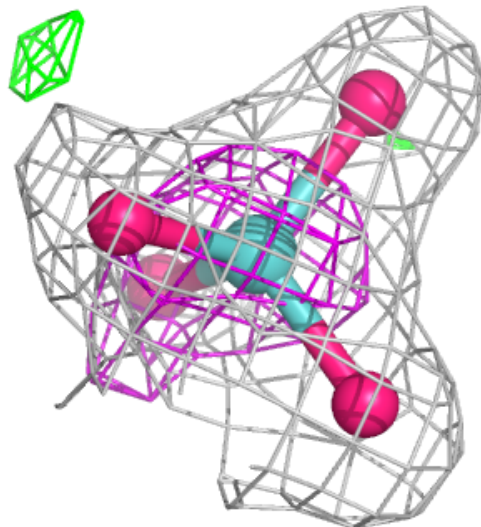
Electron density around 8M0 I 303:

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



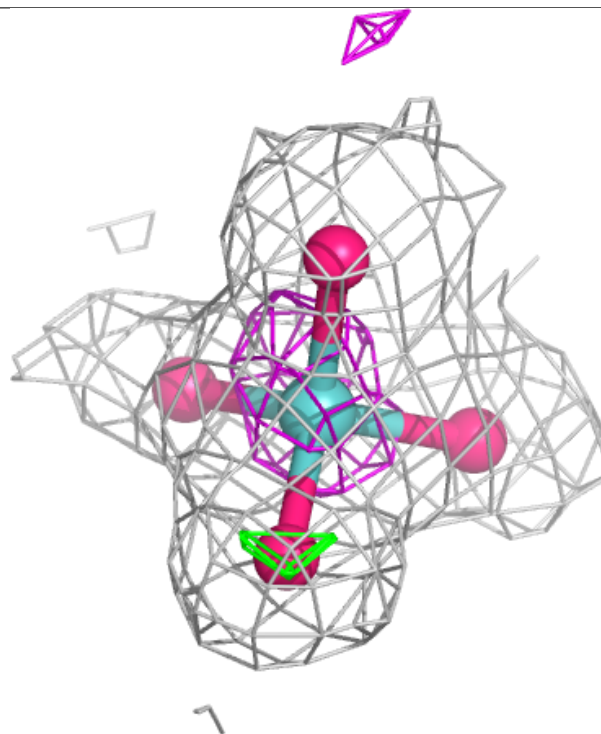
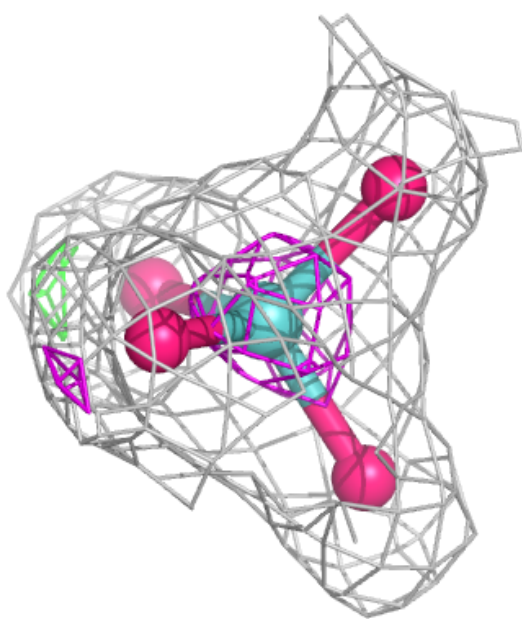
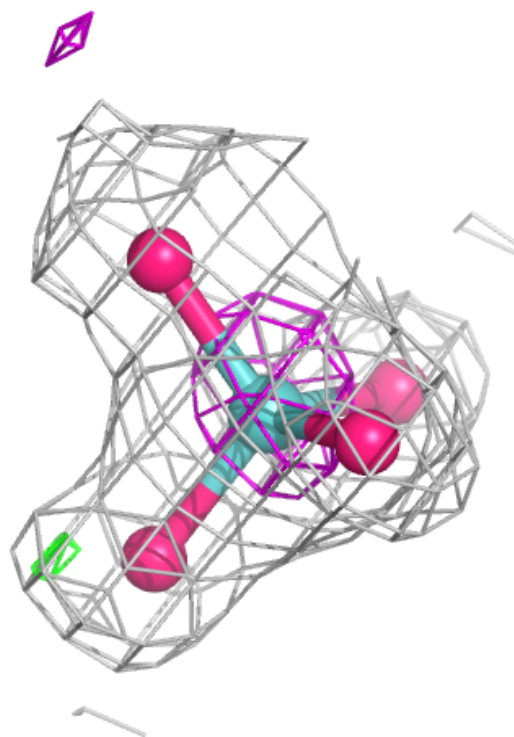
Electron density around MOO D 303 (A):

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



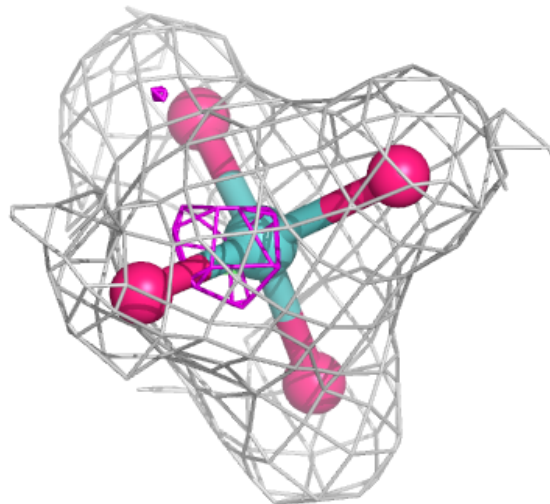
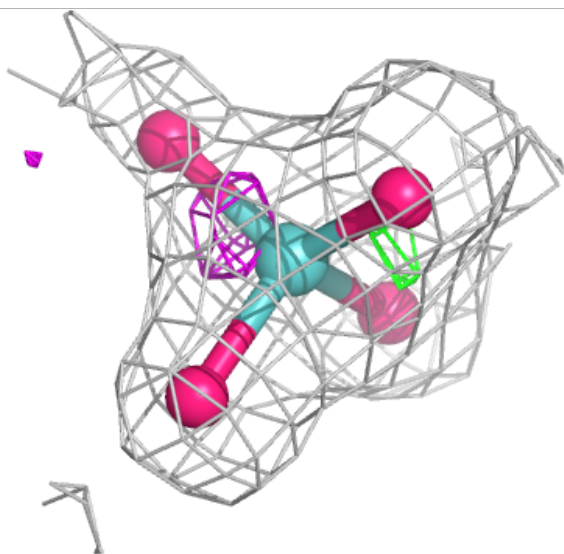
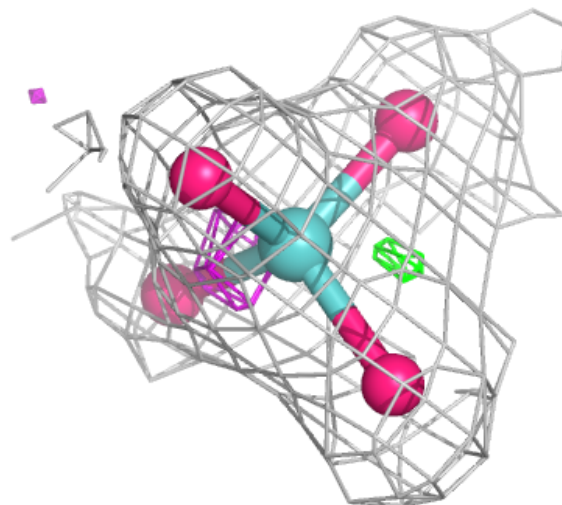
Electron density around MOO L 304 (A):

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



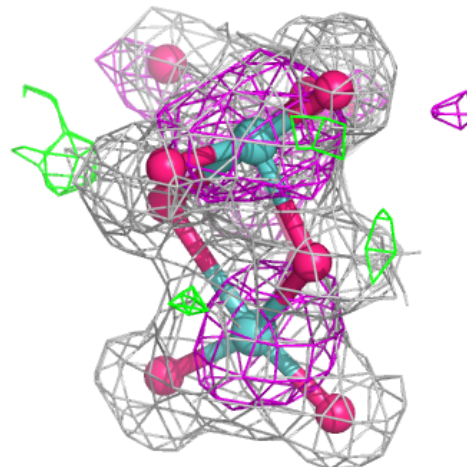
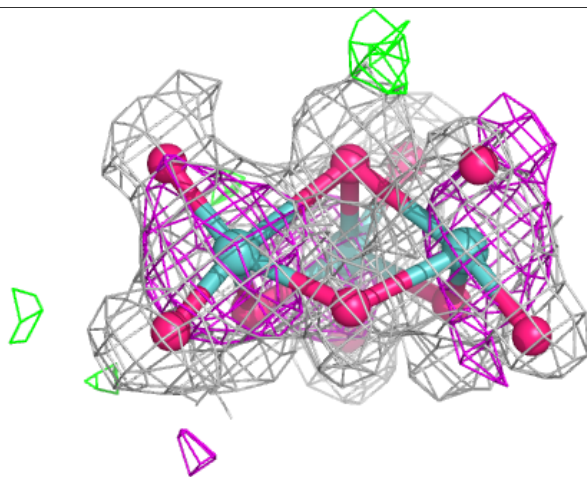
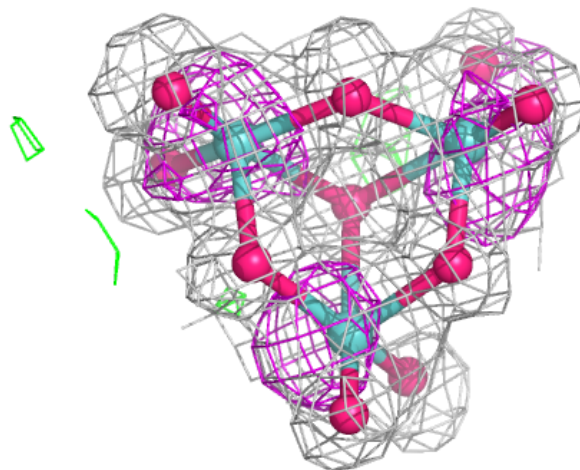
Electron density around MOO F 304 (A):

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



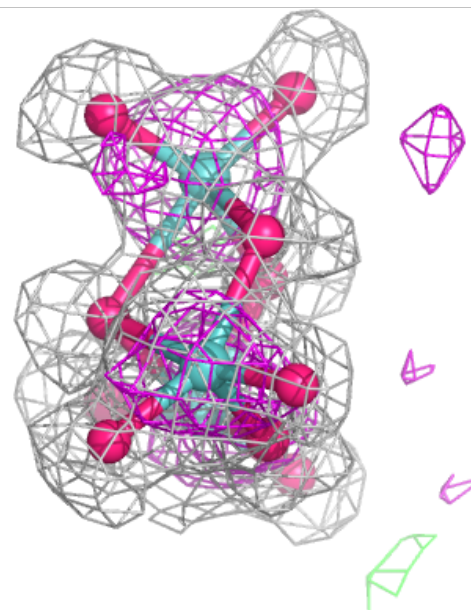
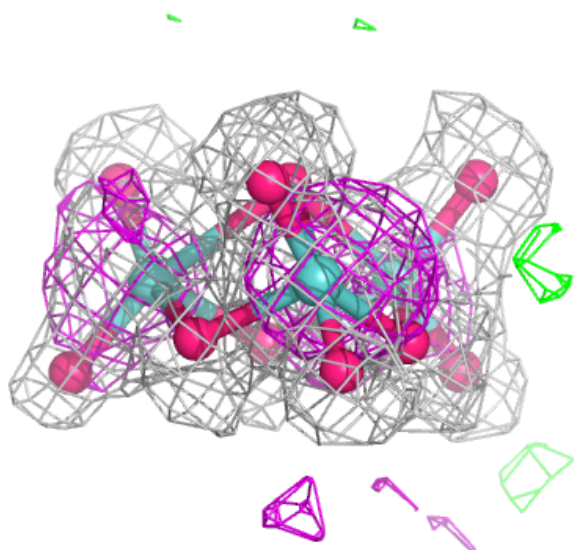
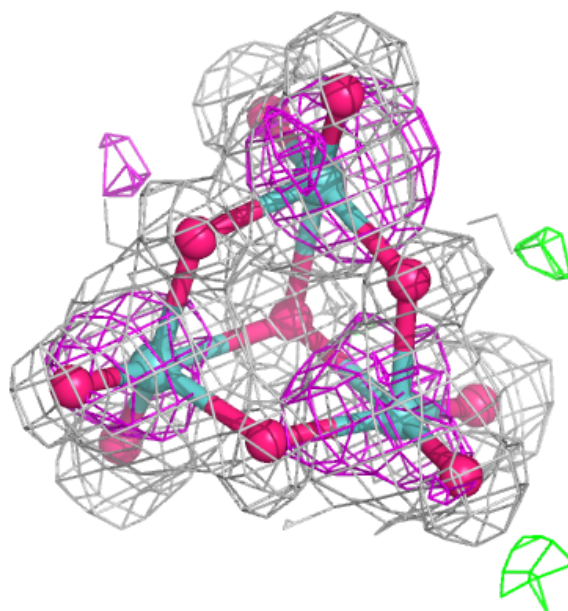
Electron density around M10 G 304:

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



Electron density around M10 A 304:

$2mF_o-DF_c$ (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.