



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 05:07 PM EDT

PDB ID : 7T8S
Title : Light Harvesting complex phycoerythrin PE 566, from the cryptophyte *Cryptomonas pyrenoidifera*
Authors : Michie, K.A.; Harrop, S.J.; Rathbone, H.W.; Wilk, K.E.; Curmi, P.M.G.
Deposited on : 2021-12-17
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

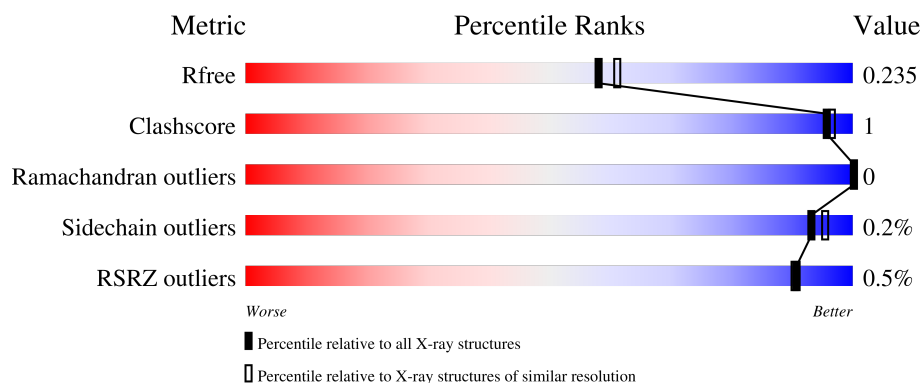
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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






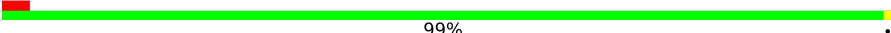
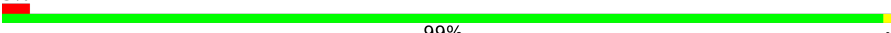
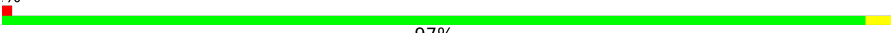
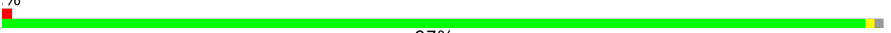

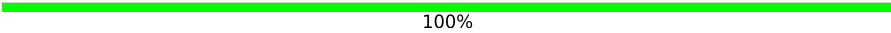
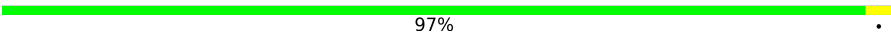

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	178	<div> <div>%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
1	C	178	<div> <div></div> <div>89%</div> <div></div> <div>8%</div> </div>
1	E	178	<div> <div></div> <div>96%</div> <div></div> <div></div> </div>
1	G	178	<div> <div></div> <div>90%</div> <div></div> <div>8%</div> </div>
1	I	178	<div> <div></div> <div>90%</div> <div></div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	178	 89% . 8%
1	M	178	 92% . .
1	O	178	 89% . 8%
2	B	78	 99% .
2	F	78	 99% .
2	J	78	 97% .
2	N	78	 97% ..
3	D	70	 100%
3	H	70	 100%
3	L	70	 97% .
3	P	70	 99% .

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 32622 atoms, of which 15539 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 Phycoerythrin beta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	171	Total	C	H	N	O	S	0	6	0
			2522	784	1254	219	255	10			
1	C	164	Total	C	H	N	O	S	0	4	0
			2410	740	1207	211	242	10			
1	E	172	Total	C	H	N	O	S	0	4	0
			2533	784	1266	219	254	10			
1	G	164	Total	C	H	N	O	S	0	6	0
			2433	749	1215	214	245	10			
1	I	172	Total	C	H	N	O	S	0	7	0
			2561	794	1278	223	256	10			
1	K	164	Total	C	H	N	O	S	0	6	0
			2448	750	1227	215	246	10			
1	M	171	Total	C	H	N	O	S	0	4	0
			2519	780	1257	219	253	10			
1	O	164	Total	C	H	N	O	S	0	4	0
			2409	739	1208	210	242	10			

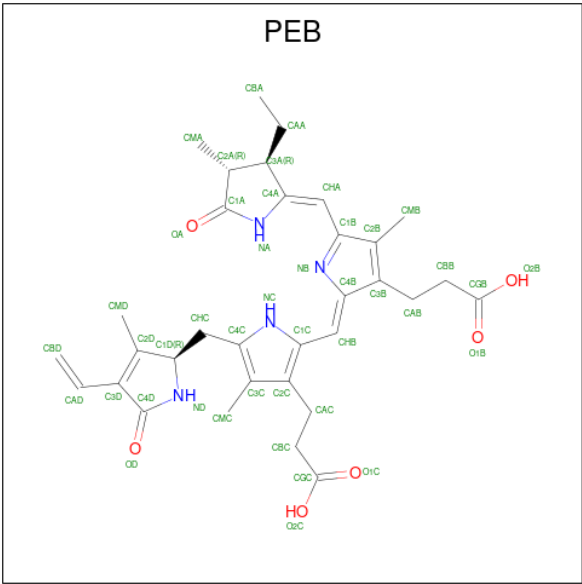
- Molecule 2 is a protein called phycoerythrin alpha-1 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	78	Total	C	H	N	O	S	0	1	0
			1198	374	600	103	118	3			
2	F	78	Total	C	H	N	O	S	0	0	0
			1177	371	584	102	117	3			
2	J	78	Total	C	H	N	O	S	0	0	0
			1177	371	584	102	117	3			
2	N	77	Total	C	H	N	O	S	0	0	0
			1176	368	588	101	116	3			

- Molecule 3 is a protein called phycoerythrin alpha-2 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	70	Total	C	H	N	O	S	0	0	0
			1058	321	531	97	106	3			
3	H	70	Total	C	H	N	O	S	0	0	0
			1036	321	509	97	106	3			
3	L	70	Total	C	H	N	O	S	0	1	0
			1043	324	511	97	108	3			
3	P	70	Total	C	H	N	O	S	0	0	0
			1047	321	520	97	106	3			

- Molecule 4 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



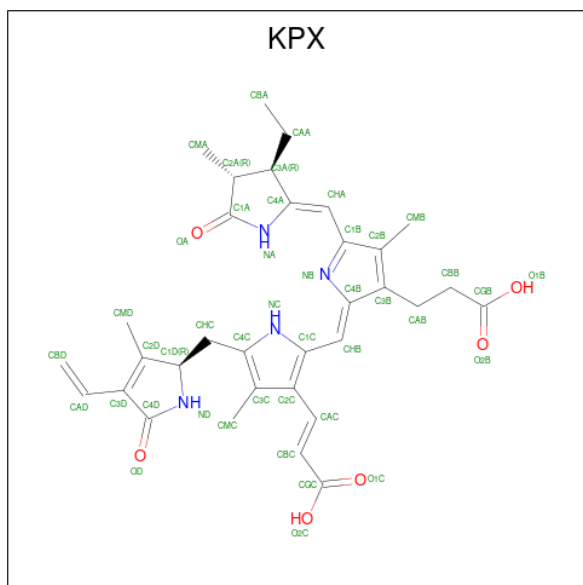
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O		0	0
			80	33	37	4	6			
4	C	1	Total	C	H	N	O		0	0
			80	33	37	4	6			
4	E	1	Total	C	H	N	O		0	0
			80	33	37	4	6			
4	G	1	Total	C	H	N	O		0	0
			80	33	37	4	6			
4	I	1	Total	C	H	N	O		0	0
			80	33	37	4	6			
4	K	1	Total	C	H	N	O		0	0
			80	33	37	4	6			
4	M	1	Total	C	H	N	O		0	0
			80	33	37	4	6			

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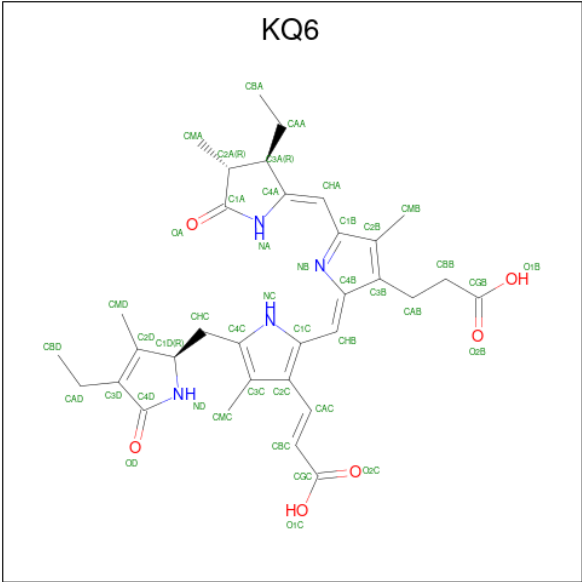
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	O	1	Total	C	H	N	O	0	0
			80	33	37	4	6		

- Molecule 5 is Bilin 584 (single linked) (three-letter code: KPX) (formula: $C_{33}H_{38}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
5	C	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
5	E	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
5	G	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
5	I	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
5	K	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
5	M	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
5	O	1	Total	C	H	N	O	0	0
			78	33	35	4	6		

- Molecule 6 is Bilin 584 (doubly linked) (three-letter code: KQ6) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



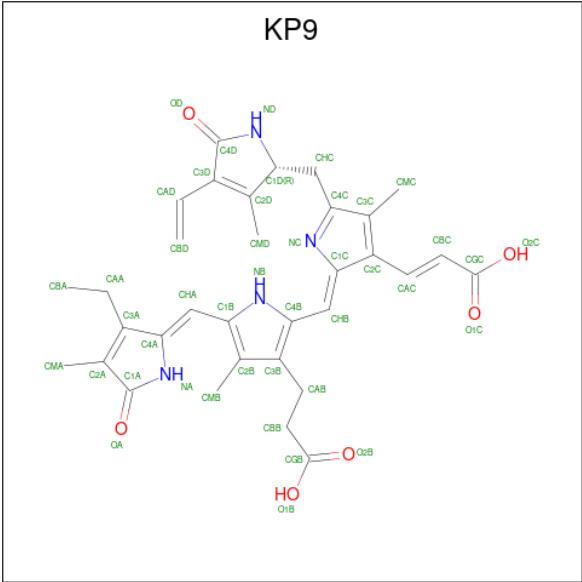
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
6	C	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
6	E	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
6	G	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
6	I	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
6	K	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
6	M	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
6	O	1	Total	C	H	N	O	0	0
			79	33	36	4	6		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	E	1	Total	C	H	O	0	0
			14	3	8	3		
7	G	1	Total	C	H	O	0	0
			14	3	8	3		
7	H	1	Total	C	H	O	0	0
			14	3	8	3		
7	I	1	Total	C	H	O	0	0
			14	3	8	3		
7	I	1	Total	C	H	O	0	0
			14	3	8	3		
7	M	1	Total	C	H	O	0	0
			14	3	8	3		
7	N	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is Bilin 618 (single linked) (three-letter code: KP9) (formula: $C_{33}H_{36}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	0	0
			76	33	33	4	6		
8	D	1	Total	C	H	N	O	0	0
			76	33	33	4	6		
8	F	1	Total	C	H	N	O	0	0
			76	33	33	4	6		
8	H	1	Total	C	H	N	O	0	0
			76	33	33	4	6		
8	J	1	Total	C	H	N	O	0	0
			76	33	33	4	6		
8	L	1	Total	C	H	N	O	0	0
			76	33	33	4	6		
8	N	1	Total	C	H	N	O	0	0
			76	33	33	4	6		
8	P	1	Total	C	H	N	O	0	0
			76	33	33	4	6		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	104	Total	O	0	0
			104	104		
9	B	69	Total	O	0	0
			69	69		
9	C	141	Total	O	0	0
			141	141		
9	D	49	Total	O	0	0
			49	49		

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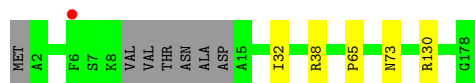
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	82	Total 82	O 82	0	0
9	F	68	Total 68	O 68	0	0
9	G	112	Total 112	O 112	0	0
9	H	36	Total 36	O 36	0	0
9	I	75	Total 75	O 75	0	0
9	J	56	Total 56	O 56	0	0
9	K	116	Total 116	O 116	0	0
9	L	36	Total 36	O 36	0	0
9	M	85	Total 85	O 85	0	0
9	N	61	Total 61	O 61	0	0
9	O	117	Total 117	O 117	0	0
9	P	38	Total 38	O 38	0	0

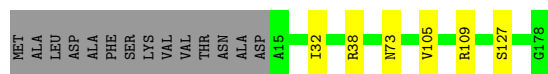
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

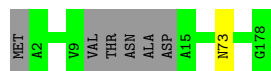
- Molecule 1: Phycoerythrin beta subunit



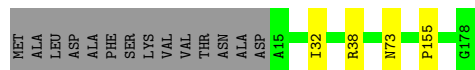
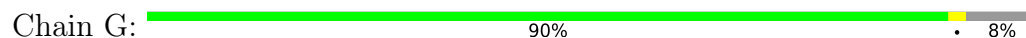
- Molecule 1: Phycoerythrin beta subunit



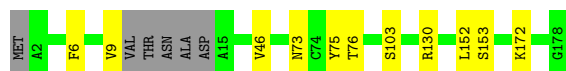
- Molecule 1: Phycoerythrin beta subunit



- Molecule 1: Phycoerythrin beta subunit

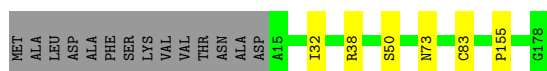


- Molecule 1: Phycoerythrin beta subunit

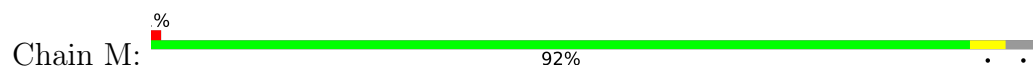


- Molecule 1: Phycoerythrin beta subunit

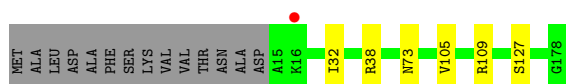
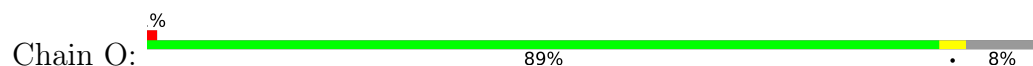




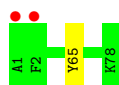
- Molecule 1: Phycoerythrin beta subunit



- Molecule 1: Phycoerythrin beta subunit



- Molecule 2: phycoerythrin alpha-1 subunit



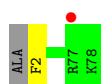
- Molecule 2: phycoerythrin alpha-1 subunit



- Molecule 2: phycoerythrin alpha-1 subunit



- Molecule 2: phycoerythrin alpha-1 subunit



- Molecule 3: phycoerythrin alpha-2 subunit

Chain D:  100%

There are no outlier residues recorded for this chain.

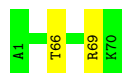
- Molecule 3: phycoerythrin alpha-2 subunit

Chain H:  100%

There are no outlier residues recorded for this chain.

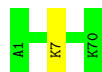
- Molecule 3: phycoerythrin alpha-2 subunit

Chain L:  97%



- Molecule 3: phycoerythrin alpha-2 subunit

Chain P:  99%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.36Å 178.36Å 173.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.77 – 2.00 63.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.77-2.00) 100.0 (63.06-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20rc2_4400	Depositor
R, R_{free}	0.203 , 0.234 0.203 , 0.235	Depositor DCC
R_{free} test set	9646 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32622	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.9393e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEB, KP9, KPX, KQ6, MEN, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.30	0/1288	0.48	0/1735
1	C	0.30	0/1218	0.49	0/1642
1	E	0.28	0/1281	0.48	0/1726
1	G	0.30	0/1236	0.50	0/1665
1	I	0.27	0/1306	0.48	0/1759
1	K	0.29	0/1236	0.49	0/1665
1	M	0.28	0/1276	0.47	0/1719
1	O	0.29	0/1216	0.49	0/1639
2	B	0.33	0/606	0.52	0/811
2	F	0.30	0/601	0.51	0/804
2	J	0.29	0/601	0.50	0/804
2	N	0.29	0/596	0.53	0/797
3	D	0.34	0/533	0.56	0/714
3	H	0.31	0/533	0.56	0/714
3	L	0.31	0/541	0.55	0/725
3	P	0.31	0/533	0.56	0/714
All	All	0.30	0/14601	0.50	0/19633

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1268	1254	1279	2	0
1	C	1203	1207	1205	3	0
1	E	1267	1266	1277	0	0
1	G	1218	1215	1222	2	0
1	I	1283	1278	1301	7	0
1	K	1221	1227	1221	5	0
1	M	1262	1257	1269	2	0
1	O	1201	1208	1204	3	0
2	B	598	600	598	1	0
2	F	593	584	594	1	0
2	J	593	584	594	3	0
2	N	588	588	586	1	0
3	D	527	531	531	0	0
3	H	527	509	531	0	0
3	L	532	511	535	2	0
3	P	527	520	531	1	0
4	A	43	37	37	1	0
4	C	43	37	37	2	0
4	E	43	37	37	1	0
4	G	43	37	37	1	0
4	I	43	37	37	1	0
4	K	43	37	37	2	0
4	M	43	37	37	2	0
4	O	43	37	37	2	0
5	A	43	35	0	0	0
5	C	43	35	0	0	0
5	E	43	35	0	0	0
5	G	43	35	0	1	0
5	I	43	35	0	0	0
5	K	43	35	0	1	0
5	M	43	35	0	0	0
5	O	43	35	0	0	0
6	A	43	36	0	0	0
6	C	43	36	0	0	0
6	E	43	36	0	0	0
6	G	43	36	0	0	0
6	I	43	36	0	0	0
6	K	43	36	0	0	0
6	M	43	36	0	0	0
6	O	43	36	0	0	0
7	A	12	16	16	0	0
7	E	6	8	8	0	0
7	G	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	6	8	8	0	0
7	I	12	16	16	0	0
7	M	6	8	8	0	0
7	N	6	8	8	0	0
8	B	43	33	0	0	0
8	D	43	33	0	0	0
8	F	43	33	0	0	0
8	H	43	33	0	0	0
8	J	43	33	0	0	0
8	L	43	33	0	0	0
8	N	43	33	0	0	0
8	P	43	33	0	0	0
9	A	104	0	0	0	0
9	B	69	0	0	0	0
9	C	141	0	0	0	0
9	D	49	0	0	0	0
9	E	82	0	0	0	0
9	F	68	0	0	1	0
9	G	112	0	0	0	0
9	H	36	0	0	0	0
9	I	75	0	0	0	0
9	J	56	0	0	0	0
9	K	116	0	0	0	0
9	L	36	0	0	0	0
9	M	85	0	0	0	0
9	N	61	0	0	0	0
9	O	117	0	0	0	0
9	P	38	0	0	0	0
All	All	17083	15539	14846	35	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 1.

The worst 5 of 35 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)
4:I:201:PEB:HMB2	4:I:201:PEB:HNA	1.57	0.70
4:E:201:PEB:HMB2	4:E:201:PEB:HNA	1.57	0.70
4:A:201:PEB:HMB2	4:A:201:PEB:HNA	1.58	0.68
4:M:201:PEB:HMB2	4:M:201:PEB:HNA	1.58	0.68
4:G:201:PEB:HNA	4:G:201:PEB:HMB2	1.61	0.66

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/178 (97%)	169 (98%)	3 (2%)	0	100	100
1	C	165/178 (93%)	163 (99%)	2 (1%)	0	100	100
1	E	171/178 (96%)	167 (98%)	4 (2%)	0	100	100
1	G	167/178 (94%)	164 (98%)	3 (2%)	0	100	100
1	I	174/178 (98%)	171 (98%)	3 (2%)	0	100	100
1	K	167/178 (94%)	165 (99%)	2 (1%)	0	100	100
1	M	170/178 (96%)	167 (98%)	3 (2%)	0	100	100
1	O	165/178 (93%)	163 (99%)	2 (1%)	0	100	100
2	B	77/78 (99%)	76 (99%)	1 (1%)	0	100	100
2	F	76/78 (97%)	75 (99%)	1 (1%)	0	100	100
2	J	76/78 (97%)	75 (99%)	1 (1%)	0	100	100
2	N	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
3	D	68/70 (97%)	68 (100%)	0	0	100	100
3	H	68/70 (97%)	68 (100%)	0	0	100	100
3	L	69/70 (99%)	69 (100%)	0	0	100	100
3	P	68/70 (97%)	68 (100%)	0	0	100	100
All	All	1928/2016 (96%)	1902 (99%)	26 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	139/139 (100%)	138 (99%)	1 (1%)	84	88
1	C	131/139 (94%)	131 (100%)	0	100	100
1	E	138/139 (99%)	138 (100%)	0	100	100
1	G	133/139 (96%)	133 (100%)	0	100	100
1	I	141/139 (101%)	141 (100%)	0	100	100
1	K	133/139 (96%)	133 (100%)	0	100	100
1	M	137/139 (99%)	135 (98%)	2 (2%)	65	69
1	O	131/139 (94%)	131 (100%)	0	100	100
2	B	61/61 (100%)	61 (100%)	0	100	100
2	F	61/61 (100%)	61 (100%)	0	100	100
2	J	61/61 (100%)	61 (100%)	0	100	100
2	N	61/61 (100%)	61 (100%)	0	100	100
3	D	57/57 (100%)	57 (100%)	0	100	100
3	H	57/57 (100%)	57 (100%)	0	100	100
3	L	58/57 (102%)	58 (100%)	0	100	100
3	P	57/57 (100%)	57 (100%)	0	100	100
All	All	1556/1584 (98%)	1553 (100%)	3 (0%)	93	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ARG
1	M	66	SER
1	M	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	48	ASN
1	K	144	ASN
1	M	26	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MEN	M	73	1	7,8,9	0.89	0	6,9,11	1.29	2 (33%)
1	MEN	I	73	1	7,8,9	0.87	0	6,9,11	1.53	2 (33%)
1	MEN	K	73	1	7,8,9	0.93	0	6,9,11	1.28	1 (16%)
1	MEN	G	73	1	7,8,9	0.92	0	6,9,11	1.38	1 (16%)
1	MEN	C	73	1	7,8,9	0.90	0	6,9,11	1.40	1 (16%)
1	MEN	A	73	1	7,8,9	0.90	0	6,9,11	1.39	1 (16%)
1	MEN	O	73	1	7,8,9	0.90	0	6,9,11	1.27	1 (16%)
1	MEN	E	73	1	7,8,9	0.84	0	6,9,11	1.38	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEN	M	73	1	-	2/7/8/10	-
1	MEN	I	73	1	-	2/7/8/10	-
1	MEN	K	73	1	-	2/7/8/10	-
1	MEN	G	73	1	-	2/7/8/10	-
1	MEN	C	73	1	-	3/7/8/10	-
1	MEN	A	73	1	-	2/7/8/10	-
1	MEN	O	73	1	-	2/7/8/10	-
1	MEN	E	73	1	-	2/7/8/10	-

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	MEN	CB-CA-C	-2.92	106.00	111.47
1	I	73	MEN	CB-CG-ND2	2.83	119.29	115.48
1	A	73	MEN	CB-CG-ND2	2.73	119.16	115.48
1	G	73	MEN	CB-CA-C	-2.70	106.41	111.47
1	O	73	MEN	CB-CA-C	-2.50	106.78	111.47

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	O	73	MEN	CA-CB-CG-OD1
1	C	73	MEN	CA-CB-CG-OD1
1	E	73	MEN	CA-CB-CG-OD1
1	G	73	MEN	CA-CB-CG-OD1
1	I	73	MEN	CA-CB-CG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

41 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	KQ6	M	203	1	42,46,46	5.11	33 (78%)	42,67,67	1.81	9 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	KPX	O	202	1	43,46,46	2.33	19 (44%)	43,67,67	1.60	9 (20%)
8	KP9	J	101	2	42,46,46	3.48	31 (73%)	39,67,67	1.79	8 (20%)
7	GOL	A	204	-	5,5,5	0.89	0	5,5,5	0.81	0
7	GOL	A	205	-	5,5,5	0.86	0	5,5,5	1.01	0
7	GOL	I	205	-	5,5,5	1.03	0	5,5,5	0.83	0
4	PEB	I	201	1	43,46,46	5.25	32 (74%)	45,67,67	1.96	12 (26%)
4	PEB	A	201	1	43,46,46	5.18	32 (74%)	45,67,67	2.02	13 (28%)
8	KP9	P	101	3	42,46,46	3.59	30 (71%)	39,67,67	1.73	9 (23%)
7	GOL	M	204	-	5,5,5	0.77	0	5,5,5	0.97	0
6	KQ6	A	203	1	42,46,46	4.96	33 (78%)	42,67,67	1.84	9 (21%)
6	KQ6	E	203	1	42,46,46	5.06	33 (78%)	42,67,67	1.80	10 (23%)
7	GOL	G	204	-	5,5,5	0.92	0	5,5,5	0.92	0
4	PEB	G	201	1	43,46,46	5.16	32 (74%)	45,67,67	1.97	11 (24%)
5	KPX	G	202	1	43,46,46	2.40	17 (39%)	43,67,67	1.61	8 (18%)
6	KQ6	G	203	1	42,46,46	4.89	33 (78%)	42,67,67	2.30	12 (28%)
8	KP9	N	101	2	42,46,46	3.46	30 (71%)	39,67,67	1.94	9 (23%)
4	PEB	M	201	1	43,46,46	5.36	32 (74%)	45,67,67	1.97	11 (24%)
7	GOL	N	102	-	5,5,5	1.07	0	5,5,5	0.75	0
5	KPX	A	202	1	43,46,46	2.30	17 (39%)	43,67,67	1.47	4 (9%)
7	GOL	H	102	-	5,5,5	0.81	0	5,5,5	1.06	0
4	PEB	E	201	1	43,46,46	5.19	32 (74%)	45,67,67	2.04	13 (28%)
6	KQ6	I	203	1	42,46,46	5.12	33 (78%)	42,67,67	1.77	7 (16%)
5	KPX	M	202	1	43,46,46	2.34	17 (39%)	43,67,67	1.51	6 (13%)
4	PEB	K	201	1	43,46,46	5.13	32 (74%)	45,67,67	1.90	12 (26%)
8	KP9	H	101	3	42,46,46	3.58	30 (71%)	39,67,67	1.79	7 (17%)
7	GOL	E	204	-	5,5,5	0.72	0	5,5,5	0.88	0
5	KPX	K	202	1	43,46,46	2.37	18 (41%)	43,67,67	1.63	8 (18%)
6	KQ6	O	203	1	42,46,46	4.89	32 (76%)	42,67,67	2.09	12 (28%)
7	GOL	I	204	-	5,5,5	0.67	0	5,5,5	0.92	0
4	PEB	C	201	1	43,46,46	5.02	32 (74%)	45,67,67	2.04	12 (26%)
8	KP9	D	101	3	42,46,46	3.53	30 (71%)	39,67,67	1.70	7 (17%)
5	KPX	I	202	1	43,46,46	2.33	16 (37%)	43,67,67	1.44	5 (11%)
6	KQ6	C	203	1	42,46,46	4.77	32 (76%)	42,67,67	2.19	12 (28%)
6	KQ6	K	203	1	42,46,46	4.81	33 (78%)	42,67,67	2.31	13 (30%)
5	KPX	C	202	1	43,46,46	2.31	19 (44%)	43,67,67	1.57	8 (18%)
8	KP9	B	101	2	42,46,46	3.43	29 (69%)	39,67,67	1.90	8 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	KP9	F	101	2	42,46,46	3.47	30 (71%)	39,67,67	1.86	5 (12%)
8	KP9	L	101	3	42,46,46	3.59	30 (71%)	39,67,67	1.82	7 (17%)
5	KPX	E	202	1	43,46,46	2.31	16 (37%)	43,67,67	1.47	6 (13%)
4	PEB	O	201	1	43,46,46	5.10	32 (74%)	45,67,67	1.98	13 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	KQ6	M	203	1	-	5/24/74/74	0/4/4/4
5	KPX	O	202	1	-	7/24/74/74	0/4/4/4
8	KP9	J	101	2	-	9/26/74/74	0/4/4/4
7	GOL	A	204	-	-	0/4/4/4	-
7	GOL	A	205	-	-	0/4/4/4	-
7	GOL	I	205	-	-	2/4/4/4	-
4	PEB	I	201	1	-	6/24/74/74	0/4/4/4
4	PEB	A	201	1	-	6/24/74/74	0/4/4/4
8	KP9	P	101	3	-	10/26/74/74	0/4/4/4
7	GOL	M	204	-	-	2/4/4/4	-
6	KQ6	A	203	1	-	6/24/74/74	0/4/4/4
6	KQ6	E	203	1	-	5/24/74/74	0/4/4/4
7	GOL	G	204	-	-	2/4/4/4	-
4	PEB	G	201	1	-	6/24/74/74	0/4/4/4
5	KPX	G	202	1	-	8/24/74/74	0/4/4/4
6	KQ6	G	203	1	-	8/24/74/74	0/4/4/4
8	KP9	N	101	2	-	10/26/74/74	0/4/4/4
4	PEB	M	201	1	-	6/24/74/74	0/4/4/4
7	GOL	N	102	-	-	0/4/4/4	-
5	KPX	A	202	1	-	9/24/74/74	0/4/4/4
7	GOL	H	102	-	-	0/4/4/4	-
4	PEB	E	201	1	-	6/24/74/74	0/4/4/4
6	KQ6	I	203	1	-	5/24/74/74	0/4/4/4
5	KPX	M	202	1	-	7/24/74/74	0/4/4/4
4	PEB	K	201	1	-	4/24/74/74	0/4/4/4
8	KP9	H	101	3	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	E	204	-	-	0/4/4/4	-
5	KPX	K	202	1	-	5/24/74/74	0/4/4/4
6	KQ6	O	203	1	-	7/24/74/74	0/4/4/4
7	GOL	I	204	-	-	0/4/4/4	-
4	PEB	C	201	1	-	5/24/74/74	0/4/4/4
8	KP9	D	101	3	-	10/26/74/74	0/4/4/4
5	KPX	I	202	1	-	7/24/74/74	0/4/4/4
6	KQ6	C	203	1	-	6/24/74/74	0/4/4/4
6	KQ6	K	203	1	-	9/24/74/74	0/4/4/4
5	KPX	C	202	1	-	6/24/74/74	0/4/4/4
8	KP9	B	101	2	-	10/26/74/74	0/4/4/4
8	KP9	F	101	2	-	9/26/74/74	0/4/4/4
8	KP9	L	101	3	-	10/26/74/74	0/4/4/4
5	KPX	E	202	1	-	9/24/74/74	0/4/4/4
4	PEB	O	201	1	-	5/24/74/74	0/4/4/4

The worst 5 of 897 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	201	PEB	CHB-C4B	15.39	1.48	1.35
4	I	201	PEB	CHB-C4B	14.65	1.47	1.35
4	A	201	PEB	CHB-C4B	14.50	1.47	1.35
4	E	201	PEB	CHB-C4B	14.40	1.47	1.35
4	K	201	PEB	CHB-C4B	14.26	1.47	1.35

The worst 5 of 295 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	203	KQ6	C1C-CHB-C4B	-9.08	117.97	128.81
6	K	203	KQ6	C1C-CHB-C4B	-8.97	118.09	128.81
4	C	201	PEB	C1C-CHB-C4B	-8.58	118.56	128.81
4	G	201	PEB	C1C-CHB-C4B	-8.22	118.99	128.81
4	E	201	PEB	C1C-CHB-C4B	-7.98	119.27	128.81

There are no chirality outliers.

5 of 237 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	PEB	NB-C1B-CHA-C4A

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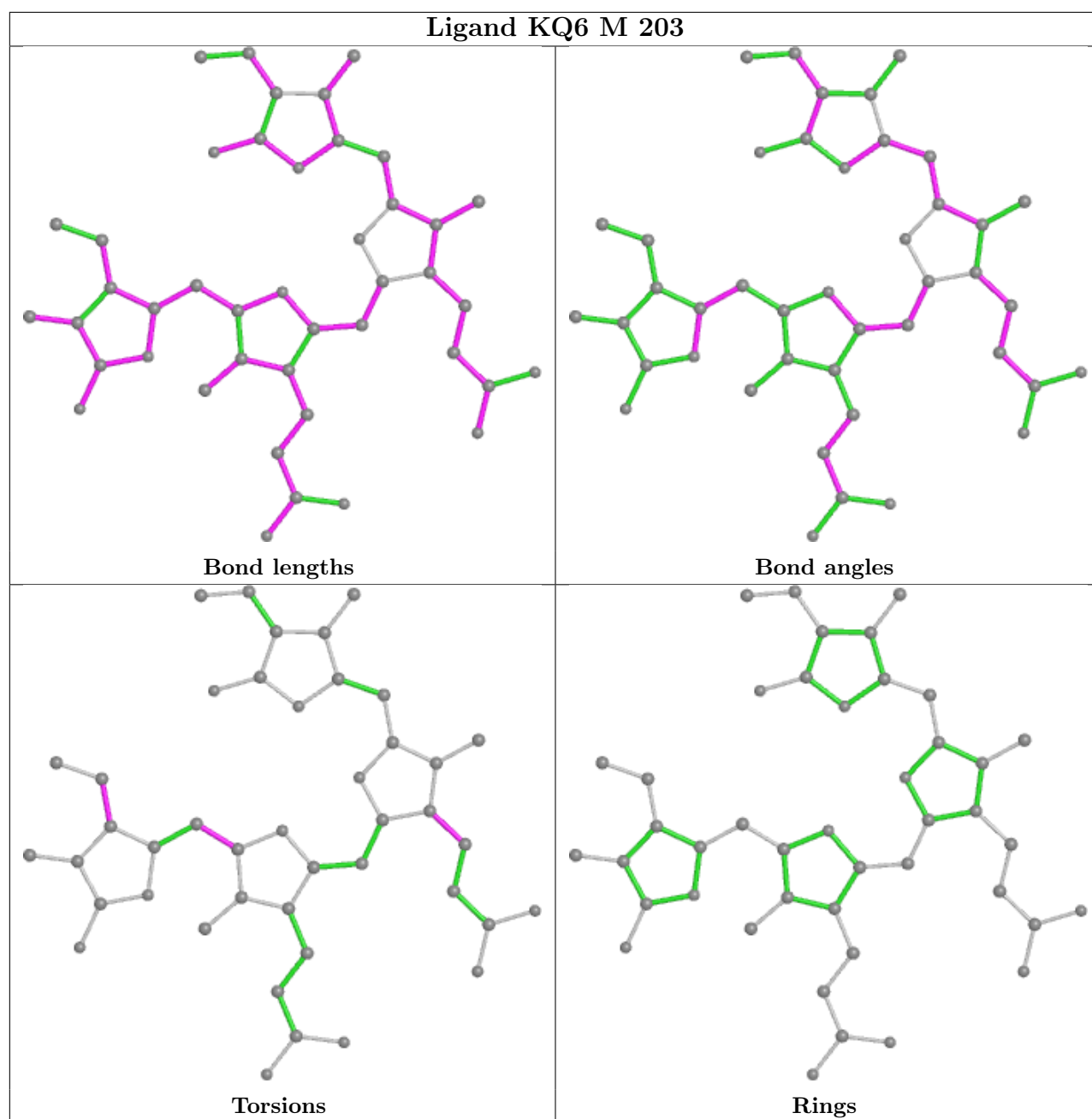
Mol	Chain	Res	Type	Atoms
4	A	201	PEB	C2B-C1B-CHA-C4A
4	C	201	PEB	NB-C1B-CHA-C4A
4	C	201	PEB	C2B-C1B-CHA-C4A
4	E	201	PEB	NB-C1B-CHA-C4A

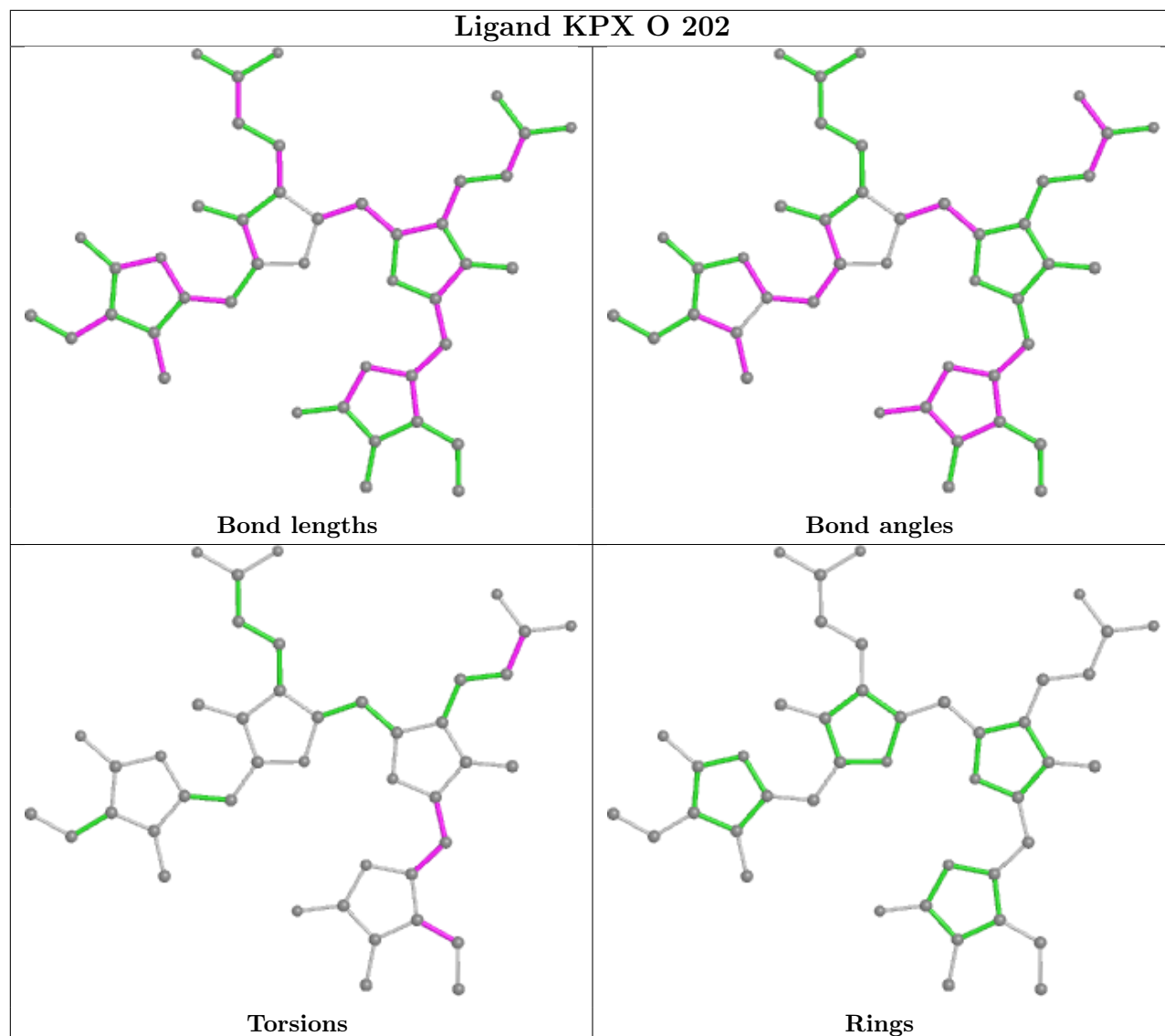
There are no ring outliers.

10 monomers are involved in 14 short contacts:

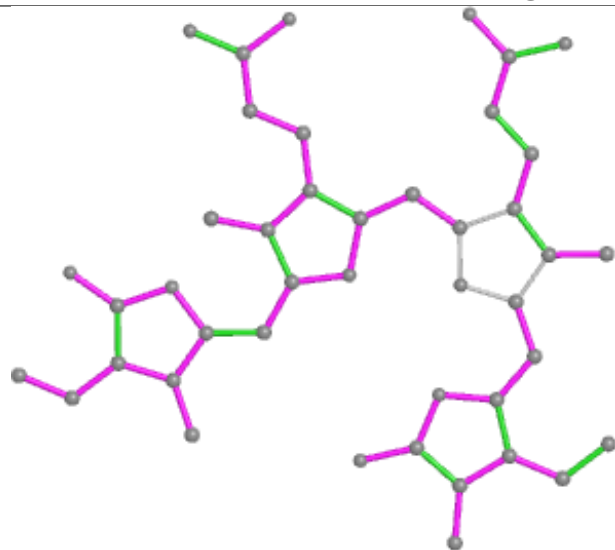
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	201	PEB	1	0
4	A	201	PEB	1	0
4	G	201	PEB	1	0
5	G	202	KPX	1	0
4	M	201	PEB	2	0
4	E	201	PEB	1	0
4	K	201	PEB	2	0
5	K	202	KPX	1	0
4	C	201	PEB	2	0
4	O	201	PEB	2	0

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.

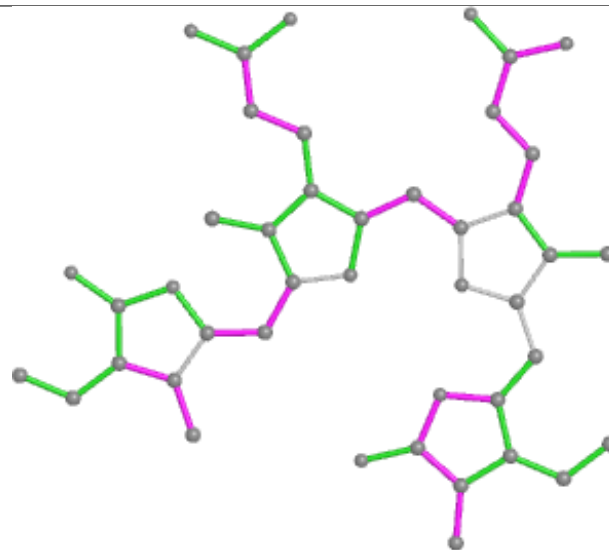




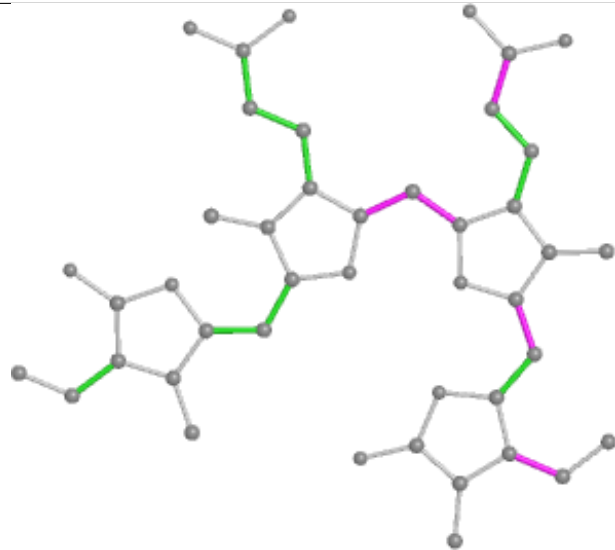
Ligand KP9 J 101



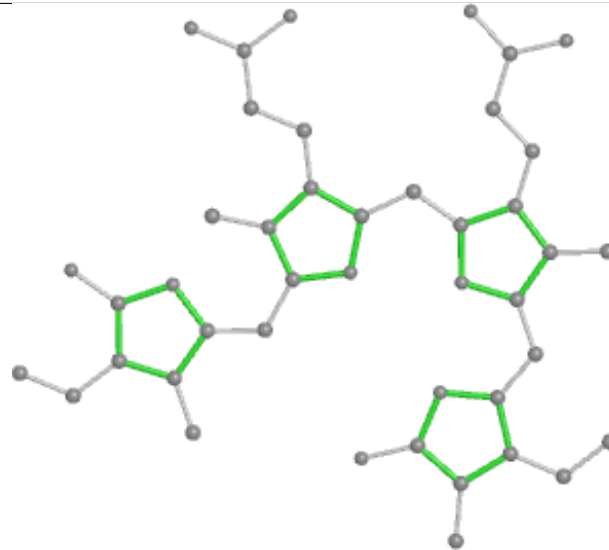
Bond lengths



Bond angles

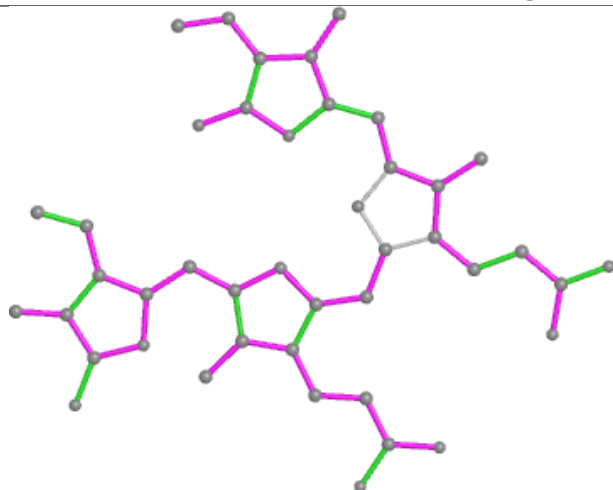


Torsions

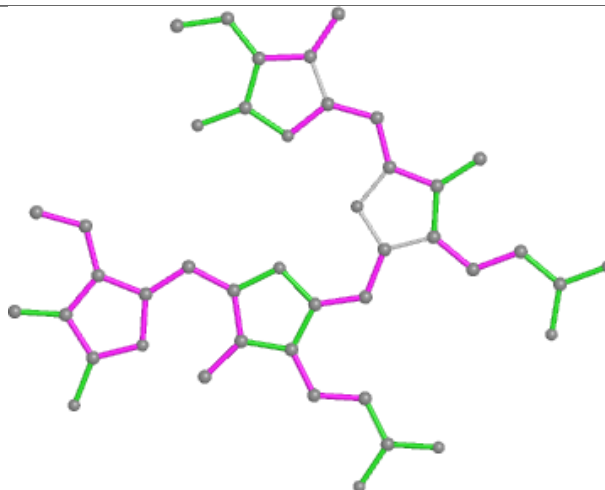


Rings

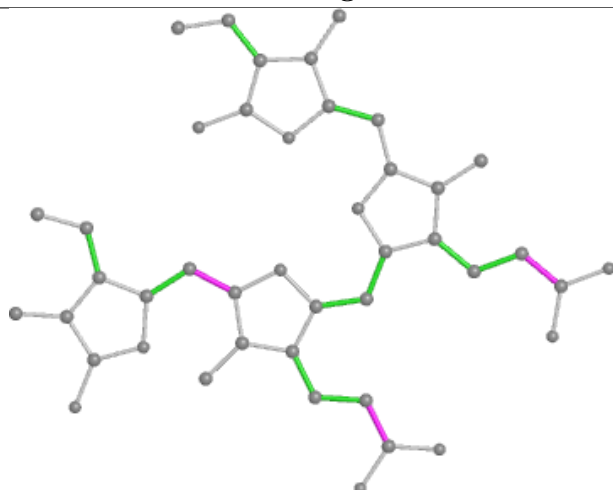
Ligand PEB I 201



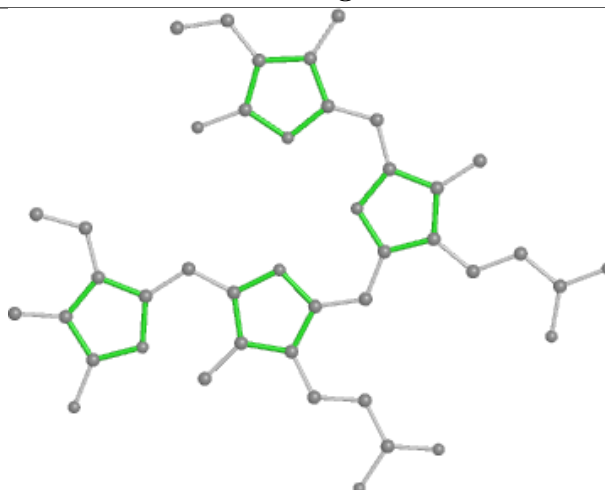
Bond lengths



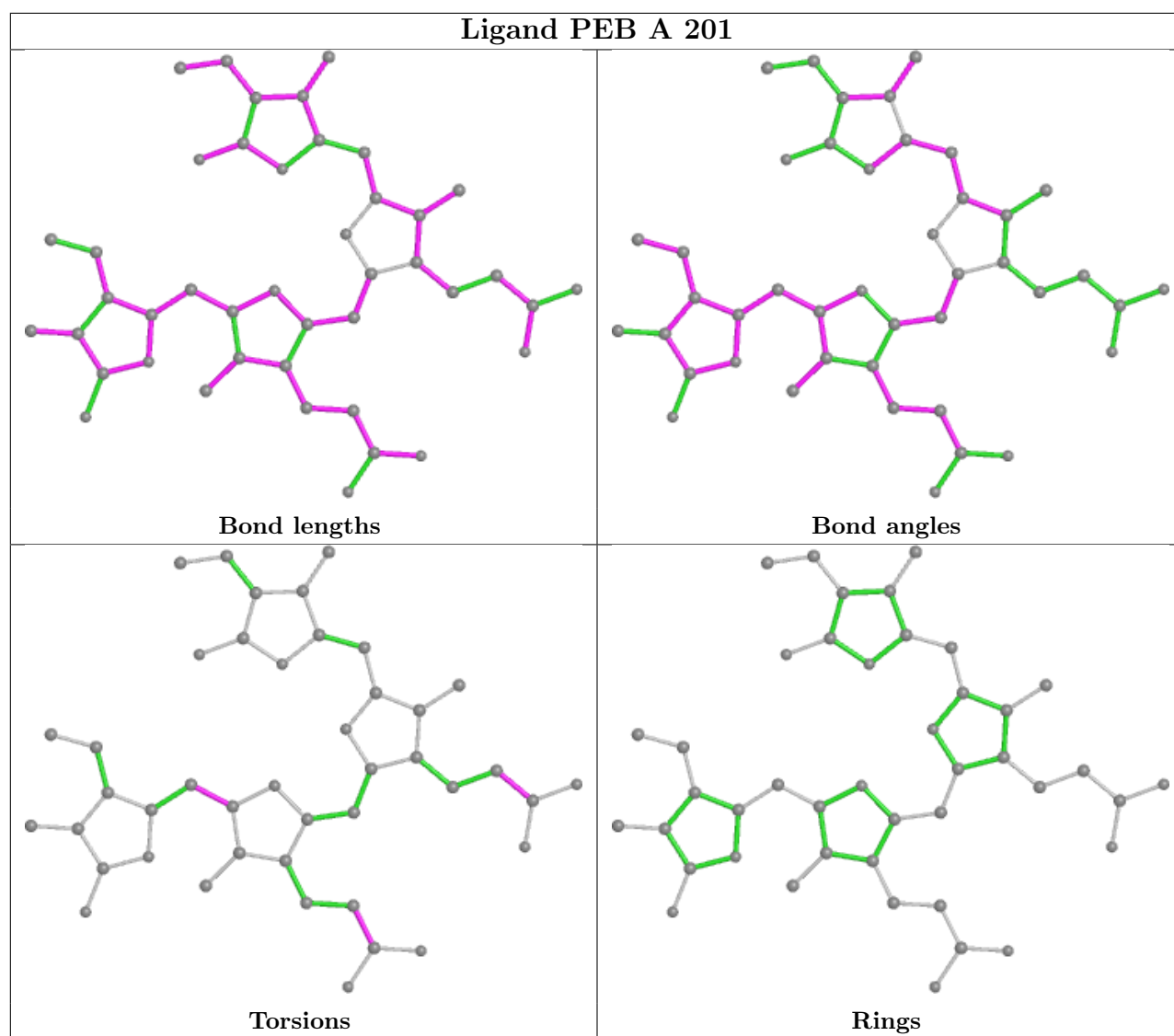
Bond angles



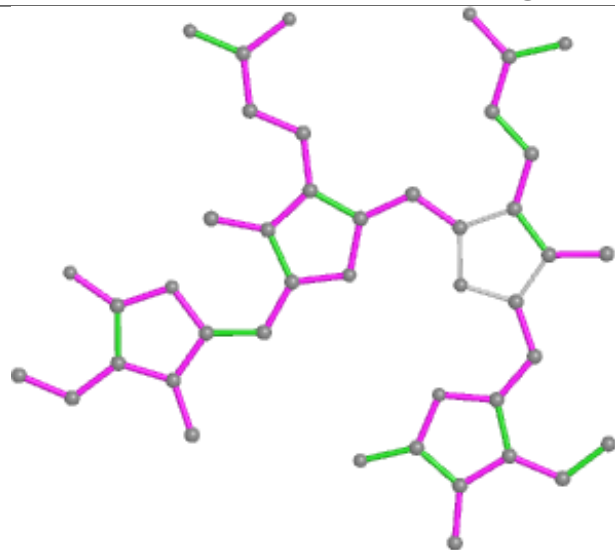
Torsions



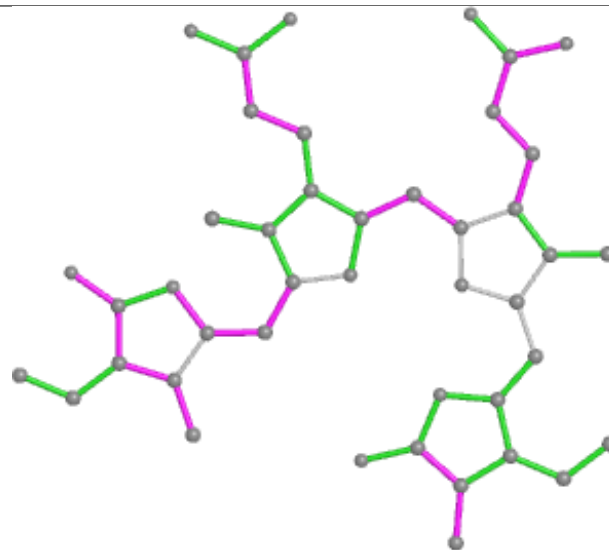
Rings



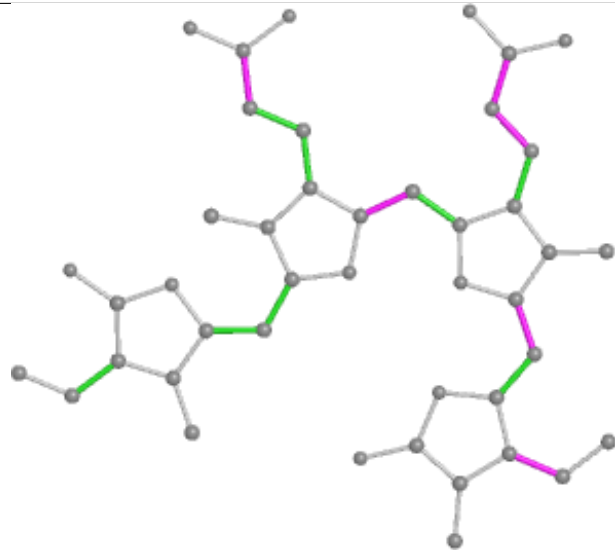
Ligand KP9 P 101



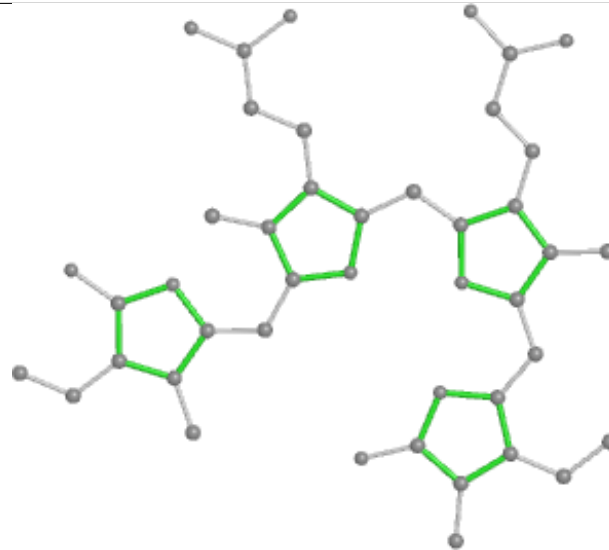
Bond lengths



Bond angles

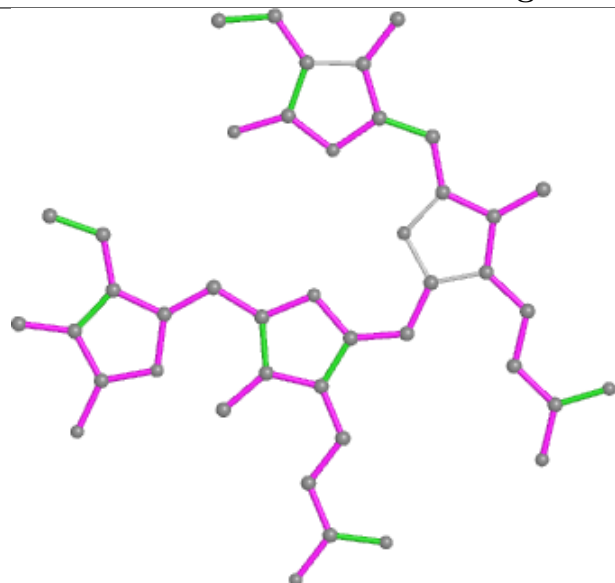


Torsions

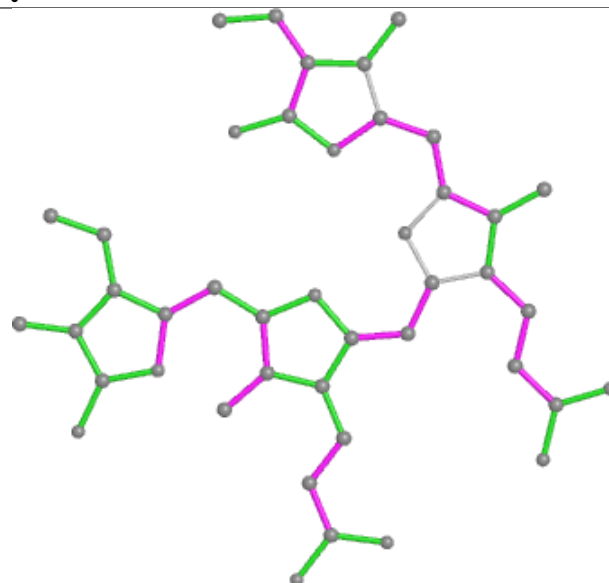


Rings

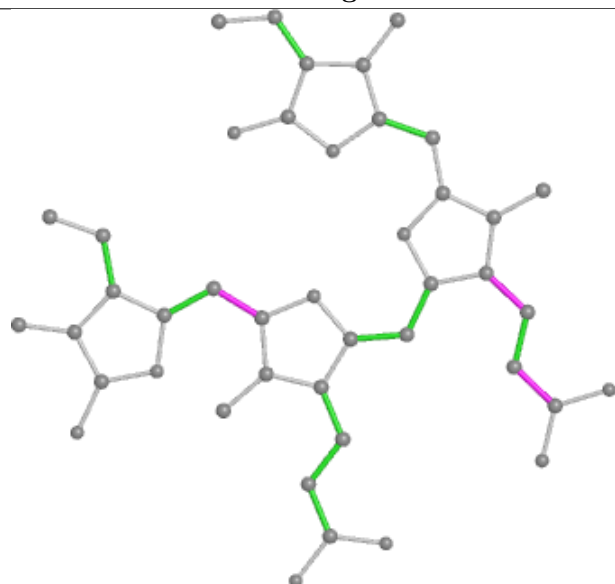
Ligand KQ6 A 203



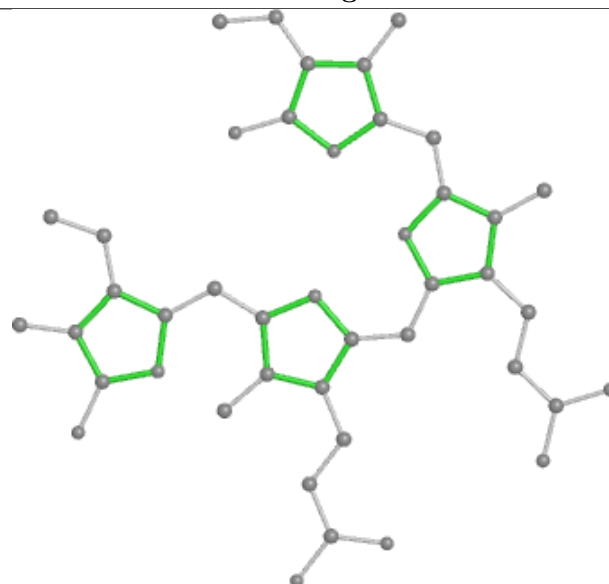
Bond lengths



Bond angles

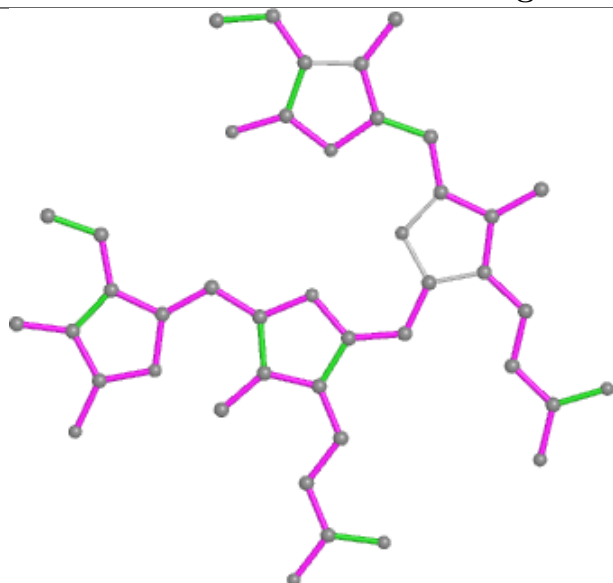


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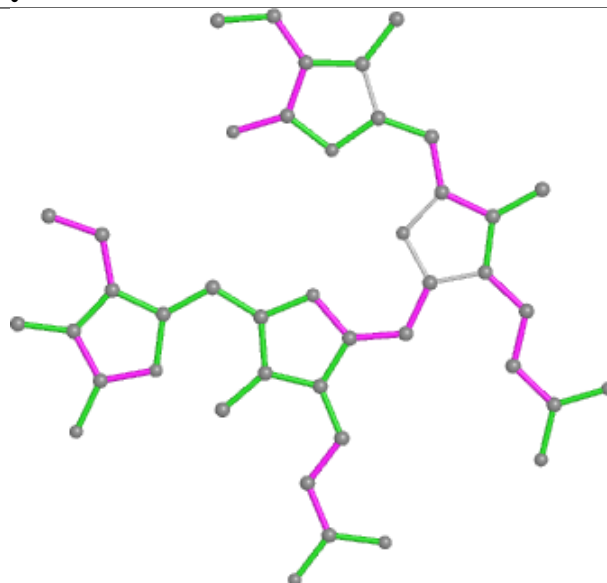


Rings

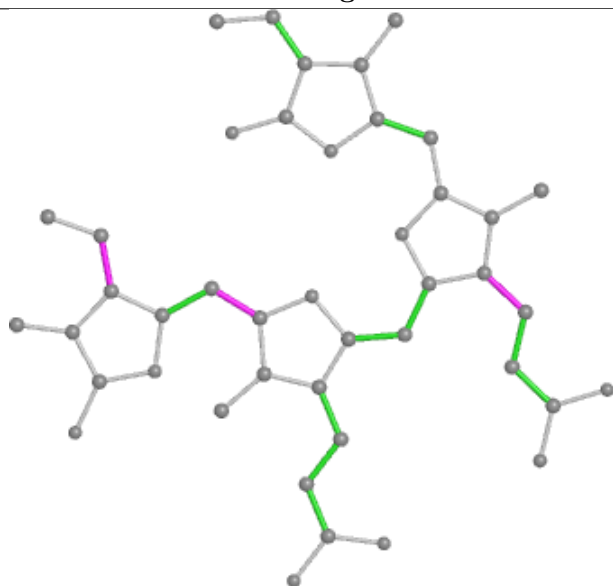
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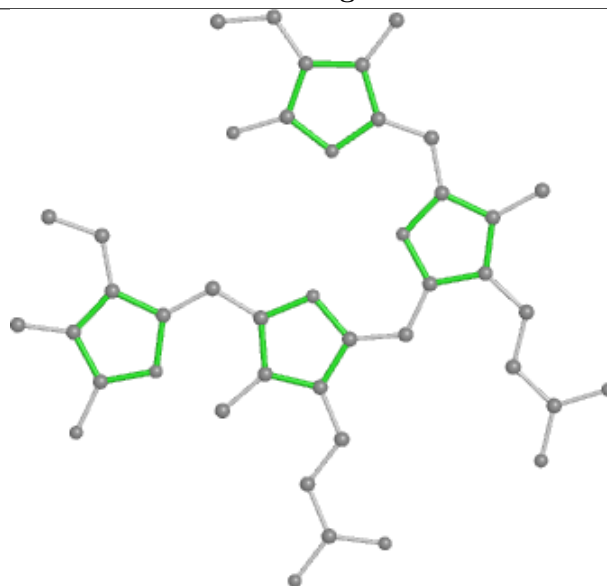
Bond lengths



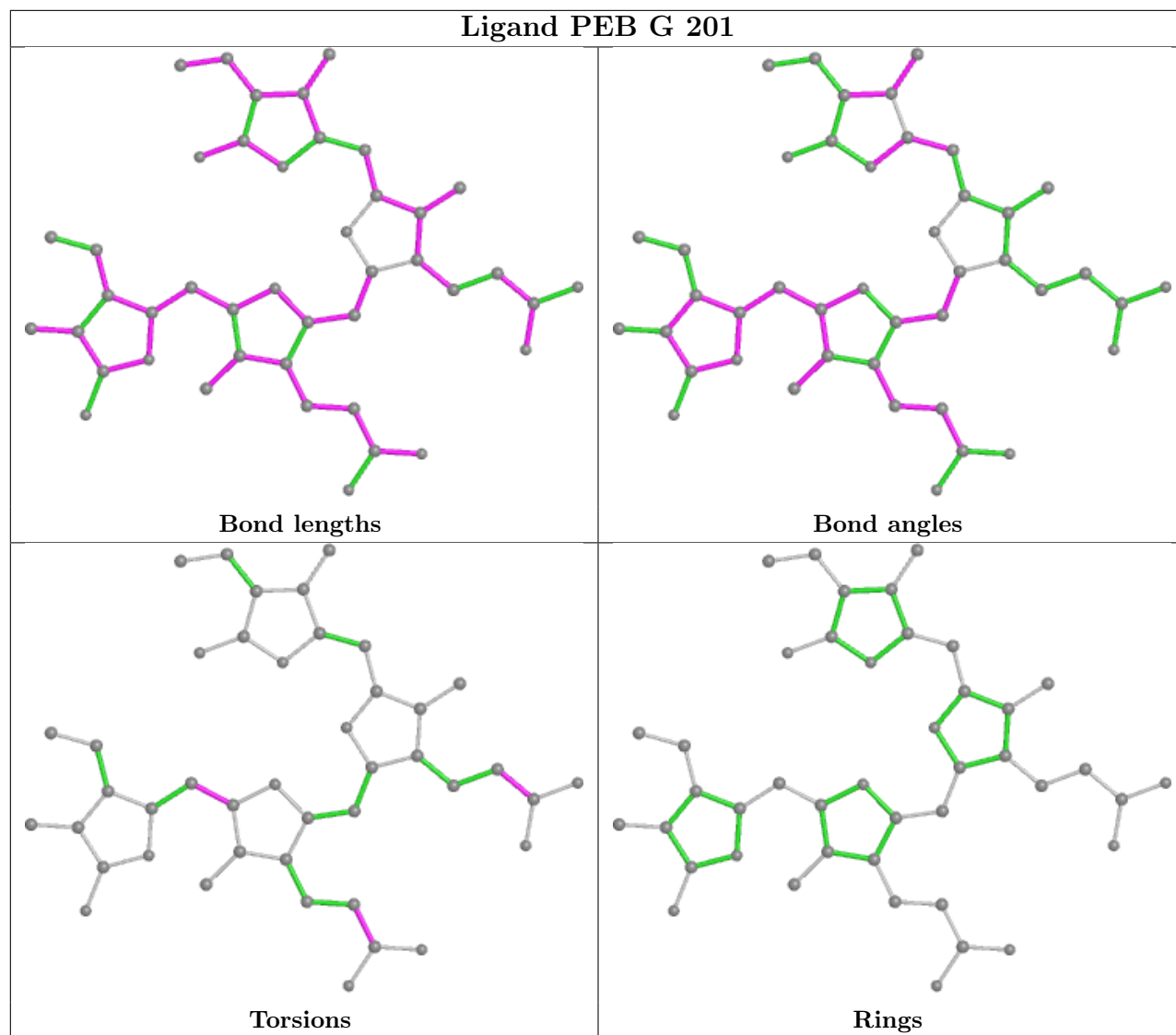
Bond angles

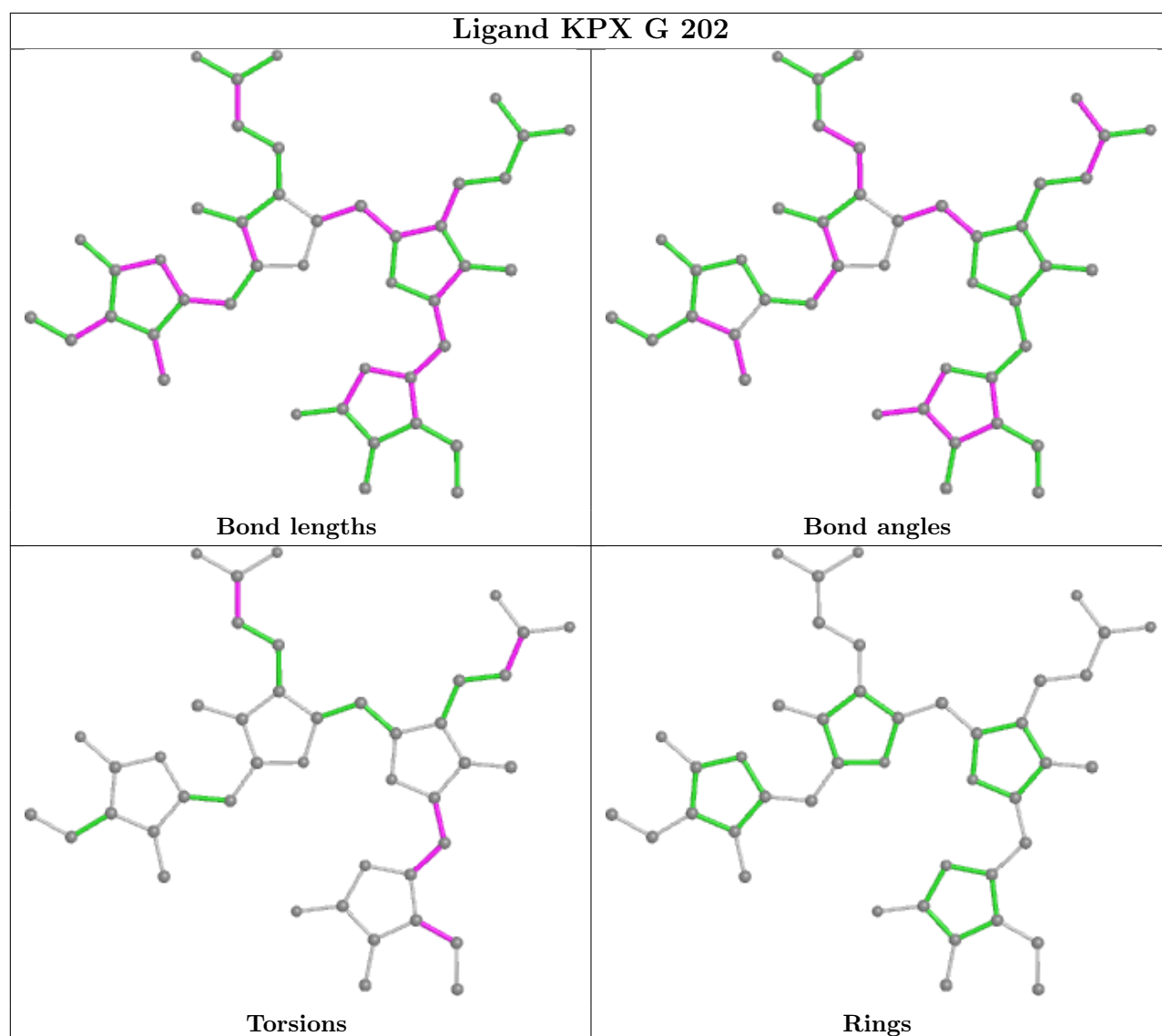


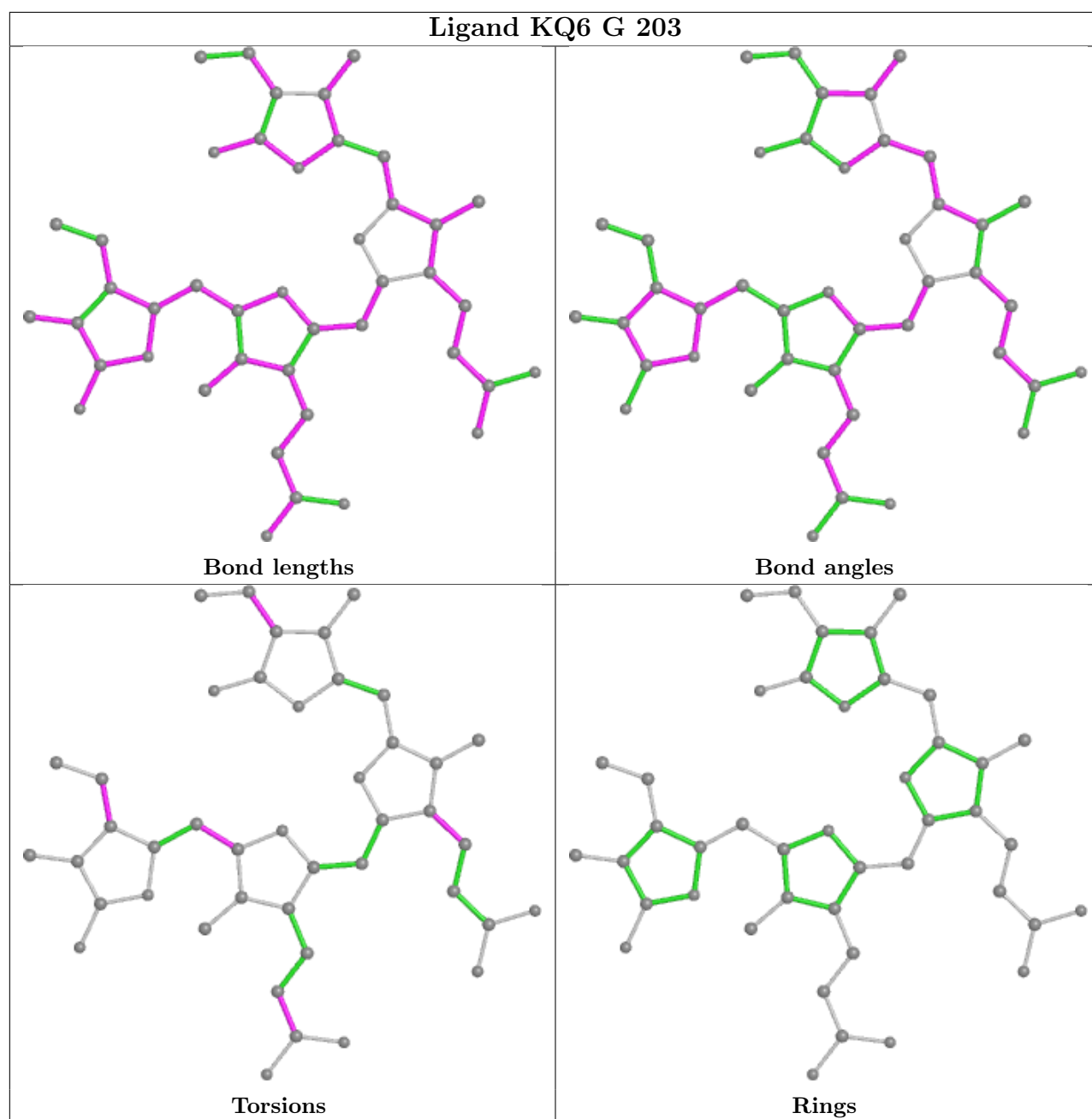
Torsions



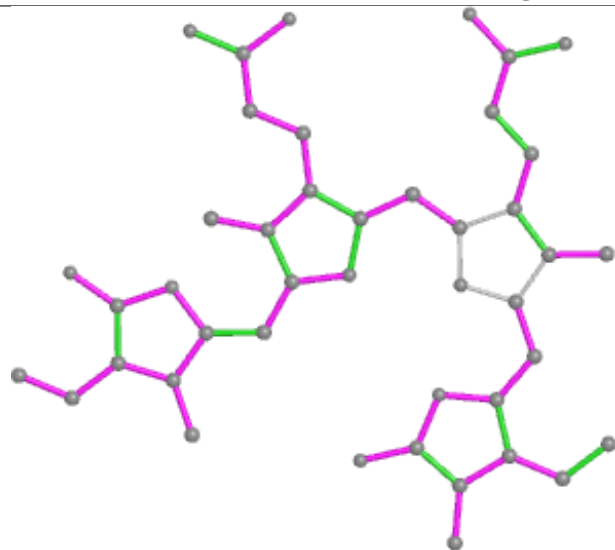
Rings



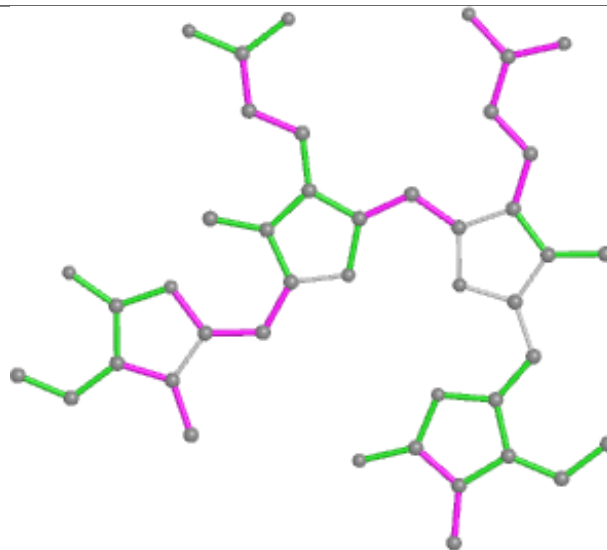




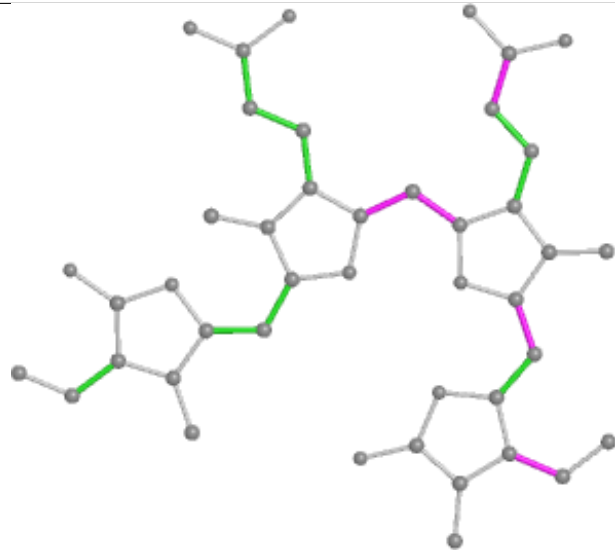
Ligand KP9 N 101



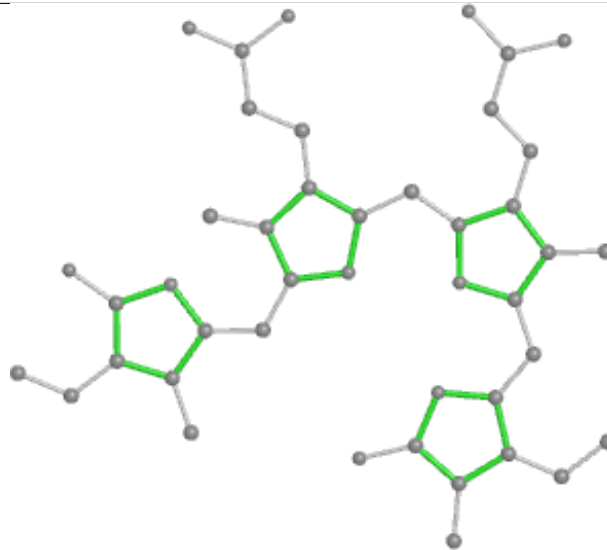
Bond lengths



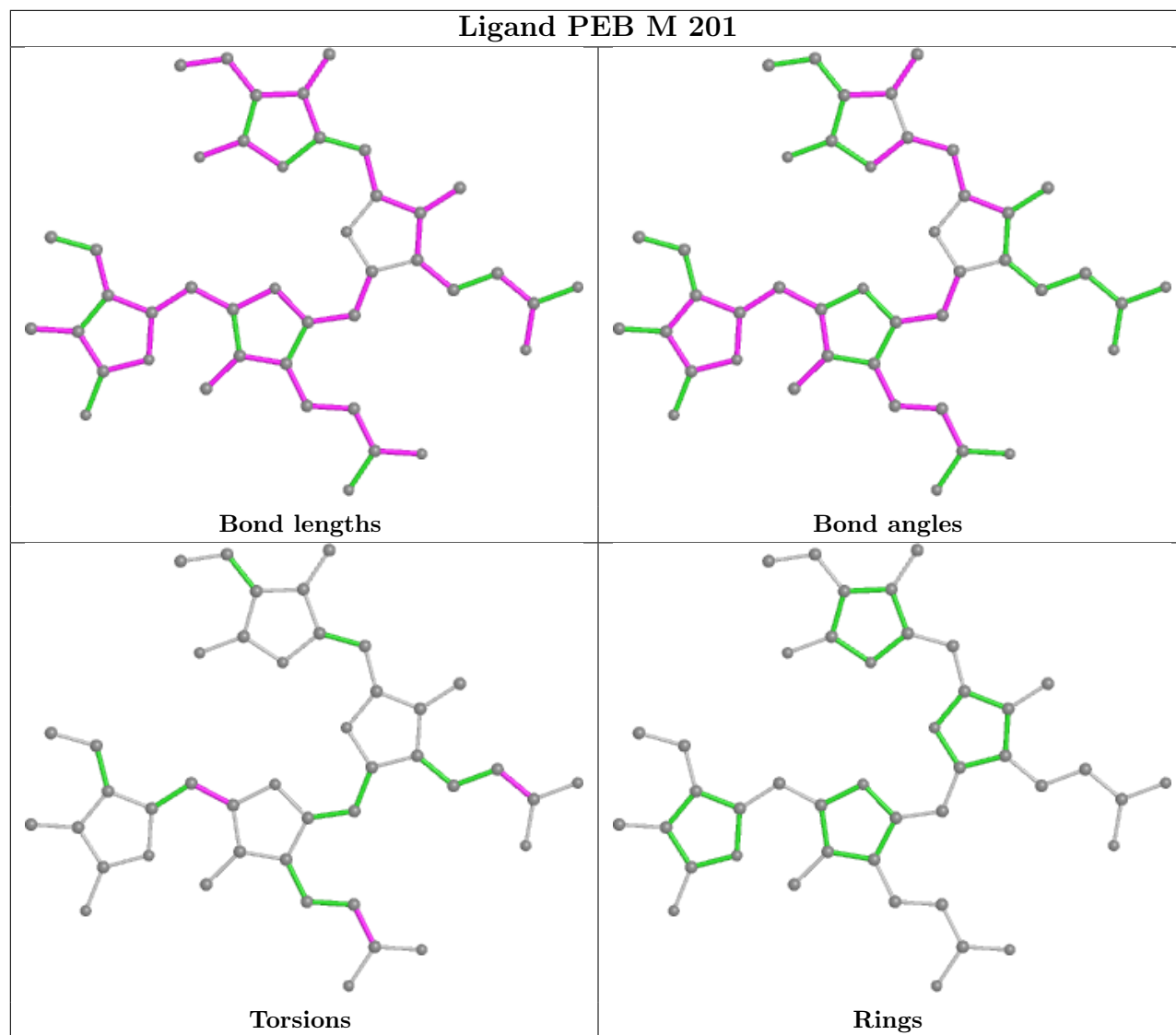
Bond angles

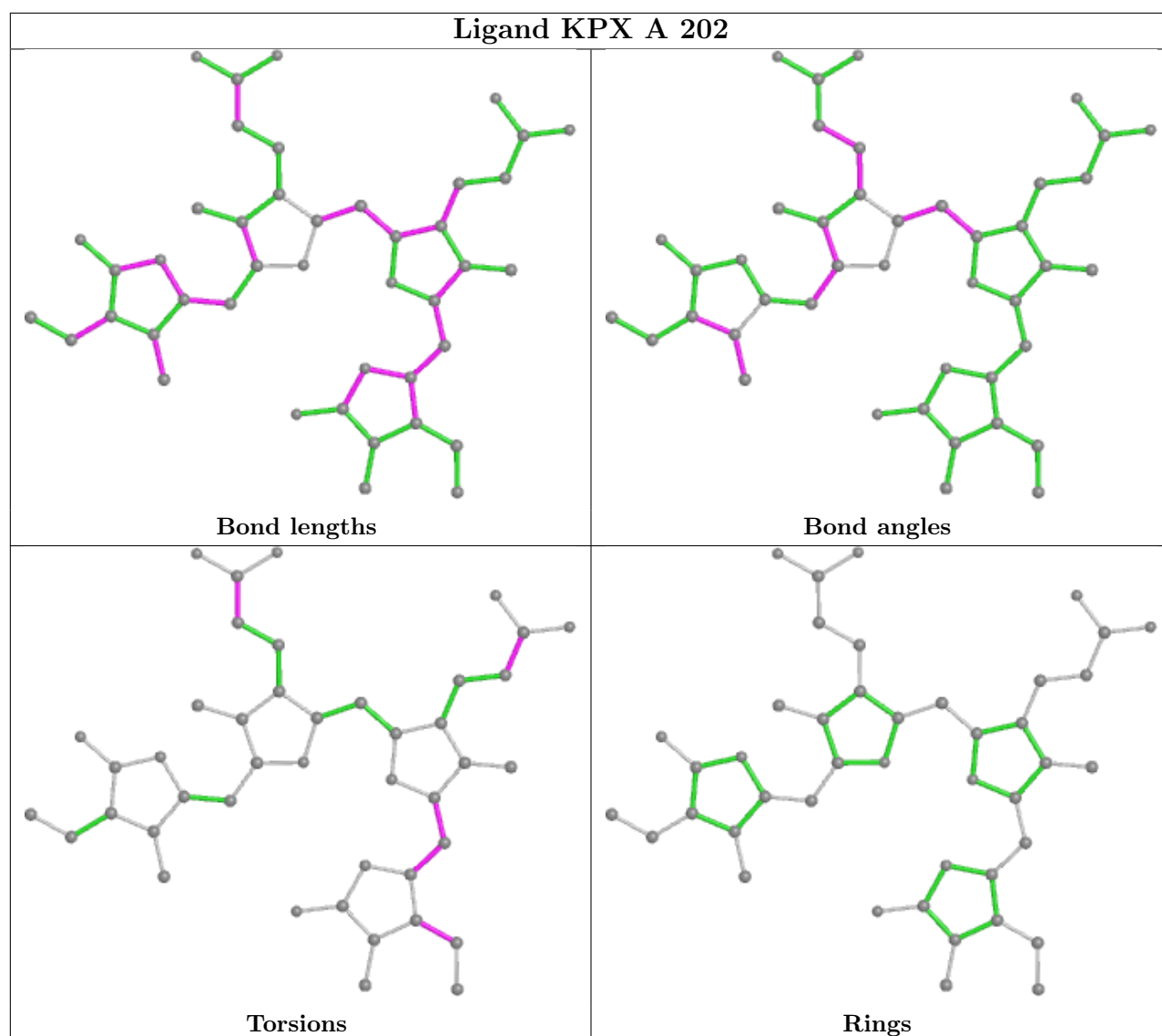


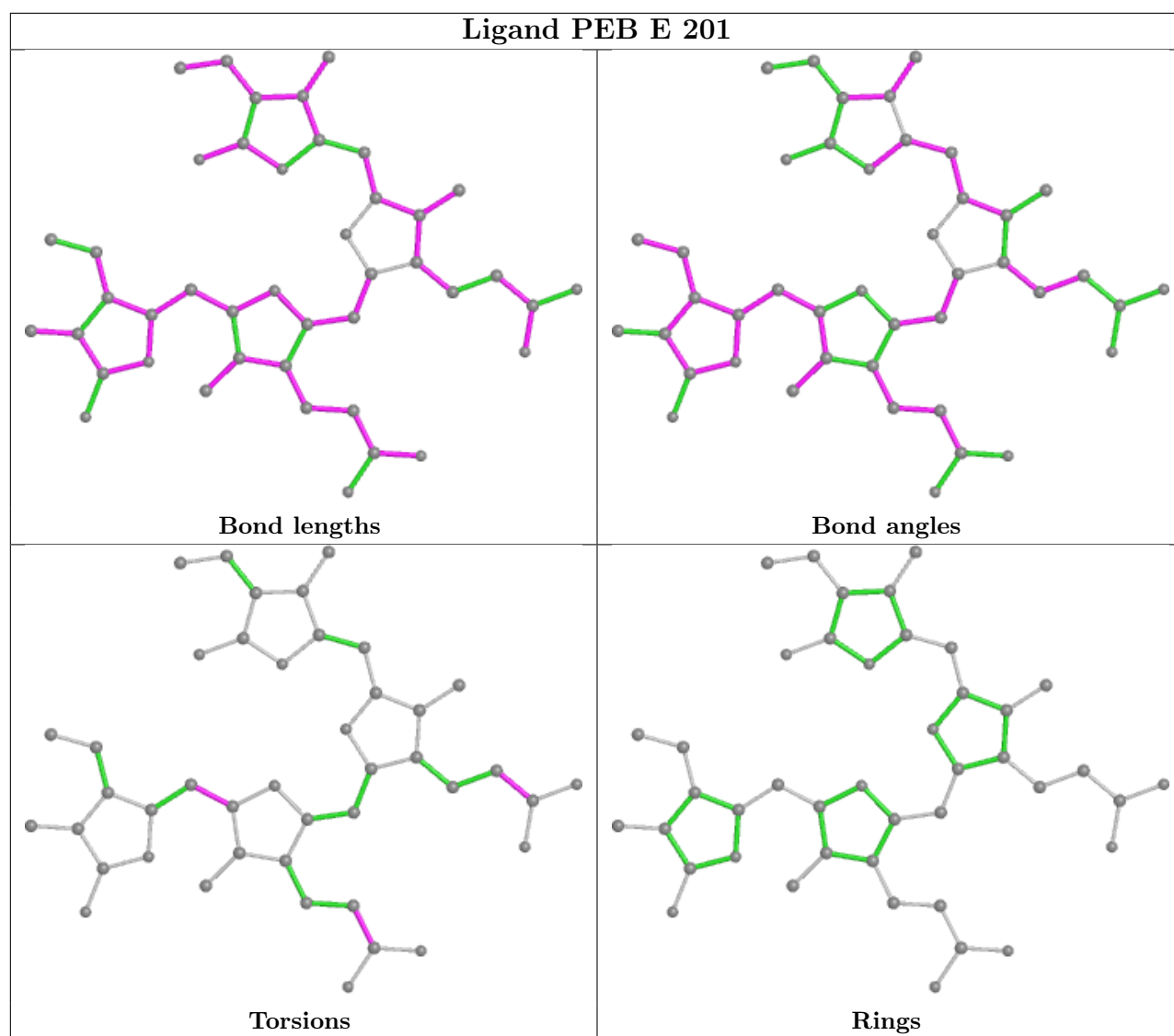
Torsions



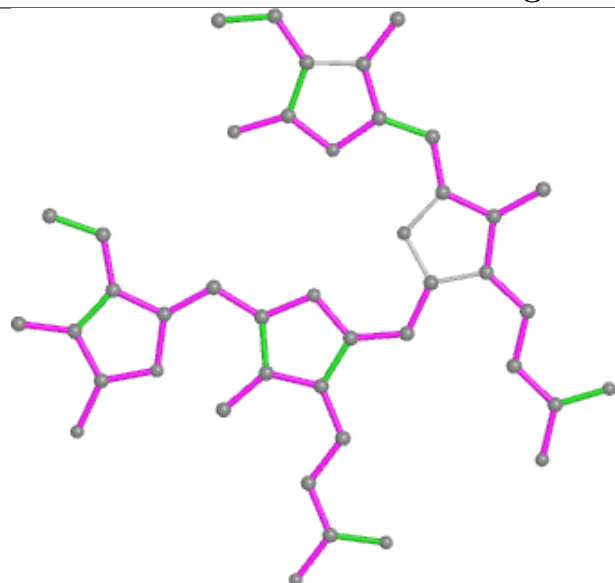
Rings



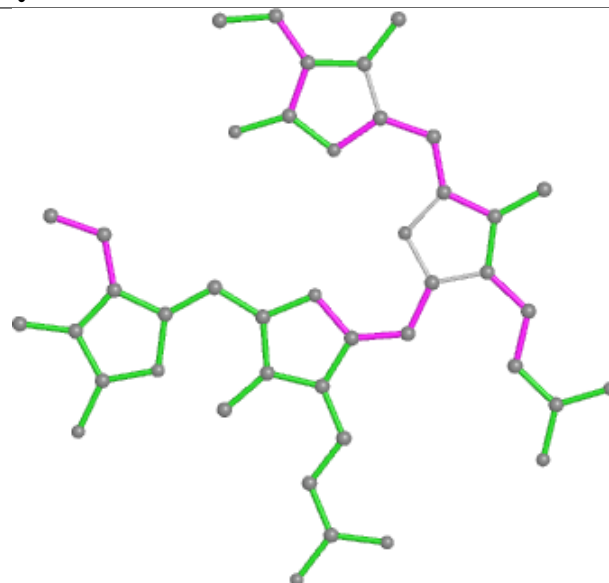




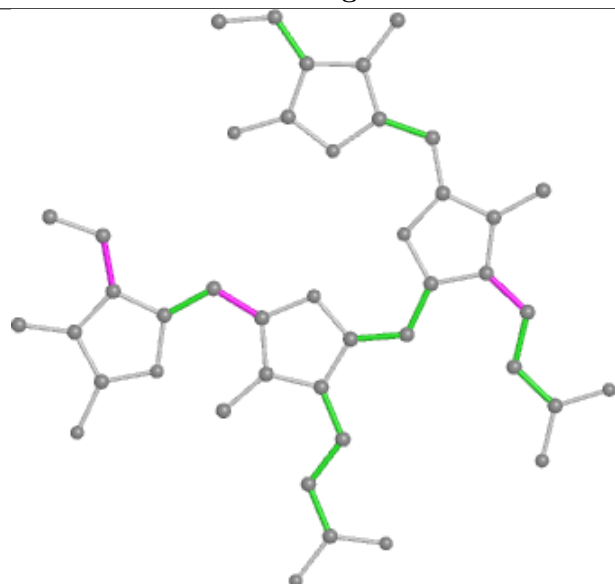
Ligand KQ6 I 203



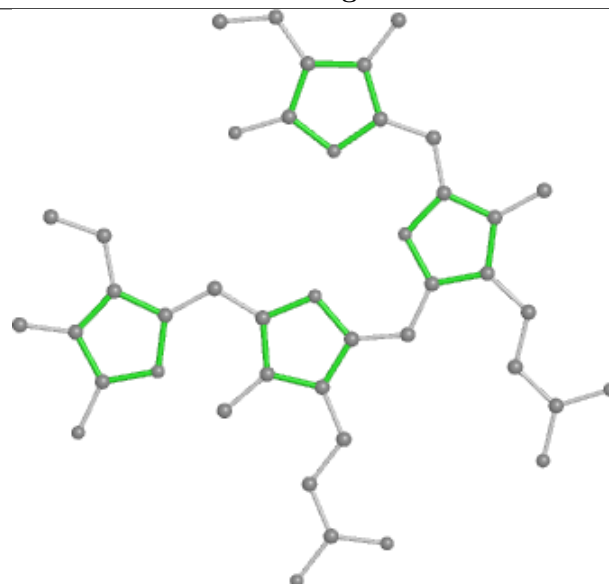
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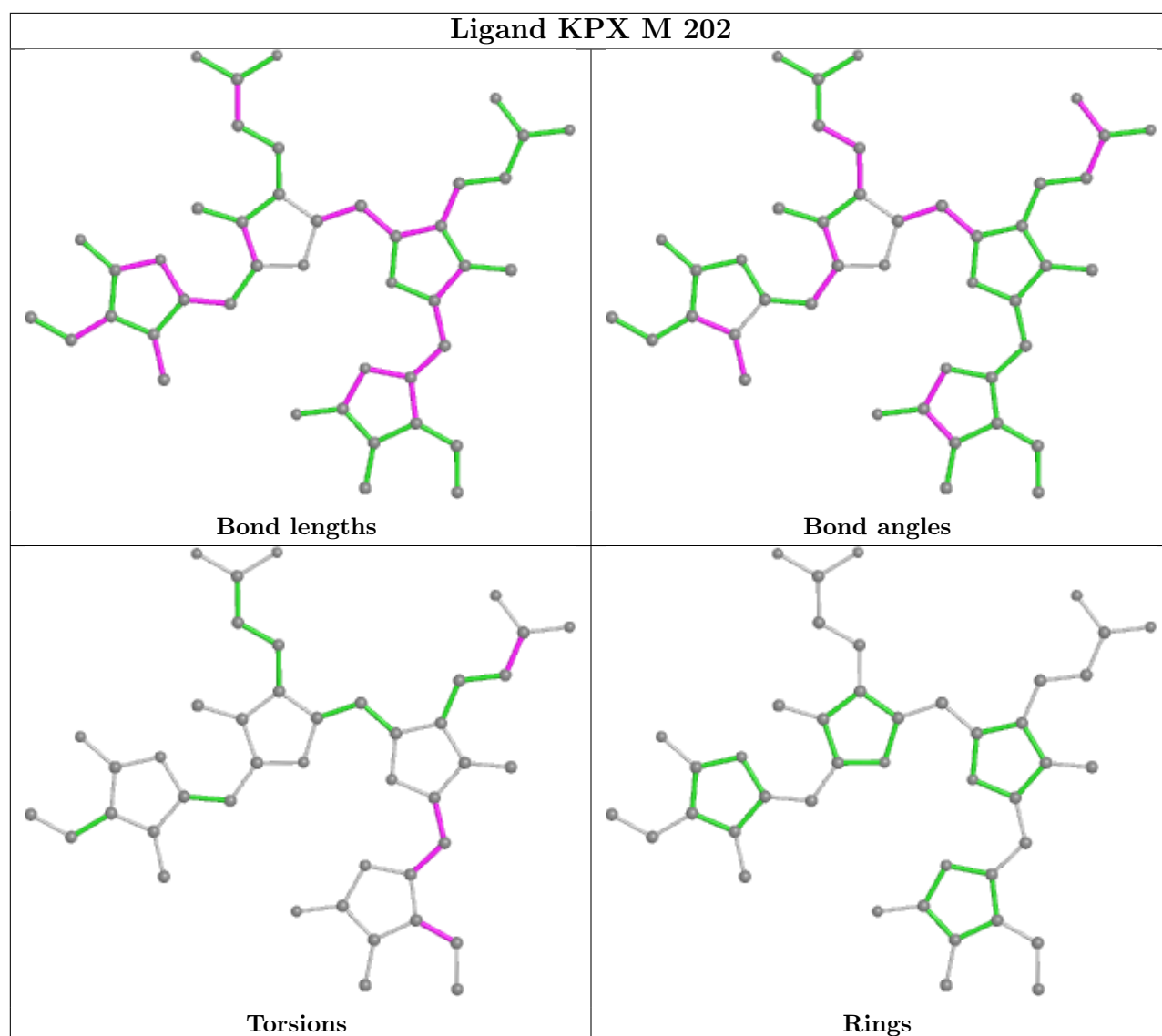
Bond angles

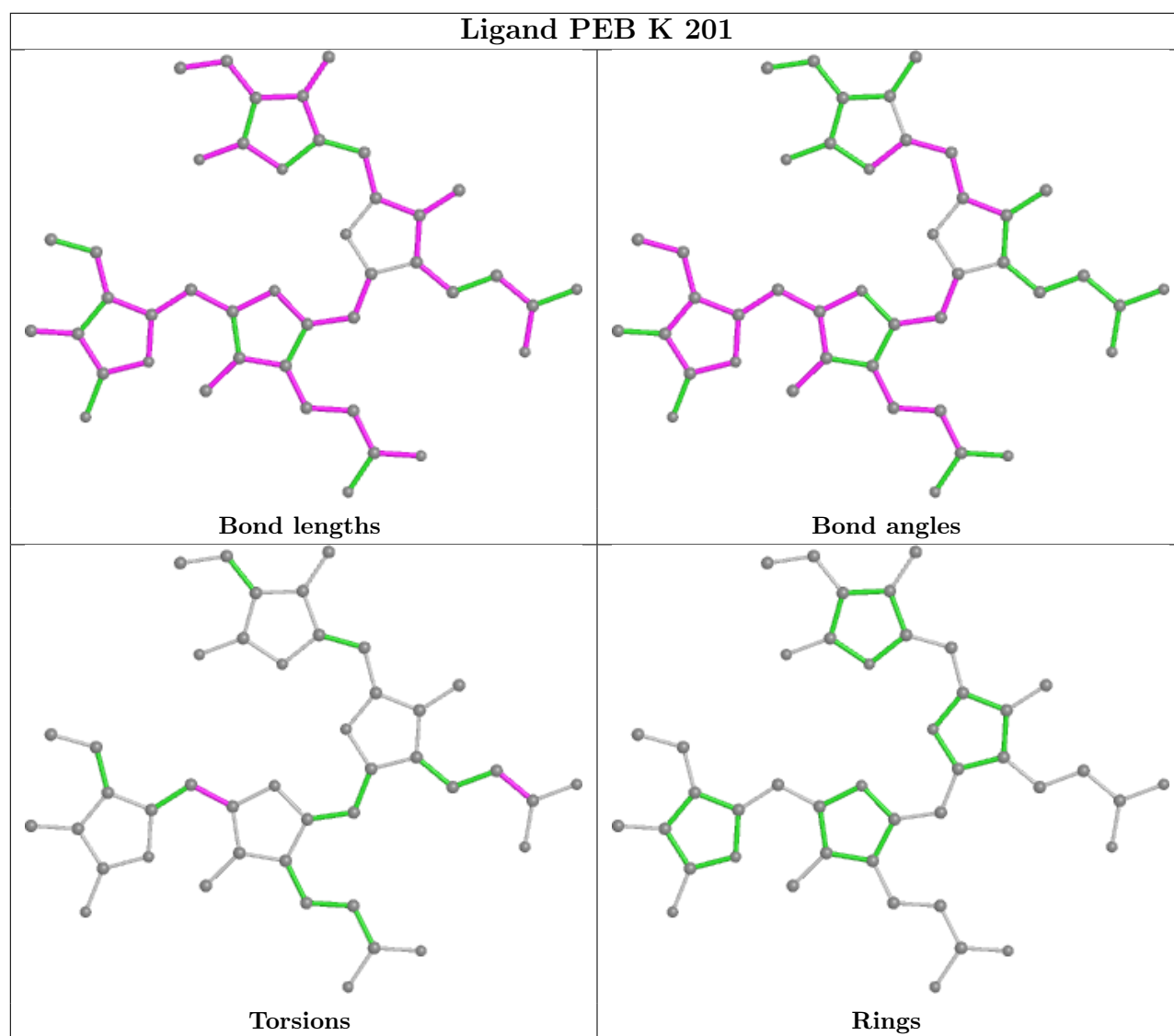


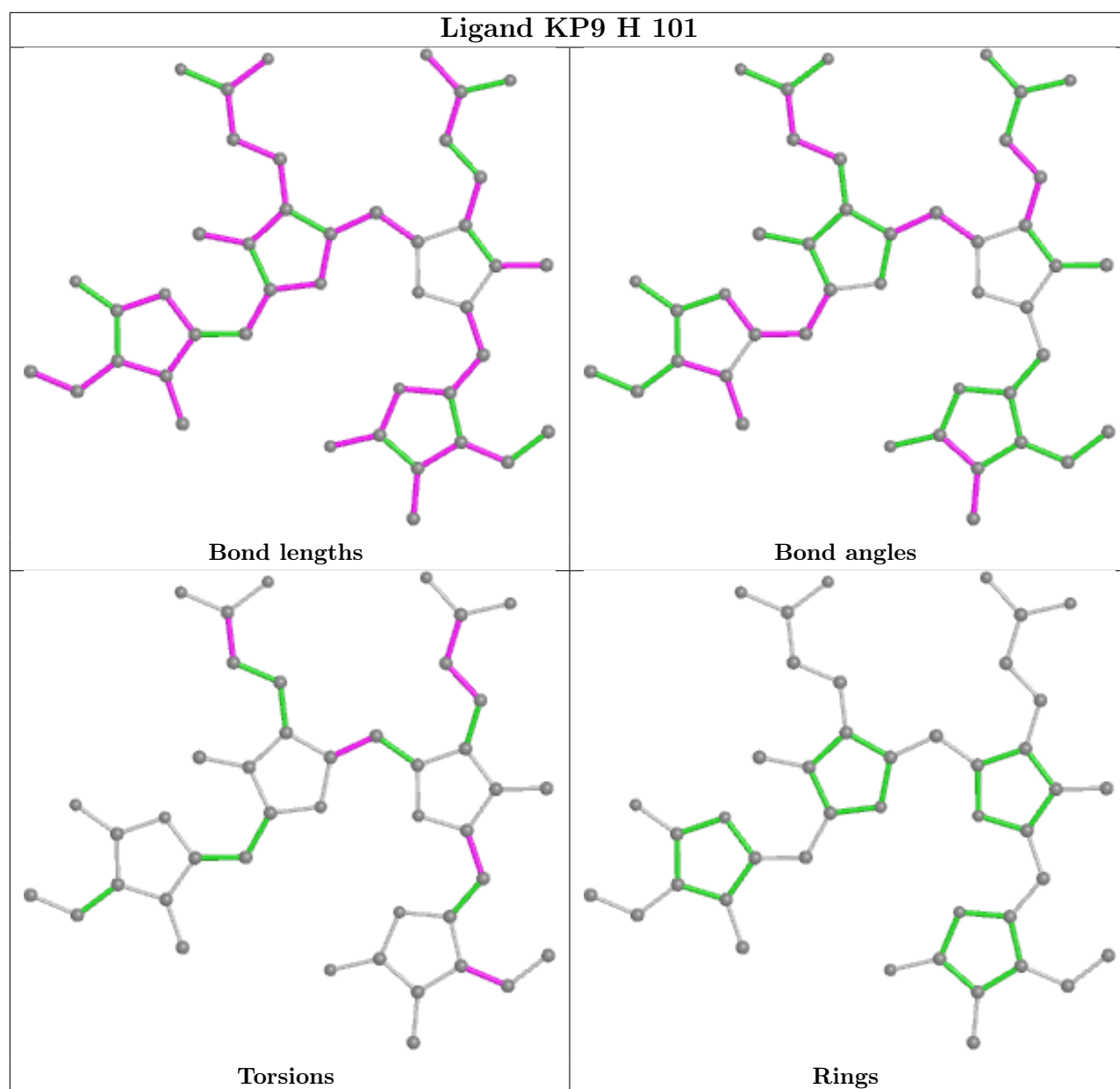
Torsions

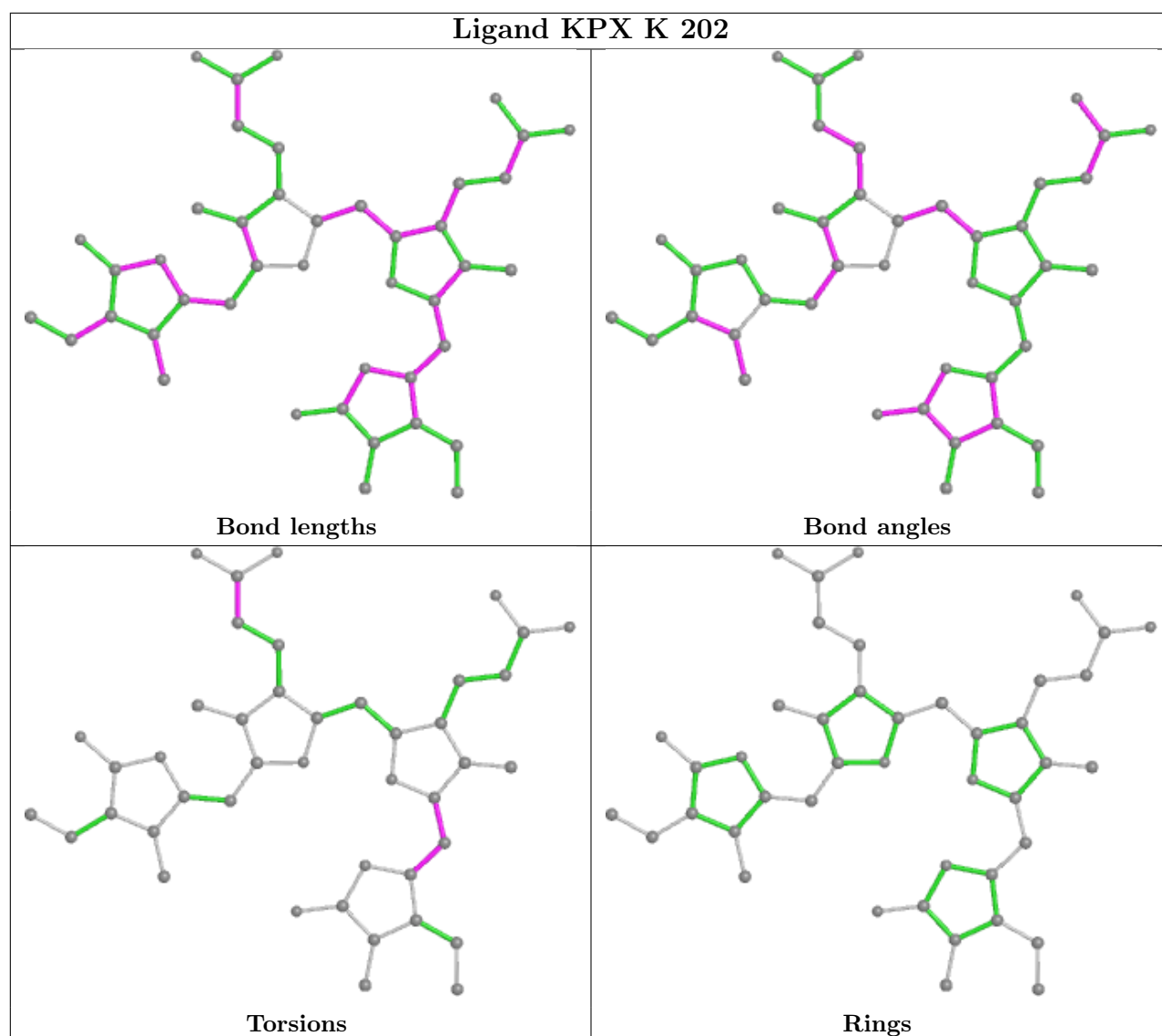


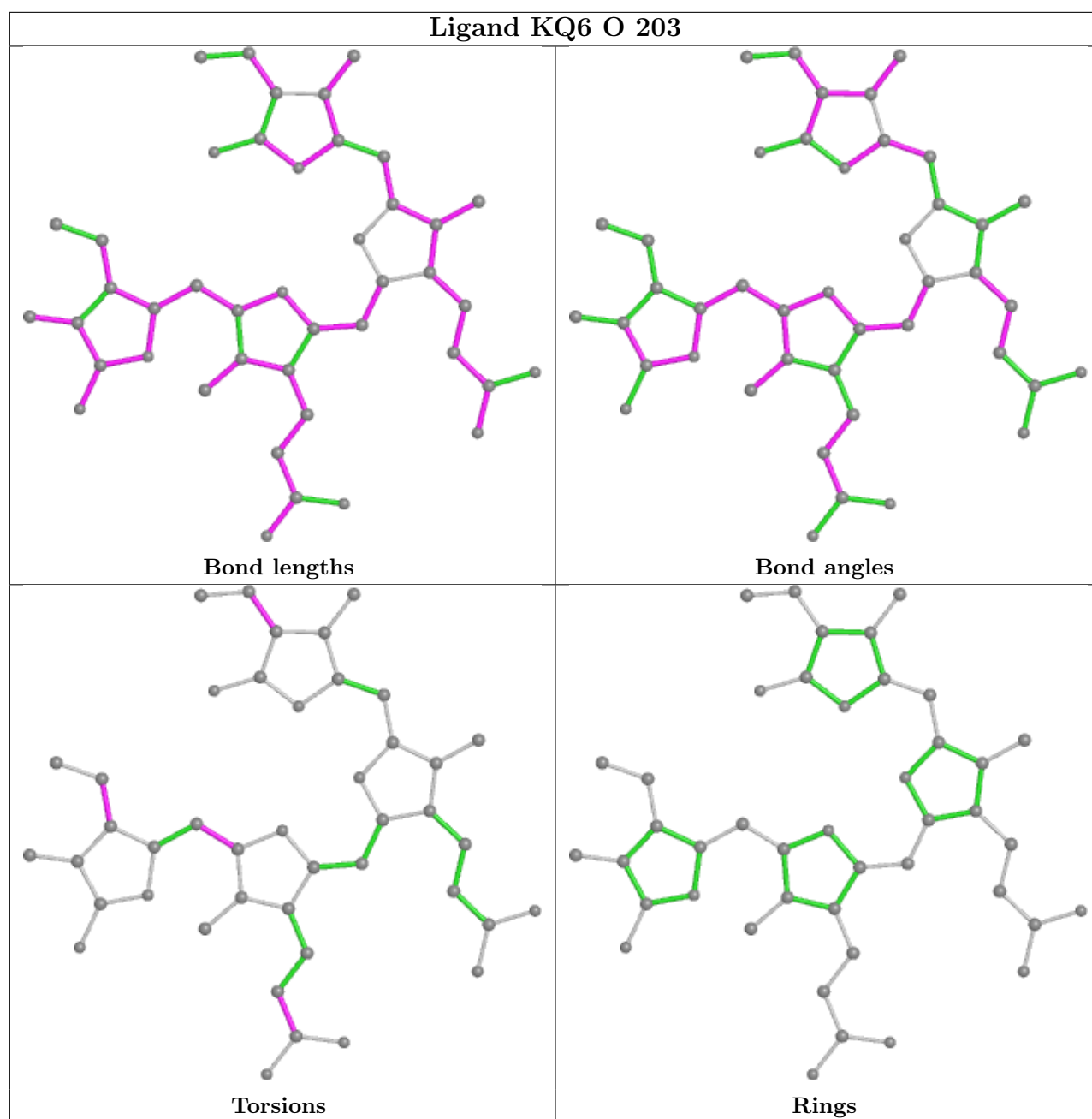
Rings

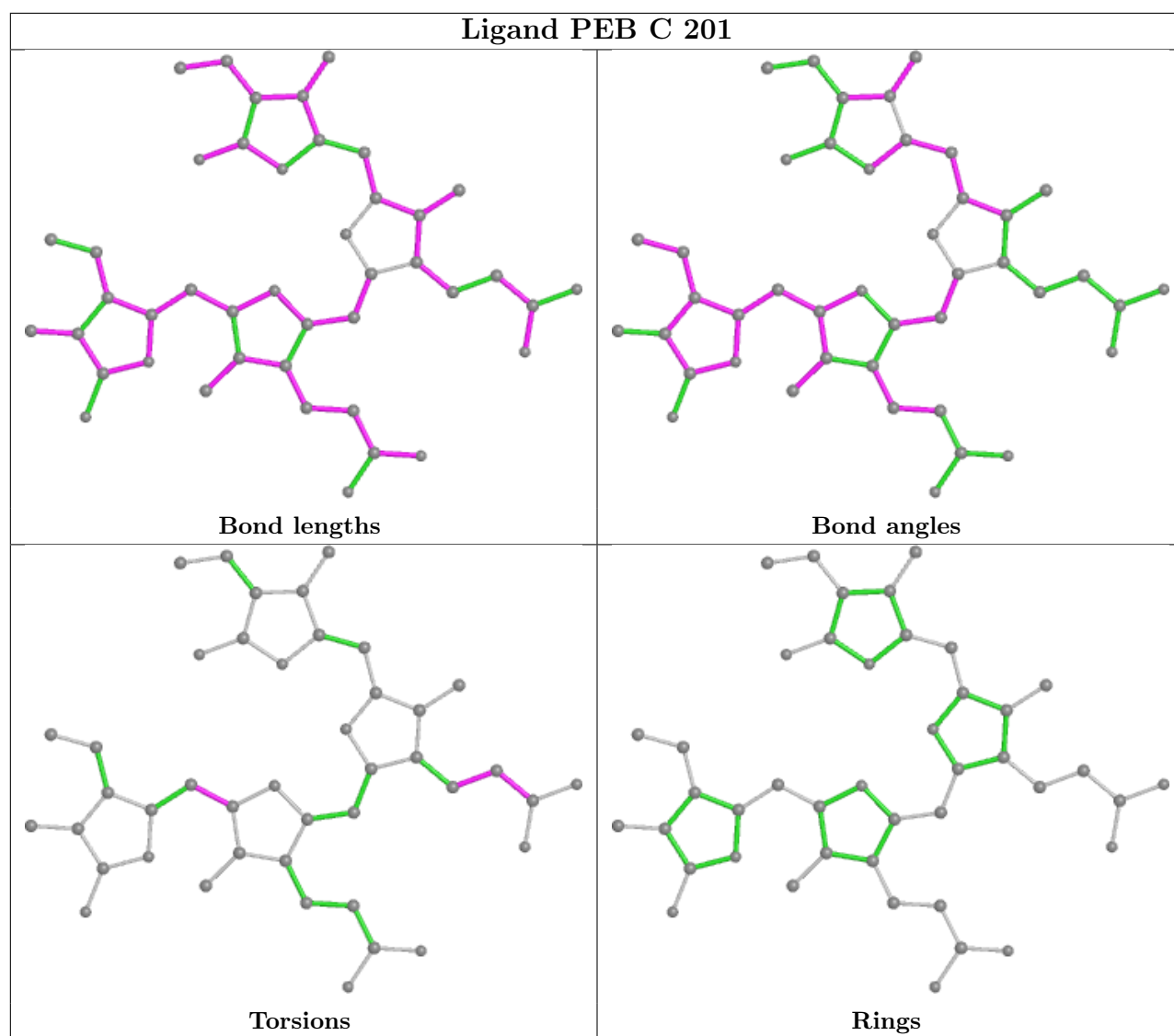


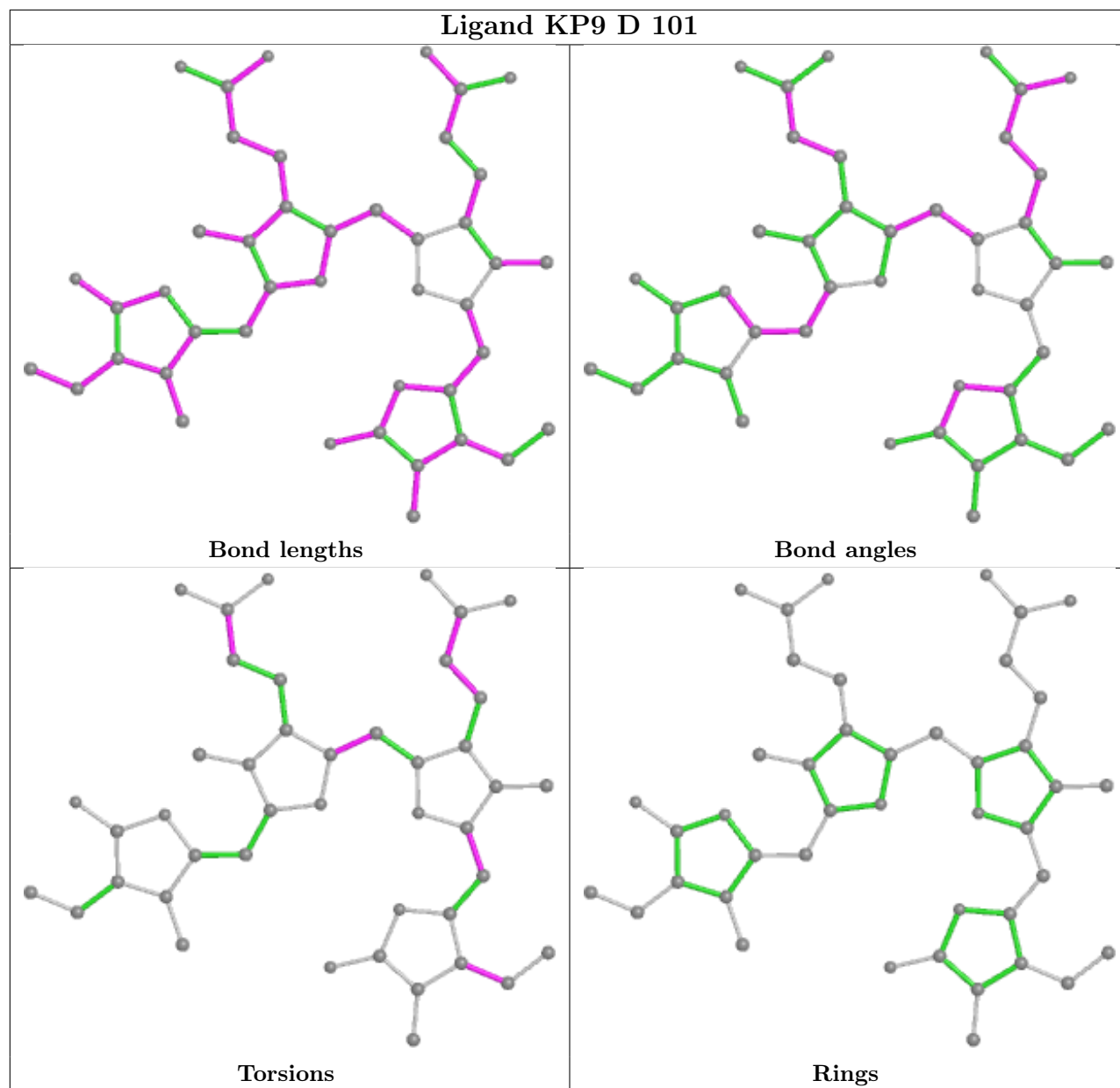




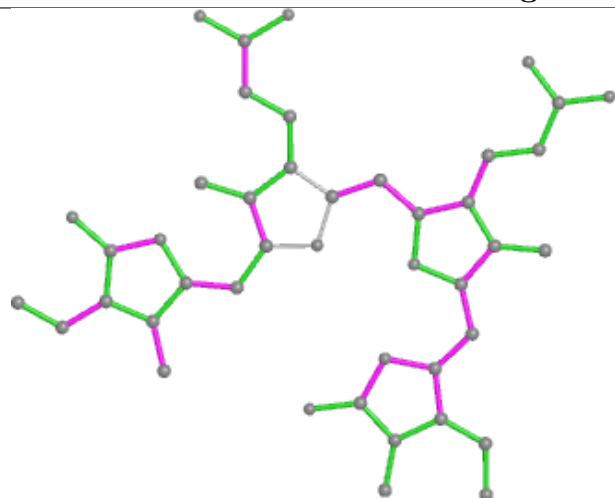




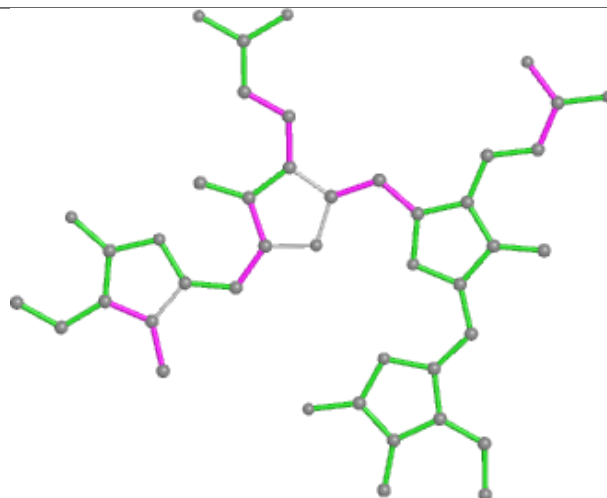




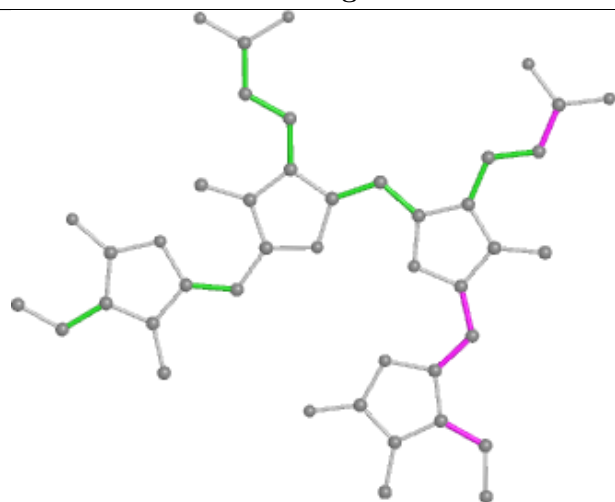
Ligand KPX I 202



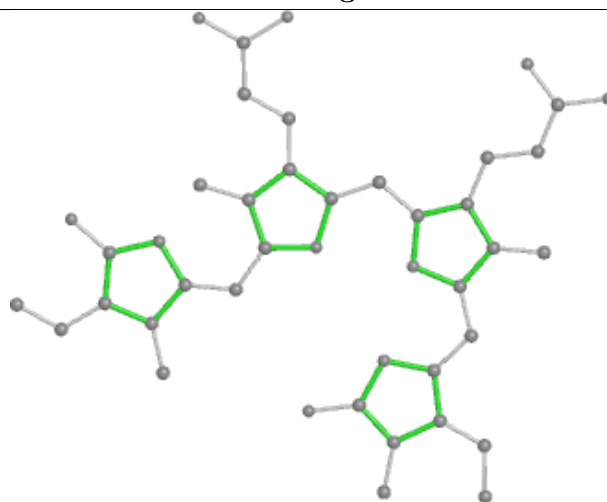
Bond lengths



Bond angles

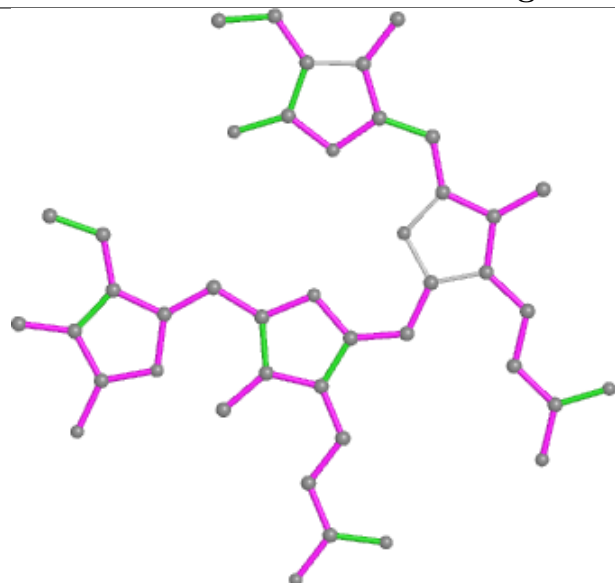


Torsions

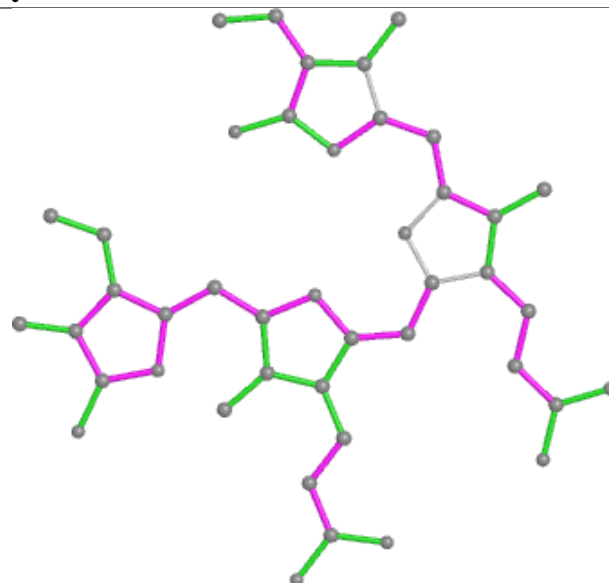


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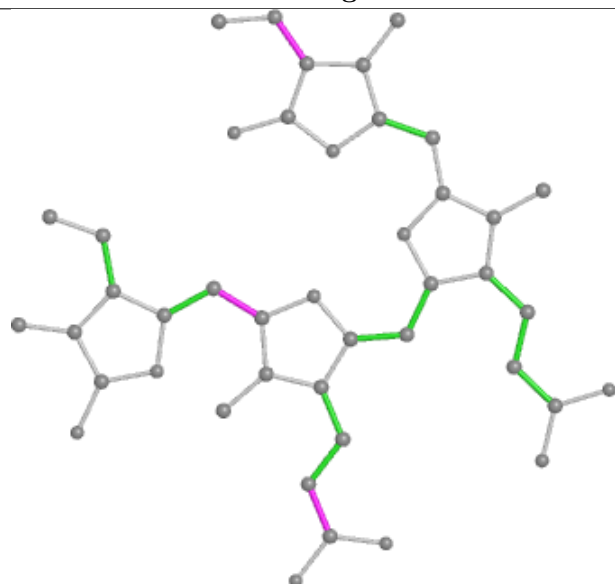
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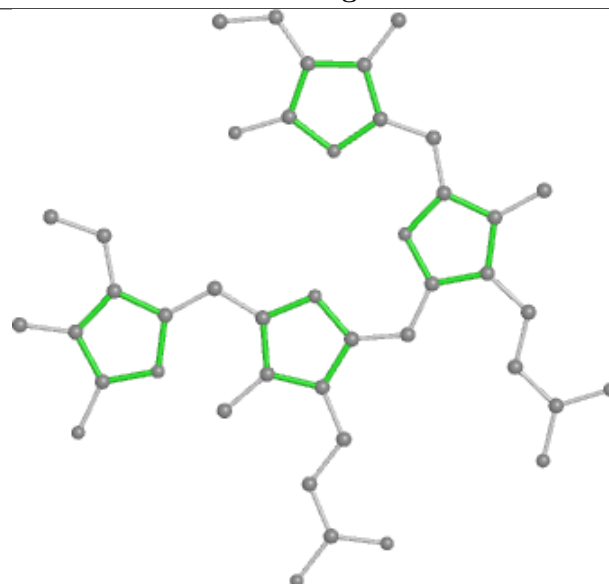
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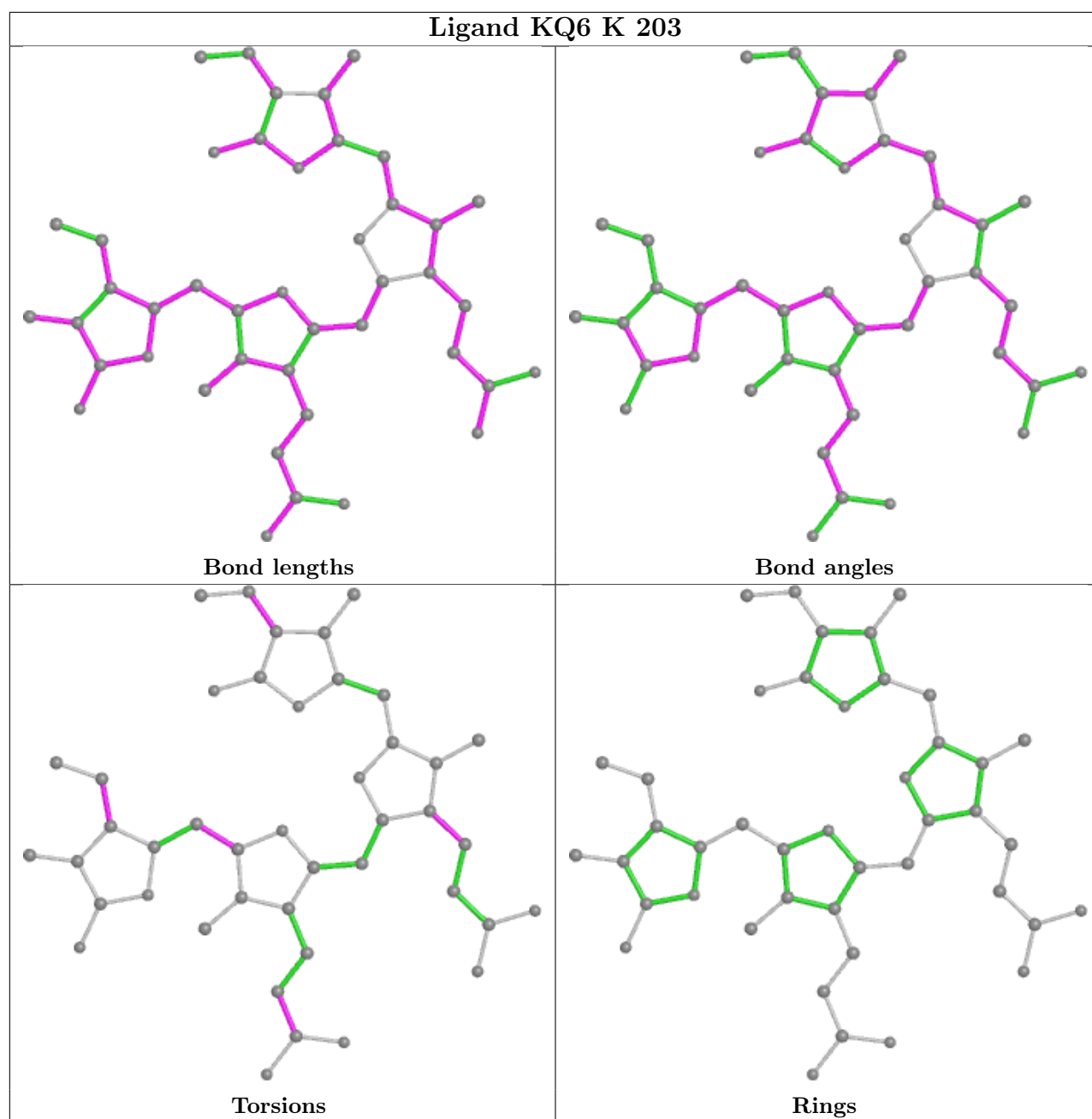
Bond angles

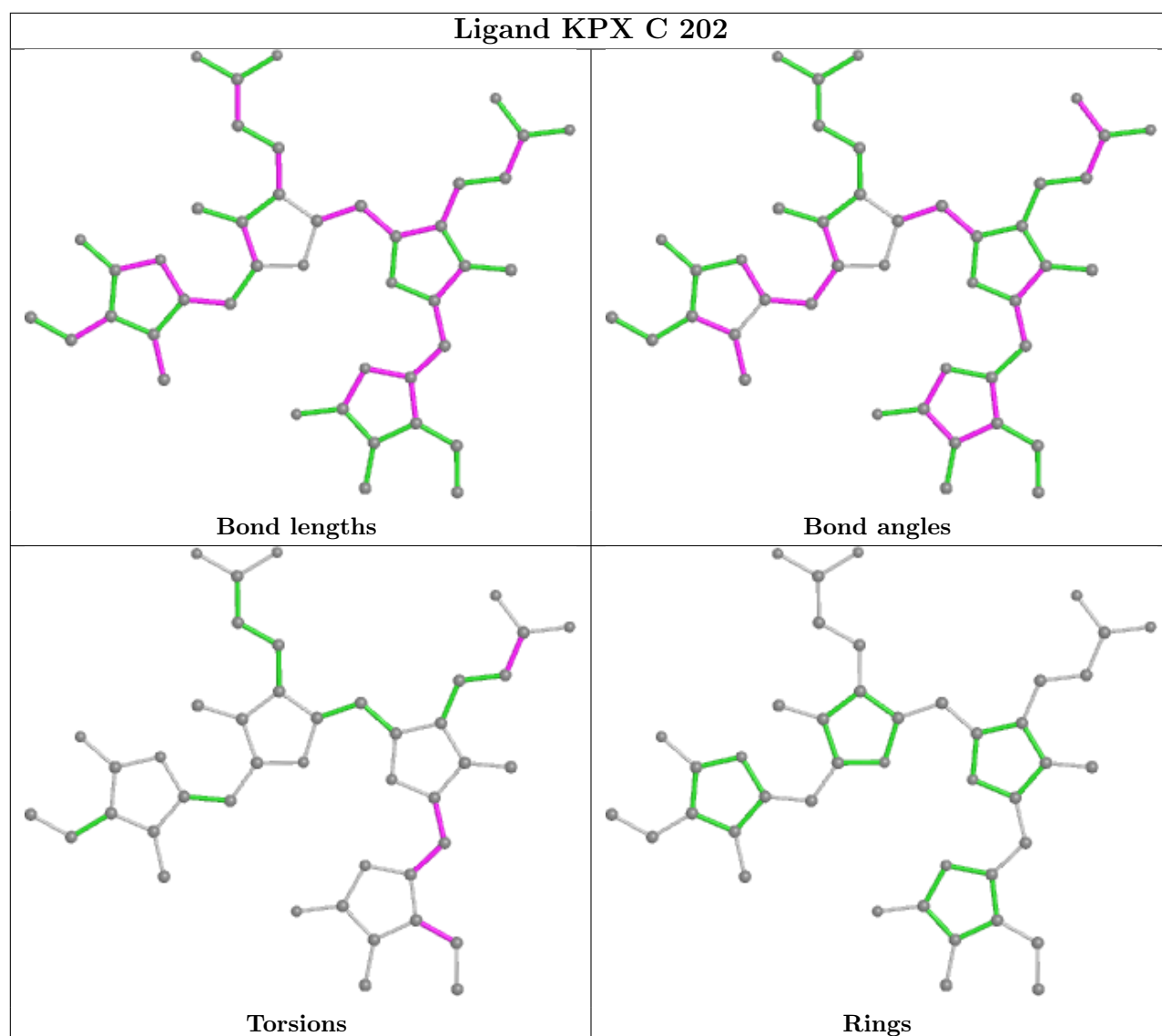


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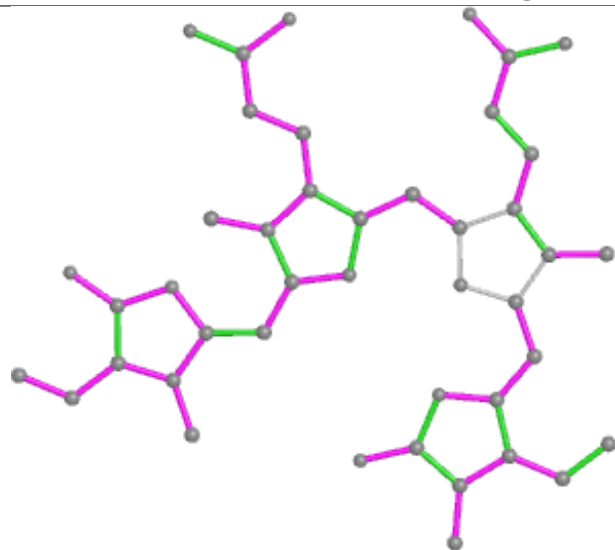


Rings

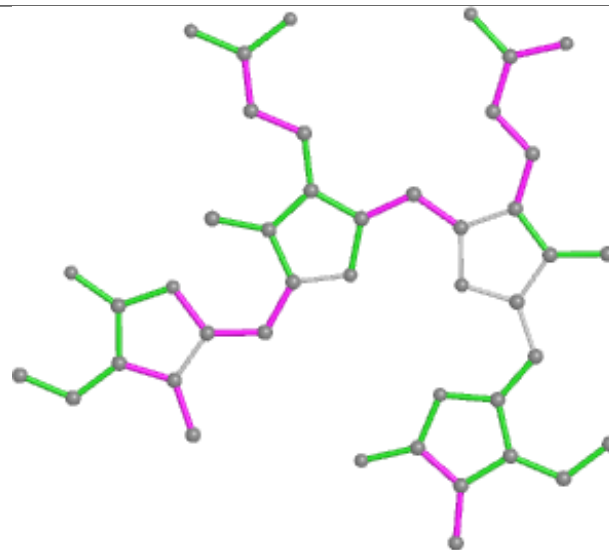




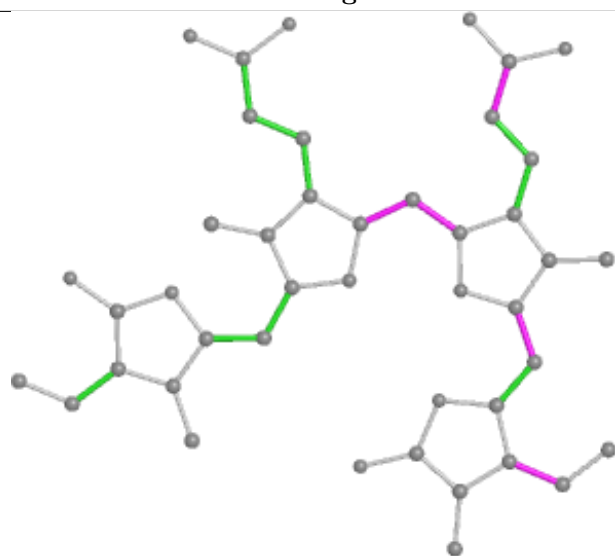
Ligand KP9 B 101



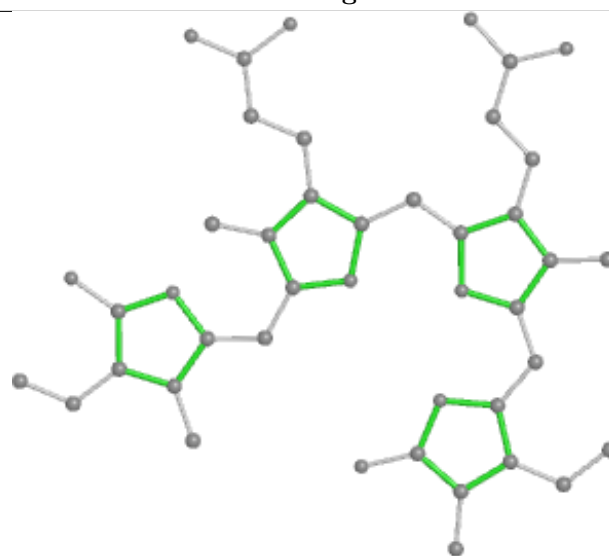
Bond lengths



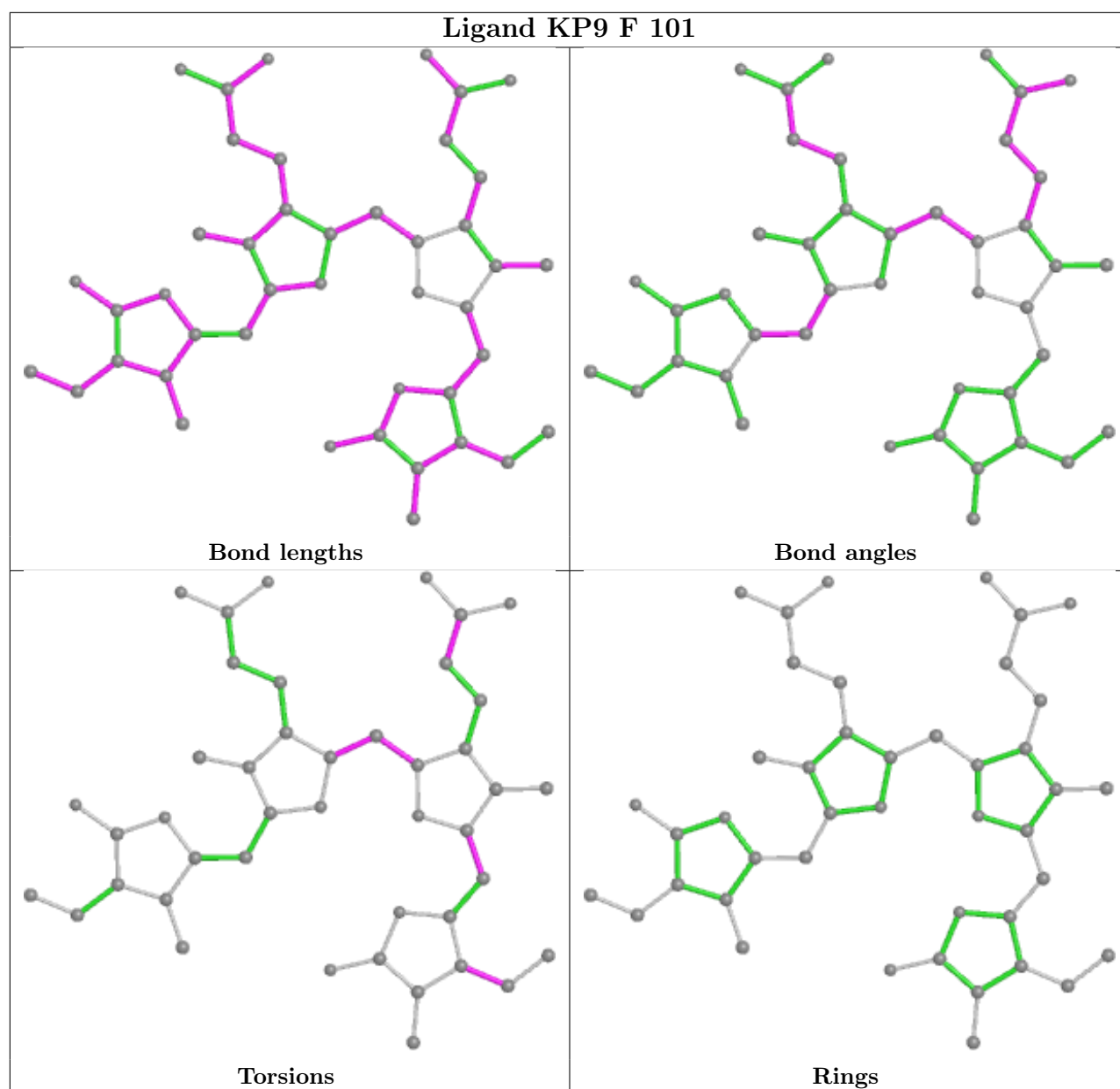
Bond angles



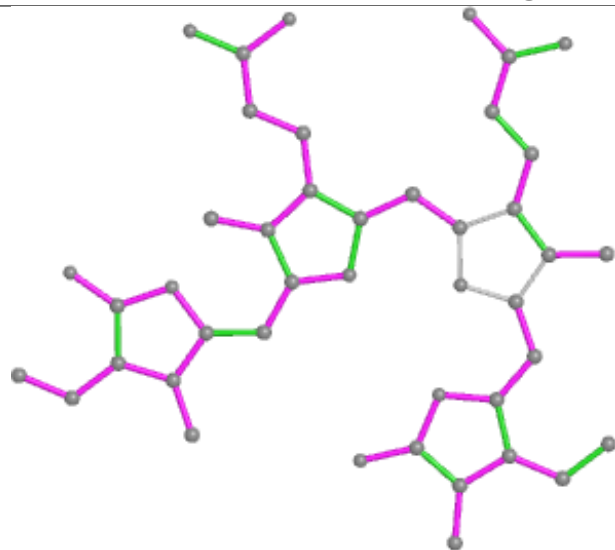
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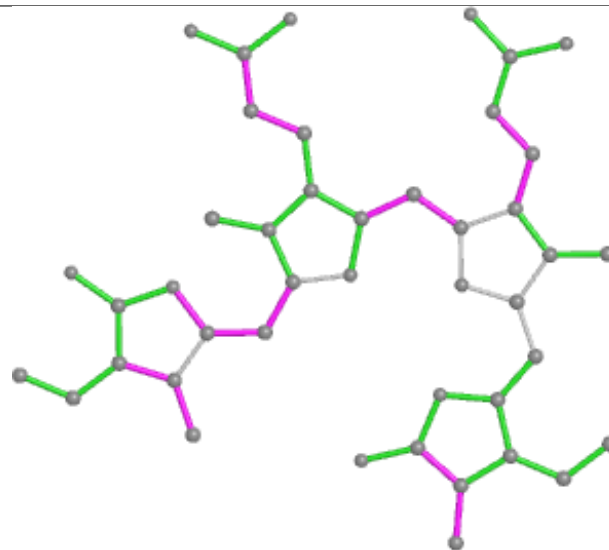
Rings



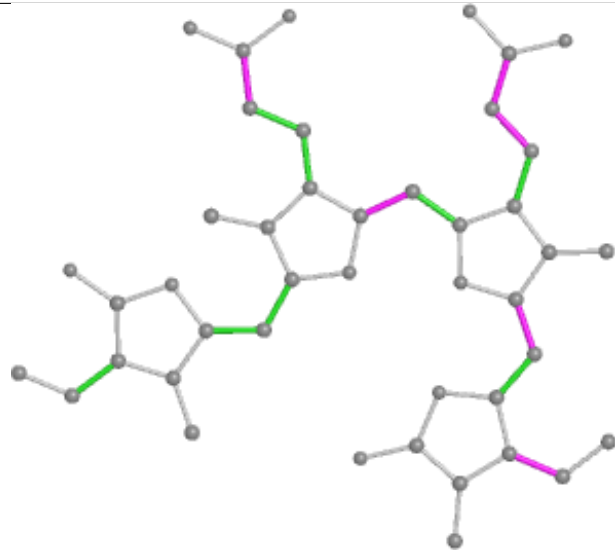
Ligand KP9 L 101



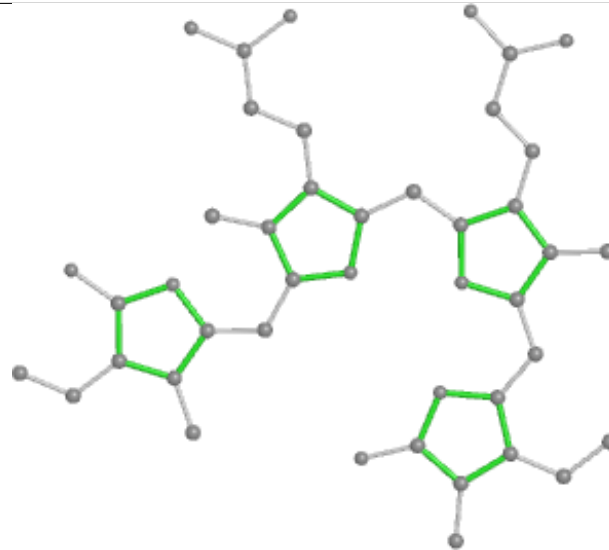
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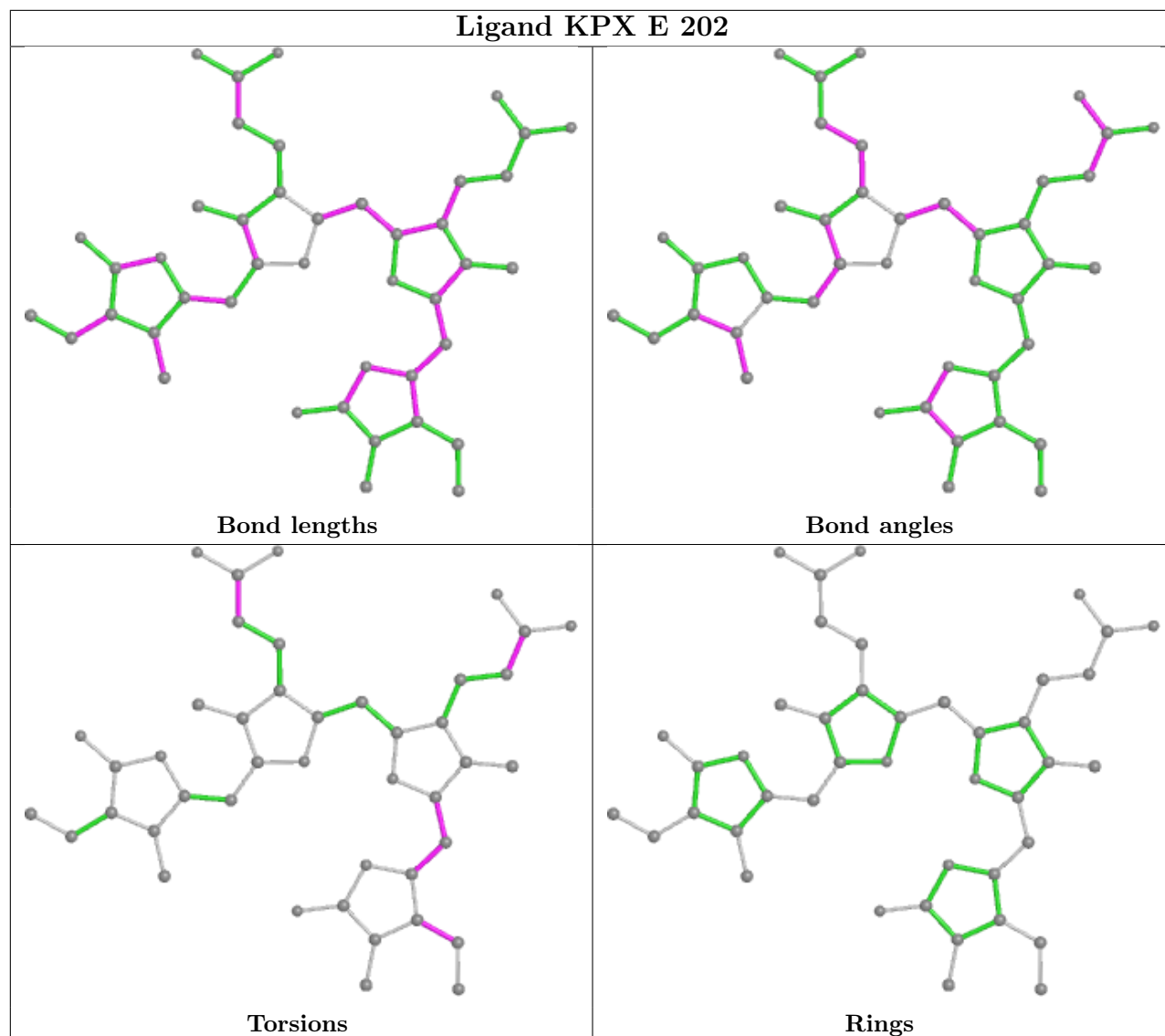
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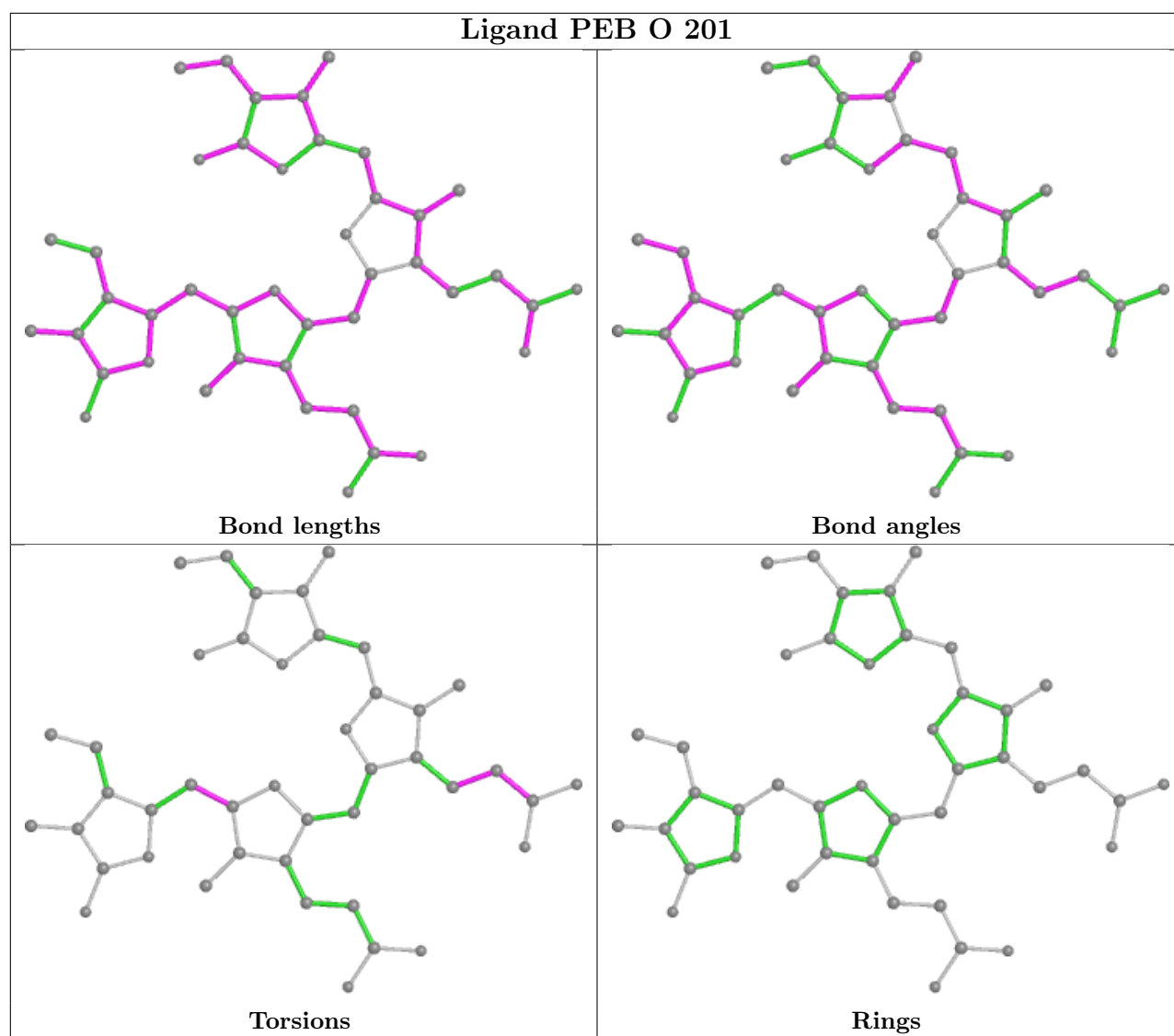


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	170/178 (95%)	-0.07	1 (0%) 89 88	20, 30, 49, 65	0
1	C	163/178 (91%)	-0.15	0 100 100	19, 25, 35, 54	0
1	E	171/178 (96%)	0.02	0 100 100	22, 32, 47, 66	0
1	G	163/178 (91%)	-0.00	0 100 100	21, 31, 43, 75	0
1	I	171/178 (96%)	0.17	0 100 100	26, 38, 53, 72	0
1	K	163/178 (91%)	-0.04	0 100 100	21, 29, 41, 71	0
1	M	170/178 (95%)	0.23	1 (0%) 89 88	29, 39, 53, 66	0
1	O	163/178 (91%)	0.17	1 (0%) 89 88	22, 34, 49, 67	0
2	B	78/78 (100%)	-0.04	2 (2%) 56 54	22, 29, 51, 62	0
2	F	78/78 (100%)	0.04	2 (2%) 56 54	24, 30, 52, 78	0
2	J	78/78 (100%)	0.14	1 (1%) 77 76	28, 35, 55, 83	0
2	N	77/78 (98%)	0.18	1 (1%) 77 76	25, 36, 54, 79	0
3	D	70/70 (100%)	-0.14	0 100 100	22, 29, 40, 62	0
3	H	70/70 (100%)	-0.08	0 100 100	22, 35, 50, 72	0
3	L	70/70 (100%)	0.05	0 100 100	25, 36, 58, 68	0
3	P	70/70 (100%)	0.16	0 100 100	27, 42, 59, 74	0
All	All	1925/2016 (95%)	0.04	9 (0%) 91 90	19, 33, 51, 83	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	PHE	2.5
2	J	2	PHE	2.5
2	N	77	ARG	2.3
2	B	2	PHE	2.3
2	F	2	PHE	2.3

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

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
1	MEN	A	73	9/10	0.95	0.14	27,29,39,39	0
1	MEN	I	73	9/10	0.95	0.14	38,42,50,50	0
1	MEN	M	73	9/10	0.95	0.16	45,48,57,57	0
1	MEN	C	73	9/10	0.96	0.12	21,24,32,32	0
1	MEN	E	73	9/10	0.96	0.11	34,37,47,47	0
1	MEN	G	73	9/10	0.97	0.13	20,25,32,32	0
1	MEN	K	73	9/10	0.98	0.12	25,27,36,36	0
1	MEN	O	73	9/10	0.98	0.11	23,27,34,34	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	M	204	6/6	0.84	0.25	32,39,44,47	0
7	GOL	I	205	6/6	0.85	0.37	32,39,45,45	0
7	GOL	A	205	6/6	0.85	0.29	28,35,39,44	0
7	GOL	G	204	6/6	0.91	0.17	26,31,33,33	14
7	GOL	H	102	6/6	0.91	0.23	38,47,57,57	0
5	KPX	K	202	43/43	0.93	0.14	29,36,45,49	0
4	PEB	E	201	43/43	0.93	0.17	28,36,47,50	0
4	PEB	M	201	43/43	0.93	0.20	33,42,56,61	0
4	PEB	I	201	43/43	0.94	0.18	30,39,52,55	0
6	KQ6	E	203	43/43	0.94	0.15	22,30,42,47	0
6	KQ6	I	203	43/43	0.94	0.16	23,31,44,51	0
6	KQ6	M	203	43/43	0.94	0.17	26,35,45,50	0
6	KQ6	O	203	43/43	0.94	0.17	22,27,32,34	0
4	PEB	C	201	43/43	0.94	0.16	21,27,36,40	0

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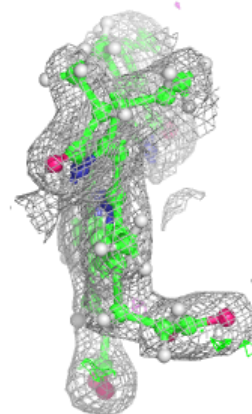
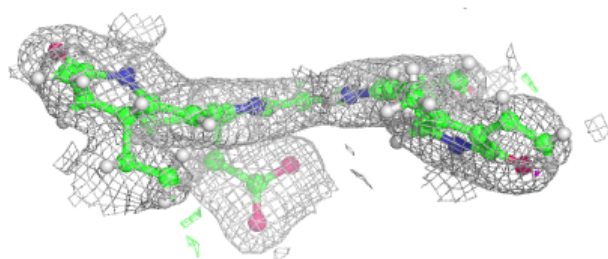
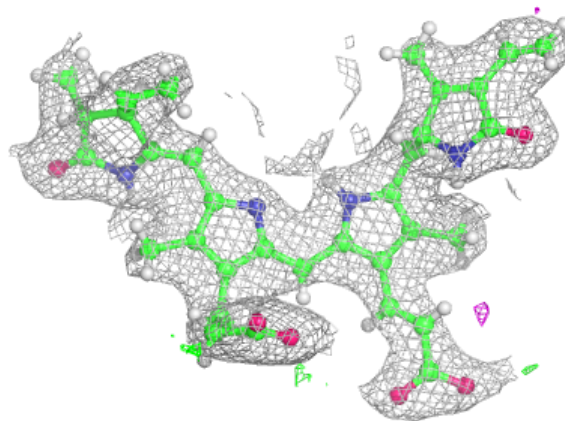
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PEB	O	201	43/43	0.94	0.16	22,31,41,44	0
5	KPX	E	202	43/43	0.94	0.14	25,31,38,46	0
5	KPX	G	202	43/43	0.94	0.13	31,38,45,50	0
5	KPX	I	202	43/43	0.94	0.15	28,36,44,49	0
8	KP9	H	101	43/43	0.94	0.16	31,36,45,49	0
8	KP9	J	101	43/43	0.94	0.15	23,29,39,42	0
8	KP9	L	101	43/43	0.94	0.15	32,39,47,52	0
8	KP9	P	101	43/43	0.94	0.19	36,41,53,56	0
6	KQ6	A	203	43/43	0.95	0.16	19,24,31,36	0
4	PEB	K	201	43/43	0.95	0.16	21,30,39,47	0
6	KQ6	G	203	43/43	0.95	0.15	22,26,32,35	0
4	PEB	G	201	43/43	0.95	0.15	20,30,38,43	0
8	KP9	B	101	43/43	0.95	0.15	21,27,34,39	0
8	KP9	D	101	43/43	0.95	0.15	23,28,33,38	0
6	KQ6	K	203	43/43	0.95	0.16	22,27,33,33	0
4	PEB	A	201	43/43	0.95	0.16	22,32,45,47	0
5	KPX	A	202	43/43	0.95	0.14	25,32,39,49	0
8	KP9	N	101	43/43	0.95	0.15	22,27,34,38	0
5	KPX	O	202	43/43	0.95	0.16	35,43,50,57	0
5	KPX	C	202	43/43	0.96	0.13	24,29,35,38	0
7	GOL	E	204	6/6	0.96	0.13	26,31,34,34	0
5	KPX	M	202	43/43	0.96	0.14	27,35,43,51	0
6	KQ6	C	203	43/43	0.96	0.15	19,23,28,29	0
8	KP9	F	101	43/43	0.96	0.14	20,25,31,32	0
7	GOL	N	102	6/6	0.97	0.13	29,36,37,38	0
7	GOL	A	204	6/6	0.97	0.12	23,28,29,29	0
7	GOL	I	204	6/6	0.97	0.15	27,33,35,35	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.

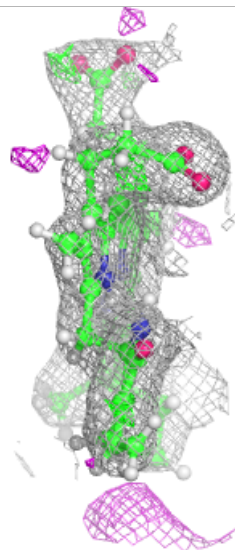
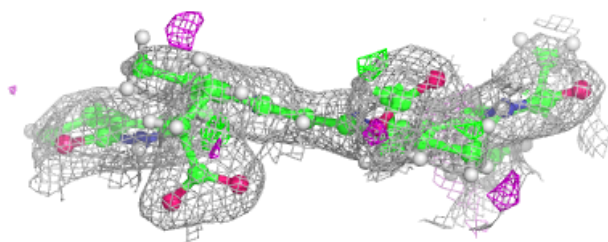
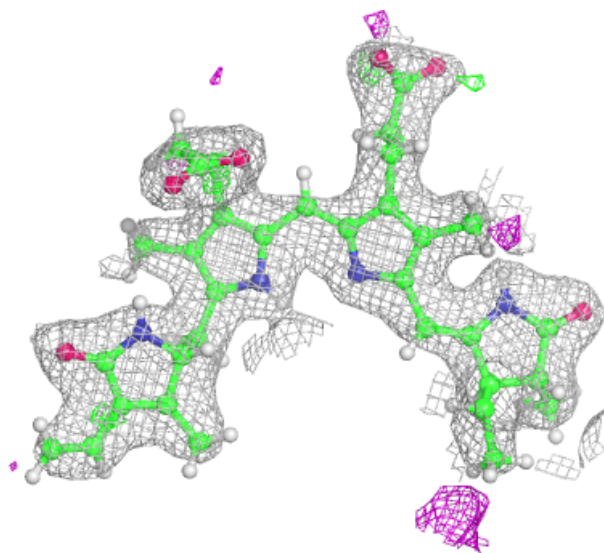
Electron density around KPX K 202:

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



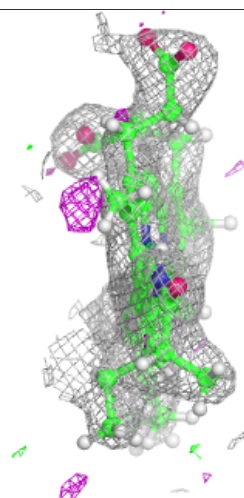
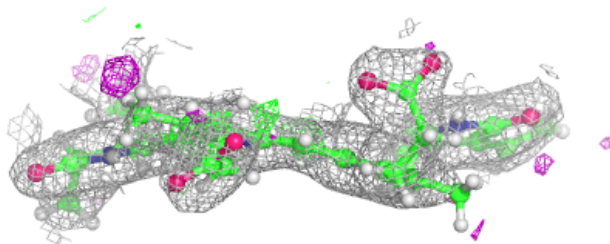
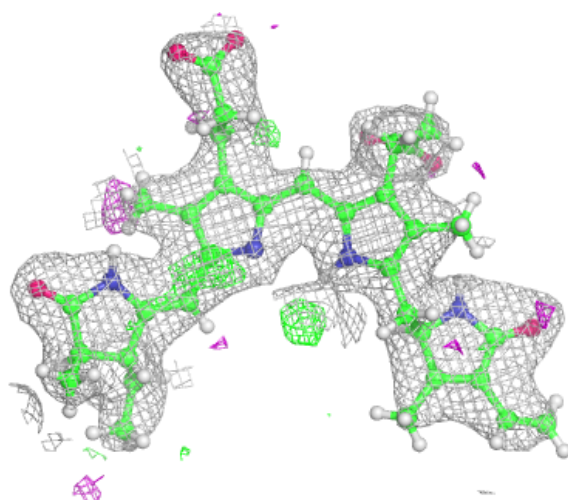
Electron density around PEB E 201:

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



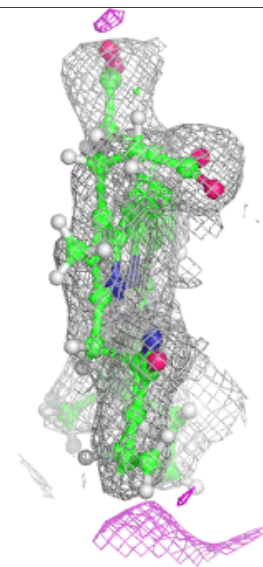
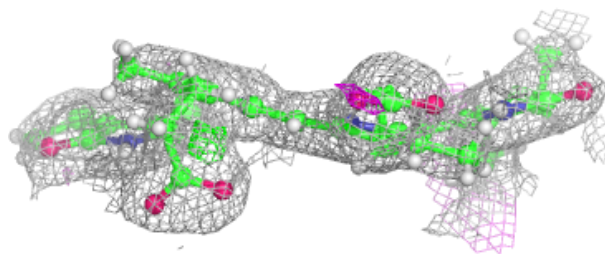
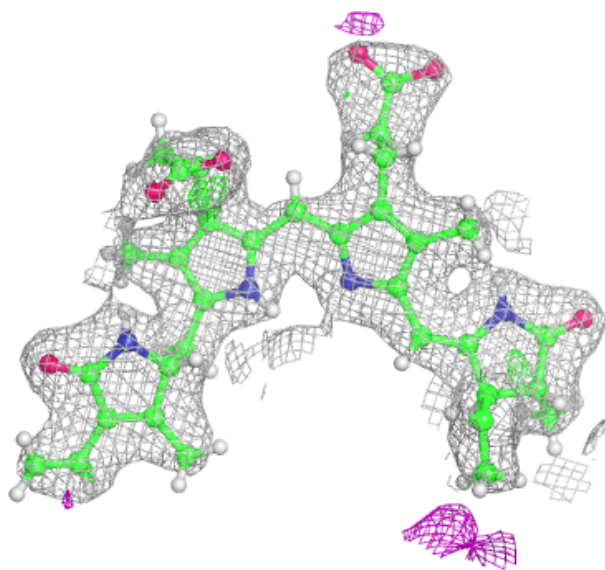
Electron density around PEB M 201:

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and green (positive)



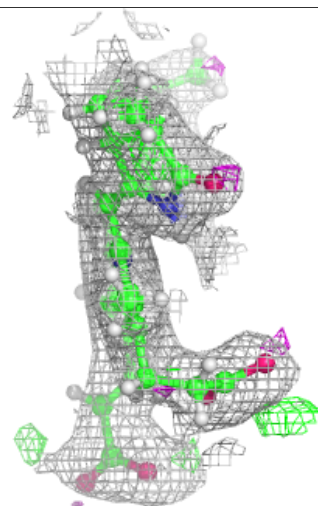
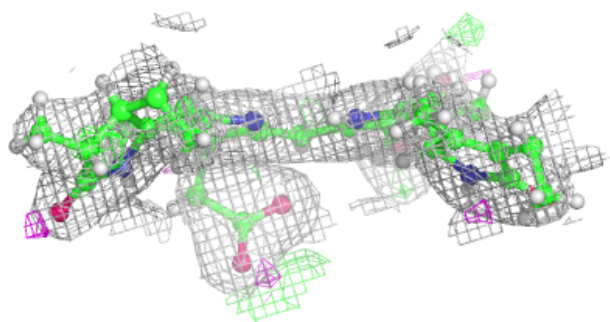
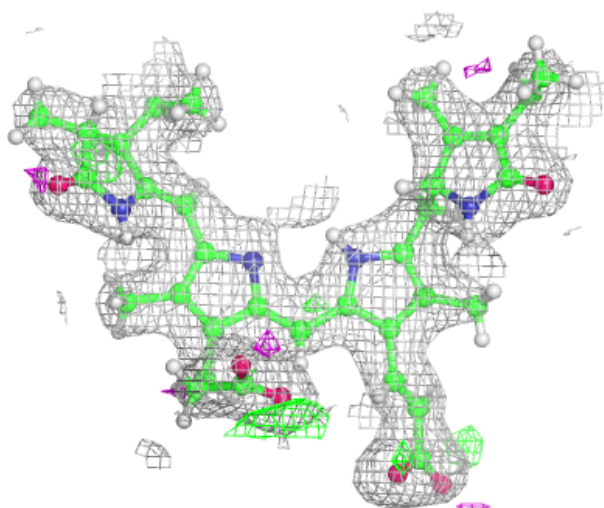
Electron density around PEB I 201:

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and green (positive)



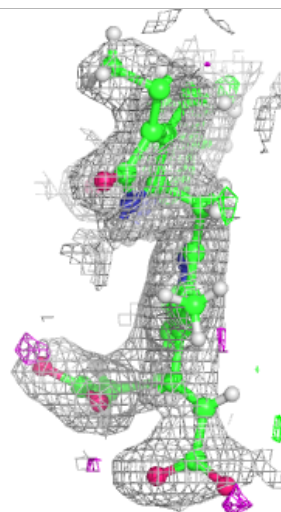
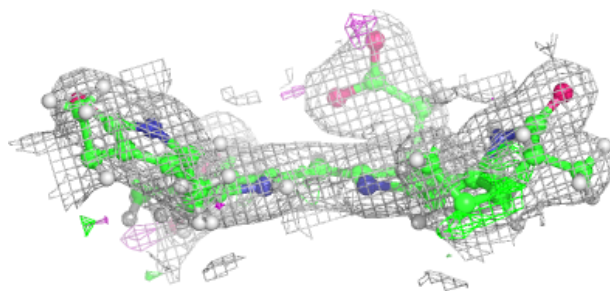
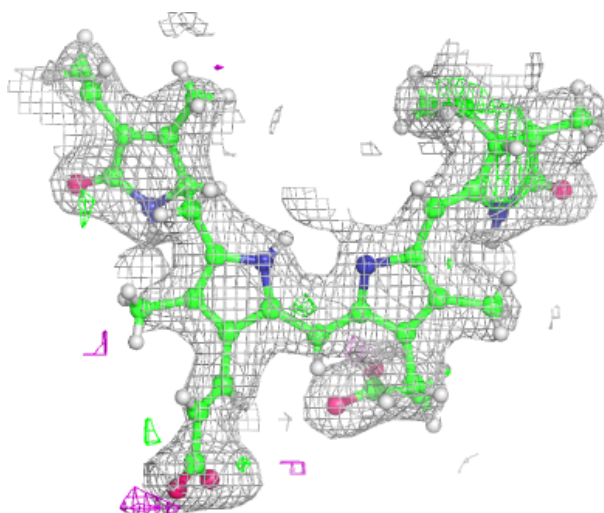
Electron density around KQ6 E 203:

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



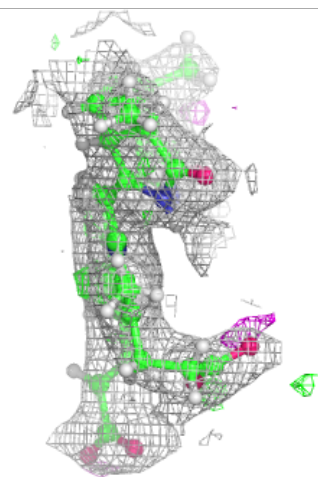
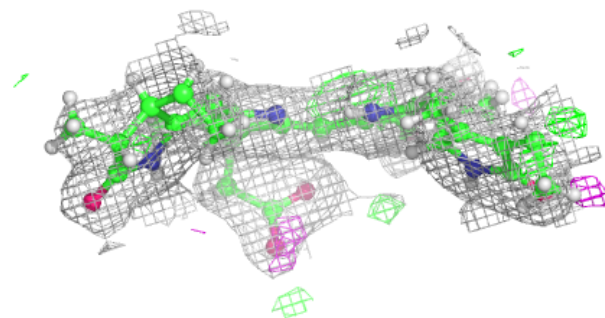
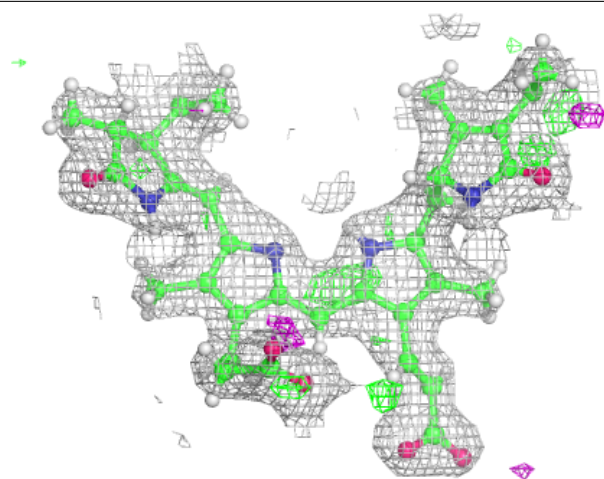
Electron density around KQ6 I 203:

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



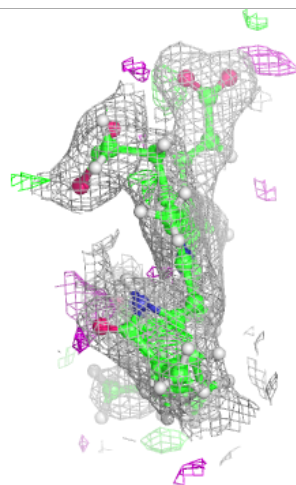
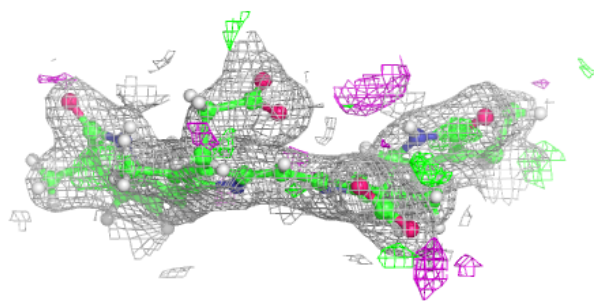
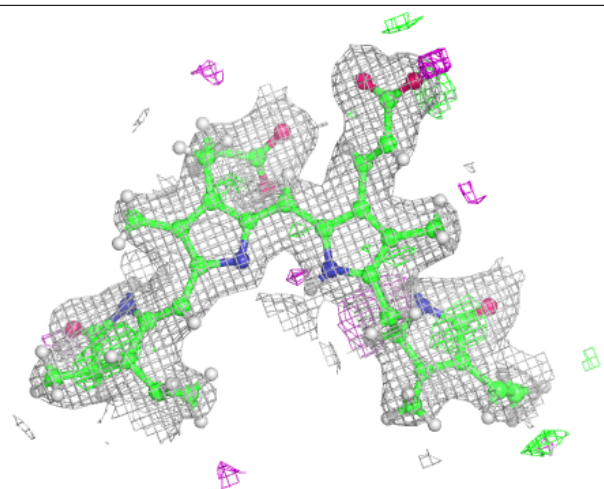
Electron density around KQ6 M 203:

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



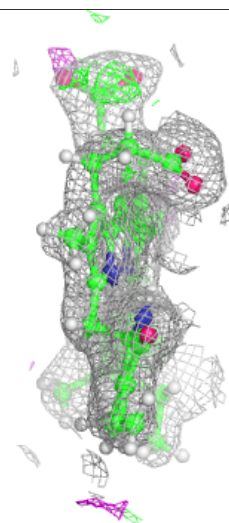
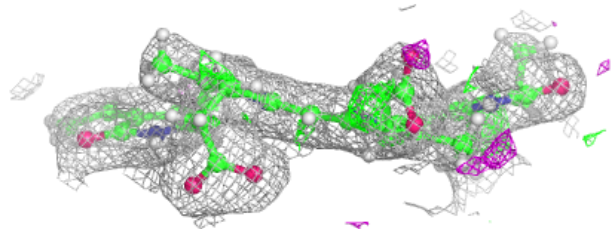
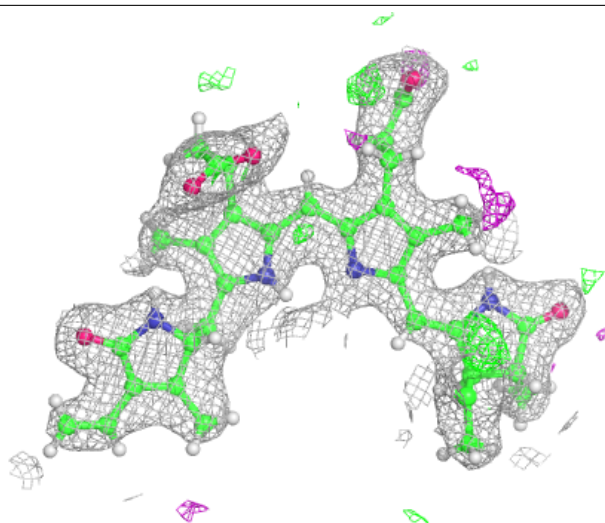
Electron density around KQ6 O 203:

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and green (positive)



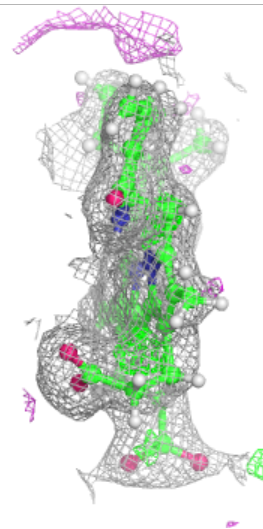
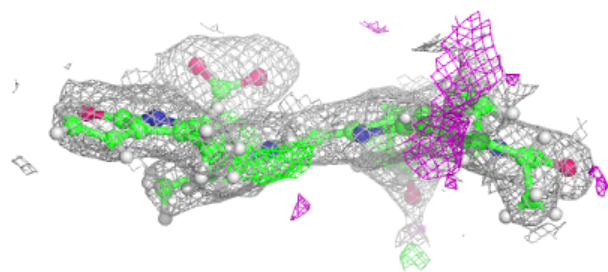
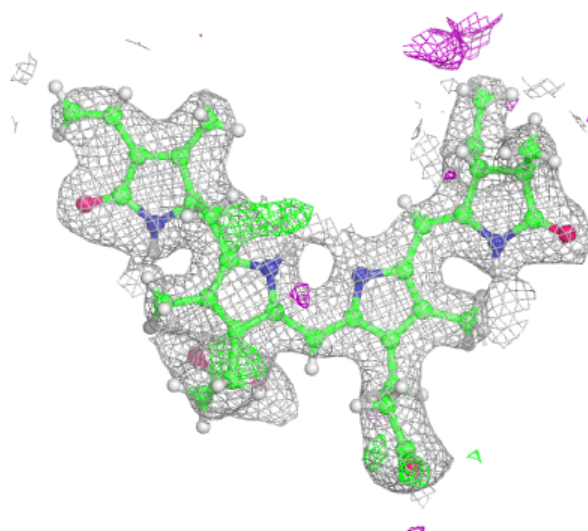
Electron density around PEB C 201:

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



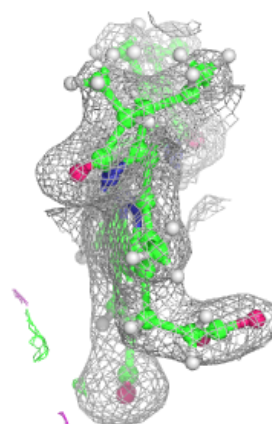
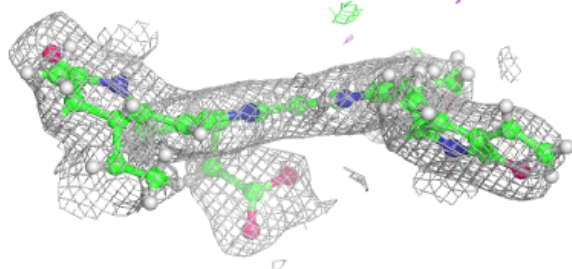
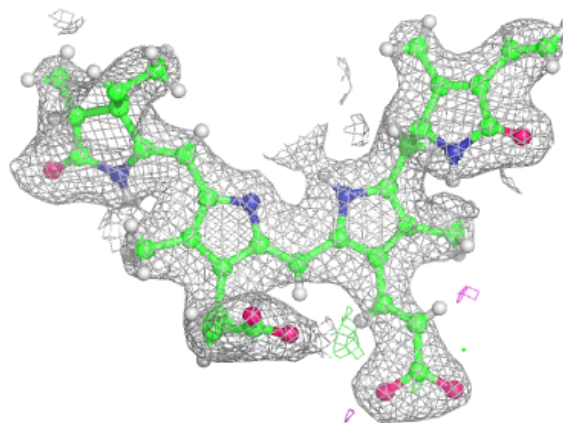
Electron density around PEB O 201:

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and green (positive)



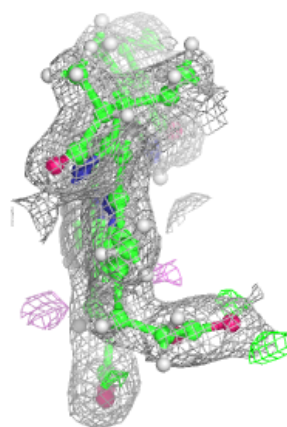
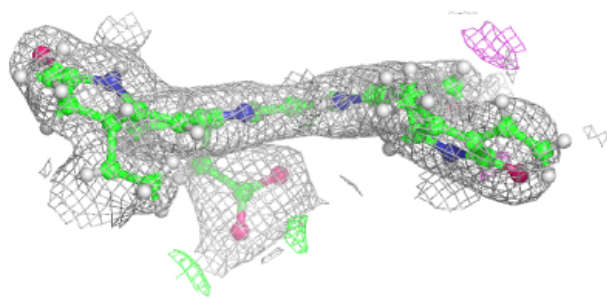
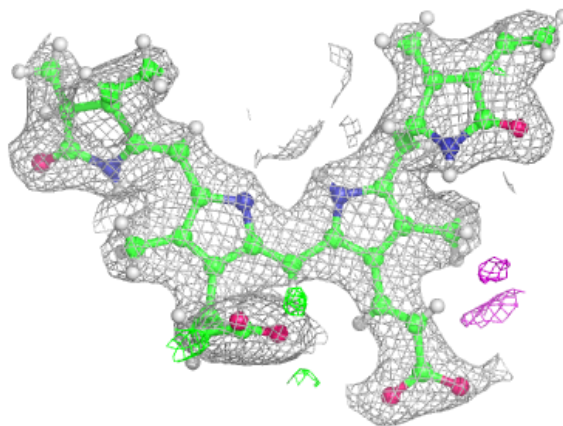
Electron density around KPX E 202:

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



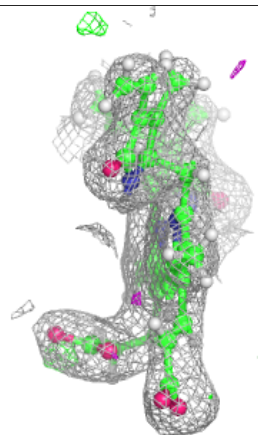
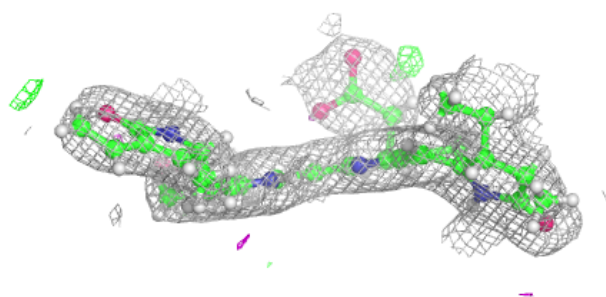
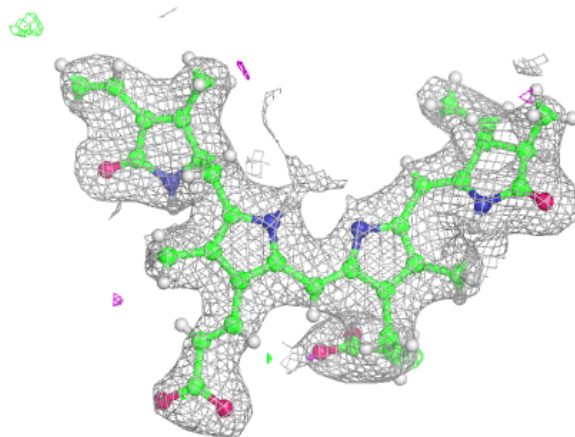
Electron density around KPX G 202:

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and green (positive)



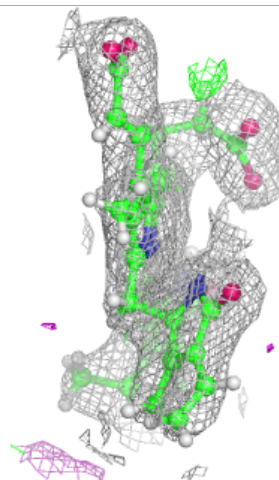
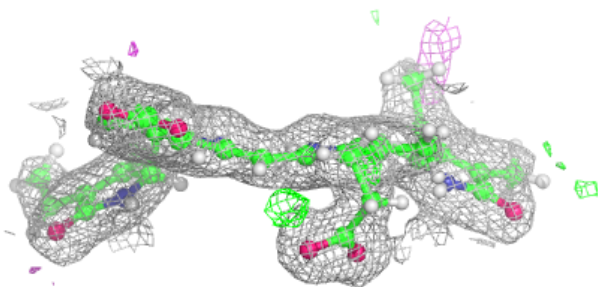
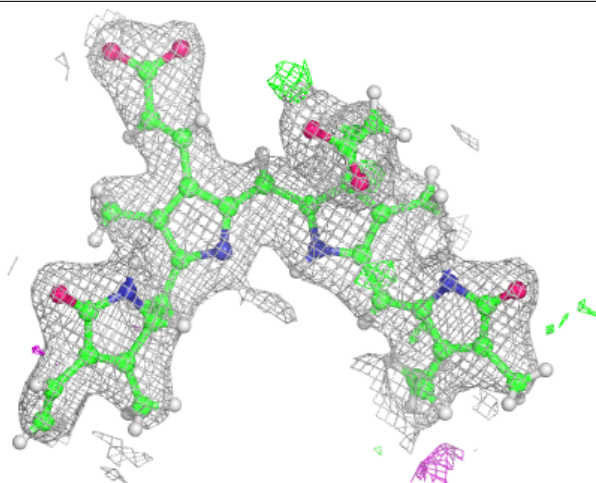
Electron density around KPX I 202:

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



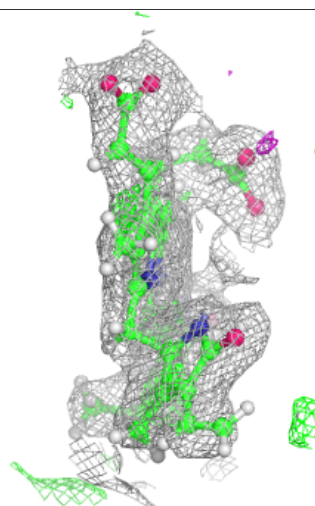
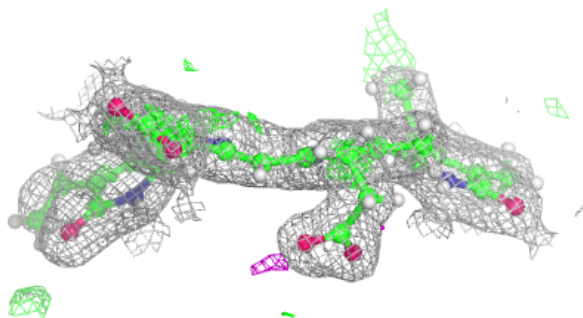
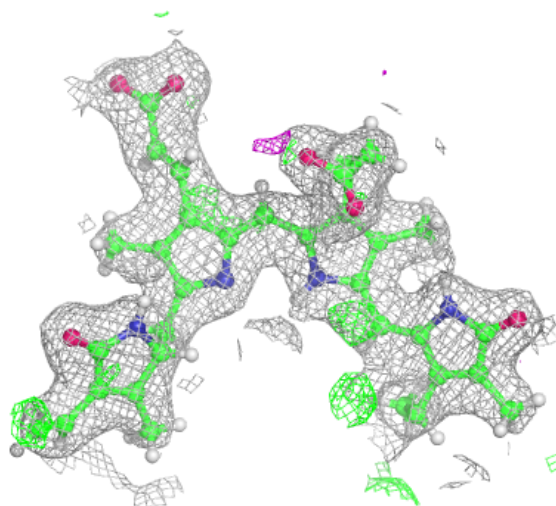
Electron density around KP9 H 101:

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



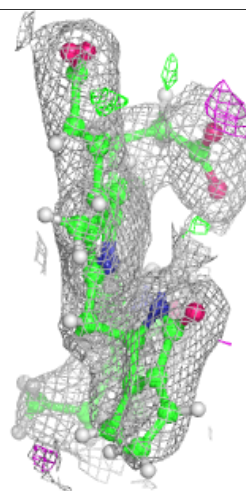
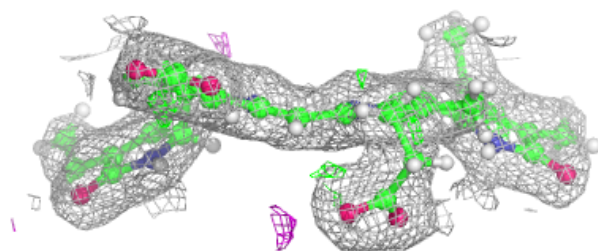
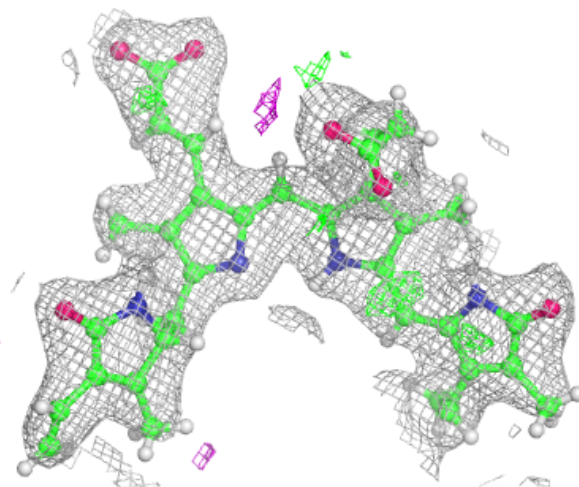
Electron density around KP9 J 101:

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



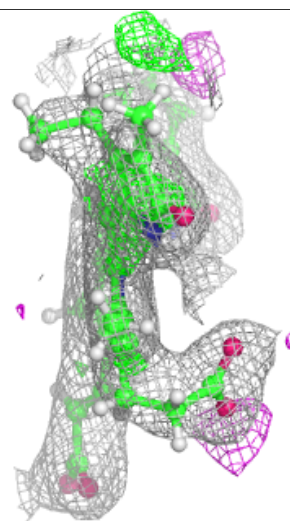
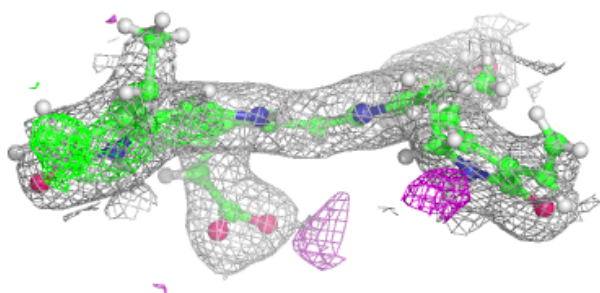
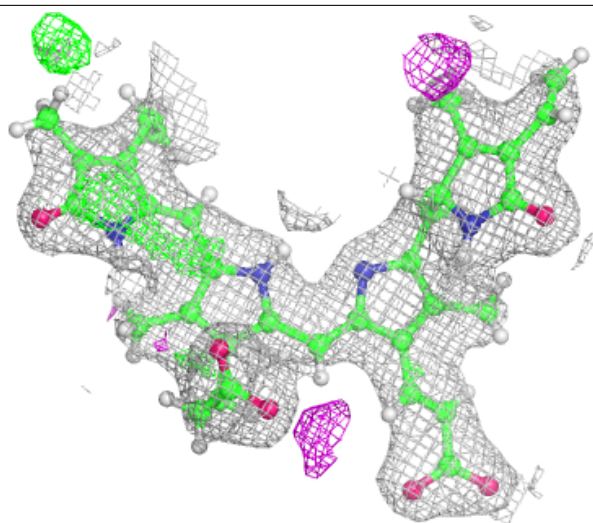
Electron density around KP9 L 101:

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



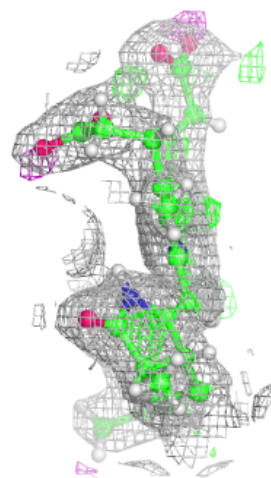
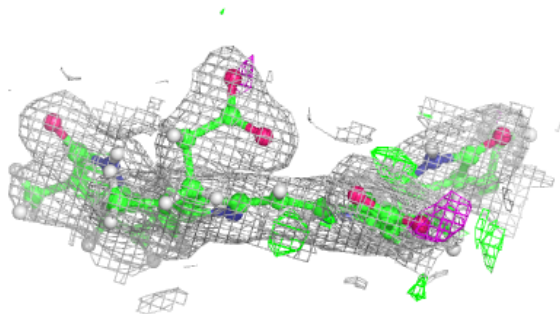
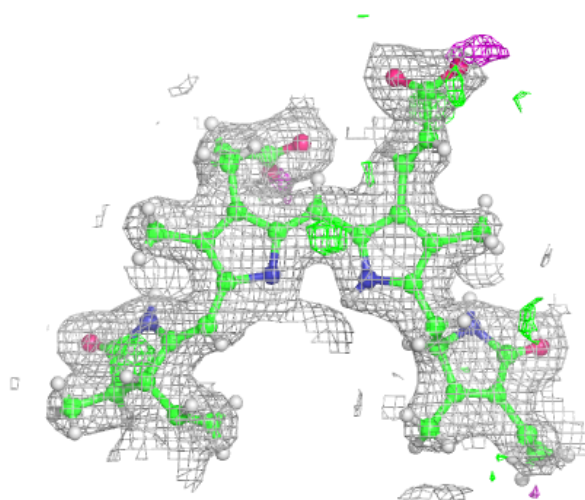
Electron density around KP9 P 101:

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and green (positive)



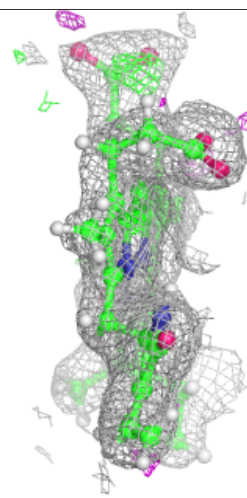
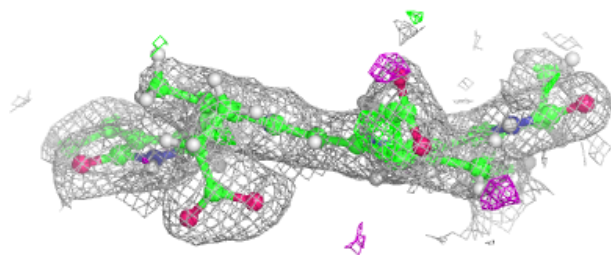
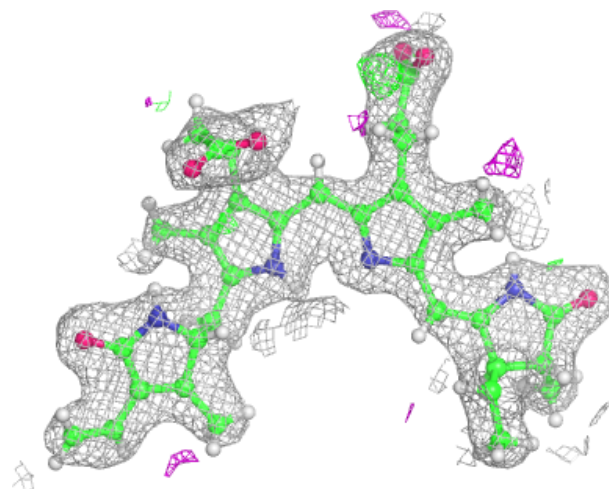
Electron density around KQ6 A 203:

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and green (positive)



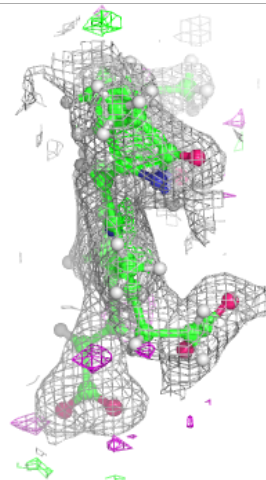
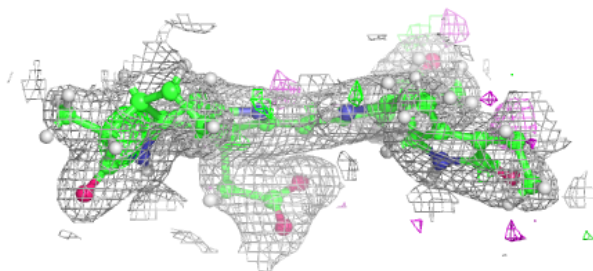
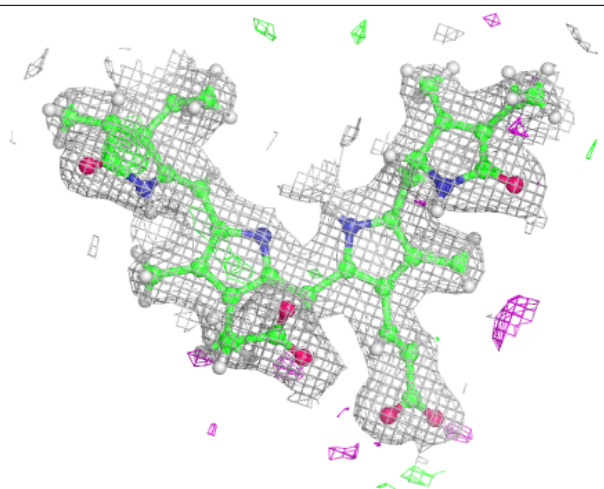
Electron density around PEB K 201:

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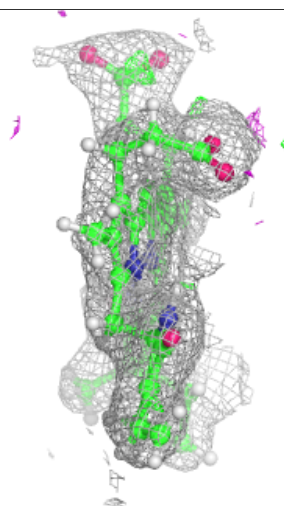
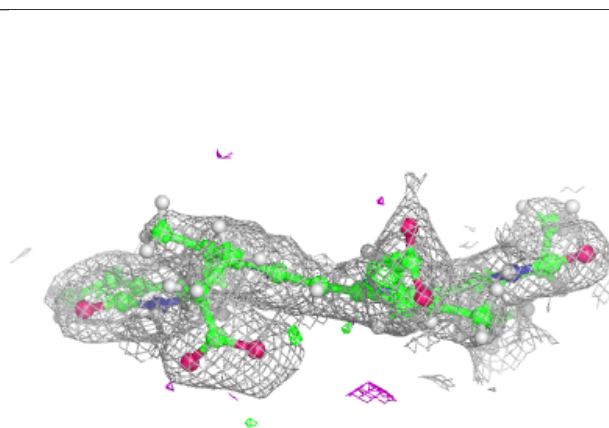
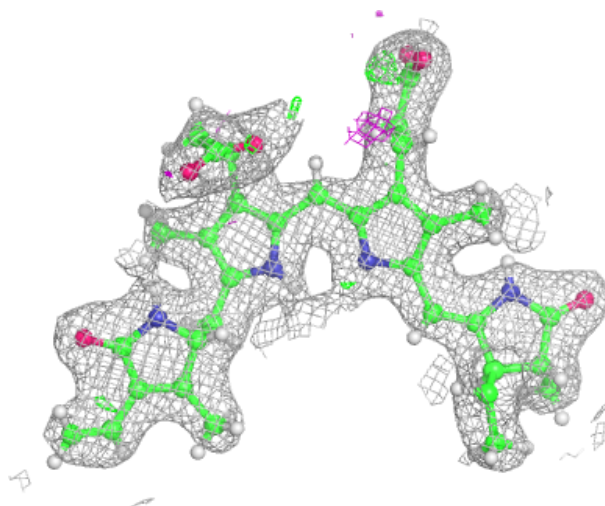
Electron density around KQ6 G 203:

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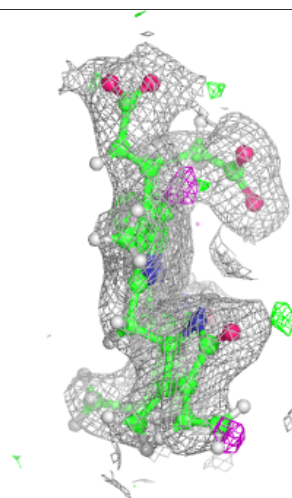
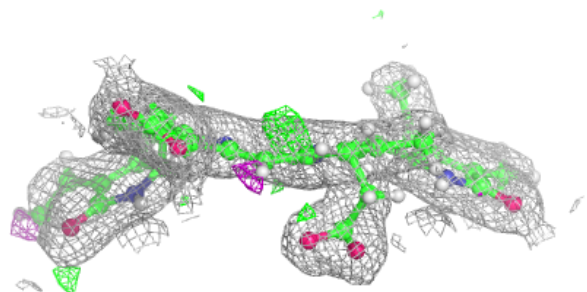
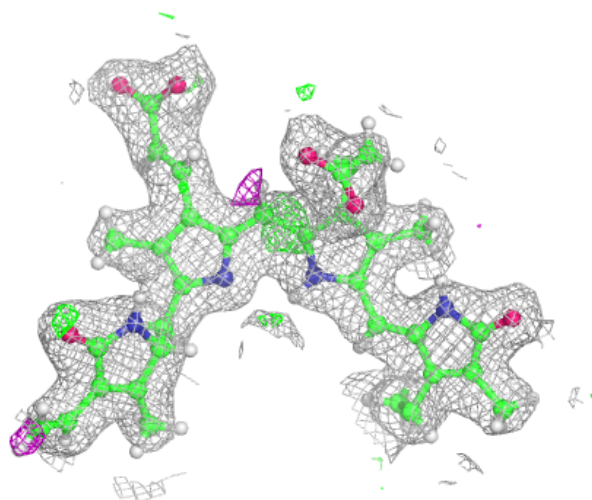
Electron density around PEB G 201:

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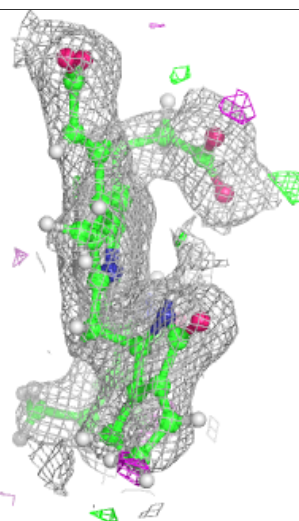
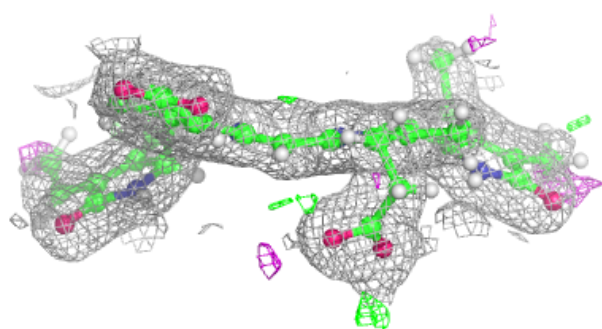
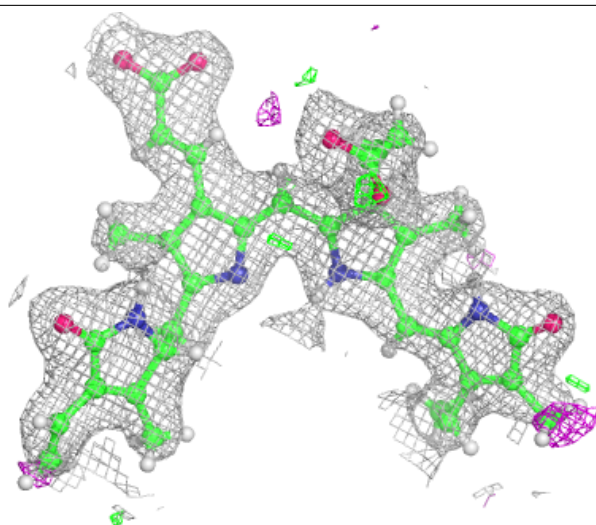
Electron density around KP9 B 101:

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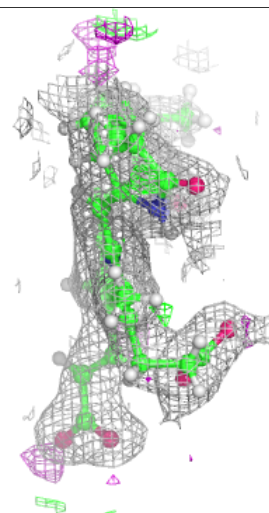
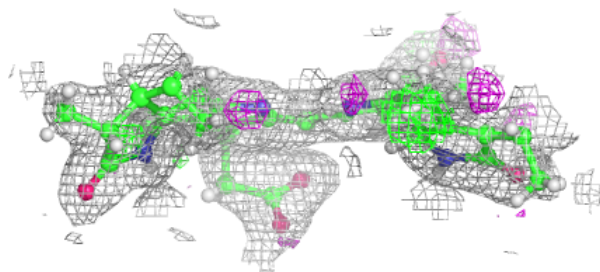
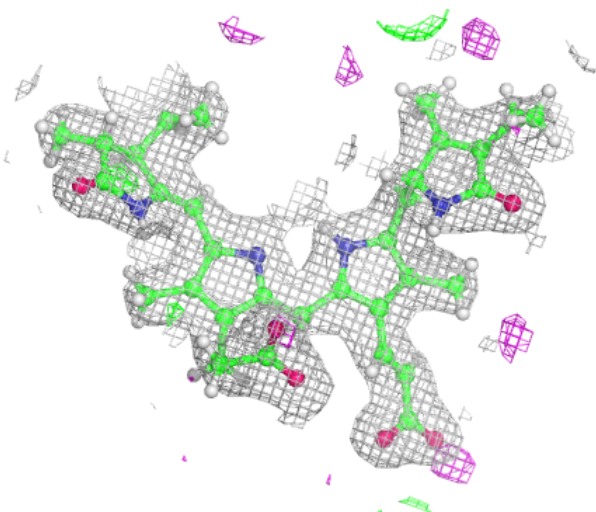
Electron density around KP9 D 101:

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and green (positive)



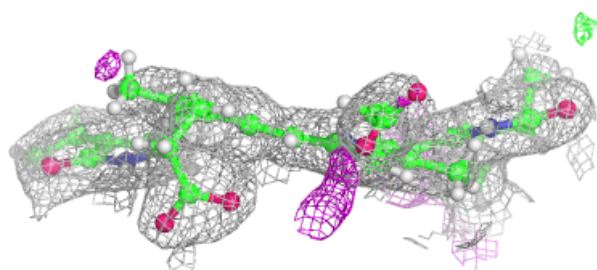
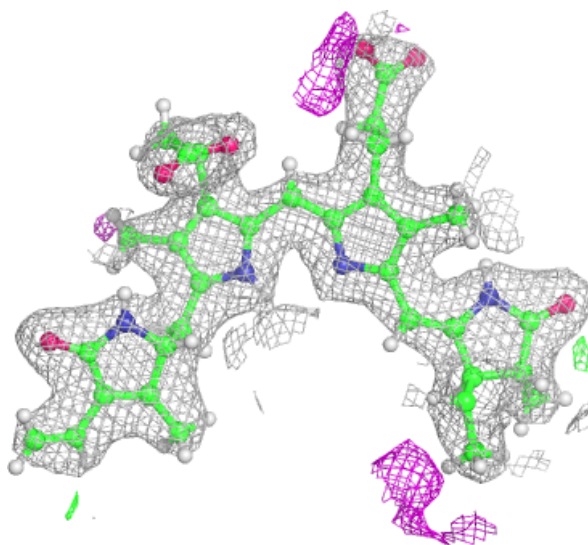
Electron density around KQ6 K 203:

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and green (positive)



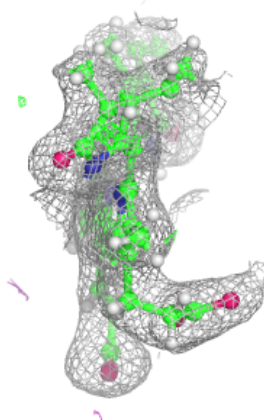
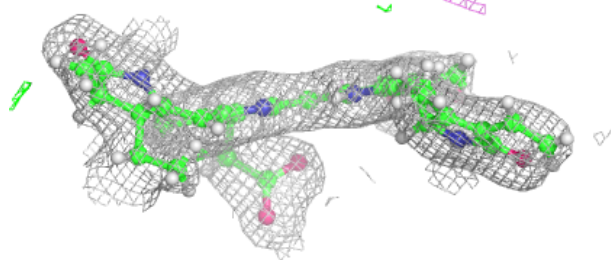
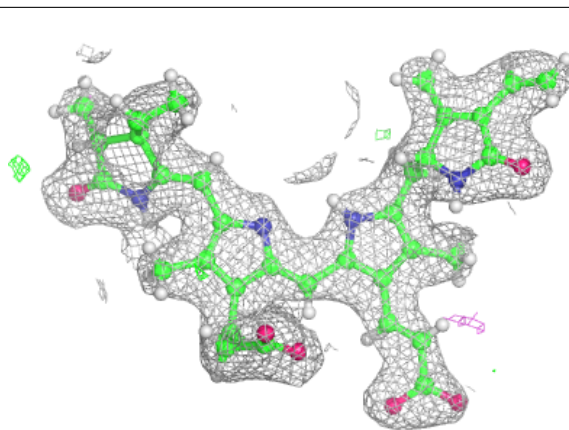
Electron density around PEB A 201:

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



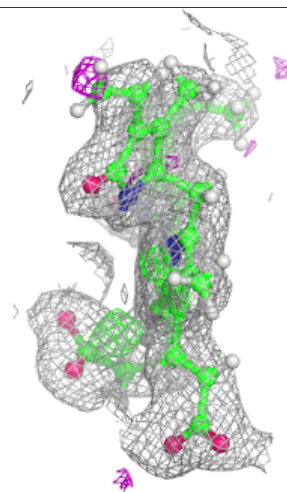
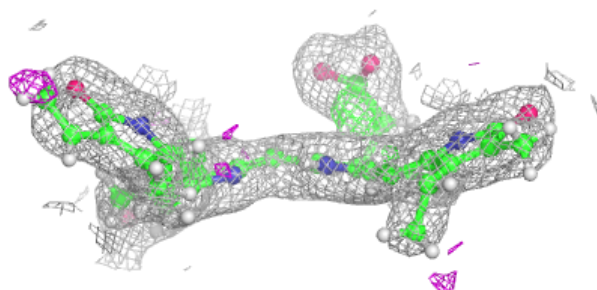
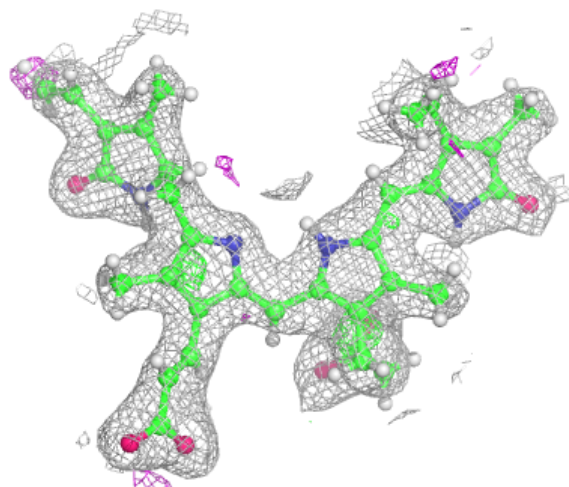
Electron density around KPX A 202:

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



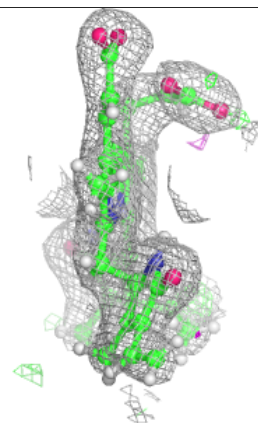
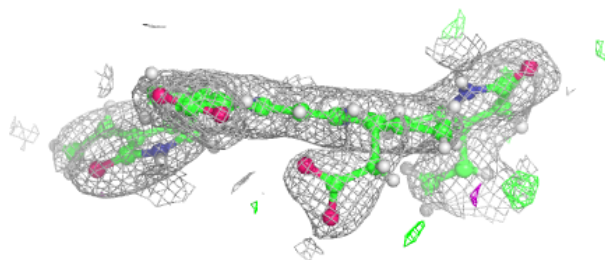
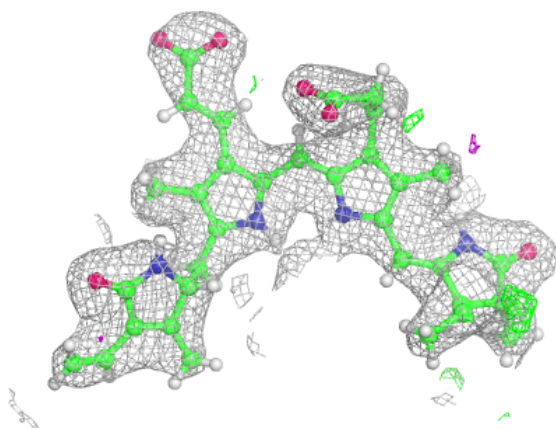
Electron density around KP9 N 101:

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



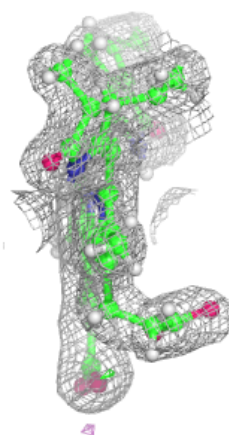
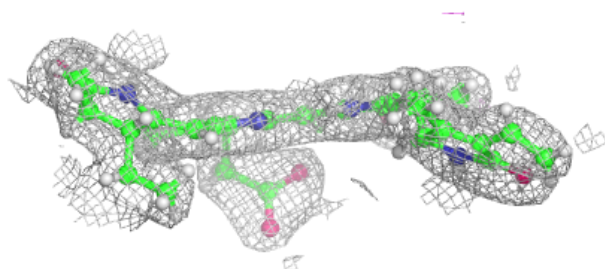
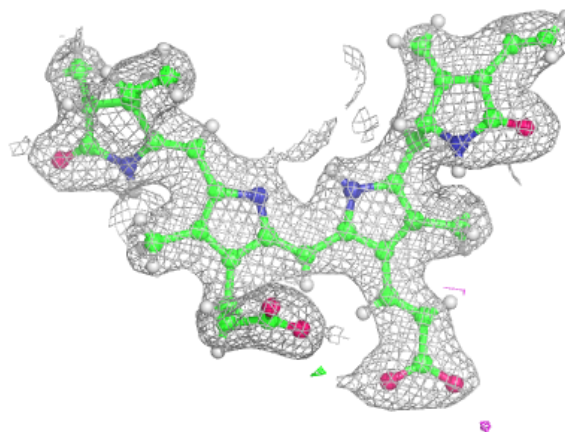
Electron density around KPX O 202:

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



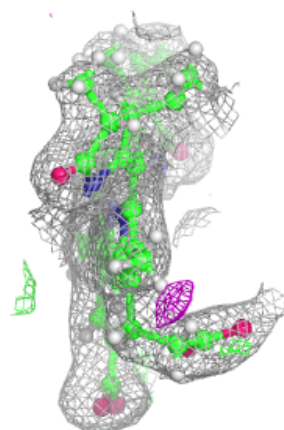
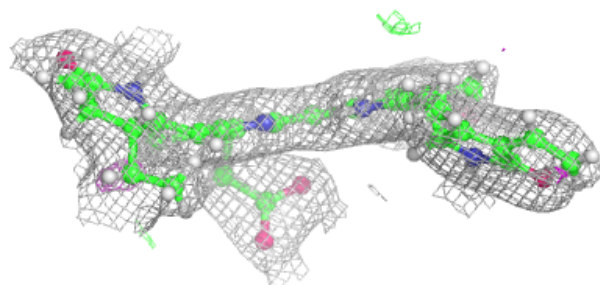
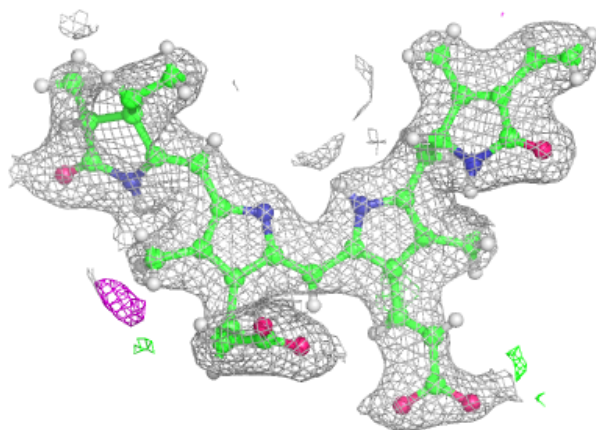
Electron density around KPX C 202:

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



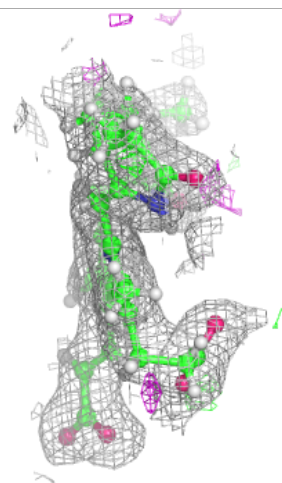
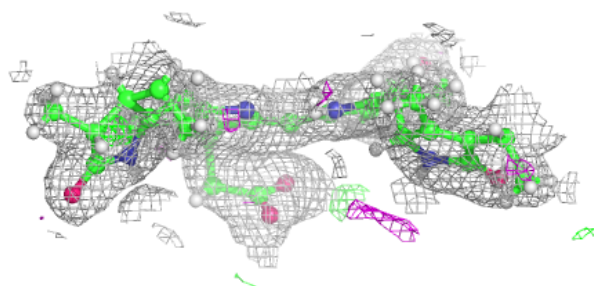
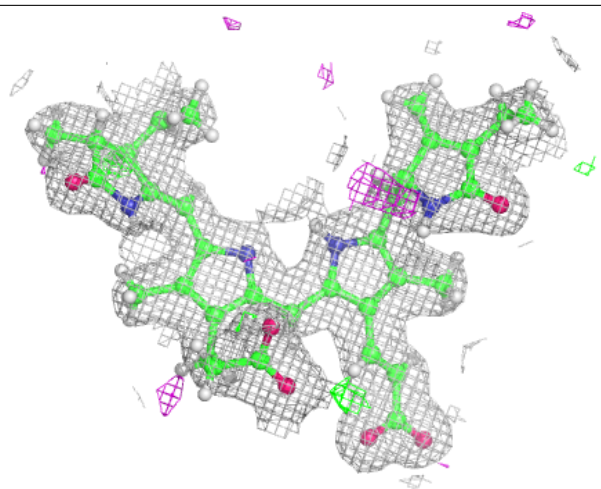
Electron density around KPX M 202:

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



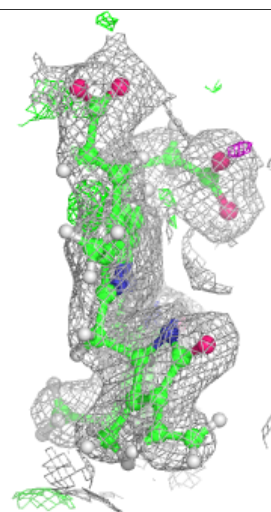
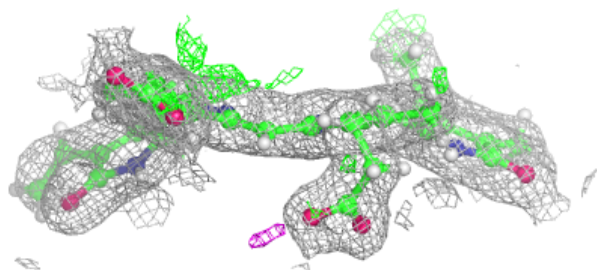
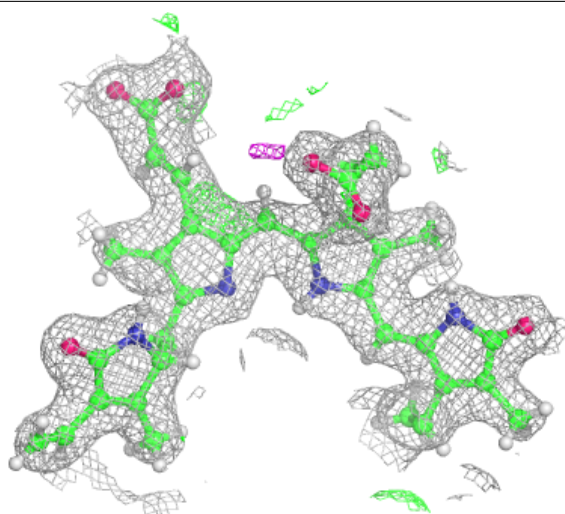
Electron density around KQ6 C 203:

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



Electron density around KP9 F 101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.