



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 3, 2022 – 06:33 PM JST

PDB ID : 7F86
Title : Crystal structure of Phycoerythrin from Halomicronema Sp. R31DM
Authors : Patel, S.N.; Gupta, G.D.; Sonani, R.R.; Singh, N.K.; Kumar, V.; Madamwar, D.
Deposited on : 2021-07-01
Resolution : 2.21 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:

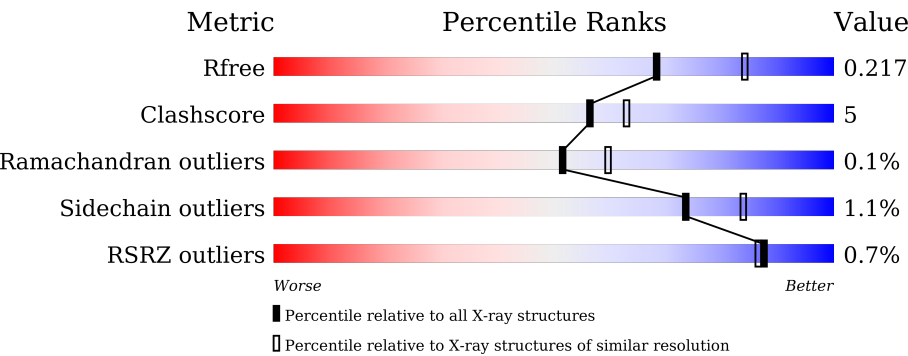
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.21 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.



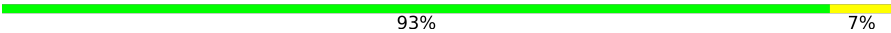
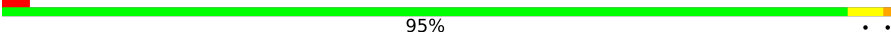

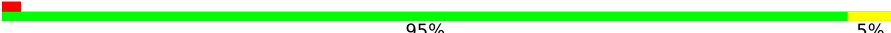










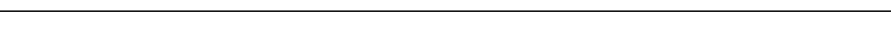
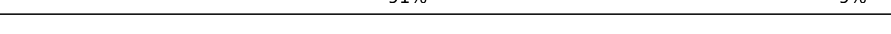
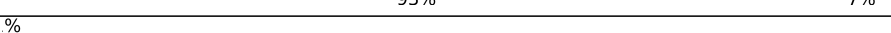

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	C	184	<div><div></div><div>95%5%</div></div>
1	E	184	<div><div>%</div><div>91%9%</div></div>
1	G	184	<div><div></div><div>95%5%</div></div>
1	I	184	<div><div>%</div><div>92%8%</div></div>
1	K	184	<div><div>%</div><div>95%5%</div></div>
1	M	184	<div><div>%</div><div>91%9%</div></div>

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Mol	Chain	Length	Quality of chain
1	N	184	 93%7%
1	P	184	 95%5%
1	R	184	 94%5%
1	T	184	 95%5%
1	V	184	 91%7%
1	X	184	 93%7%
2	A	164	 95%5%
2	B	164	 90%10%
2	D	164	 94%6%
2	F	164	 97%
2	H	164	 94%6%
2	J	164	 96%
2	L	164	 95%5%
2	O	164	 90%10%
2	Q	164	 91%9%
2	U	164	 93%7%
2	W	164	 90%10%
2	Y	164	 94%6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36454 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 Phycoerythrin beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	184	Total	C	N	O	S	0	0	0
			1348	828	245	263	12			
1	C	184	Total	C	N	O	S	0	0	0
			1348	828	245	263	12			
1	E	184	Total	C	N	O	S	0	0	0
			1348	828	245	263	12			
1	G	184	Total	C	N	O	S	0	0	0
			1344	826	245	261	12			
1	I	184	Total	C	N	O	S	0	0	0
			1348	828	245	263	12			
1	K	184	Total	C	N	O	S	0	0	0
			1348	828	245	263	12			
1	N	184	Total	C	N	O	S	0	0	0
			1344	826	245	261	12			
1	P	184	Total	C	N	O	S	0	0	0
			1348	828	245	263	12			
1	R	184	Total	C	N	O	S	0	0	0
			1348	828	245	263	12			
1	T	184	Total	C	N	O	S	0	0	0
			1344	826	245	261	12			
1	V	184	Total	C	N	O	S	0	0	0
			1348	828	245	263	12			
1	X	184	Total	C	N	O	S	0	0	0
			1348	828	245	263	12			

- Molecule 2 is a protein called Phycoerythrin alpha subunit.

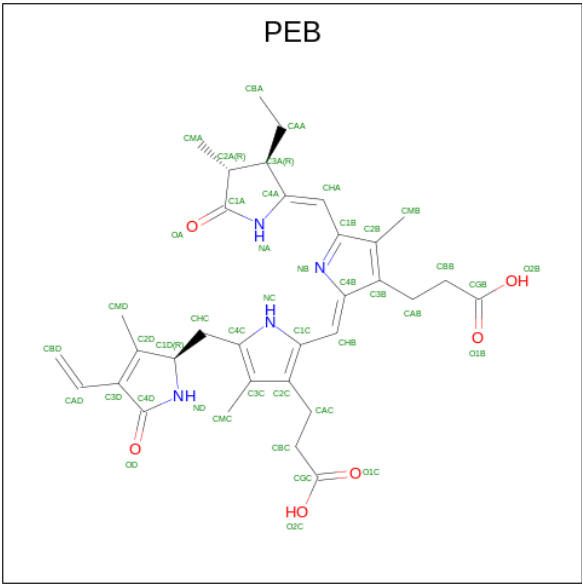
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	164	Total	C	N	O	S	0	0	0
			1245	774	220	244	7			
2	D	164	Total	C	N	O	S	0	0	0
			1245	774	220	244	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	164	Total 1245	774	220	244	7	0	0	0
2	F	164	Total 1245	774	220	244	7	0	0	0
2	H	164	Total 1245	774	218	246	7	0	1	0
2	J	164	Total 1245	774	220	244	7	0	0	0
2	L	164	Total 1245	774	220	244	7	0	0	0
2	O	164	Total 1239	771	217	244	7	0	0	0
2	Q	164	Total 1245	774	218	246	7	0	1	0
2	U	164	Total 1245	774	220	244	7	0	0	0
2	W	164	Total 1245	774	220	244	7	0	0	0
2	Y	164	Total 1245	774	220	244	7	0	0	0

- Molecule 3 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	M	1	Total 43	33	4	6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	A	1	Total 43	C 33	N 4	O 6	0	0
3	A	1	Total 43	C 33	N 4	O 6	0	0
3	D	1	Total 43	C 33	N 4	O 6	0	0
3	D	1	Total 43	C 33	N 4	O 6	0	0
3	B	1	Total 43	C 33	N 4	O 6	0	0
3	B	1	Total 43	C 33	N 4	O 6	0	0
3	F	1	Total 43	C 33	N 4	O 6	0	0
3	F	1	Total 43	C 33	N 4	O 6	0	0
3	H	1	Total 43	C 33	N 4	O 6	0	0
3	H	1	Total 43	C 33	N 4	O 6	0	0
3	J	1	Total 43	C 33	N 4	O 6	0	0
3	J	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	U	1	Total 43	C 33	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	U	1	Total	C	N	O	0	0
			43	33	4	6		
3	W	1	Total	C	N	O	0	0
			43	33	4	6		
3	W	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		
3	I	1	Total	C	N	O	0	0
			43	33	4	6		
3	I	1	Total	C	N	O	0	0
			43	33	4	6		
3	I	1	Total	C	N	O	0	0
			43	33	4	6		
3	K	1	Total	C	N	O	0	0
			43	33	4	6		
3	K	1	Total	C	N	O	0	0
			43	33	4	6		
3	K	1	Total	C	N	O	0	0
			43	33	4	6		
3	N	1	Total	C	N	O	0	0
			43	33	4	6		
3	N	1	Total	C	N	O	0	0
			43	33	4	6		
3	N	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	P	1	Total	C	N	O	0	0
			43	33	4	6		
3	P	1	Total	C	N	O	0	0
			43	33	4	6		
3	P	1	Total	C	N	O	0	0
			43	33	4	6		
3	R	1	Total	C	N	O	0	0
			43	33	4	6		
3	R	1	Total	C	N	O	0	0
			43	33	4	6		
3	R	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	V	1	Total	C	N	O	0	0
			43	33	4	6		
3	V	1	Total	C	N	O	0	0
			43	33	4	6		
3	V	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	Y	1	Total	C	N	O	0	0
			43	33	4	6		
3	Y	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	122	Total	O	0	0
			122	122		
4	A	128	Total	O	0	0
			128	128		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	116	Total 116	O 116	0	0
4	B	154	Total 154	O 154	0	0
4	F	128	Total 128	O 128	0	0
4	H	111	Total 111	O 111	0	0
4	J	129	Total 129	O 129	0	0
4	L	117	Total 117	O 117	0	0
4	O	102	Total 102	O 102	0	0
4	Q	133	Total 133	O 133	0	0
4	U	118	Total 118	O 118	0	0
4	W	108	Total 108	O 108	0	0
4	C	120	Total 120	O 120	0	0
4	E	139	Total 139	O 139	0	0
4	G	111	Total 111	O 111	0	0
4	I	82	Total 82	O 82	0	0
4	K	108	Total 108	O 108	0	0
4	N	123	Total 123	O 123	0	0
4	P	119	Total 119	O 119	0	0
4	R	122	Total 122	O 122	0	0
4	T	95	Total 95	O 95	0	0
4	V	80	Total 80	O 80	0	0
4	X	90	Total 90	O 90	0	0

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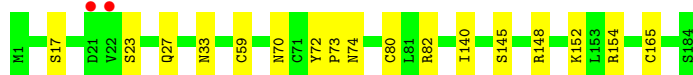
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Y	121	Total 121	O 121	0	0

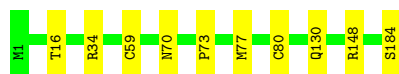
3 Residue-property plots [i](#)

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.

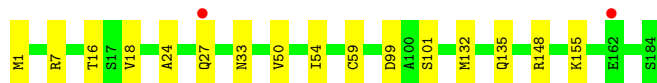
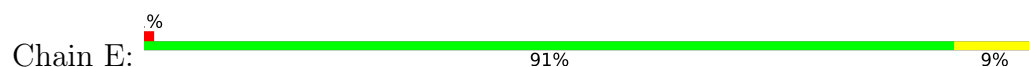
- Molecule 1: Phycoerythrin beta subunit



- Molecule 1: Phycoerythrin beta subunit



- Molecule 1: Phycoerythrin beta subunit



- Molecule 1: Phycoerythrin beta subunit



- Molecule 1: Phycoerythrin beta subunit



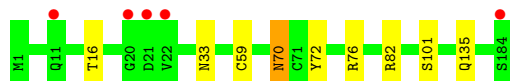
- Molecule 1: Phycoerythrin beta subunit



- Molecule 1: Phycoerythrin beta subunit



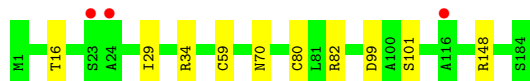
- Molecule 1: Phycoerythrin beta subunit



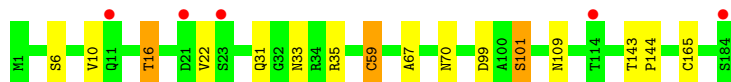
- Molecule 1: Phycoerythrin beta subunit



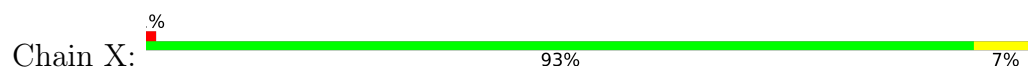
- Molecule 1: Phycoerythrin beta subunit



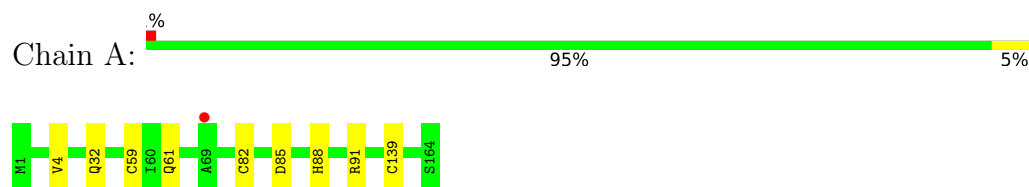
- Molecule 1: Phycoerythrin beta subunit



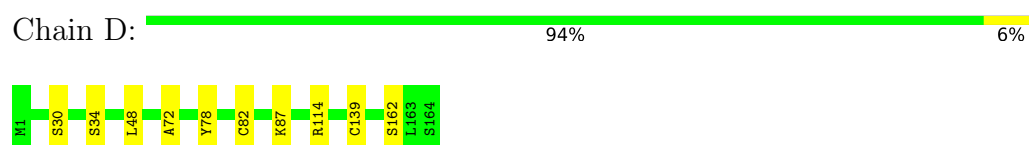
- Molecule 1: Phycoerythrin beta subunit



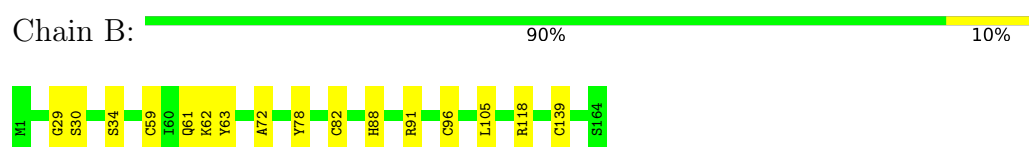
● Molecule 2: Phycoerythrin alpha subunit



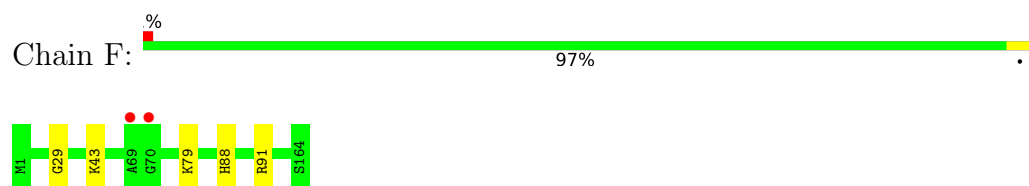
● Molecule 2: Phycoerythrin alpha subunit



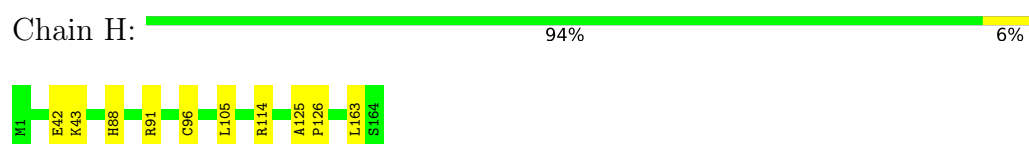
● Molecule 2: Phycoerythrin alpha subunit



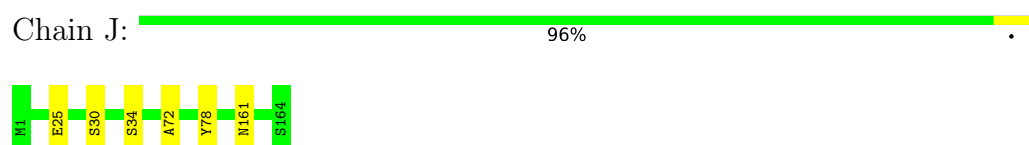
● Molecule 2: Phycoerythrin alpha subunit



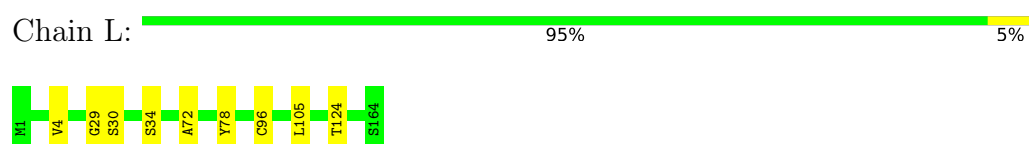
● Molecule 2: Phycoerythrin alpha subunit



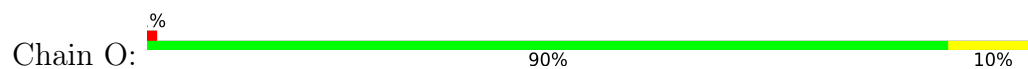
● Molecule 2: Phycoerythrin alpha subunit



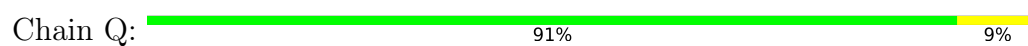
● Molecule 2: Phycoerythrin alpha subunit



• Molecule 2: Phycoerythrin alpha subunit



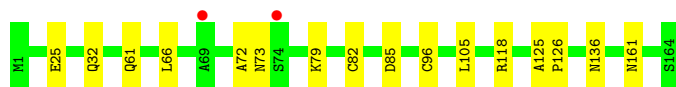
• Molecule 2: Phycoerythrin alpha subunit



• Molecule 2: Phycoerythrin alpha subunit



• Molecule 2: Phycoerythrin alpha subunit



• Molecule 2: Phycoerythrin alpha subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	108.59Å 108.63Å 116.93Å 78.37° 82.53° 62.11°	Depositor
Resolution (Å)	42.17 – 2.21 42.17 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.2 (42.17-2.21) 97.3 (42.17-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.63 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.163 , 0.210 0.173 , 0.217	Depositor DCC
R_{free} test set	11103 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	36454	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.94% 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: MEN, PEB

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	C	0.73	0/1350	0.86	0/1822
1	E	0.73	0/1350	0.85	0/1822
1	G	0.76	0/1346	0.88	0/1817
1	I	0.73	0/1350	0.84	0/1822
1	K	0.77	0/1350	0.83	0/1822
1	M	0.76	0/1350	0.85	0/1822
1	N	0.77	0/1346	0.87	0/1817
1	P	0.78	0/1350	0.84	0/1822
1	R	0.72	0/1350	0.84	0/1822
1	T	0.74	0/1346	0.84	0/1817
1	V	0.74	0/1350	0.83	0/1822
1	X	0.76	0/1350	0.85	0/1822
2	A	0.73	0/1265	0.83	0/1715
2	B	0.74	0/1265	0.85	0/1715
2	D	0.78	0/1265	0.84	0/1715
2	F	0.74	0/1265	0.86	0/1715
2	H	0.76	0/1265	0.82	0/1716
2	J	0.76	0/1265	0.85	0/1715
2	L	0.75	0/1265	0.87	0/1715
2	O	0.75	0/1259	0.84	0/1708
2	Q	0.76	0/1265	0.86	0/1716
2	U	0.74	0/1265	0.83	0/1715
2	W	0.75	0/1265	0.86	0/1715
2	Y	0.75	0/1265	0.86	0/1715
All	All	0.75	0/31362	0.85	0/42424

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	C	1348	0	1364	10	0
1	E	1348	0	1364	12	0
1	G	1344	0	1359	7	0
1	I	1348	0	1364	16	0
1	K	1348	0	1364	11	0
1	M	1348	0	1365	21	0
1	N	1344	0	1360	14	0
1	P	1348	0	1363	8	0
1	R	1348	0	1364	10	0
1	T	1344	0	1360	10	0
1	V	1348	0	1365	17	0
1	X	1348	0	1364	11	0
2	A	1245	0	1227	19	0
2	B	1245	0	1227	23	0
2	D	1245	0	1227	13	0
2	F	1245	0	1225	8	0
2	H	1245	0	1218	7	0
2	J	1245	0	1225	4	0
2	L	1245	0	1225	5	0
2	O	1239	0	1214	10	0
2	Q	1245	0	1219	14	0
2	U	1245	0	1225	11	0
2	W	1245	0	1225	16	0
2	Y	1245	0	1227	13	0
3	A	86	0	76	12	0
3	B	86	0	76	13	0
3	C	129	0	111	9	0
3	D	86	0	76	7	0
3	E	129	0	111	8	0
3	F	86	0	74	1	0
3	G	129	0	110	8	0
3	H	86	0	74	1	0
3	I	129	0	111	16	0
3	J	86	0	74	2	0
3	K	129	0	111	14	0
3	L	86	0	73	1	0
3	M	129	0	112	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	129	0	111	13	0
3	O	86	0	74	0	0
3	P	129	0	110	9	0
3	Q	86	0	75	5	0
3	R	129	0	111	10	0
3	T	129	0	111	16	0
3	U	86	0	74	2	0
3	V	129	0	112	15	0
3	W	86	0	74	4	0
3	X	129	0	111	12	0
3	Y	86	0	76	11	0
4	A	128	0	0	0	0
4	B	154	0	0	1	0
4	C	120	0	0	2	0
4	D	116	0	0	1	0
4	E	139	0	0	0	0
4	F	128	0	0	4	0
4	G	111	0	0	2	0
4	H	111	0	0	1	0
4	I	82	0	0	0	0
4	J	129	0	0	1	0
4	K	108	0	0	1	0
4	L	117	0	0	1	0
4	M	122	0	0	2	0
4	N	123	0	0	2	0
4	O	102	0	0	0	0
4	P	119	0	0	1	0
4	Q	133	0	0	3	0
4	R	122	0	0	3	0
4	T	95	0	0	2	0
4	U	118	0	0	0	0
4	V	80	0	0	1	0
4	W	108	0	0	1	0
4	X	90	0	0	1	0
4	Y	121	0	0	1	0
All	All	36454	0	33268	334	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 (334) 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:B:82:CYS:SG	3:B:201:PEB:HAA2	1.17	1.75
1:M:165:CYS:SG	3:M:301:PEB:HAA1	1.28	1.73
1:M:80:CYS:SG	3:M:303:PEB:HAA2	1.14	1.71
2:Y:82:CYS:SG	3:Y:201:PEB:HAA2	1.27	1.70
2:D:139:CYS:SG	3:D:202:PEB:HAA2	1.25	1.67
1:V:165:CYS:SG	3:V:301:PEB:HAA1	1.16	1.66
2:Y:139:CYS:SG	3:Y:202:PEB:HAA2	1.31	1.63
2:A:82:CYS:SG	3:A:201:PEB:HAA2	1.45	1.56
2:D:82:CYS:SG	3:D:201:PEB:HAA2	1.48	1.51
2:A:139:CYS:SG	3:A:202:PEB:HAA2	1.53	1.47
1:I:48:CYS:SG	3:I:302:PEB:CAA	2.02	1.46
2:B:82:CYS:SG	3:B:201:PEB:CAA	2.07	1.40
1:M:80:CYS:SG	3:M:303:PEB:CAA	2.09	1.39
1:V:165:CYS:SG	3:V:301:PEB:CAA	2.13	1.34
2:B:139:CYS:SG	3:B:202:PEB:HAA1	1.68	1.33
2:Y:82:CYS:SG	3:Y:201:PEB:CAA	2.18	1.30
1:M:165:CYS:SG	3:M:301:PEB:CAA	2.19	1.29
2:D:139:CYS:SG	3:D:202:PEB:CAA	2.21	1.27
2:Y:139:CYS:SG	3:Y:202:PEB:CAA	2.24	1.24
2:D:82:CYS:SG	3:D:201:PEB:CAA	2.27	1.21
2:A:139:CYS:SG	3:A:202:PEB:CAA	2.30	1.19
2:A:82:CYS:SG	3:A:201:PEB:CAA	2.32	1.17
1:N:59:CYS:SG	3:N:302:PEB:CAD	2.37	1.13
1:R:59:CYS:SG	3:R:302:PEB:CAD	2.37	1.12
1:K:59:CYS:SG	3:K:302:PEB:CAD	2.39	1.11
1:C:59:CYS:SG	3:C:302:PEB:CAD	2.41	1.08
1:X:59:CYS:SG	3:X:302:PEB:CAD	2.44	1.05
1:E:59:CYS:SG	3:E:302:PEB:CAD	2.45	1.05
1:I:59:CYS:SG	3:I:302:PEB:CAD	2.44	1.03
1:T:59:CYS:SG	3:T:302:PEB:CAD	2.47	1.02
2:B:139:CYS:SG	3:B:202:PEB:CAA	2.52	0.98
2:B:139:CYS:HG	3:B:202:PEB:HAA1	1.24	0.92
2:Q:139:CYS:SG	3:Q:202:PEB:CAA	2.57	0.92
1:V:59:CYS:SG	3:V:302:PEB:CAD	2.61	0.88
2:Q:139:CYS:SG	3:Q:202:PEB:HAA2	2.17	0.84
2:D:82:CYS:SG	3:D:201:PEB:CBA	2.65	0.83
2:D:114:ARG:HD3	2:W:118:ARG:CZ	2.09	0.83
1:P:82:ARG:HD3	4:P:401:HOH:O	1.81	0.79
2:A:139:CYS:SG	3:A:202:PEB:CBA	2.72	0.77
1:R:59:CYS:SG	3:R:302:PEB:CBD	2.73	0.76
3:Q:202:PEB:HBC2	3:Q:202:PEB:HHB1	1.66	0.75
1:E:59:CYS:SG	3:E:302:PEB:CBD	2.75	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:59:CYS:SG	3:X:302:PEB:HAD1	2.27	0.74
2:Y:139:CYS:CB	3:Y:202:PEB:HAA2	2.18	0.74
1:I:59:CYS:SG	3:I:302:PEB:HAD1	2.28	0.74
2:Q:139:CYS:SG	3:Q:202:PEB:HAA1	2.29	0.73
3:T:303:PEB:HMB2	3:T:303:PEB:HNA	1.53	0.71
1:C:130:GLN:NE2	4:C:401:HOH:O	2.23	0.70
1:R:59:CYS:SG	3:R:302:PEB:HAD1	2.31	0.70
2:B:82:CYS:SG	3:B:201:PEB:CBA	2.78	0.70
2:B:88:HIS:CD2	2:B:91:ARG:HH21	2.08	0.70
2:A:139:CYS:CB	3:A:202:PEB:HAA2	2.21	0.70
1:N:59:CYS:SG	3:N:302:PEB:CBD	2.80	0.70
1:K:59:CYS:SG	3:K:302:PEB:HAD1	2.31	0.69
3:V:303:PEB:HNA	3:V:303:PEB:HMB2	1.57	0.69
1:M:80:CYS:SG	3:M:303:PEB:CBA	2.81	0.68
2:Q:88:HIS:CD2	2:Q:91:ARG:HH21	2.12	0.68
3:R:303:PEB:HNA	3:R:303:PEB:HMB2	1.59	0.68
3:P:303:PEB:HNA	3:P:303:PEB:HMB2	1.59	0.67
2:Y:139:CYS:SG	3:Y:202:PEB:CBA	2.82	0.67
2:B:139:CYS:SG	3:B:202:PEB:H3A1	2.35	0.66
1:C:59:CYS:SG	3:C:302:PEB:CBD	2.83	0.66
2:B:82:CYS:SG	3:B:201:PEB:C3A	2.82	0.66
3:K:303:PEB:HMB2	3:K:303:PEB:HNA	1.60	0.66
2:A:82:CYS:SG	3:A:201:PEB:CBA	2.83	0.66
1:M:165:CYS:SG	3:M:301:PEB:CBA	2.84	0.66
3:C:303:PEB:HMB2	3:C:303:PEB:HNA	1.60	0.66
1:M:165:CYS:CB	3:M:301:PEB:HAA1	2.25	0.65
3:X:302:PEB:HNA	3:X:302:PEB:HMB3	1.60	0.65
3:G:303:PEB:HMB2	3:G:303:PEB:HNA	1.61	0.65
2:Y:82:CYS:SG	3:Y:201:PEB:CBA	2.85	0.65
1:N:59:CYS:SG	3:N:302:PEB:C3D	2.84	0.65
3:M:303:PEB:HNA	3:M:303:PEB:HMB2	1.62	0.64
3:B:202:PEB:HHB1	3:B:202:PEB:HBC2	1.80	0.64
2:F:88:HIS:CD2	2:F:91:ARG:HH21	2.16	0.64
1:K:70:MEN:HB2	3:K:303:PEB:OA	1.98	0.63
3:X:303:PEB:HMB2	3:X:303:PEB:HNA	1.63	0.63
3:E:303:PEB:HNA	3:E:303:PEB:HMB2	1.63	0.63
2:B:139:CYS:SG	3:B:202:PEB:C3A	2.86	0.63
1:P:16:THR:HG23	1:V:67:ALA:HB2	1.80	0.63
1:P:70:MEN:HB2	3:P:303:PEB:OA	1.98	0.63
3:K:301:PEB:HMB2	3:K:301:PEB:HNA	1.63	0.62
1:I:48:CYS:SG	3:I:302:PEB:CBA	2.86	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:32:GLN:HG3	2:W:32:GLN:CG	2.30	0.62
1:K:59:CYS:SG	3:K:302:PEB:CBD	2.87	0.61
2:B:88:HIS:HE1	4:N:483:HOH:O	1.84	0.61
2:O:88:HIS:HE1	4:V:462:HOH:O	1.84	0.61
2:F:88:HIS:HD2	2:F:91:ARG:HH21	1.48	0.60
1:C:16:THR:HG23	1:N:67:ALA:HB2	1.82	0.60
2:W:82:CYS:HA	3:W:201:PEB:HHA1	1.83	0.60
2:W:161:ASN:CG	4:W:307:HOH:O	2.39	0.60
2:H:88:HIS:CD2	2:H:91:ARG:HH21	2.19	0.60
1:M:72:TYR:OH	1:E:16:THR:HG22	2.02	0.59
1:M:140:ILE:O	3:M:301:PEB:HAA2	2.02	0.59
1:T:70:MEN:HB2	3:T:303:PEB:OA	2.02	0.59
3:I:303:PEB:HNA	3:I:303:PEB:HMB2	1.67	0.59
1:M:80:CYS:CB	3:M:303:PEB:HAA2	2.28	0.58
2:A:88:HIS:HD2	2:A:91:ARG:HH21	1.52	0.58
2:Q:88:HIS:HD2	2:Q:91:ARG:HH21	1.50	0.58
3:N:303:PEB:HNA	3:N:303:PEB:HMB2	1.69	0.58
3:G:301:PEB:HBA3	3:G:301:PEB:HHA1	1.86	0.57
2:U:1:MET:CE	1:V:6:SER:HB2	2.34	0.57
1:T:59:CYS:SG	3:T:302:PEB:HAD1	2.40	0.57
1:V:165:CYS:CB	3:V:301:PEB:HAA1	2.28	0.57
1:C:59:CYS:SG	3:C:302:PEB:HAD1	2.42	0.57
1:T:59:CYS:SG	3:T:302:PEB:CBD	2.93	0.57
3:T:301:PEB:HNA	3:T:301:PEB:HMB2	1.68	0.57
2:A:32:GLN:CG	2:W:32:GLN:HG3	2.34	0.57
2:Q:62:LYS:HG2	2:Q:63:TYR:CE2	2.40	0.57
2:D:82:CYS:SG	3:D:201:PEB:HBA2	2.45	0.56
1:K:133:LYS:HE3	1:K:173:SER:HB3	1.87	0.56
2:O:68:ASN:O	2:O:74:SER:HB3	2.04	0.56
1:R:148:ARG:NH1	3:R:302:PEB:HND	2.03	0.56
1:E:59:CYS:SG	3:E:302:PEB:C3D	2.93	0.56
1:X:59:CYS:SG	3:X:302:PEB:C3D	2.94	0.56
3:X:301:PEB:NA	3:X:301:PEB:HMB2	2.21	0.56
1:E:7:ARG:NH1	1:E:99:ASP:OD1	2.39	0.55
3:X:301:PEB:HMB2	3:X:301:PEB:HNA	1.71	0.55
2:A:88:HIS:CD2	2:A:91:ARG:HH21	2.25	0.55
2:A:139:CYS:SG	3:A:202:PEB:HBA2	2.46	0.55
2:F:43:LYS:HE2	4:F:415:HOH:O	2.07	0.55
1:N:59:CYS:SG	3:N:302:PEB:HAD1	2.43	0.54
1:K:59:CYS:SG	3:K:302:PEB:C3D	2.96	0.54
3:K:301:PEB:HMB2	3:K:301:PEB:NA	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:59:CYS:SG	3:V:302:PEB:CBD	2.96	0.54
2:F:79:LYS:CE	4:F:302:HOH:O	2.56	0.54
1:K:119:GLY:HA2	4:K:476:HOH:O	2.08	0.54
2:U:1:MET:HE2	1:V:6:SER:HB2	1.91	0.53
1:C:59:CYS:SG	3:C:302:PEB:C3D	2.96	0.53
1:G:148:ARG:NH2	3:G:302:PEB:HBC2	2.23	0.53
2:O:49:ASP:OD1	2:O:87:LYS:HE2	2.08	0.53
3:X:302:PEB:HMB3	3:X:302:PEB:NA	2.23	0.53
2:Q:88:HIS:CD2	4:Q:397:HOH:O	2.62	0.52
1:I:33:ASN:HB3	3:I:301:PEB:C1C	2.39	0.52
1:I:59:CYS:SG	3:I:302:PEB:CBD	2.96	0.52
1:R:80:CYS:HA	3:R:303:PEB:HHA1	1.91	0.52
1:K:67:ALA:HB2	1:V:16:THR:CG2	2.39	0.52
1:K:148:ARG:NH1	3:K:302:PEB:HND	2.07	0.52
1:M:165:CYS:SG	3:M:301:PEB:C3A	2.95	0.52
1:C:148:ARG:NH1	3:C:302:PEB:HND	2.07	0.52
3:J:202:PEB:HMB2	3:J:202:PEB:HNA	1.75	0.51
2:D:162:SER:O	2:W:118:ARG:NH2	2.43	0.51
2:Y:82:CYS:SG	3:Y:201:PEB:C3A	2.96	0.51
3:K:301:PEB:HBA3	3:K:301:PEB:HHA1	1.91	0.51
2:B:96:CYS:SG	2:B:105:LEU:HB2	2.51	0.51
1:C:80:CYS:HA	3:C:303:PEB:HHA1	1.91	0.51
2:F:88:HIS:HE1	4:C:464:HOH:O	1.93	0.50
2:L:30:SER:O	2:L:34:SER:HB3	2.11	0.50
2:Q:96:CYS:SG	2:Q:105:LEU:HB2	2.51	0.50
3:E:302:PEB:HMB3	3:E:302:PEB:HNA	1.77	0.50
3:I:302:PEB:HMB3	3:I:302:PEB:NA	2.27	0.50
1:E:148:ARG:NH1	3:E:302:PEB:HND	2.10	0.50
2:D:87:LYS:NZ	1:C:184:SER:OXT	2.33	0.50
1:R:60:GLU:OE2	4:R:401:HOH:O	2.20	0.50
1:K:67:ALA:HB2	1:V:16:THR:HG23	1.94	0.50
3:T:301:PEB:HBA3	3:T:301:PEB:HHA1	1.94	0.50
3:V:302:PEB:NA	3:V:302:PEB:HMB3	2.27	0.50
3:Y:202:PEB:HNA	3:Y:202:PEB:HMB2	1.77	0.50
2:F:79:LYS:HE3	4:F:302:HOH:O	2.11	0.50
3:R:302:PEB:HNA	3:R:302:PEB:HMB3	1.77	0.50
1:V:165:CYS:SG	3:V:301:PEB:C3A	2.95	0.49
2:A:32:GLN:CG	2:W:32:GLN:CG	2.91	0.49
3:T:301:PEB:HMB2	3:T:301:PEB:NA	2.27	0.49
3:T:302:PEB:HBB1	3:T:302:PEB:HBB1	1.95	0.49
1:X:141:LYS:O	1:X:164:ARG:NH1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:302:PEB:HMB3	3:I:302:PEB:HNA	1.77	0.49
3:P:302:PEB:HNA	3:P:302:PEB:HMB3	1.77	0.49
1:V:33:ASN:HB3	3:V:301:PEB:C1C	2.42	0.49
2:B:118:ARG:HH12	2:U:163:LEU:HA	1.76	0.49
1:R:99:ASP:OD2	1:R:101:SER:HB3	2.12	0.49
3:T:303:PEB:HBC1	4:T:408:HOH:O	2.13	0.49
3:I:301:PEB:HMB2	3:I:301:PEB:NA	2.28	0.49
2:A:139:CYS:SG	3:A:202:PEB:C3A	2.99	0.49
2:W:96:CYS:SG	2:W:105:LEU:HB2	2.53	0.49
3:C:302:PEB:NA	3:C:302:PEB:HMB3	2.28	0.49
3:X:302:PEB:HBC1	3:X:302:PEB:HHB1	1.94	0.49
2:L:72:ALA:O	2:L:78:TYR:HB3	2.13	0.49
2:J:30:SER:O	2:J:34:SER:HB3	2.13	0.49
1:N:148:ARG:NH1	3:N:302:PEB:HND	2.11	0.48
1:G:62:GLN:NE2	4:G:411:HOH:O	2.46	0.48
3:L:202:PEB:HMB2	3:L:202:PEB:NA	2.27	0.48
1:N:109:ASN:ND2	4:N:405:HOH:O	2.46	0.48
1:X:59:CYS:CB	3:X:302:PEB:HAD1	2.44	0.48
1:I:88:LEU:O	1:I:92:THR:HG23	2.14	0.48
3:C:302:PEB:HMB3	3:C:302:PEB:HNA	1.79	0.48
3:R:302:PEB:HMB3	3:R:302:PEB:NA	2.29	0.48
3:K:302:PEB:HNA	3:K:302:PEB:HMB3	1.79	0.48
1:T:148:ARG:NH1	3:T:302:PEB:HND	2.11	0.47
3:V:301:PEB:HBA3	3:V:301:PEB:HHA1	1.96	0.47
3:V:302:PEB:HMB3	3:V:302:PEB:HNA	1.79	0.47
3:V:303:PEB:HNA	3:V:303:PEB:CMB	2.27	0.47
2:O:88:HIS:CD2	2:O:91:ARG:HH21	2.32	0.47
1:G:80:CYS:HA	3:G:303:PEB:HHA1	1.95	0.47
3:N:302:PEB:HNA	3:N:302:PEB:HMB3	1.79	0.47
1:M:152:LYS:NZ	4:M:403:HOH:O	2.36	0.47
2:Q:29:GLY:HA3	2:Y:25:GLU:O	2.15	0.47
1:E:24:ALA:HA	1:E:27:GLN:OE1	2.15	0.47
2:B:29:GLY:HA3	2:J:25:GLU:O	2.15	0.47
3:J:202:PEB:HMB2	3:J:202:PEB:NA	2.30	0.47
1:M:145:SER:HB3	1:N:123:THR:OG1	2.15	0.47
2:U:96:CYS:SG	2:U:105:LEU:HB2	2.55	0.47
3:T:303:PEB:HNA	3:T:303:PEB:CMB	2.26	0.47
1:V:99:ASP:OD2	1:V:101:SER:HB3	2.14	0.47
1:V:143:THR:N	1:V:144:PRO:CD	2.77	0.47
2:H:125:ALA:N	2:H:126:PRO:CD	2.77	0.46
2:J:72:ALA:O	2:J:78:TYR:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:301:PEB:HMB2	3:I:301:PEB:HNA	1.80	0.46
3:F:201:PEB:HMC2	1:C:77:MET:HG2	1.98	0.46
2:H:42:GLU:HB2	1:I:22:VAL:HG21	1.97	0.46
1:N:91:VAL:HG11	1:N:176:PHE:CZ	2.51	0.46
1:V:31:GLN:NE2	1:V:35:ARG:HH21	2.14	0.46
1:M:23:SER:O	1:M:27:GLN:HG3	2.16	0.46
1:E:33:ASN:HB3	3:E:301:PEB:C1C	2.46	0.46
1:I:143:THR:N	1:I:144:PRO:CD	2.78	0.46
1:T:99:ASP:OD2	1:T:101:SER:HB3	2.14	0.46
3:V:301:PEB:NA	3:V:301:PEB:HMB2	2.31	0.46
2:B:118:ARG:NH1	2:U:163:LEU:HA	2.31	0.46
1:I:59:CYS:CB	3:I:302:PEB:HAD1	2.46	0.46
2:Q:35:ALA:HB3	4:Q:312:HOH:O	2.15	0.45
3:P:303:PEB:OD	3:P:303:PEB:HBD1	2.15	0.45
1:I:148:ARG:NH1	3:I:302:PEB:HND	2.15	0.45
3:K:302:PEB:HBB1	3:K:302:PEB:HBB1	1.98	0.45
3:Y:202:PEB:HMB2	3:Y:202:PEB:NA	2.32	0.45
2:H:114:ARG:NH2	2:H:163:LEU:HA	2.31	0.45
1:X:143:THR:N	1:X:144:PRO:CD	2.79	0.45
2:U:125:ALA:N	2:U:126:PRO:CD	2.80	0.45
2:A:32:GLN:HG3	2:W:32:GLN:HG2	1.99	0.45
3:A:201:PEB:HMB2	3:A:201:PEB:HNA	1.82	0.45
1:N:70:MEN:HB2	3:N:303:PEB:OA	2.17	0.45
1:T:59:CYS:SG	3:T:302:PEB:C3D	3.02	0.45
2:Y:72:ALA:O	2:Y:78:TYR:HB3	2.17	0.45
2:B:118:ARG:NH2	2:U:114:ARG:HG2	2.31	0.44
1:I:59:CYS:SG	3:I:302:PEB:C3D	3.05	0.44
1:I:135:GLN:HG2	3:I:302:PEB:C1B	2.47	0.44
1:M:148:ARG:NH2	3:M:302:PEB:HBC2	2.32	0.44
2:B:62:LYS:HD3	2:B:63:TYR:CZ	2.52	0.44
2:L:4:VAL:HG21	2:U:25:GLU:HG2	2.00	0.44
3:E:302:PEB:HMB3	3:E:302:PEB:NA	2.31	0.44
3:K:302:PEB:HMB3	3:K:302:PEB:NA	2.32	0.44
1:P:135:GLN:HG2	3:P:302:PEB:C1B	2.47	0.44
2:O:96:CYS:SG	2:O:105:LEU:HB2	2.57	0.44
2:O:39:GLU:OE1	2:O:145:SER:OG	2.30	0.44
1:G:33:ASN:HB3	3:G:301:PEB:C1C	2.47	0.44
2:O:68:ASN:O	2:O:74:SER:CB	2.65	0.44
3:I:301:PEB:HBA3	3:I:301:PEB:HHA1	2.00	0.44
1:N:59:CYS:CB	3:N:302:PEB:CAD	2.96	0.44
3:N:302:PEB:HMB3	3:N:302:PEB:NA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:301:PEB:HHA1	3:M:301:PEB:HBA3	2.00	0.44
1:R:85:GLU:HG2	4:R:478:HOH:O	2.17	0.44
2:A:82:CYS:HA	3:A:201:PEB:HHA1	1.99	0.44
2:Q:72:ALA:O	2:Q:78:TYR:HB3	2.17	0.44
1:N:132:MET:HA	1:N:135:GLN:OE1	2.18	0.44
1:M:82:ARG:NH1	4:M:401:HOH:O	2.29	0.43
1:G:148:ARG:NH1	3:G:302:PEB:HND	2.15	0.43
2:A:4:VAL:HG21	2:W:25:GLU:HG2	1.99	0.43
1:P:72:TYR:O	1:P:76:ARG:HG3	2.18	0.43
1:X:122:THR:HG23	1:X:183:LEU:O	2.18	0.43
2:B:30:SER:O	2:B:34:SER:HB3	2.18	0.43
3:V:301:PEB:HMB2	3:V:301:PEB:HNA	1.83	0.43
3:K:303:PEB:HNA	3:K:303:PEB:CMB	2.30	0.43
1:M:33:ASN:HB3	3:M:301:PEB:C1C	2.49	0.43
1:V:6:SER:O	1:V:10:VAL:HG23	2.18	0.43
2:B:118:ARG:NH1	2:U:162:SER:O	2.52	0.43
1:G:122:THR:HA	4:G:449:HOH:O	2.19	0.43
3:N:301:PEB:HBA3	3:N:301:PEB:HHA1	2.01	0.43
2:D:87:LYS:NZ	4:D:308:HOH:O	2.49	0.43
1:P:59:CYS:HB2	3:P:302:PEB:HBD2	1.94	0.43
2:Q:151:GLU:OE2	4:Q:301:HOH:O	2.22	0.42
2:W:85:ASP:OD1	3:W:201:PEB:H1D1	2.19	0.42
3:M:301:PEB:NA	3:M:301:PEB:HMB2	2.33	0.42
2:D:48:LEU:HD22	1:E:18:VAL:CG1	2.49	0.42
2:F:43:LYS:NZ	4:F:305:HOH:O	2.48	0.42
2:H:43:LYS:HE2	3:H:202:PEB:OD	2.19	0.42
3:P:302:PEB:HMB3	3:P:302:PEB:NA	2.34	0.42
3:B:202:PEB:HBA2	3:B:202:PEB:H2A1	1.67	0.42
2:Y:96:CYS:SG	2:Y:105:LEU:HB2	2.60	0.42
2:Q:1:MET:HG3	2:Q:103:GLY:HA3	2.01	0.42
2:H:114:ARG:HG3	4:H:363:HOH:O	2.19	0.42
2:L:96:CYS:SG	2:L:105:LEU:HB2	2.59	0.42
2:Q:139:CYS:SG	3:Q:202:PEB:C3A	3.07	0.42
1:P:33:ASN:HB3	3:P:301:PEB:C1C	2.50	0.42
3:P:301:PEB:HMB2	3:P:301:PEB:NA	2.34	0.42
3:X:303:PEB:HBD1	3:X:303:PEB:OD	2.19	0.42
2:O:33:ARG:NH2	2:O:147:GLN:OE1	2.49	0.42
1:M:154:ARG:NH1	2:W:136:ASN:OD1	2.53	0.42
2:B:82:CYS:CB	3:B:201:PEB:HAA2	2.32	0.42
1:N:136:ALA:O	1:N:140:ILE:HG13	2.19	0.42
3:T:302:PEB:HNA	3:T:302:PEB:HMB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:80:CYS:SG	3:M:303:PEB:C3A	3.01	0.41
3:M:301:PEB:HMB2	3:M:301:PEB:HNA	1.84	0.41
3:W:201:PEB:HAC1	1:I:77:MET:HE2	2.02	0.41
2:Y:17:ARG:HD2	4:Y:387:HOH:O	2.20	0.41
3:Y:202:PEB:HAD1	3:Y:202:PEB:HMD1	1.87	0.41
1:E:132:MET:HA	1:E:135:GLN:OE1	2.20	0.41
1:G:59:CYS:HB2	3:G:302:PEB:HBD2	1.91	0.41
1:R:184:SER:O	4:R:402:HOH:O	2.21	0.41
3:R:301:PEB:HMB2	3:R:301:PEB:HNA	1.84	0.41
1:I:67:ALA:HB2	1:X:16:THR:HG23	2.01	0.41
3:T:301:PEB:OD	2:Y:28:GLN:NE2	2.51	0.41
4:L:373:HOH:O	2:U:4:VAL:HG23	2.19	0.41
1:T:80:CYS:HA	3:T:303:PEB:HHA1	2.01	0.41
1:X:135:GLN:HG2	3:X:302:PEB:C1B	2.50	0.41
2:A:85:ASP:OD1	3:A:201:PEB:H1D1	2.21	0.41
2:J:161:ASN:CG	4:J:349:HOH:O	2.59	0.41
2:W:73:ASN:O	2:W:79:LYS:NZ	2.49	0.41
1:R:33:ASN:HB3	3:R:301:PEB:C1C	2.50	0.41
1:M:72:TYR:CZ	1:E:16:THR:HG22	2.56	0.41
2:F:29:GLY:HA3	2:O:25:GLU:O	2.21	0.41
3:G:301:PEB:NA	3:G:301:PEB:HMB2	2.35	0.41
1:V:59:CYS:CB	3:V:302:PEB:HAD1	2.51	0.41
2:L:29:GLY:HA3	2:U:25:GLU:O	2.20	0.41
3:U:201:PEB:HHC2	1:K:74:ASN:OD1	2.21	0.41
3:U:201:PEB:HMB2	3:U:201:PEB:HNA	1.86	0.41
1:X:132:MET:HA	1:X:135:GLN:OE1	2.21	0.41
2:A:32:GLN:HG2	2:W:32:GLN:HG3	2.02	0.41
2:D:72:ALA:O	2:D:78:TYR:HB3	2.20	0.41
2:B:82:CYS:HA	3:B:201:PEB:HHA1	2.02	0.41
1:T:82:ARG:HD3	4:T:453:HOH:O	2.20	0.41
2:D:30:SER:O	2:D:34:SER:HB3	2.21	0.41
2:B:61:GLN:HA	4:B:417:HOH:O	2.21	0.41
2:W:125:ALA:N	2:W:126:PRO:CD	2.84	0.41
1:X:82:ARG:HD3	4:X:401:HOH:O	2.21	0.41
2:W:66:LEU:HD22	2:W:72:ALA:HB3	2.02	0.40
3:M:302:PEB:HMB3	3:M:302:PEB:HNA	1.85	0.40
2:O:125:ALA:N	2:O:126:PRO:CD	2.84	0.40
2:H:96:CYS:SG	2:H:105:LEU:HB2	2.62	0.40
3:W:201:PEB:HMC2	1:I:77:MET:HG2	2.02	0.40
1:E:50:VAL:O	1:E:54:ILE:HG12	2.21	0.40
1:T:29:ILE:HD13	1:T:29:ILE:HA	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ALA:O	2:B:78:TYR:HB3	2.22	0.40
3:N:301:PEB:HNA	3:N:301:PEB:HMB2	1.87	0.40
1:M:74:ASN:OD1	3:D:201:PEB:HHC2	2.22	0.40
1:N:135:GLN:HG2	3:N:302:PEB:C1B	2.52	0.40
1:P:70:MEN:O	1:P:76:ARG:HB3	2.22	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	C	181/184 (98%)	174 (96%)	7 (4%)	0	100	100
1	E	181/184 (98%)	175 (97%)	6 (3%)	0	100	100
1	G	181/184 (98%)	173 (96%)	8 (4%)	0	100	100
1	I	181/184 (98%)	174 (96%)	6 (3%)	1 (1%)	25	25
1	K	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
1	M	181/184 (98%)	177 (98%)	3 (2%)	1 (1%)	25	25
1	N	181/184 (98%)	175 (97%)	6 (3%)	0	100	100
1	P	181/184 (98%)	175 (97%)	6 (3%)	0	100	100
1	R	181/184 (98%)	177 (98%)	3 (2%)	1 (1%)	25	25
1	T	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
1	V	181/184 (98%)	172 (95%)	8 (4%)	1 (1%)	25	25
1	X	181/184 (98%)	174 (96%)	7 (4%)	0	100	100
2	A	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
2	B	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
2	D	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
2	F	162/164 (99%)	159 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	163/164 (99%)	159 (98%)	4 (2%)	0	100	100
2	J	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
2	L	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
2	O	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
2	Q	163/164 (99%)	160 (98%)	3 (2%)	0	100	100
2	U	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
2	W	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
2	Y	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
All	All	4118/4176 (99%)	4010 (97%)	104 (2%)	4 (0%)	51	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	16	THR
1	M	73	PRO
1	I	73	PRO
1	R	73	PRO

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	C	139/139 (100%)	137 (99%)	2 (1%)	67	78
1	E	139/139 (100%)	136 (98%)	3 (2%)	52	64
1	G	138/139 (99%)	135 (98%)	3 (2%)	52	64
1	I	139/139 (100%)	137 (99%)	2 (1%)	67	78
1	K	139/139 (100%)	137 (99%)	2 (1%)	67	78
1	M	139/139 (100%)	137 (99%)	2 (1%)	67	78
1	N	138/139 (99%)	138 (100%)	0	100	100
1	P	139/139 (100%)	138 (99%)	1 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	139/139 (100%)	136 (98%)	3 (2%)	52	64
1	T	138/139 (99%)	136 (99%)	2 (1%)	67	78
1	V	139/139 (100%)	135 (97%)	4 (3%)	42	53
1	X	139/139 (100%)	138 (99%)	1 (1%)	84	91
2	A	128/128 (100%)	126 (98%)	2 (2%)	62	75
2	B	128/128 (100%)	127 (99%)	1 (1%)	81	89
2	D	128/128 (100%)	128 (100%)	0	100	100
2	F	128/128 (100%)	128 (100%)	0	100	100
2	H	128/128 (100%)	128 (100%)	0	100	100
2	J	128/128 (100%)	128 (100%)	0	100	100
2	L	128/128 (100%)	127 (99%)	1 (1%)	81	89
2	O	127/128 (99%)	126 (99%)	1 (1%)	81	89
2	Q	128/128 (100%)	127 (99%)	1 (1%)	81	89
2	U	128/128 (100%)	127 (99%)	1 (1%)	81	89
2	W	128/128 (100%)	127 (99%)	1 (1%)	81	89
2	Y	128/128 (100%)	127 (99%)	1 (1%)	81	89
All	All	3200/3204 (100%)	3166 (99%)	34 (1%)	73	84

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	17	SER
1	M	59	CYS
2	A	59	CYS
2	A	61	GLN
2	B	59	CYS
2	L	124	THR
2	O	48	LEU
2	Q	59	CYS
2	U	118	ARG
2	W	61	GLN
1	C	34	ARG
1	C	73	PRO
1	E	1	MET
1	E	101	SER
1	E	155	LYS

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Mol	Chain	Res	Type
1	G	73	PRO
1	G	155	LYS
1	G	158	SER
1	I	23	SER
1	I	178	ARG
1	K	122	THR
1	K	184	SER
1	P	101	SER
1	R	23	SER
1	R	73	PRO
1	R	101	SER
1	T	16	THR
1	T	34	ARG
1	V	22	VAL
1	V	59	CYS
1	V	101	SER
1	V	109	ASN
1	X	158	SER
2	Y	124	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	61	GLN
2	A	88	HIS
2	B	88	HIS
2	F	88	HIS
2	H	88	HIS
2	J	53	GLN
2	L	32	GLN
2	O	88	HIS
2	Q	88	HIS
1	G	62	GLN
1	N	109	ASN
1	T	11	GLN
1	V	31	GLN
1	X	109	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	E	70	1	7,8,9	0.65	0	6,9,11	0.66	0
1	MEN	T	70	1	7,8,9	0.65	0	6,9,11	1.10	0
1	MEN	M	70	1	7,8,9	0.73	0	6,9,11	1.19	1 (16%)
1	MEN	R	70	1	7,8,9	0.59	0	6,9,11	0.74	0
1	MEN	G	70	1	7,8,9	0.72	0	6,9,11	0.98	1 (16%)
1	MEN	P	70	1	7,8,9	0.75	0	6,9,11	1.66	1 (16%)
1	MEN	I	70	1	7,8,9	0.78	0	6,9,11	0.71	0
1	MEN	K	70	1	7,8,9	0.56	0	6,9,11	1.08	0
1	MEN	X	70	1	7,8,9	0.57	0	6,9,11	1.60	2 (33%)
1	MEN	C	70	1	7,8,9	0.95	0	6,9,11	1.36	1 (16%)
1	MEN	V	70	1	7,8,9	0.61	0	6,9,11	1.15	1 (16%)
1	MEN	N	70	1	7,8,9	0.69	0	6,9,11	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEN	E	70	1	-	3/7/8/10	-
1	MEN	T	70	1	-	4/7/8/10	-
1	MEN	M	70	1	-	3/7/8/10	-
1	MEN	R	70	1	-	3/7/8/10	-
1	MEN	G	70	1	-	3/7/8/10	-
1	MEN	P	70	1	-	4/7/8/10	-
1	MEN	I	70	1	-	3/7/8/10	-
1	MEN	K	70	1	-	3/7/8/10	-
1	MEN	X	70	1	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEN	C	70	1	-	2/7/8/10	-
1	MEN	V	70	1	-	3/7/8/10	-
1	MEN	N	70	1	-	4/7/8/10	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	70	MEN	OD1-CG-CB	3.81	127.07	121.50
1	X	70	MEN	CB-CA-C	2.91	116.92	111.47
1	M	70	MEN	CB-CA-C	2.64	116.42	111.47
1	C	70	MEN	CB-CG-ND2	-2.58	112.01	115.48
1	V	70	MEN	CB-CA-C	2.56	116.27	111.47
1	G	70	MEN	CB-CA-C	2.26	115.71	111.47
1	X	70	MEN	CB-CG-ND2	2.16	118.39	115.48

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	70	MEN	C-CA-CB-CG
1	T	70	MEN	C-CA-CB-CG
1	N	70	MEN	N-CA-CB-CG
1	P	70	MEN	N-CA-CB-CG
1	T	70	MEN	N-CA-CB-CG
1	N	70	MEN	CA-CB-CG-OD1
1	E	70	MEN	CA-CB-CG-OD1
1	P	70	MEN	CA-CB-CG-OD1
1	T	70	MEN	CA-CB-CG-OD1
1	T	70	MEN	CA-CB-CG-ND2
1	I	70	MEN	CA-CB-CG-OD1
1	K	70	MEN	CA-CB-CG-OD1
1	N	70	MEN	CA-CB-CG-ND2
1	P	70	MEN	CA-CB-CG-ND2
1	P	70	MEN	C-CA-CB-CG
1	E	70	MEN	CA-CB-CG-ND2
1	G	70	MEN	CA-CB-CG-ND2
1	I	70	MEN	CA-CB-CG-ND2
1	K	70	MEN	CA-CB-CG-ND2
1	R	70	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
1	V	70	MEN	CA-CB-CG-ND2
1	M	70	MEN	N-CA-CB-CG
1	E	70	MEN	N-CA-CB-CG
1	G	70	MEN	N-CA-CB-CG
1	I	70	MEN	N-CA-CB-CG
1	K	70	MEN	N-CA-CB-CG
1	R	70	MEN	CA-CB-CG-OD1
1	V	70	MEN	CA-CB-CG-OD1
1	C	70	MEN	CA-CB-CG-OD1
1	X	70	MEN	CA-CB-CG-OD1
1	M	70	MEN	CA-CB-CG-ND2
1	R	70	MEN	N-CA-CB-CG
1	V	70	MEN	N-CA-CB-CG
1	M	70	MEN	CA-CB-CG-OD1
1	G	70	MEN	CA-CB-CG-OD1
1	X	70	MEN	N-CA-CB-CG
1	C	70	MEN	CA-CB-CG-ND2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	T	70	MEN	1	0
1	P	70	MEN	2	0
1	K	70	MEN	1	0
1	N	70	MEN	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

60 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	$\# Z > 2$
3	PEB	Q	202	-	37,46,46	1.60	3 (8%)	39,67,67	1.28	6 (15%)
3	PEB	R	302	1	37,46,46	1.25	3 (8%)	39,67,67	1.33	7 (17%)
3	PEB	U	202	2	37,46,46	1.41	2 (5%)	39,67,67	1.11	5 (12%)
3	PEB	C	301	1	37,46,46	1.37	2 (5%)	39,67,67	1.18	3 (7%)
3	PEB	O	201	2	37,46,46	1.56	3 (8%)	39,67,67	1.33	5 (12%)
3	PEB	W	202	2	37,46,46	1.34	3 (8%)	39,67,67	1.23	6 (15%)
3	PEB	G	303	1	37,46,46	1.57	3 (8%)	39,67,67	1.52	4 (10%)
3	PEB	I	301	1	37,46,46	1.35	3 (8%)	39,67,67	0.95	3 (7%)
3	PEB	A	201	-	37,46,46	1.35	3 (8%)	39,67,67	1.39	4 (10%)
3	PEB	M	301	-	37,46,46	1.39	2 (5%)	39,67,67	1.16	5 (12%)
3	PEB	R	303	1	37,46,46	1.25	3 (8%)	39,67,67	1.38	5 (12%)
3	PEB	P	303	1	37,46,46	1.66	4 (10%)	39,67,67	1.49	8 (20%)
3	PEB	Y	201	-	37,46,46	1.28	3 (8%)	39,67,67	1.56	7 (17%)
3	PEB	K	303	1	37,46,46	1.49	3 (8%)	39,67,67	1.25	4 (10%)
3	PEB	I	302	-	37,46,46	1.93	2 (5%)	39,67,67	1.23	6 (15%)
3	PEB	D	202	-	37,46,46	1.74	2 (5%)	39,67,67	1.40	7 (17%)
3	PEB	M	302	1	37,46,46	1.53	3 (8%)	39,67,67	1.57	5 (12%)
3	PEB	Y	202	-	37,46,46	1.67	3 (8%)	39,67,67	1.63	8 (20%)
3	PEB	F	201	2	37,46,46	1.49	3 (8%)	39,67,67	1.70	3 (7%)
3	PEB	U	201	2	37,46,46	1.42	3 (8%)	39,67,67	1.43	7 (17%)
3	PEB	X	301	1	37,46,46	1.36	2 (5%)	39,67,67	0.95	3 (7%)
3	PEB	H	201	2	37,46,46	1.38	2 (5%)	39,67,67	1.44	7 (17%)
3	PEB	V	301	-	37,46,46	1.48	2 (5%)	39,67,67	0.90	1 (2%)
3	PEB	V	303	1	37,46,46	1.64	3 (8%)	39,67,67	1.36	7 (17%)
3	PEB	C	303	1	37,46,46	1.60	2 (5%)	39,67,67	1.25	4 (10%)
3	PEB	P	302	1	37,46,46	1.79	3 (8%)	39,67,67	1.24	7 (17%)
3	PEB	T	301	1	37,46,46	1.69	3 (8%)	39,67,67	1.09	3 (7%)
3	PEB	X	302	1	37,46,46	1.86	2 (5%)	39,67,67	1.30	5 (12%)
3	PEB	I	303	1	37,46,46	1.38	3 (8%)	39,67,67	1.41	8 (20%)
3	PEB	V	302	1	37,46,46	1.95	2 (5%)	39,67,67	1.30	7 (17%)
3	PEB	L	201	2	37,46,46	1.29	2 (5%)	39,67,67	1.82	8 (20%)
3	PEB	W	201	2	37,46,46	1.45	3 (8%)	39,67,67	1.29	5 (12%)
3	PEB	E	301	1	37,46,46	1.87	2 (5%)	39,67,67	1.10	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEB	C	302	1	37,46,46	1.48	2 (5%)	39,67,67	1.10	5 (12%)
3	PEB	M	303	-	37,46,46	1.66	2 (5%)	39,67,67	1.35	6 (15%)
3	PEB	T	302	1	37,46,46	1.65	3 (8%)	39,67,67	1.14	5 (12%)
3	PEB	E	302	1	37,46,46	1.85	2 (5%)	39,67,67	1.05	3 (7%)
3	PEB	T	303	1	37,46,46	1.38	2 (5%)	39,67,67	1.35	5 (12%)
3	PEB	N	303	1	37,46,46	1.44	4 (10%)	39,67,67	1.46	5 (12%)
3	PEB	B	202	-	37,46,46	1.52	3 (8%)	39,67,67	1.16	6 (15%)
3	PEB	O	202	2	37,46,46	1.30	3 (8%)	39,67,67	1.23	4 (10%)
3	PEB	X	303	1	37,46,46	1.80	3 (8%)	39,67,67	1.57	8 (20%)
3	PEB	L	202	2	37,46,46	1.52	3 (8%)	39,67,67	1.25	5 (12%)
3	PEB	Q	201	2	37,46,46	1.73	2 (5%)	39,67,67	1.49	6 (15%)
3	PEB	N	302	1	37,46,46	1.65	3 (8%)	39,67,67	1.07	3 (7%)
3	PEB	J	202	2	37,46,46	1.31	2 (5%)	39,67,67	1.22	5 (12%)
3	PEB	R	301	1	37,46,46	1.24	2 (5%)	39,67,67	1.26	2 (5%)
3	PEB	P	301	1	37,46,46	1.48	2 (5%)	39,67,67	1.05	3 (7%)
3	PEB	N	301	1	37,46,46	1.62	2 (5%)	39,67,67	0.94	3 (7%)
3	PEB	G	302	1	37,46,46	1.58	3 (8%)	39,67,67	1.37	6 (15%)
3	PEB	J	201	2	37,46,46	1.12	3 (8%)	39,67,67	1.62	5 (12%)
3	PEB	K	302	1	37,46,46	1.29	2 (5%)	39,67,67	1.05	2 (5%)
3	PEB	A	202	-	37,46,46	1.27	3 (8%)	39,67,67	1.42	6 (15%)
3	PEB	G	301	1	37,46,46	1.31	3 (8%)	39,67,67	1.01	2 (5%)
3	PEB	K	301	1	37,46,46	1.71	3 (8%)	39,67,67	1.15	4 (10%)
3	PEB	H	202	2	37,46,46	1.77	2 (5%)	39,67,67	1.11	4 (10%)
3	PEB	B	201	-	37,46,46	1.41	2 (5%)	39,67,67	1.51	6 (15%)
3	PEB	D	201	-	37,46,46	1.28	3 (8%)	39,67,67	1.61	8 (20%)
3	PEB	F	202	2	37,46,46	1.24	2 (5%)	39,67,67	1.25	3 (7%)
3	PEB	E	303	1	37,46,46	1.50	3 (8%)	39,67,67	1.53	5 (12%)

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	PEB	Q	202	-	-	6/20/74/74	0/4/4/4
3	PEB	R	302	1	-	4/20/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	U	202	2	-	5/20/74/74	0/4/4/4
3	PEB	C	301	1	-	4/20/74/74	0/4/4/4
3	PEB	O	201	2	-	5/20/74/74	0/4/4/4
3	PEB	W	202	2	-	4/20/74/74	0/4/4/4
3	PEB	G	303	1	-	8/20/74/74	0/4/4/4
3	PEB	I	301	1	-	4/20/74/74	0/4/4/4
3	PEB	A	201	-	-	4/20/74/74	0/4/4/4
3	PEB	M	301	-	-	2/20/74/74	0/4/4/4
3	PEB	R	303	1	-	6/20/74/74	0/4/4/4
3	PEB	P	303	1	-	4/20/74/74	0/4/4/4
3	PEB	Y	201	-	-	4/20/74/74	0/4/4/4
3	PEB	K	303	1	-	7/20/74/74	0/4/4/4
3	PEB	I	302	-	-	2/20/74/74	0/4/4/4
3	PEB	D	202	-	-	3/20/74/74	0/4/4/4
3	PEB	M	302	1	-	3/20/74/74	0/4/4/4
3	PEB	Y	202	-	-	4/20/74/74	0/4/4/4
3	PEB	F	201	2	-	4/20/74/74	0/4/4/4
3	PEB	U	201	2	-	4/20/74/74	0/4/4/4
3	PEB	X	301	1	-	5/20/74/74	0/4/4/4
3	PEB	H	201	2	-	4/20/74/74	0/4/4/4
3	PEB	V	301	-	-	4/20/74/74	0/4/4/4
3	PEB	V	303	1	-	6/20/74/74	0/4/4/4
3	PEB	C	303	1	-	7/20/74/74	0/4/4/4
3	PEB	P	302	1	-	4/20/74/74	0/4/4/4
3	PEB	T	301	1	-	5/20/74/74	0/4/4/4
3	PEB	X	302	1	-	4/20/74/74	0/4/4/4
3	PEB	I	303	1	-	6/20/74/74	0/4/4/4
3	PEB	V	302	1	-	3/20/74/74	0/4/4/4
3	PEB	L	201	2	-	4/20/74/74	0/4/4/4
3	PEB	W	201	2	-	6/20/74/74	0/4/4/4
3	PEB	E	301	1	-	4/20/74/74	0/4/4/4
3	PEB	C	302	1	-	3/20/74/74	0/4/4/4
3	PEB	M	303	-	-	8/20/74/74	0/4/4/4
3	PEB	T	302	1	-	3/20/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	E	302	1	-	2/20/74/74	0/4/4/4
3	PEB	T	303	1	-	6/20/74/74	0/4/4/4
3	PEB	N	303	1	-	6/20/74/74	0/4/4/4
3	PEB	B	202	-	-	6/20/74/74	0/4/4/4
3	PEB	O	202	2	-	3/20/74/74	0/4/4/4
3	PEB	X	303	1	-	2/20/74/74	0/4/4/4
3	PEB	L	202	2	-	2/20/74/74	0/4/4/4
3	PEB	Q	201	2	-	4/20/74/74	0/4/4/4
3	PEB	N	302	1	-	3/20/74/74	0/4/4/4
3	PEB	J	202	2	-	3/20/74/74	0/4/4/4
3	PEB	R	301	1	-	4/20/74/74	0/4/4/4
3	PEB	P	301	1	-	4/20/74/74	0/4/4/4
3	PEB	N	301	1	-	4/20/74/74	0/4/4/4
3	PEB	G	302	1	-	2/20/74/74	0/4/4/4
3	PEB	J	201	2	-	4/20/74/74	0/4/4/4
3	PEB	K	302	1	-	2/20/74/74	0/4/4/4
3	PEB	A	202	-	-	4/20/74/74	0/4/4/4
3	PEB	G	301	1	-	4/20/74/74	0/4/4/4
3	PEB	K	301	1	-	4/20/74/74	0/4/4/4
3	PEB	H	202	2	-	3/20/74/74	0/4/4/4
3	PEB	B	201	-	-	4/20/74/74	0/4/4/4
3	PEB	D	201	-	-	5/20/74/74	0/4/4/4
3	PEB	F	202	2	-	3/20/74/74	0/4/4/4
3	PEB	E	303	1	-	3/20/74/74	0/4/4/4

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	302	PEB	CHB-C4B	10.81	1.44	1.35
3	I	302	PEB	CHB-C4B	10.80	1.44	1.35
3	X	302	PEB	CHB-C4B	10.46	1.43	1.35
3	E	302	PEB	CHB-C4B	10.27	1.43	1.35
3	E	301	PEB	CHB-C4B	10.20	1.43	1.35
3	H	202	PEB	CHB-C4B	10.09	1.43	1.35
3	D	202	PEB	CHB-C4B	9.59	1.43	1.35
3	P	302	PEB	CHB-C4B	9.48	1.43	1.35
3	Q	201	PEB	CHB-C4B	9.16	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	303	PEB	CHB-C4B	9.09	1.42	1.35
3	N	302	PEB	CHB-C4B	9.03	1.42	1.35
3	K	301	PEB	CHB-C4B	8.86	1.42	1.35
3	M	303	PEB	CHB-C4B	8.74	1.42	1.35
3	T	301	PEB	CHB-C4B	8.71	1.42	1.35
3	T	302	PEB	CHB-C4B	8.70	1.42	1.35
3	Y	202	PEB	CHB-C4B	8.63	1.42	1.35
3	G	302	PEB	CHB-C4B	8.62	1.42	1.35
3	C	303	PEB	CHB-C4B	8.62	1.42	1.35
3	Q	202	PEB	CHB-C4B	8.47	1.42	1.35
3	V	303	PEB	CHB-C4B	8.27	1.42	1.35
3	N	301	PEB	CHB-C4B	8.21	1.42	1.35
3	M	302	PEB	CHB-C4B	8.16	1.41	1.35
3	P	303	PEB	CHB-C4B	8.00	1.41	1.35
3	G	303	PEB	CHB-C4B	7.99	1.41	1.35
3	L	202	PEB	CHB-C4B	7.92	1.41	1.35
3	V	301	PEB	CHB-C4B	7.85	1.41	1.35
3	K	303	PEB	CHB-C4B	7.83	1.41	1.35
3	P	301	PEB	CHB-C4B	7.74	1.41	1.35
3	U	202	PEB	CHB-C4B	7.63	1.41	1.35
3	B	202	PEB	CHB-C4B	7.62	1.41	1.35
3	O	201	PEB	CHB-C4B	7.53	1.41	1.35
3	C	302	PEB	CHB-C4B	7.50	1.41	1.35
3	E	303	PEB	CHB-C4B	7.38	1.41	1.35
3	U	201	PEB	CHB-C4B	7.23	1.41	1.35
3	T	303	PEB	CHB-C4B	7.22	1.41	1.35
3	C	301	PEB	CHB-C4B	7.21	1.41	1.35
3	M	301	PEB	CHB-C4B	7.08	1.41	1.35
3	B	201	PEB	CHB-C4B	7.08	1.41	1.35
3	N	303	PEB	CHB-C4B	7.07	1.41	1.35
3	F	201	PEB	CHB-C4B	7.03	1.41	1.35
3	H	201	PEB	CHB-C4B	6.92	1.40	1.35
3	I	301	PEB	CHB-C4B	6.91	1.40	1.35
3	I	303	PEB	CHB-C4B	6.78	1.40	1.35
3	W	201	PEB	CHB-C4B	6.71	1.40	1.35
3	W	202	PEB	CHB-C4B	6.71	1.40	1.35
3	J	202	PEB	CHB-C4B	6.64	1.40	1.35
3	O	202	PEB	CHB-C4B	6.42	1.40	1.35
3	X	301	PEB	CHB-C4B	6.25	1.40	1.35
3	A	201	PEB	CHB-C4B	6.21	1.40	1.35
3	D	201	PEB	CHB-C4B	6.20	1.40	1.35
3	R	301	PEB	CHB-C4B	6.20	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	PEB	CHB-C4B	6.14	1.40	1.35
3	Y	201	PEB	CHB-C4B	6.12	1.40	1.35
3	R	303	PEB	CHB-C4B	6.00	1.40	1.35
3	K	302	PEB	CHB-C4B	5.84	1.40	1.35
3	F	202	PEB	CHB-C4B	5.73	1.39	1.35
3	L	201	PEB	CHB-C4B	5.68	1.39	1.35
3	R	302	PEB	CHB-C4B	5.36	1.39	1.35
3	A	202	PEB	CHB-C4B	4.96	1.39	1.35
3	J	201	PEB	CHB-C4B	4.37	1.38	1.35
3	W	201	PEB	CHA-C4A	4.05	1.44	1.36
3	O	201	PEB	CHA-C4A	4.02	1.44	1.36
3	F	201	PEB	CHA-C4A	3.82	1.44	1.36
3	N	301	PEB	CHA-C4A	3.78	1.44	1.36
3	T	301	PEB	CHA-C4A	3.57	1.43	1.36
3	K	302	PEB	CHA-C4A	3.56	1.43	1.36
3	Q	201	PEB	CHA-C4A	3.52	1.43	1.36
3	P	302	PEB	CHA-C4A	3.44	1.43	1.36
3	V	303	PEB	CHA-C4A	3.42	1.43	1.36
3	G	301	PEB	CHA-C4A	3.42	1.43	1.36
3	L	201	PEB	CHA-C4A	3.39	1.43	1.36
3	K	301	PEB	CHA-C4A	3.34	1.43	1.36
3	B	201	PEB	CHA-C4A	3.26	1.43	1.36
3	E	301	PEB	CHA-C4A	3.26	1.43	1.36
3	A	201	PEB	CHA-C4A	3.22	1.43	1.36
3	A	202	PEB	C3C-C4C	-3.20	1.37	1.42
3	X	303	PEB	C3C-C4C	-3.20	1.37	1.42
3	P	303	PEB	CHA-C4A	3.19	1.43	1.36
3	M	301	PEB	CHA-C4A	3.18	1.43	1.36
3	A	202	PEB	CHA-C4A	3.17	1.43	1.36
3	F	202	PEB	C3C-C4C	-3.17	1.37	1.42
3	T	302	PEB	CHA-C4A	3.14	1.42	1.36
3	X	303	PEB	CHA-C4A	3.08	1.42	1.36
3	C	303	PEB	C3C-C4C	-3.05	1.37	1.42
3	M	303	PEB	CHA-C4A	3.02	1.42	1.36
3	B	202	PEB	C3C-C4C	-3.01	1.37	1.42
3	K	301	PEB	C3C-C4C	-3.00	1.37	1.42
3	Y	202	PEB	CHA-C4A	2.99	1.42	1.36
3	R	303	PEB	C3C-C4C	-2.97	1.37	1.42
3	P	303	PEB	C3C-C4C	-2.94	1.37	1.42
3	C	302	PEB	C3C-C4C	-2.91	1.37	1.42
3	B	202	PEB	CHA-C4A	2.86	1.42	1.36
3	F	201	PEB	C3C-C4C	-2.78	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	301	PEB	CHA-C4A	2.70	1.42	1.36
3	X	301	PEB	C3C-C4C	-2.69	1.37	1.42
3	G	303	PEB	CHA-C4A	2.69	1.42	1.36
3	V	301	PEB	C3C-C4C	-2.68	1.37	1.42
3	D	201	PEB	CHA-C4A	2.67	1.42	1.36
3	H	201	PEB	C3C-C4C	-2.61	1.37	1.42
3	E	303	PEB	CHA-C4A	2.60	1.41	1.36
3	M	302	PEB	C3C-C4C	-2.58	1.38	1.42
3	N	303	PEB	CHA-C4A	2.57	1.41	1.36
3	K	303	PEB	CHA-C4A	2.57	1.41	1.36
3	T	303	PEB	C3C-C4C	-2.56	1.38	1.42
3	W	202	PEB	CHA-C4A	2.52	1.41	1.36
3	O	202	PEB	CHA-C4A	2.52	1.41	1.36
3	V	302	PEB	CHA-C4A	2.52	1.41	1.36
3	T	301	PEB	C3C-C4C	-2.50	1.38	1.42
3	R	302	PEB	C3C-C4C	-2.48	1.38	1.42
3	R	302	PEB	CHA-C4A	2.48	1.41	1.36
3	O	201	PEB	C3C-C4C	-2.48	1.38	1.42
3	Y	201	PEB	C3C-C4C	-2.46	1.38	1.42
3	D	202	PEB	C3C-C4C	-2.45	1.38	1.42
3	J	202	PEB	C3C-C4C	-2.45	1.38	1.42
3	I	301	PEB	CHA-C4A	2.45	1.41	1.36
3	I	301	PEB	C3C-C4C	-2.44	1.38	1.42
3	I	303	PEB	CHA-C4A	2.43	1.41	1.36
3	H	202	PEB	C3C-C4C	-2.41	1.38	1.42
3	P	301	PEB	C3C-C4C	-2.40	1.38	1.42
3	X	302	PEB	C3C-C4C	-2.40	1.38	1.42
3	J	201	PEB	C3C-C4C	-2.38	1.38	1.42
3	K	303	PEB	C3C-C4C	-2.36	1.38	1.42
3	I	303	PEB	C3C-C4C	-2.35	1.38	1.42
3	Q	202	PEB	CHA-C4A	2.34	1.41	1.36
3	E	303	PEB	C3C-C4C	-2.34	1.38	1.42
3	U	202	PEB	C3C-C4C	-2.33	1.38	1.42
3	T	302	PEB	C3C-C4C	-2.33	1.38	1.42
3	A	201	PEB	C3C-C4C	-2.33	1.38	1.42
3	I	302	PEB	C3C-C4C	-2.30	1.38	1.42
3	Q	202	PEB	C3C-C4C	-2.28	1.38	1.42
3	V	303	PEB	C3C-C4C	-2.28	1.38	1.42
3	E	302	PEB	C3C-C4C	-2.28	1.38	1.42
3	L	202	PEB	C3C-C4C	-2.27	1.38	1.42
3	O	202	PEB	C3C-C4C	-2.27	1.38	1.42
3	R	303	PEB	CHA-C4A	2.26	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	201	PEB	CHA-C4A	2.24	1.41	1.36
3	U	201	PEB	C3C-C4C	-2.24	1.38	1.42
3	G	302	PEB	C3C-C4C	-2.22	1.38	1.42
3	M	302	PEB	CHA-C4A	2.21	1.41	1.36
3	L	202	PEB	CHA-C4A	2.19	1.41	1.36
3	D	201	PEB	C3C-C4C	-2.17	1.38	1.42
3	N	303	PEB	C3C-C4C	-2.17	1.38	1.42
3	G	303	PEB	C3C-C4C	-2.16	1.38	1.42
3	Y	202	PEB	C3C-C4C	-2.15	1.38	1.42
3	G	302	PEB	CHA-C4A	2.15	1.41	1.36
3	N	302	PEB	CHA-C4A	2.14	1.40	1.36
3	G	301	PEB	C3C-C4C	-2.13	1.38	1.42
3	N	302	PEB	C3C-C4C	-2.13	1.38	1.42
3	P	302	PEB	C3C-C4C	-2.12	1.38	1.42
3	J	201	PEB	CHA-C4A	2.11	1.40	1.36
3	W	202	PEB	C3C-C4C	-2.10	1.38	1.42
3	N	303	PEB	C2A-C1A	-2.10	1.50	1.52
3	P	303	PEB	C3D-C4D	-2.09	1.41	1.47
3	W	201	PEB	C3C-C4C	-2.09	1.38	1.42
3	C	301	PEB	C3C-C4C	-2.08	1.38	1.42
3	Y	201	PEB	CHA-C4A	2.00	1.40	1.36

All (301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	201	PEB	CHA-C4A-NA	7.19	133.75	125.20
3	L	201	PEB	CHA-C4A-NA	6.96	133.49	125.20
3	M	302	PEB	CHC-C1D-ND	-6.36	106.56	113.95
3	Y	201	PEB	CHA-C4A-NA	6.12	132.48	125.20
3	E	303	PEB	CHA-C4A-NA	5.95	132.28	125.20
3	D	201	PEB	CHA-C4A-NA	5.80	132.10	125.20
3	F	201	PEB	CHA-C4A-NA	5.64	131.91	125.20
3	H	201	PEB	CHA-C4A-NA	5.59	131.85	125.20
3	F	201	PEB	CHC-C1D-ND	-5.56	107.49	113.95
3	X	303	PEB	CHA-C4A-NA	4.96	131.10	125.20
3	Q	201	PEB	CHA-C4A-NA	4.94	131.08	125.20
3	N	303	PEB	CHA-C4A-NA	4.89	131.02	125.20
3	Y	202	PEB	CMD-C2D-C3D	-4.82	123.27	130.06
3	A	201	PEB	CHA-C4A-NA	4.69	130.79	125.20
3	G	303	PEB	OA-C1A-C2A	-4.68	122.45	126.17
3	D	202	PEB	CHC-C1D-ND	-4.51	108.71	113.95
3	T	303	PEB	CHA-C4A-NA	4.46	130.50	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	201	PEB	CHA-C4A-NA	4.45	130.50	125.20
3	P	303	PEB	CHA-C4A-NA	4.38	130.42	125.20
3	B	201	PEB	CHC-C1D-ND	-4.30	108.95	113.95
3	G	303	PEB	CHA-C4A-NA	4.29	130.31	125.20
3	Y	202	PEB	CHC-C1D-ND	-4.27	108.98	113.95
3	F	202	PEB	CHC-C1D-ND	-4.22	109.05	113.95
3	L	201	PEB	OA-C1A-C2A	-4.15	122.87	126.17
3	I	303	PEB	CHA-C4A-NA	4.14	130.13	125.20
3	R	303	PEB	CHA-C4A-NA	4.11	130.09	125.20
3	V	303	PEB	CHA-C4A-NA	4.11	130.09	125.20
3	L	202	PEB	CMD-C2D-C3D	-3.96	124.47	130.06
3	C	303	PEB	CHC-C1D-ND	-3.95	109.36	113.95
3	A	202	PEB	CAA-C3A-C2A	-3.94	104.42	114.26
3	W	201	PEB	CHC-C1D-ND	-3.93	109.38	113.95
3	M	303	PEB	CHA-C4A-NA	3.93	129.88	125.20
3	X	302	PEB	CBC-CAC-C2C	3.83	119.54	112.49
3	B	201	PEB	CHA-C4A-NA	3.82	129.75	125.20
3	O	201	PEB	CHA-C4A-NA	3.81	129.73	125.20
3	O	201	PEB	CHB-C4B-NB	-3.74	123.63	128.83
3	W	202	PEB	CHC-C1D-ND	-3.74	109.61	113.95
3	Q	201	PEB	CHC-C1D-ND	-3.73	109.61	113.95
3	U	201	PEB	CHC-C1D-ND	-3.72	109.63	113.95
3	B	201	PEB	CHB-C4B-NB	-3.71	123.68	128.83
3	M	303	PEB	OA-C1A-C2A	-3.67	123.25	126.17
3	O	202	PEB	CHC-C1D-ND	-3.57	109.80	113.95
3	D	201	PEB	CHB-C4B-NB	-3.54	123.92	128.83
3	J	202	PEB	CMD-C2D-C3D	-3.54	125.07	130.06
3	K	301	PEB	CHA-C4A-NA	3.53	129.40	125.20
3	L	201	PEB	CHB-C4B-NB	-3.52	123.95	128.83
3	G	302	PEB	CHC-C1D-ND	-3.51	109.87	113.95
3	V	302	PEB	CHA-C4A-NA	3.51	129.38	125.20
3	G	302	PEB	CBC-CAC-C2C	3.51	118.95	112.49
3	K	301	PEB	C1C-CHB-C4B	3.49	132.98	128.81
3	Q	202	PEB	C1C-CHB-C4B	3.44	132.92	128.81
3	F	201	PEB	CHB-C4B-NB	-3.44	124.06	128.83
3	O	202	PEB	CHB-C4B-NB	-3.44	124.06	128.83
3	Q	201	PEB	CHB-C4B-NB	-3.40	124.12	128.83
3	A	201	PEB	CHB-C4B-NB	-3.38	124.14	128.83
3	E	301	PEB	C1C-CHB-C4B	3.38	132.84	128.81
3	I	301	PEB	C1C-CHB-C4B	3.36	132.82	128.81
3	T	301	PEB	C1C-CHB-C4B	3.35	132.81	128.81
3	W	201	PEB	CHA-C4A-NA	3.33	129.17	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	303	PEB	C2A-C1A-NA	3.27	111.09	108.27
3	Y	201	PEB	CHC-C1D-ND	-3.26	110.17	113.95
3	I	302	PEB	CHA-C4A-NA	3.25	129.07	125.20
3	V	301	PEB	C1C-CHB-C4B	3.25	132.69	128.81
3	R	301	PEB	CHC-C1D-ND	-3.24	110.18	113.95
3	A	201	PEB	CHC-C1D-ND	-3.21	110.22	113.95
3	R	302	PEB	OA-C1A-C2A	-3.20	123.63	126.17
3	P	302	PEB	CHC-C1D-ND	-3.20	110.23	113.95
3	C	301	PEB	C1C-CHB-C4B	3.19	132.62	128.81
3	N	301	PEB	C1C-CHB-C4B	3.18	132.61	128.81
3	H	202	PEB	CHB-C4B-NB	-3.17	124.43	128.83
3	Y	201	PEB	CHB-C4B-NB	-3.17	124.43	128.83
3	J	201	PEB	CHB-C4B-NB	-3.16	124.44	128.83
3	N	303	PEB	OA-C1A-C2A	-3.15	123.67	126.17
3	Y	202	PEB	CAA-C3A-C2A	-3.13	106.44	114.26
3	Y	202	PEB	CAA-C3A-C4A	3.13	120.70	112.67
3	E	301	PEB	CHA-C4A-NA	3.12	128.91	125.20
3	T	301	PEB	CMD-C2D-C3D	-3.10	125.69	130.06
3	J	202	PEB	CHB-C4B-NB	-3.10	124.53	128.83
3	C	301	PEB	CHA-C4A-NA	3.09	128.88	125.20
3	A	202	PEB	CHB-C4B-NB	-3.09	124.54	128.83
3	L	202	PEB	CHC-C1D-ND	-3.06	110.39	113.95
3	V	303	PEB	C2A-C3A-C4A	3.06	105.92	101.34
3	Q	202	PEB	CHC-C1D-ND	-3.04	110.42	113.95
3	L	202	PEB	CHB-C4B-NB	-3.03	124.62	128.83
3	G	301	PEB	C1C-CHB-C4B	3.02	132.42	128.81
3	T	302	PEB	CHC-C1D-ND	-3.02	110.44	113.95
3	I	302	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
3	O	201	PEB	CHC-C1D-ND	-3.01	110.45	113.95
3	P	303	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
3	X	303	PEB	OA-C1A-C2A	-2.99	123.80	126.17
3	D	202	PEB	CHB-C4B-NB	-2.98	124.69	128.83
3	F	202	PEB	CHB-C4B-NB	-2.98	124.69	128.83
3	T	303	PEB	C2A-C3A-C4A	2.97	105.79	101.34
3	R	301	PEB	C1C-CHB-C4B	2.96	132.34	128.81
3	U	201	PEB	CHB-C4B-NB	-2.94	124.75	128.83
3	A	202	PEB	OA-C1A-C2A	-2.94	123.84	126.17
3	Q	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
3	A	202	PEB	C2A-C3A-C4A	2.93	105.72	101.34
3	T	302	PEB	CHA-C4A-NA	2.93	128.69	125.20
3	M	302	PEB	CMD-C2D-C3D	-2.93	125.94	130.06
3	U	202	PEB	CHC-C1D-ND	-2.91	110.56	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	303	PEB	CMB-C2B-C1B	2.91	129.55	125.06
3	U	201	PEB	CAB-CBB-CGB	2.88	117.50	112.67
3	E	303	PEB	OA-C1A-C2A	-2.87	123.89	126.17
3	D	201	PEB	CMB-C2B-C1B	2.87	129.48	125.06
3	V	302	PEB	C1C-CHB-C4B	2.87	132.24	128.81
3	G	302	PEB	CHA-C4A-NA	2.86	128.61	125.20
3	G	303	PEB	C2A-C3A-C4A	2.86	105.62	101.34
3	D	202	PEB	C2A-C3A-C4A	2.83	105.58	101.34
3	P	303	PEB	OD-C4D-C3D	-2.83	123.05	129.46
3	I	303	PEB	OA-C1A-C2A	-2.83	123.92	126.17
3	X	303	PEB	CHC-C1D-ND	-2.82	110.67	113.95
3	R	303	PEB	CHC-C1D-ND	-2.80	110.69	113.95
3	P	303	PEB	CHC-C1D-ND	-2.77	110.73	113.95
3	M	301	PEB	C1C-CHB-C4B	2.77	132.12	128.81
3	D	201	PEB	OA-C1A-C2A	-2.77	123.97	126.17
3	V	303	PEB	CHB-C4B-NB	-2.76	124.99	128.83
3	K	303	PEB	CHB-C4B-NB	-2.75	125.01	128.83
3	N	303	PEB	C2A-C3A-C4A	2.74	105.44	101.34
3	G	302	PEB	C1C-CHB-C4B	2.72	132.06	128.81
3	K	303	PEB	CHA-C4A-NA	2.71	128.43	125.20
3	J	202	PEB	CHC-C1D-ND	-2.71	110.80	113.95
3	C	302	PEB	OA-C1A-C2A	-2.71	124.02	126.17
3	I	303	PEB	CMB-C2B-C1B	2.71	129.23	125.06
3	E	303	PEB	C2A-C3A-C4A	2.70	105.39	101.34
3	U	202	PEB	CHB-C4B-NB	-2.70	125.08	128.83
3	X	303	PEB	C2A-C3A-C4A	2.69	105.38	101.34
3	C	302	PEB	C1C-CHB-C4B	2.69	132.02	128.81
3	H	202	PEB	CHC-C1D-ND	-2.69	110.82	113.95
3	T	302	PEB	C1C-CHB-C4B	2.68	132.02	128.81
3	P	303	PEB	C2A-C3A-C4A	2.68	105.35	101.34
3	E	302	PEB	CHB-C4B-NB	-2.68	125.11	128.83
3	T	303	PEB	CHB-C4B-NB	-2.68	125.12	128.83
3	D	201	PEB	C2A-C3A-C4A	2.67	105.34	101.34
3	H	201	PEB	CHB-C4B-NB	-2.67	125.12	128.83
3	L	201	PEB	CHA-C1B-C2B	2.66	131.74	124.90
3	P	302	PEB	C2A-C3A-C4A	2.66	105.32	101.34
3	W	202	PEB	C1C-CHB-C4B	2.66	131.98	128.81
3	M	302	PEB	CBC-CAC-C2C	2.65	117.38	112.49
3	M	302	PEB	CHA-C4A-NA	2.65	128.35	125.20
3	I	302	PEB	C2A-C3A-C4A	2.64	105.29	101.34
3	M	301	PEB	CAA-C3A-C4A	2.64	119.44	112.67
3	P	301	PEB	CBC-CAC-C2C	-2.63	107.64	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	201	PEB	CMB-C2B-C1B	2.63	129.11	125.06
3	C	303	PEB	CHA-C4A-NA	2.60	128.30	125.20
3	E	302	PEB	C2A-C3A-C4A	2.60	105.23	101.34
3	M	303	PEB	C2A-C1A-NA	2.59	110.51	108.27
3	B	201	PEB	CAB-CBB-CGB	2.58	117.00	112.67
3	W	202	PEB	CHB-C4B-NB	-2.57	125.27	128.83
3	B	202	PEB	C2A-C3A-C4A	2.56	105.17	101.34
3	R	303	PEB	C2A-C3A-C4A	2.56	105.17	101.34
3	N	301	PEB	C2A-C3A-C4A	2.55	105.17	101.34
3	C	301	PEB	CHC-C1D-ND	-2.55	110.99	113.95
3	P	301	PEB	C1C-CHB-C4B	2.54	131.85	128.81
3	Y	202	PEB	CHB-C4B-NB	-2.54	125.30	128.83
3	K	303	PEB	C2A-C3A-C4A	2.53	105.13	101.34
3	H	201	PEB	CMB-C2B-C1B	2.53	128.96	125.06
3	R	302	PEB	CHB-C4B-NB	-2.53	125.32	128.83
3	W	202	PEB	CMD-C2D-C3D	-2.52	126.52	130.06
3	E	303	PEB	CHC-C1D-ND	-2.51	111.03	113.95
3	Q	202	PEB	CAD-C3D-C2D	-2.50	120.37	128.60
3	O	202	PEB	C2A-C3A-C4A	2.50	105.08	101.34
3	P	303	PEB	OA-C1A-C2A	-2.48	124.20	126.17
3	R	303	PEB	CBC-CAC-C2C	2.47	117.05	112.49
3	I	303	PEB	CHB-C4B-NB	-2.47	125.40	128.83
3	X	303	PEB	CMB-C2B-C1B	2.47	128.87	125.06
3	N	302	PEB	C2A-C3A-C4A	2.47	105.03	101.34
3	O	202	PEB	CHA-C4A-NA	2.47	128.14	125.20
3	L	201	PEB	CHC-C1D-ND	-2.46	111.09	113.95
3	M	303	PEB	CHB-C4B-NB	-2.46	125.41	128.83
3	H	201	PEB	CHA-C1B-C2B	2.45	131.21	124.90
3	H	201	PEB	CHA-C1B-NB	-2.44	119.83	124.93
3	Y	201	PEB	CMB-C2B-C1B	2.44	128.82	125.06
3	X	303	PEB	CHB-C4B-NB	-2.43	125.46	128.83
3	E	302	PEB	C1C-CHB-C4B	2.43	131.71	128.81
3	B	202	PEB	CHB-C4B-NB	-2.40	125.49	128.83
3	J	201	PEB	CHA-C1B-NB	-2.40	119.91	124.93
3	W	201	PEB	CHB-C4B-NB	-2.40	125.50	128.83
3	Y	201	PEB	CHA-C1B-C2B	2.40	131.06	124.90
3	W	202	PEB	C2A-C3A-C4A	2.39	104.92	101.34
3	G	302	PEB	C2A-C3A-C4A	2.39	104.92	101.34
3	X	302	PEB	CHA-C4A-NA	2.39	128.05	125.20
3	Q	201	PEB	CHA-C1B-C2B	2.37	131.00	124.90
3	I	303	PEB	C2A-C3A-C4A	2.37	104.89	101.34
3	J	201	PEB	OA-C1A-C2A	-2.37	124.29	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	303	PEB	CMB-C2B-C1B	2.37	128.72	125.06
3	K	302	PEB	C2A-C3A-C4A	2.37	104.89	101.34
3	Y	202	PEB	CAD-C3D-C2D	-2.37	120.81	128.60
3	D	201	PEB	CHA-C1B-C2B	2.36	130.98	124.90
3	T	302	PEB	C2A-C3A-C4A	2.36	104.88	101.34
3	Y	202	PEB	OA-C1A-C2A	-2.36	124.30	126.17
3	M	301	PEB	CAA-C3A-C2A	-2.36	108.37	114.26
3	R	303	PEB	OA-C1A-C2A	-2.35	124.30	126.17
3	X	301	PEB	CMD-C2D-C3D	-2.35	126.75	130.06
3	K	302	PEB	C1C-CHB-C4B	2.35	131.61	128.81
3	J	201	PEB	CHA-C1B-C2B	2.35	130.94	124.90
3	N	303	PEB	CHB-C4B-NB	-2.35	125.57	128.83
3	P	303	PEB	CHB-C4B-NB	-2.35	125.57	128.83
3	A	201	PEB	CAB-CBB-CGB	2.35	116.61	112.67
3	I	302	PEB	C1C-CHB-C4B	2.35	131.61	128.81
3	V	302	PEB	C2A-C3A-C4A	2.34	104.85	101.34
3	M	303	PEB	C2A-C3A-C4A	2.34	104.84	101.34
3	D	201	PEB	CHA-C1B-NB	-2.33	120.06	124.93
3	L	201	PEB	C2A-C1A-NA	2.33	110.28	108.27
3	L	201	PEB	CHA-C1B-NB	-2.32	120.08	124.93
3	H	201	PEB	OA-C1A-NA	2.32	127.75	124.94
3	J	202	PEB	C2A-C3A-C4A	2.31	104.80	101.34
3	F	202	PEB	CMD-C2D-C3D	-2.31	126.81	130.06
3	N	302	PEB	CHB-C4B-NB	-2.29	125.65	128.83
3	B	202	PEB	OD-C4D-ND	-2.29	122.54	125.93
3	Q	202	PEB	C2A-C3A-C4A	2.29	104.76	101.34
3	Q	201	PEB	CHA-C1B-NB	-2.29	120.15	124.93
3	H	201	PEB	OA-C1A-C2A	-2.27	124.37	126.17
3	R	302	PEB	CHA-C4A-NA	2.26	127.90	125.20
3	X	301	PEB	CHB-C4B-NB	-2.26	125.69	128.83
3	E	301	PEB	C2A-C3A-C4A	2.26	104.73	101.34
3	Y	201	PEB	CHA-C1B-NB	-2.26	120.21	124.93
3	V	303	PEB	CAA-C3A-C4A	2.26	118.47	112.67
3	M	302	PEB	C2A-C3A-C4A	2.25	104.71	101.34
3	I	301	PEB	C2A-C3A-C4A	2.25	104.71	101.34
3	O	201	PEB	CHA-C1B-C2B	2.25	130.68	124.90
3	G	302	PEB	CHC-C4C-C3C	-2.25	126.50	130.34
3	V	303	PEB	OA-C1A-C2A	-2.24	124.39	126.17
3	R	302	PEB	CMB-C2B-C1B	2.24	128.51	125.06
3	U	202	PEB	C2A-C3A-C4A	2.22	104.67	101.34
3	C	302	PEB	CHC-C1D-ND	-2.22	111.37	113.95
3	C	303	PEB	CHB-C4B-NB	-2.21	125.76	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	202	PEB	C2A-C3A-C4A	2.21	104.65	101.34
3	A	202	PEB	CAA-C3A-C4A	2.21	118.34	112.67
3	I	302	PEB	CAC-CBC-CGC	2.20	116.37	112.67
3	P	302	PEB	CAA-C3A-C4A	2.20	118.33	112.67
3	U	201	PEB	CMB-C2B-C1B	2.19	128.44	125.06
3	Q	202	PEB	CHB-C4B-NB	-2.19	125.78	128.83
3	I	303	PEB	CHA-C1B-NB	-2.19	120.35	124.93
3	U	202	PEB	CMD-C2D-C3D	-2.19	126.97	130.06
3	T	301	PEB	C2A-C3A-C4A	2.19	104.62	101.34
3	P	301	PEB	C2A-C3A-C4A	2.18	104.61	101.34
3	A	202	PEB	CMD-C2D-C3D	-2.18	126.99	130.06
3	X	302	PEB	OA-C1A-C2A	-2.17	124.44	126.17
3	X	302	PEB	C2A-C3A-C4A	2.17	104.59	101.34
3	H	202	PEB	C2A-C3A-C4A	2.17	104.58	101.34
3	I	303	PEB	CHA-C1B-C2B	2.16	130.47	124.90
3	V	302	PEB	CAC-CBC-CGC	2.16	116.30	112.67
3	X	303	PEB	OD-C4D-C3D	-2.16	124.57	129.46
3	V	302	PEB	CHC-C1D-ND	-2.15	111.45	113.95
3	H	202	PEB	C1C-CHB-C4B	2.15	131.38	128.81
3	G	301	PEB	C2A-C3A-C4A	2.15	104.56	101.34
3	M	303	PEB	CMB-C2B-C1B	2.15	128.37	125.06
3	T	303	PEB	CMD-C2D-C3D	-2.15	127.04	130.06
3	U	201	PEB	CHA-C1B-C2B	2.14	130.41	124.90
3	M	301	PEB	CMD-C2D-C3D	-2.14	127.04	130.06
3	M	301	PEB	C2A-C3A-C4A	2.13	104.53	101.34
3	P	302	PEB	CHC-C4C-C3C	-2.13	126.70	130.34
3	C	303	PEB	C2A-C3A-C4A	2.13	104.53	101.34
3	Q	201	PEB	CAB-CBB-CGB	2.13	116.24	112.67
3	D	202	PEB	CAA-C3A-C4A	2.13	118.13	112.67
3	I	301	PEB	CHA-C4A-NA	2.12	127.73	125.20
3	D	201	PEB	CAB-CBB-CGB	2.12	116.22	112.67
3	B	201	PEB	OA-C1A-C2A	-2.11	124.49	126.17
3	W	201	PEB	C2A-C3A-C4A	2.11	104.49	101.34
3	U	202	PEB	C1C-CHB-C4B	2.10	131.31	128.81
3	W	201	PEB	CMB-C2B-C1B	2.09	128.28	125.06
3	B	201	PEB	CHA-C1B-C2B	2.09	130.27	124.90
3	C	302	PEB	CHA-C4A-NA	2.09	127.69	125.20
3	N	301	PEB	CHA-C4A-NA	2.09	127.69	125.20
3	I	302	PEB	CHB-C4B-NB	-2.08	125.94	128.83
3	X	303	PEB	CHA-C1B-C2B	2.08	130.25	124.90
3	R	302	PEB	C2A-C3A-C4A	2.08	104.46	101.34
3	V	303	PEB	CMB-C2B-C1B	2.08	128.26	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	302	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
3	U	201	PEB	CHA-C1B-NB	-2.07	120.60	124.93
3	W	202	PEB	CHA-C4A-NA	2.07	127.66	125.20
3	J	202	PEB	CAD-C3D-C2D	-2.07	121.80	128.60
3	Y	201	PEB	C2A-C3A-C4A	2.06	104.43	101.34
3	B	202	PEB	C1C-CHB-C4B	2.06	131.27	128.81
3	V	302	PEB	OD-C4D-C3D	-2.06	124.79	129.46
3	L	202	PEB	OD-C4D-C3D	-2.06	124.79	129.46
3	O	201	PEB	CHA-C1B-NB	-2.06	120.62	124.93
3	I	303	PEB	CHC-C1D-ND	-2.06	111.56	113.95
3	N	303	PEB	CHC-C1D-ND	-2.05	111.56	113.95
3	V	303	PEB	CHA-C1B-C2B	2.05	130.17	124.90
3	D	202	PEB	OD-C4D-ND	-2.05	122.90	125.93
3	B	202	PEB	CAD-C3D-C2D	-2.05	121.86	128.60
3	L	202	PEB	C2A-C3A-C4A	2.05	104.40	101.34
3	V	302	PEB	CMD-C2D-C3D	-2.04	127.18	130.06
3	B	202	PEB	C2A-C1A-NA	2.04	110.03	108.27
3	P	302	PEB	CHB-C4B-NB	-2.04	125.99	128.83
3	K	301	PEB	CAD-C3D-C2D	-2.04	121.88	128.60
3	P	302	PEB	C1C-CHB-C4B	2.04	131.25	128.81
3	E	303	PEB	CHA-C1B-C2B	2.04	130.14	124.90
3	D	202	PEB	CMB-C2B-C1B	2.04	128.20	125.06
3	T	302	PEB	OD-C4D-ND	-2.04	122.91	125.93
3	X	302	PEB	CHC-C1D-ND	-2.03	111.59	113.95
3	R	302	PEB	CAC-CBC-CGC	2.03	116.08	112.67
3	X	301	PEB	C1C-CHB-C4B	2.03	131.23	128.81
3	C	302	PEB	C2A-C3A-C4A	2.02	104.37	101.34
3	R	302	PEB	CHC-C1D-ND	-2.02	111.60	113.95
3	P	302	PEB	CHA-C4A-NA	2.02	127.61	125.20
3	D	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
3	K	301	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
3	P	303	PEB	CMB-C2B-C1B	2.00	128.14	125.06

There are no chirality outliers.

All (250) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	301	PEB	NB-C1B-CHA-C4A
3	M	301	PEB	C2B-C1B-CHA-C4A
3	M	302	PEB	NB-C1B-CHA-C4A
3	M	302	PEB	C2B-C1B-CHA-C4A
3	M	303	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
3	M	303	PEB	C2C-C1C-CHB-C4B
3	M	303	PEB	NA-C4A-CHA-C1B
3	M	303	PEB	C3A-C4A-CHA-C1B
3	M	303	PEB	NB-C1B-CHA-C4A
3	M	303	PEB	C2B-C1B-CHA-C4A
3	A	201	PEB	NA-C4A-CHA-C1B
3	A	201	PEB	C3A-C4A-CHA-C1B
3	A	201	PEB	NB-C1B-CHA-C4A
3	A	201	PEB	C2B-C1B-CHA-C4A
3	A	202	PEB	C2A-C3A-CAA-CBA
3	A	202	PEB	C4A-C3A-CAA-CBA
3	A	202	PEB	NB-C1B-CHA-C4A
3	A	202	PEB	C2B-C1B-CHA-C4A
3	D	201	PEB	C2A-C3A-CAA-CBA
3	D	201	PEB	NA-C4A-CHA-C1B
3	D	201	PEB	C3A-C4A-CHA-C1B
3	D	201	PEB	C2B-C1B-CHA-C4A
3	D	202	PEB	NB-C1B-CHA-C4A
3	D	202	PEB	C2B-C1B-CHA-C4A
3	B	201	PEB	NA-C4A-CHA-C1B
3	B	201	PEB	C3A-C4A-CHA-C1B
3	B	201	PEB	NB-C1B-CHA-C4A
3	B	201	PEB	C2B-C1B-CHA-C4A
3	B	202	PEB	C1C-C2C-CAC-CBC
3	B	202	PEB	C3C-C2C-CAC-CBC
3	B	202	PEB	C2A-C3A-CAA-CBA
3	B	202	PEB	C4A-C3A-CAA-CBA
3	B	202	PEB	NB-C1B-CHA-C4A
3	B	202	PEB	C2B-C1B-CHA-C4A
3	F	201	PEB	NA-C4A-CHA-C1B
3	F	201	PEB	C3A-C4A-CHA-C1B
3	F	201	PEB	NB-C1B-CHA-C4A
3	F	201	PEB	C2B-C1B-CHA-C4A
3	F	202	PEB	C2A-C3A-CAA-CBA
3	F	202	PEB	NB-C1B-CHA-C4A
3	F	202	PEB	C2B-C1B-CHA-C4A
3	H	201	PEB	NA-C4A-CHA-C1B
3	H	201	PEB	C3A-C4A-CHA-C1B
3	H	202	PEB	NB-C1B-CHA-C4A
3	H	202	PEB	C2B-C1B-CHA-C4A
3	J	201	PEB	NA-C4A-CHA-C1B
3	J	201	PEB	C3A-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
3	J	202	PEB	NB-C1B-CHA-C4A
3	J	202	PEB	C2B-C1B-CHA-C4A
3	L	201	PEB	NA-C4A-CHA-C1B
3	L	201	PEB	C3A-C4A-CHA-C1B
3	L	202	PEB	NB-C1B-CHA-C4A
3	L	202	PEB	C2B-C1B-CHA-C4A
3	O	201	PEB	C2C-C1C-CHB-C4B
3	O	201	PEB	NA-C4A-CHA-C1B
3	O	201	PEB	C3A-C4A-CHA-C1B
3	O	201	PEB	NB-C1B-CHA-C4A
3	O	201	PEB	C2B-C1B-CHA-C4A
3	O	202	PEB	NB-C1B-CHA-C4A
3	O	202	PEB	C2B-C1B-CHA-C4A
3	Q	201	PEB	NA-C4A-CHA-C1B
3	Q	201	PEB	C3A-C4A-CHA-C1B
3	Q	202	PEB	C1C-C2C-CAC-CBC
3	Q	202	PEB	C3C-C2C-CAC-CBC
3	Q	202	PEB	C2A-C3A-CAA-CBA
3	Q	202	PEB	C4A-C3A-CAA-CBA
3	Q	202	PEB	NB-C1B-CHA-C4A
3	Q	202	PEB	C2B-C1B-CHA-C4A
3	U	201	PEB	NA-C4A-CHA-C1B
3	U	201	PEB	C3A-C4A-CHA-C1B
3	U	201	PEB	NB-C1B-CHA-C4A
3	U	201	PEB	C2B-C1B-CHA-C4A
3	U	202	PEB	C2A-C3A-CAA-CBA
3	U	202	PEB	C4A-C3A-CAA-CBA
3	U	202	PEB	NB-C1B-CHA-C4A
3	U	202	PEB	C2B-C1B-CHA-C4A
3	W	201	PEB	NC-C1C-CHB-C4B
3	W	201	PEB	C2C-C1C-CHB-C4B
3	W	201	PEB	NA-C4A-CHA-C1B
3	W	201	PEB	C3A-C4A-CHA-C1B
3	W	201	PEB	NB-C1B-CHA-C4A
3	W	201	PEB	C2B-C1B-CHA-C4A
3	W	202	PEB	NB-C1B-CHA-C4A
3	W	202	PEB	C2B-C1B-CHA-C4A
3	C	301	PEB	C2A-C3A-CAA-CBA
3	C	301	PEB	C4A-C3A-CAA-CBA
3	C	301	PEB	NB-C1B-CHA-C4A
3	C	301	PEB	C2B-C1B-CHA-C4A
3	C	302	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
3	C	302	PEB	C2B-C1B-CHA-C4A
3	C	303	PEB	NC-C1C-CHB-C4B
3	C	303	PEB	C2C-C1C-CHB-C4B
3	C	303	PEB	C3A-C4A-CHA-C1B
3	C	303	PEB	NB-C1B-CHA-C4A
3	C	303	PEB	C2B-C1B-CHA-C4A
3	E	301	PEB	C2A-C3A-CAA-CBA
3	E	301	PEB	C4A-C3A-CAA-CBA
3	E	301	PEB	NB-C1B-CHA-C4A
3	E	301	PEB	C2B-C1B-CHA-C4A
3	E	302	PEB	NB-C1B-CHA-C4A
3	E	302	PEB	C2B-C1B-CHA-C4A
3	G	301	PEB	NB-C1B-CHA-C4A
3	G	301	PEB	C2B-C1B-CHA-C4A
3	G	302	PEB	NB-C1B-CHA-C4A
3	G	302	PEB	C2B-C1B-CHA-C4A
3	G	303	PEB	NC-C1C-CHB-C4B
3	G	303	PEB	C2C-C1C-CHB-C4B
3	G	303	PEB	NA-C4A-CHA-C1B
3	G	303	PEB	C3A-C4A-CHA-C1B
3	G	303	PEB	NB-C1B-CHA-C4A
3	G	303	PEB	C2B-C1B-CHA-C4A
3	I	301	PEB	NB-C1B-CHA-C4A
3	I	301	PEB	C2B-C1B-CHA-C4A
3	I	302	PEB	NB-C1B-CHA-C4A
3	I	302	PEB	C2B-C1B-CHA-C4A
3	I	303	PEB	NC-C1C-CHB-C4B
3	I	303	PEB	C2C-C1C-CHB-C4B
3	I	303	PEB	NB-C1B-CHA-C4A
3	I	303	PEB	C2B-C1B-CHA-C4A
3	K	301	PEB	C2A-C3A-CAA-CBA
3	K	301	PEB	NB-C1B-CHA-C4A
3	K	301	PEB	C2B-C1B-CHA-C4A
3	K	302	PEB	NB-C1B-CHA-C4A
3	K	302	PEB	C2B-C1B-CHA-C4A
3	K	303	PEB	NC-C1C-CHB-C4B
3	K	303	PEB	C2C-C1C-CHB-C4B
3	K	303	PEB	NB-C1B-CHA-C4A
3	K	303	PEB	C2B-C1B-CHA-C4A
3	N	301	PEB	C2A-C3A-CAA-CBA
3	N	301	PEB	NB-C1B-CHA-C4A
3	N	301	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
3	N	302	PEB	NB-C1B-CHA-C4A
3	N	302	PEB	C2B-C1B-CHA-C4A
3	N	303	PEB	NC-C1C-CHB-C4B
3	N	303	PEB	C2C-C1C-CHB-C4B
3	N	303	PEB	NB-C1B-CHA-C4A
3	N	303	PEB	C2B-C1B-CHA-C4A
3	P	301	PEB	C2A-C3A-CAA-CBA
3	P	301	PEB	C4A-C3A-CAA-CBA
3	P	301	PEB	NB-C1B-CHA-C4A
3	P	301	PEB	C2B-C1B-CHA-C4A
3	P	302	PEB	C2D-C3D-CAD-CBD
3	P	302	PEB	NB-C1B-CHA-C4A
3	P	302	PEB	C2B-C1B-CHA-C4A
3	P	303	PEB	NC-C1C-CHB-C4B
3	P	303	PEB	C2C-C1C-CHB-C4B
3	P	303	PEB	NB-C1B-CHA-C4A
3	P	303	PEB	C2B-C1B-CHA-C4A
3	R	301	PEB	NB-C1B-CHA-C4A
3	R	301	PEB	C2B-C1B-CHA-C4A
3	R	302	PEB	C4A-C3A-CAA-CBA
3	R	302	PEB	NB-C1B-CHA-C4A
3	R	302	PEB	C2B-C1B-CHA-C4A
3	R	303	PEB	NC-C1C-CHB-C4B
3	R	303	PEB	C3A-C4A-CHA-C1B
3	R	303	PEB	NB-C1B-CHA-C4A
3	R	303	PEB	C2B-C1B-CHA-C4A
3	T	301	PEB	NB-C1B-CHA-C4A
3	T	301	PEB	C2B-C1B-CHA-C4A
3	T	302	PEB	NB-C1B-CHA-C4A
3	T	302	PEB	C2B-C1B-CHA-C4A
3	T	303	PEB	NC-C1C-CHB-C4B
3	T	303	PEB	C2C-C1C-CHB-C4B
3	T	303	PEB	NB-C1B-CHA-C4A
3	T	303	PEB	C2B-C1B-CHA-C4A
3	V	301	PEB	NB-C1B-CHA-C4A
3	V	301	PEB	C2B-C1B-CHA-C4A
3	V	302	PEB	NB-C1B-CHA-C4A
3	V	302	PEB	C2B-C1B-CHA-C4A
3	V	303	PEB	NC-C1C-CHB-C4B
3	V	303	PEB	C2C-C1C-CHB-C4B
3	V	303	PEB	NB-C1B-CHA-C4A
3	V	303	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
3	X	301	PEB	C2C-CAC-CBC-CGC
3	X	301	PEB	NB-C1B-CHA-C4A
3	X	301	PEB	C2B-C1B-CHA-C4A
3	X	302	PEB	C1C-C2C-CAC-CBC
3	X	302	PEB	C3C-C2C-CAC-CBC
3	X	302	PEB	NB-C1B-CHA-C4A
3	X	302	PEB	C2B-C1B-CHA-C4A
3	Y	201	PEB	NA-C4A-CHA-C1B
3	Y	201	PEB	C3A-C4A-CHA-C1B
3	Y	201	PEB	C2B-C1B-CHA-C4A
3	Y	202	PEB	C4A-C3A-CAA-CBA
3	Y	202	PEB	NB-C1B-CHA-C4A
3	Y	202	PEB	C2B-C1B-CHA-C4A
3	D	201	PEB	NB-C1B-CHA-C4A
3	J	201	PEB	C2B-C1B-CHA-C4A
3	Q	201	PEB	C2B-C1B-CHA-C4A
3	E	303	PEB	C2B-C1B-CHA-C4A
3	M	303	PEB	NB-C4B-CHB-C1C
3	C	303	PEB	NB-C4B-CHB-C1C
3	G	303	PEB	NB-C4B-CHB-C1C
3	I	303	PEB	NB-C4B-CHB-C1C
3	K	303	PEB	NB-C4B-CHB-C1C
3	T	303	PEB	NB-C4B-CHB-C1C
3	V	303	PEB	NB-C4B-CHB-C1C
3	H	201	PEB	NB-C1B-CHA-C4A
3	J	201	PEB	NB-C1B-CHA-C4A
3	L	201	PEB	NB-C1B-CHA-C4A
3	Q	201	PEB	NB-C1B-CHA-C4A
3	E	303	PEB	NB-C1B-CHA-C4A
3	X	303	PEB	NB-C1B-CHA-C4A
3	Y	201	PEB	NB-C1B-CHA-C4A
3	H	201	PEB	C2B-C1B-CHA-C4A
3	L	201	PEB	C2B-C1B-CHA-C4A
3	X	303	PEB	C2B-C1B-CHA-C4A
3	R	303	PEB	NA-C4A-CHA-C1B
3	P	302	PEB	C4D-C3D-CAD-CBD
3	M	303	PEB	C3B-C4B-CHB-C1C
3	G	303	PEB	C3B-C4B-CHB-C1C
3	G	301	PEB	C2A-C3A-CAA-CBA
3	I	301	PEB	C2A-C3A-CAA-CBA
3	C	303	PEB	NA-C4A-CHA-C1B
3	V	303	PEB	C3B-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
3	W	202	PEB	C3B-CAB-CBB-CGB
3	T	301	PEB	NB-C4B-CHB-C1C
3	J	202	PEB	C4D-C3D-CAD-CBD
3	D	202	PEB	C4A-C3A-CAA-CBA
3	C	302	PEB	C4A-C3A-CAA-CBA
3	G	301	PEB	C4A-C3A-CAA-CBA
3	I	301	PEB	C4A-C3A-CAA-CBA
3	K	301	PEB	C4A-C3A-CAA-CBA
3	N	301	PEB	C4A-C3A-CAA-CBA
3	R	301	PEB	C4A-C3A-CAA-CBA
3	T	301	PEB	C4A-C3A-CAA-CBA
3	V	302	PEB	C4A-C3A-CAA-CBA
3	X	301	PEB	C4A-C3A-CAA-CBA
3	K	303	PEB	NA-C4A-CHA-C1B
3	R	301	PEB	C2A-C3A-CAA-CBA
3	X	301	PEB	C2A-C3A-CAA-CBA
3	N	302	PEB	C3C-C2C-CAC-CBC
3	I	303	PEB	C3B-C4B-CHB-C1C
3	Y	202	PEB	C3B-CAB-CBB-CGB
3	R	303	PEB	NB-C4B-CHB-C1C
3	R	302	PEB	C2B-C3B-CAB-CBB
3	T	302	PEB	C2B-C3B-CAB-CBB
3	O	202	PEB	C3B-CAB-CBB-CGB
3	T	301	PEB	C2A-C3A-CAA-CBA
3	K	303	PEB	C3B-C4B-CHB-C1C
3	T	303	PEB	C3B-C4B-CHB-C1C
3	E	303	PEB	NB-C4B-CHB-C1C
3	V	301	PEB	C4A-C3A-CAA-CBA
3	N	303	PEB	NB-C4B-CHB-C1C
3	M	302	PEB	C3B-CAB-CBB-CGB
3	H	202	PEB	C3B-CAB-CBB-CGB
3	N	303	PEB	NA-C4A-CHA-C1B
3	W	202	PEB	C2C-CAC-CBC-CGC
3	U	202	PEB	C3B-CAB-CBB-CGB
3	V	301	PEB	C2A-C3A-CAA-CBA

There are no ring outliers.

50 monomers are involved in 207 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	202	PEB	5	0
3	R	302	PEB	6	0

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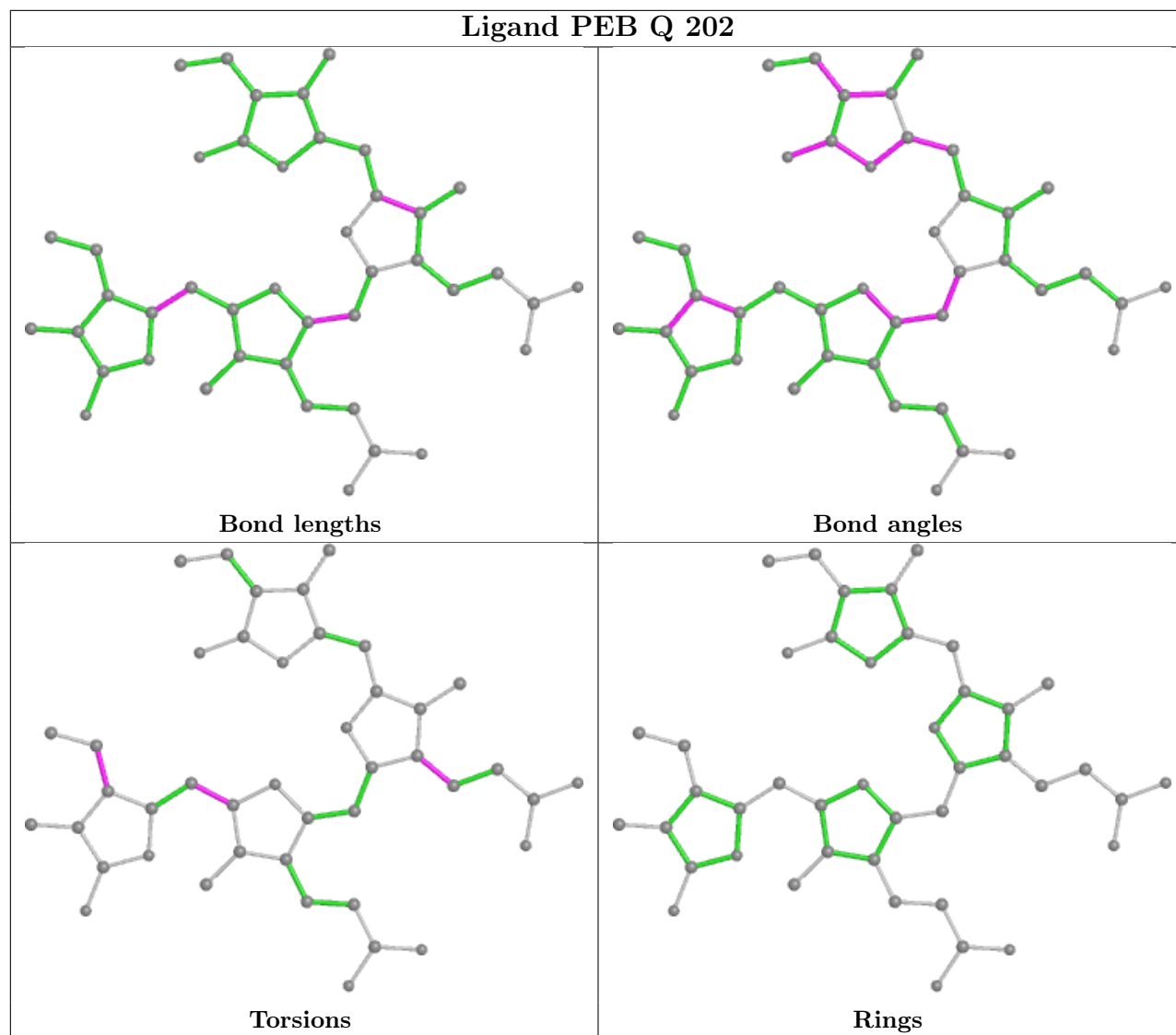
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	303	PEB	2	0
3	I	301	PEB	4	0
3	A	201	PEB	6	0
3	M	301	PEB	10	0
3	R	303	PEB	2	0
3	P	303	PEB	3	0
3	Y	201	PEB	4	0
3	K	303	PEB	3	0
3	I	302	PEB	11	0
3	D	202	PEB	2	0
3	M	302	PEB	2	0
3	Y	202	PEB	7	0
3	F	201	PEB	1	0
3	U	201	PEB	2	0
3	X	301	PEB	2	0
3	V	301	PEB	8	0
3	V	303	PEB	2	0
3	C	303	PEB	2	0
3	P	302	PEB	4	0
3	T	301	PEB	4	0
3	X	302	PEB	8	0
3	I	303	PEB	1	0
3	V	302	PEB	5	0
3	W	201	PEB	4	0
3	E	301	PEB	1	0
3	C	302	PEB	7	0
3	M	303	PEB	6	0
3	T	302	PEB	7	0
3	E	302	PEB	6	0
3	T	303	PEB	5	0
3	N	303	PEB	2	0
3	B	202	PEB	7	0
3	X	303	PEB	2	0
3	L	202	PEB	1	0
3	N	302	PEB	9	0
3	J	202	PEB	2	0
3	R	301	PEB	2	0
3	P	301	PEB	2	0
3	N	301	PEB	2	0
3	G	302	PEB	3	0
3	K	302	PEB	8	0
3	A	202	PEB	6	0

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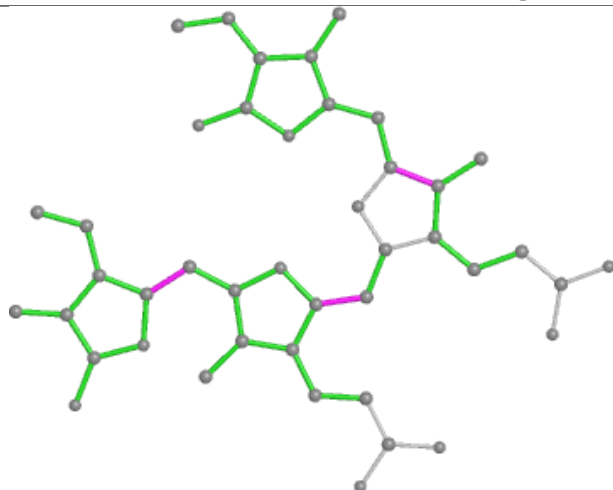
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	301	PEB	3	0
3	K	301	PEB	3	0
3	H	202	PEB	1	0
3	B	201	PEB	6	0
3	D	201	PEB	5	0
3	E	303	PEB	1	0

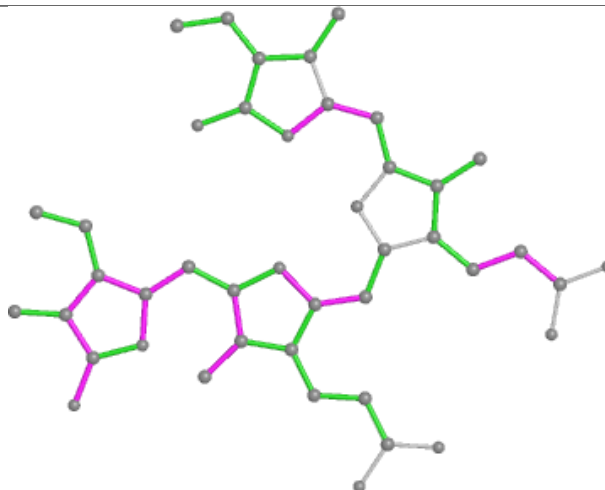
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



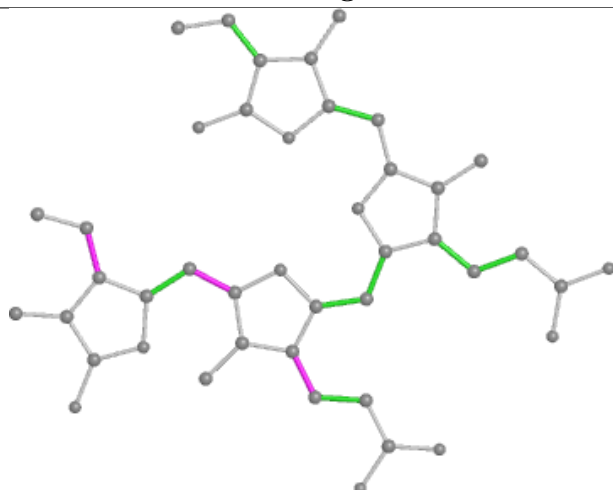
Ligand PEB R 302



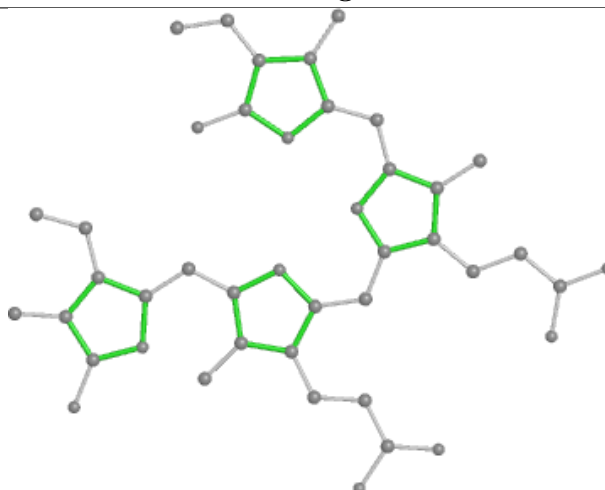
Bond lengths



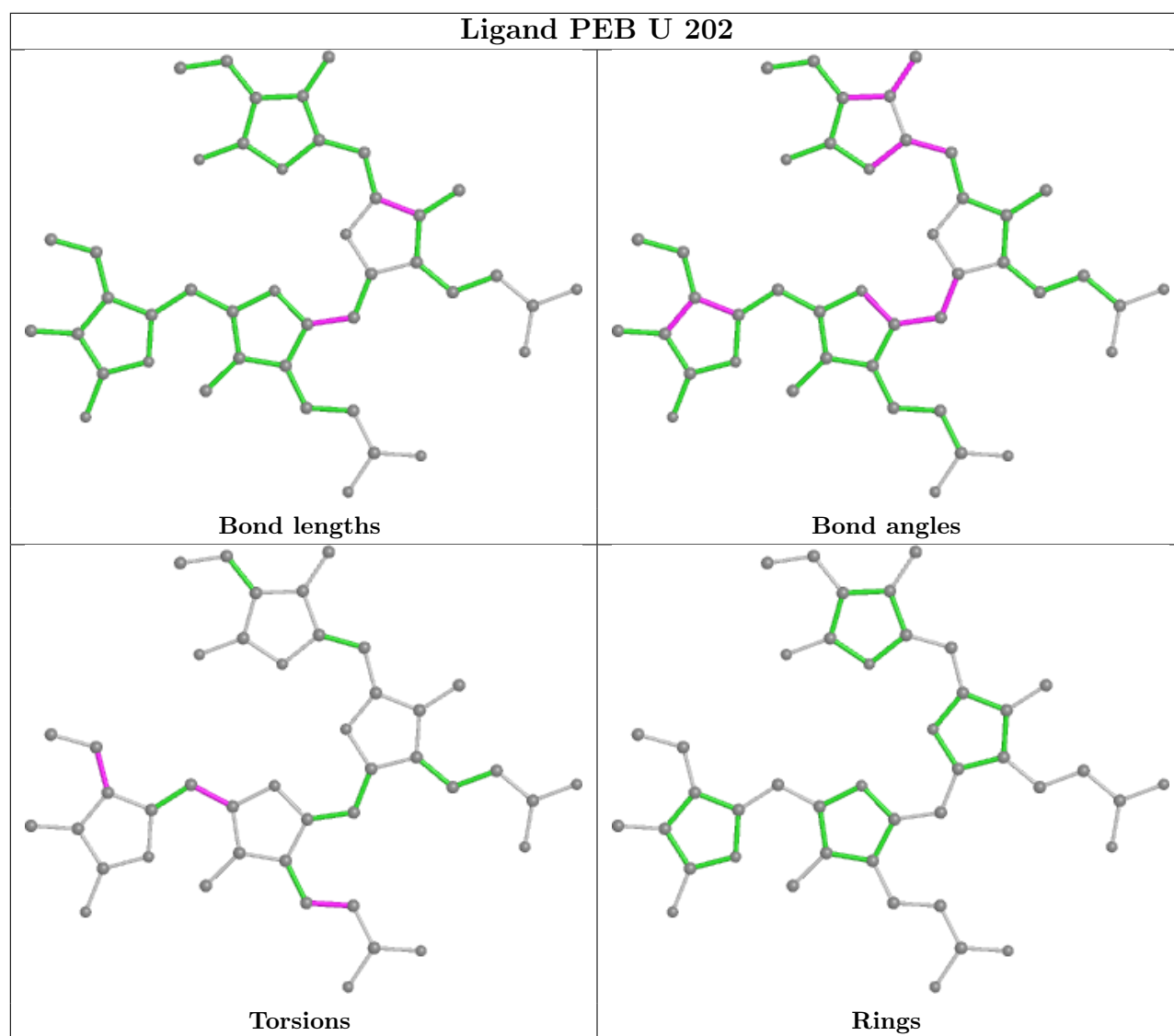
Bond angles

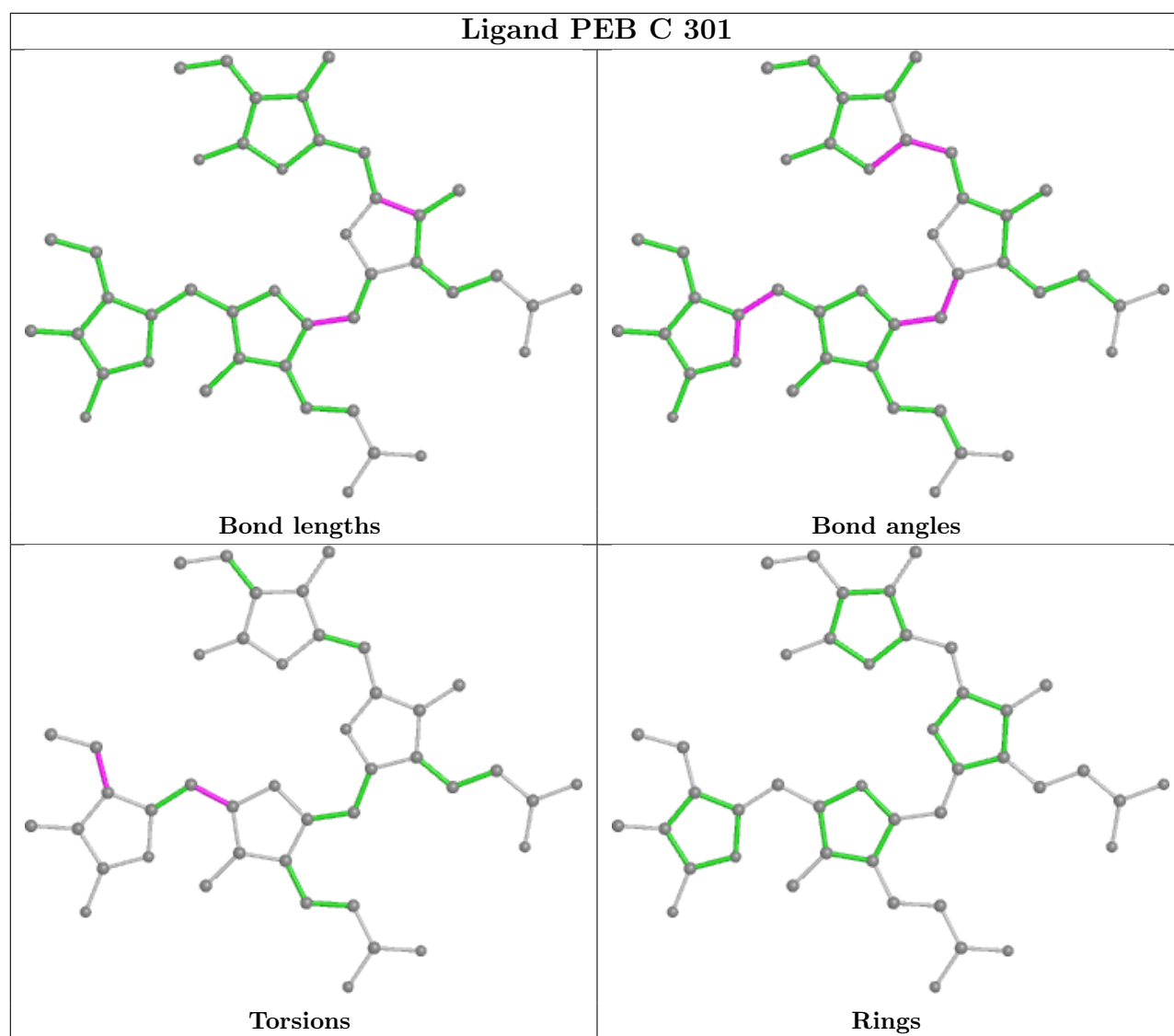


Torsions

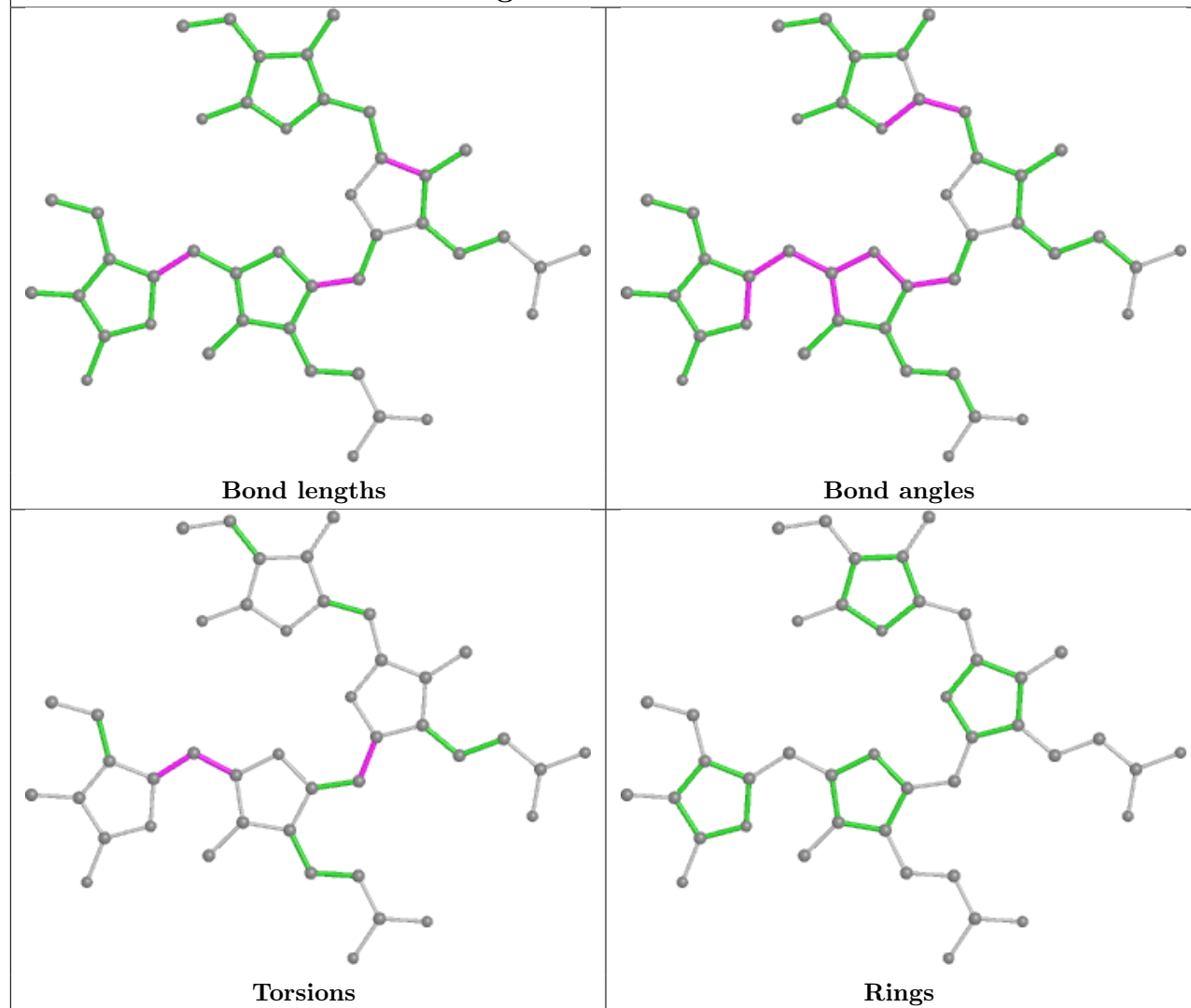


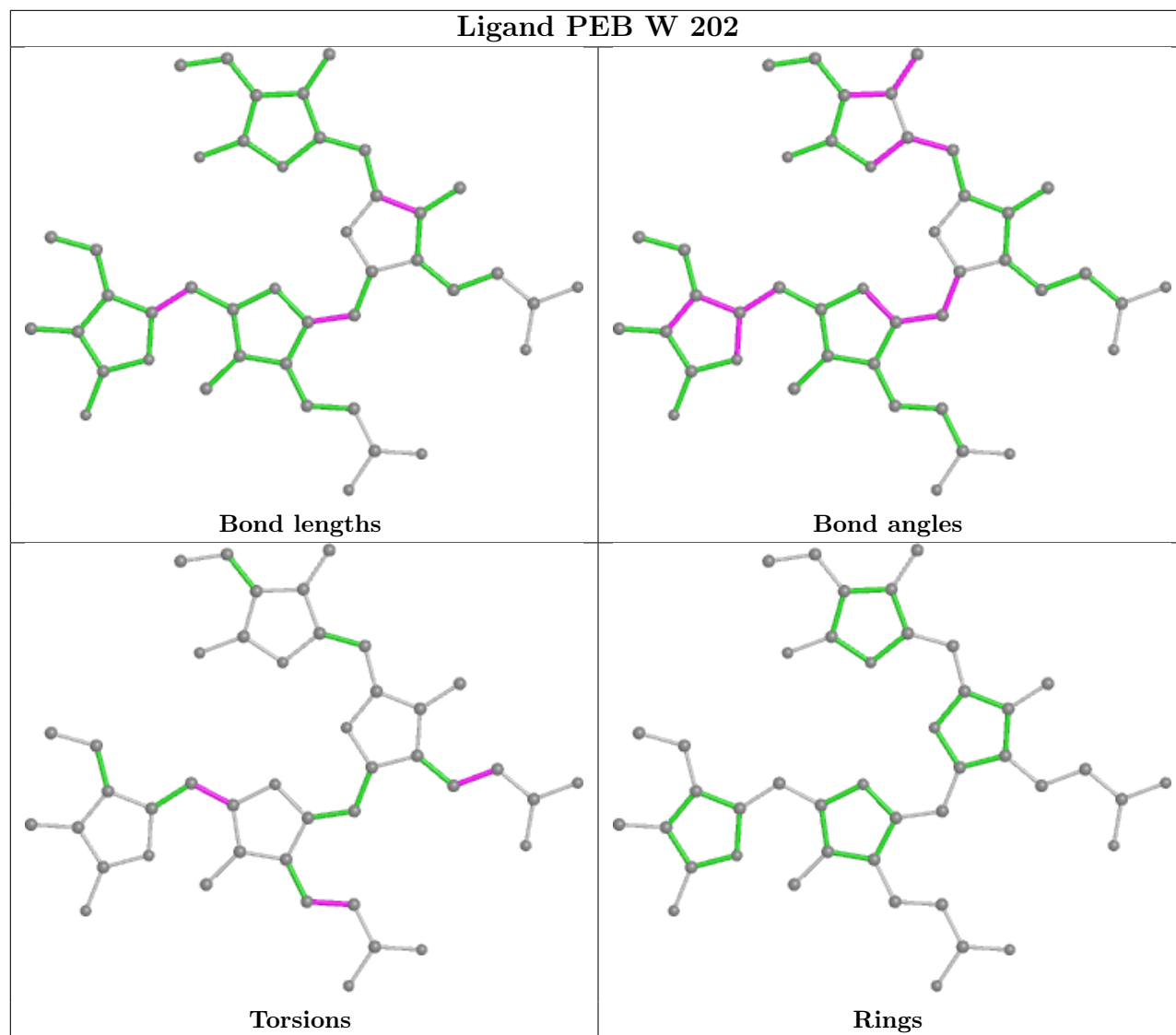
Rings



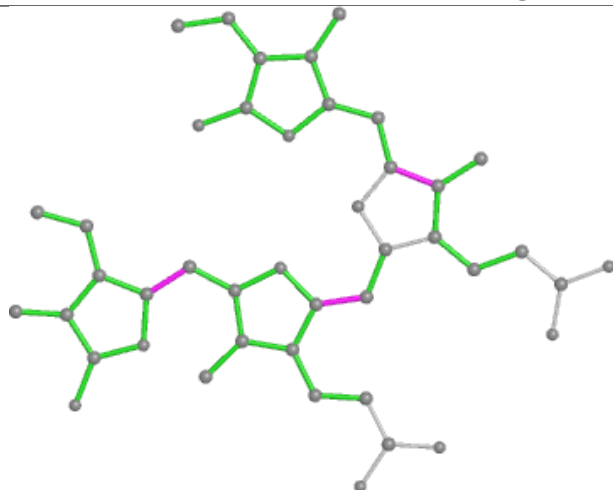


Ligand PEB O 201

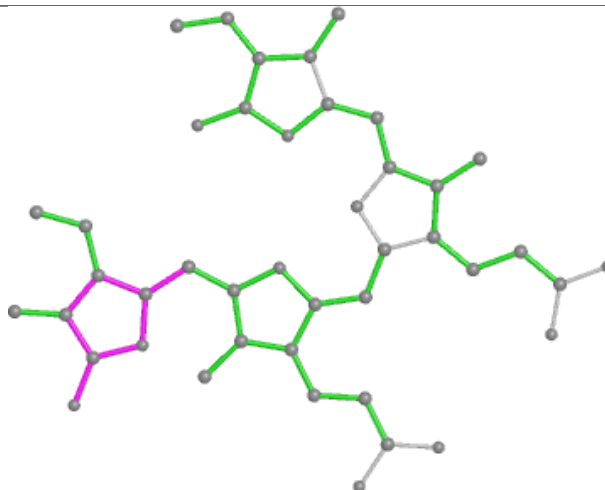




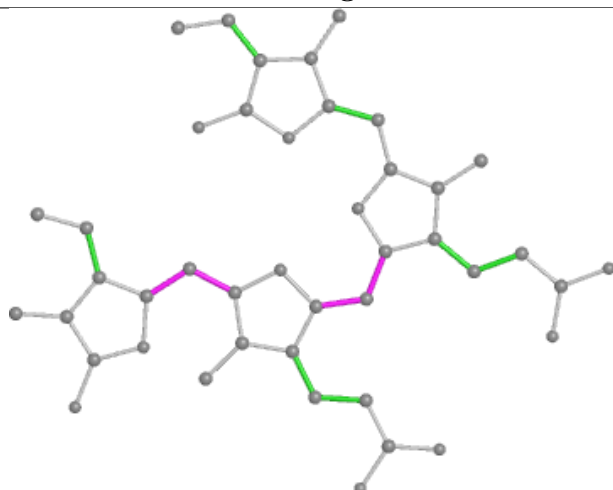
Ligand PEB G 303



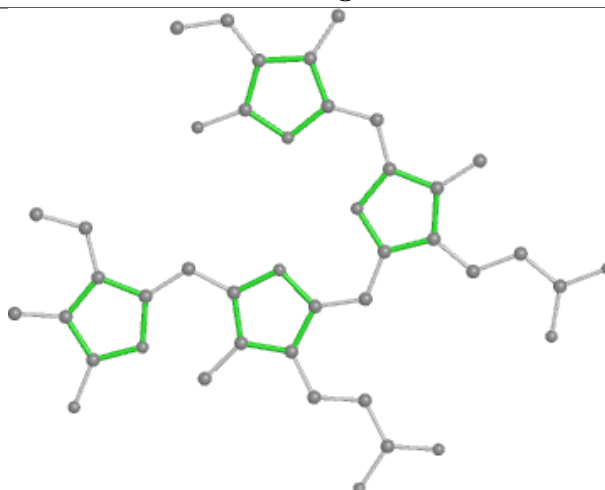
Bond lengths



Bond angles

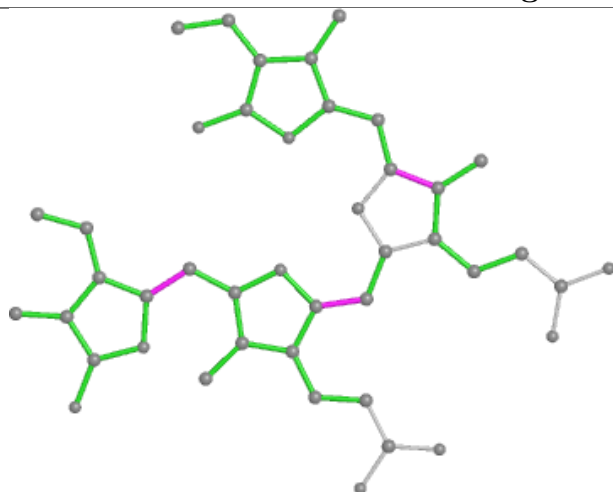


Torsions

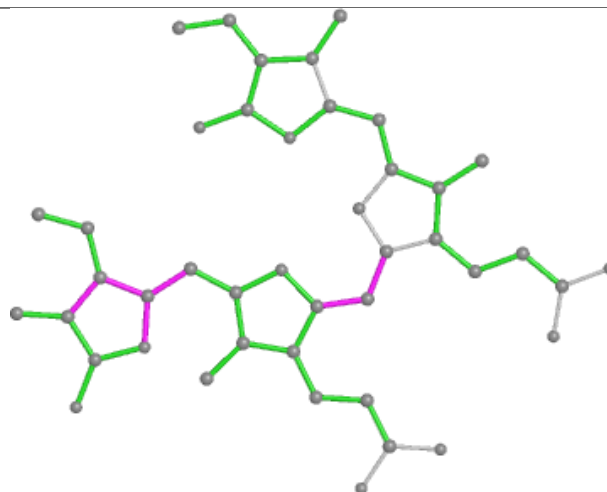


Rings

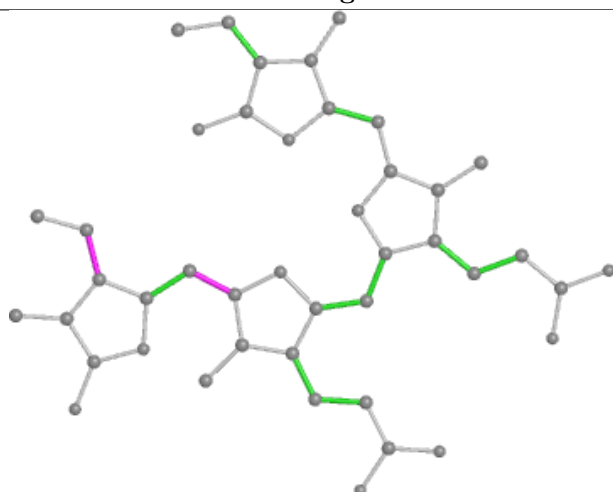
Ligand PEB I 301



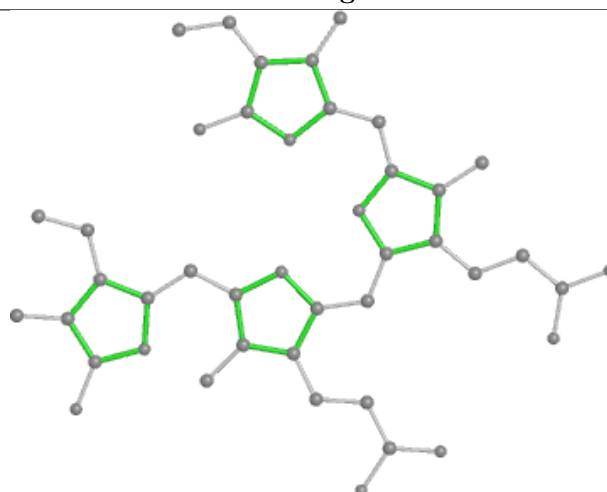
Bond lengths



Bond angles

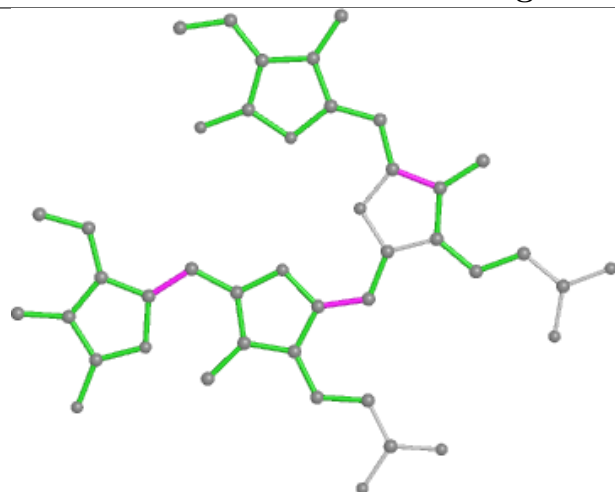


Torsions

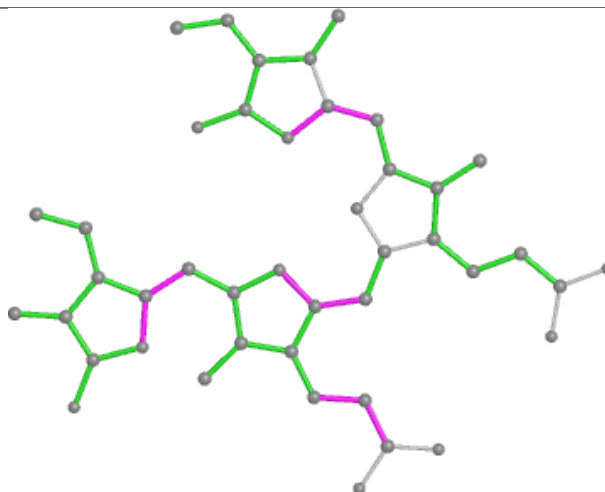


Rings

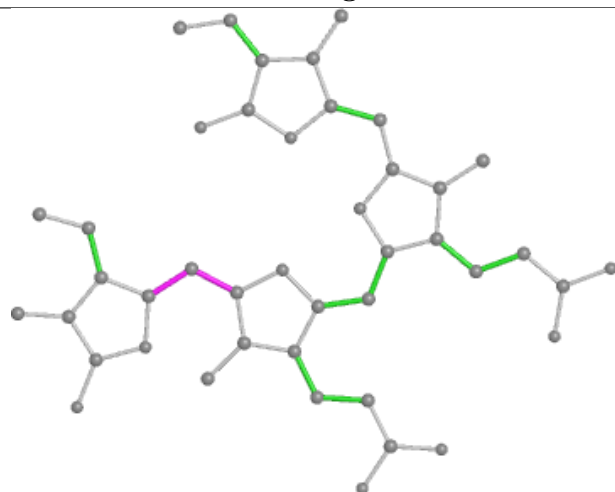
Ligand PEB A 201



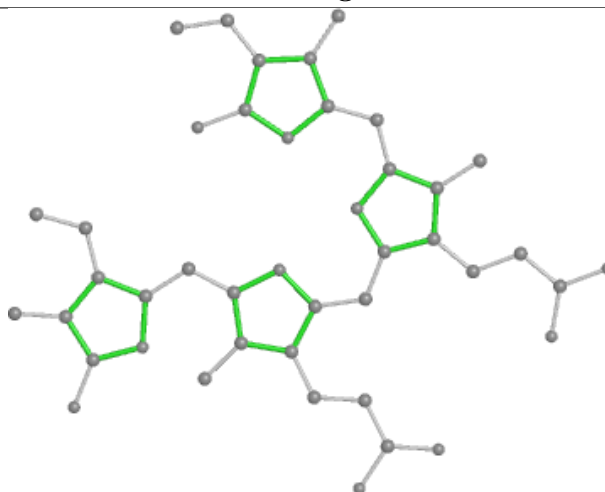
Bond lengths



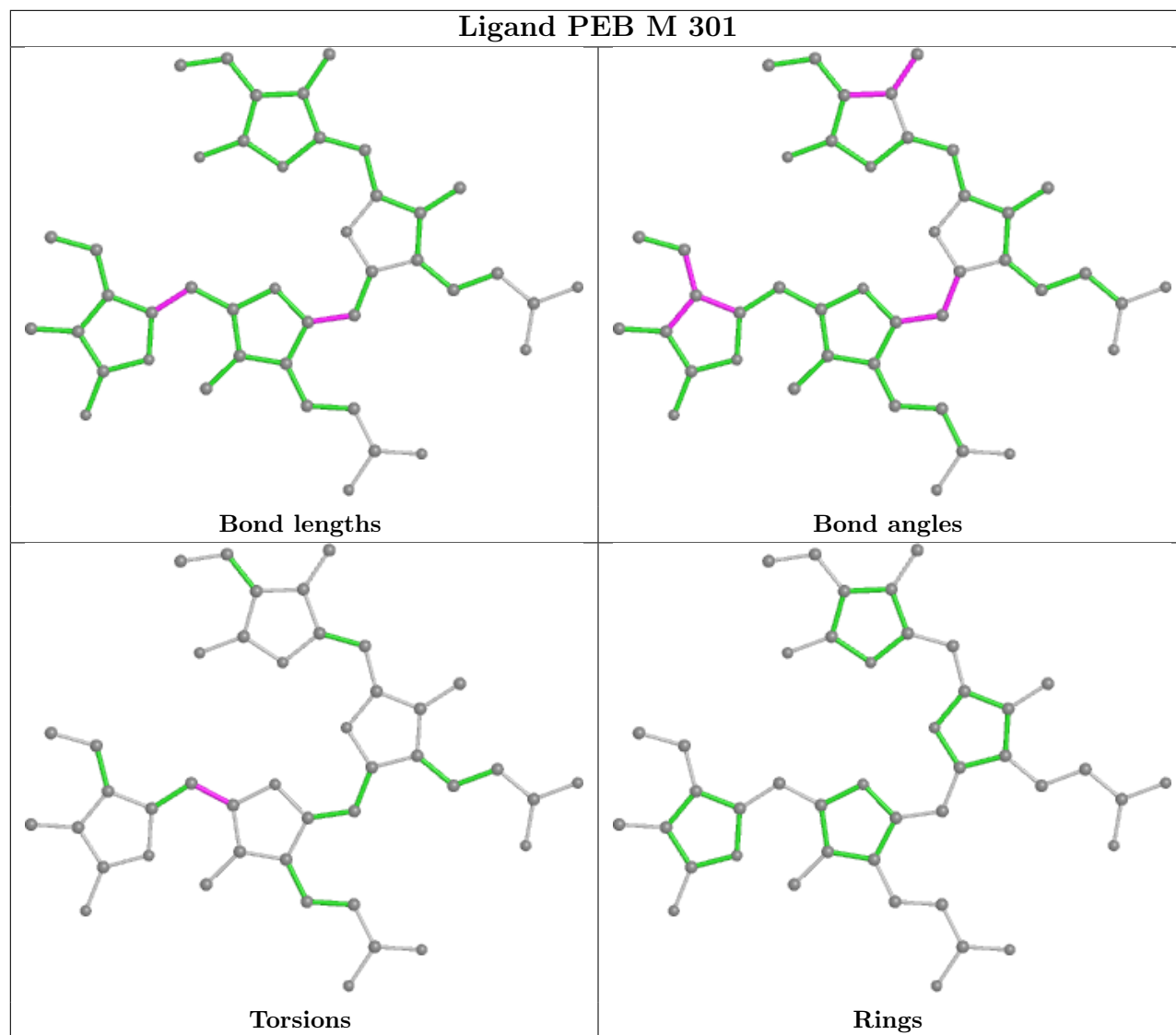
Bond angles



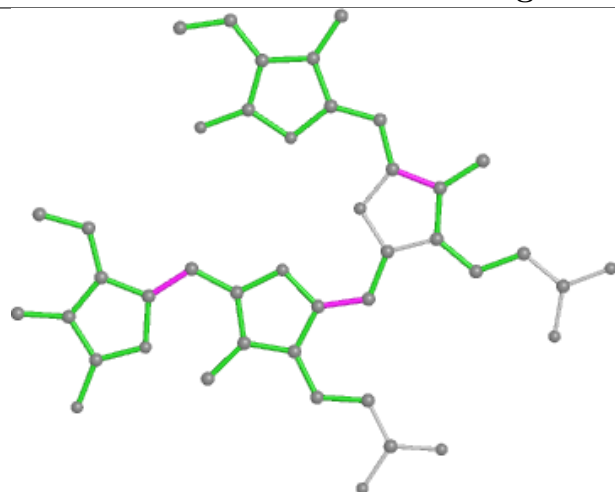
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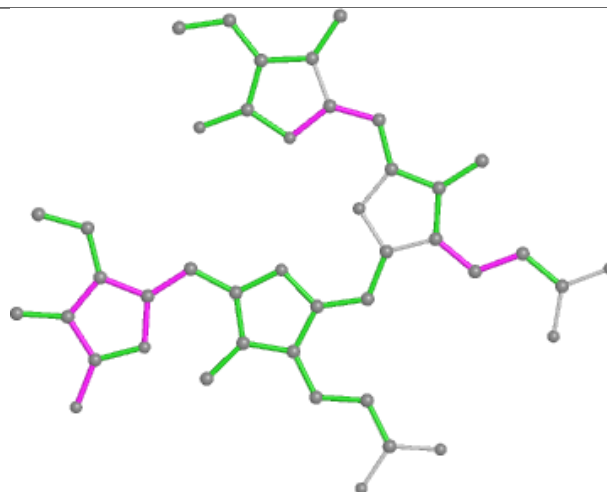
Rings



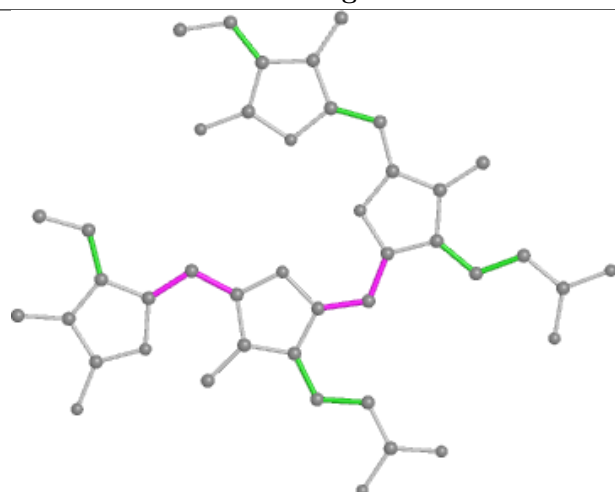
Ligand PEB R 303



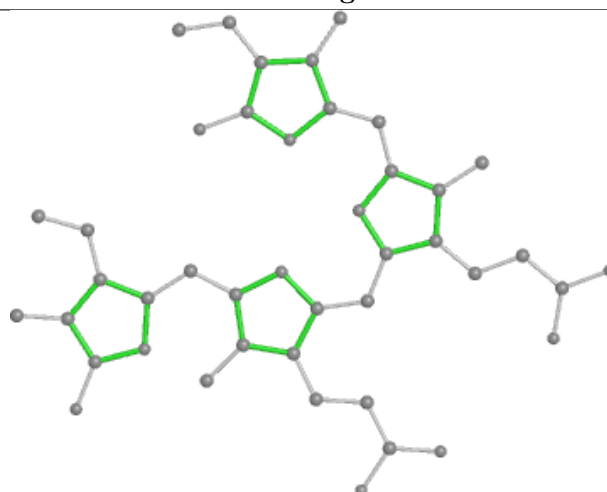
Bond lengths



Bond angles

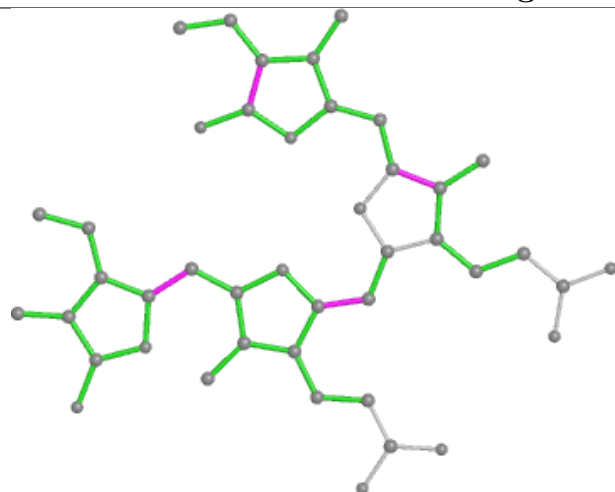


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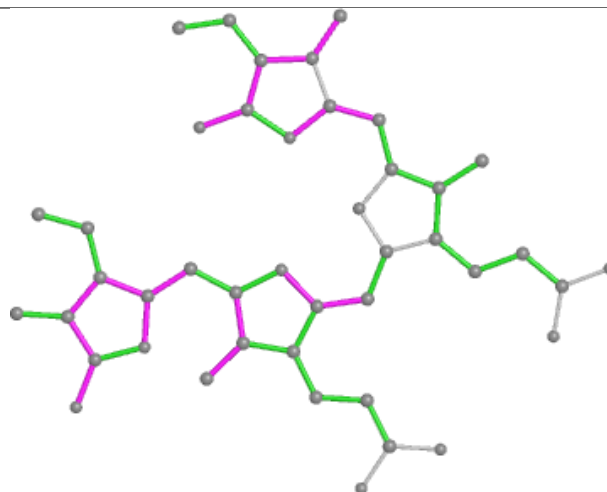


Rings

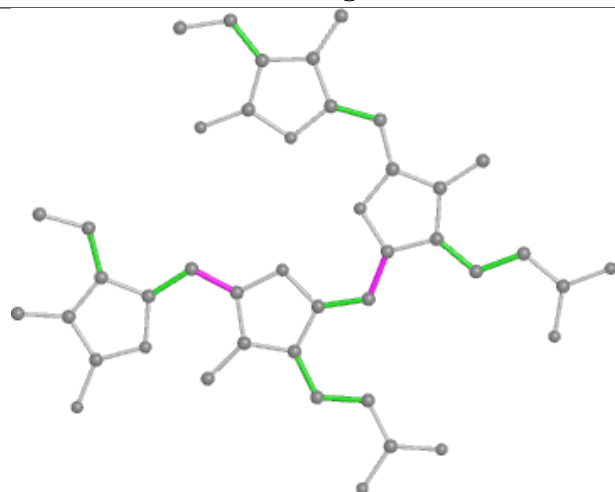
Ligand PEB P 303



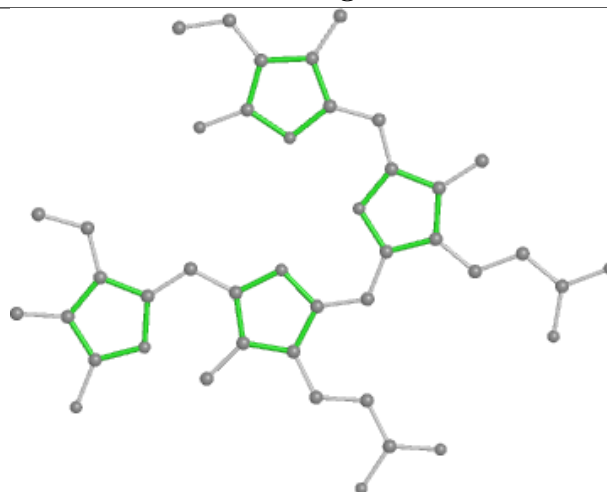
Bond lengths



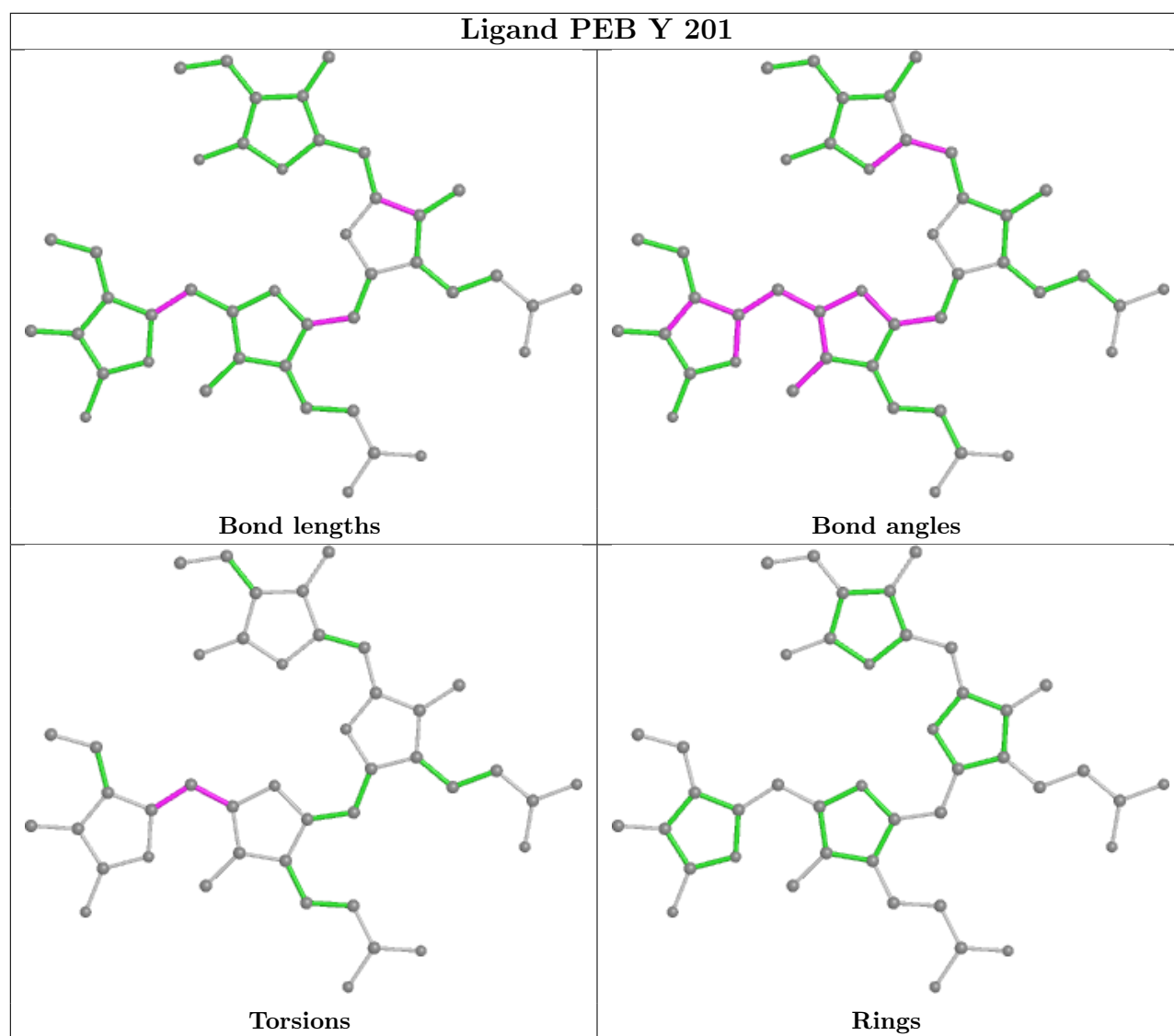
Bond angles

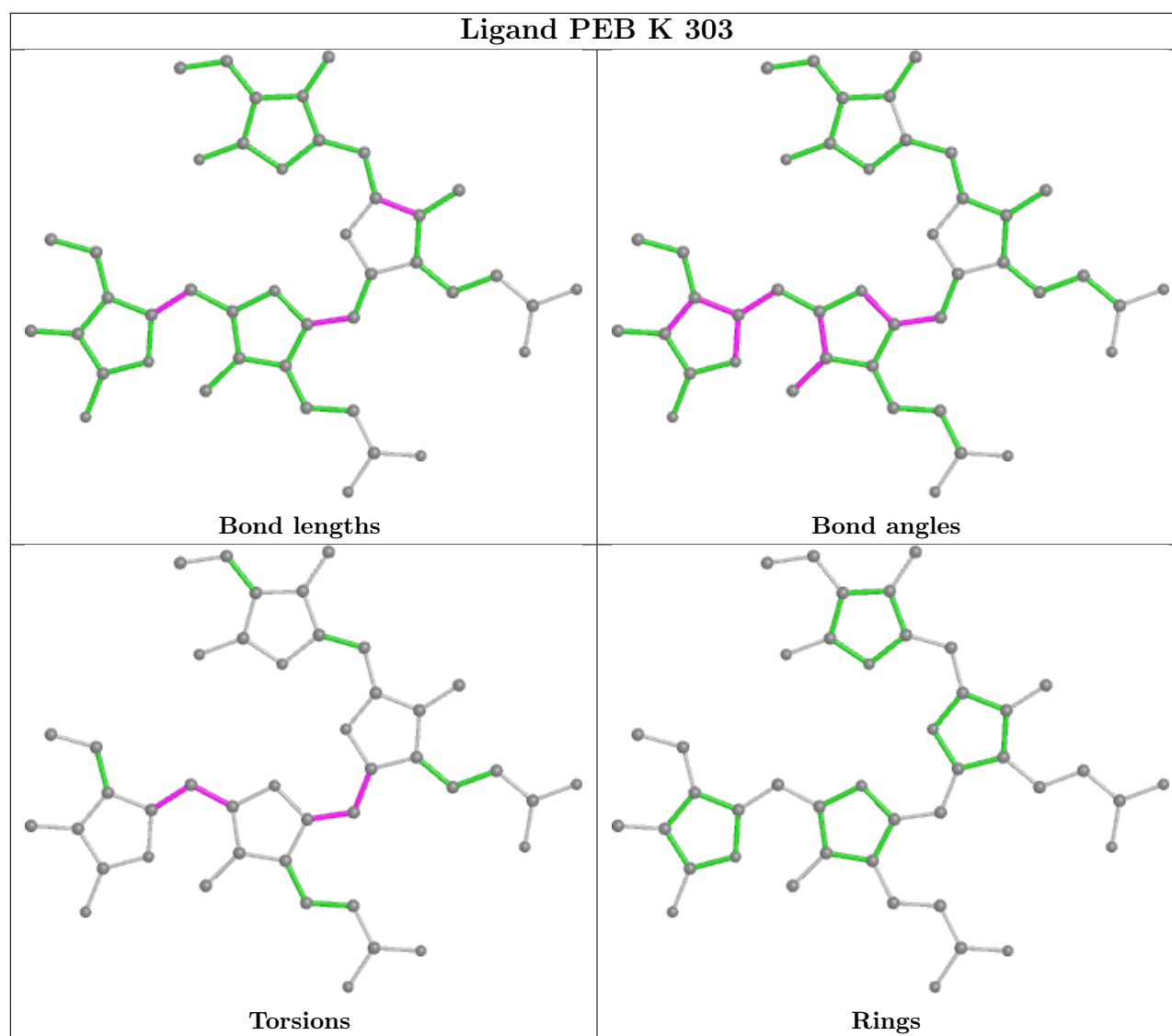


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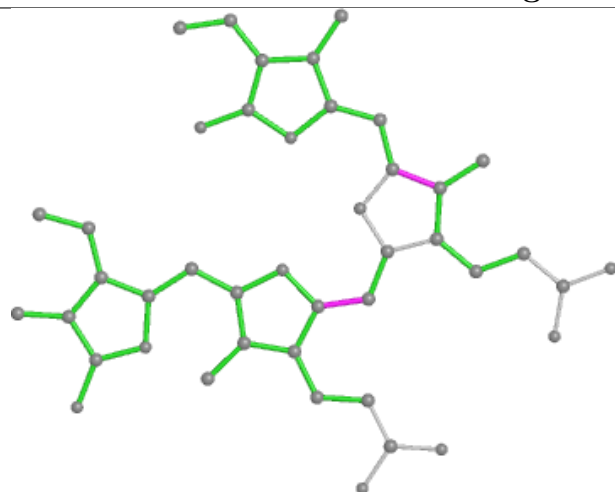


Rings

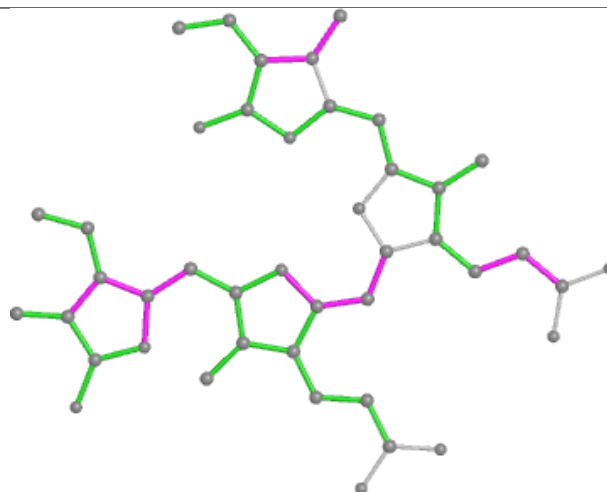




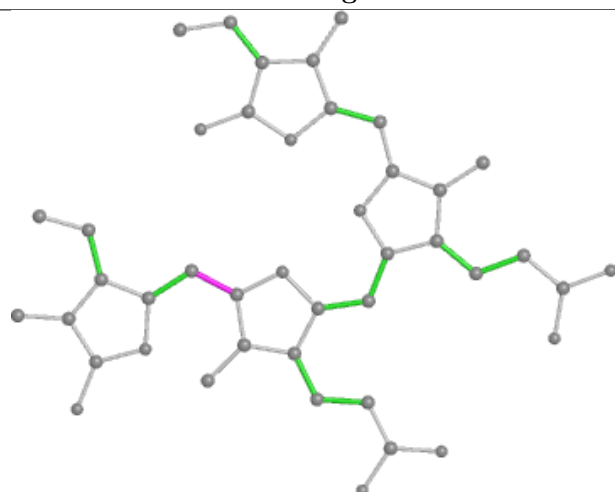
Ligand PEB I 302



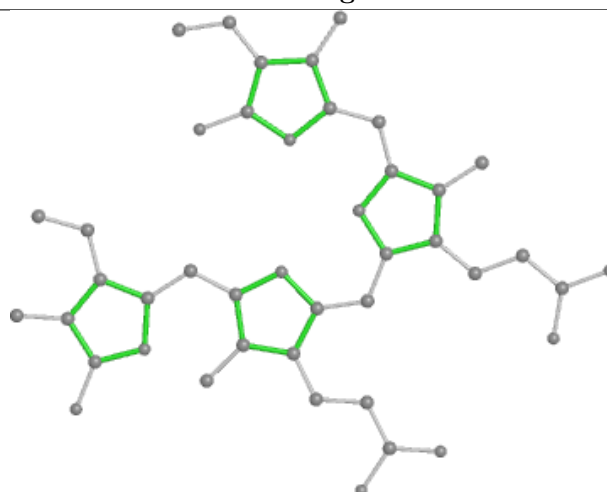
Bond lengths



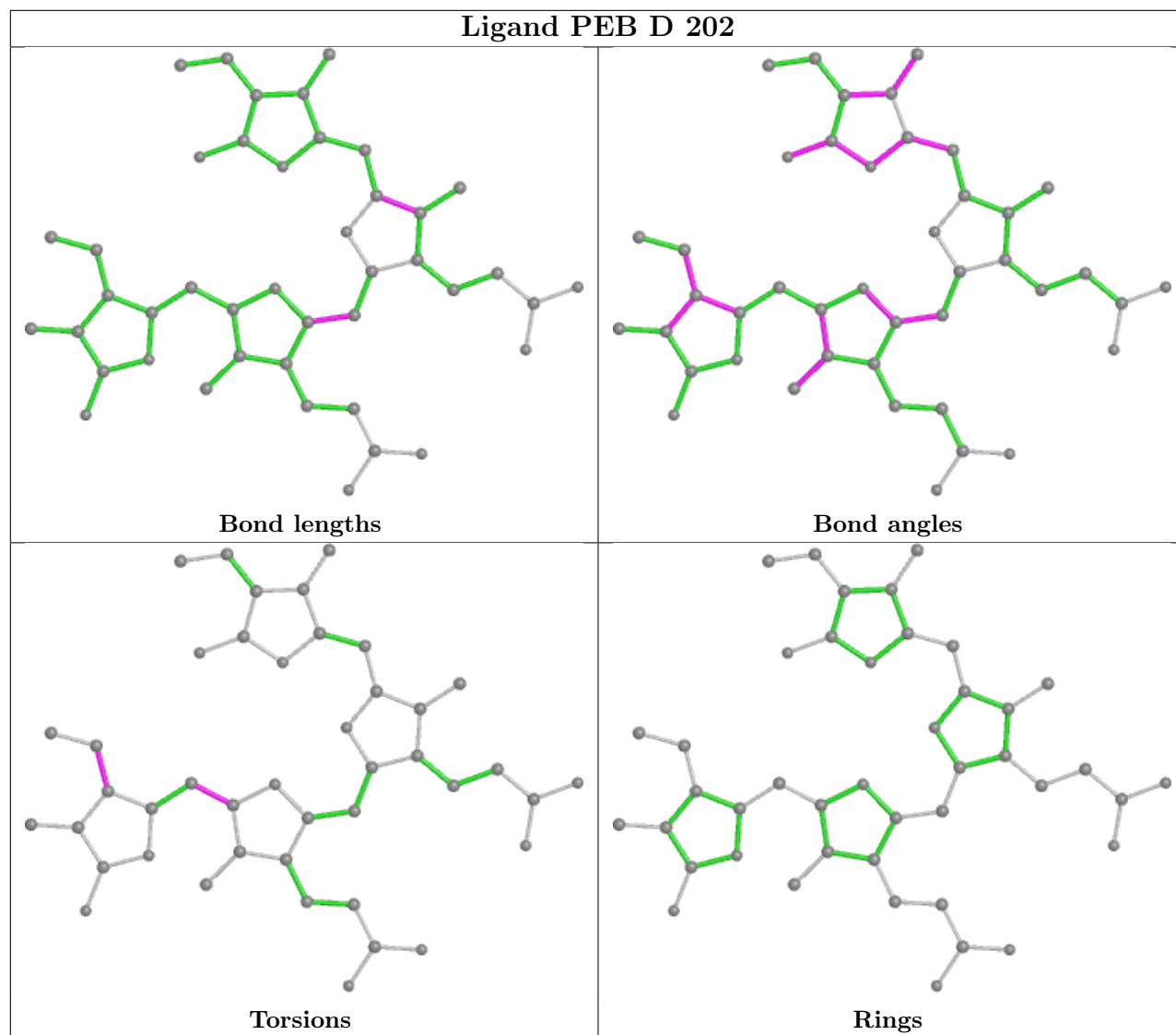
Bond angles

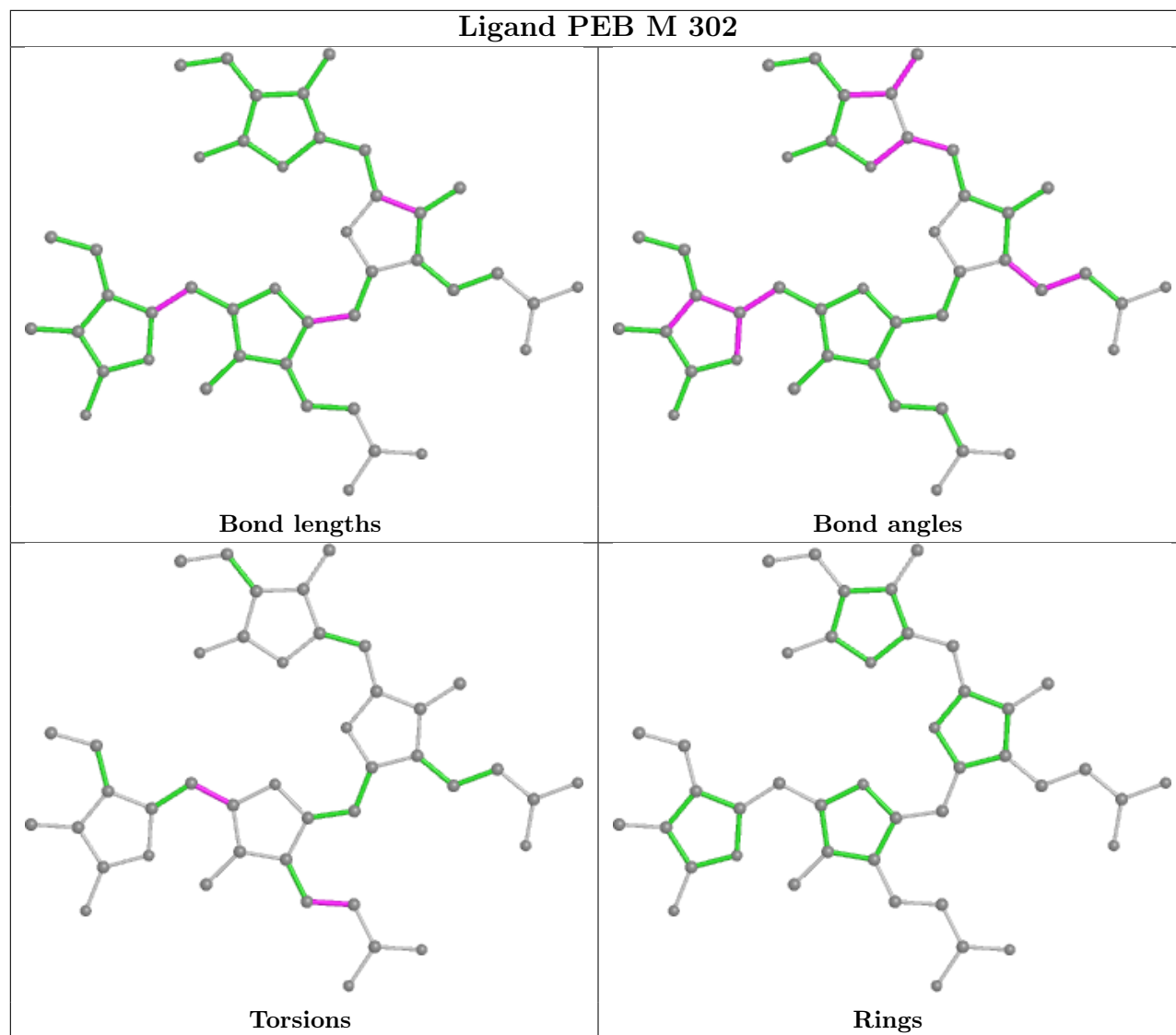


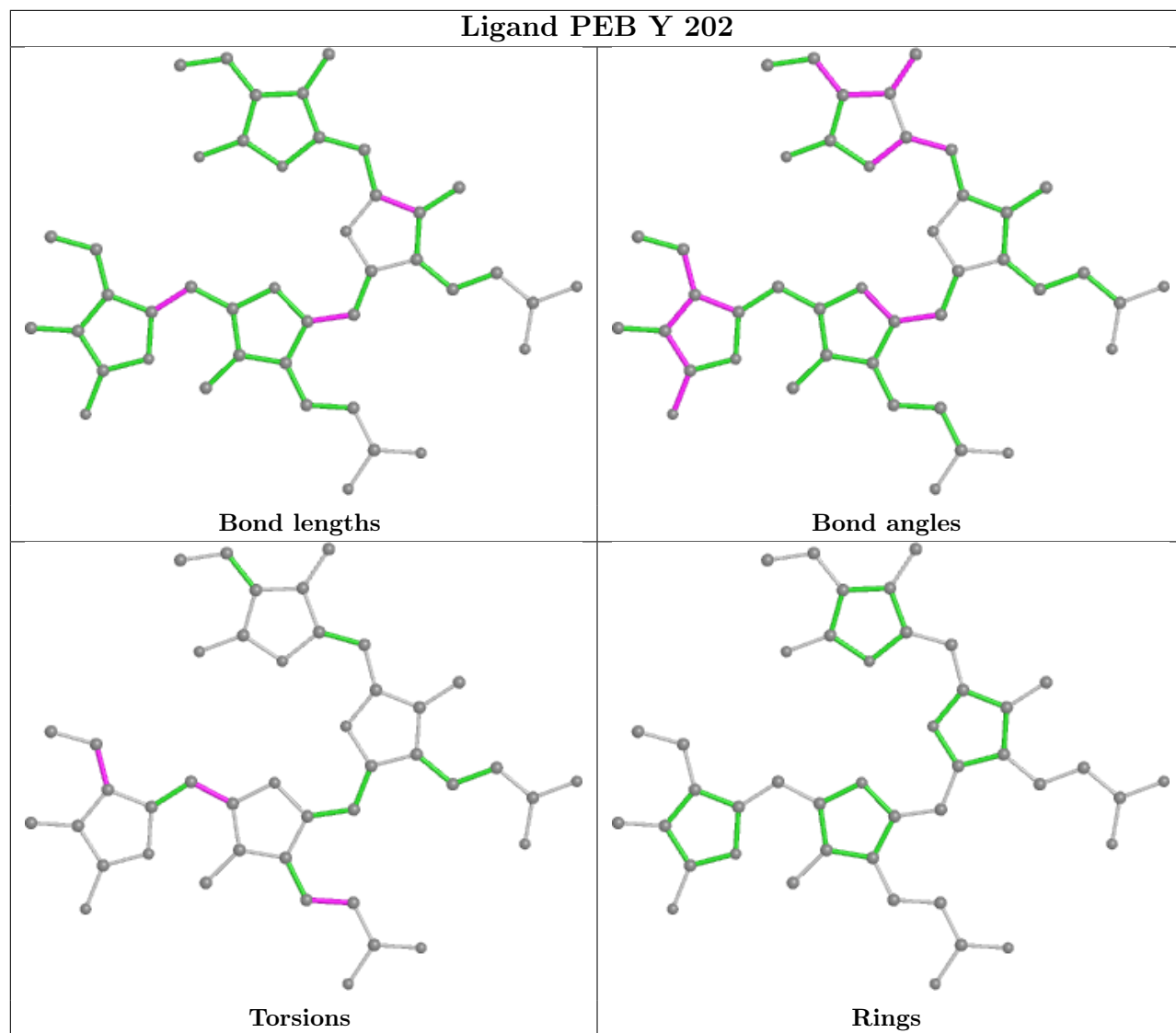
Torsions



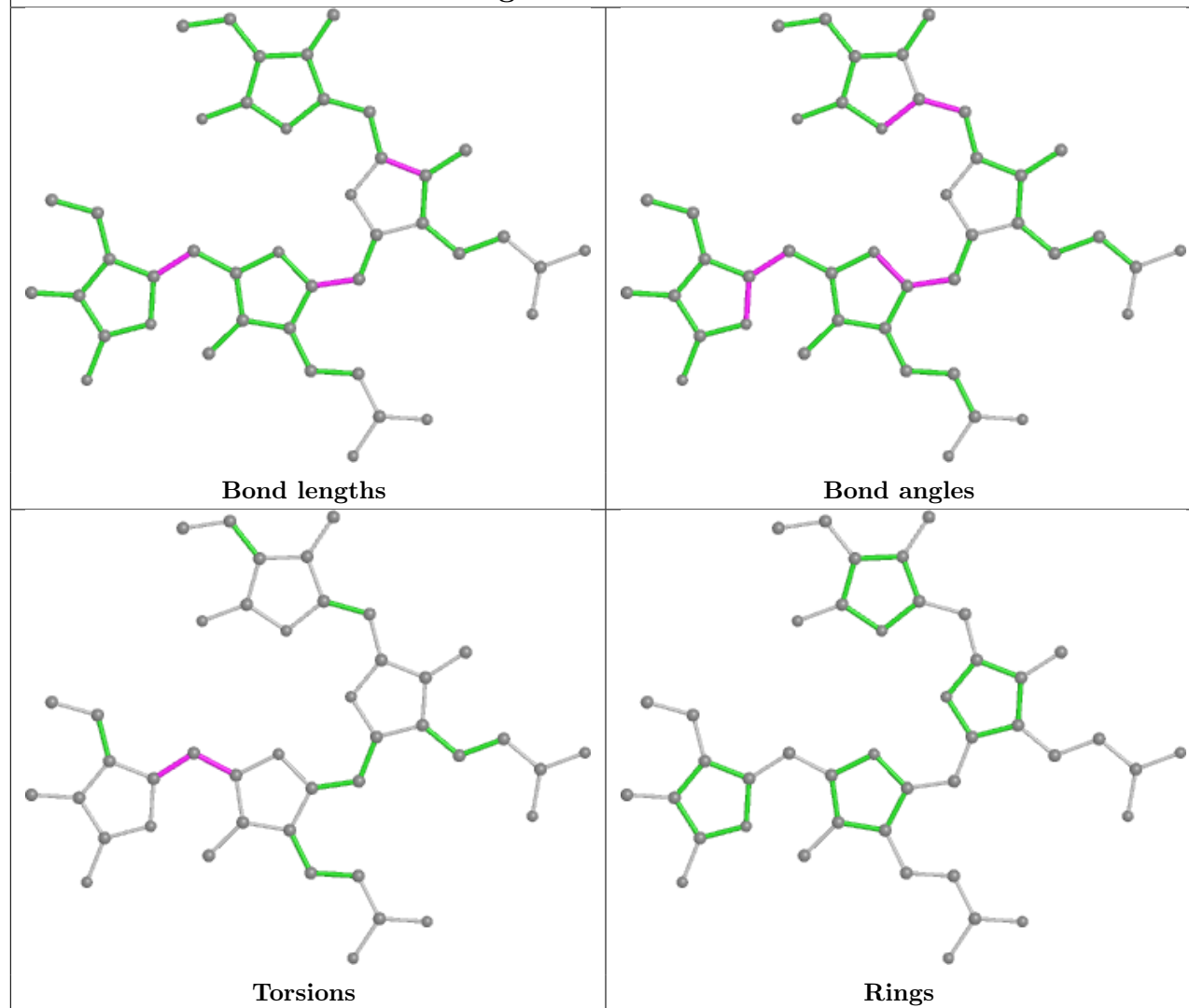
Rings

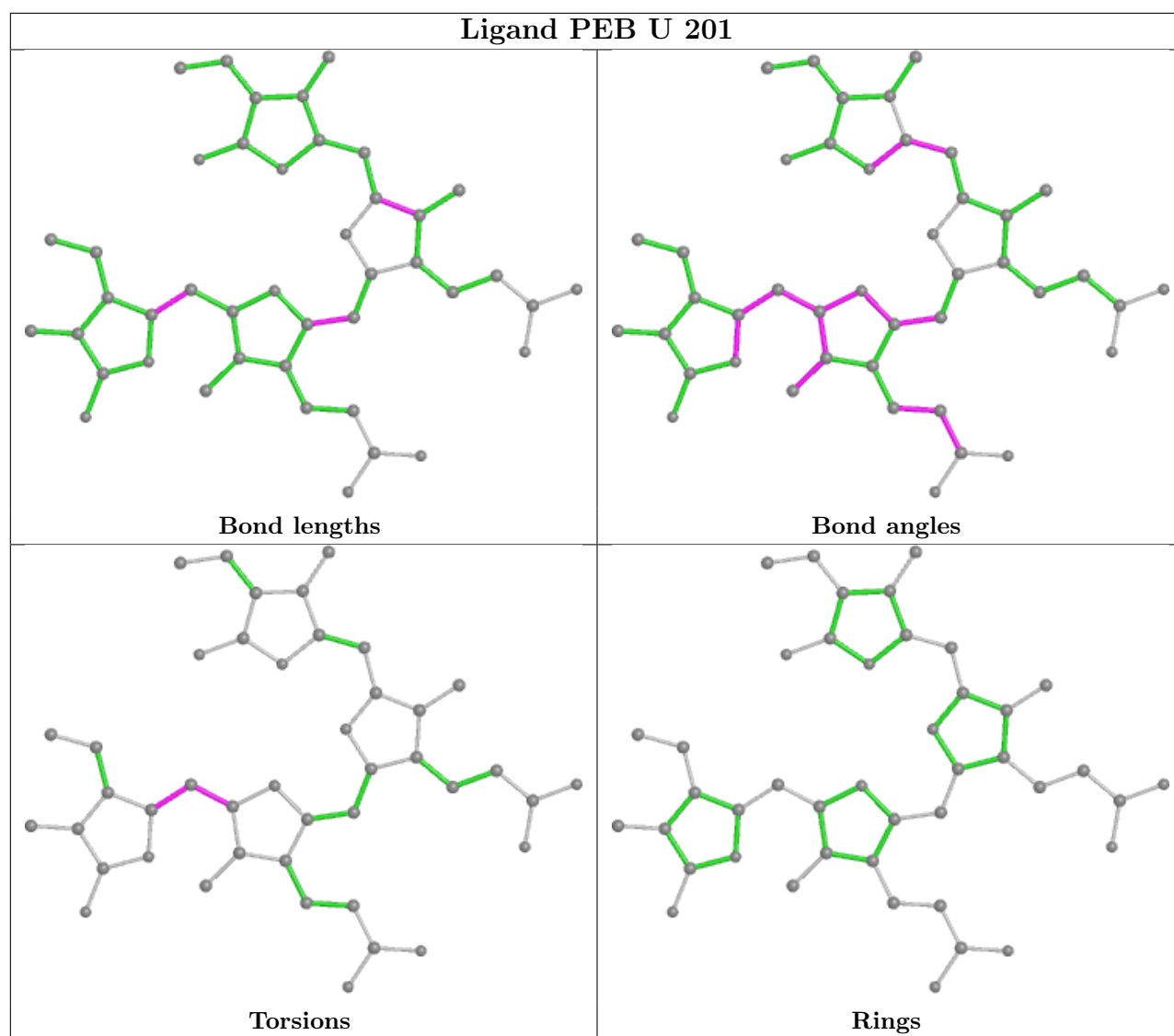


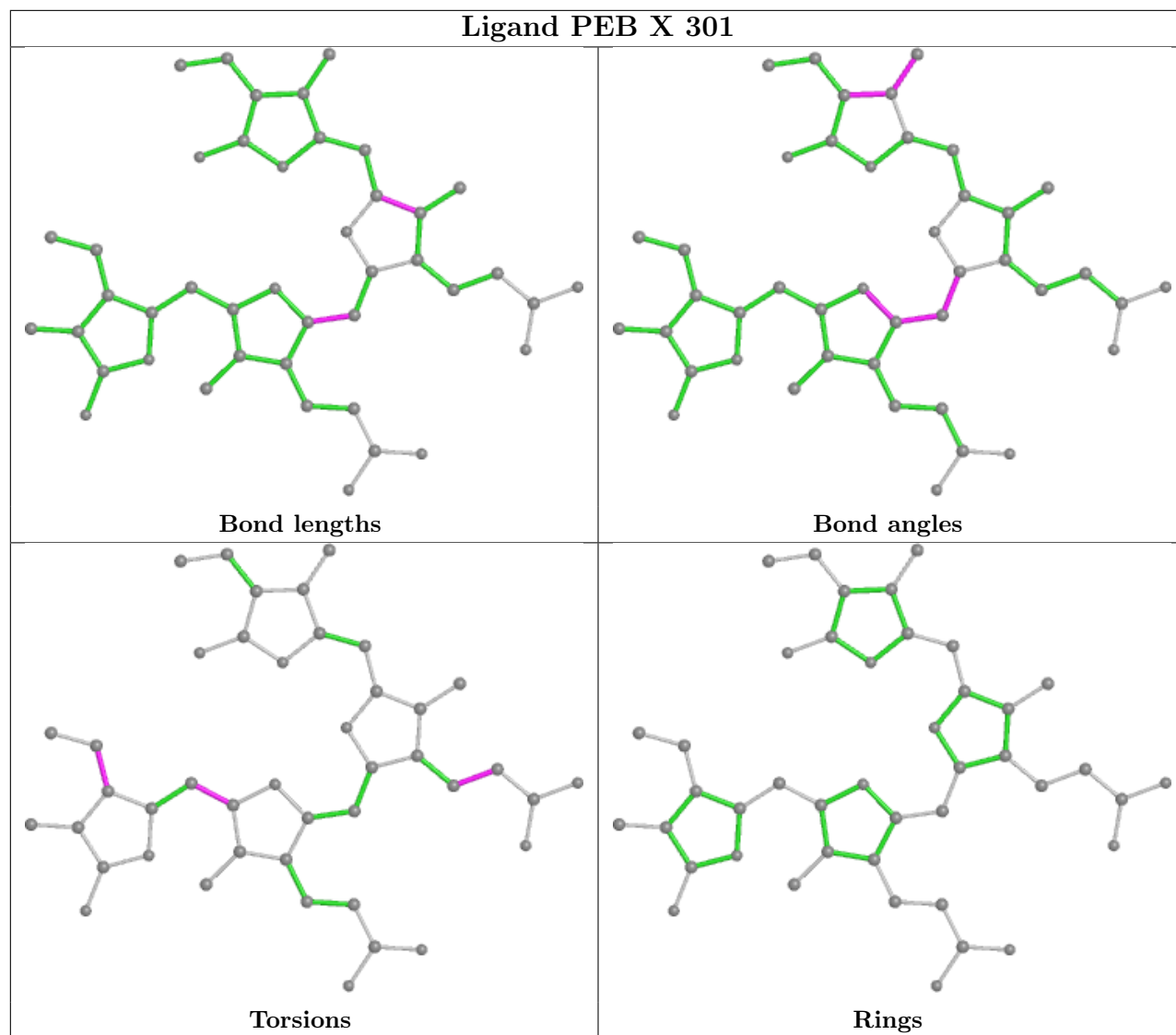




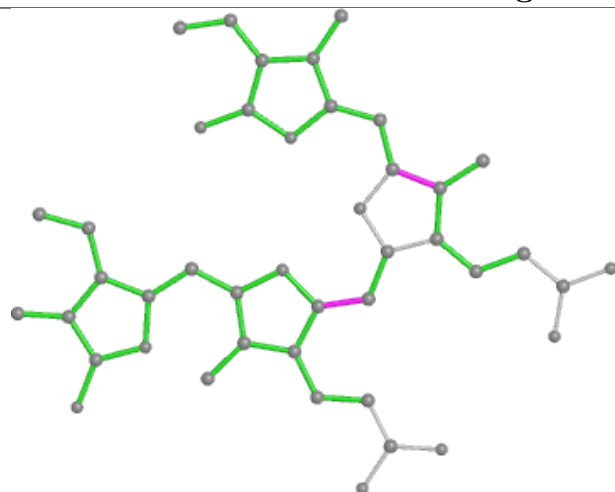
Ligand PEB F 201



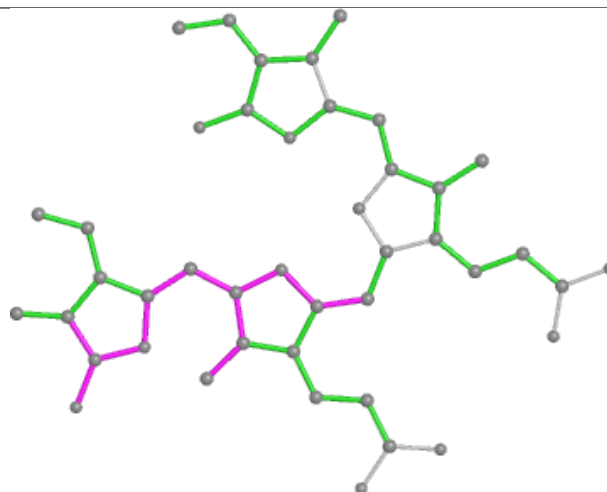




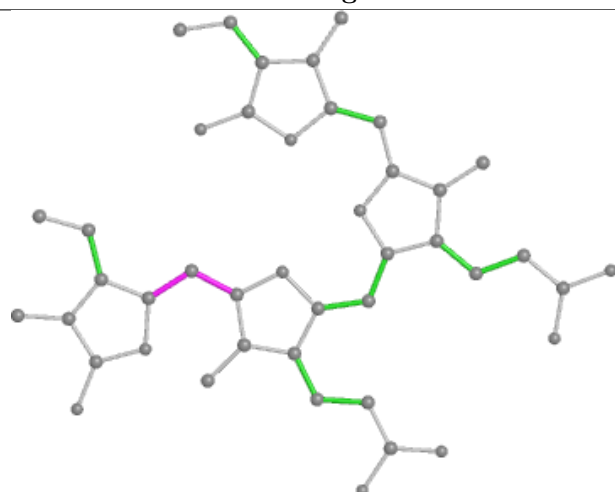
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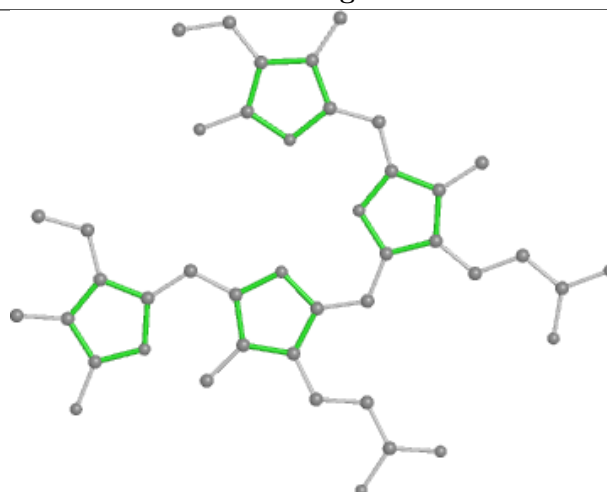
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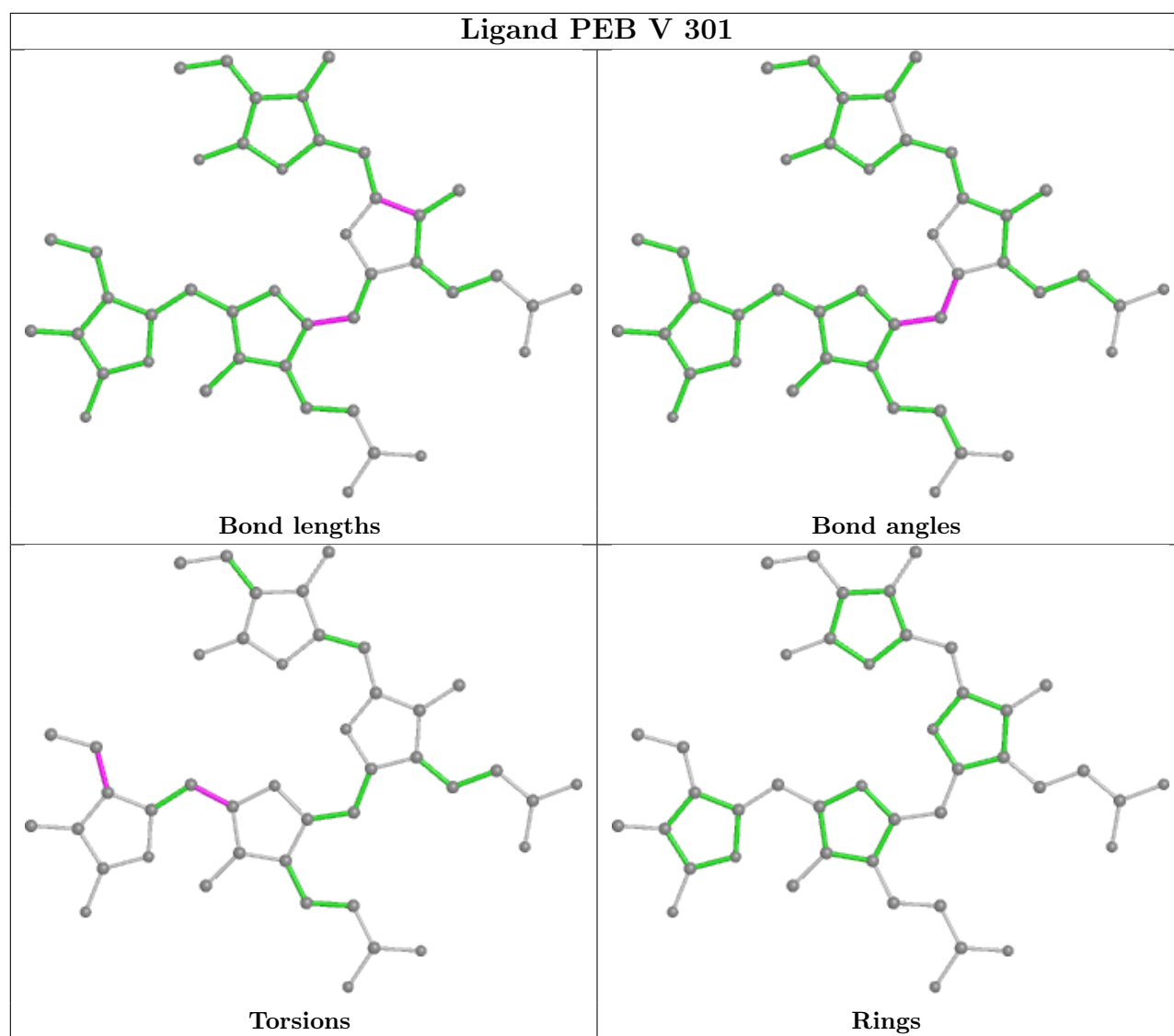
Bond angles



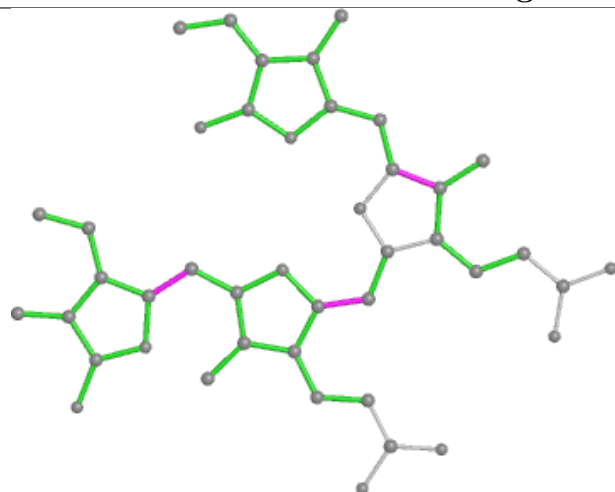
Torsions



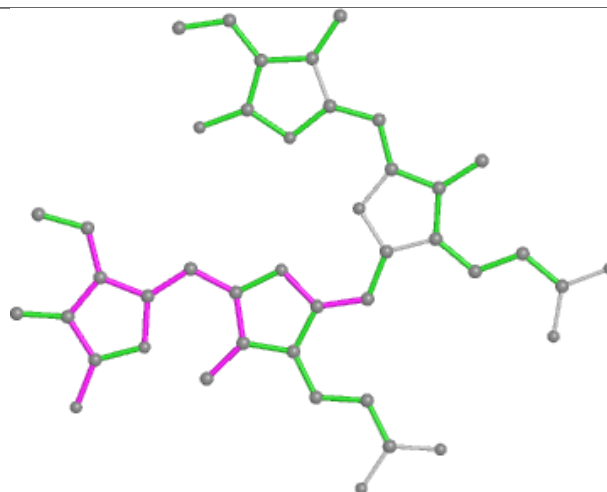
Rings



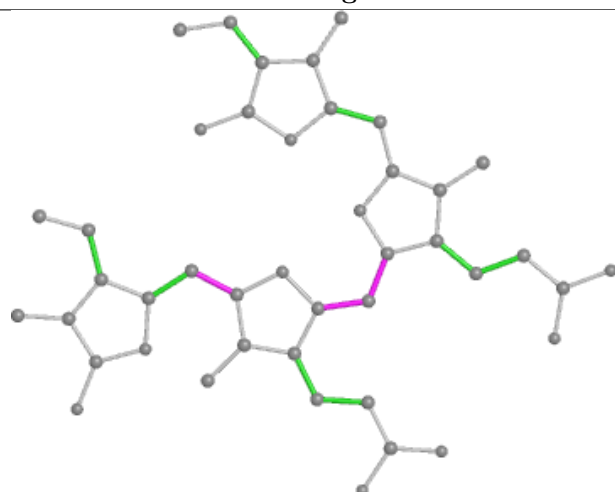
Ligand PEB V 303



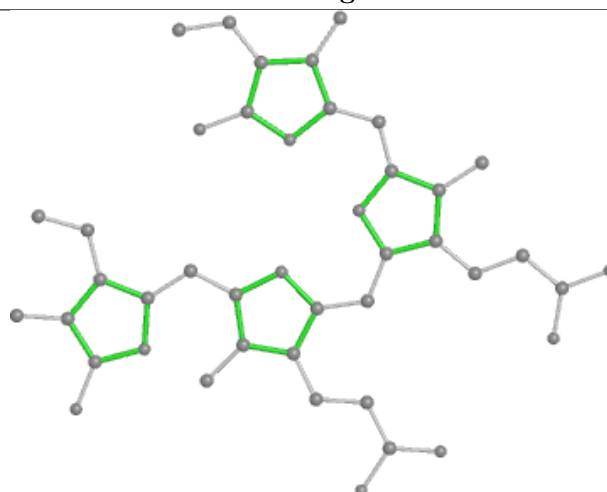
Bond lengths



Bond angles

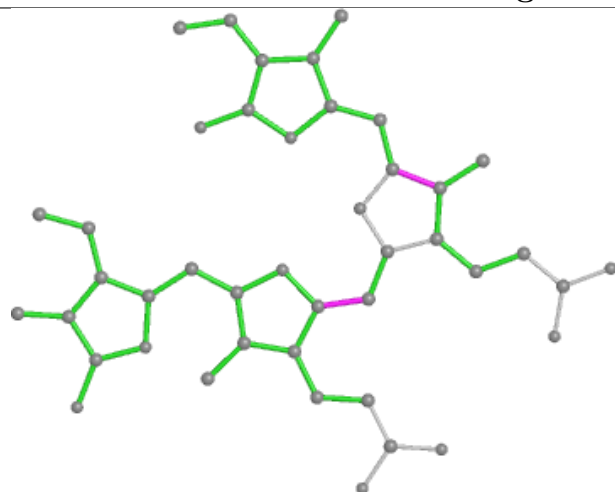


Torsions

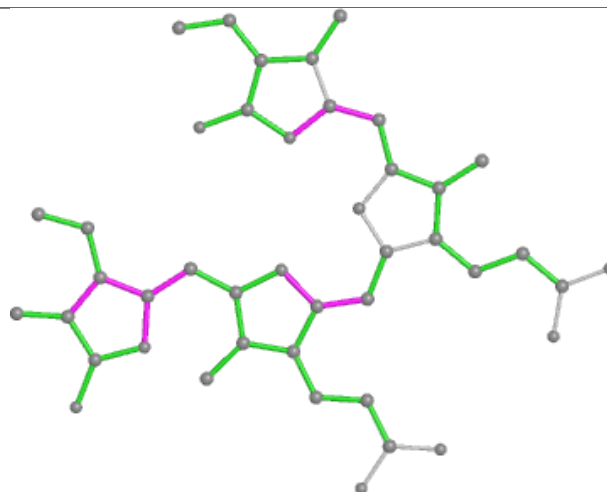


Rings

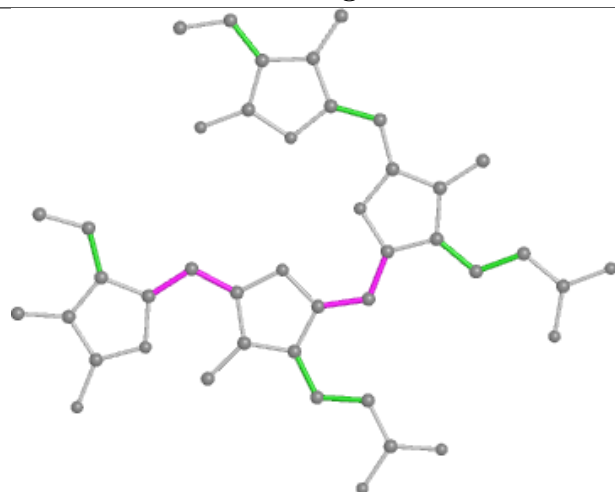
Ligand PEB C 303



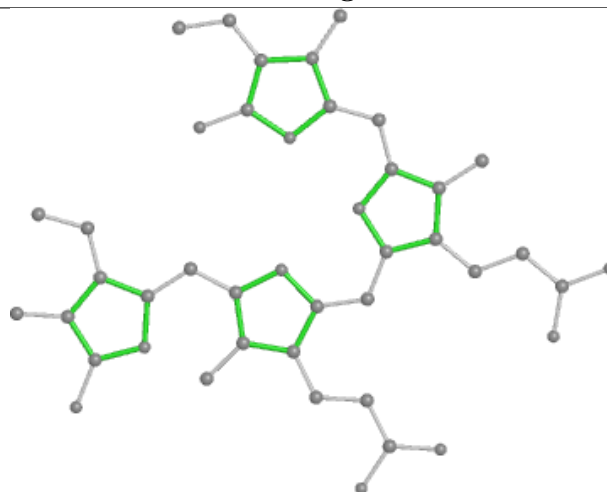
Bond lengths



Bond angles

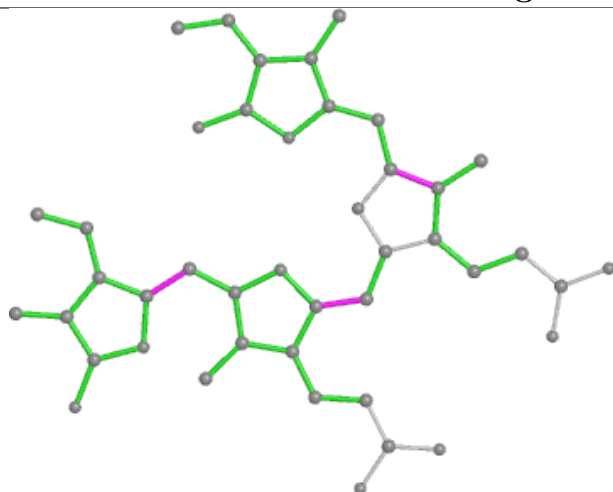


Torsions

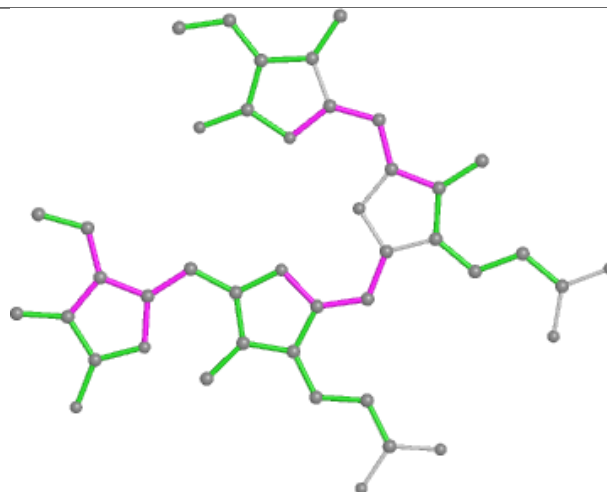


Rings

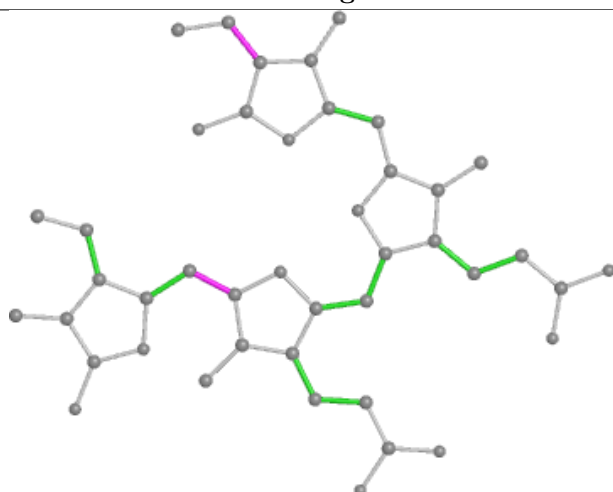
Ligand PEB P 302



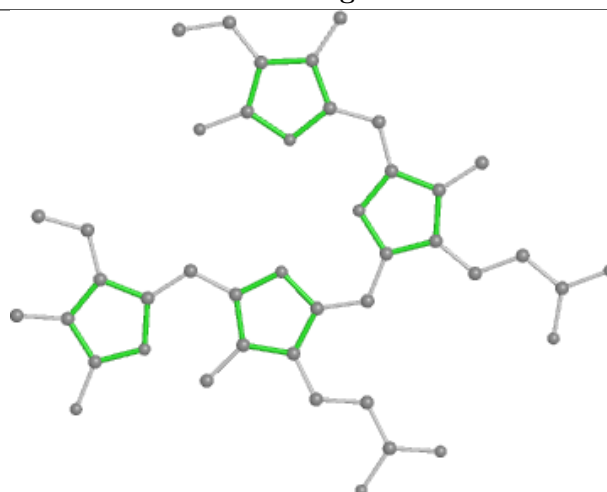
Bond lengths



Bond angles

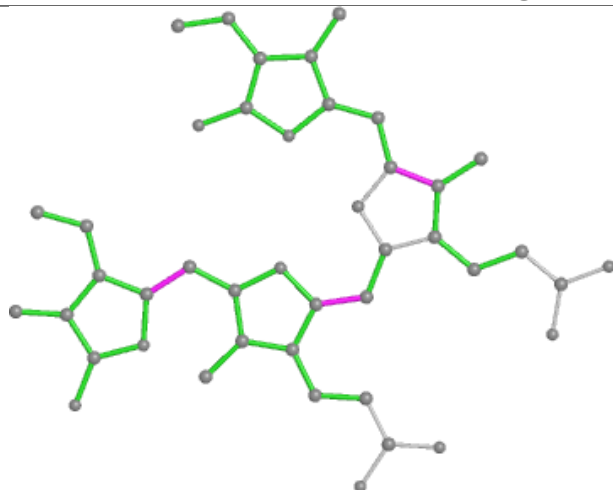


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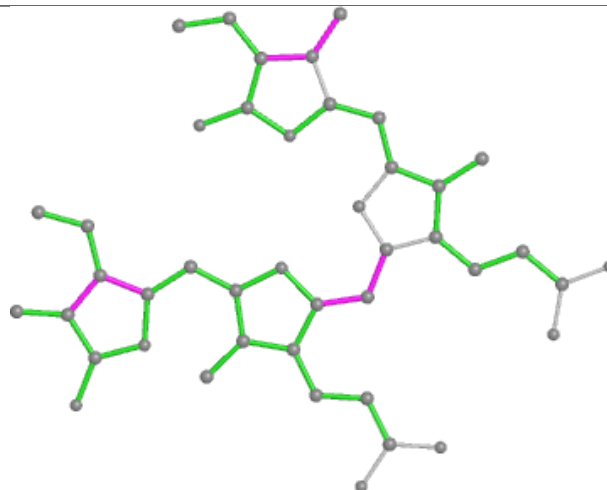


Rings

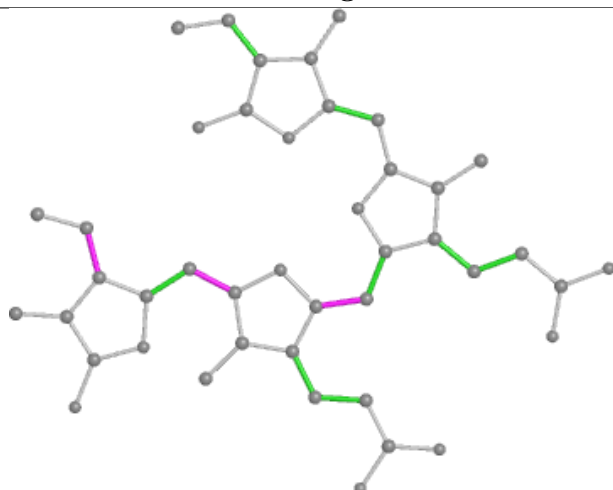
Ligand PEB T 301



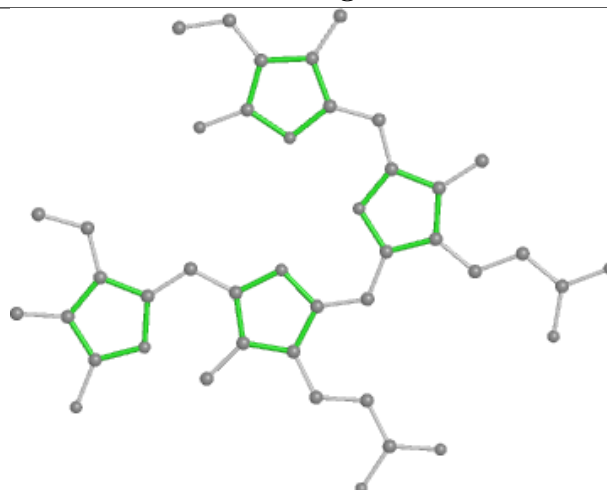
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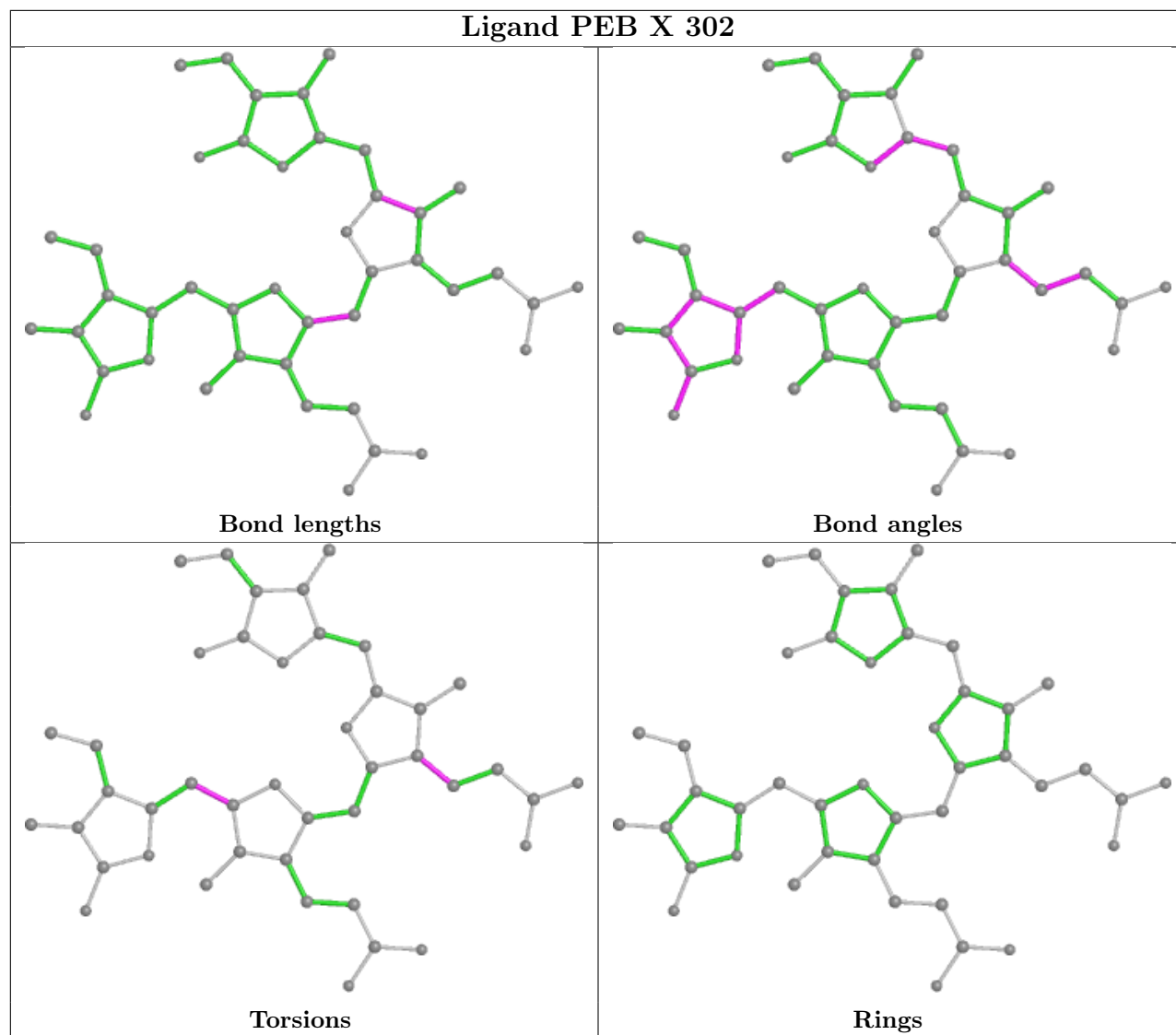
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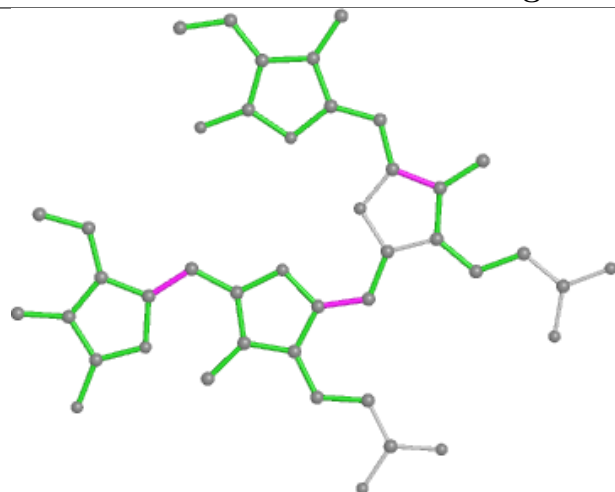
Torsions



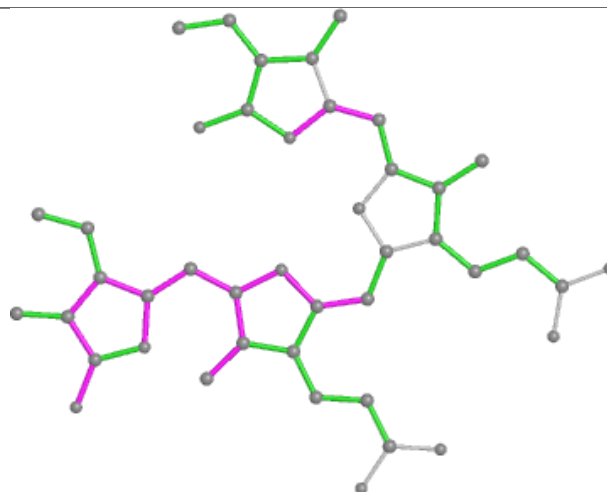
Rings



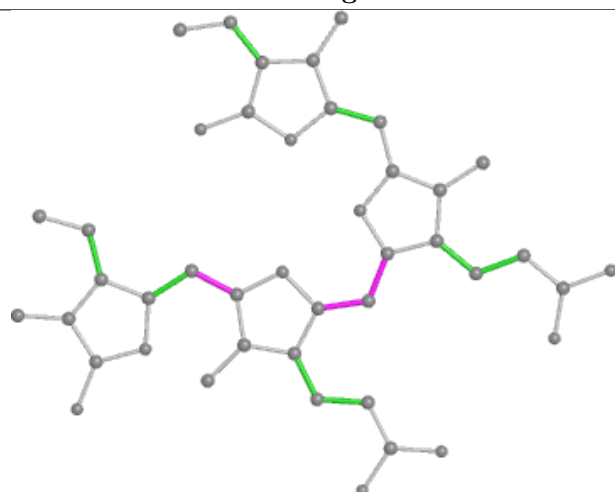
Ligand PEB I 303



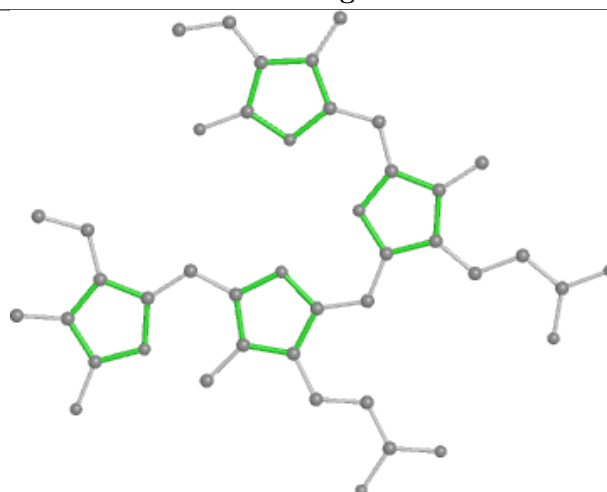
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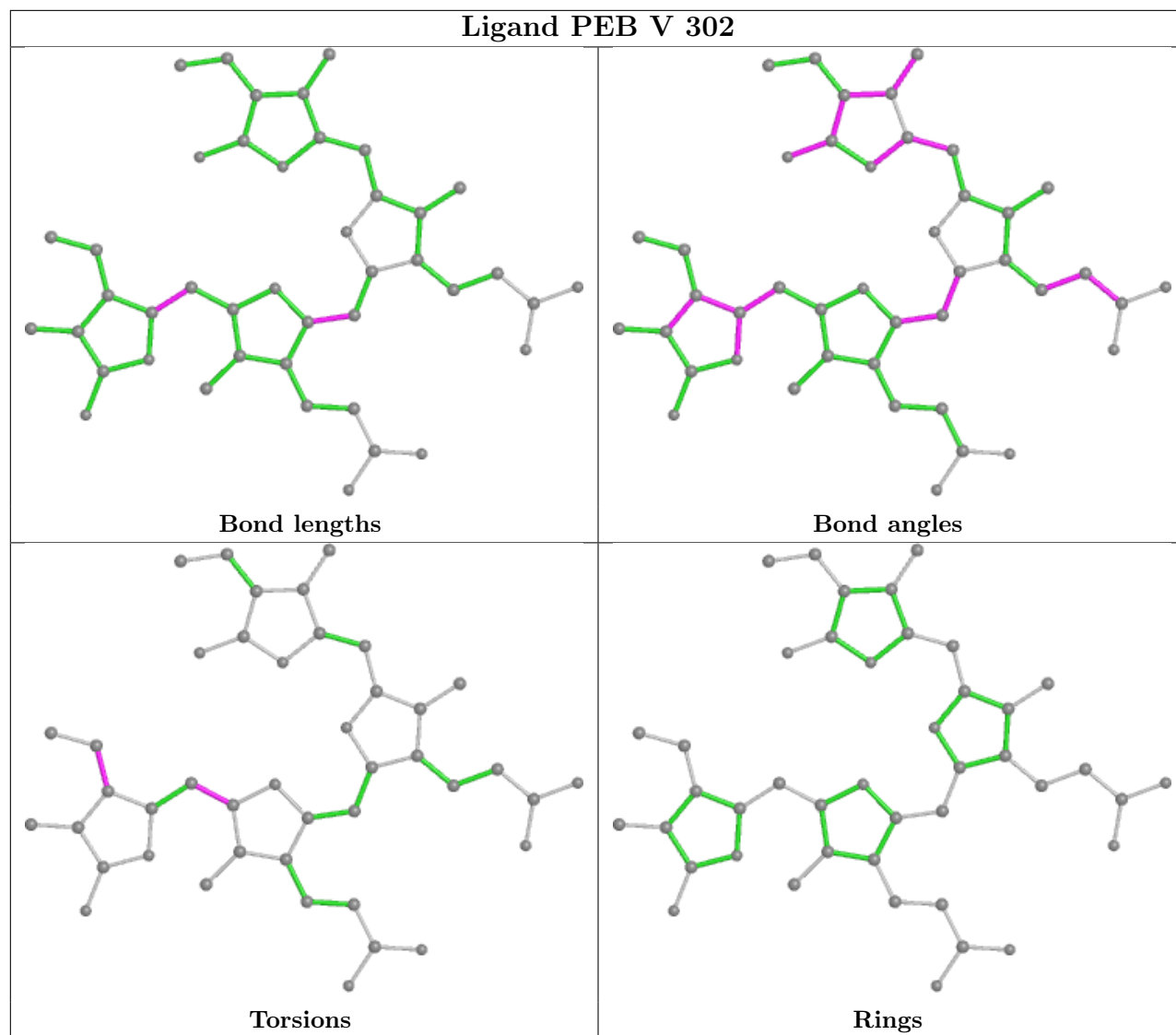
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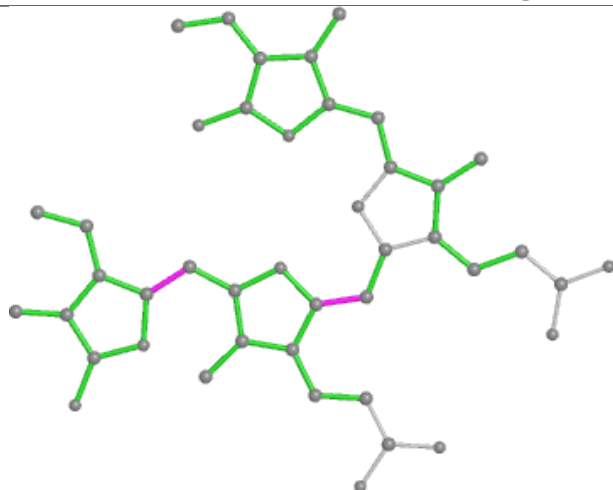
Torsions



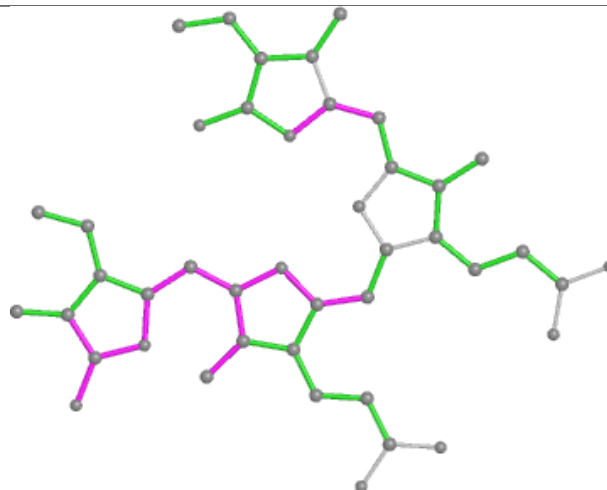
Rings



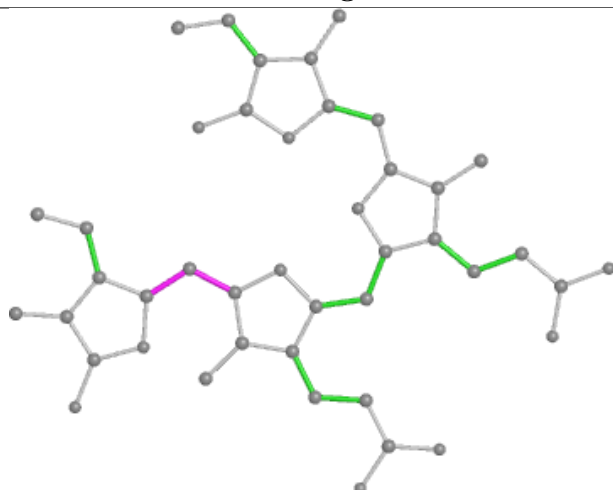
Ligand PEB L 201



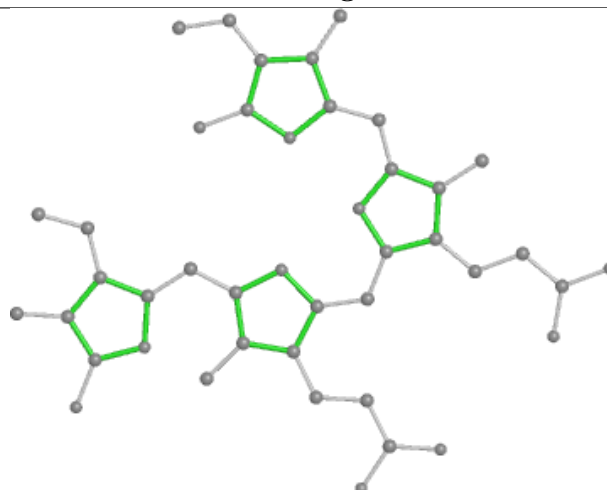
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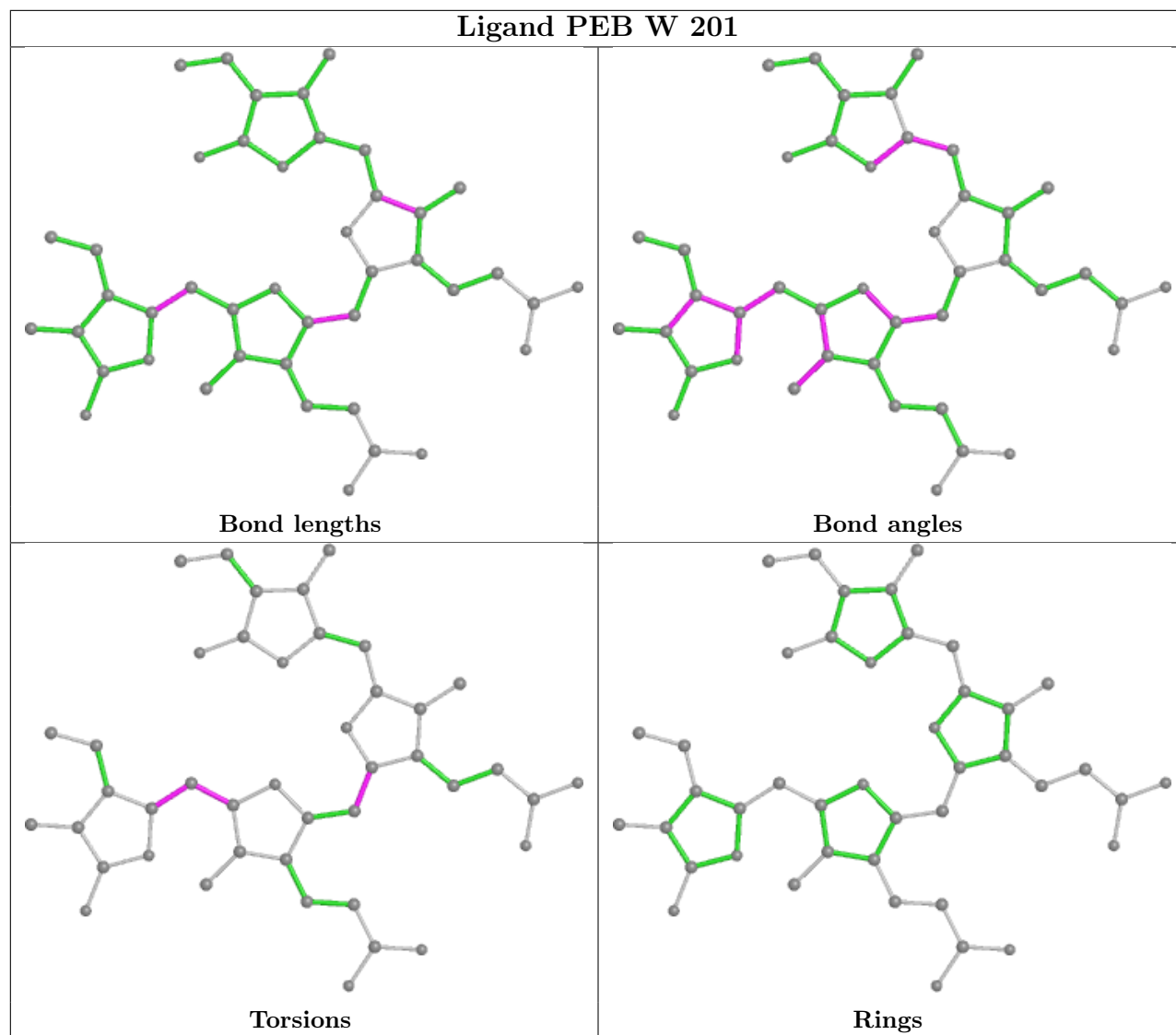
Bond angles



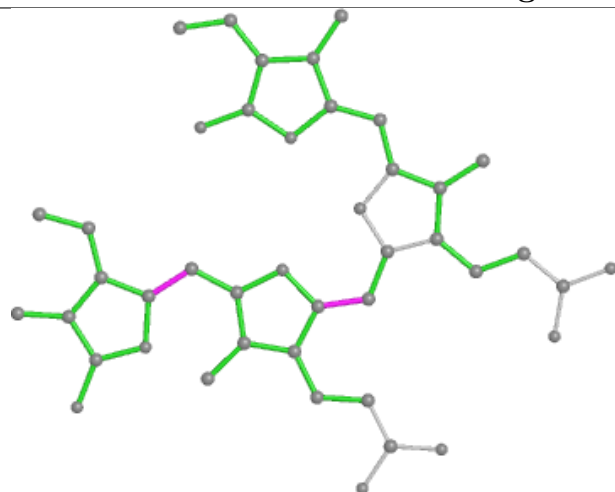
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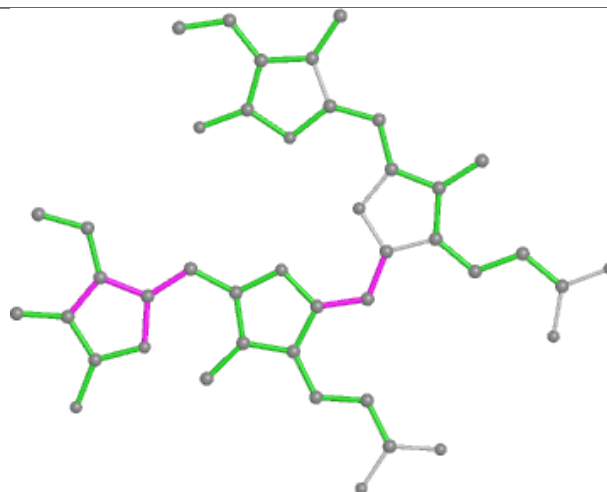
Rings



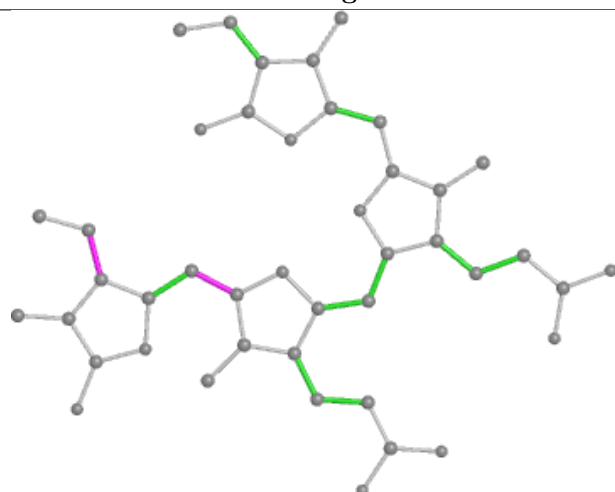
Ligand PEB E 301



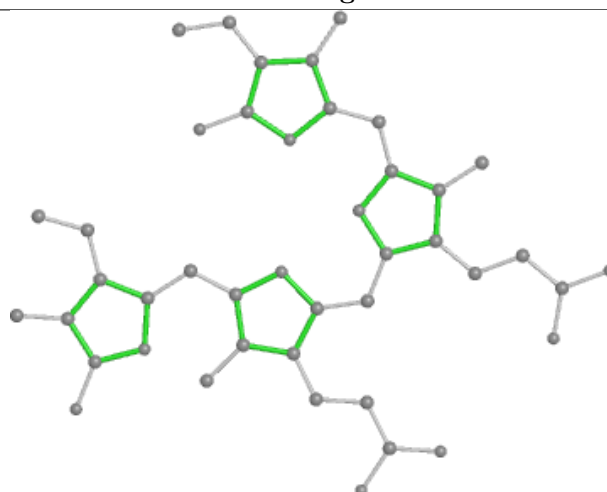
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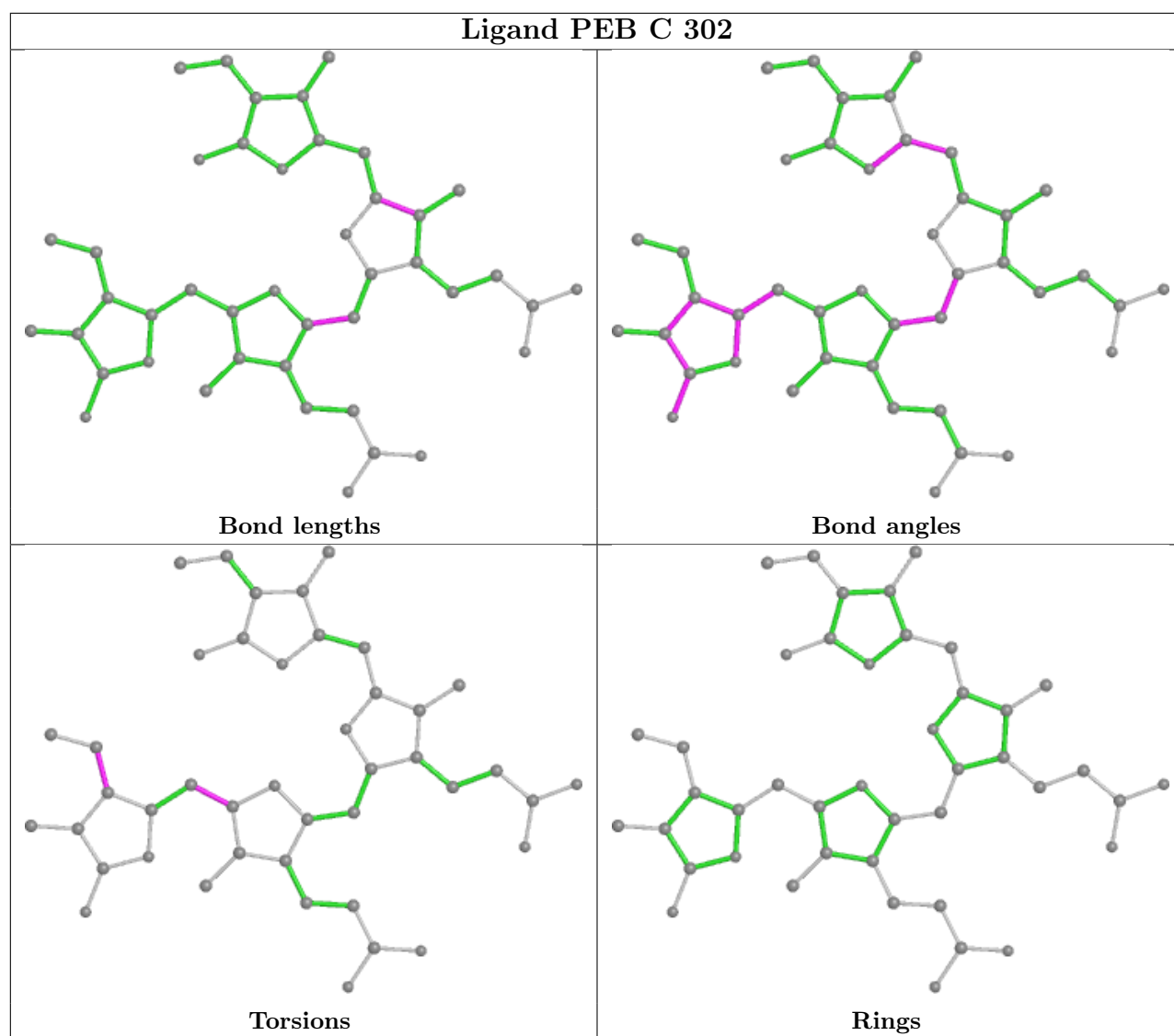
Bond angles

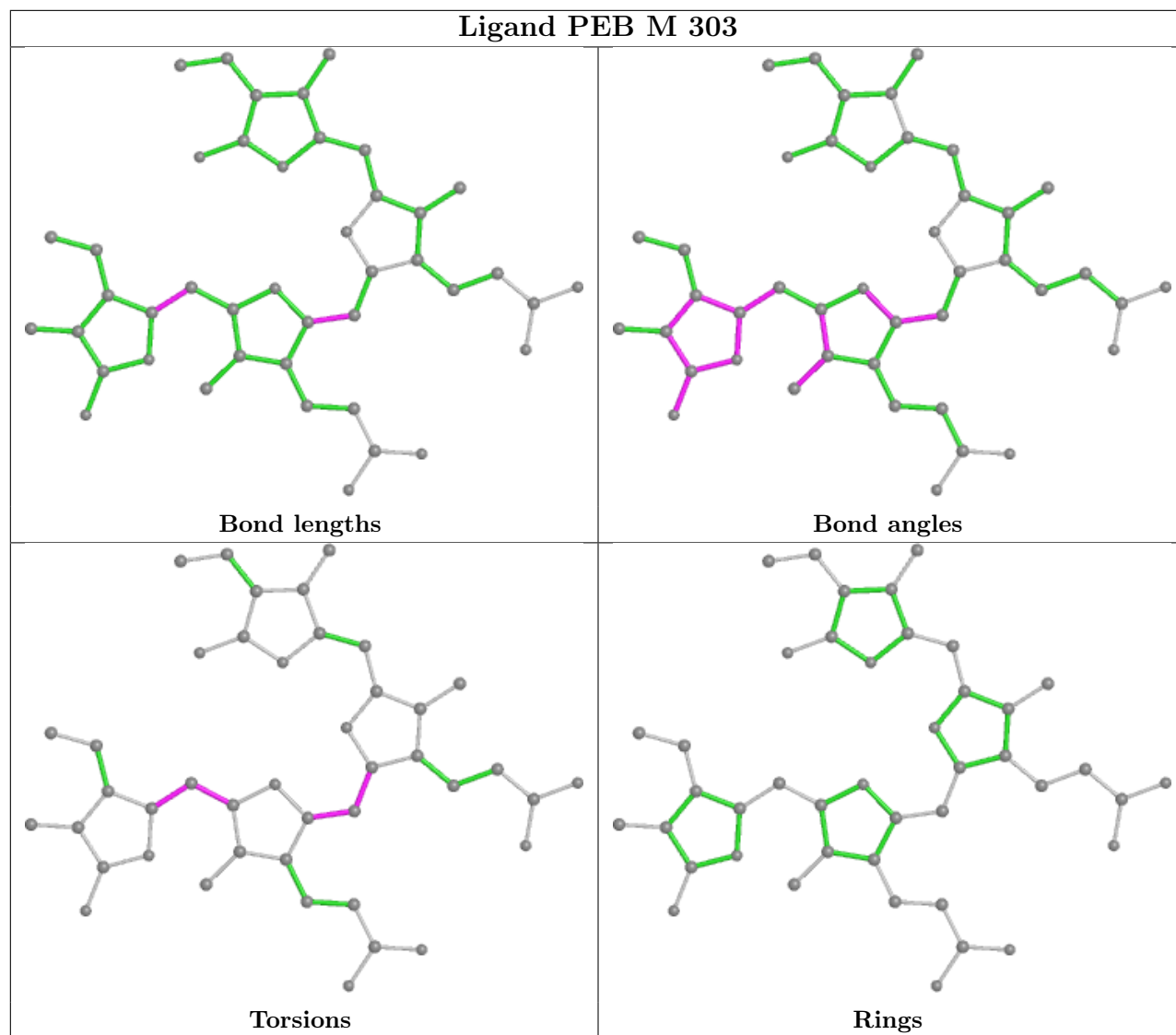


Torsions

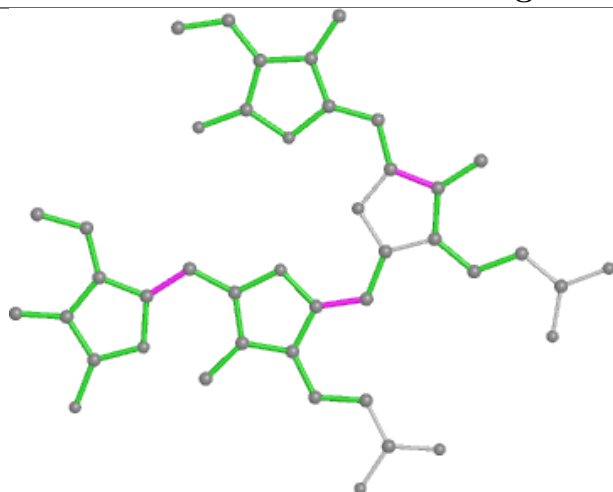


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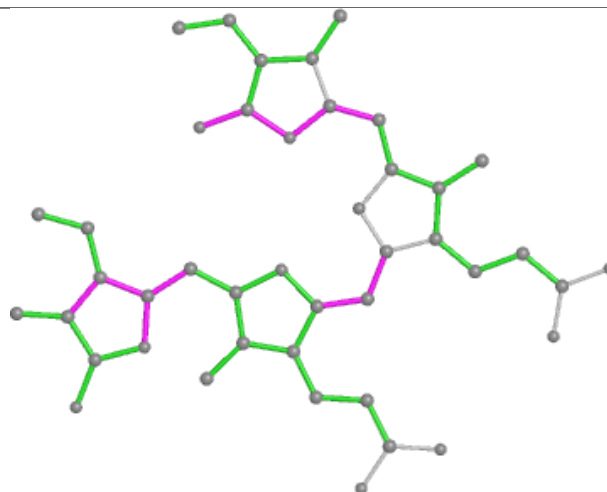




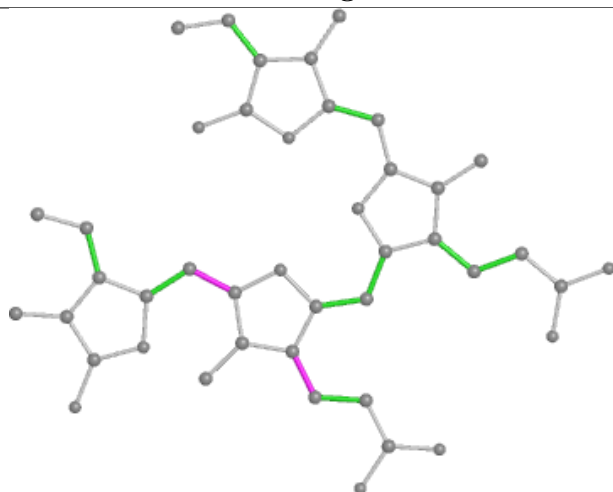
Ligand PEB T 302



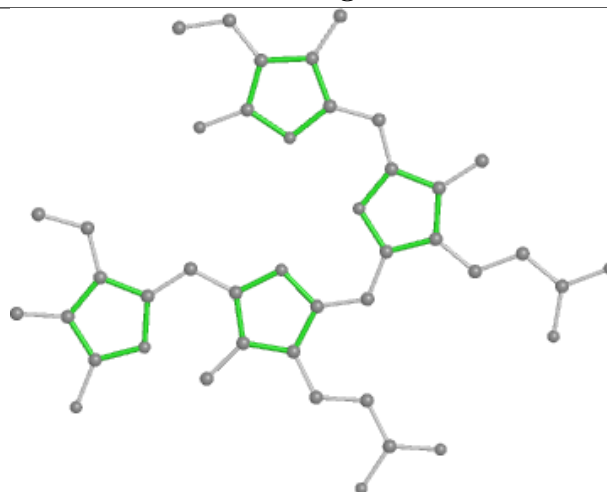
Bond lengths



Bond angles

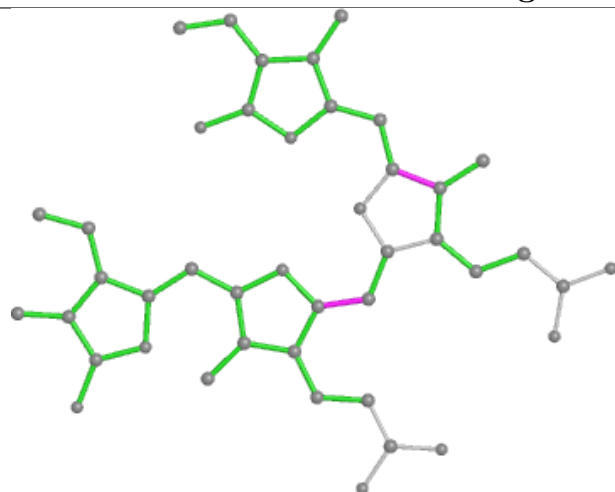


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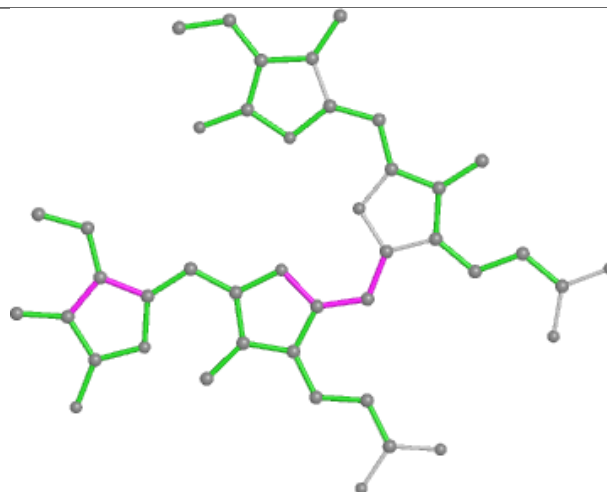


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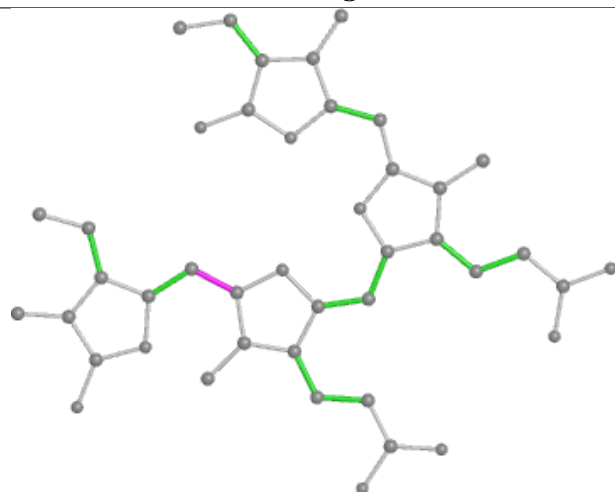
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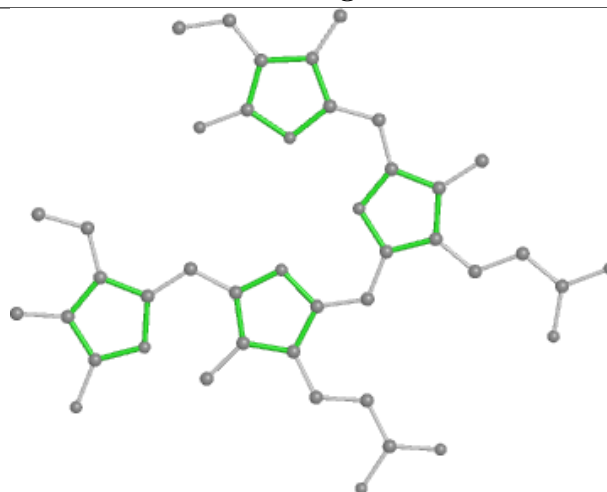
Bond lengths



Bond angles

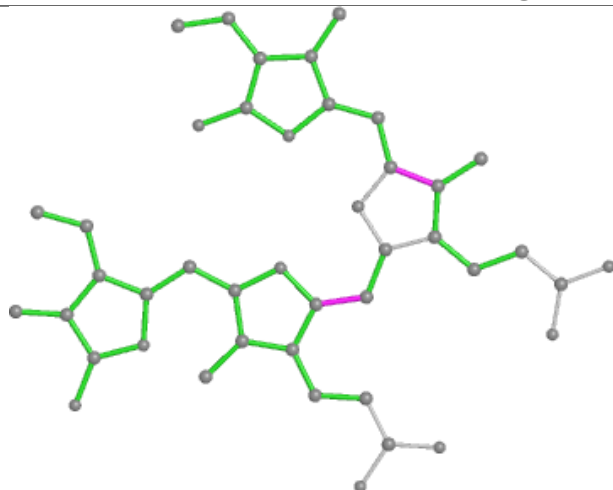


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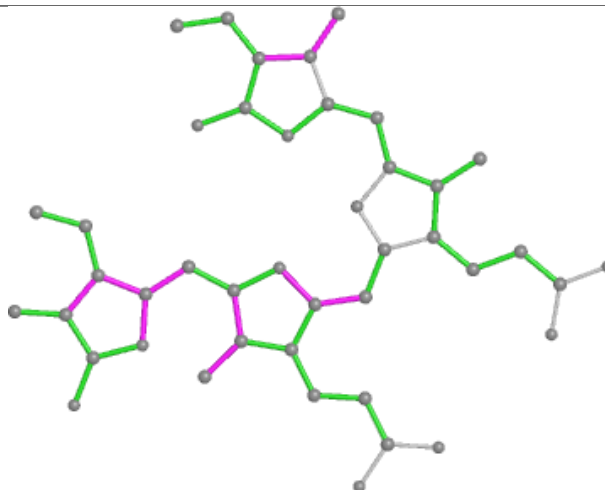


Rings

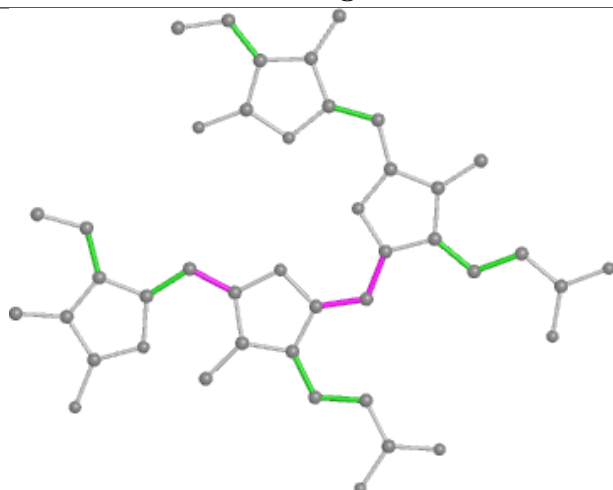
Ligand PEB T 303



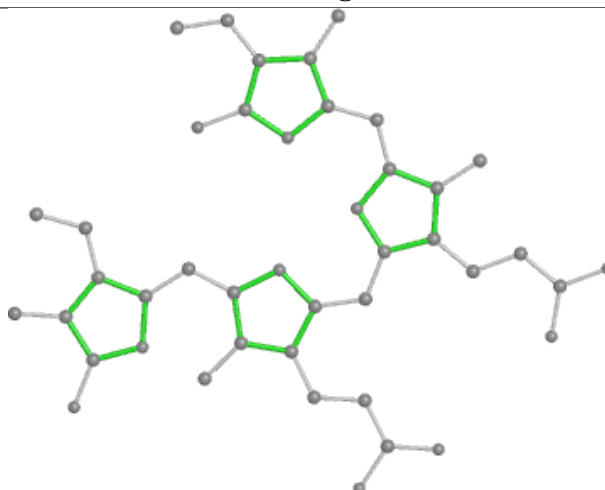
Bond lengths



Bond angles

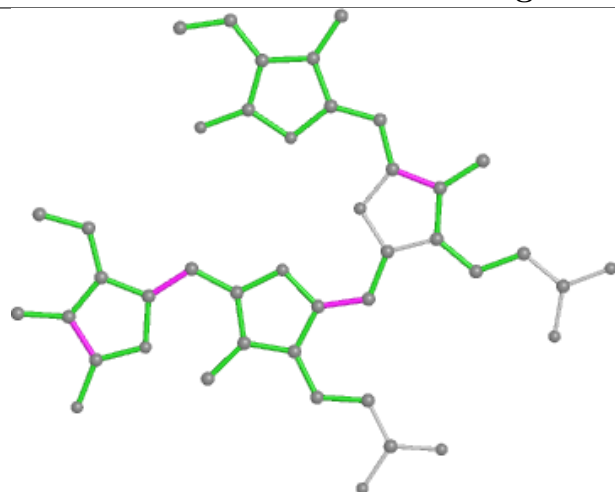


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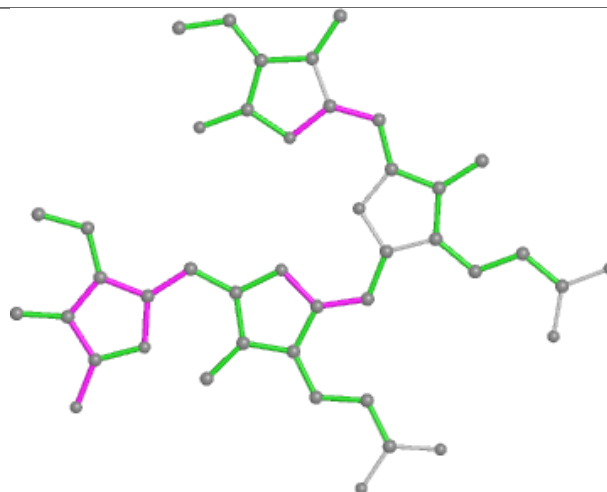


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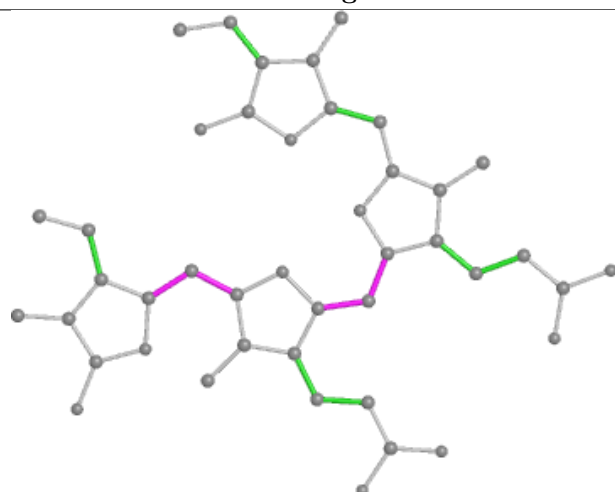
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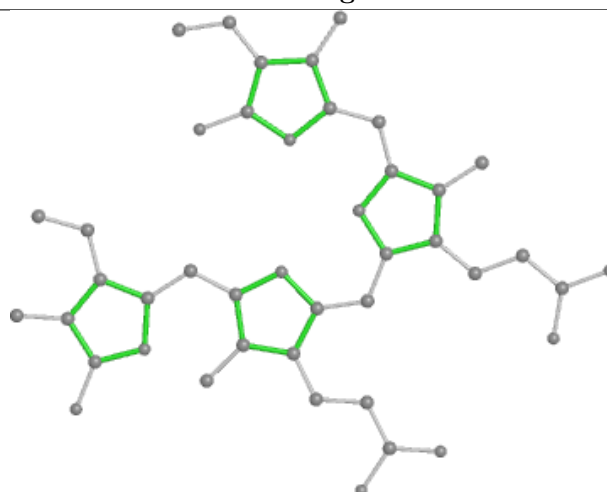
Bond lengths



Bond angles

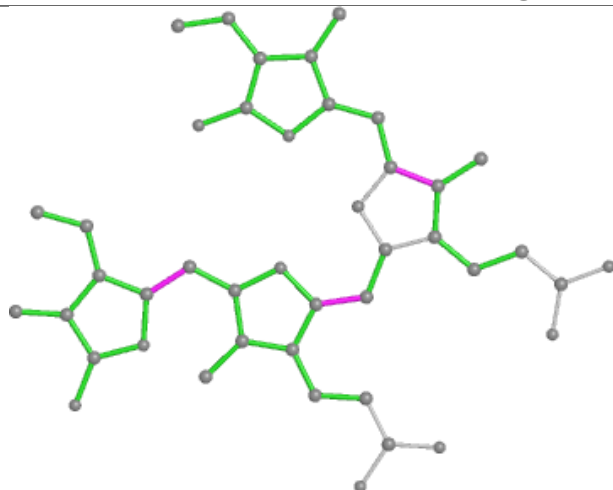


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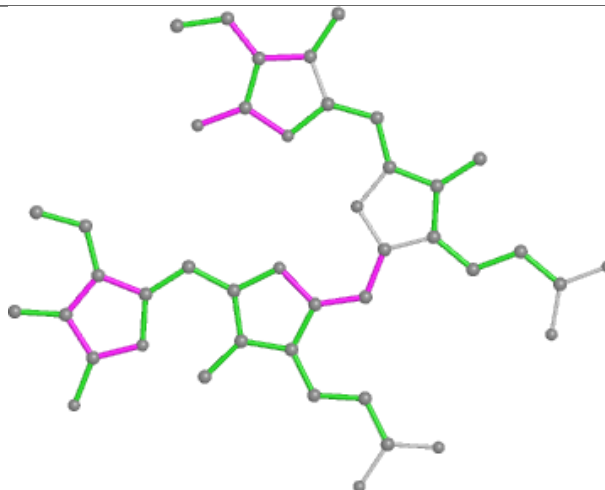


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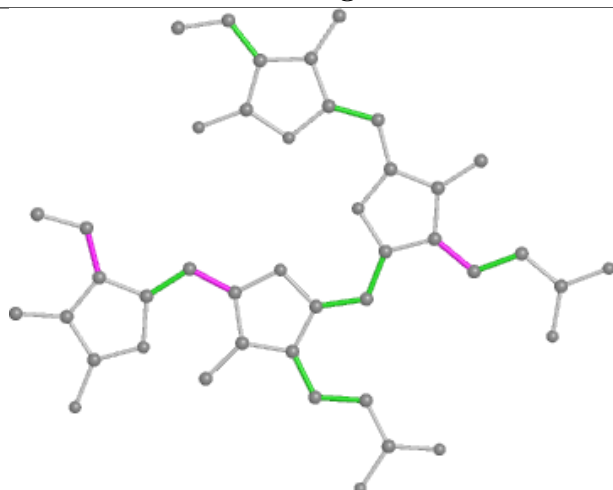
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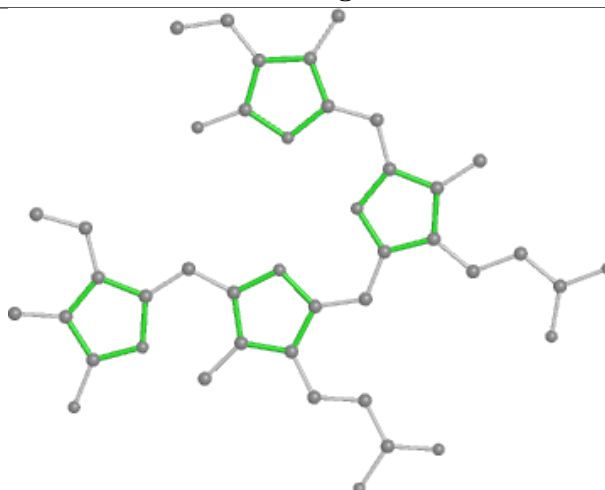
Bond lengths



Bond angles

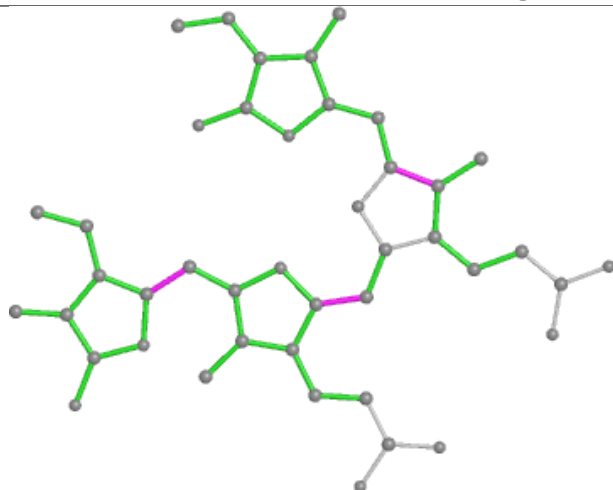


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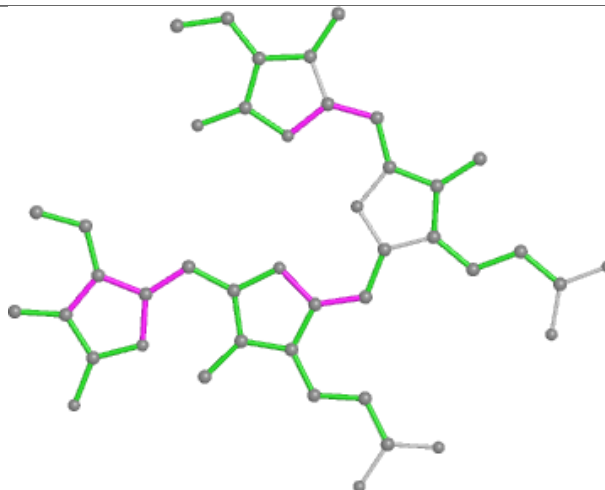


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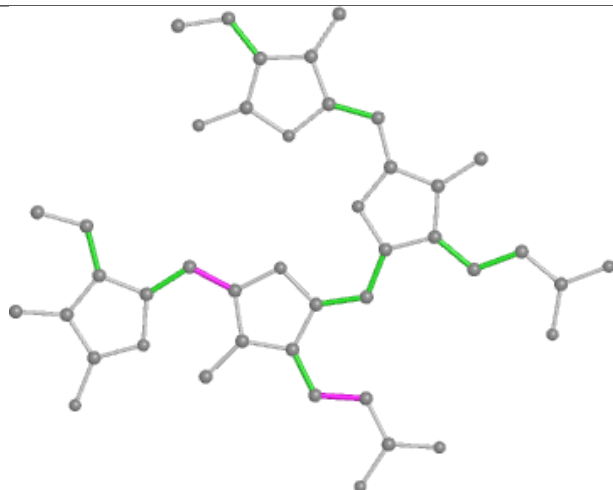
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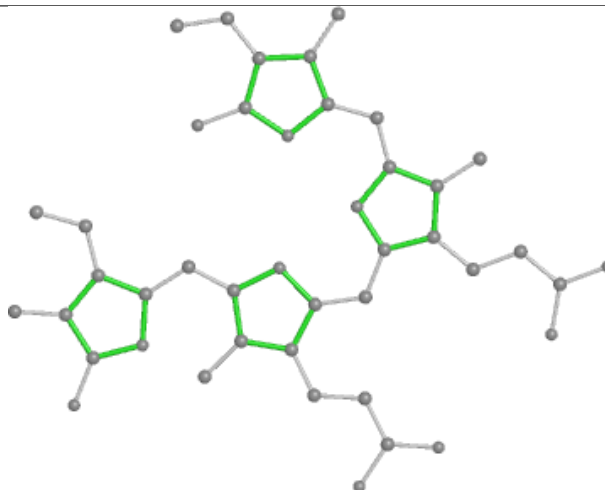
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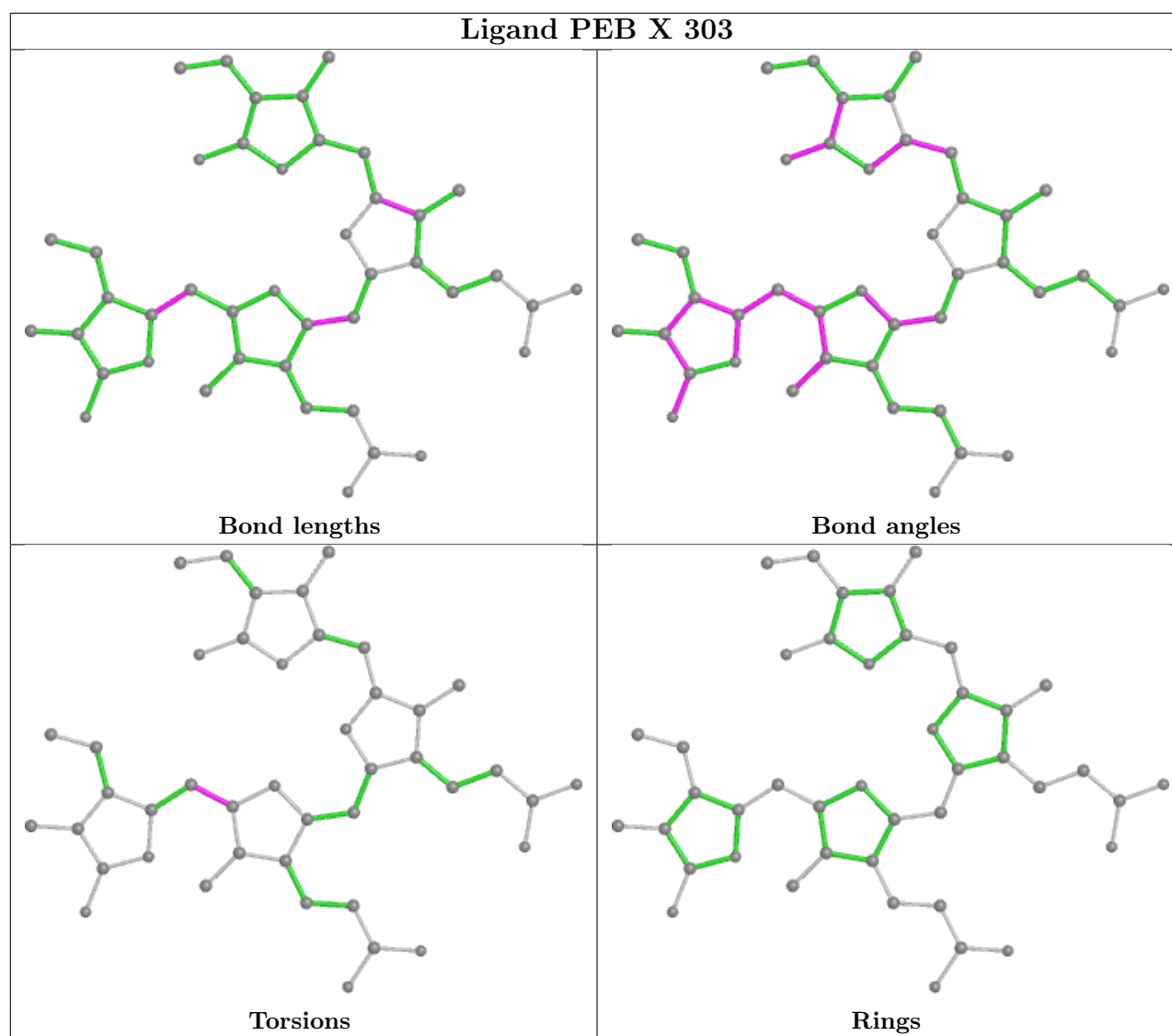
Bond angles



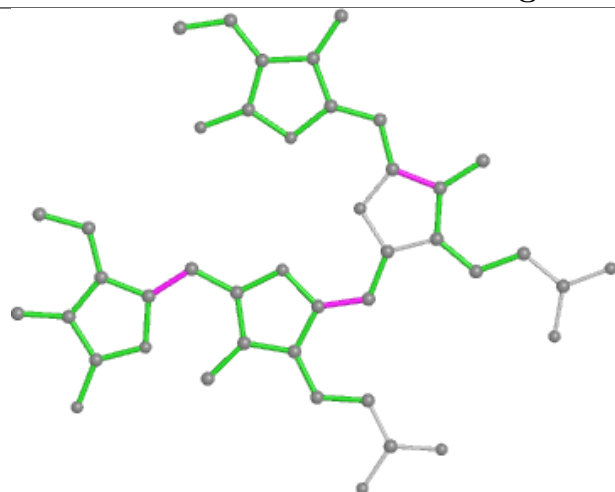
Torsions



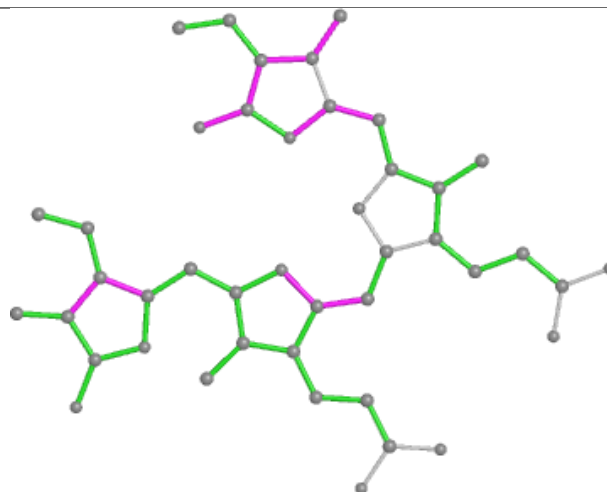
Rings



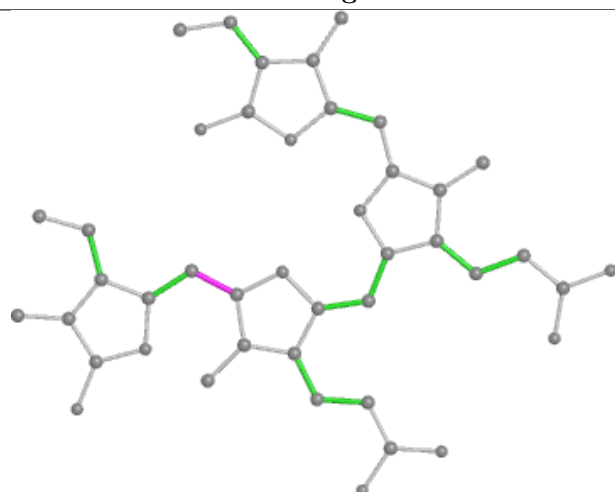
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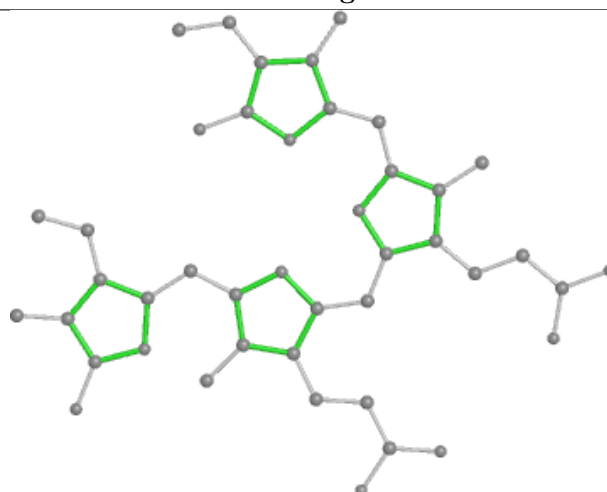
Bond lengths



Bond angles

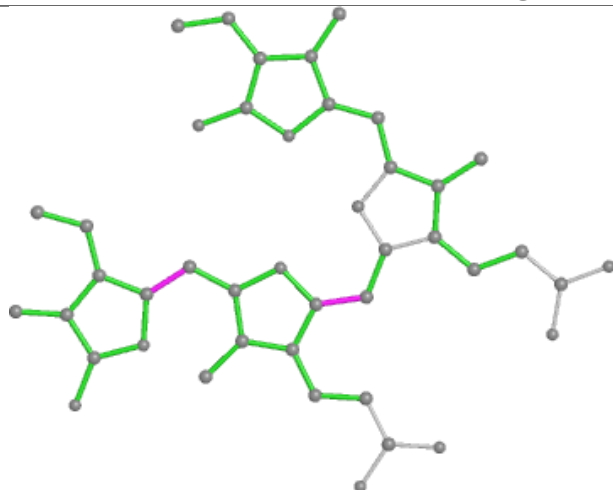


Torsions

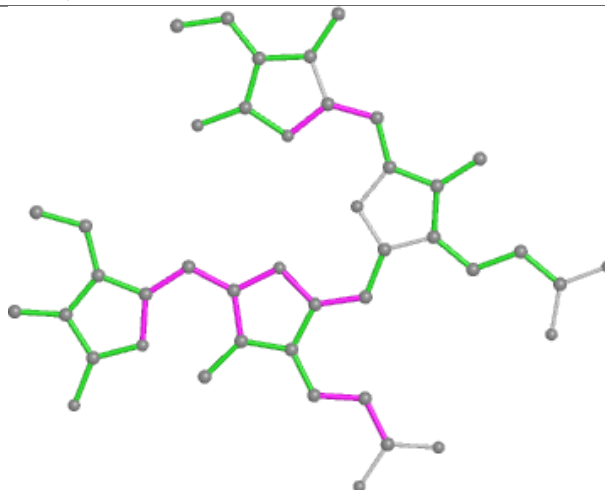


Rings

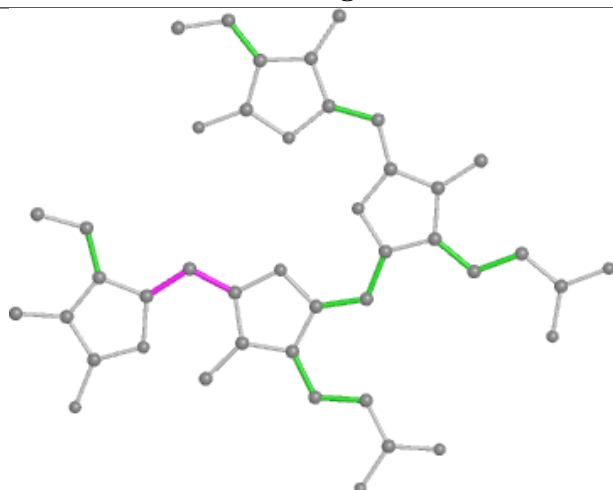
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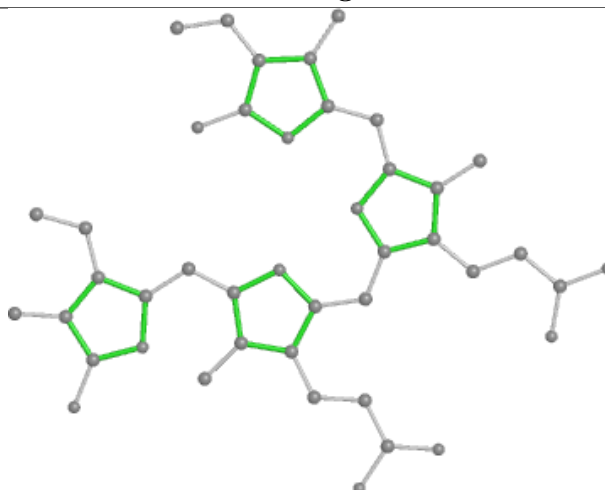
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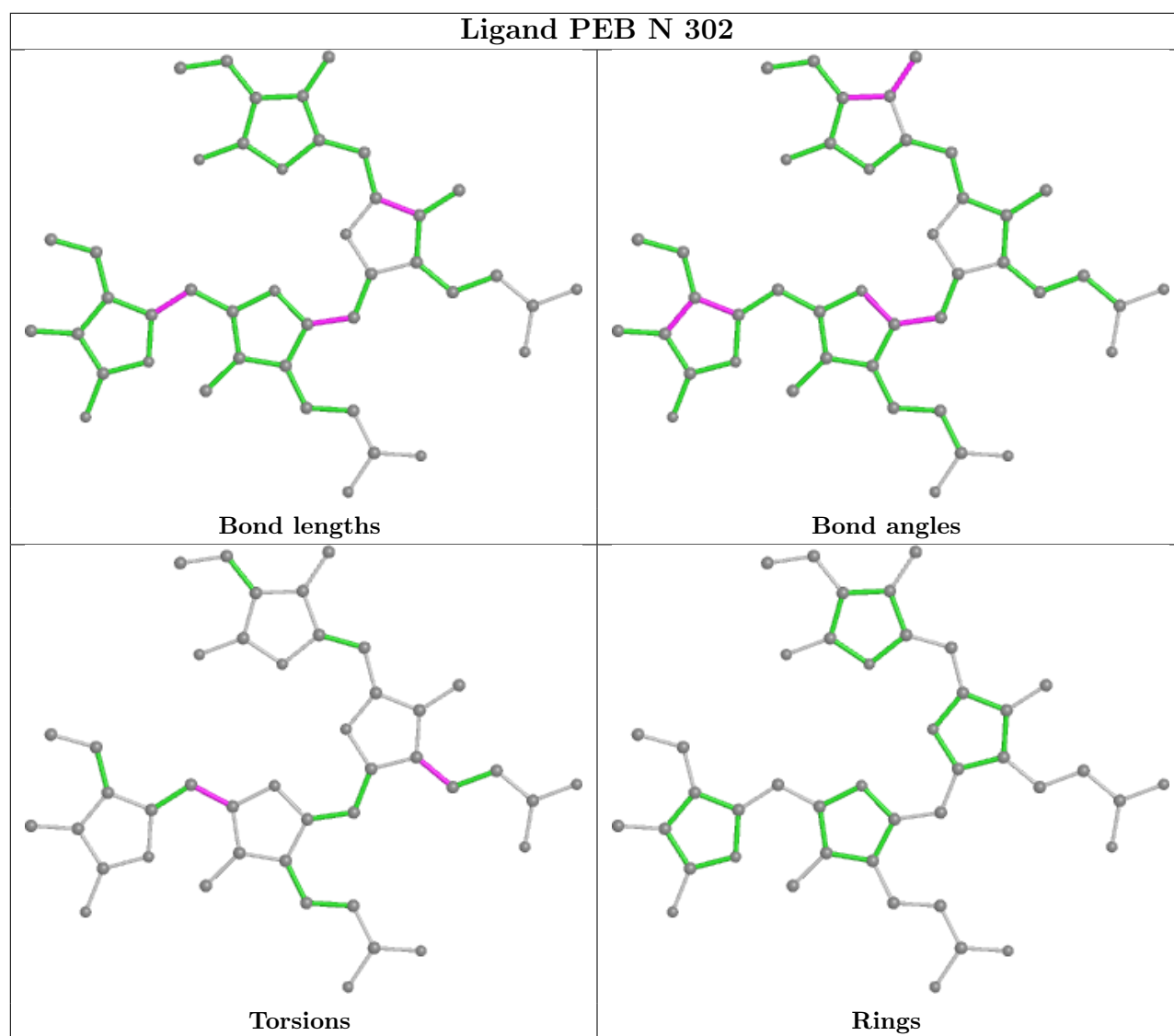
Bond angles



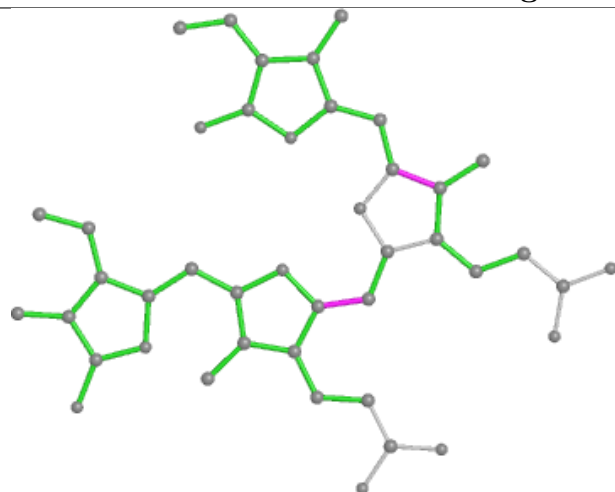
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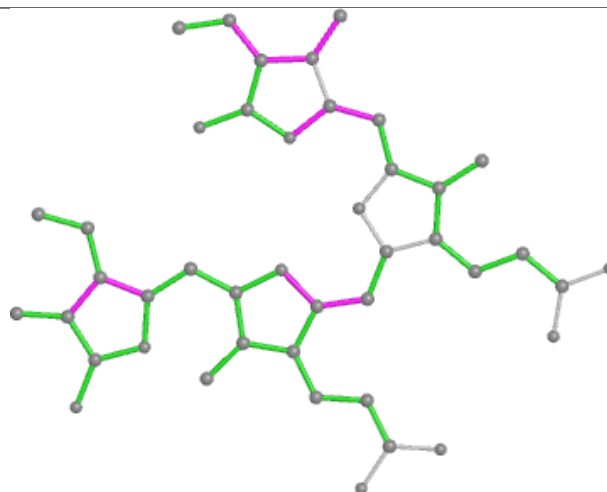
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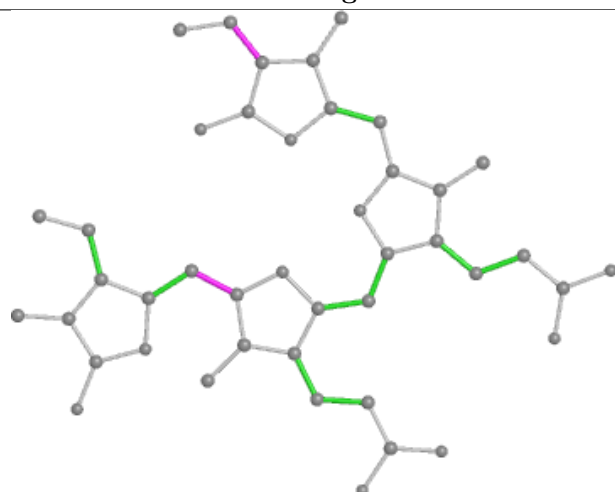
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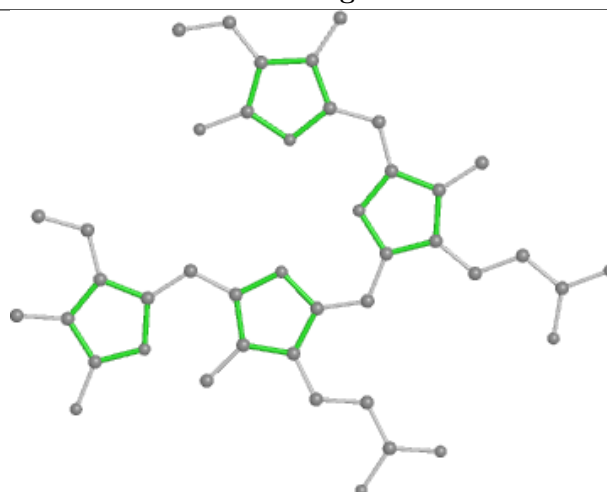
Bond lengths



Bond angles

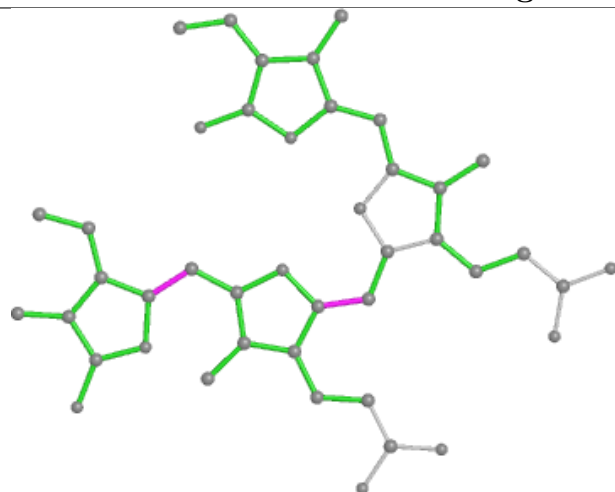


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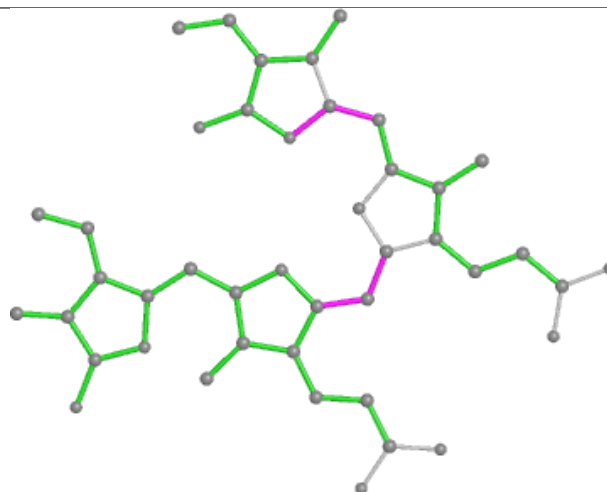


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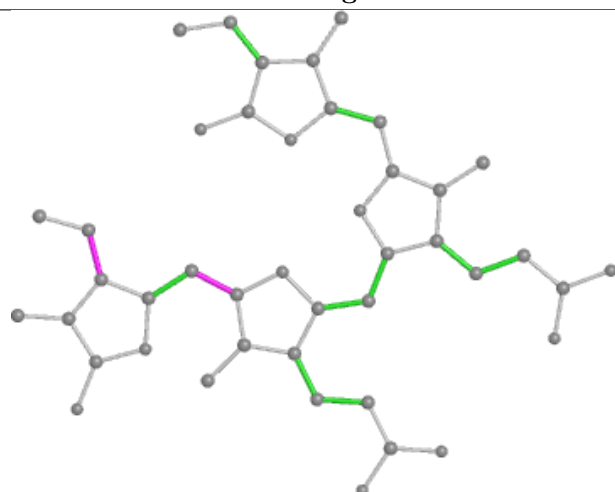
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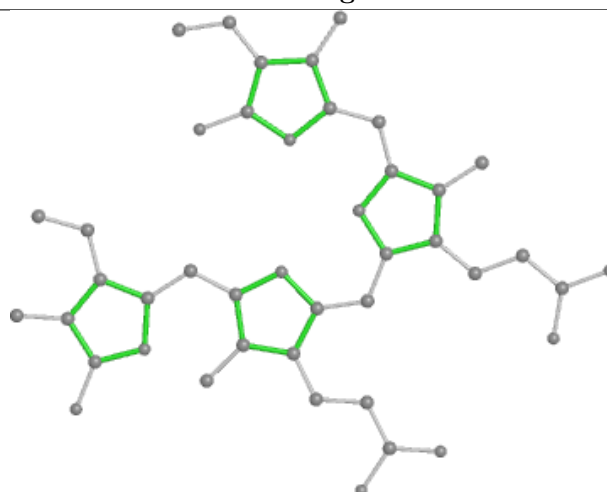
Bond lengths



Bond angles

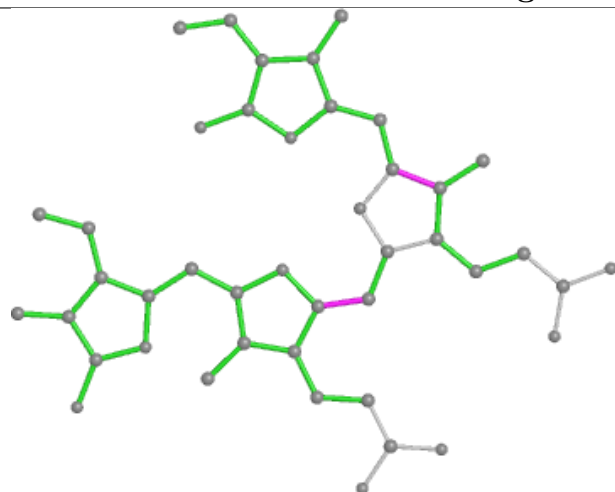


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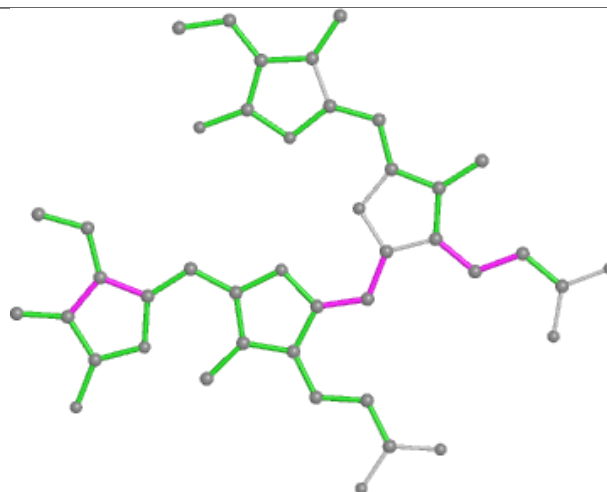


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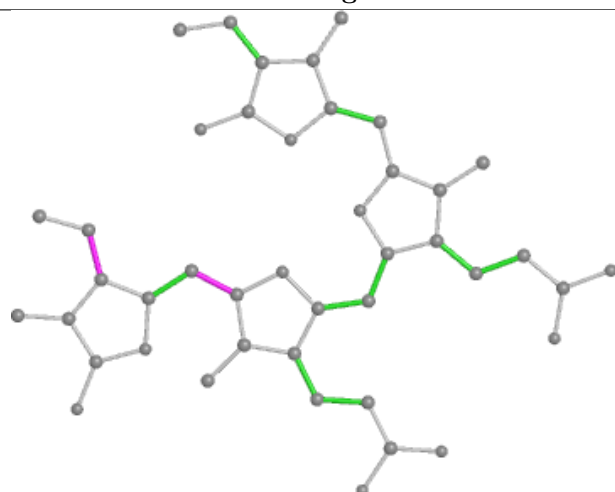
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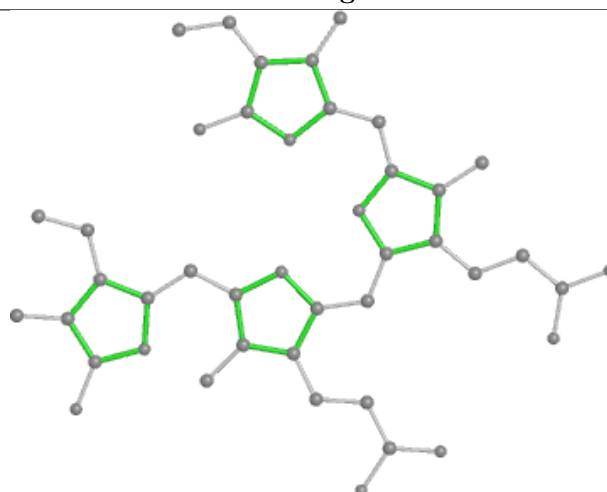
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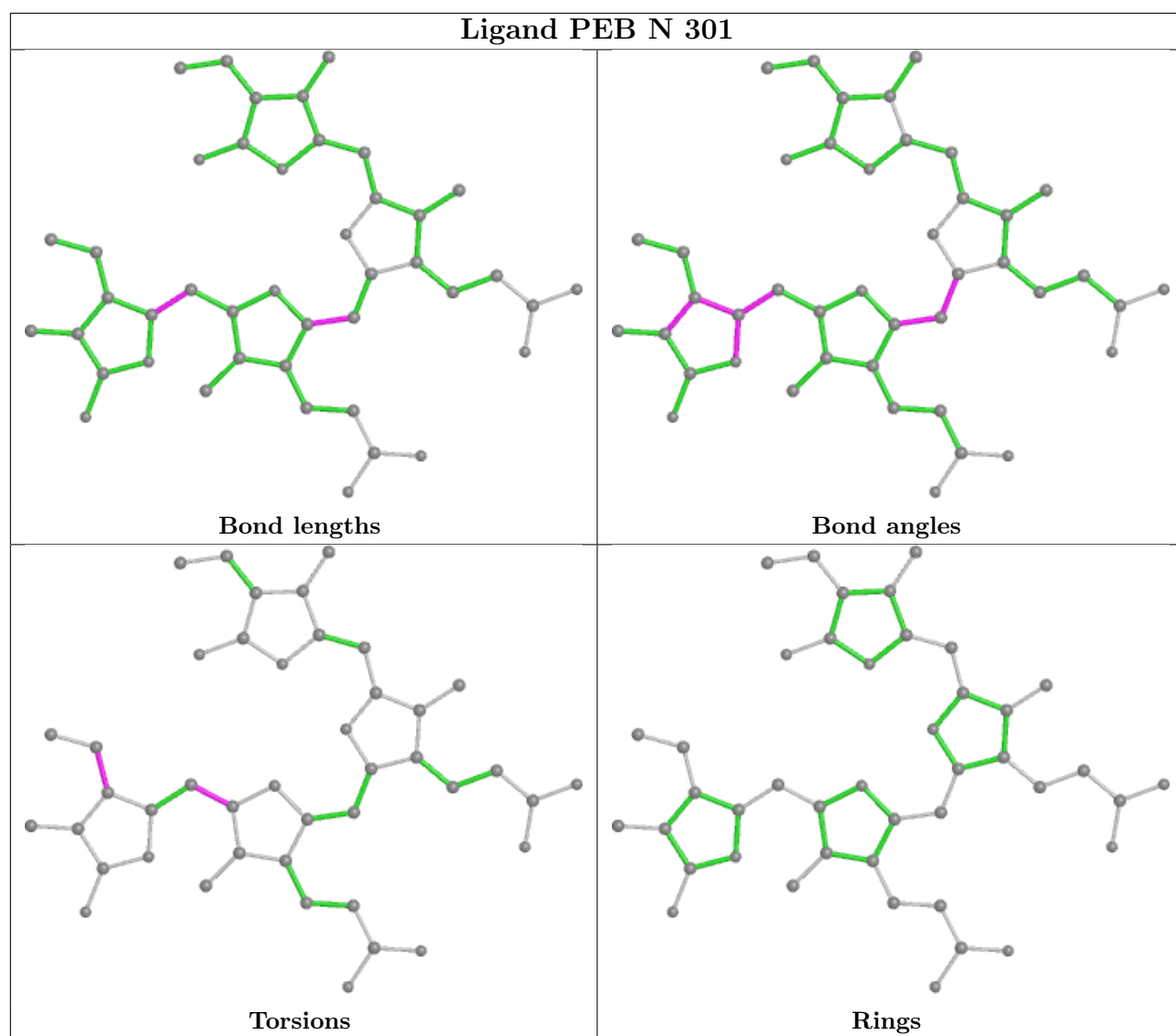
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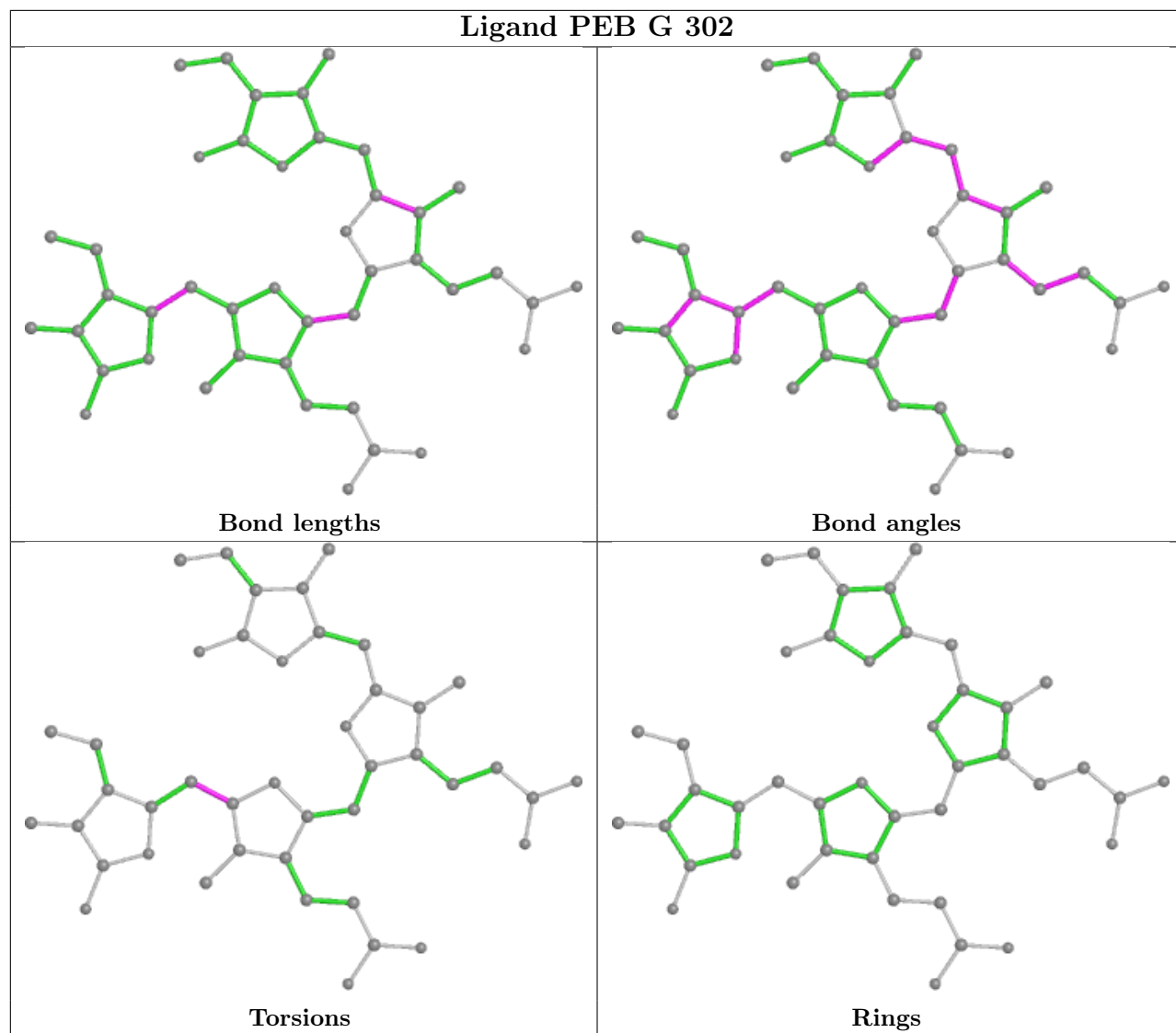


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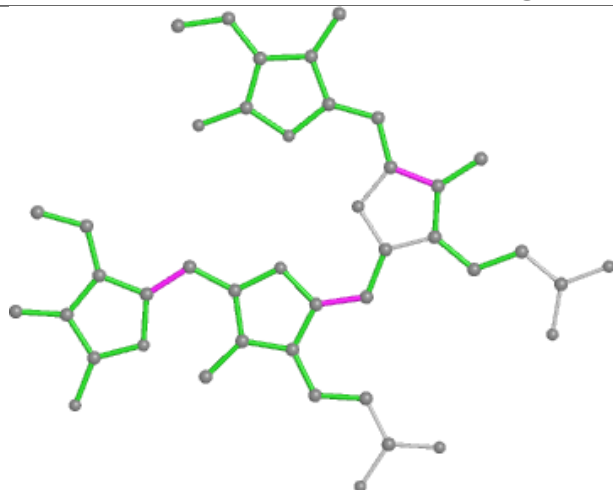


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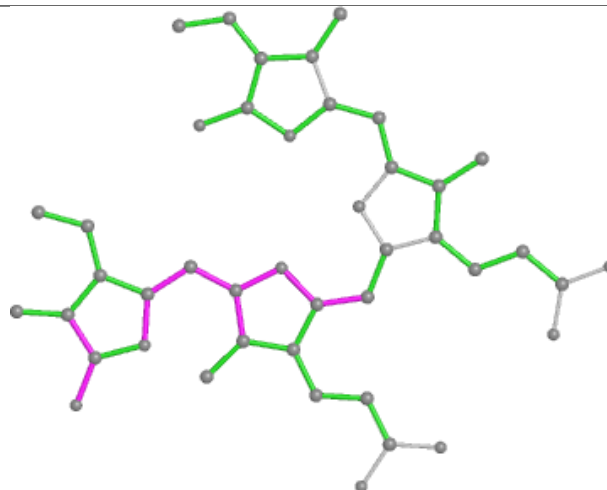




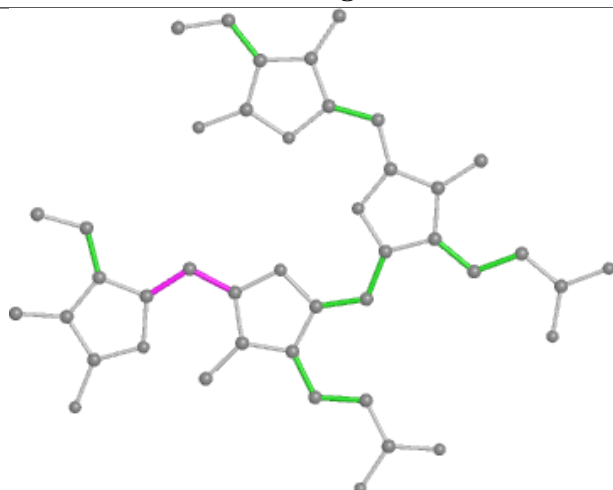
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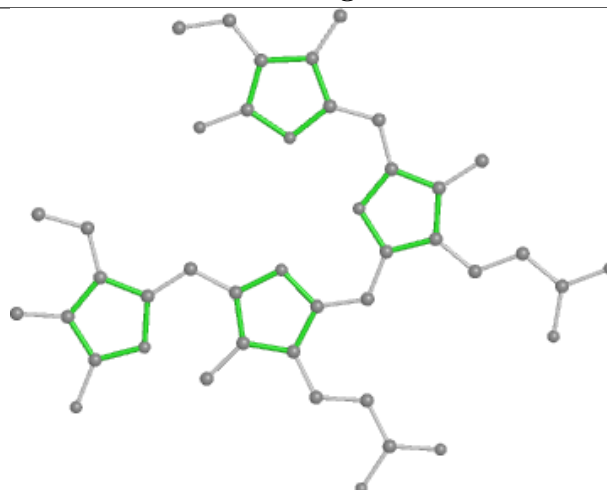
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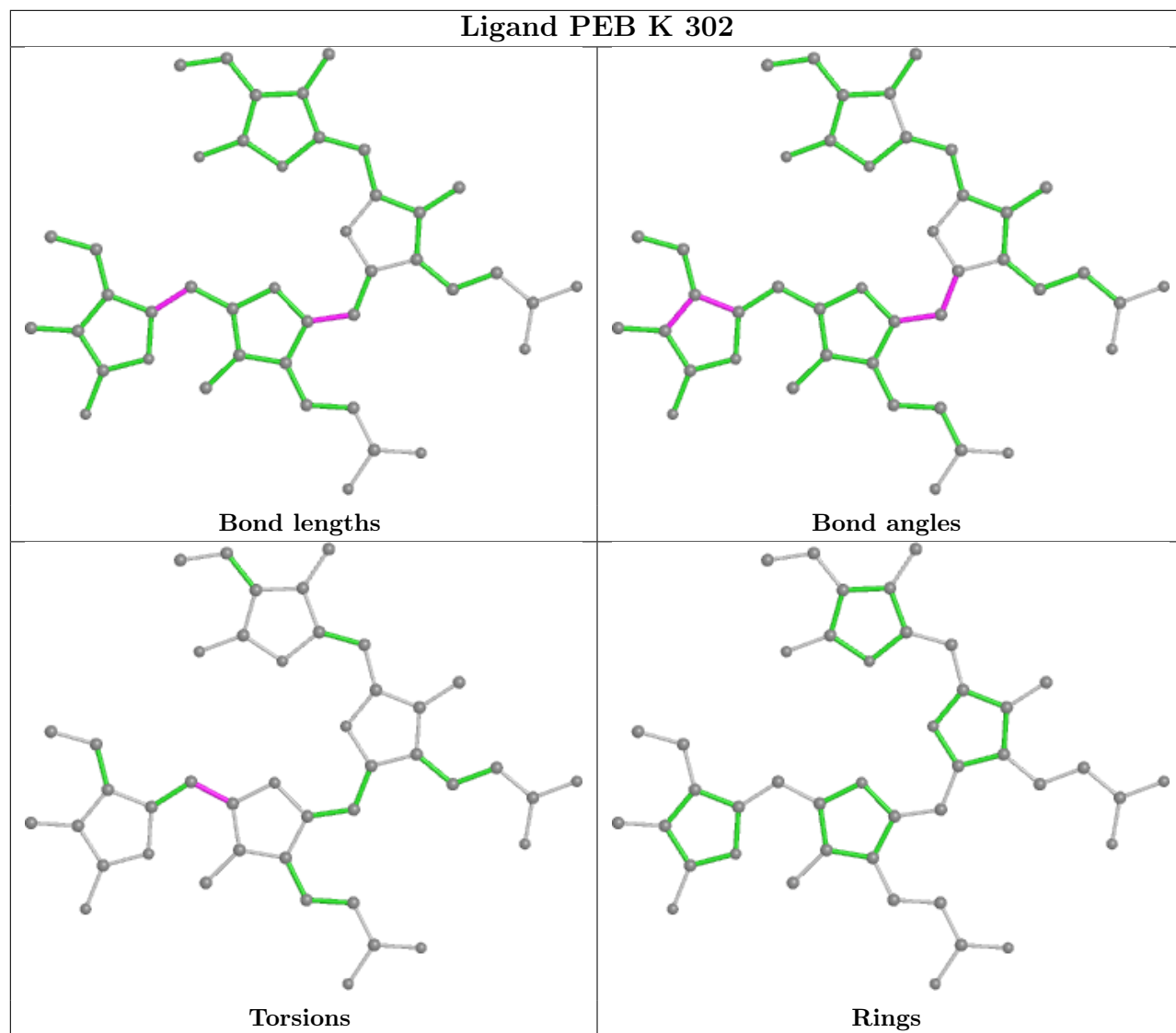
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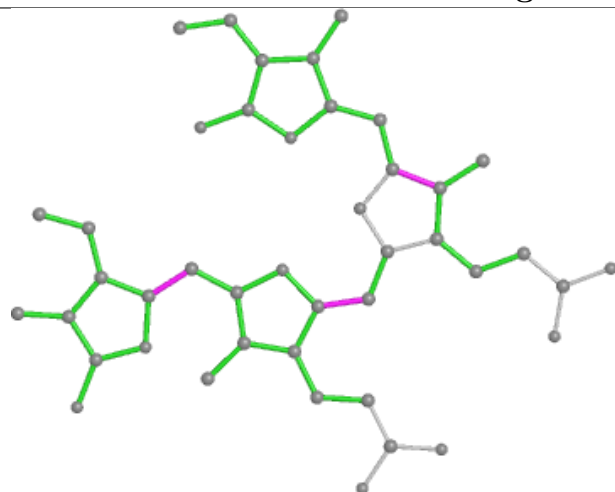
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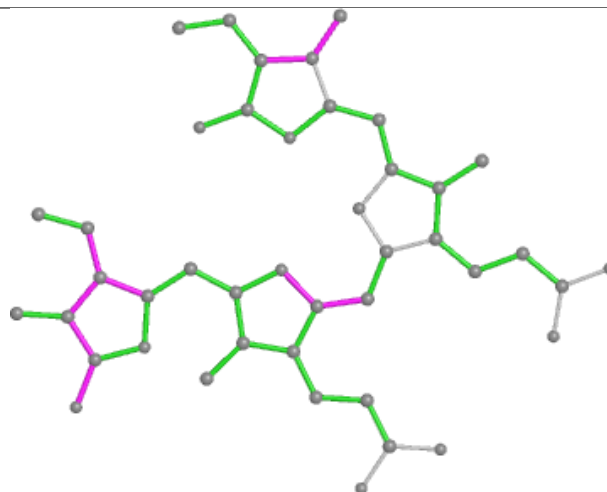
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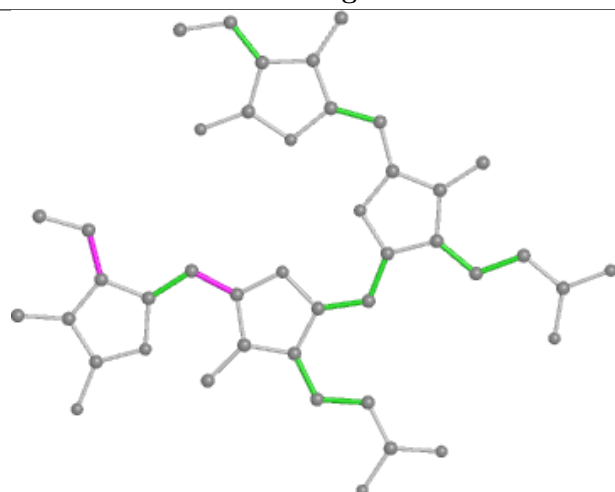
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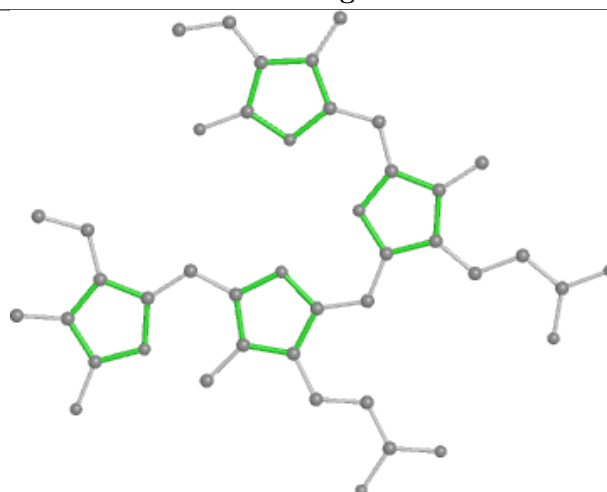
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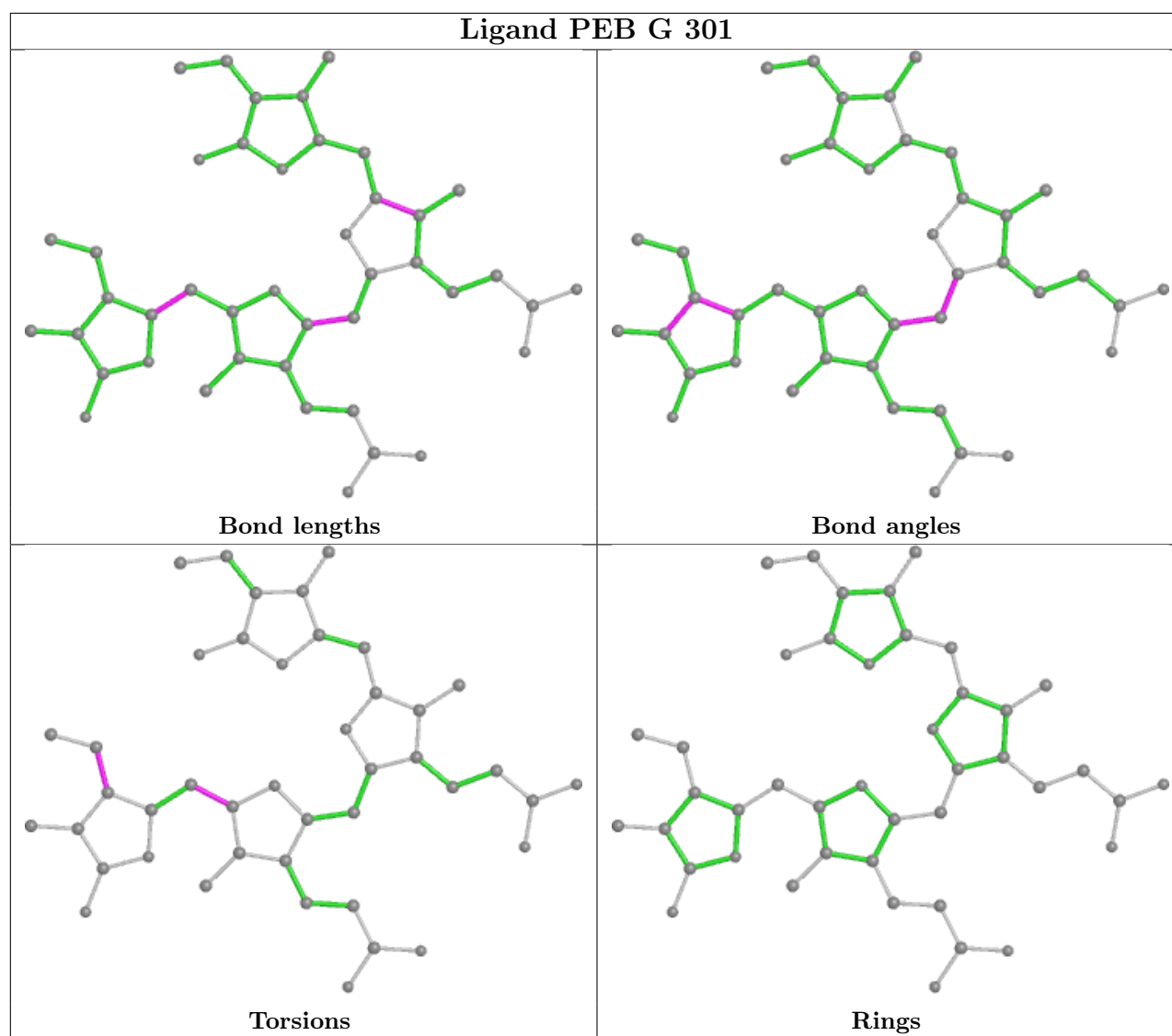
Bond angles

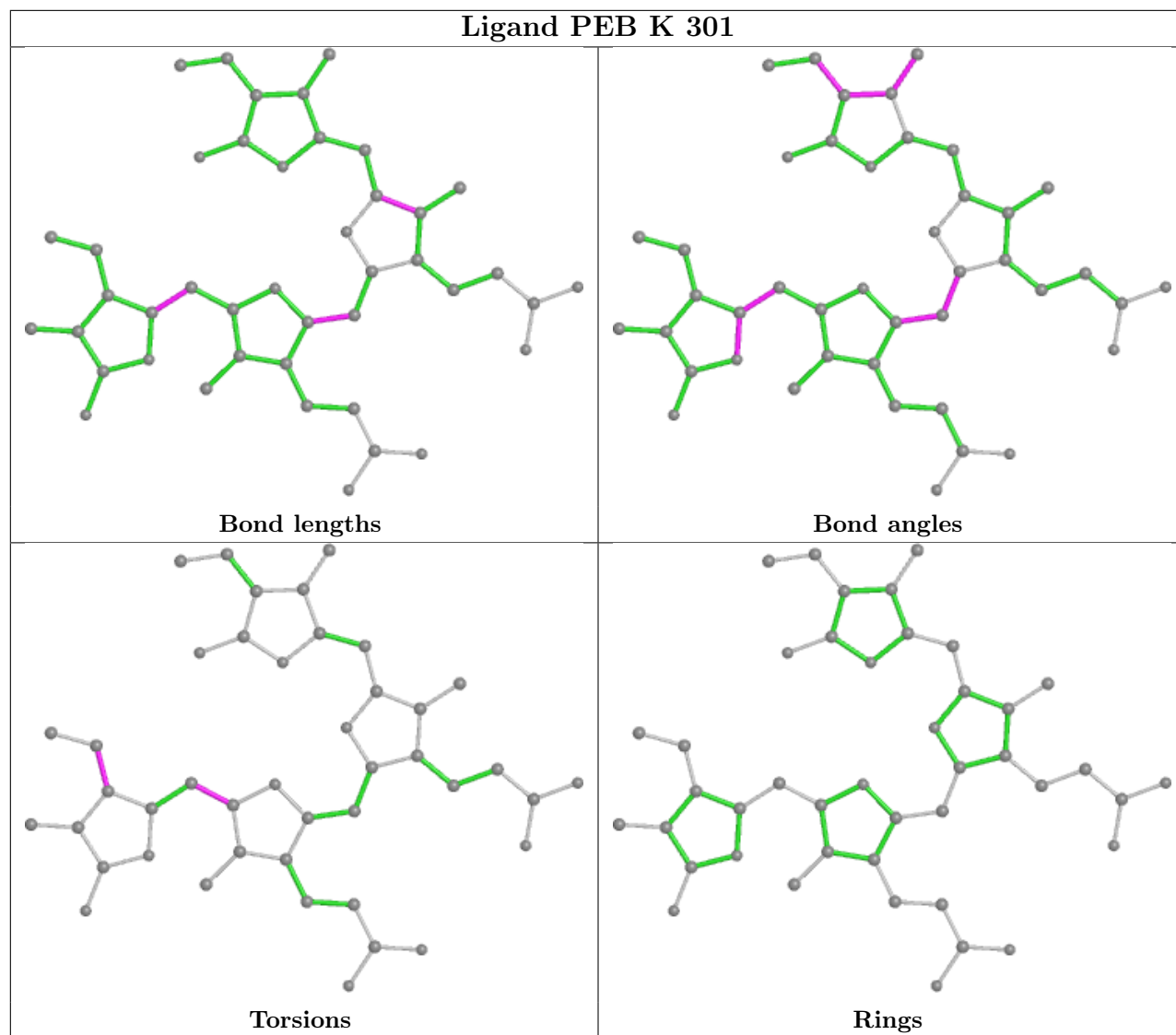


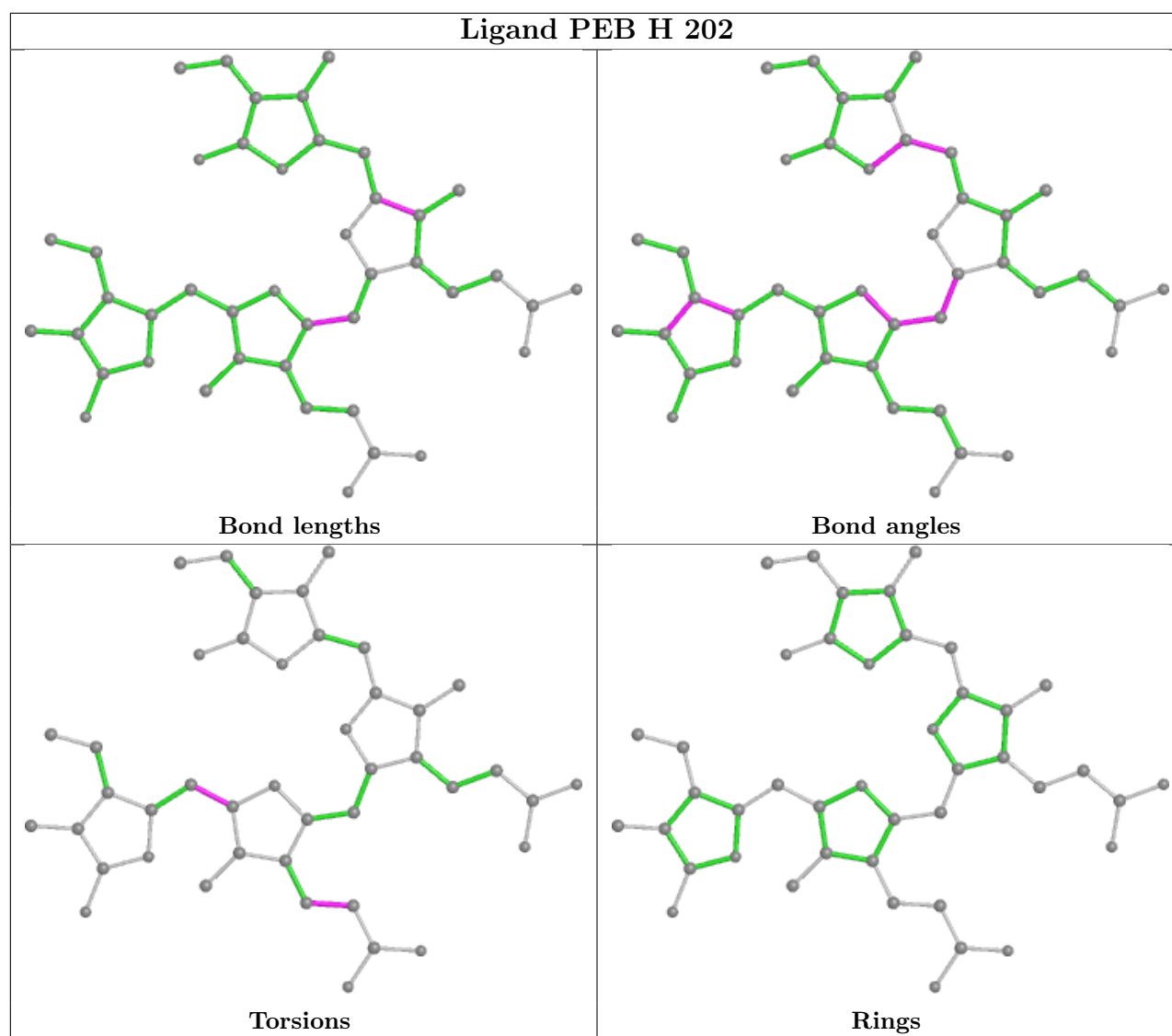
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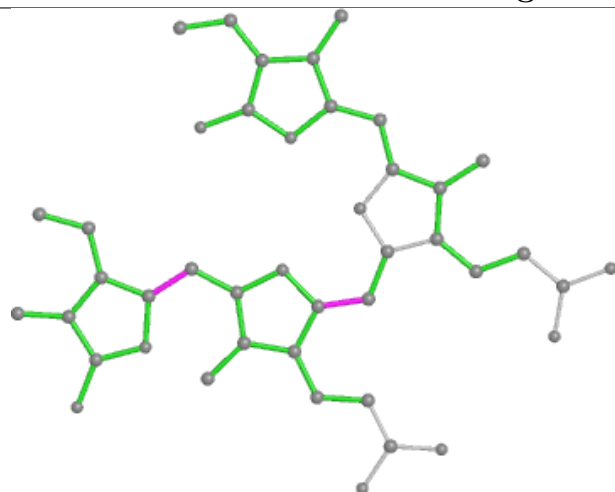
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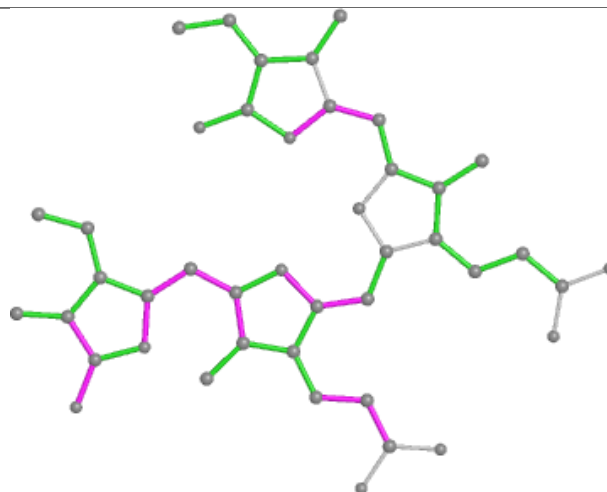




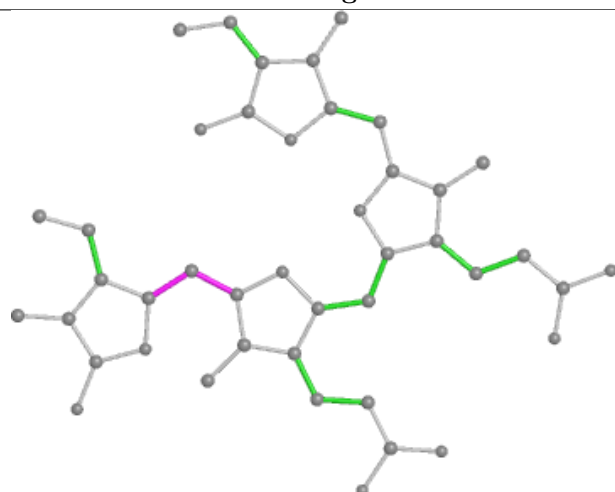
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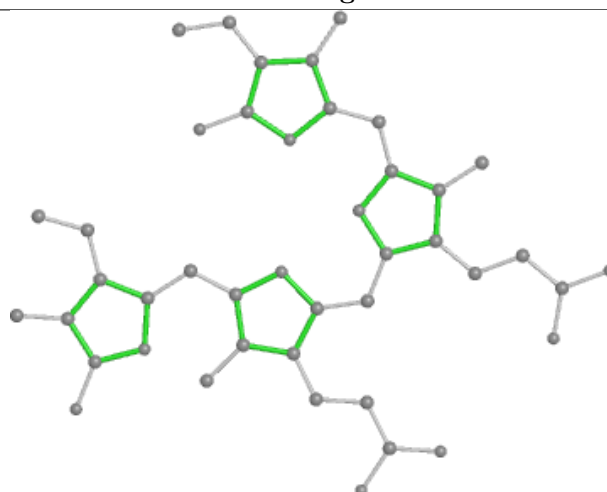
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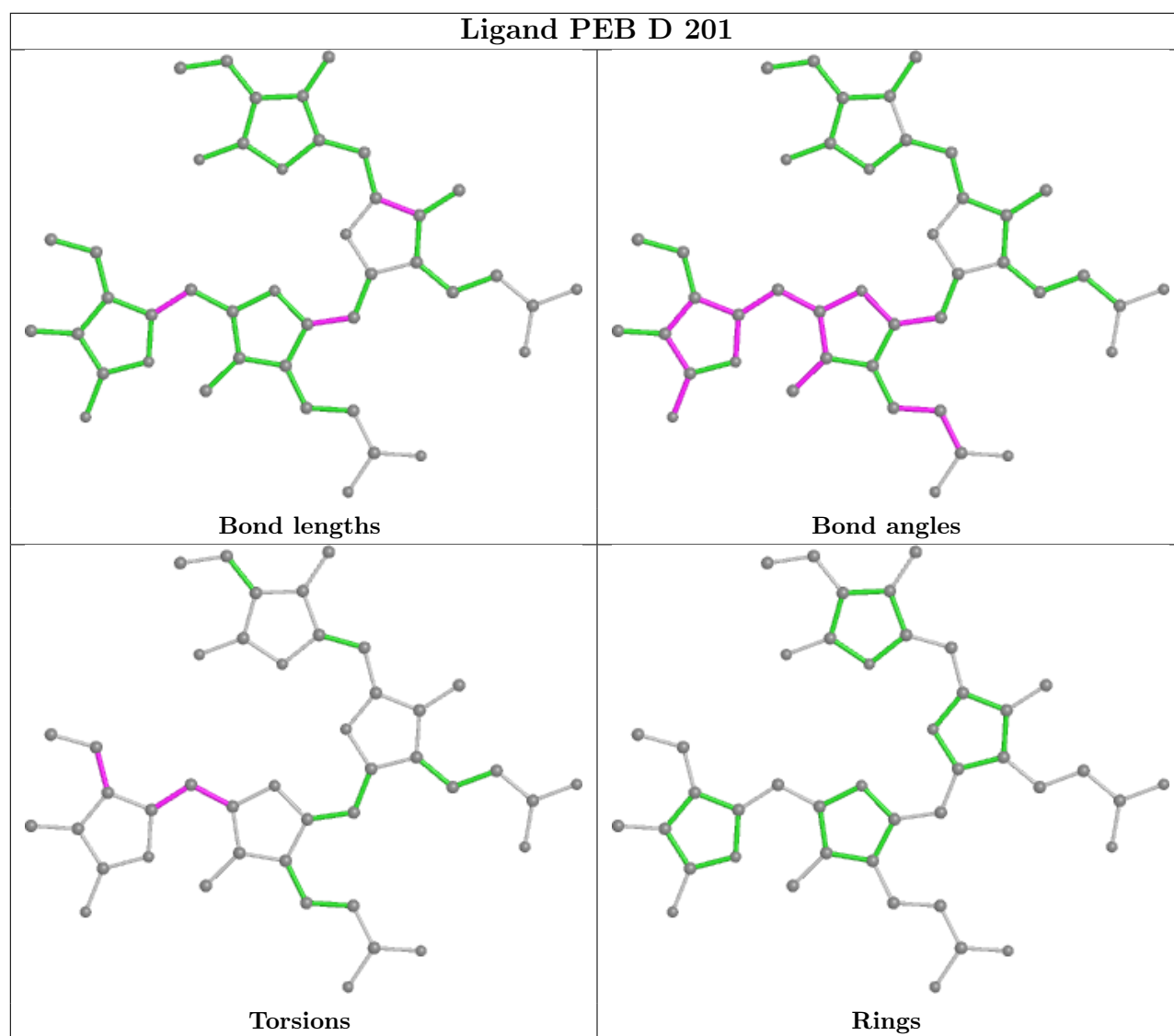
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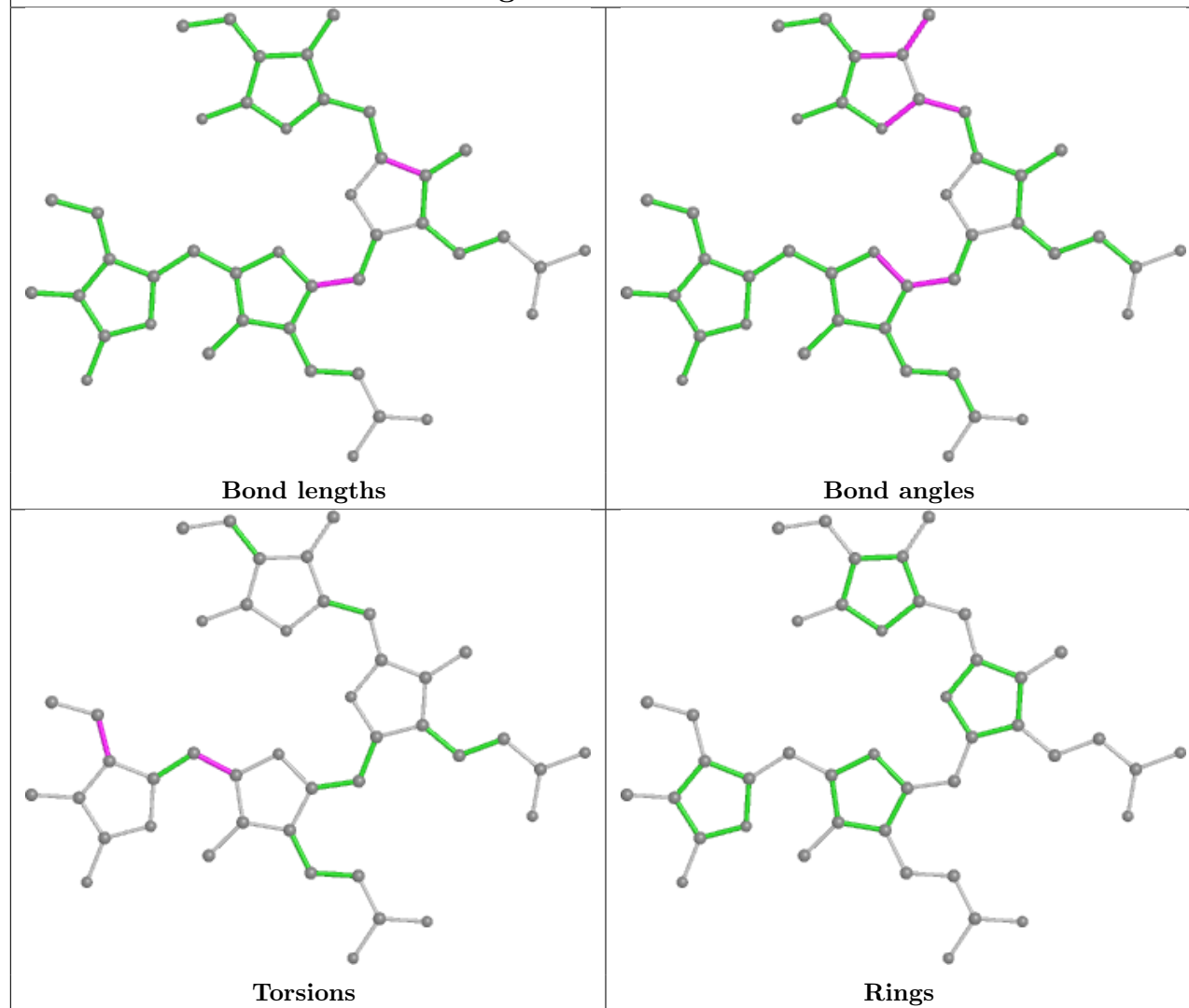
Torsions

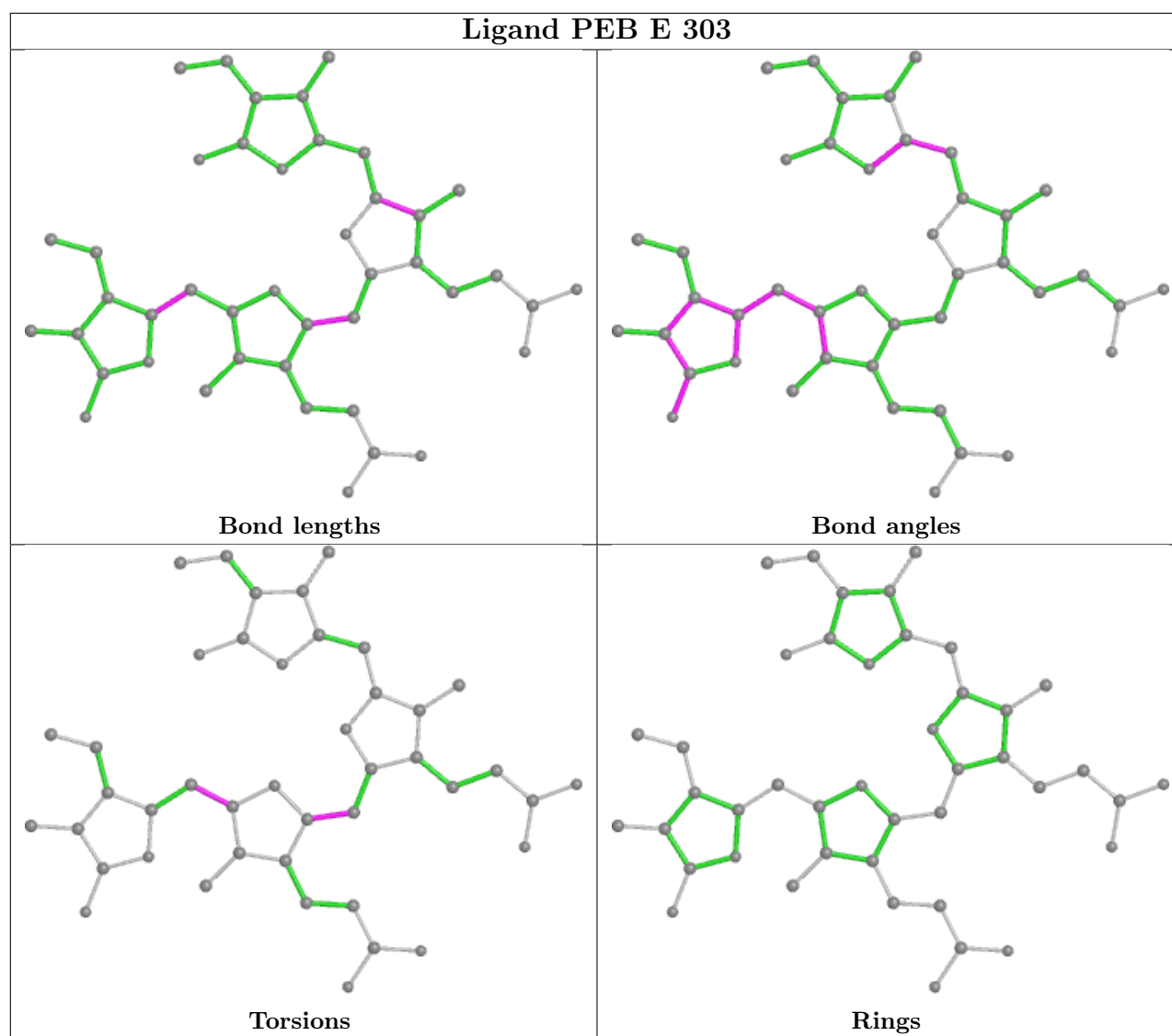


Rings



Ligand PEB F 202





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	C	183/184 (99%)	-0.50	0 100 100	10, 16, 31, 40	0
1	E	183/184 (99%)	-0.43	2 (1%) 80 79	11, 16, 31, 42	0
1	G	183/184 (99%)	-0.44	0 100 100	10, 16, 32, 47	0
1	I	183/184 (99%)	-0.43	1 (0%) 91 90	11, 21, 35, 58	0
1	K	183/184 (99%)	-0.39	1 (0%) 91 90	10, 19, 32, 43	0
1	M	183/184 (99%)	-0.39	2 (1%) 80 79	9, 16, 31, 47	0
1	N	183/184 (99%)	-0.42	0 100 100	10, 17, 31, 45	0
1	P	183/184 (99%)	-0.26	5 (2%) 54 52	10, 18, 37, 51	0
1	R	183/184 (99%)	-0.52	1 (0%) 91 90	10, 17, 31, 45	0
1	T	183/184 (99%)	-0.28	3 (1%) 72 70	12, 21, 34, 46	0
1	V	183/184 (99%)	-0.15	5 (2%) 54 52	13, 26, 42, 71	0
1	X	183/184 (99%)	-0.38	1 (0%) 91 90	10, 18, 36, 50	0
2	A	164/164 (100%)	-0.49	1 (0%) 89 88	9, 13, 28, 46	0
2	B	164/164 (100%)	-0.68	0 100 100	9, 13, 24, 36	0
2	D	164/164 (100%)	-0.53	0 100 100	8, 14, 29, 37	0
2	F	164/164 (100%)	-0.49	2 (1%) 79 77	9, 14, 27, 47	0
2	H	164/164 (100%)	-0.52	0 100 100	9, 16, 29, 38	0
2	J	164/164 (100%)	-0.58	0 100 100	9, 15, 25, 34	0
2	L	164/164 (100%)	-0.41	0 100 100	9, 15, 29, 38	0
2	O	164/164 (100%)	-0.28	2 (1%) 79 77	10, 22, 38, 49	0
2	Q	164/164 (100%)	-0.60	0 100 100	9, 14, 22, 33	0
2	U	164/164 (100%)	-0.47	0 100 100	11, 18, 29, 40	0
2	W	164/164 (100%)	-0.34	2 (1%) 79 77	10, 20, 36, 48	0
2	Y	164/164 (100%)	-0.55	0 100 100	10, 15, 24, 31	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4164/4176 (99%)	-0.44	28 (0%) 87 86	8, 17, 33, 71	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	23	SER	3.8
1	I	23	SER	3.7
1	T	23	SER	3.6
2	F	69	ALA	3.6
1	P	184	SER	3.3
1	V	184	SER	3.1
2	O	74	SER	3.0
2	W	69	ALA	2.9
1	M	21	ASP	2.9
2	A	69	ALA	2.7
1	P	20	GLY	2.7
1	T	116	ALA	2.7
1	P	22	VAL	2.6
2	O	69	ALA	2.5
2	W	74	SER	2.4
1	V	11	GLN	2.4
1	E	162	GLU	2.3
1	V	114	THR	2.3
2	F	70	GLY	2.3
1	M	22	VAL	2.2
1	K	114	THR	2.2
1	T	24	ALA	2.1
1	V	21	ASP	2.1
1	X	23	SER	2.1
1	P	11	GLN	2.1
1	P	21	ASP	2.1
1	R	162	GLU	2.1
1	E	27	GLN	2.0

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(\AA^2)	Q<0.9
1	MEN	V	70	9/10	0.92	0.14	27,30,32,34	0
1	MEN	P	70	9/10	0.94	0.11	13,14,14,16	0
1	MEN	K	70	9/10	0.94	0.16	21,23,26,26	0
1	MEN	T	70	9/10	0.95	0.15	20,22,24,24	0
1	MEN	I	70	9/10	0.95	0.11	20,22,23,23	0
1	MEN	C	70	9/10	0.96	0.10	16,18,18,19	0
1	MEN	E	70	9/10	0.96	0.09	14,15,17,18	0
1	MEN	N	70	9/10	0.96	0.09	12,12,13,13	0
1	MEN	M	70	9/10	0.97	0.09	11,14,17,18	0
1	MEN	R	70	9/10	0.97	0.10	15,15,17,18	0
1	MEN	G	70	9/10	0.98	0.10	13,14,15,15	0
1	MEN	X	70	9/10	0.98	0.10	13,14,16,18	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
3	PEB	O	201	43/43	0.89	0.15	25,31,36,45	0
3	PEB	K	303	43/43	0.89	0.16	15,18,34,56	0
3	PEB	V	303	43/43	0.89	0.16	21,26,36,49	0
3	PEB	V	301	43/43	0.90	0.15	15,22,31,41	0
3	PEB	W	201	43/43	0.90	0.14	21,26,32,39	0
3	PEB	X	302	43/43	0.90	0.14	13,18,28,30	0
3	PEB	O	202	43/43	0.91	0.16	22,35,38,43	0
3	PEB	N	302	43/43	0.91	0.14	16,19,26,32	0
3	PEB	T	301	43/43	0.91	0.12	13,19,24,31	0
3	PEB	U	202	43/43	0.91	0.14	18,25,39,41	0
3	PEB	M	303	43/43	0.91	0.14	11,16,23,33	0
3	PEB	E	301	43/43	0.91	0.14	12,20,26,29	0
3	PEB	J	202	43/43	0.92	0.14	22,26,28,31	0
3	PEB	C	301	43/43	0.92	0.12	14,17,28,40	0
3	PEB	N	303	43/43	0.92	0.13	14,18,28,37	0
3	PEB	P	303	43/43	0.92	0.15	12,18,31,49	0
3	PEB	M	301	43/43	0.92	0.11	11,16,22,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEB	T	302	43/43	0.92	0.11	15,22,30,33	0
3	PEB	T	303	43/43	0.92	0.15	17,20,32,51	0
3	PEB	E	303	43/43	0.92	0.12	13,16,25,40	0
3	PEB	V	302	43/43	0.92	0.13	21,26,30,33	0
3	PEB	I	301	43/43	0.92	0.13	11,18,34,40	0
3	PEB	I	303	43/43	0.92	0.14	17,20,33,46	0
3	PEB	B	201	43/43	0.93	0.12	12,15,20,21	0
3	PEB	K	301	43/43	0.93	0.12	12,18,23,30	0
3	PEB	B	202	43/43	0.93	0.15	14,19,28,35	0
3	PEB	N	301	43/43	0.93	0.13	14,20,24,30	0
3	PEB	F	202	43/43	0.93	0.13	13,16,27,33	0
3	PEB	W	202	43/43	0.93	0.13	21,32,35,50	0
3	PEB	P	301	43/43	0.93	0.12	11,18,25,35	0
3	PEB	H	201	43/43	0.93	0.13	18,21,26,28	0
3	PEB	R	301	43/43	0.93	0.11	13,18,26,37	0
3	PEB	R	302	43/43	0.93	0.13	15,21,27,32	0
3	PEB	R	303	43/43	0.93	0.13	14,16,27,37	0
3	PEB	C	303	43/43	0.93	0.12	13,16,26,37	0
3	PEB	H	202	43/43	0.93	0.13	20,23,29,39	0
3	PEB	E	302	43/43	0.93	0.13	16,20,24,31	0
3	PEB	M	302	43/43	0.93	0.12	13,18,31,38	0
3	PEB	G	301	43/43	0.93	0.12	14,18,23,29	0
3	PEB	D	201	43/43	0.93	0.12	12,14,18,19	0
3	PEB	I	302	43/43	0.93	0.12	14,20,24,32	0
3	PEB	A	201	43/43	0.94	0.11	14,16,24,28	0
3	PEB	P	302	43/43	0.94	0.12	12,17,22,27	0
3	PEB	G	302	43/43	0.94	0.11	12,18,30,47	0
3	PEB	G	303	43/43	0.94	0.15	13,18,27,43	0
3	PEB	F	201	43/43	0.94	0.11	13,15,22,29	0
3	PEB	L	202	43/43	0.94	0.11	15,20,26,26	0
3	PEB	D	202	43/43	0.94	0.11	15,19,28,30	0
3	PEB	C	302	43/43	0.94	0.13	15,21,27,28	0
3	PEB	K	302	43/43	0.94	0.10	12,18,24,26	0
3	PEB	A	202	43/43	0.94	0.11	12,16,21,26	0
3	PEB	Q	201	43/43	0.94	0.12	10,14,18,20	0
3	PEB	Q	202	43/43	0.94	0.14	16,21,31,47	0
3	PEB	X	301	43/43	0.94	0.11	12,18,26,41	0
3	PEB	U	201	43/43	0.94	0.12	17,20,27,28	0
3	PEB	X	303	43/43	0.94	0.12	13,16,28,46	0
3	PEB	Y	201	43/43	0.94	0.11	12,15,18,24	0
3	PEB	Y	202	43/43	0.94	0.14	18,23,30,31	0
3	PEB	J	201	43/43	0.95	0.10	14,17,23,27	0

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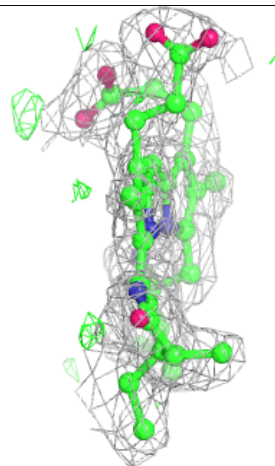
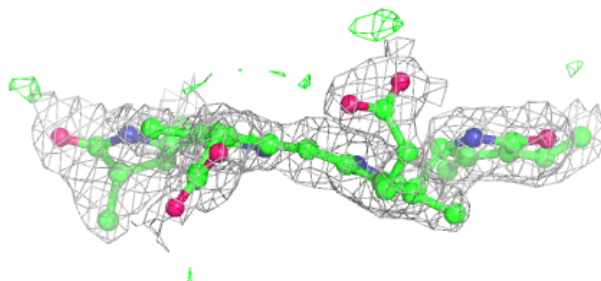
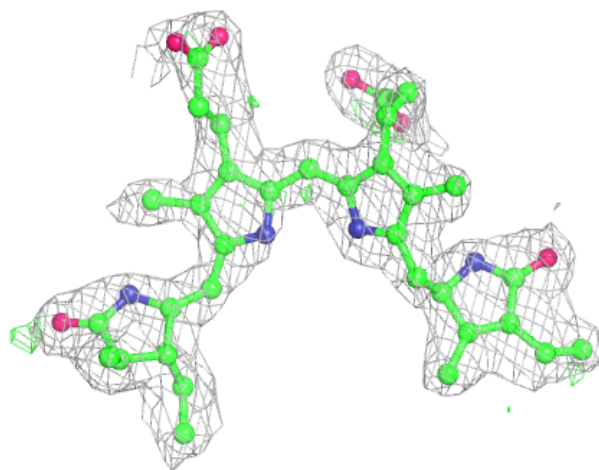
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEB	L	201	43/43	0.95	0.11	13,16,20,22	0

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.

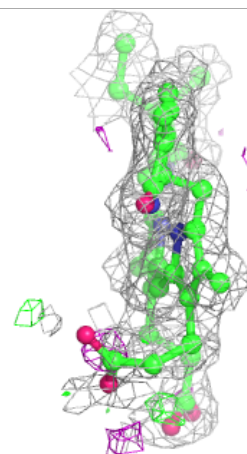
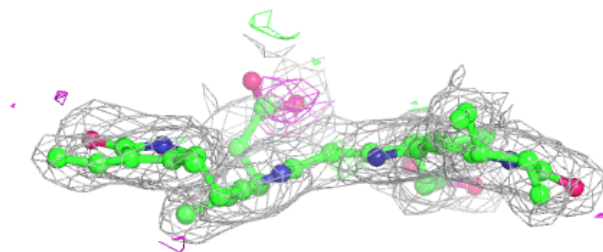
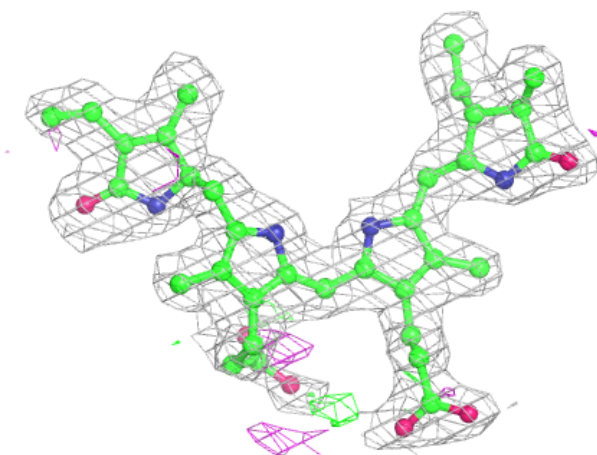
Electron density around PEB O 201:

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



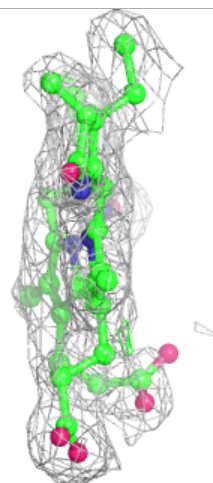
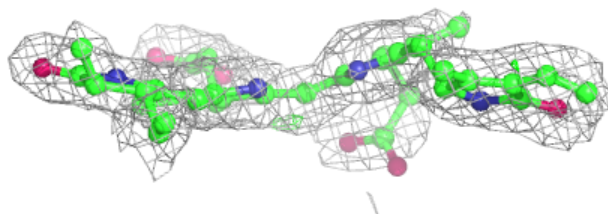
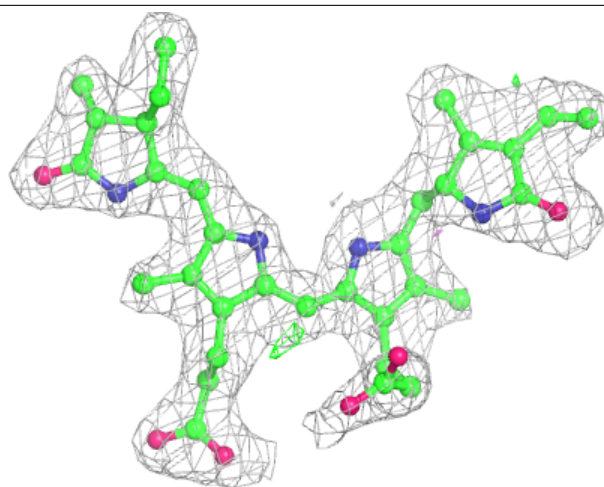
Electron density around PEB K 303:

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



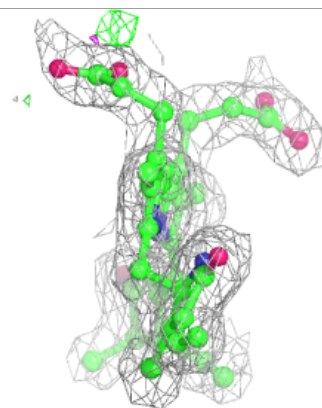
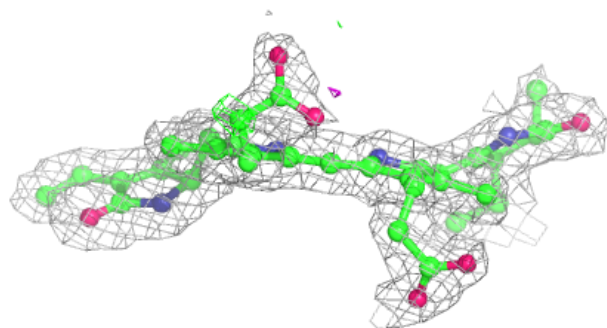
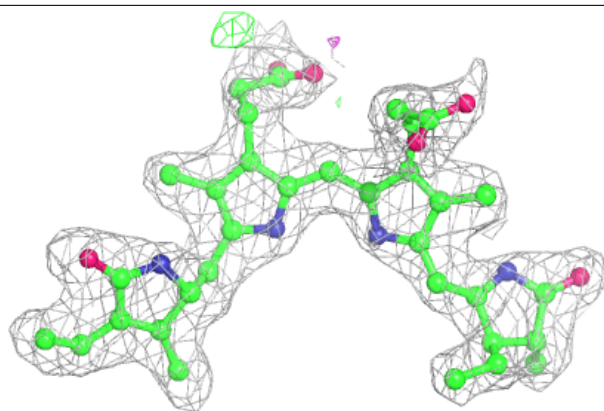
Electron density around PEB V 303:

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



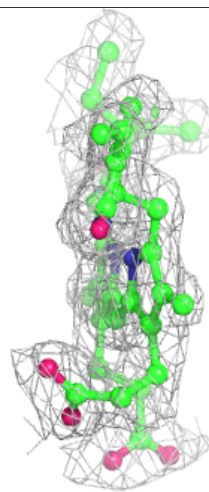
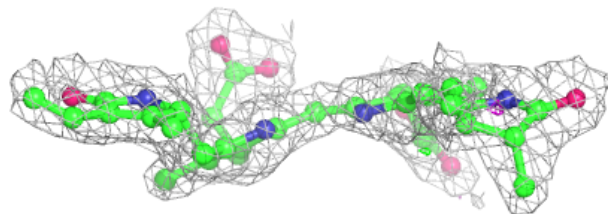
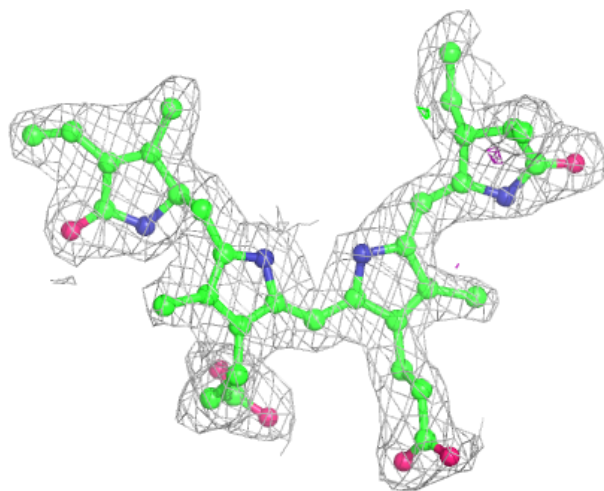
Electron density around PEB V 301:

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



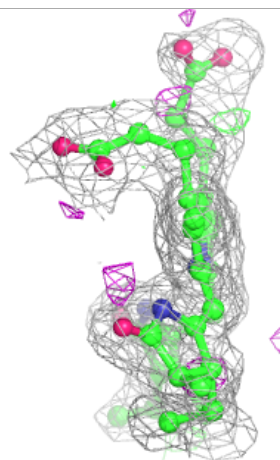
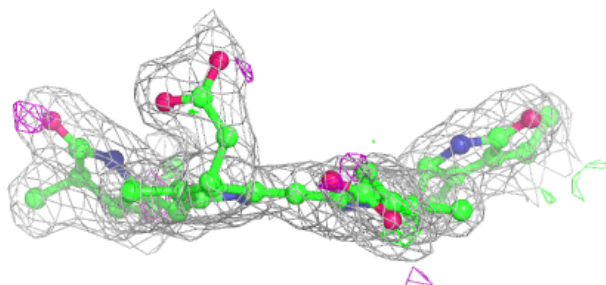
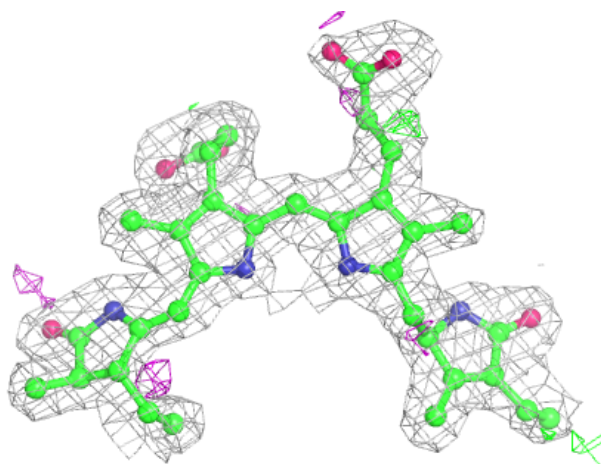
Electron density around PEB W 201:

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and green (positive)



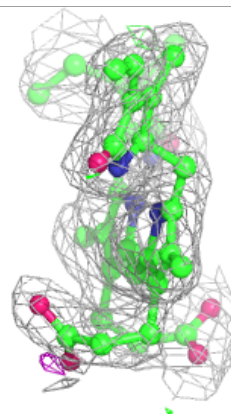
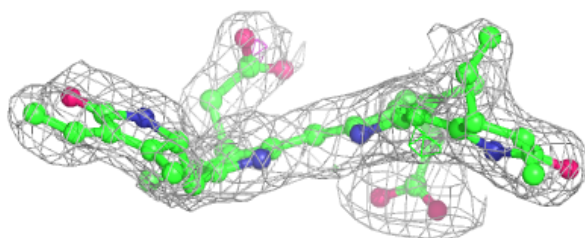
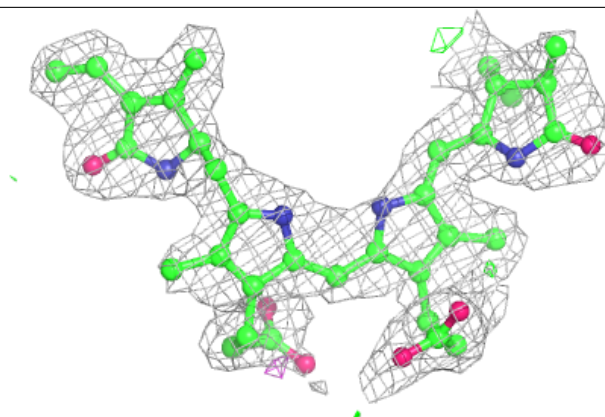
Electron density around PEB X 302:

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



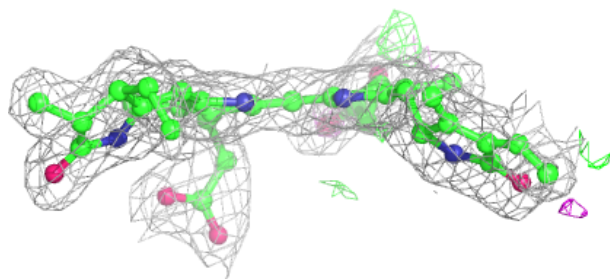
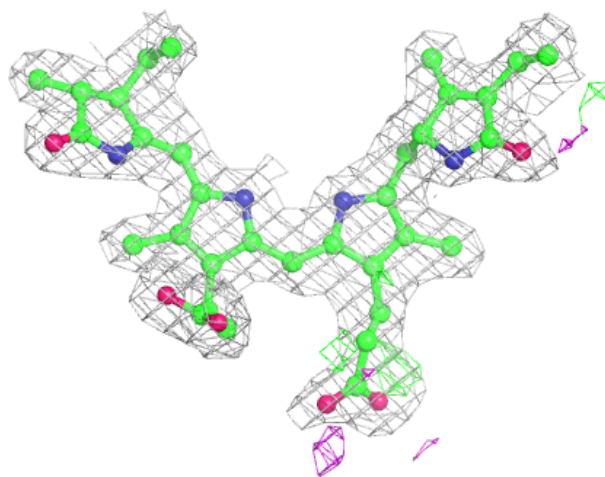
Electron density around PEB O 202:

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



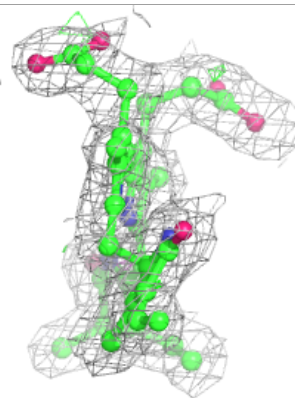
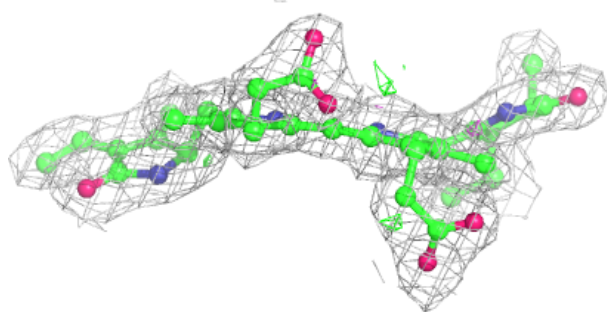
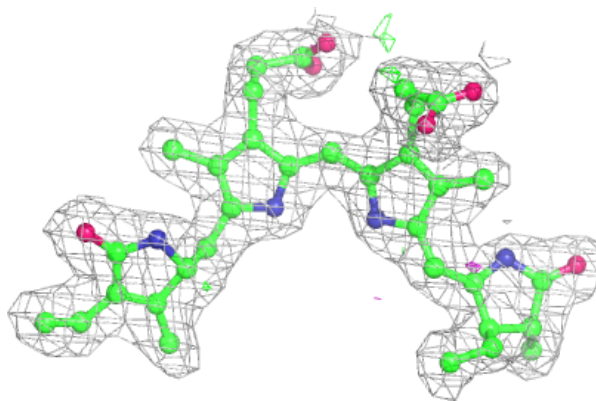
Electron density around PEB N 302:

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and green (positive)

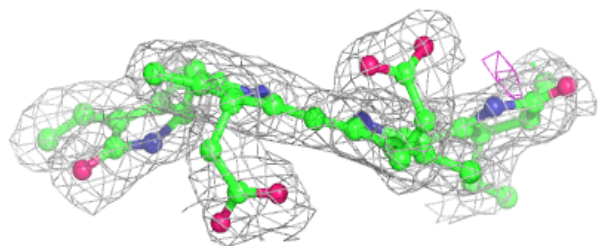
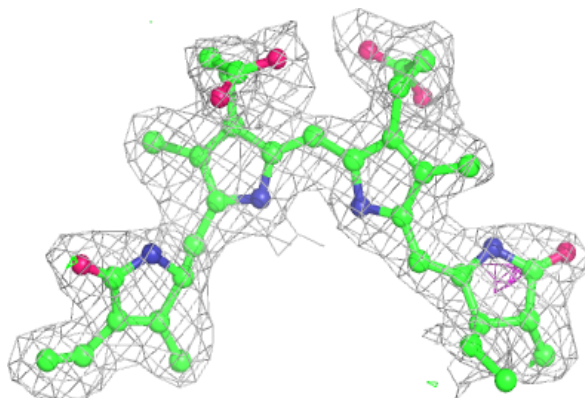


Electron density around PEB T 301:

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

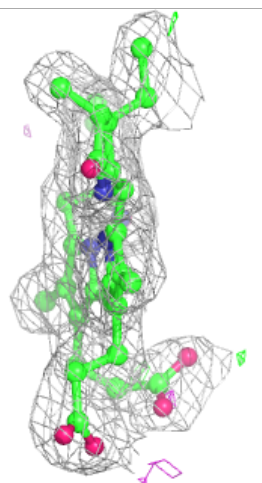
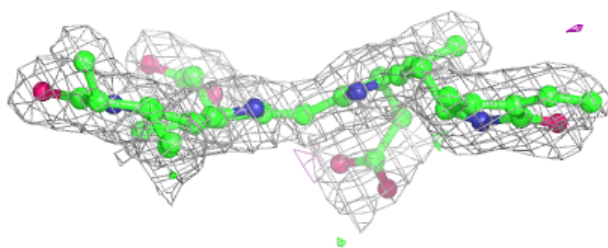
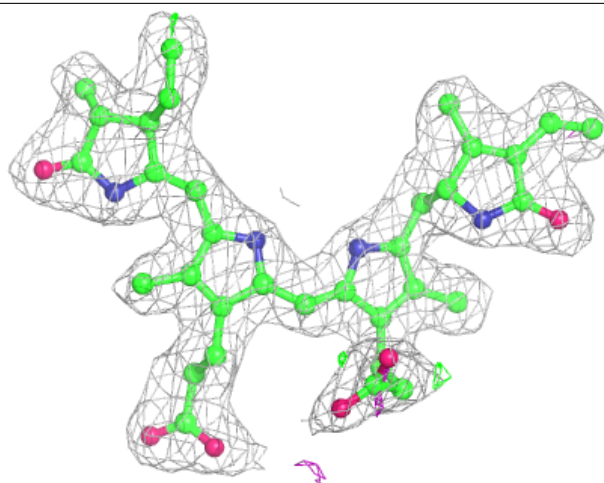
**Electron density around PEB U 202:**

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



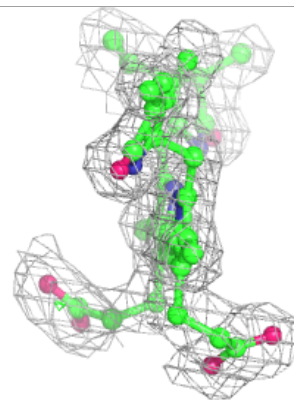
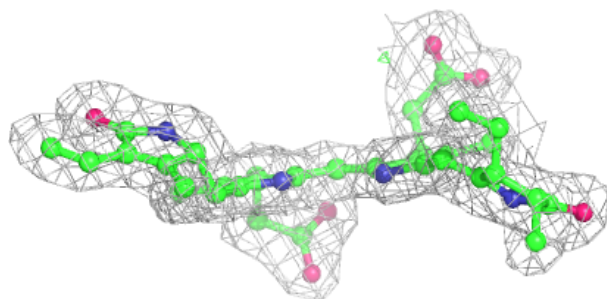
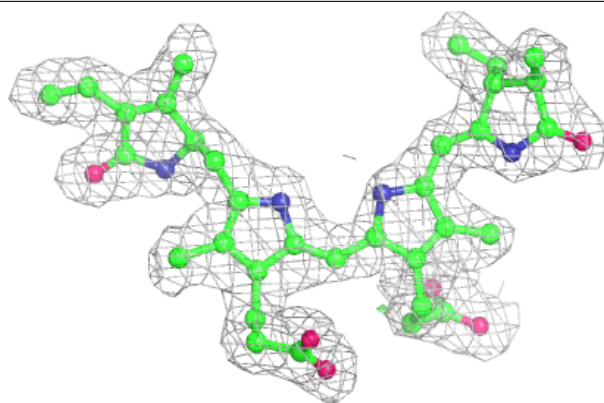
Electron density around PEB M 303:

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

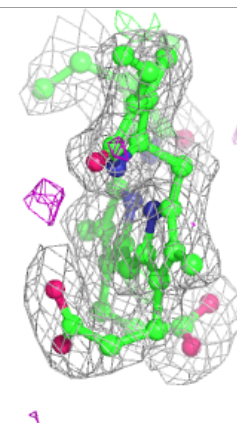
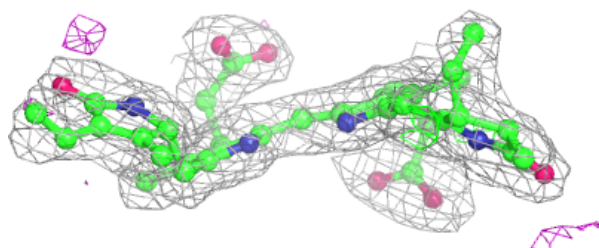
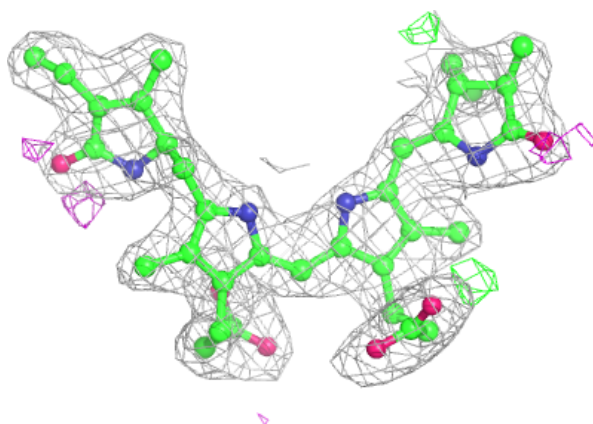


Electron density around PEB E 301:

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

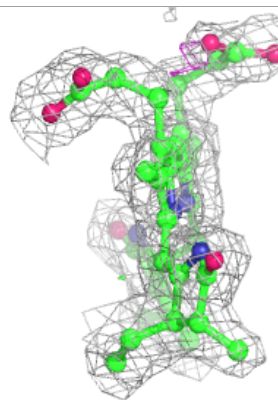
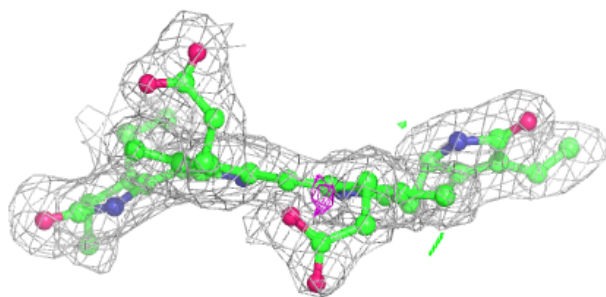
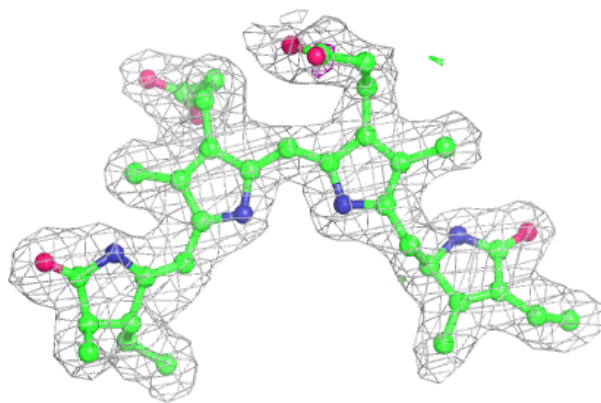
**Electron density around PEB J 202:**

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



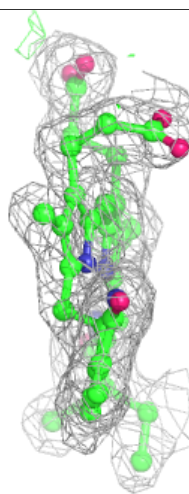
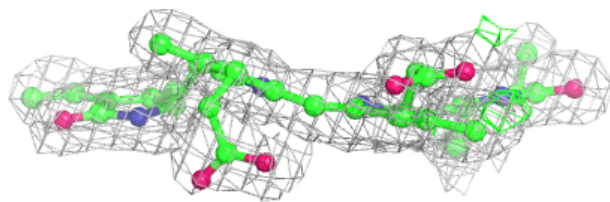
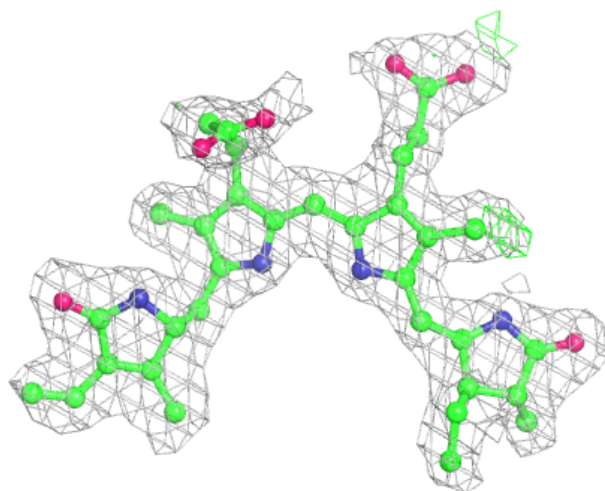
Electron density around PEB C 301:

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



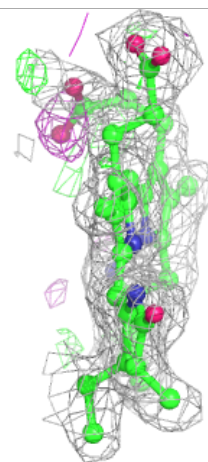
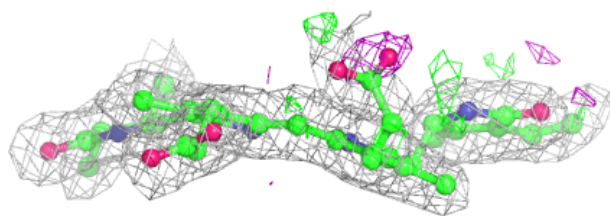
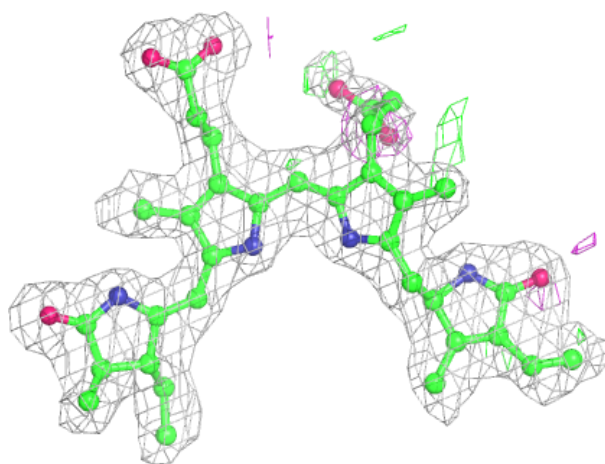
Electron density around PEB N 303:

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



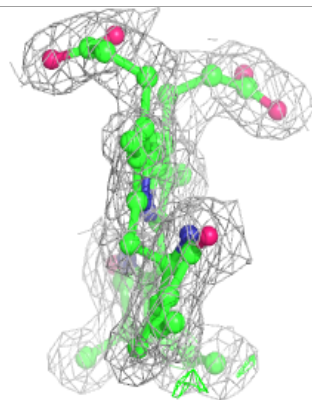
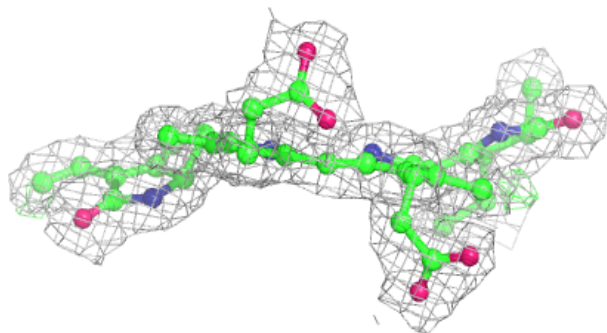
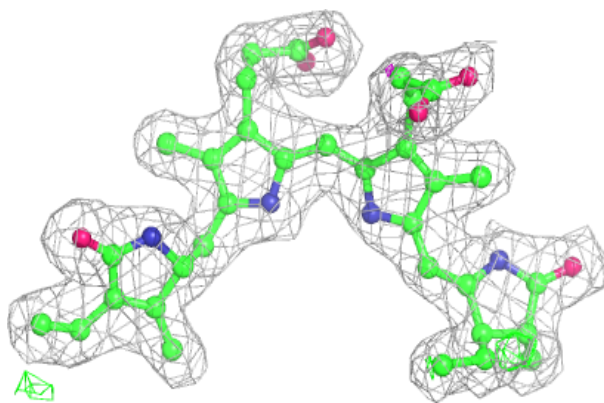
Electron density around PEB P 303:

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



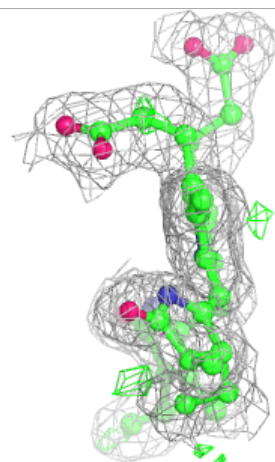
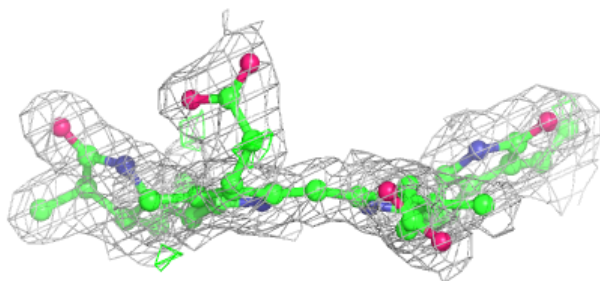
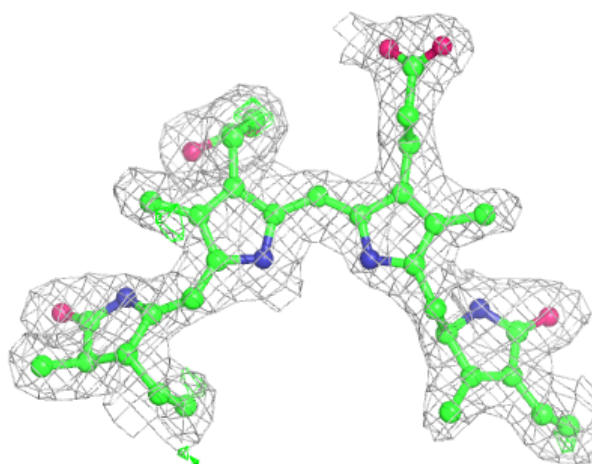
Electron density around PEB M 301:

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



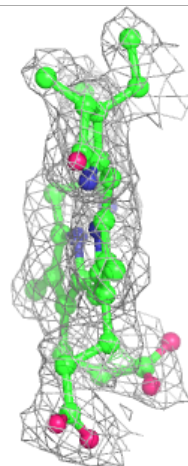
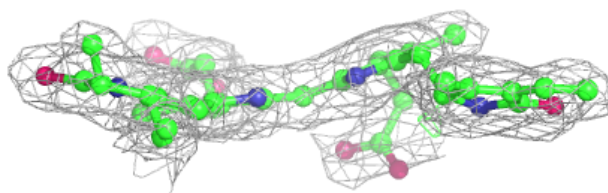
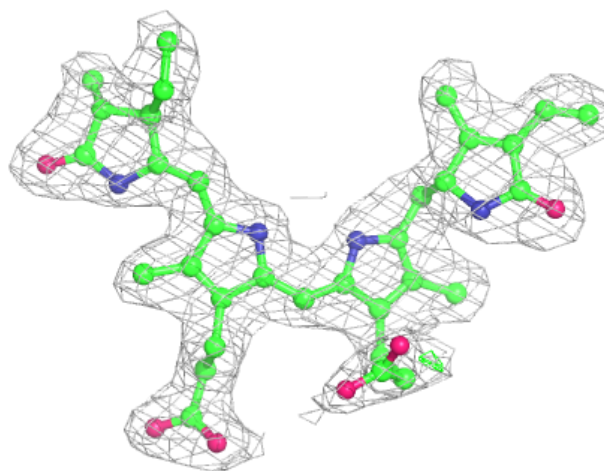
Electron density around PEB T 302:

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



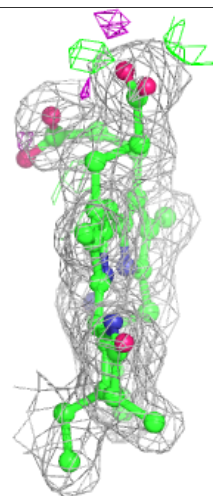
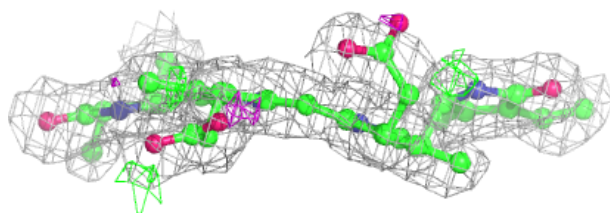
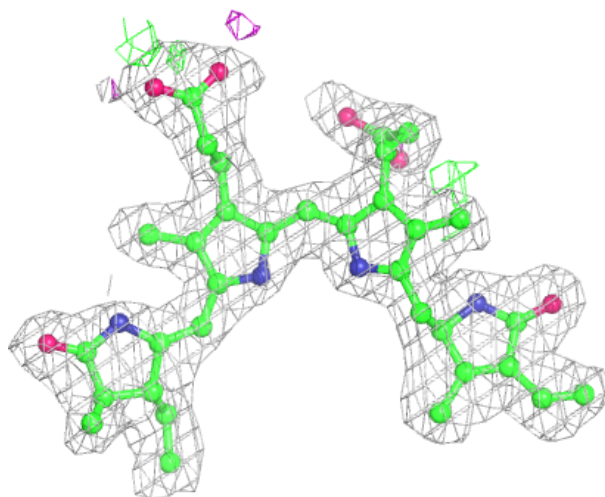
Electron density around PEB T 303:

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



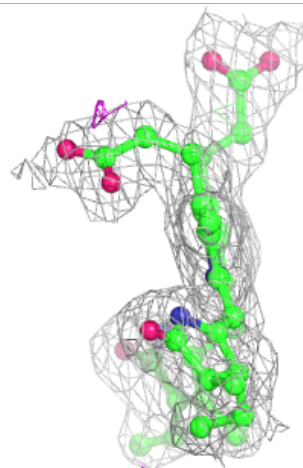
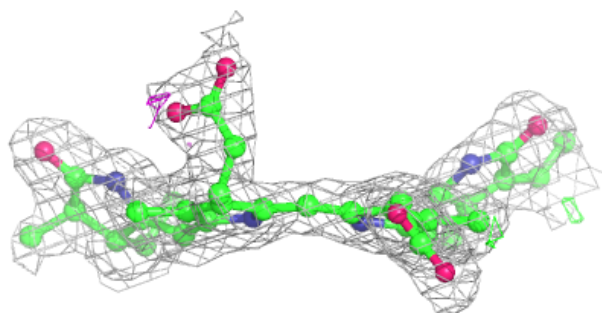
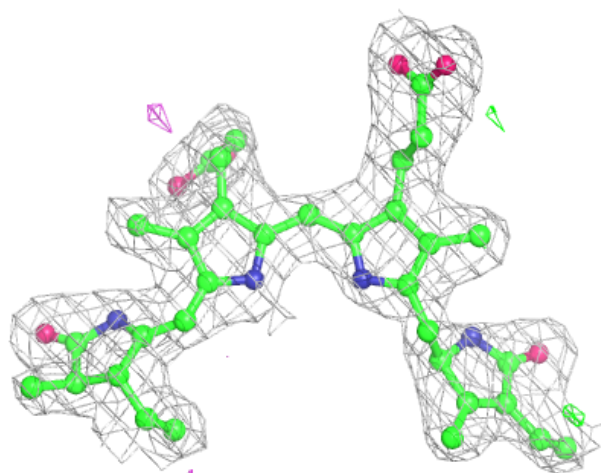
Electron density around PEB E 303:

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



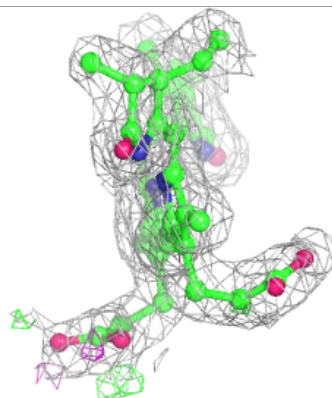
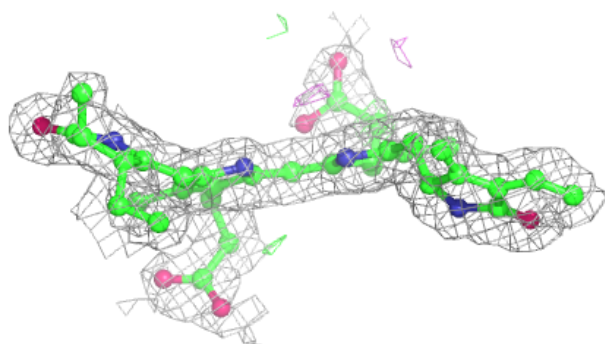
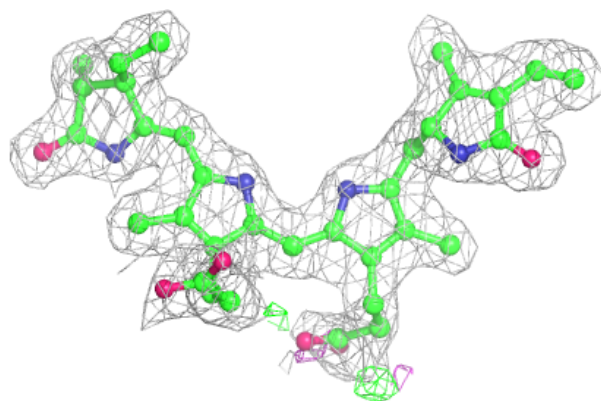
Electron density around PEB V 302:

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



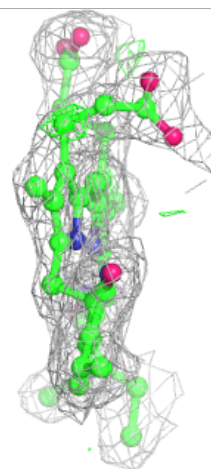
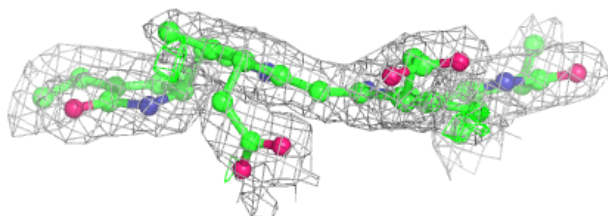
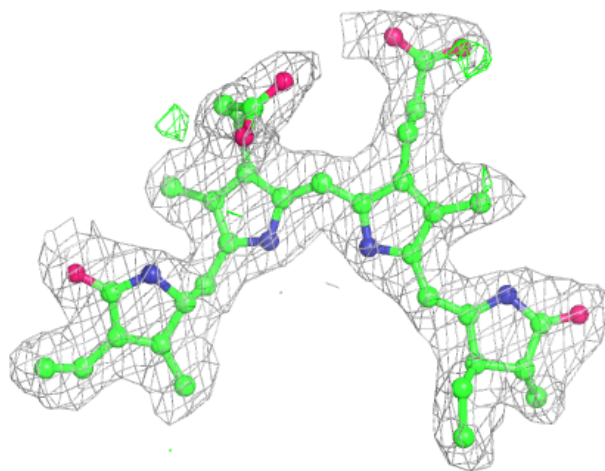
Electron density around PEB I 301:

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



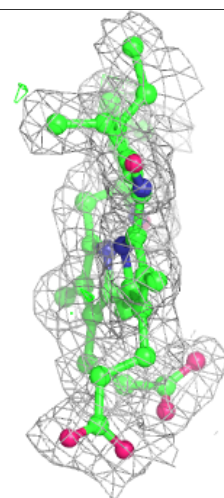
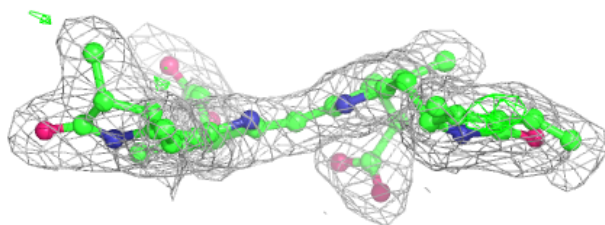
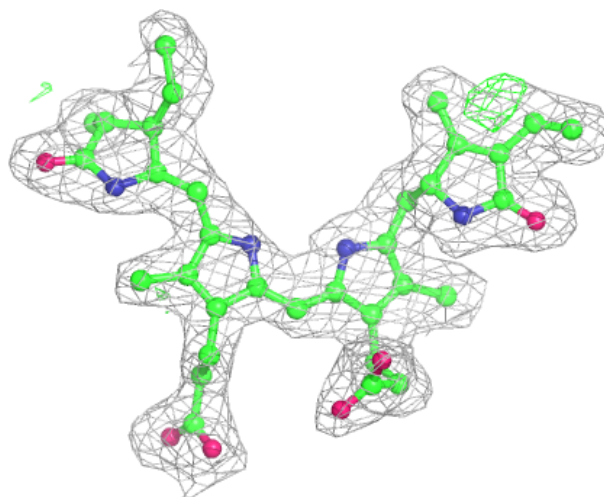
Electron density around PEB I 303:

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



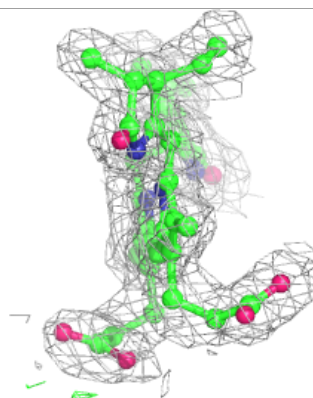
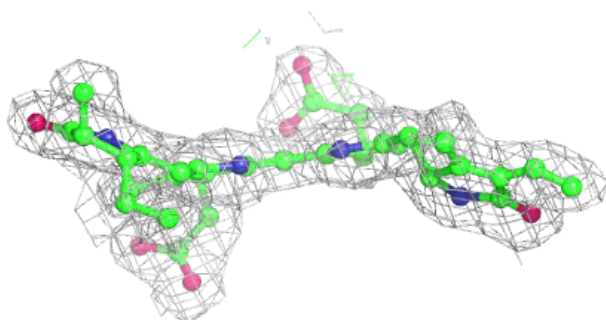
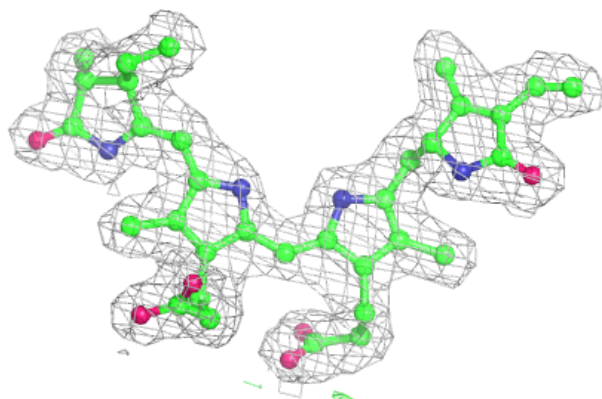
Electron density around PEB B 201:

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

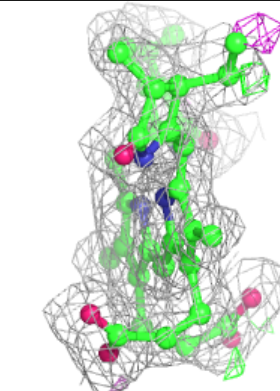
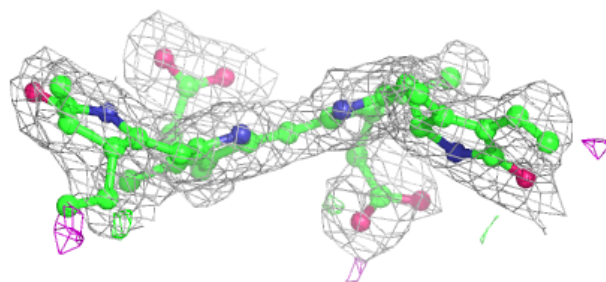
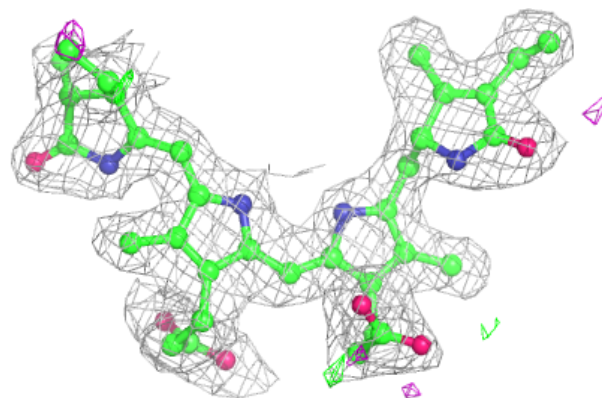


Electron density around PEB K 301:

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

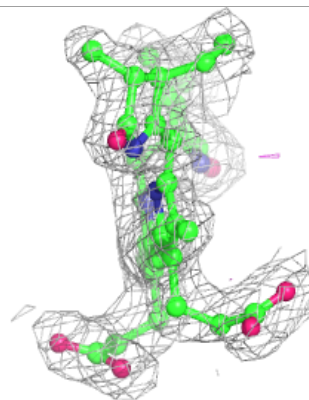
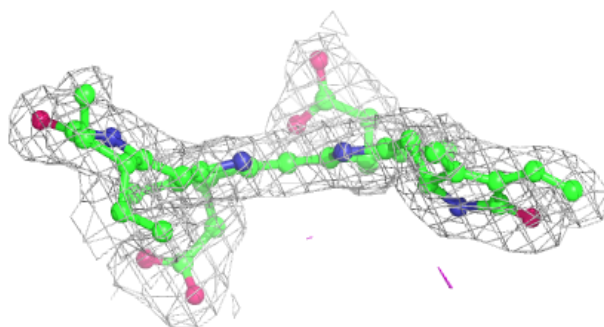
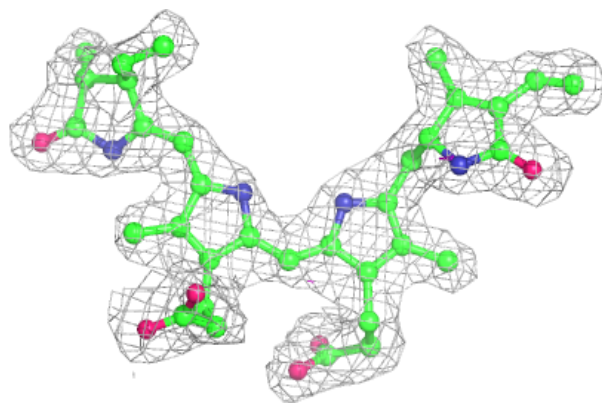
**Electron density around PEB B 202:**

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



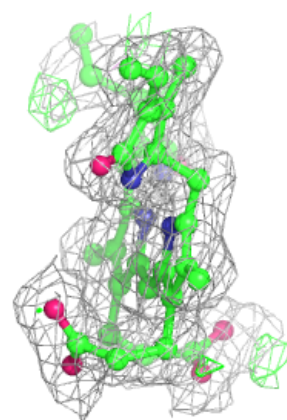
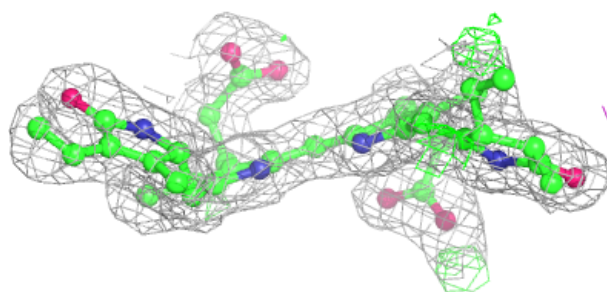
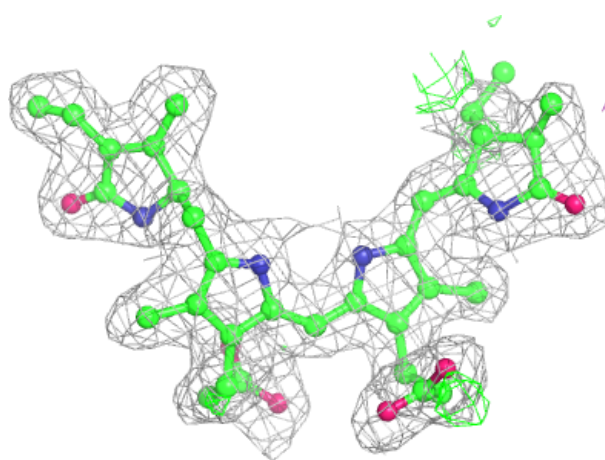
Electron density around PEB N 301:

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



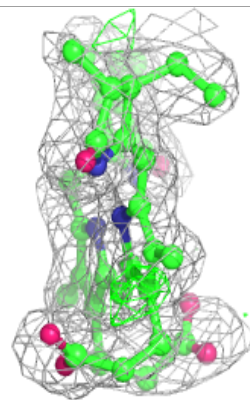
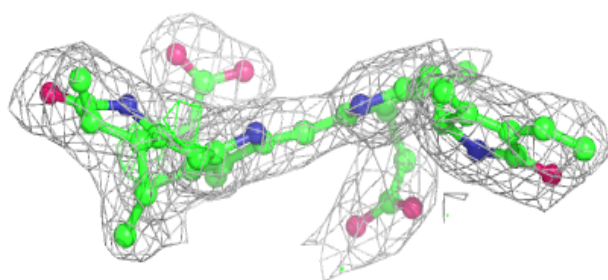
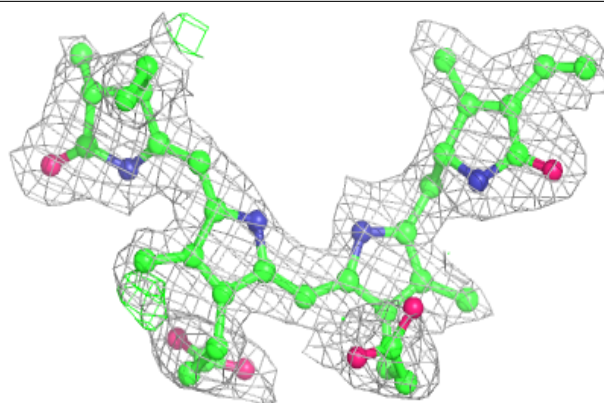
Electron density around PEB F 202:

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

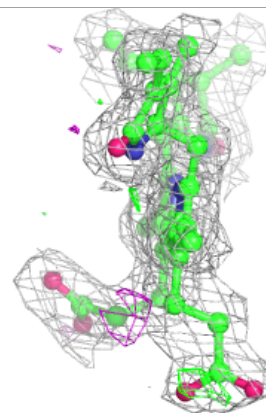
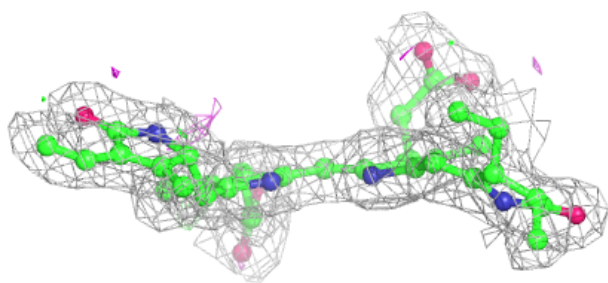
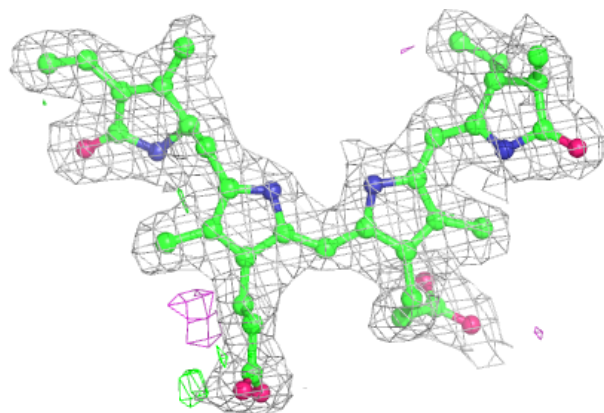


Electron density around PEB W 202:

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

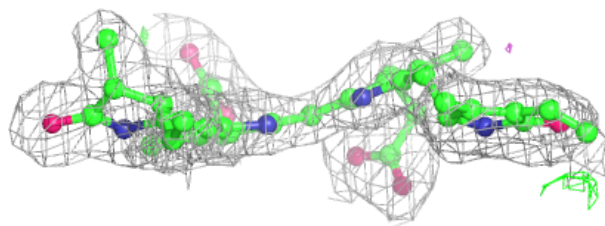
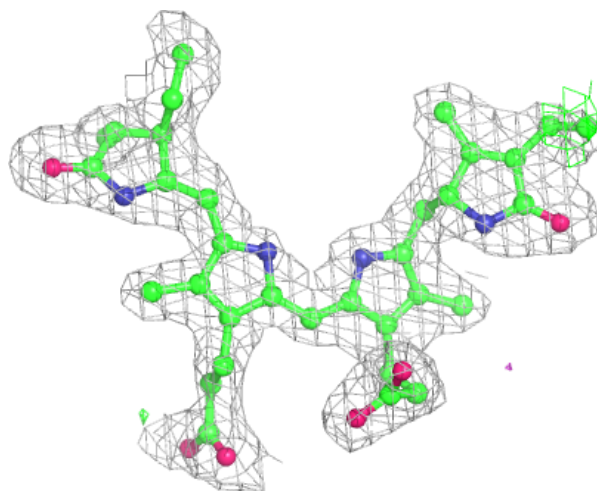
**Electron density around PEB P 301:**

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



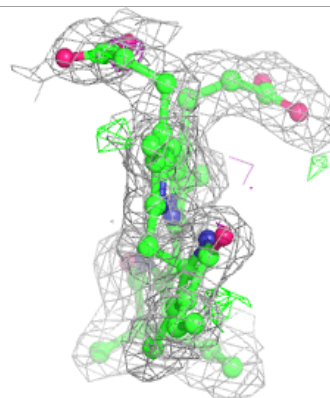
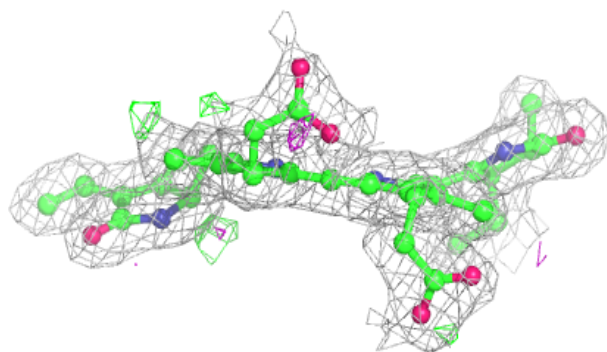
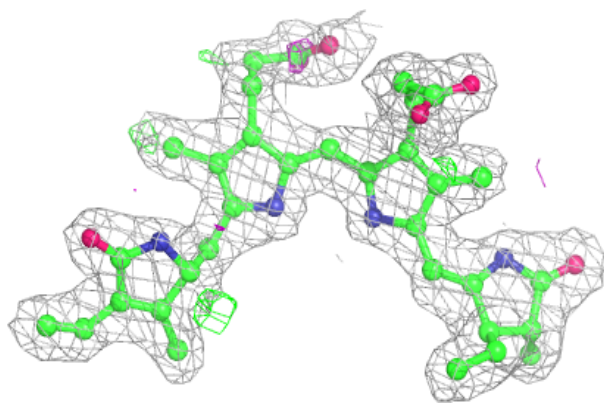
Electron density around PEB H 201:

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

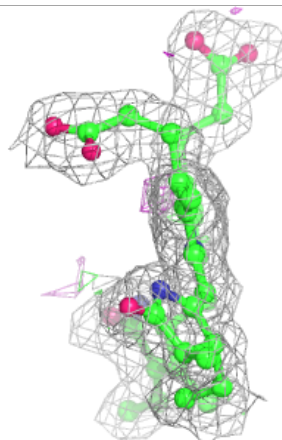
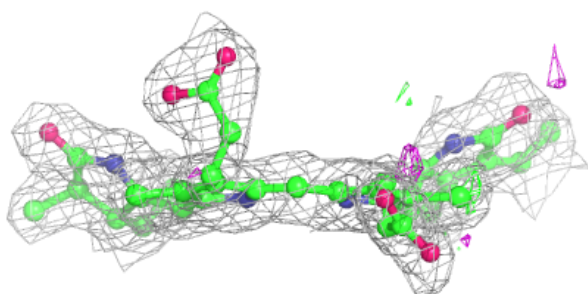
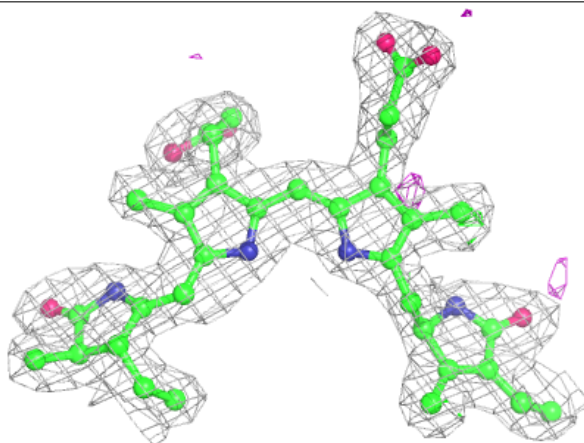


Electron density around PEB R 301:

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

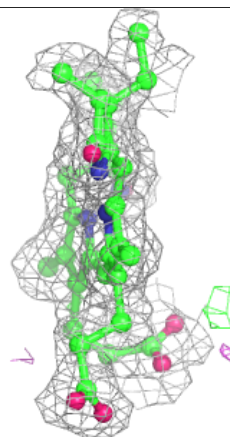
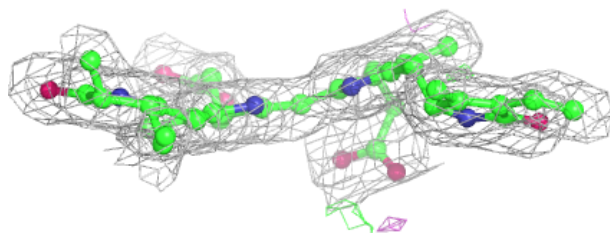
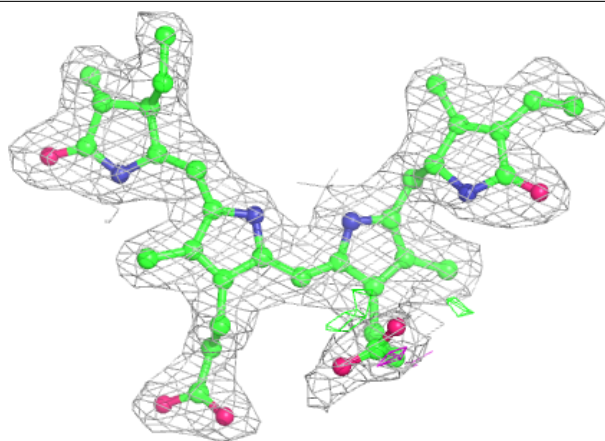
**Electron density around PEB R 302:**

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



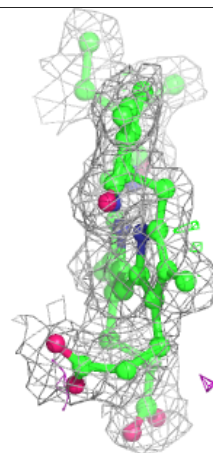
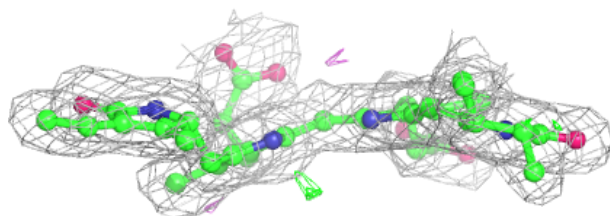
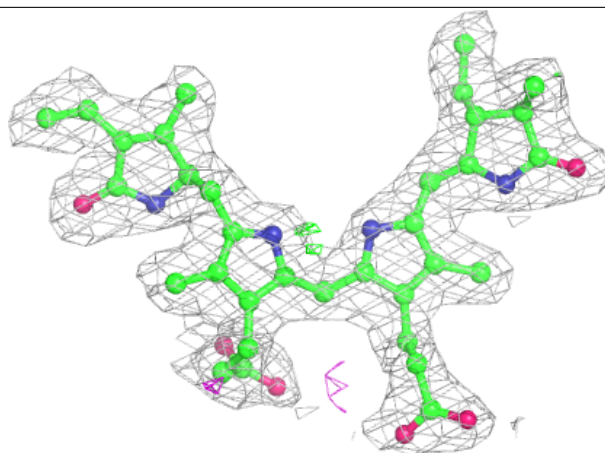
Electron density around PEB R 303:

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

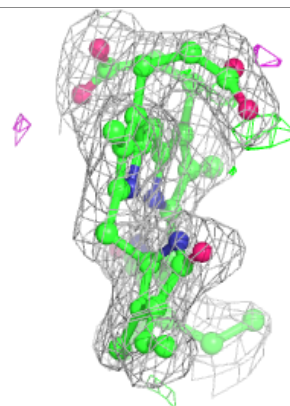
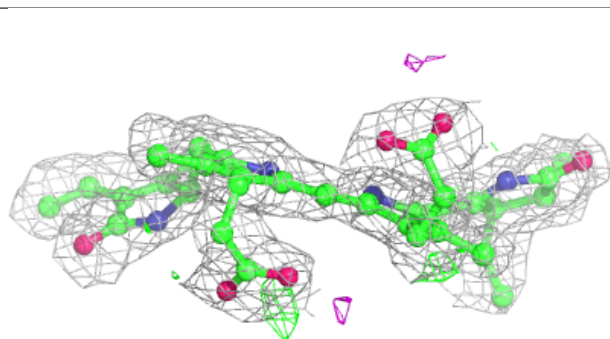
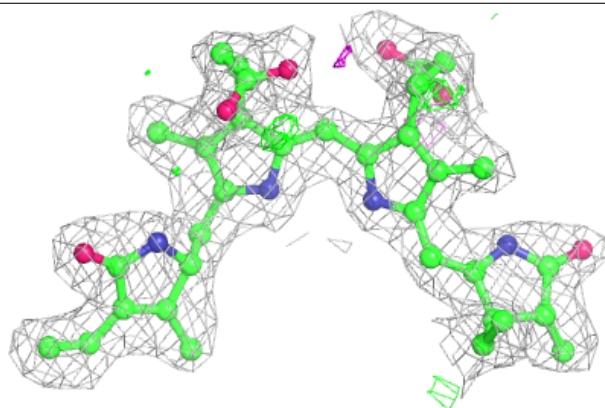


Electron density around PEB C 303:

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

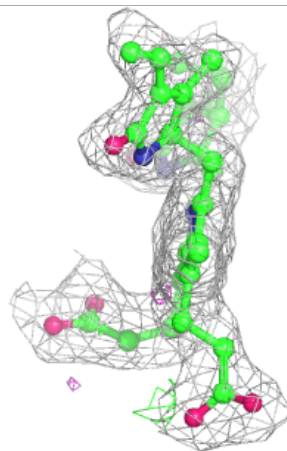
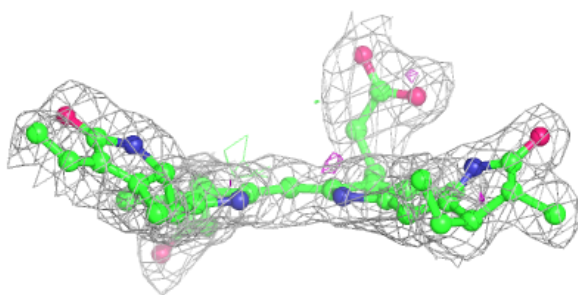
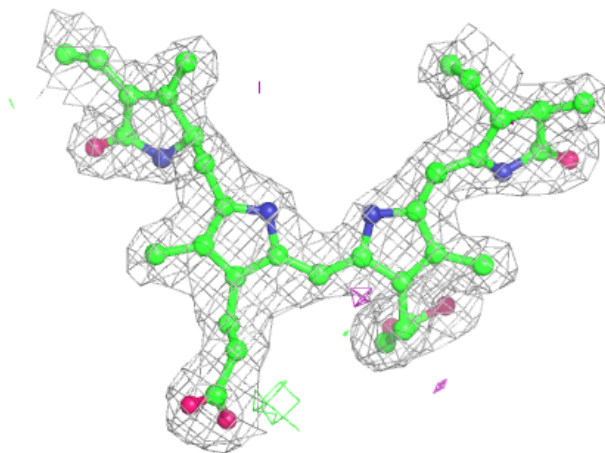
**Electron density around PEB H 202:**

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



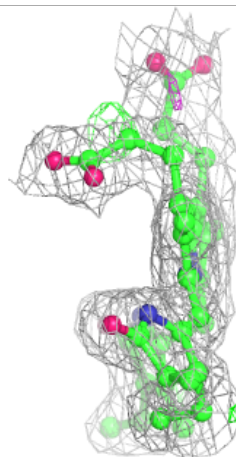
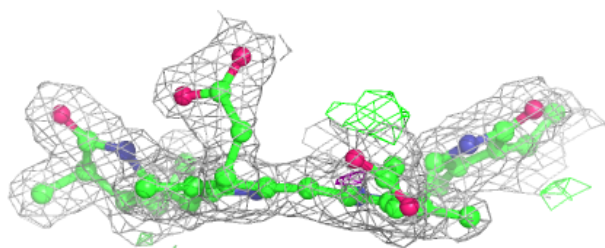
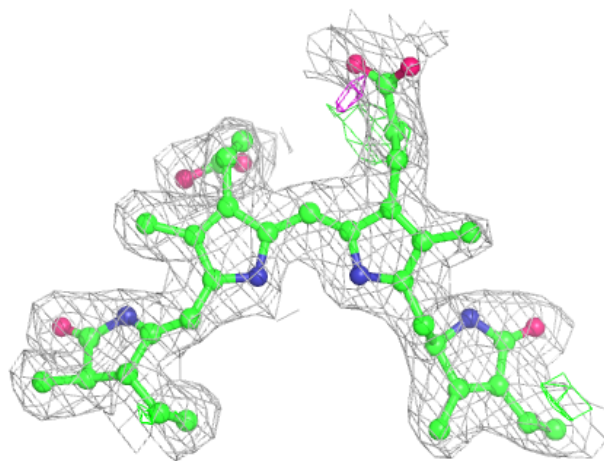
Electron density around PEB E 302:

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



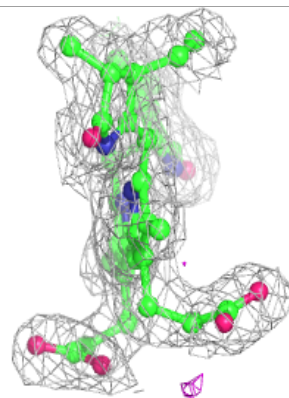
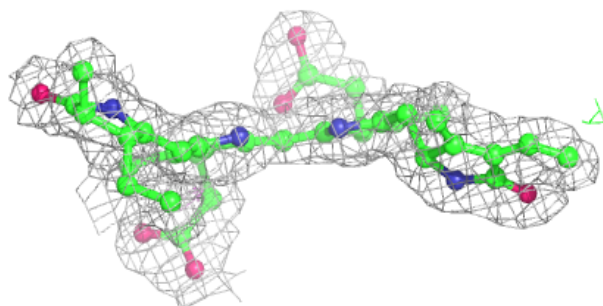
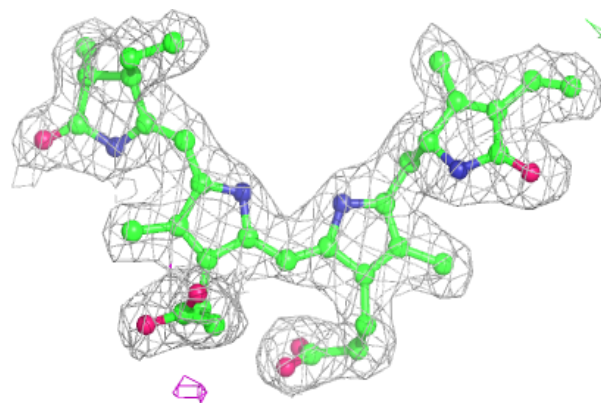
Electron density around PEB M 302:

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



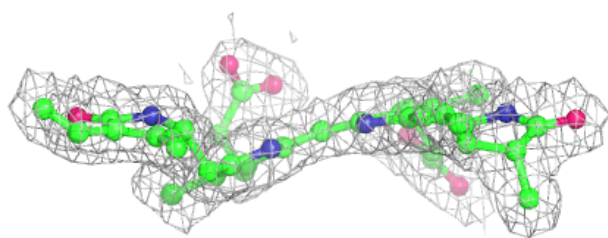
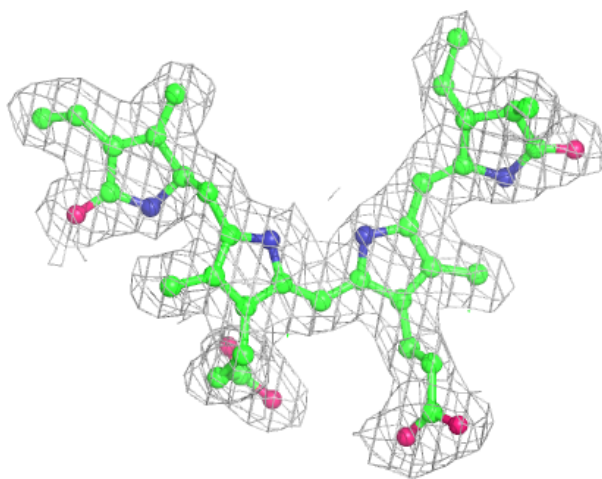
Electron density around PEB G 301:

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



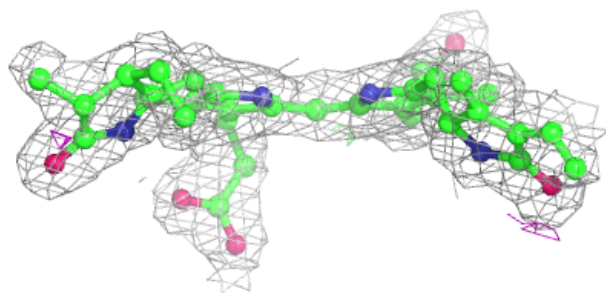
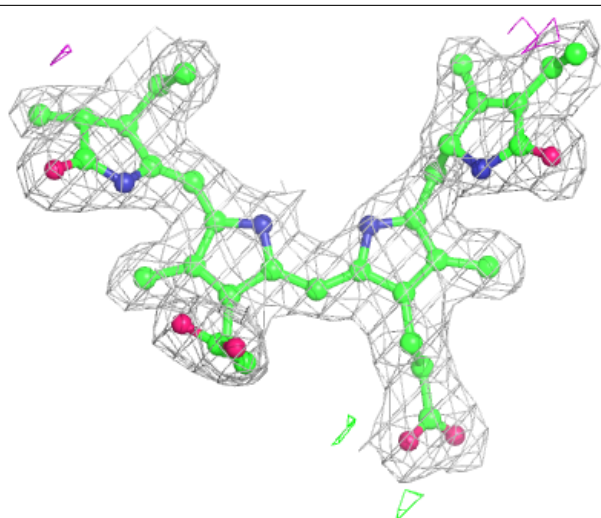
Electron density around PEB D 201:

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



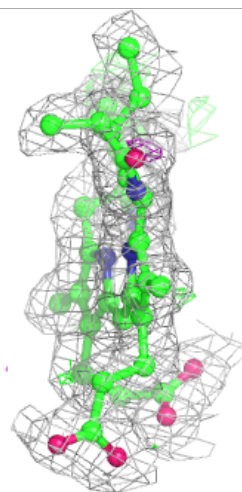
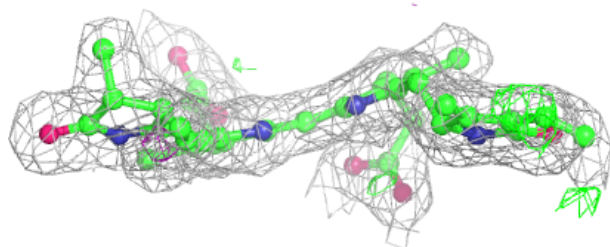
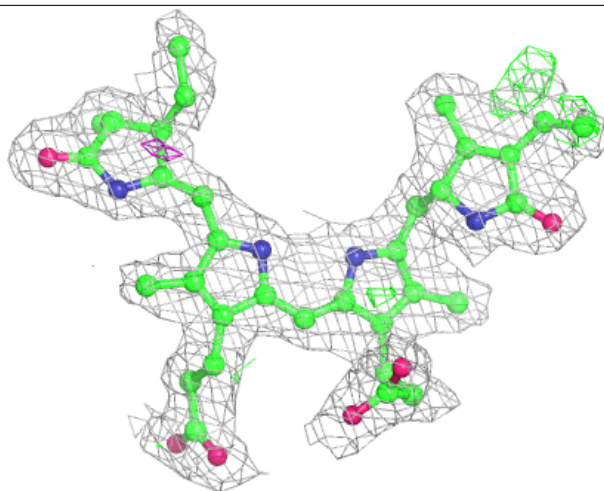
Electron density around PEB I 302:

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



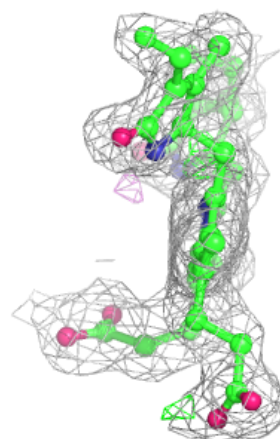
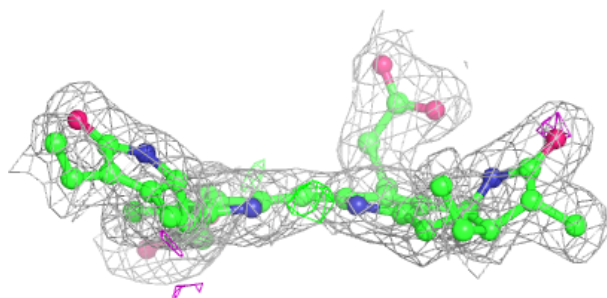
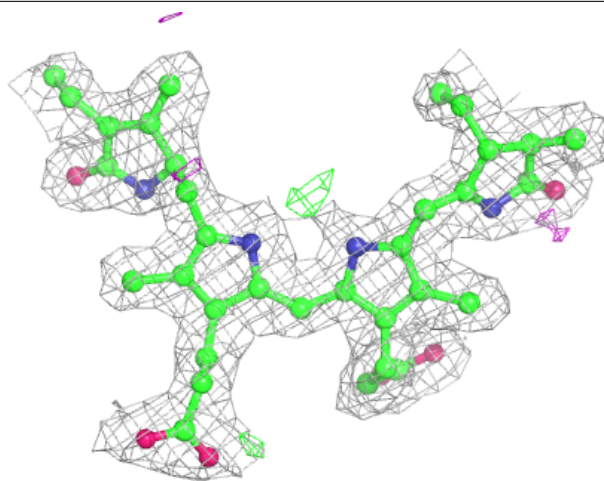
Electron density around PEB A 201:

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



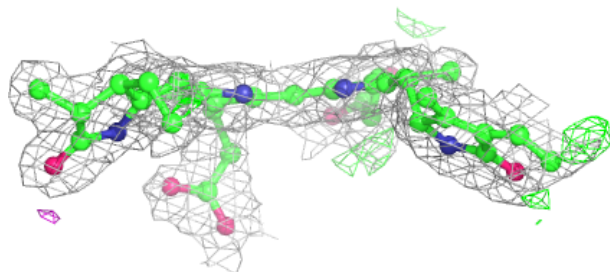
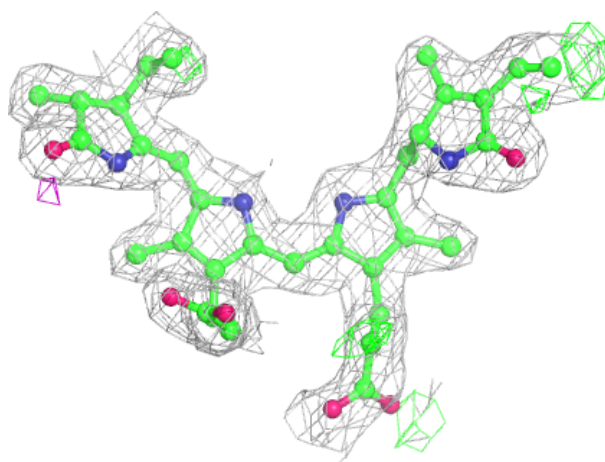
Electron density around PEB P 302:

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



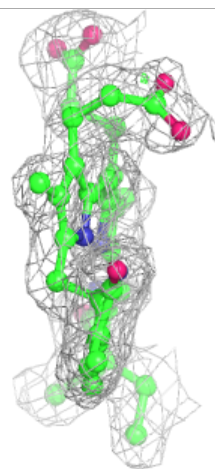
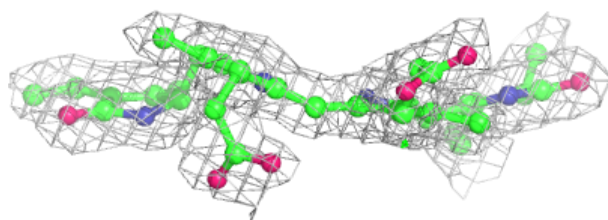
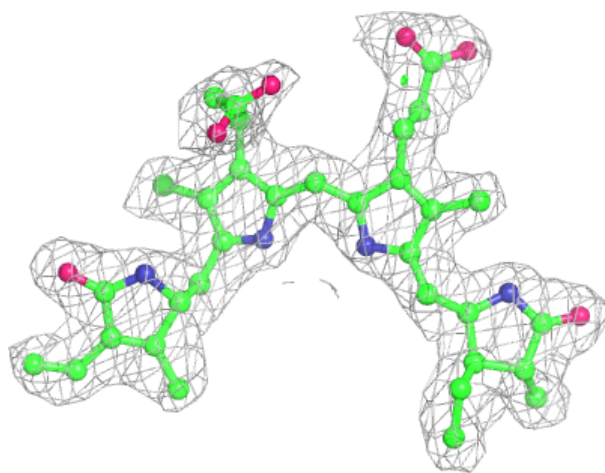
Electron density around PEB G 302:

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



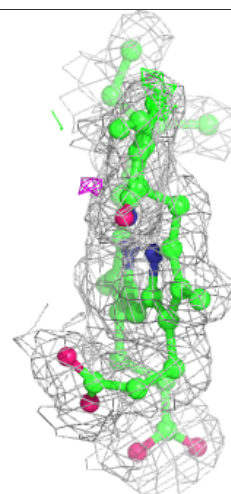
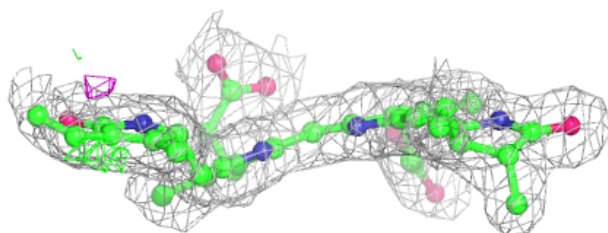
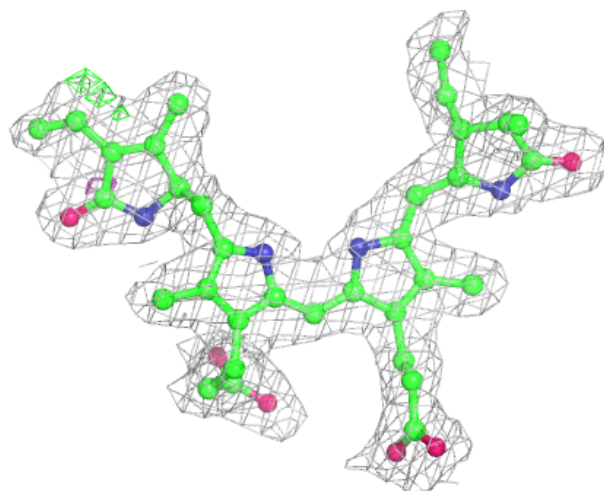
Electron density around PEB G 303:

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



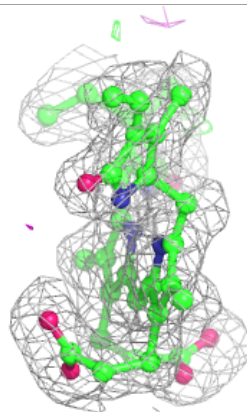
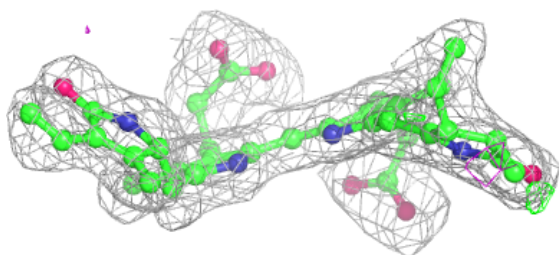
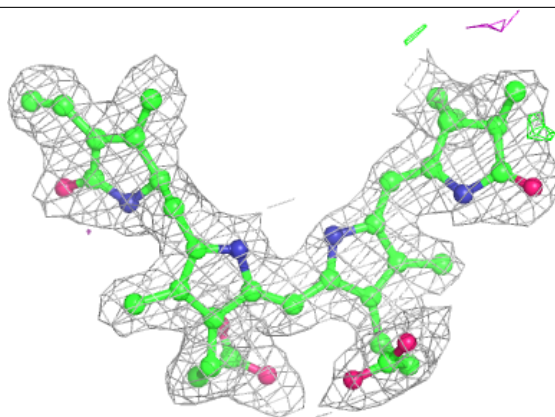
Electron density around PEB F 201:

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

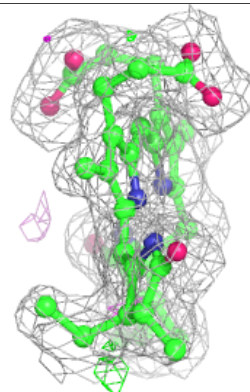
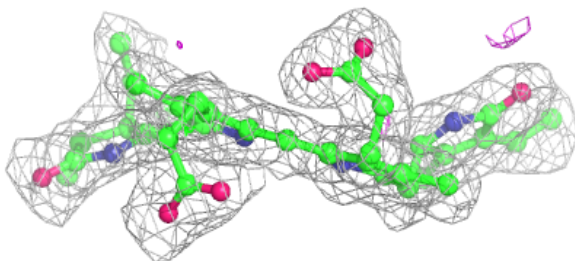
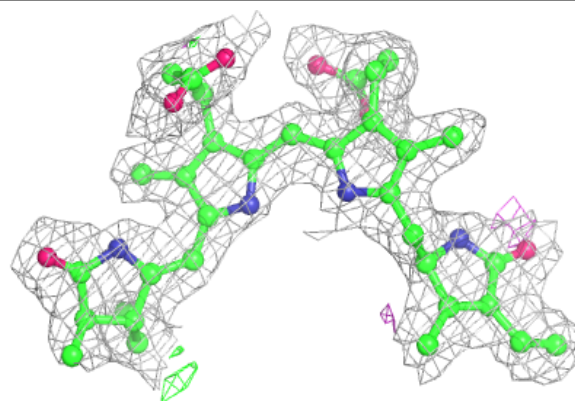


Electron density around PEB L 202:

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

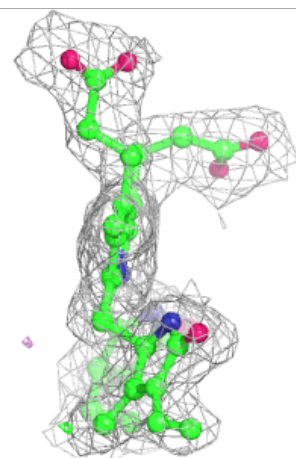
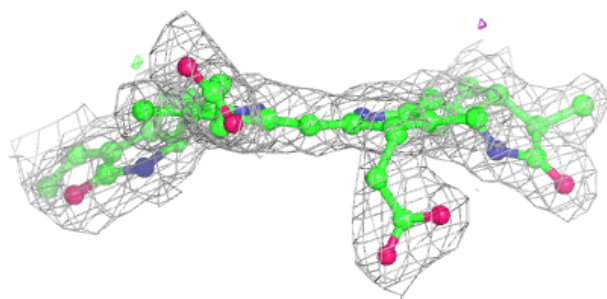
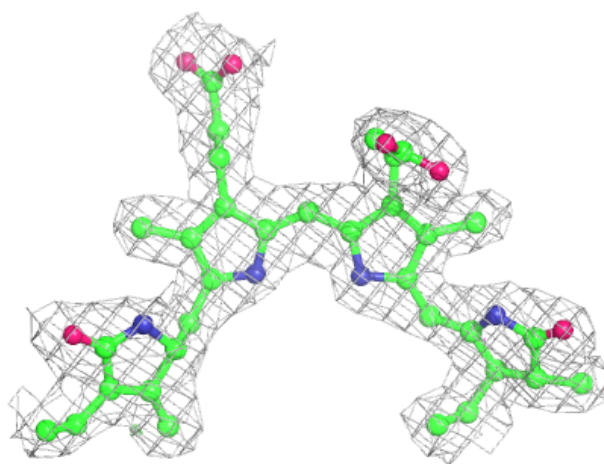
**Electron density around PEB D 202:**

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



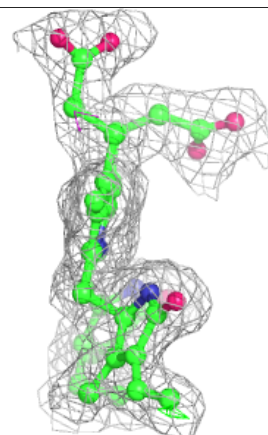
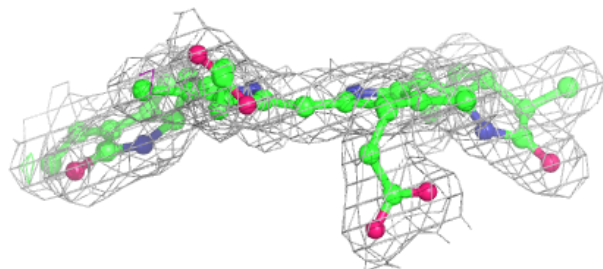
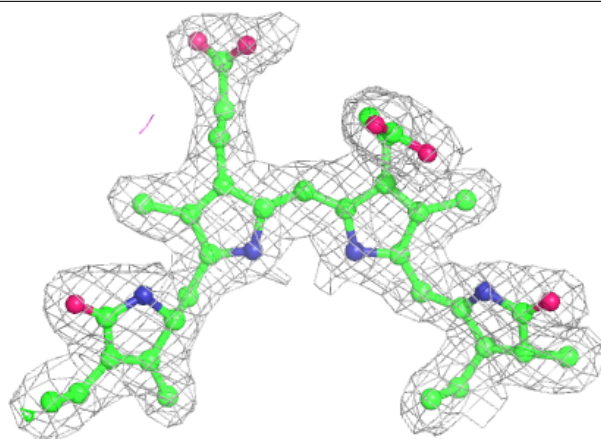
Electron density around PEB C 302:

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



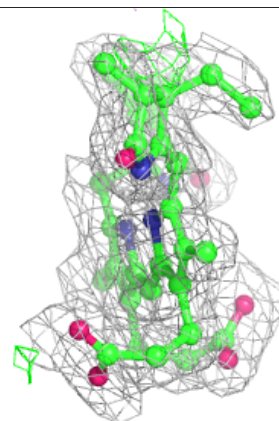
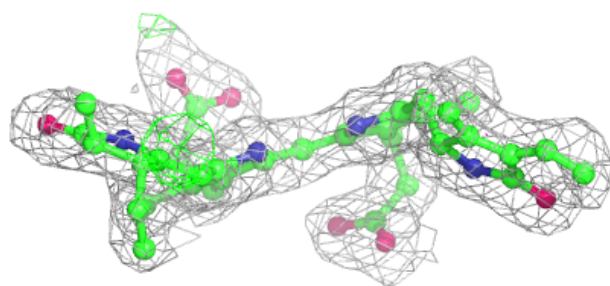
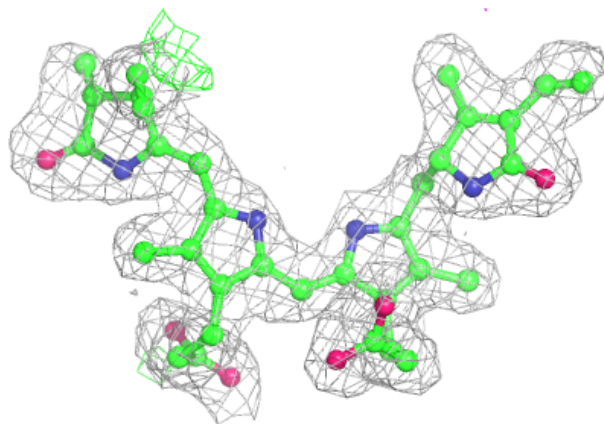
Electron density around PEB K 302:

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



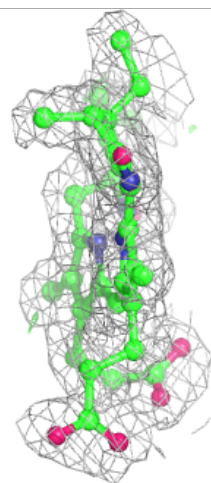
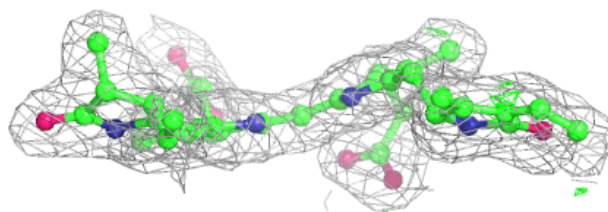
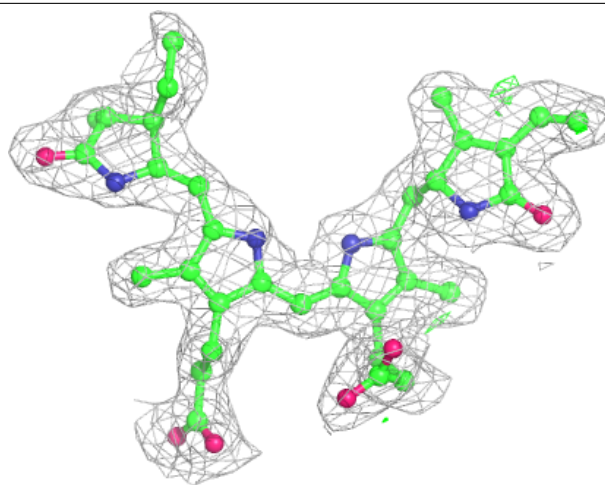
Electron density around PEB A 202:

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



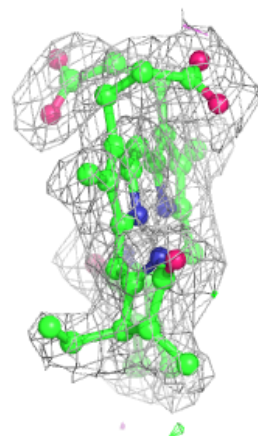
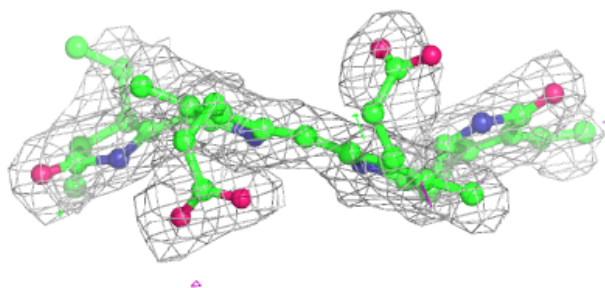
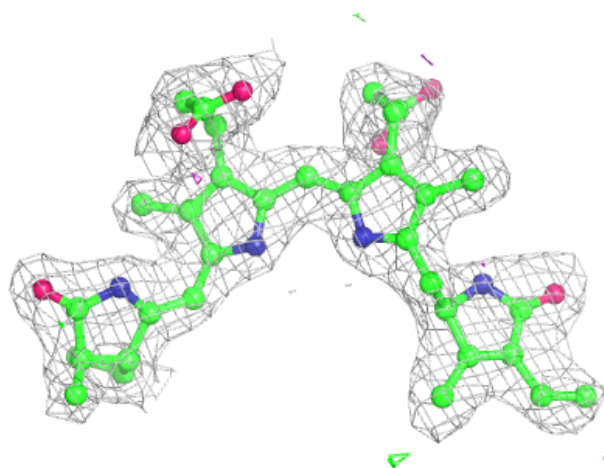
Electron density around PEB Q 201:

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



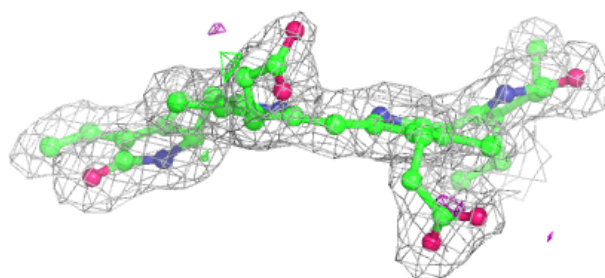
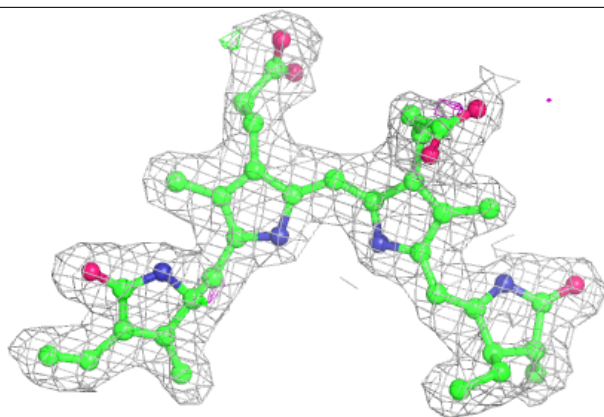
Electron density around PEB Q 202:

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



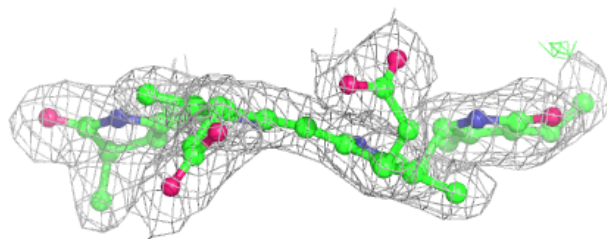
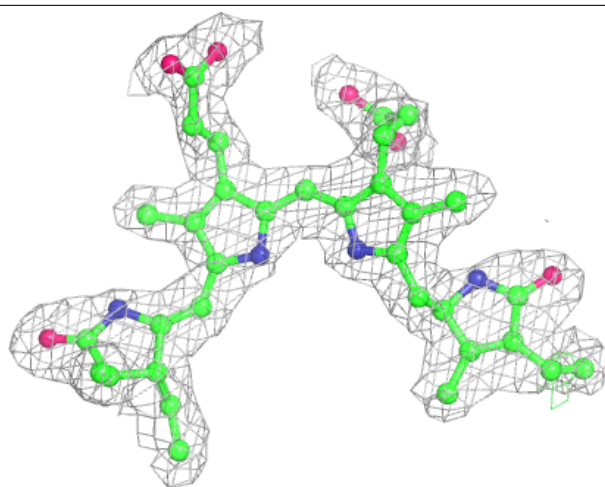
Electron density around PEB X 301:

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



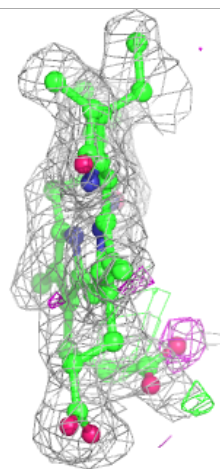
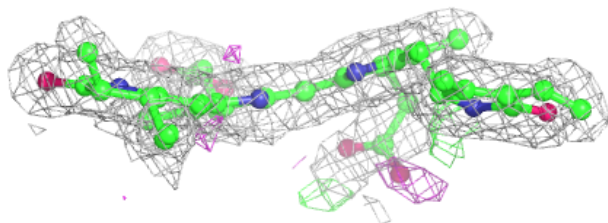
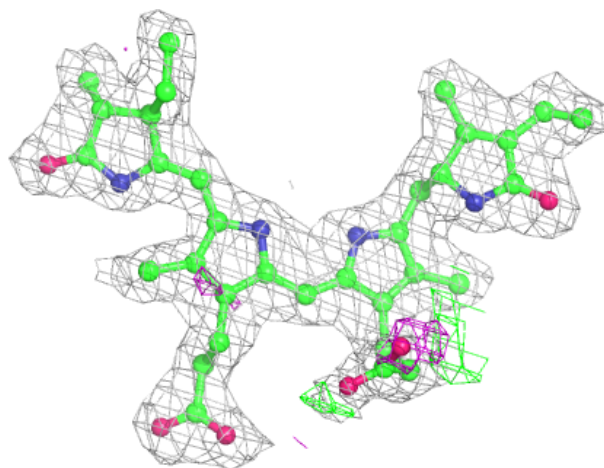
Electron density around PEB U 201:

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



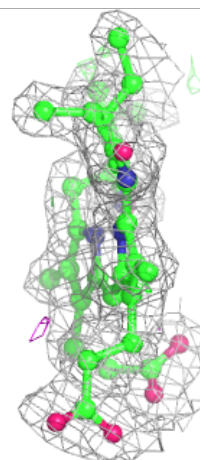
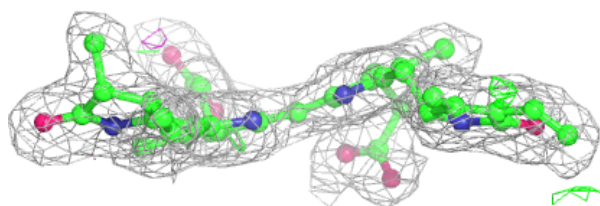
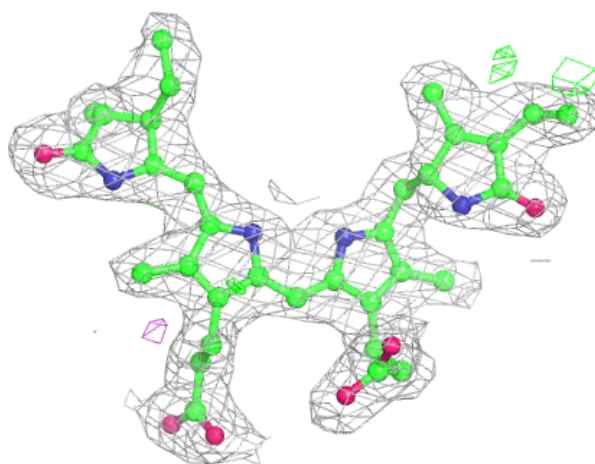
Electron density around PEB X 303:

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



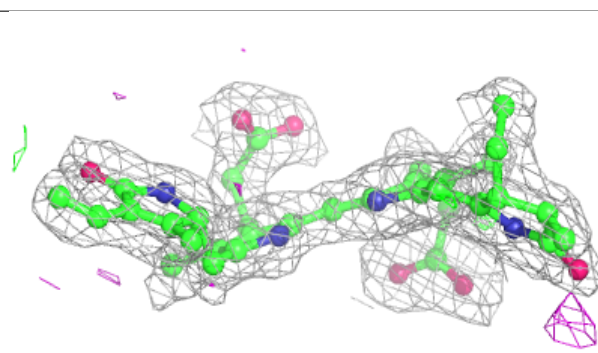
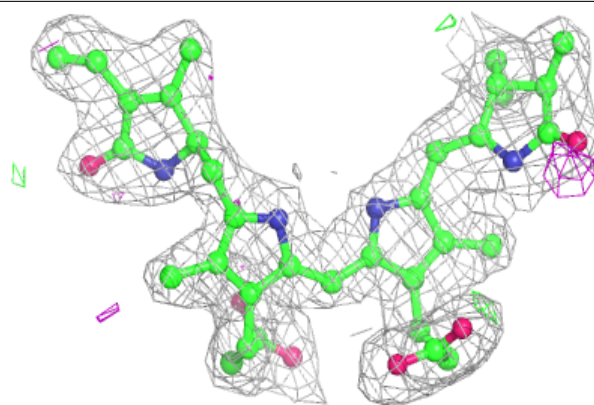
Electron density around PEB Y 201:

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



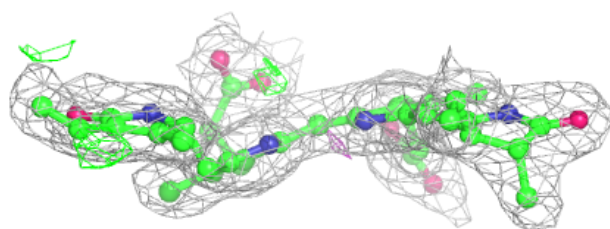
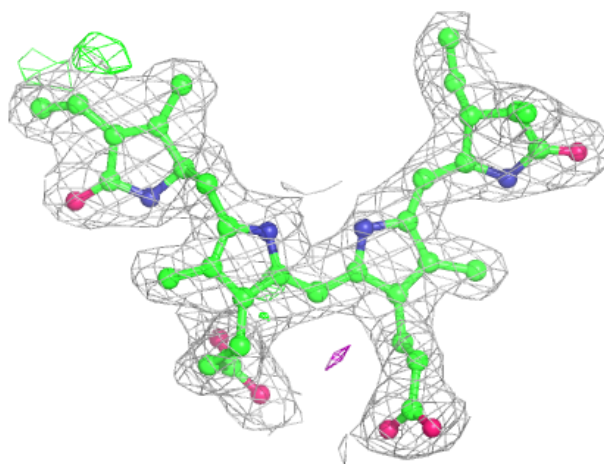
Electron density around PEB Y 202:

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



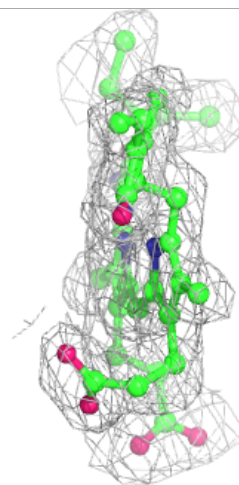
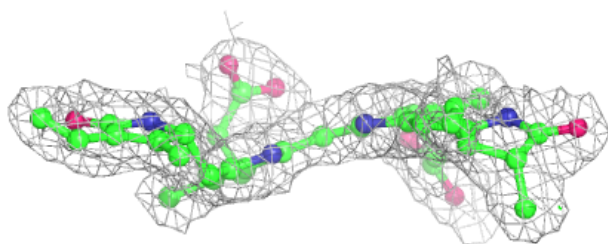
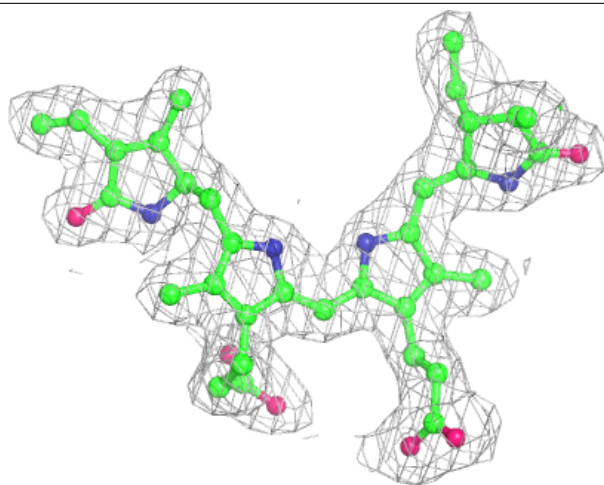
Electron density around PEB J 201:

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



Electron density around PEB L 201:

$2mF_o-DF_c$ (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.