



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2026 – 10:59 PM UTC

PDB ID : 5NB4 / pdb_00005nb4
Title : Atomic resolution structure of C-phycoerythrin from marine cyanobacterium
Phormidium sp. A09DM at pH 7.5
Authors : Sonani, R.R.; Roszak, A.W.; Ortmann de Percin Northumberland, C.;
Madamwar, D.; Cogdell, R.J.
Deposited on : 2017-03-01
Resolution : 1.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

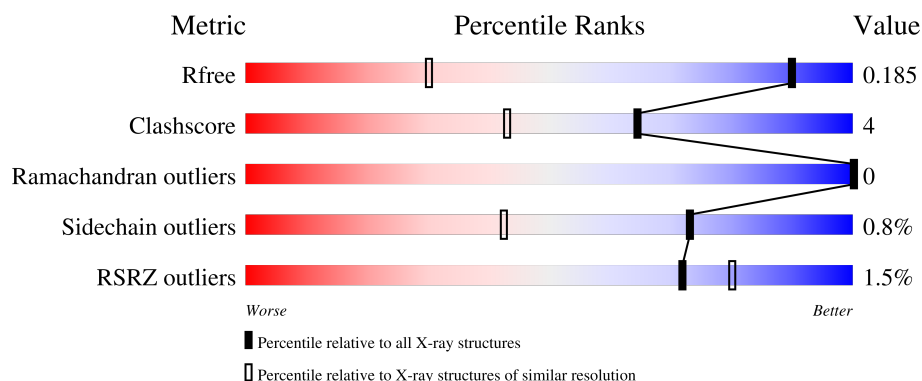
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

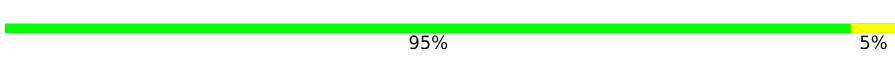
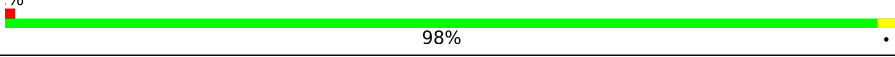
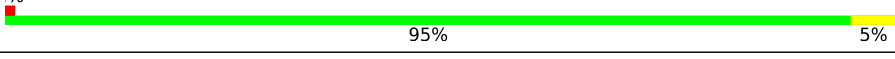
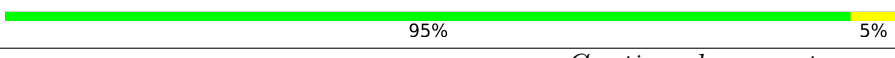
The reported resolution of this entry is 1.14 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1380 (1.16-1.12)
Clashscore	190562	1393 (1.16-1.12)
Ramachandran outliers	187476	1369 (1.16-1.12)
Sidechain outliers	187428	1369 (1.16-1.12)
RSRZ outliers	180081	1379 (1.16-1.12)

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

Mol	Chain	Length	Quality of chain
1	A	164	
1	B	164	
1	C	164	
1	D	164	

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Mol	Chain	Length	Quality of chain
1	E	164	% 95% • •
1	F	164	% 87% 11% •
1	G	164	% 95% 5%
1	H	164	2% 94% 6%
1	I	164	95% 5%
1	J	164	95% 5%
1	K	164	95% • •
1	L	164	96% •
2	M	184	2% 96% • •
2	N	184	% 94% 5% •
2	O	184	2% 93% 7%
2	P	184	3% 91% 9%
2	Q	184	2% 94% 6%
2	R	184	5% 89% 11% •
2	S	184	3% 94% 6%
2	T	184	5% 91% 9% •
2	U	184	4% 90% 9% •
2	V	184	% 95% 5% •
2	W	184	% 93% 7%
2	X	184	% 93% 7%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 43607 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 Alpha subunit,Phycoerythrin Alpha subunit,P hycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	10	0
			1300	812	229	252	7			
1	B	164	Total	C	N	O	S	0	8	0
			1292	805	227	253	7			
1	C	164	Total	C	N	O	S	0	9	0
			1298	810	227	254	7			
1	D	164	Total	C	N	O	S	0	10	0
			1314	822	233	252	7			
1	E	164	Total	C	N	O	S	0	8	0
			1292	805	227	253	7			
1	F	164	Total	C	N	O	S	0	11	0
			1316	820	230	259	7			
1	G	164	Total	C	N	O	S	0	8	0
			1301	811	228	255	7			
1	H	164	Total	C	N	O	S	0	10	0
			1316	820	231	258	7			
1	I	164	Total	C	N	O	S	0	12	0
			1315	823	229	256	7			
1	J	164	Total	C	N	O	S	0	10	0
			1306	816	228	255	7			
1	K	164	Total	C	N	O	S	0	10	0
			1304	813	228	256	7			
1	L	164	Total	C	N	O	S	0	8	0
			1300	811	230	252	7			

- Molecule 2 is a protein called Phycoerythrin Beta subunit,Phycoerythrin Beta subunit.

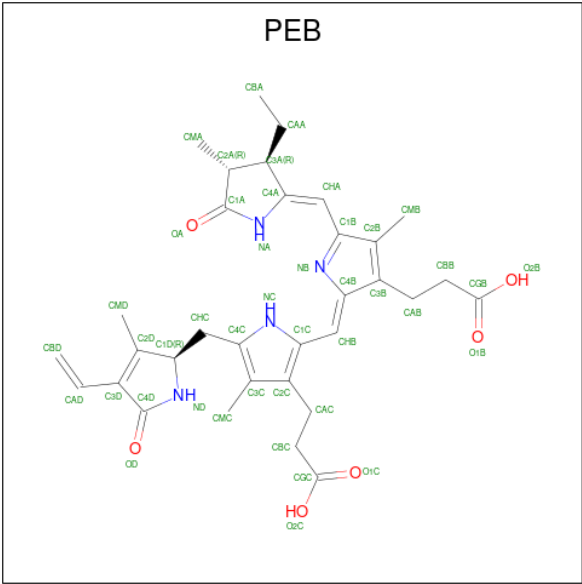
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	184	Total	C	N	O	S	0	12	0
			1416	876	254	273	13			
2	N	184	Total	C	N	O	S	0	12	0
			1411	868	252	277	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	O	184	Total 1400	867	252	268	13	0	9	0
2	P	184	Total 1401	865	249	273	14	0	11	0
2	Q	184	Total 1394	862	248	271	13	0	10	0
2	R	184	Total 1402	867	251	271	13	0	10	0
2	S	184	Total 1410	870	251	275	14	0	12	0
2	T	184	Total 1407	871	247	276	13	0	12	0
2	U	184	Total 1441	892	257	279	13	0	16	0
2	V	184	Total 1437	888	255	280	14	0	16	0
2	W	184	Total 1423	880	251	278	14	0	15	0
2	X	184	Total 1401	865	251	272	13	0	11	0

- Molecule 3 is PHYCOERYTHROBILIN (CCD ID: PEB) (formula: C₃₃H₄₀N₄O₆).



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

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

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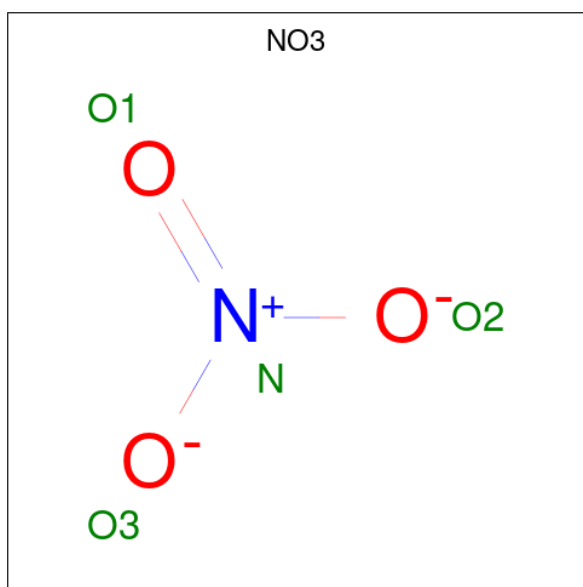
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	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	O	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	P	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	Q	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	S	1	Total 49	C 37	N 4	O 8	0	1

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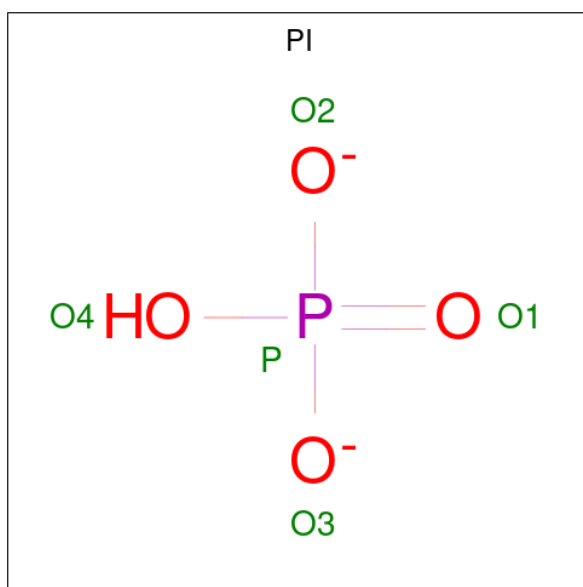
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	S	1	Total	C	N	O	0	0
			43	33	4	6		
3	S	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	U	1	Total	C	N	O	0	0
			43	33	4	6		
3	U	1	Total	C	N	O	0	0
			43	33	4	6		
3	U	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	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	W	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		

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	C	1	Total	N	O	0	0
			4	1	3		
4	D	1	Total	N	O	0	0
			4	1	3		
4	I	1	Total	N	O	0	0
			4	1	3		
4	J	1	Total	N	O	0	0
			4	1	3		
4	L	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is HYDROGENPHOSPHATE ION (CCD ID: PI) (formula: HO₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	I	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	K	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	M	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	O	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	Q	1	Total	O	P	0	0
			5	4	1		
5	R	1	Total	O	P	0	0
			5	4	1		
5	S	1	Total	O	P	0	0
			5	4	1		
5	T	1	Total	O	P	0	0
			5	4	1		
5	U	1	Total	O	P	0	0
			5	4	1		
5	V	1	Total	O	P	0	0
			5	4	1		
5	W	1	Total	O	P	0	0
			5	4	1		
5	X	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

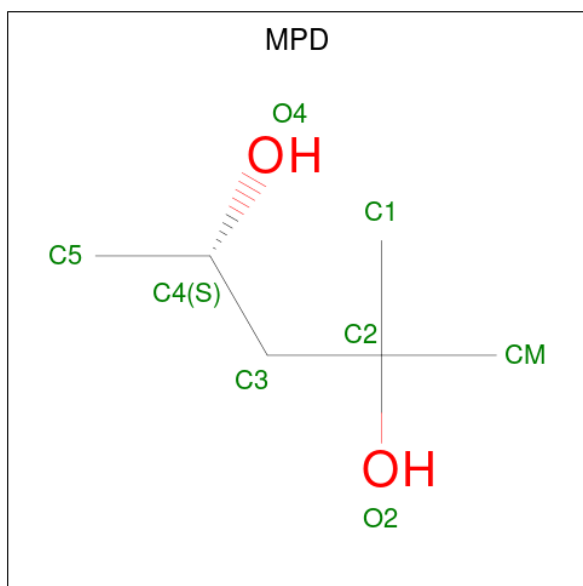
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		
6	E	1	Total	Na	0	0
			1	1		
6	F	1	Total	Na	0	0
			1	1		
6	G	1	Total	Na	0	0
			1	1		
6	H	1	Total	Na	0	0
			1	1		
6	I	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Na	0	0
			1	1		
6	K	1	Total	Na	0	0
			1	1		
6	L	1	Total	Na	0	0
			1	1		
6	N	1	Total	Na	0	0
			1	1		
6	S	1	Total	Na	0	0
			1	1		
6	V	1	Total	Na	0	0
			1	1		
6	W	1	Total	Na	0	0
			1	1		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



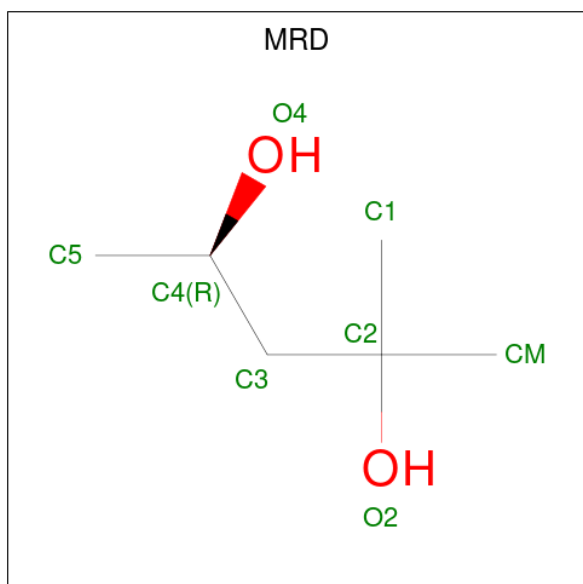
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			8	6	2		
7	M	1	Total	C	O	0	0
			8	6	2		
7	O	1	Total	C	O	0	0
			8	6	2		
7	P	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	Q	1	Total	C	O	0	0
			8	6	2		
7	R	1	Total	C	O	0	0
			8	6	2		
7	S	1	Total	C	O	0	0
			8	6	2		
7	U	1	Total	C	O	0	0
			8	6	2		
7	W	1	Total	C	O	0	0
			8	6	2		
7	X	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	T	1	Total	C	O	0	0
			8	6	2		
8	V	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	356	Total	O	0	0
			356	356		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	312	Total 312	O 312	0	0
9	C	341	Total 341	O 341	0	0
9	D	363	Total 363	O 363	0	0
9	E	319	Total 319	O 319	0	0
9	F	345	Total 345	O 345	0	0
9	G	350	Total 350	O 350	0	0
9	H	324	Total 324	O 324	0	0
9	I	351	Total 351	O 351	0	0
9	J	345	Total 345	O 345	0	0
9	K	319	Total 319	O 319	0	0
9	L	355	Total 355	O 355	0	0
9	M	362	Total 362	O 362	0	0
9	N	359	Total 359	O 359	0	0
9	O	362	Total 362	O 362	0	0
9	P	330	Total 330	O 330	0	0
9	Q	322	Total 322	O 322	0	0
9	R	297	Total 297	O 297	0	0
9	S	318	Total 318	O 318	0	0
9	T	312	Total 312	O 312	0	0
9	U	340	Total 340	O 340	0	0
9	V	361	Total 361	O 361	0	0

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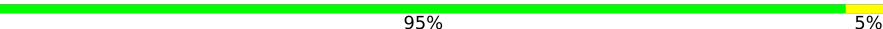
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	W	368	Total 368	O 368	0	0
9	X	357	Total 357	O 357	0	0

3 Residue-property plots [i](#)

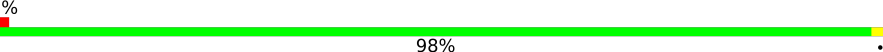
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A: 

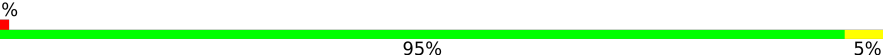


- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain B: 

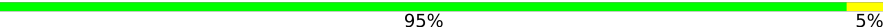


- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain C: 

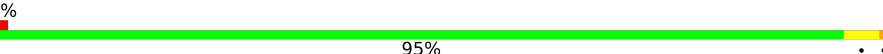


- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain D: 

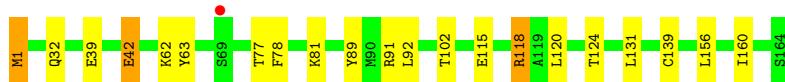
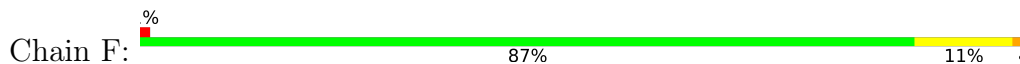


- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain E: 



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit





- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain L: 96%



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain M: 96%



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain N: 94%



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain O: 93%



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain P: 91%

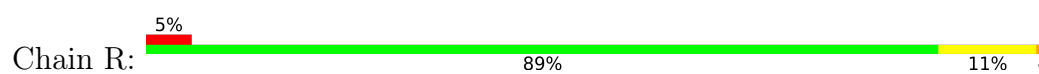


- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

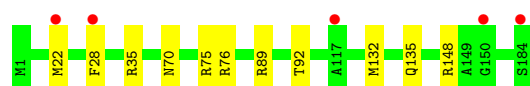
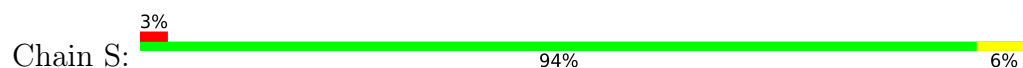
Chain Q: 94%



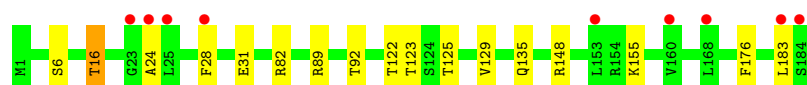
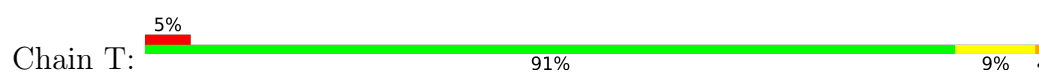
- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



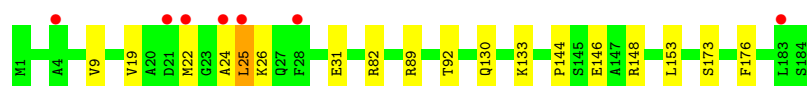
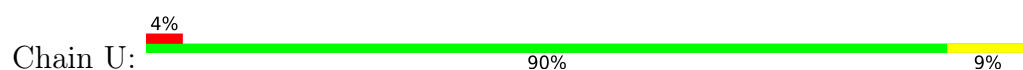
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	109.05Å 109.09Å 117.37Å 78.78° 82.32° 60.26°	Depositor
Resolution (Å)	94.62 – 1.14 94.62 – 1.14	Depositor EDS
% Data completeness (in resolution range)	93.8 (94.62-1.14) 93.8 (94.62-1.14)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.14Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.147 , 0.184 0.149 , 0.185	Depositor DCC
R_{free} test set	79190 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.014 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	43607	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, NA, PI, PEB, MRD, MEN, NO3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	0/1344	0.97	0/1816
1	B	0.96	1/1327 (0.1%)	0.93	0/1795
1	C	0.93	0/1336	0.94	0/1806
1	D	0.93	1/1364 (0.1%)	0.93	0/1841
1	E	0.91	0/1327	0.96	0/1795
1	F	0.97	0/1354	0.94	0/1830
1	G	0.93	2/1336 (0.1%)	0.97	0/1806
1	H	0.90	0/1354	0.93	0/1830
1	I	0.98	0/1365	0.95	0/1843
1	J	0.94	0/1344	0.97	0/1817
1	K	1.01	0/1342	0.96	1/1814 (0.1%)
1	L	0.96	0/1338	0.95	0/1808
2	M	0.91	0/1455	0.93	0/1959
2	N	0.96	0/1439	0.94	0/1937
2	O	0.95	0/1427	0.97	0/1921
2	P	1.03	1/1434 (0.1%)	1.06	2/1933 (0.1%)
2	Q	0.93	0/1427	0.95	0/1925
2	R	0.96	1/1432 (0.1%)	1.03	2/1929 (0.1%)
2	S	0.88	0/1443	0.96	0/1945
2	T	0.94	0/1442	0.98	0/1942
2	U	1.01	1/1488 (0.1%)	1.02	0/2002
2	V	0.94	0/1478	0.91	0/1989
2	W	0.94	0/1464	0.91	0/1971
2	X	0.90	0/1437	0.96	0/1937
All	All	0.95	7/33497 (0.0%)	0.96	5/45191 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	131	LEU	C-O	7.41	1.32	1.24
2	P	47	SER	N-CA	-6.38	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	102	THR	C-O	-6.10	1.15	1.24
1	B	12	ALA	N-CA	-5.72	1.39	1.46
2	U	176	PHE	C-O	-5.12	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	23	GLY	N-CA-C	7.13	120.77	112.50
2	P	34	ARG	CB-CA-C	-5.50	101.66	110.79
2	P	34	ARG	CG-CD-NE	-5.30	100.34	112.00
2	R	27	GLN	CA-C-O	-5.28	115.21	120.76
1	K	93	ILE	N-CA-C	-5.16	105.68	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1300	0	1313	12	0
1	B	1292	0	1289	4	0
1	C	1298	0	1301	13	0
1	D	1314	0	1339	14	0
1	E	1292	0	1289	11	0
1	F	1316	0	1314	30	0
1	G	1301	0	1300	13	0
1	H	1316	0	1316	12	0
1	I	1315	0	1334	10	0
1	J	1306	0	1311	12	0
1	K	1304	0	1305	14	0
1	L	1300	0	1307	12	0
2	M	1416	0	1462	6	0
2	N	1411	0	1444	12	0
2	O	1400	0	1443	10	0
2	P	1401	0	1432	9	0
2	Q	1394	0	1428	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	1402	0	1439	17	0
2	S	1410	0	1439	9	0
2	T	1407	0	1443	17	0
2	U	1441	0	1488	16	0
2	V	1437	0	1476	8	0
2	W	1423	0	1466	18	0
2	X	1401	0	1437	13	0
3	A	86	0	74	1	0
3	B	86	0	74	0	0
3	C	86	0	74	0	0
3	D	86	0	74	0	0
3	E	86	0	74	0	0
3	F	86	0	74	2	0
3	G	86	0	74	0	0
3	H	86	0	74	0	0
3	I	86	0	74	0	0
3	J	86	0	74	0	0
3	K	86	0	74	1	0
3	L	86	0	74	0	0
3	M	129	0	110	1	0
3	N	129	0	110	2	0
3	O	129	0	110	3	0
3	P	129	0	110	3	0
3	Q	129	0	110	4	0
3	R	129	0	111	7	0
3	S	135	0	87	1	0
3	T	129	0	110	4	0
3	U	129	0	110	3	0
3	V	129	0	110	2	0
3	W	129	0	110	2	0
3	X	129	0	110	2	0
4	A	4	0	0	1	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	I	4	0	0	1	0
4	J	4	0	0	0	0
4	L	4	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	5	0	0	0	0
5	G	5	0	0	0	0
5	H	5	0	0	1	0
5	I	5	0	0	0	0
5	J	5	0	0	0	0
5	K	5	0	0	0	0
5	L	5	0	0	0	0
5	M	5	0	0	0	0
5	N	5	0	0	0	0
5	O	5	0	0	0	0
5	P	5	0	0	0	0
5	Q	5	0	0	0	0
5	R	5	0	0	0	0
5	S	5	0	0	0	0
5	T	5	0	0	0	0
5	U	5	0	0	0	0
5	V	5	0	0	0	0
5	W	5	0	0	0	0
5	X	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	N	1	0	0	0	0
6	S	1	0	0	0	0
6	V	1	0	0	0	0
6	W	1	0	0	0	0
7	B	8	0	14	0	0
7	M	8	0	12	0	0
7	O	8	0	10	3	0
7	P	8	0	11	0	0
7	Q	8	0	11	2	0
7	R	8	0	14	0	0
7	S	8	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	U	8	0	12	0	0
7	W	8	0	11	1	0
7	X	8	0	14	0	0
8	T	8	0	11	0	0
8	V	8	0	11	0	0
9	A	356	0	0	5	0
9	B	312	0	0	1	0
9	C	341	0	0	6	0
9	D	363	0	0	4	1
9	E	319	0	0	6	0
9	F	345	0	0	17	0
9	G	350	0	0	6	0
9	H	324	0	0	5	0
9	I	351	0	0	5	0
9	J	345	0	0	6	0
9	K	319	0	0	2	0
9	L	355	0	0	2	0
9	M	362	0	0	1	1
9	N	359	0	0	2	1
9	O	362	0	0	4	1
9	P	330	0	0	4	0
9	Q	322	0	0	6	0
9	R	297	0	0	11	1
9	S	318	0	0	7	0
9	T	312	0	0	9	1
9	U	340	0	0	6	0
9	V	361	0	0	3	0
9	W	368	0	0	5	1
9	X	357	0	0	10	1
All	All	43607	0	35446	280	4

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 4.

The worst 5 of 280 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115[A]:GLU:OE1	9:M:301:HOH:O	1.60	1.19
1:C:32[A]:GLN:HG3	1:F:32[A]:GLN:HG3	1.20	1.19
1:H:32[A]:GLN:HG3	1:K:32[A]:GLN:HG3	1.25	1.14
1:I:32[A]:GLN:HG3	1:L:32[A]:GLN:HG3	1.17	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32[A]:GLN:HG3	1:E:32[A]:GLN:HG3	1.24	1.14

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:484:HOH:O	9:W:355:HOH:O[1_654]	2.12	0.08
9:R:491:HOH:O	9:T:570:HOH:O[1_565]	2.17	0.03
9:N:329:HOH:O	9:X:463:HOH:O[1_564]	2.18	0.02
9:D:636:HOH:O	9:O:484:HOH:O[1_645]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	B	169/164 (103%)	167 (99%)	2 (1%)	0	100	100
1	C	170/164 (104%)	168 (99%)	2 (1%)	0	100	100
1	D	173/164 (106%)	171 (99%)	2 (1%)	0	100	100
1	E	169/164 (103%)	166 (98%)	3 (2%)	0	100	100
1	F	172/164 (105%)	170 (99%)	2 (1%)	0	100	100
1	G	170/164 (104%)	168 (99%)	2 (1%)	0	100	100
1	H	172/164 (105%)	169 (98%)	3 (2%)	0	100	100
1	I	174/164 (106%)	172 (99%)	2 (1%)	0	100	100
1	J	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	K	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	L	170/164 (104%)	168 (99%)	2 (1%)	0	100	100
2	M	194/184 (105%)	188 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	192/184 (104%)	185 (96%)	7 (4%)	0	100	100
2	O	190/184 (103%)	185 (97%)	5 (3%)	0	100	100
2	P	192/184 (104%)	188 (98%)	4 (2%)	0	100	100
2	Q	191/184 (104%)	187 (98%)	4 (2%)	0	100	100
2	R	191/184 (104%)	187 (98%)	4 (2%)	0	100	100
2	S	193/184 (105%)	189 (98%)	4 (2%)	0	100	100
2	T	192/184 (104%)	186 (97%)	6 (3%)	0	100	100
2	U	197/184 (107%)	194 (98%)	3 (2%)	0	100	100
2	V	196/184 (106%)	192 (98%)	4 (2%)	0	100	100
2	W	195/184 (106%)	190 (97%)	5 (3%)	0	100	100
2	X	192/184 (104%)	189 (98%)	3 (2%)	0	100	100
All	All	4367/4176 (105%)	4286 (98%)	81 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/127 (108%)	137 (100%)	0	100	100
1	B	135/127 (106%)	133 (98%)	2 (2%)	57	19
1	C	136/127 (107%)	136 (100%)	0	100	100
1	D	139/127 (109%)	139 (100%)	0	100	100
1	E	135/127 (106%)	133 (98%)	2 (2%)	57	19
1	F	138/127 (109%)	132 (96%)	6 (4%)	26	1
1	G	136/127 (107%)	136 (100%)	0	100	100
1	H	138/127 (109%)	136 (99%)	2 (1%)	59	21
1	I	140/127 (110%)	140 (100%)	0	100	100
1	J	137/127 (108%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	137/127 (108%)	133 (97%)	4 (3%)	37	4
1	L	136/127 (107%)	136 (100%)	0	100	100
2	M	151/138 (109%)	149 (99%)	2 (1%)	61	23
2	N	150/138 (109%)	147 (98%)	3 (2%)	48	9
2	O	147/138 (106%)	147 (100%)	0	100	100
2	P	149/138 (108%)	145 (97%)	4 (3%)	39	5
2	Q	148/138 (107%)	148 (100%)	0	100	100
2	R	148/138 (107%)	146 (99%)	2 (1%)	59	21
2	S	150/138 (109%)	150 (100%)	0	100	100
2	T	150/138 (109%)	147 (98%)	3 (2%)	48	9
2	U	155/138 (112%)	152 (98%)	3 (2%)	50	11
2	V	154/138 (112%)	151 (98%)	3 (2%)	50	11
2	W	153/138 (111%)	152 (99%)	1 (1%)	76	48
2	X	149/138 (108%)	149 (100%)	0	100	100
All	All	3448/3180 (108%)	3411 (99%)	37 (1%)	73	31

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	123	THR
2	V	162	GLU
2	T	155	LYS
2	U	26[B]	LYS
1	K	1[A]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	61	GLN
1	L	61	GLN
2	X	45	ASN
1	K	28	GLN
1	L	28	GLN

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
2	MEN	U	70	2	7,8,9	0.79	0	4,9,11	1.11	0
2	MEN	O	70	2	7,8,9	0.48	0	4,9,11	1.44	1 (25%)
2	MEN	P	70	2	7,8,9	0.60	0	4,9,11	0.67	0
2	MEN	Q	70	2	7,8,9	0.46	0	4,9,11	1.14	0
2	MEN	T	70	2	7,8,9	0.47	0	4,9,11	0.85	0
2	MEN	R	70	2	7,8,9	0.50	0	4,9,11	2.07	2 (50%)
2	MEN	M	70	2	7,8,9	0.46	0	4,9,11	0.41	0
2	MEN	V	70	2	7,8,9	0.70	0	4,9,11	0.83	0
2	MEN	N	70	2	7,8,9	0.67	0	4,9,11	0.70	0
2	MEN	X	70	2	7,8,9	0.48	0	4,9,11	0.41	0
2	MEN	S	70	2	7,8,9	0.35	0	4,9,11	1.92	1 (25%)
2	MEN	W	70	2	7,8,9	0.69	0	4,9,11	0.49	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
2	MEN	U	70	2	-	2/7/8/10	-
2	MEN	O	70	2	-	3/7/8/10	-
2	MEN	P	70	2	-	3/7/8/10	-
2	MEN	Q	70	2	-	3/7/8/10	-
2	MEN	T	70	2	-	3/7/8/10	-
2	MEN	R	70	2	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	M	70	2	-	3/7/8/10	-
2	MEN	V	70	2	-	3/7/8/10	-
2	MEN	N	70	2	-	2/7/8/10	-
2	MEN	X	70	2	-	3/7/8/10	-
2	MEN	S	70	2	-	2/7/8/10	-
2	MEN	W	70	2	-	2/7/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	70	MEN	OD1-CG-CB	-3.38	116.59	121.54
2	R	70	MEN	OD1-CG-CB	-3.22	116.83	121.54
2	R	70	MEN	CB-CG-ND2	2.57	118.89	115.53
2	O	70	MEN	OD1-CG-CB	-2.12	118.44	121.54

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	70	MEN	N-CA-CB-CG
2	Q	70	MEN	N-CA-CB-CG
2	T	70	MEN	N-CA-CB-CG
2	T	70	MEN	CA-CB-CG-OD1
2	V	70	MEN	CA-CB-CG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 119 ligands modelled in this entry, 16 are monoatomic - leaving 103 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PI	E	203	-	4,4,4	0.88	0	6,6,6	0.71	0
3	PEB	O	187	2	46,46,46	2.05	10 (21%)	56,67,67	1.24	6 (10%)
3	PEB	T	188	2	46,46,46	1.97	13 (28%)	56,67,67	1.84	16 (28%)
4	NO3	J	203	-	1,3,3	1.47	0	0,3,3	-	-
3	PEB	N	187	2	46,46,46	1.68	7 (15%)	56,67,67	1.59	14 (25%)
3	PEB	M	187	2	46,46,46	1.77	10 (21%)	56,67,67	1.55	13 (23%)
4	NO3	L	203	-	1,3,3	1.71	0	0,3,3	-	-
7	MPD	O	204	-	7,7,7	0.94	0	9,10,10	1.34	1 (11%)
5	PI	U	205	-	4,4,4	1.37	1 (25%)	6,6,6	0.59	0
5	PI	X	205	-	4,4,4	0.86	0	6,6,6	0.83	0
5	PI	I	204	-	4,4,4	1.11	0	6,6,6	1.12	0
3	PEB	W	187	2	46,46,46	1.91	7 (15%)	56,67,67	1.52	11 (19%)
3	PEB	V	187	2	46,46,46	1.86	8 (17%)	56,67,67	1.47	9 (16%)
3	PEB	M	188	2	46,46,46	1.97	9 (19%)	56,67,67	1.65	13 (23%)
3	PEB	A	166	1	46,46,46	1.43	6 (13%)	56,67,67	1.69	7 (12%)
3	PEB	O	188	2	46,46,46	2.19	14 (30%)	56,67,67	1.55	12 (21%)
5	PI	H	203	-	4,4,4	1.42	0	6,6,6	1.20	1 (16%)
3	PEB	D	166	1	46,46,46	1.98	8 (17%)	56,67,67	1.78	10 (17%)
7	MPD	S	204	-	7,7,7	0.28	0	9,10,10	0.73	0
5	PI	K	203	-	4,4,4	1.06	0	6,6,6	0.93	0
3	PEB	S	186[B]	-	46,46,46	1.88	10 (21%)	56,67,67	2.32	20 (35%)
7	MPD	X	204	-	7,7,7	0.39	0	9,10,10	0.84	1 (11%)
3	PEB	G	166	1	46,46,46	1.72	8 (17%)	56,67,67	1.88	9 (16%)
3	PEB	P	188	2	46,46,46	1.89	7 (15%)	56,67,67	1.70	14 (25%)
3	PEB	N	186	2	46,46,46	1.84	9 (19%)	56,67,67	1.82	18 (32%)
7	MPD	R	204	-	7,7,7	0.21	0	9,10,10	1.63	2 (22%)
7	MPD	Q	204	-	7,7,7	0.64	0	9,10,10	1.00	0
4	NO3	I	203	-	1,3,3	1.68	0	0,3,3	-	-
3	PEB	G	167	1	46,46,46	1.98	12 (26%)	56,67,67	1.48	7 (12%)
3	PEB	L	167	1	46,46,46	1.70	8 (17%)	56,67,67	1.50	10 (17%)
3	PEB	X	188	2	46,46,46	2.15	9 (19%)	56,67,67	1.62	13 (23%)
3	PEB	S	188	2	46,46,46	1.84	10 (21%)	56,67,67	1.49	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PI	S	205	-	4,4,4	0.86	0	6,6,6	0.41	0
3	PEB	J	167	1	46,46,46	1.79	10 (21%)	56,67,67	1.90	17 (30%)
3	PEB	O	186	2	46,46,46	1.81	10 (21%)	56,67,67	1.73	13 (23%)
3	PEB	X	186	2	46,46,46	1.91	10 (21%)	56,67,67	1.76	16 (28%)
3	PEB	C	167	1	46,46,46	1.96	11 (23%)	56,67,67	1.94	18 (32%)
5	PI	F	203	-	4,4,4	1.08	0	6,6,6	0.51	0
3	PEB	R	186	2	46,46,46	2.16	13 (28%)	56,67,67	2.10	15 (26%)
5	PI	R	205	-	4,4,4	0.71	0	6,6,6	0.66	0
3	PEB	Q	186	2	46,46,46	2.05	10 (21%)	56,67,67	1.92	16 (28%)
5	PI	J	204	-	4,4,4	1.24	0	6,6,6	0.72	0
3	PEB	F	166	1	46,46,46	1.77	6 (13%)	56,67,67	1.78	10 (17%)
3	PEB	R	187	2	46,46,46	1.97	8 (17%)	56,67,67	1.74	17 (30%)
3	PEB	U	186	2	46,46,46	2.01	13 (28%)	56,67,67	2.08	17 (30%)
3	PEB	E	167	1	46,46,46	1.94	11 (23%)	56,67,67	1.32	6 (10%)
3	PEB	T	187	2	46,46,46	1.71	10 (21%)	56,67,67	1.73	10 (17%)
3	PEB	W	186	2	46,46,46	1.93	12 (26%)	56,67,67	2.07	21 (37%)
8	MRD	T	204	-	7,7,7	0.50	0	9,10,10	0.55	0
5	PI	O	205	-	4,4,4	0.95	0	6,6,6	1.06	0
5	PI	A	204	-	4,4,4	1.16	0	6,6,6	0.99	0
3	PEB	U	188	2	46,46,46	1.98	11 (23%)	56,67,67	1.43	9 (16%)
5	PI	B	204	-	4,4,4	1.25	0	6,6,6	1.93	2 (33%)
5	PI	N	204	-	4,4,4	0.80	0	6,6,6	1.33	1 (16%)
4	NO3	D	203	-	1,3,3	2.01	1 (100%)	0,3,3	-	-
5	PI	Q	205	-	4,4,4	0.93	0	6,6,6	1.22	0
3	PEB	C	166	1	46,46,46	2.03	10 (21%)	56,67,67	2.08	15 (26%)
3	PEB	E	166	1	46,46,46	2.39	14 (30%)	56,67,67	2.10	13 (23%)
3	PEB	B	167	1	46,46,46	1.84	9 (19%)	56,67,67	1.80	12 (21%)
7	MPD	W	204	-	7,7,7	0.25	0	9,10,10	1.07	0
3	PEB	R	188	2	46,46,46	2.00	11 (23%)	56,67,67	1.60	8 (14%)
3	PEB	H	167	1	46,46,46	1.85	10 (21%)	56,67,67	1.54	8 (14%)
5	PI	L	204	-	4,4,4	1.15	0	6,6,6	0.92	0
3	PEB	I	166	1	46,46,46	2.02	10 (21%)	56,67,67	1.86	11 (19%)
3	PEB	Q	188	2	46,46,46	1.72	8 (17%)	56,67,67	1.54	12 (21%)
7	MPD	U	204	-	7,7,7	0.38	0	9,10,10	0.94	0
3	PEB	L	166	1	46,46,46	1.74	9 (19%)	56,67,67	1.85	10 (17%)
3	PEB	P	187	2	46,46,46	1.65	8 (17%)	56,67,67	1.55	9 (16%)
3	PEB	M	186	2	46,46,46	1.91	11 (23%)	56,67,67	1.81	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PI	G	203	-	4,4,4	0.99	0	6,6,6	0.87	0
4	NO3	A	203	-	1,3,3	1.61	0	0,3,3	-	-
3	PEB	X	187	2	46,46,46	1.78	10 (21%)	56,67,67	1.54	10 (17%)
3	PEB	V	188	2	46,46,46	1.90	11 (23%)	56,67,67	1.40	7 (12%)
3	PEB	B	166	1	46,46,46	1.93	11 (23%)	56,67,67	1.82	9 (16%)
3	PEB	V	186	2	46,46,46	1.67	10 (21%)	56,67,67	1.83	14 (25%)
3	PEB	W	188	2	46,46,46	2.10	8 (17%)	56,67,67	1.83	15 (26%)
3	PEB	U	187	2	46,46,46	1.87	8 (17%)	56,67,67	1.42	11 (19%)
5	PI	W	205	-	4,4,4	1.03	0	6,6,6	1.17	0
5	PI	P	205	-	4,4,4	0.50	0	6,6,6	1.40	1 (16%)
3	PEB	K	166	1	46,46,46	1.93	11 (23%)	56,67,67	1.91	11 (19%)
7	MPD	M	204	-	7,7,7	0.20	0	9,10,10	1.17	1 (11%)
3	PEB	S	186[A]	-	46,46,46	1.90	10 (21%)	56,67,67	2.31	21 (37%)
3	PEB	K	167	1	46,46,46	2.20	11 (23%)	56,67,67	1.76	17 (30%)
8	MRD	V	204	-	7,7,7	0.30	0	9,10,10	1.17	0
3	PEB	T	186	2	46,46,46	2.19	11 (23%)	56,67,67	2.09	19 (33%)
5	PI	M	205	-	4,4,4	1.15	0	6,6,6	1.18	0
5	PI	C	204	-	4,4,4	1.20	0	6,6,6	1.49	1 (16%)
5	PI	V	205	-	4,4,4	0.85	0	6,6,6	0.89	0
3	PEB	N	188	2	46,46,46	1.90	8 (17%)	56,67,67	1.66	16 (28%)
7	MPD	P	204	-	7,7,7	0.31	0	9,10,10	0.92	0
3	PEB	Q	187	2	46,46,46	1.70	9 (19%)	56,67,67	1.56	10 (17%)
5	PI	T	205	-	4,4,4	0.92	0	6,6,6	1.39	0
3	PEB	I	167	1	46,46,46	1.87	9 (19%)	56,67,67	1.73	13 (23%)
3	PEB	D	167	1	46,46,46	1.69	8 (17%)	56,67,67	1.61	15 (26%)
3	PEB	P	186	2	46,46,46	2.26	14 (30%)	56,67,67	1.76	14 (25%)
3	PEB	A	167	1	46,46,46	1.68	9 (19%)	56,67,67	1.46	12 (21%)
5	PI	D	204	-	4,4,4	1.20	0	6,6,6	0.46	0
3	PEB	J	166	1	46,46,46	1.63	8 (17%)	56,67,67	1.78	9 (16%)
4	NO3	C	203	-	1,3,3	1.22	0	0,3,3	-	-
7	MPD	B	203	-	7,7,7	0.64	0	9,10,10	1.79	2 (22%)
3	PEB	F	167	1	46,46,46	1.96	12 (26%)	56,67,67	1.66	11 (19%)
3	PEB	S	187	2	46,46,46	1.80	10 (21%)	56,67,67	1.62	12 (21%)
3	PEB	H	166	1	46,46,46	2.11	8 (17%)	56,67,67	2.09	16 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MPD	R	204	-	-	2/5/5/5	-
3	PEB	U	188	2	-	5/26/74/74	0/4/4/4
7	MPD	Q	204	-	-	0/5/5/5	-
3	PEB	O	187	2	-	6/26/74/74	0/4/4/4
3	PEB	T	188	2	-	5/26/74/74	0/4/4/4
3	PEB	G	167	1	-	6/26/74/74	0/4/4/4
3	PEB	K	166	1	-	4/26/74/74	0/4/4/4
3	PEB	N	187	2	-	7/26/74/74	0/4/4/4
3	PEB	S	186[A]	-	-	7/26/74/74	0/4/4/4
7	MPD	M	204	-	-	0/5/5/5	-
3	PEB	K	167	1	-	6/26/74/74	0/4/4/4
3	PEB	L	167	1	-	6/26/74/74	0/4/4/4
8	MRD	V	204	-	-	3/5/5/5	-
3	PEB	T	186	2	-	6/26/74/74	0/4/4/4
3	PEB	C	166	1	-	4/26/74/74	0/4/4/4
3	PEB	M	187	2	-	8/26/74/74	0/4/4/4
3	PEB	E	166	1	-	4/26/74/74	0/4/4/4
3	PEB	B	167	1	-	7/26/74/74	0/4/4/4
3	PEB	X	188	2	-	5/26/74/74	0/4/4/4
7	MPD	W	204	-	-	0/5/5/5	-
7	MPD	O	204	-	-	0/5/5/5	-
3	PEB	N	188	2	-	5/26/74/74	0/4/4/4
3	PEB	S	188	2	-	6/26/74/74	0/4/4/4
3	PEB	R	188	2	-	4/26/74/74	0/4/4/4
7	MPD	P	204	-	-	1/5/5/5	-
3	PEB	Q	187	2	-	9/26/74/74	0/4/4/4
3	PEB	H	167	1	-	6/26/74/74	0/4/4/4
3	PEB	J	167	1	-	6/26/74/74	0/4/4/4
3	PEB	O	186	2	-	6/26/74/74	0/4/4/4
3	PEB	W	187	2	-	7/26/74/74	0/4/4/4
3	PEB	I	166	1	-	4/26/74/74	0/4/4/4
3	PEB	Q	188	2	-	5/26/74/74	0/4/4/4
3	PEB	C	167	1	-	6/26/74/74	0/4/4/4
3	PEB	I	167	1	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	X	186	2	-	6/26/74/74	0/4/4/4
3	PEB	D	167	1	-	6/26/74/74	0/4/4/4
3	PEB	P	186	2	-	6/26/74/74	0/4/4/4
3	PEB	V	187	2	-	6/26/74/74	0/4/4/4
3	PEB	R	186	2	-	6/26/74/74	0/4/4/4
3	PEB	M	188	2	-	5/26/74/74	0/4/4/4
3	PEB	F	167	1	-	6/26/74/74	0/4/4/4
7	MPD	U	204	-	-	0/5/5/5	-
3	PEB	L	166	1	-	4/26/74/74	0/4/4/4
3	PEB	A	167	1	-	7/26/74/74	0/4/4/4
3	PEB	A	166	1	-	4/26/74/74	0/4/4/4
3	PEB	O	188	2	-	6/26/74/74	0/4/4/4
3	PEB	P	187	2	-	6/26/74/74	0/4/4/4
3	PEB	Q	186	2	-	6/26/74/74	0/4/4/4
3	PEB	M	186	2	-	6/26/74/74	0/4/4/4
3	PEB	F	166	1	-	4/26/74/74	0/4/4/4
3	PEB	D	166	1	-	4/26/74/74	0/4/4/4
3	PEB	J	166	1	-	4/26/74/74	0/4/4/4
3	PEB	R	187	2	-	6/26/74/74	0/4/4/4
3	PEB	U	186	2	-	6/26/74/74	0/4/4/4
3	PEB	X	187	2	-	7/26/74/74	0/4/4/4
3	PEB	V	188	2	-	5/26/74/74	0/4/4/4
3	PEB	B	166	1	-	4/26/74/74	0/4/4/4
3	PEB	E	167	1	-	7/26/74/74	0/4/4/4
3	PEB	T	187	2	-	8/26/74/74	0/4/4/4
3	PEB	S	186[B]	-	-	7/26/74/74	0/4/4/4
3	PEB	W	186	2	-	6/26/74/74	0/4/4/4
7	MPD	B	203	-	-	3/5/5/5	-
7	MPD	S	204	-	-	1/5/5/5	-
3	PEB	V	186	2	-	6/26/74/74	0/4/4/4
7	MPD	X	204	-	-	1/5/5/5	-
3	PEB	W	188	2	-	5/26/74/74	0/4/4/4
3	PEB	U	187	2	-	7/26/74/74	0/4/4/4
8	MRD	T	204	-	-	0/5/5/5	-
3	PEB	G	166	1	-	4/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	P	188	2	-	3/26/74/74	0/4/4/4
3	PEB	S	187	2	-	7/26/74/74	0/4/4/4
3	PEB	N	186	2	-	6/26/74/74	0/4/4/4
3	PEB	H	166	1	-	4/26/74/74	0/4/4/4

The worst 5 of 598 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	188	PEB	C2D-C3D	9.37	1.46	1.34
3	P	186	PEB	C2D-C3D	8.88	1.46	1.34
3	O	187	PEB	C2D-C3D	8.31	1.45	1.34
3	V	187	PEB	C2D-C3D	8.25	1.45	1.34
3	H	166	PEB	C4C-C3C	8.13	1.49	1.38

The worst 5 of 786 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	166	PEB	CHA-C4A-NA	8.26	135.95	125.63
3	L	166	PEB	CHA-C4A-NA	7.22	134.64	125.63
3	I	166	PEB	CHA-C4A-NA	7.19	134.61	125.63
3	F	166	PEB	CHA-C4A-NA	6.99	134.35	125.63
3	H	166	PEB	CHA-C4A-NA	6.97	134.34	125.63

There are no chirality outliers.

5 of 358 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	166	PEB	C2B-C1B-CHA-C4A
3	A	167	PEB	NB-C1B-CHA-C4A
3	A	167	PEB	C2B-C1B-CHA-C4A
3	B	166	PEB	C2B-C1B-CHA-C4A
3	B	167	PEB	NB-C1B-CHA-C4A

There are no ring outliers.

37 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	188	PEB	2	0
4	L	203	NO3	1	0
7	O	204	MPD	3	0

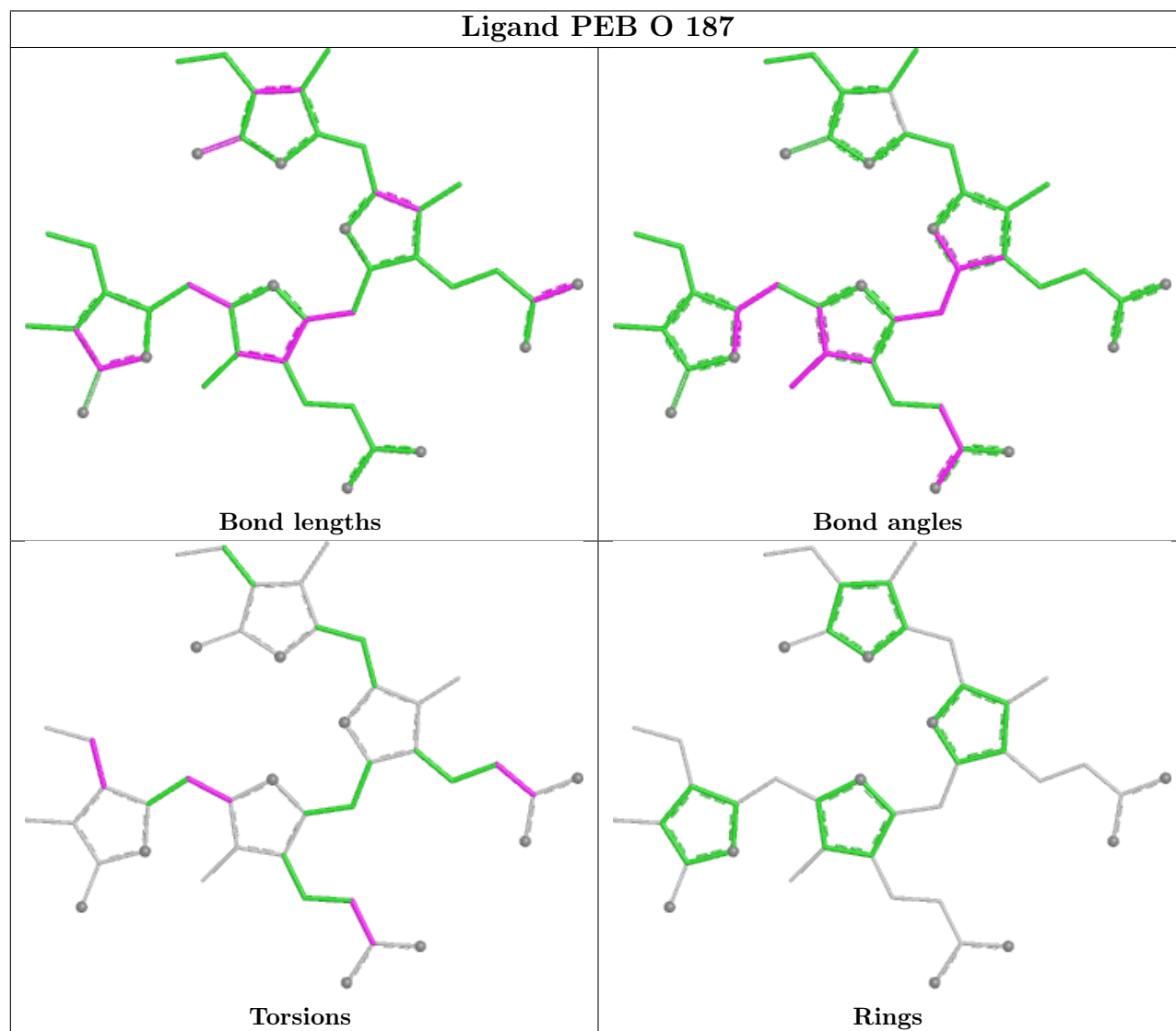
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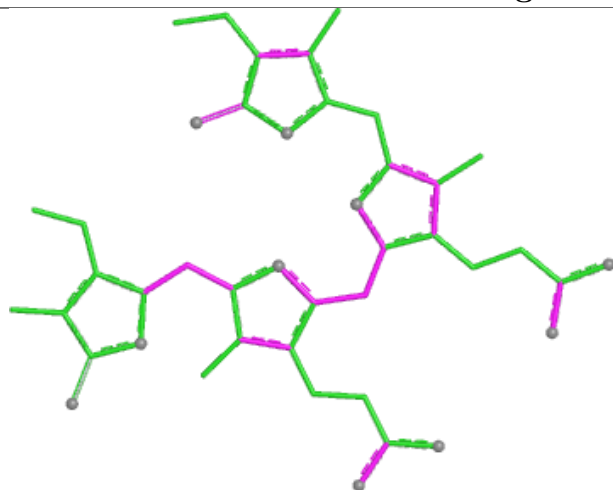
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	188	PEB	2	0
5	H	203	PI	1	0
3	P	188	PEB	1	0
3	N	186	PEB	1	0
7	Q	204	MPD	2	0
4	I	203	NO3	1	0
3	S	188	PEB	1	0
3	O	186	PEB	1	0
3	X	186	PEB	1	0
3	R	186	PEB	1	0
3	Q	186	PEB	2	0
3	F	166	PEB	1	0
3	R	187	PEB	2	0
3	U	186	PEB	1	0
3	T	187	PEB	1	0
3	W	186	PEB	1	0
3	U	188	PEB	1	0
7	W	204	MPD	1	0
3	R	188	PEB	4	0
3	Q	188	PEB	2	0
3	P	187	PEB	1	0
3	M	186	PEB	1	0
4	A	203	NO3	1	0
3	X	187	PEB	1	0
3	V	188	PEB	1	0
3	V	186	PEB	1	0
3	W	188	PEB	1	0
3	U	187	PEB	1	0
3	K	166	PEB	1	0
3	T	186	PEB	1	0
3	N	188	PEB	1	0
3	P	186	PEB	1	0
3	A	167	PEB	1	0
3	F	167	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

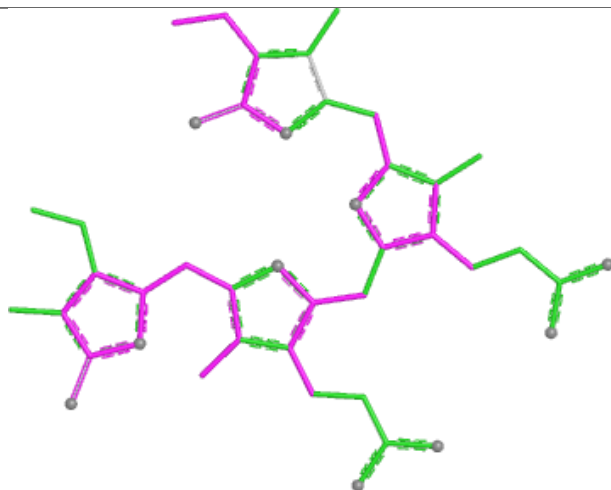
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



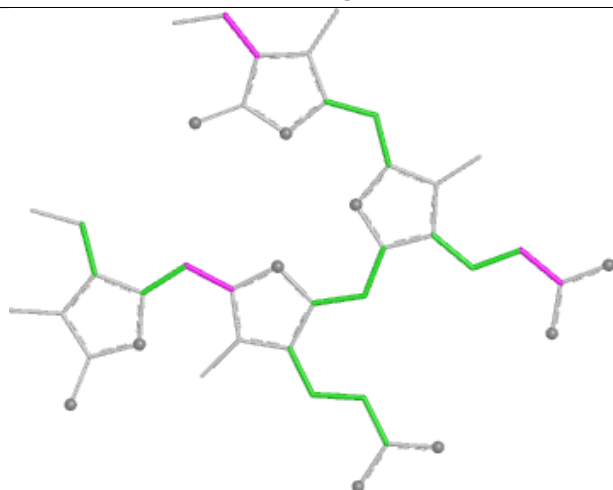
Ligand PEB T 188



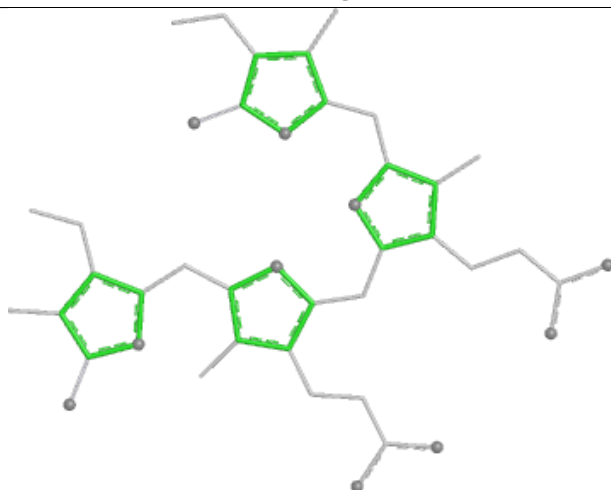
Bond lengths



Bond angles

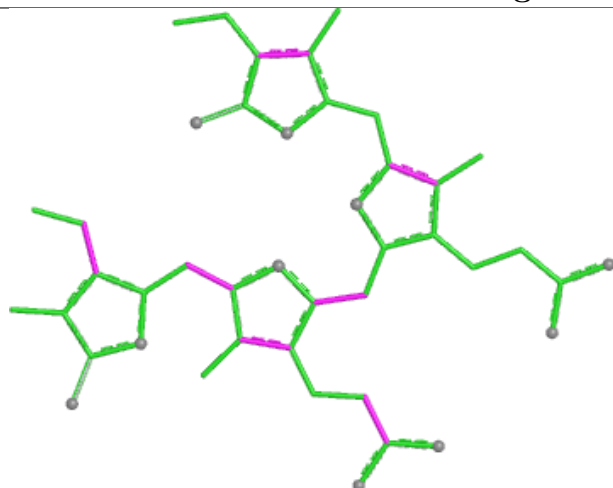


Torsions

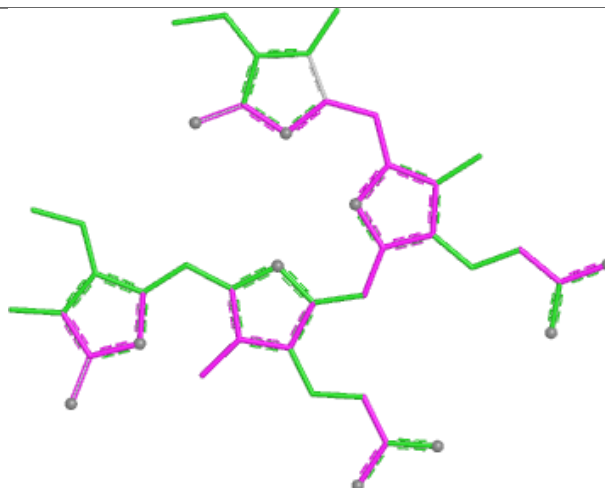


Rings

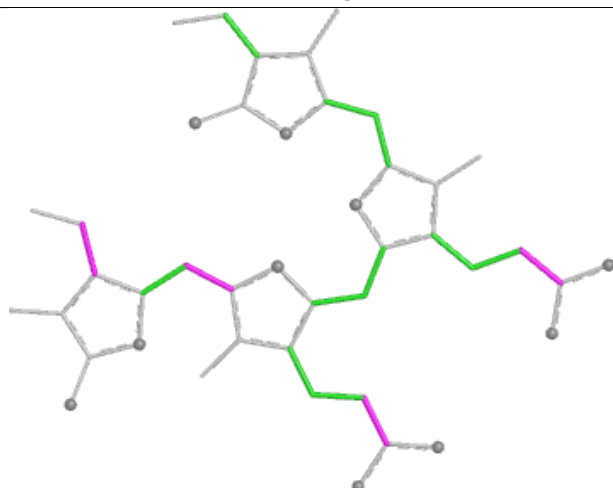
Ligand PEB N 187



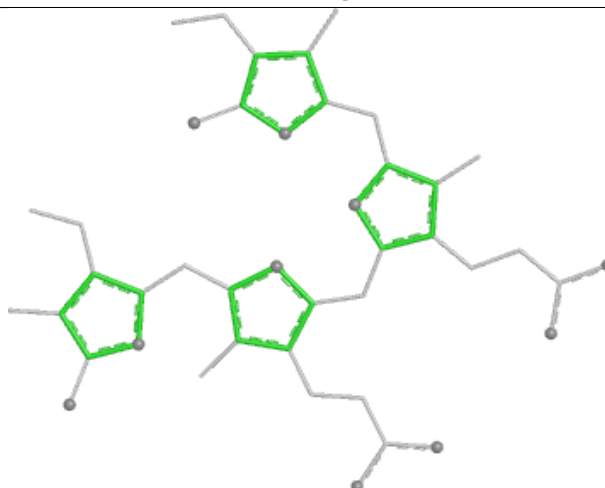
Bond lengths



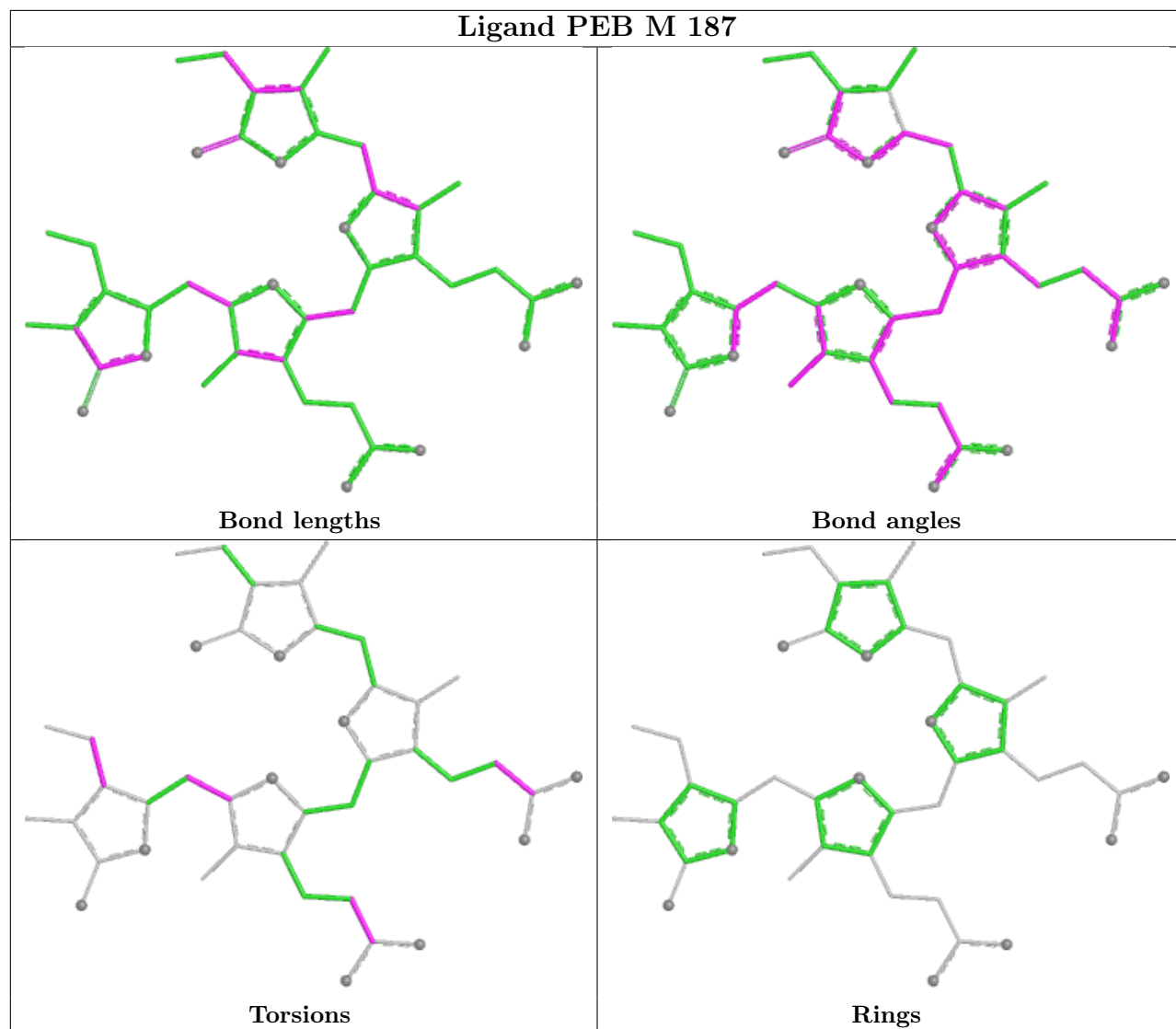
Bond angles

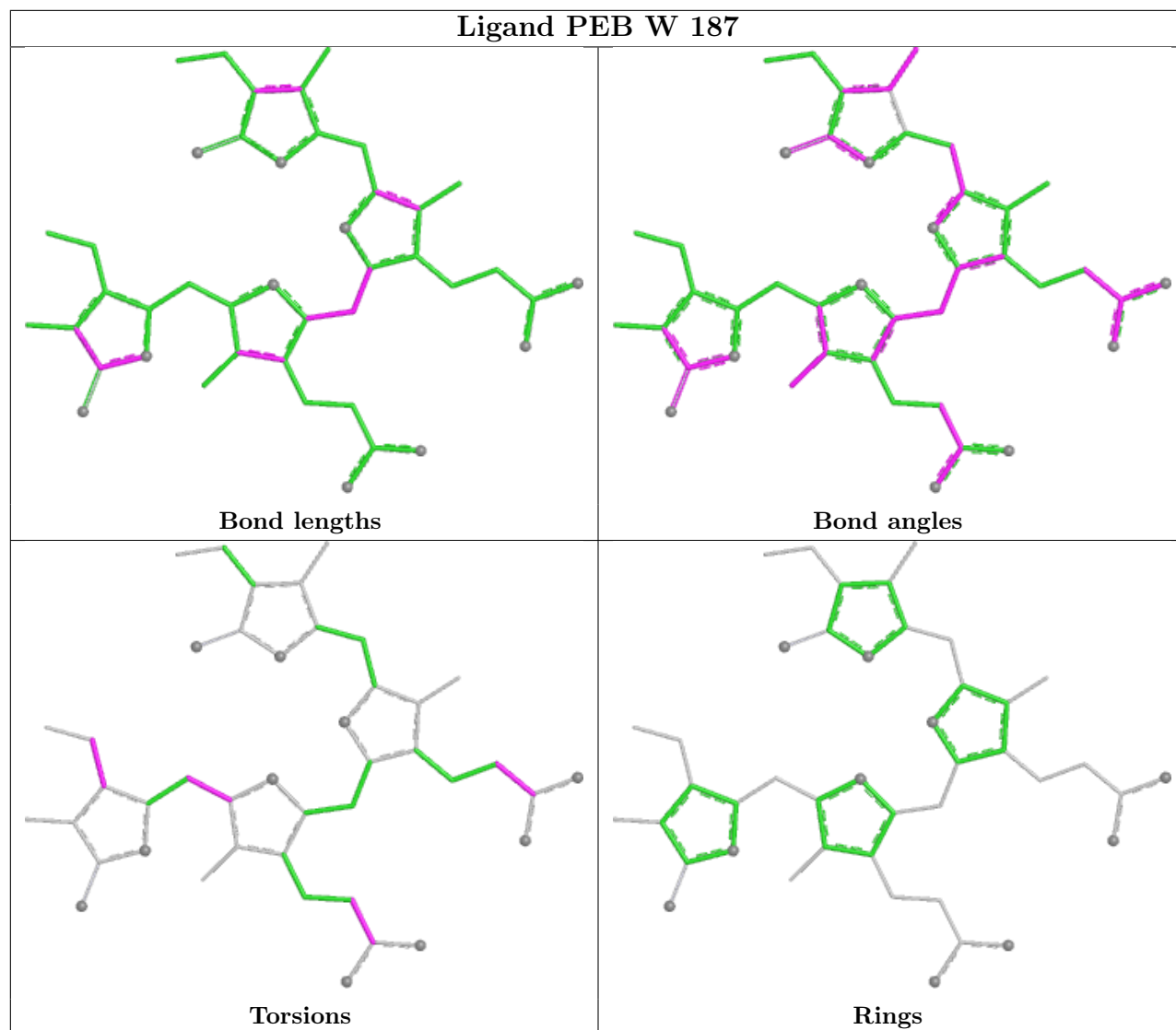


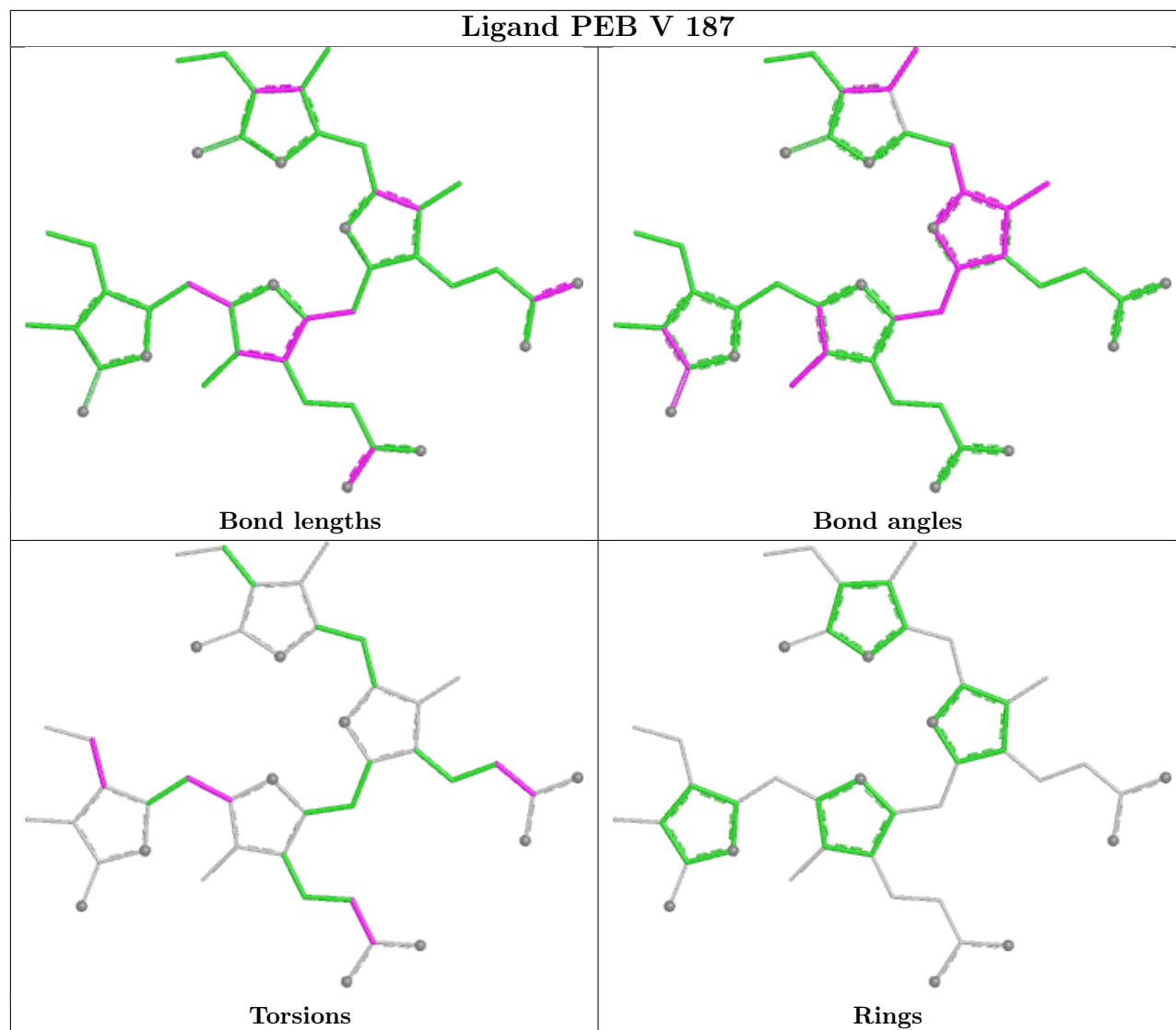
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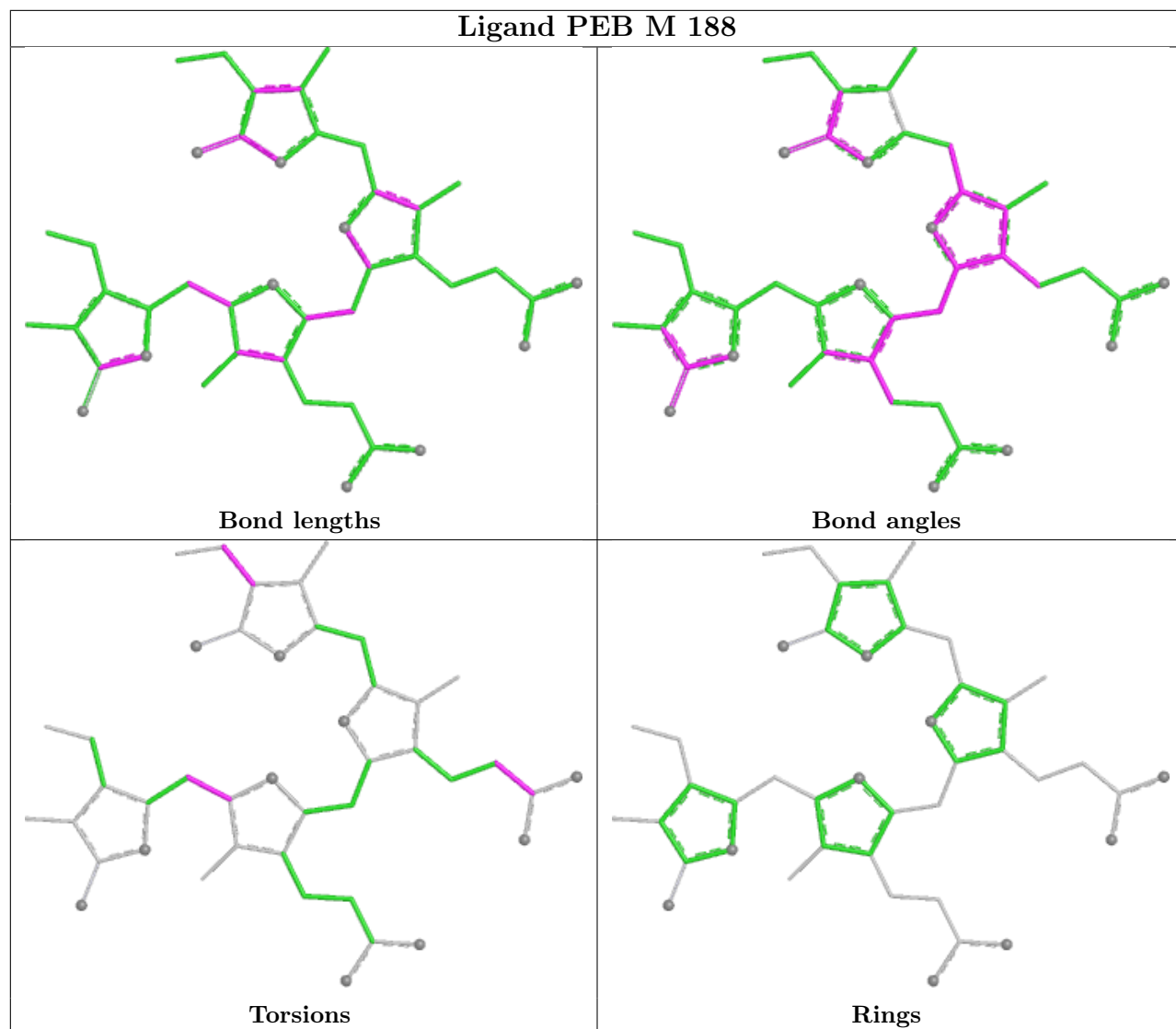


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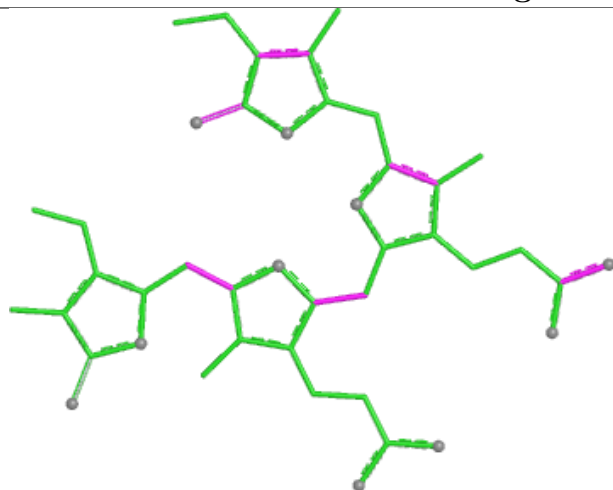




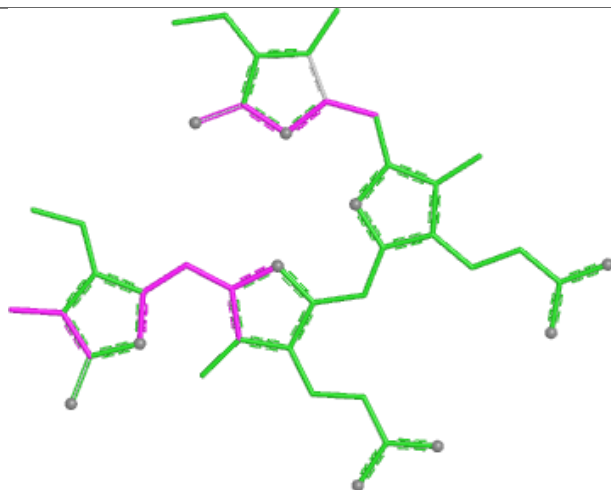




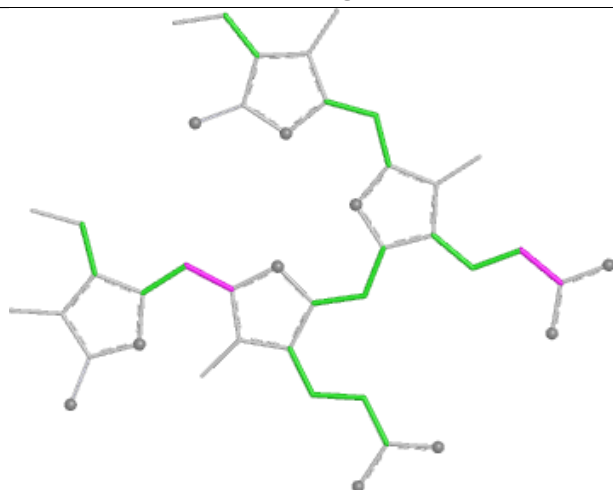
Ligand PEB A 166



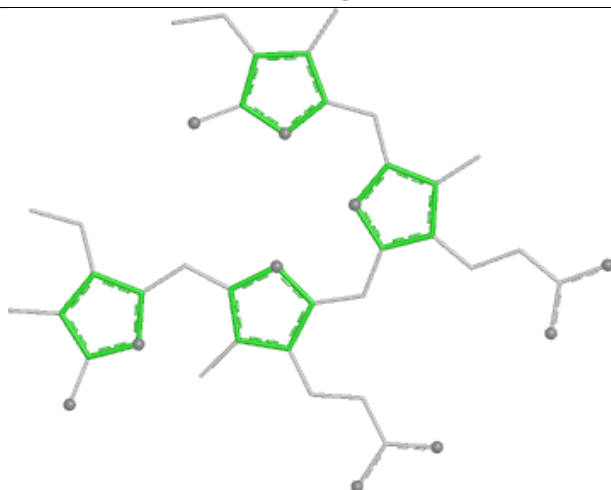
Bond lengths



Bond angles

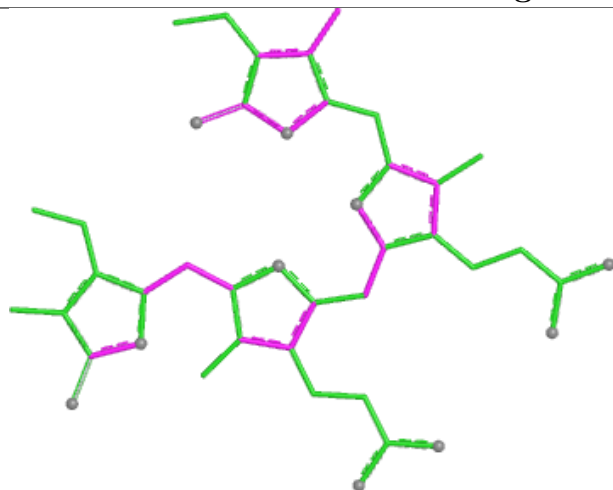


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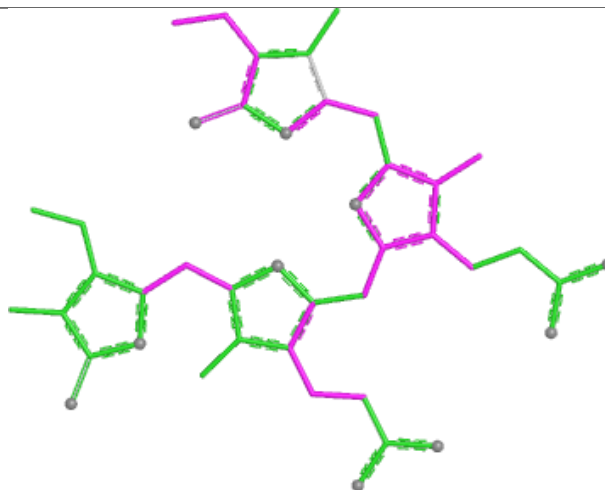


Rings

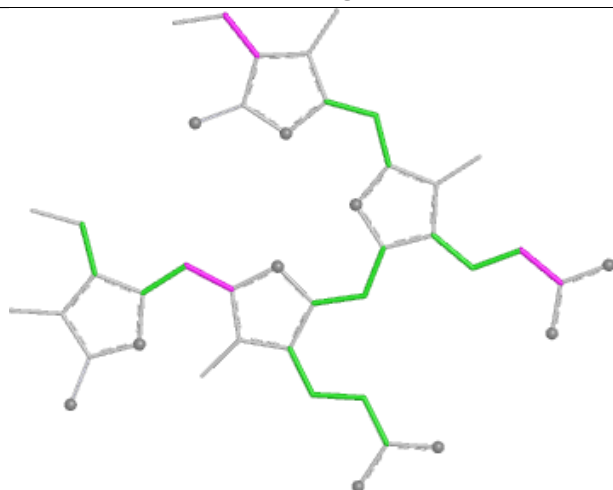
Ligand PEB O 188



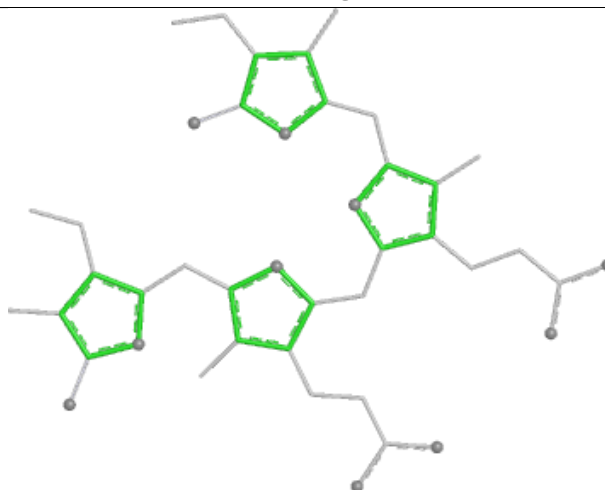
Bond lengths



Bond angles

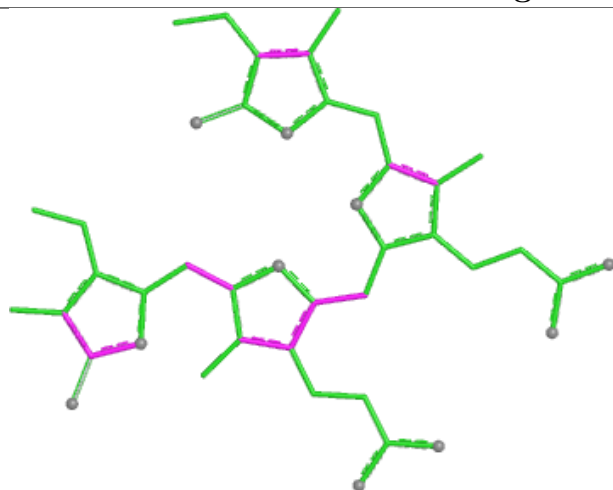


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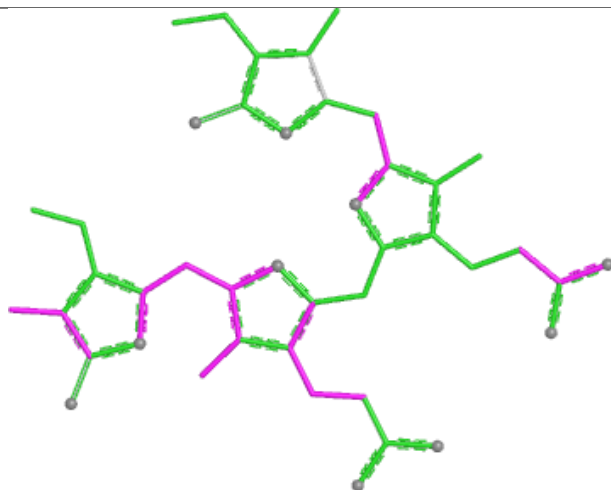


Rings

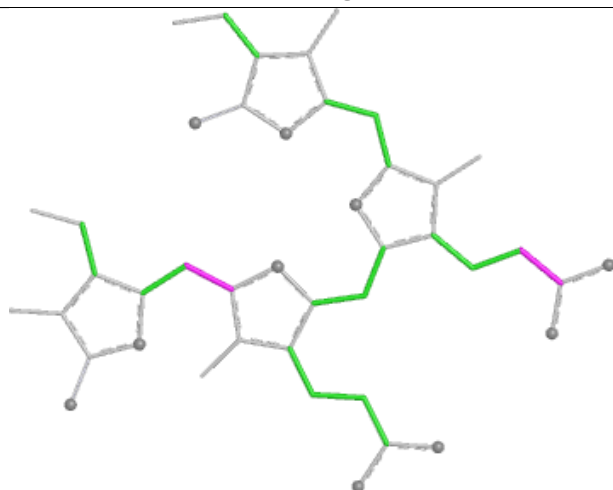
Ligand PEB D 166



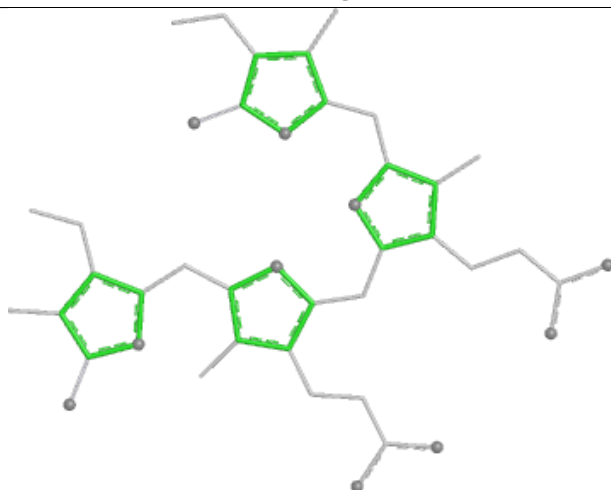
Bond lengths



Bond angles

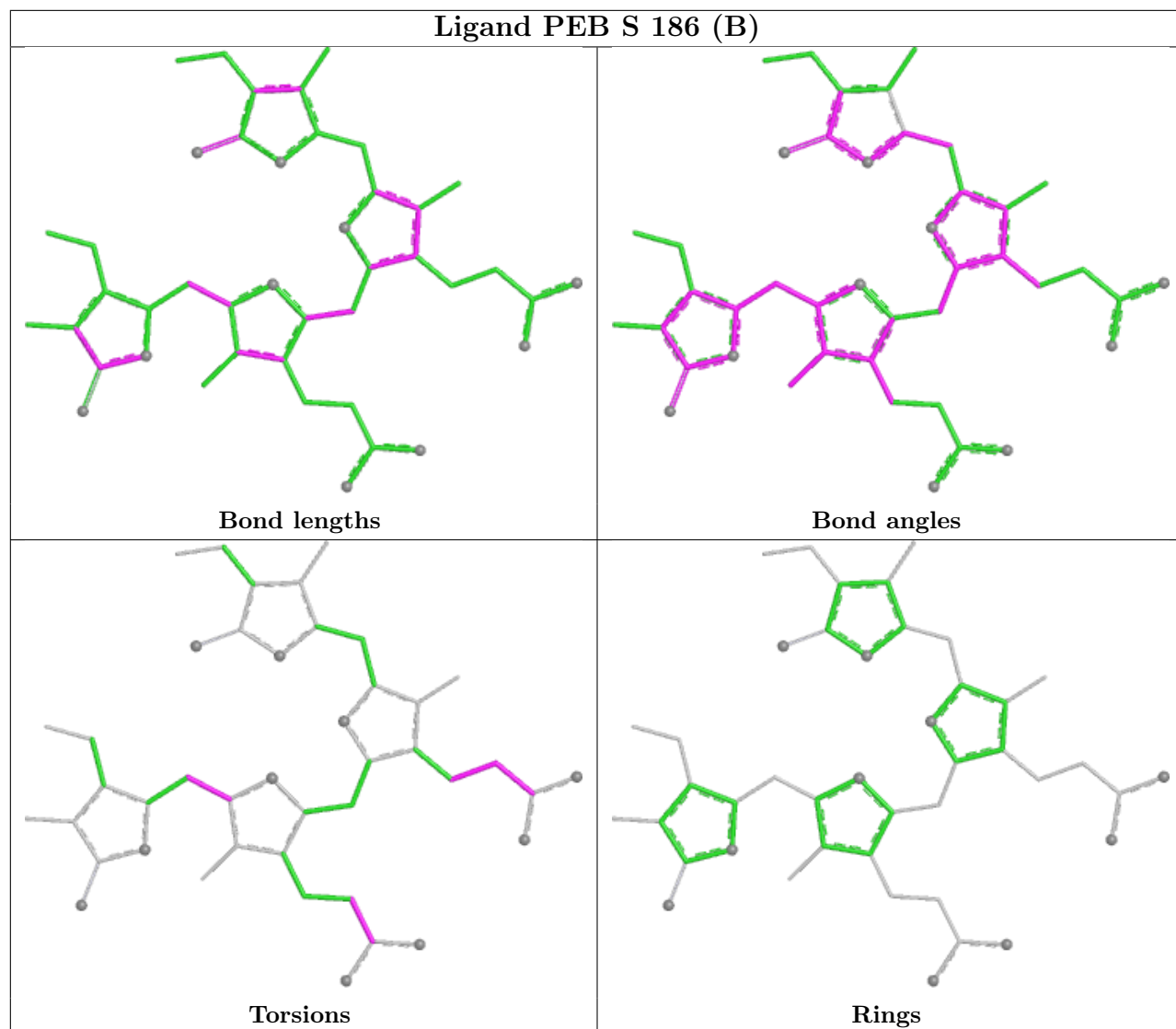


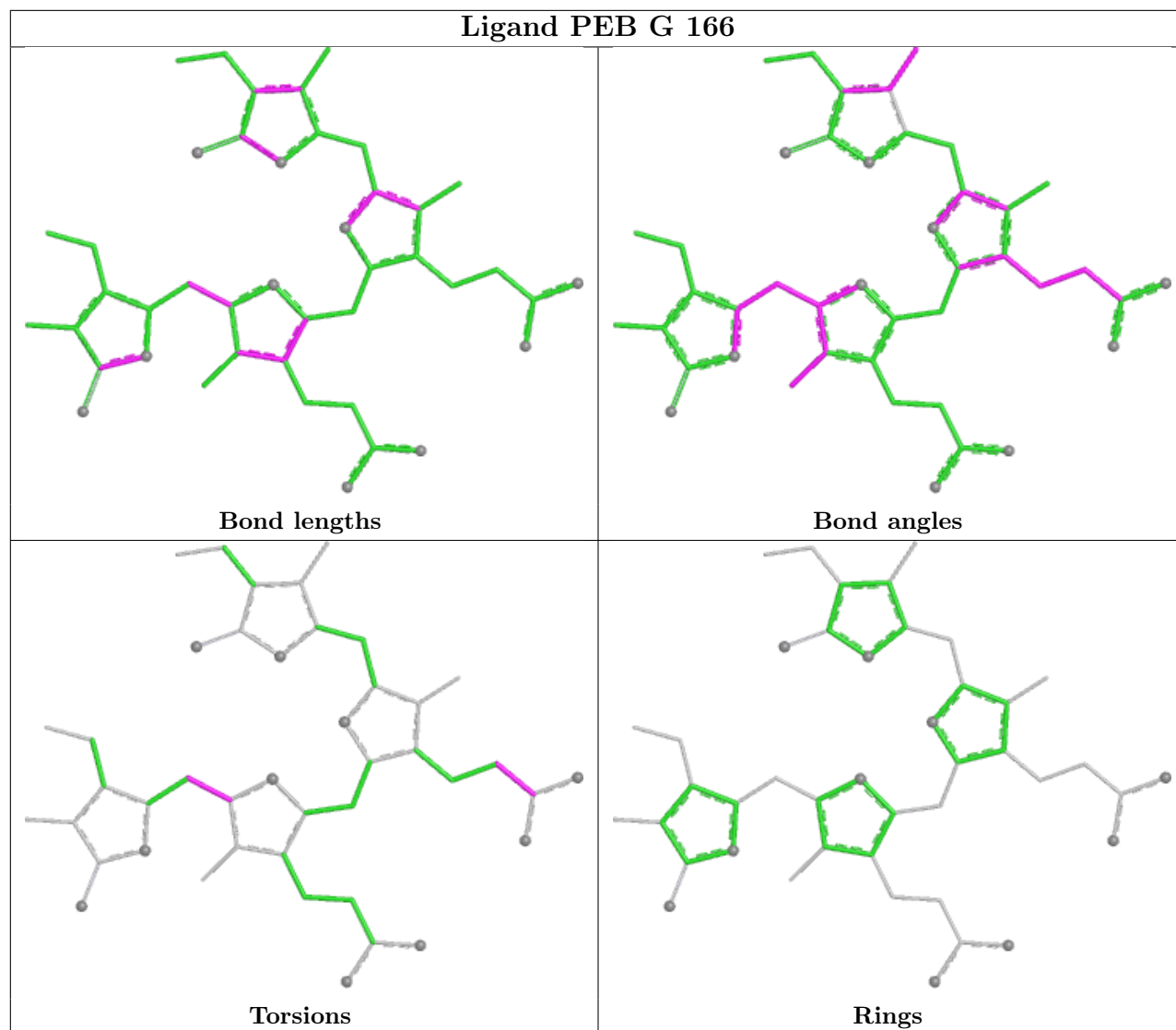
Torsions



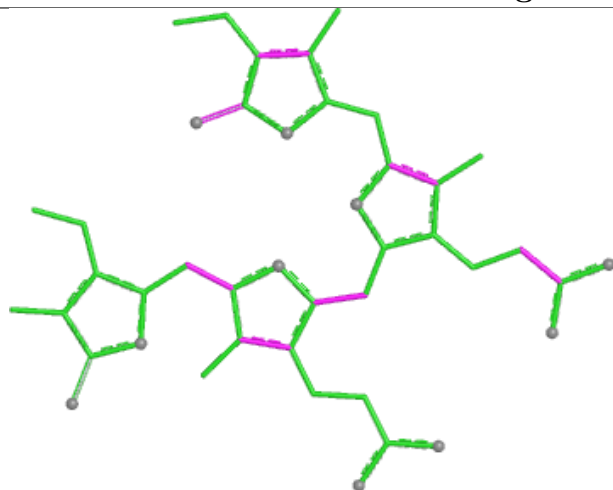
Rings

Ligand PEB S 186 (B)

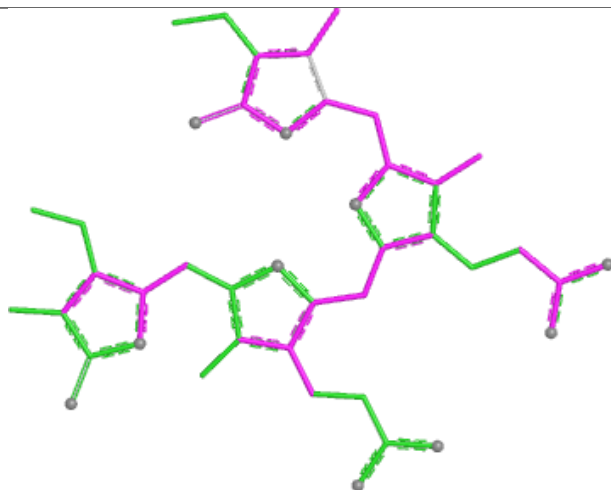




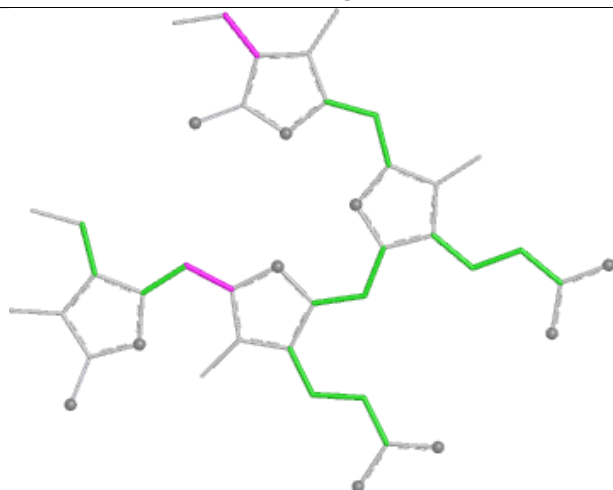
Ligand PEB P 188



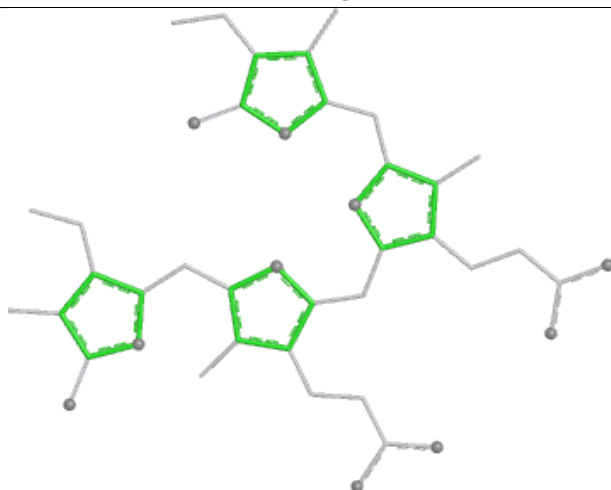
Bond lengths



Bond angles

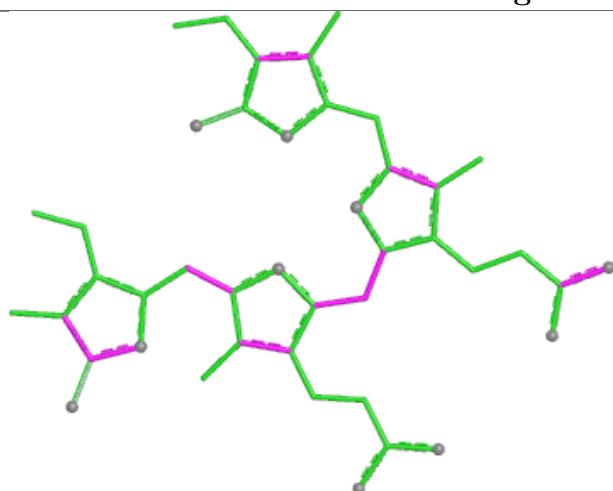


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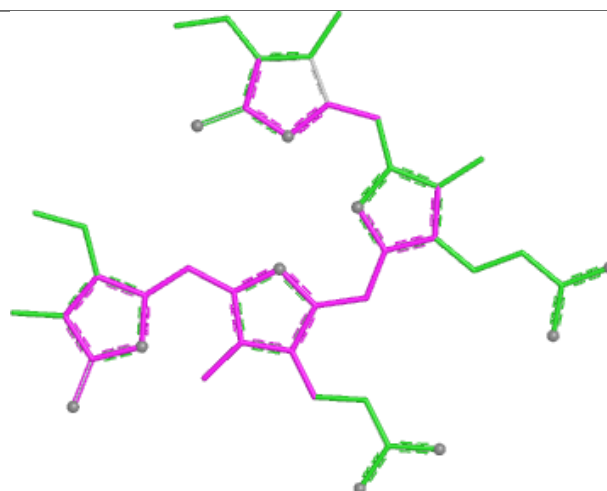


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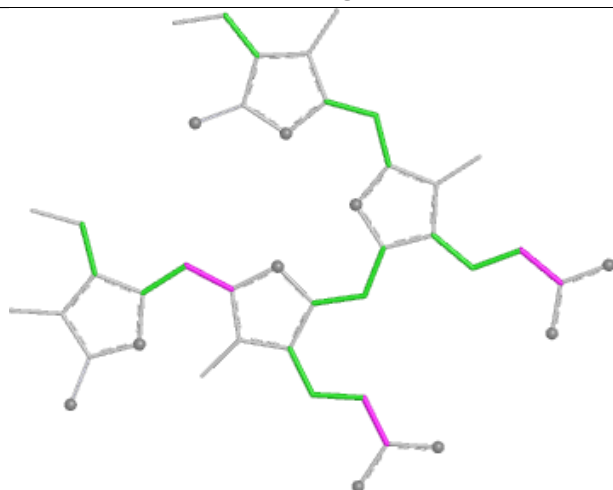
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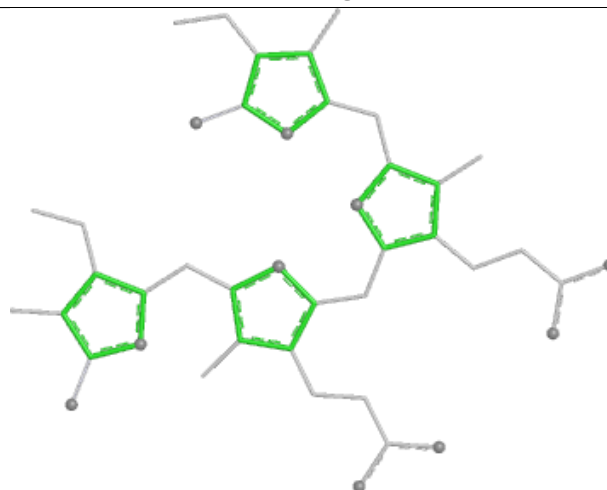
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Bond angles

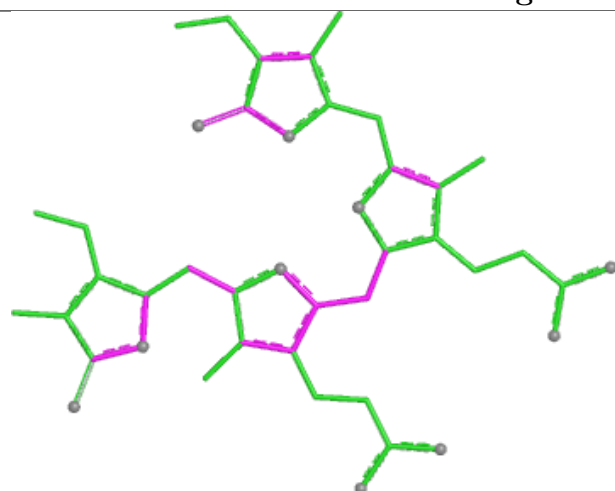


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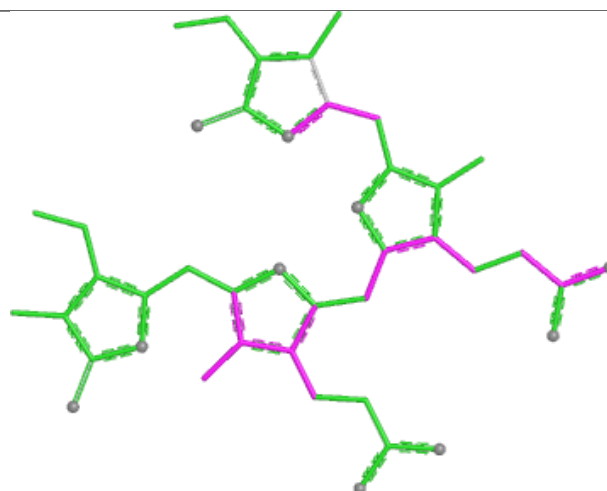


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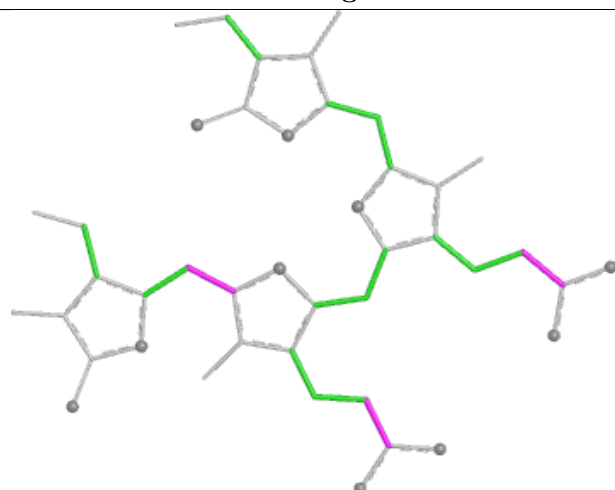
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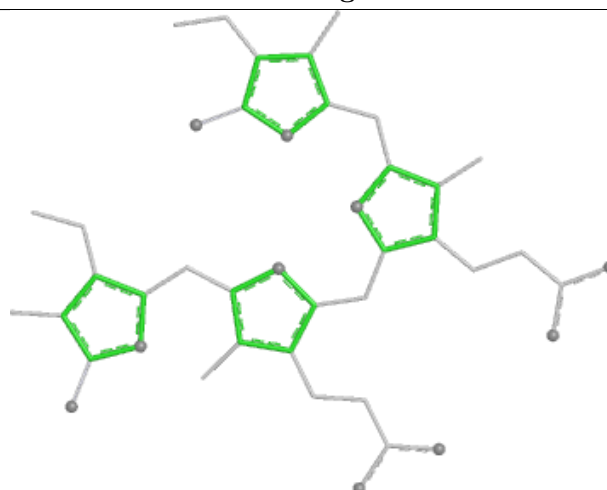
Bond lengths



Bond angles

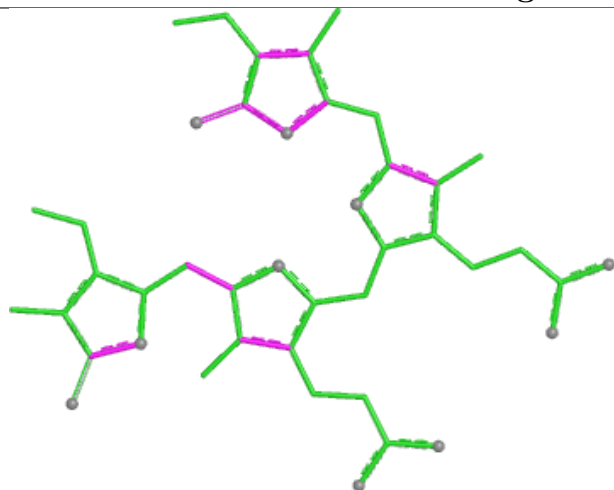


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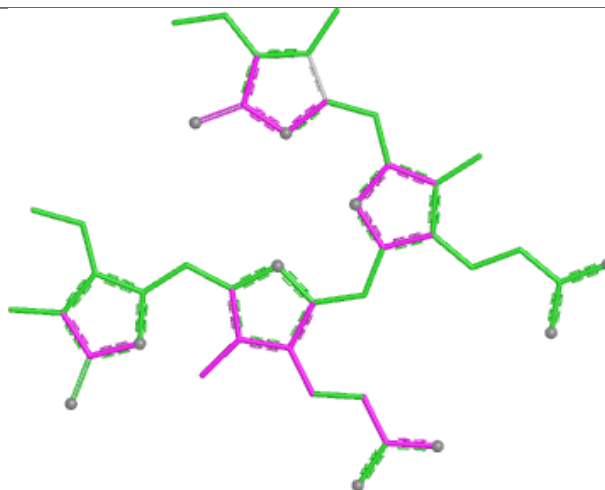


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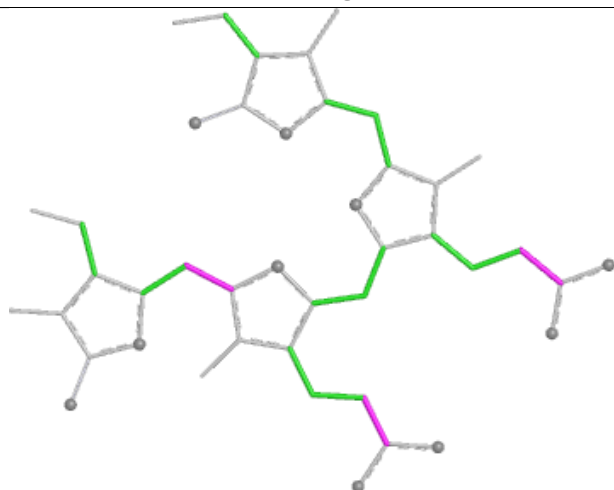
Ligand PEB L 167



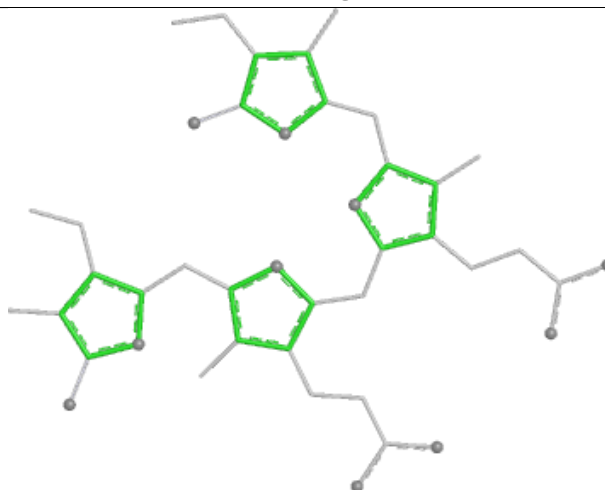
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Bond angles

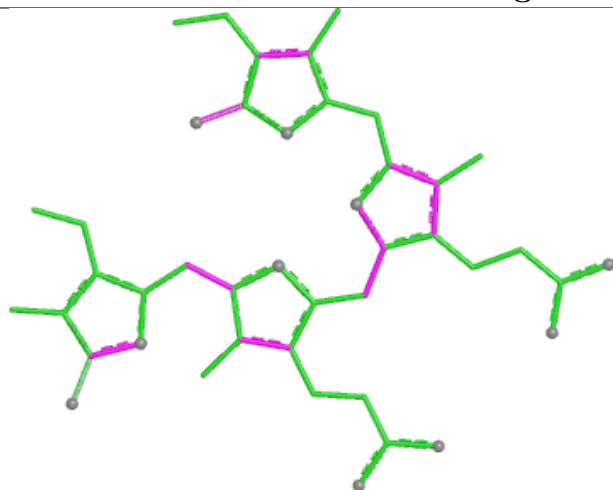


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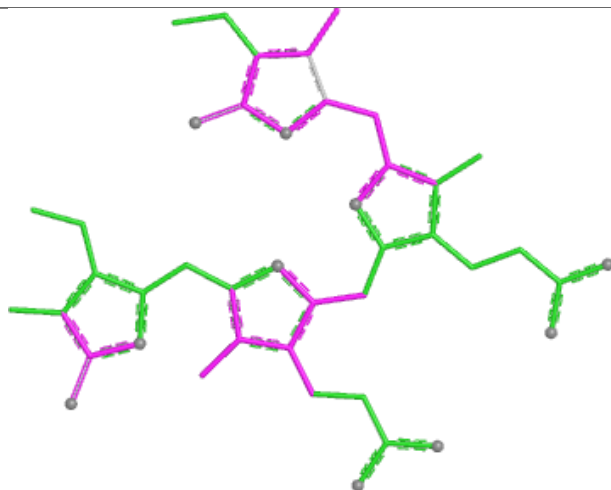


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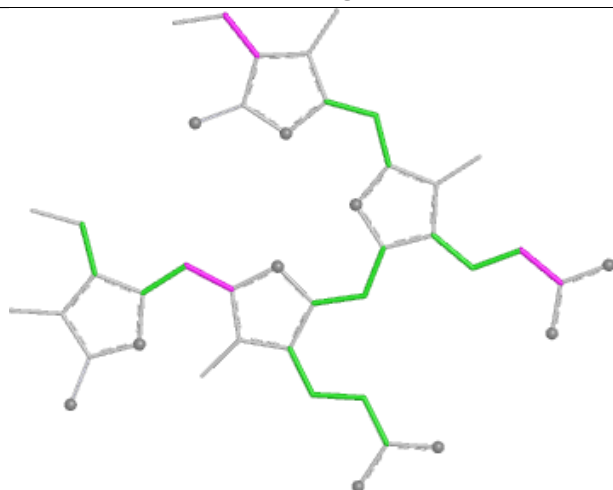
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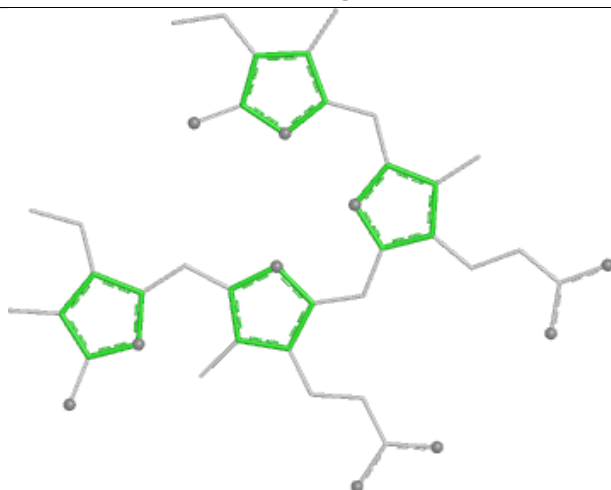
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Bond angles

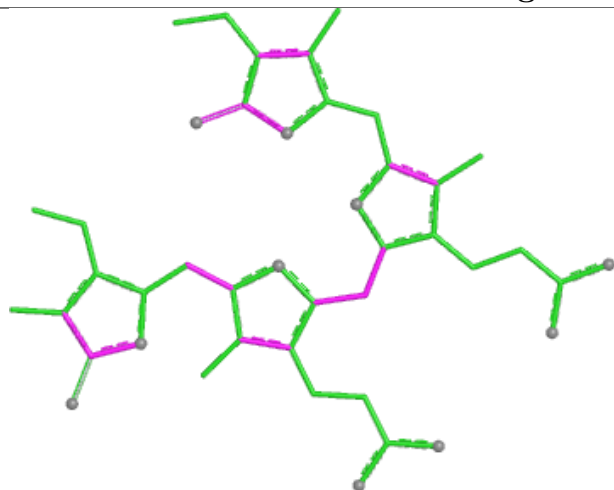


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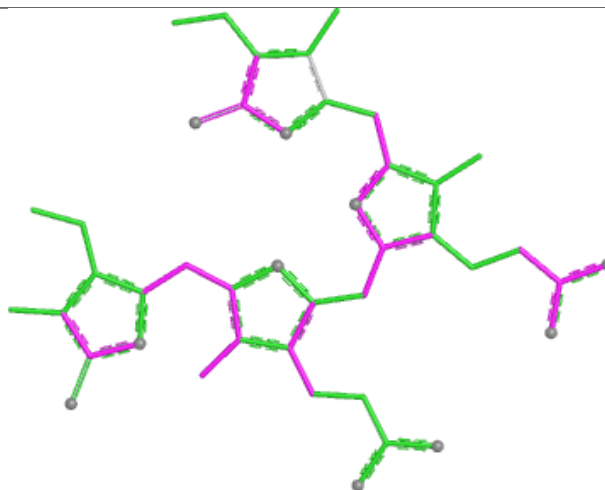


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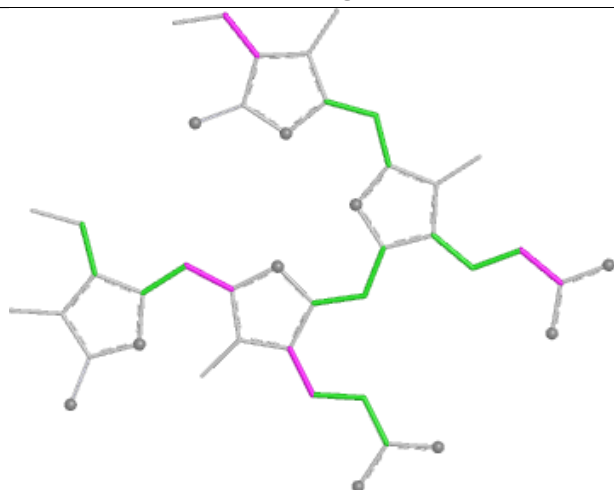
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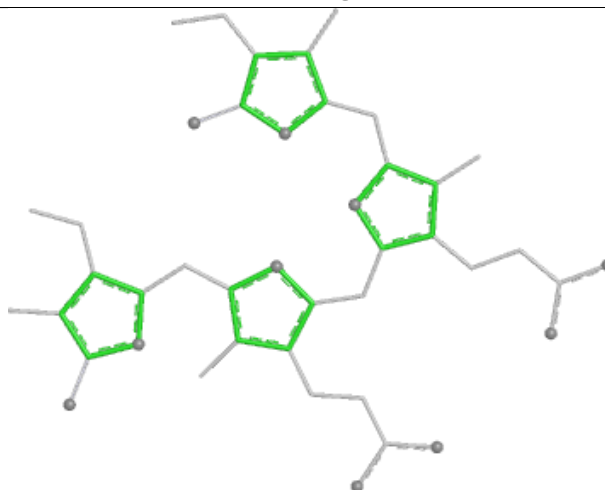
Bond lengths



Bond angles

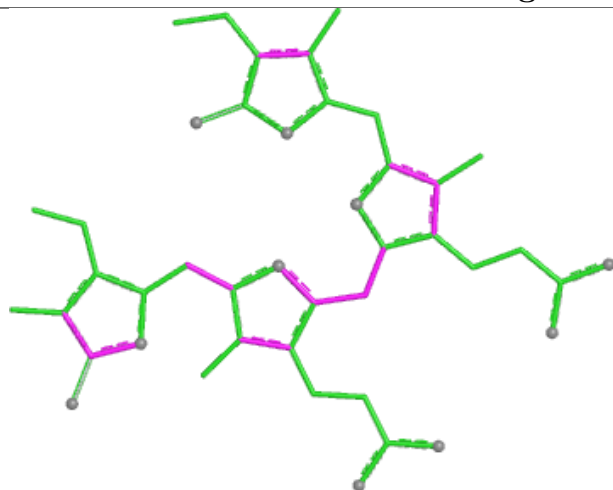


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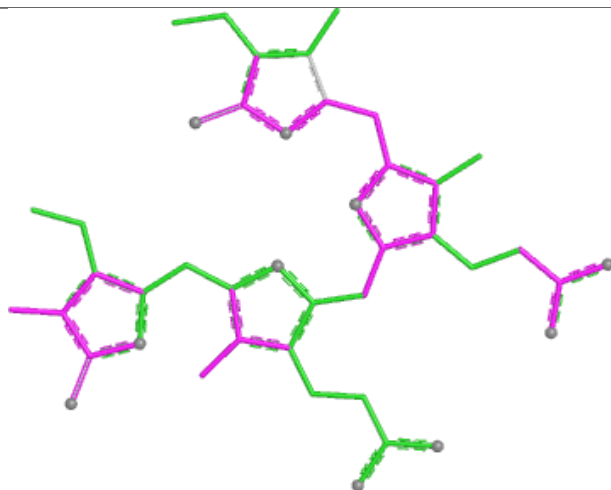


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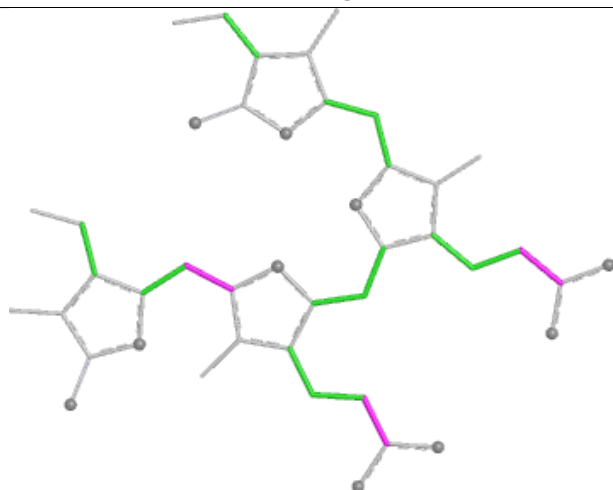
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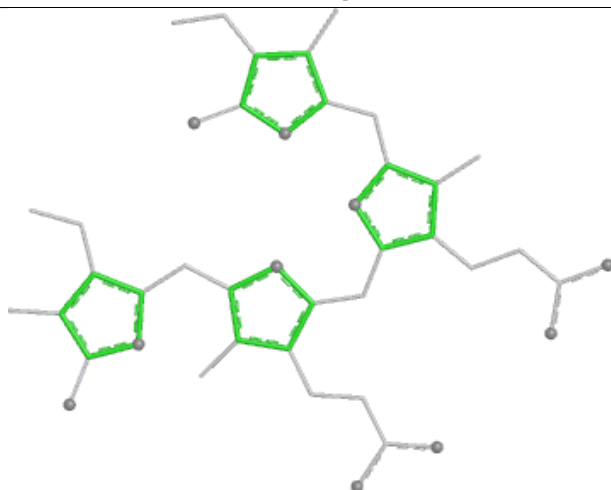
Bond lengths



Bond angles

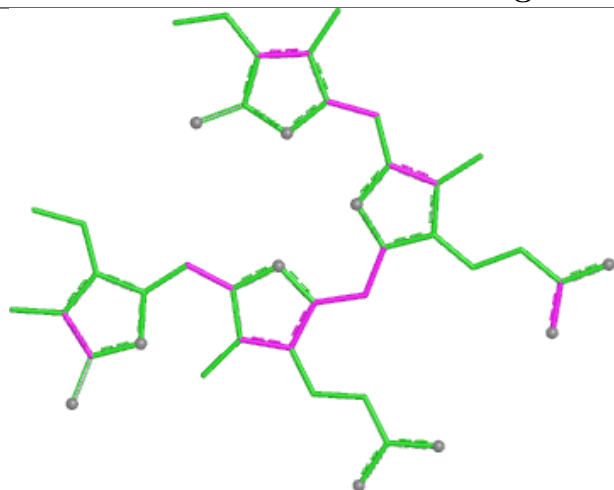


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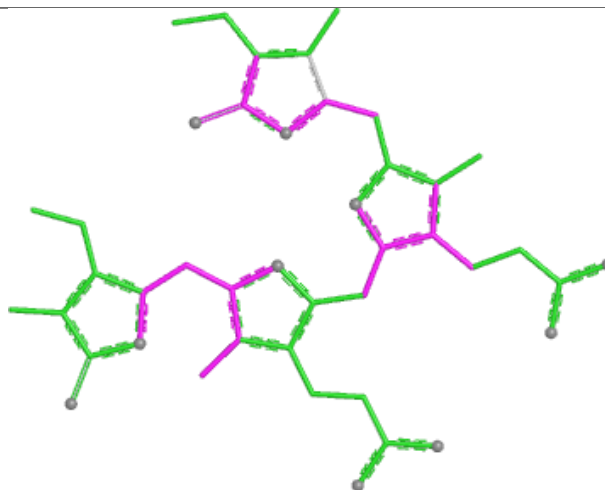


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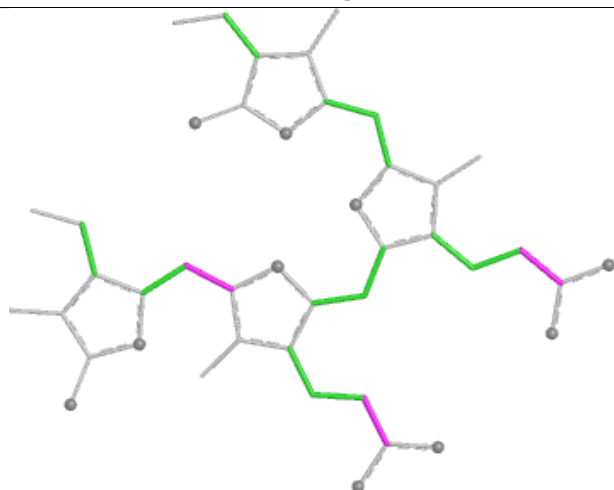
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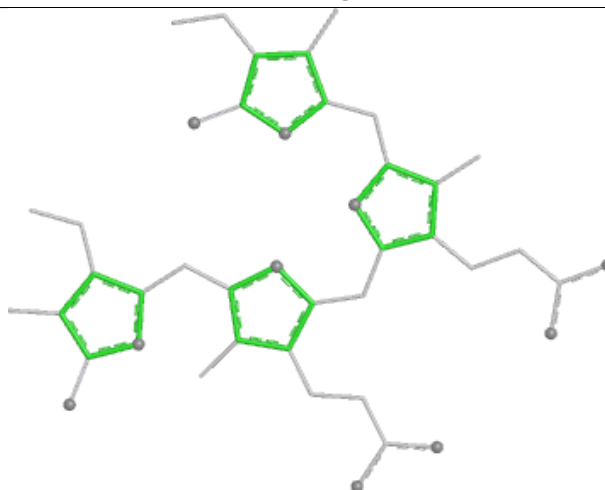
Bond lengths



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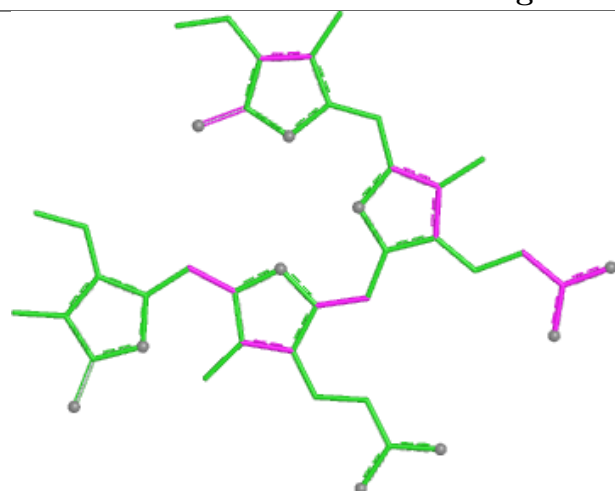


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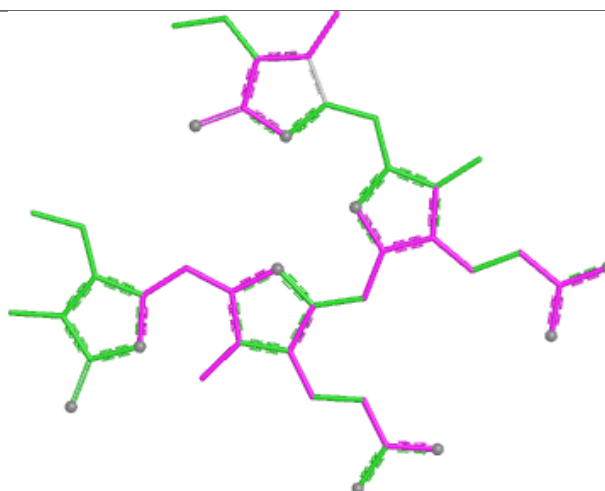


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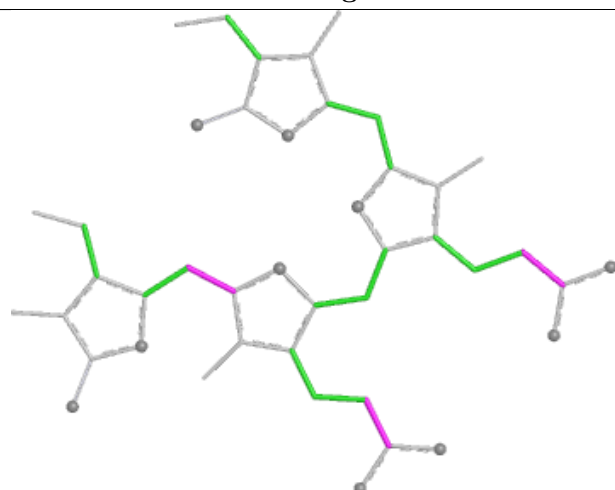
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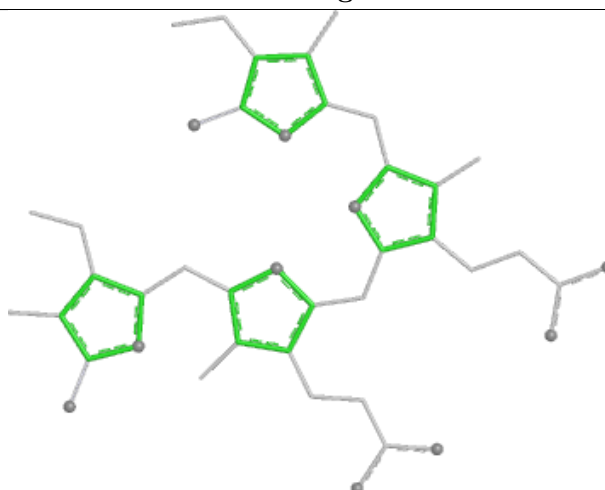
Bond lengths



Bond angles

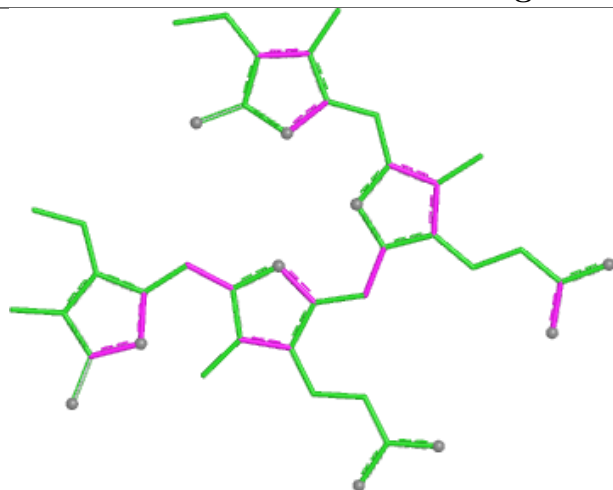


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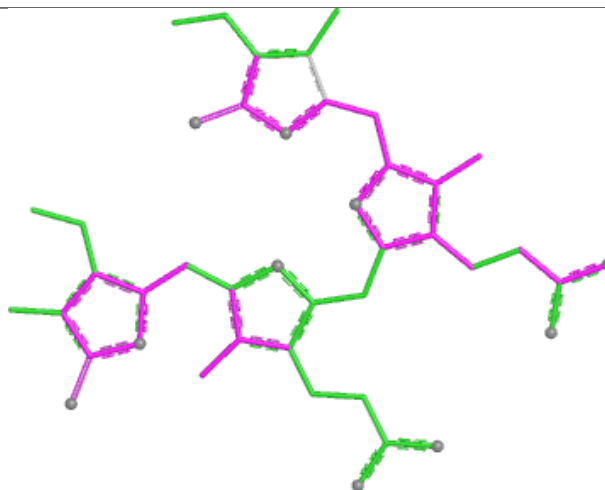


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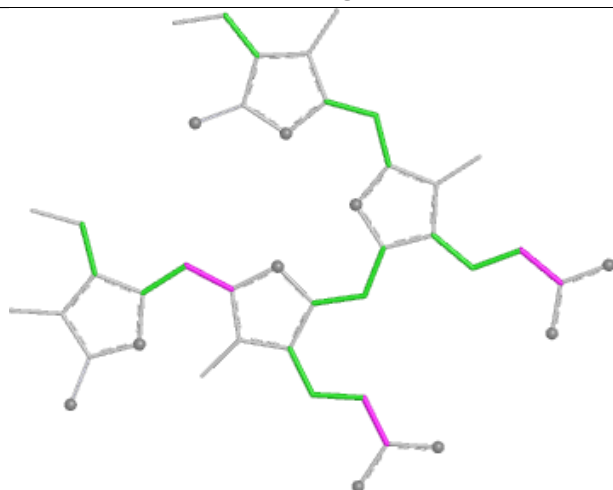
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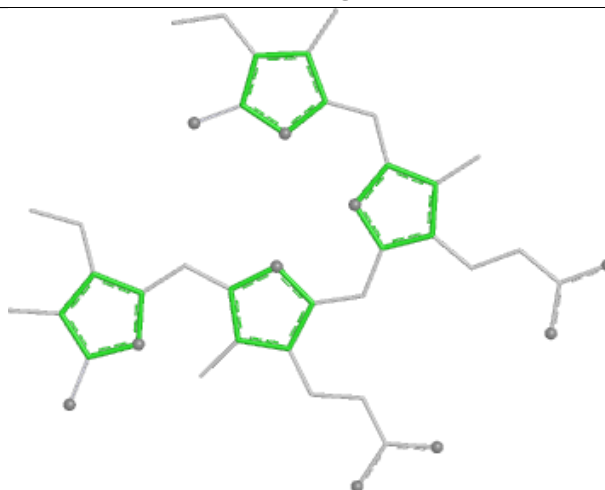
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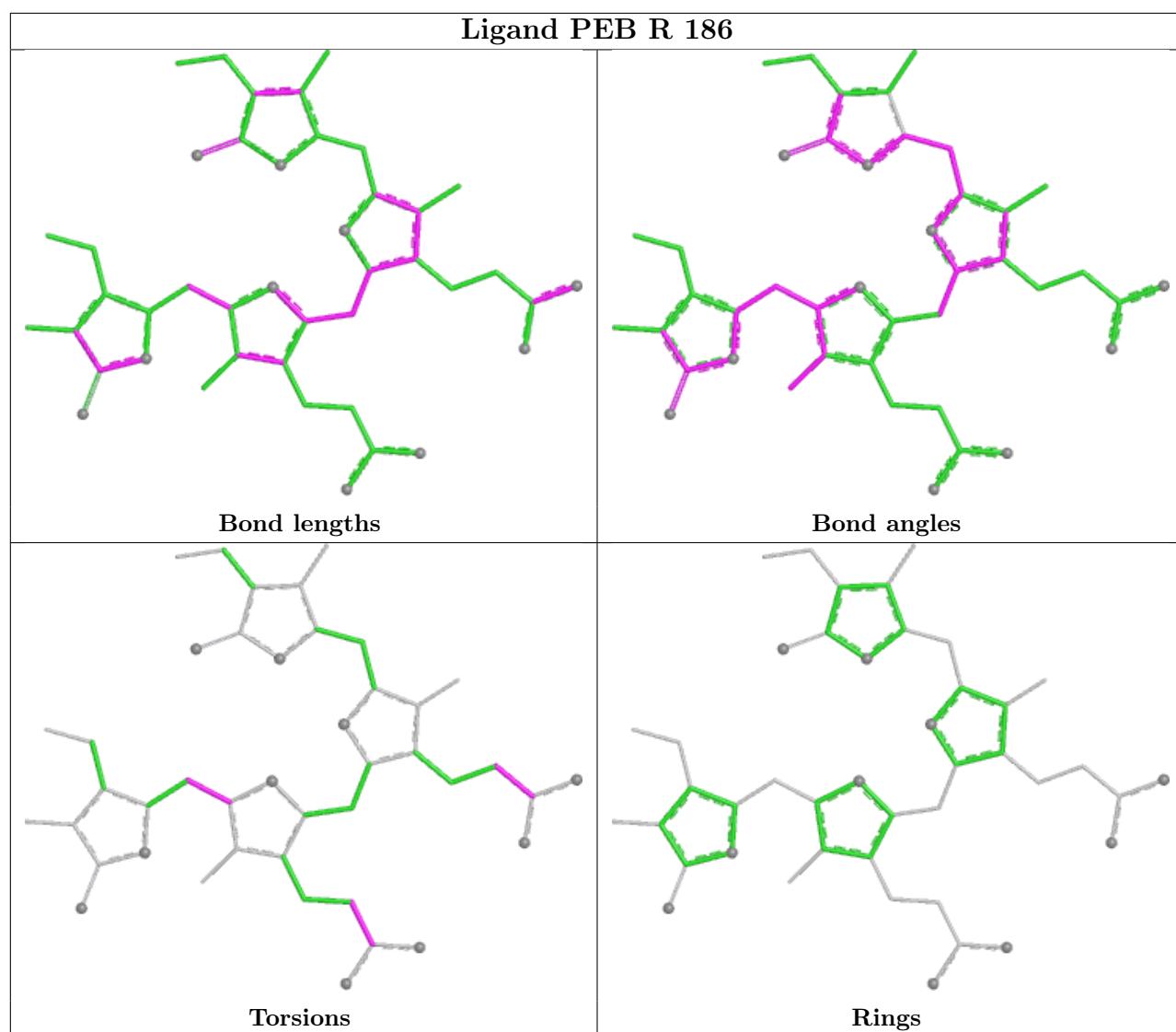
Bond angles

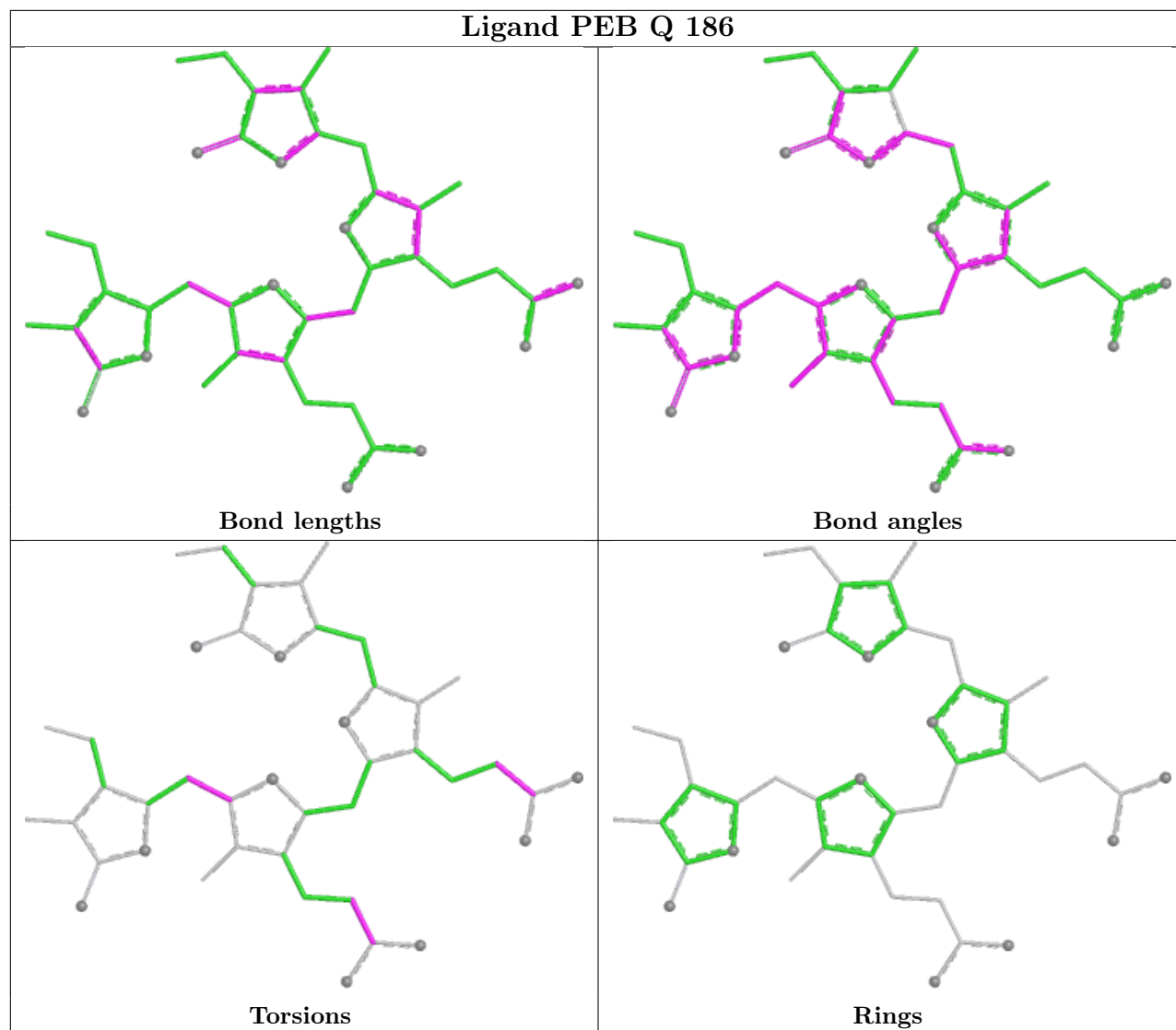


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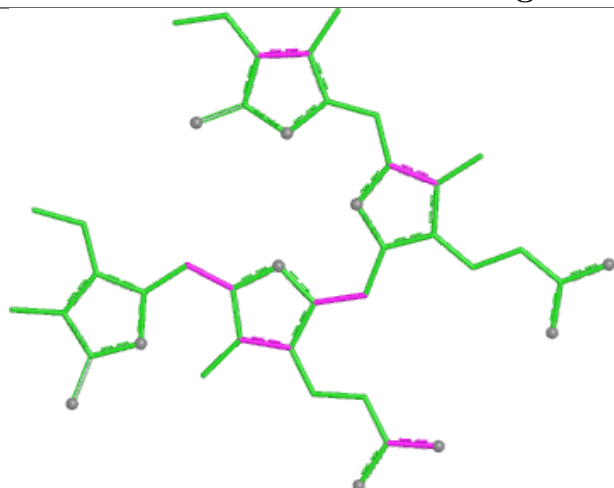


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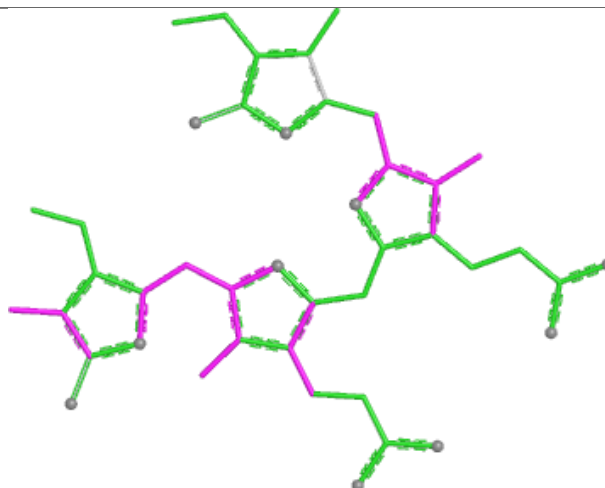




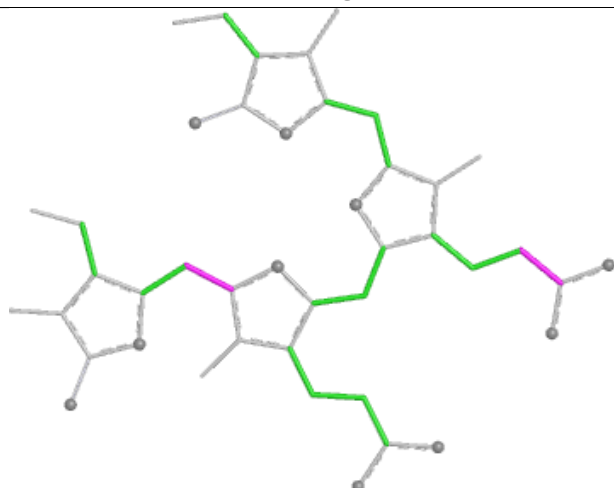
Ligand PEB F 166



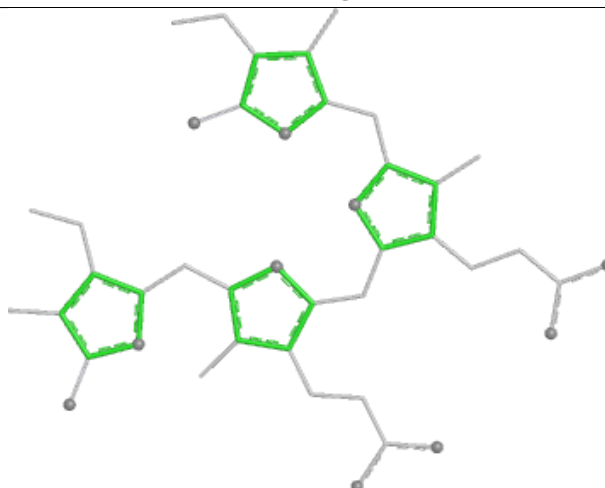
Bond lengths



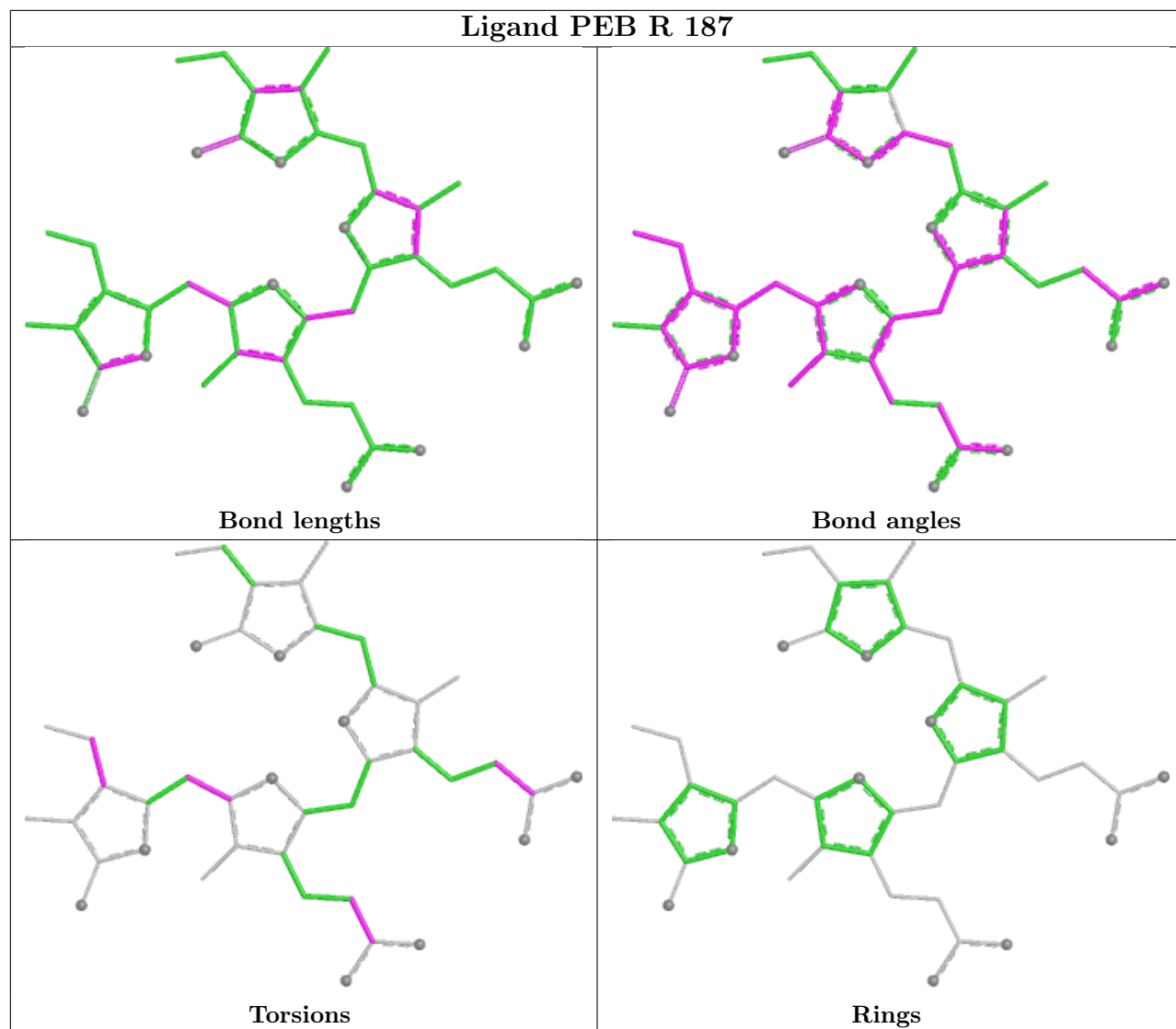
Bond angles

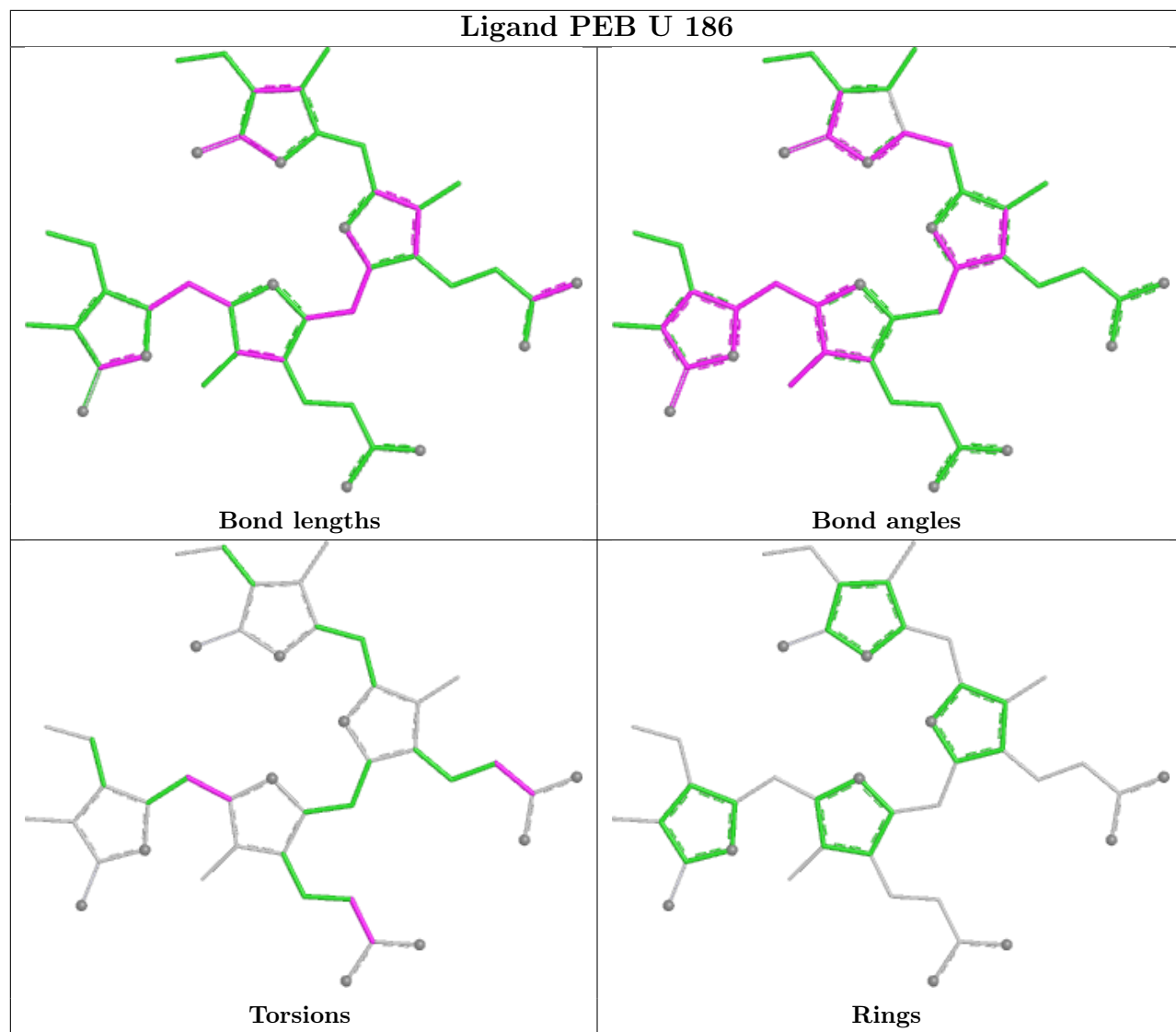


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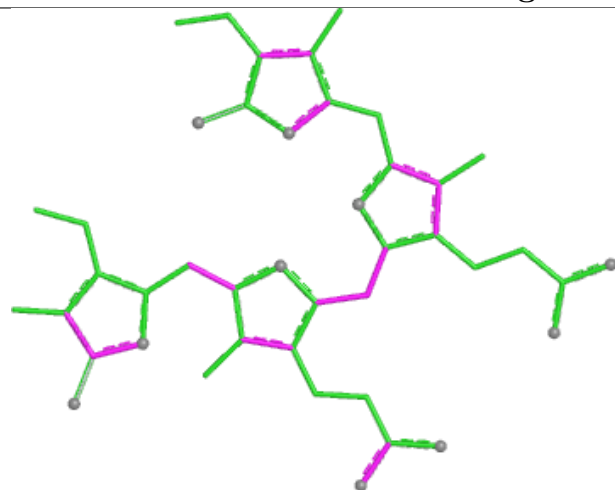


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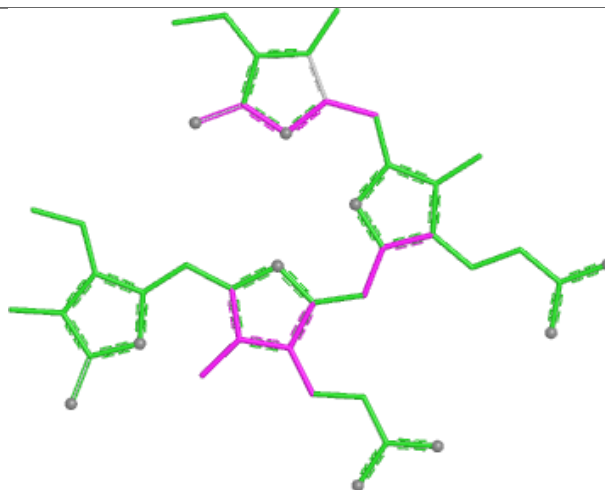




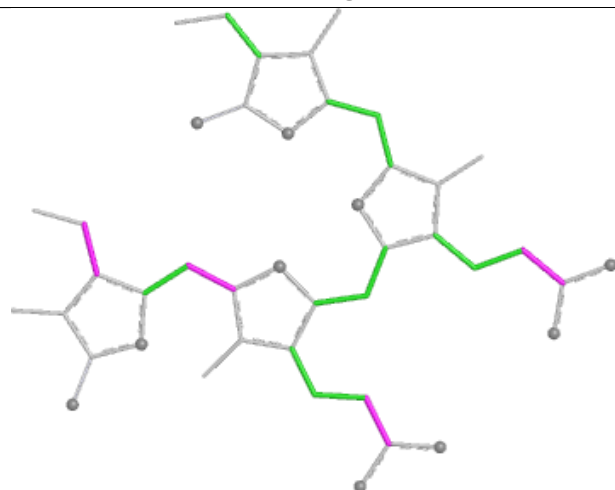
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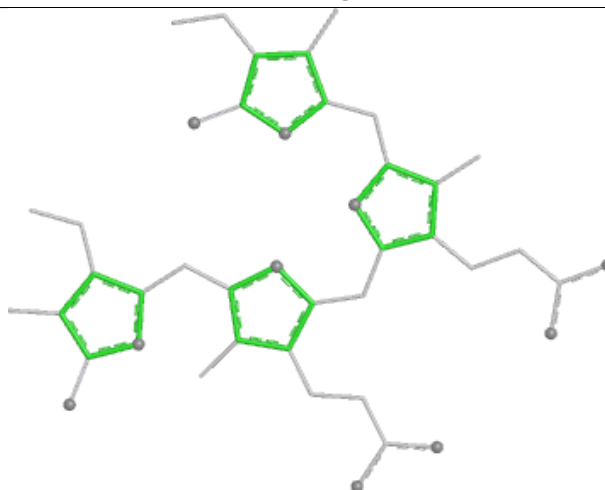
Bond lengths



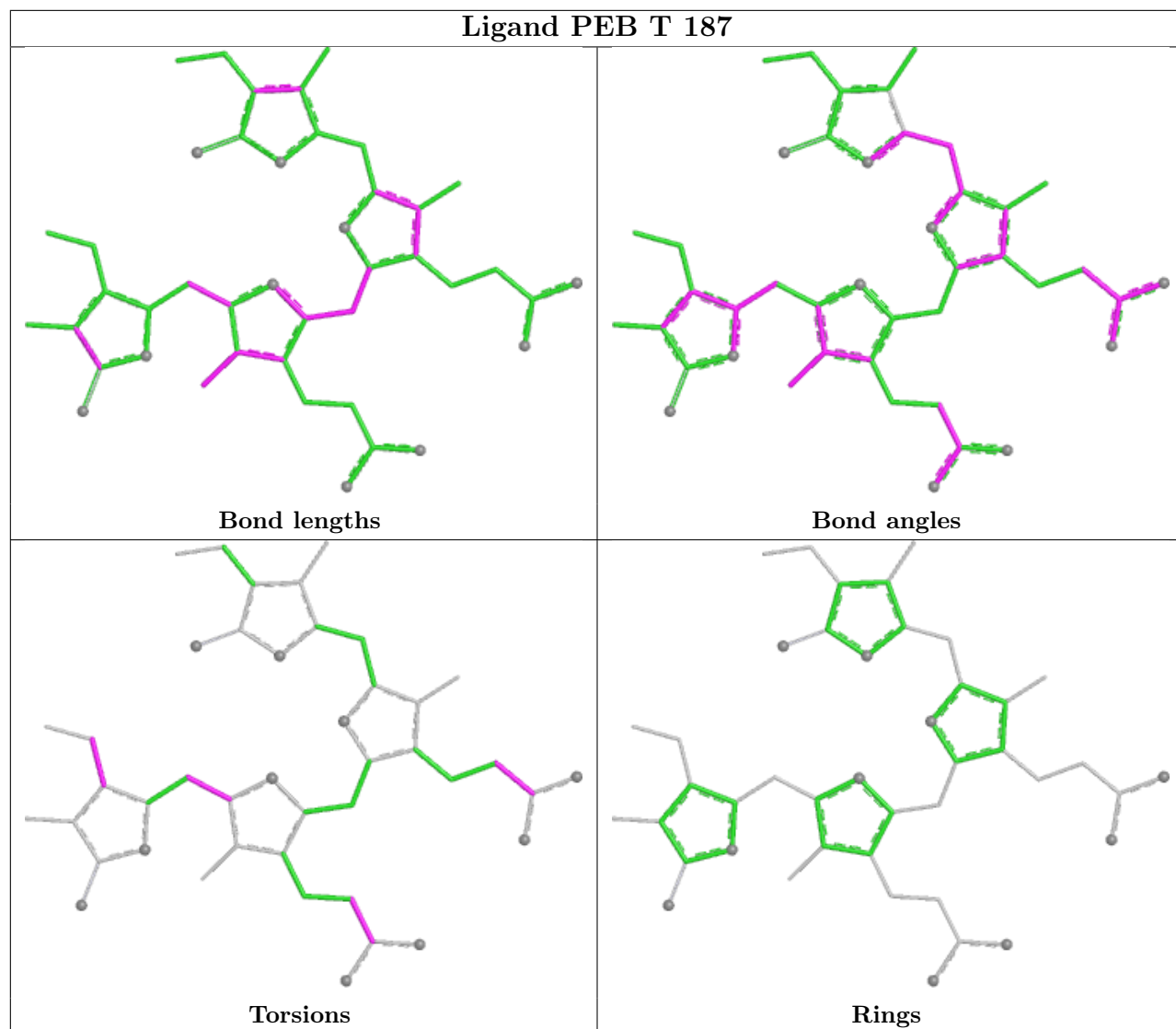
Bond angles

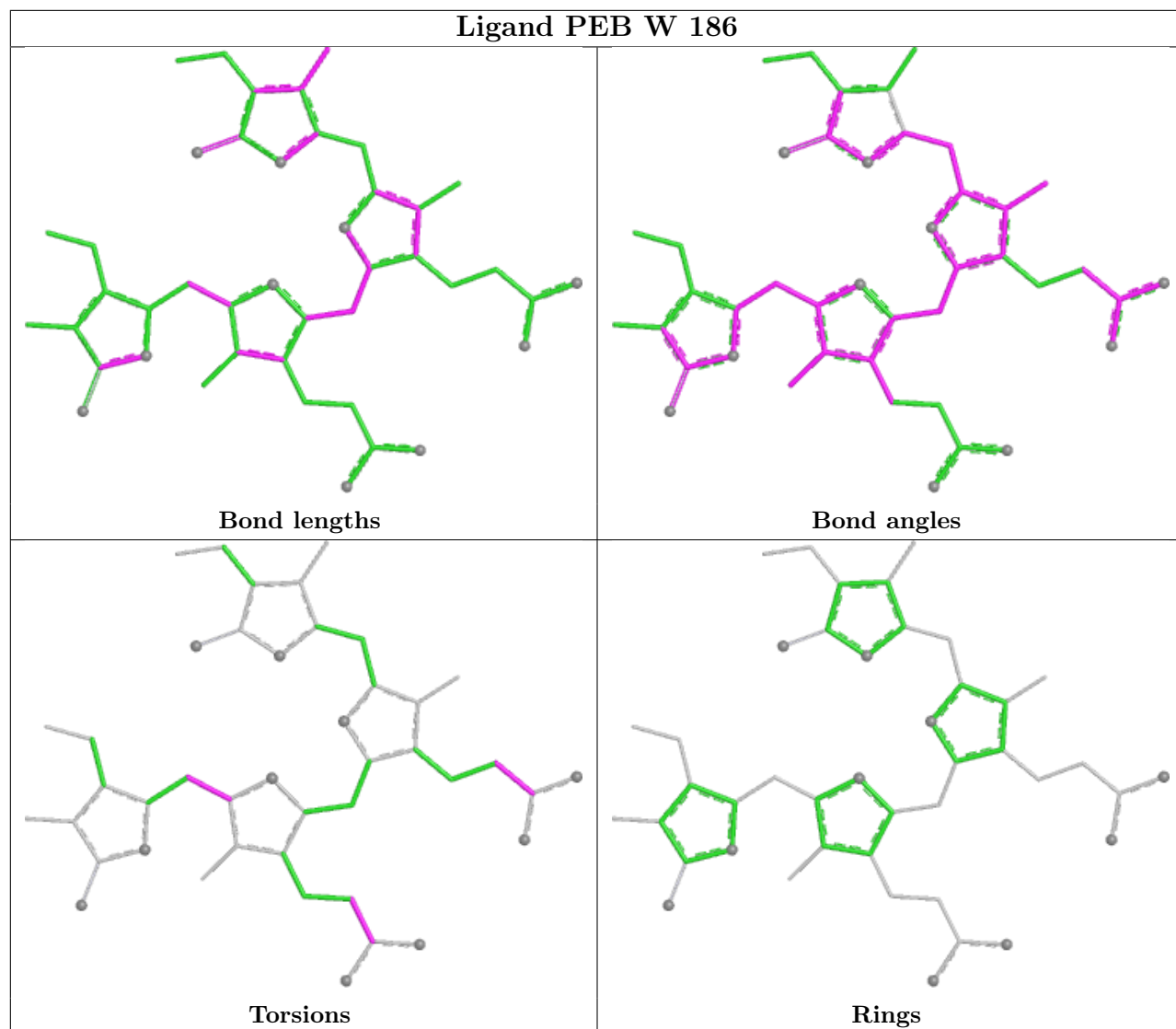


Torsions

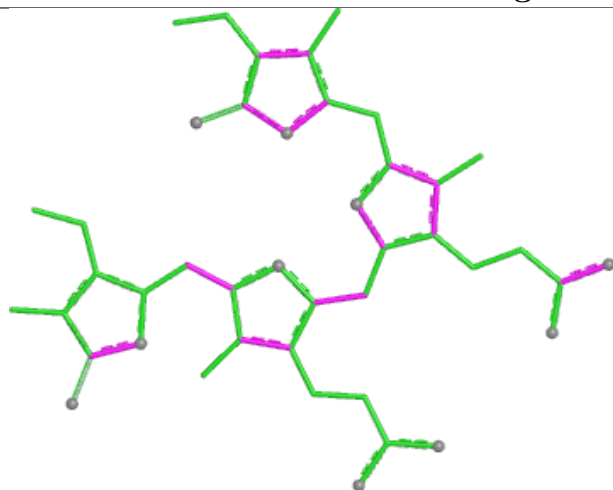


Rings

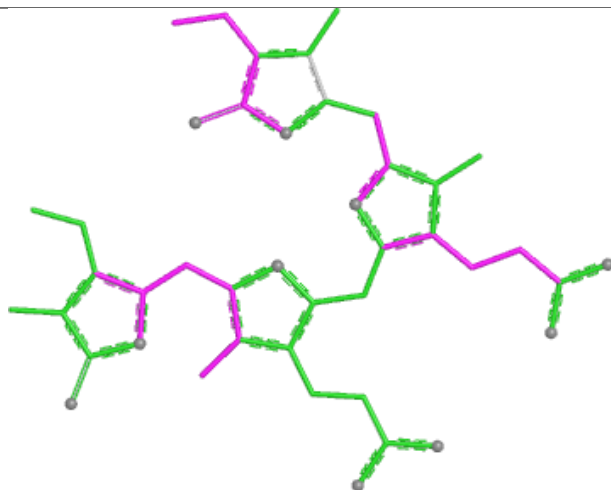




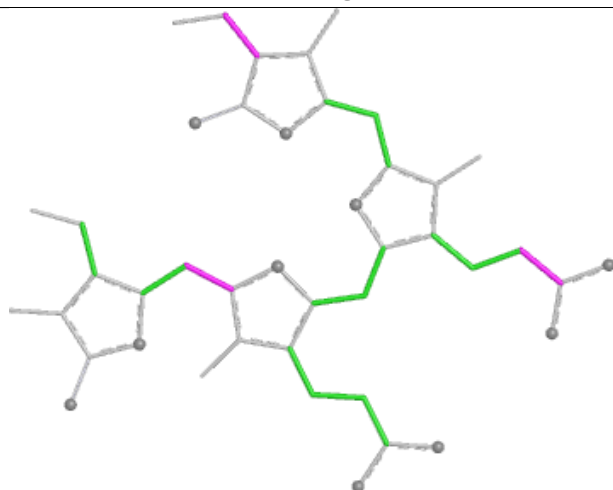
Ligand PEB U 188



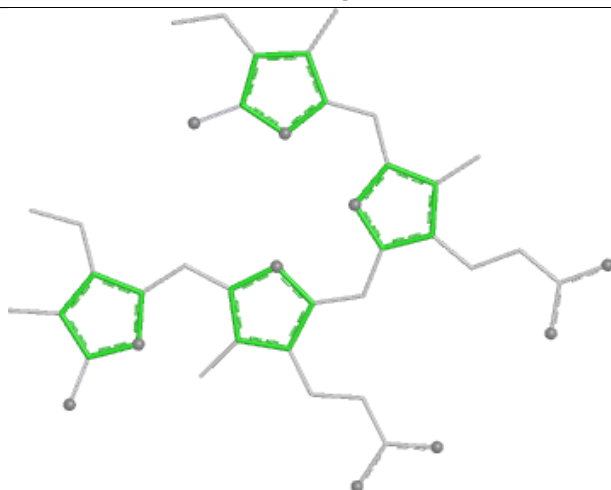
Bond lengths



Bond angles

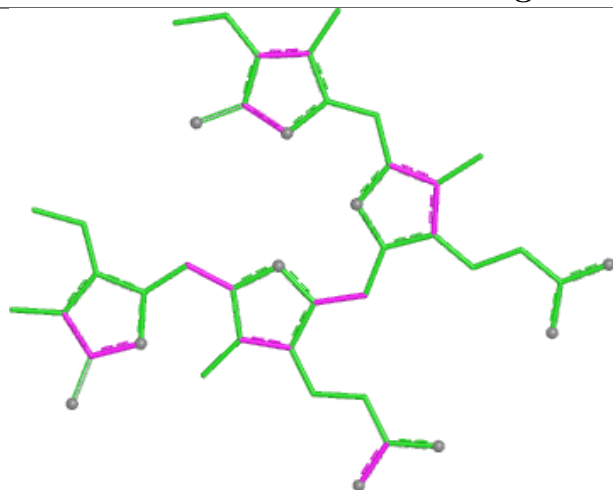


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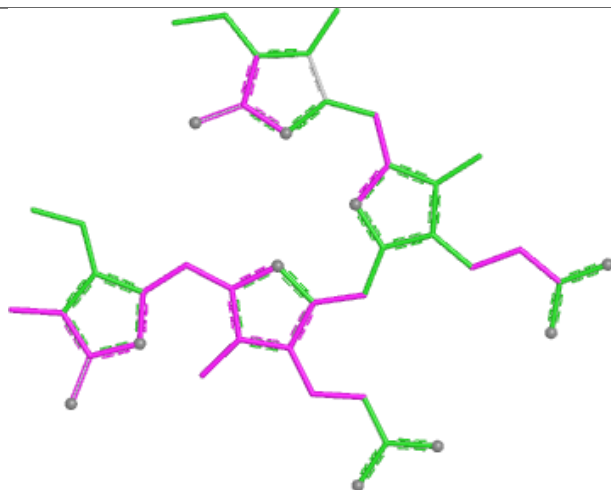


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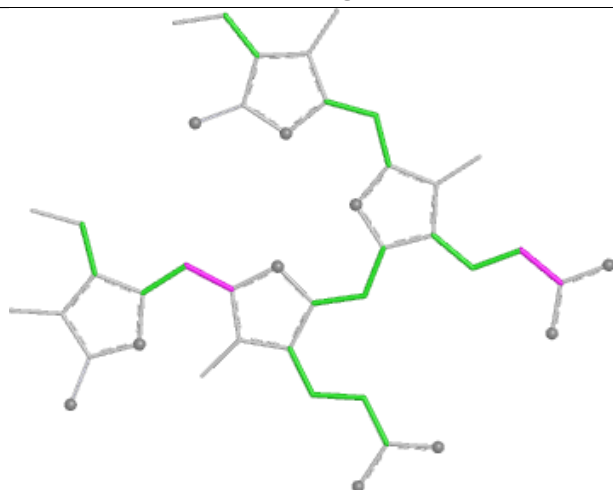
Ligand PEB C 166



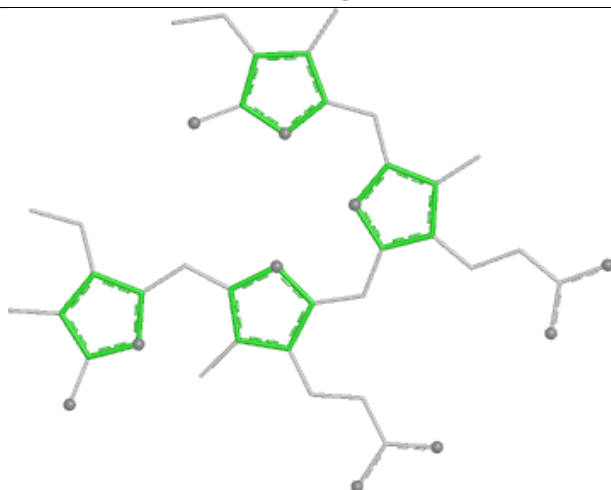
Bond lengths



Bond angles

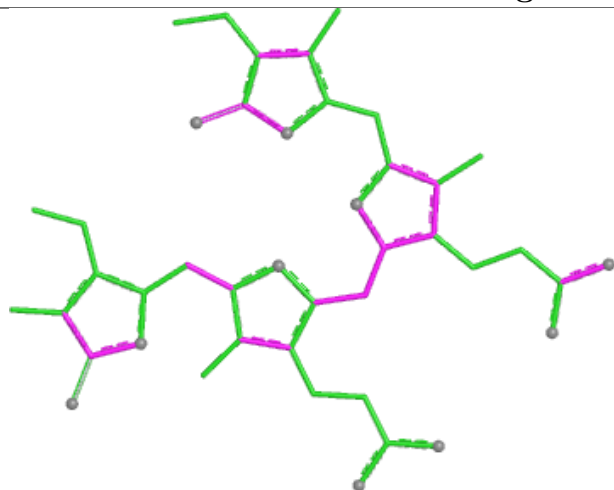


Torsions

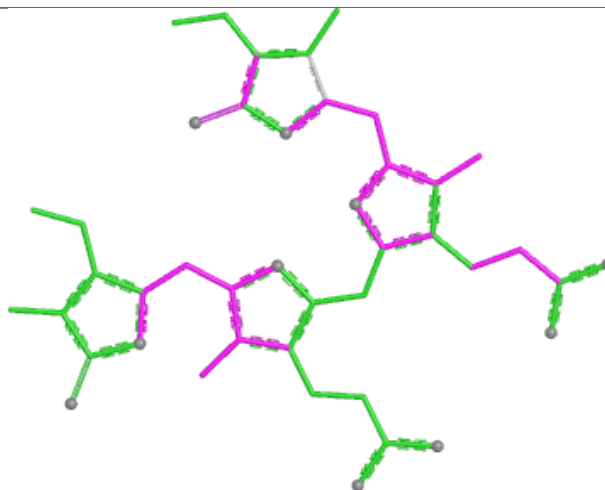


Rings

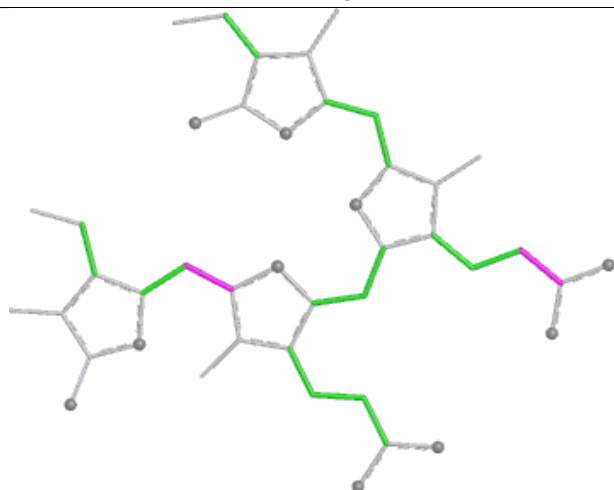
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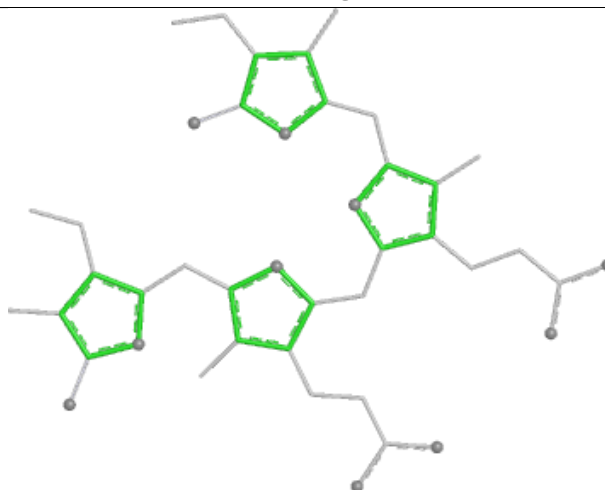
Bond lengths



Bond angles

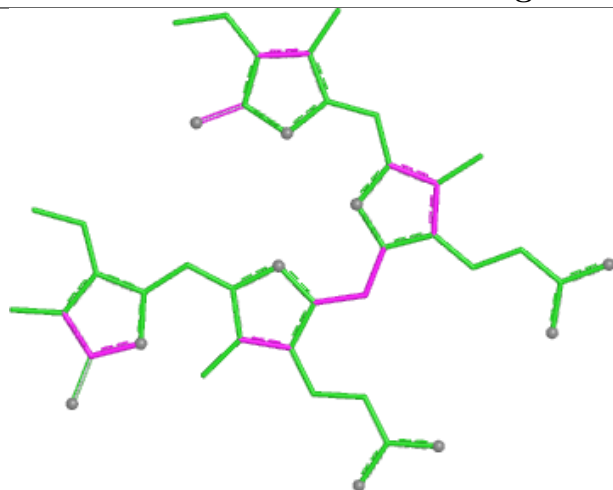


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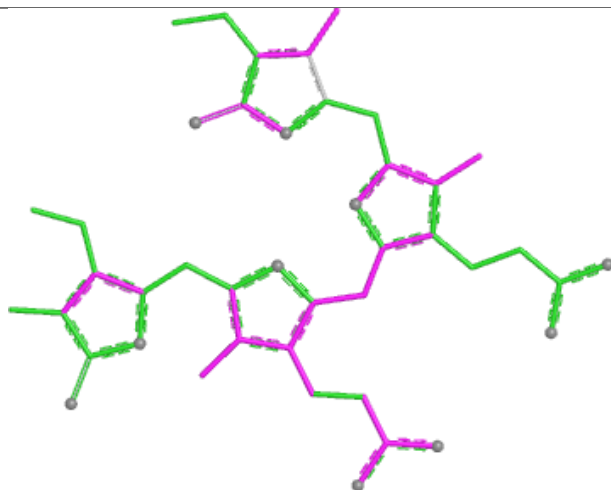


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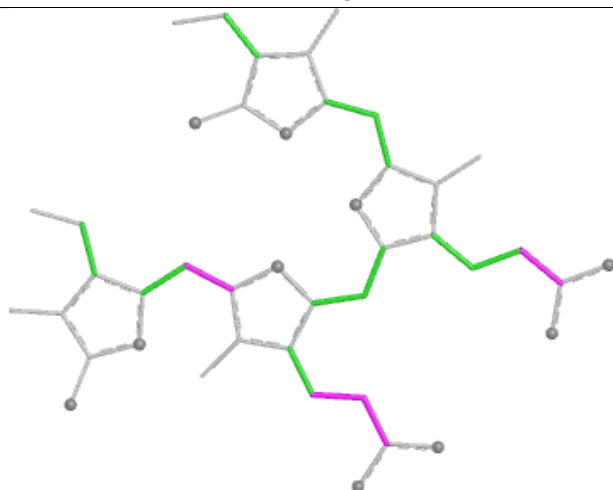
Ligand PEB B 167



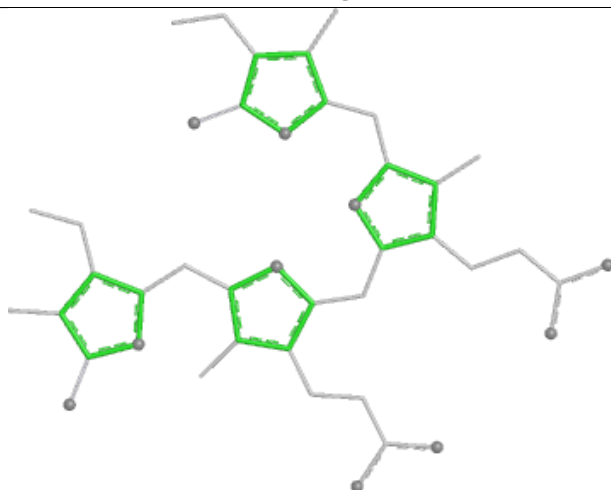
Bond lengths



Bond angles

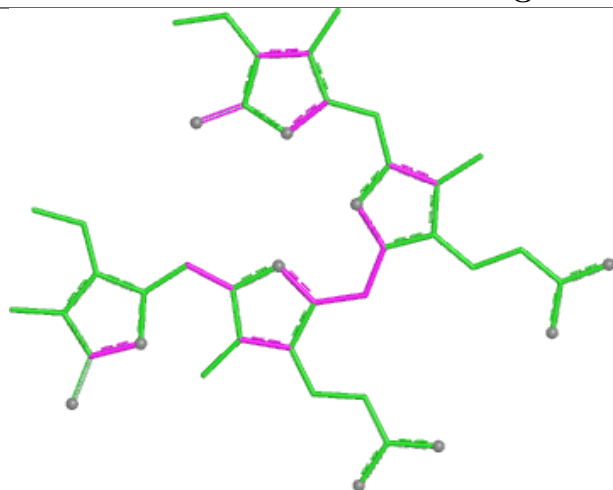


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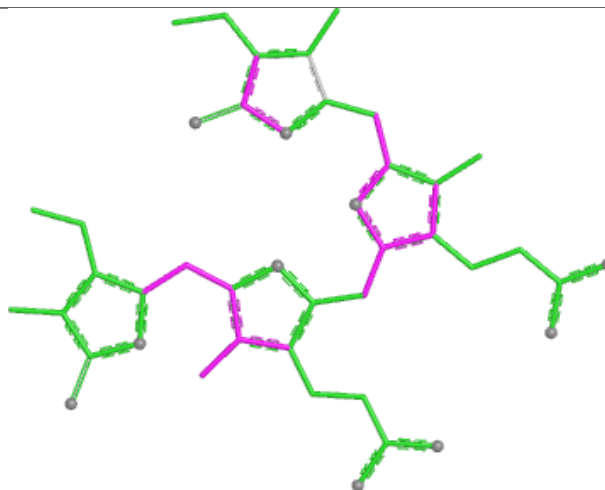


Rings

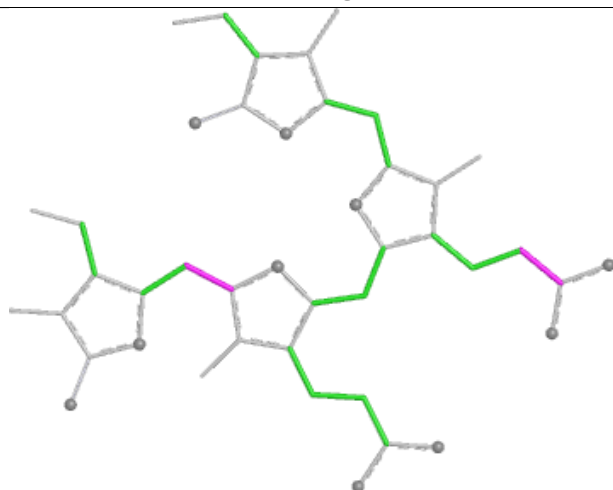
Ligand PEB R 188



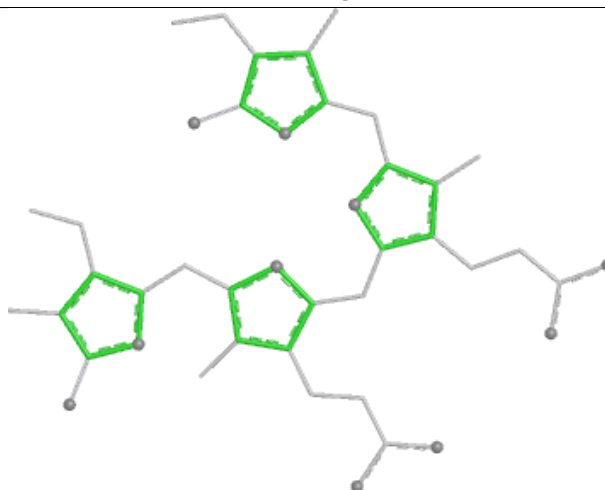
Bond lengths



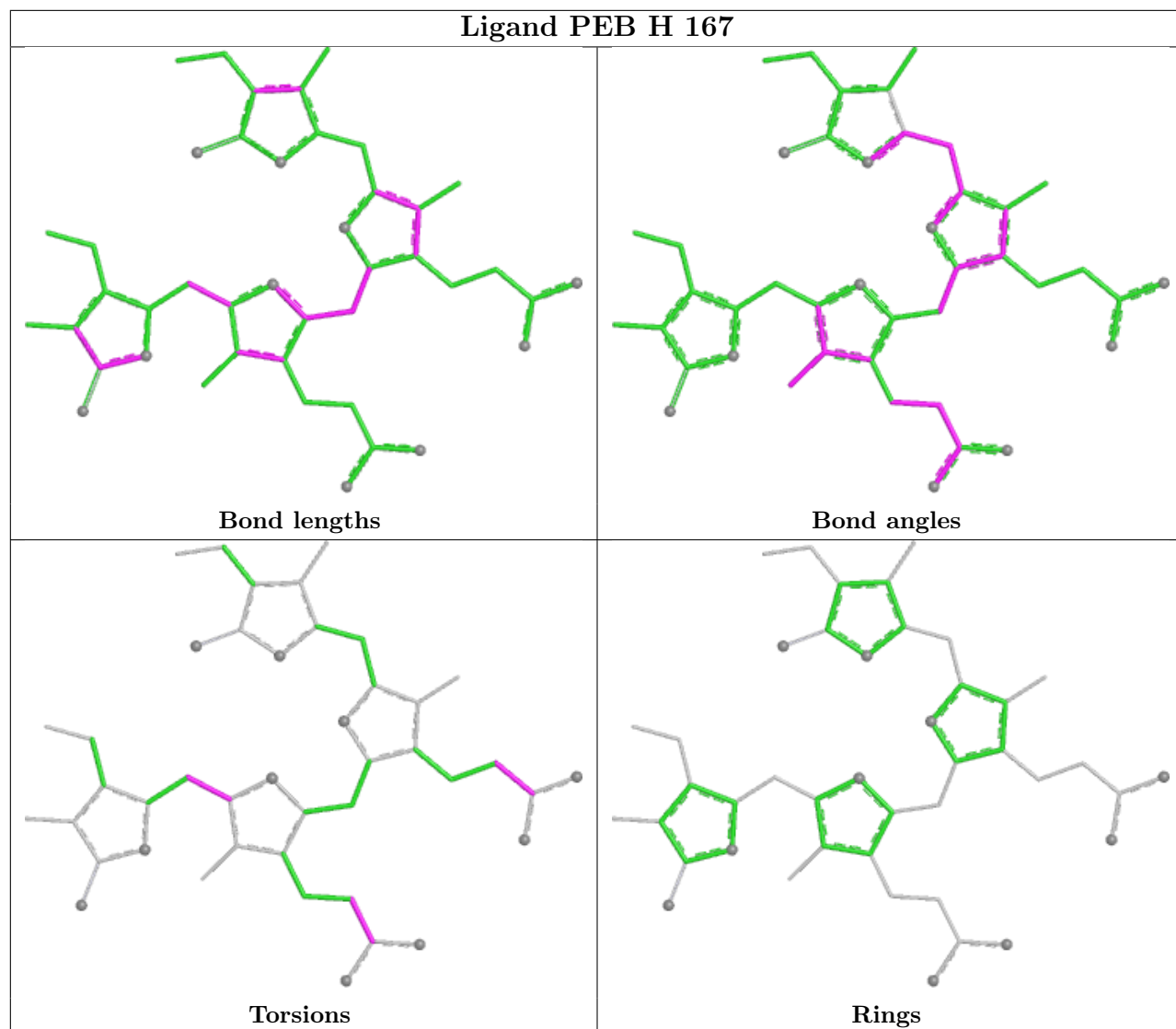
Bond angles



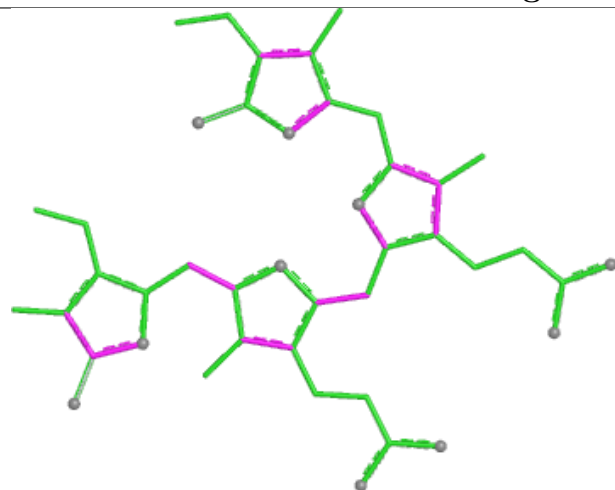
Torsions



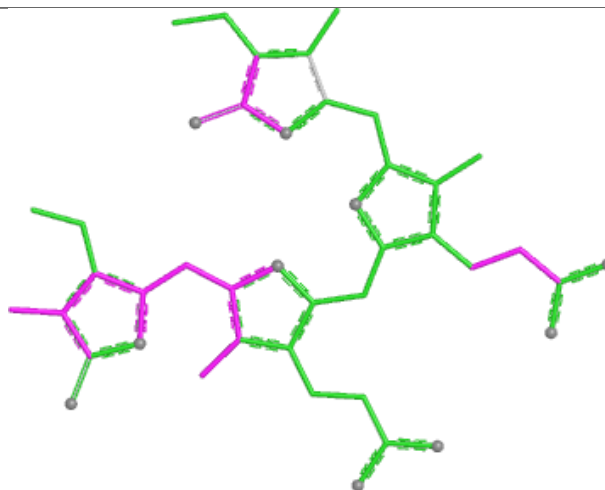
Rings



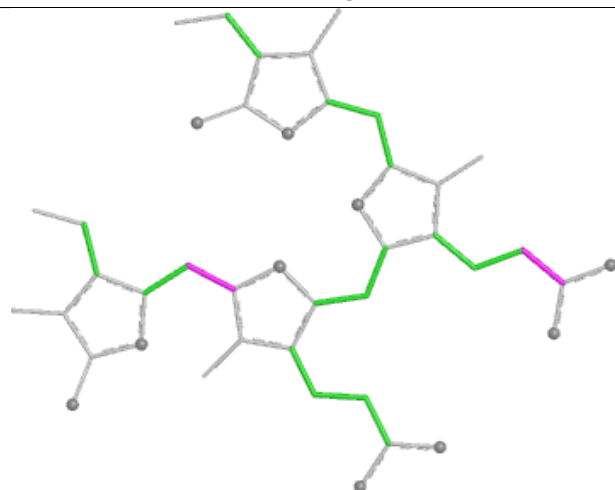
Ligand PEB I 166



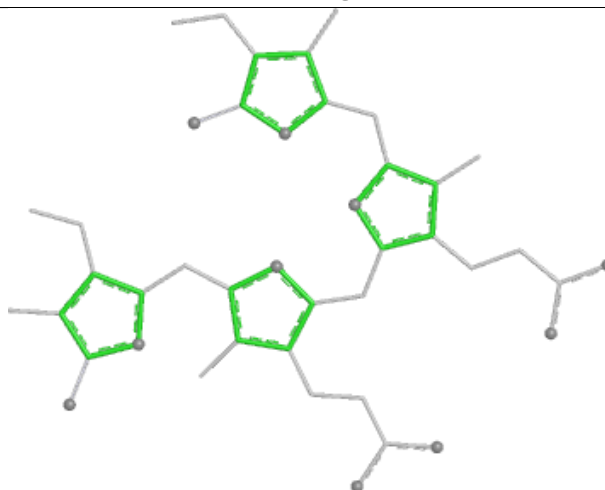
Bond lengths



Bond angles

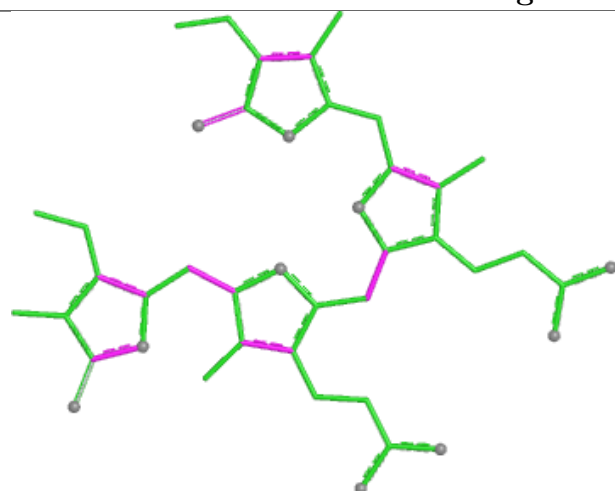


Torsions

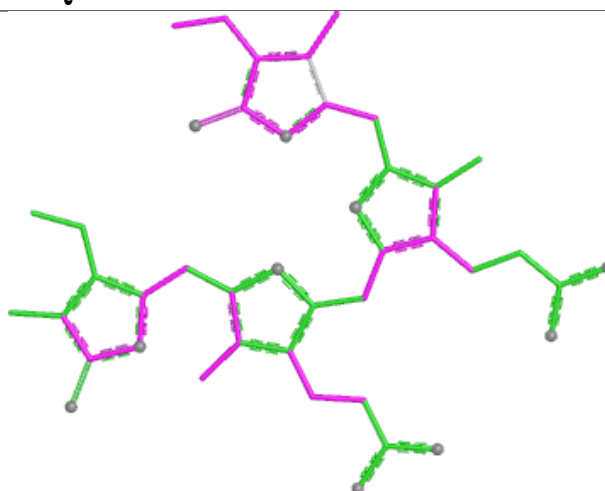


Rings

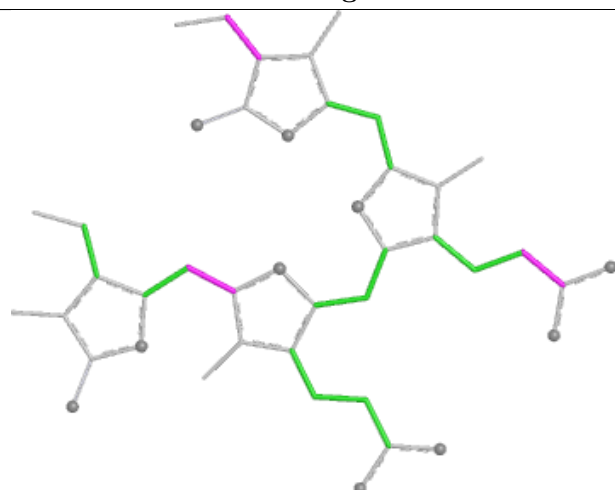
Ligand PEB Q 188



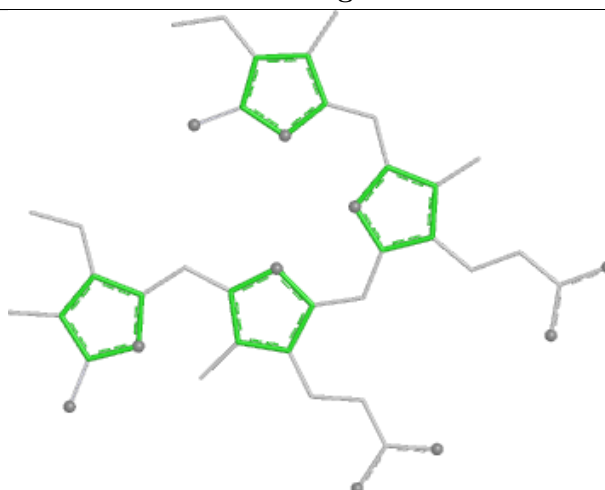
Bond lengths



Bond angles

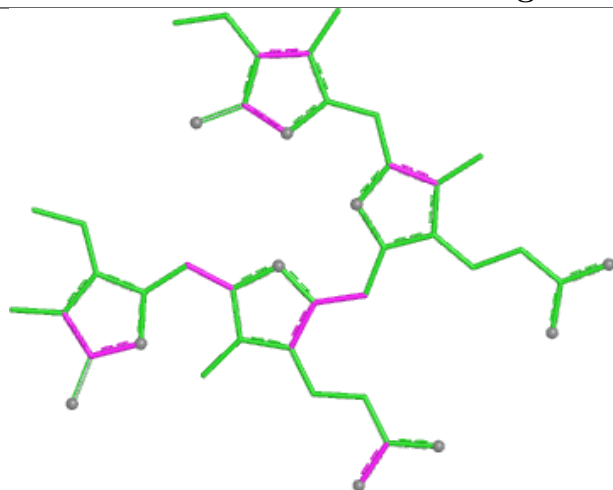


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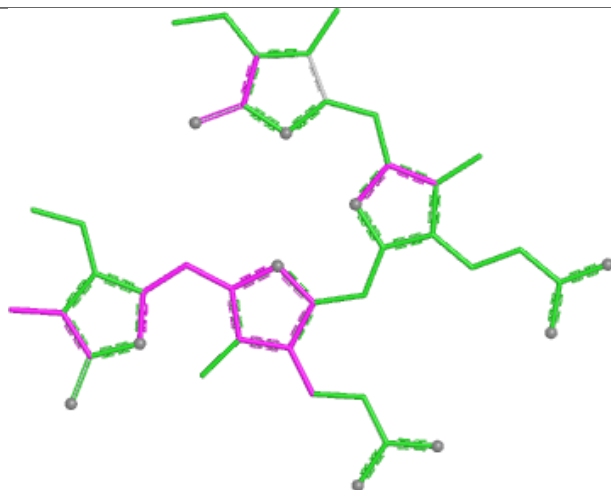


Rings

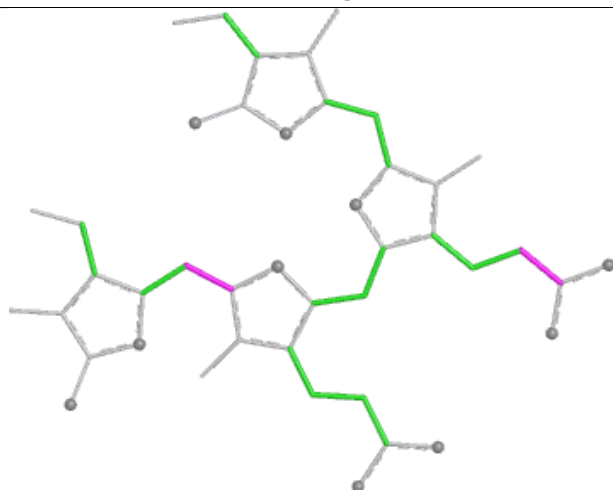
Ligand PEB L 166



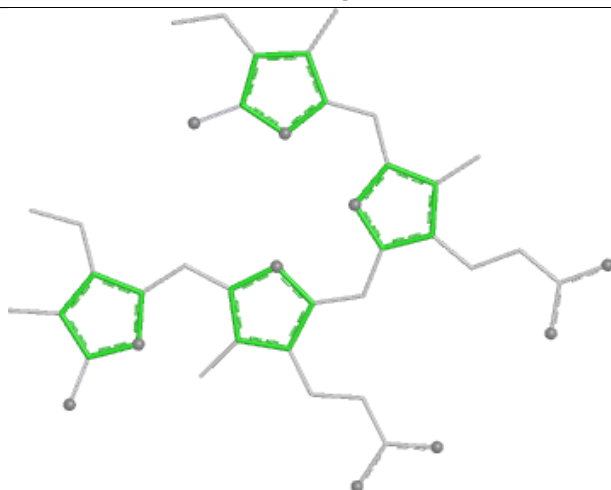
Bond lengths



Bond angles

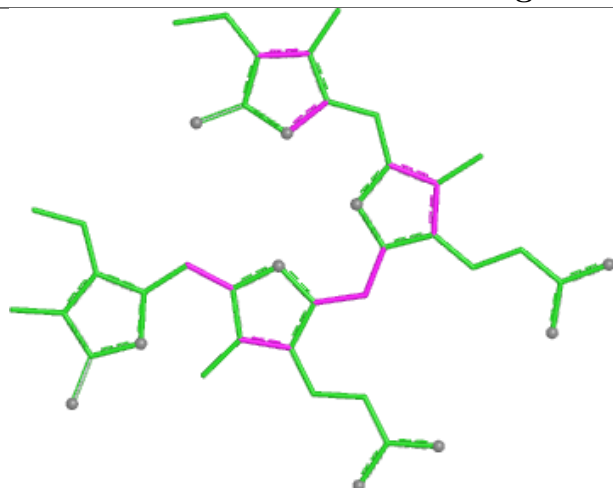


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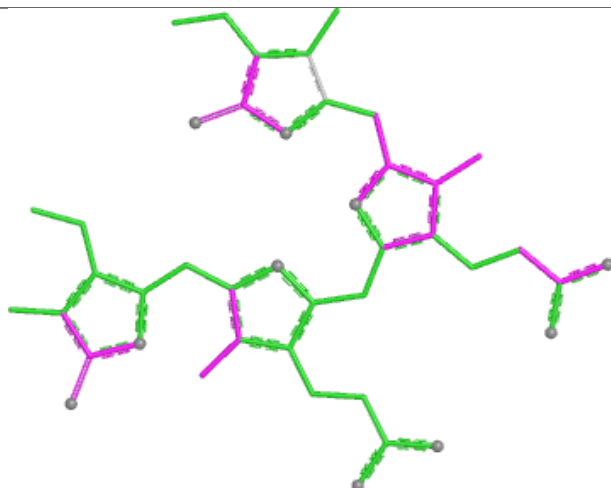


Rings

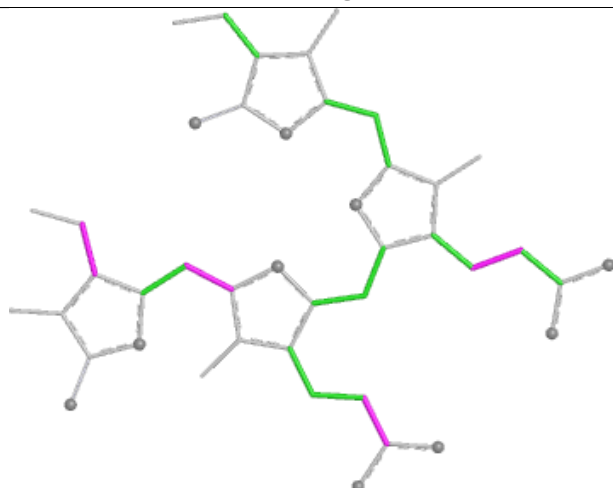
Ligand PEB P 187



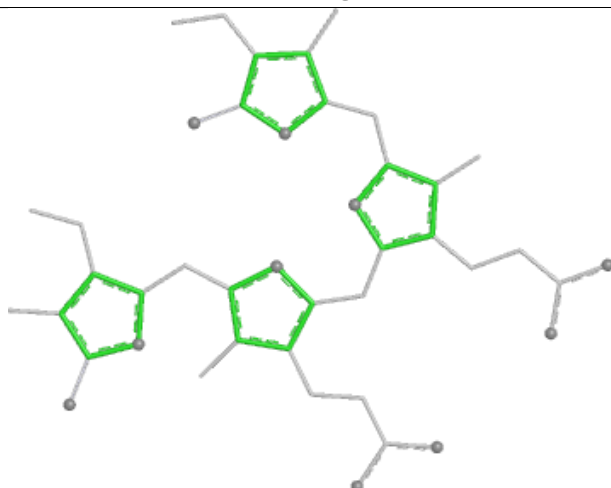
Bond lengths



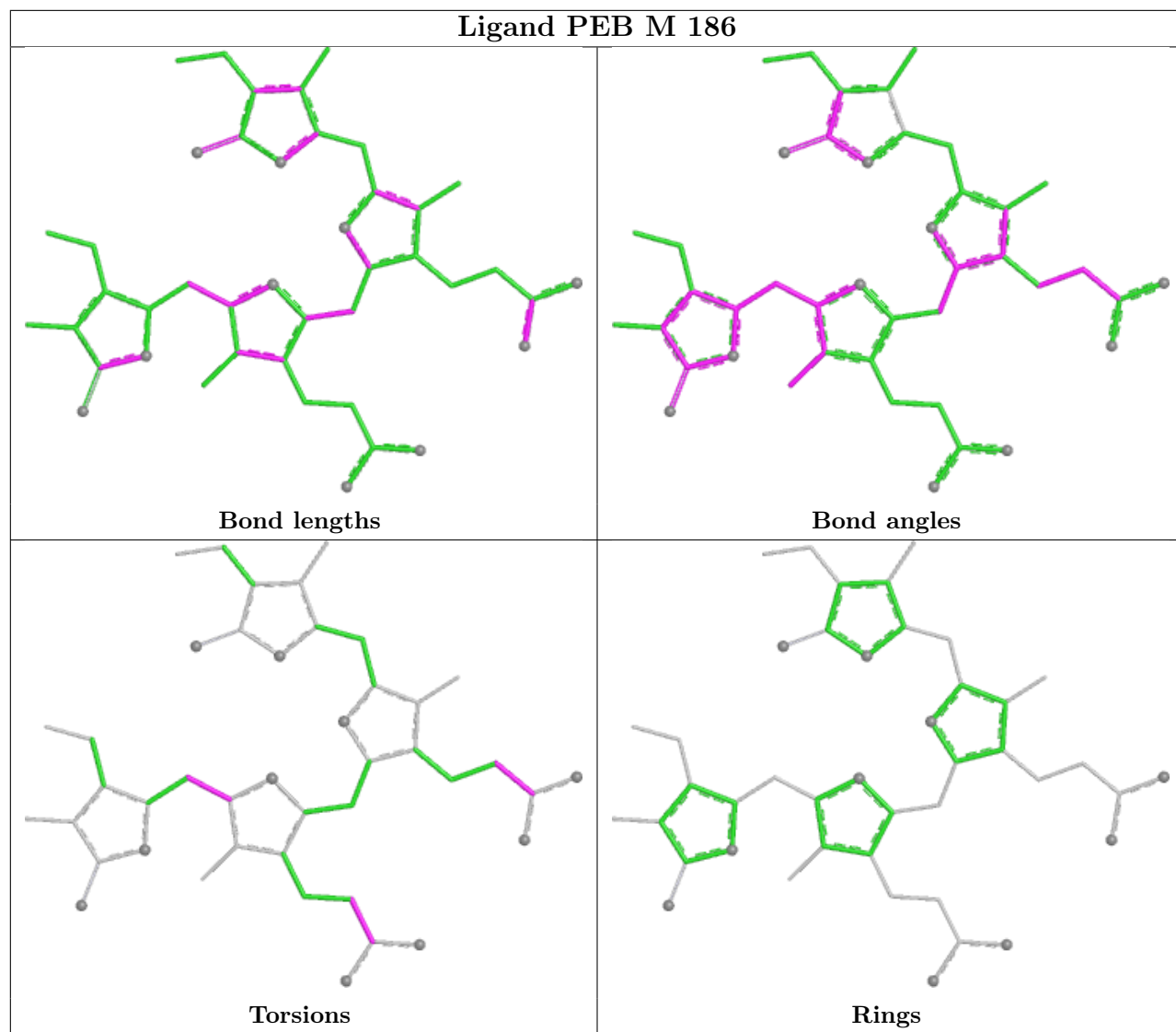
Bond angles

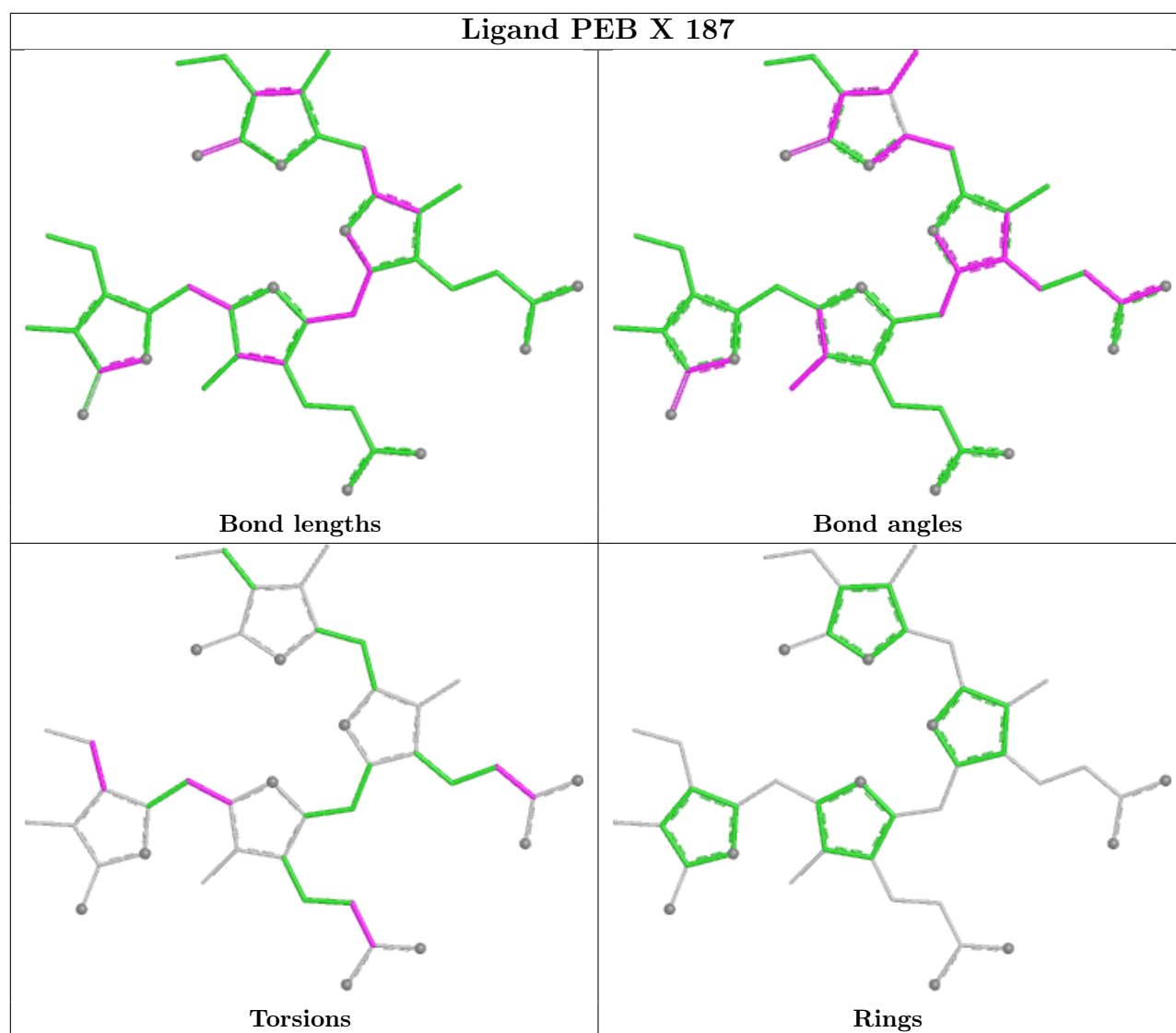


Torsions

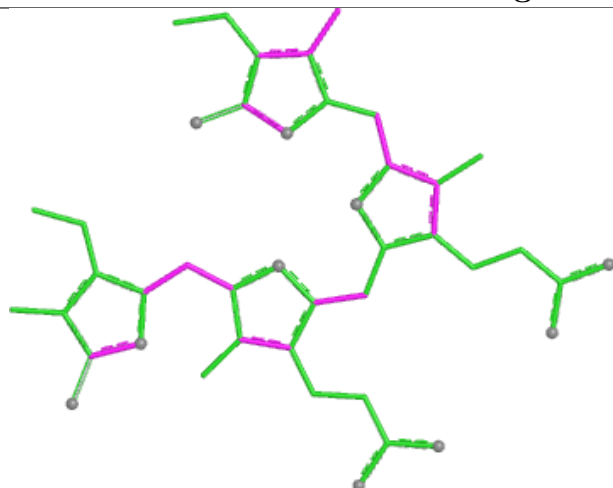


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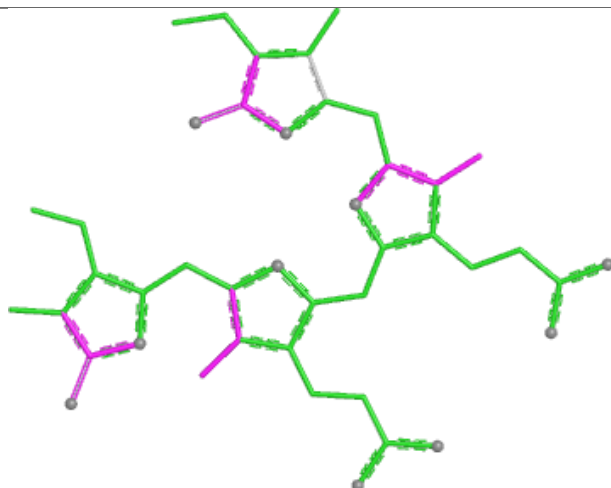




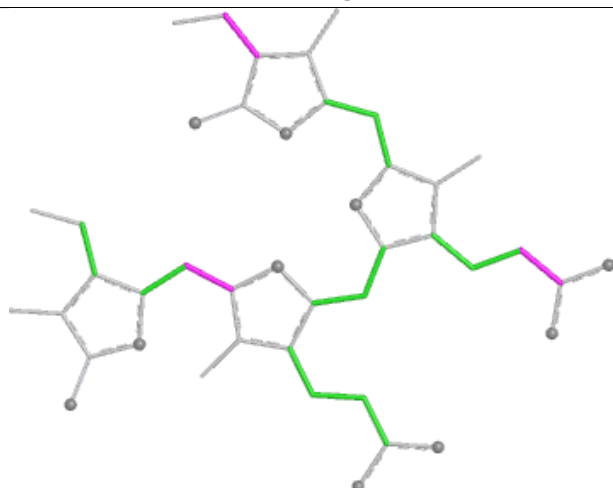
Ligand PEB V 188



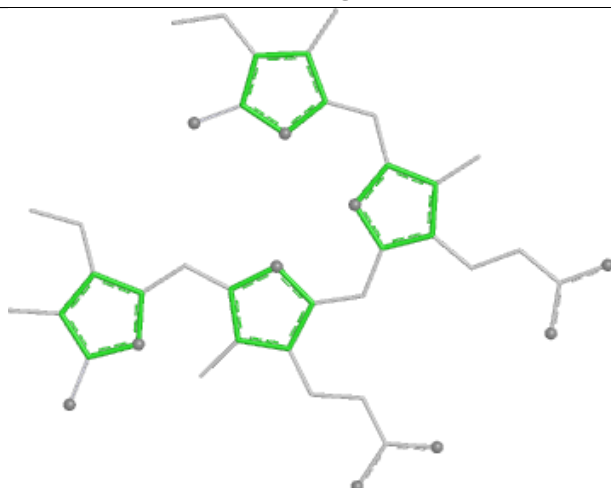
Bond lengths



Bond angles

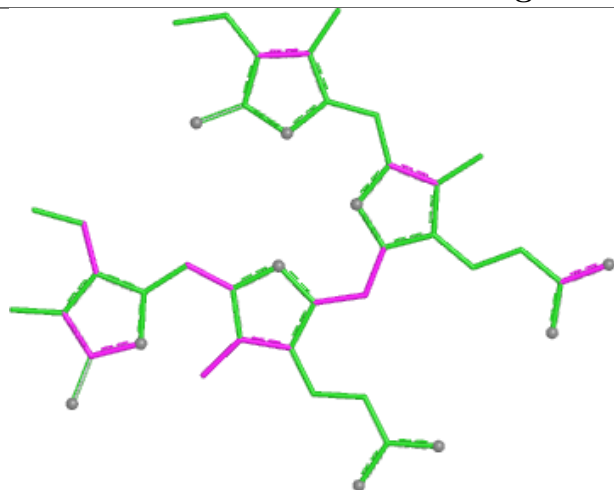


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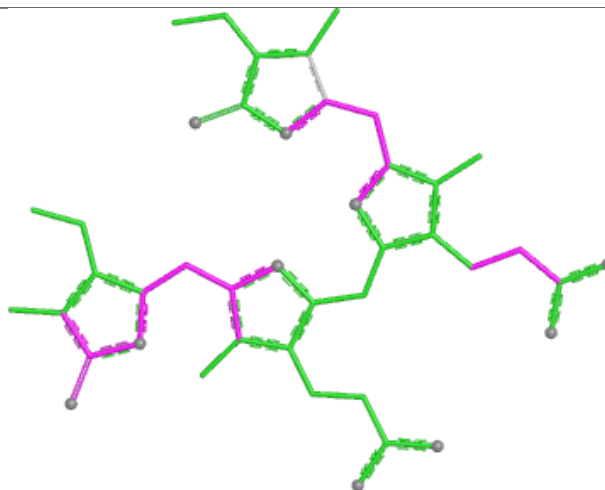


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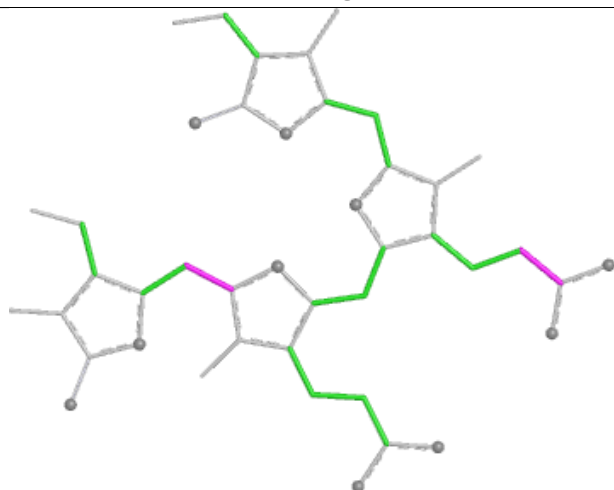
Ligand PEB B 166



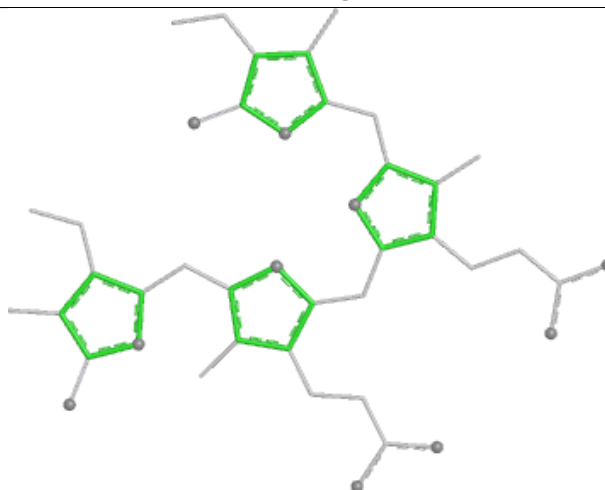
Bond lengths



Bond angles

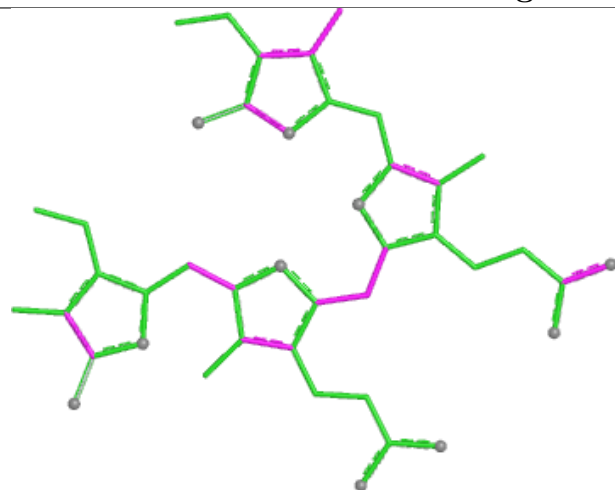


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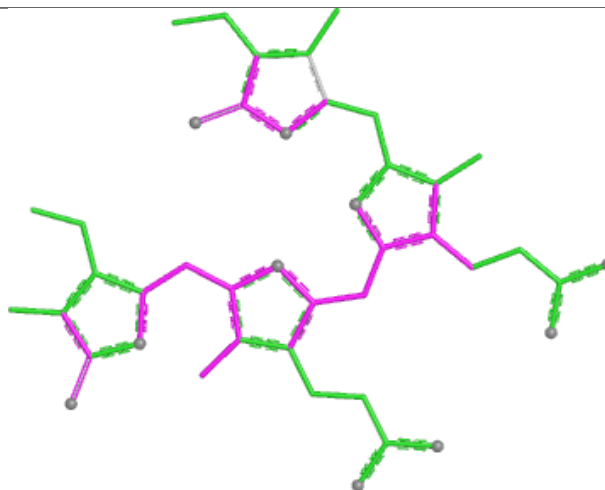


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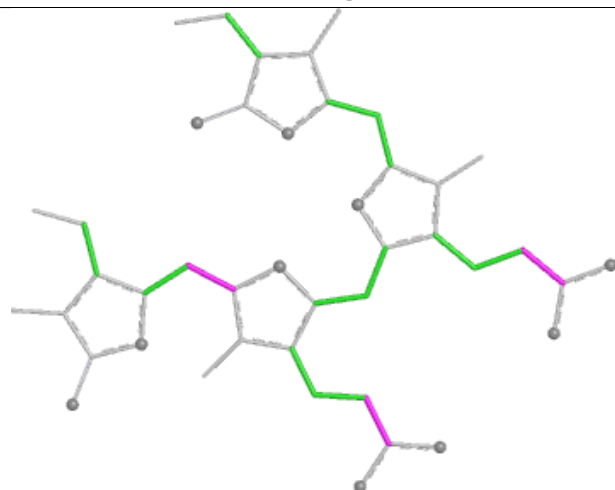
Ligand PEB V 186



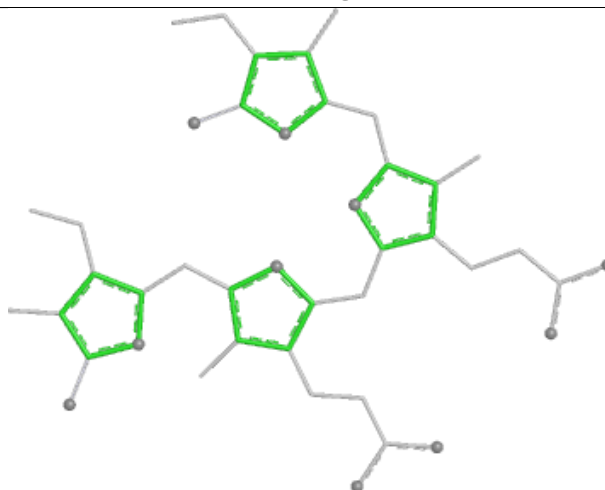
Bond lengths



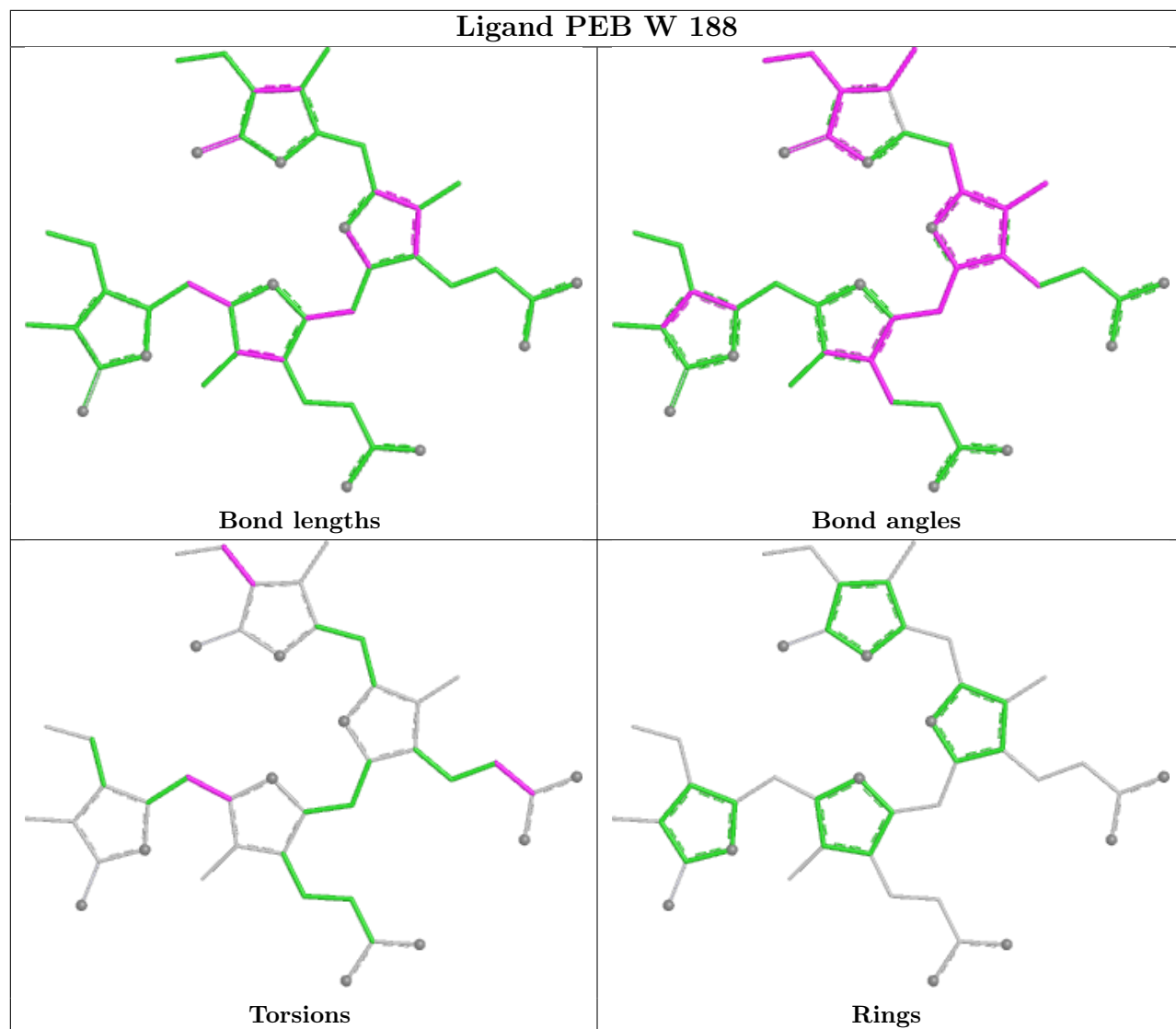
Bond angles



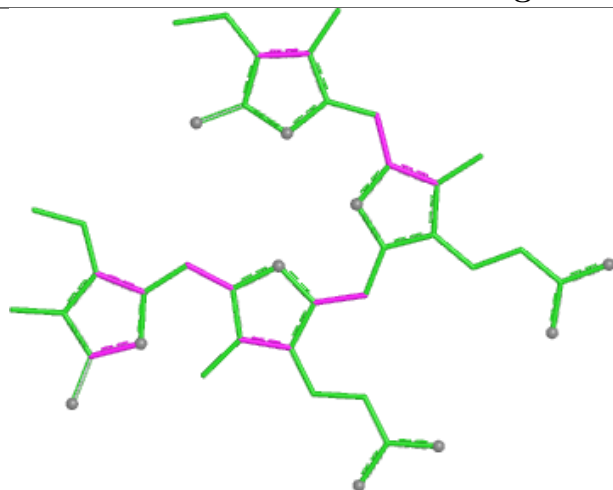
Torsions



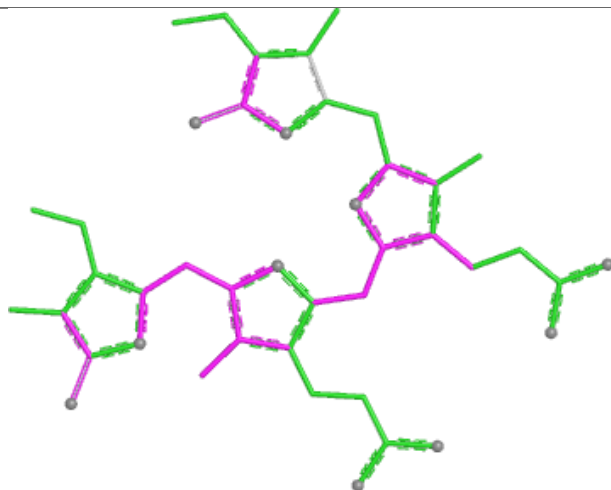
Rings



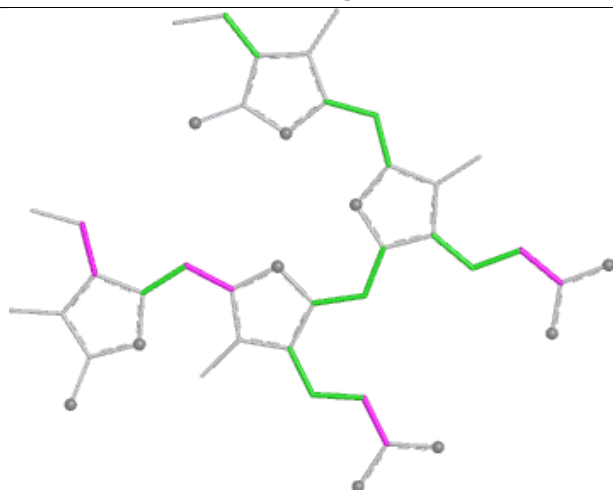
Ligand PEB U 187



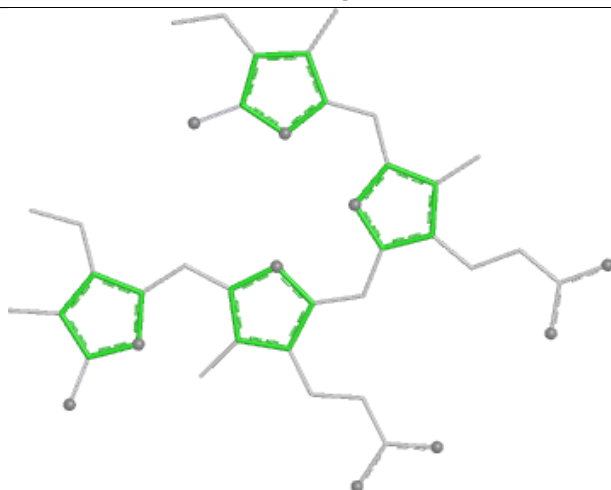
Bond lengths



Bond angles

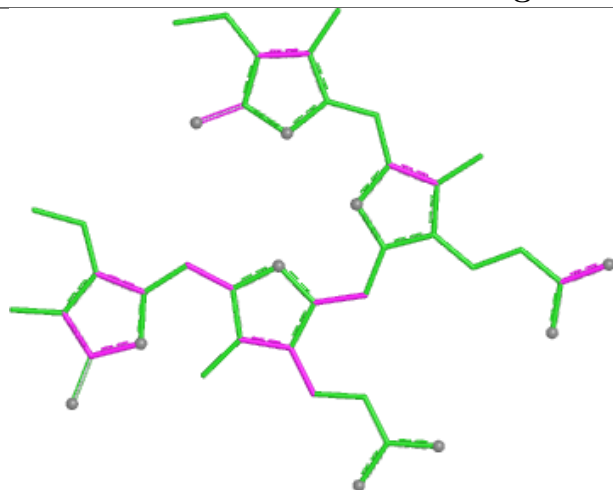


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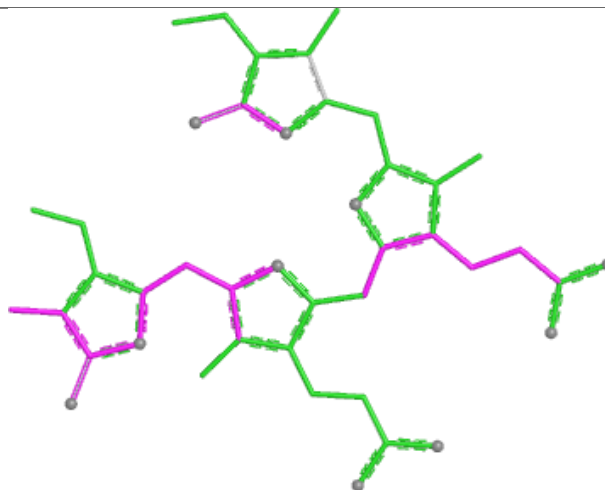


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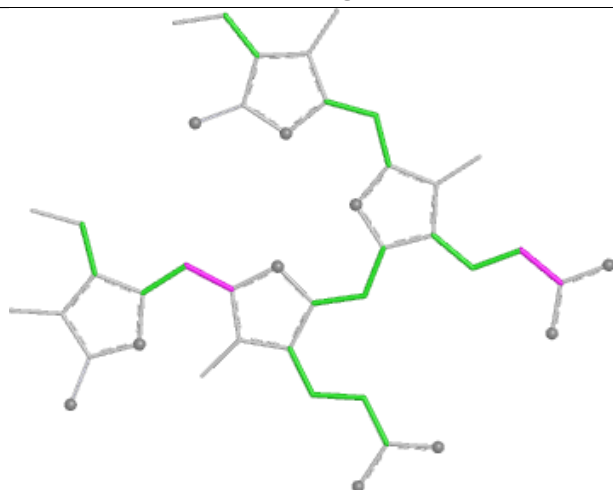
Ligand PEB K 166



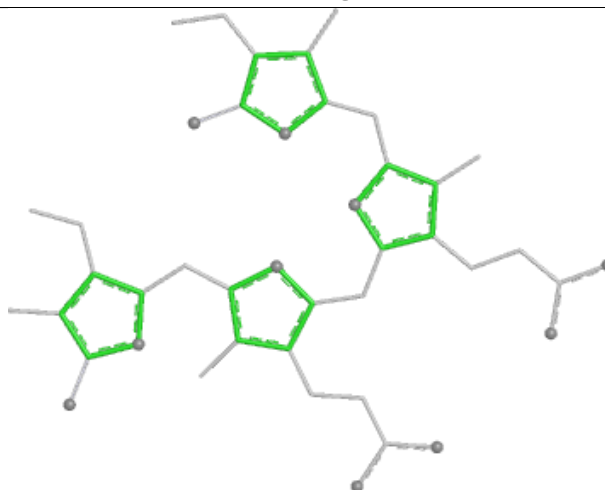
Bond lengths



Bond angles

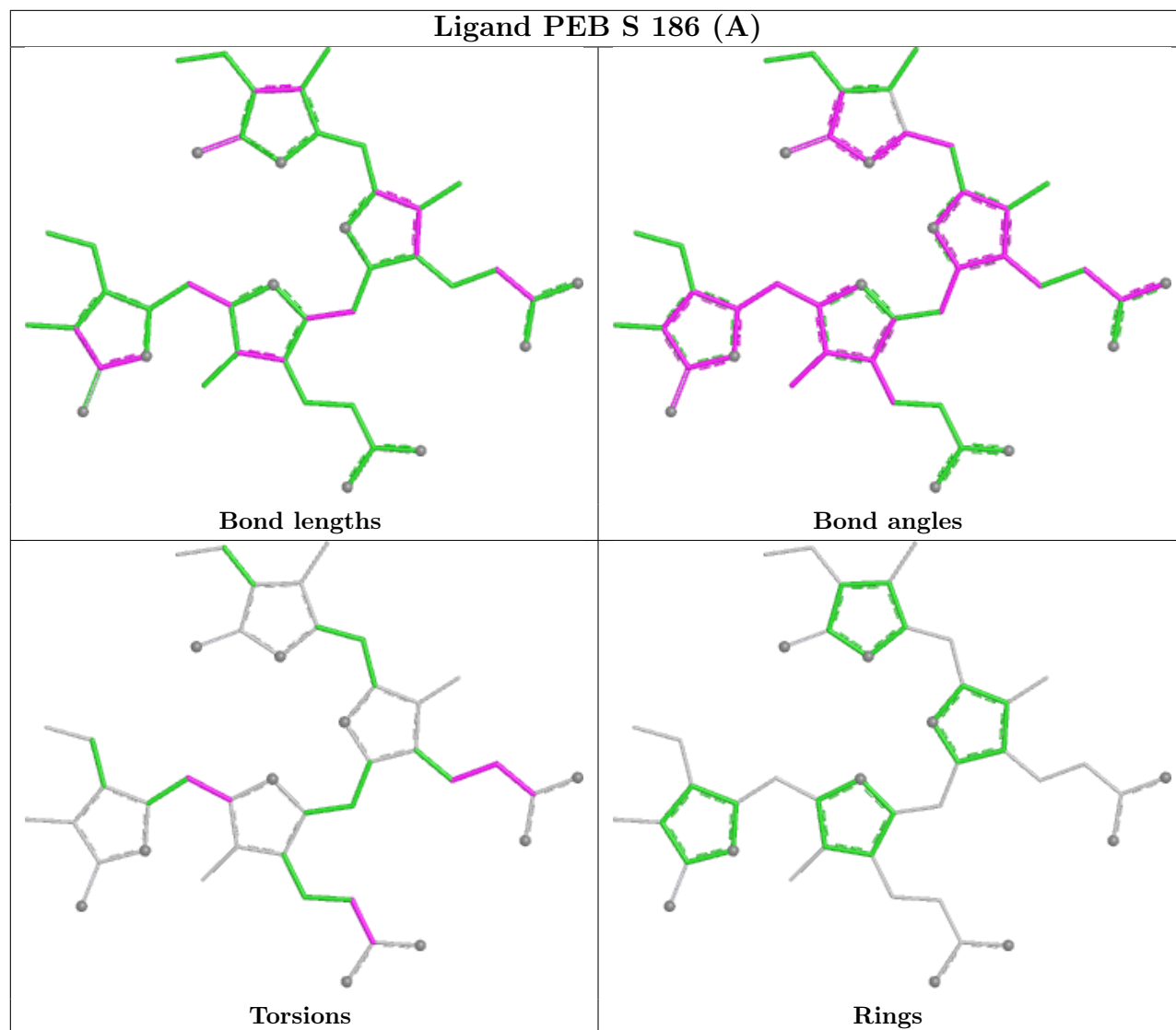


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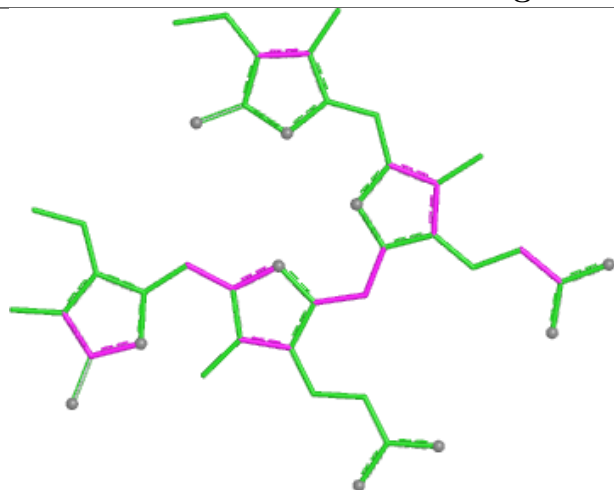


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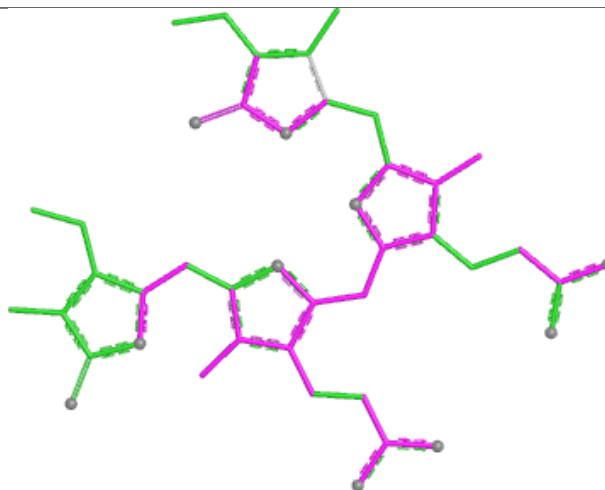
Ligand PEB S 186 (A)



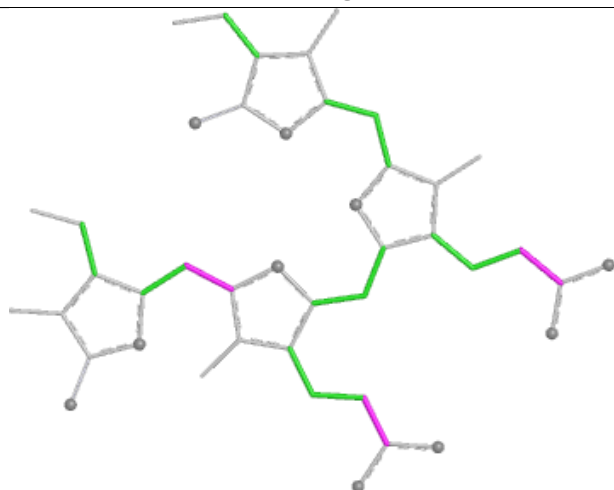
Ligand PEB K 167



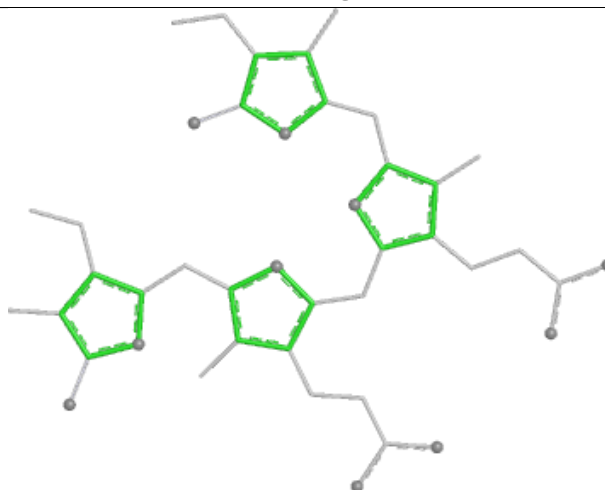
Bond lengths



Bond angles

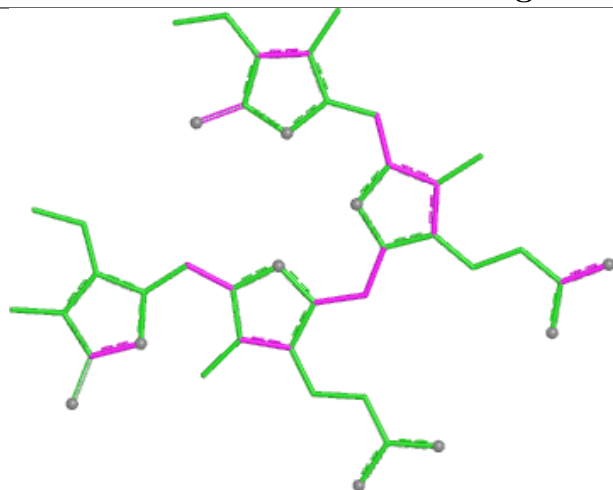


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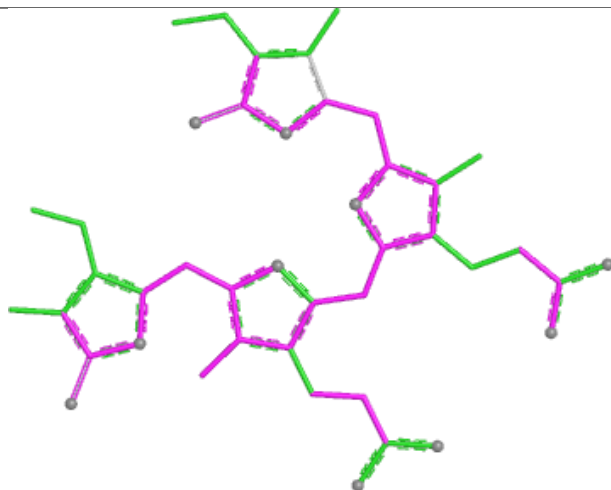


Rings

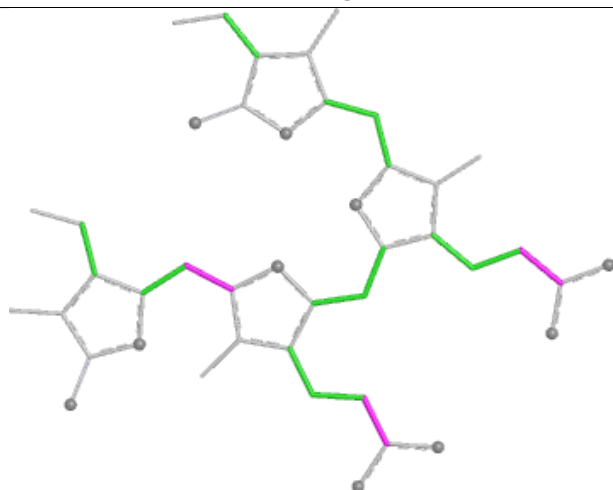
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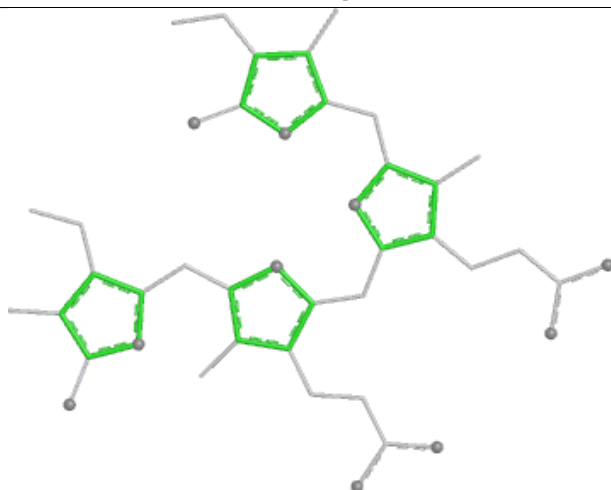
Bond lengths



Bond angles

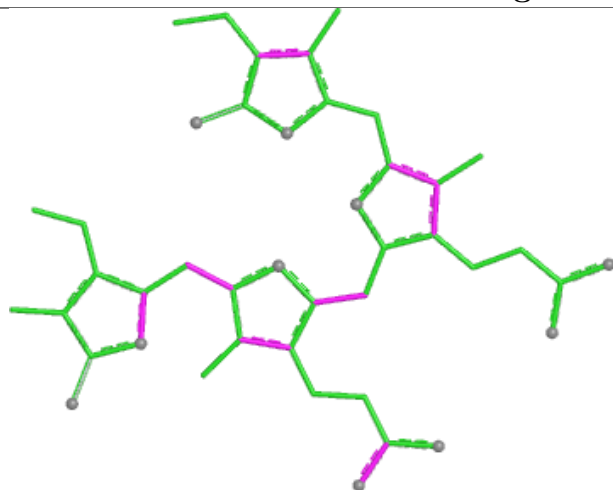


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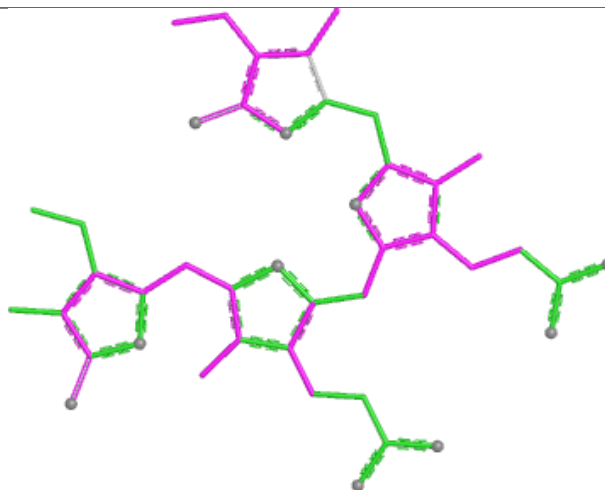


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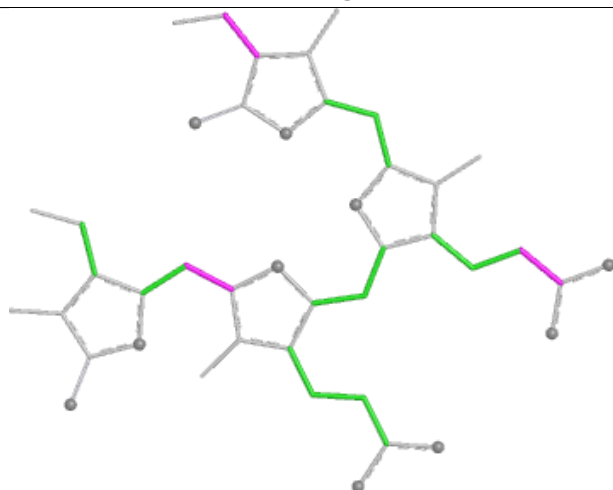
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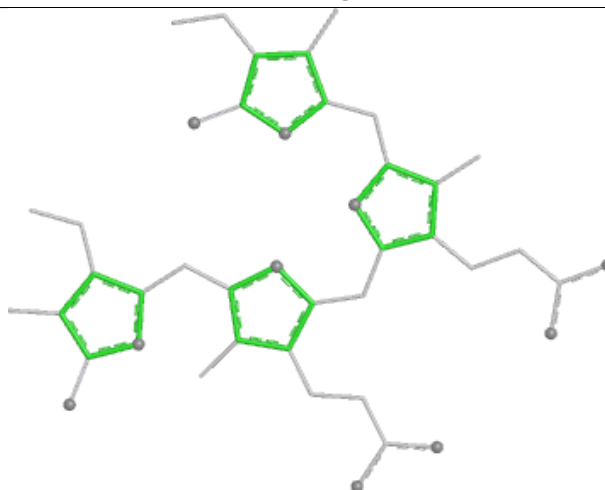
Bond lengths



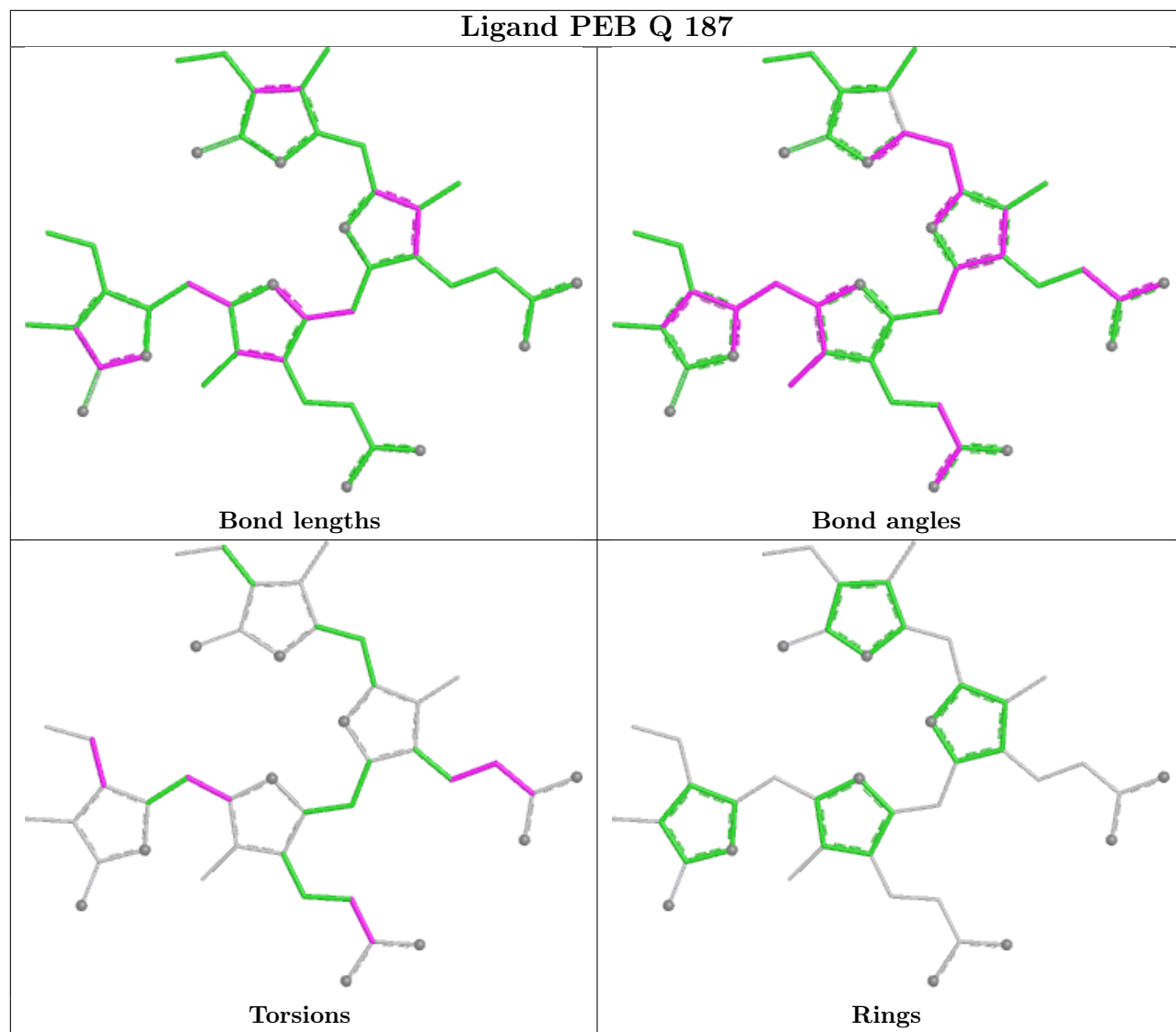
Bond angles



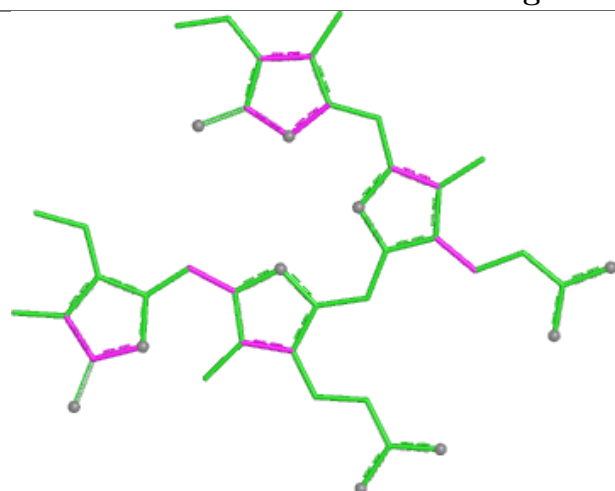
Torsions



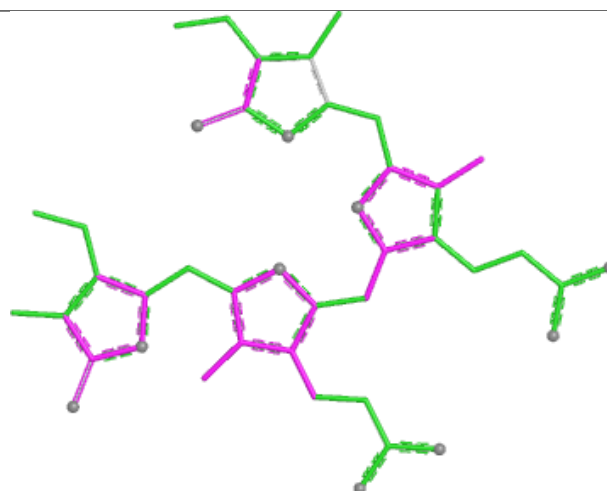
Rings



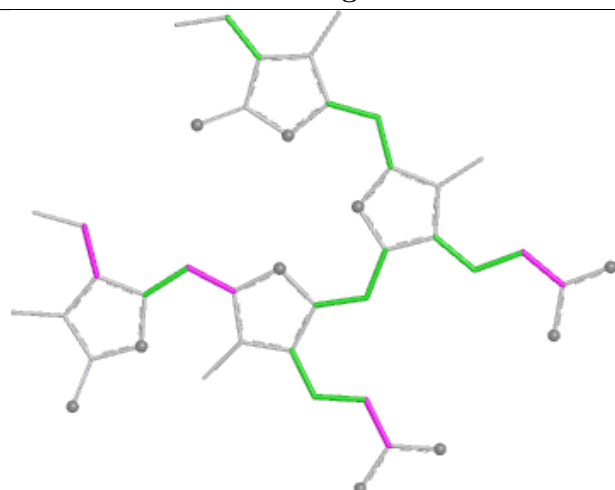
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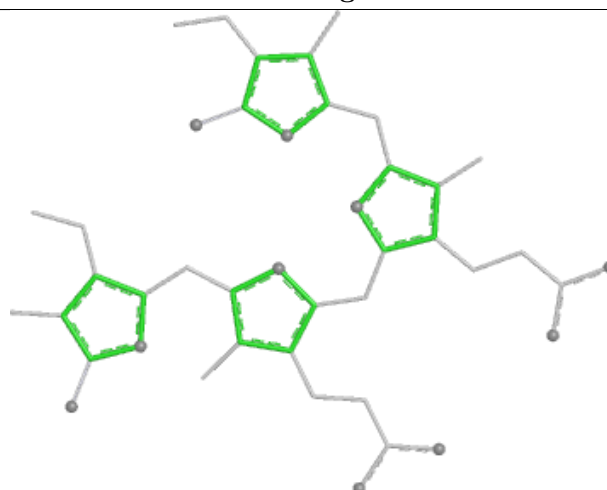
Bond lengths



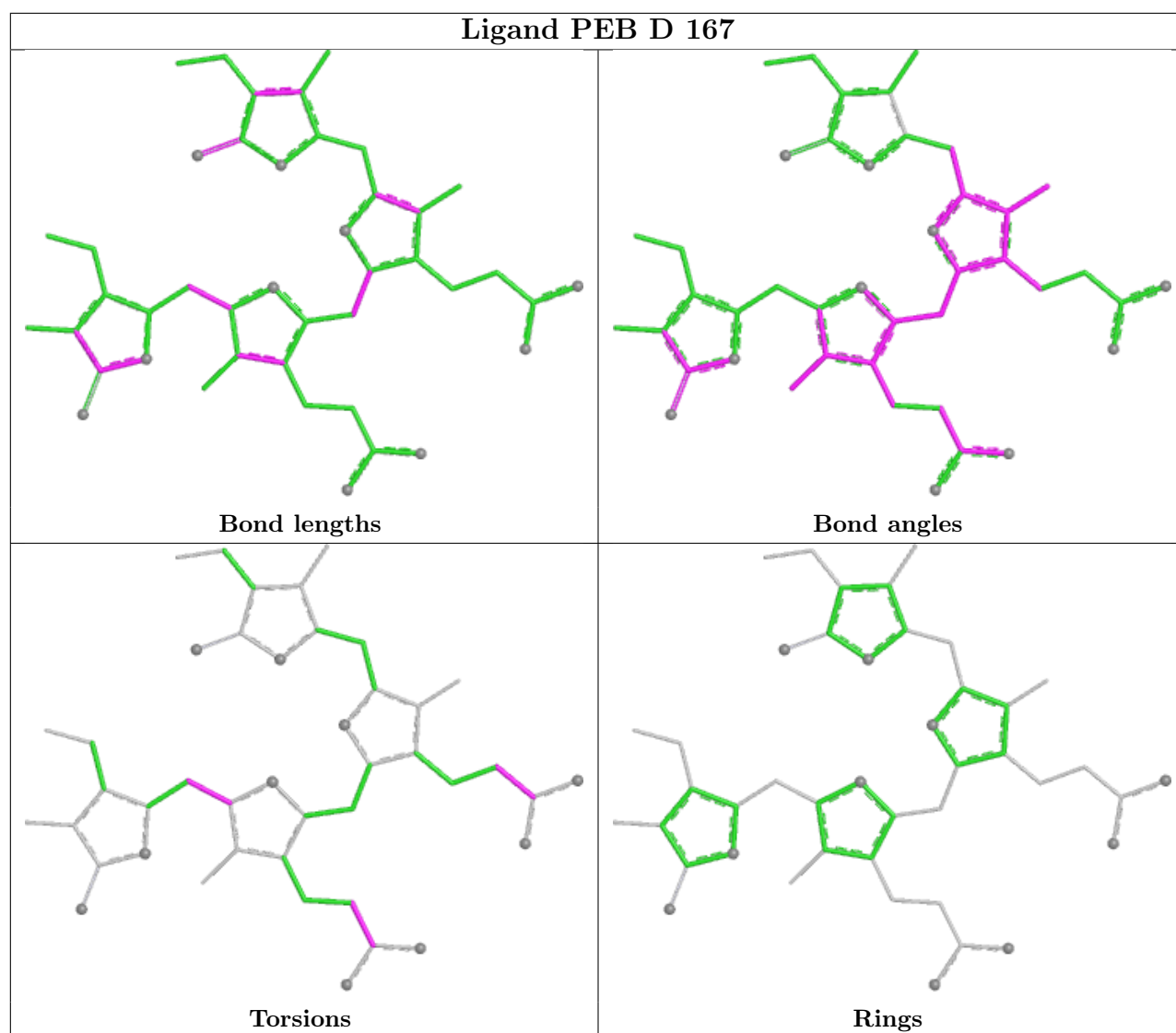
Bond angles



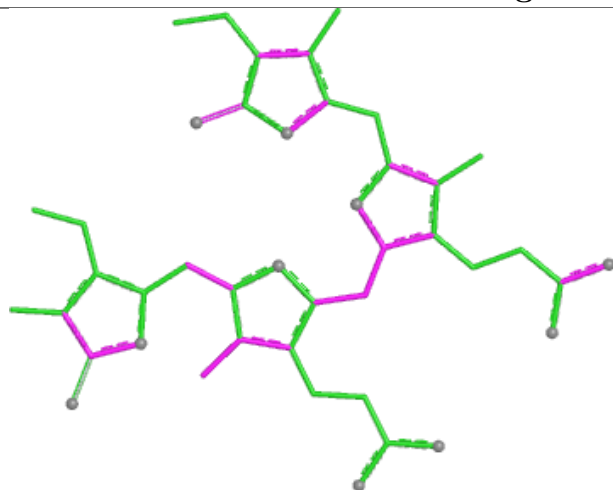
Torsions



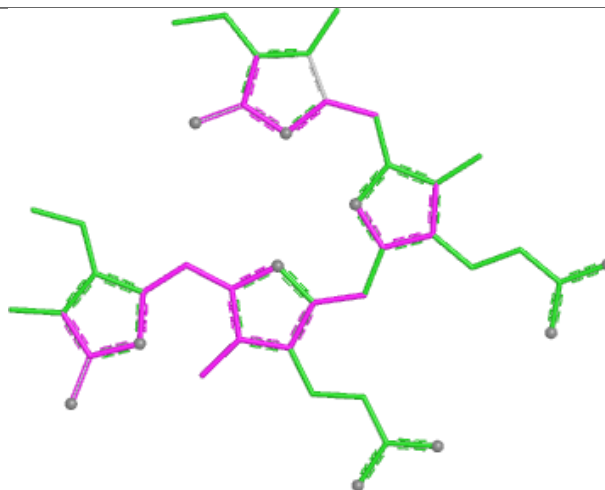
Rings



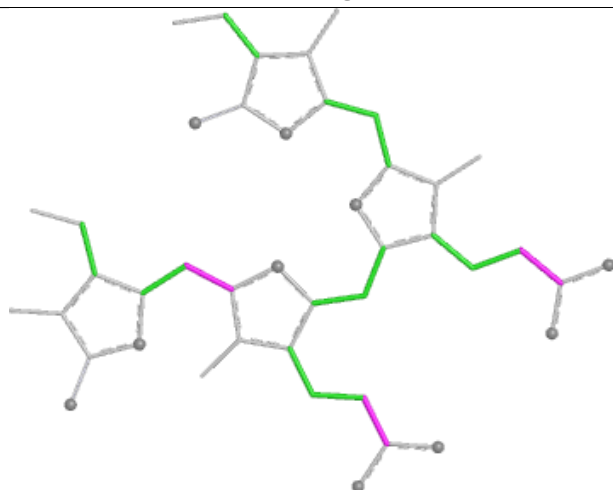
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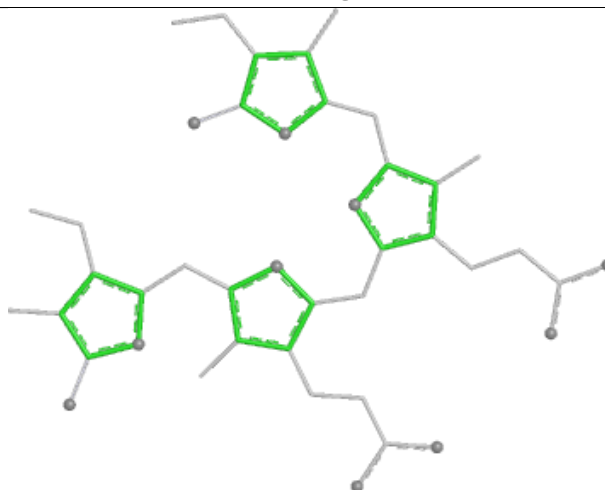
Bond lengths



Bond angles

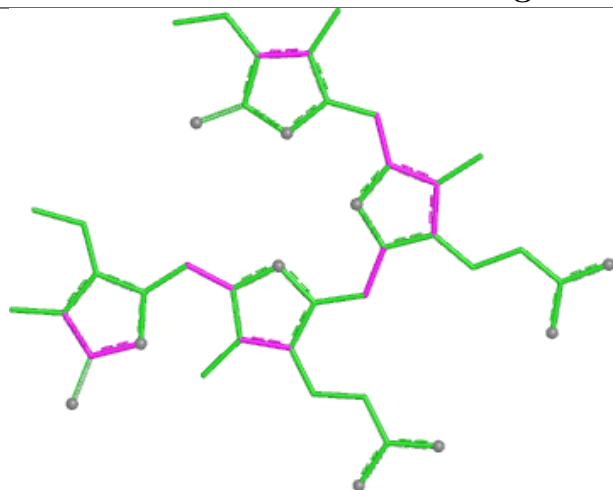


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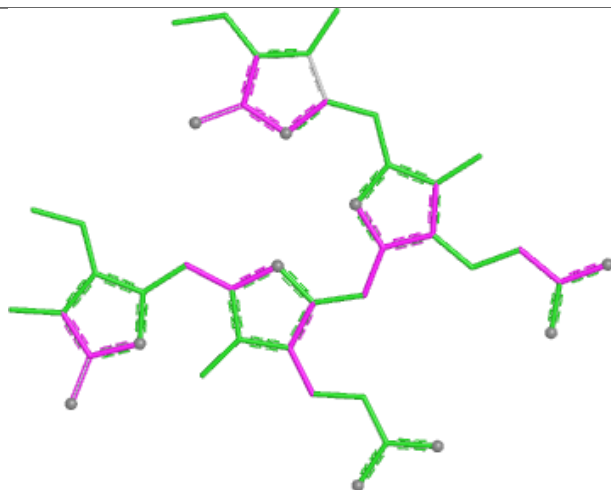


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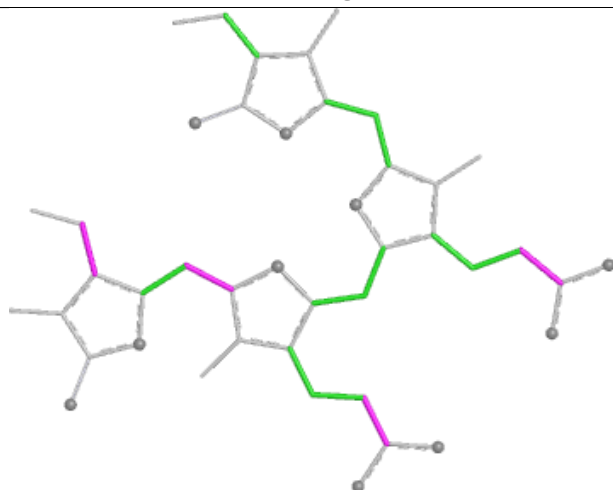
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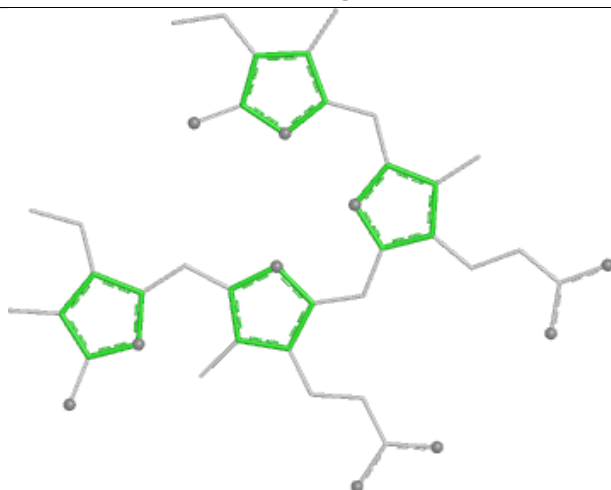
Bond lengths



Bond angles

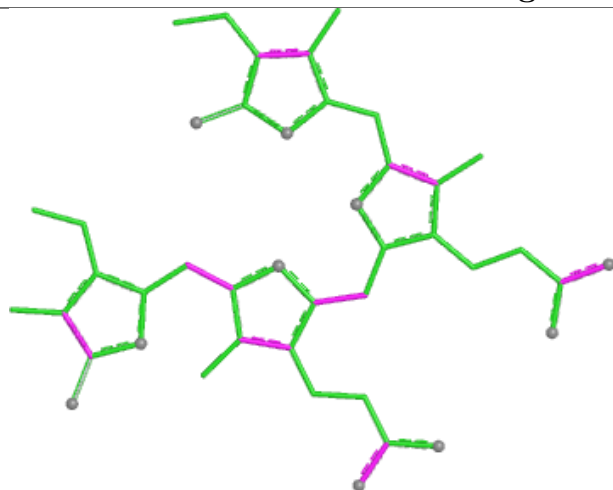


Torsions

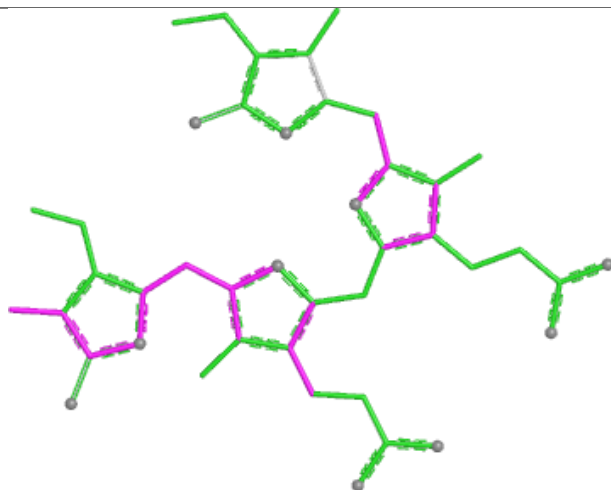


Rings

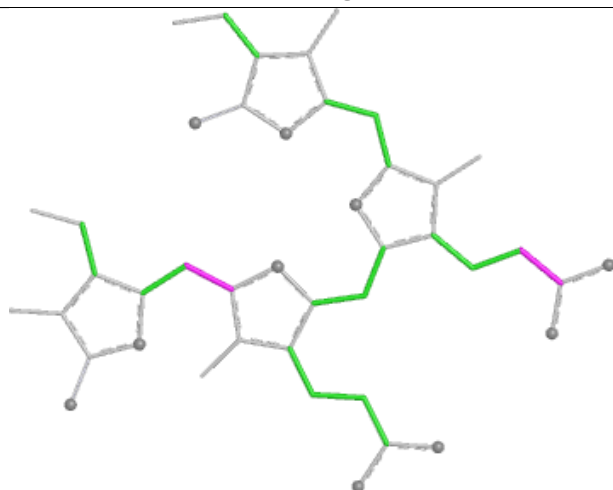
Ligand PEB J 166



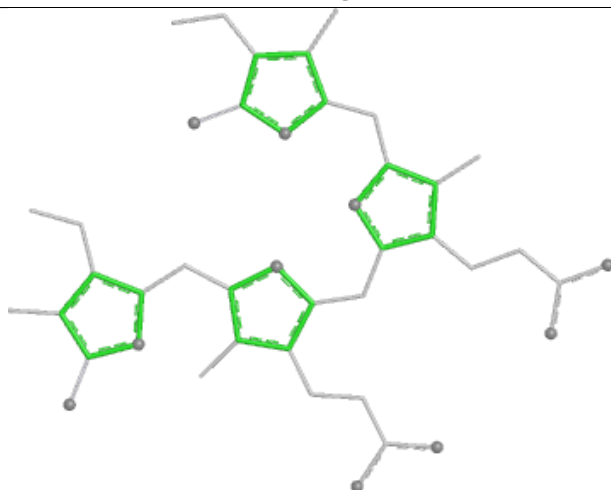
Bond lengths



Bond angles

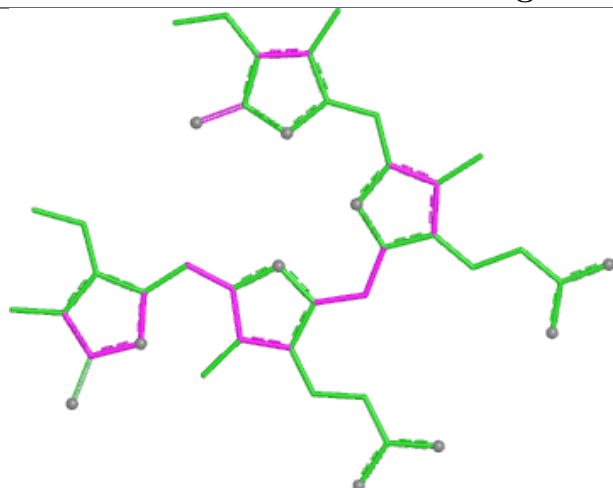


Torsions

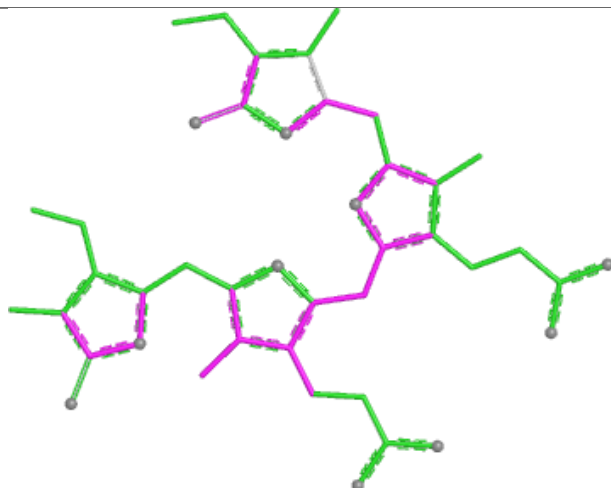


Rings

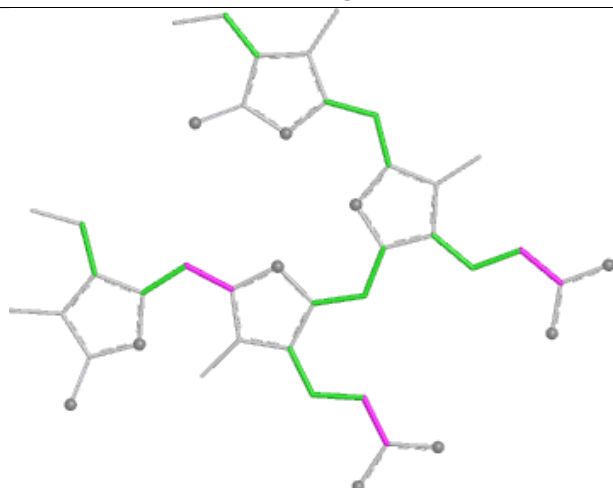
Ligand PEB F 167



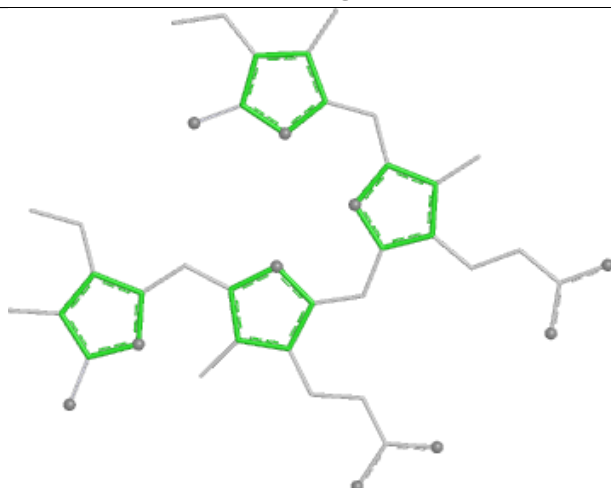
Bond lengths



Bond angles

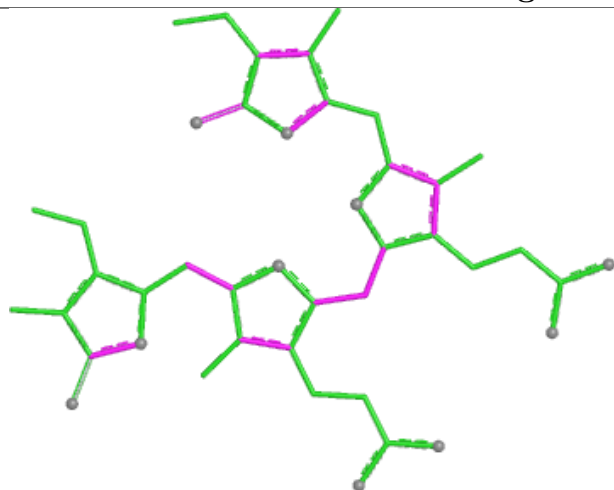


Torsions

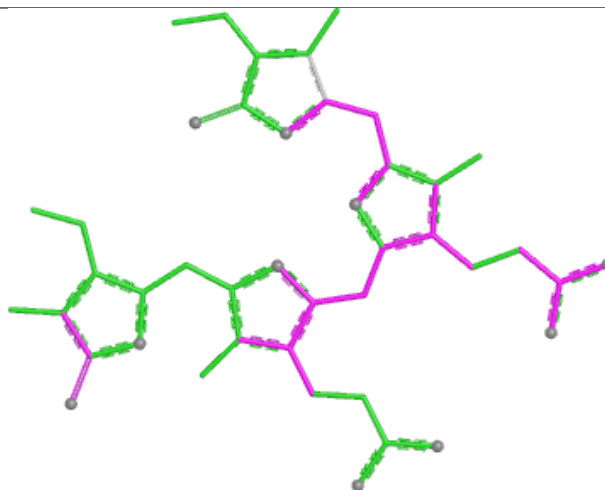


Rings

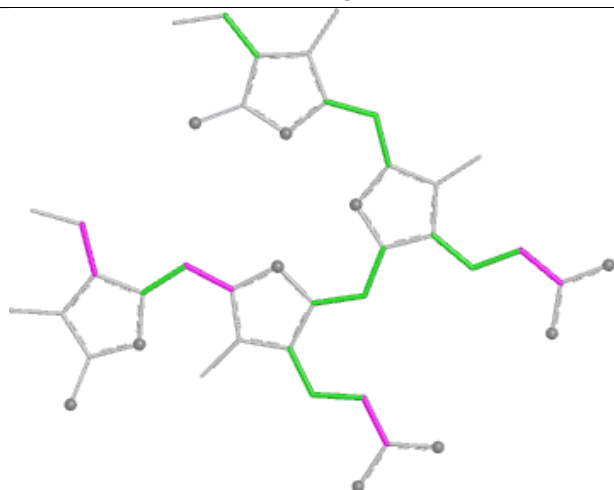
Ligand PEB S 187



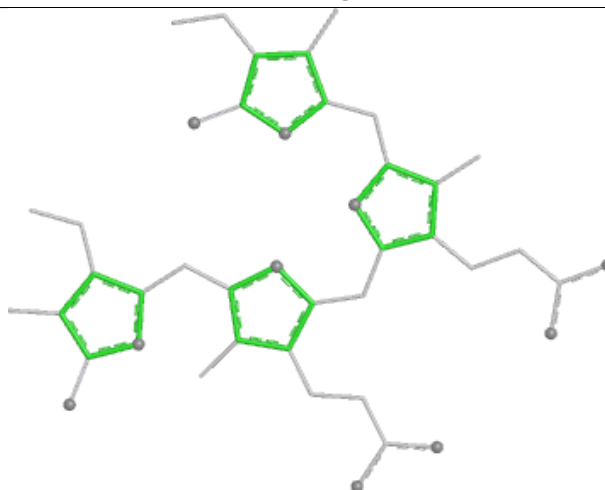
Bond lengths



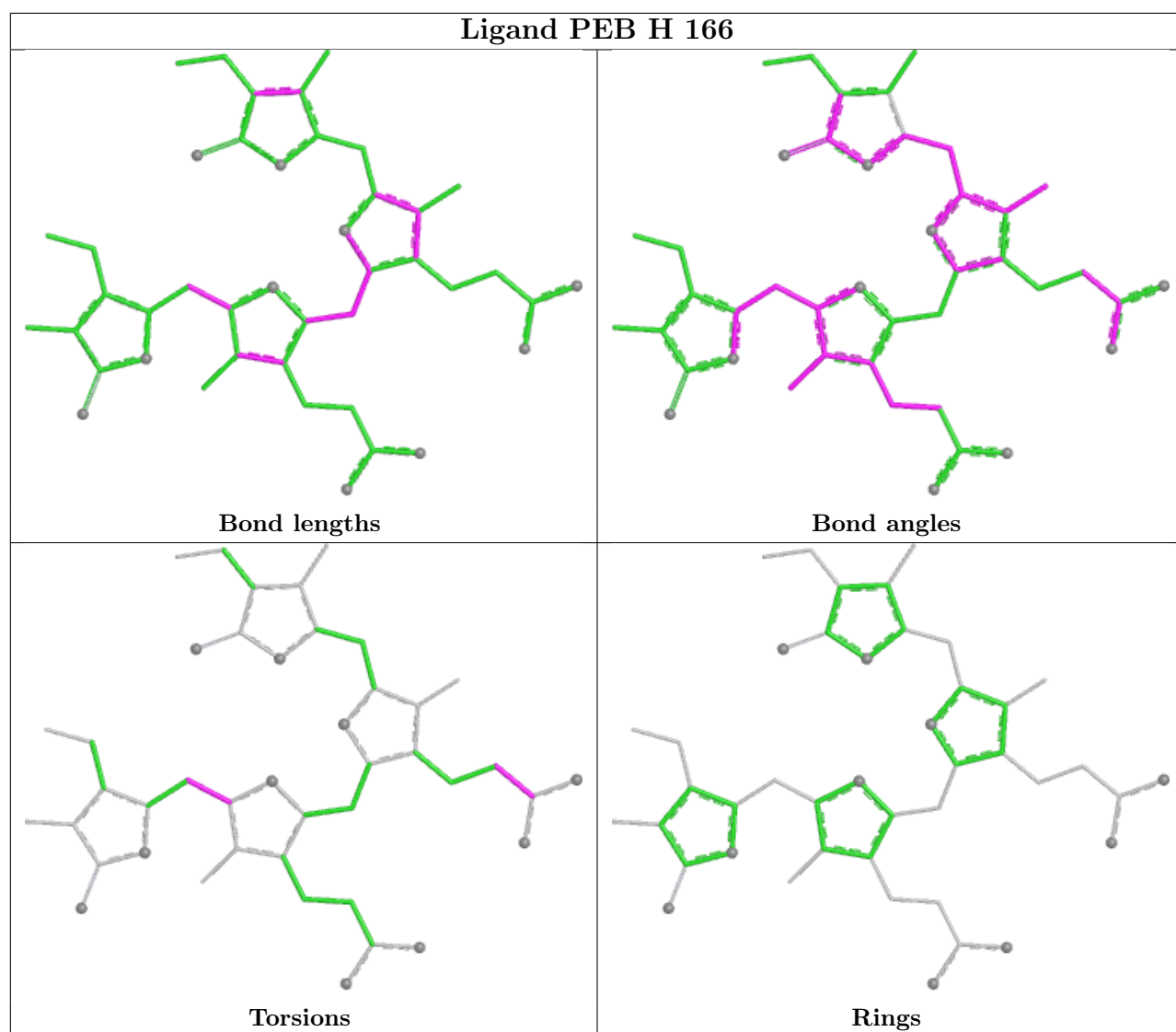
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	164/164 (100%)	-0.35	0 100 100	4, 9, 15, 23	10 (6%)
1	B	164/164 (100%)	-0.30	1 (0%) 85 91	5, 10, 17, 24	8 (4%)
1	C	164/164 (100%)	-0.03	1 (0%) 85 91	6, 12, 18, 25	9 (5%)
1	D	164/164 (100%)	-0.22	0 100 100	4, 10, 18, 28	10 (6%)
1	E	164/164 (100%)	0.04	1 (0%) 85 91	4, 12, 28, 38	8 (4%)
1	F	164/164 (100%)	-0.06	1 (0%) 85 91	5, 12, 16, 23	11 (6%)
1	G	164/164 (100%)	-0.20	1 (0%) 85 91	5, 10, 17, 22	8 (4%)
1	H	164/164 (100%)	0.08	3 (1%) 67 76	5, 12, 25, 45	10 (6%)
1	I	164/164 (100%)	-0.03	0 100 100	4, 11, 20, 31	12 (7%)
1	J	164/164 (100%)	-0.11	0 100 100	5, 11, 17, 25	10 (6%)
1	K	164/164 (100%)	-0.01	0 100 100	5, 11, 18, 26	10 (6%)
1	L	164/164 (100%)	-0.27	0 100 100	5, 10, 15, 23	8 (4%)
2	M	183/184 (99%)	-0.15	3 (1%) 70 78	5, 11, 21, 34	12 (6%)
2	N	183/184 (99%)	-0.02	1 (0%) 87 92	7, 12, 20, 34	12 (6%)
2	O	183/184 (99%)	0.03	4 (2%) 62 70	7, 12, 24, 42	9 (4%)
2	P	183/184 (99%)	0.00	5 (2%) 56 64	6, 12, 23, 45	11 (6%)
2	Q	183/184 (99%)	0.08	4 (2%) 62 70	7, 13, 24, 62	10 (5%)
2	R	183/184 (99%)	0.50	10 (5%) 30 39	8, 17, 31, 44	10 (5%)
2	S	183/184 (99%)	0.13	5 (2%) 56 64	7, 13, 26, 38	12 (6%)
2	T	183/184 (99%)	0.58	9 (4%) 35 43	8, 16, 31, 100	12 (6%)
2	U	183/184 (99%)	0.16	7 (3%) 44 51	5, 13, 23, 41	16 (8%)
2	V	183/184 (99%)	-0.15	2 (1%) 78 86	6, 11, 20, 39	16 (8%)
2	W	183/184 (99%)	0.01	2 (1%) 78 86	7, 12, 21, 36	15 (8%)
2	X	183/184 (99%)	-0.02	2 (1%) 78 86	6, 11, 22, 34	11 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4164/4176 (99%)	-0.01	62 (1%) 72 80	4, 12, 23, 100	260 (6%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	23	GLY	5.8
2	U	28[A]	PHE	5.2
2	T	24	ALA	5.1
2	X	150	GLY	4.2
2	T	28[A]	PHE	3.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MEN	R	70	9/10	0.97	0.07	17,20,22,26	0
2	MEN	U	70	9/10	0.97	0.06	11,11,14,15	0
2	MEN	N	70	9/10	0.98	0.05	11,11,12,15	0
2	MEN	S	70	9/10	0.98	0.06	14,14,17,20	0
2	MEN	T	70	9/10	0.98	0.06	14,15,18,20	0
2	MEN	P	70	9/10	0.98	0.05	11,13,15,16	0
2	MEN	M	70	9/10	0.99	0.04	9,9,11,13	0
2	MEN	Q	70	9/10	0.99	0.04	11,12,14,16	0
2	MEN	O	70	9/10	0.99	0.04	10,10,14,15	0
2	MEN	V	70	9/10	0.99	0.03	9,10,14,15	0
2	MEN	W	70	9/10	0.99	0.04	10,11,13,14	0
2	MEN	X	70	9/10	0.99	0.04	10,11,12,14	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MPD	R	204	8/8	0.76	0.23	10,18,21,21	8
7	MPD	O	204	8/8	0.79	0.20	9,20,24,27	8
7	MPD	Q	204	8/8	0.82	0.15	12,15,16,17	8
7	MPD	B	203	8/8	0.82	0.17	13,13,18,23	8
7	MPD	S	204	8/8	0.83	0.14	15,17,19,20	8
8	MRD	V	204	8/8	0.83	0.13	12,16,19,20	8
7	MPD	P	204	8/8	0.85	0.14	12,15,16,17	8
8	MRD	T	204	8/8	0.86	0.12	12,14,18,23	8
7	MPD	M	204	8/8	0.86	0.14	12,14,16,17	8
5	PI	W	205	5/5	0.87	0.12	19,22,26,29	5
7	MPD	U	204	8/8	0.87	0.16	16,18,27,28	8
5	PI	R	205	5/5	0.88	0.12	21,23,24,25	5
7	MPD	W	204	8/8	0.88	0.14	12,14,16,16	8
7	MPD	X	204	8/8	0.90	0.11	13,15,18,18	8
5	PI	N	204	5/5	0.90	0.10	18,20,21,27	5
5	PI	U	205	5/5	0.90	0.11	17,19,20,25	5
5	PI	P	205	5/5	0.91	0.10	18,18,21,22	5
5	PI	E	203	5/5	0.92	0.09	20,20,22,23	5
5	PI	X	205	5/5	0.92	0.11	20,23,26,28	5
5	PI	J	204	5/5	0.93	0.10	16,19,21,25	5
5	PI	M	205	5/5	0.93	0.09	20,22,23,25	5
5	PI	G	203	5/5	0.93	0.10	18,20,23,24	5
5	PI	I	204	5/5	0.93	0.09	14,16,17,18	5
5	PI	O	205	5/5	0.94	0.10	19,20,22,22	5
5	PI	V	205	5/5	0.94	0.09	17,17,20,23	5
5	PI	A	204	5/5	0.94	0.09	15,16,19,23	5
5	PI	C	204	5/5	0.94	0.09	18,18,23,26	5
5	PI	K	203	5/5	0.95	0.08	15,17,18,21	5
5	PI	L	204	5/5	0.95	0.09	16,18,19,22	5
4	NO3	L	203	4/4	0.95	0.08	13,15,22,24	0
3	PEB	J	167	43/43	0.95	0.07	11,16,22,31	0
3	PEB	R	186	43/43	0.95	0.07	15,18,31,46	0
3	PEB	R	188	43/43	0.95	0.08	12,16,31,43	0
5	PI	F	203	5/5	0.95	0.08	17,18,22,24	5
5	PI	T	205	5/5	0.95	0.07	26,27,29,30	5
3	PEB	U	187	43/43	0.95	0.07	8,12,17,33	0
5	PI	H	203	5/5	0.95	0.10	17,18,20,21	5
4	NO3	A	203	4/4	0.95	0.08	11,15,19,21	0
4	NO3	C	203	4/4	0.95	0.07	16,21,22,23	0
5	PI	B	204	5/5	0.96	0.07	14,14,15,19	5
3	PEB	I	167	43/43	0.96	0.07	9,12,18,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEB	S	186[A]	43/43	0.96	0.07	12,14,26,32	6
3	PEB	S	186[B]	43/43	0.96	0.07	12,14,20,33	6
3	PEB	T	186	43/43	0.96	0.07	14,17,27,44	0
3	PEB	T	187	43/43	0.96	0.07	10,14,23,39	0
3	PEB	T	188	43/43	0.96	0.07	12,15,23,26	0
3	PEB	C	167	43/43	0.96	0.07	12,18,26,32	0
3	PEB	X	188	43/43	0.96	0.07	9,11,16,19	0
3	PEB	K	167	43/43	0.96	0.07	11,14,21,27	0
3	PEB	Q	187	43/43	0.96	0.07	10,12,20,38	0
4	NO3	I	203	4/4	0.96	0.06	13,20,22,22	0
4	NO3	J	203	4/4	0.96	0.07	12,20,20,23	0
3	PEB	E	166	43/43	0.96	0.07	14,18,26,35	0
5	PI	Q	205	5/5	0.96	0.07	22,23,24,25	5
3	PEB	R	187	43/43	0.96	0.06	13,15,23,32	0
5	PI	S	205	5/5	0.96	0.08	18,18,21,22	5
3	PEB	P	186	43/43	0.97	0.06	9,13,24,40	0
5	PI	D	204	5/5	0.97	0.06	13,13,16,16	5
3	PEB	P	187	43/43	0.97	0.06	9,11,18,31	0
3	PEB	P	188	43/43	0.97	0.05	8,10,17,22	0
3	PEB	Q	186	43/43	0.97	0.06	10,13,25,45	0
3	PEB	B	167	43/43	0.97	0.06	9,13,19,26	0
3	PEB	F	166	43/43	0.97	0.05	9,11,14,21	0
3	PEB	F	167	43/43	0.97	0.05	10,12,16,21	0
3	PEB	G	166	43/43	0.97	0.05	8,11,13,18	0
3	PEB	I	166	43/43	0.97	0.06	10,12,17,24	0
3	PEB	C	166	43/43	0.97	0.05	10,12,14,18	0
3	PEB	S	187	43/43	0.97	0.06	11,13,20,33	0
3	PEB	S	188	43/43	0.97	0.05	11,12,17,21	0
3	PEB	J	166	43/43	0.97	0.05	10,11,14,19	0
3	PEB	B	166	43/43	0.97	0.05	9,10,12,21	0
3	PEB	K	166	43/43	0.97	0.06	10,12,14,25	0
3	PEB	U	186	43/43	0.97	0.06	9,13,21,41	0
3	PEB	D	167	43/43	0.97	0.06	9,13,17,24	0
3	PEB	U	188	43/43	0.97	0.06	9,11,18,34	0
3	PEB	V	186	43/43	0.97	0.06	8,11,21,32	0
3	PEB	V	187	43/43	0.97	0.05	10,11,17,26	0
3	PEB	W	186	43/43	0.97	0.06	9,13,21,34	0
6	NA	V	206	1/1	0.97	0.20	25,25,25,25	1
3	PEB	W	187	43/43	0.97	0.06	9,11,19,28	0
3	PEB	W	188	43/43	0.97	0.05	10,12,16,23	0
3	PEB	X	186	43/43	0.97	0.06	9,12,24,36	0
3	PEB	L	167	43/43	0.97	0.06	9,12,17,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEB	M	186	43/43	0.97	0.06	8,11,20,37	0
3	PEB	M	188	43/43	0.97	0.06	8,10,14,18	0
4	NO3	D	203	4/4	0.97	0.07	12,16,19,23	0
3	PEB	N	186	43/43	0.97	0.06	9,13,23,32	0
3	PEB	N	187	43/43	0.97	0.05	9,11,17,27	0
3	PEB	N	188	43/43	0.97	0.05	10,12,17,22	0
3	PEB	O	186	43/43	0.97	0.06	8,12,20,33	0
3	PEB	O	187	43/43	0.97	0.06	10,13,20,25	0
6	NA	A	205	1/1	0.98	0.12	18,18,18,18	0
6	NA	S	206	1/1	0.98	0.17	29,29,29,29	0
3	PEB	H	166	43/43	0.98	0.06	13,16,22,29	0
3	PEB	L	166	43/43	0.98	0.04	8,9,12,18	0
3	PEB	V	188	43/43	0.98	0.04	8,10,14,16	0
3	PEB	O	188	43/43	0.98	0.05	9,11,15,16	0
3	PEB	H	167	43/43	0.98	0.05	11,12,16,21	0
3	PEB	E	167	43/43	0.98	0.05	11,13,16,20	0
3	PEB	M	187	43/43	0.98	0.05	9,10,16,26	0
3	PEB	X	187	43/43	0.98	0.05	9,11,19,29	0
3	PEB	D	166	43/43	0.98	0.05	9,11,15,20	0
3	PEB	A	166	43/43	0.98	0.05	8,9,13,19	0
3	PEB	Q	188	43/43	0.98	0.04	10,13,17,19	0
3	PEB	A	167	43/43	0.98	0.05	9,11,17,27	0
3	PEB	G	167	43/43	0.98	0.05	9,12,16,22	0
6	NA	G	204	1/1	0.99	0.09	16,16,16,16	0
6	NA	H	204	1/1	0.99	0.19	21,21,21,21	0
6	NA	I	205	1/1	0.99	0.12	20,20,20,20	0
6	NA	J	205	1/1	0.99	0.12	17,17,17,17	0
6	NA	K	204	1/1	0.99	0.13	22,22,22,22	0
6	NA	L	205	1/1	0.99	0.13	17,17,17,17	0
6	NA	N	205	1/1	0.99	0.17	28,28,28,28	0
6	NA	B	205	1/1	0.99	0.16	21,21,21,21	0
6	NA	C	205	1/1	0.99	0.14	19,19,19,19	0
6	NA	W	206	1/1	0.99	0.13	25,25,25,25	0
6	NA	E	204	1/1	0.99	0.12	19,19,19,19	0
6	NA	D	205	1/1	1.00	0.13	18,18,18,18	0
6	NA	F	204	1/1	1.00	0.13	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.