



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2021 – 05:21 pm GMT

PDB ID : 7AP5  
Title : Crystal structure of phycoerythrin from cyanobacterium Nostoc sp. WR13 contains multiple stacks of hexameric assemblies which resemble the rods of phycobilisome.  
Authors : Patel, H.M.; Roszak, A.W.; Cogdell, R.J.; Madamwar, D.; Liu, H.; Gross, M.L.; Blankenship, R.E.  
Deposited on : 2020-10-15  
Resolution : 2.13 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

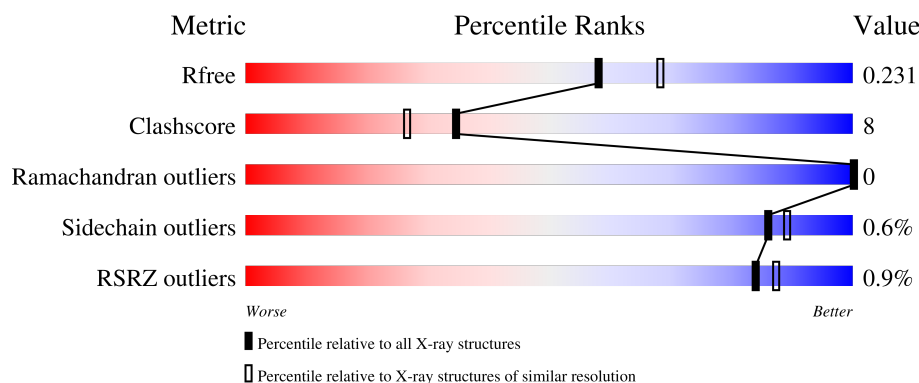
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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  $\geq 3$ , 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	AAA	164	<div><div></div><div>93%</div><div>7%</div></div>
1	CCC	164	<div><div></div><div>95%</div><div>• •</div></div>
1	EEE	164	<div><div></div><div>98%</div><div>•</div></div>
1	GGG	164	<div><div></div><div>92%</div><div>8%</div></div>
1	III	164	<div><div></div><div>95%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
1	KKK	164	
1	MMM	164	
1	OOO	164	
2	BBB	184	
2	DDD	184	
2	FFF	184	
2	HHH	184	
2	JJJ	184	
2	LLL	184	
2	NNN	184	
2	PPP	184	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	1PE	JJJ	308	-	-	X	-
14	EDO	NNN	219	-	-	X	-
4	PG4	AAA	203	-	-	X	-
4	PG4	AAA	204	-	-	X	-
4	PG4	CCC	203	-	-	X	-
4	PG4	KKK	204	-	-	X	-
4	PG4	MMM	203	-	-	X	-
4	PG4	MMM	205	-	-	-	X
5	PGE	BBB	209	-	-	-	X
5	PGE	HHH	310	-	-	-	X
5	PGE	HHH	313	-	-	-	X
5	PGE	JJJ	310	-	-	X	-
6	PEG	CCC	210	-	-	X	-
6	PEG	CCC	214	-	-	-	X
6	PEG	CCC	219	-	-	X	-
6	PEG	EEE	212	-	-	-	X
6	PEG	GGG	211	-	-	X	-
6	PEG	III	201	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PEG	LLL	215	-	-	-	X
6	PEG	LLL	217	-	-	X	-
6	PEG	MMM	209	-	-	X	-
6	PEG	PPP	212	-	-	-	X
7	PO4	AAA	214	-	-	X	-
7	PO4	CCC	217	-	-	X	-
7	PO4	GGG	214	-	-	X	-
7	PO4	KKK	215	-	-	X	-
7	PO4	PPP	217	-	-	X	-
8	NO3	LLL	223	-	-	X	-
8	NO3	LLL	224	-	-	X	-



## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 26483 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 Alpha subunit of cyanobacterial protein phycoerythrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	164	Total	C	N	O	S	0	4	0
			1257	785	220	245	7			
1	CCC	164	Total	C	N	O	S	0	4	0
			1256	785	219	245	7			
1	EEE	164	Total	C	N	O	S	0	4	0
			1254	784	219	244	7			
1	GGG	164	Total	C	N	O	S	0	2	0
			1244	777	218	242	7			
1	III	164	Total	C	N	O	S	0	2	0
			1244	777	218	242	7			
1	KKK	164	Total	C	N	O	S	0	3	0
			1245	780	217	241	7			
1	MMM	164	Total	C	N	O	S	0	3	0
			1247	780	217	243	7			
1	OOO	164	Total	C	N	O	S	0	1	0
			1238	774	217	240	7			

- Molecule 2 is a protein called Beta subunit of cyanobacterial protein phycoerythrin.

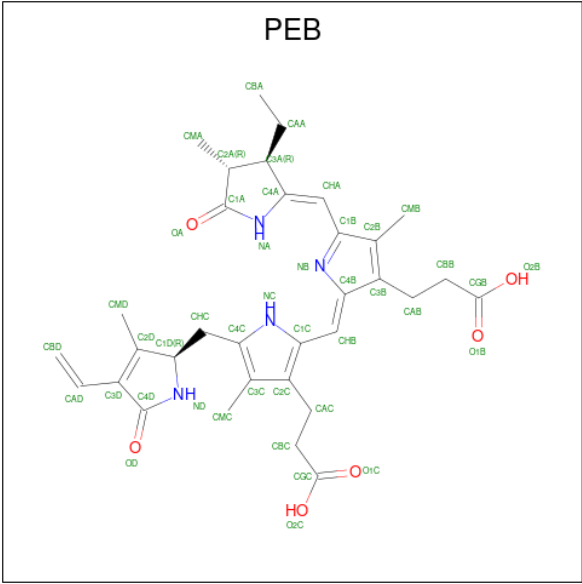
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	184	Total	C	N	O	S	0	6	0
			1378	845	253	268	12			
2	DDD	184	Total	C	N	O	S	0	9	0
			1382	849	251	270	12			
2	FFF	184	Total	C	N	O	S	0	6	0
			1370	840	250	268	12			
2	HHH	184	Total	C	N	O	S	0	7	0
			1368	839	247	270	12			
2	JJJ	184	Total	C	N	O	S	0	8	0
			1376	844	250	270	12			
2	LLL	184	Total	C	N	O	S	0	7	0
			1381	847	253	269	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	NNN	184	Total	C	N	O	S	0	3	0
			1355	830	247	266	12			
2	PPP	184	Total	C	N	O	S	0	4	0
			1363	835	250	266	12			

- Molecule 3 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O		0	0
			43	33	4	6			
3	AAA	1	Total	C	N	O		0	0
			43	33	4	6			
3	BBB	1	Total	C	N	O		0	0
			43	33	4	6			
3	BBB	1	Total	C	N	O		0	0
			43	33	4	6			
3	BBB	1	Total	C	N	O		0	0
			43	33	4	6			
3	CCC	1	Total	C	N	O		0	0
			43	33	4	6			
3	CCC	1	Total	C	N	O		0	0
			43	33	4	6			
3	DDD	1	Total	C	N	O		0	0
			43	33	4	6			
3	DDD	1	Total	C	N	O		0	0
			43	33	4	6			

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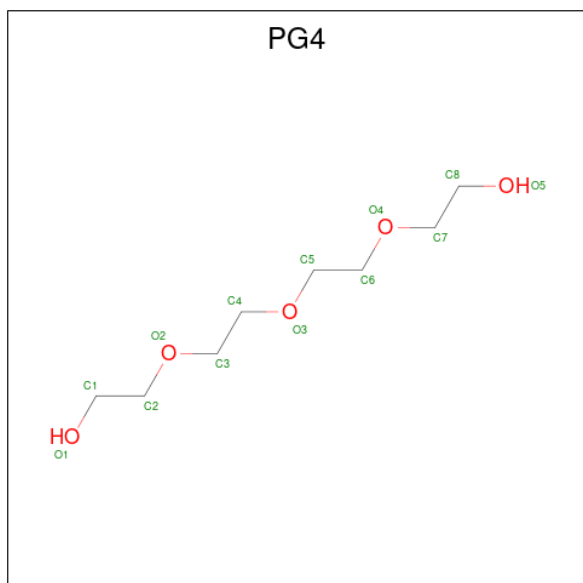
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	DDD	1	Total	C	N	O	0	0
			43	33	4	6		
3	EEE	1	Total	C	N	O	0	0
			43	33	4	6		
3	EEE	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		
3	GGG	1	Total	C	N	O	0	0
			43	33	4	6		
3	GGG	1	Total	C	N	O	0	0
			43	33	4	6		
3	HHH	1	Total	C	N	O	0	0
			43	33	4	6		
3	HHH	1	Total	C	N	O	0	0
			43	33	4	6		
3	HHH	1	Total	C	N	O	0	0
			43	33	4	6		
3	III	1	Total	C	N	O	0	0
			43	33	4	6		
3	III	1	Total	C	N	O	0	0
			43	33	4	6		
3	JJJ	1	Total	C	N	O	0	0
			43	33	4	6		
3	JJJ	1	Total	C	N	O	0	0
			43	33	4	6		
3	JJJ	1	Total	C	N	O	0	0
			43	33	4	6		
3	KKK	1	Total	C	N	O	0	0
			43	33	4	6		
3	KKK	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	MMM	1	Total	C	N	O	0	0
			43	33	4	6		
3	MMM	1	Total	C	N	O	0	0
			43	33	4	6		
3	NNN	1	Total	C	N	O	0	0
			43	33	4	6		
3	NNN	1	Total	C	N	O	0	0
			43	33	4	6		
3	NNN	1	Total	C	N	O	0	0
			43	33	4	6		
3	OOO	1	Total	C	N	O	0	0
			43	33	4	6		
3	OOO	1	Total	C	N	O	0	0
			43	33	4	6		
3	PPP	1	Total	C	N	O	0	0
			43	33	4	6		
3	PPP	1	Total	C	N	O	0	0
			43	33	4	6		
3	PPP	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			13	8	5		

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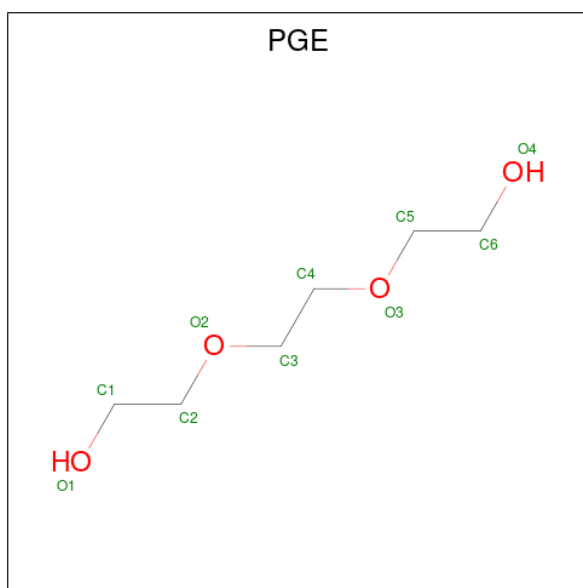
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			13	8	5		
4	AAA	1	Total	C	O	0	0
			13	8	5		
4	CCC	1	Total	C	O	0	0
			13	8	5		
4	DDD	1	Total	C	O	0	0
			13	8	5		
4	DDD	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	GGG	1	Total	C	O	0	0
			13	8	5		
4	GGG	1	Total	C	O	0	0
			13	8	5		
4	GGG	1	Total	C	O	0	0
			13	8	5		
4	HHH	1	Total	C	O	0	0
			13	8	5		
4	HHH	1	Total	C	O	0	0
			13	8	5		
4	JJJ	1	Total	C	O	0	0
			13	8	5		
4	KKK	1	Total	C	O	0	0
			13	8	5		
4	KKK	1	Total	C	O	0	0
			13	8	5		
4	KKK	1	Total	C	O	0	0
			13	8	5		
4	LLL	1	Total	C	O	0	0
			13	8	5		
4	LLL	1	Total	C	O	0	0
			13	8	5		
4	LLL	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	MMM	1	Total	C	O	0	0
			13	8	5		
4	MMM	1	Total	C	O	0	0
			13	8	5		
4	MMM	1	Total	C	O	0	0
			13	8	5		
4	MMM	1	Total	C	O	0	0
			13	8	5		
4	NNN	1	Total	C	O	0	0
			13	8	5		
4	NNN	1	Total	C	O	0	0
			13	8	5		
4	NNN	1	Total	C	O	0	0
			13	8	5		
4	NNN	1	Total	C	O	0	0
			13	8	5		
4	NNN	1	Total	C	O	0	0
			13	8	5		
4	OOO	1	Total	C	O	0	0
			13	8	5		
4	PPP	1	Total	C	O	0	0
			13	8	5		
4	PPP	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 10 6 4	0	0
5	AAA	1	Total C O 10 6 4	0	0
5	AAA	1	Total C O 10 6 4	0	0
5	AAA	1	Total C O 10 6 4	0	0
5	AAA	1	Total C O 10 6 4	0	0
5	AAA	1	Total C O 10 6 4	0	0
5	BBB	1	Total C O 10 6 4	0	0
5	BBB	1	Total C O 10 6 4	0	0
5	BBB	1	Total C O 10 6 4	0	0
5	CCC	1	Total C O 10 6 4	0	0
5	CCC	1	Total C O 10 6 4	0	0
5	CCC	1	Total C O 10 6 4	0	0
5	CCC	1	Total C O 10 6 4	0	0
5	CCC	1	Total C O 10 6 4	0	0
5	DDD	1	Total C O 10 6 4	0	0
5	DDD	1	Total C O 10 6 4	0	0
5	DDD	1	Total C O 10 6 4	0	0
5	EEE	1	Total C O 10 6 4	0	0
5	EEE	1	Total C O 10 6 4	0	0
5	EEE	1	Total C O 10 6 4	0	0
5	EEE	1	Total C O 10 6 4	0	0
5	FFF	1	Total C O 10 6 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	FFF	1	Total	C	O	0	0
			10	6	4		
5	FFF	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	III	1	Total	C	O	0	0
			10	6	4		
5	III	1	Total	C	O	0	0
			10	6	4		
5	III	1	Total	C	O	0	0
			10	6	4		
5	III	1	Total	C	O	0	0
			10	6	4		
5	JJJ	1	Total	C	O	0	0
			10	6	4		
5	JJJ	1	Total	C	O	0	0
			10	6	4		
5	JJJ	1	Total	C	O	0	0
			10	6	4		
5	KKK	1	Total	C	O	0	0
			10	6	4		
5	KKK	1	Total	C	O	0	0
			10	6	4		

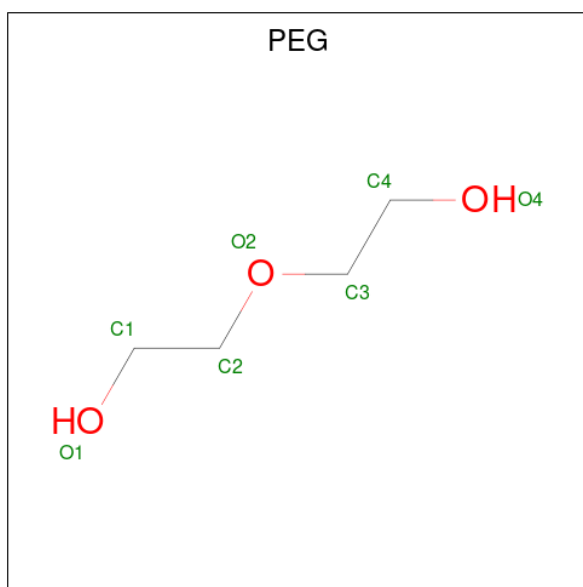
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	LLL	1	Total	C	O	0	0
			10	6	4		
5	LLL	1	Total	C	O	0	0
			10	6	4		
5	LLL	1	Total	C	O	0	0
			10	6	4		
5	LLL	1	Total	C	O	0	0
			10	6	4		
5	MMM	1	Total	C	O	0	0
			10	6	4		
5	MMM	1	Total	C	O	0	0
			10	6	4		
5	NNN	1	Total	C	O	0	0
			10	6	4		
5	NNN	1	Total	C	O	0	0
			10	6	4		
5	NNN	1	Total	C	O	0	0
			10	6	4		
5	NNN	1	Total	C	O	0	0
			10	6	4		
5	OOO	1	Total	C	O	0	0
			10	6	4		
5	OOO	1	Total	C	O	0	0
			10	6	4		
5	OOO	1	Total	C	O	0	0
			10	6	4		
5	PPP	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			7	4	3		
6	AAA	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	EEE	1	Total	C	O	0	0
			7	4	3		
6	EEE	1	Total	C	O	0	0
			7	4	3		
6	FFF	1	Total	C	O	0	0
			7	4	3		
6	FFF	1	Total	C	O	0	0
			7	4	3		
6	FFF	1	Total	C	O	0	0
			7	4	3		
6	FFF	1	Total	C	O	0	0
			7	4	3		
6	FFF	1	Total	C	O	0	0
			7	4	3		
6	GGG	1	Total	C	O	0	0
			7	4	3		
6	GGG	1	Total	C	O	0	0
			7	4	3		
6	GGG	1	Total	C	O	0	0
			7	4	3		
6	GGG	1	Total	C	O	0	0
			7	4	3		
6	GGG	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	HHH	1	Total	C	O	0	0
			7	4	3		
6	HHH	1	Total	C	O	0	0
			7	4	3		
6	HHH	1	Total	C	O	0	0
			7	4	3		
6	HHH	1	Total	C	O	0	0
			7	4	3		
6	HHH	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	JJJ	1	Total	C	O	0	0
			7	4	3		
6	JJJ	1	Total	C	O	0	0
			7	4	3		
6	JJJ	1	Total	C	O	0	0
			7	4	3		
6	KKK	1	Total	C	O	0	0
			7	4	3		
6	KKK	1	Total	C	O	0	0
			7	4	3		
6	KKK	1	Total	C	O	0	0
			7	4	3		
6	KKK	1	Total	C	O	0	0
			7	4	3		
6	KKK	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		

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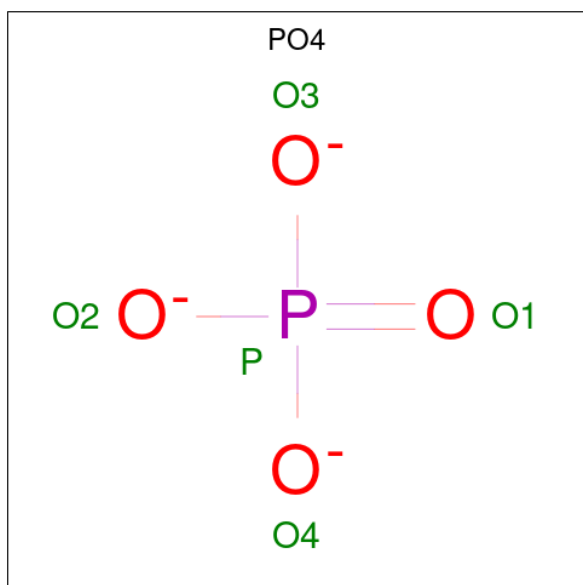
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	1
			14	8	6		
6	MMM	1	Total	C	O	0	0
			7	4	3		
6	MMM	1	Total	C	O	0	0
			7	4	3		
6	MMM	1	Total	C	O	0	0
			7	4	3		
6	NNN	1	Total	C	O	0	0
			7	4	3		
6	NNN	1	Total	C	O	0	0
			7	4	3		
6	NNN	1	Total	C	O	0	0
			7	4	3		
6	OOO	1	Total	C	O	0	0
			7	4	3		
6	OOO	1	Total	C	O	0	0
			7	4	3		
6	OOO	1	Total	C	O	0	0
			7	4	3		
6	OOO	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	PPP	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	O	P	0	0
			5	4	1		
7	AAA	1	Total	O	P	0	0
			5	4	1		
7	BBB	1	Total	O	P	0	0
			5	4	1		
7	BBB	1	Total	O	P	0	0
			5	4	1		
7	BBB	1	Total	O	P	0	0
			5	4	1		
7	BBB	1	Total	O	P	0	0
			5	4	1		
7	CCC	1	Total	O	P	0	0
			5	4	1		
7	CCC	1	Total	O	P	0	0
			5	4	1		
7	CCC	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	4	1		
7	GGG	1	Total	O	P	0	0
			5	4	1		
7	GGG	1	Total	O	P	0	0
			5	4	1		
7	HHH	1	Total	O	P	0	0
			5	4	1		
7	HHH	1	Total	O	P	0	0
			5	4	1		
7	HHH	1	Total	O	P	0	0
			5	4	1		
7	HHH	1	Total	O	P	0	0
			5	4	1		
7	III	1	Total	O	P	0	0
			5	4	1		
7	III	1	Total	O	P	0	0
			5	4	1		
7	III	1	Total	O	P	0	0
			5	4	1		
7	JJJ	1	Total	O	P	0	0
			5	4	1		

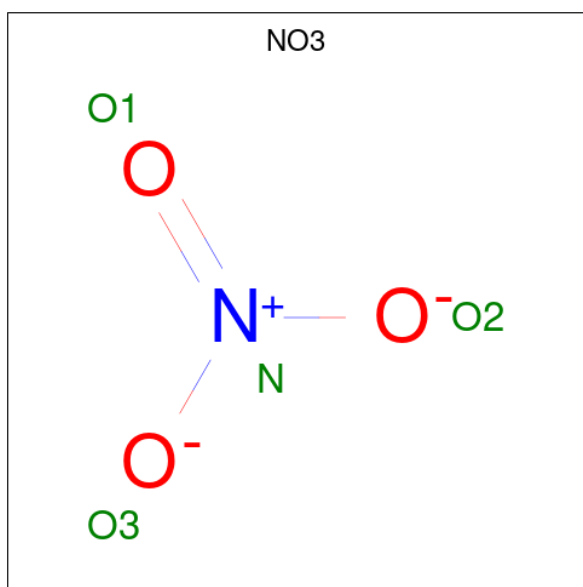
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	JJJ	1	Total	O	P	0	0
			5	4	1		
7	JJJ	1	Total	O	P	0	0
			5	4	1		
7	JJJ	1	Total	O	P	0	0
			5	4	1		
7	JJJ	1	Total	O	P	0	0
			5	4	1		
7	JJJ	1	Total	O	P	0	0
			5	4	1		
7	KKK	1	Total	O	P	0	0
			5	4	1		
7	KKK	1	Total	O	P	0	0
			5	4	1		
7	KKK	1	Total	O	P	0	0
			5	4	1		
7	LLL	1	Total	O	P	0	0
			5	4	1		
7	LLL	1	Total	O	P	0	0
			5	4	1		
7	NNN	1	Total	O	P	0	0
			5	4	1		
7	NNN	1	Total	O	P	0	0
			5	4	1		
7	NNN	1	Total	O	P	0	0
			5	4	1		
7	NNN	1	Total	O	P	0	0
			5	4	1		
7	NNN	1	Total	O	P	0	0
			5	4	1		
7	OOO	1	Total	O	P	0	0
			5	4	1		
7	PPP	1	Total	O	P	0	0
			5	4	1		
7	PPP	1	Total	O	P	0	0
			5	4	1		
7	PPP	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).





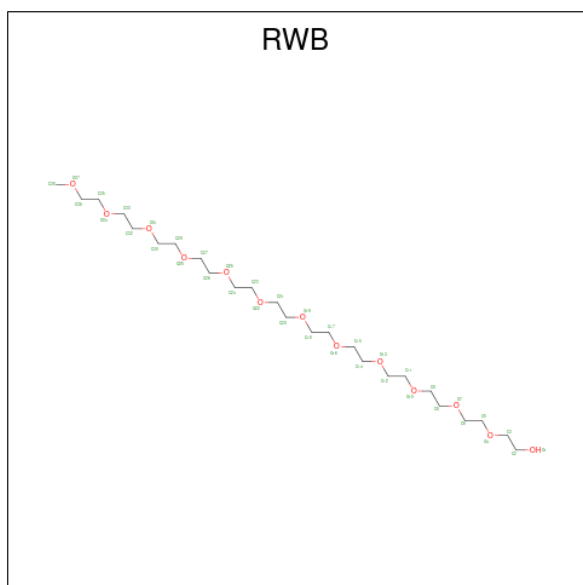
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	N	O	0	0
			4	1	3		
8	AAA	1	Total	N	O	0	0
			4	1	3		
8	BBB	1	Total	N	O	0	0
			4	1	3		
8	CCC	1	Total	N	O	0	0
			4	1	3		
8	DDD	1	Total	N	O	0	0
			4	1	3		
8	DDD	1	Total	N	O	0	0
			4	1	3		
8	EEE	1	Total	N	O	0	0
			4	1	3		
8	EEE	1	Total	N	O	0	0
			4	1	3		
8	FFF	1	Total	N	O	0	0
			4	1	3		
8	GGG	1	Total	N	O	0	0
			4	1	3		
8	HHH	1	Total	N	O	0	0
			4	1	3		
8	HHH	1	Total	N	O	0	0
			4	1	3		
8	III	1	Total	N	O	0	0
			4	1	3		
8	JJJ	1	Total	N	O	0	0
			4	1	3		

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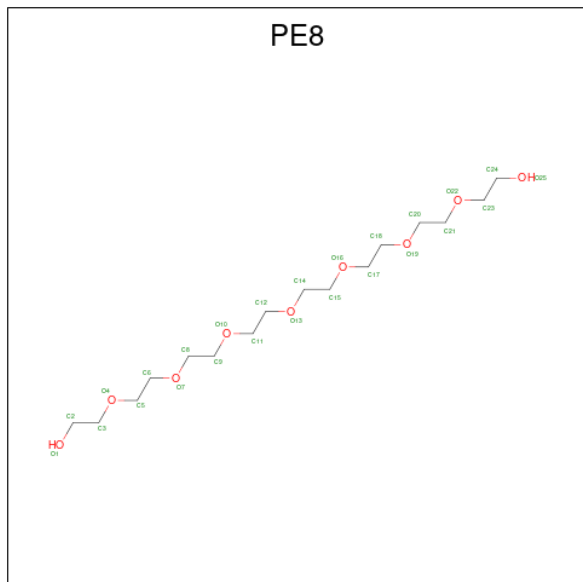
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	JJJ	1	Total	N	O	0	0
			4	1	3		
8	KKK	1	Total	N	O	0	0
			4	1	3		
8	KKK	1	Total	N	O	0	0
			4	1	3		
8	LLL	1	Total	N	O	0	0
			4	1	3		
8	LLL	1	Total	N	O	0	0
			4	1	3		
8	LLL	1	Total	N	O	0	0
			4	1	3		
8	MMM	1	Total	N	O	0	0
			4	1	3		
8	OOO	1	Total	N	O	0	0
			4	1	3		
8	PPP	1	Total	N	O	0	0
			4	1	3		

- Molecule 9 is dodecaethylene glycol monomethyl ether (three-letter code: RWB) (formula:  $C_{25}H_{52}O_{13}$ ).



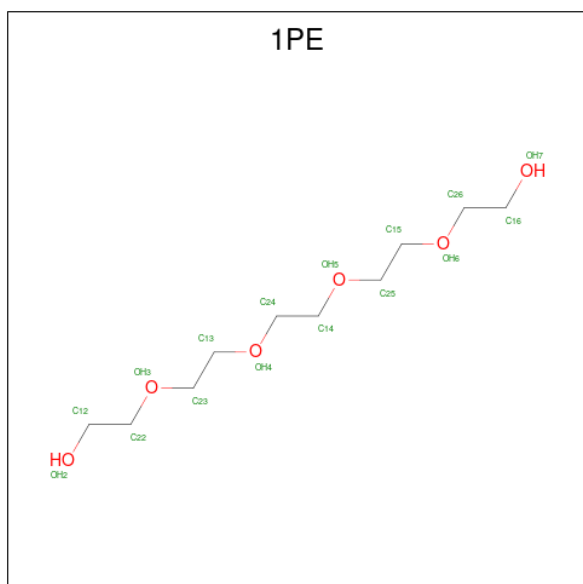
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	BBB	1	Total	C	O	0	0
			38	25	13		
9	LLL	1	Total	C	O	0	0
			38	25	13		

- Molecule 10 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula:  $C_{16}H_{34}O_9$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	BBB	1	Total	C	O	0	0
			25	16	9		

- Molecule 11 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



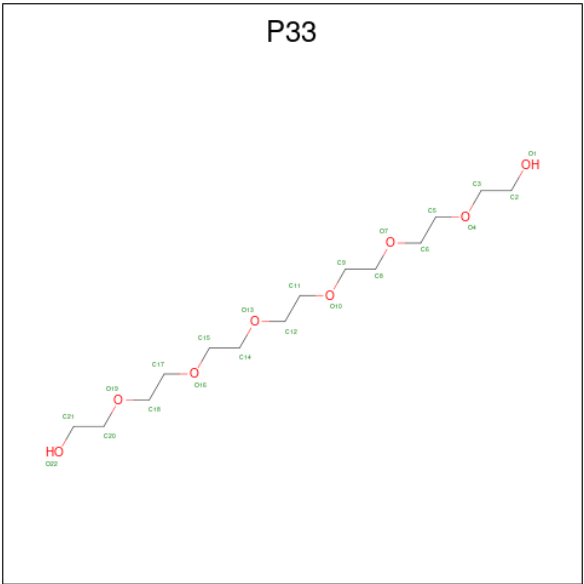
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	BBB	1	Total	C	O	0	0
			16	10	6		

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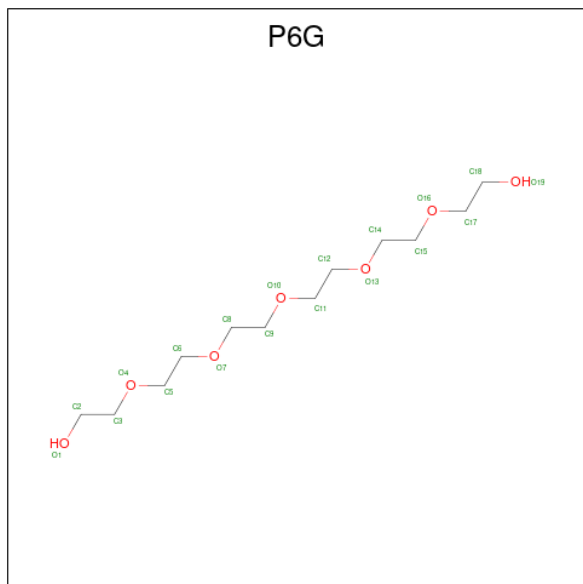
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	BBB	1	Total	C	O	0	0
			16	10	6		
11	BBB	1	Total	C	O	0	0
			16	10	6		
11	DDD	1	Total	C	O	0	0
			16	10	6		
11	EEE	1	Total	C	O	0	0
			16	10	6		
11	FFF	1	Total	C	O	0	0
			16	10	6		
11	HHH	1	Total	C	O	0	0
			16	10	6		
11	JJJ	1	Total	C	O	0	0
			16	10	6		
11	JJJ	1	Total	C	O	0	0
			16	10	6		
11	JJJ	1	Total	C	O	0	0
			16	10	6		
11	LLL	1	Total	C	O	0	0
			16	10	6		
11	PPP	1	Total	C	O	0	0
			16	10	6		

- Molecule 12 is 3,6,9,12,15,18-HEXAOSAICOSANE-1,20-DIOL (three-letter code: P33) (formula: C<sub>14</sub>H<sub>30</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	DDD	1	Total	C	O	0	0
			22	14	8		
12	DDD	1	Total	C	O	0	0
			22	14	8		
12	FFF	1	Total	C	O	0	0
			22	14	8		
12	HHH	1	Total	C	O	0	0
			22	14	8		
12	HHH	1	Total	C	O	0	0
			22	14	8		
12	JJJ	1	Total	C	O	0	0
			22	14	8		

- Molecule 13 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	DDD	1	Total	C	O	0	0
			19	12	7		

- Molecule 14 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



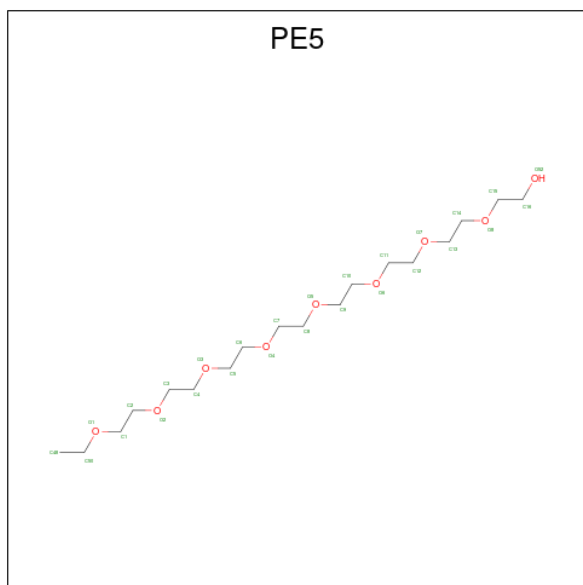
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	DDD	1	Total	C	O	0	0
			4	2	2		
14	DDD	1	Total	C	O	0	0
			4	2	2		
14	EEE	1	Total	C	O	0	0
			4	2	2		
14	EEE	1	Total	C	O	0	0
			4	2	2		
14	FFF	1	Total	C	O	0	0
			4	2	2		
14	FFF	1	Total	C	O	0	0
			4	2	2		
14	HHH	1	Total	C	O	0	0
			4	2	2		
14	HHH	1	Total	C	O	0	0
			4	2	2		
14	III	1	Total	C	O	0	0
			4	2	2		
14	III	1	Total	C	O	0	0
			4	2	2		
14	LLL	1	Total	C	O	0	0
			4	2	2		
14	NNN	1	Total	C	O	0	0
			4	2	2		
14	NNN	1	Total	C	O	0	0
			4	2	2		
14	NNN	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	PPP	1	Total	C	O	0	0
			4	2	2		

- Molecule 15 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	NNN	1	Total	C	O	0	0
			27	18	9		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	AAA	93	Total	O	0	0
			93	93		
16	BBB	90	Total	O	0	0
			90	90		
16	CCC	90	Total	O	0	0
			90	90		
16	DDD	97	Total	O	0	0
			97	97		
16	EEE	82	Total	O	0	0
			82	82		
16	FFF	110	Total	O	0	0
			110	110		
16	GGG	77	Total	O	0	0
			77	77		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	HHH	92	Total 92	O 92	0	0
16	III	79	Total 79	O 79	0	0
16	JJJ	106	Total 106	O 106	0	0
16	KKK	86	Total 86	O 86	0	0
16	LLL	97	Total 97	O 97	0	0
16	MMM	76	Total 76	O 76	0	0
16	NNN	76	Total 76	O 76	0	0
16	OOO	57	Total 57	O 57	0	0
16	PPP	57	Total 57	O 57	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.

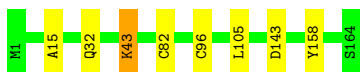
- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain AAA:  93% 7%



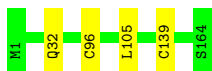
- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain CCC:  95% ..



- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain EEE:  98% .



- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain GGG:  92% 8%



- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain III:  95% 5%



- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain KKK:  90% 10%



- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain MMM: 93% 7%



- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain OOO: 2% 92% 8%



- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin

Chain BBB: 95% 5%



- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin

Chain DDD: 92% 8%



- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin

Chain FFF: 91% 9%



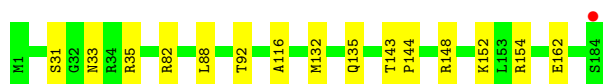
- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin

Chain HHH: 93% 7%

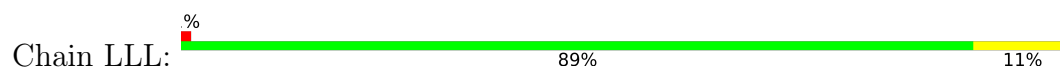


- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin

Chain JJJ: % 92% 8%



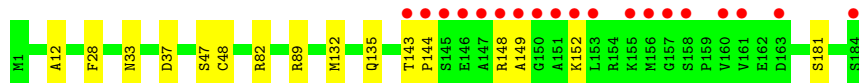
- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin



- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin



- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.76Å 192.76Å 524.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.01 – 2.13 174.83 – 2.13	Depositor EDS
% Data completeness (in resolution range)	75.0 (49.01-2.13) 75.0 (174.83-2.13)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.177 , 0.225 0.188 , 0.231	Depositor DCC
$R_{free}$ test set	7767 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PE8, MEN, P6G, PGE, 1PE, PEB, RWB, NO3, EDO, PEG, PG4, P33, PE5, PO4

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	AAA	0.74	0/1283	0.83	1/1739 (0.1%)
1	CCC	0.70	0/1285	0.80	0/1741
1	EEE	0.71	0/1283	0.80	0/1739
1	GGG	0.70	0/1267	0.81	0/1717
1	III	0.69	0/1267	0.79	0/1717
1	KKK	0.69	0/1274	0.81	0/1727
1	MMM	0.72	0/1276	0.81	0/1729
1	OOO	0.72	1/1261 (0.1%)	0.81	0/1709
2	BBB	0.71	0/1401	0.81	1/1892 (0.1%)
2	DDD	0.69	0/1411	0.80	0/1905
2	FFF	0.73	1/1390 (0.1%)	0.80	1/1878 (0.1%)
2	HHH	0.70	0/1391	0.81	0/1880
2	JJJ	0.71	0/1402	0.84	0/1894
2	LLL	0.70	0/1407	0.80	1/1900 (0.1%)
2	NNN	0.70	0/1366	0.81	0/1846
2	PPP	0.71	0/1377	0.81	0/1860
All	All	0.71	2/21341 (0.0%)	0.81	4/28873 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	FFF	113	GLU	CD-OE1	6.99	1.33	1.25
1	OOO	115	GLU	CD-OE1	5.42	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	37	ARG	NE-CZ-NH2	-5.91	117.34	120.30
2	LLL	154	ARG	CG-CD-NE	-5.32	100.64	111.80
2	FFF	154	ARG	CG-CD-NE	-5.14	101.00	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	154	ARG	CG-CD-NE	-5.01	101.28	111.80

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	AAA	1257	0	1252	20	0
1	CCC	1256	0	1252	12	0
1	EEE	1254	0	1253	5	0
1	GGG	1244	0	1238	12	0
1	III	1244	0	1238	10	0
1	KKK	1245	0	1248	18	0
1	MMM	1247	0	1245	25	0
1	OOO	1238	0	1234	6	0
2	BBB	1378	0	1410	8	0
2	DDD	1382	0	1420	13	0
2	FFF	1370	0	1397	14	0
2	HHH	1368	0	1394	20	0
2	JJJ	1376	0	1407	15	0
2	LLL	1381	0	1415	23	0
2	NNN	1355	0	1372	17	0
2	PPP	1363	0	1385	18	0
3	AAA	86	0	74	1	0
3	BBB	129	0	110	10	0
3	CCC	86	0	74	2	0
3	DDD	129	0	110	7	0
3	EEE	86	0	74	3	0
3	FFF	129	0	110	6	0
3	GGG	86	0	74	1	0
3	HHH	129	0	110	5	0
3	III	86	0	74	0	0
3	JJJ	129	0	110	6	0
3	KKK	86	0	74	2	0
3	LLL	129	0	110	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	MMM	86	0	74	4	0
3	NNN	129	0	110	8	0
3	OOO	86	0	74	5	0
3	PPP	129	0	110	16	0
4	AAA	39	0	54	18	0
4	CCC	13	0	18	7	0
4	DDD	26	0	36	1	0
4	FFF	52	0	72	9	0
4	GGG	39	0	54	4	0
4	HHH	26	0	36	4	0
4	JJJ	13	0	18	3	0
4	KKK	39	0	54	9	0
4	LLL	39	0	54	6	0
4	MMM	52	0	72	27	0
4	NNN	65	0	90	4	0
4	OOO	13	0	18	0	0
4	PPP	26	0	36	5	0
5	AAA	60	0	84	3	0
5	BBB	30	0	42	1	0
5	CCC	50	0	70	3	0
5	DDD	30	0	42	12	0
5	EEE	40	0	56	0	0
5	FFF	30	0	42	6	0
5	GGG	40	0	56	5	0
5	HHH	60	0	84	9	0
5	III	40	0	56	6	0
5	JJJ	30	0	42	7	0
5	KKK	20	0	28	4	0
5	LLL	40	0	56	12	0
5	MMM	20	0	28	0	0
5	NNN	40	0	56	4	0
5	OOO	30	0	42	1	0
5	PPP	10	0	14	1	0
6	AAA	14	0	20	0	0
6	BBB	49	0	70	1	0
6	CCC	63	0	90	16	0
6	DDD	35	0	50	3	0
6	EEE	14	0	20	0	0
6	FFF	35	0	50	0	0
6	GGG	35	0	50	7	0
6	HHH	35	0	50	3	0
6	III	42	0	60	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	JJJ	21	0	30	2	0
6	KKK	35	0	50	6	0
6	LLL	63	0	90	7	0
6	MMM	21	0	30	8	0
6	NNN	21	0	30	3	0
6	OOO	28	0	40	1	0
6	PPP	49	0	70	3	0
7	AAA	10	0	0	2	0
7	BBB	20	0	0	0	0
7	CCC	15	0	0	2	0
7	DDD	30	0	0	1	0
7	FFF	25	0	0	0	0
7	GGG	10	0	0	2	0
7	HHH	20	0	0	0	0
7	III	15	0	0	0	0
7	JJJ	30	0	0	0	0
7	KKK	15	0	0	2	0
7	LLL	10	0	0	1	0
7	NNN	25	0	0	0	0
7	OOO	5	0	0	1	0
7	PPP	15	0	0	3	0
8	AAA	8	0	0	0	0
8	BBB	4	0	0	0	0
8	CCC	4	0	0	0	0
8	DDD	8	0	0	0	0
8	EEE	8	0	0	0	0
8	FFF	4	0	0	0	0
8	GGG	4	0	0	0	0
8	HHH	8	0	0	0	0
8	III	4	0	0	0	0
8	JJJ	8	0	0	1	0
8	KKK	8	0	0	1	0
8	LLL	12	0	0	2	0
8	MMM	4	0	0	0	0
8	OOO	4	0	0	1	0
8	PPP	4	0	0	0	0
9	BBB	38	0	0	0	0
9	LLL	38	0	0	2	0
10	BBB	25	0	34	0	0
11	BBB	48	0	66	3	0
11	DDD	16	0	22	5	0
11	EEE	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	FFF	16	0	22	1	0
11	HHH	16	0	22	2	0
11	JJJ	48	0	66	11	0
11	LLL	16	0	22	0	0
11	PPP	16	0	22	1	0
12	DDD	44	0	60	6	0
12	FFF	22	0	30	2	0
12	HHH	44	0	60	4	0
12	JJJ	22	0	30	4	0
13	DDD	19	0	26	2	0
14	DDD	8	0	12	0	0
14	EEE	8	0	12	0	0
14	FFF	8	0	12	0	0
14	HHH	8	0	12	0	0
14	III	8	0	12	1	0
14	LLL	4	0	6	0	0
14	NNN	12	0	18	5	0
14	PPP	4	0	6	0	0
15	NNN	27	0	38	6	0
16	AAA	93	0	0	2	0
16	BBB	90	0	0	2	0
16	CCC	90	0	0	0	0
16	DDD	97	0	0	7	0
16	EEE	82	0	0	0	0
16	FFF	110	0	0	2	0
16	GGG	77	0	0	1	0
16	HHH	92	0	0	1	0
16	III	79	0	0	0	0
16	JJJ	106	0	0	7	0
16	KKK	86	0	0	4	0
16	LLL	97	0	0	1	0
16	MMM	76	0	0	3	0
16	NNN	76	0	0	3	0
16	OOO	57	0	0	1	0
16	PPP	57	0	0	4	0
All	All	26483	0	25474	419	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 8.

All (419) 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)
6:CCC:219:PEG:C1	5:DDD:212:PGE:H62	1.53	1.35
7:AAA:214:PO4:O4	16:AAA:301:HOH:O	1.53	1.25
6:CCC:219:PEG:H12	5:DDD:212:PGE:C6	1.77	1.15
1:AAA:47:ASN:HA	4:AAA:203:PG4:H52	1.34	1.08
1:GGG:49:ASP:HB2	5:GGG:208:PGE:H1	1.28	1.08
5:DDD:210:PGE:H62	5:DDD:210:PGE:H2	1.32	1.08
7:PPP:217:PO4:O4	16:PPP:301:HOH:O	1.69	1.07
8:KKK:216:NO3:O1	16:KKK:801:HOH:O	1.69	1.06
4:MMM:205:PG4:H21	6:MMM:210:PEG:H11	1.09	1.05
4:CCC:203:PG4:H41	7:CCC:217:PO4:O4	1.57	1.03
8:OOO:212:NO3:O1	16:OOO:301:HOH:O	1.75	1.03
6:CCC:219:PEG:H12	5:DDD:212:PGE:H62	1.02	1.02
5:DDD:210:PGE:H2	5:DDD:210:PGE:C6	1.88	1.02
7:DDD:223:PO4:O1	16:DDD:301:HOH:O	1.79	1.00
4:CCC:203:PG4:H11	4:CCC:203:PG4:H61	1.42	0.99
6:MMM:209:PEG:H11	16:MMM:361:HOH:O	1.64	0.97
1:AAA:49:ASP:HB2	4:AAA:203:PG4:H61	1.47	0.93
7:AAA:214:PO4:P	16:AAA:301:HOH:O	2.17	0.91
1:MMM:115[B]:GLU:OE1	16:MMM:301:HOH:O	1.88	0.91
1:CCC:32[A]:GLN:HG3	1:EEE:32[A]:GLN:HG3	1.50	0.91
7:PPP:217:PO4:O2	16:PPP:302:HOH:O	1.86	0.91
6:CCC:219:PEG:C1	5:DDD:212:PGE:C6	2.43	0.89
1:GGG:32:GLN:HG3	1:III:32:GLN:HG3	1.55	0.88
6:CCC:219:PEG:H11	5:DDD:212:PGE:H62	1.52	0.87
1:AAA:47:ASN:CA	4:AAA:203:PG4:H52	2.05	0.86
4:GGG:205:PG4:H81	4:GGG:205:PG4:H51	1.56	0.86
2:HHH:148[B]:ARG:HG2	2:HHH:148[B]:ARG:HH11	1.40	0.86
1:KKK:32:GLN:HG3	1:MMM:32:GLN:HG3	1.57	0.86
12:DDD:205:P33:C15	16:DDD:304:HOH:O	2.24	0.85
5:NNN:211:PGE:H62	11:PPP:205:1PE:H142	1.60	0.84
4:CCC:203:PG4:H11	4:CCC:203:PG4:C6	2.08	0.82
1:KKK:115:GLU:OE2	7:KKK:215:PO4:O1	1.98	0.82
2:FFF:116:ALA:HA	5:FFF:212:PGE:H5	1.61	0.82
5:HHH:310:PGE:O4	5:HHH:310:PGE:H42	1.79	0.82
5:JJJ:310:PGE:H52	5:JJJ:310:PGE:O2	1.80	0.82
4:PPP:206:PG4:H51	4:PPP:206:PG4:O2	1.76	0.81
2:JJJ:88:LEU:O	2:JJJ:92[B]:THR:HG23	1.81	0.81
3:PPP:202:PEB:HMB2	3:PPP:202:PEB:HNA	1.45	0.81
5:KKK:206:PGE:H62	5:KKK:207:PGE:O1	1.80	0.80
2:PPP:28:PHE:HB3	4:PPP:207:PG4:H51	1.62	0.80
1:AAA:47:ASN:HA	4:AAA:203:PG4:C5	2.11	0.80
4:MMM:205:PG4:H21	6:MMM:210:PEG:C1	2.04	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:KKK:204:PG4:H42	4:KKK:204:PG4:O4	1.83	0.78
2:JJJ:31[B]:SER:OG	16:JJJ:401:HOH:O	2.00	0.78
2:HHH:89:ARG:HH22	5:HHH:312:PGE:H22	1.48	0.77
12:DDD:205:P33:C14	16:DDD:304:HOH:O	2.32	0.77
11:DDD:207:1PE:C15	11:DDD:207:1PE:H241	2.15	0.77
4:GGG:204:PG4:H32	6:GGG:211:PEG:H42	1.67	0.76
7:GGG:214:PO4:O3	16:GGG:301:HOH:O	2.02	0.76
3:LLL:201:PEB:HNA	3:LLL:201:PEB:HMB2	1.51	0.75
5:JJJ:311:PGE:H5	6:JJJ:314:PEG:H21	1.67	0.75
2:PPP:148[A]:ARG:HD2	3:PPP:204:PEB:O2B	1.86	0.74
2:JJJ:116:ALA:HB2	4:JJJ:309:PG4:H52	1.68	0.74
3:NNN:205:PEB:HMB3	3:NNN:205:PEB:HNA	1.52	0.74
5:FFF:213:PGE:H12	11:HHH:301:1PE:H132	1.69	0.74
2:JJJ:116:ALA:HB2	4:JJJ:309:PG4:C5	2.19	0.73
2:NNN:113:GLU:OE1	16:NNN:301:HOH:O	2.05	0.72
2:LLL:148[B]:ARG:NH1	6:LLL:217:PEG:H11	2.04	0.72
1:AAA:49:ASP:CB	4:AAA:203:PG4:H61	2.19	0.72
4:CCC:203:PG4:H61	4:CCC:203:PG4:C1	2.18	0.72
1:GGG:49:ASP:CB	5:GGG:208:PGE:H1	2.15	0.72
5:OOO:206:PGE:O1	5:OOO:206:PGE:H32	1.87	0.71
3:BBB:201:PEB:HMB2	3:BBB:201:PEB:HNA	1.55	0.71
2:JJJ:82[C]:ARG:NH2	16:JJJ:402:HOH:O	2.22	0.71
2:LLL:148[B]:ARG:HH11	6:LLL:217:PEG:C1	2.04	0.71
3:NNN:204:PEB:HMB2	3:NNN:204:PEB:HNA	1.56	0.70
1:CCC:32[B]:GLN:OE1	6:CCC:214:PEG:H31	1.91	0.70
3:FFF:204:PEB:HNA	3:FFF:204:PEB:HMB2	1.56	0.70
11:DDD:207:1PE:H241	11:DDD:207:1PE:H151	1.74	0.70
6:NNN:214:PEG:H41	16:NNN:365:HOH:O	1.92	0.69
2:NNN:82[C]:ARG:NH2	14:NNN:219:EDO:H12	2.08	0.69
2:LLL:152:LYS:NZ	9:LLL:204:RWB:O19	2.26	0.68
4:CCC:203:PG4:C4	7:CCC:217:PO4:O4	2.39	0.68
2:LLL:148[B]:ARG:NH1	6:LLL:217:PEG:C1	2.56	0.68
3:HHH:302:PEB:HNA	3:HHH:302:PEB:HMB2	1.58	0.68
5:JJJ:310:PGE:C3	4:LLL:208:PG4:H22	2.24	0.68
1:MMM:21[A]:SER:H	4:MMM:203:PG4:H81	1.59	0.67
11:JJJ:308:1PE:OH3	16:JJJ:402:HOH:O	2.11	0.67
8:LLL:223:NO3:O1	8:LLL:224:NO3:O2	2.13	0.67
2:PPP:12:ALA:HB2	6:PPP:214:PEG:H42	1.75	0.67
5:JJJ:310:PGE:H3	4:LLL:208:PG4:H22	1.77	0.67
2:NNN:82[C]:ARG:HH22	14:NNN:219:EDO:H12	1.59	0.67
3:DDD:201:PEB:HNA	3:DDD:201:PEB:HMB2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:NNN:206:PE5:C16	15:NNN:206:PE5:H31	2.25	0.66
4:KKK:204:PG4:O4	4:KKK:204:PG4:C4	2.44	0.65
2:DDD:116:ALA:HB2	13:DDD:206:P6G:H91	1.77	0.65
11:JJJ:308:1PE:H262	11:JJJ:308:1PE:OH5	1.97	0.65
2:PPP:148[A]:ARG:CD	3:PPP:204:PEB:O2B	2.45	0.65
11:JJJ:308:1PE:C23	16:JJJ:402:HOH:O	2.46	0.64
1:MMM:20:SER:HB2	4:MMM:203:PG4:H82	1.78	0.64
1:AAA:114:ARG:HG3	4:AAA:204:PG4:H12	1.80	0.64
2:LLL:148[B]:ARG:HH11	6:LLL:217:PEG:H11	1.60	0.64
1:MMM:19:PRO:O	4:MMM:203:PG4:H52	1.97	0.64
1:KKK:145:SER:HB2	6:KKK:209:PEG:H12	1.79	0.64
1:MMM:61:LYS:NZ	4:MMM:205:PG4:O2	2.30	0.64
5:FFF:213:PGE:C4	2:HHH:130:GLN:HG2	2.27	0.63
16:KKK:832:HOH:O	4:MMM:203:PG4:H31	1.98	0.63
2:LLL:82[B]:ARG:NH2	16:LLL:301:HOH:O	2.28	0.63
1:KKK:115:GLU:OE2	7:KKK:215:PO4:P	2.57	0.63
3:BBB:202:PEB:HMB2	3:BBB:202:PEB:HNA	1.62	0.63
3:FFF:205:PEB:HMB2	3:FFF:205:PEB:HNA	1.63	0.63
1:MMM:18:PHE:O	4:MMM:203:PG4:H41	1.99	0.62
1:MMM:21[B]:SER:H	4:MMM:203:PG4:H81	1.61	0.62
5:HHH:310:PGE:O4	5:HHH:310:PGE:C4	2.46	0.62
2:LLL:157:GLY:HA3	5:LLL:225:PGE:C2	2.30	0.62
3:FFF:204:PEB:HNA	3:FFF:204:PEB:CMB	2.12	0.62
6:GGG:211:PEG:C3	6:III:201:PEG:O4	2.48	0.61
1:AAA:114:ARG:CG	4:AAA:204:PG4:H12	2.31	0.61
1:MMM:18:PHE:N	4:MMM:203:PG4:O2	2.33	0.61
1:GGG:39:GLU:O	1:GGG:43:LYS:HG2	1.99	0.60
1:MMM:19:PRO:O	4:MMM:203:PG4:C5	2.49	0.60
3:OOO:202:PEB:HMB2	3:OOO:202:PEB:HNA	1.67	0.60
3:PPP:203:PEB:NA	3:PPP:203:PEB:HMB2	2.16	0.60
2:FFF:28:PHE:HB3	4:FFF:209:PG4:H51	1.83	0.60
11:JJJ:308:1PE:OH5	11:JJJ:308:1PE:C26	2.49	0.60
1:AAA:47:ASN:C	4:AAA:203:PG4:H52	2.22	0.59
3:DDD:202:PEB:HMB2	3:DDD:202:PEB:HNA	1.66	0.59
1:III:161:ASN:HB3	5:III:204:PGE:H1	1.84	0.59
1:KKK:161:ASN:HB3	6:KKK:208:PEG:H22	1.84	0.58
4:PPP:206:PG4:O2	4:PPP:206:PG4:C5	2.51	0.58
4:FFF:202:PG4:O4	4:FFF:202:PG4:H31	2.03	0.58
3:FFF:205:PEB:HMB2	3:FFF:205:PEB:NA	2.18	0.58
12:HHH:306:P33:H151	12:HHH:306:P33:H111	1.85	0.58
1:MMM:43:LYS:HG2	3:MMM:202:PEB:HBD1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:82:CYS:HA	3:CCC:201:PEB:HHA1	1.86	0.58
1:GGG:32:GLN:CG	1:III:32:GLN:HG3	2.30	0.58
2:LLL:157:GLY:HA3	5:LLL:225:PGE:H2	1.85	0.58
1:KKK:32:GLN:CG	1:MMM:32:GLN:HG3	2.31	0.58
5:DDD:210:PGE:H62	5:DDD:210:PGE:C2	2.22	0.58
5:FFF:213:PGE:H42	2:HHH:130:GLN:HG2	1.86	0.58
5:LLL:210:PGE:H1	5:LLL:210:PGE:C4	2.33	0.57
5:LLL:226:PGE:H3	1:MMM:161:ASN:HB3	1.86	0.57
1:OOO:136:ASN:ND2	7:OOO:211:PO4:O1	2.36	0.57
1:GGG:32:GLN:HG3	1:III:32:GLN:CG	2.31	0.57
2:PPP:149:ALA:HB2	3:PPP:204:PEB:C1A	2.34	0.57
1:OOO:82:CYS:HA	3:OOO:201:PEB:HHA1	1.85	0.57
6:GGG:211:PEG:H32	6:III:201:PEG:O4	2.05	0.57
5:FFF:213:PGE:H2	2:HHH:180:ILE:HG21	1.86	0.57
3:NNN:205:PEB:HMB3	3:NNN:205:PEB:NA	2.18	0.57
6:JJJ:312:PEG:H42	16:JJJ:437:HOH:O	2.05	0.56
1:OOO:17:ARG:HG3	1:OOO:18:PHE:O	2.05	0.56
16:KKK:811:HOH:O	4:MMM:203:PG4:H62	2.04	0.56
3:BBB:202:PEB:HMB2	3:BBB:202:PEB:NA	2.20	0.56
1:CCC:143:ASP:HA	6:CCC:210:PEG:H22	1.88	0.56
5:LLL:225:PGE:H1	1:MMM:149:LEU:HD23	1.87	0.56
11:JJJ:308:1PE:H232	16:JJJ:402:HOH:O	2.06	0.56
5:JJJ:310:PGE:O2	5:JJJ:310:PGE:C5	2.53	0.56
6:GGG:211:PEG:H32	6:III:201:PEG:C4	2.35	0.56
1:III:84:ARG:HG3	11:JJJ:302:1PE:H241	1.87	0.56
2:NNN:152:LYS:HE3	15:NNN:206:PE5:H61	1.87	0.56
2:FFF:4:ALA:HB2	4:FFF:209:PG4:H41	1.88	0.56
1:MMM:21[A]:SER:H	4:MMM:203:PG4:C8	2.18	0.56
2:NNN:82[C]:ARG:HH12	14:NNN:219:EDO:H22	1.71	0.56
14:III:217:EDO:O2	11:JJJ:308:1PE:H151	2.06	0.55
3:JJJ:303:PEB:HNA	3:JJJ:303:PEB:HMB2	1.71	0.55
2:LLL:118:LEU:HD11	3:LLL:201:PEB:HAC1	1.87	0.55
2:FFF:28:PHE:HB3	4:FFF:209:PG4:C5	2.37	0.55
5:FFF:213:PGE:H4	2:HHH:130:GLN:HG2	1.88	0.55
1:CCC:15:ALA:HB2	5:CCC:208:PGE:H4	1.89	0.55
1:KKK:32:GLN:HG3	1:MMM:32:GLN:CG	2.33	0.55
1:MMM:20:SER:CB	4:MMM:203:PG4:H82	2.36	0.55
2:JJJ:154:ARG:NH2	12:JJJ:306:P33:H52	2.23	0.54
2:BBB:113:GLU:OE2	11:BBB:206:1PE:H161	2.07	0.54
1:KKK:18:PHE:CD1	5:LLL:226:PGE:H5	2.43	0.54
1:MMM:20:SER:HB3	4:MMM:203:PG4:H42	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:NNN:28:PHE:CE1	5:NNN:212:PGE:H5	2.42	0.54
3:PPP:203:PEB:HMB2	3:PPP:203:PEB:HNA	1.71	0.54
1:CCC:32[A]:GLN:CG	1:EEE:32[A]:GLN:HG3	2.31	0.54
1:MMM:21[B]:SER:H	4:MMM:203:PG4:C8	2.20	0.54
2:PPP:135:GLN:HG2	3:PPP:204:PEB:C1B	2.38	0.54
4:KKK:204:PG4:H82	4:KKK:204:PG4:O1	2.08	0.54
3:HHH:302:PEB:HNA	3:HHH:302:PEB:CMB	2.21	0.53
2:HHH:148[B]:ARG:HH11	2:HHH:148[B]:ARG:CG	2.18	0.52
3:OOO:202:PEB:HMB2	3:OOO:202:PEB:NA	2.23	0.52
6:CCC:213:PEG:C3	6:CCC:213:PEG:O1	2.57	0.52
1:MMM:17:ARG:HA	4:MMM:203:PG4:H11	1.92	0.52
5:AAA:208:PGE:H3	5:AAA:210:PGE:H5	1.91	0.52
2:NNN:152:LYS:HG2	15:NNN:206:PE5:H151	1.91	0.52
1:AAA:115:GLU:OE2	4:AAA:204:PG4:O2	2.28	0.52
2:PPP:149:ALA:CB	3:PPP:204:PEB:C1A	2.88	0.52
1:AAA:115:GLU:OE2	4:AAA:204:PG4:C3	2.57	0.52
6:III:211:PEG:C4	11:JJJ:308:1PE:H142	2.40	0.52
2:FFF:157:GLY:O	11:FFF:201:1PE:H232	2.10	0.52
5:JJJ:310:PGE:H32	4:LLL:208:PG4:H22	1.92	0.52
6:PPP:214:PEG:H41	16:PPP:337:HOH:O	2.10	0.52
3:HHH:304:PEB:HNA	3:HHH:304:PEB:HMB3	1.75	0.51
6:CCC:213:PEG:O1	6:CCC:213:PEG:C4	2.57	0.51
6:KKK:208:PEG:H32	4:MMM:203:PG4:H32	1.93	0.51
1:MMM:43:LYS:HG2	3:MMM:202:PEB:CBD	2.39	0.51
3:EEE:202:PEB:HBD1	3:EEE:202:PEB:OD	2.10	0.51
5:JJJ:310:PGE:H22	4:LLL:208:PG4:H31	1.92	0.51
2:LLL:88:LEU:O	2:LLL:92[B]:THR:HG23	2.09	0.51
2:NNN:170:ALA:HB1	4:NNN:208:PG4:H81	1.91	0.51
3:CCC:202:PEB:C4D	6:CCC:210:PEG:H21	2.40	0.51
4:GGG:205:PG4:H51	4:GGG:205:PG4:C8	2.36	0.51
3:JJJ:305:PEB:HNA	3:JJJ:305:PEB:HMB3	1.76	0.51
2:LLL:116:ALA:HB2	4:LLL:207:PG4:H32	1.93	0.51
1:CCC:32[A]:GLN:HG3	1:EEE:32[A]:GLN:CG	2.33	0.50
2:DDD:28:PHE:HB3	6:DDD:213:PEG:H12	1.92	0.50
2:JJJ:152:LYS:HE3	12:JJJ:306:P33:H141	1.93	0.50
1:AAA:112:GLY:H	4:AAA:204:PG4:C4	2.25	0.50
1:CCC:143:ASP:HA	6:CCC:210:PEG:C2	2.42	0.50
5:LLL:210:PGE:H1	5:LLL:210:PGE:H42	1.93	0.50
4:DDD:209:PG4:H52	16:DDD:317:HOH:O	2.12	0.50
2:LLL:86:ILE:HG21	3:LLL:201:PEB:CAD	2.41	0.50
2:PPP:152:LYS:O	3:PPP:204:PEB:HMA2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:DDD:207:1PE:C15	11:DDD:207:1PE:C24	2.89	0.49
3:NNN:203:PEB:HMB2	3:NNN:203:PEB:HNA	1.76	0.49
3:DDD:202:PEB:HMB2	3:DDD:202:PEB:NA	2.27	0.49
12:DDD:205:P33:H151	16:DDD:304:HOH:O	2.03	0.49
1:AAA:113:GLN:N	4:AAA:204:PG4:H21	2.28	0.49
1:AAA:115:GLU:OE2	4:AAA:204:PG4:H32	2.12	0.49
1:KKK:128:VAL:HG12	15:NNN:206:PE5:H141	1.94	0.49
1:GGG:2:LYS:HD2	6:III:201:PEG:H11	1.95	0.49
1:KKK:158:TYR:HD1	4:MMM:203:PG4:H61	1.77	0.49
5:LLL:210:PGE:C4	5:LLL:210:PGE:C1	2.91	0.49
5:AAA:208:PGE:C3	5:AAA:210:PGE:H5	2.42	0.48
3:NNN:204:PEB:HMB2	3:NNN:204:PEB:NA	2.26	0.48
1:CCC:143:ASP:CA	6:CCC:210:PEG:H22	2.43	0.48
2:HHH:98:GLY:HA3	5:HHH:309:PGE:H6	1.95	0.48
2:FFF:153:LEU:HB3	4:FFF:202:PG4:H72	1.95	0.48
1:AAA:114:ARG:H	4:AAA:204:PG4:H21	1.78	0.48
12:DDD:205:P33:H112	12:DDD:205:P33:H182	1.95	0.48
2:PPP:149:ALA:HB2	3:PPP:204:PEB:OA	2.12	0.48
12:DDD:205:P33:H142	16:DDD:304:HOH:O	2.08	0.48
3:LLL:201:PEB:HNA	3:LLL:201:PEB:CMB	2.22	0.48
6:OOO:207:PEG:H32	6:OOO:207:PEG:H11	1.41	0.48
1:AAA:57:ASN:HB3	5:AAA:207:PGE:H6	1.94	0.48
3:BBB:203:PEB:HMB3	3:BBB:203:PEB:HNA	1.79	0.48
2:FFF:152:LYS:HE3	12:FFF:207:P33:O13	2.13	0.48
4:FFF:210:PG4:H31	4:FFF:210:PG4:H11	1.66	0.48
1:GGG:48:ILE:N	5:GGG:208:PGE:H22	2.29	0.48
1:GGG:115:GLU:OE2	7:GGG:214:PO4:O1	2.31	0.48
4:MMM:205:PG4:H62	4:MMM:205:PG4:H42	1.54	0.48
2:BBB:148[B]:ARG:CD	16:BBB:364:HOH:O	2.61	0.48
6:GGG:211:PEG:H31	6:III:201:PEG:O4	2.13	0.47
6:GGG:211:PEG:C3	6:III:201:PEG:C4	2.92	0.47
2:BBB:148[B]:ARG:HD2	16:BBB:364:HOH:O	2.15	0.47
5:BBB:222:PGE:H3	5:BBB:222:PGE:H52	1.24	0.47
16:KKK:811:HOH:O	4:MMM:203:PG4:C6	2.60	0.47
6:MMM:209:PEG:C1	16:MMM:361:HOH:O	2.41	0.47
2:HHH:27:ALA:HA	5:HHH:311:PGE:H32	1.96	0.47
2:HHH:35:ARG:CZ	5:HHH:309:PGE:H62	2.45	0.47
11:BBB:208:1PE:H242	11:BBB:208:1PE:H251	1.48	0.47
11:DDD:207:1PE:H261	11:DDD:207:1PE:H251	1.48	0.47
8:JJJ:322:NO3:O3	16:JJJ:403:HOH:O	2.18	0.47
1:MMM:18:PHE:C	4:MMM:203:PG4:H41	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:PPP:217:PO4:P	16:PPP:302:HOH:O	2.67	0.47
2:FFF:163:ASP:OD1	16:FFF:301:HOH:O	2.20	0.46
2:DDD:155[B]:LYS:HG2	5:DDD:211:PGE:H2	1.97	0.46
2:JJJ:152:LYS:HE3	12:JJJ:306:P33:C14	2.45	0.46
3:DDD:201:PEB:HNA	3:DDD:201:PEB:CMB	2.24	0.46
2:FFF:35:ARG:NH2	4:FFF:209:PG4:H42	2.29	0.46
3:HHH:304:PEB:HMB3	3:HHH:304:PEB:NA	2.31	0.46
12:HHH:305:P33:O22	12:HHH:305:P33:H112	2.16	0.46
3:NNN:204:PEB:HBD1	3:NNN:204:PEB:OD	2.15	0.46
1:AAA:49:ASP:HB2	4:AAA:203:PG4:H31	1.97	0.46
2:LLL:46:ALA:HB3	5:LLL:226:PGE:H62	1.97	0.46
5:NNN:212:PGE:H1	16:NNN:362:HOH:O	2.15	0.46
2:HHH:112:LYS:HG2	4:HHH:307:PG4:H71	1.98	0.46
3:LLL:203:PEB:NA	3:LLL:203:PEB:HMB3	2.29	0.46
1:KKK:83:ALA:HB3	6:KKK:212:PEG:H12	1.98	0.46
1:KKK:116:VAL:HG11	3:KKK:201:PEB:HMC2	1.97	0.46
3:NNN:203:PEB:HBD1	3:NNN:203:PEB:OD	2.15	0.46
3:DDD:201:PEB:OD	3:DDD:201:PEB:HBD1	2.16	0.46
5:III:206:PGE:H2	5:III:206:PGE:H4	1.25	0.46
3:PPP:202:PEB:HMC3	3:PPP:202:PEB:CGC	2.46	0.46
3:BBB:201:PEB:HNA	3:BBB:201:PEB:CMB	2.24	0.45
11:BBB:208:1PE:H262	11:BBB:208:1PE:H252	1.04	0.45
3:FFF:206:PEB:HMB3	3:FFF:206:PEB:NA	2.31	0.45
2:PPP:33:ASN:HB3	3:PPP:203:PEB:C1C	2.45	0.45
6:LLL:214:PEG:H41	6:LLL:214:PEG:H21	1.53	0.45
2:LLL:157:GLY:HA3	5:LLL:225:PGE:H22	1.99	0.45
2:PPP:48:CYS:SG	3:PPP:204:PEB:HMA1	2.56	0.45
1:AAA:49:ASP:HB2	4:AAA:203:PG4:C6	2.33	0.45
6:DDD:215:PEG:H12	6:DDD:215:PEG:H32	1.42	0.45
5:GGG:207:PGE:H22	5:III:204:PGE:H62	1.98	0.45
4:KKK:204:PG4:H22	4:KKK:204:PG4:C8	2.47	0.45
5:LLL:210:PGE:H42	5:LLL:210:PGE:C1	2.46	0.45
2:NNN:168:LEU:HG	6:NNN:214:PEG:C1	2.46	0.45
1:AAA:112:GLY:H	4:AAA:204:PG4:H41	1.81	0.45
2:DDD:7:ARG:HH22	11:DDD:207:1PE:H261	1.82	0.45
3:BBB:203:PEB:HBC1	3:BBB:203:PEB:HMC2	1.98	0.45
5:DDD:211:PGE:H1	5:DDD:211:PGE:H3	1.82	0.45
2:FFF:152:LYS:NZ	12:FFF:207:P33:O4	2.45	0.45
1:III:161:ASN:CB	5:III:204:PGE:H32	2.47	0.45
2:BBB:33:ASN:HB3	3:BBB:202:PEB:C1C	2.47	0.45
4:CCC:203:PG4:H12	4:FFF:202:PG4:H21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DDD:155[A]:LYS:HG2	5:DDD:211:PGE:H2	1.99	0.45
3:LLL:203:PEB:HMB3	3:LLL:203:PEB:HNA	1.82	0.45
1:CCC:43:LYS:HG3	6:CCC:210:PEG:O1	2.17	0.44
2:HHH:152:LYS:HE3	12:HHH:305:P33:H141	1.99	0.44
2:HHH:181[A]:SER:OG	11:HHH:301:1PE:H141	2.17	0.44
2:FFF:164:ARG:NH2	16:FFF:307:HOH:O	2.41	0.44
2:HHH:148[B]:ARG:HG2	16:HHH:420:HOH:O	2.17	0.44
4:HHH:307:PG4:H31	4:HHH:307:PG4:H51	1.81	0.44
1:OOO:13:ASP:OD1	2:PPP:89:ARG:NH1	2.45	0.44
2:DDD:152:LYS:NZ	12:DDD:204:P33:O4	2.49	0.44
8:LLL:223:NO3:O2	8:LLL:224:NO3:O2	2.35	0.44
4:GGG:204:PG4:H11	6:GGG:211:PEG:H21	1.99	0.44
3:MMM:202:PEB:NA	3:MMM:202:PEB:HMB2	2.33	0.44
15:NNN:206:PE5:H31	15:NNN:206:PE5:H161	1.96	0.44
2:PPP:28:PHE:HB3	4:PPP:207:PG4:C5	2.42	0.44
5:DDD:210:PGE:H2	5:DDD:210:PGE:C5	2.47	0.44
6:HHH:316:PEG:C4	6:HHH:316:PEG:H11	2.48	0.44
2:PPP:132:MET:HA	2:PPP:135:GLN:OE1	2.18	0.44
3:BBB:203:PEB:HMB3	3:BBB:203:PEB:NA	2.33	0.44
2:BBB:132:MET:HA	2:BBB:135:GLN:OE1	2.18	0.43
1:MMM:20:SER:HA	4:MMM:203:PG4:C8	2.47	0.43
3:AAA:202:PEB:HBD1	3:AAA:202:PEB:OD	2.18	0.43
2:FFF:132:MET:HA	2:FFF:135:GLN:OE1	2.19	0.43
2:NNN:82[C]:ARG:HH12	14:NNN:219:EDO:C2	2.31	0.43
4:FFF:202:PG4:H42	4:FFF:202:PG4:H22	1.56	0.43
2:LLL:33:ASN:HB3	3:LLL:202:PEB:C1C	2.49	0.43
1:OOO:96:CYS:SG	1:OOO:105:LEU:HB2	2.57	0.43
2:DDD:33:ASN:HB3	3:DDD:202:PEB:C1C	2.49	0.43
6:DDD:214:PEG:H12	6:DDD:214:PEG:H42	2.01	0.43
1:EEE:96:CYS:SG	1:EEE:105:LEU:HB2	2.59	0.43
2:JJJ:152:LYS:HZ2	12:JJJ:306:P33:C6	2.32	0.43
1:KKK:149:LEU:HD23	4:NNN:201:PG4:H41	2.00	0.43
1:KKK:61:LYS:NZ	5:KKK:206:PGE:O2	2.44	0.43
3:PPP:202:PEB:HMC3	3:PPP:202:PEB:O2C	2.19	0.43
4:KKK:205:PG4:H71	4:KKK:205:PG4:H52	1.75	0.43
1:AAA:110:ILE:O	4:AAA:204:PG4:H22	2.19	0.43
6:CCC:210:PEG:H21	6:CCC:210:PEG:H42	1.77	0.43
2:DDD:31[B]:SER:OG	16:DDD:302:HOH:O	2.21	0.43
2:HHH:82:ARG:HH22	3:HHH:302:PEB:C1C	2.32	0.43
2:JJJ:116:ALA:HB2	4:JJJ:309:PG4:H51	1.96	0.43
2:JJJ:132:MET:HA	2:JJJ:135:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KKK:10:ALA:HB1	4:KKK:204:PG4:H81	2.00	0.43
4:KKK:204:PG4:O1	4:KKK:204:PG4:H71	2.18	0.43
2:LLL:152:LYS:HE3	9:LLL:204:RWB:C27	2.49	0.43
3:MMM:202:PEB:HBB1	3:MMM:202:PEB:HMB1	2.00	0.43
2:PPP:28:PHE:CB	4:PPP:207:PG4:H51	2.42	0.43
2:BBB:37:ASP:OD2	3:BBB:202:PEB:NB	2.52	0.42
1:CCC:158:TYR:CD1	5:CCC:205:PGE:H42	2.54	0.42
4:CCC:203:PG4:H51	4:CCC:203:PG4:H71	1.56	0.42
1:GGG:56:TYR:HB2	1:GGG:86:ILE:HD12	2.01	0.42
1:MMM:19:PRO:O	4:MMM:203:PG4:H51	2.18	0.42
2:BBB:143:THR:N	2:BBB:144:PRO:CD	2.83	0.42
2:HHH:27:ALA:N	5:HHH:311:PGE:H22	2.33	0.42
2:LLL:132:MET:HA	2:LLL:135:GLN:OE1	2.19	0.42
3:NNN:205:PEB:HBC1	3:NNN:205:PEB:HMC2	2.01	0.42
2:LLL:47:SER:OG	6:MMM:209:PEG:H21	2.19	0.42
6:LLL:218[A]:PEG:O4	7:LLL:221:PO4:O1	2.31	0.42
1:OOO:85:ASP:OD1	3:OOO:201:PEB:H1D1	2.19	0.42
5:PPP:208:PGE:H1	5:PPP:208:PGE:H3	1.78	0.42
1:GGG:96:CYS:SG	1:GGG:105:LEU:HB2	2.59	0.42
5:GGG:206:PGE:H12	5:GGG:206:PGE:H32	1.81	0.42
4:HHH:308:PG4:H21	4:HHH:308:PG4:H42	1.75	0.42
1:III:56:TYR:HB2	1:III:86:ILE:HD12	2.01	0.42
1:GGG:116:VAL:HG11	3:GGG:201:PEB:HMC2	2.01	0.42
2:JJJ:35:ARG:CZ	11:JJJ:307:1PE:H141	2.50	0.42
2:JJJ:82[A]:ARG:HH22	3:JJJ:303:PEB:C1C	2.32	0.42
2:DDD:132:MET:HA	2:DDD:135:GLN:OE1	2.19	0.42
3:EEE:202:PEB:HNA	3:EEE:202:PEB:HMB2	1.84	0.42
5:HHH:310:PGE:H42	5:HHH:310:PGE:HO4	1.81	0.42
6:III:211:PEG:H41	11:JJJ:308:1PE:H142	2.01	0.42
2:LLL:47:SER:OG	6:MMM:209:PEG:C2	2.67	0.42
2:NNN:132:MET:HA	2:NNN:135:GLN:OE1	2.20	0.42
2:NNN:143:THR:N	2:NNN:144:PRO:CD	2.83	0.42
6:HHH:318:PEG:H11	6:HHH:318:PEG:H32	1.62	0.42
11:JJJ:308:1PE:H132	11:JJJ:308:1PE:H141	1.77	0.42
4:NNN:208:PG4:H81	4:NNN:208:PG4:H61	1.38	0.42
2:PPP:82[A]:ARG:NH2	3:PPP:202:PEB:O1C	2.52	0.42
2:BBB:82[A]:ARG:HH22	3:BBB:201:PEB:C1C	2.32	0.42
2:FFF:82[A]:ARG:HH22	3:FFF:204:PEB:C1C	2.33	0.42
3:LLL:202:PEB:HNA	3:LLL:202:PEB:HMB2	1.83	0.42
3:JJJ:303:PEB:HBD1	3:JJJ:303:PEB:OD	2.18	0.42
2:NNN:82[C]:ARG:CZ	14:NNN:219:EDO:H12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:NNN:206:PE5:C16	15:NNN:206:PE5:C3	2.94	0.42
1:MMM:61:LYS:HE2	6:MMM:210:PEG:H42	2.02	0.42
2:HHH:132:MET:HA	2:HHH:135:GLN:OE1	2.19	0.41
5:KKK:206:PGE:C6	5:KKK:207:PGE:O1	2.60	0.41
3:OOO:201:PEB:CMB	3:OOO:201:PEB:HNA	2.33	0.41
6:BBB:223:PEG:H21	6:BBB:223:PEG:H41	1.78	0.41
5:CCC:204:PGE:H22	6:CCC:210:PEG:H12	2.02	0.41
1:III:96:CYS:SG	1:III:105:LEU:HB2	2.60	0.41
1:III:161:ASN:HB2	5:III:204:PGE:H32	2.02	0.41
2:NNN:112:LYS:HZ1	5:NNN:210:PGE:H1	1.85	0.41
2:DDD:113:GLU:HA	13:DDD:206:P6G:H142	2.01	0.41
6:HHH:314:PEG:H22	6:HHH:314:PEG:H42	1.70	0.41
1:KKK:96:CYS:SG	1:KKK:105:LEU:HB2	2.60	0.41
5:KKK:207:PGE:H3	5:KKK:207:PGE:H52	1.46	0.41
6:KKK:208:PEG:H21	4:MMM:203:PG4:H21	2.03	0.41
2:DDD:143:THR:N	2:DDD:144:PRO:CD	2.84	0.41
2:HHH:89:ARG:NH2	5:HHH:312:PGE:H22	2.25	0.41
2:HHH:112:LYS:HE3	4:HHH:307:PG4:H71	2.03	0.41
2:HHH:152:LYS:HE3	12:HHH:305:P33:C14	2.51	0.41
1:CCC:96:CYS:SG	1:CCC:105:LEU:HB2	2.60	0.41
3:JJJ:304:PEB:HNA	3:JJJ:304:PEB:HMB2	1.84	0.41
6:CCC:215:PEG:H21	6:CCC:215:PEG:H41	1.57	0.41
3:KKK:202:PEB:NA	3:KKK:202:PEB:HMB2	2.36	0.41
2:LLL:82[A]:ARG:HH22	3:LLL:201:PEB:C1C	2.34	0.41
2:LLL:143:THR:N	2:LLL:144:PRO:CD	2.84	0.41
6:LLL:212:PEG:H22	6:LLL:212:PEG:H41	1.42	0.41
4:MMM:203:PG4:H51	2:NNN:43:ALA:HB1	2.03	0.41
4:NNN:207:PG4:H32	4:NNN:207:PG4:H81	2.03	0.41
2:PPP:143:THR:N	2:PPP:144:PRO:CD	2.84	0.41
2:DDD:70:MEN:O	2:DDD:76:ARG:HB3	2.21	0.41
1:III:158:TYR:CD1	5:III:204:PGE:H4	2.56	0.41
2:JJJ:143:THR:N	2:JJJ:144:PRO:CD	2.84	0.41
2:LLL:98:GLY:HA3	4:LLL:206:PG4:C3	2.51	0.41
5:LLL:210:PGE:H62	5:LLL:210:PGE:H4	1.59	0.41
2:PPP:37:ASP:OD2	3:PPP:203:PEB:NB	2.54	0.41
1:AAA:96:CYS:SG	1:AAA:105:LEU:HB2	2.61	0.40
1:KKK:10:ALA:CB	4:KKK:204:PG4:H81	2.51	0.40
2:FFF:143:THR:N	2:FFF:144:PRO:CD	2.84	0.40
2:JJJ:33:ASN:HB3	3:JJJ:304:PEB:C1C	2.52	0.40
1:KKK:84:ARG:HA	6:KKK:212:PEG:H21	2.02	0.40
4:KKK:204:PG4:H11	4:KKK:204:PG4:H31	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LLL:70:MEN:O	2:LLL:76:ARG:HB3	2.22	0.40
2:DDD:37:ASP:OD2	3:DDD:202:PEB:NB	2.54	0.40
6:MMM:208:PEG:H12	6:MMM:208:PEG:H31	1.28	0.40
2:NNN:70:MEN:O	2:NNN:76:ARG:HB3	2.22	0.40
1:EEE:139:CYS:SG	3:EEE:202:PEB:HHA1	2.62	0.40
2:NNN:168:LEU:HG	6:NNN:214:PEG:H12	2.03	0.40
6:PPP:210:PEG:H41	6:PPP:210:PEG:H21	1.84	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	AAA	165/164 (101%)	162 (98%)	3 (2%)	0	100	100
1	CCC	165/164 (101%)	162 (98%)	3 (2%)	0	100	100
1	EEE	165/164 (101%)	162 (98%)	3 (2%)	0	100	100
1	GGG	163/164 (99%)	160 (98%)	3 (2%)	0	100	100
1	III	163/164 (99%)	160 (98%)	3 (2%)	0	100	100
1	KKK	164/164 (100%)	161 (98%)	3 (2%)	0	100	100
1	MMM	164/164 (100%)	161 (98%)	3 (2%)	0	100	100
1	OOO	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
2	BBB	188/184 (102%)	184 (98%)	4 (2%)	0	100	100
2	DDD	190/184 (103%)	186 (98%)	4 (2%)	0	100	100
2	FFF	187/184 (102%)	183 (98%)	4 (2%)	0	100	100
2	HHH	188/184 (102%)	183 (97%)	5 (3%)	0	100	100
2	JJJ	189/184 (103%)	184 (97%)	5 (3%)	0	100	100
2	LLL	189/184 (103%)	185 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	NNN	184/184 (100%)	180 (98%)	4 (2%)	0	100	100
2	PPP	185/184 (100%)	181 (98%)	4 (2%)	0	100	100
All	All	2811/2784 (101%)	2753 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	128/124 (103%)	128 (100%)	0	100	100
1	CCC	128/124 (103%)	127 (99%)	1 (1%)	81	85
1	EEE	128/124 (103%)	128 (100%)	0	100	100
1	GGG	126/124 (102%)	124 (98%)	2 (2%)	62	65
1	III	126/124 (102%)	126 (100%)	0	100	100
1	KKK	127/124 (102%)	126 (99%)	1 (1%)	81	85
1	MMM	127/124 (102%)	127 (100%)	0	100	100
1	OOO	125/124 (101%)	121 (97%)	4 (3%)	39	37
2	BBB	145/138 (105%)	145 (100%)	0	100	100
2	DDD	147/138 (106%)	145 (99%)	2 (1%)	67	70
2	FFF	144/138 (104%)	144 (100%)	0	100	100
2	HHH	145/138 (105%)	145 (100%)	0	100	100
2	JJJ	146/138 (106%)	143 (98%)	3 (2%)	53	54
2	LLL	146/138 (106%)	146 (100%)	0	100	100
2	NNN	141/138 (102%)	140 (99%)	1 (1%)	84	87
2	PPP	142/138 (103%)	140 (99%)	2 (1%)	67	70
All	All	2171/2096 (104%)	2155 (99%)	16 (1%)	86	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	43	LYS
2	DDD	155[A]	LYS
2	DDD	155[B]	LYS
1	GGG	1[A]	MET
1	GGG	1[B]	MET
2	JJJ	148[A]	ARG
2	JJJ	148[B]	ARG
2	JJJ	162	GLU
1	KKK	43	LYS
2	NNN	167	SER
1	OOO	25	GLU
1	OOO	43	LYS
1	OOO	114	ARG
1	OOO	118	ARG
2	PPP	47	SER
2	PPP	181	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

321 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

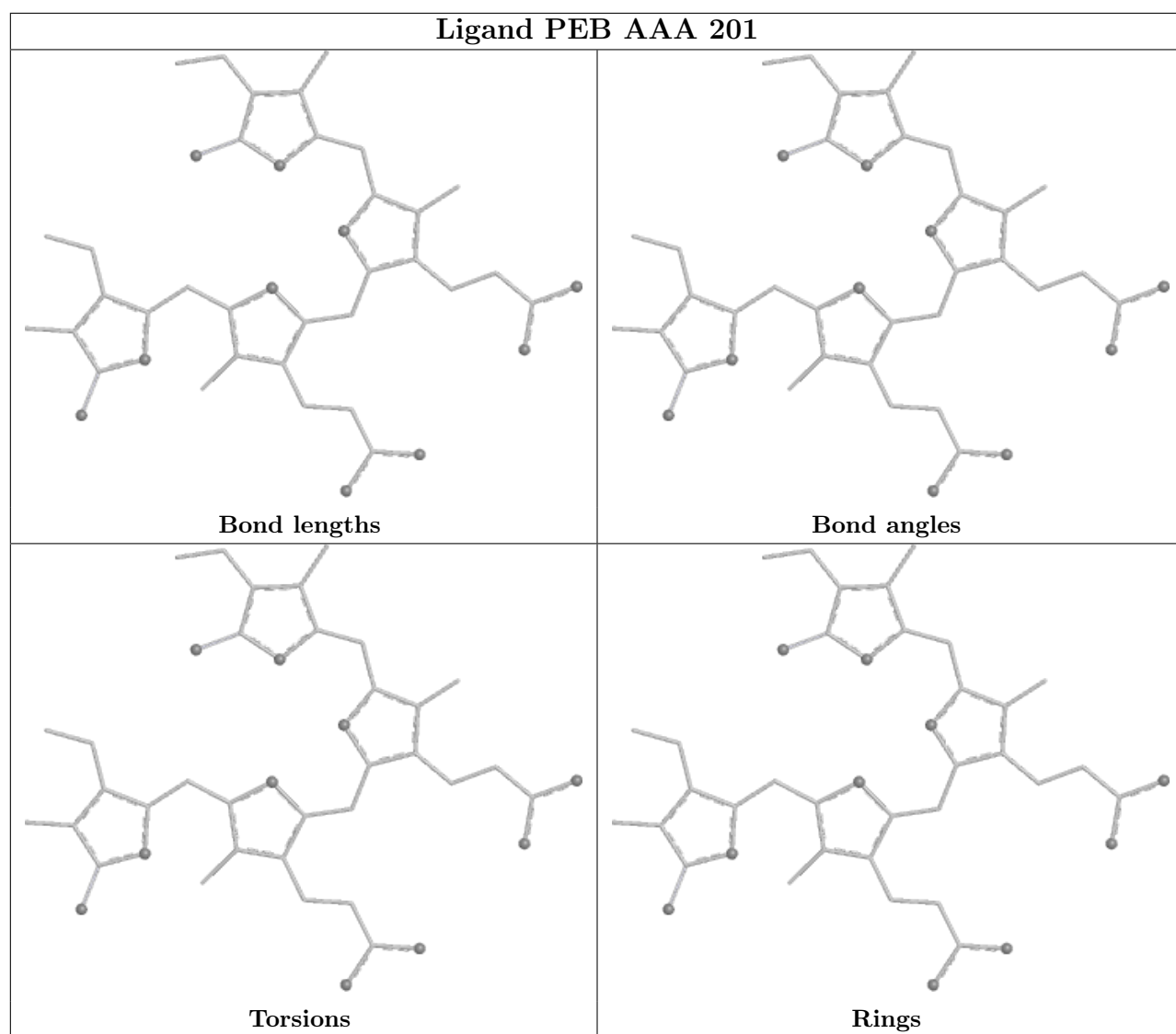
There are no chirality outliers.

There are no torsion outliers.

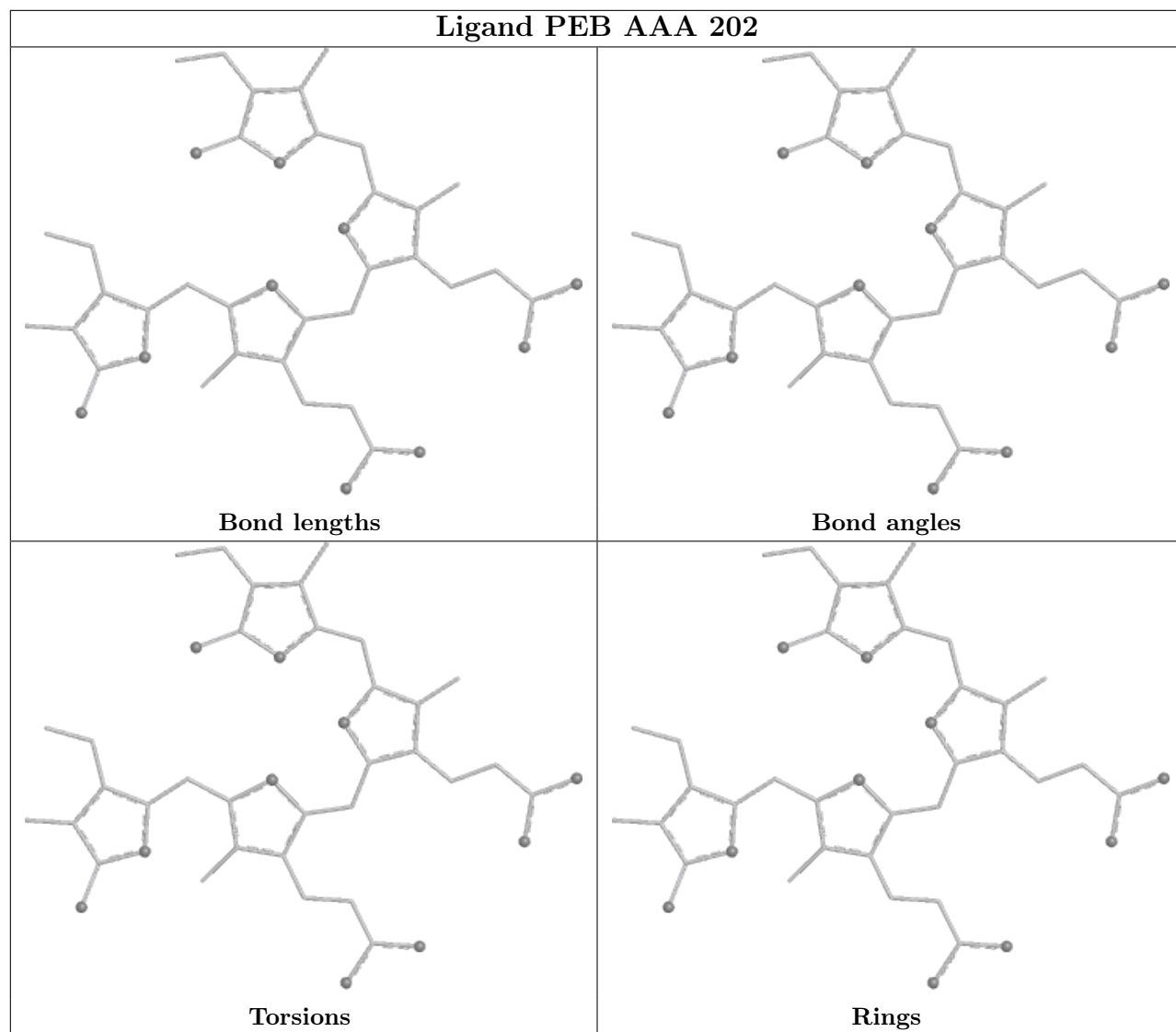
There are no ring outliers.

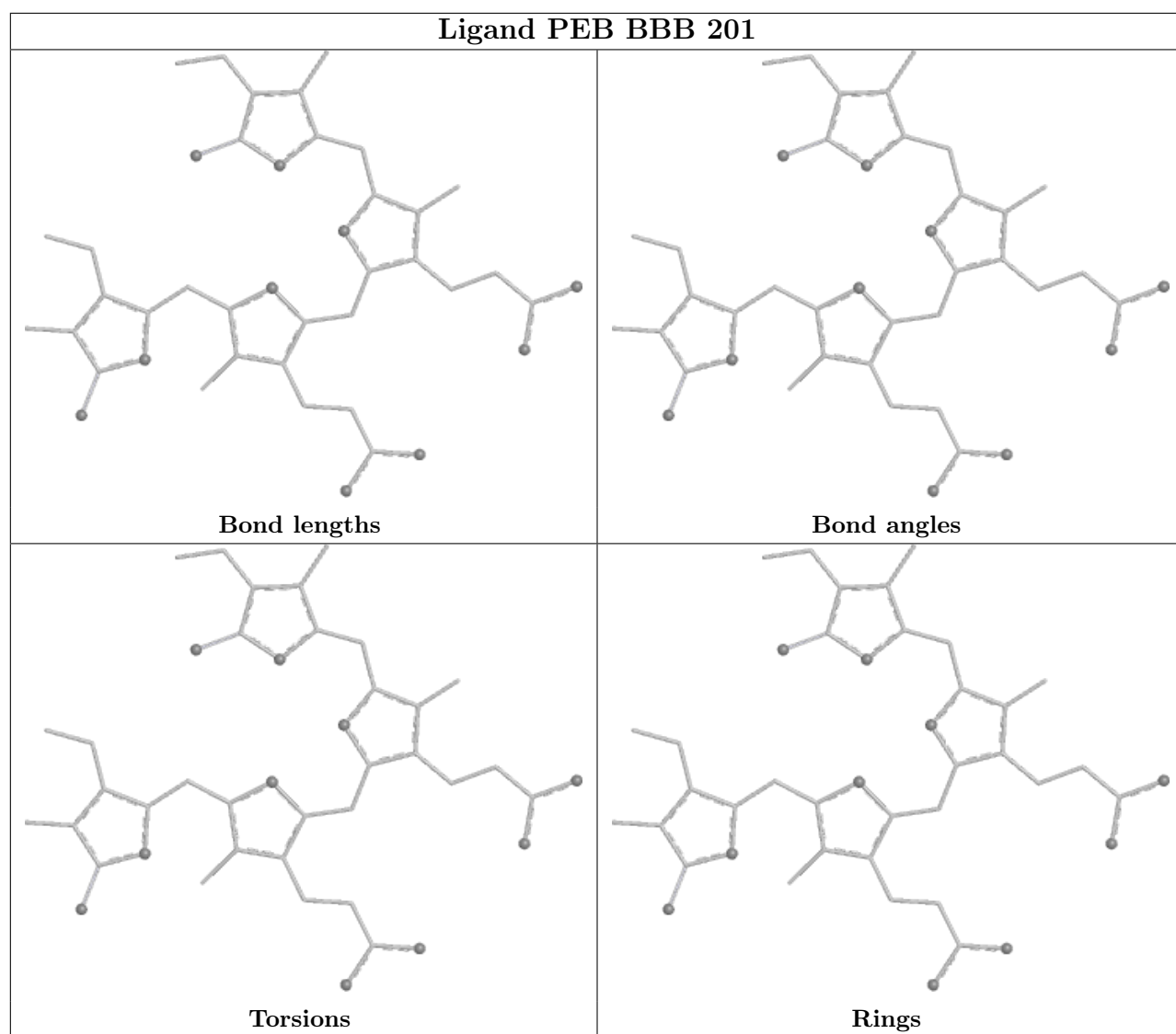
No monomer is involved in short contacts.

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.

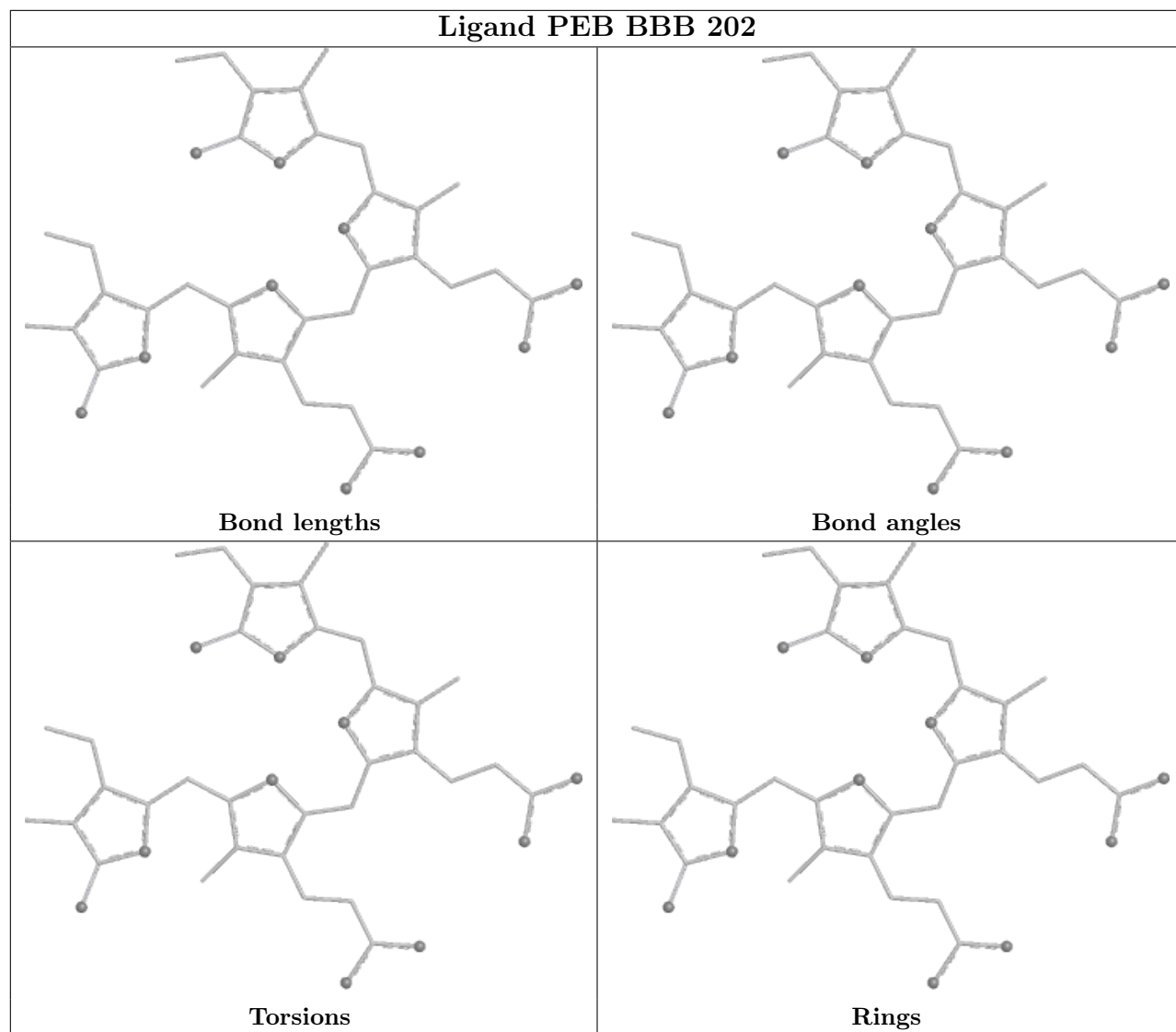


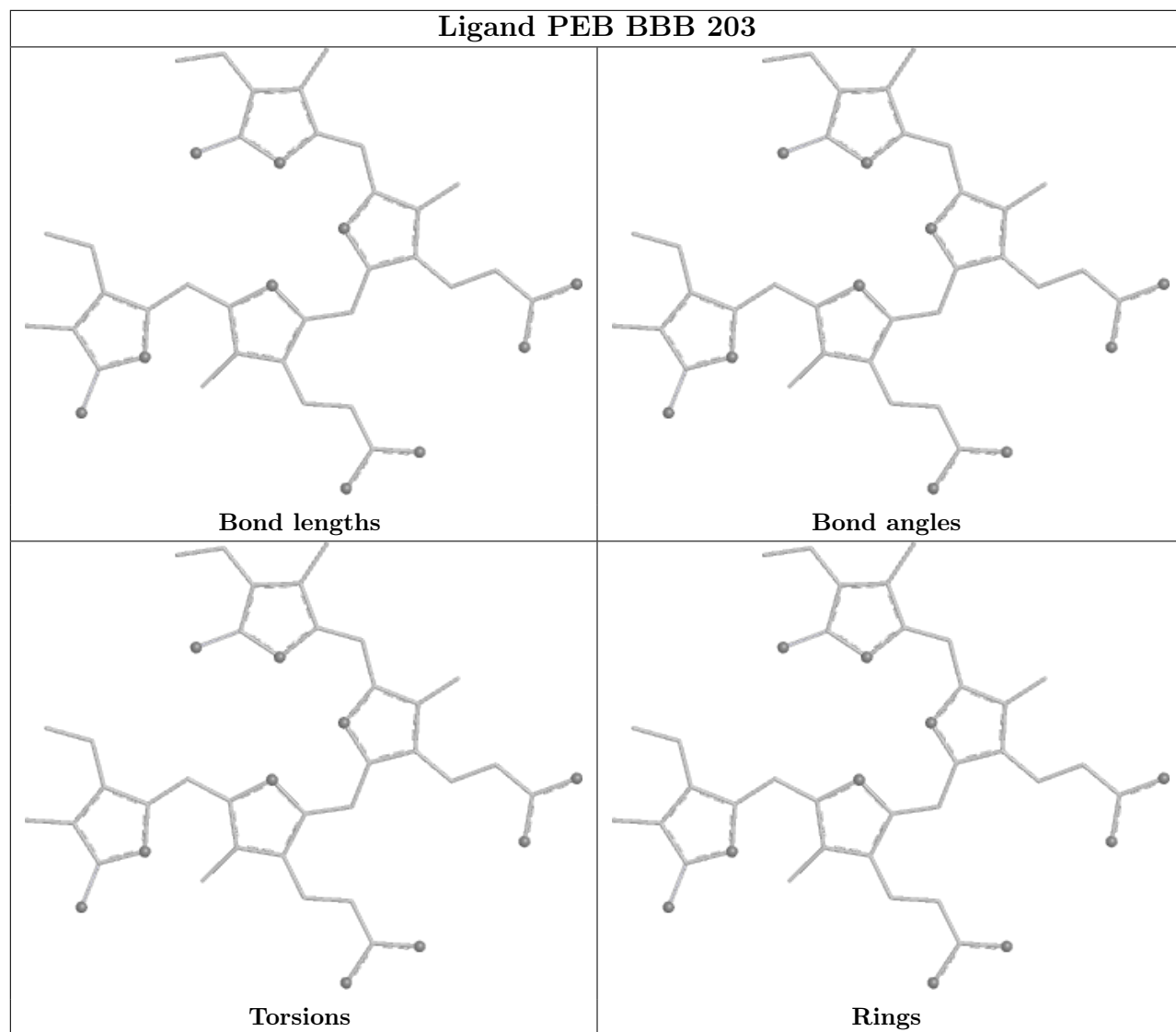




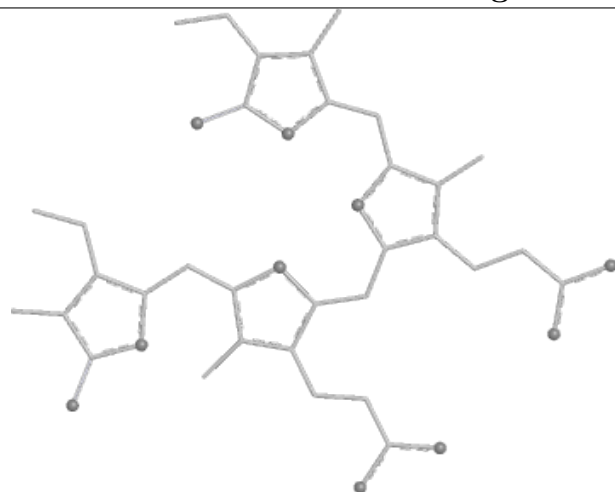


## Ligand PEB BBB 202

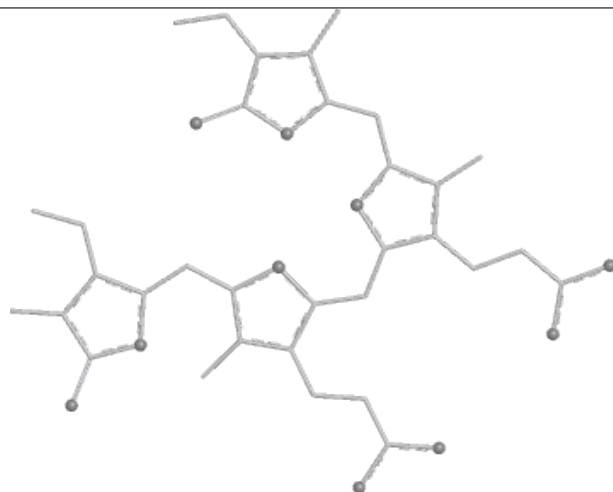




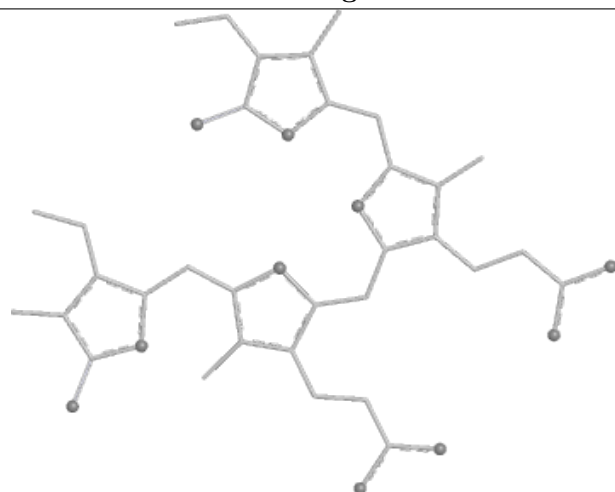
## Ligand PEB CCC 201



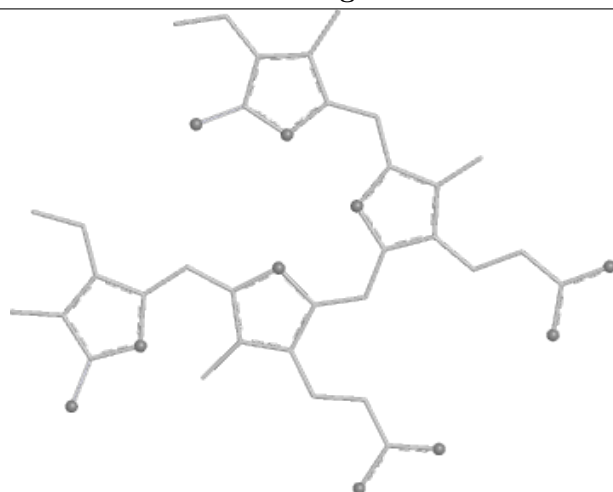
Bond lengths



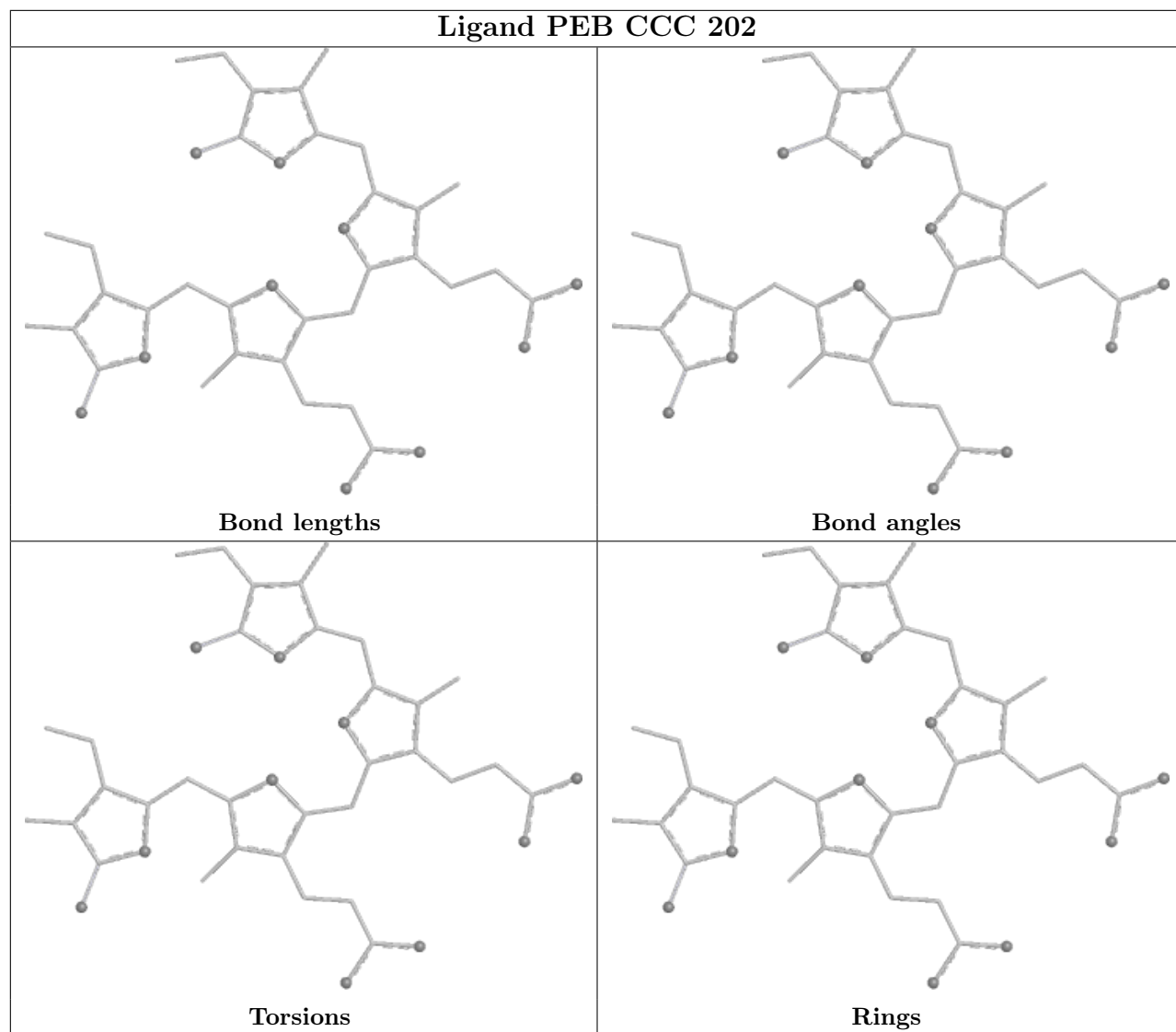
Bond angles

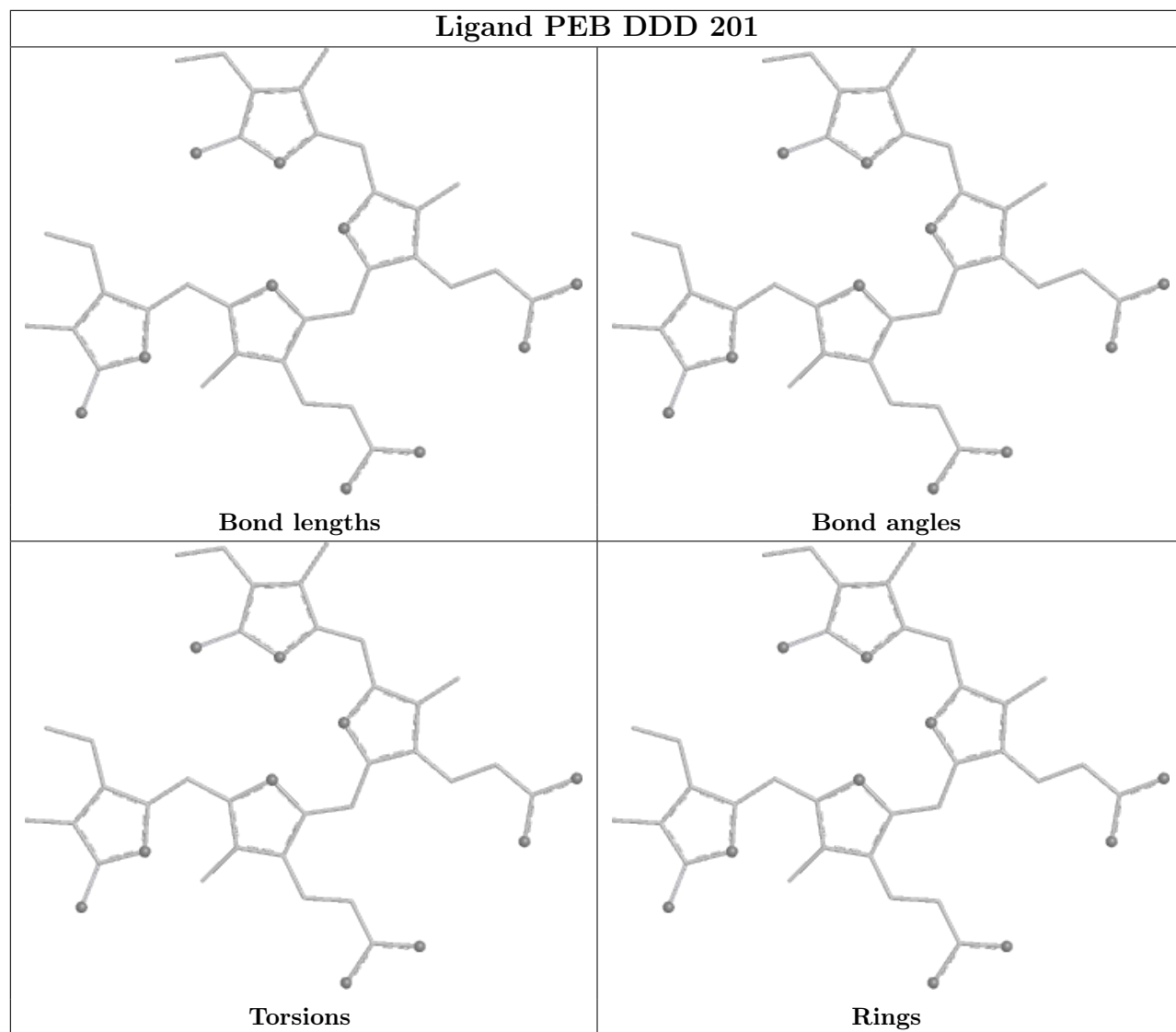


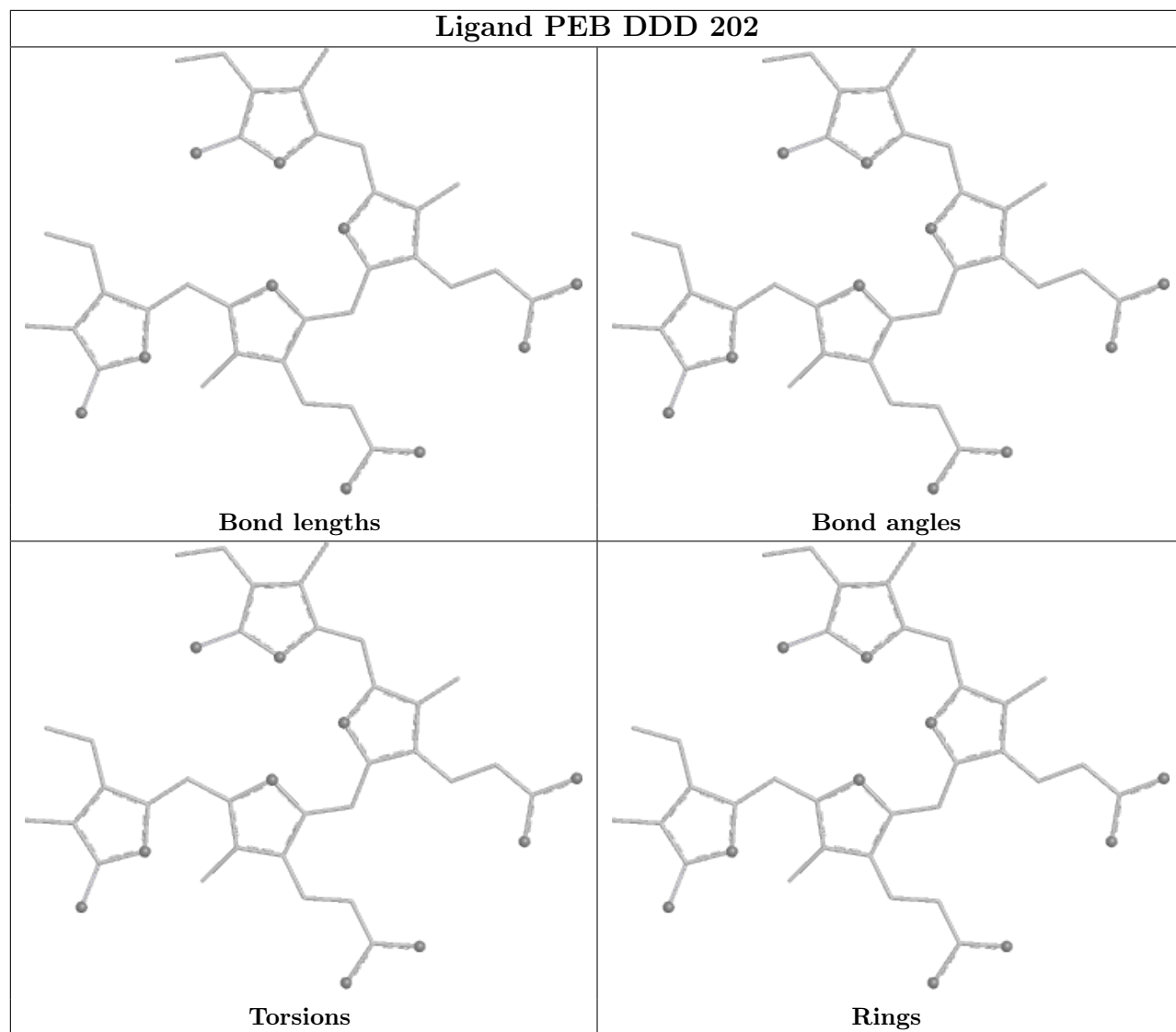
Torsions



Rings

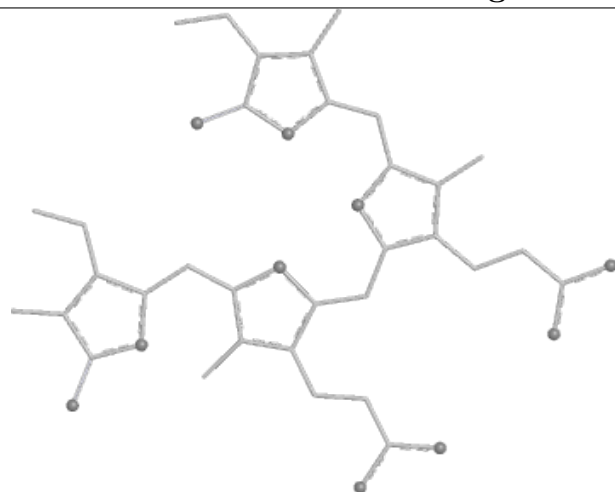




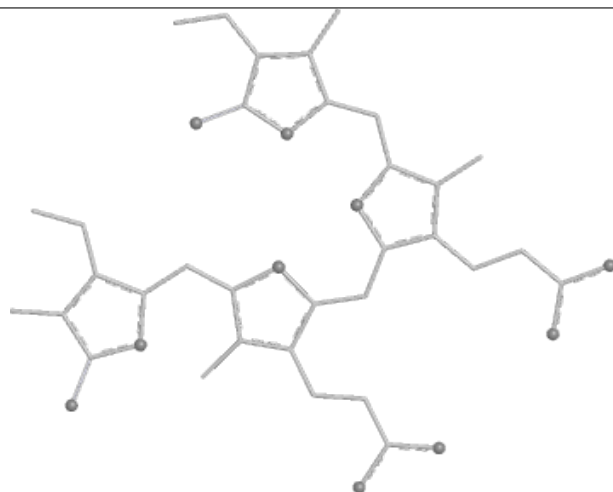




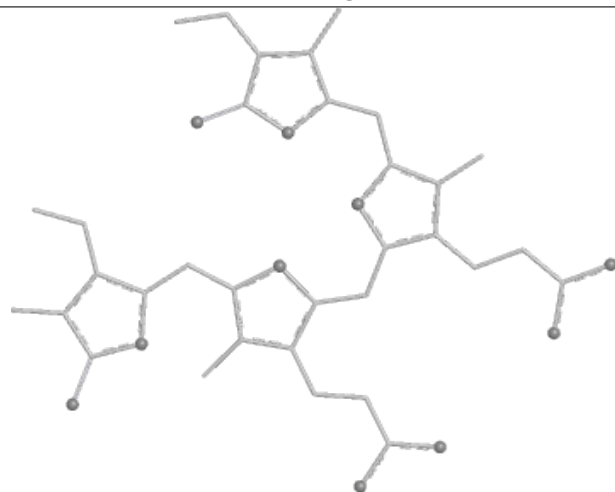
## Ligand PEB DDD 203



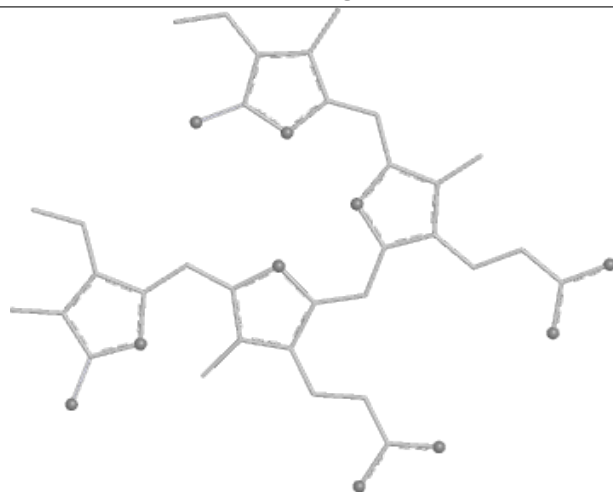
Bond lengths



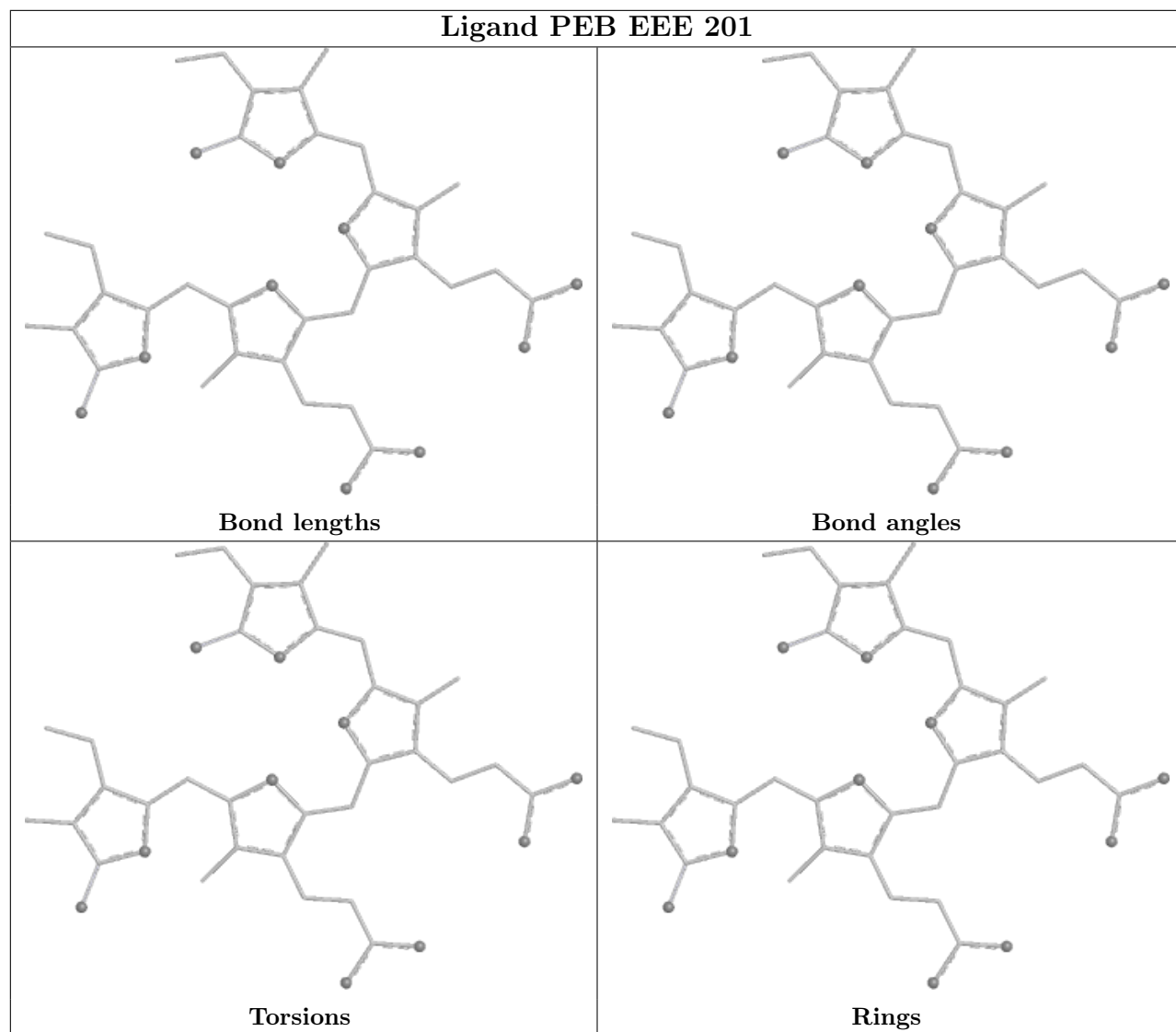
Bond angles

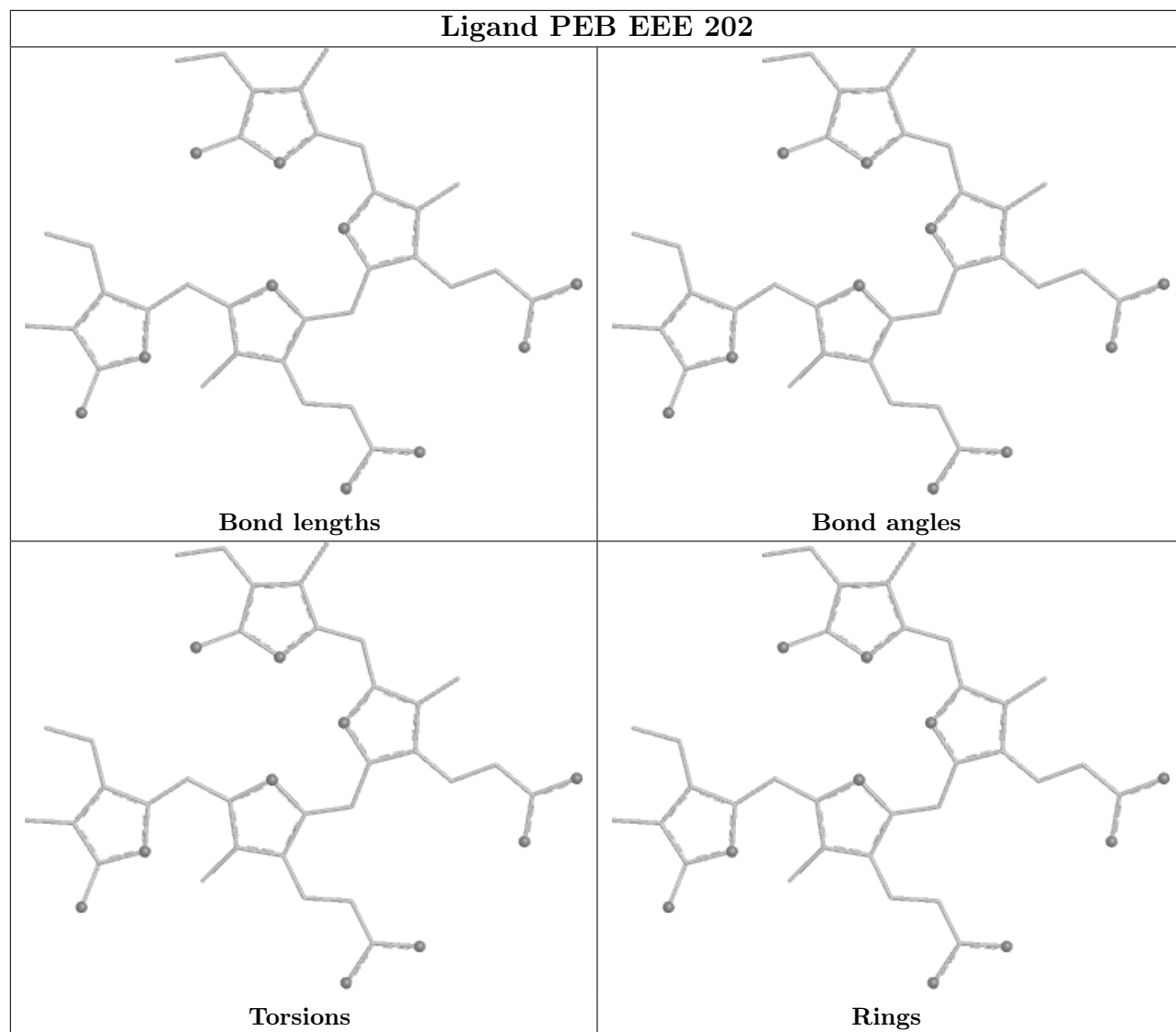


Torsions

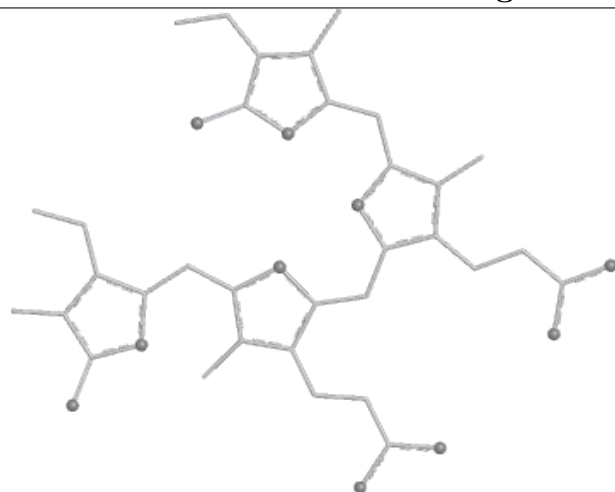


Rings

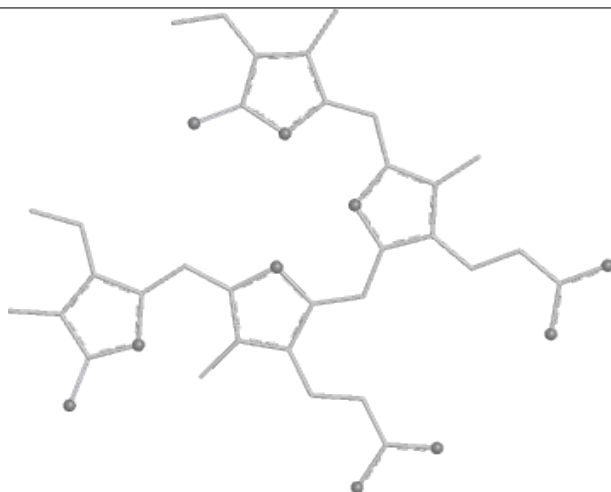




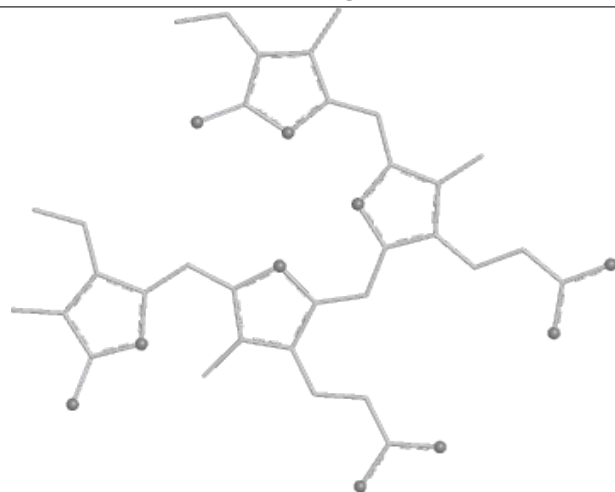
## Ligand PEB FFF 204



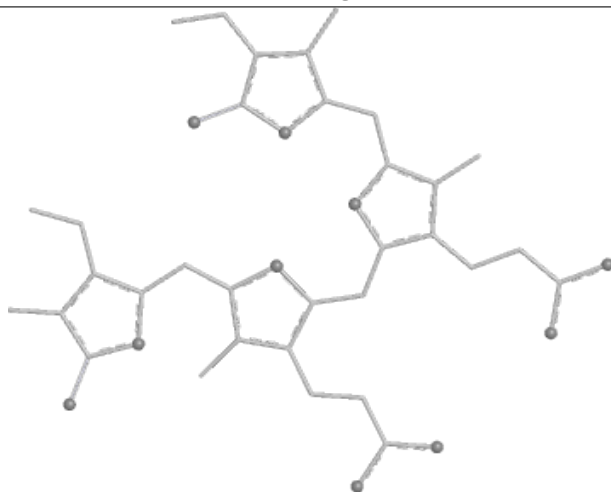
Bond lengths



Bond angles

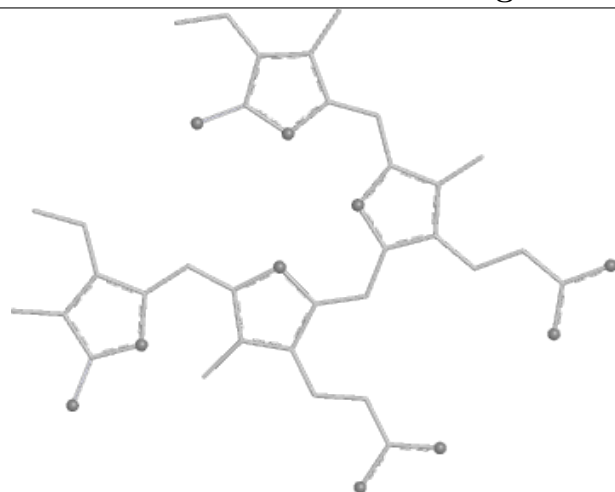


Torsions

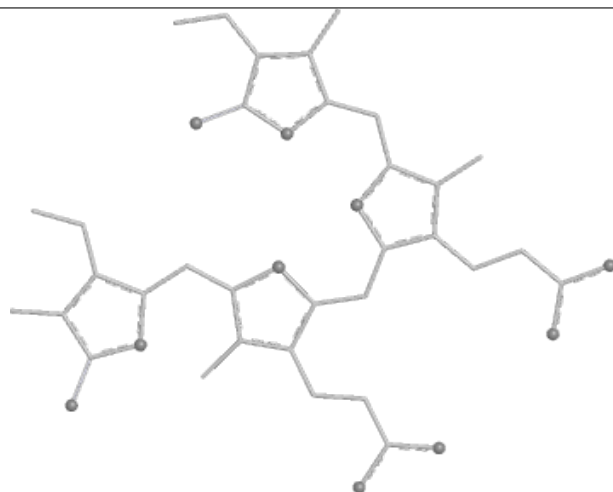


Rings

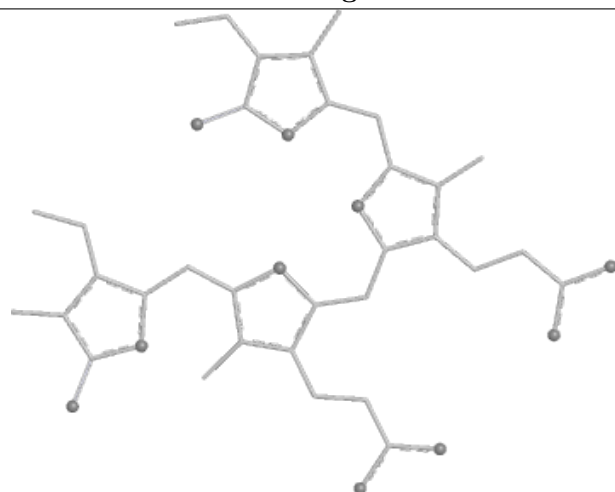
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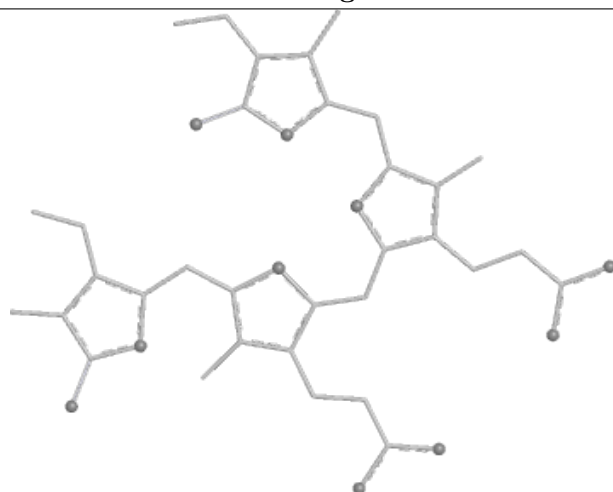
Bond lengths



Bond angles

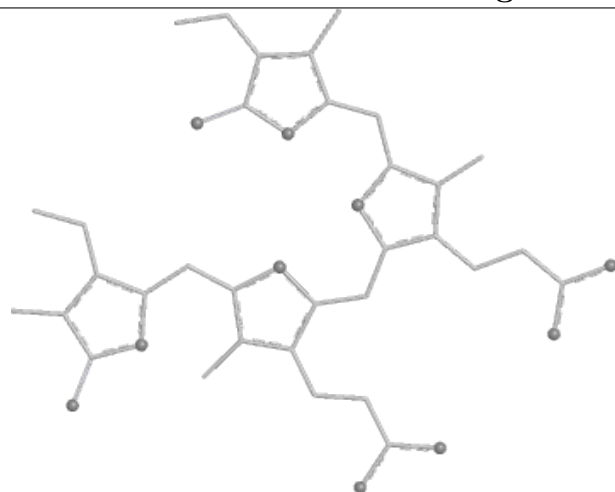


Torsions

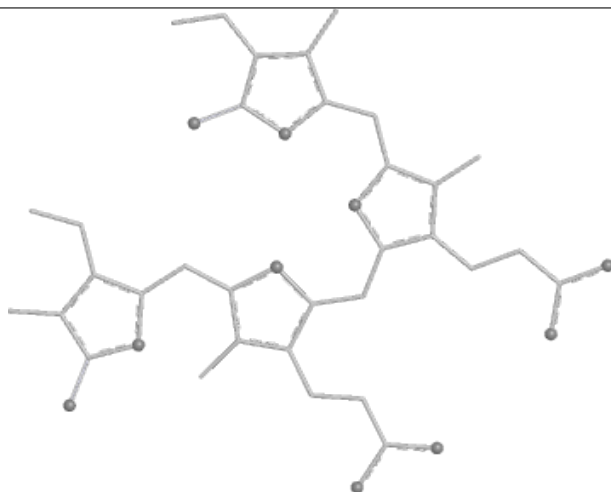


Rings

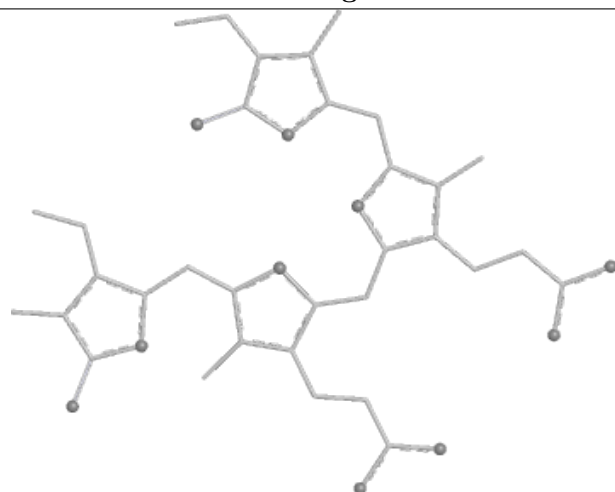
## Ligand PEB FFF 206



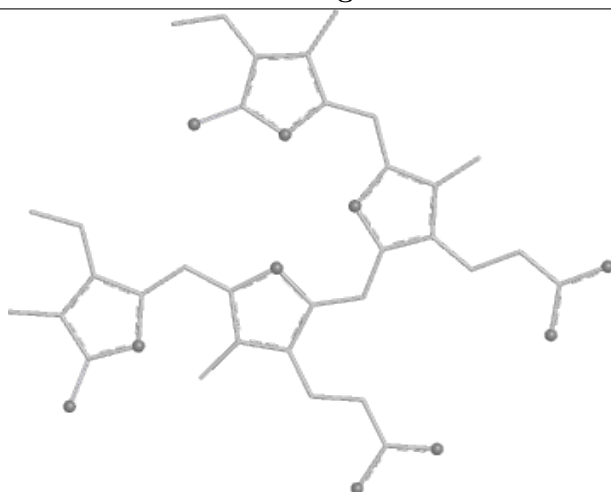
Bond lengths



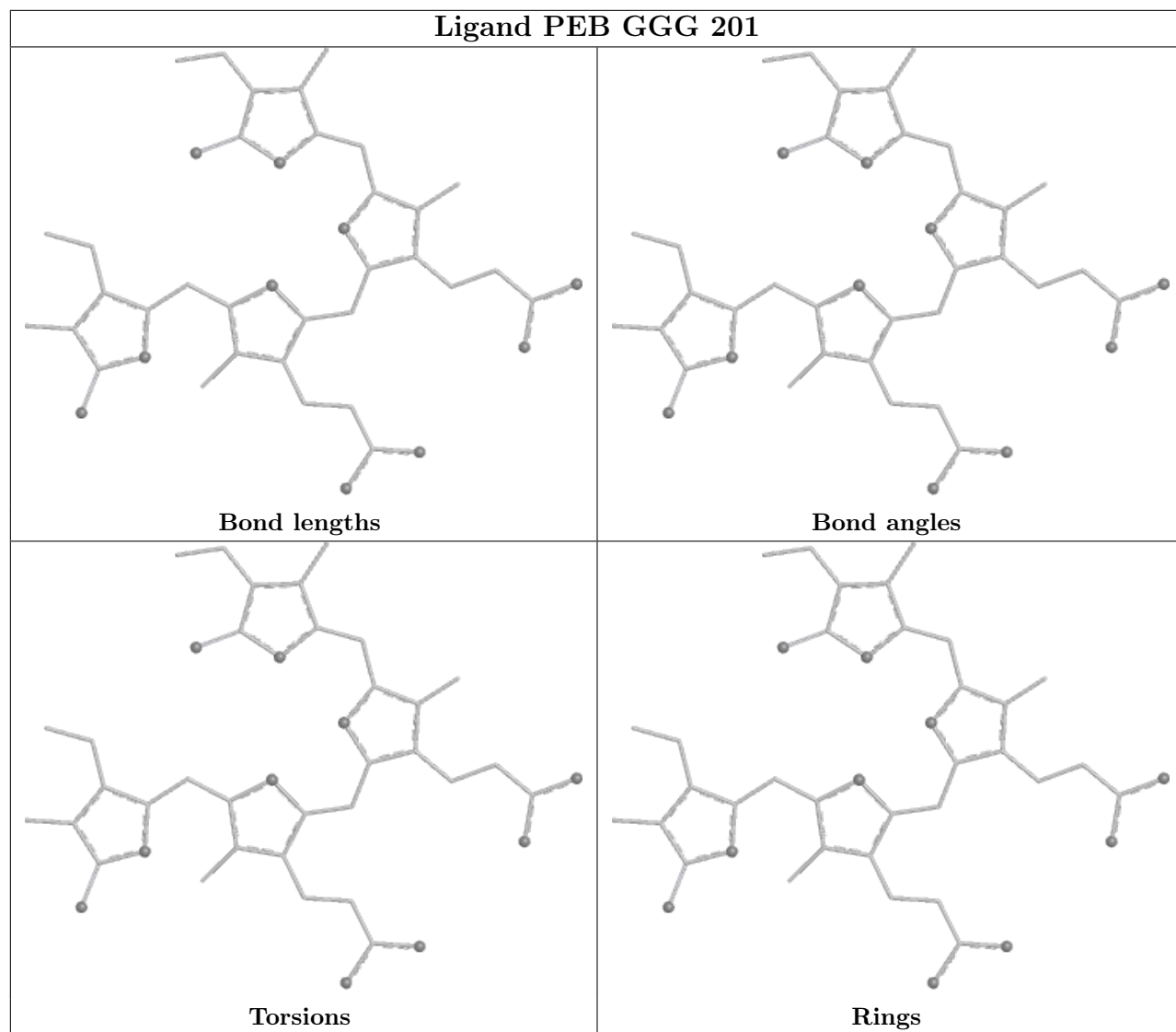
Bond angles

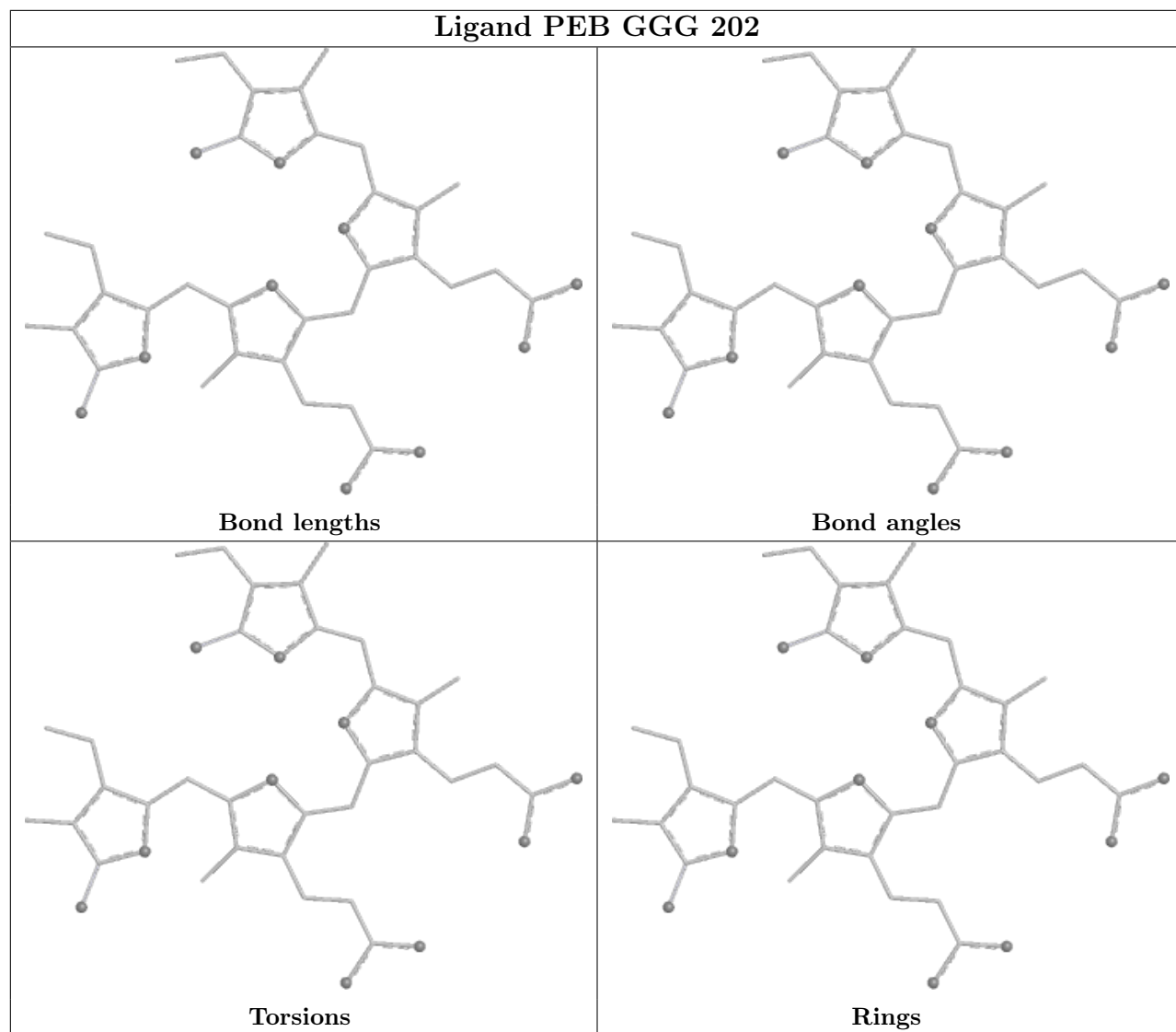


Torsions

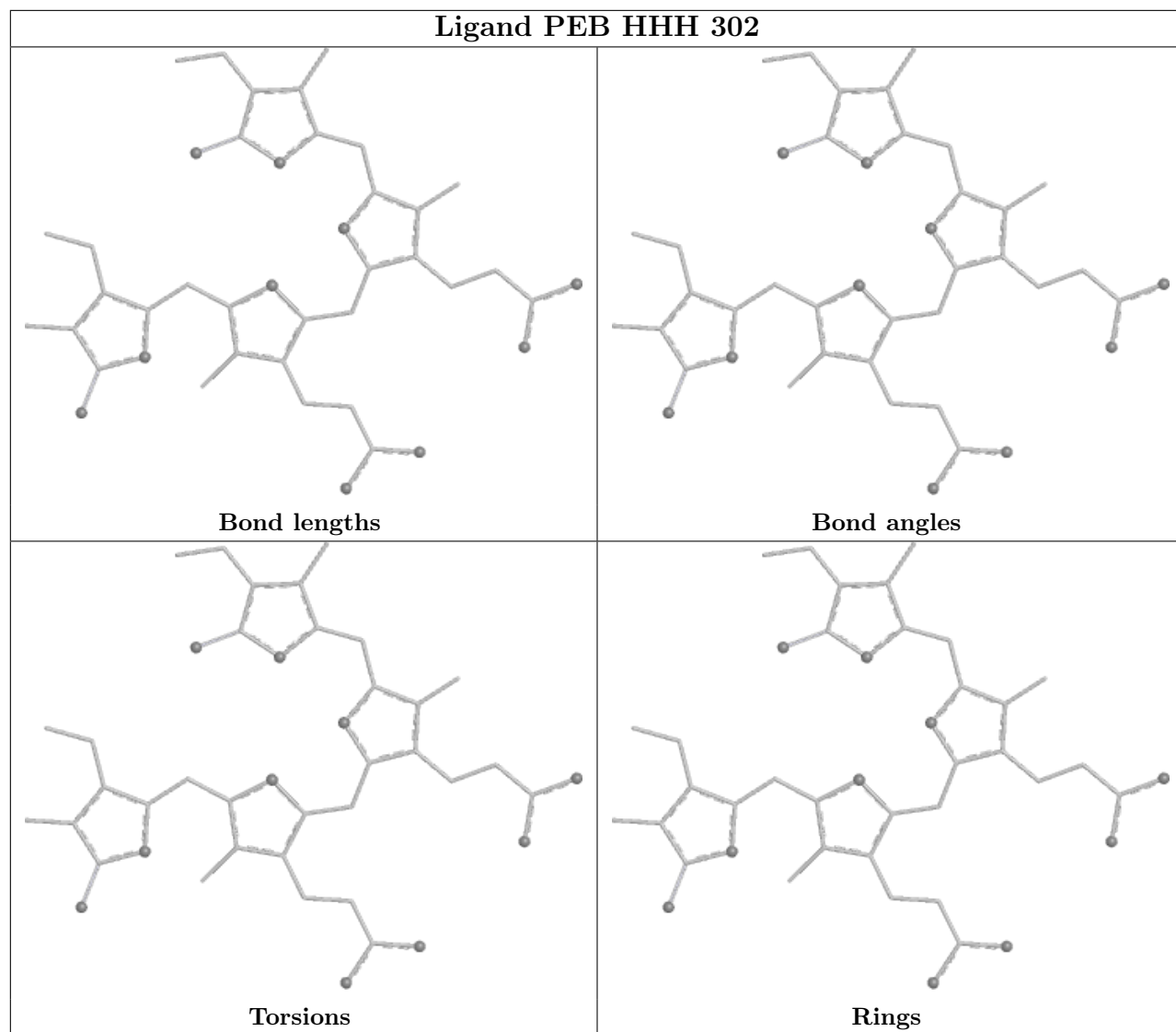


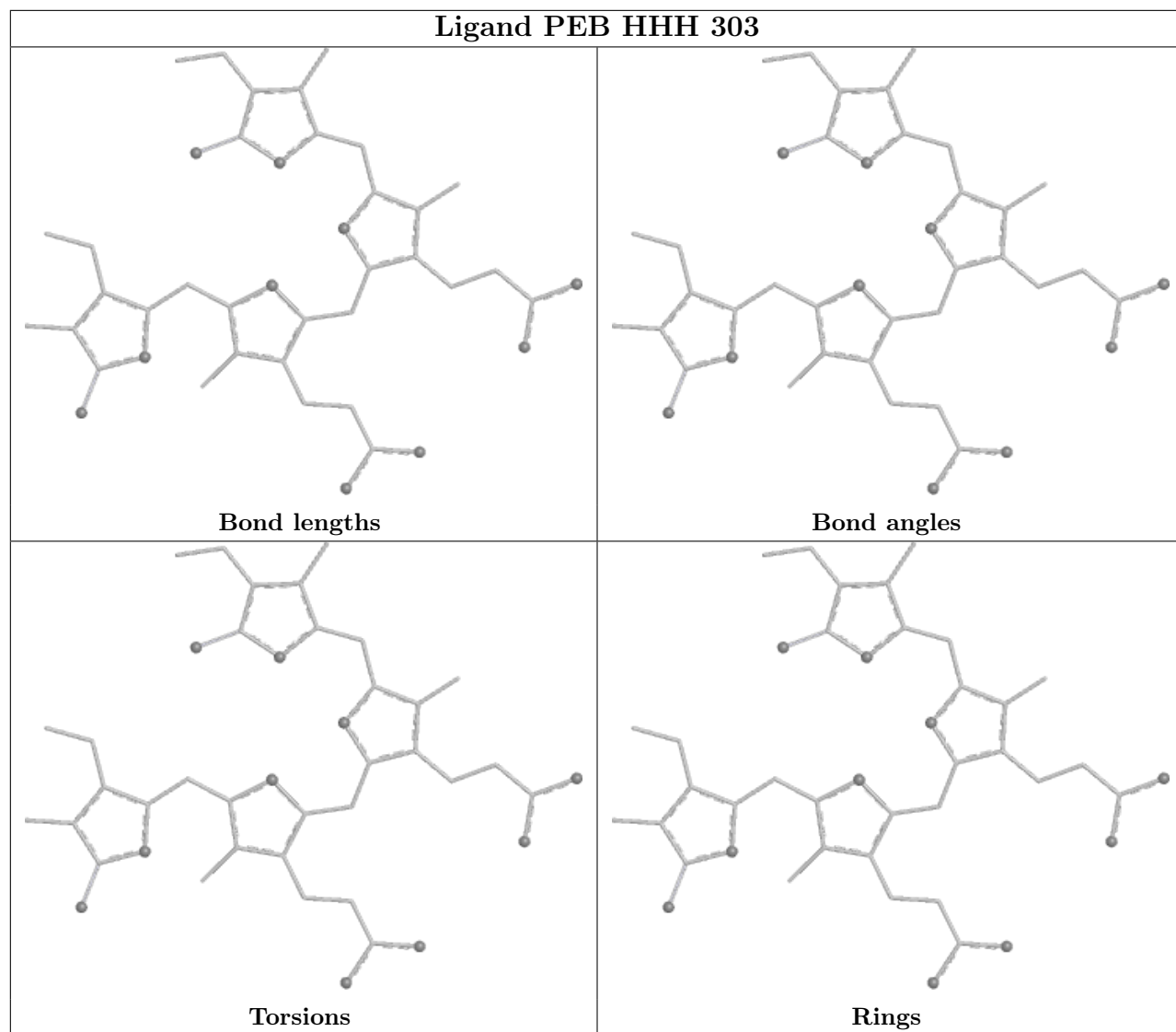
Rings



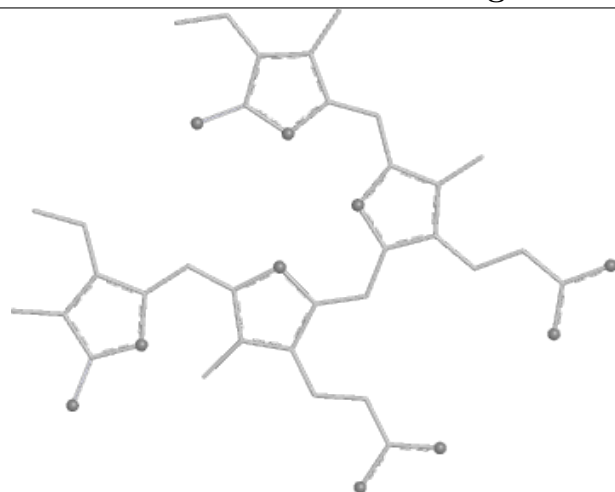




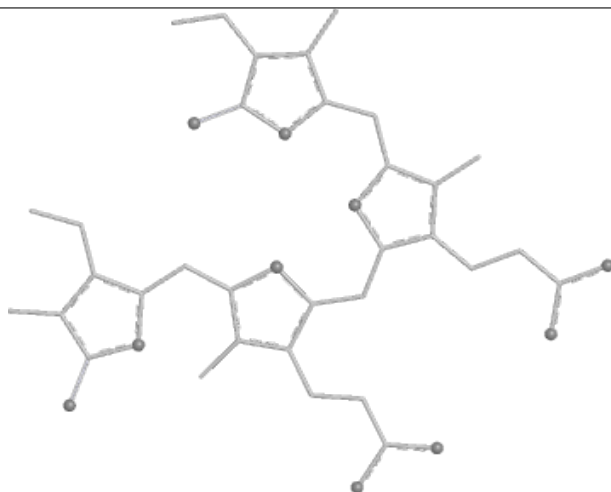




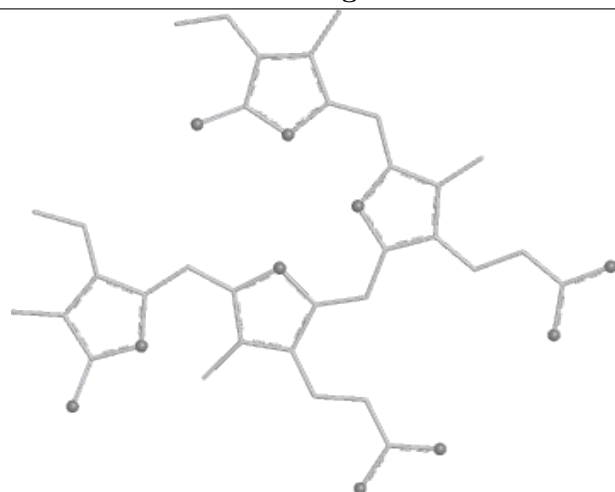
## Ligand PEB HHH 304



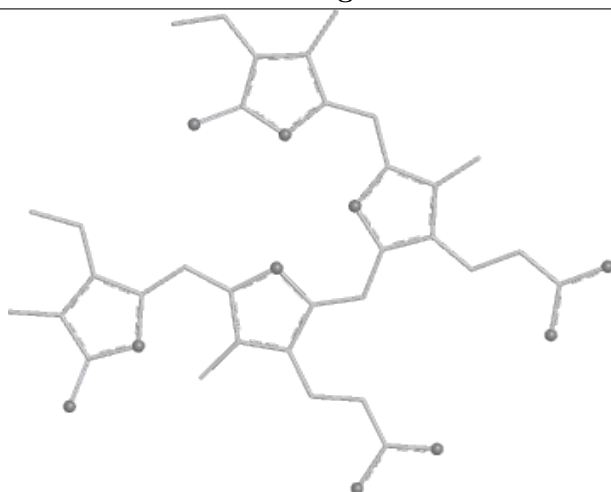
Bond lengths



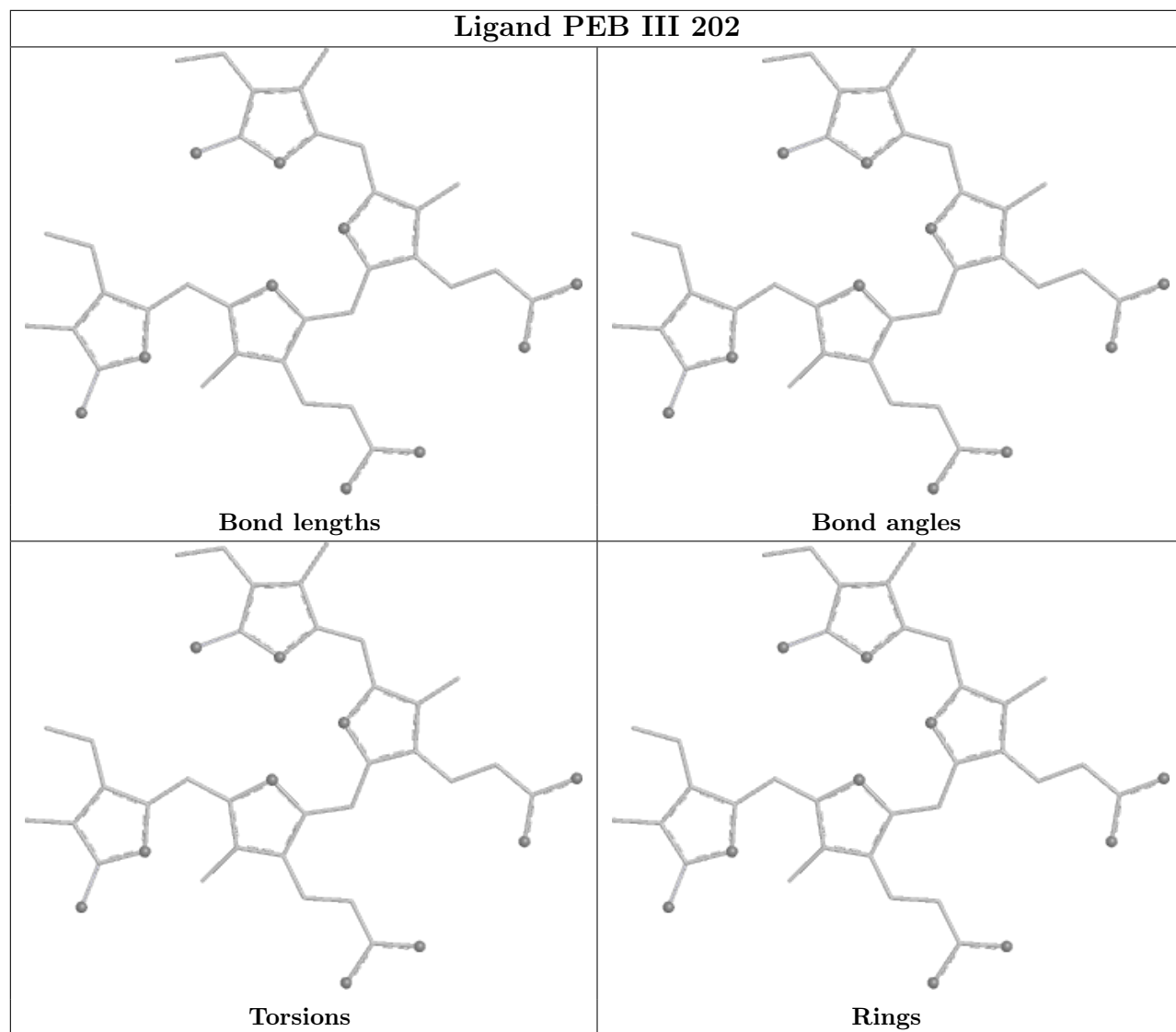
Bond angles

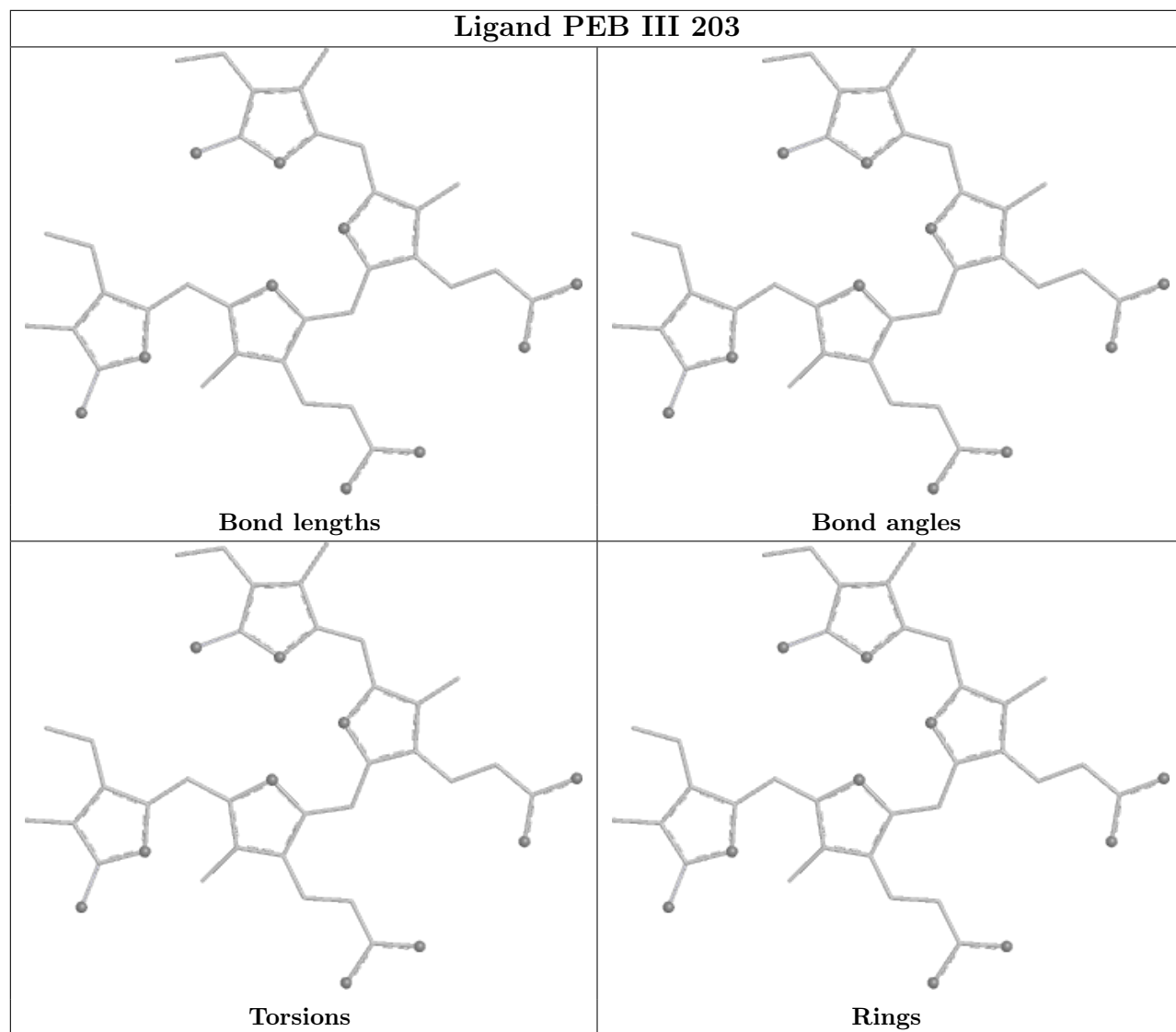


Torsions

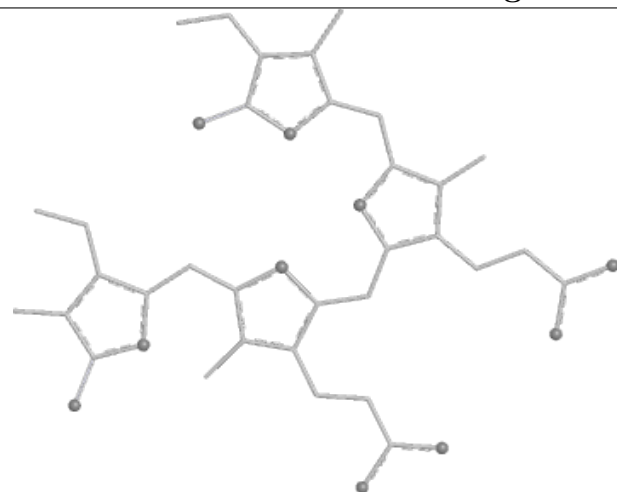


Rings

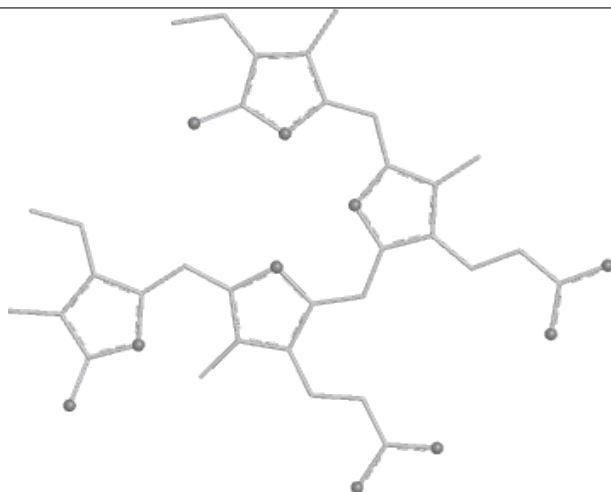




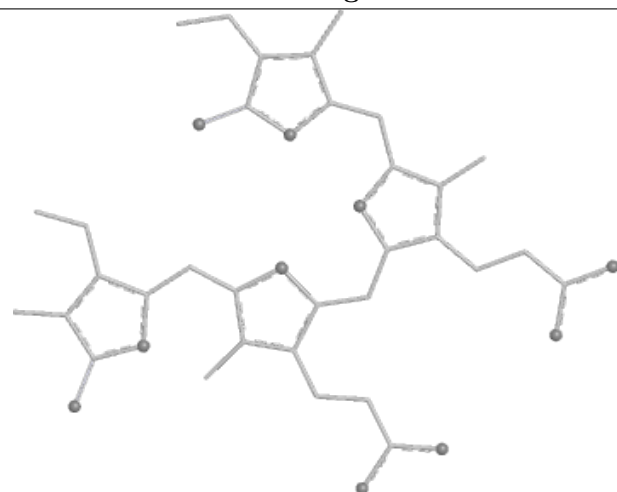
## Ligand PEB JJJ 303



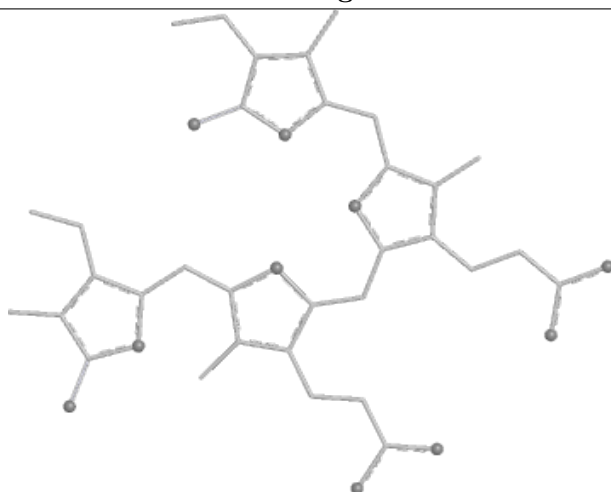
Bond lengths



Bond angles

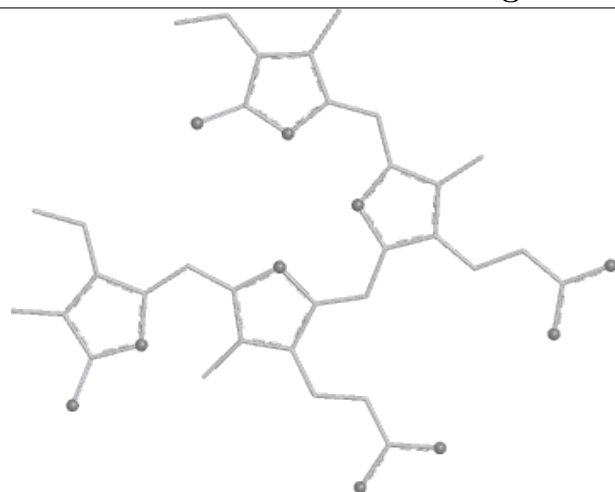


Torsions

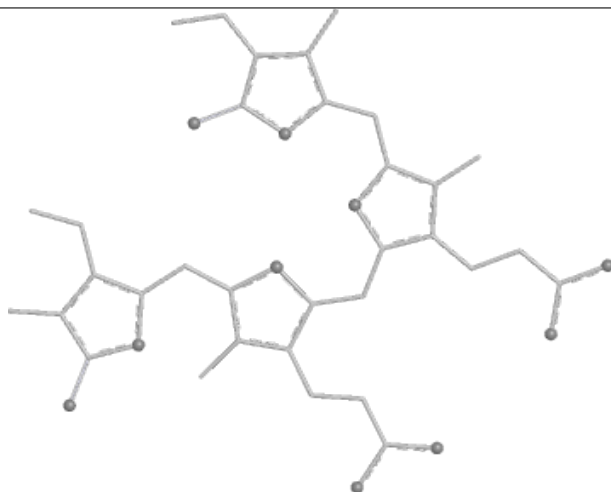


Rings

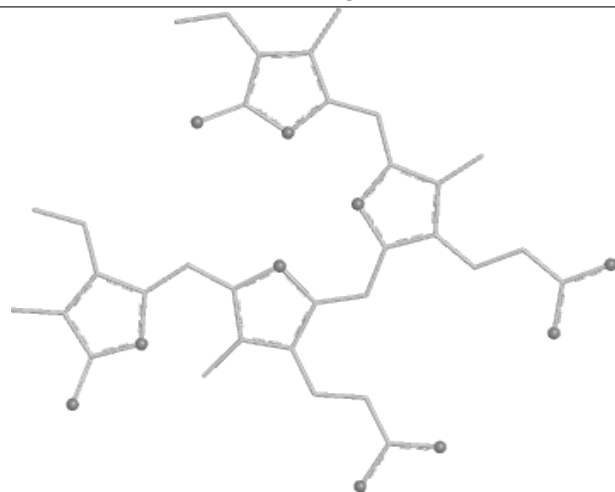
## Ligand PEB JJJ 304



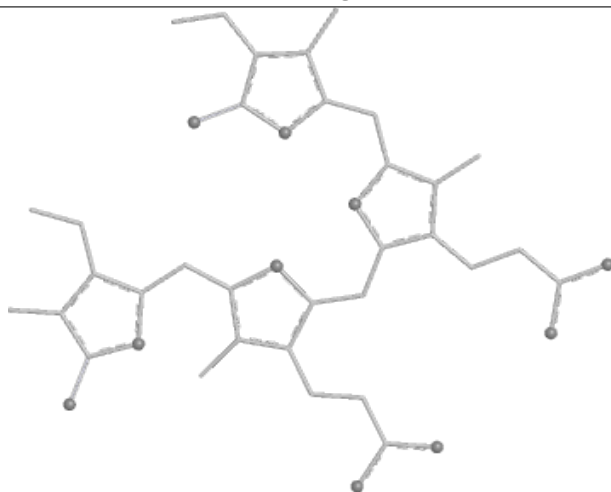
Bond lengths



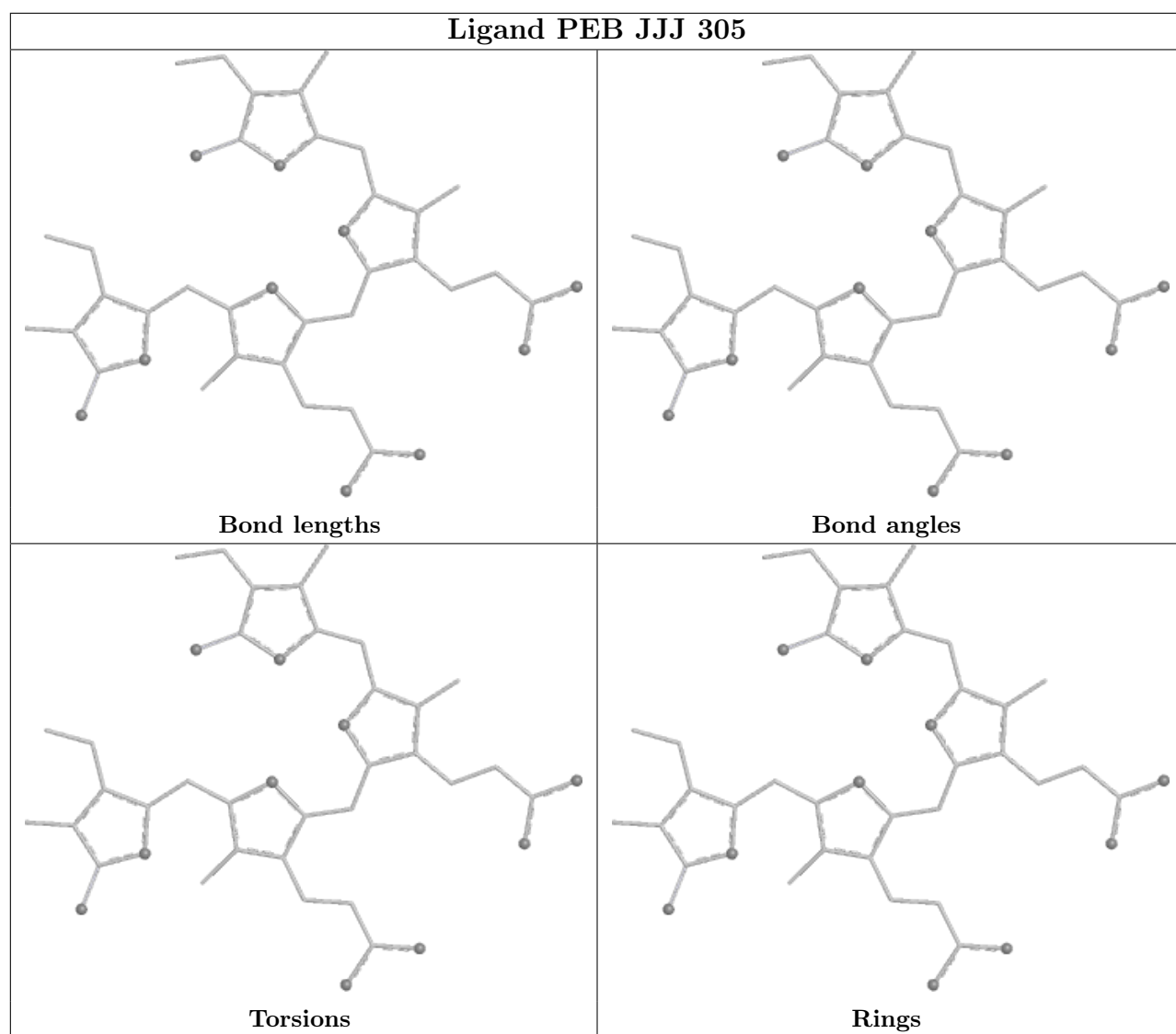
Bond angles



Torsions

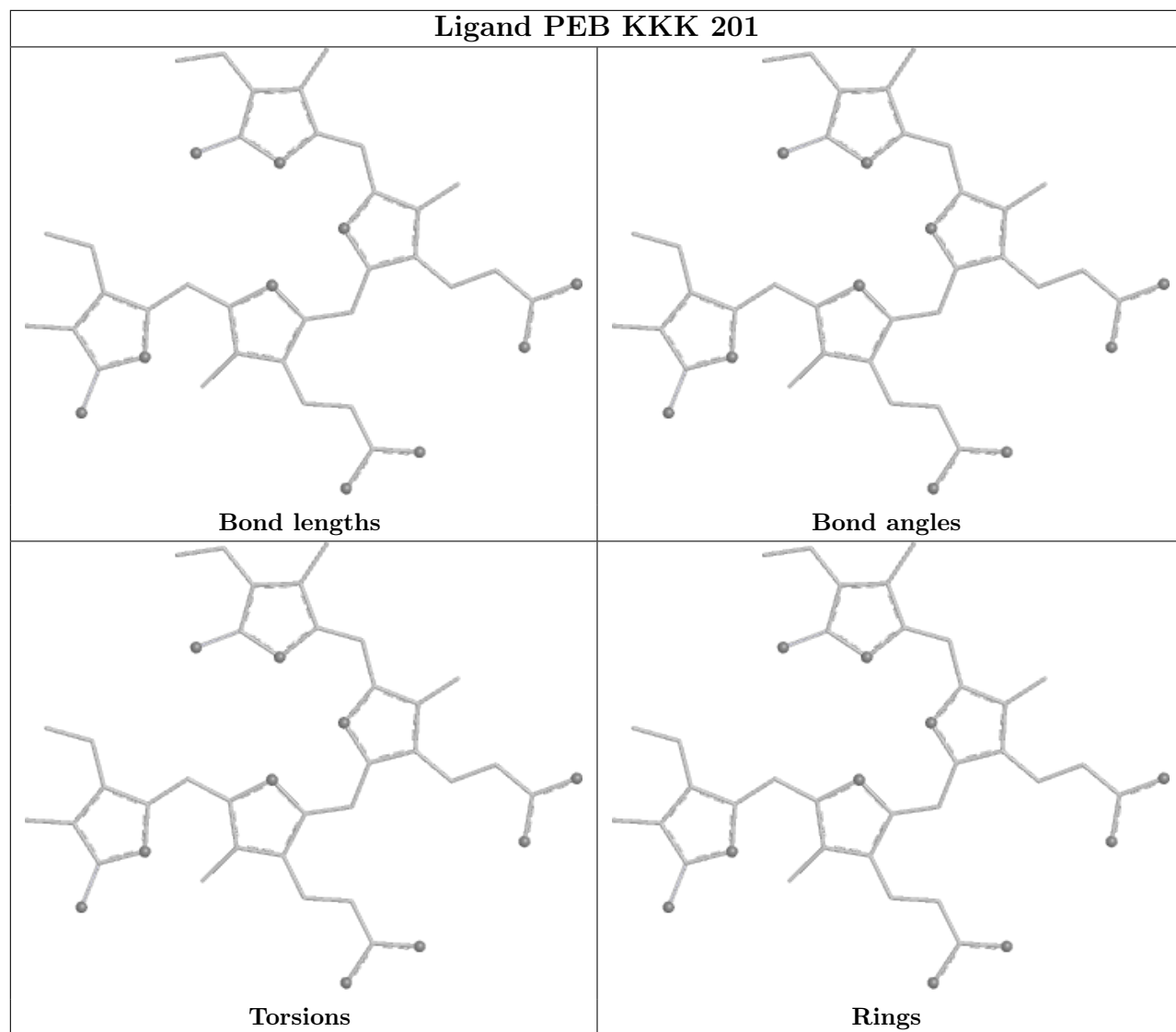


Rings

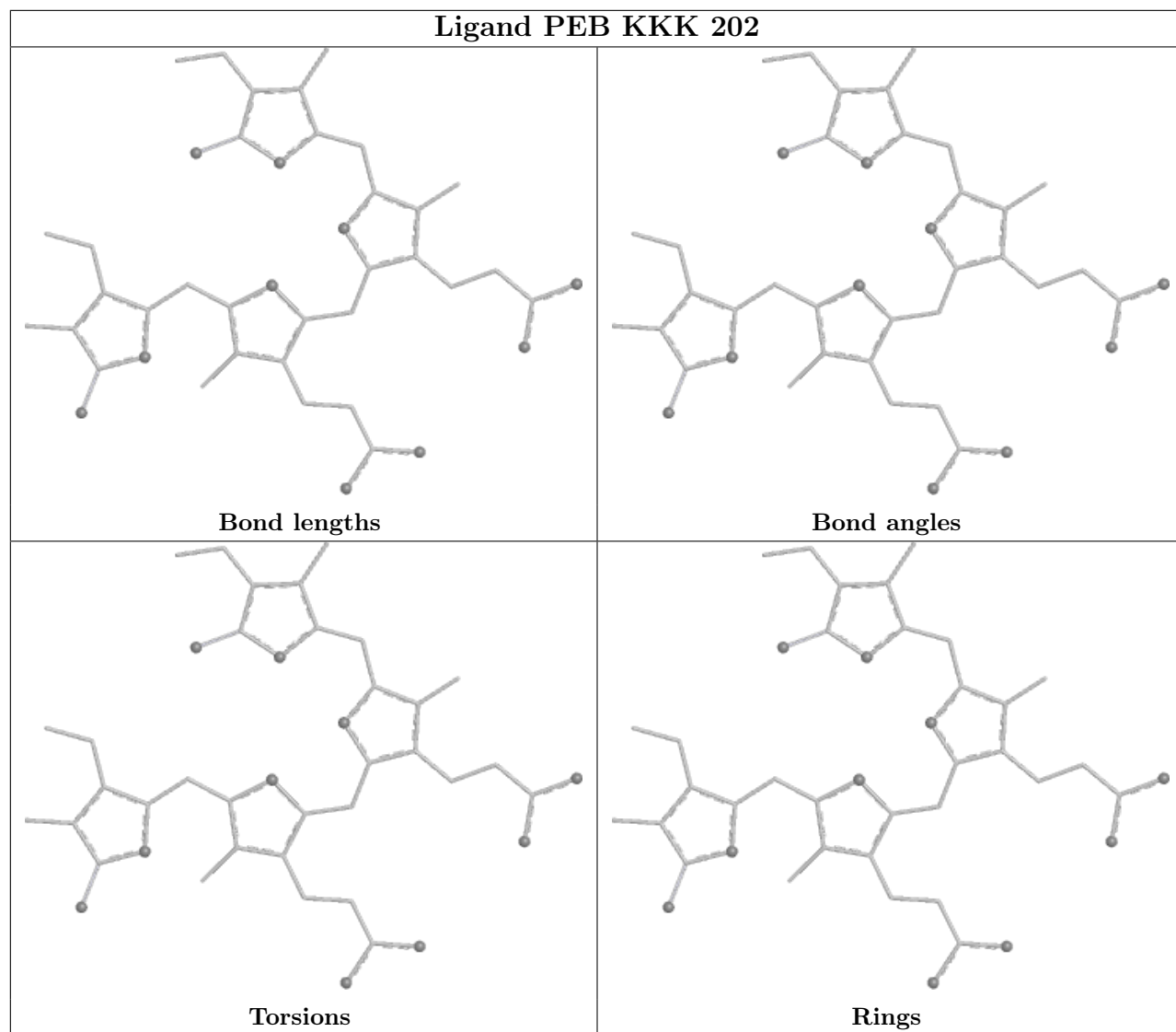




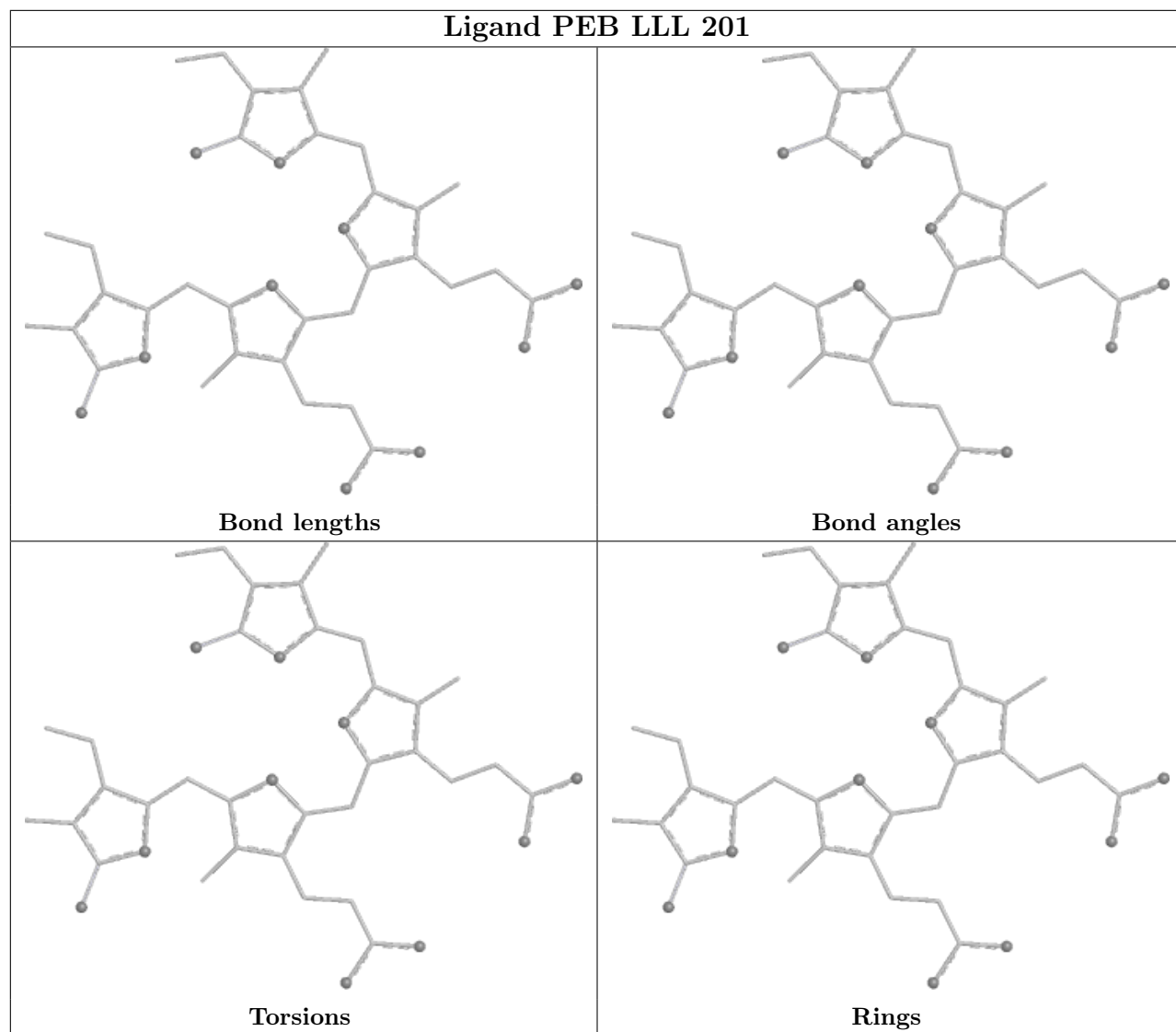
## Ligand PEB KKK 201



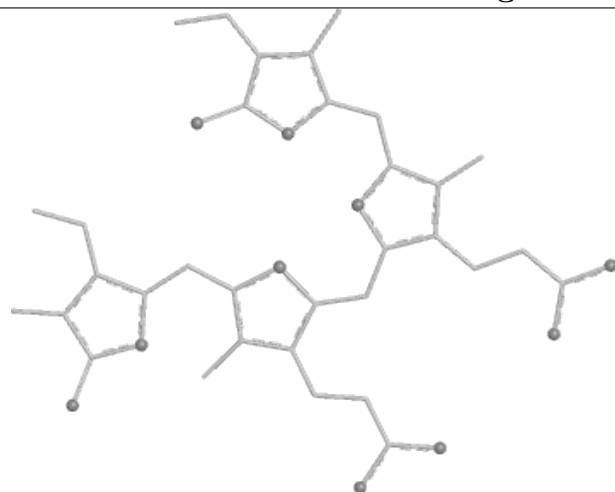
## Ligand PEB KKK 202



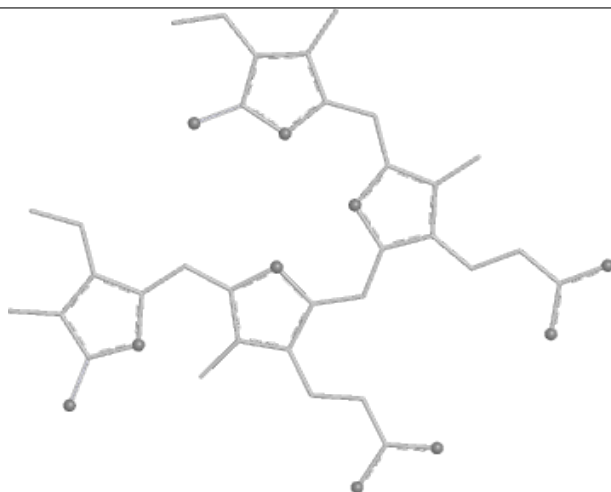
## Ligand PEB LLL 201



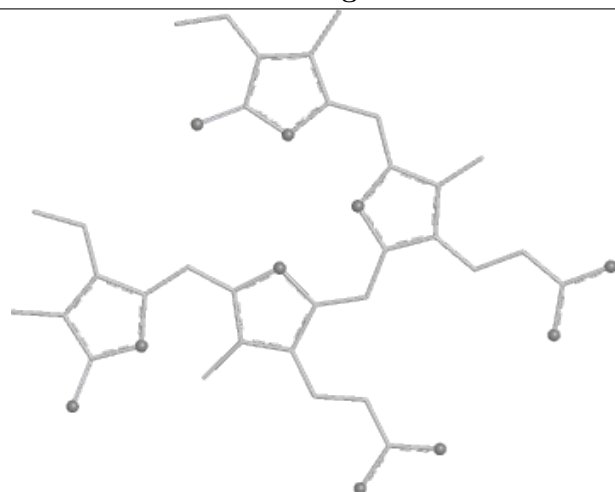
## Ligand PEB LLL 202



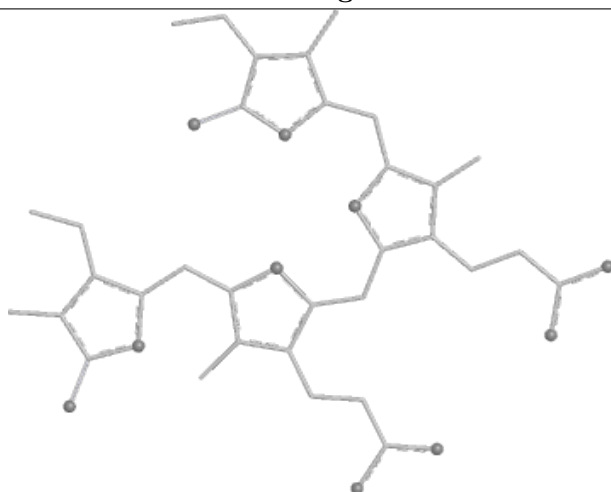
Bond lengths



Bond angles

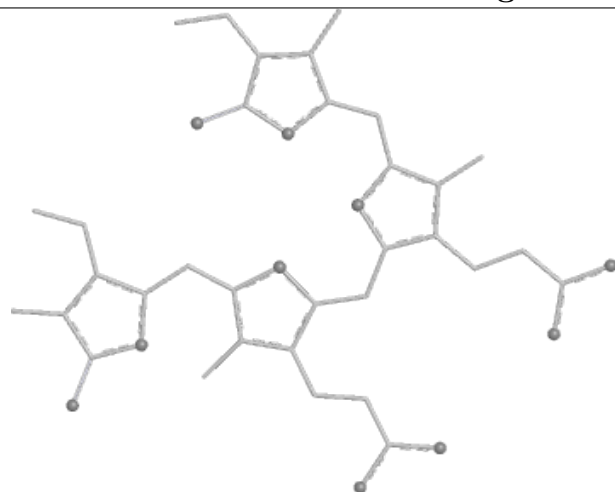


Torsions

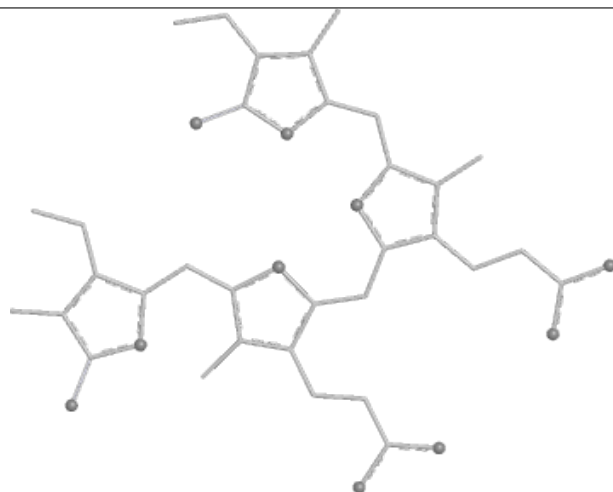


Rings

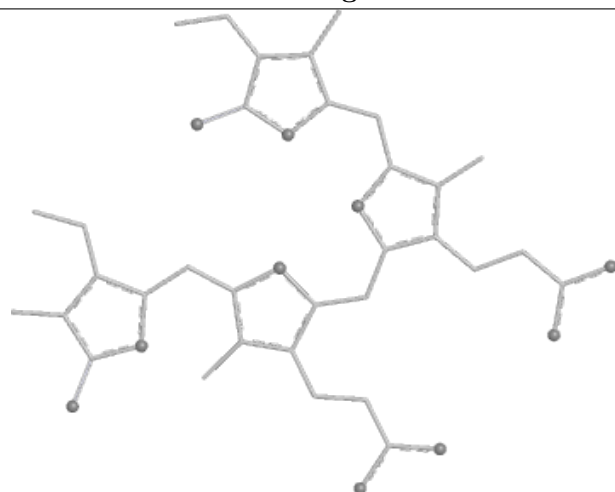
## Ligand PEB LLL 203



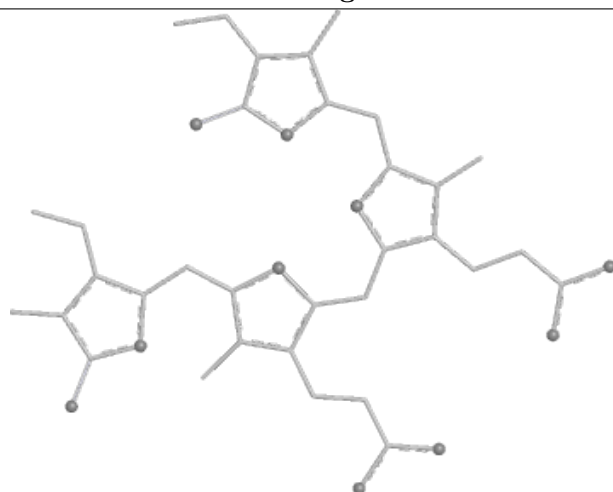
Bond lengths



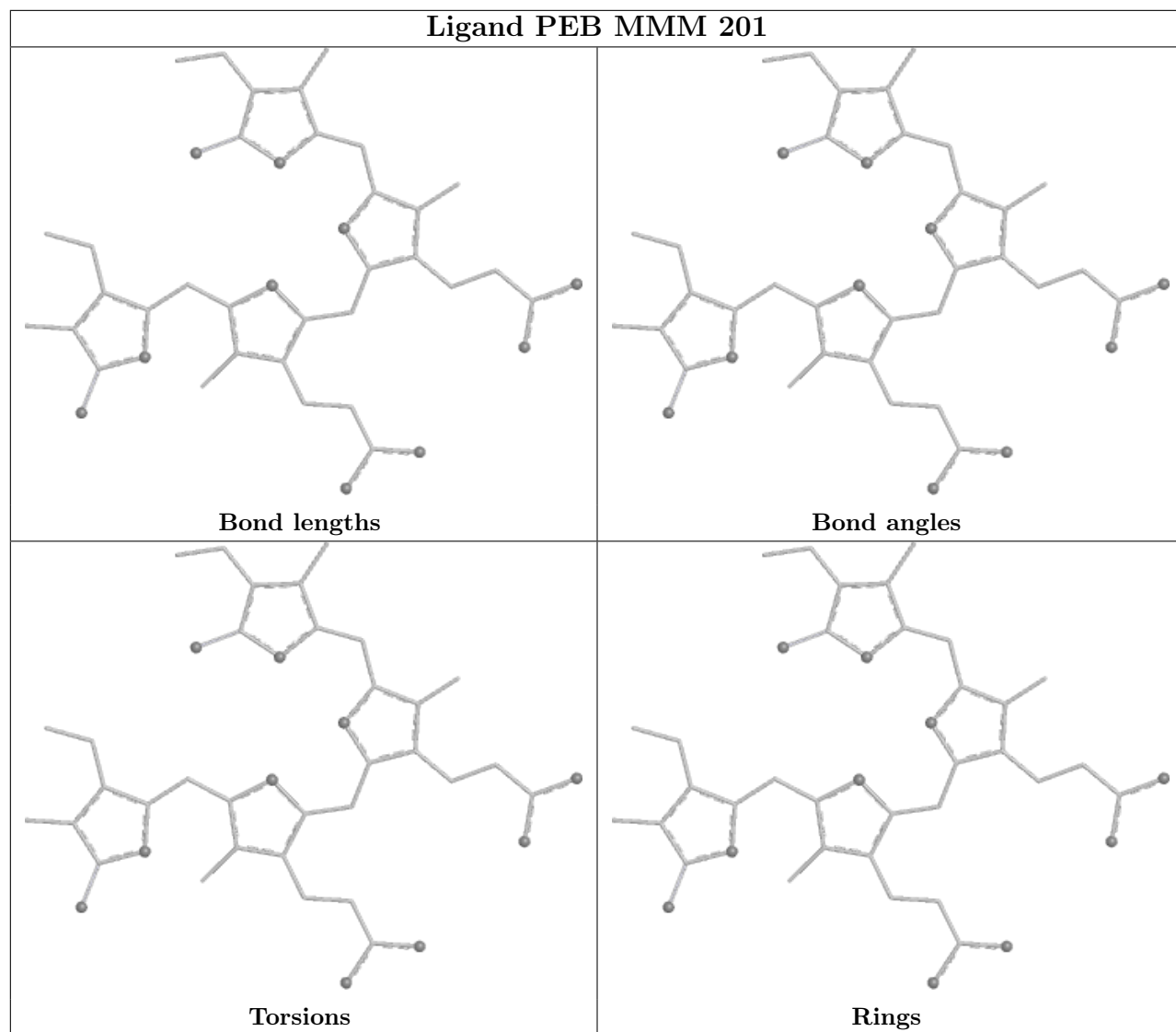
Bond angles

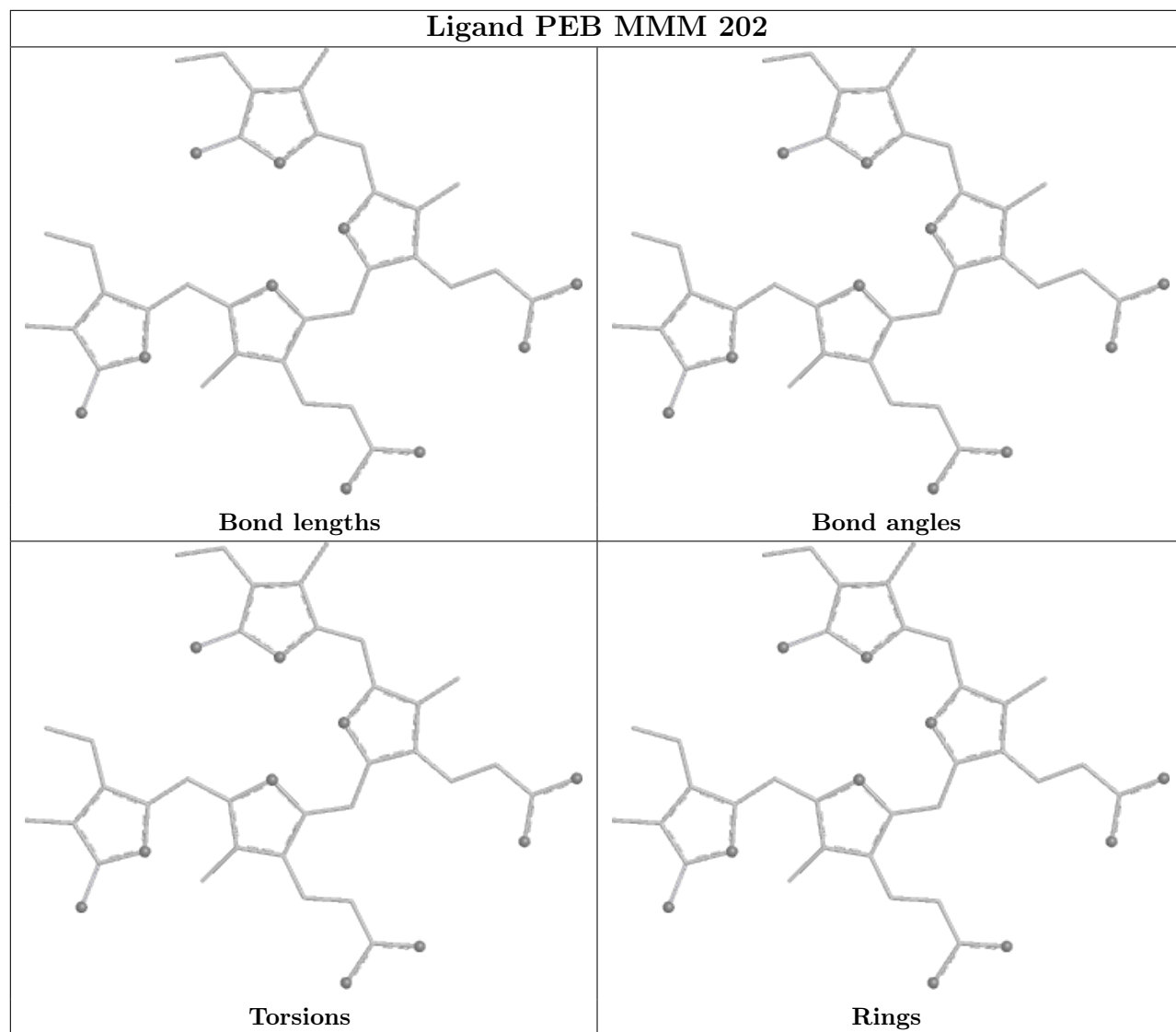


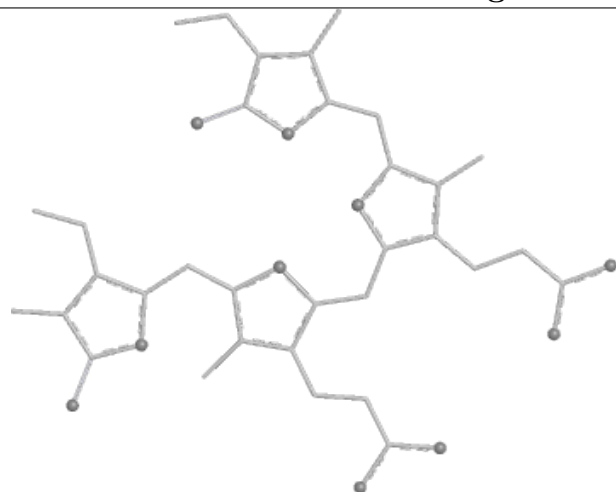
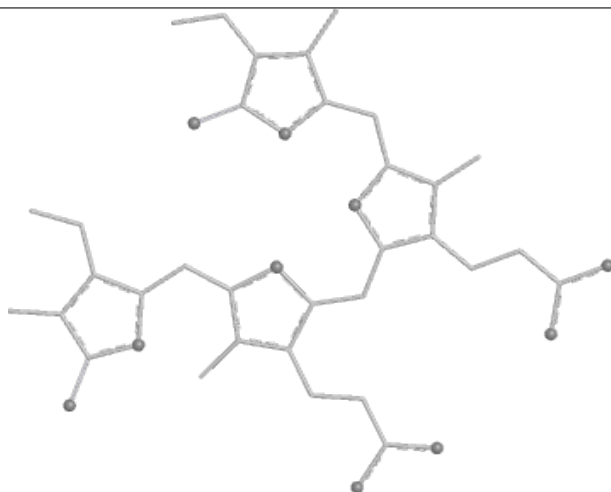
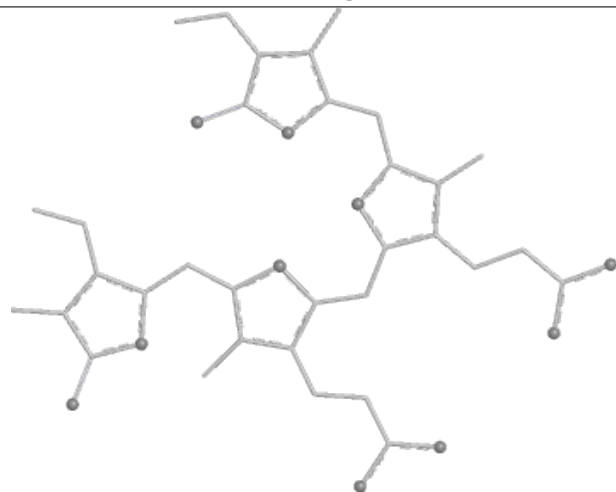
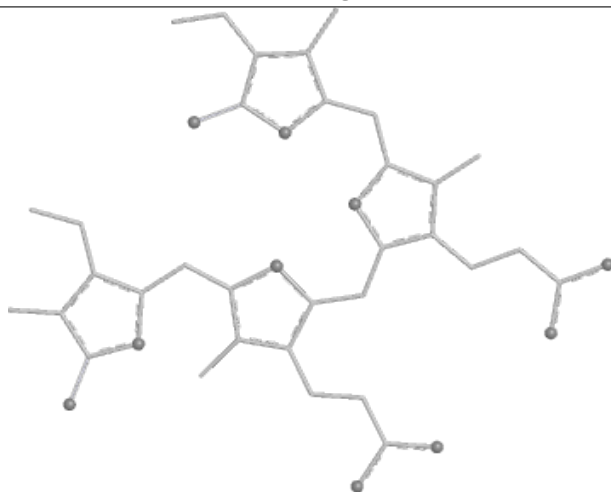
Torsions



Rings

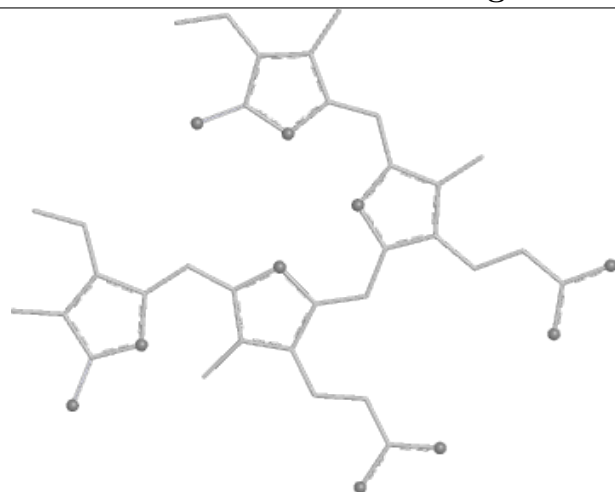




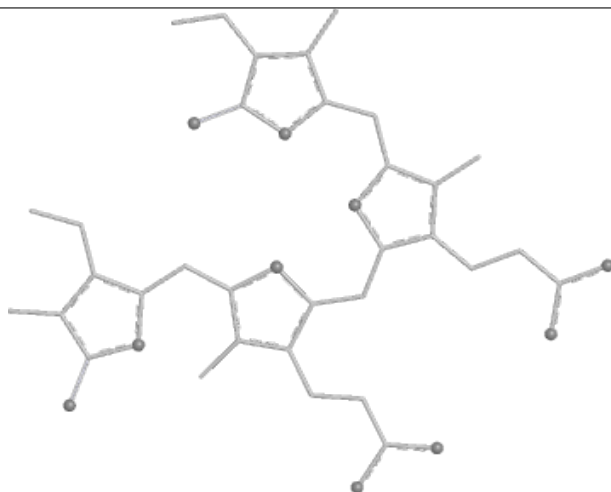
**Ligand PEB NNN 203****Bond lengths****Bond angles****Torsions****Rings**



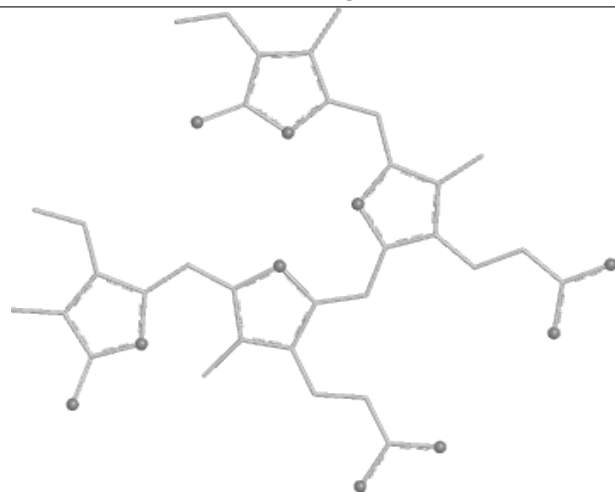
## Ligand PEB NNN 204



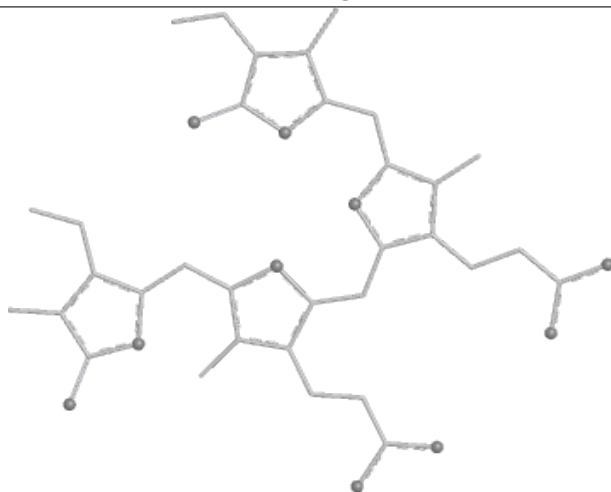
Bond lengths



Bond angles

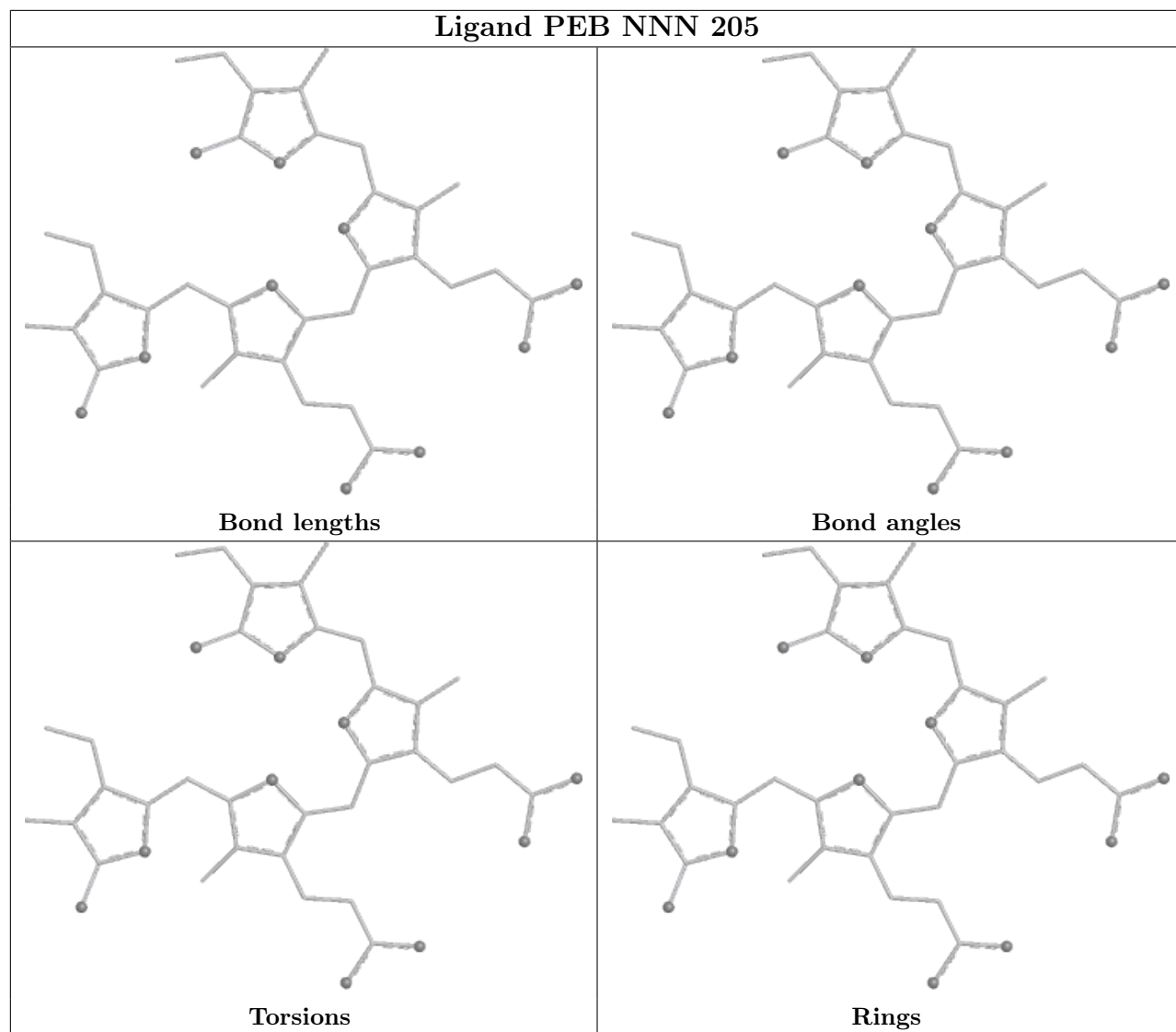


Torsions

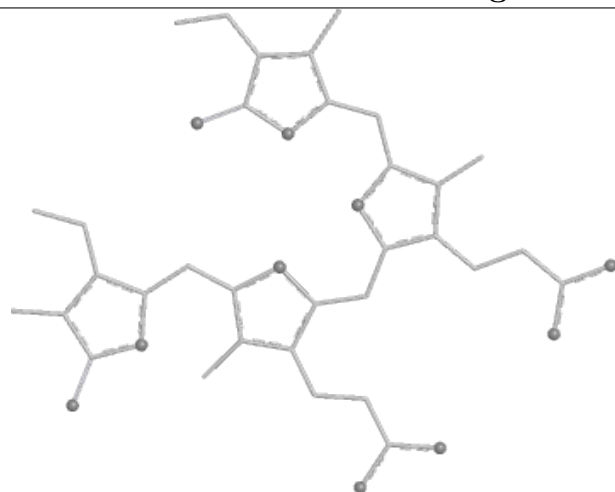


Rings

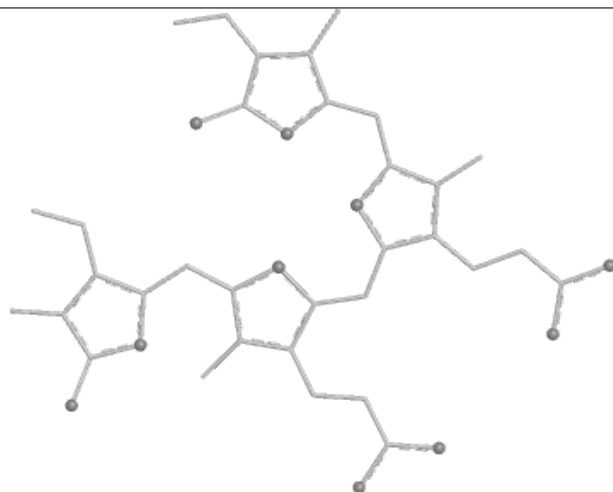
## Ligand PEB NNN 205



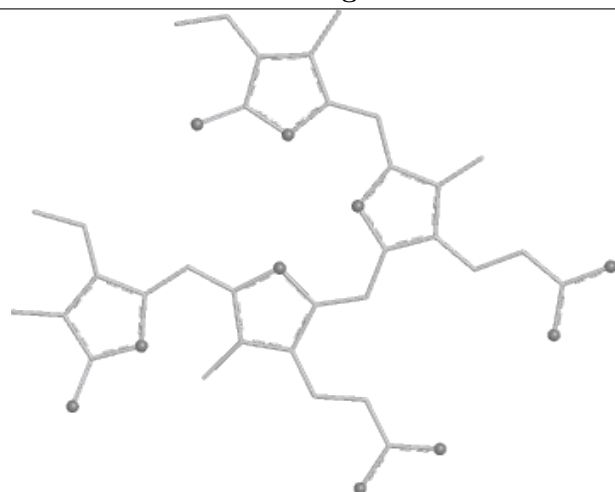
## Ligand PEB OOO 201



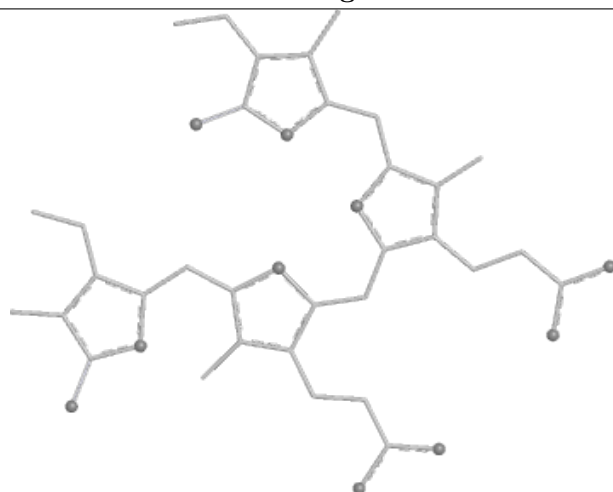
Bond lengths



Bond angles

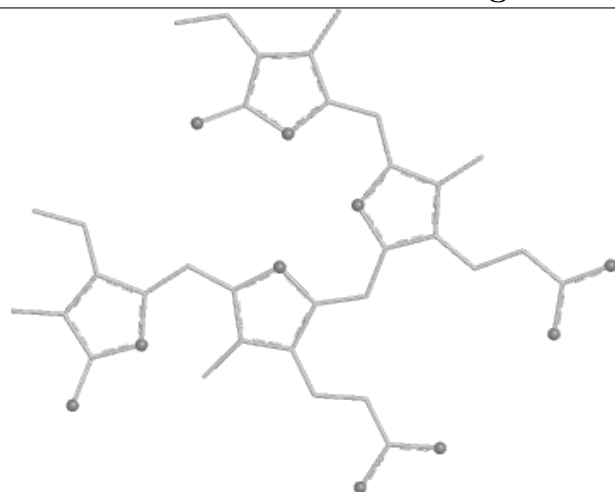


Torsions

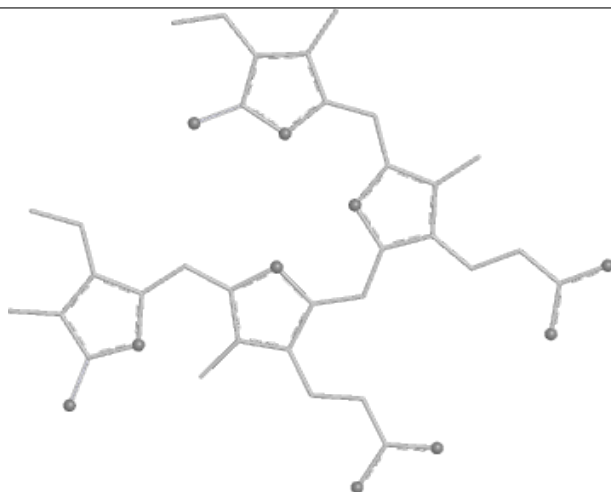


Rings

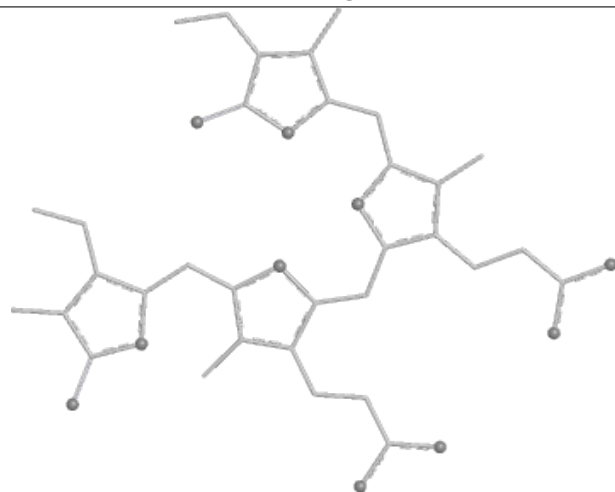
## Ligand PEB OOO 202



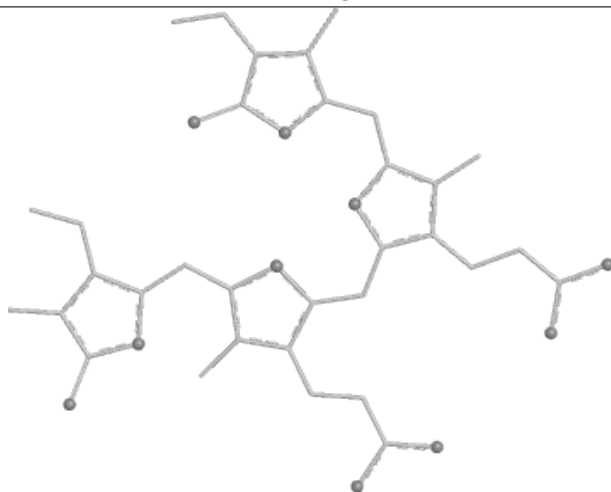
Bond lengths



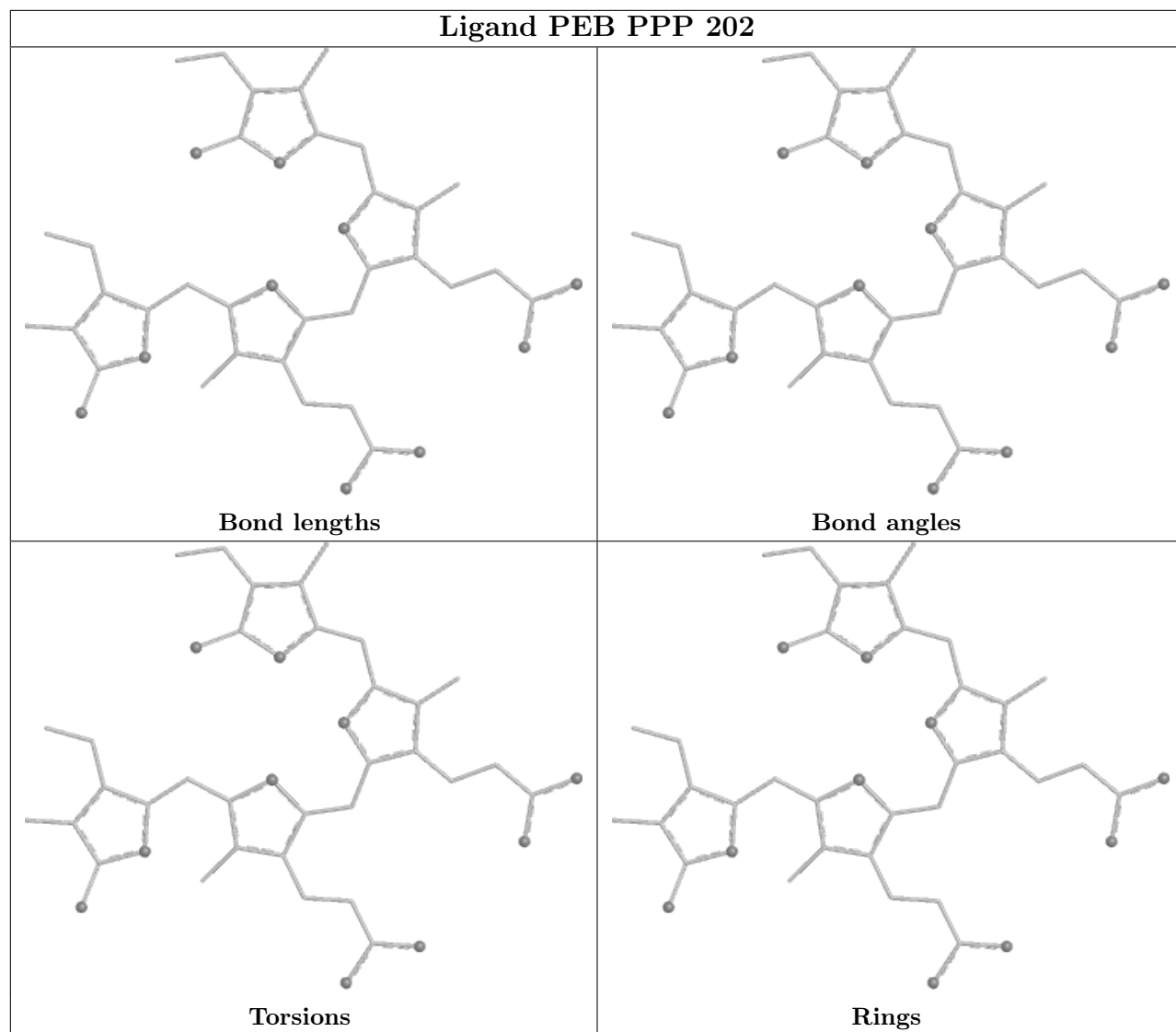
Bond angles



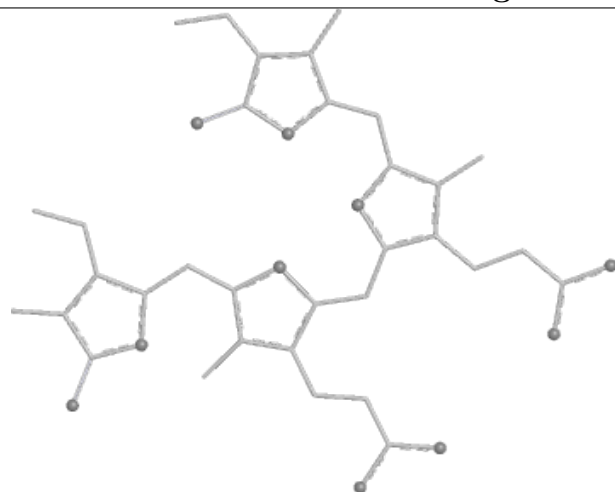
Torsions



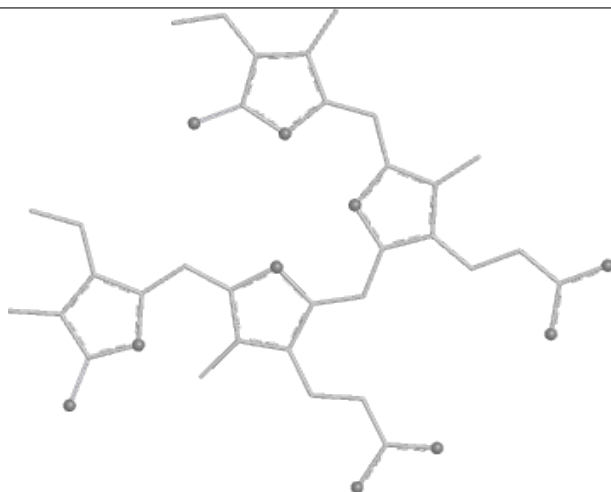
Rings



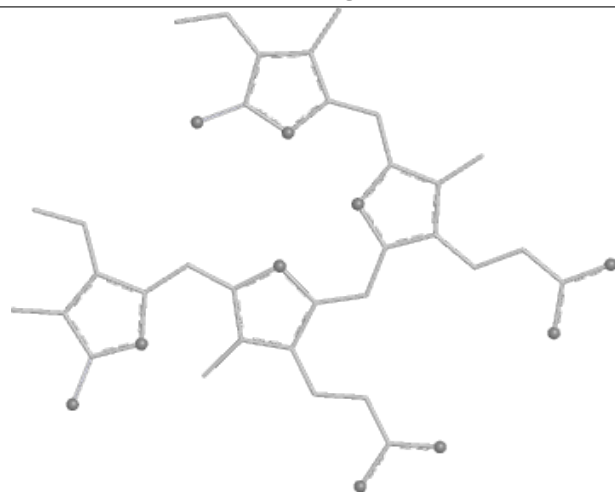
## Ligand PEB PPP 203



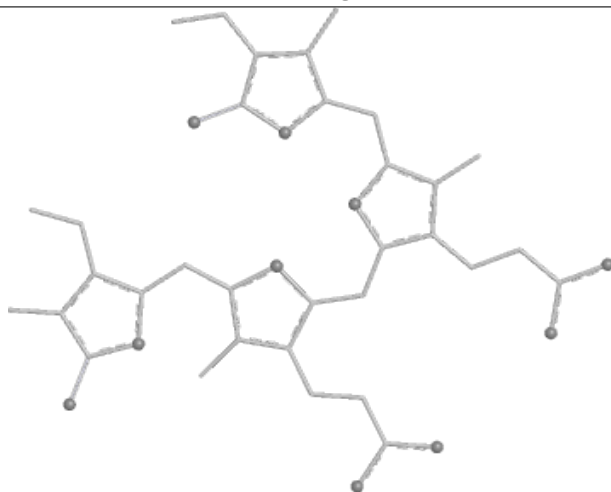
Bond lengths



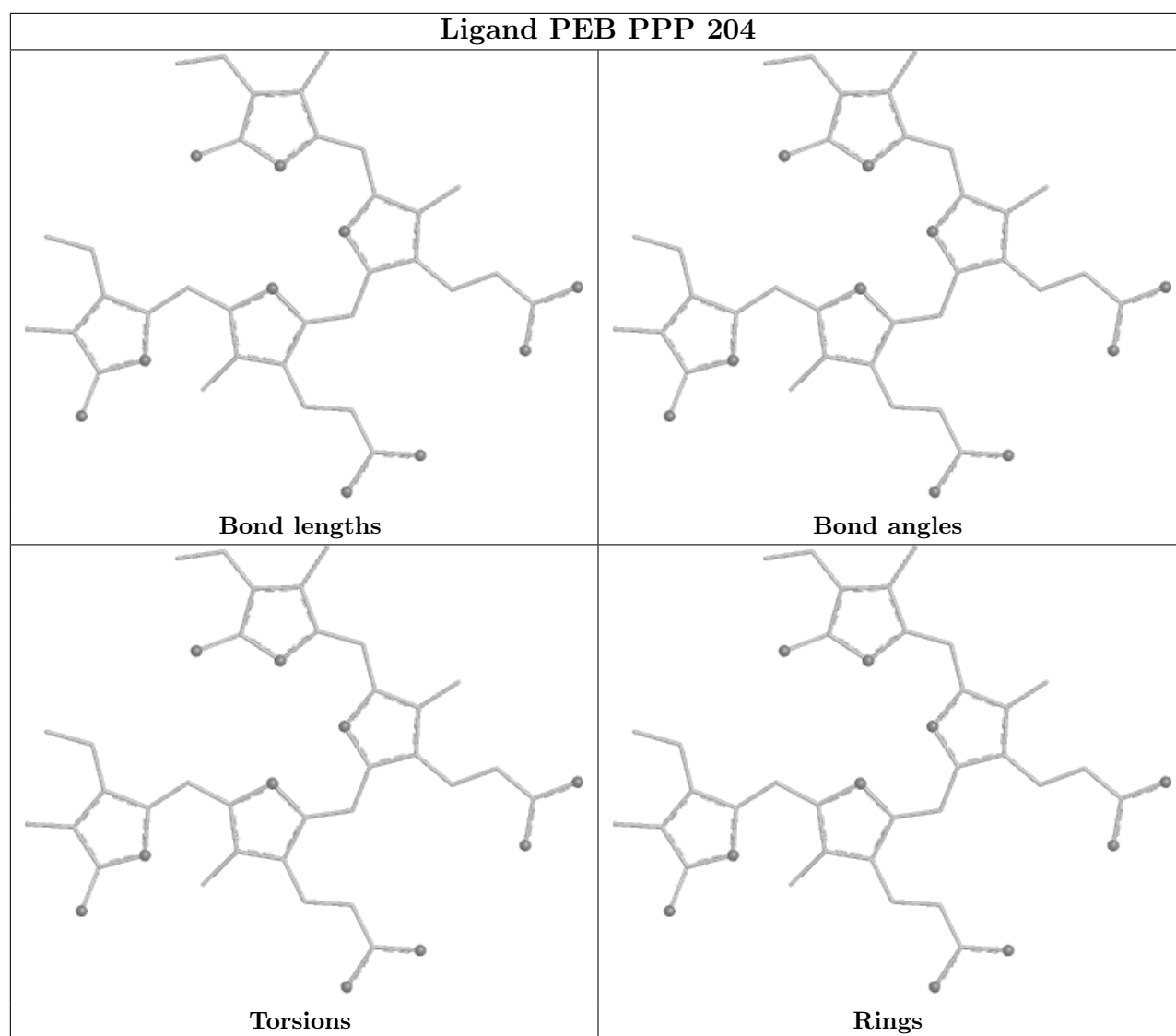
Bond angles



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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	164/164 (100%)	-0.43	0 100 100	29, 36, 47, 55	0
1	CCC	164/164 (100%)	-0.45	0 100 100	30, 38, 49, 57	0
1	EEE	164/164 (100%)	-0.43	0 100 100	30, 39, 52, 59	0
1	GGG	164/164 (100%)	-0.44	0 100 100	32, 39, 55, 63	0
1	III	164/164 (100%)	-0.43	0 100 100	30, 39, 52, 61	0
1	KKK	164/164 (100%)	-0.45	0 100 100	32, 40, 52, 59	0
1	MMM	164/164 (100%)	-0.46	0 100 100	32, 39, 54, 65	0
1	OOO	164/164 (100%)	0.19	4 (2%) 59 65	45, 58, 80, 92	0
2	BBB	183/184 (99%)	-0.43	0 100 100	29, 36, 48, 74	0
2	DDD	183/184 (99%)	-0.45	0 100 100	30, 36, 51, 77	0
2	FFF	183/184 (99%)	-0.41	0 100 100	31, 38, 51, 75	0
2	HHH	183/184 (99%)	-0.43	0 100 100	33, 38, 52, 78	0
2	JJJ	183/184 (99%)	-0.41	1 (0%) 91 93	32, 37, 54, 67	0
2	LLL	183/184 (99%)	-0.43	1 (0%) 91 93	31, 38, 51, 67	0
2	NNN	183/184 (99%)	-0.41	1 (0%) 91 93	35, 41, 56, 73	0
2	PPP	183/184 (99%)	0.47	19 (10%) 6 8	41, 54, 137, 182	1 (0%)
All	All	2776/2784 (99%)	-0.34	26 (0%) 84 87	29, 39, 61, 182	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	PPP	150	GLY	12.3
2	PPP	153	LEU	9.5
2	PPP	147	ALA	8.1
2	PPP	151	ALA	7.6
2	PPP	145	SER	6.5

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Mol	Chain	Res	Type	RSRZ
2	PPP	152	LYS	5.8
2	PPP	163	ASP	5.6
2	PPP	144	PRO	5.5
2	PPP	149	ALA	4.7
2	PPP	148[A]	ARG	4.4
2	PPP	158	SER	4.3
2	PPP	143	THR	4.3
2	PPP	146	GLU	4.2
2	PPP	161	VAL	3.5
2	PPP	160	VAL	3.3
1	OOO	164	SER	3.1
1	OOO	67	ASN	3.0
2	PPP	155	LYS	2.6
2	LLL	184	SER	2.6
2	JJJ	184	SER	2.5
2	PPP	156	MET	2.4
2	PPP	157	GLY	2.4
1	OOO	71	GLU	2.3
2	PPP	184	SER	2.2
2	NNN	184	SER	2.2
1	OOO	161	ASN	2.1

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MEN	PPP	70	9/10	0.92	0.14	44,45,47,50	0
2	MEN	FFF	70	9/10	0.96	0.11	33,36,37,39	0
2	MEN	JJJ	70	9/10	0.97	0.11	30,33,37,37	0
2	MEN	LLL	70	9/10	0.97	0.12	29,31,35,36	0
2	MEN	NNN	70	9/10	0.97	0.10	38,40,42,45	0
2	MEN	BBB	70	9/10	0.97	0.09	31,33,34,35	0
2	MEN	DDD	70	9/10	0.98	0.11	31,33,37,38	0
2	MEN	HHH	70	9/10	0.98	0.10	31,33,35,36	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	PEG	PPP	212	7/7	0.54	0.54	45,47,48,48	7
14	EDO	FFF	203	4/4	0.62	0.38	51,51,51,53	4
5	PGE	AAA	210	10/10	0.63	0.37	50,57,57,58	10
5	PGE	OOO	206	10/10	0.64	0.33	63,68,69,71	10
6	PEG	PPP	211	7/7	0.64	0.30	48,48,51,51	7
11	1PE	JJJ	308	16/16	0.66	0.33	42,50,52,52	16
8	NO3	AAA	217	4/4	0.66	0.20	45,48,55,57	4
7	PO4	NNN	224	5/5	0.67	0.27	62,63,65,71	5
5	PGE	BBB	209	10/10	0.68	0.50	45,47,48,49	10
7	PO4	III	216	5/5	0.68	0.32	49,51,55,58	5
6	PEG	CCC	214	7/7	0.69	0.43	43,49,54,54	7
8	NO3	CCC	218	4/4	0.69	0.18	47,48,51,57	4
8	NO3	DDD	226	4/4	0.69	0.26	43,43,44,46	4
6	PEG	JJJ	314	7/7	0.69	0.35	51,53,56,57	7
8	NO3	AAA	216	4/4	0.69	0.18	38,39,42,47	4
14	EDO	NNN	219	4/4	0.69	0.27	48,49,50,51	4
5	PGE	KKK	206	10/10	0.70	0.24	47,51,54,55	10
11	1PE	PPP	205	16/16	0.70	0.37	47,53,56,57	16
12	P33	HHH	306	22/22	0.70	0.38	47,51,58,59	22
4	PG4	MMM	205	13/13	0.70	0.43	48,49,53,53	13
8	NO3	JJJ	320	4/4	0.70	0.19	54,55,60,62	4
6	PEG	LLL	212	7/7	0.71	0.34	43,46,49,49	7
11	1PE	DDD	207	16/16	0.72	0.31	46,52,53,54	16
6	PEG	OOO	208	7/7	0.72	0.28	51,54,56,56	7
6	PEG	HHH	317	7/7	0.72	0.28	43,48,52,52	7
6	PEG	III	209	7/7	0.73	0.30	49,51,54,54	7
5	PGE	CCC	208	10/10	0.74	0.36	42,50,51,51	10
5	PGE	AAA	209	10/10	0.74	0.31	50,53,57,58	10
6	PEG	NNN	215	7/7	0.74	0.36	41,44,49,50	7
8	NO3	MMM	211	4/4	0.74	0.21	40,46,49,53	4
7	PO4	DDD	224	5/5	0.74	0.38	58,59,60,62	5
7	PO4	CCC	217	5/5	0.75	0.23	55,56,58,59	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PEG	DDD	216	7/7	0.75	0.30	47,48,50,51	7
4	PG4	AAA	205	13/13	0.75	0.38	46,48,49,49	13
4	PG4	DDD	208	13/13	0.75	0.36	37,49,54,54	13
6	PEG	EEE	212	7/7	0.76	0.43	45,47,47,48	7
4	PG4	NNN	208	13/13	0.76	0.26	49,55,58,58	13
6	PEG	CCC	209	7/7	0.76	0.31	40,43,46,47	7
5	PGE	DDD	211	10/10	0.76	0.37	47,53,55,56	10
4	PG4	NNN	207	13/13	0.76	0.33	42,47,55,55	13
5	PGE	HHH	310	10/10	0.77	0.41	48,52,55,55	10
6	PEG	LLL	217	7/7	0.77	0.23	46,48,50,50	7
6	PEG	CCC	219	7/7	0.78	0.28	46,48,49,50	7
4	PG4	KKK	204	13/13	0.78	0.33	40,48,54,54	13
7	PO4	JJJ	321	5/5	0.78	0.15	41,44,47,53	5
5	PGE	NNN	210	10/10	0.78	0.23	42,49,51,51	10
4	PG4	GGG	205	13/13	0.78	0.28	50,53,56,56	13
4	PG4	OOO	203	13/13	0.78	0.33	49,51,55,56	13
5	PGE	HHH	313	10/10	0.78	0.42	41,45,48,49	10
14	EDO	III	217	4/4	0.78	0.28	42,43,43,44	4
6	PEG	KKK	210	7/7	0.78	0.23	43,45,49,50	7
6	PEG	BBB	213	7/7	0.79	0.32	38,44,46,47	7
6	PEG	III	201	7/7	0.79	0.26	35,36,38,39	7
8	NO3	EEE	210	4/4	0.79	0.13	40,42,45,49	4
5	PGE	JJJ	311	10/10	0.79	0.27	47,53,59,59	10
8	NO3	LLL	223	4/4	0.79	0.17	48,51,51,53	4
5	PGE	FFF	212	10/10	0.79	0.33	43,46,49,52	10
8	NO3	OOO	212	4/4	0.79	0.17	44,47,49,49	4
11	1PE	BBB	207	16/16	0.79	0.32	41,50,57,58	16
5	PGE	BBB	210	10/10	0.79	0.20	41,45,50,50	10
5	PGE	OOO	204	10/10	0.79	0.33	49,54,57,57	10
11	1PE	LLL	205	16/16	0.79	0.24	38,56,63,63	16
6	PEG	LLL	215	7/7	0.79	0.41	47,48,51,51	7
5	PGE	EEE	205	10/10	0.79	0.26	44,46,51,52	10
7	PO4	OOO	211	5/5	0.79	0.39	125,128,132,132	0
6	PEG	MMM	209	7/7	0.79	0.25	37,41,42,44	7
6	PEG	EEE	213	7/7	0.79	0.24	46,49,50,50	7
8	NO3	FFF	225	4/4	0.80	0.16	43,43,44,50	4
8	NO3	HHH	325	4/4	0.80	0.13	38,42,43,46	4
6	PEG	III	211	7/7	0.80	0.24	37,39,40,41	7
4	PG4	MMM	212	13/13	0.80	0.25	42,47,60,60	13
5	PGE	DDD	210	10/10	0.80	0.28	39,48,57,58	10
5	PGE	NNN	213	10/10	0.80	0.24	42,48,53,54	10
5	PGE	HHH	312	10/10	0.80	0.29	41,47,49,49	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PEG	LLL	216	7/7	0.80	0.23	49,52,54,57	7
5	PGE	OOO	205	10/10	0.80	0.37	45,47,49,50	10
7	PO4	PPP	218	5/5	0.80	0.24	46,47,49,51	5
6	PEG	GGG	211	7/7	0.80	0.35	29,31,33,33	7
4	PG4	CCC	203	13/13	0.80	0.26	43,46,50,51	13
5	PGE	JJJ	310	10/10	0.80	0.32	38,42,46,47	10
6	PEG	OOO	209	7/7	0.80	0.26	53,55,56,56	7
5	PGE	BBB	222	10/10	0.80	0.25	47,48,49,50	10
7	PO4	III	215	5/5	0.81	0.28	48,51,52,53	5
5	PGE	III	207	10/10	0.81	0.22	42,48,49,50	10
4	PG4	KKK	205	13/13	0.81	0.24	39,47,52,53	13
7	PO4	NNN	223	5/5	0.81	0.28	46,49,51,52	5
6	PEG	CCC	221	7/7	0.81	0.32	41,42,44,46	7
6	PEG	OOO	207	7/7	0.81	0.54	43,45,47,47	7
4	PG4	HHH	308	13/13	0.81	0.31	49,51,54,55	13
5	PGE	DDD	212	10/10	0.81	0.28	39,53,55,56	10
6	PEG	PPP	210	7/7	0.81	0.24	49,52,54,54	7
8	NO3	BBB	221	4/4	0.81	0.12	41,43,45,48	4
6	PEG	LLL	211	7/7	0.81	0.20	41,44,49,50	7
4	PG4	GGG	203	13/13	0.81	0.26	50,52,55,55	13
6	PEG	BBB	216	7/7	0.81	0.34	39,43,45,45	7
5	PGE	NNN	212	10/10	0.81	0.20	46,51,54,57	10
5	PGE	LLL	209	10/10	0.82	0.30	47,51,53,53	10
4	PG4	LLL	208	13/13	0.82	0.31	40,42,49,50	13
4	PG4	PPP	206	13/13	0.82	0.40	40,48,50,51	13
6	PEG	HHH	316	7/7	0.82	0.21	40,48,53,53	7
4	PG4	PPP	207	13/13	0.82	0.21	44,46,52,53	13
11	1PE	BBB	208	16/16	0.82	0.32	37,48,54,55	16
4	PG4	NNN	202	13/13	0.82	0.21	47,53,57,59	13
5	PGE	GGG	217	10/10	0.82	0.35	51,53,58,60	10
7	PO4	GGG	215	5/5	0.82	0.25	43,46,47,49	5
8	NO3	DDD	225	4/4	0.82	0.10	43,44,46,48	4
6	PEG	NNN	214	7/7	0.82	0.30	38,50,57,57	7
6	PEG	DDD	214	7/7	0.82	0.23	45,48,50,51	7
4	PG4	NNN	209	13/13	0.82	0.28	44,49,57,58	13
7	PO4	KKK	213	5/5	0.82	0.19	42,46,49,49	5
6	PEG	III	210	7/7	0.83	0.25	48,48,49,49	7
4	PG4	AAA	204	13/13	0.83	0.26	46,51,60,61	13
4	PG4	HHH	307	13/13	0.83	0.27	39,43,46,48	13
6	PEG	LLL	218[A]	7/7	0.83	0.33	40,44,46,46	7
6	PEG	OOO	210	7/7	0.83	0.22	40,42,43,43	7
11	1PE	HHH	301	16/16	0.83	0.25	43,48,51,52	16

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PEG	LLL	218[B]	7/7	0.83	0.33	45,48,50,50	7
7	PO4	KKK	214	5/5	0.83	0.17	50,50,52,56	5
6	PEG	LLL	213	7/7	0.83	0.20	46,49,52,53	7
12	P33	DDD	205	22/22	0.83	0.22	39,51,57,58	22
6	PEG	MMM	210	7/7	0.83	0.24	50,51,54,54	7
14	EDO	DDD	218	4/4	0.83	0.39	38,38,39,39	4
8	NO3	III	218	4/4	0.83	0.16	41,41,46,48	4
6	PEG	PPP	214	7/7	0.83	0.31	42,48,50,50	7
6	PEG	LLL	214	7/7	0.83	0.30	48,49,50,51	7
6	PEG	PPP	209	7/7	0.84	0.30	47,47,50,51	7
6	PEG	FFF	218	7/7	0.84	0.25	40,43,46,47	7
6	PEG	CCC	212	7/7	0.84	0.23	54,56,58,59	7
4	PG4	FFF	210	13/13	0.84	0.23	43,51,55,56	13
5	PGE	GGG	208	10/10	0.84	0.21	34,50,56,57	10
4	PG4	LLL	207	13/13	0.84	0.25	39,42,48,48	13
4	PG4	JJJ	309	13/13	0.84	0.27	44,47,60,61	13
7	PO4	FFF	224	5/5	0.84	0.29	51,51,52,54	5
5	PGE	HHH	311	10/10	0.84	0.27	47,54,60,61	10
4	PG4	FFF	202	13/13	0.84	0.28	42,44,46,46	13
8	NO3	PPP	219	4/4	0.84	0.18	39,40,41,42	4
5	PGE	AAA	208	10/10	0.84	0.36	41,43,45,46	10
6	PEG	MMM	208	7/7	0.85	0.27	42,46,49,50	7
4	PG4	MMM	203	13/13	0.85	0.26	38,44,55,57	13
6	PEG	PPP	213	7/7	0.85	0.24	43,47,50,50	7
10	PE8	BBB	205	25/25	0.85	0.20	44,50,68,71	25
5	PGE	LLL	210	10/10	0.85	0.43	43,45,47,48	10
7	PO4	AAA	215	5/5	0.85	0.27	49,51,53,53	5
6	PEG	HHH	314	7/7	0.85	0.33	46,47,48,50	7
7	PO4	DDD	220	5/5	0.85	0.23	44,48,52,53	5
11	1PE	JJJ	302	16/16	0.85	0.22	37,45,48,49	16
4	PG4	AAA	203	13/13	0.85	0.23	42,46,51,51	13
5	PGE	PPP	208	10/10	0.85	0.22	45,50,51,51	10
6	PEG	BBB	211	7/7	0.85	0.31	46,48,52,52	7
7	PO4	HHH	324	5/5	0.85	0.34	40,42,45,47	5
5	PGE	NNN	211	10/10	0.85	0.32	43,43,48,49	10
5	PGE	CCC	204	10/10	0.85	0.18	43,53,58,58	10
6	PEG	PPP	201	7/7	0.85	0.34	43,47,51,52	7
14	EDO	FFF	219	4/4	0.85	0.22	49,50,53,53	4
14	EDO	HHH	320	4/4	0.85	0.23	51,52,52,52	4
5	PGE	III	206	10/10	0.85	0.37	47,49,50,51	10
6	PEG	FFF	217	7/7	0.85	0.33	43,45,46,46	7
11	1PE	BBB	206	16/16	0.86	0.25	40,44,49,50	16

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PGE	EEE	206	10/10	0.86	0.18	43,50,56,57	10
4	PG4	KKK	203	13/13	0.86	0.20	41,55,66,67	13
5	PGE	GGG	206	10/10	0.86	0.27	45,52,54,54	10
7	PO4	NNN	221	5/5	0.86	0.20	49,50,50,52	5
6	PEG	CCC	215	7/7	0.86	0.21	35,38,38,38	7
11	1PE	JJJ	307	16/16	0.86	0.17	41,43,48,48	16
9	RWB	BBB	204	38/38	0.86	0.25	34,48,59,61	38
6	PEG	HHH	318	7/7	0.86	0.34	41,44,47,47	7
5	PGE	HHH	309	10/10	0.87	0.21	46,49,52,52	10
6	PEG	HHH	315	7/7	0.87	0.23	42,45,46,48	7
5	PGE	FFF	211	10/10	0.87	0.26	42,43,48,49	10
5	PGE	AAA	206	10/10	0.87	0.22	37,42,55,56	10
12	P33	FFF	207	22/22	0.87	0.17	43,46,65,69	22
7	PO4	DDD	222	5/5	0.87	0.31	48,49,51,52	5
12	P33	JJJ	306	22/22	0.87	0.19	44,48,73,75	22
13	P6G	DDD	206	19/19	0.87	0.27	35,37,54,54	19
4	PG4	DDD	209	13/13	0.87	0.25	48,52,53,55	13
5	PGE	CCC	207	10/10	0.87	0.19	46,51,57,59	10
6	PEG	III	208	7/7	0.87	0.25	44,44,45,46	7
6	PEG	GGG	210	7/7	0.87	0.31	48,49,51,51	7
7	PO4	III	214	5/5	0.87	0.19	45,48,56,59	5
14	EDO	NNN	217	4/4	0.87	0.15	48,49,50,51	4
14	EDO	NNN	218	4/4	0.87	0.29	44,44,45,45	4
5	PGE	EEE	207	10/10	0.87	0.16	47,49,55,56	10
6	PEG	DDD	215	7/7	0.88	0.41	53,56,57,59	7
4	PG4	LLL	206	13/13	0.88	0.18	45,49,64,66	13
6	PEG	GGG	209	7/7	0.88	0.23	43,47,57,59	7
7	PO4	FFF	223	5/5	0.88	0.23	42,46,47,47	5
5	PGE	MMM	206	10/10	0.88	0.17	44,48,51,52	10
6	PEG	III	212	7/7	0.88	0.22	34,37,41,42	7
6	PEG	CCC	211	7/7	0.88	0.29	42,42,46,47	7
6	PEG	KKK	209	7/7	0.88	0.17	42,52,55,55	7
6	PEG	GGG	213	7/7	0.88	0.21	46,47,50,52	7
6	PEG	KKK	211	7/7	0.88	0.28	43,44,46,47	7
7	PO4	JJJ	317	5/5	0.88	0.16	43,44,45,49	5
7	PO4	JJJ	319	5/5	0.88	0.16	62,62,65,67	5
4	PG4	FFF	209	13/13	0.89	0.20	41,44,48,51	13
7	PO4	BBB	220	5/5	0.89	0.17	46,47,52,53	5
5	PGE	EEE	204	10/10	0.89	0.24	40,45,49,49	10
6	PEG	KKK	212	7/7	0.89	0.18	41,42,43,43	7
8	NO3	KKK	216	4/4	0.89	0.14	42,42,49,49	4
5	PGE	LLL	226	10/10	0.89	0.18	46,49,50,50	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NO3	LLL	224	4/4	0.89	0.12	43,45,45,46	4
6	PEG	FFF	216	7/7	0.89	0.27	43,44,45,45	7
6	PEG	CCC	213	7/7	0.89	0.20	38,40,44,44	7
4	PG4	NNN	201	13/13	0.89	0.22	43,48,62,62	13
14	EDO	DDD	217	4/4	0.89	0.22	37,38,38,39	4
5	PGE	MMM	207	10/10	0.89	0.23	41,42,43,45	10
9	RWB	LLL	204	38/38	0.89	0.20	38,47,69,70	38
5	PGE	FFF	213	10/10	0.89	0.22	41,42,53,53	10
4	PG4	GGG	204	13/13	0.89	0.21	30,35,56,59	13
6	PEG	GGG	212	7/7	0.89	0.25	41,42,44,44	7
6	PEG	JJJ	313	7/7	0.89	0.28	41,44,46,47	7
5	PGE	GGG	207	10/10	0.89	0.22	41,46,49,50	10
6	PEG	BBB	223	7/7	0.89	0.35	42,46,51,51	7
14	EDO	PPP	215	4/4	0.89	0.25	51,52,52,53	4
7	PO4	CCC	216	5/5	0.90	0.23	46,47,51,52	5
14	EDO	EEE	209	4/4	0.90	0.33	53,53,54,54	4
7	PO4	PPP	216	5/5	0.90	0.17	48,48,51,52	5
7	PO4	FFF	222	5/5	0.90	0.24	46,46,47,50	5
8	NO3	EEE	211	4/4	0.90	0.27	40,41,42,45	4
5	PGE	AAA	207	10/10	0.90	0.18	45,47,51,53	10
11	1PE	EEE	203	16/16	0.90	0.18	47,60,64,67	16
6	PEG	KKK	208	7/7	0.90	0.18	39,41,41,42	7
4	PG4	FFF	208	13/13	0.90	0.23	40,43,45,45	13
7	PO4	HHH	322	5/5	0.90	0.26	37,39,41,41	5
6	PEG	NNN	216	7/7	0.91	0.38	42,46,46,48	7
7	PO4	BBB	218	5/5	0.91	0.27	43,45,48,51	5
5	PGE	III	205	10/10	0.91	0.25	42,43,45,45	10
14	EDO	EEE	208	4/4	0.91	0.17	38,39,40,41	4
6	PEG	FFF	215	7/7	0.91	0.19	43,50,52,54	7
7	PO4	KKK	215	5/5	0.91	0.19	45,47,50,51	5
6	PEG	AAA	212	7/7	0.91	0.21	44,45,47,48	7
14	EDO	HHH	319	4/4	0.91	0.28	38,39,41,42	4
12	P33	DDD	204	22/22	0.91	0.17	44,47,65,67	22
8	NO3	KKK	217	4/4	0.91	0.14	36,39,41,41	4
7	PO4	CCC	220	5/5	0.91	0.17	43,47,49,50	5
12	P33	HHH	305	22/22	0.91	0.15	45,48,56,57	22
7	PO4	GGG	214	5/5	0.91	0.24	42,49,49,52	5
7	PO4	JJJ	318	5/5	0.91	0.15	43,44,45,49	5
5	PGE	KKK	207	10/10	0.92	0.34	40,43,46,46	10
7	PO4	DDD	223	5/5	0.92	0.18	45,52,53,53	5
5	PGE	III	204	10/10	0.92	0.17	44,47,55,59	10
7	PO4	FFF	221	5/5	0.92	0.19	39,42,44,45	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PEG	DDD	213	7/7	0.92	0.18	42,43,54,58	7
4	PG4	MMM	204	13/13	0.92	0.18	44,49,51,52	13
3	PEB	PPP	204	43/43	0.92	0.12	49,60,81,87	0
8	NO3	HHH	326	4/4	0.92	0.10	47,47,49,51	4
7	PO4	AAA	214	5/5	0.92	0.24	47,47,49,49	5
11	1PE	FFF	201	16/16	0.92	0.20	38,51,63,64	16
3	PEB	OOO	202	43/43	0.92	0.13	56,63,73,74	0
8	NO3	JJJ	322	4/4	0.92	0.13	41,45,46,46	4
3	PEB	PPP	202	43/43	0.92	0.14	49,55,74,88	0
6	PEG	JJJ	312	7/7	0.92	0.27	43,44,46,46	7
14	EDO	LLL	219	4/4	0.92	0.24	33,34,34,35	4
5	PGE	AAA	211	10/10	0.92	0.22	27,28,29,31	10
6	PEG	FFF	214	7/7	0.92	0.28	40,43,48,48	7
5	PGE	HHH	327	10/10	0.92	0.18	44,50,66,67	10
6	PEG	BBB	212	7/7	0.92	0.21	40,42,51,51	7
6	PEG	AAA	213	7/7	0.93	0.20	37,37,38,40	7
3	PEB	PPP	203	43/43	0.93	0.15	55,65,80,97	0
14	EDO	III	213	4/4	0.93	0.18	43,43,45,45	4
3	PEB	III	203	43/43	0.93	0.11	47,52,58,60	0
6	PEG	DDD	227	7/7	0.93	0.13	45,46,51,54	7
6	PEG	CCC	210	7/7	0.93	0.25	41,42,43,43	7
3	PEB	KKK	202	43/43	0.93	0.13	45,54,59,63	0
6	PEG	BBB	214	7/7	0.93	0.15	43,44,46,47	7
8	NO3	GGG	216	4/4	0.93	0.14	41,42,44,44	4
15	PE5	NNN	206	27/27	0.93	0.18	33,43,71,74	27
5	PGE	CCC	205	10/10	0.94	0.13	45,46,55,63	0
8	NO3	LLL	222	4/4	0.94	0.18	43,46,46,47	4
3	PEB	OOO	201	43/43	0.94	0.12	45,51,56,60	0
5	PGE	CCC	206	10/10	0.95	0.13	45,48,58,58	10
7	PO4	NNN	220	5/5	0.95	0.20	41,46,47,48	5
5	PGE	LLL	225	10/10	0.95	0.14	41,47,62,64	10
3	PEB	EEE	202	43/43	0.95	0.12	45,55,60,64	0
3	PEB	AAA	202	43/43	0.95	0.10	41,45,52,64	0
5	PGE	JJJ	301	10/10	0.95	0.15	37,44,56,56	10
3	PEB	JJJ	304	43/43	0.95	0.10	36,39,46,59	0
7	PO4	PPP	217	5/5	0.95	0.19	31,33,35,35	5
7	PO4	FFF	220	5/5	0.95	0.10	44,47,48,51	5
3	PEB	BBB	202	43/43	0.95	0.10	32,36,44,55	0
3	PEB	LLL	202	43/43	0.95	0.10	36,41,52,72	0
3	PEB	NNN	204	43/43	0.95	0.10	34,40,53,68	0
6	PEG	BBB	215	7/7	0.95	0.19	46,49,49,50	7
3	PEB	EEE	201	43/43	0.95	0.10	33,36,42,45	0

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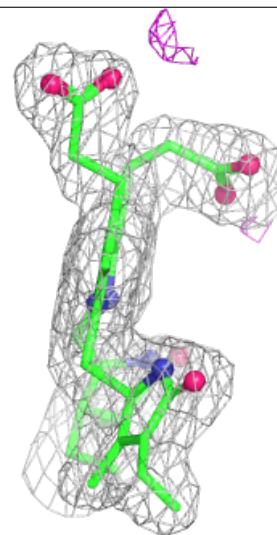
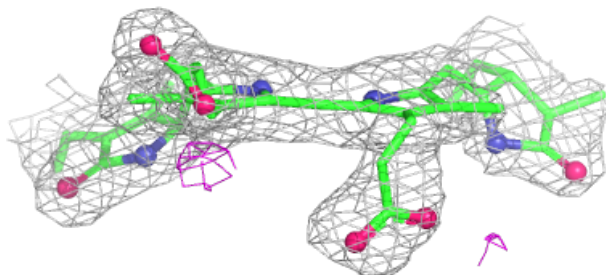
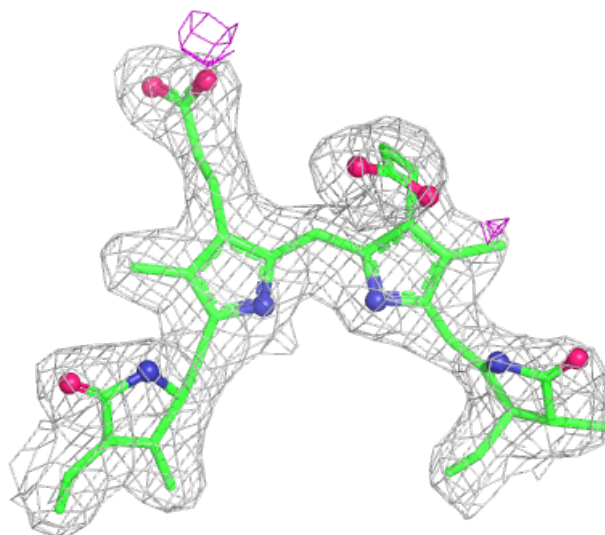
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEB	DDD	201	43/43	0.96	0.10	30,35,55,69	0
3	PEB	LLL	203	43/43	0.96	0.09	30,35,48,51	0
7	PO4	LLL	220	5/5	0.96	0.14	46,47,48,51	5
3	PEB	MMM	202	43/43	0.96	0.12	44,50,56,58	0
3	PEB	NNN	203	43/43	0.96	0.10	40,47,58,72	0
3	PEB	DDD	202	43/43	0.96	0.10	37,40,47,60	0
3	PEB	NNN	205	43/43	0.96	0.09	37,42,46,50	0
3	PEB	BBB	201	43/43	0.96	0.10	32,37,49,64	0
3	PEB	AAA	201	43/43	0.96	0.09	32,35,41,43	0
3	PEB	FFF	205	43/43	0.96	0.09	36,41,47,58	0
3	PEB	FFF	206	43/43	0.96	0.09	33,37,44,51	0
7	PO4	HHH	321	5/5	0.96	0.15	35,37,40,40	5
3	PEB	GGG	202	43/43	0.96	0.12	45,51,57,60	0
3	PEB	HHH	302	43/43	0.96	0.10	33,37,44,63	0
3	PEB	HHH	303	43/43	0.96	0.09	37,41,51,58	0
3	PEB	HHH	304	43/43	0.96	0.09	31,38,43,50	0
3	PEB	BBB	203	43/43	0.96	0.08	31,36,42,46	0
7	PO4	JJJ	315	5/5	0.96	0.16	48,51,52,53	5
7	PO4	JJJ	316	5/5	0.96	0.19	43,43,46,49	5
3	PEB	CCC	201	43/43	0.96	0.10	32,37,40,42	0
3	PEB	JJJ	305	43/43	0.96	0.09	32,36,41,42	0
3	PEB	KKK	201	43/43	0.96	0.09	32,37,40,42	0
3	PEB	CCC	202	43/43	0.96	0.11	34,41,47,50	0
7	PO4	DDD	221	5/5	0.96	0.12	47,51,53,53	5
3	PEB	DDD	203	43/43	0.97	0.08	33,36,42,48	0
3	PEB	III	202	43/43	0.97	0.09	31,35,41,43	0
7	PO4	HHH	323	5/5	0.97	0.12	40,41,43,45	5
3	PEB	FFF	204	43/43	0.97	0.10	32,38,51,73	0
3	PEB	LLL	201	43/43	0.97	0.09	32,36,47,68	0
3	PEB	JJJ	303	43/43	0.97	0.10	34,38,49,75	0
7	PO4	DDD	219	5/5	0.97	0.17	37,39,40,41	5
3	PEB	GGG	201	43/43	0.97	0.09	33,37,41,49	0
3	PEB	MMM	201	43/43	0.97	0.09	36,39,43,49	0
7	PO4	NNN	222	5/5	0.97	0.20	40,42,42,46	5
7	PO4	BBB	217	5/5	0.97	0.12	42,43,44,45	5
7	PO4	LLL	221	5/5	0.98	0.14	42,43,46,48	5
7	PO4	BBB	219	5/5	0.99	0.12	41,41,44,45	5

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.

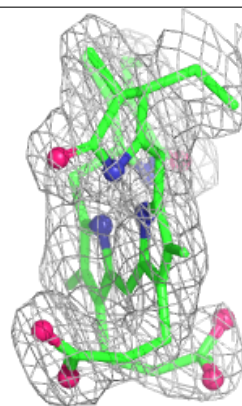
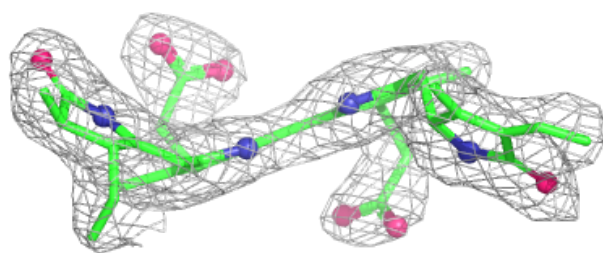
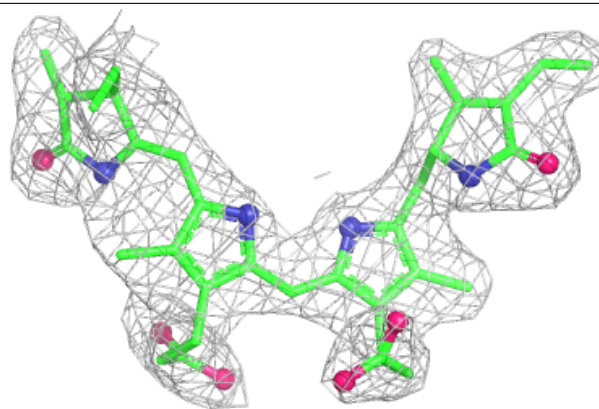
**Electron density around PEB PPP 204:**

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



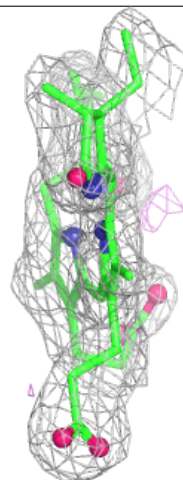
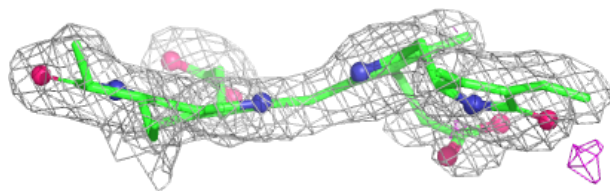
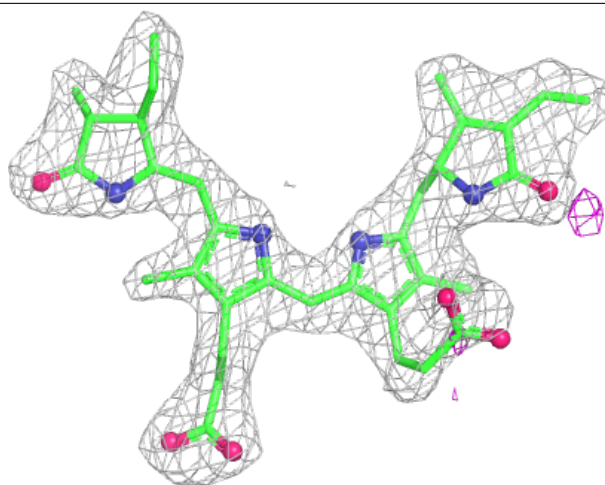
**Electron density around PEB OOO 202:**

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



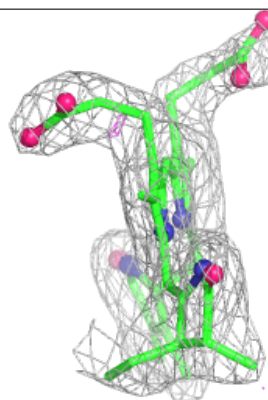
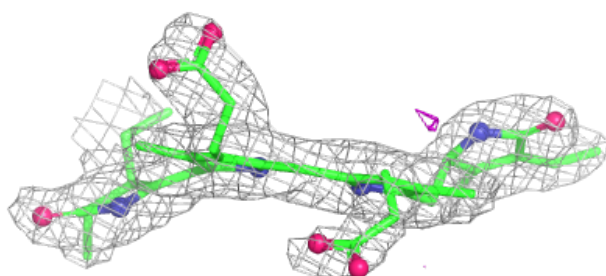
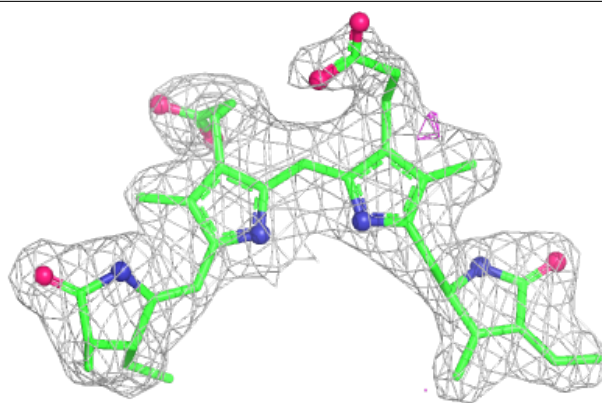
**Electron density around PEB PPP 202:**

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

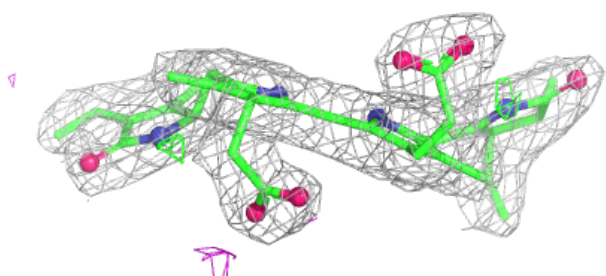
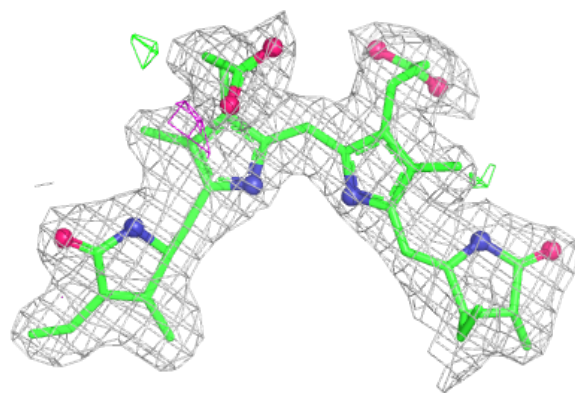


**Electron density around PEB PPP 203:**

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

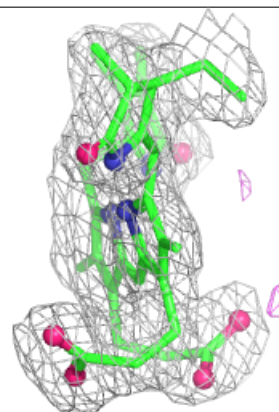
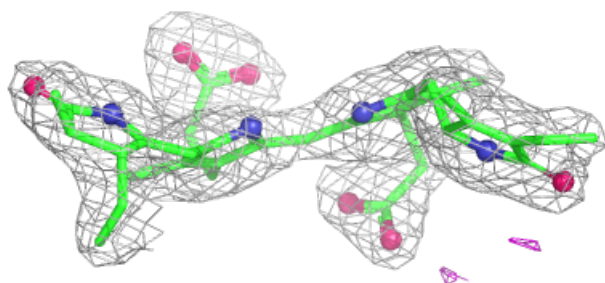
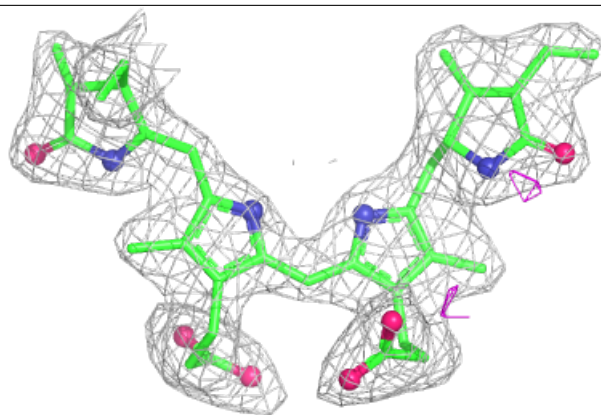
**Electron density around PEB III 203:**

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



**Electron density around PEB KKK 202:**

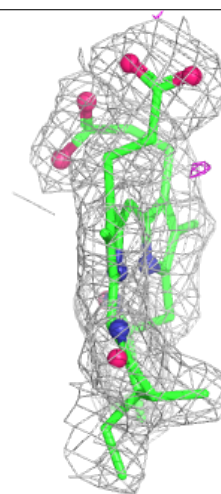
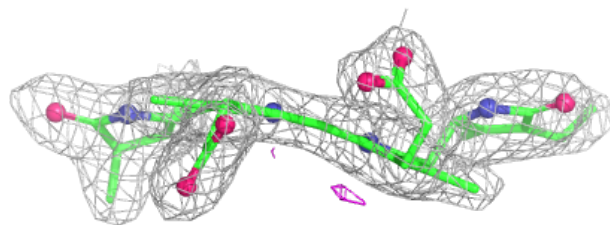
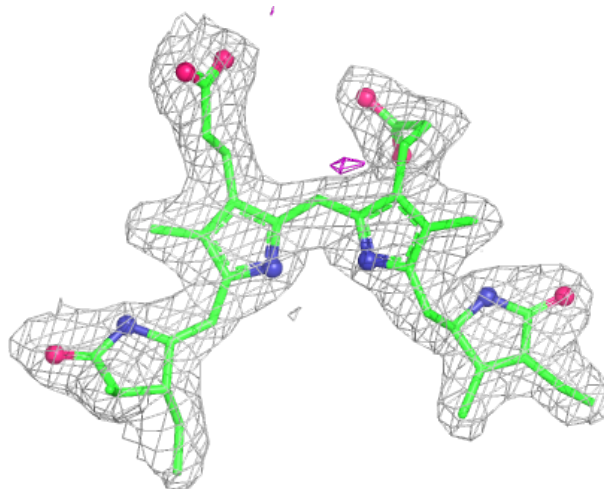
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





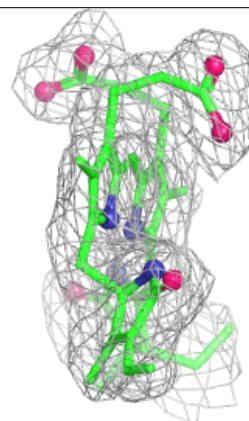
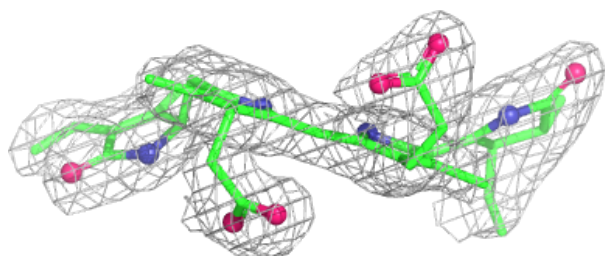
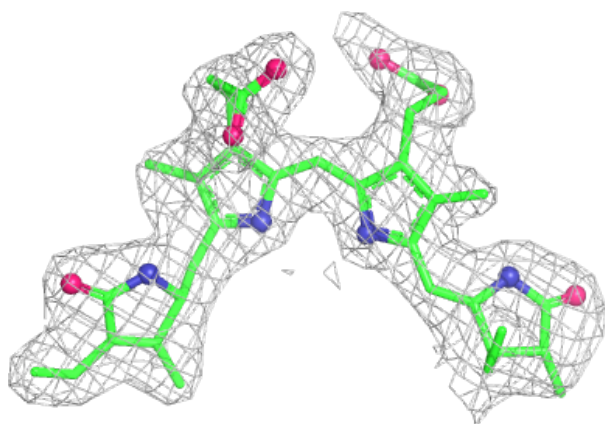
**Electron density around PEB OOO 201:**

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

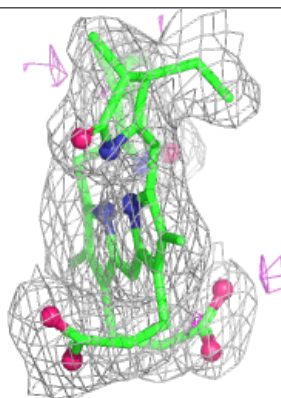
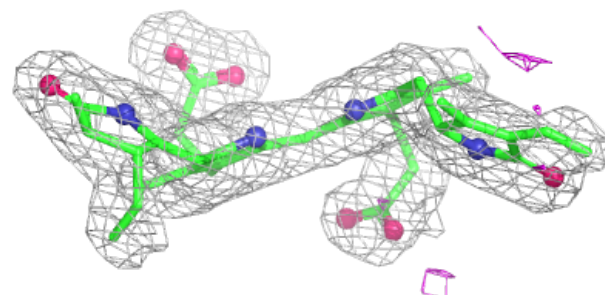
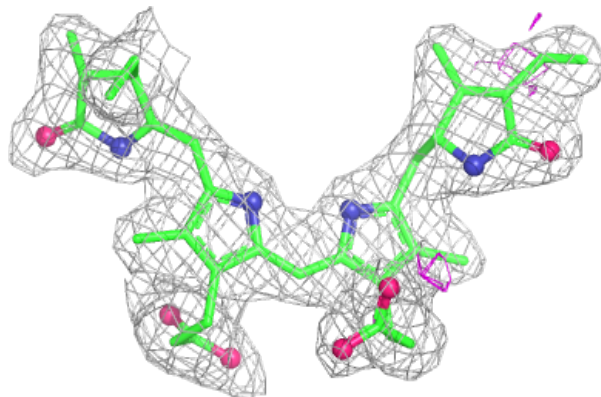


**Electron density around PEB EEE 202:**

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

**Electron density around PEB AAA 202:**

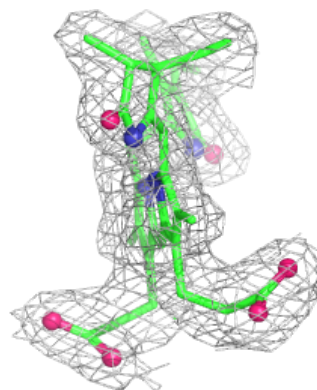
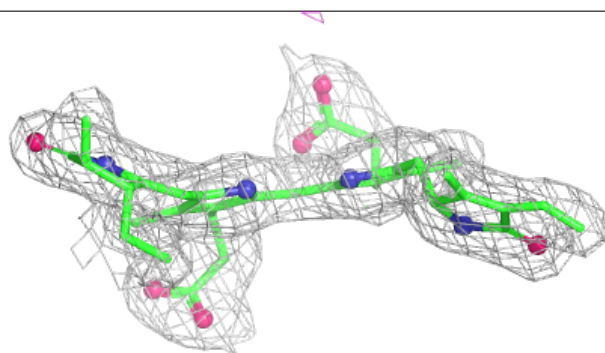
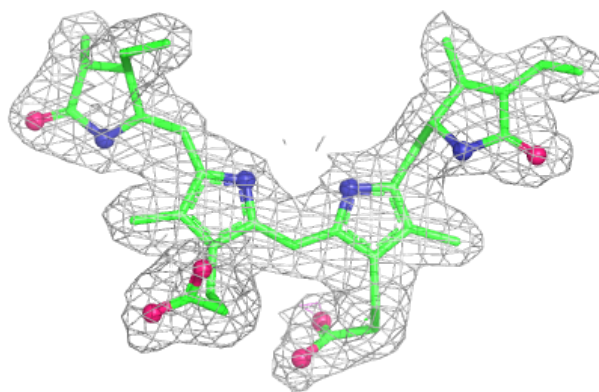
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



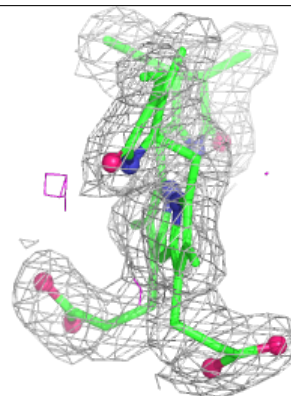
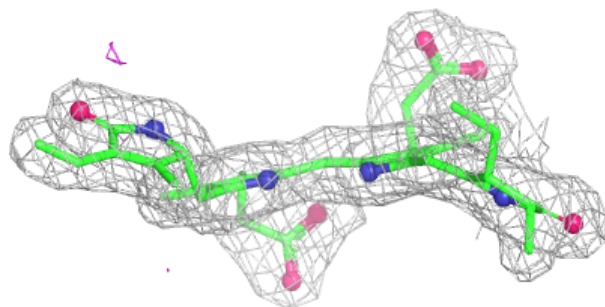
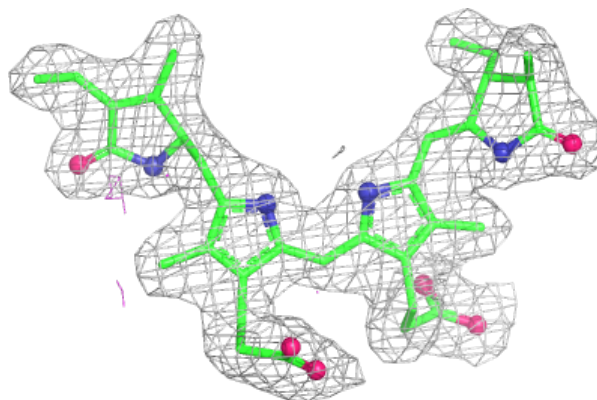


**Electron density around PEB JJJ 304:**

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

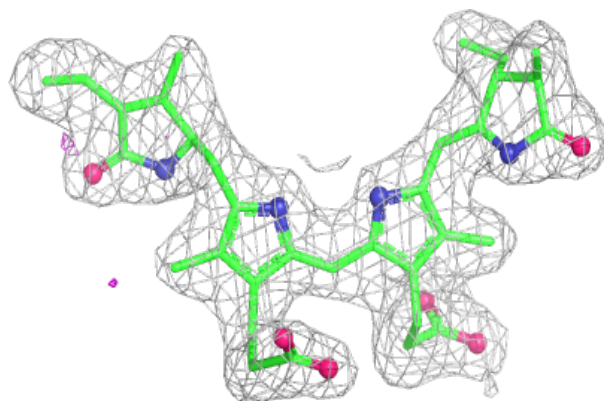
**Electron density around PEB BBB 202:**

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

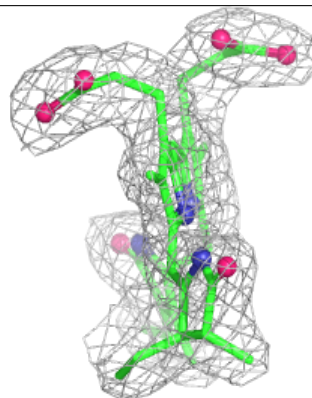
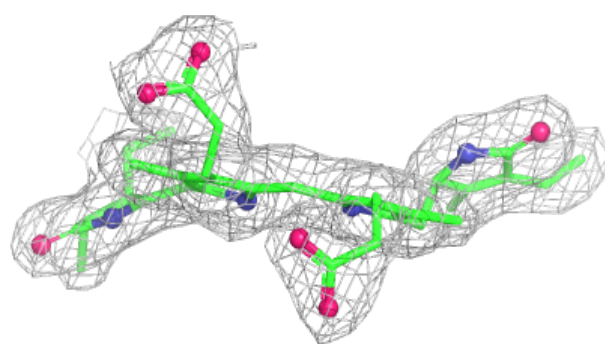
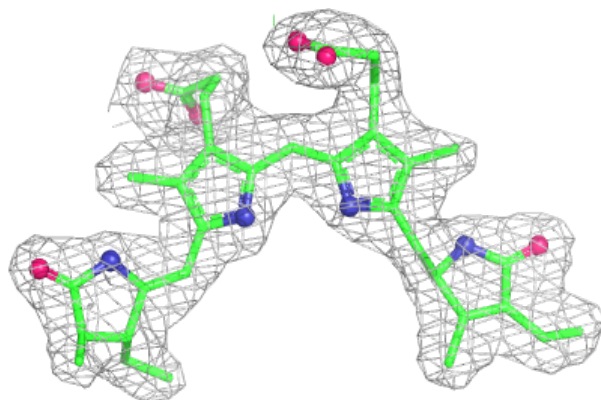


**Electron density around PEB LLL 202:**

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

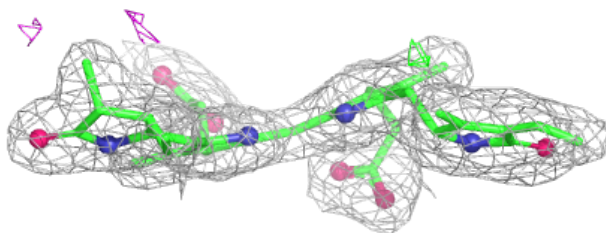
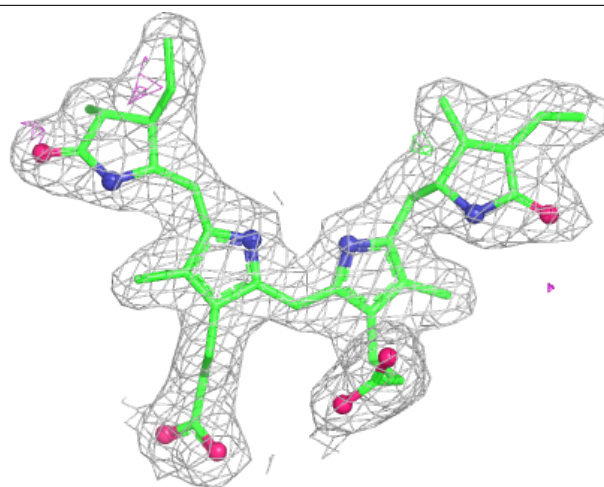
**Electron density around PEB NNN 204:**

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



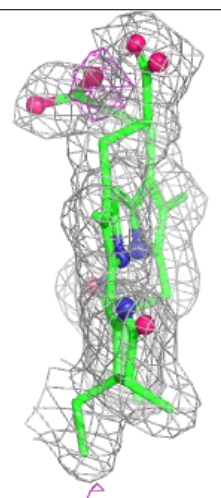
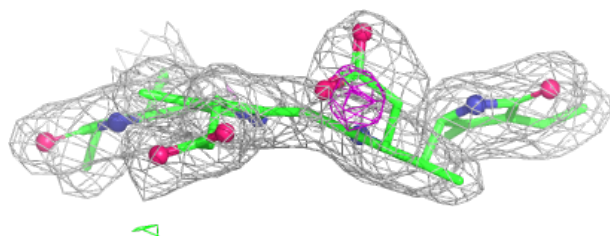
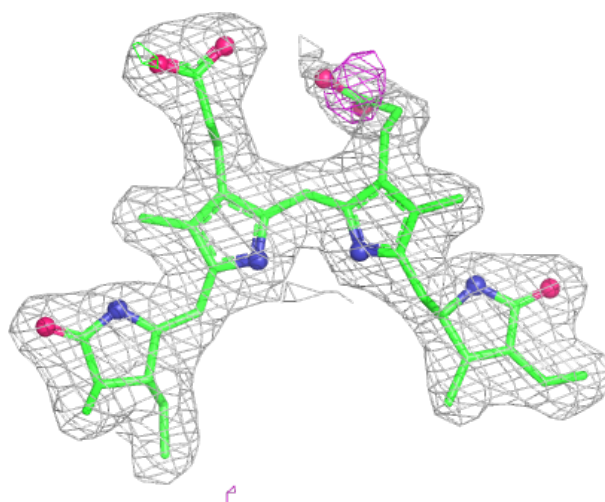
**Electron density around PEB EEE 201:**

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



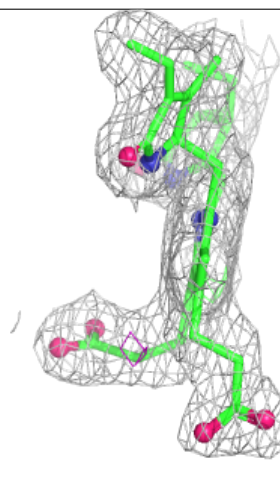
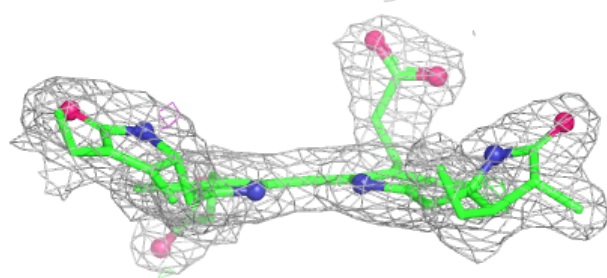
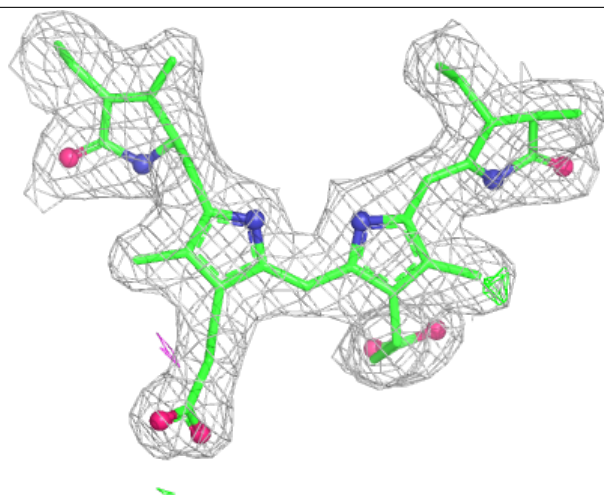
**Electron density around PEB DDD 201:**

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



**Electron density around PEB LLL 203:**

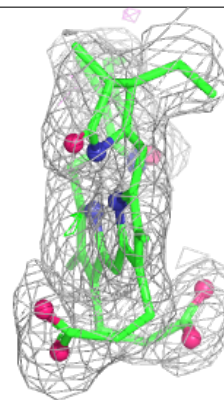
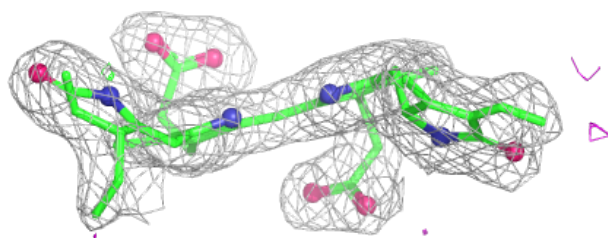
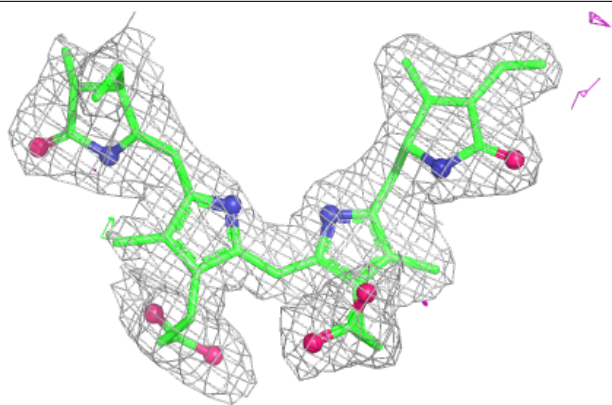
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





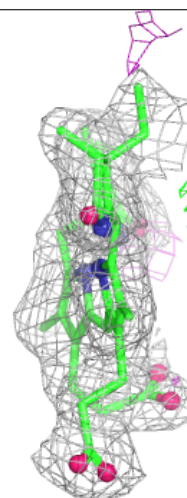
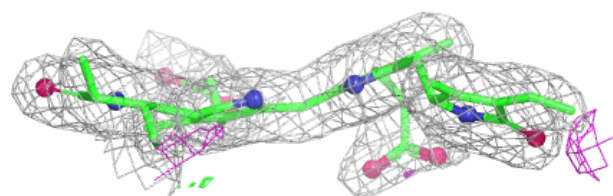
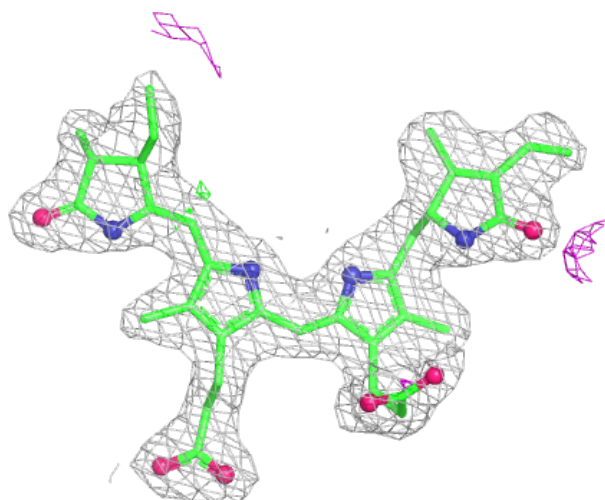
**Electron density around PEB MMM 202:**

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



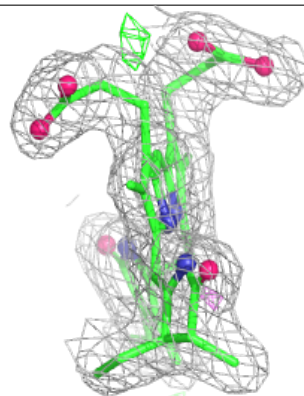
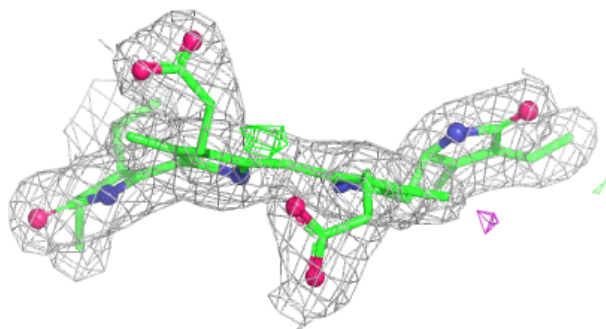
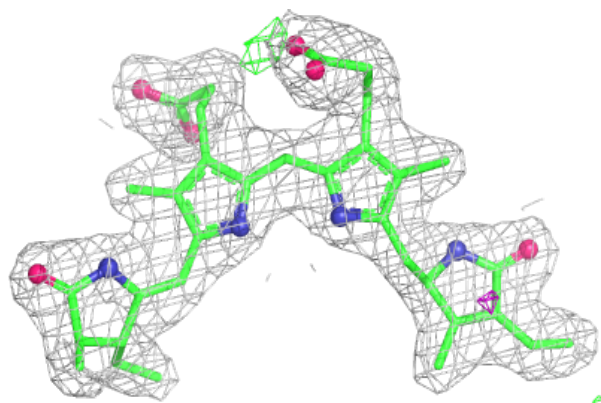
**Electron density around PEB NNN 203:**

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



**Electron density around PEB DDD 202:**

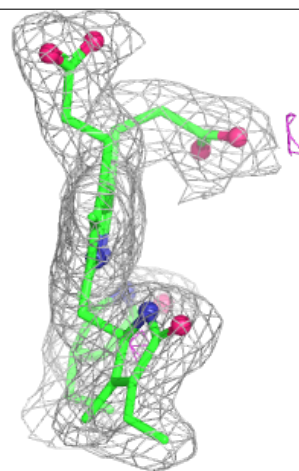
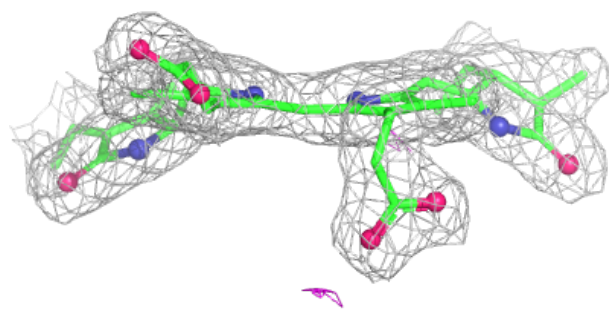
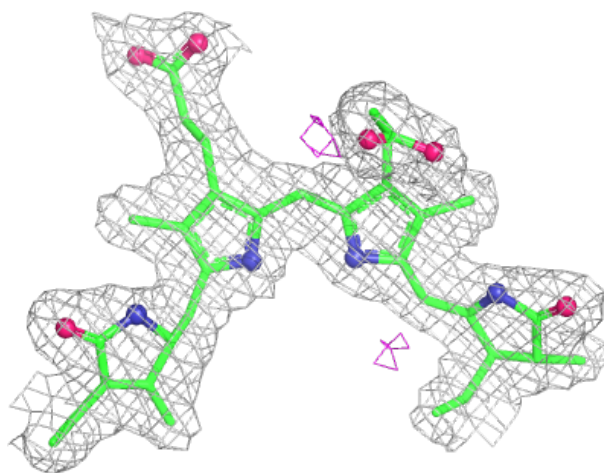
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





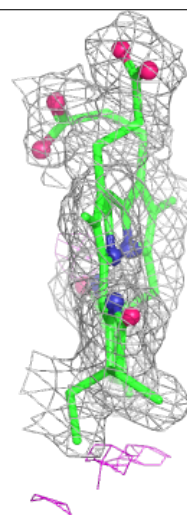
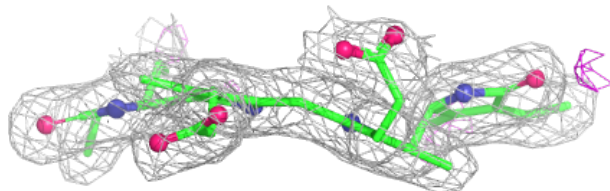
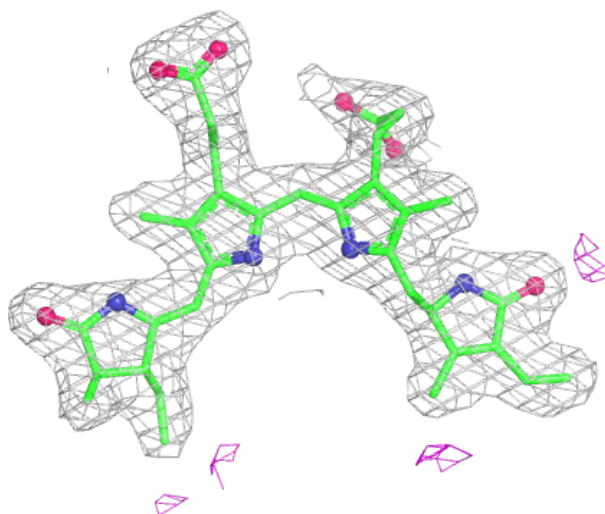
**Electron density around PEB NNN 205:**

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



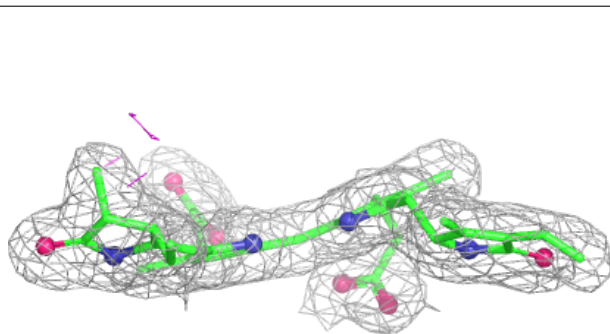
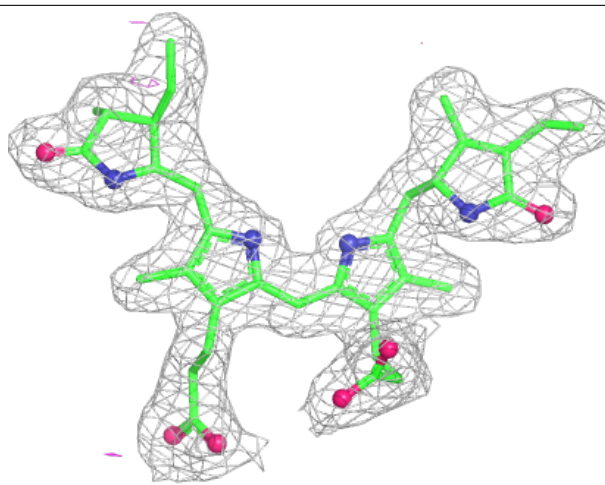
**Electron density around PEB BBB 201:**

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



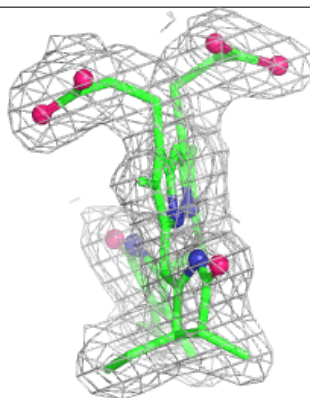
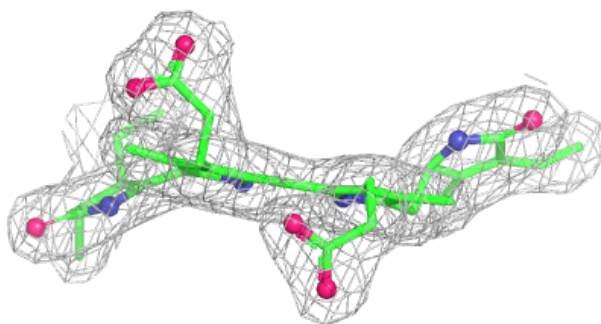
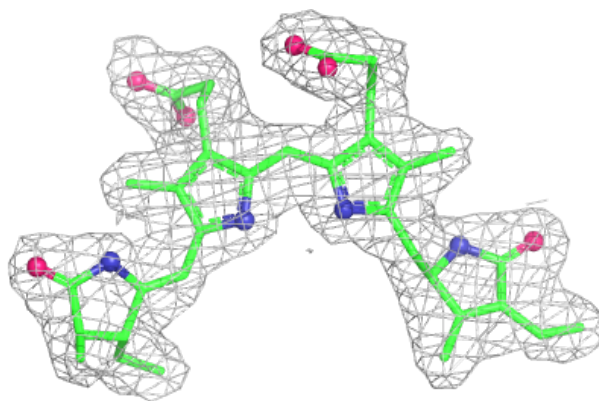
**Electron density around PEB AAA 201:**

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

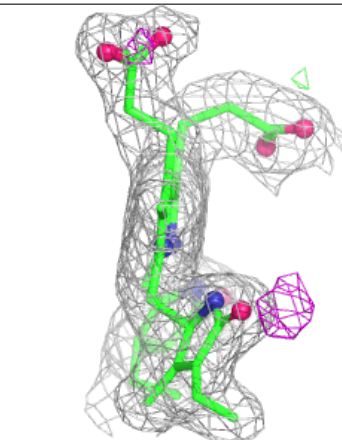
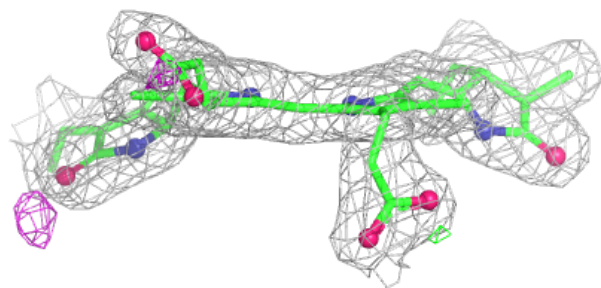
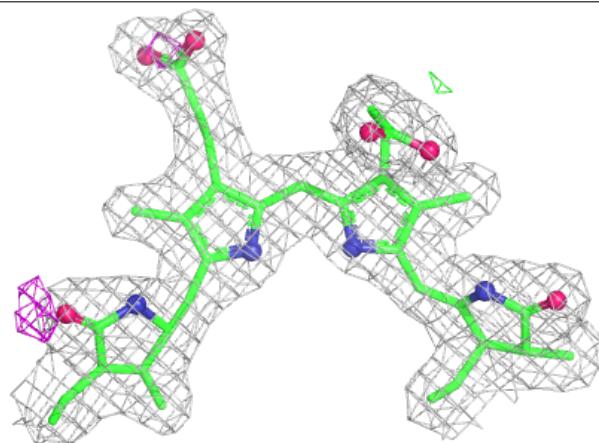


**Electron density around PEB FFF 205:**

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

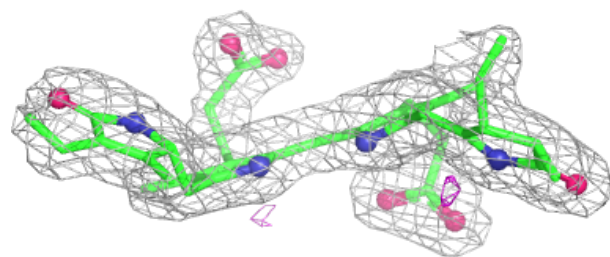
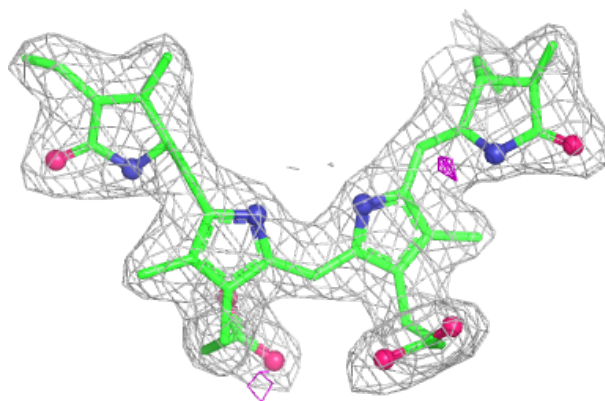
**Electron density around PEB FFF 206:**

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



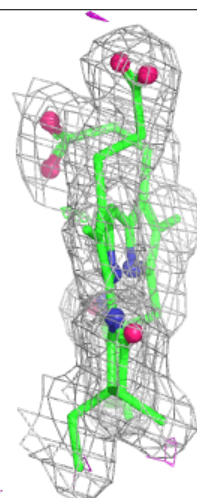
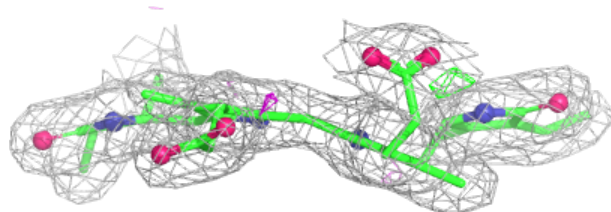
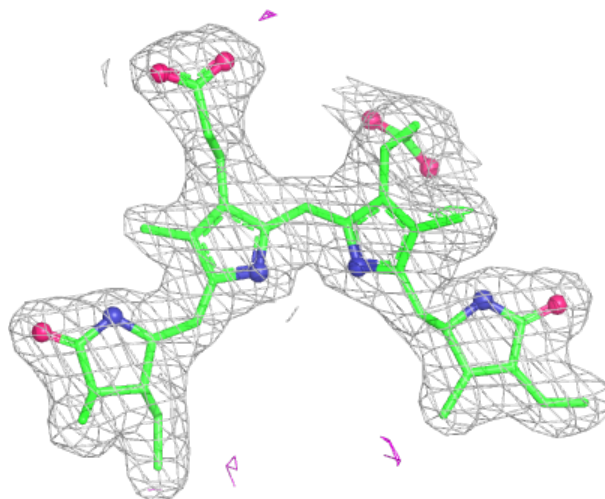
**Electron density around PEB GGG 202:**

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



**Electron density around PEB HHH 302:**

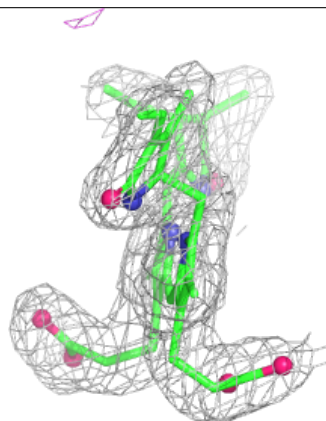
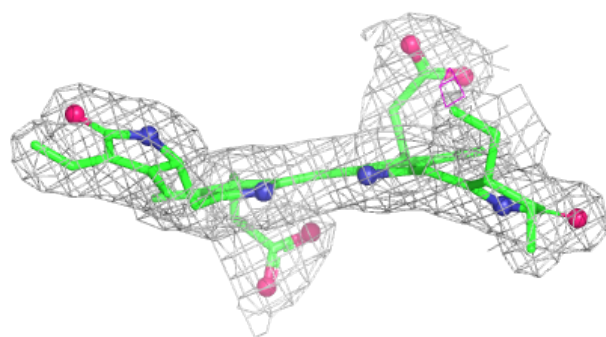
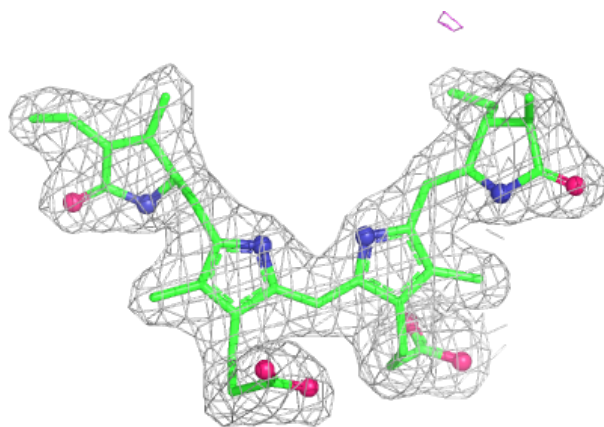
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





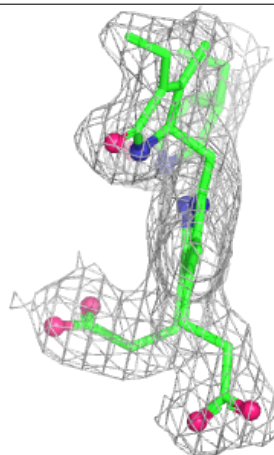
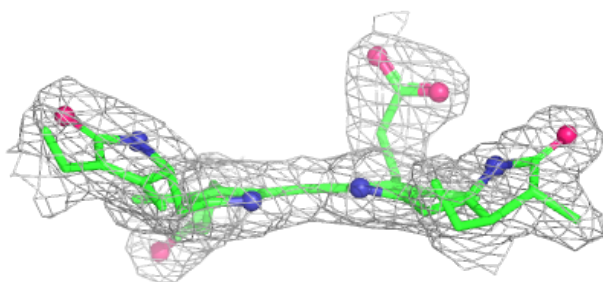
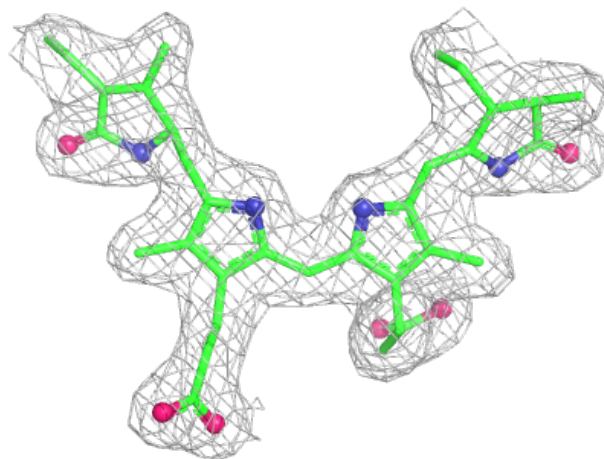
**Electron density around PEB HHH 303:**

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



**Electron density around PEB HHH 304:**

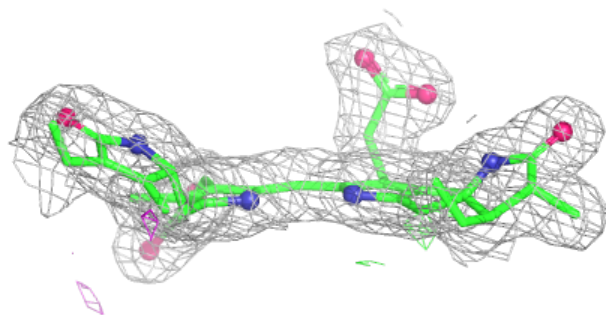
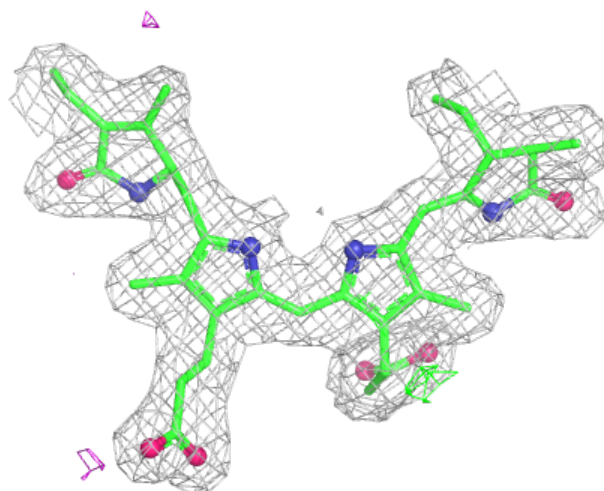
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





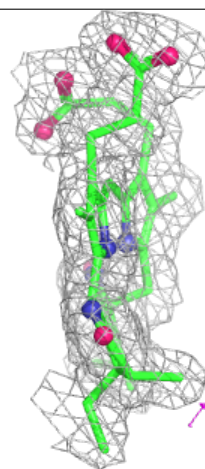
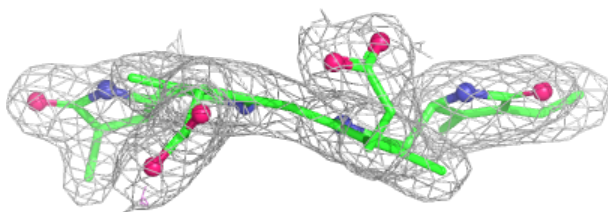
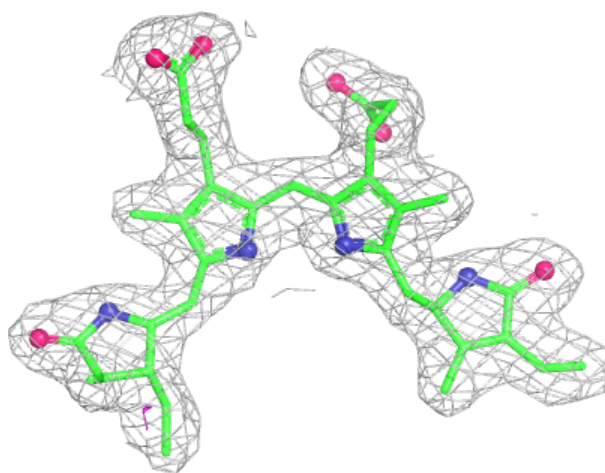
**Electron density around PEB BBB 203:**

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



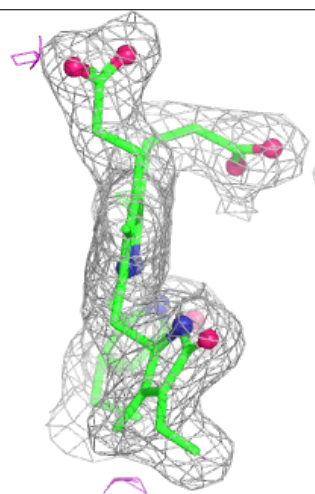
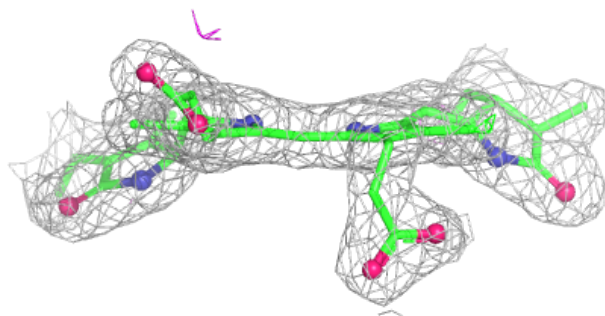
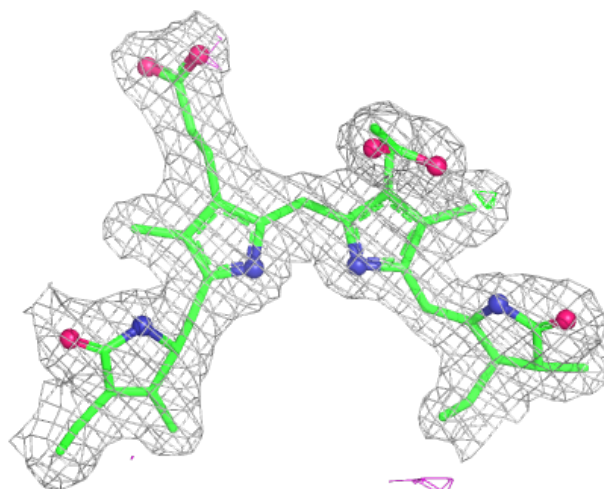
**Electron density around PEB CCC 201:**

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



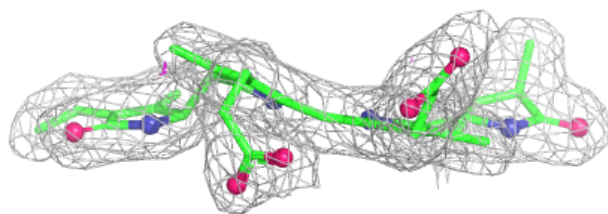
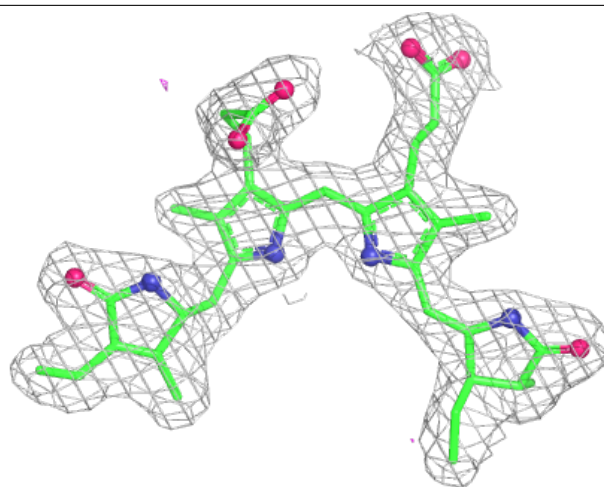
**Electron density around PEB JJJ 305:**

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



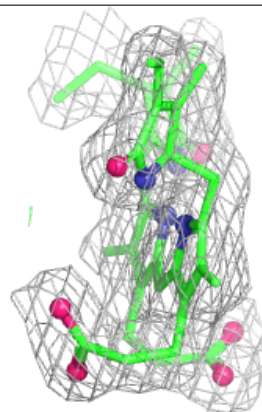
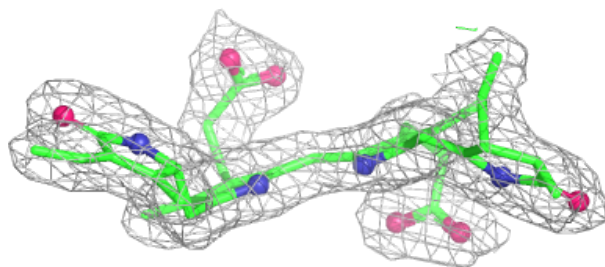
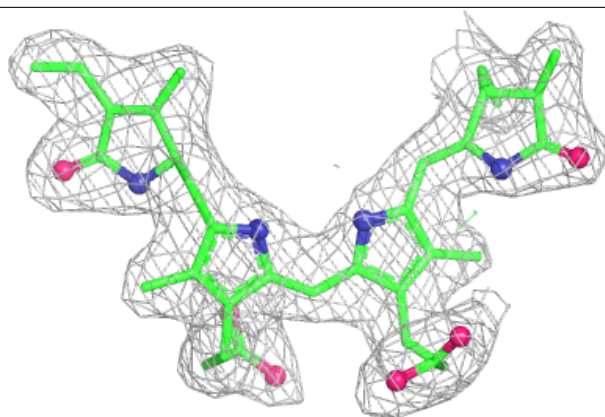
**Electron density around PEB KKK 201:**

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



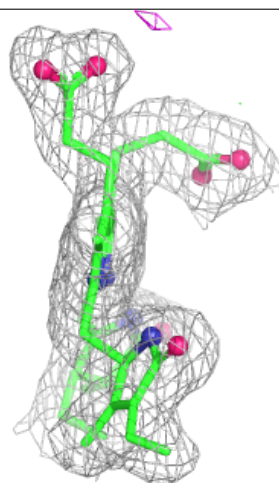
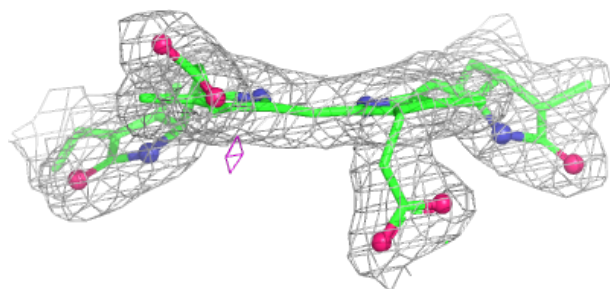
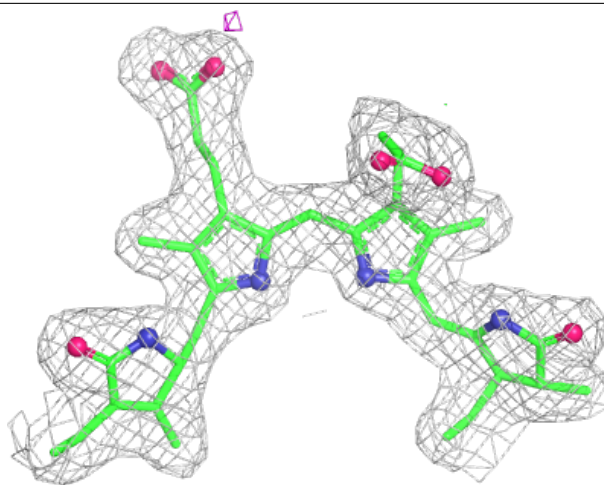
**Electron density around PEB CCC 202:**

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



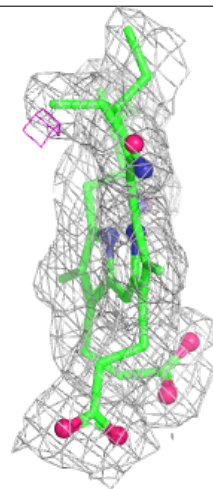
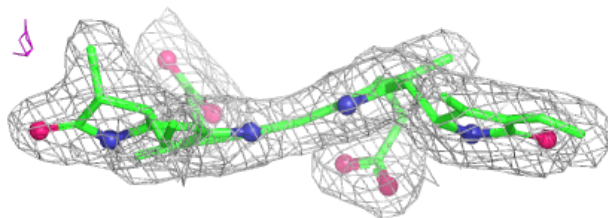
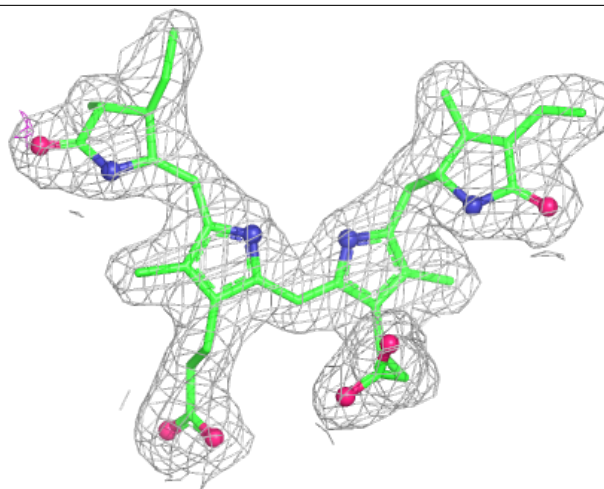
**Electron density around PEB DDD 203:**

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



**Electron density around PEB III 202:**

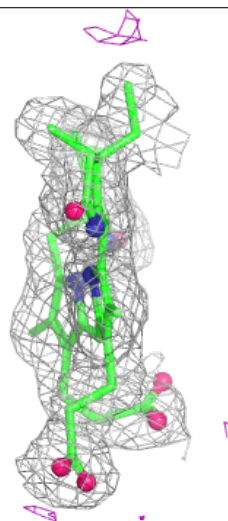
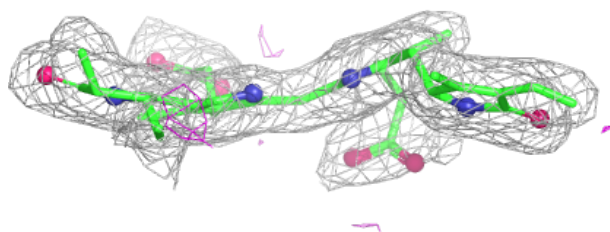
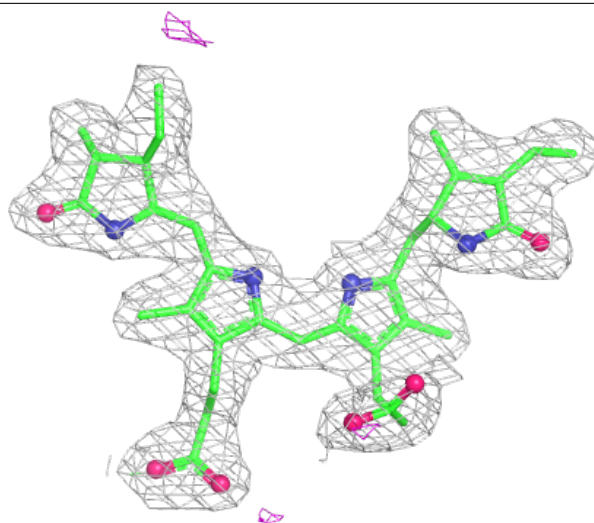
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PEB FFF 204:**

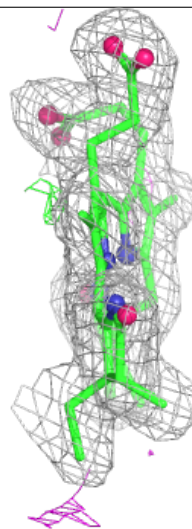
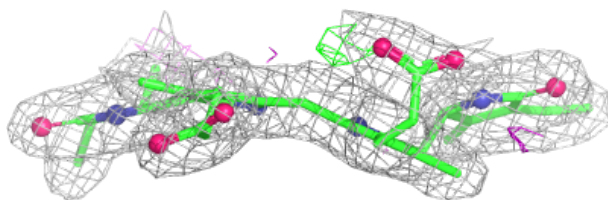
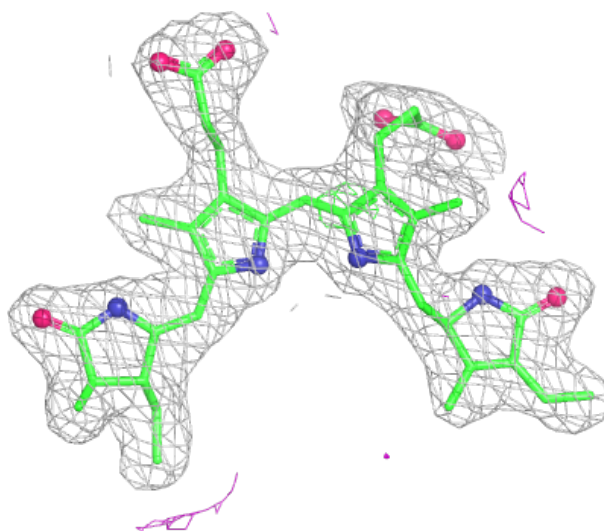
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





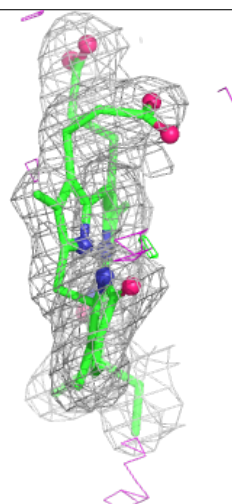
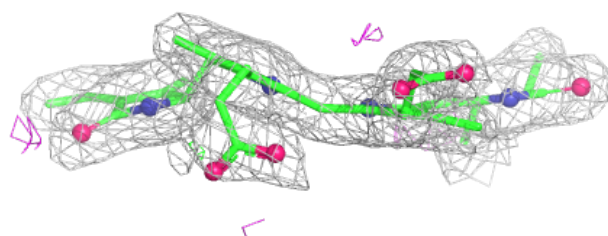
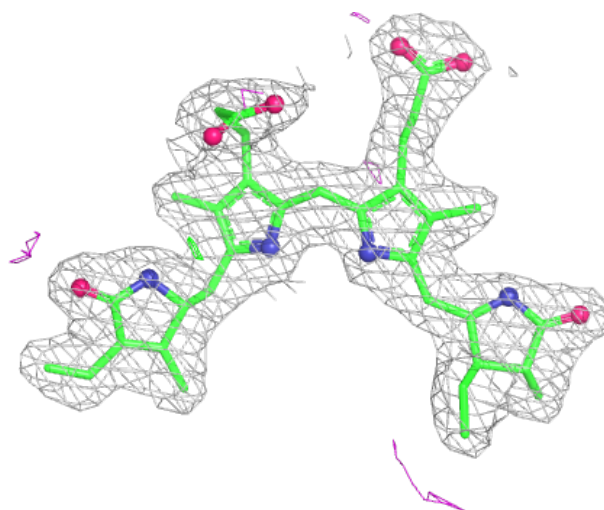
**Electron density around PEB LLL 201:**

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



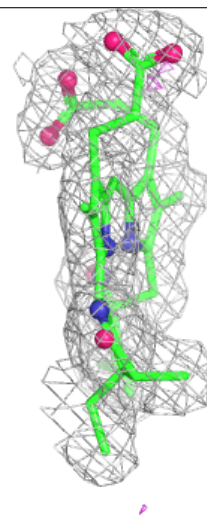
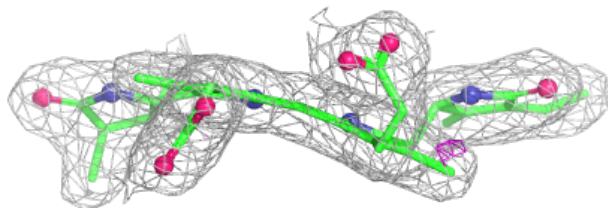
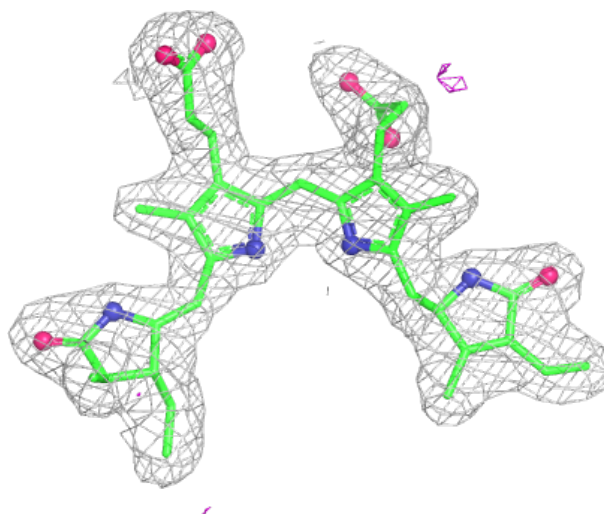
**Electron density around PEB JJJ 303:**

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



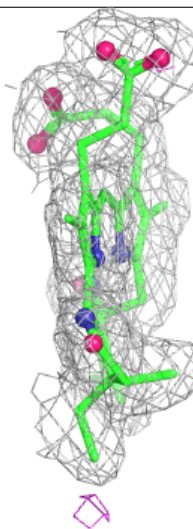
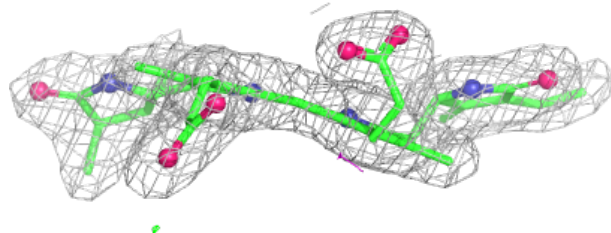
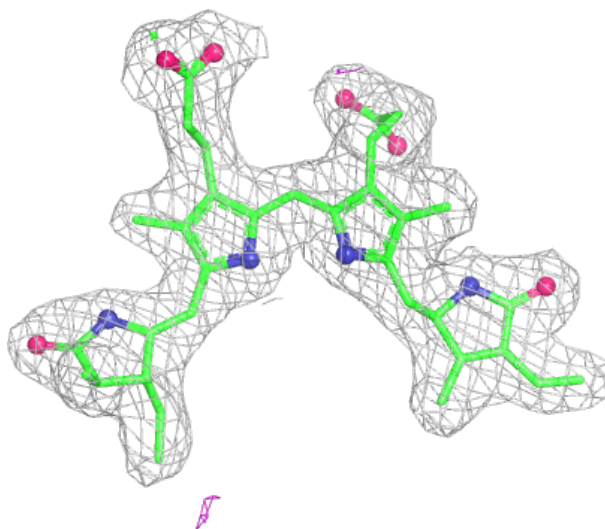
**Electron density around PEB GGG 201:**

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



**Electron density around PEB MMM 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 ⓘ

There are no such residues in this entry.