



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 11:04 PM UTC

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

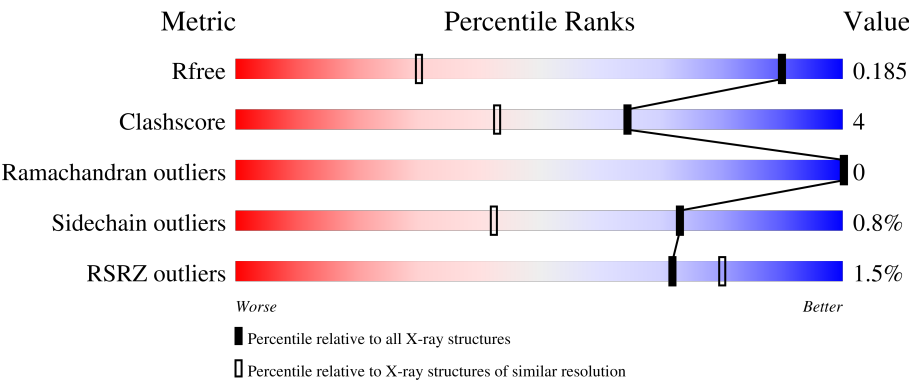
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.14 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	164	95%5%
1	B	164	% 98%.
1	C	164	% 95%5%
1	D	164	95%5%

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

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 43607 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,P hycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit.

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

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

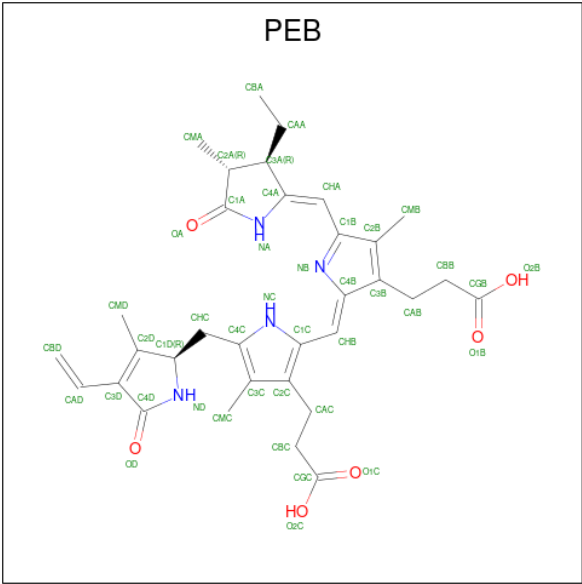
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	184	Total	C	N	O	S	0	12	0
			1416	876	254	273	13			
2	N	184	Total	C	N	O	S	0	12	0
			1411	868	252	277	14			

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

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



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

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

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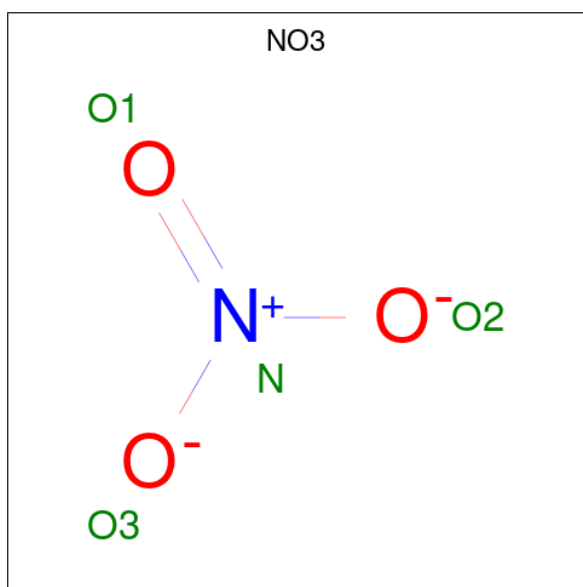
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3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

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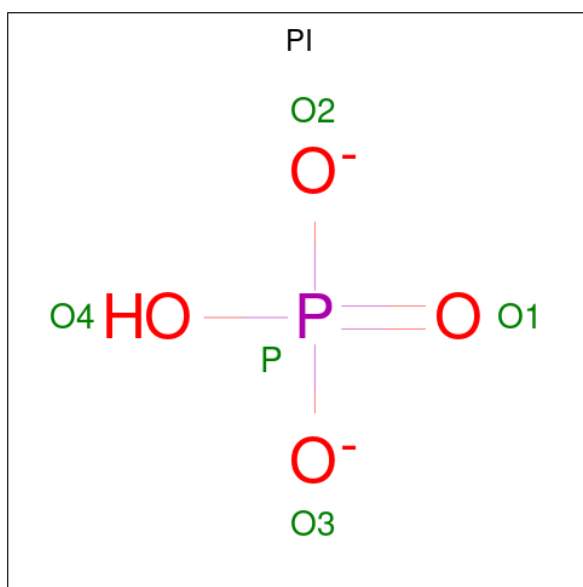
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	S	1	Total	C	N	O	0	0
			43	33	4	6		
3	S	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	U	1	Total	C	N	O	0	0
			43	33	4	6		
3	U	1	Total	C	N	O	0	0
			43	33	4	6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

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



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

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



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

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

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

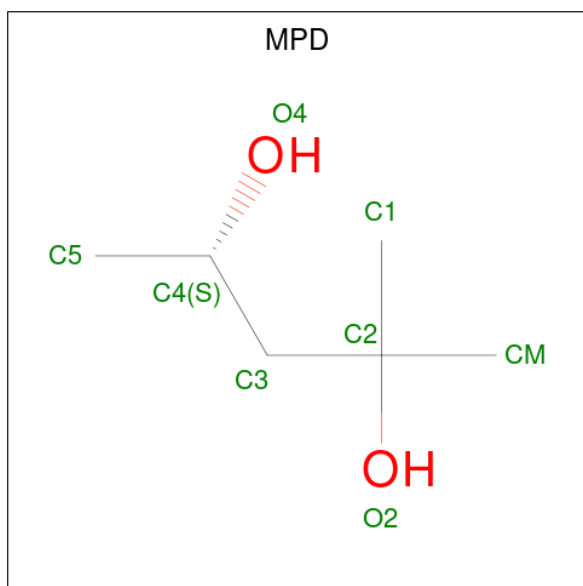
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		
6	E	1	Total	Na	0	0
			1	1		
6	F	1	Total	Na	0	0
			1	1		
6	G	1	Total	Na	0	0
			1	1		
6	H	1	Total	Na	0	0
			1	1		
6	I	1	Total	Na	0	0
			1	1		

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

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



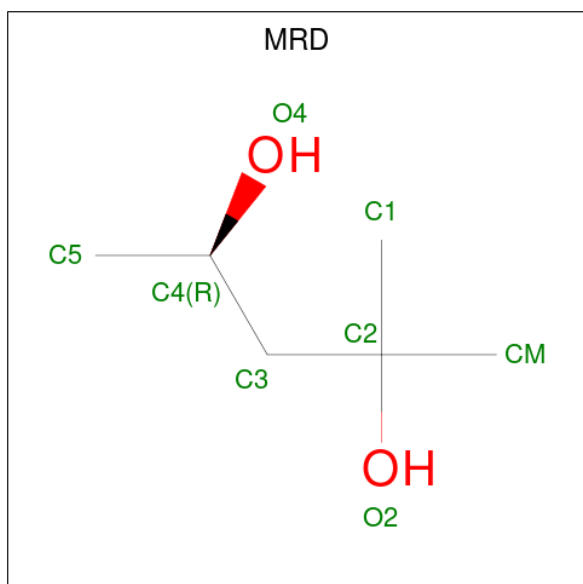
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			8	6	2		
7	M	1	Total	C	O	0	0
			8	6	2		
7	O	1	Total	C	O	0	0
			8	6	2		
7	P	1	Total	C	O	0	0
			8	6	2		

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

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



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

- Molecule 9 is water.

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

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

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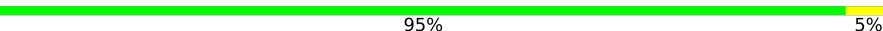
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	W	368	Total 368	O 368	0	0
9	X	357	Total 357	O 357	0	0

3 Residue-property plots

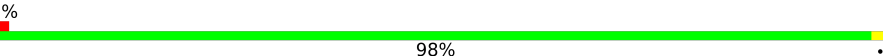
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

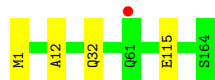
- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain A: 

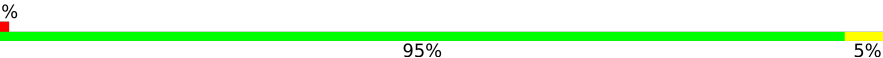


- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain B: 

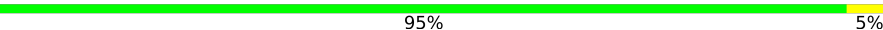


- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain C: 

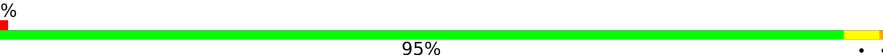


- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain D: 

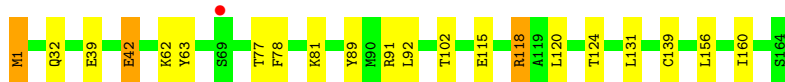
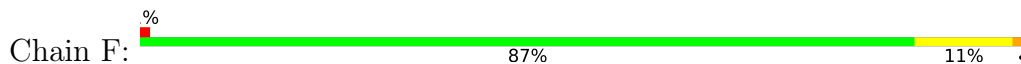


- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain E: 



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



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



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



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



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



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





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

Chain L: 96%



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain M: 96%



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain N: 94% 5%



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain O: 93% 7%



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain P: 91% 9%

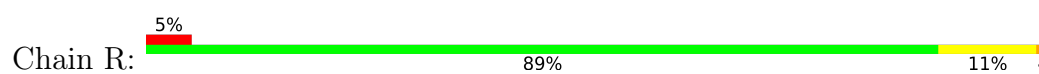


- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

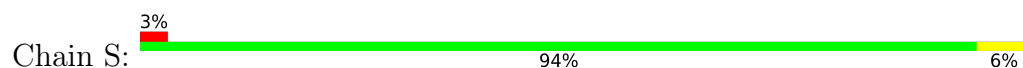
Chain Q: 94% 6%



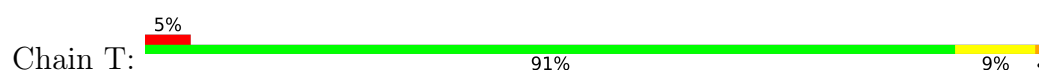
- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



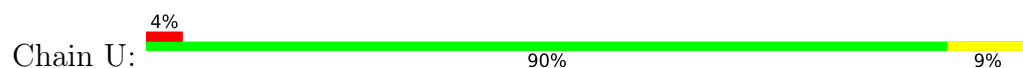
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



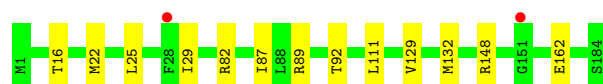
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



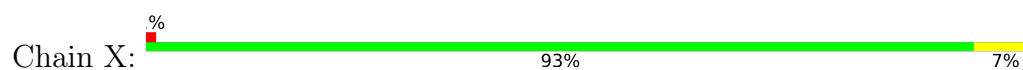
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



4 Data and refinement statistics

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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

All (7) bond length outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	102	THR	C-O	-6.10	1.15	1.24
1	B	12	ALA	N-CA	-5.72	1.39	1.46
2	U	176	PHE	C-O	-5.12	1.18	1.24
2	R	176	PHE	C-O	5.08	1.30	1.24
1	G	121	GLY	CA-C	-5.03	1.44	1.51

All (5) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1401	0	1432	9	0
2	Q	1394	0	1428	15	0
2	R	1402	0	1439	17	0
2	S	1410	0	1439	9	0
2	T	1407	0	1443	17	0
2	U	1441	0	1488	16	0
2	V	1437	0	1476	8	0
2	W	1423	0	1466	18	0
2	X	1401	0	1437	13	0
3	A	86	0	74	1	0
3	B	86	0	74	0	0
3	C	86	0	74	0	0
3	D	86	0	74	0	0
3	E	86	0	74	0	0
3	F	86	0	74	2	0
3	G	86	0	74	0	0
3	H	86	0	74	0	0
3	I	86	0	74	0	0
3	J	86	0	74	0	0
3	K	86	0	74	1	0
3	L	86	0	74	0	0
3	M	129	0	110	1	0
3	N	129	0	110	2	0
3	O	129	0	110	3	0
3	P	129	0	110	3	0
3	Q	129	0	110	4	0
3	R	129	0	111	7	0
3	S	135	0	87	1	0
3	T	129	0	110	4	0
3	U	129	0	110	3	0
3	V	129	0	110	2	0
3	W	129	0	110	2	0
3	X	129	0	110	2	0
4	A	4	0	0	1	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	I	4	0	0	1	0
4	J	4	0	0	0	0
4	L	4	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (280) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32[A]:GLN:HG3	1:K:32[A]:GLN:HG3	1.25	1.14
1:I:32[A]:GLN:HG3	1:L:32[A]:GLN:HG3	1.17	1.14
1:B:32[A]:GLN:HG3	1:E:32[A]:GLN:HG3	1.24	1.14
1:A:32[A]:GLN:HG3	1:D:32[A]:GLN:HG3	1.25	1.12
1:G:115[C]:GLU:OE1	2:U:82[C]:ARG:NH2	1.87	1.07
1:C:32[A]:GLN:HG3	1:F:32[A]:GLN:CG	1.83	1.07
1:C:32[A]:GLN:CG	1:F:32[A]:GLN:HG3	1.85	1.06
2:S:22[B]:MET:HA	2:S:22[B]:MET:HE2	1.34	1.06
1:A:32[A]:GLN:HG3	1:D:32[A]:GLN:CG	1.88	1.03
1:I:32[A]:GLN:CG	1:L:32[A]:GLN:HG3	1.89	1.02
1:I:32[A]:GLN:HG3	1:L:32[A]:GLN:CG	1.90	1.02
1:B:32[A]:GLN:HG3	1:E:32[A]:GLN:CG	1.90	1.01
1:B:32[A]:GLN:CG	1:E:32[A]:GLN:HG3	1.90	0.99
1:A:32[A]:GLN:CG	1:D:32[A]:GLN:HG3	1.92	0.99
1:K:42[A]:GLU:CG	2:W:22[A]:MET:HG3	1.94	0.97
9:I:579:HOH:O	3:X:187:PEB:HAD1	1.63	0.96
2:X:24:ALA:HB3	9:X:307:HOH:O	1.65	0.96
1:H:32[A]:GLN:HG3	1:K:32[A]:GLN:CG	1.96	0.95
9:G:321:HOH:O	1:L:118[B]:ARG:HD2	1.69	0.93
1:G:120:LEU:HA	9:G:313:HOH:O	1.67	0.93
1:D:114[B]:ARG:HG3	1:D:114[B]:ARG:HH11	1.34	0.92
1:H:32[A]:GLN:CG	1:K:32[A]:GLN:HG3	1.98	0.92
9:S:463:HOH:O	2:T:16:THR:HB	1.69	0.92
1:D:114[B]:ARG:HG3	1:D:114[B]:ARG:NH1	1.86	0.90
1:D:33:ARG:HB2	9:D:506:HOH:O	1.71	0.90
2:N:16[B]:THR:HG21	9:N:440:HOH:O	1.72	0.89
1:G:124[A]:THR:HG23	4:L:203:NO3:O2	1.73	0.88
3:R:188:PEB:HBA1	9:R:330:HOH:O	1.74	0.88
1:F:78:PHE:HA	9:F:513:HOH:O	1.70	0.87
2:R:170:ALA:HB2	9:R:498:HOH:O	1.74	0.86
1:A:132:SER:HB2	9:A:390:HOH:O	1.74	0.86
2:S:22[B]:MET:HA	2:S:22[B]:MET:CE	2.05	0.86
2:X:2:LEU:HD13	9:X:302:HOH:O	1.74	0.86
2:X:156:MET:HB3	9:X:322:HOH:O	1.75	0.85
2:M:67:ALA:HB2	2:N:16[B]:THR:HG22	1.59	0.85
1:J:118[A]:ARG:HD2	9:J:333:HOH:O	1.78	0.84
1:F:39:GLU:O	1:F:42[A]:GLU:HG3	1.78	0.83
2:T:129:VAL:HG13	9:T:467:HOH:O	1.78	0.83
1:D:113:GLN:HE21	1:D:114[B]:ARG:HH12	1.23	0.81
2:W:111:LEU:HD21	9:W:344:HOH:O	1.79	0.81
1:I:154:ALA:HB1	9:I:458:HOH:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:188:PEB:CBA	9:R:330:HOH:O	2.27	0.80
1:D:114[B]:ARG:HH11	1:D:114[B]:ARG:CG	1.93	0.79
1:K:42[A]:GLU:HG2	2:W:22[A]:MET:HG3	1.66	0.76
1:H:99:VAL:HG13	9:T:335:HOH:O	1.84	0.76
2:P:16:THR:HG23	2:Q:67:ALA:HB2	1.66	0.76
4:A:203:NO3:O2	1:F:118[A]:ARG:NH2	2.19	0.76
2:P:82[A]:ARG:NH1	3:P:186:PEB:O2C	2.16	0.75
3:R:187:PEB:HBA2	9:R:354:HOH:O	1.87	0.75
2:N:83:ASP:HB3	9:N:320:HOH:O	1.86	0.75
2:U:89:ARG:O	2:U:92[B]:THR:HG22	1.88	0.74
1:F:78:PHE:HD1	9:F:503:HOH:O	1.70	0.73
2:W:87:ILE:HD11	9:W:344:HOH:O	1.87	0.73
1:F:115[B]:GLU:HG3	1:F:118[B]:ARG:NH2	2.04	0.72
1:F:115[B]:GLU:HG3	1:F:118[B]:ARG:HH22	1.55	0.72
2:R:129:VAL:HG11	9:R:320:HOH:O	1.90	0.72
1:F:81:LYS:HB2	9:F:513:HOH:O	1.88	0.72
1:F:91:ARG:HG2	9:F:350:HOH:O	1.90	0.71
2:V:82[A]:ARG:NH1	3:V:186:PEB:O2C	2.23	0.71
1:I:159:ALA:HB3	9:I:309:HOH:O	1.88	0.71
1:I:118[B]:ARG:HD2	9:K:325:HOH:O	1.91	0.71
2:N:22[A]:MET:HE2	2:N:25:LEU:HD12	1.72	0.71
2:X:153:LEU:HD22	9:X:436:HOH:O	1.90	0.70
2:R:180:ILE:HG13	9:R:320:HOH:O	1.92	0.70
1:A:124[A]:THR:HG21	9:A:486:HOH:O	1.90	0.70
2:X:82[A]:ARG:NH1	3:X:186:PEB:O2C	2.23	0.70
2:O:89:ARG:O	2:O:92[A]:THR:HG22	1.92	0.69
1:F:120:LEU:HD22	9:F:502:HOH:O	1.94	0.68
1:F:89:TYR:HB2	9:F:532:HOH:O	1.93	0.67
2:P:65:ILE:O	9:P:302:HOH:O	2.13	0.67
2:R:155[B]:LYS:HA	2:R:155[B]:LYS:HE2	1.77	0.66
2:O:82[A]:ARG:NH1	3:O:186:PEB:O2C	2.23	0.66
2:P:74:ASN:HA	9:P:329:HOH:O	1.95	0.66
2:W:16[B]:THR:HG21	9:W:354:HOH:O	1.95	0.66
2:T:82:ARG:NH1	3:T:186:PEB:O2C	2.27	0.66
1:K:42[A]:GLU:HG2	2:W:22[A]:MET:CG	2.25	0.66
1:G:28:GLN:HG2	9:S:503:HOH:O	1.96	0.66
2:R:38:ALA:HA	9:R:354:HOH:O	1.97	0.65
2:S:89:ARG:O	2:S:92[B]:THR:HG22	1.96	0.65
1:K:42[A]:GLU:HG3	2:W:22[A]:MET:HG3	1.77	0.65
2:N:89:ARG:O	2:N:92[A]:THR:HG22	1.97	0.64
2:T:148:ARG:NH1	9:T:305:HOH:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:89:ARG:O	2:V:92[B]:THR:HG22	1.97	0.64
1:E:118[B]:ARG:NH2	9:E:307:HOH:O	2.26	0.64
1:H:27:VAL:HG12	9:T:505:HOH:O	1.98	0.64
2:R:155[B]:LYS:HE2	2:R:155[B]:LYS:CA	2.28	0.64
1:F:131:LEU:HB3	9:F:347:HOH:O	1.98	0.63
2:S:76:ARG:NH2	9:S:305:HOH:O	2.25	0.63
1:H:31:ILE:HD11	9:T:505:HOH:O	1.97	0.63
2:U:146:GLU:OE2	2:U:153[A]:LEU:HD22	1.99	0.63
2:W:22[A]:MET:SD	2:W:25:LEU:HD12	2.38	0.63
1:G:115[C]:GLU:CD	2:U:82[C]:ARG:NH2	2.55	0.62
1:F:77:THR:HG22	9:F:503:HOH:O	2.00	0.62
2:X:89:ARG:O	2:X:92[B]:THR:HG22	1.99	0.62
2:U:82[A]:ARG:NH1	3:U:186:PEB:O2C	2.24	0.62
1:J:33:ARG:HB2	9:S:503:HOH:O	2.01	0.61
1:A:128:VAL:HG12	9:A:390:HOH:O	2.00	0.61
2:T:89:ARG:O	2:T:92[B]:THR:HG22	2.01	0.61
9:B:326:HOH:O	1:D:118[B]:ARG:HD3	2.01	0.60
2:O:141[B]:LYS:HE3	2:O:164:ARG:HB2	1.82	0.60
1:J:102:THR:N	9:J:305:HOH:O	2.34	0.60
2:Q:16:THR:HG23	2:R:67:ALA:HB2	1.82	0.59
2:M:82[A]:ARG:NH1	3:M:186:PEB:O2C	2.30	0.59
1:F:120:LEU:CD2	9:F:502:HOH:O	2.51	0.58
1:I:156:LEU:HA	9:I:309:HOH:O	2.04	0.58
2:Q:168:LEU:HD11	9:Q:360:HOH:O	2.04	0.58
2:V:155:LYS:NZ	9:V:305:HOH:O	2.33	0.58
1:J:114:ARG:HG3	9:J:473:HOH:O	2.03	0.58
2:V:22[A]:MET:HE3	9:V:422:HOH:O	2.03	0.58
2:N:82[A]:ARG:NH1	3:N:186:PEB:O2C	2.26	0.58
1:G:118[B]:ARG:HD2	9:G:306:HOH:O	2.03	0.58
2:N:22[A]:MET:CE	2:N:25:LEU:HD12	2.34	0.58
2:T:6:SER:HB3	9:T:335:HOH:O	2.04	0.57
2:W:89:ARG:O	2:W:92[B]:THR:HG22	2.04	0.57
2:U:9:VAL:HG23	9:U:369:HOH:O	2.04	0.57
1:E:70:GLY:O	9:E:306:HOH:O	2.16	0.57
2:W:29:ILE:HD13	7:W:204:MPD:H52	1.87	0.57
2:X:153:LEU:HB2	9:X:436:HOH:O	2.04	0.56
1:L:118[A]:ARG:NH1	9:L:307:HOH:O	2.39	0.56
2:U:24:ALA:HB3	9:U:496:HOH:O	2.06	0.56
2:W:82[A]:ARG:NH1	3:W:186:PEB:O1C	2.36	0.56
5:H:203:PI:O4	9:H:307:HOH:O	2.17	0.55
2:X:146:GLU:HA	9:X:436:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:52:ASP:HB2	9:R:330:HOH:O	2.06	0.55
2:Q:82[A]:ARG:NH2	3:Q:186:PEB:O2C	2.40	0.55
2:Q:29:ILE:HD13	7:Q:204:MPD:H52	1.89	0.55
2:W:132:MET:HB2	9:W:307:HOH:O	2.05	0.54
2:X:156:MET:HE3	9:X:322:HOH:O	2.07	0.54
1:C:33:ARG:HG2	9:F:366:HOH:O	2.08	0.54
1:D:118[B]:ARG:HD2	9:D:388:HOH:O	2.06	0.54
2:O:76:ARG:NH2	9:O:306:HOH:O	2.40	0.54
2:V:178[B]:ARG:NH2	2:V:178[B]:ARG:HG3	2.22	0.54
1:G:118[A]:ARG:NH1	9:G:309:HOH:O	2.40	0.53
2:R:28[B]:PHE:HA	2:R:31[B]:GLU:HG2	1.89	0.53
2:T:176:PHE:HD1	9:T:467:HOH:O	1.91	0.53
2:P:148:ARG:NH1	3:P:188:PEB:HND	2.07	0.53
1:J:33:ARG:HD3	9:S:503:HOH:O	2.08	0.52
2:R:179:VAL:HG12	9:R:320:HOH:O	2.08	0.52
2:U:148:ARG:NH1	3:U:188:PEB:HND	2.07	0.52
2:R:163:ASP:HB3	9:R:443:HOH:O	2.10	0.52
2:U:19:VAL:HG21	9:U:369:HOH:O	2.10	0.52
2:R:82:ARG:NH1	3:R:186:PEB:O2C	2.40	0.51
2:O:22:MET:HE3	9:O:341:HOH:O	2.11	0.51
2:S:22[B]:MET:CE	2:S:22[B]:MET:CA	2.83	0.51
1:C:5:VAL:HG11	7:O:204:MPD:H13	1.91	0.51
2:R:135:GLN:HG2	3:R:188:PEB:C1B	2.41	0.51
1:K:1[A]:MET:HE1	1:K:104:PRO:HG3	1.91	0.51
1:A:128:VAL:CG1	9:A:390:HOH:O	2.59	0.51
2:U:130[B]:GLN:HA	2:U:130[B]:GLN:HE21	1.76	0.50
2:X:7:ARG:HA	9:X:302:HOH:O	2.10	0.50
2:T:148:ARG:NH1	3:T:188:PEB:HND	2.10	0.50
1:A:118[A]:ARG:NH1	1:F:124[A]:THR:OG1	2.45	0.50
1:C:102:THR:N	9:C:307:HOH:O	2.41	0.50
1:C:114:ARG:HG3	9:C:413:HOH:O	2.11	0.50
1:C:118[A]:ARG:NH1	1:E:124[A]:THR:OG1	2.45	0.50
2:O:31:GLU:OE2	9:O:304:HOH:O	2.19	0.49
2:Q:148:ARG:NH1	9:Q:303:HOH:O	2.46	0.49
9:I:579:HOH:O	1:L:24:LEU:HD12	2.11	0.49
9:H:372:HOH:O	1:J:118[A]:ARG:HD3	2.12	0.49
1:C:32[A]:GLN:HG3	1:F:32[A]:GLN:HG2	1.86	0.49
1:F:102:THR:N	9:F:308:HOH:O	2.43	0.49
1:H:118[A]:ARG:NH1	1:J:124[A]:THR:OG1	2.46	0.49
1:C:118[A]:ARG:NH2	9:C:305:HOH:O	2.36	0.48
1:D:113:GLN:HE21	1:D:114[B]:ARG:NH1	2.03	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124[A]:THR:HG21	9:E:492:HOH:O	2.13	0.48
2:Q:168:LEU:HD21	9:Q:360:HOH:O	2.13	0.48
1:F:1[A]:MET:HE3	1:F:1[A]:MET:HB2	1.57	0.48
2:W:22[B]:MET:HE2	2:W:25:LEU:HD12	1.96	0.48
2:S:75:ARG:NH2	9:S:312:HOH:O	2.45	0.48
1:E:114:ARG:HG3	9:E:450:HOH:O	2.14	0.48
1:F:156:LEU:HB3	9:F:347:HOH:O	2.14	0.48
1:E:1[A]:MET:HG3	1:E:103:GLY:HA3	1.95	0.48
2:R:148:ARG:NH1	3:R:188:PEB:HND	2.11	0.48
2:M:27:GLN:HE21	2:M:31[A]:GLU:HG3	1.79	0.48
2:P:89:ARG:NH2	9:P:306:HOH:O	2.45	0.48
2:Q:29:ILE:HD13	7:Q:204:MPD:C5	2.44	0.47
2:U:133:LYS:HE3	2:U:173:SER:HB3	1.96	0.47
2:N:148:ARG:NH1	3:N:188:PEB:HND	2.13	0.47
2:T:122[B]:THR:HG22	9:T:477:HOH:O	2.14	0.47
2:W:148:ARG:NH1	3:W:188:PEB:HND	2.13	0.47
1:F:62[A]:LYS:NZ	9:F:305:HOH:O	2.03	0.47
3:R:187:PEB:HBA3	3:R:187:PEB:HHA1	1.96	0.47
1:K:42[A]:GLU:CD	2:W:22[A]:MET:HG3	2.39	0.47
1:J:43[B]:LYS:NZ	9:J:307:HOH:O	2.47	0.47
2:T:28[B]:PHE:HA	2:T:31[B]:GLU:HG2	1.96	0.46
1:G:28:GLN:HG3	1:J:32[B]:GLN:HG2	1.97	0.46
2:S:148:ARG:NH1	3:S:188:PEB:HND	2.12	0.46
1:D:51:VAL:HG21	9:D:413:HOH:O	2.15	0.46
2:U:144:PRO:HG2	2:U:153[B]:LEU:HD21	1.97	0.46
1:K:62[B]:LYS:NZ	9:K:309:HOH:O	2.49	0.46
2:M:67:ALA:HB2	2:N:16[A]:THR:HG23	1.97	0.46
2:O:148:ARG:NH1	3:O:188:PEB:HND	2.14	0.46
2:W:129:VAL:HG13	9:W:307:HOH:O	2.15	0.46
1:A:124[A]:THR:OG1	1:F:118[A]:ARG:NH1	2.49	0.45
1:G:124[A]:THR:OG1	1:L:118[A]:ARG:NH1	2.50	0.45
2:P:146:GLU:OE1	2:P:153:LEU:HD22	2.17	0.45
1:H:43[A]:LYS:HD3	9:H:492:HOH:O	2.16	0.45
1:F:92:LEU:HD23	9:F:350:HOH:O	2.16	0.45
2:W:16[A]:THR:HG23	2:X:67:ALA:HB2	1.97	0.45
1:F:160:ILE:CD1	9:F:347:HOH:O	2.64	0.45
1:G:28:GLN:CG	1:J:32[B]:GLN:HG2	2.47	0.45
2:Q:135:GLN:HG2	3:Q:188:PEB:C1B	2.46	0.45
1:F:160:ILE:HD11	9:F:347:HOH:O	2.17	0.45
1:H:42[A]:GLU:HG2	9:H:492:HOH:O	2.15	0.45
2:M:5:PHE:HE1	2:M:28[A]:PHE:CD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:148:ARG:NH1	3:Q:188:PEB:HND	2.14	0.45
1:K:62[B]:LYS:HG2	1:K:63:TYR:CE2	2.52	0.45
2:V:178[B]:ARG:HG3	2:V:178[B]:ARG:HH21	1.81	0.45
2:V:148:ARG:NH1	3:V:188:PEB:HND	2.15	0.45
2:N:82[B]:ARG:NH1	2:N:82[B]:ARG:HB2	2.32	0.44
2:O:27:GLN:NE2	2:O:31:GLU:OE2	2.44	0.44
2:P:22[A]:MET:HE2	2:P:25:LEU:HD12	1.98	0.44
1:A:121:GLY:HA2	9:A:394:HOH:O	2.16	0.44
3:F:166:PEB:HMB1	9:F:513:HOH:O	2.16	0.44
1:G:163:LEU:O	1:L:118[A]:ARG:HD2	2.18	0.44
1:H:62[C]:LYS:NZ	9:H:309:HOH:O	2.33	0.44
1:D:113:GLN:NE2	1:D:114[B]:ARG:HH12	2.03	0.44
2:X:10:VAL:CG2	9:X:302:HOH:O	2.66	0.44
3:T:187:PEB:HBA3	3:T:187:PEB:HHA1	2.00	0.44
9:G:321:HOH:O	1:L:118[B]:ARG:CD	2.45	0.44
2:U:31[B]:GLU:HG3	9:U:349:HOH:O	2.18	0.44
1:J:118[A]:ARG:CD	9:J:333:HOH:O	2.52	0.44
2:T:125:THR:HG21	2:T:183:LEU:HD13	1.99	0.44
2:N:22[A]:MET:HE2	2:N:25:LEU:CD1	2.44	0.44
2:T:24:ALA:HB3	9:T:402:HOH:O	2.17	0.44
1:E:61[A]:GLN:NE2	9:E:313:HOH:O	2.50	0.43
1:L:1[A]:MET:HG3	1:L:103:GLY:HA3	2.00	0.43
2:U:22:MET:HE2	2:U:25:LEU:CD2	2.48	0.43
2:U:31[B]:GLU:HG3	9:U:458:HOH:O	2.18	0.43
2:V:183:LEU:HD22	9:V:481:HOH:O	2.18	0.43
1:C:32[A]:GLN:CD	1:F:32[A]:GLN:HG3	2.41	0.43
9:C:342:HOH:O	7:O:204:MPD:CM	2.66	0.43
2:Q:24:ALA:HB3	9:Q:364:HOH:O	2.19	0.43
2:U:31[B]:GLU:CG	9:U:458:HOH:O	2.67	0.43
1:E:118[A]:ARG:NH1	9:E:314:HOH:O	2.51	0.43
3:P:187:PEB:HBA3	3:P:187:PEB:HHA1	2.00	0.43
4:I:203:NO3:O2	1:K:118[A]:ARG:NH2	2.51	0.43
1:C:2:LYS:HB3	9:C:307:HOH:O	2.18	0.43
2:O:31:GLU:HB3	9:O:358:HOH:O	2.18	0.42
2:Q:26:LYS:NZ	9:Q:302:HOH:O	2.42	0.42
2:R:159:PRO:HB3	9:R:574:HOH:O	2.18	0.42
1:C:1[B]:MET:HG3	1:C:103:GLY:HA3	2.01	0.42
2:N:146:GLU:OE2	2:N:153:LEU:HD22	2.19	0.42
1:L:87:LYS:HE2	9:X:366:HOH:O	2.20	0.42
2:P:66:GLN:HA	9:P:302:HOH:O	2.19	0.42
1:G:118[A]:ARG:HA	1:G:118[A]:ARG:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1[A]:MET:HG3	1:I:103:GLY:HA3	2.02	0.42
1:F:118[A]:ARG:HH11	1:F:118[A]:ARG:HD3	1.71	0.41
9:S:418:HOH:O	2:T:16:THR:HG21	2.19	0.41
1:A:1[B]:MET:HE3	1:A:1[B]:MET:HB2	1.67	0.41
2:Q:31[B]:GLU:CD	9:Q:360:HOH:O	2.63	0.41
2:Q:82[A]:ARG:NH1	3:Q:186:PEB:O2C	2.53	0.41
2:R:155[B]:LYS:HA	2:R:155[B]:LYS:CE	2.49	0.41
1:H:19:PRO:CD	2:T:92[B]:THR:HG23	2.50	0.41
1:I:118[A]:ARG:NH1	1:K:124[A]:THR:OG1	2.53	0.41
2:T:16:THR:O	2:T:16:THR:OG1	2.35	0.41
1:F:62[A]:LYS:HE2	1:F:63:TYR:OH	2.20	0.41
3:K:166:PEB:HNA	3:K:166:PEB:HMB3	1.85	0.41
2:O:135:GLN:HG2	3:O:188:PEB:C1B	2.51	0.41
2:Q:27:GLN:NE2	2:Q:31[A]:GLU:OE2	2.53	0.41
1:I:27:VAL:O	1:I:30[B]:SER:HB3	2.21	0.41
2:T:135:GLN:HG2	3:T:188:PEB:C1B	2.50	0.41
1:J:2:LYS:HB3	9:J:305:HOH:O	2.19	0.41
2:X:27:GLN:NE2	2:X:31[A]:GLU:OE1	2.54	0.41
9:C:342:HOH:O	7:O:204:MPD:HM3	2.20	0.40
1:D:87:LYS:NZ	9:D:312:HOH:O	2.53	0.40
1:G:35:ALA:HB1	9:G:580:HOH:O	2.22	0.40
2:S:132:MET:HA	2:S:135:GLN:OE1	2.21	0.40
1:A:43[A]:LYS:HG3	3:A:167:PEB:CBD	2.51	0.40
1:F:139:CYS:SG	3:F:167:PEB:HHA1	2.61	0.40
1:K:1[A]:MET:HE3	1:K:1[A]:MET:HB3	1.86	0.40
2:R:144:PRO:HG2	2:R:153:LEU:HD11	2.03	0.40
2:S:28[A]:PHE:CZ	2:S:35:ARG:NH2	2.89	0.40
3:U:187:PEB:HBA3	3:U:187:PEB:HHA1	2.03	0.40
1:H:19:PRO:HD2	2:T:92[B]:THR:HG21	2.04	0.40
1:L:118[A]:ARG:NH2	9:L:305:HOH:O	2.23	0.40
2:M:155[A]:LYS:CA	2:M:155[A]:LYS:HE2	2.44	0.40
2:W:22[B]:MET:CE	2:W:25:LEU:HD12	2.51	0.40

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	B	169/164 (103%)	167 (99%)	2 (1%)	0	100	100
1	C	170/164 (104%)	168 (99%)	2 (1%)	0	100	100
1	D	173/164 (106%)	171 (99%)	2 (1%)	0	100	100
1	E	169/164 (103%)	166 (98%)	3 (2%)	0	100	100
1	F	172/164 (105%)	170 (99%)	2 (1%)	0	100	100
1	G	170/164 (104%)	168 (99%)	2 (1%)	0	100	100
1	H	172/164 (105%)	169 (98%)	3 (2%)	0	100	100
1	I	174/164 (106%)	172 (99%)	2 (1%)	0	100	100
1	J	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	K	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	L	170/164 (104%)	168 (99%)	2 (1%)	0	100	100
2	M	194/184 (105%)	188 (97%)	6 (3%)	0	100	100
2	N	192/184 (104%)	185 (96%)	7 (4%)	0	100	100
2	O	190/184 (103%)	185 (97%)	5 (3%)	0	100	100
2	P	192/184 (104%)	188 (98%)	4 (2%)	0	100	100
2	Q	191/184 (104%)	187 (98%)	4 (2%)	0	100	100
2	R	191/184 (104%)	187 (98%)	4 (2%)	0	100	100
2	S	193/184 (105%)	189 (98%)	4 (2%)	0	100	100
2	T	192/184 (104%)	186 (97%)	6 (3%)	0	100	100
2	U	197/184 (107%)	194 (98%)	3 (2%)	0	100	100
2	V	196/184 (106%)	192 (98%)	4 (2%)	0	100	100
2	W	195/184 (106%)	190 (97%)	5 (3%)	0	100	100
2	X	192/184 (104%)	189 (98%)	3 (2%)	0	100	100
All	All	4367/4176 (105%)	4286 (98%)	81 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/127 (108%)	137 (100%)	0	100	100
1	B	135/127 (106%)	133 (98%)	2 (2%)	57	19
1	C	136/127 (107%)	136 (100%)	0	100	100
1	D	139/127 (109%)	139 (100%)	0	100	100
1	E	135/127 (106%)	133 (98%)	2 (2%)	57	19
1	F	138/127 (109%)	132 (96%)	6 (4%)	26	1
1	G	136/127 (107%)	136 (100%)	0	100	100
1	H	138/127 (109%)	136 (99%)	2 (1%)	59	21
1	I	140/127 (110%)	140 (100%)	0	100	100
1	J	137/127 (108%)	137 (100%)	0	100	100
1	K	137/127 (108%)	133 (97%)	4 (3%)	37	4
1	L	136/127 (107%)	136 (100%)	0	100	100
2	M	151/138 (109%)	149 (99%)	2 (1%)	61	23
2	N	150/138 (109%)	147 (98%)	3 (2%)	48	9
2	O	147/138 (106%)	147 (100%)	0	100	100
2	P	149/138 (108%)	145 (97%)	4 (3%)	39	5
2	Q	148/138 (107%)	148 (100%)	0	100	100
2	R	148/138 (107%)	146 (99%)	2 (1%)	59	21
2	S	150/138 (109%)	150 (100%)	0	100	100
2	T	150/138 (109%)	147 (98%)	3 (2%)	48	9
2	U	155/138 (112%)	152 (98%)	3 (2%)	50	11
2	V	154/138 (112%)	151 (98%)	3 (2%)	50	11
2	W	153/138 (111%)	152 (99%)	1 (1%)	76	48
2	X	149/138 (108%)	149 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3448/3180 (108%)	3411 (99%)	37 (1%)	73	31

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1[A]	MET
1	B	1[B]	MET
1	E	1[A]	MET
1	E	1[B]	MET
1	F	1[A]	MET
1	F	1[B]	MET
1	F	42[A]	GLU
1	F	42[B]	GLU
1	F	118[A]	ARG
1	F	118[B]	ARG
1	H	1[A]	MET
1	H	1[B]	MET
1	K	1[A]	MET
1	K	1[B]	MET
1	K	118[A]	ARG
1	K	118[B]	ARG
2	M	155[A]	LYS
2	M	155[B]	LYS
2	N	73	PRO
2	N	92[A]	THR
2	N	92[B]	THR
2	P	26	LYS
2	P	27	GLN
2	P	31[A]	GLU
2	P	31[B]	GLU
2	R	28[A]	PHE
2	R	28[B]	PHE
2	T	16	THR
2	T	123	THR
2	T	155	LYS
2	U	25	LEU
2	U	26[A]	LYS
2	U	26[B]	LYS
2	V	9	VAL
2	V	155	LYS
2	V	162	GLU
2	W	162	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	53	GLN
1	A	57	ASN
1	A	61	GLN
1	A	68	ASN
1	B	28	GLN
1	B	53	GLN
1	B	57	ASN
1	C	28	GLN
1	C	53	GLN
1	C	57	ASN
1	D	53	GLN
1	D	61	GLN
1	D	113	GLN
1	E	28	GLN
1	F	28	GLN
1	F	53	GLN
1	F	57	ASN
1	G	28	GLN
1	G	57	ASN
1	H	53	GLN
1	H	57	ASN
1	I	28	GLN
1	I	53	GLN
1	I	61	GLN
1	J	28	GLN
1	J	53	GLN
1	J	57	ASN
1	J	61	GLN
1	K	28	GLN
1	K	53	GLN
1	K	57	ASN
1	L	28	GLN
1	L	53	GLN
1	L	57	ASN
1	L	61	GLN
2	M	27	GLN
2	M	45	ASN
2	N	45	ASN
2	P	27	GLN
2	P	45	ASN

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Mol	Chain	Res	Type
2	Q	45	ASN
2	R	11	GLN
2	R	45	ASN
2	T	45	ASN
2	T	130	GLN
2	V	45	ASN
2	W	45	ASN
2	X	11	GLN
2	X	45	ASN
2	X	61	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	U	70	2	7,8,9	0.79	0	4,9,11	1.11	0
2	MEN	O	70	2	7,8,9	0.48	0	4,9,11	1.44	1 (25%)
2	MEN	P	70	2	7,8,9	0.60	0	4,9,11	0.67	0
2	MEN	Q	70	2	7,8,9	0.46	0	4,9,11	1.14	0
2	MEN	T	70	2	7,8,9	0.47	0	4,9,11	0.85	0
2	MEN	R	70	2	7,8,9	0.50	0	4,9,11	2.07	2 (50%)
2	MEN	M	70	2	7,8,9	0.46	0	4,9,11	0.41	0
2	MEN	V	70	2	7,8,9	0.70	0	4,9,11	0.83	0
2	MEN	N	70	2	7,8,9	0.67	0	4,9,11	0.70	0
2	MEN	X	70	2	7,8,9	0.48	0	4,9,11	0.41	0
2	MEN	S	70	2	7,8,9	0.35	0	4,9,11	1.92	1 (25%)
2	MEN	W	70	2	7,8,9	0.69	0	4,9,11	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	U	70	2	-	2/7/8/10	-
2	MEN	O	70	2	-	3/7/8/10	-
2	MEN	P	70	2	-	3/7/8/10	-
2	MEN	Q	70	2	-	3/7/8/10	-
2	MEN	T	70	2	-	3/7/8/10	-
2	MEN	R	70	2	-	3/7/8/10	-
2	MEN	M	70	2	-	3/7/8/10	-
2	MEN	V	70	2	-	3/7/8/10	-
2	MEN	N	70	2	-	2/7/8/10	-
2	MEN	X	70	2	-	3/7/8/10	-
2	MEN	S	70	2	-	2/7/8/10	-
2	MEN	W	70	2	-	2/7/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

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

There are no chirality outliers.

All (32) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	Q	70	MEN	CA-CB-CG-OD1
2	R	70	MEN	CA-CB-CG-OD1
2	W	70	MEN	CA-CB-CG-OD1
2	X	70	MEN	CA-CB-CG-OD1
2	V	70	MEN	N-CA-CB-CG
2	X	70	MEN	N-CA-CB-CG
2	S	70	MEN	CA-CB-CG-OD1
2	P	70	MEN	CA-CB-CG-ND2
2	Q	70	MEN	CA-CB-CG-ND2
2	T	70	MEN	CA-CB-CG-ND2
2	M	70	MEN	CA-CB-CG-ND2
2	N	70	MEN	CA-CB-CG-ND2
2	O	70	MEN	CA-CB-CG-ND2
2	R	70	MEN	CA-CB-CG-ND2
2	S	70	MEN	CA-CB-CG-ND2
2	U	70	MEN	CA-CB-CG-ND2
2	V	70	MEN	CA-CB-CG-ND2
2	W	70	MEN	CA-CB-CG-ND2
2	X	70	MEN	CA-CB-CG-ND2
2	U	70	MEN	CA-CB-CG-OD1
2	M	70	MEN	N-CA-CB-CG
2	P	70	MEN	N-CA-CB-CG
2	R	70	MEN	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PI	E	203	-	4,4,4	0.88	0	6,6,6	0.71	0
3	PEB	O	187	2	46,46,46	2.05	10 (21%)	56,67,67	1.24	6 (10%)
3	PEB	T	188	2	46,46,46	1.97	13 (28%)	56,67,67	1.84	16 (28%)
4	NO3	J	203	-	1,3,3	1.47	0	0,3,3	-	-
3	PEB	N	187	2	46,46,46	1.68	7 (15%)	56,67,67	1.59	14 (25%)
3	PEB	M	187	2	46,46,46	1.77	10 (21%)	56,67,67	1.55	13 (23%)
4	NO3	L	203	-	1,3,3	1.71	0	0,3,3	-	-
7	MPD	O	204	-	7,7,7	0.94	0	9,10,10	1.34	1 (11%)
5	PI	U	205	-	4,4,4	1.37	1 (25%)	6,6,6	0.59	0
5	PI	X	205	-	4,4,4	0.86	0	6,6,6	0.83	0
5	PI	I	204	-	4,4,4	1.11	0	6,6,6	1.12	0
3	PEB	W	187	2	46,46,46	1.91	7 (15%)	56,67,67	1.52	11 (19%)
3	PEB	V	187	2	46,46,46	1.86	8 (17%)	56,67,67	1.47	9 (16%)
3	PEB	M	188	2	46,46,46	1.97	9 (19%)	56,67,67	1.65	13 (23%)
3	PEB	A	166	1	46,46,46	1.43	6 (13%)	56,67,67	1.69	7 (12%)
3	PEB	O	188	2	46,46,46	2.19	14 (30%)	56,67,67	1.55	12 (21%)
5	PI	H	203	-	4,4,4	1.42	0	6,6,6	1.20	1 (16%)
3	PEB	D	166	1	46,46,46	1.98	8 (17%)	56,67,67	1.78	10 (17%)
7	MPD	S	204	-	7,7,7	0.28	0	9,10,10	0.73	0
5	PI	K	203	-	4,4,4	1.06	0	6,6,6	0.93	0
3	PEB	S	186[B]	-	46,46,46	1.88	10 (21%)	56,67,67	2.32	20 (35%)
7	MPD	X	204	-	7,7,7	0.39	0	9,10,10	0.84	1 (11%)
3	PEB	G	166	1	46,46,46	1.72	8 (17%)	56,67,67	1.88	9 (16%)
3	PEB	P	188	2	46,46,46	1.89	7 (15%)	56,67,67	1.70	14 (25%)
3	PEB	N	186	2	46,46,46	1.84	9 (19%)	56,67,67	1.82	18 (32%)
7	MPD	R	204	-	7,7,7	0.21	0	9,10,10	1.63	2 (22%)
7	MPD	Q	204	-	7,7,7	0.64	0	9,10,10	1.00	0
4	NO3	I	203	-	1,3,3	1.68	0	0,3,3	-	-
3	PEB	G	167	1	46,46,46	1.98	12 (26%)	56,67,67	1.48	7 (12%)
3	PEB	L	167	1	46,46,46	1.70	8 (17%)	56,67,67	1.50	10 (17%)
3	PEB	X	188	2	46,46,46	2.15	9 (19%)	56,67,67	1.62	13 (23%)
3	PEB	S	188	2	46,46,46	1.84	10 (21%)	56,67,67	1.49	11 (19%)
5	PI	S	205	-	4,4,4	0.86	0	6,6,6	0.41	0
3	PEB	J	167	1	46,46,46	1.79	10 (21%)	56,67,67	1.90	17 (30%)
3	PEB	O	186	2	46,46,46	1.81	10 (21%)	56,67,67	1.73	13 (23%)
3	PEB	X	186	2	46,46,46	1.91	10 (21%)	56,67,67	1.76	16 (28%)
3	PEB	C	167	1	46,46,46	1.96	11 (23%)	56,67,67	1.94	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PI	F	203	-	4,4,4	1.08	0	6,6,6	0.51	0
3	PEB	R	186	2	46,46,46	2.16	13 (28%)	56,67,67	2.10	15 (26%)
5	PI	R	205	-	4,4,4	0.71	0	6,6,6	0.66	0
3	PEB	Q	186	2	46,46,46	2.05	10 (21%)	56,67,67	1.92	16 (28%)
5	PI	J	204	-	4,4,4	1.24	0	6,6,6	0.72	0
3	PEB	F	166	1	46,46,46	1.77	6 (13%)	56,67,67	1.78	10 (17%)
3	PEB	R	187	2	46,46,46	1.97	8 (17%)	56,67,67	1.74	17 (30%)
3	PEB	U	186	2	46,46,46	2.01	13 (28%)	56,67,67	2.08	17 (30%)
3	PEB	E	167	1	46,46,46	1.94	11 (23%)	56,67,67	1.32	6 (10%)
3	PEB	T	187	2	46,46,46	1.71	10 (21%)	56,67,67	1.73	10 (17%)
3	PEB	W	186	2	46,46,46	1.93	12 (26%)	56,67,67	2.07	21 (37%)
8	MRD	T	204	-	7,7,7	0.50	0	9,10,10	0.55	0
5	PI	O	205	-	4,4,4	0.95	0	6,6,6	1.06	0
5	PI	A	204	-	4,4,4	1.16	0	6,6,6	0.99	0
3	PEB	U	188	2	46,46,46	1.98	11 (23%)	56,67,67	1.43	9 (16%)
5	PI	B	204	-	4,4,4	1.25	0	6,6,6	1.93	2 (33%)
5	PI	N	204	-	4,4,4	0.80	0	6,6,6	1.33	1 (16%)
4	NO3	D	203	-	1,3,3	2.01	1 (100%)	0,3,3	-	-
5	PI	Q	205	-	4,4,4	0.93	0	6,6,6	1.22	0
3	PEB	C	166	1	46,46,46	2.03	10 (21%)	56,67,67	2.08	15 (26%)
3	PEB	E	166	1	46,46,46	2.39	14 (30%)	56,67,67	2.10	13 (23%)
3	PEB	B	167	1	46,46,46	1.84	9 (19%)	56,67,67	1.80	12 (21%)
7	MPD	W	204	-	7,7,7	0.25	0	9,10,10	1.07	0
3	PEB	R	188	2	46,46,46	2.00	11 (23%)	56,67,67	1.60	8 (14%)
3	PEB	H	167	1	46,46,46	1.85	10 (21%)	56,67,67	1.54	8 (14%)
5	PI	L	204	-	4,4,4	1.15	0	6,6,6	0.92	0
3	PEB	I	166	1	46,46,46	2.02	10 (21%)	56,67,67	1.86	11 (19%)
3	PEB	Q	188	2	46,46,46	1.72	8 (17%)	56,67,67	1.54	12 (21%)
7	MPD	U	204	-	7,7,7	0.38	0	9,10,10	0.94	0
3	PEB	L	166	1	46,46,46	1.74	9 (19%)	56,67,67	1.85	10 (17%)
3	PEB	P	187	2	46,46,46	1.65	8 (17%)	56,67,67	1.55	9 (16%)
3	PEB	M	186	2	46,46,46	1.91	11 (23%)	56,67,67	1.81	15 (26%)
5	PI	G	203	-	4,4,4	0.99	0	6,6,6	0.87	0
4	NO3	A	203	-	1,3,3	1.61	0	0,3,3	-	-
3	PEB	X	187	2	46,46,46	1.78	10 (21%)	56,67,67	1.54	10 (17%)
3	PEB	V	188	2	46,46,46	1.90	11 (23%)	56,67,67	1.40	7 (12%)
3	PEB	B	166	1	46,46,46	1.93	11 (23%)	56,67,67	1.82	9 (16%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MPD	R	204	-	-	2/5/5/5	-

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

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

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

All (598) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	188	PEB	C2D-C3D	9.37	1.46	1.34
3	P	186	PEB	C2D-C3D	8.88	1.46	1.34
3	O	187	PEB	C2D-C3D	8.31	1.45	1.34
3	V	187	PEB	C2D-C3D	8.25	1.45	1.34
3	H	166	PEB	C4C-C3C	8.13	1.49	1.38
3	P	188	PEB	C2D-C3D	8.07	1.44	1.34
3	E	166	PEB	C4C-C3C	8.03	1.49	1.38
3	W	188	PEB	C2D-C3D	8.00	1.44	1.34
3	T	186	PEB	C4C-C3C	8.00	1.49	1.38
3	V	188	PEB	C2D-C3D	7.74	1.44	1.34
3	O	188	PEB	C2D-C3D	7.72	1.44	1.34
3	Q	186	PEB	C2D-C3D	7.71	1.44	1.34
3	R	186	PEB	C4C-C3C	7.55	1.48	1.38
3	N	188	PEB	C2D-C3D	7.53	1.44	1.34
3	M	188	PEB	C2D-C3D	7.41	1.44	1.34
3	U	188	PEB	C2D-C3D	7.28	1.43	1.34
3	I	166	PEB	C2D-C3D	7.27	1.43	1.34
3	R	187	PEB	C2D-C3D	7.17	1.43	1.34
3	H	166	PEB	C2D-C3D	7.09	1.43	1.34
3	W	187	PEB	C4C-C3C	7.06	1.48	1.38
3	K	167	PEB	C2D-C3D	6.94	1.43	1.34
3	X	186	PEB	C2D-C3D	6.88	1.43	1.34
3	D	166	PEB	C2D-C3D	6.76	1.43	1.34
3	S	187	PEB	C2D-C3D	6.68	1.43	1.34
3	U	186	PEB	C2D-C3D	6.67	1.43	1.34
3	C	167	PEB	C4C-C3C	6.58	1.47	1.38
3	T	186	PEB	C2D-C3D	6.54	1.43	1.34
3	T	188	PEB	C2D-C3D	6.54	1.43	1.34
3	C	166	PEB	C2D-C3D	6.54	1.43	1.34
3	F	167	PEB	C4C-C3C	6.52	1.47	1.38
3	B	166	PEB	C4C-C3C	6.48	1.47	1.38
3	M	186	PEB	C2D-C3D	6.37	1.42	1.34
3	I	167	PEB	C2D-C3D	6.33	1.42	1.34
3	D	167	PEB	C4C-C3C	6.29	1.46	1.38
3	Q	188	PEB	C2D-C3D	6.28	1.42	1.34
3	W	186	PEB	C2D-C3D	6.28	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	187	PEB	C2D-C3D	6.24	1.42	1.34
3	K	167	PEB	C4C-C3C	6.22	1.46	1.38
3	E	167	PEB	C4C-C3C	6.20	1.46	1.38
3	F	166	PEB	C4C-C3C	6.17	1.46	1.38
3	F	166	PEB	C2D-C3D	6.16	1.42	1.34
3	E	166	PEB	C2D-C3D	6.15	1.42	1.34
3	H	167	PEB	C2D-C3D	6.06	1.42	1.34
3	U	187	PEB	C2D-C3D	6.02	1.42	1.34
3	R	186	PEB	C2D-C3D	5.91	1.42	1.34
3	C	166	PEB	C4C-C3C	5.90	1.46	1.38
3	Q	186	PEB	C4C-C3C	5.86	1.46	1.38
3	S	188	PEB	C2D-C3D	5.86	1.42	1.34
3	K	167	PEB	C1A-NA	-5.79	1.30	1.37
3	I	166	PEB	C4C-C3C	5.74	1.46	1.38
3	U	186	PEB	C4C-C3C	5.73	1.46	1.38
3	R	188	PEB	C2D-C3D	5.73	1.41	1.34
3	G	167	PEB	C4C-C3C	5.72	1.46	1.38
3	I	167	PEB	C4C-C3C	5.68	1.46	1.38
3	F	167	PEB	C2D-C3D	5.61	1.41	1.34
3	W	186	PEB	C4C-C3C	5.59	1.45	1.38
3	B	167	PEB	C4C-C3C	5.58	1.45	1.38
3	D	166	PEB	C4C-C3C	5.58	1.45	1.38
3	L	167	PEB	C4C-C3C	5.58	1.45	1.38
3	N	186	PEB	C2D-C3D	5.57	1.41	1.34
3	E	167	PEB	C2D-C3D	5.55	1.41	1.34
3	R	188	PEB	C4C-C3C	5.52	1.45	1.38
3	N	187	PEB	C2D-C3D	5.52	1.41	1.34
3	K	166	PEB	C2D-C3D	5.50	1.41	1.34
3	O	186	PEB	C4C-C3C	5.48	1.45	1.38
3	M	187	PEB	C4C-C3C	5.47	1.45	1.38
3	R	187	PEB	C4C-C3C	5.45	1.45	1.38
3	G	166	PEB	C4C-C3C	5.44	1.45	1.38
3	E	166	PEB	CHB-C4B	5.43	1.49	1.38
3	A	167	PEB	C4C-C3C	5.42	1.45	1.38
3	P	187	PEB	C2D-C3D	5.42	1.41	1.34
3	O	187	PEB	C4C-C3C	5.34	1.45	1.38
3	T	188	PEB	C4C-C3C	5.30	1.45	1.38
3	Q	187	PEB	C2D-C3D	5.29	1.41	1.34
3	E	166	PEB	C3B-C2B	5.29	1.48	1.36
3	U	188	PEB	C4C-C3C	5.28	1.45	1.38
3	H	167	PEB	C4C-C3C	5.27	1.45	1.38
3	S	188	PEB	C4C-C3C	5.27	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	186	PEB	C2D-C3D	5.26	1.41	1.34
3	P	188	PEB	C4C-C3C	5.25	1.45	1.38
3	S	186[A]	PEB	C2D-C3D	5.22	1.41	1.34
3	S	186[B]	PEB	C2D-C3D	5.22	1.41	1.34
3	X	186	PEB	C4C-C3C	5.19	1.45	1.38
3	O	188	PEB	C4C-C3C	5.16	1.45	1.38
3	M	188	PEB	C4C-C3C	5.16	1.45	1.38
3	T	187	PEB	C4C-C3C	5.13	1.45	1.38
3	X	188	PEB	C4C-C3C	5.12	1.45	1.38
3	W	187	PEB	C2D-C3D	5.11	1.41	1.34
3	N	186	PEB	C4C-C3C	5.10	1.45	1.38
3	G	166	PEB	C2D-C3D	5.06	1.41	1.34
3	K	166	PEB	C2A-C1A	-5.06	1.47	1.52
3	L	166	PEB	C2D-C3D	5.02	1.41	1.34
3	M	187	PEB	C2D-C3D	4.97	1.41	1.34
3	C	166	PEB	CHB-C4B	4.94	1.48	1.38
3	K	166	PEB	C4C-C3C	4.93	1.45	1.38
3	G	167	PEB	C2D-C3D	4.82	1.40	1.34
3	N	187	PEB	C4C-C3C	4.79	1.44	1.38
3	R	188	PEB	CHA-C1B	4.77	1.51	1.40
3	B	167	PEB	C1A-NA	-4.74	1.31	1.37
3	C	166	PEB	C3B-C2B	4.73	1.47	1.36
3	T	186	PEB	C3B-C2B	4.69	1.46	1.36
3	J	167	PEB	C4C-C3C	4.67	1.44	1.38
3	P	186	PEB	CHB-C4B	4.64	1.47	1.38
3	J	167	PEB	C2D-C3D	4.62	1.40	1.34
3	J	166	PEB	C3B-C2B	4.60	1.46	1.36
3	S	186[A]	PEB	C4C-C3C	4.54	1.44	1.38
3	S	186[B]	PEB	C4C-C3C	4.54	1.44	1.38
3	P	186	PEB	C4C-C3C	4.54	1.44	1.38
3	B	167	PEB	C2A-C1A	-4.52	1.48	1.52
3	N	188	PEB	C4C-C3C	4.51	1.44	1.38
3	D	166	PEB	C2A-C1A	-4.46	1.48	1.52
3	W	186	PEB	CHB-C4B	4.46	1.47	1.38
3	J	166	PEB	C4C-C3C	4.45	1.44	1.38
3	T	187	PEB	C2D-C3D	4.40	1.40	1.34
3	R	187	PEB	C3B-C2B	4.40	1.46	1.36
3	K	167	PEB	C2A-C1A	-4.39	1.48	1.52
3	S	186[A]	PEB	CHB-C4B	4.39	1.47	1.38
3	S	186[B]	PEB	CHB-C4B	4.39	1.47	1.38
3	I	166	PEB	CHB-C4B	4.38	1.47	1.38
3	R	186	PEB	CHB-C4B	4.37	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	167	PEB	C2D-C3D	4.37	1.40	1.34
3	R	187	PEB	CHB-C4B	4.36	1.46	1.38
3	J	167	PEB	C3B-C2B	4.35	1.46	1.36
3	X	188	PEB	C1A-NA	-4.34	1.32	1.37
3	M	186	PEB	CHB-C4B	4.33	1.46	1.38
3	A	166	PEB	C2D-C3D	4.32	1.40	1.34
3	B	166	PEB	C2D-C3D	4.32	1.40	1.34
3	U	187	PEB	C4C-C3C	4.31	1.44	1.38
3	A	166	PEB	C4C-C3C	4.28	1.44	1.38
3	W	188	PEB	C3B-C2B	4.26	1.46	1.36
3	V	187	PEB	C4C-C3C	4.24	1.44	1.38
3	T	188	PEB	CHA-C1B	4.23	1.50	1.40
3	Q	188	PEB	C4C-C3C	4.20	1.44	1.38
3	N	188	PEB	C3B-C2B	4.20	1.45	1.36
3	L	166	PEB	C4D-ND	-4.19	1.29	1.35
3	N	186	PEB	CHA-C1B	4.14	1.50	1.40
3	W	187	PEB	C1A-NA	-4.13	1.32	1.37
3	W	188	PEB	C4C-C3C	4.13	1.43	1.38
3	E	167	PEB	C1A-NA	-4.10	1.32	1.37
3	C	167	PEB	C1A-NA	-4.08	1.32	1.37
3	H	166	PEB	C3B-C2B	4.07	1.45	1.36
3	U	186	PEB	C3B-C2B	4.07	1.45	1.36
3	T	186	PEB	CHB-C4B	4.06	1.46	1.38
3	R	188	PEB	C3B-C2B	4.04	1.45	1.36
3	T	186	PEB	CHA-C1B	4.03	1.49	1.40
3	G	167	PEB	C1A-NA	-4.02	1.32	1.37
3	G	166	PEB	C3B-C2B	4.01	1.45	1.36
3	S	187	PEB	C4C-C3C	3.99	1.43	1.38
3	L	166	PEB	CHA-C1B	3.97	1.49	1.40
3	O	188	PEB	CHA-C1B	3.96	1.49	1.40
3	Q	186	PEB	CHB-C4B	3.96	1.46	1.38
3	V	186	PEB	C2D-C3D	3.95	1.39	1.34
3	N	186	PEB	CHB-C4B	3.95	1.46	1.38
3	W	188	PEB	CHB-C4B	3.94	1.46	1.38
3	B	166	PEB	C3B-C2B	3.94	1.45	1.36
3	O	187	PEB	C1A-NA	-3.92	1.32	1.37
3	V	186	PEB	C4C-C3C	3.90	1.43	1.38
3	X	187	PEB	C4C-C3C	3.90	1.43	1.38
3	L	166	PEB	C4B-C3B	-3.88	1.39	1.45
3	H	167	PEB	CHA-C1B	3.87	1.49	1.40
3	V	188	PEB	C4C-C3C	3.86	1.43	1.38
3	A	167	PEB	C1A-NA	-3.85	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	167	PEB	C1A-NA	-3.81	1.32	1.37
3	Q	186	PEB	CHA-C1B	3.80	1.49	1.40
3	P	188	PEB	C3B-C2B	3.78	1.44	1.36
3	L	167	PEB	C1A-NA	-3.78	1.32	1.37
3	M	186	PEB	C4C-C3C	3.78	1.43	1.38
3	I	166	PEB	C3B-C2B	3.77	1.44	1.36
3	E	166	PEB	CHB-C1C	3.77	1.48	1.40
3	W	187	PEB	C3B-C2B	3.76	1.44	1.36
3	U	187	PEB	CHA-C1B	3.75	1.49	1.40
3	S	188	PEB	CHB-C4B	3.71	1.45	1.38
3	Q	186	PEB	C3B-C2B	3.71	1.44	1.36
3	S	186[A]	PEB	C3B-C2B	3.70	1.44	1.36
3	S	186[B]	PEB	C3B-C2B	3.70	1.44	1.36
3	H	166	PEB	CHB-C4B	3.68	1.45	1.38
3	A	167	PEB	C2D-C3D	3.68	1.39	1.34
3	K	166	PEB	C3B-C2B	3.67	1.44	1.36
3	R	186	PEB	C3B-C2B	3.66	1.44	1.36
3	M	188	PEB	C1A-NA	-3.66	1.32	1.37
3	B	167	PEB	C2D-C3D	3.65	1.39	1.34
3	N	187	PEB	CHA-C1B	3.64	1.49	1.40
3	Q	187	PEB	CHB-C4B	3.64	1.45	1.38
3	X	187	PEB	C3B-C2B	3.63	1.44	1.36
3	U	188	PEB	C1A-NA	-3.62	1.33	1.37
3	O	186	PEB	C2A-C1A	-3.62	1.48	1.52
3	O	186	PEB	C3B-C2B	3.61	1.44	1.36
3	P	187	PEB	CHA-C1B	3.61	1.48	1.40
3	W	188	PEB	C1C-NC	-3.60	1.31	1.37
3	O	188	PEB	C1D-ND	3.60	1.50	1.45
3	U	188	PEB	CHA-C1B	3.59	1.48	1.40
3	L	166	PEB	C4C-C3C	3.59	1.43	1.38
3	O	187	PEB	C3B-C2B	3.58	1.44	1.36
3	S	188	PEB	C3B-C2B	3.58	1.44	1.36
3	T	188	PEB	C3B-C2B	3.56	1.44	1.36
3	G	166	PEB	C4C-NC	-3.56	1.29	1.37
3	U	187	PEB	CHB-C4B	3.56	1.45	1.38
3	Q	187	PEB	C4C-C3C	3.56	1.43	1.38
3	X	188	PEB	C3B-C2B	3.55	1.44	1.36
3	X	186	PEB	CHA-C1B	3.55	1.48	1.40
3	W	186	PEB	C3B-C2B	3.53	1.44	1.36
3	U	187	PEB	C1A-NA	-3.52	1.33	1.37
3	D	167	PEB	C1A-NA	-3.52	1.33	1.37
3	R	188	PEB	C1A-NA	-3.51	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	167	PEB	C3B-C2B	3.51	1.44	1.36
3	M	186	PEB	C3B-C2B	3.51	1.44	1.36
3	Q	187	PEB	C2A-C1A	-3.51	1.49	1.52
3	R	187	PEB	CHA-C1B	3.50	1.48	1.40
3	O	186	PEB	CHB-C4B	3.48	1.45	1.38
3	V	187	PEB	CHB-C4B	3.48	1.45	1.38
3	S	187	PEB	CHB-C4B	3.48	1.45	1.38
3	O	187	PEB	C2A-C1A	-3.47	1.49	1.52
3	S	188	PEB	C2A-C1A	-3.47	1.49	1.52
3	R	186	PEB	CHA-C1B	3.47	1.48	1.40
3	Q	187	PEB	CHA-C1B	3.47	1.48	1.40
3	R	188	PEB	C1C-NC	-3.46	1.31	1.37
3	E	167	PEB	CHB-C4B	3.46	1.45	1.38
3	C	167	PEB	CHA-C1B	3.46	1.48	1.40
3	W	188	PEB	CHA-C1B	3.45	1.48	1.40
3	W	188	PEB	C2C-C3C	3.44	1.47	1.38
3	E	166	PEB	C1A-NA	-3.44	1.33	1.37
3	T	187	PEB	CHA-C1B	3.44	1.48	1.40
3	P	186	PEB	C3B-C2B	3.43	1.44	1.36
3	U	188	PEB	O2C-CGC	-3.43	1.19	1.30
3	H	167	PEB	C2A-C1A	-3.42	1.49	1.52
3	G	167	PEB	CHB-C4B	3.41	1.45	1.38
3	M	186	PEB	CHA-C1B	3.41	1.48	1.40
3	D	166	PEB	C1A-NA	-3.41	1.33	1.37
3	N	188	PEB	CHB-C4B	3.40	1.45	1.38
3	O	188	PEB	C3B-C2B	3.39	1.44	1.36
3	J	166	PEB	C2D-C3D	3.38	1.39	1.34
3	B	166	PEB	C1A-NA	-3.38	1.33	1.37
3	D	167	PEB	C3B-C2B	3.37	1.44	1.36
3	I	167	PEB	C1A-NA	-3.36	1.33	1.37
3	E	166	PEB	OD-C4D	3.35	1.29	1.23
3	O	188	PEB	C4D-ND	-3.35	1.30	1.35
3	G	167	PEB	C3B-C2B	3.32	1.43	1.36
3	P	187	PEB	C4C-C3C	3.32	1.42	1.38
3	D	166	PEB	C3B-C2B	3.31	1.43	1.36
3	P	187	PEB	C3B-C2B	3.31	1.43	1.36
3	C	167	PEB	C4A-NA	-3.31	1.31	1.37
3	Q	187	PEB	C3B-C2B	3.28	1.43	1.36
3	C	167	PEB	C3B-C2B	3.27	1.43	1.36
3	M	187	PEB	C3B-C2B	3.27	1.43	1.36
3	Q	188	PEB	C1A-NA	-3.27	1.33	1.37
3	A	167	PEB	CHA-C1B	3.26	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	166	PEB	CHA-C1B	3.26	1.48	1.40
3	X	186	PEB	CHB-C4B	3.25	1.44	1.38
3	K	166	PEB	OD-C4D	3.25	1.29	1.23
3	T	187	PEB	CHB-C4B	3.24	1.44	1.38
3	C	167	PEB	C2C-C3C	3.24	1.47	1.38
3	B	166	PEB	CHA-C1B	3.22	1.48	1.40
3	O	188	PEB	OD-C4D	3.21	1.29	1.23
3	O	187	PEB	CHA-C1B	3.21	1.48	1.40
3	U	187	PEB	C3B-C2B	3.21	1.43	1.36
3	V	186	PEB	CHA-C1B	3.21	1.48	1.40
3	U	188	PEB	C3B-C2B	3.20	1.43	1.36
3	P	186	PEB	CMB-C2B	-3.20	1.44	1.50
3	N	187	PEB	C3B-C2B	3.20	1.43	1.36
3	C	166	PEB	C2A-C1A	-3.19	1.49	1.52
3	U	186	PEB	CHA-C1B	3.18	1.48	1.40
3	S	186[A]	PEB	C2C-C3C	3.18	1.47	1.38
3	P	188	PEB	CHA-C1B	3.18	1.47	1.40
3	V	188	PEB	C3B-C2B	3.17	1.43	1.36
3	D	166	PEB	CHA-C1B	3.16	1.47	1.40
3	R	186	PEB	C2C-C3C	3.14	1.47	1.38
3	E	166	PEB	CHA-C1B	3.13	1.47	1.40
3	B	167	PEB	C3B-C2B	3.13	1.43	1.36
3	U	186	PEB	CHB-C4B	3.13	1.44	1.38
3	X	188	PEB	CHA-C1B	3.12	1.47	1.40
3	K	167	PEB	C2C-C3C	3.11	1.47	1.38
3	N	186	PEB	O2C-CGC	-3.11	1.20	1.30
3	S	187	PEB	CHA-C1B	3.10	1.47	1.40
3	V	186	PEB	C3B-C2B	3.09	1.43	1.36
3	S	186[A]	PEB	CHA-C1B	3.08	1.47	1.40
3	S	186[B]	PEB	CHA-C1B	3.08	1.47	1.40
3	U	187	PEB	C3A-C4A	3.07	1.57	1.50
3	N	186	PEB	C3B-C2B	3.07	1.43	1.36
3	I	167	PEB	CHA-C1B	3.07	1.47	1.40
3	G	167	PEB	C4D-ND	-3.06	1.31	1.35
3	F	166	PEB	C3B-C2B	3.06	1.43	1.36
3	J	166	PEB	C2A-C1A	-3.03	1.49	1.52
3	V	186	PEB	CHB-C4B	3.03	1.44	1.38
3	W	186	PEB	CHA-C1B	3.03	1.47	1.40
3	D	167	PEB	CHA-C1B	3.03	1.47	1.40
3	V	188	PEB	C1A-NA	-3.03	1.33	1.37
3	I	166	PEB	CHA-C1B	3.02	1.47	1.40
3	F	167	PEB	C2A-C1A	-3.02	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	186	PEB	CHB-C1C	3.01	1.47	1.40
3	R	186	PEB	CHB-C1C	3.00	1.47	1.40
3	O	188	PEB	C1A-NA	-3.00	1.33	1.37
3	G	167	PEB	CHA-C1B	3.00	1.47	1.40
3	V	187	PEB	C3B-C2B	2.99	1.43	1.36
3	V	188	PEB	CHA-C1B	2.99	1.47	1.40
3	P	186	PEB	CHA-C1B	2.99	1.47	1.40
3	Q	188	PEB	C3B-C2B	2.98	1.43	1.36
3	B	166	PEB	CHB-C4B	2.98	1.44	1.38
3	C	166	PEB	C1A-NA	-2.97	1.33	1.37
3	R	188	PEB	CHB-C4B	2.97	1.44	1.38
3	H	167	PEB	C2C-C3C	2.96	1.46	1.38
3	P	186	PEB	C1D-ND	2.96	1.50	1.45
3	O	188	PEB	CHB-C1C	2.96	1.47	1.40
3	K	166	PEB	CHA-C1B	2.95	1.47	1.40
3	P	186	PEB	C2A-C1A	-2.95	1.49	1.52
3	V	187	PEB	CHA-C1B	2.95	1.47	1.40
3	J	167	PEB	CHB-C1C	2.94	1.47	1.40
3	R	186	PEB	C2A-C1A	-2.94	1.49	1.52
3	L	167	PEB	CHA-C1B	2.94	1.47	1.40
3	E	166	PEB	C4D-ND	-2.92	1.31	1.35
3	L	167	PEB	C4D-ND	-2.91	1.31	1.35
3	M	188	PEB	C3B-C2B	2.90	1.43	1.36
3	W	186	PEB	OD-C4D	2.89	1.29	1.23
3	K	167	PEB	C3B-C2B	2.89	1.43	1.36
3	Q	188	PEB	OD-C4D	2.89	1.29	1.23
3	X	187	PEB	CHC-C4C	2.89	1.53	1.50
3	C	167	PEB	CHB-C1C	2.89	1.46	1.40
3	I	167	PEB	C3B-C2B	2.88	1.43	1.36
3	M	187	PEB	CHA-C1B	2.88	1.47	1.40
3	R	187	PEB	OD-C4D	2.87	1.29	1.23
3	R	186	PEB	OD-C4D	2.86	1.29	1.23
3	M	188	PEB	C1C-NC	-2.86	1.32	1.37
3	C	166	PEB	C4D-ND	-2.85	1.31	1.35
3	S	188	PEB	CHA-C1B	2.85	1.47	1.40
3	W	187	PEB	C2A-C1A	-2.85	1.49	1.52
3	P	186	PEB	OD-C4D	2.85	1.29	1.23
3	O	187	PEB	CHB-C4B	2.85	1.44	1.38
3	S	186[A]	PEB	OD-C4D	2.85	1.29	1.23
3	S	186[B]	PEB	OD-C4D	2.85	1.29	1.23
3	U	187	PEB	CHC-C4C	2.83	1.53	1.50
3	S	187	PEB	C1D-ND	2.82	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	166	PEB	C1D-ND	2.82	1.49	1.45
3	E	167	PEB	CHA-C1B	2.82	1.47	1.40
3	A	166	PEB	CHA-C1B	2.82	1.47	1.40
3	A	167	PEB	CHC-C4C	-2.82	1.46	1.50
3	J	167	PEB	CHA-C1B	2.82	1.47	1.40
3	F	167	PEB	CHB-C4B	2.81	1.44	1.38
3	X	186	PEB	C3B-C2B	2.81	1.42	1.36
3	C	167	PEB	C4B-NB	-2.81	1.32	1.38
3	P	188	PEB	OD-C4D	2.81	1.28	1.23
3	G	167	PEB	C4A-NA	-2.80	1.31	1.37
3	N	188	PEB	C2C-C3C	2.80	1.46	1.38
3	K	167	PEB	CHB-C1C	2.79	1.46	1.40
3	L	166	PEB	C2A-C1A	-2.79	1.49	1.52
3	J	167	PEB	CHB-C4B	2.79	1.44	1.38
3	D	166	PEB	C4B-C3B	-2.79	1.41	1.45
3	F	166	PEB	O1B-CGB	2.78	1.31	1.22
3	G	167	PEB	OD-C4D	2.78	1.28	1.23
3	F	167	PEB	CHA-C1B	2.77	1.47	1.40
3	O	188	PEB	C2C-C3C	2.77	1.46	1.38
3	P	186	PEB	C1A-NA	-2.75	1.34	1.37
3	D	167	PEB	C2A-C1A	-2.75	1.49	1.52
3	J	166	PEB	CHA-C1B	2.74	1.46	1.40
3	K	166	PEB	CHB-C4B	2.74	1.43	1.38
3	V	188	PEB	C4D-ND	-2.74	1.31	1.35
3	A	167	PEB	CHB-C1C	2.73	1.46	1.40
3	S	186[B]	PEB	C1C-C2C	2.72	1.48	1.42
3	Q	186	PEB	C2C-C3C	2.72	1.46	1.38
3	L	167	PEB	C1D-ND	2.72	1.49	1.45
3	H	167	PEB	C1A-NA	-2.71	1.34	1.37
3	R	187	PEB	C2C-C3C	2.71	1.46	1.38
3	N	188	PEB	C4A-NA	-2.70	1.32	1.37
3	L	167	PEB	OD-C4D	2.70	1.28	1.23
3	H	167	PEB	C3B-C2B	2.70	1.42	1.36
3	L	167	PEB	C3B-C2B	2.69	1.42	1.36
3	Q	188	PEB	CHA-C1B	2.68	1.46	1.40
3	I	167	PEB	C1D-ND	-2.67	1.42	1.45
3	W	186	PEB	C1C-NC	-2.67	1.33	1.37
3	T	188	PEB	CHB-C1C	2.67	1.46	1.40
3	D	166	PEB	CHB-C4B	2.67	1.43	1.38
3	T	187	PEB	C3B-C2B	2.67	1.42	1.36
3	S	186[A]	PEB	C2A-C1A	-2.67	1.49	1.52
3	S	186[B]	PEB	C2A-C1A	-2.67	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	187	PEB	C1A-NA	-2.66	1.34	1.37
3	T	188	PEB	C2C-C3C	2.66	1.45	1.38
3	W	187	PEB	CHB-C4B	2.66	1.43	1.38
3	H	166	PEB	C1C-NC	-2.66	1.33	1.37
3	L	167	PEB	C2D-C3D	2.66	1.38	1.34
3	H	166	PEB	CHB-C1C	2.65	1.46	1.40
3	X	187	PEB	CHA-C1B	2.65	1.46	1.40
3	O	186	PEB	O1C-CGC	2.64	1.30	1.22
3	E	167	PEB	C2A-C1A	-2.64	1.49	1.52
3	M	188	PEB	CHA-C1B	2.64	1.46	1.40
3	N	187	PEB	CAA-C3A	2.62	1.59	1.54
3	X	186	PEB	O1C-CGC	2.62	1.30	1.22
3	F	166	PEB	CHA-C1B	2.61	1.46	1.40
3	T	186	PEB	OD-C4D	2.61	1.28	1.23
3	P	186	PEB	CHB-C1C	2.61	1.46	1.40
3	B	166	PEB	O2C-CGC	-2.61	1.22	1.30
3	E	166	PEB	C2C-C3C	2.60	1.45	1.38
3	V	186	PEB	CHB-C1C	2.60	1.46	1.40
3	J	166	PEB	CHB-C4B	2.60	1.43	1.38
3	E	167	PEB	C3B-C2B	2.60	1.42	1.36
3	U	186	PEB	CHA-C4A	-2.59	1.32	1.36
3	S	187	PEB	C3B-C2B	2.59	1.42	1.36
3	M	186	PEB	C1C-NC	-2.57	1.33	1.37
3	S	186[A]	PEB	C1A-NA	-2.57	1.34	1.37
3	S	186[B]	PEB	C1A-NA	-2.57	1.34	1.37
3	X	187	PEB	C1A-NA	-2.57	1.34	1.37
3	T	187	PEB	C2C-C3C	2.57	1.45	1.38
3	S	187	PEB	OD-C4D	2.57	1.28	1.23
3	F	167	PEB	C1A-NA	-2.57	1.34	1.37
3	R	188	PEB	CHB-C1C	2.56	1.46	1.40
3	C	166	PEB	O2B-CGB	-2.56	1.22	1.30
3	W	188	PEB	OD-C4D	2.56	1.28	1.23
3	U	188	PEB	C1C-NC	-2.56	1.33	1.37
3	M	186	PEB	C1B-NB	2.56	1.42	1.36
3	T	186	PEB	O2C-CGC	-2.55	1.22	1.30
3	M	186	PEB	O1C-CGC	2.54	1.30	1.22
3	U	186	PEB	C2C-C3C	2.54	1.45	1.38
3	W	187	PEB	CHB-C1C	2.53	1.46	1.40
3	H	167	PEB	CHB-C4B	2.53	1.43	1.38
3	X	188	PEB	C2C-C3C	2.53	1.45	1.38
3	K	166	PEB	C1A-NA	-2.53	1.34	1.37
3	X	188	PEB	C1C-NC	-2.52	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	167	PEB	OD-C4D	2.52	1.28	1.23
3	P	186	PEB	C1C-NC	-2.52	1.33	1.37
3	V	188	PEB	CHA-C4A	-2.52	1.32	1.36
3	J	167	PEB	C2A-C1A	-2.52	1.49	1.52
3	S	188	PEB	OD-C4D	2.51	1.28	1.23
3	Q	186	PEB	OD-C4D	2.51	1.28	1.23
3	M	187	PEB	CHB-C4B	2.51	1.43	1.38
3	T	186	PEB	C2C-C3C	2.51	1.45	1.38
3	M	186	PEB	OD-C4D	2.51	1.28	1.23
3	V	188	PEB	CHB-C4B	2.51	1.43	1.38
3	P	187	PEB	CHB-C4B	2.51	1.43	1.38
3	F	167	PEB	C4A-NA	-2.50	1.32	1.37
3	M	188	PEB	C4D-ND	-2.49	1.31	1.35
3	X	186	PEB	C2C-C3C	2.49	1.45	1.38
3	R	187	PEB	C1A-NA	-2.49	1.34	1.37
5	U	205	PI	P-O1	2.48	1.56	1.50
3	E	167	PEB	C1D-ND	2.48	1.49	1.45
3	I	167	PEB	C4D-ND	-2.48	1.31	1.35
3	V	187	PEB	O2B-CGB	-2.48	1.22	1.30
3	H	167	PEB	CHB-C1C	2.48	1.45	1.40
3	B	167	PEB	C2C-C3C	2.48	1.45	1.38
3	S	187	PEB	CHB-C1C	2.47	1.45	1.40
3	S	186[B]	PEB	C2C-C3C	2.47	1.45	1.38
3	K	167	PEB	CHB-C4B	2.47	1.43	1.38
3	T	187	PEB	CHB-C1C	2.46	1.45	1.40
3	G	166	PEB	C4B-C3B	-2.46	1.41	1.45
3	U	188	PEB	CHB-C4B	2.44	1.43	1.38
3	S	187	PEB	C1A-NA	-2.44	1.34	1.37
3	W	186	PEB	CMD-C2D	-2.44	1.46	1.50
3	F	167	PEB	CHB-C1C	2.43	1.45	1.40
3	G	167	PEB	C4B-NB	-2.42	1.33	1.38
3	N	188	PEB	CHA-C1B	2.41	1.46	1.40
3	S	188	PEB	CHB-C1C	2.41	1.45	1.40
3	K	166	PEB	O2C-CGC	-2.41	1.22	1.30
3	T	188	PEB	O1C-CGC	2.41	1.30	1.22
3	X	187	PEB	OD-C4D	2.40	1.28	1.23
3	X	187	PEB	CHB-C4B	2.40	1.43	1.38
3	V	187	PEB	C4B-C3B	-2.40	1.42	1.45
3	E	166	PEB	C2A-C1A	-2.40	1.49	1.52
3	T	187	PEB	C2A-C1A	-2.40	1.50	1.52
3	Q	186	PEB	C2A-C1A	-2.39	1.50	1.52
3	E	167	PEB	C2C-C3C	2.38	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	188	PEB	CHB-C4B	2.37	1.43	1.38
3	T	186	PEB	C1A-NA	-2.37	1.34	1.37
3	W	186	PEB	C1A-NA	-2.37	1.34	1.37
3	T	188	PEB	C4B-NB	-2.37	1.33	1.38
3	W	186	PEB	C2C-C3C	2.37	1.45	1.38
3	F	167	PEB	C2C-C3C	2.36	1.45	1.38
3	E	166	PEB	O2C-CGC	-2.36	1.23	1.30
3	T	188	PEB	O2B-CGB	-2.36	1.23	1.30
3	N	186	PEB	C1A-NA	-2.36	1.34	1.37
3	C	167	PEB	O1C-CGC	2.35	1.29	1.22
3	X	186	PEB	OD-C4D	2.35	1.28	1.23
3	G	166	PEB	CHA-C1B	2.34	1.46	1.40
3	T	188	PEB	C1C-NC	-2.34	1.33	1.37
3	G	167	PEB	CHB-C1C	2.34	1.45	1.40
3	D	167	PEB	C2D-C3D	2.33	1.37	1.34
3	X	186	PEB	CBC-CGC	2.33	1.56	1.50
3	V	188	PEB	CHC-C4C	2.32	1.52	1.50
3	M	187	PEB	C2A-C1A	-2.32	1.50	1.52
3	M	187	PEB	C1A-NA	-2.32	1.34	1.37
3	U	186	PEB	C1A-NA	-2.31	1.34	1.37
3	K	167	PEB	CHA-C1B	2.31	1.45	1.40
3	R	186	PEB	C1A-NA	-2.31	1.34	1.37
3	V	187	PEB	O2C-CGC	-2.31	1.23	1.30
3	V	188	PEB	C2C-C3C	2.30	1.44	1.38
3	R	188	PEB	C4B-NB	-2.30	1.33	1.38
3	M	186	PEB	C1A-NA	-2.30	1.34	1.37
3	E	166	PEB	C1C-C2C	2.29	1.47	1.42
3	V	186	PEB	CMD-C2D	-2.29	1.46	1.50
3	X	187	PEB	CHB-C1C	2.29	1.45	1.40
3	B	166	PEB	C2A-C1A	-2.28	1.50	1.52
3	P	187	PEB	C1D-ND	2.27	1.49	1.45
3	T	186	PEB	CHB-C1C	2.27	1.45	1.40
3	Q	188	PEB	CHB-C1C	2.26	1.45	1.40
3	A	166	PEB	O2C-CGC	-2.26	1.23	1.30
3	A	167	PEB	C2C-C3C	2.26	1.44	1.38
3	E	167	PEB	O2B-CGB	-2.26	1.23	1.30
3	V	186	PEB	O2C-CGC	-2.25	1.23	1.30
3	B	167	PEB	CHB-C4B	2.24	1.42	1.38
3	X	188	PEB	OD-C4D	2.24	1.27	1.23
3	I	166	PEB	C2A-C1A	-2.23	1.50	1.52
3	M	187	PEB	OD-C4D	2.23	1.27	1.23
3	F	167	PEB	OD-C4D	2.23	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	186	PEB	C1C-C2C	2.23	1.47	1.42
3	G	167	PEB	C4B-C3B	-2.23	1.42	1.45
3	I	167	PEB	C2A-C1A	-2.23	1.50	1.52
3	M	188	PEB	CHB-C4B	2.23	1.42	1.38
3	R	188	PEB	C1D-ND	2.22	1.48	1.45
3	N	187	PEB	CBB-CGB	2.22	1.55	1.50
3	N	187	PEB	CHB-C4B	2.22	1.42	1.38
3	O	188	PEB	CMD-C2D	2.22	1.54	1.50
3	T	188	PEB	OD-C4D	2.22	1.27	1.23
3	U	186	PEB	C1C-NC	-2.22	1.34	1.37
3	V	186	PEB	C2A-C1A	-2.21	1.50	1.52
3	G	166	PEB	C4D-ND	-2.20	1.32	1.35
3	P	186	PEB	O2C-CGC	-2.20	1.23	1.30
3	X	187	PEB	C1C-NC	-2.20	1.34	1.37
3	U	188	PEB	C4D-ND	-2.20	1.32	1.35
3	Q	188	PEB	C3A-C4A	2.20	1.55	1.50
3	R	186	PEB	C4B-NB	-2.19	1.33	1.38
3	S	186[A]	PEB	CBC-CGC	2.19	1.55	1.50
3	O	188	PEB	C1C-NC	-2.19	1.34	1.37
3	C	166	PEB	CHA-C1B	2.19	1.45	1.40
3	K	167	PEB	C1B-NB	-2.19	1.31	1.36
3	Q	186	PEB	O2C-CGC	-2.19	1.23	1.30
3	O	187	PEB	O2C-CGC	-2.19	1.23	1.30
3	U	186	PEB	O2C-CGC	-2.18	1.23	1.30
3	V	186	PEB	C4D-ND	-2.18	1.32	1.35
3	W	186	PEB	CHB-C1C	2.18	1.45	1.40
3	K	167	PEB	CBC-CGC	2.17	1.55	1.50
3	O	187	PEB	OD-C4D	2.17	1.27	1.23
3	V	188	PEB	CMD-C2D	2.17	1.54	1.50
3	O	186	PEB	CHB-C1C	2.17	1.45	1.40
3	R	186	PEB	C1C-C2C	2.17	1.47	1.42
3	L	166	PEB	CHB-C4B	2.17	1.42	1.38
3	B	167	PEB	OD-C4D	2.16	1.27	1.23
3	T	187	PEB	CMB-C2B	-2.16	1.46	1.50
3	B	167	PEB	CHB-C1C	2.16	1.45	1.40
3	M	188	PEB	OD-C4D	2.16	1.27	1.23
3	M	187	PEB	CHC-C4C	2.15	1.52	1.50
3	S	188	PEB	C4D-ND	-2.14	1.32	1.35
3	I	166	PEB	C2C-C3C	2.14	1.44	1.38
3	P	187	PEB	C2C-C3C	2.14	1.44	1.38
3	O	186	PEB	CHA-C1B	2.13	1.45	1.40
3	T	188	PEB	CHA-C4A	-2.13	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	166	PEB	OD-C4D	2.13	1.27	1.23
3	D	167	PEB	CHB-C1C	2.13	1.45	1.40
3	U	188	PEB	C1D-ND	2.13	1.48	1.45
3	P	188	PEB	CBC-CGC	2.13	1.55	1.50
3	O	188	PEB	CHA-C4A	-2.12	1.33	1.36
3	J	167	PEB	C2C-C3C	2.12	1.44	1.38
3	Q	187	PEB	C4B-NB	-2.12	1.34	1.38
3	U	186	PEB	C4D-ND	-2.12	1.32	1.35
3	R	188	PEB	OD-C4D	2.11	1.27	1.23
3	A	166	PEB	CHB-C4B	2.11	1.42	1.38
3	J	167	PEB	C4B-NB	-2.11	1.34	1.38
3	X	188	PEB	CHB-C1C	2.10	1.45	1.40
3	N	186	PEB	CHB-C1C	2.10	1.45	1.40
3	W	186	PEB	C1D-ND	2.09	1.48	1.45
3	L	166	PEB	O2B-CGB	-2.09	1.23	1.30
3	I	167	PEB	CAC-C2C	-2.08	1.46	1.51
3	T	186	PEB	CHC-C4C	2.08	1.52	1.50
3	I	166	PEB	C1A-NA	-2.08	1.35	1.37
3	B	166	PEB	CMB-C2B	-2.08	1.46	1.50
3	T	187	PEB	C4B-NB	-2.08	1.34	1.38
3	U	188	PEB	C2C-C3C	2.08	1.44	1.38
3	A	167	PEB	C3B-C2B	2.07	1.41	1.36
3	K	166	PEB	CAB-C3B	-2.07	1.46	1.51
3	S	187	PEB	C2C-C3C	2.07	1.44	1.38
3	P	187	PEB	CHB-C1C	2.06	1.45	1.40
3	S	188	PEB	C1A-NA	-2.06	1.35	1.37
3	O	188	PEB	C4B-C3B	-2.06	1.42	1.45
3	H	166	PEB	C2C-C3C	2.06	1.44	1.38
3	E	167	PEB	CHB-C1C	2.06	1.45	1.40
3	O	187	PEB	C4B-C3B	-2.05	1.42	1.45
3	A	167	PEB	C2A-C1A	-2.05	1.50	1.52
3	F	167	PEB	C1B-C2B	2.05	1.50	1.45
3	X	186	PEB	O2C-CGC	-2.05	1.24	1.30
3	B	166	PEB	CHB-C1C	2.04	1.44	1.40
3	M	186	PEB	C1D-ND	2.03	1.48	1.45
3	N	188	PEB	O2B-CGB	-2.03	1.24	1.30
3	K	166	PEB	C3A-C4A	2.03	1.55	1.50
3	R	186	PEB	O2C-CGC	-2.03	1.24	1.30
3	C	166	PEB	C2C-C3C	2.03	1.44	1.38
3	I	166	PEB	C1C-NC	-2.03	1.34	1.37
3	L	166	PEB	C1A-NA	-2.03	1.35	1.37
3	Q	186	PEB	C1D-ND	2.03	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	166	PEB	CHB-C4B	2.02	1.42	1.38
3	G	166	PEB	C1A-NA	-2.02	1.35	1.37
3	O	186	PEB	CHC-C1D	2.02	1.57	1.53
3	J	166	PEB	O2B-CGB	-2.02	1.24	1.30
3	Q	187	PEB	C2C-C3C	2.02	1.44	1.38
3	H	167	PEB	C4B-NB	-2.02	1.34	1.38
3	N	186	PEB	C2A-C1A	-2.02	1.50	1.52
3	E	166	PEB	C1C-NC	-2.01	1.34	1.37
3	U	186	PEB	OD-C4D	2.01	1.27	1.23
3	M	187	PEB	CAD-C3D	-2.01	1.42	1.47
3	P	188	PEB	CHB-C4B	2.01	1.42	1.38
3	C	167	PEB	C1D-ND	2.01	1.48	1.45
4	D	203	NO3	O1-N	2.01	1.34	1.24
3	B	166	PEB	CAA-C3A	-2.01	1.50	1.54
3	J	166	PEB	O2C-CGC	-2.01	1.24	1.30
3	O	186	PEB	C4B-C3B	-2.00	1.42	1.45

All (786) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	166	PEB	CHA-C4A-NA	8.26	135.95	125.63
3	L	166	PEB	CHA-C4A-NA	7.22	134.64	125.63
3	I	166	PEB	CHA-C4A-NA	7.19	134.61	125.63
3	F	166	PEB	CHA-C4A-NA	6.99	134.35	125.63
3	H	166	PEB	CHA-C4A-NA	6.97	134.34	125.63
3	K	166	PEB	CHA-C4A-NA	6.75	134.06	125.63
3	C	166	PEB	CHA-C4A-NA	6.60	133.87	125.63
3	S	186[B]	PEB	C1C-C2C-C3C	-6.58	99.96	107.62
3	S	186[A]	PEB	C1C-C2C-C3C	-6.58	99.97	107.62
3	E	166	PEB	CHA-C4A-NA	6.40	133.62	125.63
3	B	166	PEB	CHA-C4A-NA	6.34	133.55	125.63
3	D	166	PEB	CHA-C4A-NA	6.23	133.41	125.63
3	V	186	PEB	CHA-C4A-NA	6.05	133.18	125.63
3	I	167	PEB	C3C-C4C-NC	5.75	112.96	108.31
3	W	188	PEB	CMC-C3C-C4C	5.75	133.14	126.97
3	J	167	PEB	CMB-C2B-C1B	5.66	133.89	125.10
3	J	166	PEB	CHA-C1B-NB	-5.49	113.09	124.95
3	C	167	PEB	C2A-C1A-NA	5.41	112.79	108.29
3	H	166	PEB	CHA-C1B-NB	-5.29	113.52	124.95
3	S	186[A]	PEB	OA-C1A-C2A	-5.24	122.00	126.17
3	S	186[B]	PEB	OA-C1A-C2A	-5.24	122.00	126.17
3	C	167	PEB	CMB-C2B-C1B	5.24	133.24	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	166	PEB	CHA-C4A-NA	5.19	132.11	125.63
3	E	166	PEB	C3C-C4C-NC	5.18	112.51	108.31
3	O	186	PEB	CHA-C4A-NA	5.15	132.06	125.63
3	R	186	PEB	C1C-C2C-C3C	-5.13	101.65	107.62
3	C	166	PEB	CHA-C1B-NB	-5.11	113.91	124.95
3	S	186[B]	PEB	CAC-C2C-C1C	5.11	133.88	125.77
3	U	186	PEB	OA-C1A-C2A	-5.02	122.18	126.17
3	T	186	PEB	C2C-C1C-NC	4.95	113.77	107.57
3	E	166	PEB	C1B-C2B-C3B	-4.94	100.87	106.48
3	U	186	PEB	CHA-C4A-NA	4.92	131.77	125.63
3	Q	186	PEB	C1C-C2C-C3C	-4.90	101.91	107.62
3	W	188	PEB	CHC-C4C-NC	4.90	127.66	121.10
3	E	166	PEB	CHA-C1B-NB	-4.87	114.43	124.95
3	W	186	PEB	O2C-CGC-CBC	4.86	129.36	114.00
3	J	166	PEB	CHA-C4A-NA	4.84	131.67	125.63
3	U	186	PEB	CMB-C2B-C1B	4.79	132.54	125.10
3	R	186	PEB	CHA-C4A-NA	4.76	131.57	125.63
3	D	166	PEB	C1B-CHA-C4A	4.75	136.90	127.25
3	S	186[A]	PEB	C2C-C1C-NC	4.73	113.50	107.57
3	R	186	PEB	C2C-C1C-NC	4.71	113.47	107.57
3	Q	186	PEB	C2C-C1C-NC	4.70	113.47	107.57
3	T	186	PEB	CMB-C2B-C1B	4.68	132.37	125.10
3	J	166	PEB	C1B-CHA-C4A	4.63	136.65	127.25
3	A	166	PEB	CHA-C1B-NB	-4.62	114.98	124.95
3	C	167	PEB	CHC-C1D-ND	-4.60	108.08	113.73
3	S	186[A]	PEB	CHA-C4A-NA	4.60	131.38	125.63
3	S	186[B]	PEB	CHA-C4A-NA	4.60	131.38	125.63
3	P	186	PEB	C1C-C2C-C3C	-4.58	102.29	107.62
3	B	167	PEB	CMC-C3C-C4C	4.57	131.88	126.97
3	H	167	PEB	CMB-C2B-C1B	4.56	132.19	125.10
3	X	186	PEB	CMB-C2B-C1B	4.52	132.12	125.10
3	K	166	PEB	C2A-C1A-NA	4.48	112.01	108.29
3	R	188	PEB	CHC-C4C-NC	4.47	127.08	121.10
3	A	166	PEB	C1B-CHA-C4A	4.46	136.31	127.25
3	T	188	PEB	C2A-C1A-NA	4.45	111.99	108.29
3	C	166	PEB	C1B-CHA-C4A	4.45	136.28	127.25
3	K	166	PEB	CHA-C1B-NB	-4.42	115.41	124.95
3	F	166	PEB	CHA-C1B-NB	-4.37	115.52	124.95
3	F	167	PEB	CMB-C2B-C1B	4.34	131.84	125.10
3	I	166	PEB	CHA-C1B-NB	-4.33	115.61	124.95
3	C	166	PEB	CAB-C3B-C4B	4.31	132.59	125.02
3	Q	186	PEB	CHA-C4A-NA	4.31	131.01	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	166	PEB	C1B-CHA-C4A	4.29	135.97	127.25
3	R	186	PEB	OA-C1A-C2A	-4.26	122.78	126.17
3	I	167	PEB	CMC-C3C-C4C	4.26	131.55	126.97
3	A	166	PEB	CHA-C1B-C2B	4.26	135.82	124.87
3	S	186[B]	PEB	C2C-C1C-NC	4.26	112.91	107.57
3	O	186	PEB	CMB-C2B-C1B	4.25	131.70	125.10
3	J	167	PEB	C1C-C2C-C3C	-4.22	102.70	107.62
3	K	167	PEB	CAB-C3B-C4B	4.20	132.40	125.02
3	T	187	PEB	CHA-C4A-NA	4.20	130.87	125.63
3	G	166	PEB	CHA-C1B-NB	-4.20	115.89	124.95
3	X	188	PEB	OA-C1A-C2A	-4.19	122.84	126.17
3	W	186	PEB	CHA-C1B-NB	-4.19	115.91	124.95
3	K	166	PEB	C1B-CHA-C4A	4.17	135.73	127.25
3	F	166	PEB	C1B-CHA-C4A	4.17	135.73	127.25
3	M	186	PEB	CHA-C1B-NB	-4.16	115.96	124.95
3	T	187	PEB	CMB-C2B-C1B	4.16	131.57	125.10
3	T	187	PEB	CHC-C1D-ND	-4.16	108.62	113.73
3	L	166	PEB	C3C-C4C-NC	4.15	111.67	108.31
3	H	166	PEB	CMB-C2B-C1B	4.13	131.52	125.10
3	T	188	PEB	C2A-C3A-C4A	4.13	107.53	101.34
3	W	186	PEB	O1C-CGC-CBC	-4.12	110.01	123.09
3	T	186	PEB	OA-C1A-C2A	-4.12	122.90	126.17
3	O	188	PEB	CHC-C1D-ND	-4.11	108.68	113.73
3	G	167	PEB	CMB-C2B-C1B	4.11	131.48	125.10
3	Q	187	PEB	CHC-C1D-ND	-4.10	108.70	113.73
3	D	166	PEB	CHA-C1B-NB	-4.09	116.12	124.95
3	P	186	PEB	CMB-C2B-C1B	4.08	131.44	125.10
3	B	166	PEB	C1B-CHA-C4A	4.07	135.52	127.25
3	D	167	PEB	OA-C1A-C2A	-4.07	122.94	126.17
3	B	167	PEB	CMB-C2B-C1B	4.06	131.41	125.10
3	V	187	PEB	CMB-C2B-C1B	4.06	131.41	125.10
3	B	166	PEB	CHA-C1B-NB	-4.02	116.27	124.95
3	N	188	PEB	C3C-C4C-NC	4.02	111.56	108.31
3	O	188	PEB	CMC-C3C-C4C	4.00	131.27	126.97
3	R	188	PEB	C2C-C1C-NC	3.99	112.58	107.57
3	S	187	PEB	C4B-C3B-C2B	-3.98	102.42	106.73
3	L	166	PEB	CHA-C1B-NB	-3.98	116.36	124.95
3	R	187	PEB	CMB-C2B-C1B	3.96	131.26	125.10
3	X	187	PEB	CHC-C1D-ND	-3.96	108.87	113.73
3	M	186	PEB	CHA-C4A-NA	3.95	130.56	125.63
3	W	186	PEB	CHA-C4A-NA	3.92	130.53	125.63
3	W	186	PEB	C2C-C1C-NC	3.91	112.48	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	186	PEB	C2A-C1A-NA	3.91	111.54	108.29
3	R	186	PEB	C3D-C4D-ND	3.90	114.65	107.33
3	E	166	PEB	CMB-C2B-C1B	3.89	131.14	125.10
3	N	188	PEB	CMD-C2D-C3D	-3.89	124.43	129.95
3	X	186	PEB	C1C-C2C-C3C	-3.89	103.10	107.62
3	S	186[A]	PEB	CHC-C1D-ND	-3.88	108.97	113.73
3	S	186[B]	PEB	CHC-C1D-ND	-3.88	108.97	113.73
3	V	186	PEB	CHA-C1B-C2B	3.87	134.82	124.87
3	K	167	PEB	C4B-C3B-C2B	-3.87	102.54	106.73
3	L	167	PEB	OD-C4D-ND	-3.84	120.74	126.02
3	N	186	PEB	CHA-C1B-NB	-3.84	116.66	124.95
3	L	166	PEB	CHA-C1B-C2B	3.84	134.73	124.87
3	P	188	PEB	CMD-C2D-C3D	-3.81	124.53	129.95
3	C	166	PEB	C4B-C3B-C2B	-3.81	102.61	106.73
3	W	186	PEB	C1C-C2C-C3C	-3.78	103.22	107.62
3	U	186	PEB	CHA-C1B-NB	-3.77	116.82	124.95
3	B	167	PEB	O1B-CGB-CBB	-3.75	111.19	123.09
3	K	167	PEB	OD-C4D-ND	-3.75	120.87	126.02
3	S	186[A]	PEB	C3D-C4D-ND	3.74	114.34	107.33
3	S	186[B]	PEB	C3D-C4D-ND	3.74	114.34	107.33
3	T	187	PEB	C2A-C3A-C4A	3.74	106.94	101.34
3	G	166	PEB	CHA-C1B-C2B	3.74	134.48	124.87
3	M	186	PEB	CMB-C2B-C1B	3.73	130.90	125.10
3	C	166	PEB	CHA-C1B-C2B	3.73	134.46	124.87
3	B	167	PEB	CAB-C3B-C4B	3.71	131.53	125.02
3	B	166	PEB	CHC-C1D-ND	-3.70	109.19	113.73
3	L	166	PEB	C1B-CHA-C4A	3.70	134.76	127.25
3	O	186	PEB	C1C-C2C-C3C	-3.69	103.33	107.62
3	T	186	PEB	C1C-C2C-C3C	-3.67	103.34	107.62
3	N	187	PEB	CHC-C4C-NC	3.67	126.01	121.10
3	F	167	PEB	C1A-NA-C4A	3.67	118.01	113.41
3	Q	187	PEB	CHC-C4C-NC	3.67	126.00	121.10
3	R	188	PEB	CHB-C1C-C2C	-3.66	119.34	127.22
3	B	166	PEB	CHC-C4C-NC	3.66	126.00	121.10
3	B	166	PEB	OA-C1A-C2A	-3.65	123.27	126.17
3	M	186	PEB	C2C-C1C-NC	3.65	112.15	107.57
3	R	188	PEB	C1C-C2C-C3C	-3.65	103.37	107.62
3	M	188	PEB	C1C-C2C-C3C	-3.65	103.37	107.62
3	U	186	PEB	C2A-C3A-C4A	3.64	106.79	101.34
3	P	186	PEB	C2A-C1A-NA	3.64	111.31	108.29
3	R	186	PEB	CMB-C2B-C1B	3.63	130.73	125.10
3	V	188	PEB	CMC-C3C-C4C	3.61	130.85	126.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	188	PEB	CHC-C1D-ND	-3.61	109.30	113.73
3	A	166	PEB	CHC-C1D-ND	-3.60	109.32	113.73
3	M	188	PEB	C2A-C1A-NA	3.58	111.27	108.29
3	U	187	PEB	C3C-C4C-NC	3.58	111.21	108.31
3	S	186[A]	PEB	CMB-C2B-C1B	3.57	130.64	125.10
3	S	186[B]	PEB	CMB-C2B-C1B	3.57	130.64	125.10
3	B	166	PEB	C2A-C1A-NA	3.57	111.25	108.29
3	X	186	PEB	C1B-CHA-C4A	3.56	134.49	127.25
3	H	166	PEB	C3D-C4D-ND	3.54	113.96	107.33
3	N	186	PEB	CHA-C4A-NA	3.52	130.03	125.63
3	J	167	PEB	OA-C1A-C2A	-3.50	123.39	126.17
3	X	187	PEB	CAC-C2C-C1C	3.50	131.32	125.77
3	C	166	PEB	CHC-C4C-NC	3.49	125.77	121.10
3	U	188	PEB	CHC-C4C-NC	3.48	125.76	121.10
3	M	188	PEB	C2C-C1C-NC	3.47	111.92	107.57
3	A	167	PEB	C3D-C4D-ND	3.47	113.83	107.33
3	J	167	PEB	C1B-C2B-C3B	-3.47	102.54	106.48
3	H	167	PEB	C1B-C2B-C3B	-3.47	102.54	106.48
3	S	187	PEB	CAB-C3B-C4B	3.47	131.11	125.02
3	J	166	PEB	CHA-C1B-C2B	3.47	133.78	124.87
3	P	188	PEB	CMC-C3C-C4C	3.46	130.69	126.97
3	F	167	PEB	C4B-C3B-C2B	-3.46	102.98	106.73
3	X	188	PEB	C3C-C4C-NC	3.45	111.11	108.31
3	C	167	PEB	C1B-C2B-C3B	-3.45	102.56	106.48
3	N	186	PEB	CHC-C1D-ND	-3.45	109.50	113.73
3	H	166	PEB	OD-C4D-C3D	-3.45	121.39	129.71
3	R	186	PEB	C1D-ND-C4D	-3.44	108.12	113.42
3	Q	188	PEB	CAC-C2C-C1C	3.44	131.23	125.77
3	T	187	PEB	CHC-C4C-NC	3.44	125.70	121.10
3	M	188	PEB	OD-C4D-C3D	-3.44	121.41	129.71
3	T	188	PEB	OD-C4D-ND	-3.44	121.30	126.02
3	N	186	PEB	CAB-C3B-C4B	3.43	131.04	125.02
3	U	186	PEB	C1C-C2C-C3C	-3.42	103.64	107.62
3	S	188	PEB	CHC-C4C-NC	3.41	125.67	121.10
3	O	187	PEB	CMB-C2B-C1B	3.41	130.40	125.10
3	U	186	PEB	C2C-C1C-NC	3.41	111.84	107.57
3	H	166	PEB	C1B-C2B-C3B	-3.41	102.61	106.48
3	P	187	PEB	CMB-C2B-C1B	3.41	130.39	125.10
3	Q	186	PEB	CHB-C1C-C2C	-3.41	119.90	127.22
3	U	186	PEB	CHC-C1D-ND	-3.40	109.56	113.73
3	H	166	PEB	C1B-CHA-C4A	3.39	134.15	127.25
3	M	187	PEB	CHA-C4A-NA	3.39	129.86	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	167	PEB	OD-C4D-ND	-3.38	121.37	126.02
3	X	188	PEB	C2A-C1A-NA	3.38	111.10	108.29
3	S	186[A]	PEB	C1D-ND-C4D	-3.38	108.22	113.42
3	S	186[B]	PEB	C1D-ND-C4D	-3.38	108.22	113.42
3	T	188	PEB	CHC-C4C-NC	3.38	125.62	121.10
3	Q	186	PEB	CHA-C1B-NB	-3.37	117.68	124.95
3	M	186	PEB	CHA-C1B-C2B	3.36	133.51	124.87
3	T	186	PEB	CHA-C1B-NB	-3.36	117.70	124.95
3	Q	188	PEB	CHC-C1D-ND	-3.35	109.62	113.73
3	C	167	PEB	CHC-C4C-NC	3.35	125.59	121.10
3	P	188	PEB	O2C-CGC-CBC	3.34	124.56	114.00
3	J	167	PEB	OD-C4D-ND	-3.34	121.42	126.02
3	M	187	PEB	C2C-C1C-NC	3.33	111.74	107.57
3	Q	187	PEB	CHA-C4A-NA	3.33	129.79	125.63
3	V	186	PEB	CHA-C1B-NB	-3.32	117.79	124.95
3	P	186	PEB	CHA-C1B-NB	-3.31	117.80	124.95
3	S	187	PEB	C1C-C2C-C3C	-3.31	103.76	107.62
3	P	187	PEB	C1C-C2C-C3C	-3.31	103.77	107.62
3	W	188	PEB	CAB-C3B-C4B	3.30	130.82	125.02
3	O	188	PEB	C3C-C4C-NC	3.30	110.98	108.31
3	D	166	PEB	CHA-C1B-C2B	3.30	133.34	124.87
3	I	166	PEB	CMB-C2B-C1B	3.29	130.21	125.10
3	K	166	PEB	CHA-C1B-C2B	3.29	133.31	124.87
3	Q	188	PEB	C2A-C1A-NA	3.28	111.02	108.29
3	E	166	PEB	C2C-C1C-NC	3.28	111.68	107.57
3	J	167	PEB	C2C-C1C-NC	3.28	111.68	107.57
3	E	166	PEB	C1B-CHA-C4A	3.28	133.91	127.25
5	B	204	PI	O2-P-O1	-3.26	99.41	110.95
3	R	186	PEB	CHA-C1B-NB	-3.26	117.90	124.95
3	L	167	PEB	CMB-C2B-C1B	3.26	130.16	125.10
3	V	187	PEB	C2C-C1C-NC	3.26	111.65	107.57
3	F	167	PEB	CHC-C1D-ND	-3.25	109.75	113.73
3	E	166	PEB	CHC-C4C-NC	3.25	125.44	121.10
3	S	188	PEB	CMB-C2B-C1B	3.24	130.13	125.10
3	A	167	PEB	C1D-ND-C4D	-3.24	108.44	113.42
3	W	186	PEB	CMB-C2B-C1B	3.24	130.13	125.10
3	L	167	PEB	CAB-C3B-C4B	3.24	130.70	125.02
3	E	166	PEB	CHC-C1D-ND	-3.23	109.76	113.73
3	X	186	PEB	CHA-C4A-NA	3.23	129.66	125.63
3	T	188	PEB	C3D-C4D-ND	3.23	113.38	107.33
3	W	186	PEB	CHA-C1B-C2B	3.22	133.15	124.87
3	W	186	PEB	CHC-C1D-ND	-3.22	109.78	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	188	PEB	O1C-CGC-CBC	-3.22	112.88	123.09
3	X	188	PEB	CMB-C2B-C1B	3.22	130.10	125.10
3	S	188	PEB	CHB-C1C-C2C	-3.22	120.30	127.22
3	P	188	PEB	CHC-C4C-NC	3.22	125.40	121.10
3	K	166	PEB	OA-C1A-C2A	-3.22	123.62	126.17
3	R	187	PEB	C1C-C2C-C3C	-3.21	103.88	107.62
3	R	186	PEB	CHC-C1D-ND	-3.21	109.79	113.73
3	H	166	PEB	C2C-C1C-NC	3.21	111.59	107.57
3	M	188	PEB	CAC-C2C-C1C	3.20	130.86	125.77
3	U	186	PEB	CHB-C1C-C2C	-3.20	120.35	127.22
3	T	186	PEB	CHA-C4A-NA	3.19	129.61	125.63
3	W	187	PEB	C2A-C1A-NA	3.18	110.94	108.29
3	N	186	PEB	CHB-C4B-C3B	-3.17	118.09	125.40
3	S	186[A]	PEB	CAB-C3B-C4B	3.16	130.58	125.02
3	S	186[B]	PEB	CAB-C3B-C4B	3.16	130.58	125.02
3	W	187	PEB	CHC-C4C-NC	3.16	125.33	121.10
3	M	186	PEB	OA-C1A-C2A	-3.16	123.66	126.17
3	E	166	PEB	CMC-C3C-C4C	3.15	130.36	126.97
3	W	187	PEB	OD-C4D-ND	-3.15	121.69	126.02
3	B	167	PEB	C3C-C4C-NC	3.15	110.86	108.31
3	K	167	PEB	O1B-CGB-CBB	-3.14	113.12	123.09
3	D	167	PEB	CMC-C3C-C4C	3.14	130.35	126.97
3	T	186	PEB	CHC-C4C-NC	3.14	125.30	121.10
3	R	186	PEB	OD-C4D-ND	-3.14	121.70	126.02
3	P	188	PEB	C4B-C3B-C2B	-3.13	103.34	106.73
3	M	186	PEB	C1C-C2C-C3C	-3.12	103.99	107.62
3	V	186	PEB	C1C-C2C-C3C	-3.12	103.99	107.62
3	L	167	PEB	C3D-C4D-ND	3.12	113.17	107.33
3	N	188	PEB	OA-C1A-C2A	-3.11	123.70	126.17
3	V	188	PEB	OD-C4D-C3D	-3.11	122.20	129.71
3	W	188	PEB	C1C-C2C-C3C	-3.11	104.00	107.62
3	P	186	PEB	CHA-C1B-C2B	3.11	132.85	124.87
3	M	188	PEB	CHB-C1C-C2C	-3.11	120.54	127.22
3	H	166	PEB	C3C-C4C-NC	3.11	110.83	108.31
3	V	186	PEB	OD-C4D-ND	-3.11	121.75	126.02
3	Q	186	PEB	CHC-C1D-ND	-3.10	109.92	113.73
7	R	204	MPD	C5-C4-C3	-3.10	97.27	111.67
3	B	166	PEB	CHA-C1B-C2B	3.10	132.83	124.87
3	T	188	PEB	CAC-C2C-C1C	3.10	130.69	125.77
3	N	186	PEB	CHA-C1B-C2B	3.10	132.83	124.87
3	J	166	PEB	CHC-C4C-NC	3.08	125.22	121.10
3	L	166	PEB	CMA-C2A-C1A	-3.08	105.77	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	186	PEB	C3D-C4D-ND	3.07	113.09	107.33
3	V	187	PEB	OA-C1A-C2A	3.07	128.62	126.17
3	S	186[A]	PEB	CHB-C1C-C2C	-3.07	120.62	127.22
3	T	188	PEB	CAB-C3B-C4B	3.06	130.39	125.02
3	F	166	PEB	CHA-C1B-C2B	3.06	132.72	124.87
3	J	167	PEB	CHC-C1D-ND	-3.05	109.98	113.73
3	D	166	PEB	CMB-C2B-C1B	3.05	129.84	125.10
3	T	188	PEB	OA-C1A-NA	-3.05	121.34	124.93
3	W	187	PEB	CMB-C2B-C1B	3.03	129.81	125.10
3	I	166	PEB	CHA-C1B-C2B	3.03	132.65	124.87
3	M	188	PEB	OA-C1A-C2A	-3.01	123.78	126.17
3	R	187	PEB	CAB-C3B-C4B	3.01	130.31	125.02
3	H	167	PEB	CHB-C1C-C2C	-3.01	120.75	127.22
3	U	188	PEB	CAC-C2C-C1C	3.01	130.54	125.77
7	B	203	MPD	C1-C2-C3	-3.00	97.24	110.20
3	G	166	PEB	C1B-CHA-C4A	3.00	133.35	127.25
3	N	186	PEB	C2C-C1C-NC	2.99	111.32	107.57
3	I	167	PEB	C2A-C1A-NA	2.99	110.78	108.29
3	R	186	PEB	CHC-C4C-NC	2.99	125.10	121.10
3	G	167	PEB	CHC-C1D-ND	-2.99	110.06	113.73
3	J	166	PEB	CAB-C3B-C4B	2.98	130.25	125.02
3	S	188	PEB	C3D-C4D-ND	2.98	112.91	107.33
3	X	186	PEB	C2C-C1C-NC	2.98	111.30	107.57
3	D	167	PEB	CMB-C2B-C1B	2.97	129.72	125.10
3	P	187	PEB	CHC-C4C-NC	2.96	125.06	121.10
3	M	188	PEB	CAB-C3B-C4B	2.96	130.21	125.02
3	W	188	PEB	C4B-C3B-C2B	-2.95	103.53	106.73
3	V	188	PEB	C2A-C1A-NA	2.95	110.74	108.29
3	K	167	PEB	CMB-C2B-C1B	2.95	129.68	125.10
3	N	186	PEB	C1C-C2C-C3C	-2.95	104.19	107.62
3	T	186	PEB	OD-C4D-C3D	-2.94	122.61	129.71
3	G	167	PEB	CAC-C2C-C1C	2.93	130.42	125.77
3	G	167	PEB	CHB-C1C-C2C	-2.93	120.92	127.22
3	T	186	PEB	CHB-C1C-C2C	-2.93	120.93	127.22
3	H	167	PEB	CHC-C1D-ND	-2.91	110.16	113.73
3	M	188	PEB	C3D-C4D-ND	2.91	112.79	107.33
3	D	167	PEB	O1B-CGB-CBB	-2.90	113.90	123.09
3	L	166	PEB	C4B-C3B-C2B	2.89	109.85	106.73
3	N	187	PEB	C2A-C1A-NA	-2.88	105.89	108.29
3	W	186	PEB	C4B-C3B-C2B	-2.88	103.62	106.73
3	S	186[A]	PEB	CHA-C1B-NB	-2.87	118.75	124.95
3	S	186[B]	PEB	CHA-C1B-NB	-2.87	118.75	124.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	188	PEB	CHA-C4A-NA	2.87	129.21	125.63
3	H	166	PEB	CHA-C1B-C2B	2.86	132.23	124.87
3	V	187	PEB	C3C-C4C-NC	2.86	110.63	108.31
3	S	188	PEB	OD-C4D-C3D	-2.86	122.81	129.71
3	W	188	PEB	CAC-C2C-C1C	2.86	130.31	125.77
3	U	188	PEB	C1B-CHA-C4A	2.86	133.06	127.25
3	U	186	PEB	C1B-C2B-C3B	-2.86	103.24	106.48
3	S	187	PEB	C3B-C4B-NB	2.85	114.08	110.04
3	K	167	PEB	CHA-C4A-NA	2.85	129.18	125.63
3	R	187	PEB	OA-C1A-NA	2.85	128.28	124.93
3	S	187	PEB	CHC-C4C-NC	2.84	124.90	121.10
3	D	166	PEB	CHC-C4C-NC	2.84	124.90	121.10
3	N	188	PEB	OD-C4D-C3D	-2.84	122.86	129.71
3	S	187	PEB	OA-C1A-C2A	-2.83	123.92	126.17
3	S	186[A]	PEB	OD-C4D-C3D	-2.83	122.86	129.71
3	S	186[B]	PEB	OD-C4D-C3D	-2.83	122.86	129.71
3	O	186	PEB	CHC-C1D-ND	-2.83	110.26	113.73
3	S	186[A]	PEB	OA-C1A-NA	2.83	128.26	124.93
3	S	186[B]	PEB	OA-C1A-NA	2.83	128.26	124.93
3	A	166	PEB	CMA-C2A-C1A	-2.83	106.31	112.40
3	K	167	PEB	CHB-C1C-C2C	-2.82	121.17	127.22
3	U	186	PEB	C1A-NA-C4A	2.81	116.93	113.41
3	S	186[A]	PEB	O2C-CGC-CBC	2.81	122.89	114.00
7	B	203	MPD	O4-C4-C3	-2.81	100.19	111.35
3	T	188	PEB	C1C-C2C-C3C	-2.80	104.37	107.62
3	T	187	PEB	O2C-CGC-CBC	2.79	122.83	114.00
3	R	187	PEB	CHA-C4A-NA	2.79	129.11	125.63
3	K	167	PEB	C1C-C2C-C3C	-2.79	104.38	107.62
3	N	186	PEB	CMB-C2B-C1B	2.79	129.43	125.10
3	E	167	PEB	CAB-C3B-C4B	2.78	129.91	125.02
3	X	187	PEB	CMD-C2D-C3D	-2.78	126.00	129.95
3	O	186	PEB	C1D-ND-C4D	-2.77	109.16	113.42
3	K	166	PEB	CMA-C2A-C1A	-2.76	106.45	112.40
3	S	186[B]	PEB	CHB-C1C-C2C	-2.76	121.28	127.22
3	O	186	PEB	C2C-C1C-NC	2.76	111.03	107.57
3	M	187	PEB	CHC-C1D-ND	-2.75	110.36	113.73
3	D	167	PEB	C4B-C3B-C2B	-2.75	103.75	106.73
3	D	167	PEB	CHB-C1C-C2C	-2.75	121.32	127.22
3	D	167	PEB	C2C-C1C-NC	2.75	111.01	107.57
3	V	186	PEB	CHB-C1C-C2C	-2.74	121.32	127.22
3	N	187	PEB	C1C-C2C-C3C	-2.74	104.43	107.62
3	P	187	PEB	OD-C4D-C3D	-2.74	123.09	129.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	186	PEB	C1B-CHA-C4A	2.74	132.82	127.25
3	G	167	PEB	CAB-C3B-C4B	2.74	129.82	125.02
3	L	167	PEB	C1D-ND-C4D	-2.74	109.21	113.42
3	Q	187	PEB	CMB-C2B-C1B	2.73	129.34	125.10
3	X	186	PEB	OD-C4D-C3D	-2.73	123.12	129.71
3	U	186	PEB	OA-C1A-NA	2.73	128.14	124.93
3	G	166	PEB	C3C-C4C-NC	2.73	110.52	108.31
5	C	204	PI	O3-P-O1	-2.72	101.32	110.95
3	R	186	PEB	CHA-C1B-C2B	2.72	131.87	124.87
3	F	167	PEB	CHB-C1C-C2C	-2.72	121.37	127.22
3	H	166	PEB	O1C-CGC-CBC	-2.72	114.47	123.09
3	K	167	PEB	CMC-C3C-C4C	2.72	129.89	126.97
3	I	167	PEB	C2C-C1C-NC	2.71	110.96	107.57
3	N	186	PEB	OA-C1A-C2A	-2.70	124.02	126.17
3	N	188	PEB	CAC-C2C-C1C	2.70	130.06	125.77
3	Q	188	PEB	CMB-C2B-C1B	2.69	129.28	125.10
3	E	166	PEB	OD-C4D-C3D	-2.69	123.21	129.71
3	I	167	PEB	CAB-C3B-C2B	-2.69	122.83	127.87
3	R	188	PEB	C1B-CHA-C4A	2.69	132.72	127.25
3	J	167	PEB	C3D-C4D-ND	2.69	112.37	107.33
3	W	188	PEB	CMD-C2D-C3D	-2.69	126.14	129.95
3	C	167	PEB	C3D-C4D-ND	2.68	112.36	107.33
3	V	188	PEB	CMB-C2B-C1B	2.68	129.27	125.10
3	C	167	PEB	OA-C1A-NA	-2.68	121.77	124.93
3	X	187	PEB	CHB-C1C-C2C	-2.68	121.46	127.22
3	D	166	PEB	CMA-C2A-C1A	-2.68	106.63	112.40
3	J	166	PEB	CMA-C2A-C1A	-2.68	106.63	112.40
3	W	188	PEB	CBD-CAD-C3D	-2.68	114.15	127.53
3	N	186	PEB	CHB-C1C-C2C	-2.68	121.47	127.22
3	I	166	PEB	C2A-C3A-C4A	2.67	105.34	101.34
3	Q	186	PEB	OA-C1A-C2A	-2.67	124.05	126.17
3	X	186	PEB	C3D-C4D-ND	2.67	112.33	107.33
3	W	186	PEB	CAB-C3B-C4B	2.67	129.71	125.02
3	F	167	PEB	OD-C4D-C3D	-2.67	123.26	129.71
3	F	167	PEB	CAB-C3B-C4B	2.66	129.69	125.02
5	B	204	PI	O4-P-O3	2.66	116.19	107.91
3	R	186	PEB	CHB-C1C-C2C	-2.66	121.50	127.22
3	H	167	PEB	CAB-CBB-CGB	-2.66	106.61	113.67
3	R	186	PEB	OD-C4D-C3D	-2.65	123.30	129.71
3	X	187	PEB	CMB-C2B-C1B	2.65	129.21	125.10
3	Q	186	PEB	C2A-C1A-NA	2.64	110.48	108.29
3	R	188	PEB	C1B-C2B-C3B	-2.64	103.48	106.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	188	PEB	CAB-C3B-C4B	2.64	129.65	125.02
3	N	187	PEB	C2C-C1C-NC	2.64	110.87	107.57
3	B	167	PEB	CHB-C4B-C3B	-2.63	119.32	125.40
3	P	187	PEB	C3D-C4D-ND	2.63	112.26	107.33
3	T	188	PEB	C3B-C4B-NB	2.63	113.76	110.04
3	S	187	PEB	CHB-C4B-C3B	-2.63	119.33	125.40
3	C	167	PEB	C2A-C3A-C4A	2.62	105.27	101.34
3	V	186	PEB	CHB-C4B-NB	2.62	130.11	124.60
3	C	166	PEB	CMB-C2B-C1B	2.62	129.17	125.10
3	C	166	PEB	C3D-C4D-ND	2.62	112.23	107.33
3	A	167	PEB	OA-C1A-C2A	-2.61	124.10	126.17
3	W	187	PEB	O2C-CGC-CBC	2.61	122.25	114.00
3	X	187	PEB	C2C-C1C-NC	2.61	110.84	107.57
3	O	188	PEB	CHB-C1C-C2C	-2.61	121.61	127.22
3	S	187	PEB	O2C-CGC-CBC	2.61	122.23	114.00
3	Q	186	PEB	OD-C4D-ND	-2.60	122.44	126.02
3	V	186	PEB	CAC-C2C-C1C	2.60	129.89	125.77
3	B	167	PEB	OD-C4D-ND	-2.60	122.45	126.02
3	O	188	PEB	CAC-C2C-C1C	2.59	129.88	125.77
3	M	187	PEB	CMB-C2B-C1B	2.59	129.12	125.10
3	O	186	PEB	CHA-C1B-C2B	2.59	131.53	124.87
3	O	188	PEB	C1B-CHA-C4A	2.59	132.51	127.25
3	K	166	PEB	OD-C4D-ND	-2.59	122.46	126.02
3	U	188	PEB	CAC-CBC-CGC	2.59	120.52	113.67
3	V	186	PEB	C3D-C4D-ND	2.58	112.17	107.33
3	J	167	PEB	CHC-C4C-NC	2.58	124.56	121.10
3	S	186[A]	PEB	C4B-C3B-C2B	-2.58	103.93	106.73
3	S	186[B]	PEB	C4B-C3B-C2B	-2.58	103.93	106.73
3	K	167	PEB	CHB-C4B-C3B	-2.58	119.43	125.40
3	Q	186	PEB	C3D-C4D-ND	2.58	112.17	107.33
3	P	186	PEB	C1B-CHA-C4A	2.58	132.50	127.25
3	E	167	PEB	CHC-C1D-ND	-2.58	110.56	113.73
3	Q	186	PEB	CHA-C1B-C2B	2.58	131.50	124.87
3	B	167	PEB	CMD-C2D-C3D	-2.58	126.29	129.95
3	U	187	PEB	C1B-C2B-C3B	-2.57	103.56	106.48
3	C	166	PEB	OD-C4D-C3D	-2.57	123.50	129.71
3	I	167	PEB	C3A-C4A-NA	2.57	111.25	107.94
3	N	188	PEB	CHB-C1C-C2C	-2.56	121.71	127.22
3	R	186	PEB	OA-C1A-NA	2.56	127.94	124.93
3	T	186	PEB	CHB-C4B-C3B	-2.56	119.49	125.40
3	R	187	PEB	OA-C1A-C2A	-2.56	124.14	126.17
3	X	188	PEB	OD-C4D-C3D	-2.55	123.56	129.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	187	PEB	C1C-CHB-C4B	2.55	133.78	128.22
3	N	186	PEB	C1B-CHA-C4A	2.54	132.42	127.25
3	G	166	PEB	CAC-C2C-C1C	2.54	129.81	125.77
3	X	187	PEB	O2C-CGC-CBC	2.54	122.04	114.00
3	S	187	PEB	CHB-C1C-C2C	-2.54	121.76	127.22
3	U	186	PEB	CHA-C1B-C2B	2.54	131.39	124.87
3	U	187	PEB	CHA-C4A-NA	2.54	128.80	125.63
3	N	186	PEB	CHB-C4B-NB	2.54	129.93	124.60
3	N	188	PEB	CMC-C3C-C4C	2.54	129.70	126.97
3	Q	188	PEB	OD-C4D-ND	-2.53	122.53	126.02
3	N	188	PEB	CBD-CAD-C3D	-2.53	114.87	127.53
3	J	167	PEB	C2A-C1A-NA	2.53	110.39	108.29
3	R	187	PEB	OD-C4D-C3D	-2.52	123.61	129.71
3	T	186	PEB	C3C-C4C-NC	2.52	110.35	108.31
3	P	186	PEB	OA-C1A-C2A	-2.52	124.17	126.17
3	O	188	PEB	OD-C4D-C3D	-2.52	123.63	129.71
3	Q	188	PEB	C3D-C4D-ND	2.51	112.04	107.33
3	C	167	PEB	C1C-C2C-C3C	-2.51	104.69	107.62
3	V	187	PEB	C1C-CHB-C4B	2.51	133.71	128.22
3	I	167	PEB	C4B-NB-C1B	2.51	111.12	106.52
3	S	186[A]	PEB	CAC-C2C-C3C	2.51	132.69	127.07
3	L	167	PEB	C2A-C1A-NA	2.50	110.37	108.29
3	X	186	PEB	CMD-C2D-C3D	-2.50	126.40	129.95
3	S	188	PEB	C1B-CHA-C4A	2.50	132.34	127.25
5	P	205	PI	O3-P-O2	2.50	115.68	107.91
3	B	167	PEB	O2B-CGB-CBB	2.50	121.88	114.00
3	K	166	PEB	CAC-C2C-C1C	2.50	129.73	125.77
3	G	166	PEB	CMB-C2B-C1B	2.49	128.97	125.10
3	S	187	PEB	CHC-C1D-ND	-2.49	110.67	113.73
3	D	167	PEB	CAC-C2C-C1C	2.49	129.73	125.77
3	V	188	PEB	OA-C1A-C2A	-2.49	124.19	126.17
3	P	187	PEB	CMC-C3C-C4C	2.48	129.64	126.97
3	J	167	PEB	C1D-ND-C4D	-2.48	109.60	113.42
3	O	186	PEB	C3D-C4D-ND	2.48	111.98	107.33
3	D	166	PEB	CAB-C3B-C4B	2.48	129.37	125.02
3	C	167	PEB	C3C-C4C-NC	2.48	110.32	108.31
3	V	186	PEB	CMB-C2B-C1B	2.47	128.94	125.10
3	S	186[A]	PEB	CHA-C1B-C2B	2.47	131.22	124.87
3	S	186[B]	PEB	CHA-C1B-C2B	2.47	131.22	124.87
3	T	186	PEB	CHC-C1D-ND	-2.47	110.70	113.73
3	W	186	PEB	C3D-C4D-ND	2.47	111.95	107.33
3	M	186	PEB	C1B-CHA-C4A	2.46	132.26	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	166	PEB	CAC-CBC-CGC	-2.46	107.14	113.67
3	B	167	PEB	CHB-C1C-C2C	-2.46	121.93	127.22
3	S	186[A]	PEB	C1B-CHA-C4A	2.45	132.24	127.25
3	S	186[B]	PEB	C1B-CHA-C4A	2.45	132.24	127.25
3	R	187	PEB	O2C-CGC-CBC	2.45	121.74	114.00
3	X	186	PEB	CHB-C1C-C2C	-2.45	121.95	127.22
3	E	167	PEB	CHB-C1C-C2C	-2.45	121.96	127.22
3	N	188	PEB	CMB-C2B-C1B	2.44	128.89	125.10
3	C	167	PEB	C2C-C1C-NC	2.44	110.62	107.57
3	Q	186	PEB	CMB-C2B-C1B	2.44	128.88	125.10
3	I	167	PEB	CAB-C3B-C4B	2.44	129.30	125.02
3	N	187	PEB	C4B-C3B-C2B	-2.44	104.09	106.73
3	P	188	PEB	C2A-C3A-C4A	2.43	104.98	101.34
3	O	187	PEB	CHA-C4A-NA	2.43	128.67	125.63
3	P	187	PEB	O2C-CGC-CBC	2.43	121.69	114.00
3	W	186	PEB	OD-C4D-C3D	-2.43	123.84	129.71
3	F	166	PEB	CMA-C2A-C1A	-2.43	107.16	112.40
3	W	187	PEB	CMD-C2D-C3D	-2.43	126.50	129.95
3	I	166	PEB	OD-C4D-C3D	-2.43	123.84	129.71
3	N	187	PEB	CHC-C1D-ND	-2.43	110.75	113.73
3	W	186	PEB	CHB-C1C-C2C	-2.43	122.00	127.22
3	F	167	PEB	C2A-C1A-NA	-2.43	106.27	108.29
3	O	188	PEB	C1C-C2C-C3C	-2.43	104.80	107.62
3	S	188	PEB	CHB-C1C-NC	2.42	130.76	125.29
3	M	186	PEB	CAC-CBC-CGC	2.42	120.09	113.67
3	N	187	PEB	O2B-CGB-CBB	2.42	121.64	114.00
3	J	167	PEB	O1C-CGC-CBC	-2.42	115.42	123.09
3	R	188	PEB	CMB-C2B-C1B	2.41	128.85	125.10
3	G	167	PEB	C1B-C2B-C3B	-2.41	103.74	106.48
3	X	188	PEB	CMD-C2D-C3D	-2.41	126.53	129.95
3	Q	188	PEB	CMD-C2D-C3D	-2.41	126.53	129.95
3	N	187	PEB	O2C-CGC-CBC	2.41	121.60	114.00
3	I	167	PEB	C1B-C2B-C3B	-2.40	103.75	106.48
3	P	186	PEB	CHA-C4A-NA	2.40	128.63	125.63
3	N	188	PEB	C2C-C1C-NC	2.40	110.58	107.57
3	X	186	PEB	O1B-CGB-CBB	-2.40	115.49	123.09
3	U	188	PEB	C3D-C4D-ND	2.40	111.82	107.33
3	O	187	PEB	C1C-CHB-C4B	2.40	133.46	128.22
3	H	167	PEB	CHC-C4C-NC	2.39	124.30	121.10
3	Q	188	PEB	C1C-C2C-C3C	-2.39	104.84	107.62
3	S	186[A]	PEB	OD-C4D-ND	-2.39	122.74	126.02
3	S	186[B]	PEB	OD-C4D-ND	-2.39	122.74	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	188	PEB	C2A-C3A-C4A	2.39	104.91	101.34
3	U	188	PEB	C3A-C4A-NA	2.39	111.01	107.94
3	V	188	PEB	C3D-C4D-ND	2.38	111.79	107.33
3	M	186	PEB	OD-C4D-ND	-2.38	122.74	126.02
3	W	186	PEB	CHB-C4B-C3B	-2.38	119.90	125.40
3	U	187	PEB	C1C-CHB-C4B	2.38	133.42	128.22
3	S	188	PEB	O1C-CGC-CBC	-2.38	115.55	123.09
3	V	187	PEB	CMC-C3C-C4C	2.37	129.52	126.97
3	A	167	PEB	CAB-C3B-C4B	2.37	129.18	125.02
3	R	187	PEB	C2C-C1C-NC	2.37	110.54	107.57
3	W	188	PEB	C2C-C1C-NC	2.37	110.54	107.57
3	A	167	PEB	C2C-C1C-NC	2.37	110.54	107.57
3	O	187	PEB	O2B-CGB-CBB	2.36	121.47	114.00
3	H	166	PEB	C1D-ND-C4D	-2.36	109.79	113.42
3	M	188	PEB	CHC-C4C-NC	2.36	124.26	121.10
3	O	186	PEB	CHB-C1C-C2C	-2.36	122.15	127.22
3	U	186	PEB	C3A-C4A-NA	-2.36	104.90	107.94
3	R	187	PEB	C2A-C3A-C4A	2.36	104.87	101.34
3	X	188	PEB	CHC-C1D-ND	-2.36	110.84	113.73
3	N	188	PEB	C1B-CHA-C4A	2.36	132.04	127.25
3	T	188	PEB	C1B-CHA-C4A	2.35	132.04	127.25
3	U	186	PEB	C3D-C4D-ND	2.35	111.74	107.33
3	X	188	PEB	CAB-C3B-C4B	2.35	129.15	125.02
3	F	167	PEB	C2C-C1C-NC	2.35	110.51	107.57
3	W	188	PEB	C3D-C4D-ND	2.35	111.73	107.33
3	A	166	PEB	OD-C4D-ND	-2.35	122.79	126.02
3	C	166	PEB	CAC-CBC-CGC	-2.35	107.44	113.67
3	N	188	PEB	C1C-C2C-C3C	-2.35	104.89	107.62
3	H	166	PEB	CMC-C3C-C4C	2.35	129.49	126.97
3	K	167	PEB	C1D-ND-C4D	-2.34	109.81	113.42
3	C	167	PEB	CHA-C4A-NA	2.34	128.56	125.63
3	D	167	PEB	CAB-C3B-C4B	2.34	129.13	125.02
3	B	167	PEB	C4B-C3B-C2B	-2.34	104.19	106.73
3	C	167	PEB	CAC-C2C-C1C	2.34	129.49	125.77
3	O	186	PEB	OD-C4D-C3D	-2.33	124.07	129.71
3	A	167	PEB	CHB-C1C-C2C	-2.33	122.20	127.22
3	L	166	PEB	C4B-NB-C1B	2.33	110.80	106.52
3	P	186	PEB	CHC-C1D-ND	-2.33	110.88	113.73
3	Q	186	PEB	C1B-CHA-C4A	2.33	131.98	127.25
3	W	186	PEB	C1B-CHA-C4A	2.33	131.98	127.25
3	U	187	PEB	CMB-C2B-C1B	2.32	128.71	125.10
3	X	187	PEB	C1C-C2C-C3C	-2.32	104.92	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	188	PEB	CBD-CAD-C3D	-2.32	115.93	127.53
3	A	167	PEB	C2A-C1A-NA	2.32	110.22	108.29
3	N	187	PEB	CMB-C2B-C1B	2.32	128.70	125.10
3	E	166	PEB	CHA-C1B-C2B	2.32	130.83	124.87
3	T	188	PEB	C2C-C1C-NC	2.32	110.47	107.57
3	F	166	PEB	CMB-C2B-C1B	2.32	128.70	125.10
3	M	186	PEB	OD-C4D-C3D	-2.32	124.12	129.71
3	W	187	PEB	O1C-CGC-CBC	-2.31	115.75	123.09
3	K	166	PEB	CAC-CBC-CGC	-2.31	107.53	113.67
3	L	167	PEB	C2C-C1C-NC	2.31	110.46	107.57
3	O	188	PEB	C2C-C1C-NC	2.31	110.46	107.57
3	R	188	PEB	C3D-C4D-ND	2.31	111.65	107.33
3	N	188	PEB	CBC-CAC-C2C	-2.30	106.16	112.53
3	O	187	PEB	C1B-C2B-C3B	-2.30	103.86	106.48
3	N	188	PEB	C2A-C3A-C4A	2.30	104.78	101.34
3	U	186	PEB	OD-C4D-ND	-2.29	122.86	126.02
3	P	186	PEB	CHB-C4B-C3B	-2.29	120.11	125.40
3	Q	188	PEB	CHA-C4A-NA	2.29	128.49	125.63
5	N	204	PI	O4-P-O1	-2.29	102.86	110.95
7	O	204	MPD	O2-C2-C1	2.29	115.11	107.99
3	T	186	PEB	CAB-CBB-CGB	-2.29	107.60	113.67
3	J	167	PEB	CHB-C1C-C2C	-2.28	122.31	127.22
3	K	167	PEB	C3D-C4D-ND	2.28	111.61	107.33
3	M	187	PEB	O2B-CGB-CBB	2.28	121.21	114.00
3	X	186	PEB	CHA-C1B-NB	-2.28	120.03	124.95
3	S	188	PEB	CAB-C3B-C4B	2.28	129.02	125.02
3	U	187	PEB	CAC-C2C-C1C	2.28	129.39	125.77
3	M	186	PEB	C2A-C3A-C4A	2.28	104.75	101.34
3	V	186	PEB	C1D-ND-C4D	-2.28	109.92	113.42
3	Q	187	PEB	C1C-C2C-C3C	-2.27	104.97	107.62
3	C	166	PEB	CBB-CAB-C3B	-2.27	106.26	112.53
3	U	188	PEB	CMB-C2B-C1B	2.27	128.62	125.10
3	P	188	PEB	CHB-C1C-C2C	-2.26	122.35	127.22
3	V	187	PEB	C1C-C2C-C3C	-2.26	104.98	107.62
3	C	167	PEB	C1D-ND-C4D	-2.26	109.94	113.42
3	X	188	PEB	CHB-C4B-C3B	-2.26	120.17	125.40
3	O	186	PEB	CHA-C1B-NB	-2.26	120.07	124.95
3	M	186	PEB	CHB-C1C-C2C	-2.26	122.36	127.22
3	N	188	PEB	CAB-C3B-C4B	2.26	128.99	125.02
3	T	186	PEB	CHA-C1B-C2B	2.26	130.68	124.87
3	D	167	PEB	C3B-C4B-NB	2.26	113.25	110.04
7	R	204	MPD	O2-C2-CM	2.26	115.03	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	186[A]	PEB	C2A-C3A-C4A	2.26	104.72	101.34
3	S	186[B]	PEB	C2A-C3A-C4A	2.26	104.72	101.34
3	O	188	PEB	CAB-C3B-C4B	2.25	128.98	125.02
3	H	166	PEB	CHC-C1D-ND	-2.25	110.97	113.73
3	P	186	PEB	C3D-C4D-ND	2.25	111.55	107.33
3	U	188	PEB	OD-C4D-C3D	-2.25	124.27	129.71
3	P	188	PEB	OD-C4D-ND	-2.25	122.93	126.02
3	C	167	PEB	CMC-C3C-C4C	2.25	129.38	126.97
3	T	187	PEB	C1B-C2B-C3B	-2.24	103.93	106.48
3	V	187	PEB	CMD-C2D-C3D	-2.24	126.77	129.95
3	H	167	PEB	O2B-CGB-CBB	2.24	121.07	114.00
3	T	187	PEB	O2B-CGB-CBB	2.24	121.07	114.00
3	R	187	PEB	CHA-C1B-NB	-2.24	120.12	124.95
3	P	188	PEB	CHB-C4B-C3B	-2.24	120.23	125.40
3	V	186	PEB	C2C-C1C-NC	2.24	110.37	107.57
3	X	186	PEB	O1C-CGC-CBC	2.23	130.18	123.09
3	L	167	PEB	O1B-CGB-CBB	-2.23	116.02	123.09
3	W	186	PEB	C1D-ND-C4D	-2.23	109.99	113.42
3	M	187	PEB	CAC-C2C-C1C	2.23	129.31	125.77
3	K	167	PEB	C3C-C4C-NC	2.23	110.11	108.31
3	Q	187	PEB	C2A-C3A-C4A	2.23	104.68	101.34
3	J	166	PEB	C1C-C2C-C3C	-2.23	105.03	107.62
3	T	188	PEB	CHB-C4B-C3B	-2.23	120.26	125.40
3	C	166	PEB	CHB-C4B-C3B	-2.23	120.26	125.40
3	T	187	PEB	O1C-CGC-CBC	-2.22	116.04	123.09
7	M	204	MPD	CM-C2-C1	-2.22	105.65	110.63
3	G	166	PEB	CMD-C2D-C3D	-2.22	126.80	129.95
3	R	187	PEB	C3D-C4D-ND	2.22	111.49	107.33
3	Q	188	PEB	CHB-C1C-C2C	-2.22	122.45	127.22
3	P	188	PEB	CHA-C4A-NA	2.22	128.40	125.63
3	F	166	PEB	CMC-C3C-C4C	-2.22	124.59	126.97
3	W	187	PEB	OA-C1A-NA	-2.21	122.32	124.93
3	T	186	PEB	C3D-C4D-ND	2.21	111.48	107.33
3	I	167	PEB	OD-C4D-C3D	-2.21	124.38	129.71
3	L	166	PEB	OD-C4D-C3D	-2.20	124.39	129.71
3	X	187	PEB	OA-C1A-NA	2.20	127.53	124.93
3	I	166	PEB	CAC-CBC-CGC	-2.20	107.82	113.67
3	K	166	PEB	CHB-C1C-C2C	-2.20	122.49	127.22
3	X	186	PEB	CHA-C1B-C2B	2.20	130.52	124.87
3	J	167	PEB	O2C-CGC-CBC	2.20	120.94	114.00
3	O	187	PEB	C2C-C1C-NC	2.20	110.32	107.57
3	S	188	PEB	C2A-C1A-NA	2.20	110.11	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	188	PEB	CBD-CAD-C3D	-2.19	116.56	127.53
3	S	188	PEB	O2C-CGC-CBC	2.19	120.92	114.00
3	T	186	PEB	O1C-CGC-CBC	2.19	130.04	123.09
3	N	187	PEB	CHB-C1C-C2C	-2.18	122.53	127.22
3	V	188	PEB	C3C-C4C-NC	2.18	110.08	108.31
3	C	167	PEB	OD-C4D-C3D	-2.18	124.44	129.71
3	P	186	PEB	OD-C4D-ND	-2.18	123.02	126.02
3	Q	187	PEB	O2B-CGB-CBB	2.18	120.89	114.00
3	G	167	PEB	O2C-CGC-CBC	2.18	120.89	114.00
3	O	188	PEB	CBD-CAD-C3D	-2.18	116.63	127.53
3	D	167	PEB	C3C-C4C-NC	2.18	110.07	108.31
3	D	166	PEB	CBB-CAB-C3B	-2.18	106.52	112.53
3	U	186	PEB	C1B-CHA-C4A	2.17	131.67	127.25
3	N	187	PEB	C3C-C4C-NC	-2.17	106.55	108.31
3	D	166	PEB	O2C-CGC-CBC	2.17	120.87	114.00
3	M	187	PEB	CAB-C3B-C4B	2.17	128.84	125.02
3	T	186	PEB	C4B-C3B-C2B	-2.17	104.38	106.73
3	W	187	PEB	CHB-C4B-C3B	-2.17	120.39	125.40
3	V	186	PEB	OA-C1A-C2A	-2.17	124.45	126.17
3	K	167	PEB	O2B-CGB-CBB	2.17	120.84	114.00
3	N	186	PEB	C1D-ND-C4D	-2.17	110.09	113.42
3	J	167	PEB	C2A-C3A-C4A	2.17	104.58	101.34
3	Q	187	PEB	CHA-C1B-NB	-2.16	120.28	124.95
3	R	187	PEB	O1B-CGB-CBB	-2.16	116.24	123.09
3	H	166	PEB	CHC-C4C-NC	2.16	123.99	121.10
3	S	187	PEB	CAC-C2C-C1C	2.16	129.20	125.77
3	F	166	PEB	CHC-C4C-NC	2.16	123.98	121.10
3	M	187	PEB	O1C-CGC-CBC	-2.16	116.25	123.09
3	D	167	PEB	C1C-C2C-C3C	-2.16	105.11	107.62
3	P	187	PEB	OA-C1A-C2A	-2.16	124.46	126.17
3	N	187	PEB	C1A-NA-C4A	2.15	116.11	113.41
3	M	187	PEB	C3C-C4C-NC	2.15	110.06	108.31
3	Q	186	PEB	O1B-CGB-CBB	-2.15	116.27	123.09
3	E	167	PEB	C4B-C3B-C2B	-2.15	104.40	106.73
3	U	187	PEB	OA-C1A-C2A	-2.15	124.46	126.17
3	I	166	PEB	CMA-C2A-C1A	-2.15	107.77	112.40
3	M	188	PEB	C3C-C4C-NC	2.15	110.05	108.31
3	N	186	PEB	C2A-C3A-C4A	2.14	104.55	101.34
3	W	188	PEB	C3C-C4C-NC	2.14	110.04	108.31
3	K	167	PEB	O2C-CGC-CBC	2.14	120.76	114.00
3	W	187	PEB	O2B-CGB-CBB	2.14	120.75	114.00
3	I	166	PEB	C3D-C4D-ND	2.14	111.33	107.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	167	PEB	O2C-CGC-CBC	2.13	120.74	114.00
3	L	167	PEB	C3C-C4C-NC	2.13	110.04	108.31
3	O	186	PEB	C1B-CHA-C4A	2.13	131.59	127.25
3	S	187	PEB	O1C-CGC-CBC	-2.13	116.33	123.09
3	P	186	PEB	C4B-C3B-C2B	-2.13	104.42	106.73
3	U	187	PEB	OD-C4D-C3D	-2.13	124.56	129.71
3	P	187	PEB	OA-C1A-NA	2.13	127.43	124.93
3	P	186	PEB	C2C-C1C-NC	2.12	110.23	107.57
3	K	167	PEB	C2C-C1C-NC	2.12	110.23	107.57
3	M	188	PEB	CAB-C3B-C2B	-2.12	123.89	127.87
3	L	167	PEB	CAB-C3B-C2B	-2.12	123.89	127.87
3	C	166	PEB	CMA-C2A-C1A	-2.12	107.83	112.40
3	W	186	PEB	CHC-C4C-NC	2.12	123.93	121.10
3	W	188	PEB	OD-C4D-ND	-2.11	123.12	126.02
3	U	187	PEB	CHA-C1B-NB	-2.11	120.39	124.95
3	V	186	PEB	CHB-C4B-C3B	-2.11	120.53	125.40
3	W	186	PEB	OA-C1A-C2A	-2.10	124.50	126.17
3	U	187	PEB	C2C-C1C-NC	2.10	110.20	107.57
3	J	167	PEB	C3C-C4C-NC	2.10	110.01	108.31
3	W	187	PEB	CHB-C1C-C2C	-2.10	122.71	127.22
3	W	188	PEB	CHB-C1C-C2C	-2.10	122.71	127.22
3	Q	188	PEB	CBB-CAB-C3B	2.10	118.33	112.53
3	M	187	PEB	CHB-C1C-C2C	-2.09	122.72	127.22
3	I	167	PEB	OA-C1A-C2A	-2.09	124.51	126.17
3	I	167	PEB	CHB-C1C-C2C	-2.09	122.72	127.22
3	N	187	PEB	OA-C1A-C2A	2.09	127.84	126.17
3	A	167	PEB	O2C-CGC-CBC	2.09	120.61	114.00
3	I	167	PEB	CMB-C2B-C1B	2.09	128.34	125.10
3	F	166	PEB	CMC-C3C-C2C	2.09	130.05	125.62
3	U	187	PEB	C3D-C4D-ND	2.09	111.24	107.33
3	N	186	PEB	C4B-C3B-C2B	-2.08	104.47	106.73
3	H	167	PEB	C1C-C2C-C3C	-2.08	105.20	107.62
3	E	167	PEB	OD-C4D-ND	-2.08	123.16	126.02
3	D	167	PEB	CHC-C4C-NC	2.08	123.88	121.10
3	Q	186	PEB	CAB-C3B-C4B	2.08	128.67	125.02
3	N	186	PEB	C2A-C1A-NA	2.08	110.02	108.29
3	X	186	PEB	O2C-CGC-O1C	-2.08	117.98	123.33
3	Q	187	PEB	CHB-C1C-C2C	-2.08	122.75	127.22
3	X	186	PEB	CAC-C2C-C1C	2.08	129.07	125.77
3	W	186	PEB	C2A-C1A-NA	2.07	110.01	108.29
3	R	187	PEB	CHC-C1D-ND	-2.07	111.19	113.73
3	X	187	PEB	OD-C4D-C3D	-2.07	124.70	129.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	187	PEB	C1C-C2C-C3C	-2.07	105.21	107.62
3	P	188	PEB	C3D-C4D-ND	2.07	111.21	107.33
3	F	167	PEB	C3C-C4C-NC	2.07	109.99	108.31
3	X	186	PEB	CAB-C3B-C4B	2.07	128.65	125.02
3	X	188	PEB	C3D-C4D-ND	2.07	111.20	107.33
3	J	166	PEB	C2A-C1A-NA	2.07	110.00	108.29
3	T	188	PEB	CMB-C2B-C1B	2.06	128.30	125.10
3	V	187	PEB	CHC-C4C-NC	2.06	123.86	121.10
3	C	167	PEB	OD-C4D-ND	-2.06	123.19	126.02
5	H	203	PI	O2-P-O1	-2.06	103.67	110.95
3	K	167	PEB	C3B-C4B-NB	2.06	112.95	110.04
3	Q	187	PEB	O2C-CGC-CBC	2.06	120.49	114.00
3	C	166	PEB	OA-C1A-NA	2.05	127.35	124.93
7	X	204	MPD	CM-C2-C1	-2.05	106.03	110.63
3	O	186	PEB	CAC-C2C-C1C	2.05	129.03	125.77
3	R	187	PEB	CHB-C4B-C3B	-2.05	120.67	125.40
3	L	166	PEB	CAB-C3B-C2B	-2.05	124.03	127.87
3	A	167	PEB	OD-C4D-C3D	-2.05	124.77	129.71
3	M	187	PEB	C3D-C4D-ND	2.05	111.17	107.33
3	W	186	PEB	CMC-C3C-C4C	2.05	129.17	126.97
3	F	166	PEB	CAB-C3B-C4B	2.05	128.61	125.02
3	H	166	PEB	CBB-CAB-C3B	-2.04	106.88	112.53
3	A	167	PEB	CHA-C1B-NB	-2.04	120.54	124.95
3	E	167	PEB	CMB-C2B-C1B	2.04	128.27	125.10
3	X	188	PEB	CHC-C4C-NC	2.04	123.83	121.10
3	F	167	PEB	CHB-C4B-C3B	-2.04	120.68	125.40
3	X	188	PEB	C1B-C2B-C3B	-2.04	104.16	106.48
3	B	167	PEB	C2A-C3A-C4A	2.04	104.40	101.34
3	D	167	PEB	OA-C1A-NA	2.04	127.33	124.93
3	R	187	PEB	CBA-CAA-C3A	2.04	117.73	113.41
3	U	188	PEB	CBD-CAD-C3D	-2.04	117.35	127.53
3	M	187	PEB	OD-C4D-ND	-2.04	123.22	126.02
3	D	167	PEB	CHB-C4B-C3B	-2.03	120.70	125.40
3	M	187	PEB	CHB-C4B-C3B	-2.03	120.70	125.40
3	G	166	PEB	CAC-CBC-CGC	-2.03	108.27	113.67
3	O	188	PEB	CBB-CAB-C3B	2.03	118.16	112.53
3	S	186[A]	PEB	C3C-C4C-NC	2.03	109.96	108.31
3	S	186[B]	PEB	C3C-C4C-NC	2.03	109.96	108.31
3	I	166	PEB	C3A-C4A-NA	-2.03	105.33	107.94
3	W	188	PEB	CHB-C4B-C3B	-2.03	120.71	125.40
3	N	188	PEB	C3D-C4D-ND	2.03	111.13	107.33
3	E	166	PEB	CAC-CBC-CGC	-2.03	108.29	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	186	PEB	C1D-ND-C4D	-2.03	110.31	113.42
3	M	188	PEB	CHB-C4B-C3B	-2.02	120.72	125.40
3	N	186	PEB	C3D-C4D-ND	2.02	111.11	107.33
3	M	186	PEB	OA-C1A-NA	2.01	127.30	124.93
3	J	167	PEB	CMA-C2A-C1A	2.01	116.74	112.40
3	X	188	PEB	CHB-C4B-NB	2.01	128.83	124.60
3	N	187	PEB	OD-C4D-ND	-2.01	123.26	126.02
3	A	167	PEB	C1C-C2C-C3C	-2.01	105.28	107.62

There are no chirality outliers.

All (358) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	166	PEB	C2B-C1B-CHA-C4A
3	A	167	PEB	NB-C1B-CHA-C4A
3	A	167	PEB	C2B-C1B-CHA-C4A
3	B	166	PEB	C2B-C1B-CHA-C4A
3	B	167	PEB	NB-C1B-CHA-C4A
3	B	167	PEB	C2B-C1B-CHA-C4A
3	C	166	PEB	C2B-C1B-CHA-C4A
3	C	167	PEB	NB-C1B-CHA-C4A
3	C	167	PEB	C2B-C1B-CHA-C4A
3	D	166	PEB	C2B-C1B-CHA-C4A
3	D	167	PEB	NB-C1B-CHA-C4A
3	D	167	PEB	C2B-C1B-CHA-C4A
3	E	166	PEB	C2B-C1B-CHA-C4A
3	E	167	PEB	NB-C1B-CHA-C4A
3	E	167	PEB	C2B-C1B-CHA-C4A
3	F	167	PEB	NB-C1B-CHA-C4A
3	F	167	PEB	C2B-C1B-CHA-C4A
3	G	166	PEB	C2B-C1B-CHA-C4A
3	G	167	PEB	NB-C1B-CHA-C4A
3	G	167	PEB	C2B-C1B-CHA-C4A
3	H	166	PEB	C2B-C1B-CHA-C4A
3	H	167	PEB	NB-C1B-CHA-C4A
3	H	167	PEB	C2B-C1B-CHA-C4A
3	I	166	PEB	C2B-C1B-CHA-C4A
3	I	167	PEB	NB-C1B-CHA-C4A
3	I	167	PEB	C2B-C1B-CHA-C4A
3	J	166	PEB	C2B-C1B-CHA-C4A
3	J	167	PEB	NB-C1B-CHA-C4A
3	J	167	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
3	K	166	PEB	C2B-C1B-CHA-C4A
3	K	167	PEB	NB-C1B-CHA-C4A
3	K	167	PEB	C2B-C1B-CHA-C4A
3	L	166	PEB	C2B-C1B-CHA-C4A
3	L	167	PEB	NB-C1B-CHA-C4A
3	L	167	PEB	C2B-C1B-CHA-C4A
3	M	187	PEB	NB-C1B-CHA-C4A
3	M	187	PEB	C2B-C1B-CHA-C4A
3	M	188	PEB	NB-C1B-CHA-C4A
3	M	188	PEB	C2B-C1B-CHA-C4A
3	N	187	PEB	NB-C1B-CHA-C4A
3	N	187	PEB	C2B-C1B-CHA-C4A
3	N	188	PEB	C2D-C3D-CAD-CBD
3	N	188	PEB	NB-C1B-CHA-C4A
3	N	188	PEB	C2B-C1B-CHA-C4A
3	O	186	PEB	NB-C1B-CHA-C4A
3	O	187	PEB	NB-C1B-CHA-C4A
3	O	187	PEB	C2B-C1B-CHA-C4A
3	O	188	PEB	C2D-C3D-CAD-CBD
3	O	188	PEB	NB-C1B-CHA-C4A
3	O	188	PEB	C2B-C1B-CHA-C4A
3	P	187	PEB	NB-C1B-CHA-C4A
3	P	187	PEB	C2B-C1B-CHA-C4A
3	P	188	PEB	NB-C1B-CHA-C4A
3	P	188	PEB	C2B-C1B-CHA-C4A
3	Q	187	PEB	NB-C1B-CHA-C4A
3	Q	187	PEB	C2B-C1B-CHA-C4A
3	Q	188	PEB	NB-C1B-CHA-C4A
3	Q	188	PEB	C2B-C1B-CHA-C4A
3	R	186	PEB	NB-C1B-CHA-C4A
3	R	187	PEB	NB-C1B-CHA-C4A
3	R	187	PEB	C2B-C1B-CHA-C4A
3	R	188	PEB	NB-C1B-CHA-C4A
3	R	188	PEB	C2B-C1B-CHA-C4A
3	S	186[A]	PEB	NB-C1B-CHA-C4A
3	S	186[B]	PEB	NB-C1B-CHA-C4A
3	S	187	PEB	NB-C1B-CHA-C4A
3	S	187	PEB	C2B-C1B-CHA-C4A
3	S	188	PEB	NB-C1B-CHA-C4A
3	S	188	PEB	C2B-C1B-CHA-C4A
3	T	187	PEB	NB-C1B-CHA-C4A
3	T	187	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
3	T	188	PEB	NB-C1B-CHA-C4A
3	T	188	PEB	C2B-C1B-CHA-C4A
3	U	187	PEB	NB-C1B-CHA-C4A
3	U	187	PEB	C2B-C1B-CHA-C4A
3	U	188	PEB	NB-C1B-CHA-C4A
3	U	188	PEB	C2B-C1B-CHA-C4A
3	V	187	PEB	NB-C1B-CHA-C4A
3	V	187	PEB	C2B-C1B-CHA-C4A
3	V	188	PEB	C2D-C3D-CAD-CBD
3	V	188	PEB	NB-C1B-CHA-C4A
3	V	188	PEB	C2B-C1B-CHA-C4A
3	W	187	PEB	NB-C1B-CHA-C4A
3	W	187	PEB	C2B-C1B-CHA-C4A
3	W	188	PEB	NB-C1B-CHA-C4A
3	W	188	PEB	C2B-C1B-CHA-C4A
3	X	187	PEB	NB-C1B-CHA-C4A
3	X	187	PEB	C2B-C1B-CHA-C4A
3	X	188	PEB	NB-C1B-CHA-C4A
3	X	188	PEB	C2B-C1B-CHA-C4A
7	R	204	MPD	C2-C3-C4-O4
7	R	204	MPD	C2-C3-C4-C5
3	Q	186	PEB	NB-C1B-CHA-C4A
3	F	166	PEB	C2B-C1B-CHA-C4A
3	A	166	PEB	NB-C1B-CHA-C4A
3	B	166	PEB	NB-C1B-CHA-C4A
3	C	166	PEB	NB-C1B-CHA-C4A
3	D	166	PEB	NB-C1B-CHA-C4A
3	E	166	PEB	NB-C1B-CHA-C4A
3	F	166	PEB	NB-C1B-CHA-C4A
3	G	166	PEB	NB-C1B-CHA-C4A
3	H	166	PEB	NB-C1B-CHA-C4A
3	I	166	PEB	NB-C1B-CHA-C4A
3	J	166	PEB	NB-C1B-CHA-C4A
3	K	166	PEB	NB-C1B-CHA-C4A
3	L	166	PEB	NB-C1B-CHA-C4A
3	M	186	PEB	NB-C1B-CHA-C4A
3	N	186	PEB	NB-C1B-CHA-C4A
3	P	186	PEB	NB-C1B-CHA-C4A
3	T	186	PEB	NB-C1B-CHA-C4A
3	U	186	PEB	NB-C1B-CHA-C4A
3	V	186	PEB	NB-C1B-CHA-C4A
3	W	186	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
3	X	186	PEB	NB-C1B-CHA-C4A
3	S	186[A]	PEB	C2C-CAC-CBC-CGC
3	M	186	PEB	C2B-C1B-CHA-C4A
3	N	186	PEB	C2B-C1B-CHA-C4A
3	O	186	PEB	C2B-C1B-CHA-C4A
3	P	186	PEB	C2B-C1B-CHA-C4A
3	Q	186	PEB	C2B-C1B-CHA-C4A
3	R	186	PEB	C2B-C1B-CHA-C4A
3	S	186[A]	PEB	C2B-C1B-CHA-C4A
3	S	186[B]	PEB	C2B-C1B-CHA-C4A
3	T	186	PEB	C2B-C1B-CHA-C4A
3	U	186	PEB	C2B-C1B-CHA-C4A
3	V	186	PEB	C2B-C1B-CHA-C4A
3	W	186	PEB	C2B-C1B-CHA-C4A
3	X	186	PEB	C2B-C1B-CHA-C4A
3	M	188	PEB	C2D-C3D-CAD-CBD
3	P	188	PEB	C2D-C3D-CAD-CBD
3	Q	188	PEB	C2D-C3D-CAD-CBD
3	U	188	PEB	C2D-C3D-CAD-CBD
3	W	188	PEB	C2D-C3D-CAD-CBD
3	X	188	PEB	C2D-C3D-CAD-CBD
3	O	188	PEB	C4D-C3D-CAD-CBD
3	A	167	PEB	C4A-C3A-CAA-CBA
3	E	167	PEB	C4A-C3A-CAA-CBA
3	I	167	PEB	C4A-C3A-CAA-CBA
3	M	187	PEB	C4A-C3A-CAA-CBA
3	N	187	PEB	C4A-C3A-CAA-CBA
3	O	187	PEB	C4A-C3A-CAA-CBA
3	P	187	PEB	C4A-C3A-CAA-CBA
3	Q	187	PEB	C4A-C3A-CAA-CBA
3	R	187	PEB	C4A-C3A-CAA-CBA
3	S	187	PEB	C4A-C3A-CAA-CBA
3	T	187	PEB	C4A-C3A-CAA-CBA
3	U	187	PEB	C4A-C3A-CAA-CBA
3	V	187	PEB	C4A-C3A-CAA-CBA
3	W	187	PEB	C4A-C3A-CAA-CBA
3	X	187	PEB	C4A-C3A-CAA-CBA
3	S	188	PEB	C2D-C3D-CAD-CBD
8	V	204	MRD	C2-C3-C4-O4
7	B	203	MPD	C1-C2-C3-C4
7	B	203	MPD	CM-C2-C3-C4
3	Q	187	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	V	204	MRD	C2-C3-C4-C5
3	L	167	PEB	CAB-CBB-CGB-O2B
3	C	167	PEB	CAC-CBC-CGC-O1C
3	T	186	PEB	CAC-CBC-CGC-O1C
3	C	166	PEB	CAC-CBC-CGC-O1C
3	G	166	PEB	CAC-CBC-CGC-O1C
3	I	166	PEB	CAC-CBC-CGC-O1C
3	K	167	PEB	CAC-CBC-CGC-O2C
3	S	186[B]	PEB	CAC-CBC-CGC-O1C
3	X	186	PEB	CAC-CBC-CGC-O2C
3	D	167	PEB	CAC-CBC-CGC-O2C
3	E	167	PEB	CAC-CBC-CGC-O1C
3	F	167	PEB	CAC-CBC-CGC-O1C
3	H	167	PEB	CAC-CBC-CGC-O1C
3	M	188	PEB	CAC-CBC-CGC-O2C
3	A	166	PEB	CAC-CBC-CGC-O1C
3	D	166	PEB	CAC-CBC-CGC-O1C
3	F	166	PEB	CAC-CBC-CGC-O1C
3	I	167	PEB	CAC-CBC-CGC-O2C
3	J	166	PEB	CAC-CBC-CGC-O1C
3	J	167	PEB	CAC-CBC-CGC-O1C
3	X	186	PEB	CAC-CBC-CGC-O1C
3	S	188	PEB	C2B-C3B-CAB-CBB
3	B	166	PEB	CAC-CBC-CGC-O1C
3	I	167	PEB	CAC-CBC-CGC-O1C
3	L	166	PEB	CAC-CBC-CGC-O1C
3	M	188	PEB	CAC-CBC-CGC-O1C
3	S	186[A]	PEB	CAB-CBB-CGB-O1B
3	S	186[B]	PEB	CAB-CBB-CGB-O1B
3	E	166	PEB	CAC-CBC-CGC-O1C
3	H	166	PEB	CAC-CBC-CGC-O1C
3	M	186	PEB	CAC-CBC-CGC-O1C
3	B	167	PEB	CAB-CBB-CGB-O2B
3	F	167	PEB	CAC-CBC-CGC-O2C
3	R	186	PEB	CAC-CBC-CGC-O1C
3	T	186	PEB	CAB-CBB-CGB-O1B
3	V	187	PEB	CAB-CBB-CGB-O1B
3	A	167	PEB	CAC-CBC-CGC-O1C
3	L	167	PEB	CAC-CBC-CGC-O1C
3	O	186	PEB	CAB-CBB-CGB-O1B
3	T	187	PEB	CAB-CBB-CGB-O1B
3	W	186	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
3	B	167	PEB	CAC-CBC-CGC-O1C
3	E	167	PEB	CAC-CBC-CGC-O2C
3	I	166	PEB	CAC-CBC-CGC-O2C
3	K	167	PEB	CAC-CBC-CGC-O1C
3	T	186	PEB	CAC-CBC-CGC-O2C
3	U	186	PEB	CAB-CBB-CGB-O1B
3	U	188	PEB	CAC-CBC-CGC-O1C
3	A	166	PEB	CAC-CBC-CGC-O2C
3	D	166	PEB	CAC-CBC-CGC-O2C
3	H	167	PEB	CAC-CBC-CGC-O2C
3	J	167	PEB	CAC-CBC-CGC-O2C
3	P	187	PEB	CAB-CBB-CGB-O2B
3	S	186[B]	PEB	CAC-CBC-CGC-O2C
3	W	186	PEB	CAC-CBC-CGC-O1C
3	X	187	PEB	CAB-CBB-CGB-O2B
3	B	166	PEB	CAC-CBC-CGC-O2C
3	B	167	PEB	CAC-CBC-CGC-O2C
3	H	166	PEB	CAC-CBC-CGC-O2C
3	M	186	PEB	CAB-CBB-CGB-O1B
3	N	186	PEB	CAB-CBB-CGB-O1B
3	R	186	PEB	CAB-CBB-CGB-O1B
3	S	187	PEB	CAB-CBB-CGB-O2B
3	V	186	PEB	CAB-CBB-CGB-O1B
3	K	166	PEB	CAC-CBC-CGC-O1C
3	L	167	PEB	CAB-CBB-CGB-O1B
3	M	187	PEB	CAB-CBB-CGB-O2B
3	R	186	PEB	CAC-CBC-CGC-O2C
3	V	187	PEB	CAB-CBB-CGB-O2B
3	W	186	PEB	CAB-CBB-CGB-O1B
3	W	187	PEB	CAB-CBB-CGB-O1B
3	A	167	PEB	CAB-CBB-CGB-O1B
3	A	167	PEB	CAB-CBB-CGB-O2B
3	D	167	PEB	CAC-CBC-CGC-O1C
3	L	166	PEB	CAC-CBC-CGC-O2C
3	L	167	PEB	CAC-CBC-CGC-O2C
3	M	186	PEB	CAC-CBC-CGC-O2C
3	M	187	PEB	CAB-CBB-CGB-O1B
3	N	187	PEB	CAB-CBB-CGB-O2B
3	Q	187	PEB	CAB-CBB-CGB-O2B
3	T	187	PEB	CAB-CBB-CGB-O2B
3	M	187	PEB	C2A-C3A-CAA-CBA
3	A	167	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
3	C	167	PEB	CAC-CBC-CGC-O2C
3	G	167	PEB	CAC-CBC-CGC-O2C
3	K	166	PEB	CAC-CBC-CGC-O2C
3	X	187	PEB	CAB-CBB-CGB-O1B
3	D	167	PEB	CAB-CBB-CGB-O2B
3	F	166	PEB	CAC-CBC-CGC-O2C
3	F	167	PEB	CAB-CBB-CGB-O2B
3	G	167	PEB	CAB-CBB-CGB-O2B
3	J	166	PEB	CAC-CBC-CGC-O2C
3	P	186	PEB	CAB-CBB-CGB-O1B
3	P	187	PEB	CAB-CBB-CGB-O1B
3	R	188	PEB	CAC-CBC-CGC-O1C
3	X	186	PEB	CAB-CBB-CGB-O1B
3	C	167	PEB	CAB-CBB-CGB-O2B
3	N	187	PEB	CAB-CBB-CGB-O1B
3	U	187	PEB	CAB-CBB-CGB-O2B
3	C	166	PEB	CAC-CBC-CGC-O2C
3	E	166	PEB	CAC-CBC-CGC-O2C
3	G	167	PEB	CAC-CBC-CGC-O1C
3	O	187	PEB	CAB-CBB-CGB-O2B
3	Q	186	PEB	CAB-CBB-CGB-O1B
3	S	187	PEB	CAB-CBB-CGB-O1B
3	U	187	PEB	CAB-CBB-CGB-O1B
3	B	167	PEB	CAB-CBB-CGB-O1B
3	O	186	PEB	CAB-CBB-CGB-O2B
3	P	186	PEB	CAB-CBB-CGB-O2B
3	Q	187	PEB	CAB-CBB-CGB-O1B
3	U	188	PEB	CAC-CBC-CGC-O2C
3	G	166	PEB	CAC-CBC-CGC-O2C
3	R	186	PEB	CAB-CBB-CGB-O2B
3	T	186	PEB	CAB-CBB-CGB-O2B
3	V	186	PEB	CAC-CBC-CGC-O2C
3	V	186	PEB	CAB-CBB-CGB-O2B
3	W	186	PEB	CAB-CBB-CGB-O2B
3	B	167	PEB	C3B-CAB-CBB-CGB
3	M	186	PEB	CAB-CBB-CGB-O2B
3	Q	186	PEB	CAB-CBB-CGB-O2B
3	U	186	PEB	CAB-CBB-CGB-O2B
3	X	186	PEB	CAB-CBB-CGB-O2B
3	N	186	PEB	CAB-CBB-CGB-O2B
3	W	187	PEB	CAB-CBB-CGB-O2B
3	H	167	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
3	O	186	PEB	CAC-CBC-CGC-O2C
3	Q	188	PEB	CAC-CBC-CGC-O2C
3	R	187	PEB	CAB-CBB-CGB-O2B
3	U	186	PEB	CAC-CBC-CGC-O2C
3	W	188	PEB	CAC-CBC-CGC-O1C
3	X	188	PEB	CAC-CBC-CGC-O2C
3	F	167	PEB	CAB-CBB-CGB-O1B
3	K	167	PEB	CAB-CBB-CGB-O2B
3	O	187	PEB	CAB-CBB-CGB-O1B
3	Q	188	PEB	CAC-CBC-CGC-O1C
3	S	188	PEB	CAC-CBC-CGC-O1C
3	W	188	PEB	CAC-CBC-CGC-O2C
3	Q	186	PEB	CAC-CBC-CGC-O2C
3	E	167	PEB	CAB-CBB-CGB-O2B
3	I	167	PEB	CAB-CBB-CGB-O2B
3	S	186[A]	PEB	CAB-CBB-CGB-O2B
3	S	186[B]	PEB	CAB-CBB-CGB-O2B
3	D	167	PEB	CAB-CBB-CGB-O1B
3	X	188	PEB	CAC-CBC-CGC-O1C
3	P	186	PEB	CAC-CBC-CGC-O2C
3	Q	186	PEB	CAC-CBC-CGC-O1C
3	R	188	PEB	CAC-CBC-CGC-O2C
3	G	167	PEB	CAB-CBB-CGB-O1B
3	J	167	PEB	CAB-CBB-CGB-O2B
3	K	167	PEB	CAB-CBB-CGB-O1B
3	E	167	PEB	CAB-CBB-CGB-O1B
3	N	186	PEB	CAC-CBC-CGC-O2C
3	I	167	PEB	CAB-CBB-CGB-O1B
3	N	186	PEB	CAC-CBC-CGC-O1C
3	T	188	PEB	C2D-C3D-CAD-CBD
3	C	167	PEB	CAB-CBB-CGB-O1B
3	T	187	PEB	CAC-CBC-CGC-O2C
3	U	186	PEB	CAC-CBC-CGC-O1C
3	O	186	PEB	CAC-CBC-CGC-O1C
3	J	167	PEB	CAB-CBB-CGB-O1B
3	P	186	PEB	CAC-CBC-CGC-O1C
3	R	187	PEB	CAB-CBB-CGB-O1B
3	V	186	PEB	CAC-CBC-CGC-O1C
3	H	167	PEB	CAB-CBB-CGB-O1B
3	Q	187	PEB	C2C-CAC-CBC-CGC
3	N	188	PEB	CAC-CBC-CGC-O1C
3	S	188	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
3	P	187	PEB	C2C-CAC-CBC-CGC
3	S	186[B]	PEB	C2C-CAC-CBC-CGC
3	T	187	PEB	CAC-CBC-CGC-O1C
3	N	188	PEB	CAC-CBC-CGC-O2C
7	B	203	MPD	O2-C2-C3-C4
8	V	204	MRD	O2-C2-C3-C4
3	S	187	PEB	CAC-CBC-CGC-O1C
7	P	204	MPD	C2-C3-C4-O4
7	S	204	MPD	C2-C3-C4-O4
7	X	204	MPD	C2-C3-C4-O4
3	M	187	PEB	CAC-CBC-CGC-O1C
3	M	187	PEB	CAC-CBC-CGC-O2C
3	N	187	PEB	CAC-CBC-CGC-O2C
3	O	187	PEB	CAC-CBC-CGC-O1C
3	Q	187	PEB	CAC-CBC-CGC-O1C
3	V	187	PEB	CAC-CBC-CGC-O1C
3	V	188	PEB	CAC-CBC-CGC-O1C
3	T	188	PEB	CAC-CBC-CGC-O1C
3	V	188	PEB	CAC-CBC-CGC-O2C
3	X	187	PEB	CAC-CBC-CGC-O1C
3	X	187	PEB	CAC-CBC-CGC-O2C
3	N	187	PEB	CAC-CBC-CGC-O1C
3	T	187	PEB	C2A-C3A-CAA-CBA
3	O	188	PEB	CAC-CBC-CGC-O1C
3	O	188	PEB	CAC-CBC-CGC-O2C
3	Q	187	PEB	CAC-CBC-CGC-O2C
3	S	187	PEB	CAC-CBC-CGC-O2C
3	W	187	PEB	CAC-CBC-CGC-O1C
3	T	188	PEB	CAC-CBC-CGC-O2C
3	U	187	PEB	CAC-CBC-CGC-O2C
3	S	186[A]	PEB	CAC-CBC-CGC-O2C
3	R	187	PEB	CAC-CBC-CGC-O1C
3	S	186[A]	PEB	CAC-CBC-CGC-O1C
3	U	187	PEB	CAC-CBC-CGC-O1C
3	W	187	PEB	CAC-CBC-CGC-O2C

There are no ring outliers.

37 monomers are involved in 48 short contacts:

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

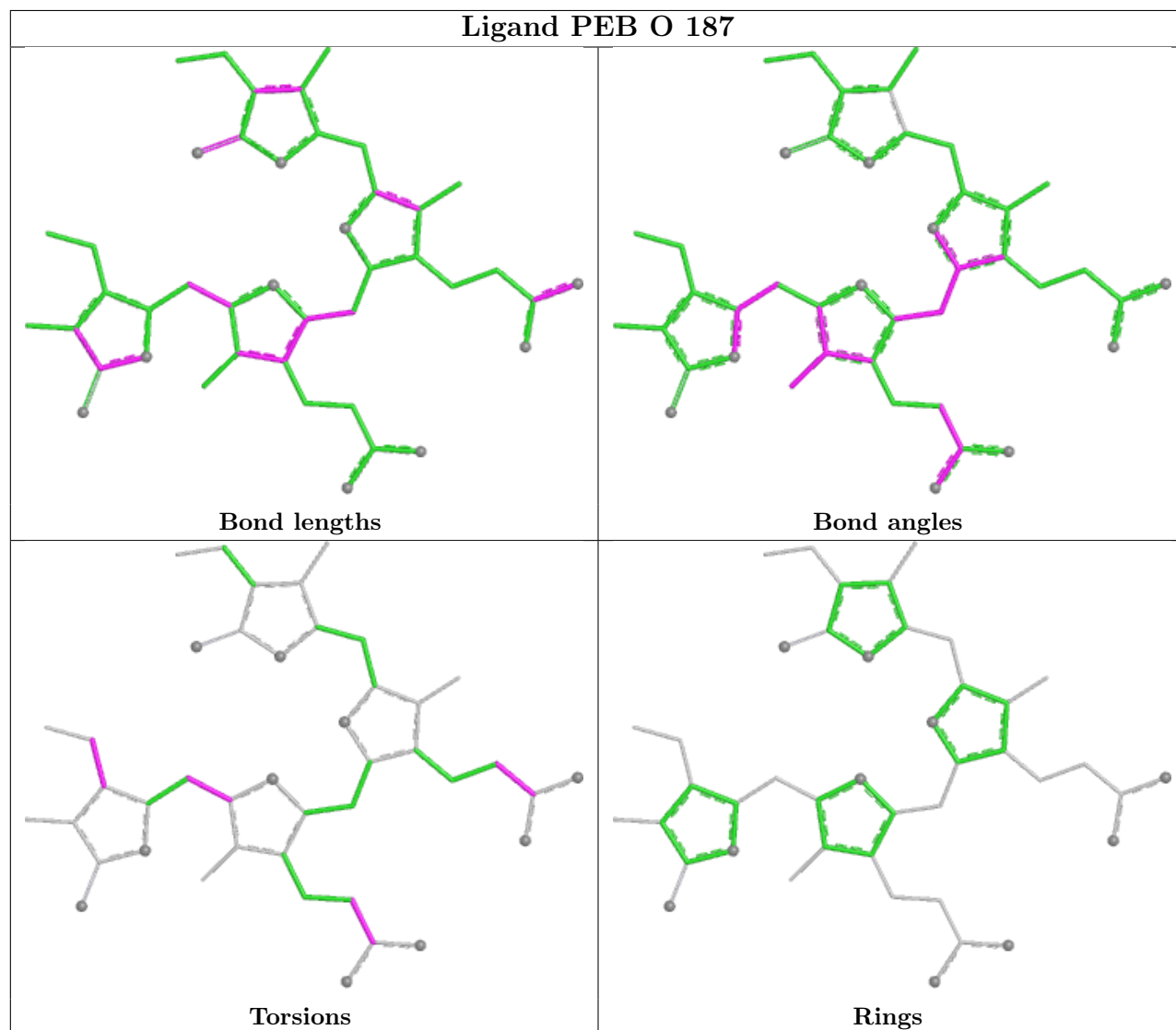
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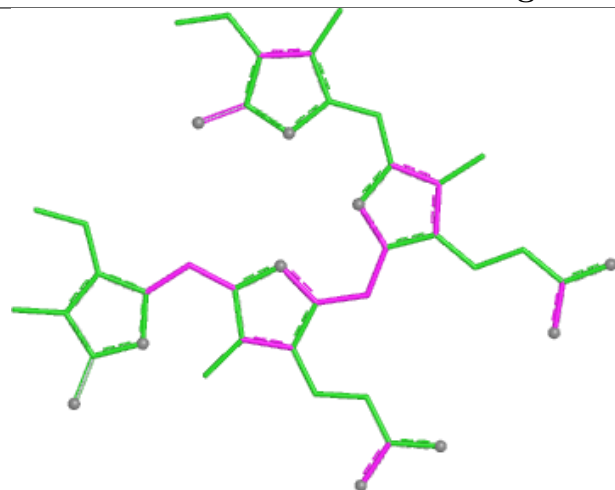
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	O	204	MPD	3	0
3	O	188	PEB	2	0
5	H	203	PI	1	0
3	P	188	PEB	1	0
3	N	186	PEB	1	0
7	Q	204	MPD	2	0
4	I	203	NO3	1	0
3	S	188	PEB	1	0
3	O	186	PEB	1	0
3	X	186	PEB	1	0
3	R	186	PEB	1	0
3	Q	186	PEB	2	0
3	F	166	PEB	1	0
3	R	187	PEB	2	0
3	U	186	PEB	1	0
3	T	187	PEB	1	0
3	W	186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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

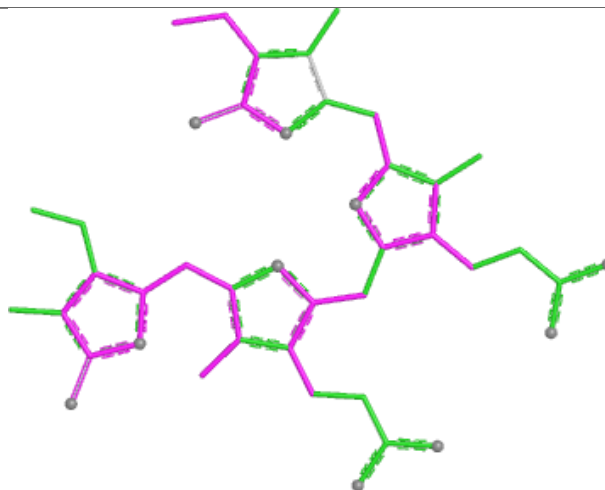
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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



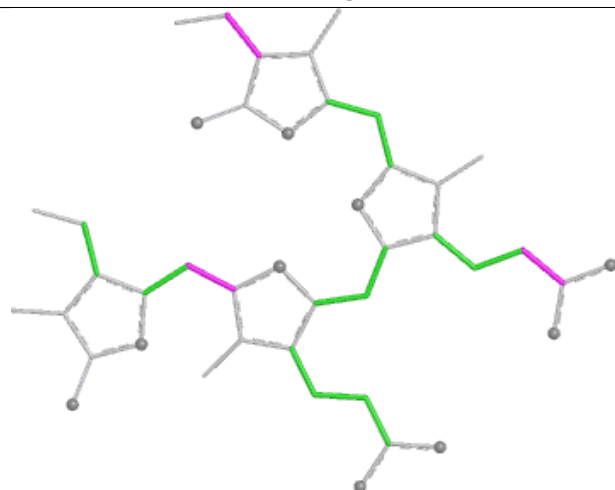
Ligand PEB T 188



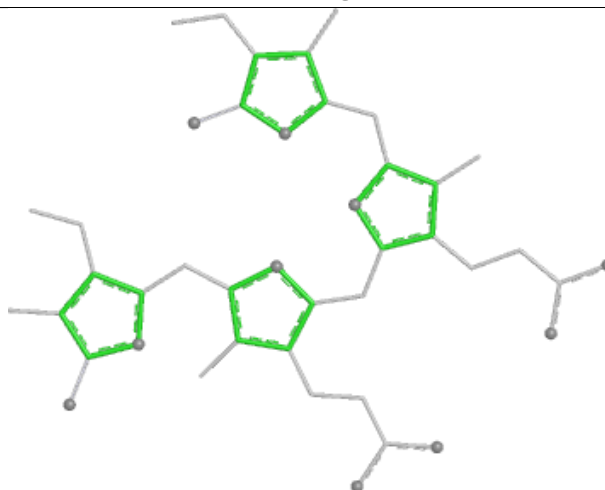
Bond lengths



Bond angles

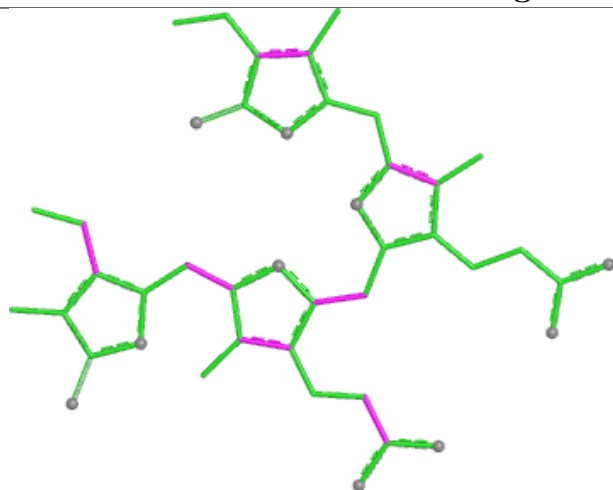


Torsions

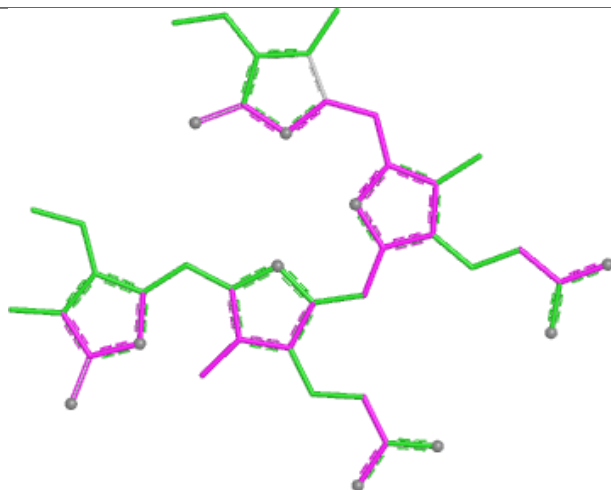


Rings

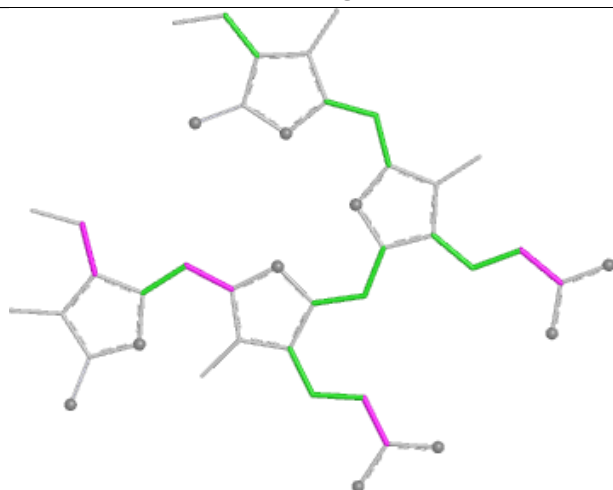
Ligand PEB N 187



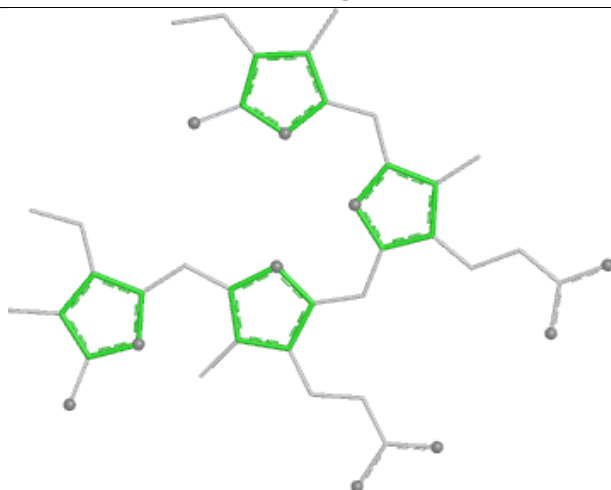
Bond lengths



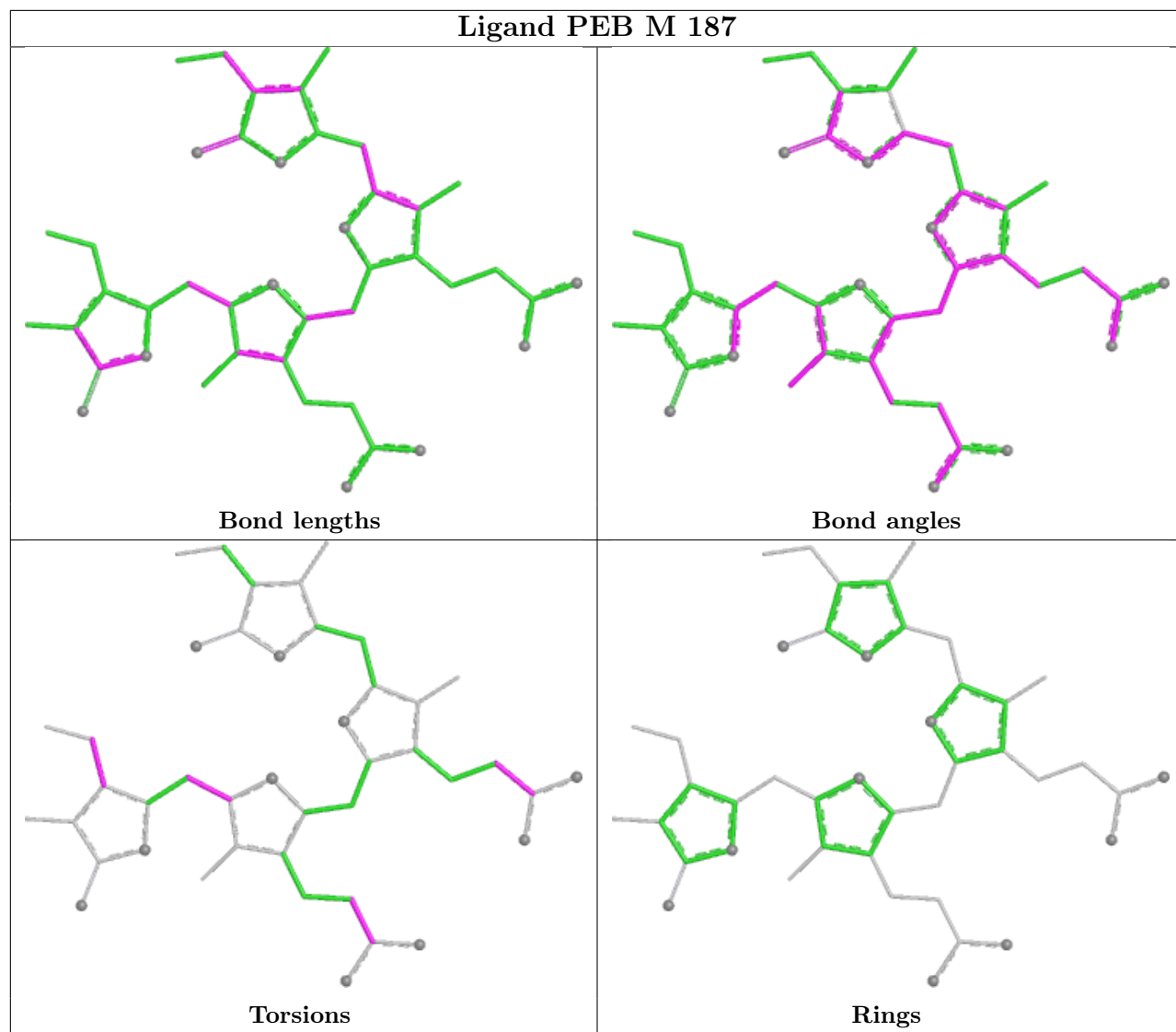
Bond angles

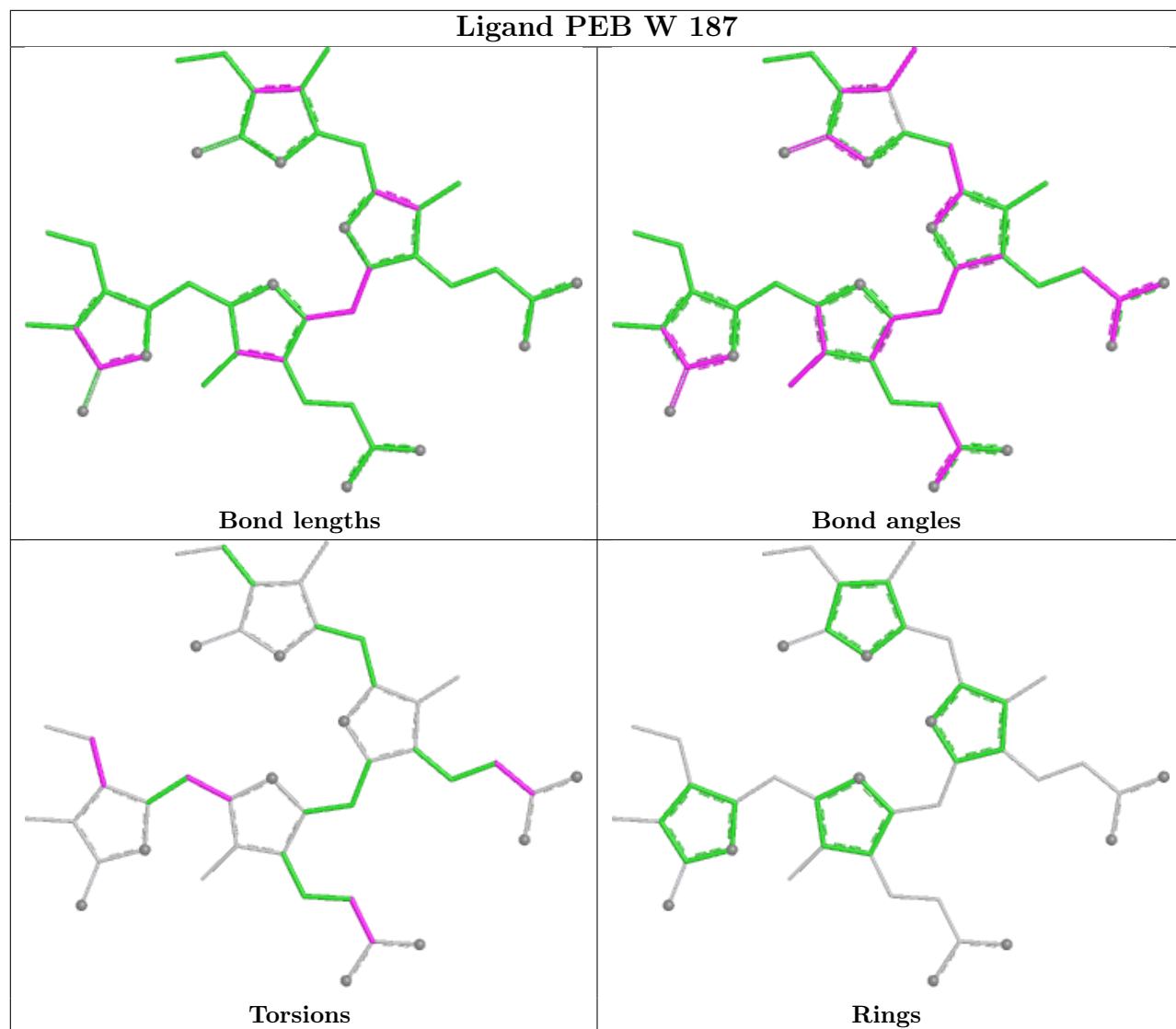


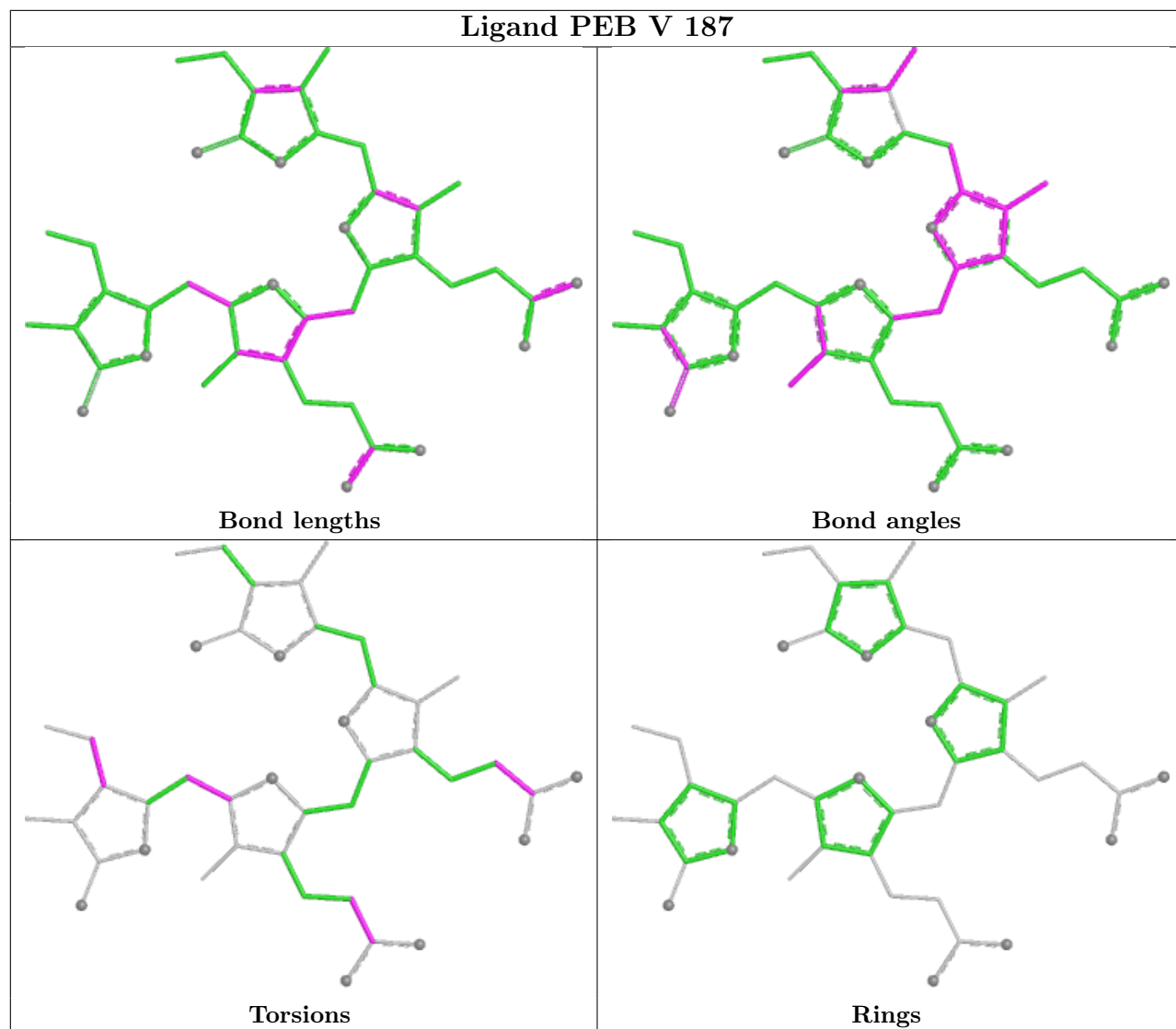
Torsions

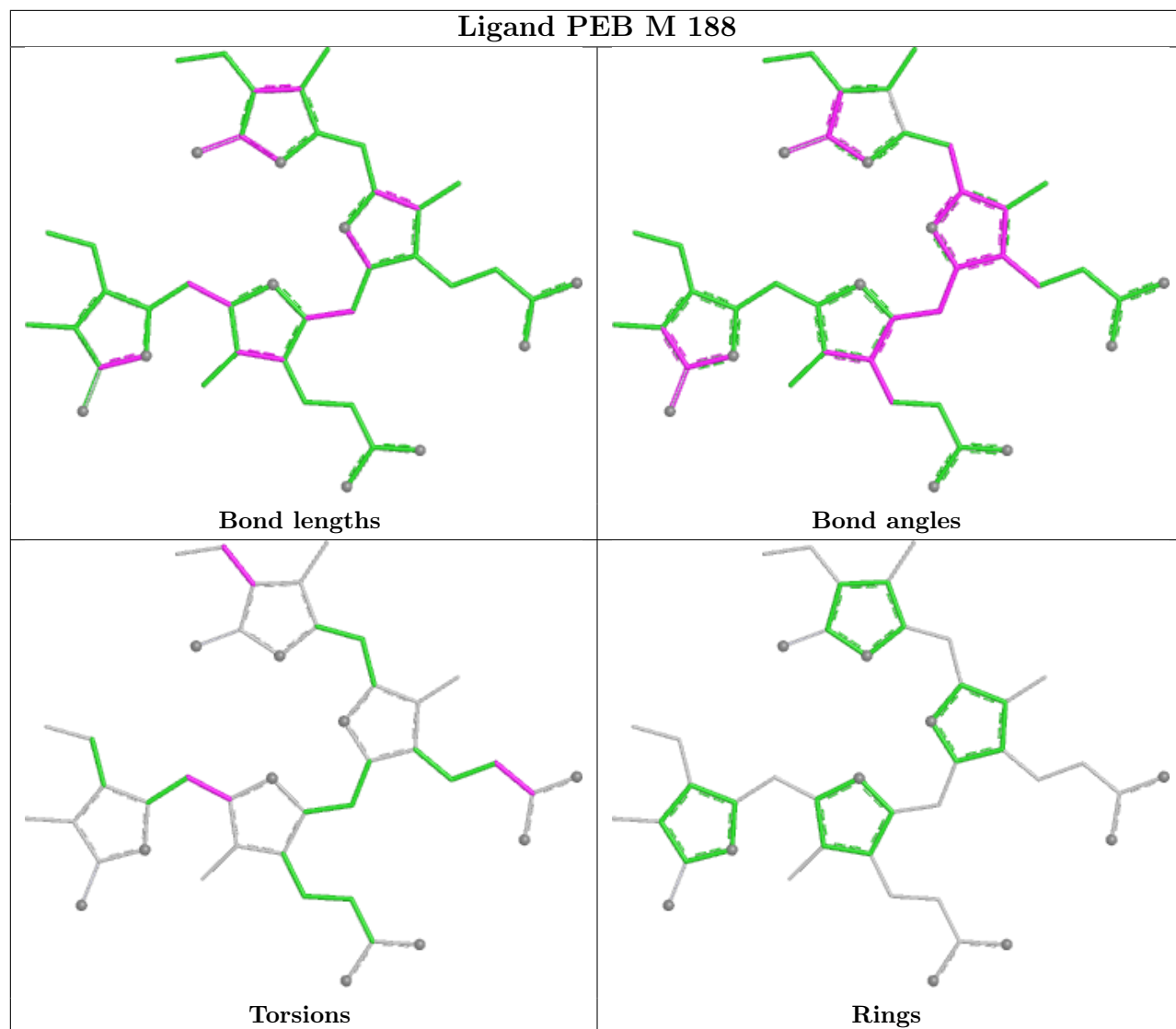


Rings

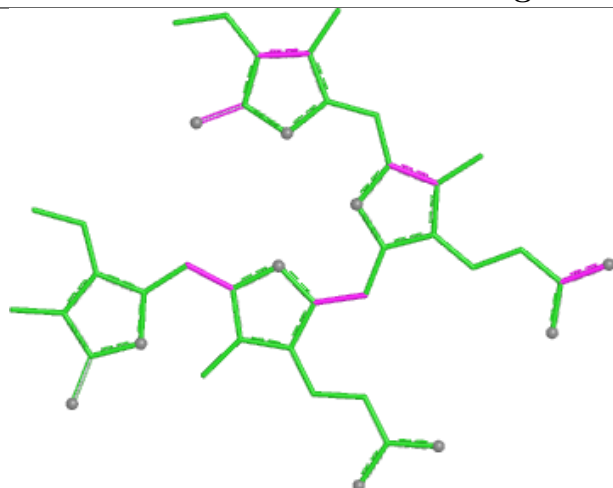




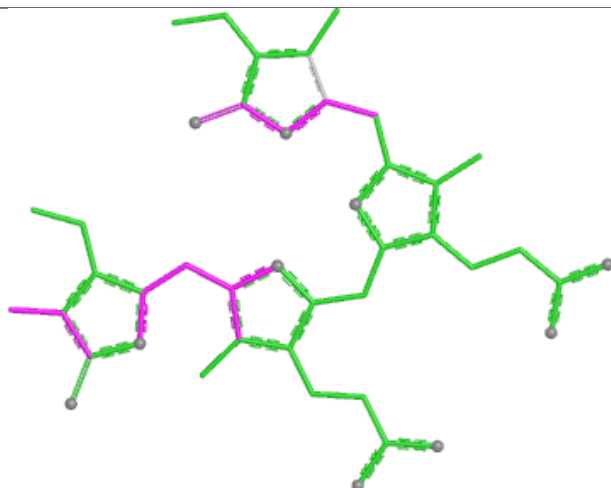




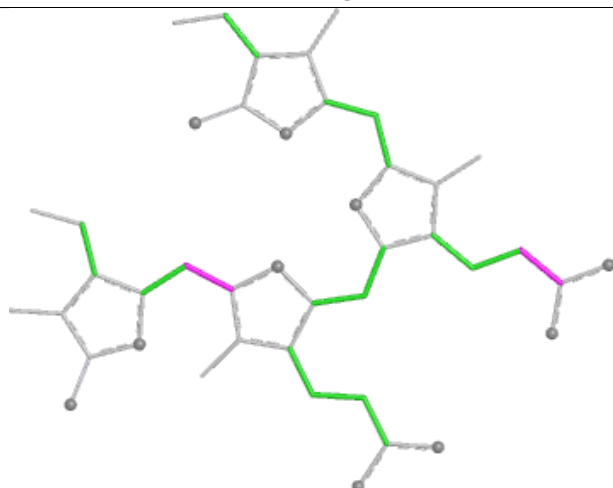
Ligand PEB A 166



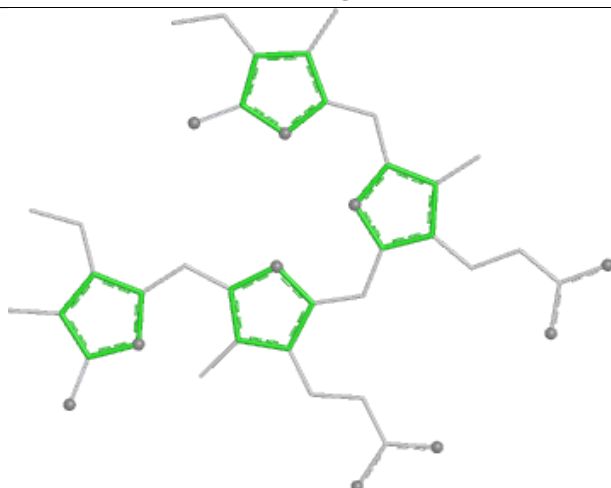
Bond lengths



Bond angles

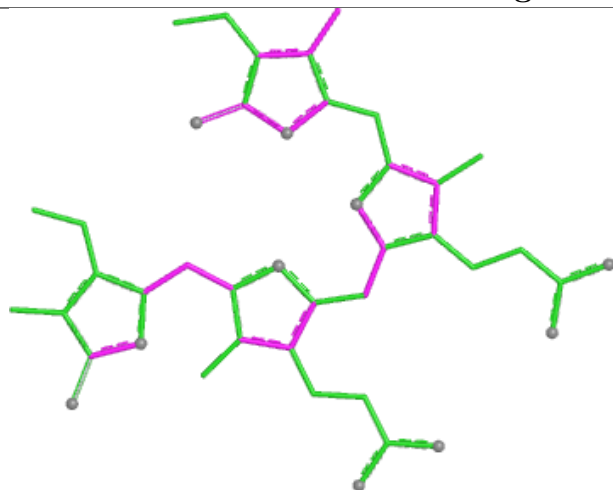


Torsions

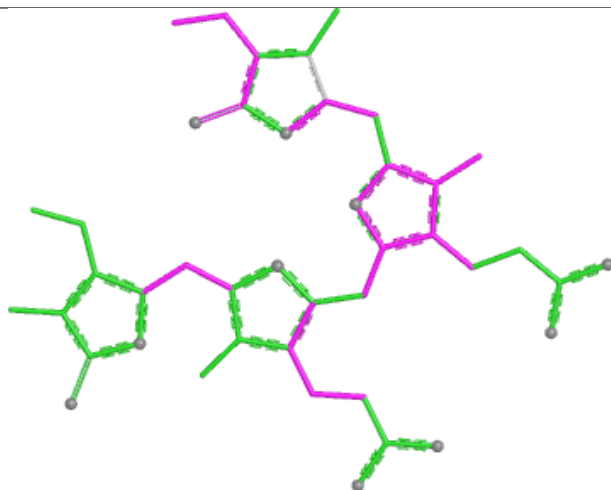


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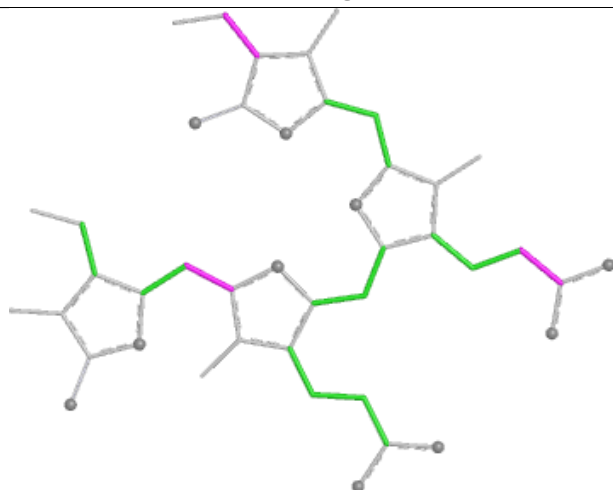
Ligand PEB O 188



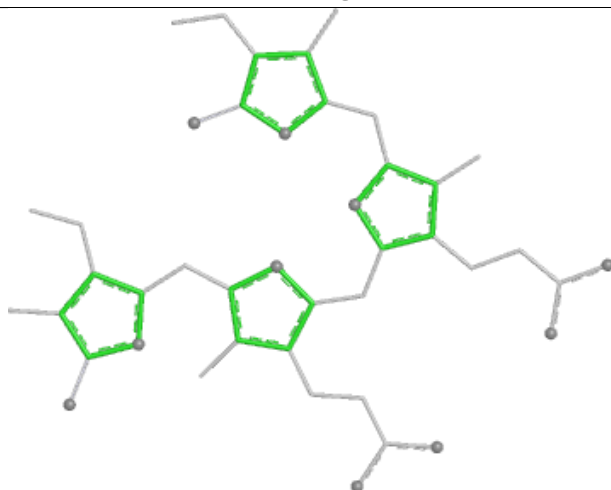
Bond lengths



Bond angles

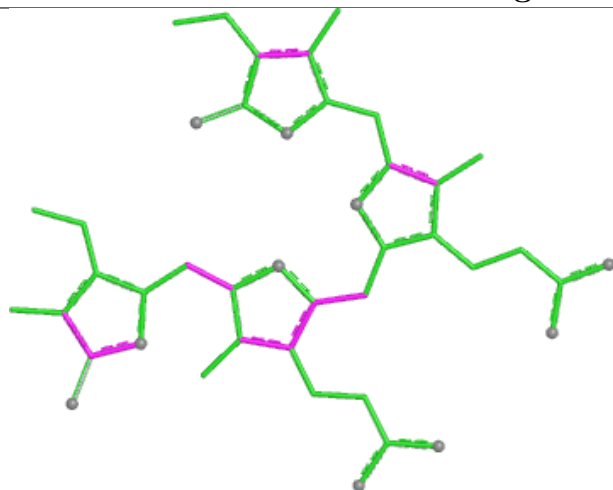


Torsions

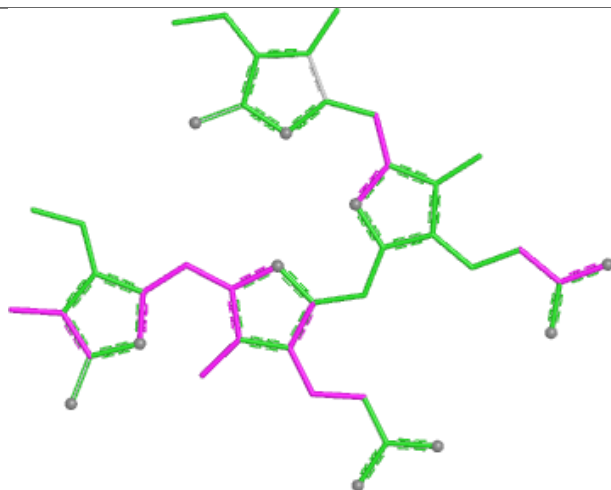


Rings

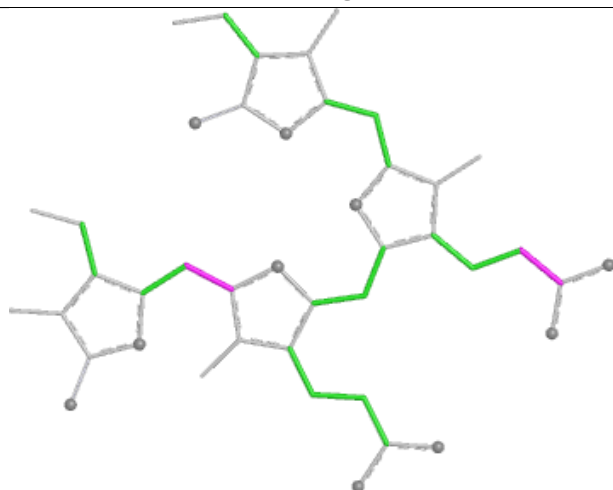
Ligand PEB D 166



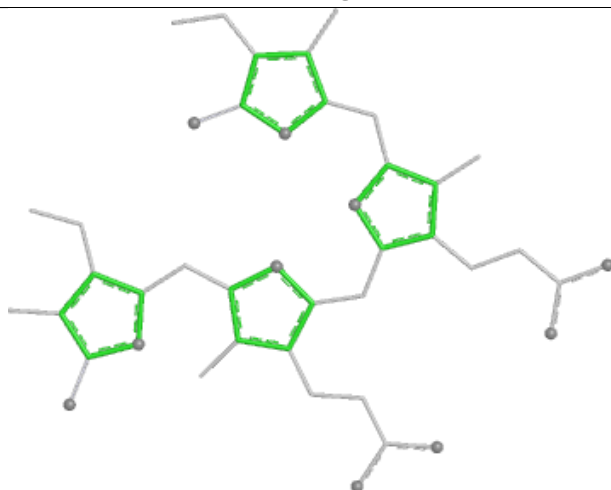
Bond lengths



Bond angles

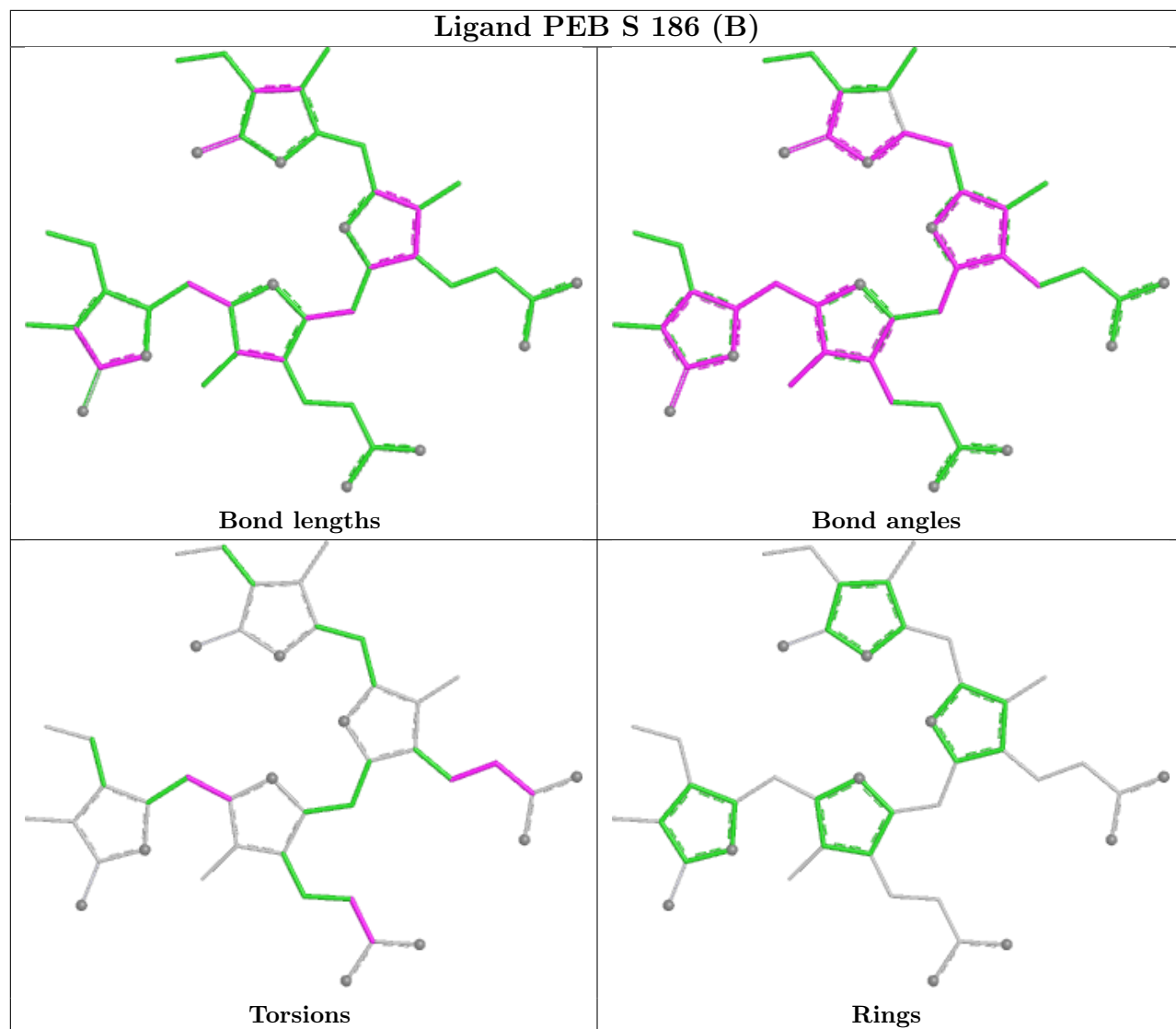


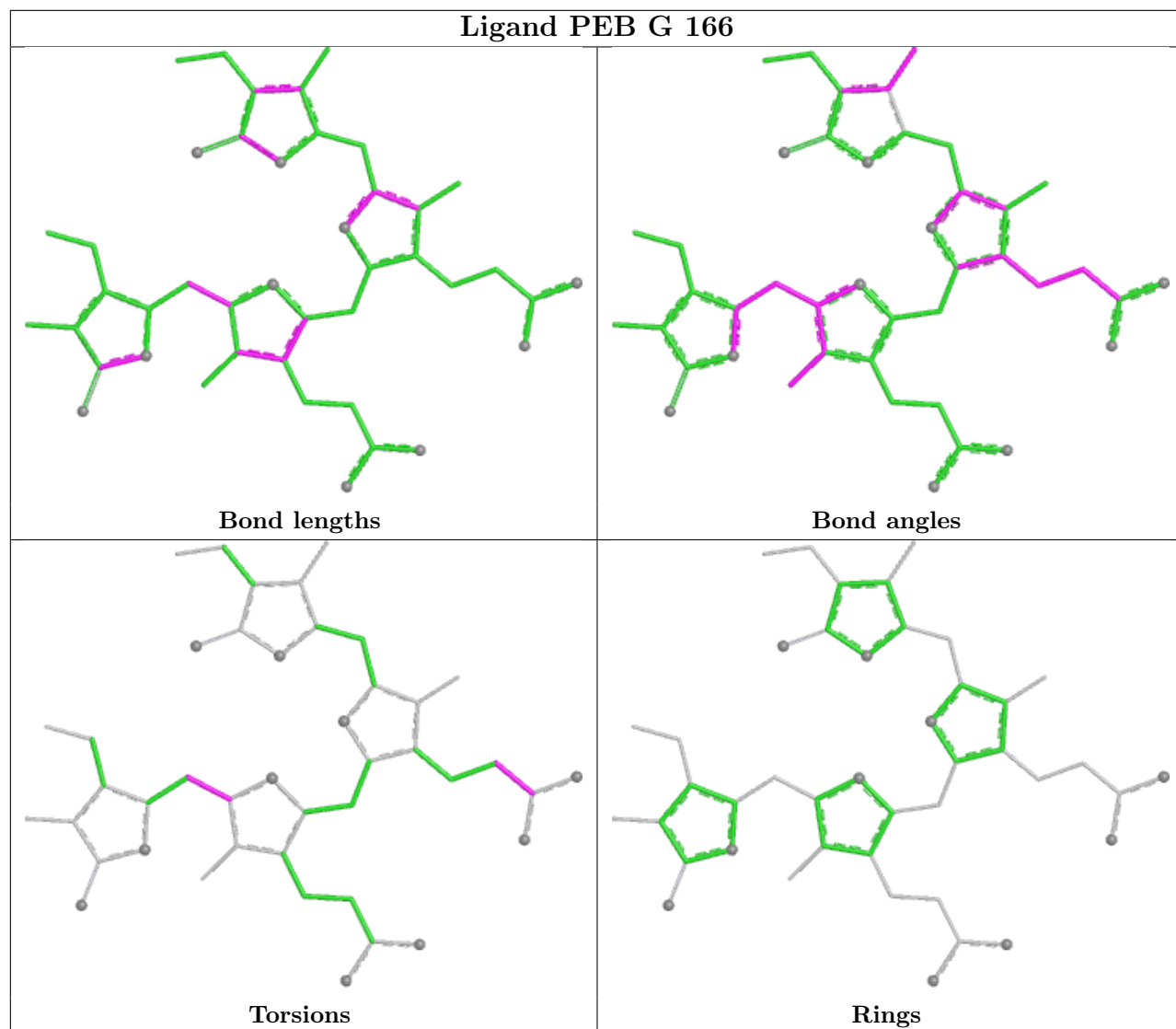
Torsions



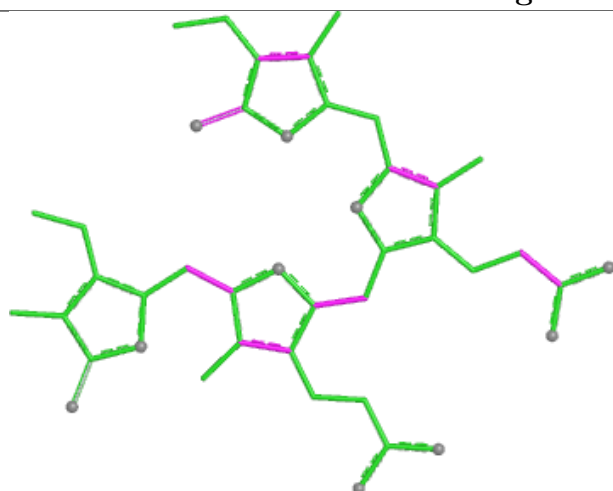
Rings

Ligand PEB S 186 (B)

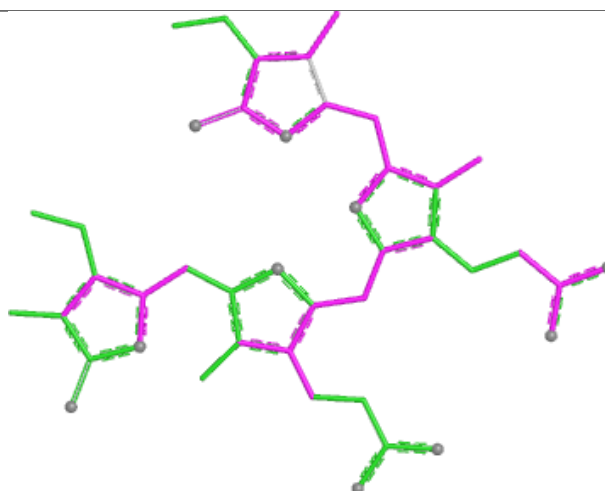




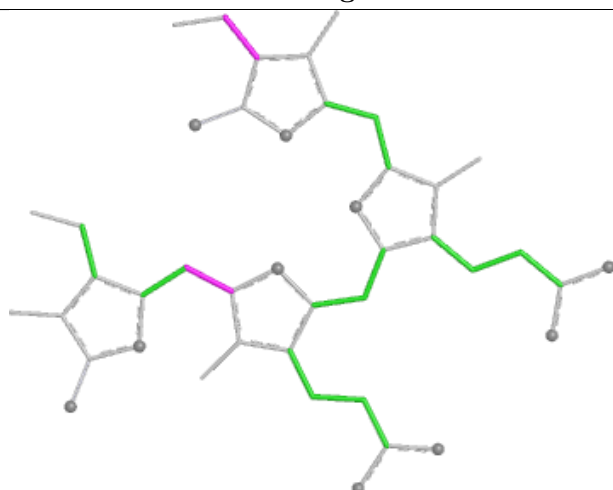
Ligand PEB P 188



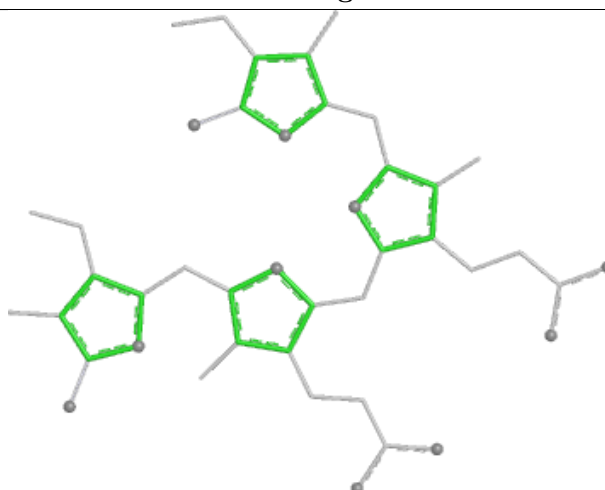
Bond lengths



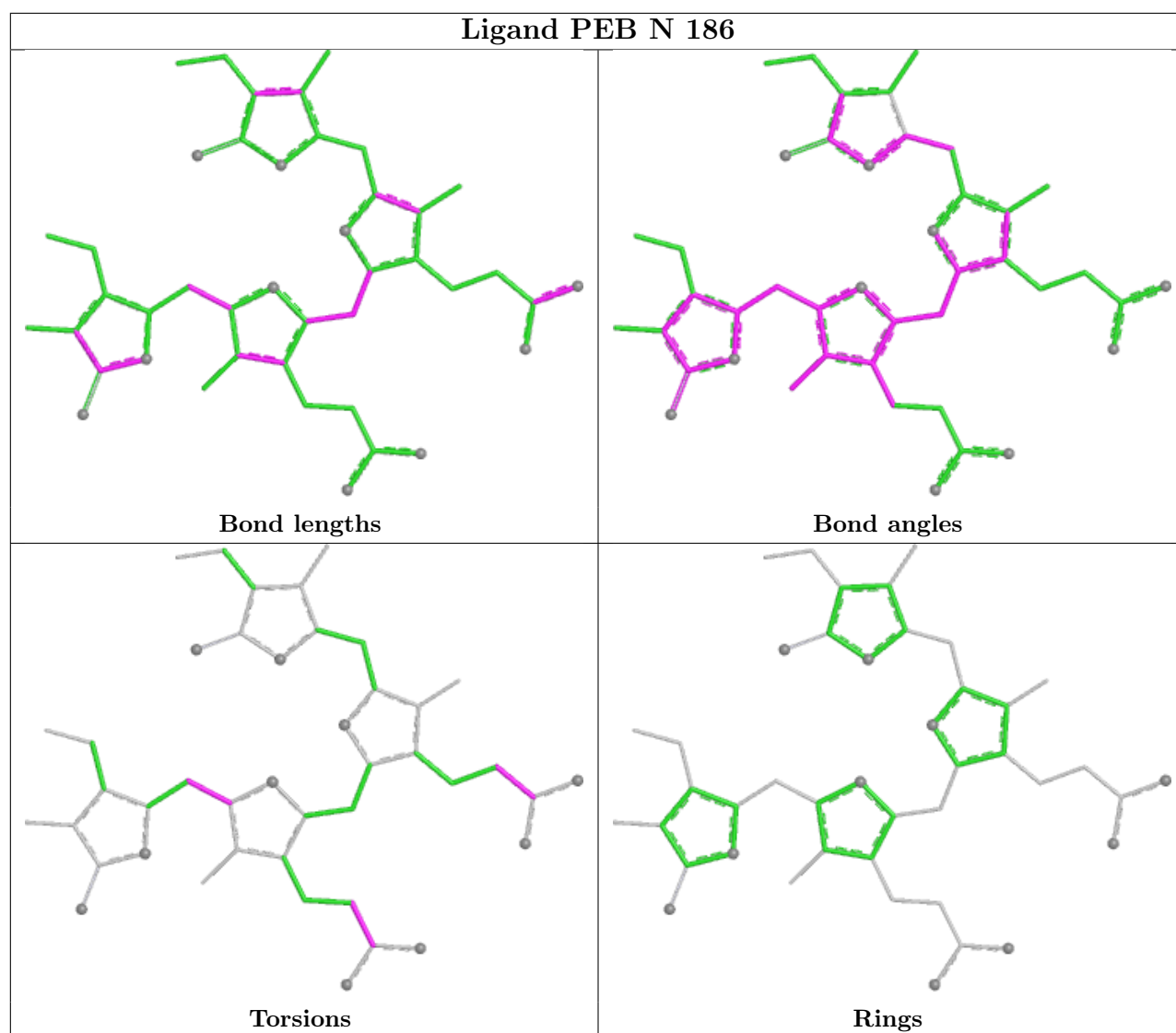
Bond angles

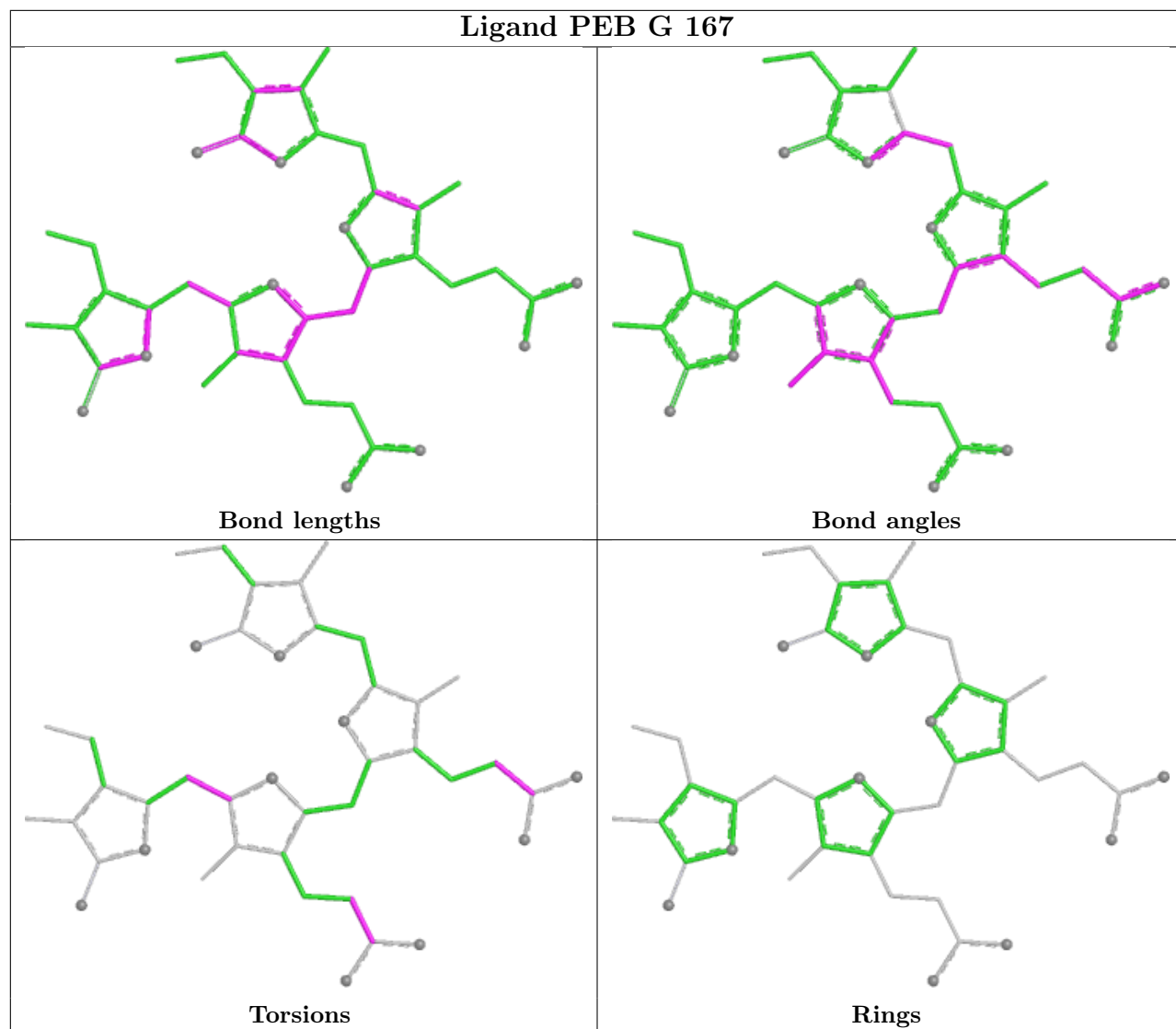


Torsions

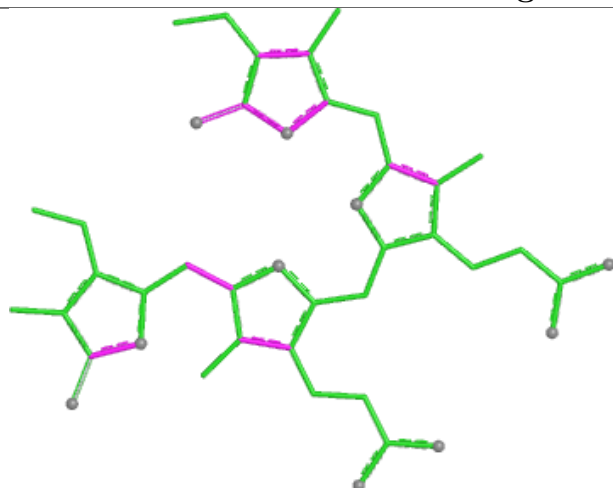


Rings

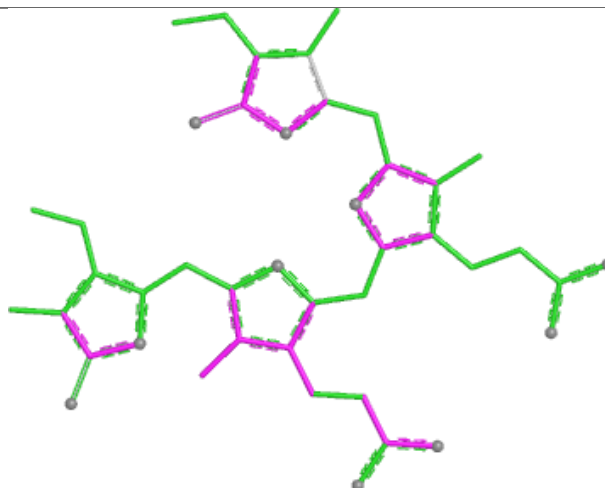




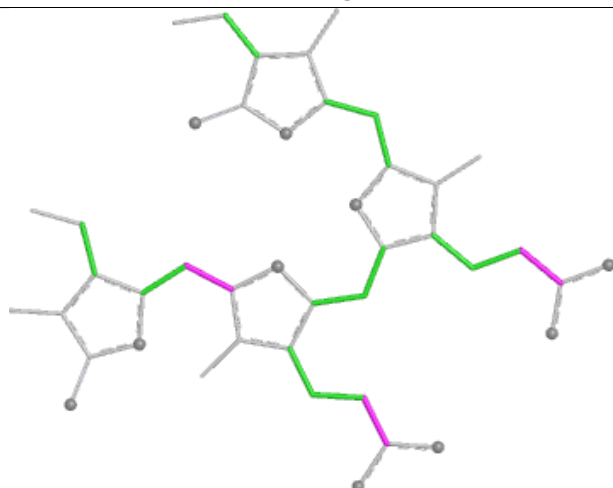
Ligand PEB L 167



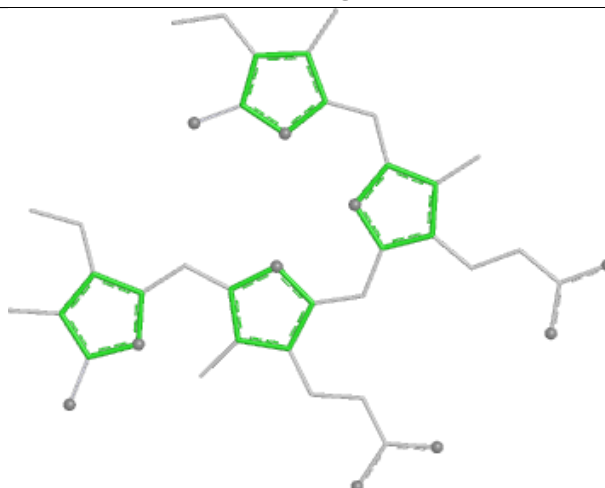
Bond lengths



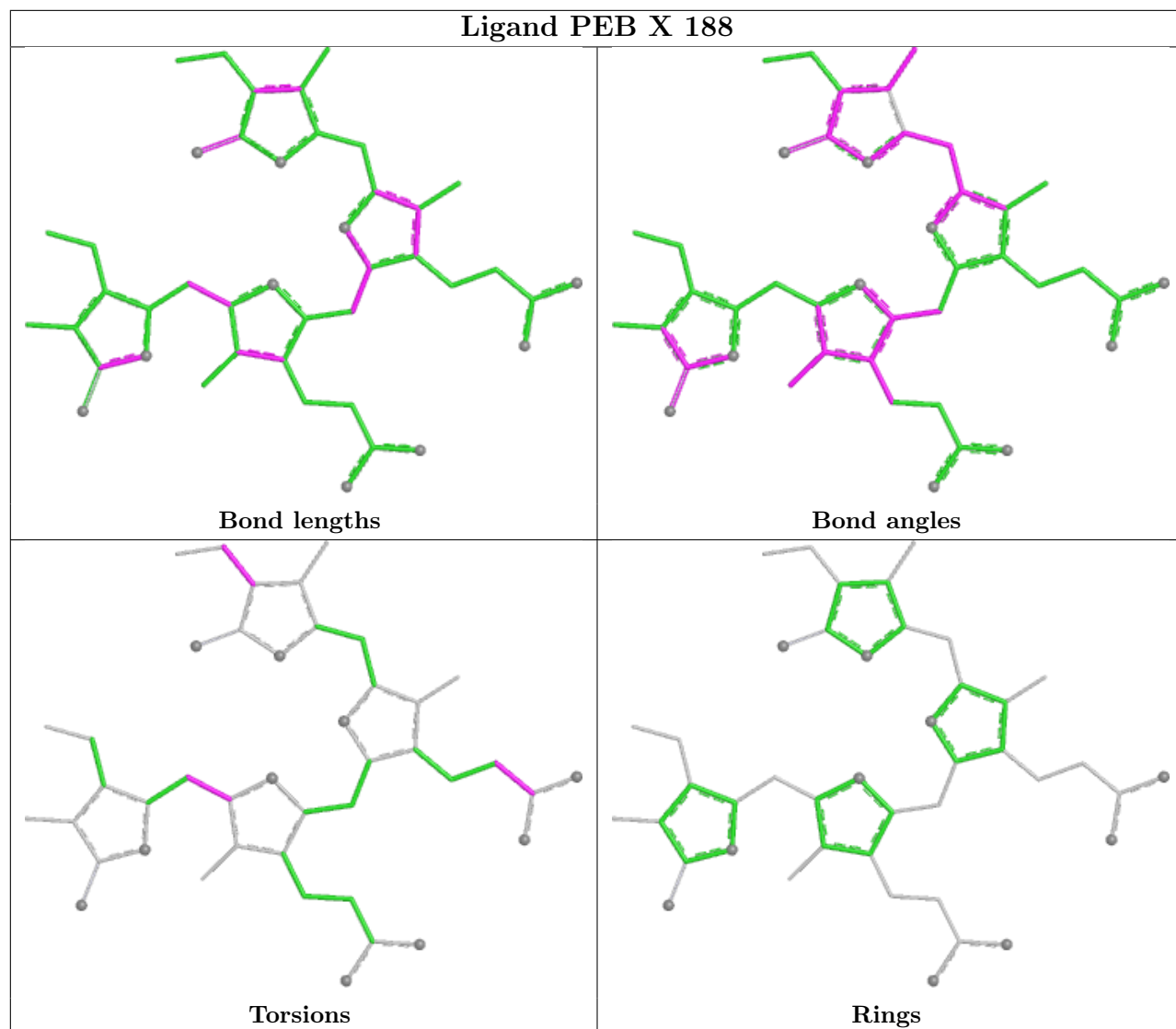
Bond angles



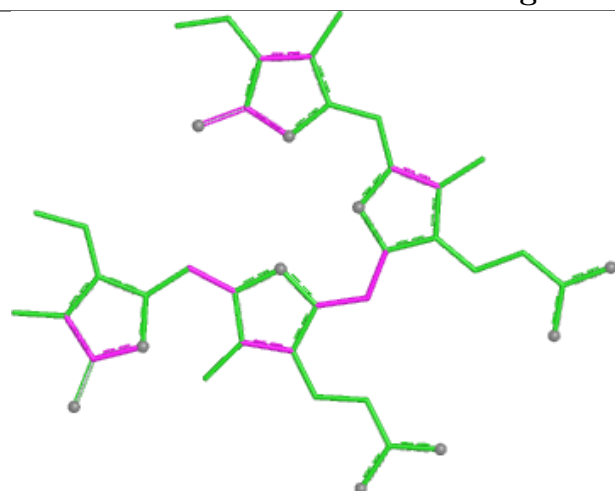
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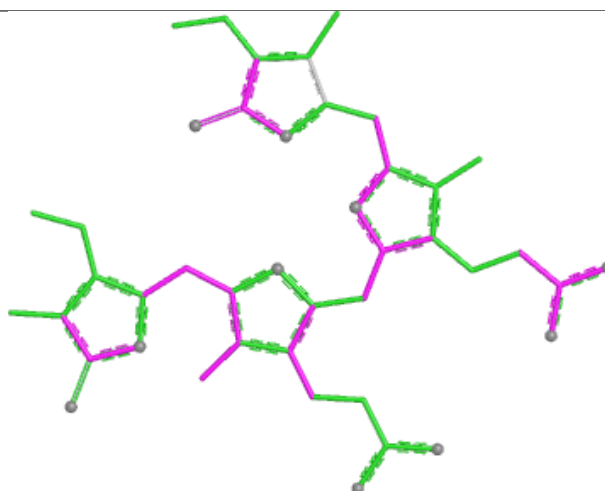
Rings



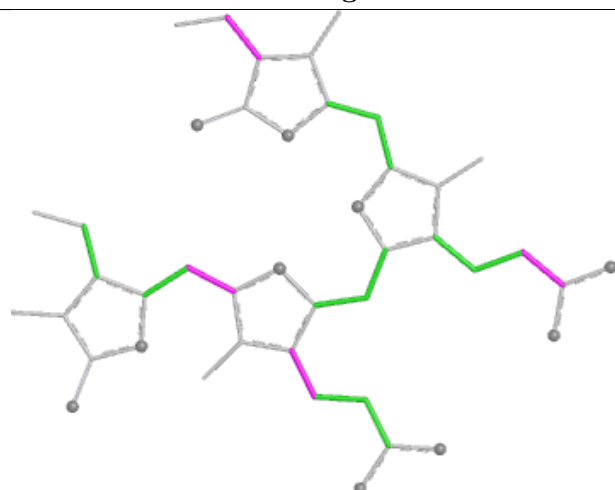
Ligand PEB S 188



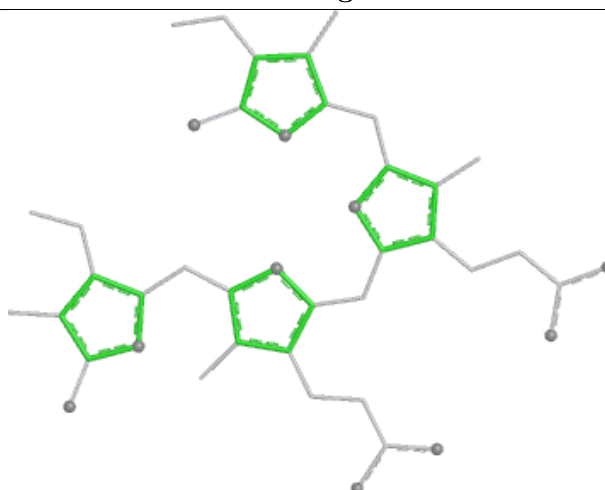
Bond lengths



Bond angles

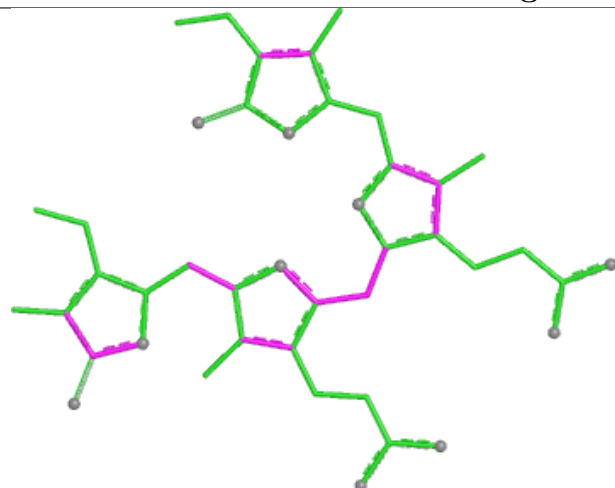


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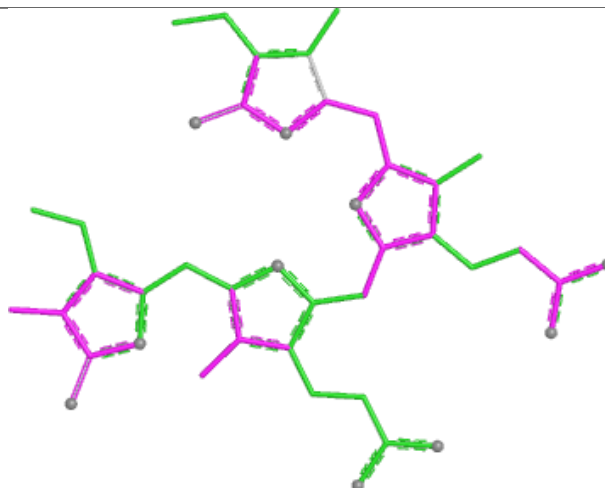


Rings

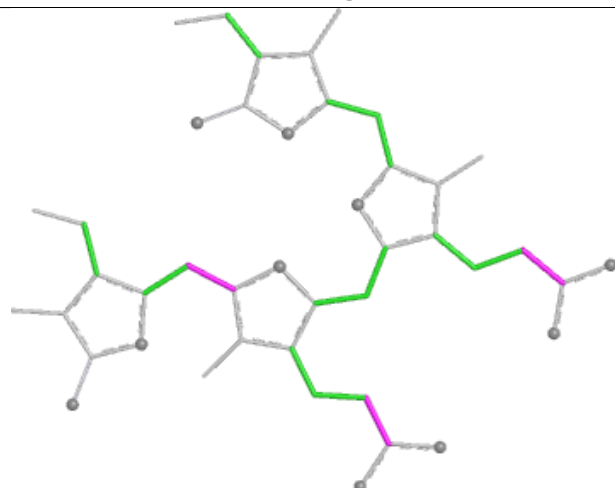
Ligand PEB J 167



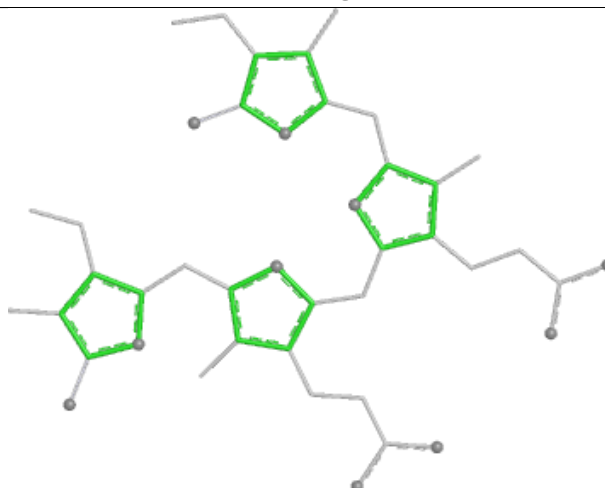
Bond lengths



Bond angles

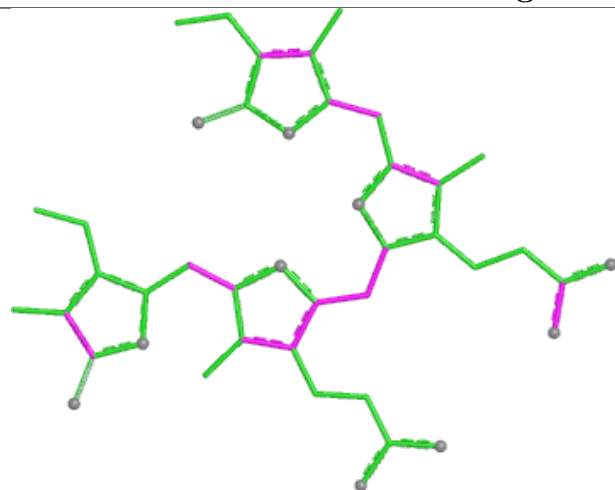


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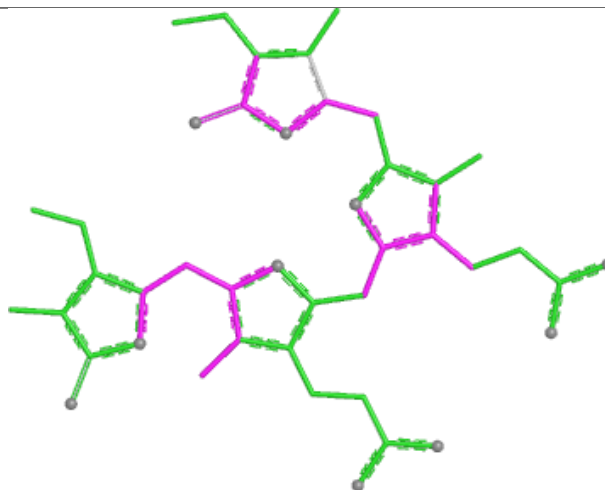


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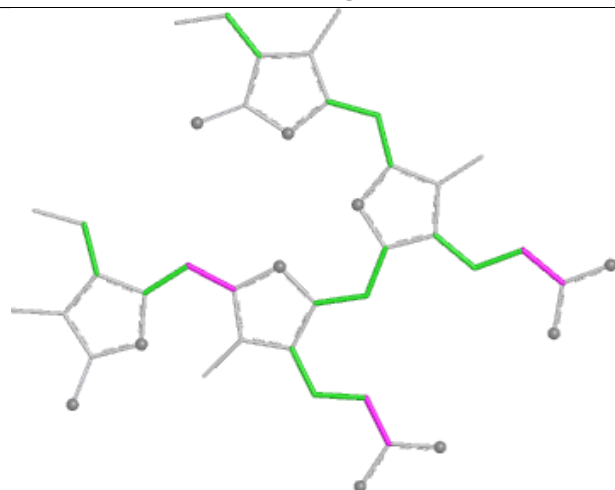
Ligand PEB O 186



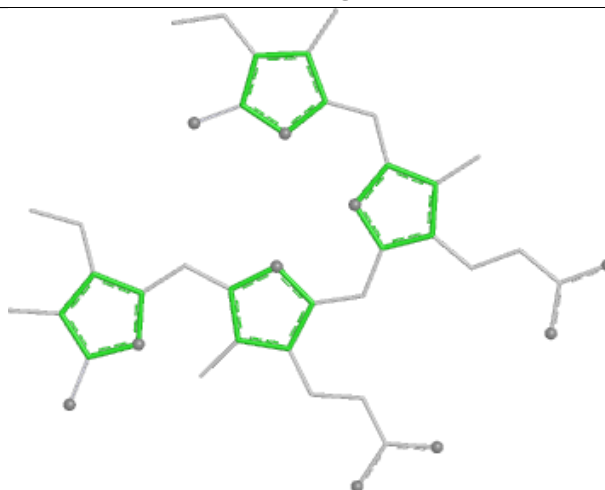
Bond lengths



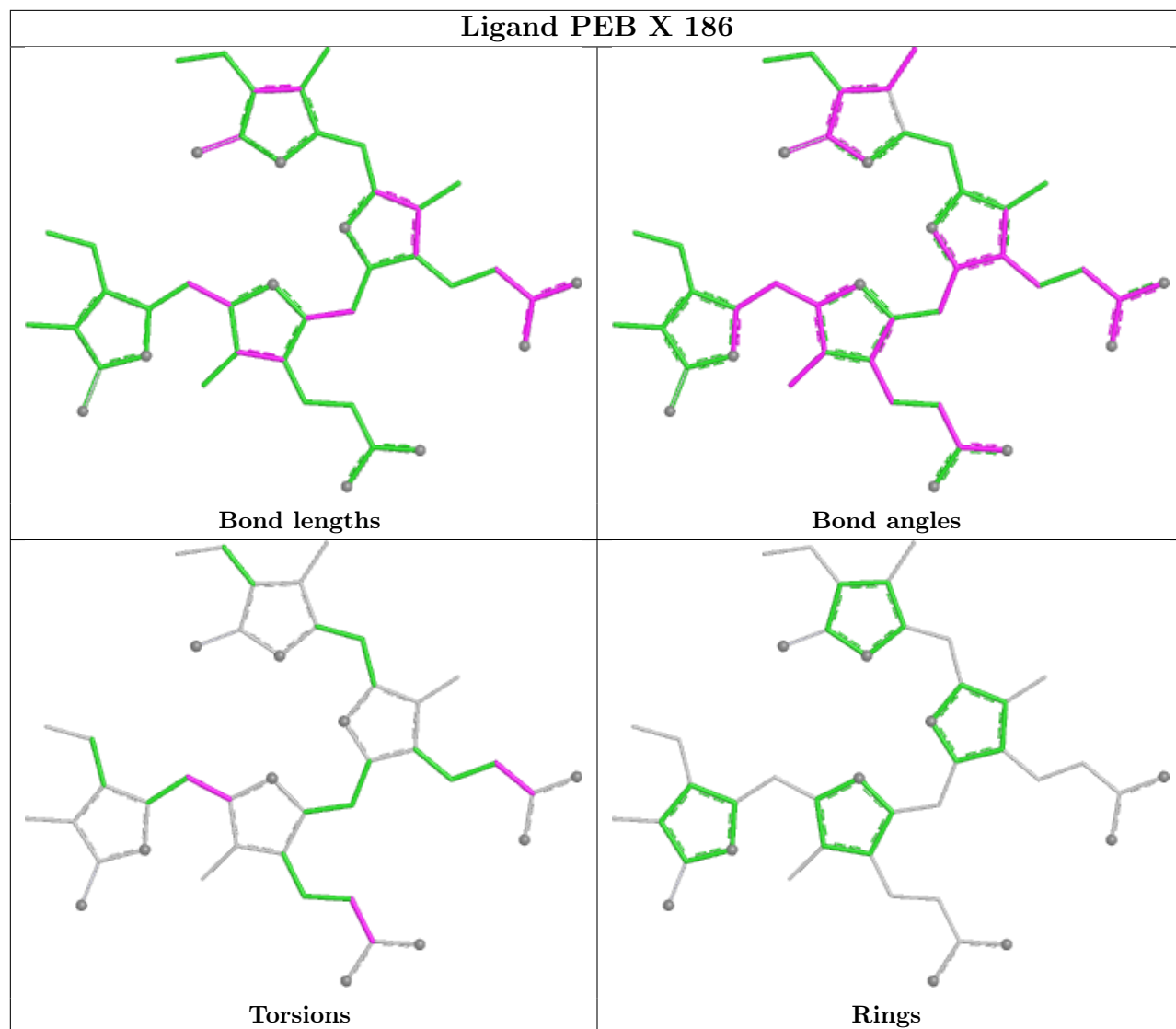
Bond angles



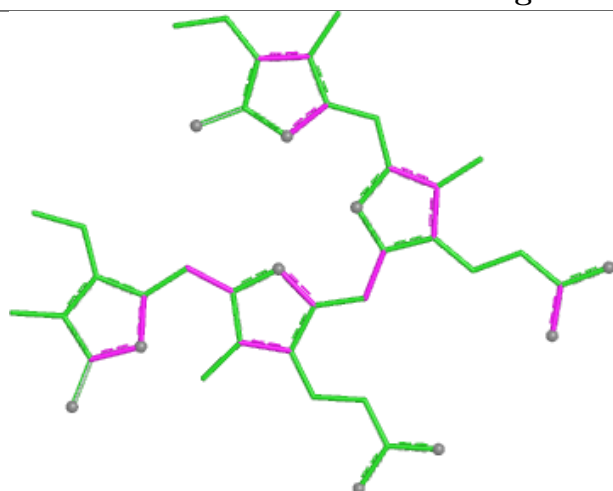
Torsions



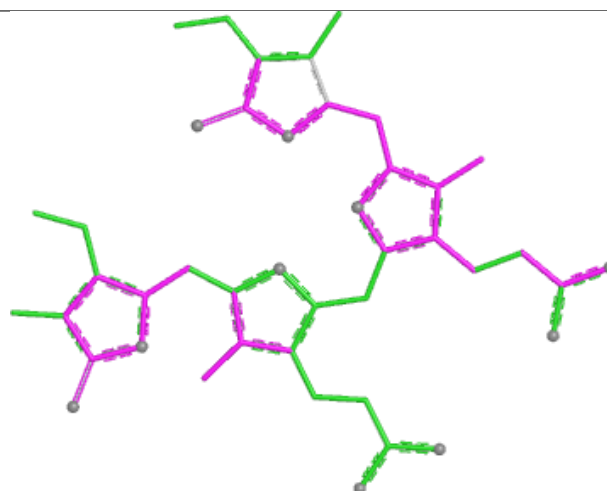
Rings



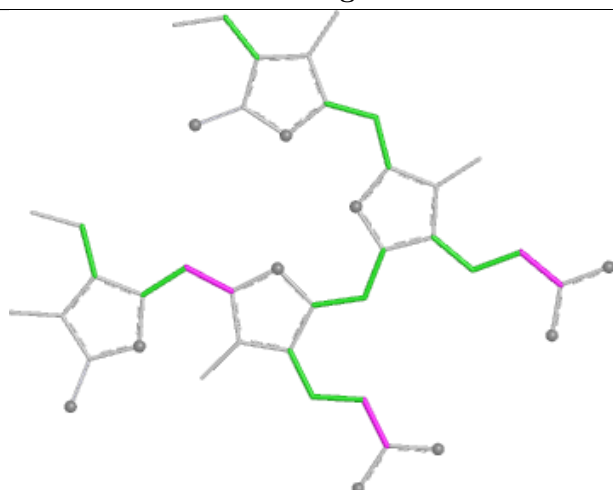
Ligand PEB C 167



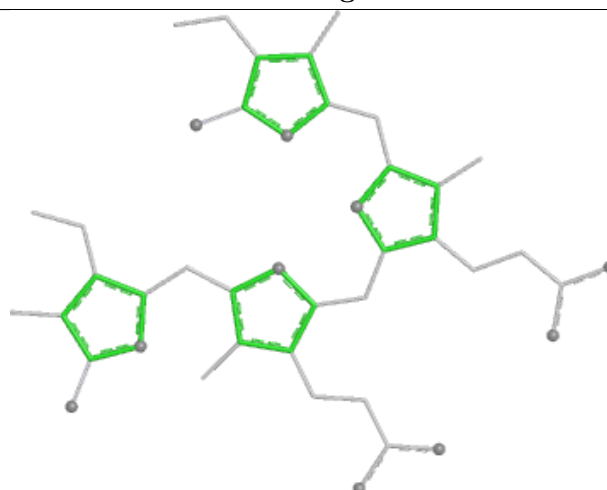
Bond lengths



Bond angles

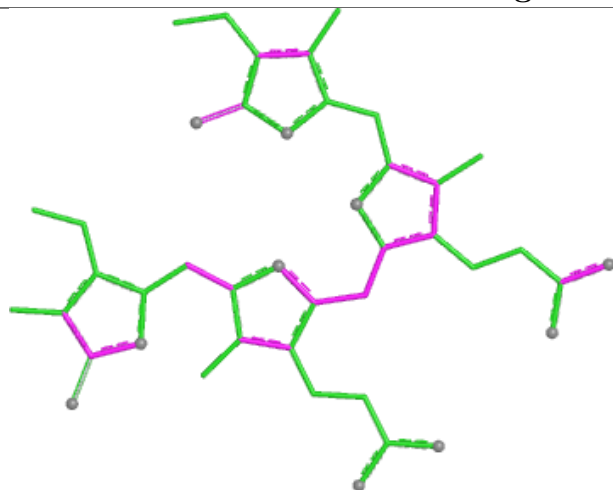


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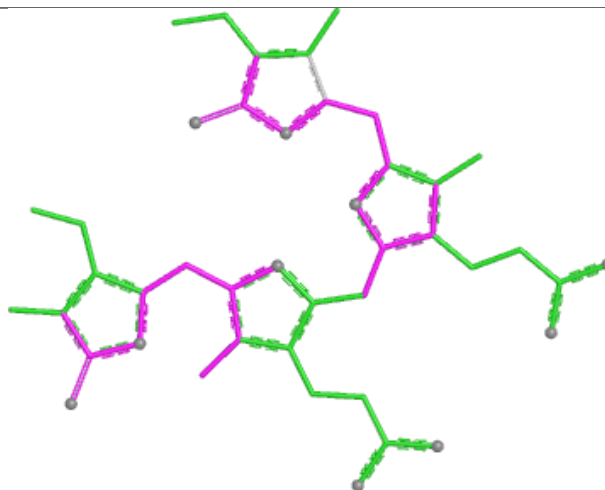


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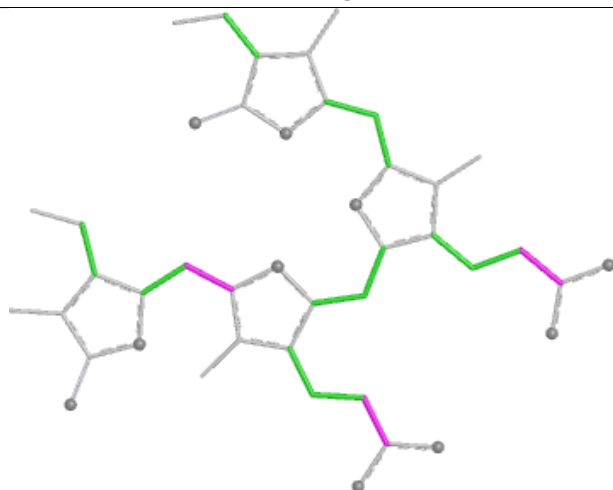
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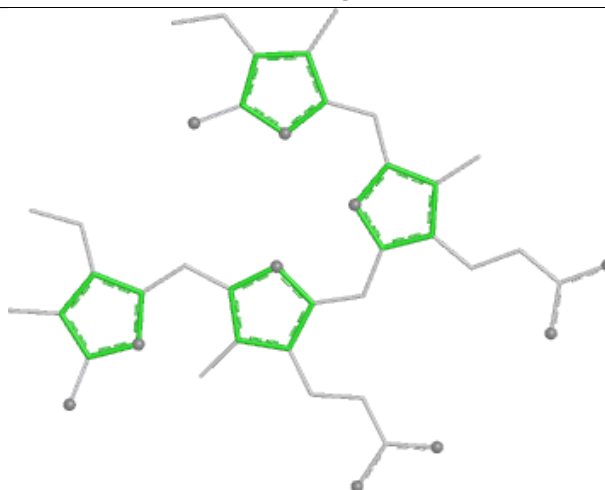
Bond lengths



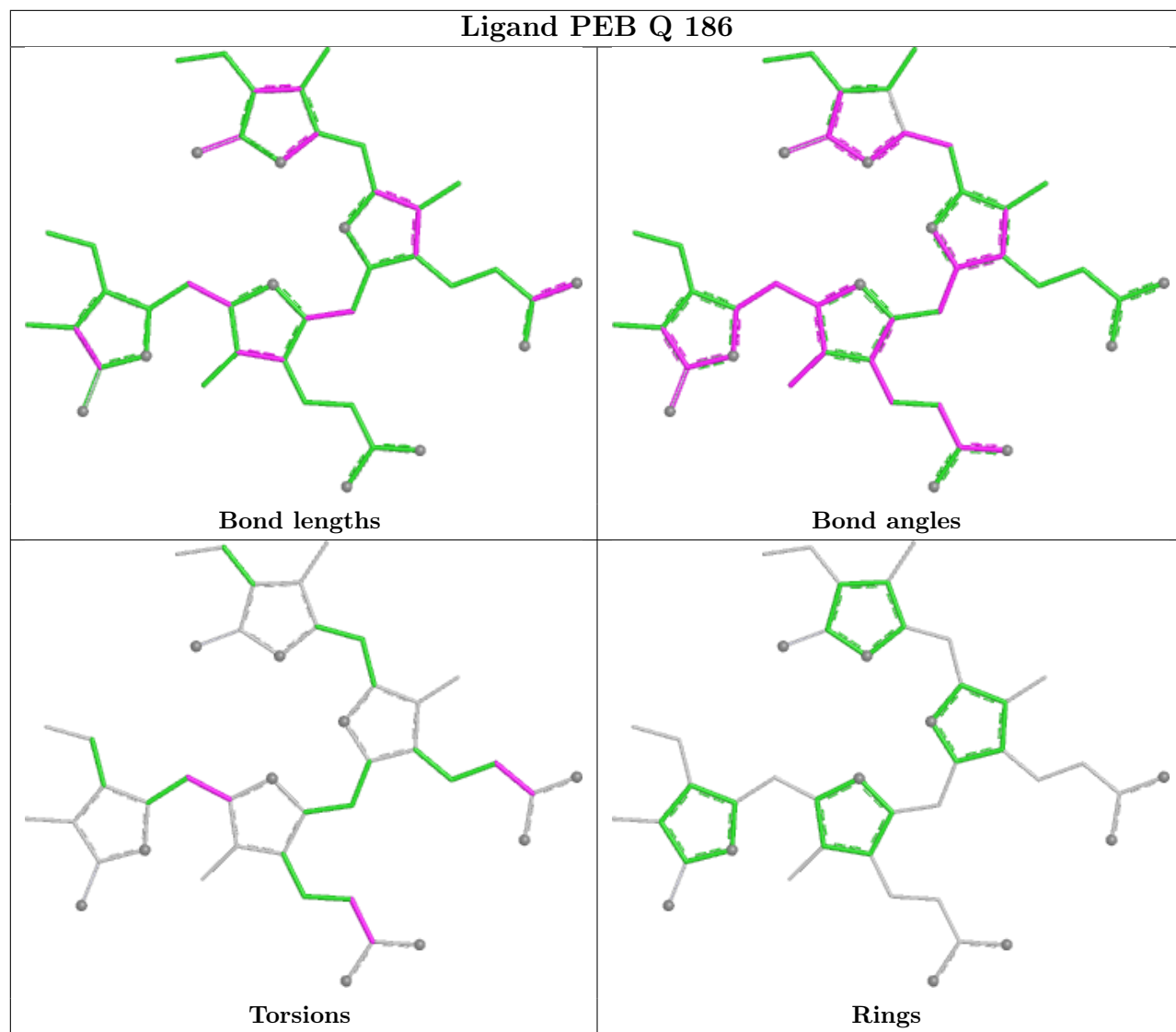
Bond angles



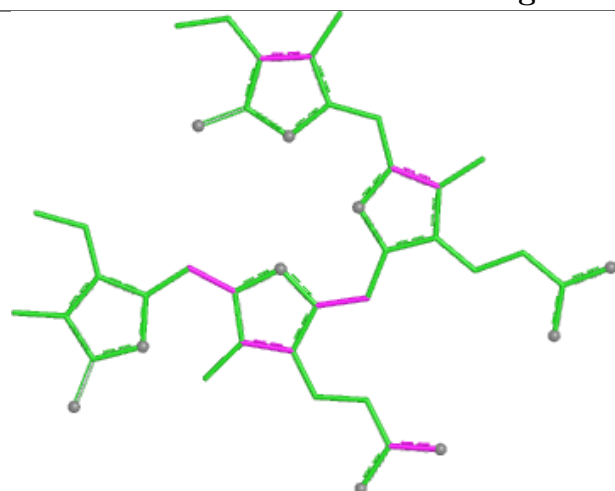
Torsions



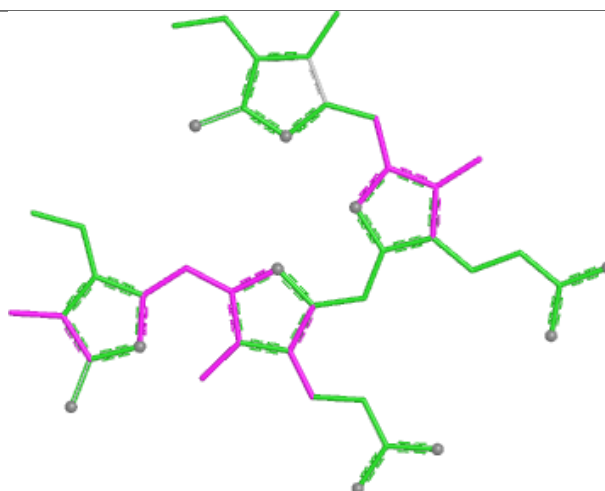
Rings



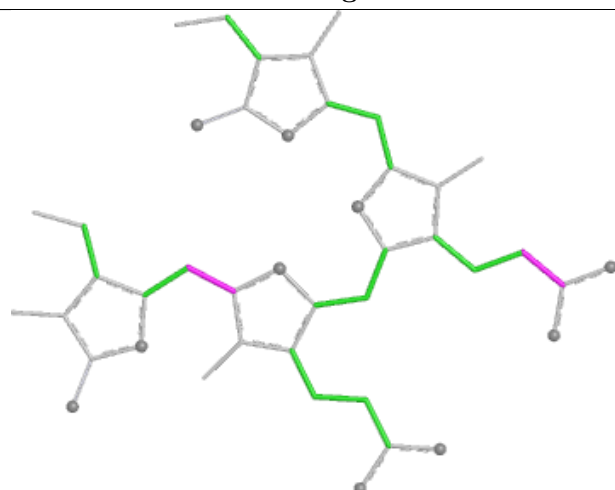
Ligand PEB F 166



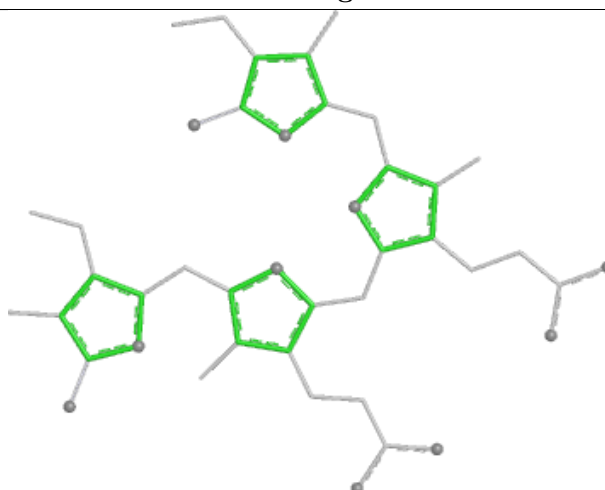
Bond lengths



Bond angles

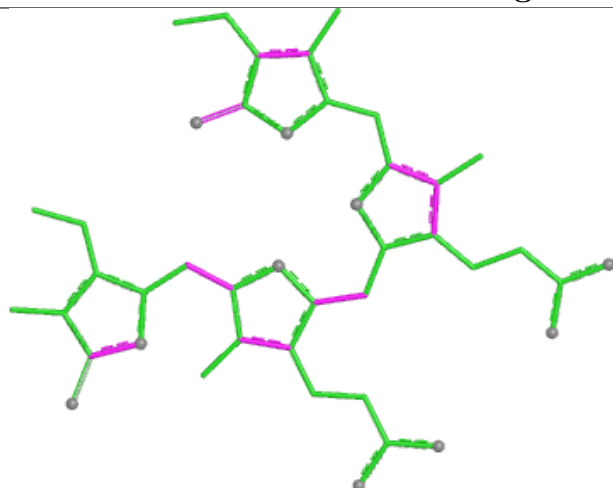


Torsions

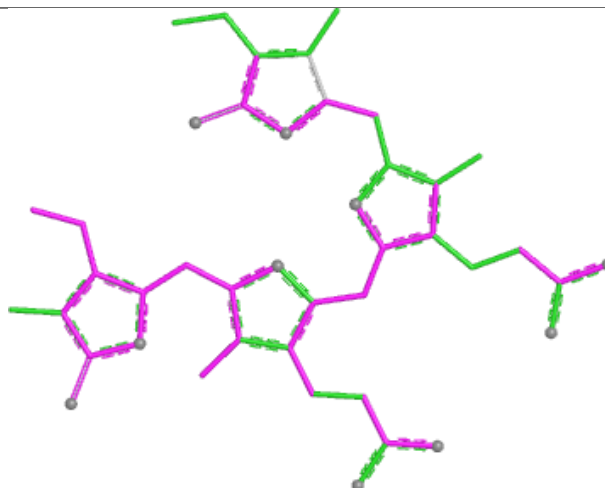


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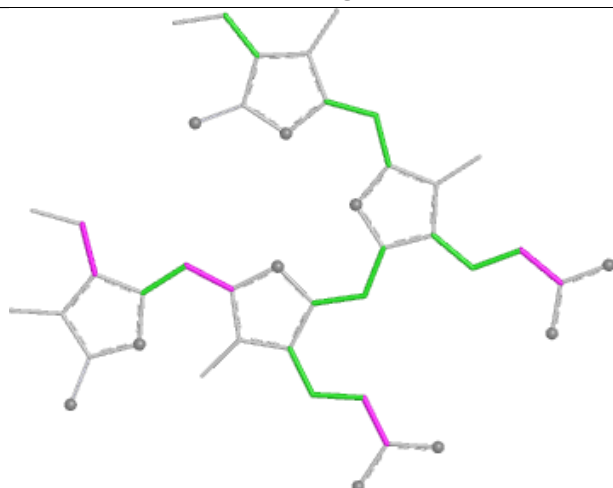
Ligand PEB R 187



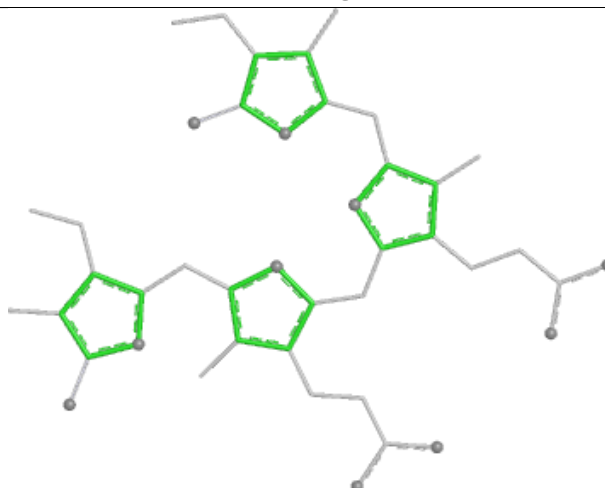
Bond lengths



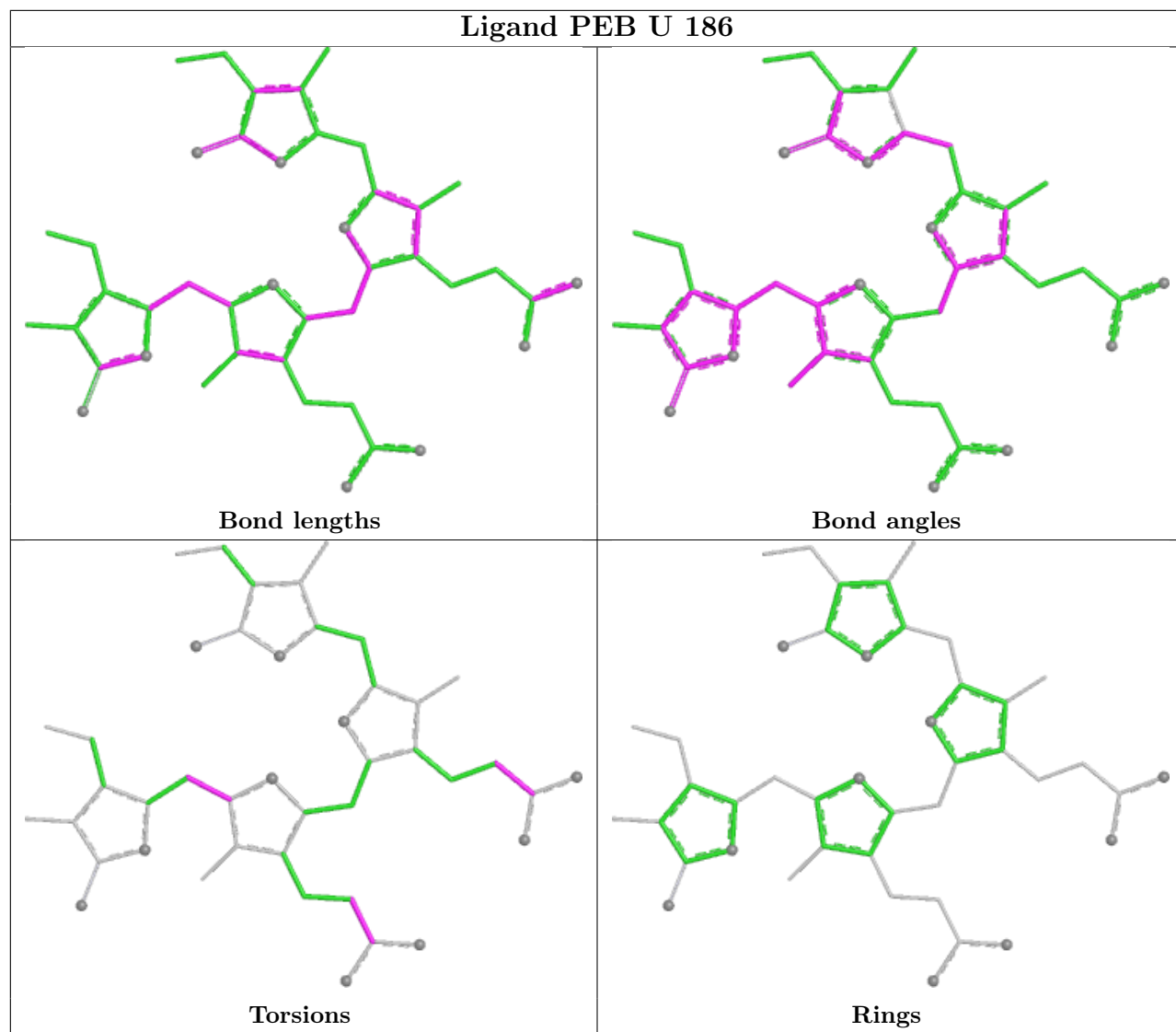
Bond angles



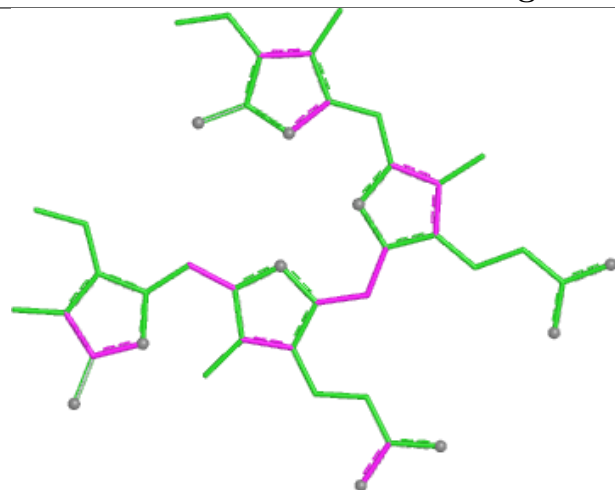
Torsions



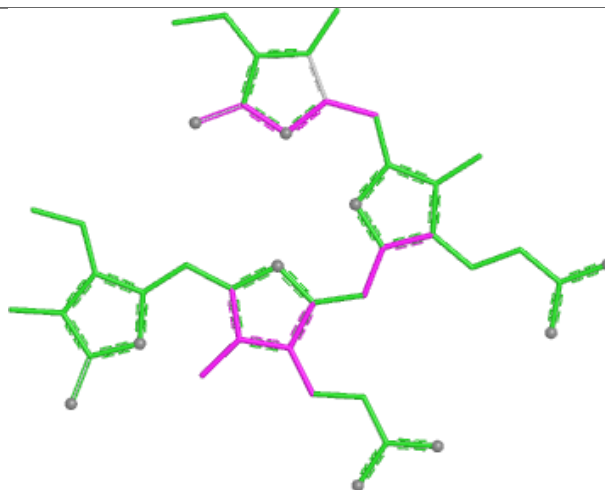
Rings



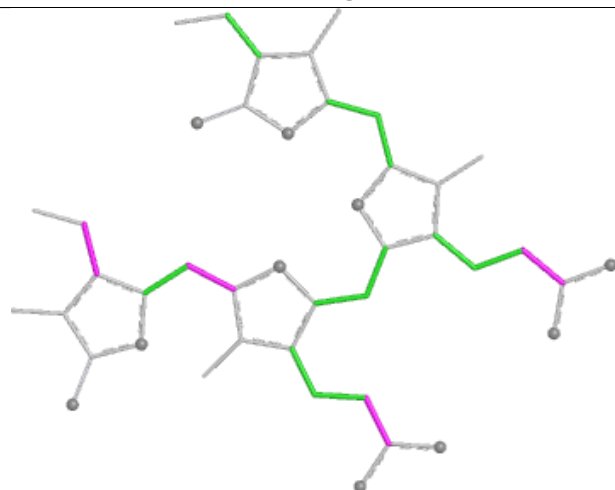
Ligand PEB E 167



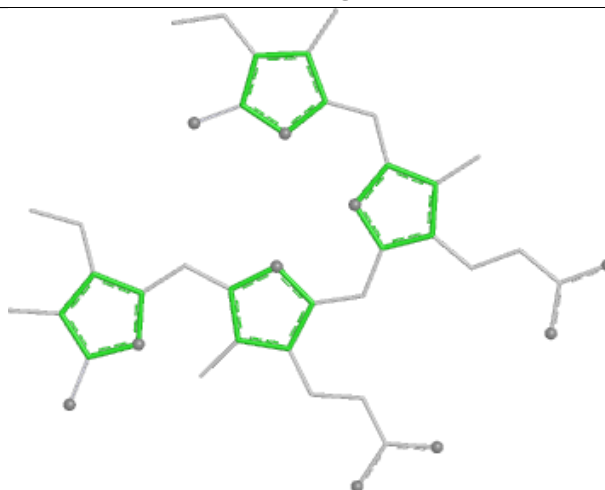
Bond lengths



Bond angles

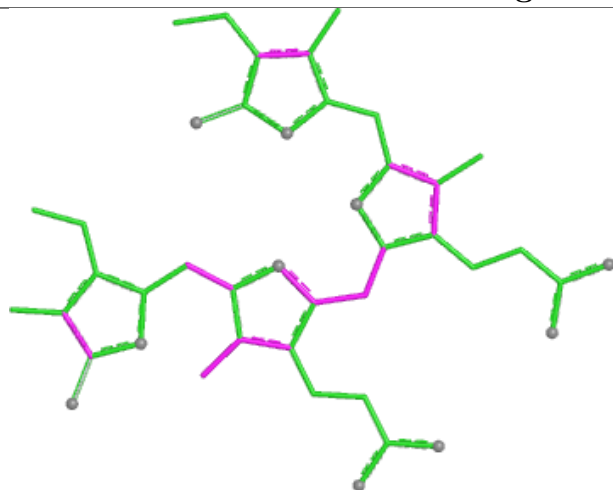


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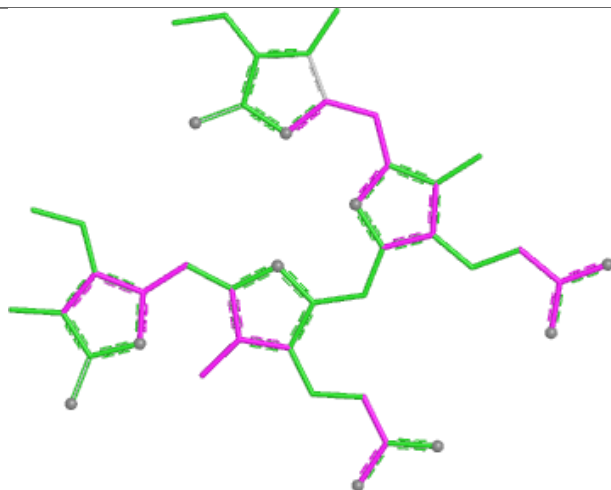


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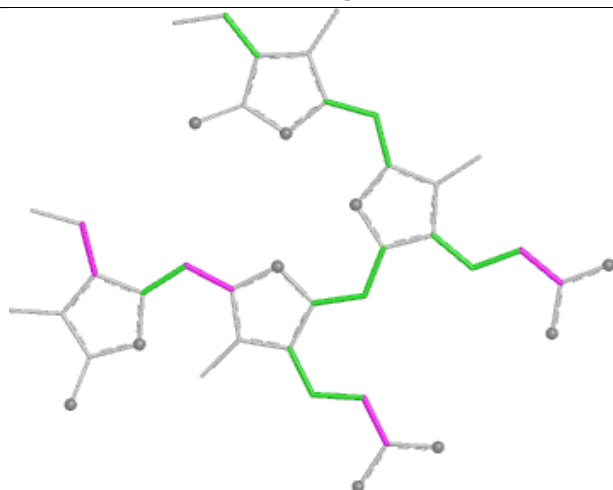
Ligand PEB T 187



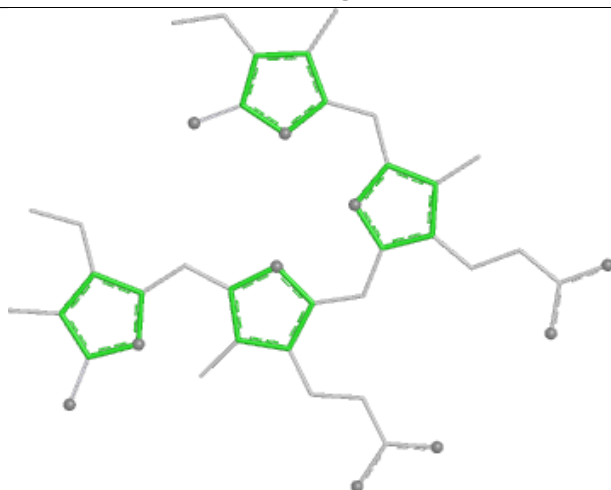
Bond lengths



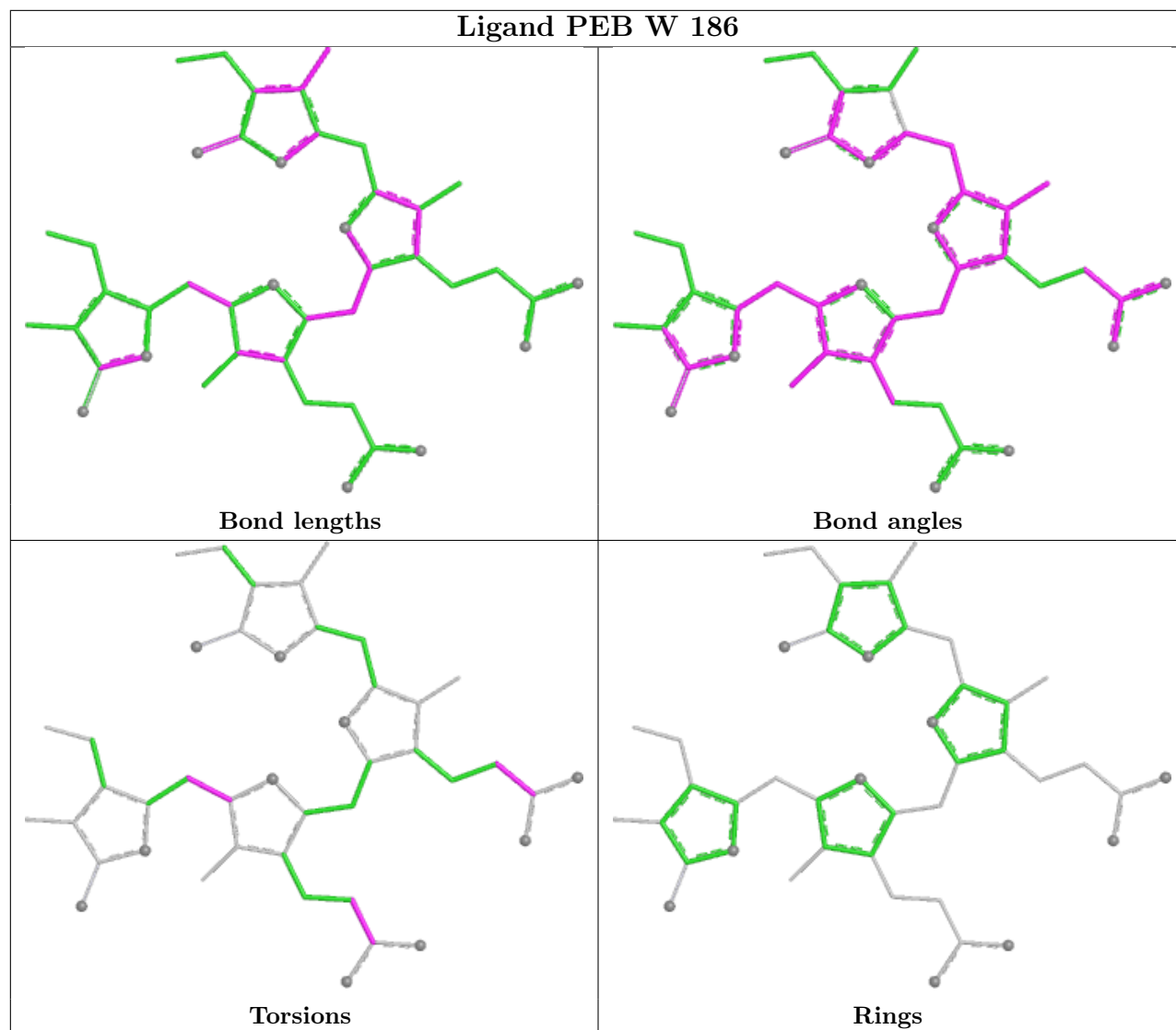
Bond angles



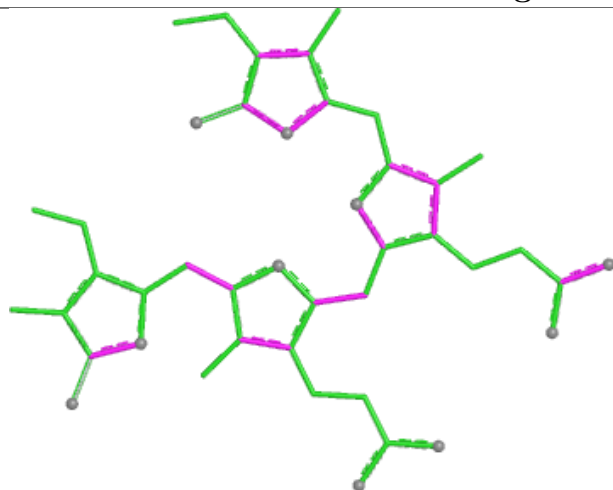
Torsions



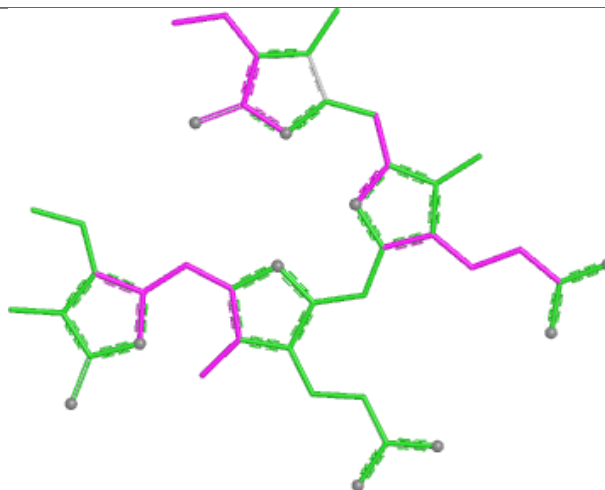
Rings



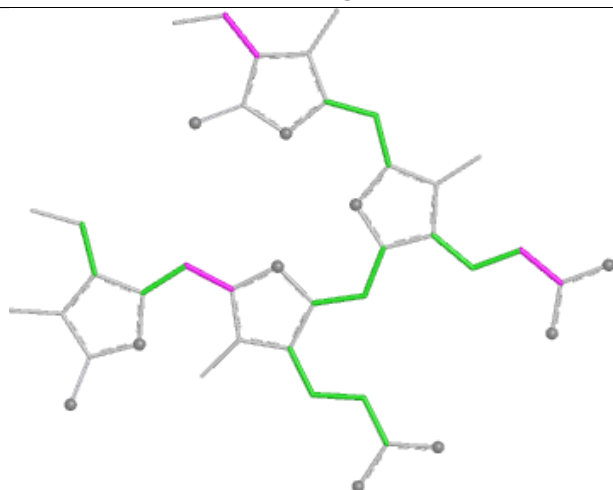
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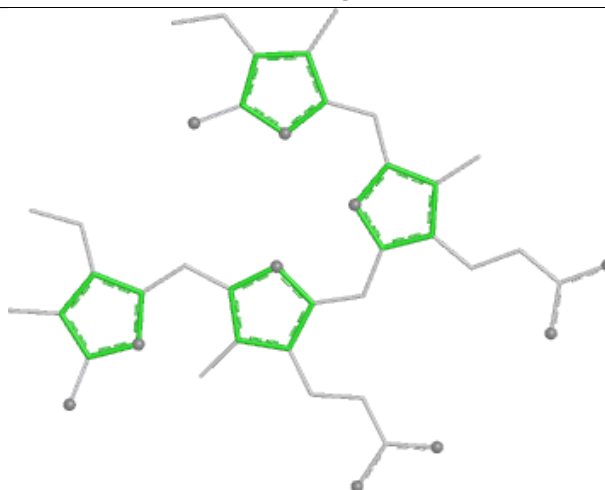
Bond lengths



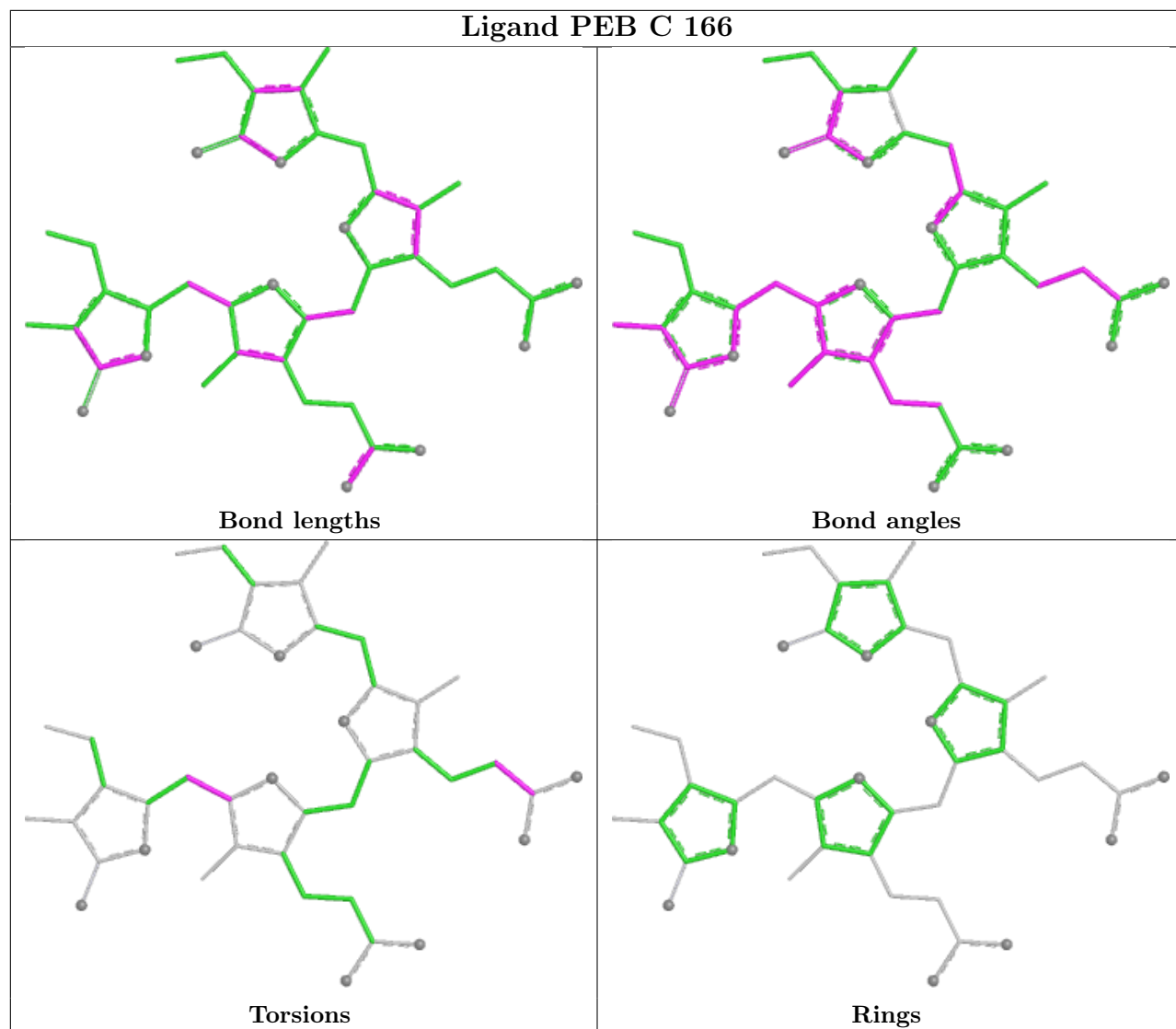
Bond angles



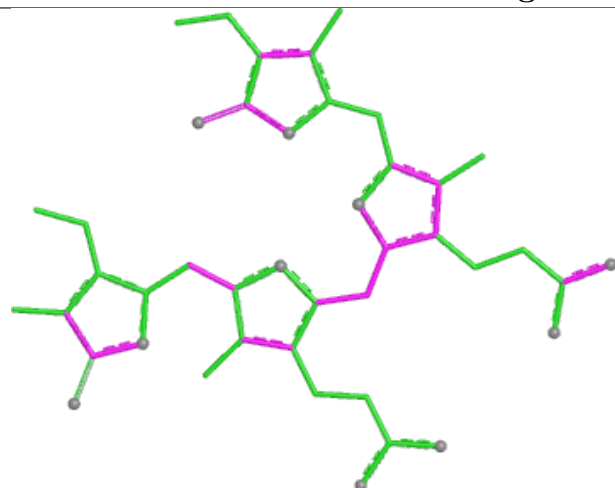
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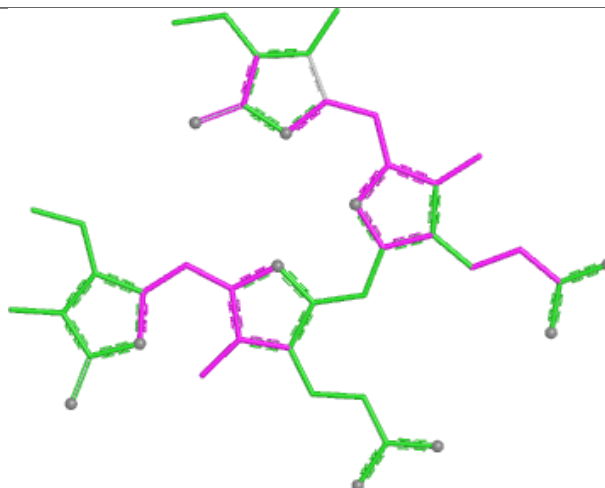
Rings



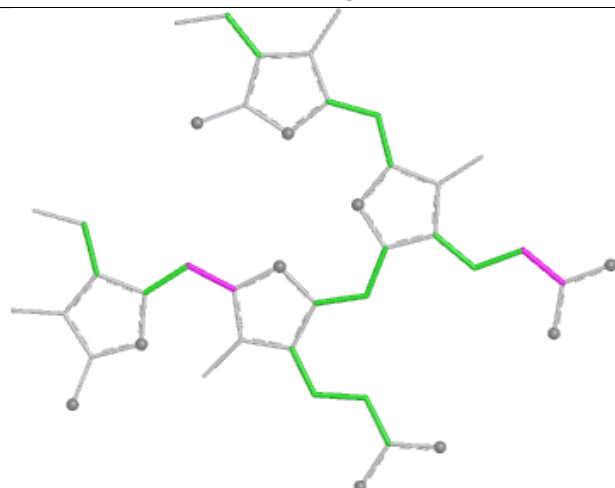
Ligand PEB E 166



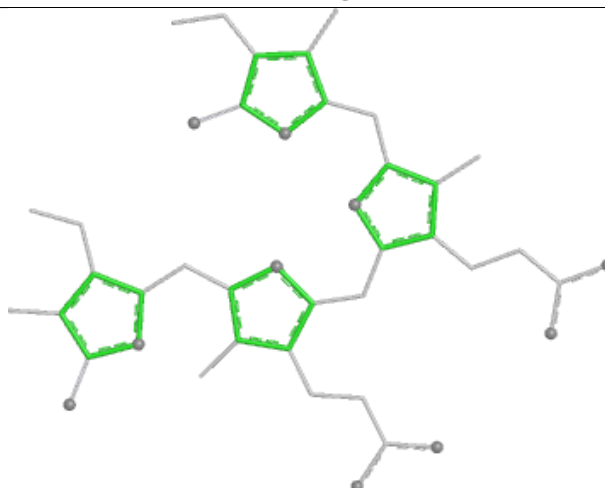
Bond lengths



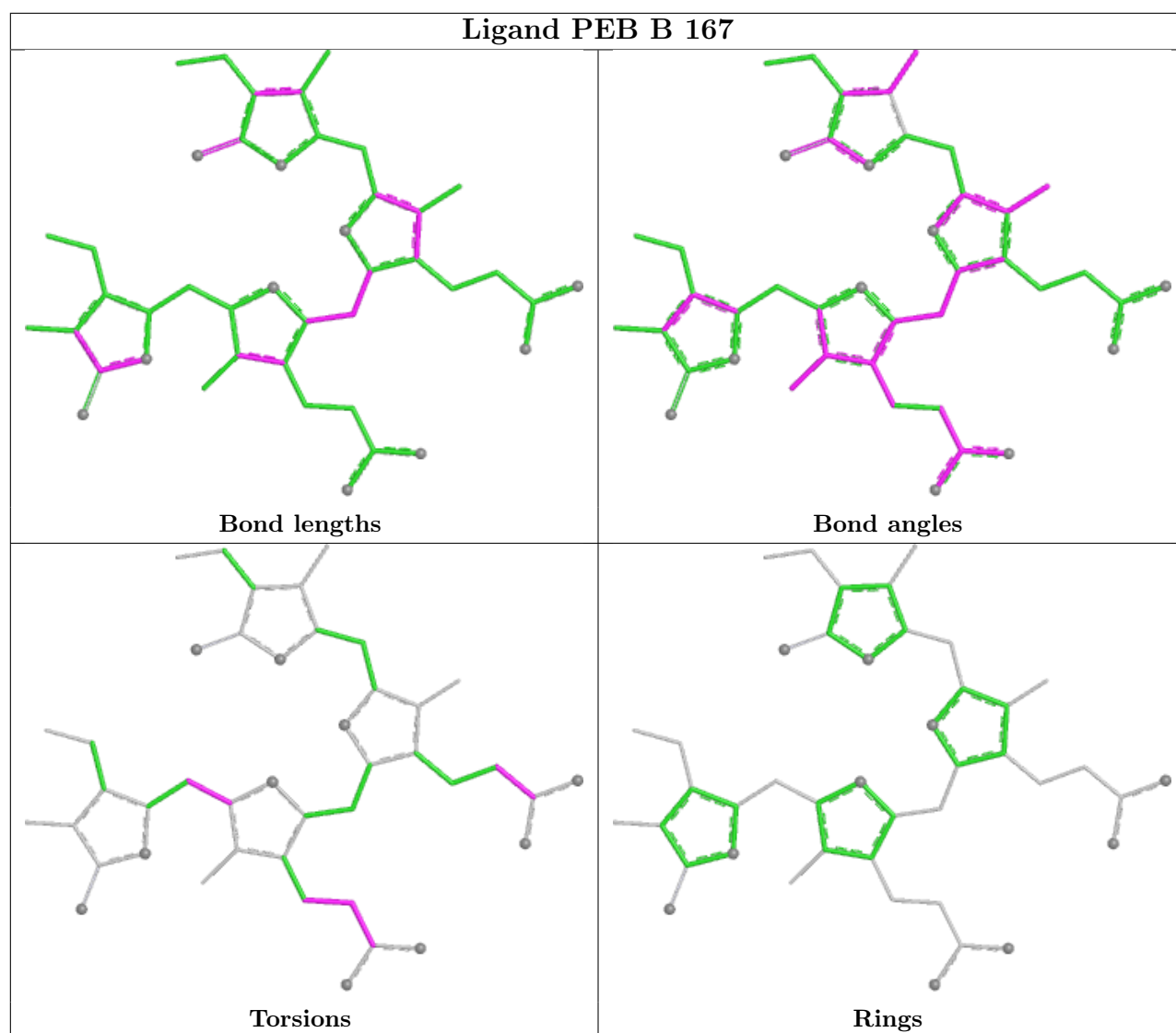
Bond angles



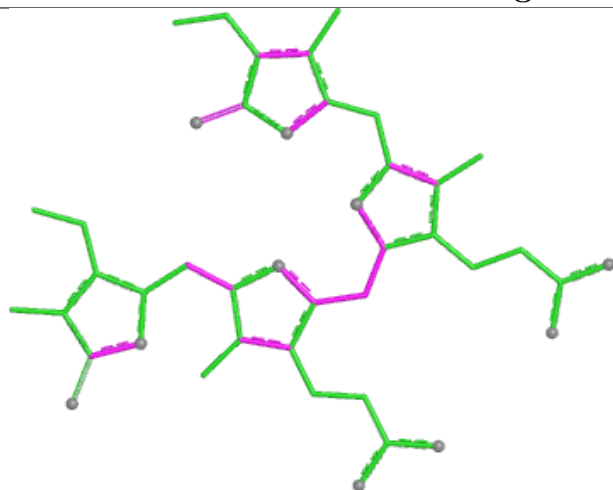
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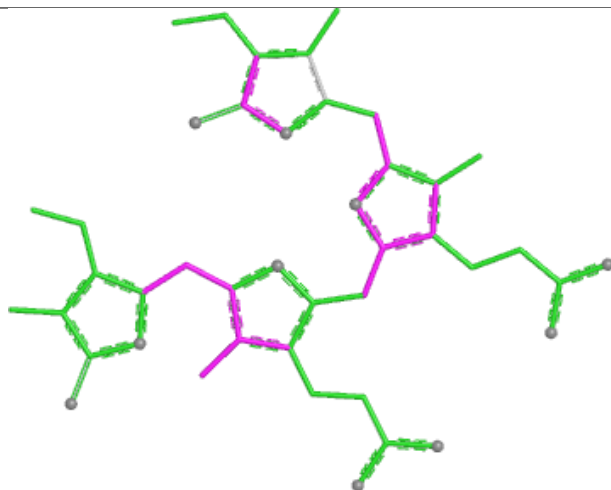
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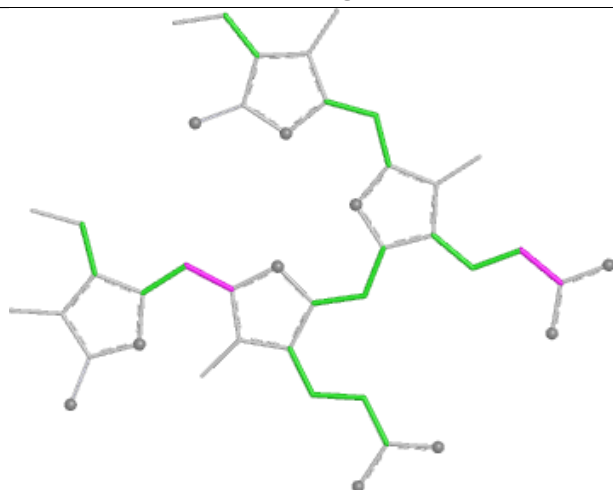
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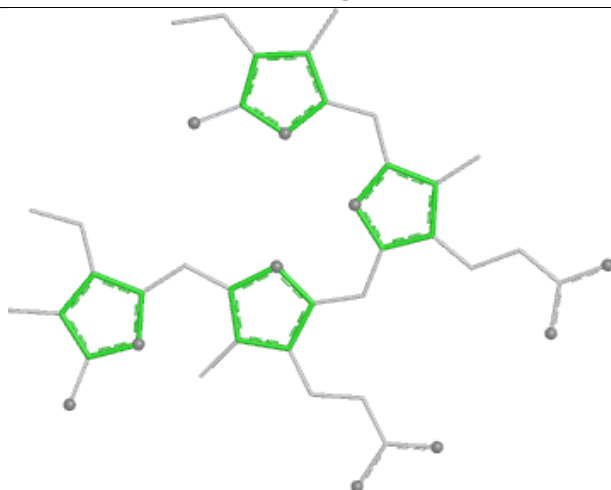
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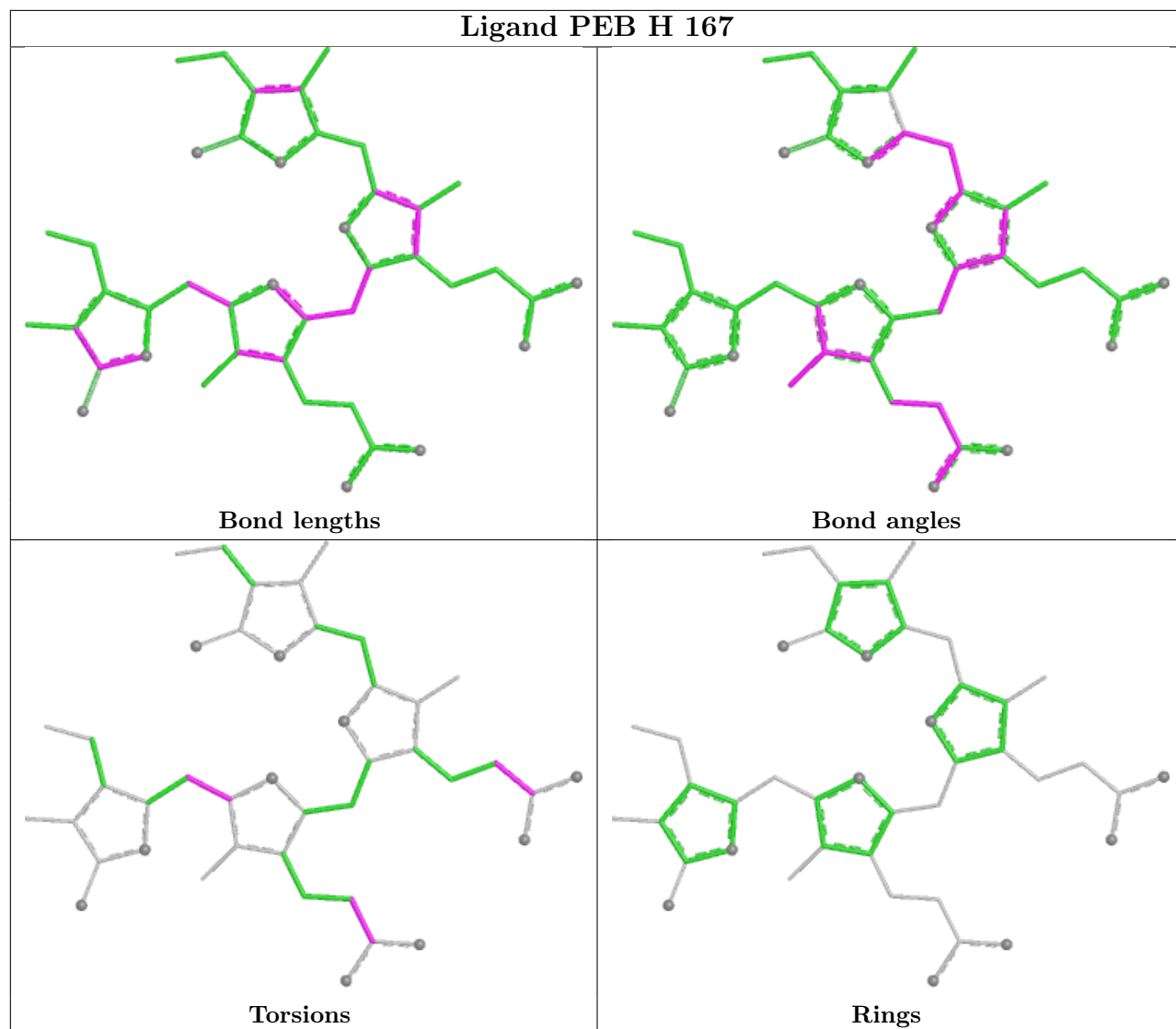
Bond angles



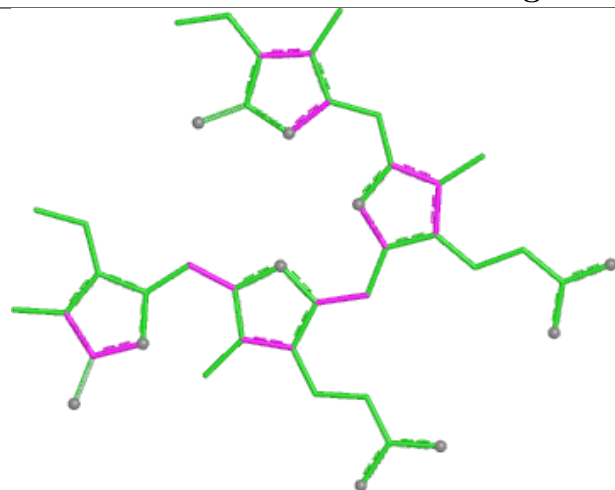
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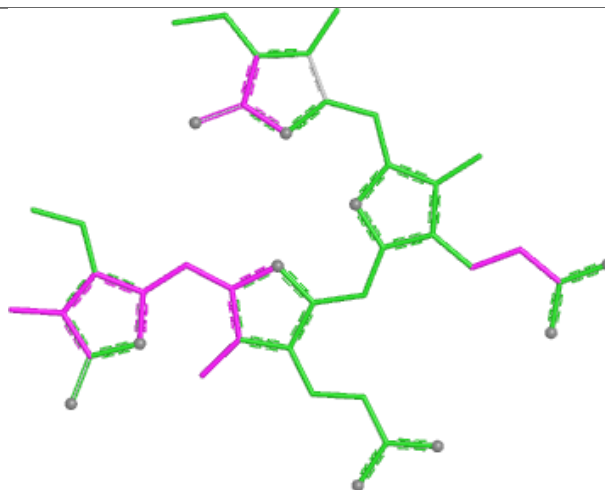
Rings



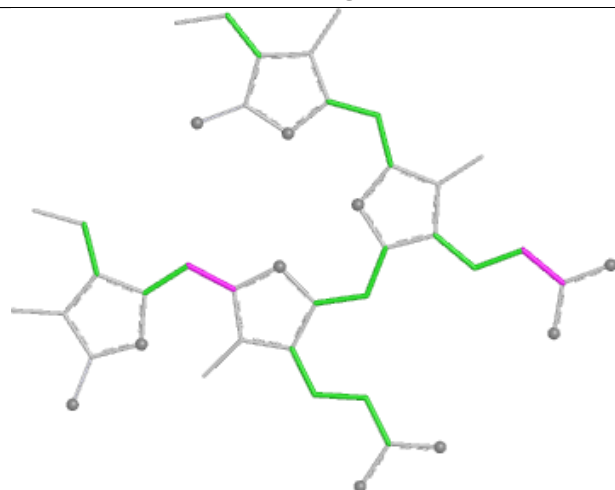
Ligand PEB I 166



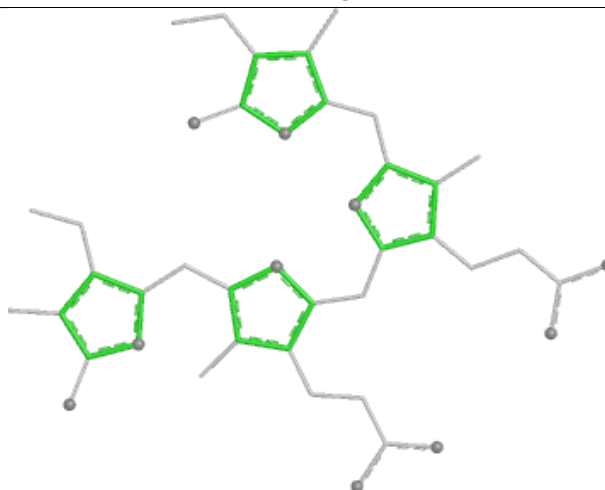
Bond lengths



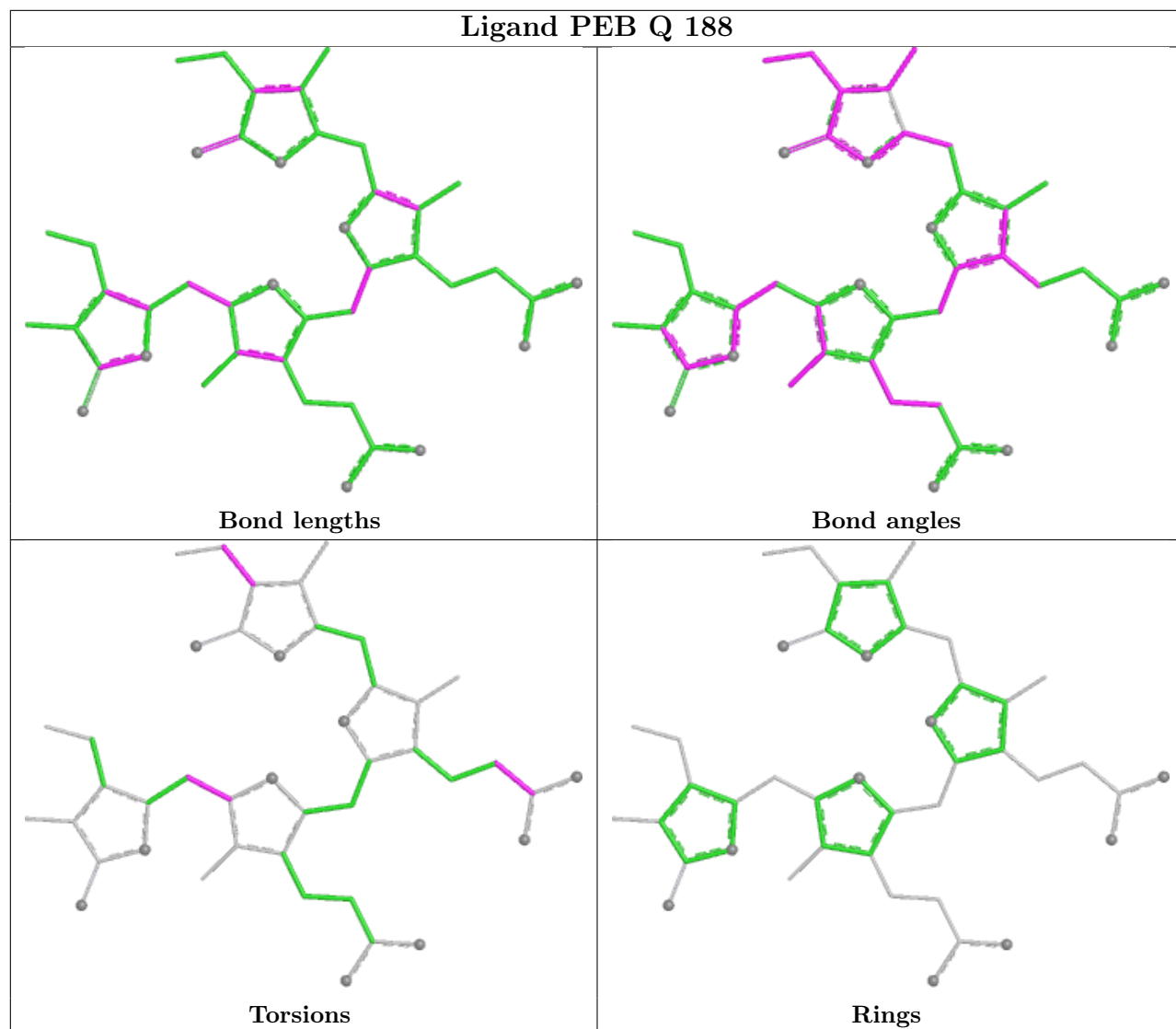
Bond angles



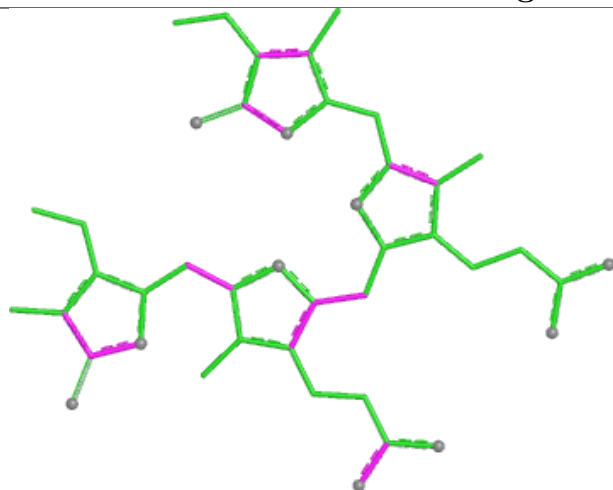
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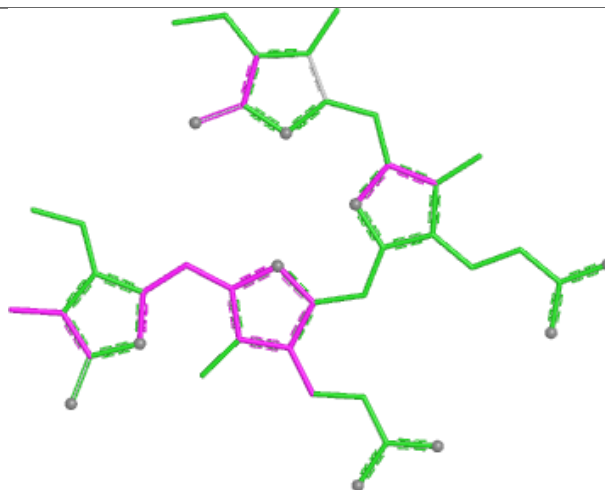
Rings



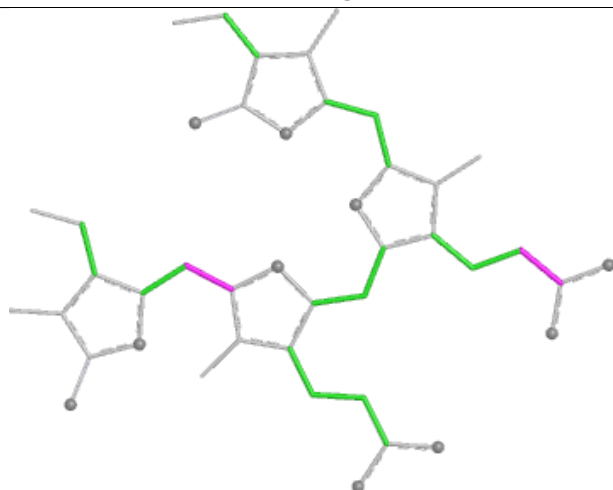
Ligand PEB L 166



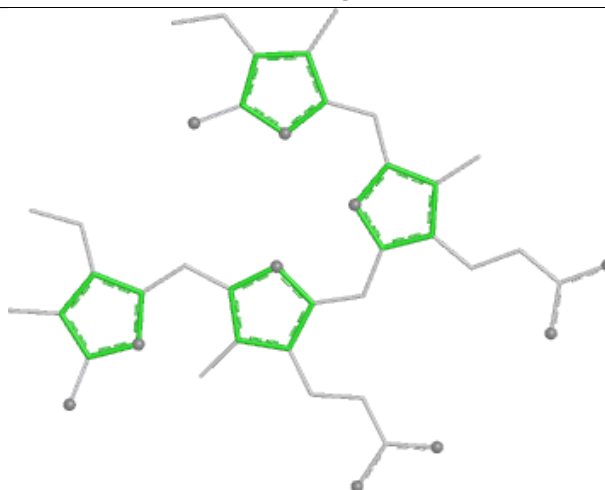
Bond lengths



Bond angles

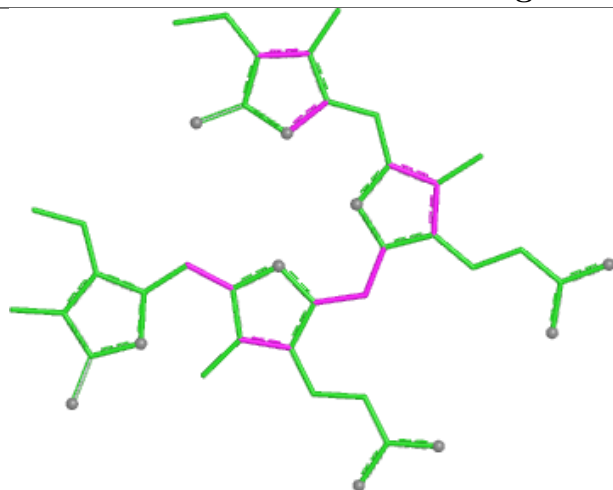


Torsions

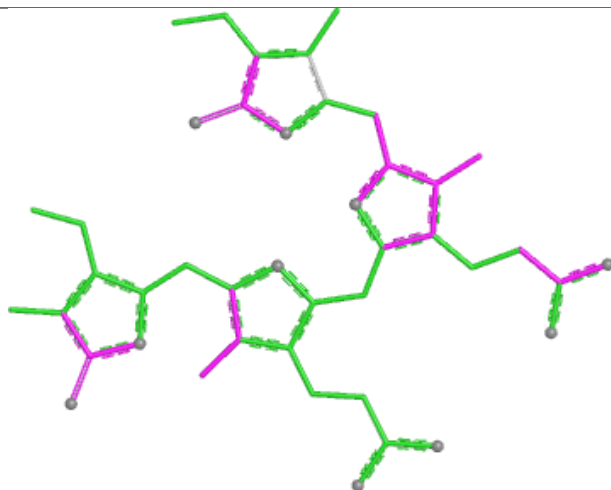


Rings

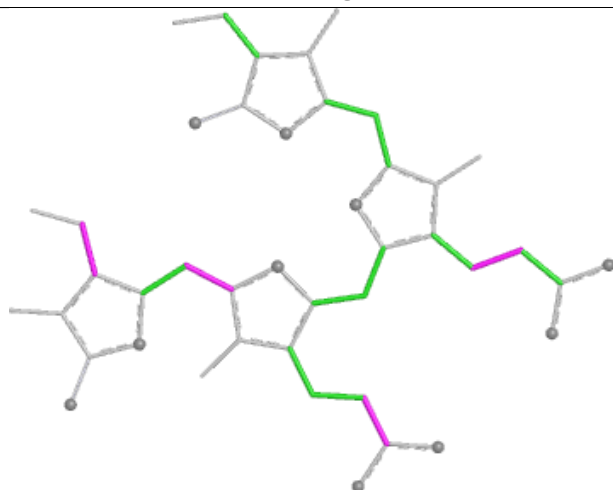
Ligand PEB P 187



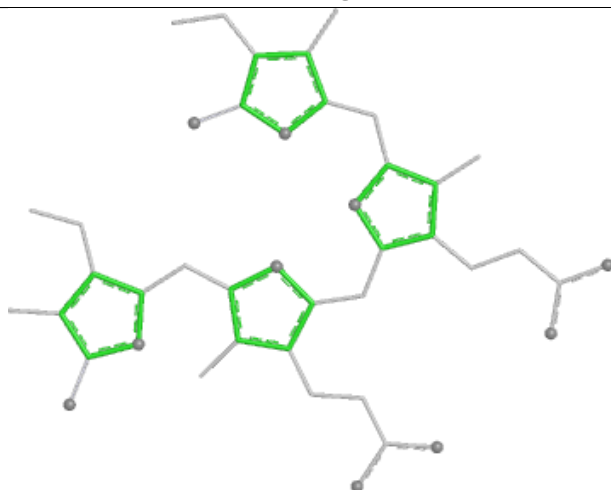
Bond lengths



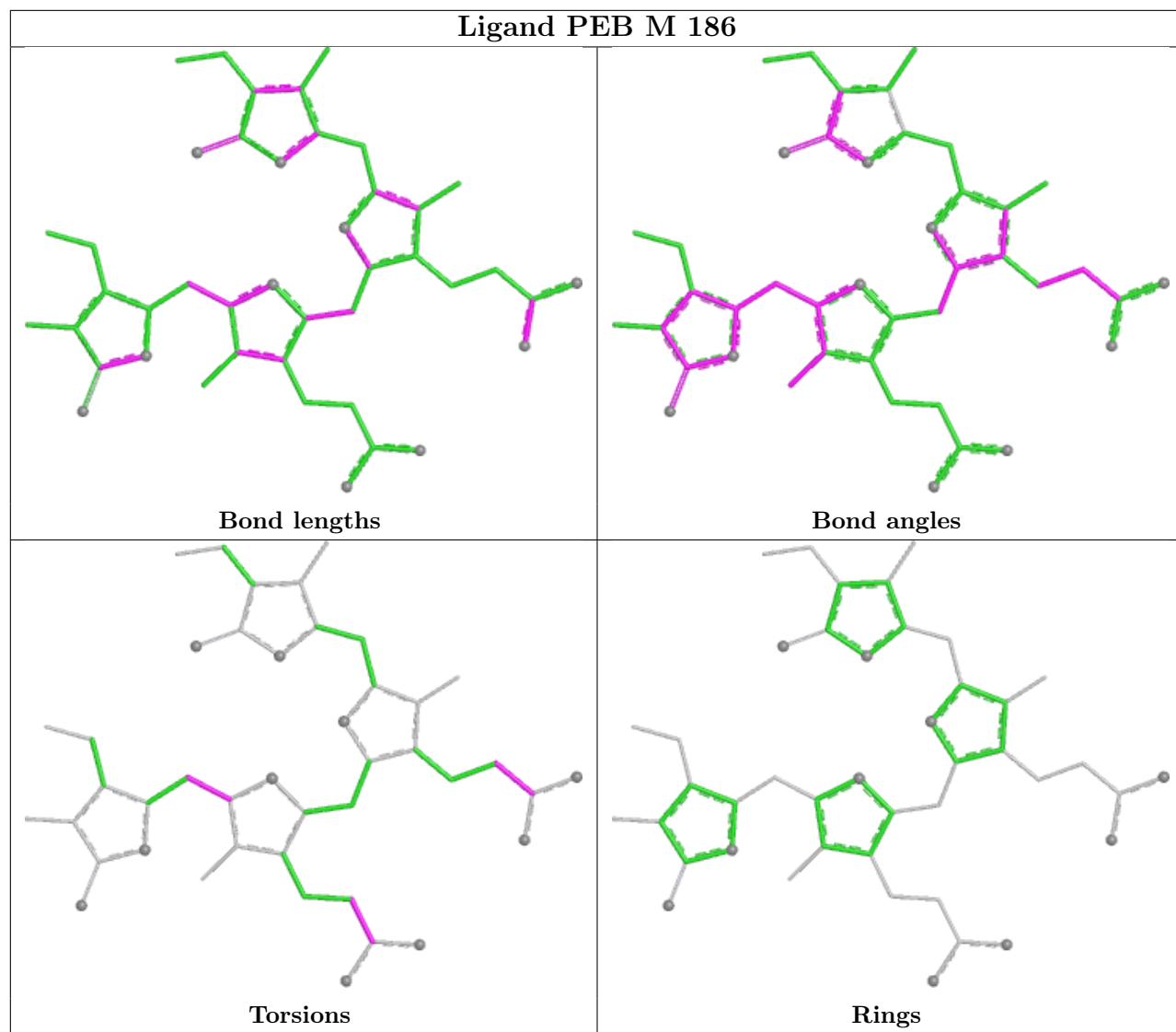
Bond angles

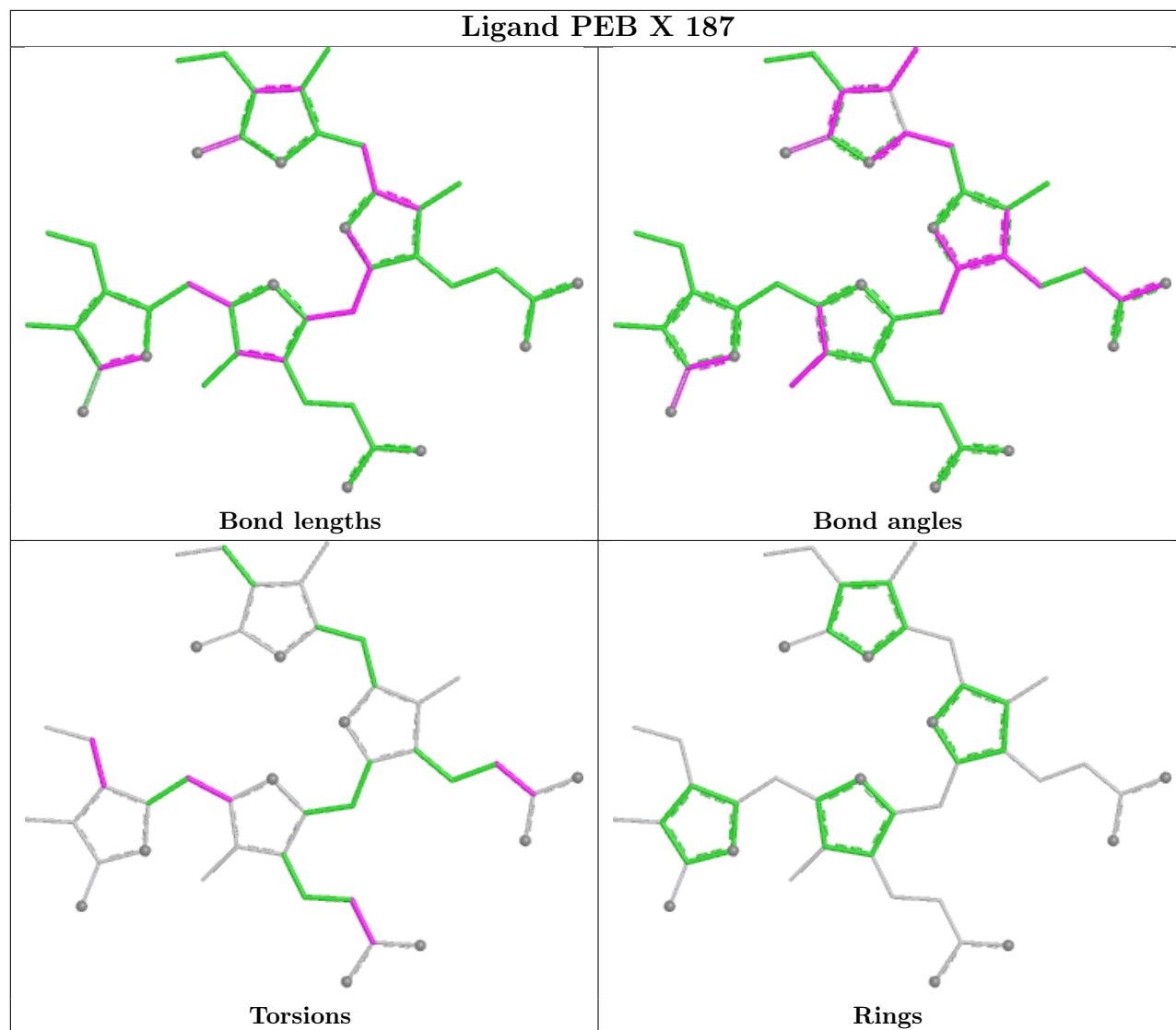


Torsions

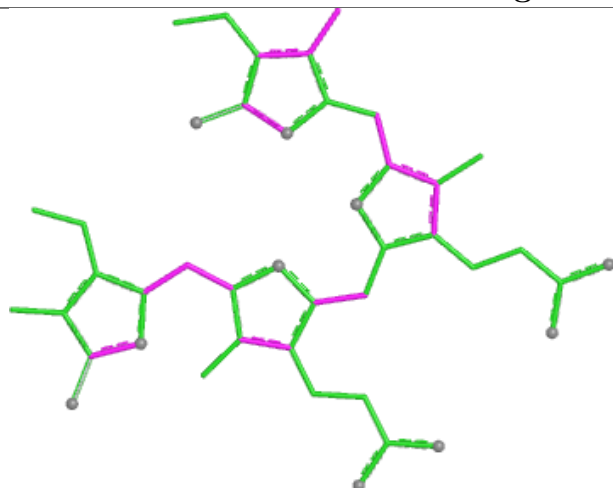


Rings

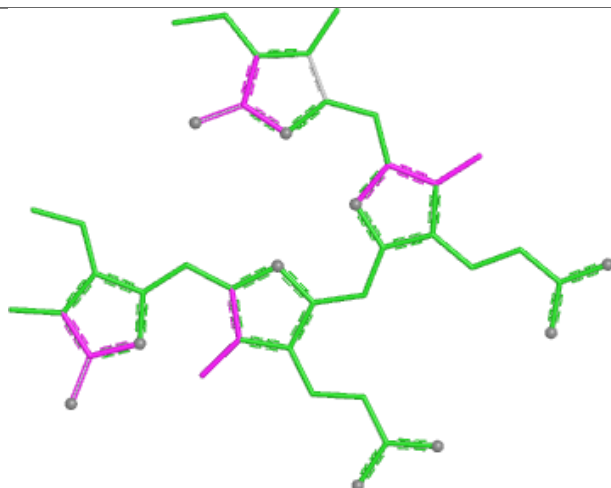




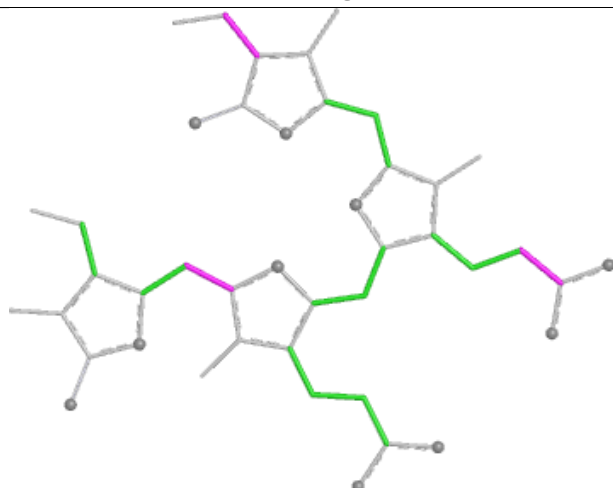
Ligand PEB V 188



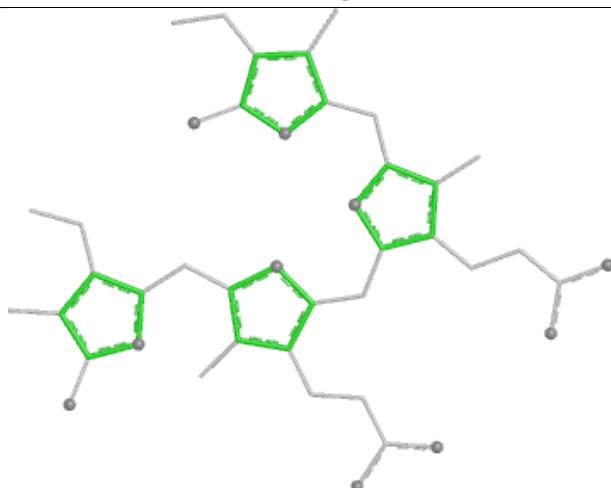
Bond lengths



Bond angles

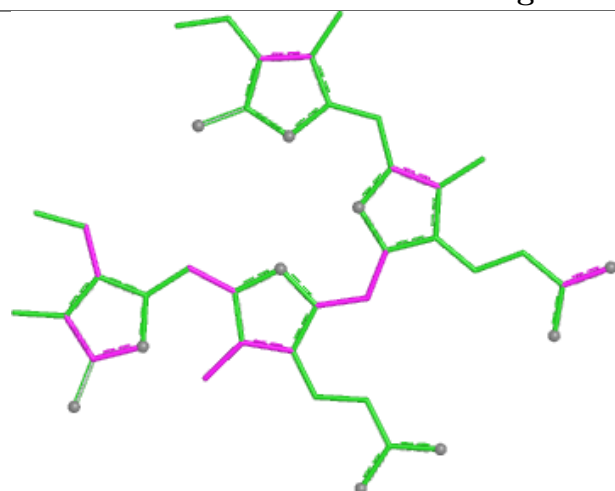


Torsions

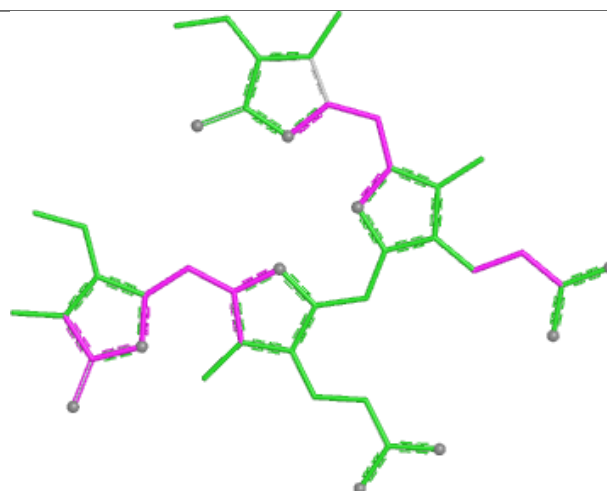


Rings

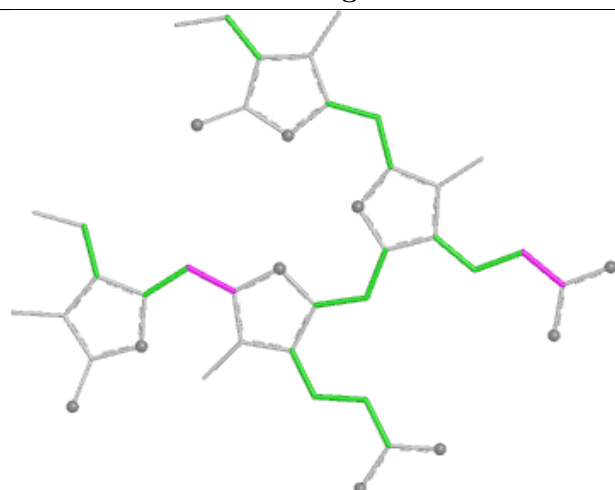
Ligand PEB B 166



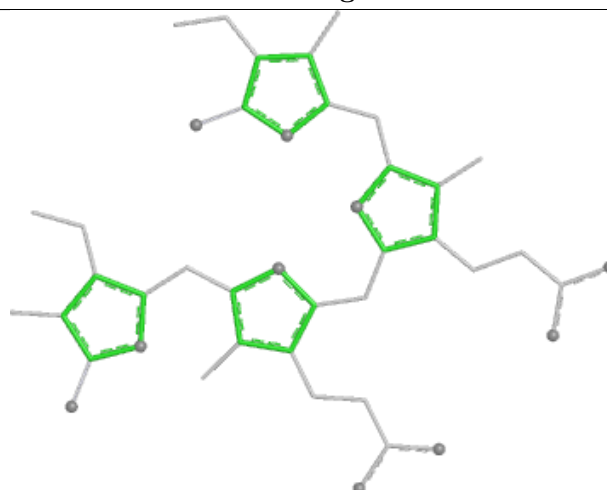
Bond lengths



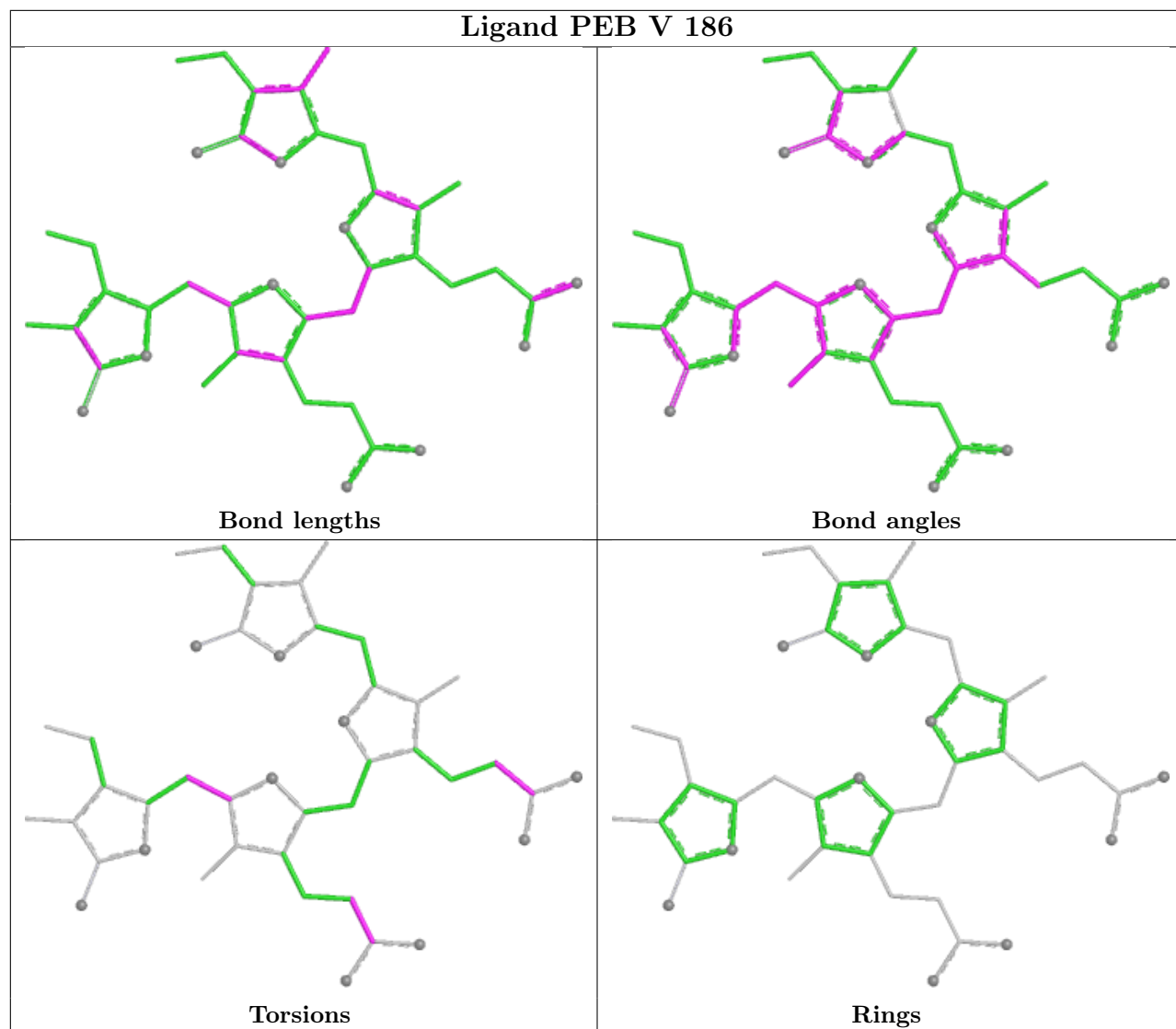
Bond angles

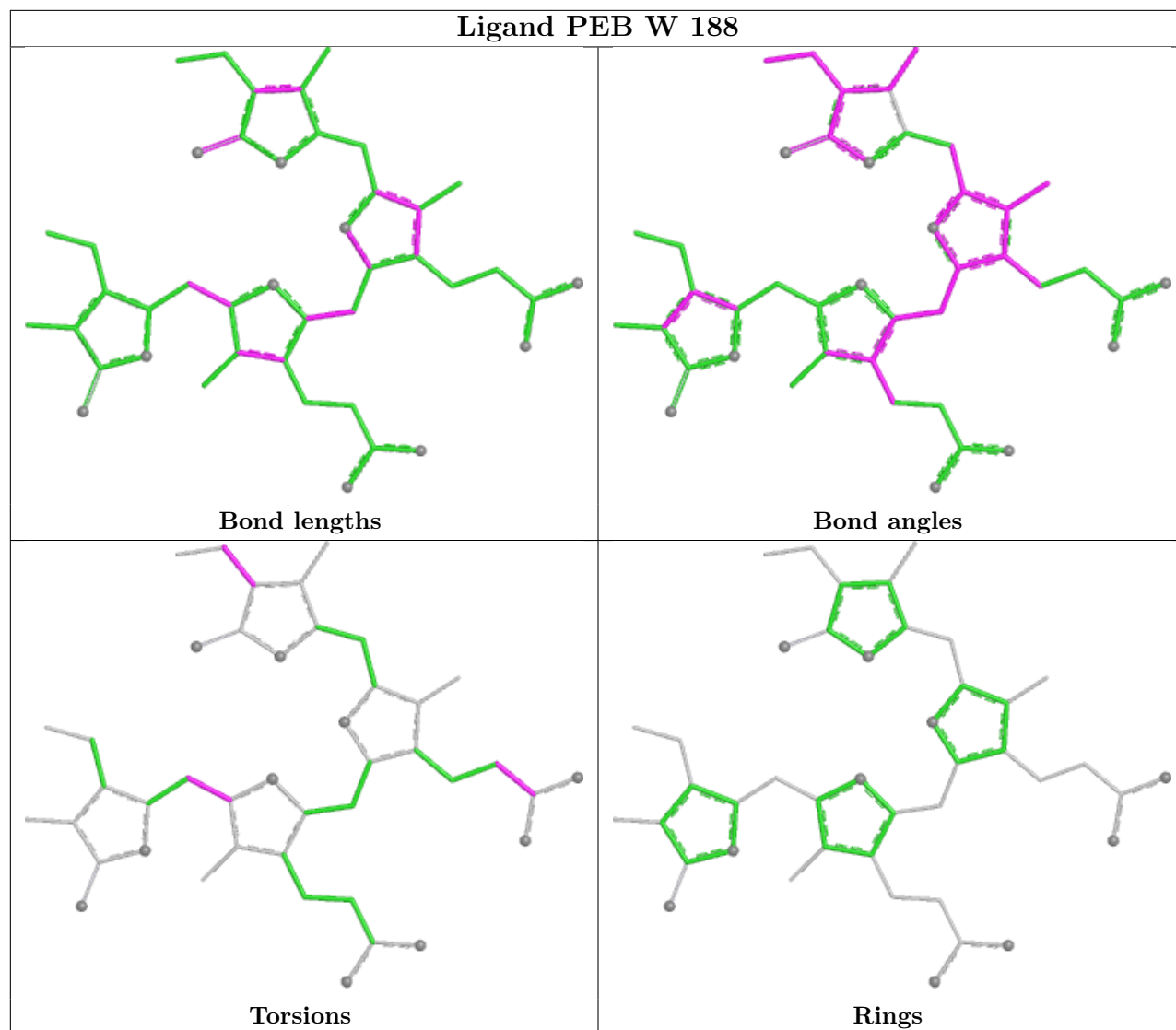


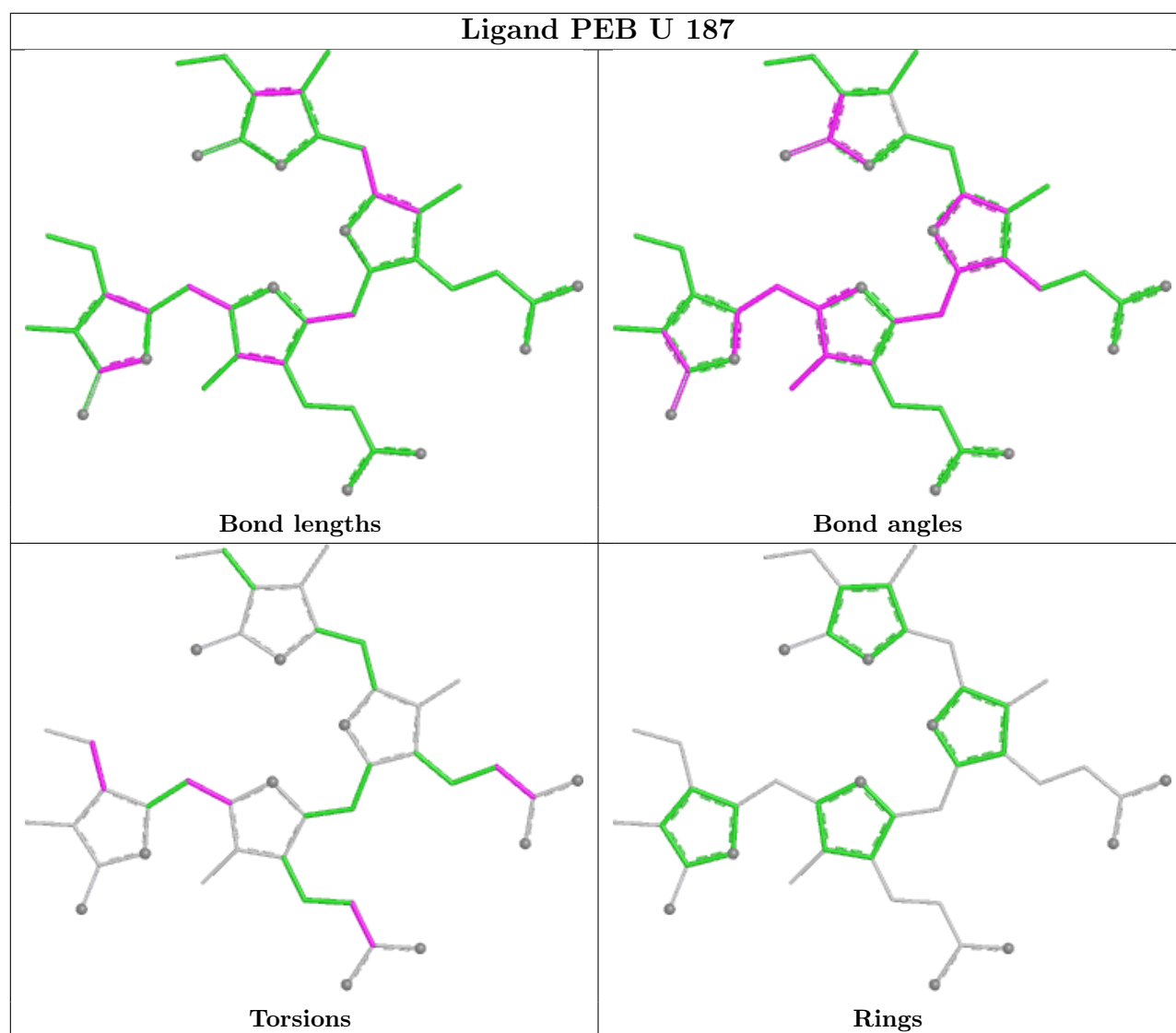
Torsions



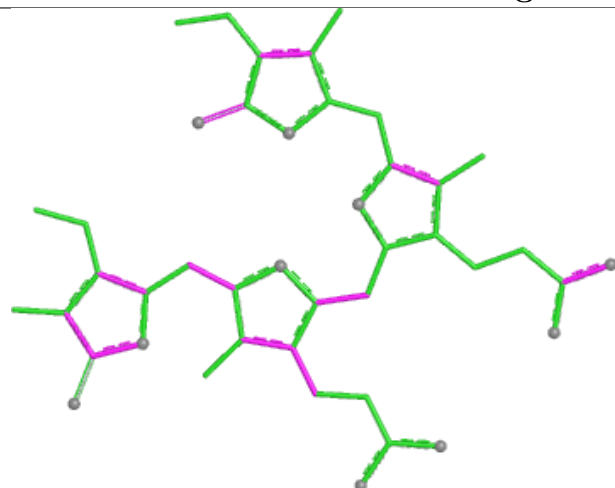
Rings



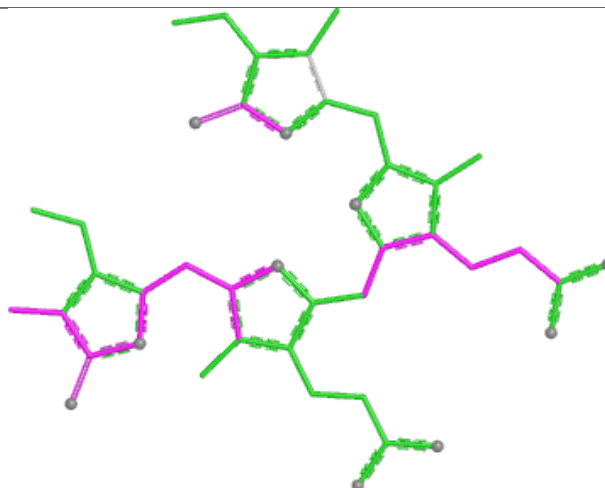




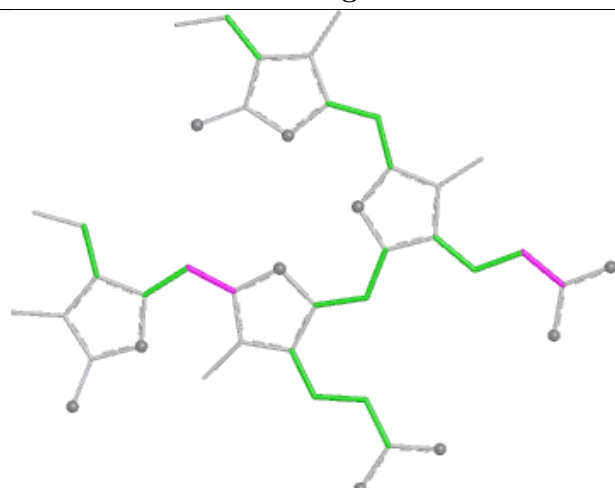
Ligand PEB K 166



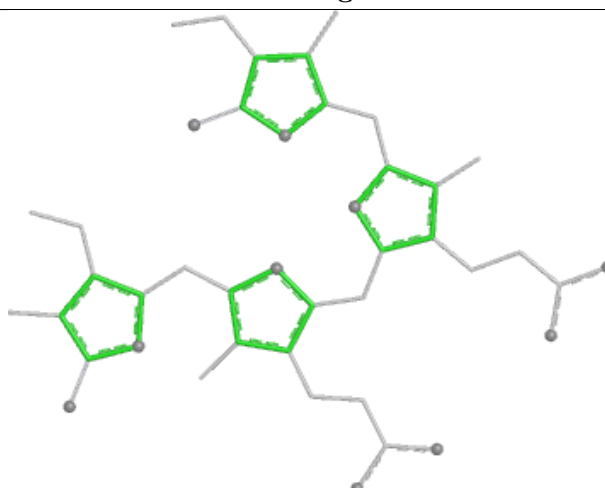
Bond lengths



Bond angles

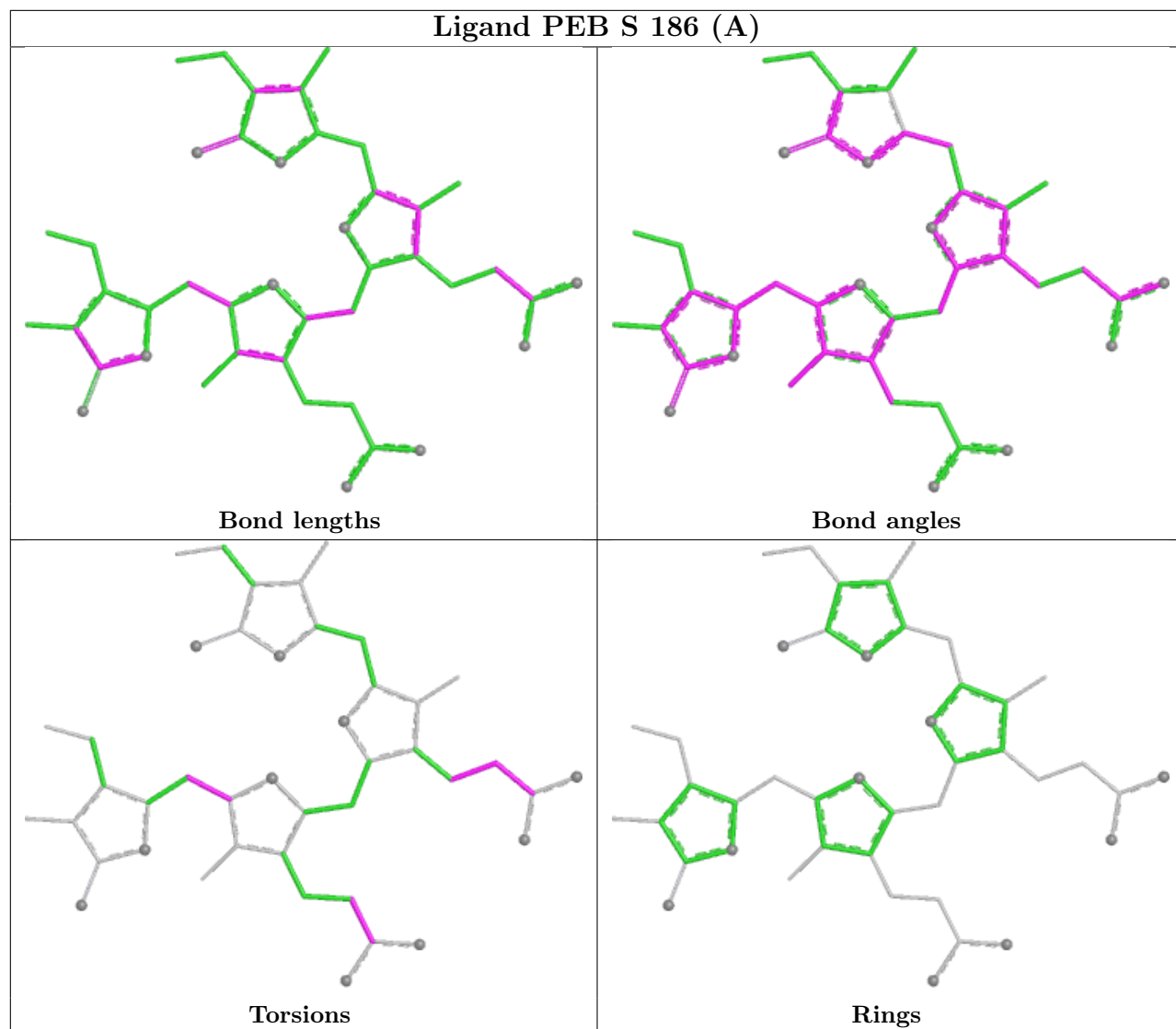


Torsions

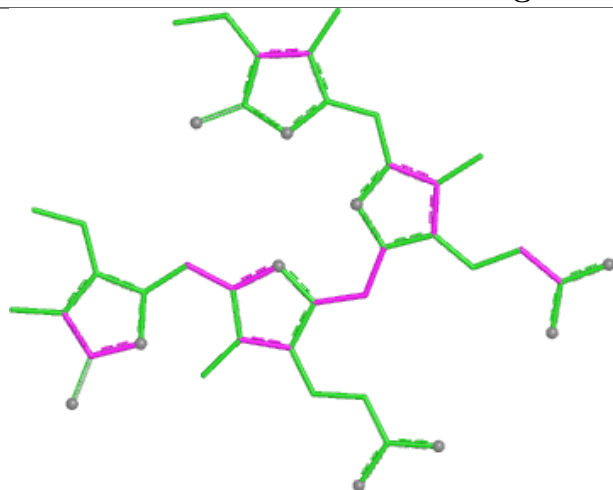


Rings

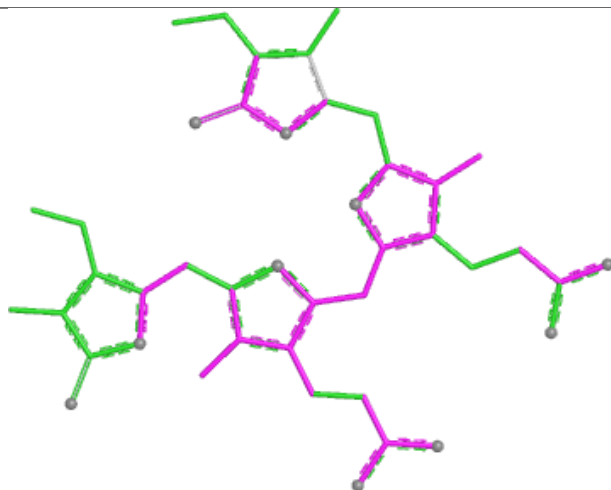
Ligand PEB S 186 (A)



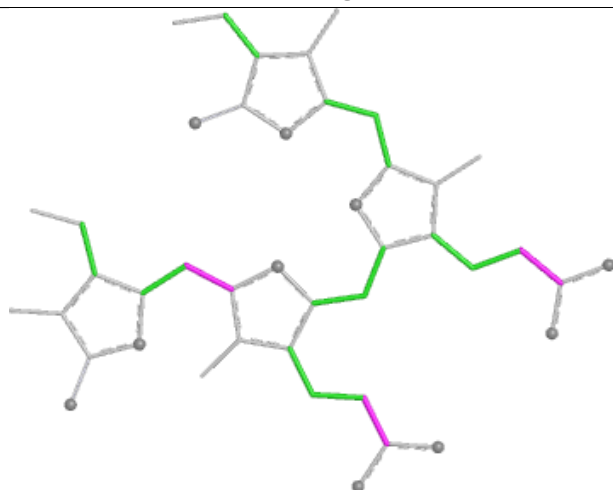
Ligand PEB K 167



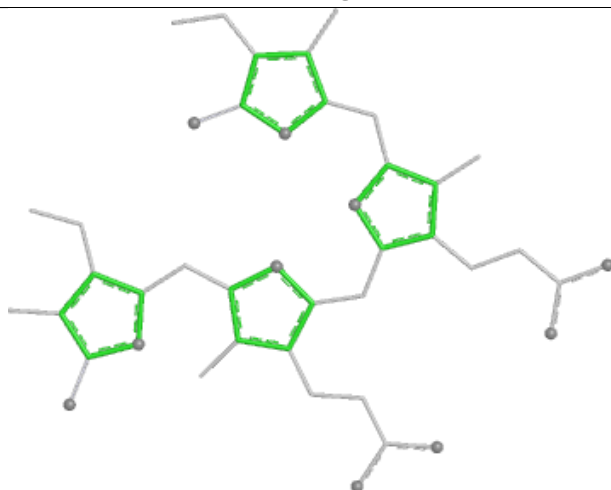
Bond lengths



Bond angles

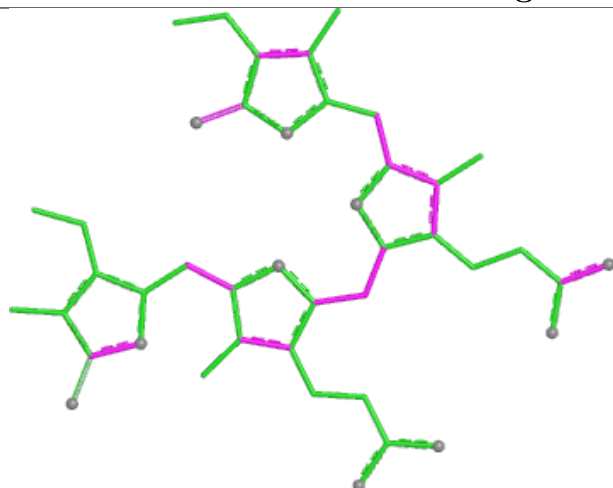


Torsions

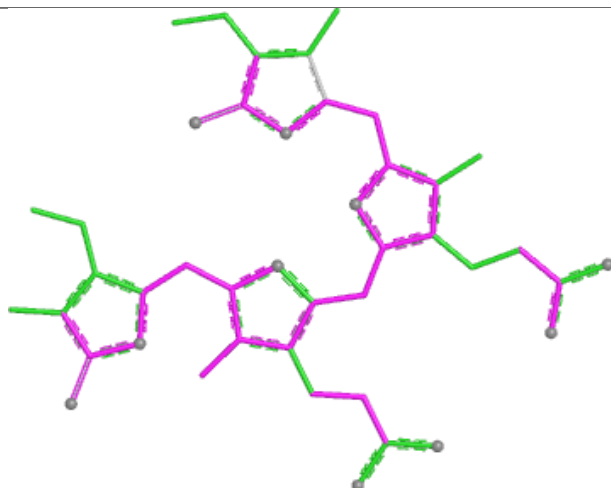


Rings

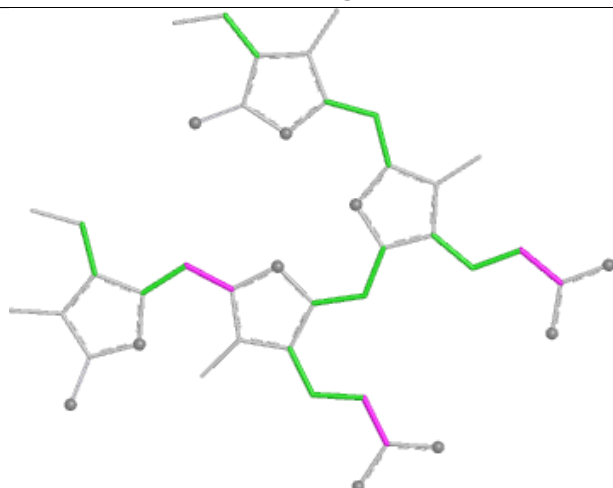
Ligand PEB T 186



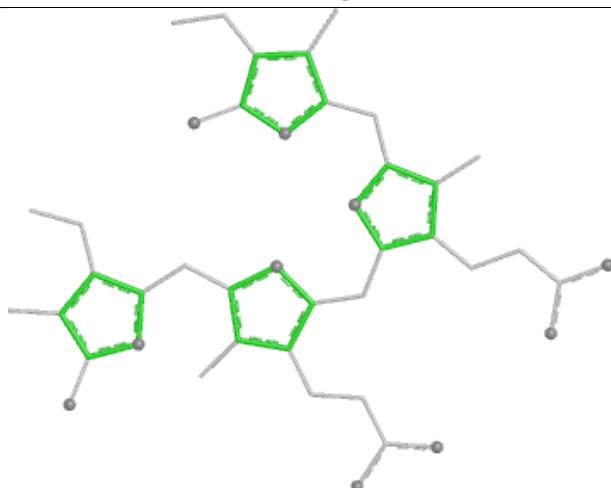
Bond lengths



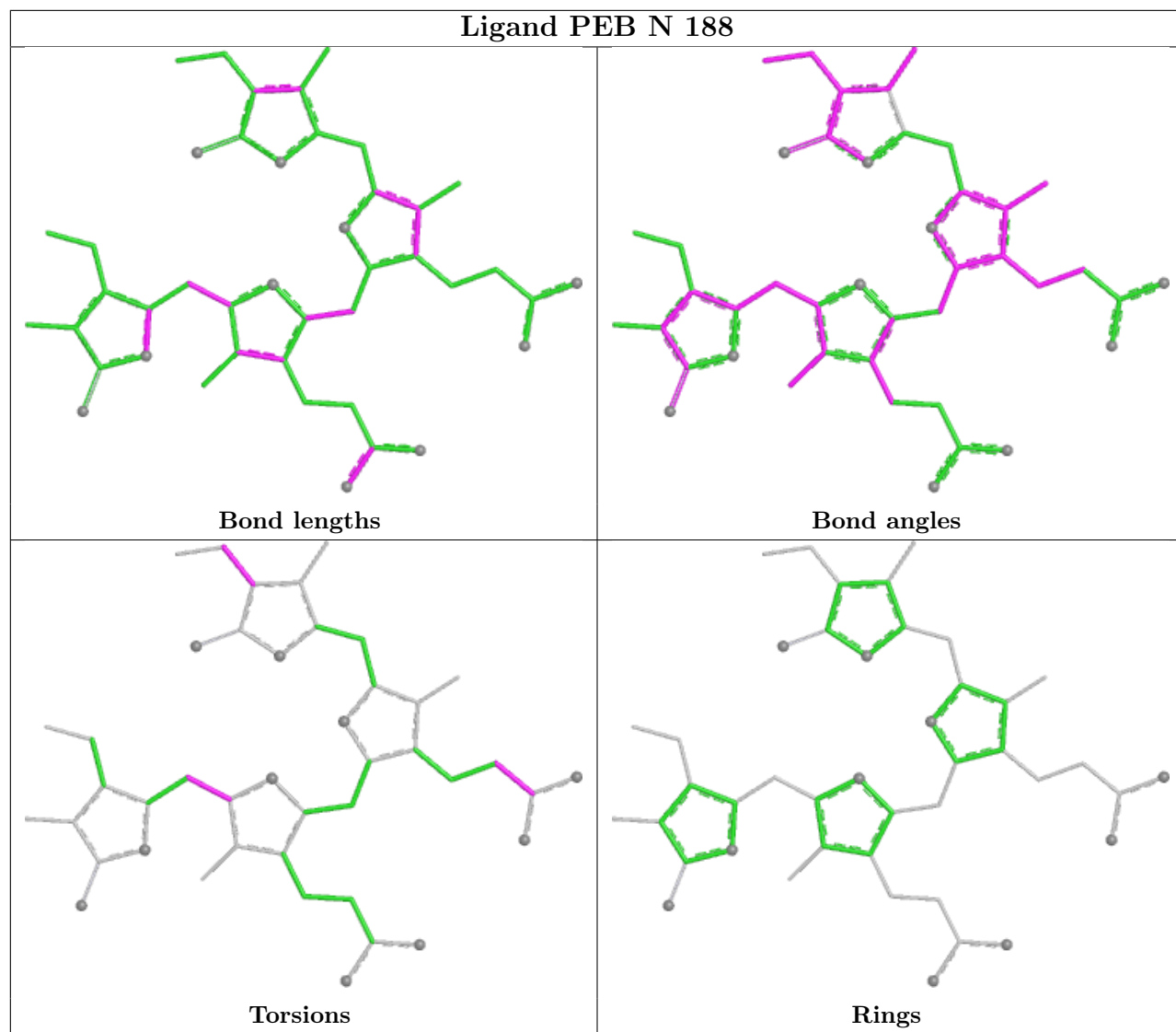
Bond angles

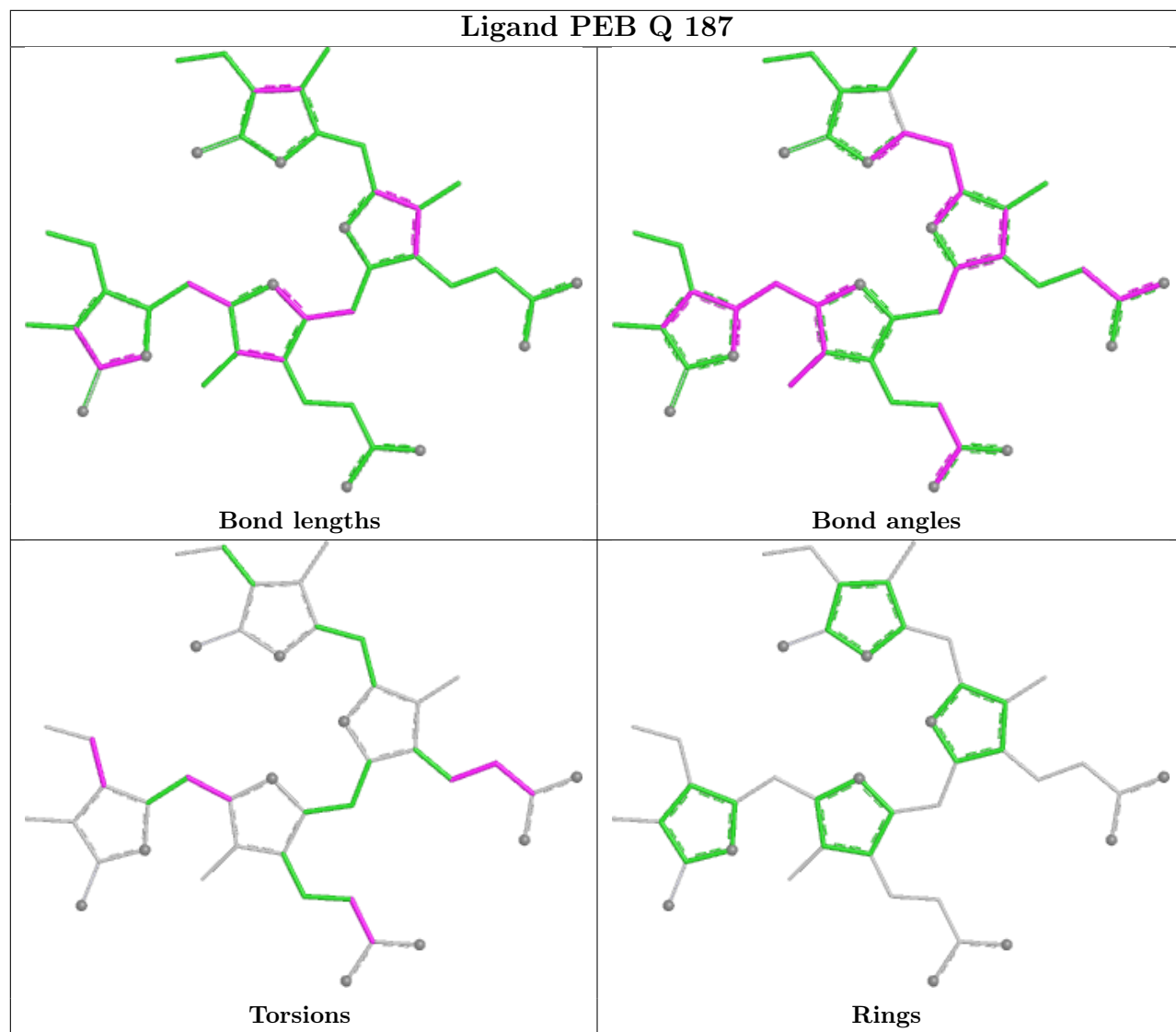


Torsions

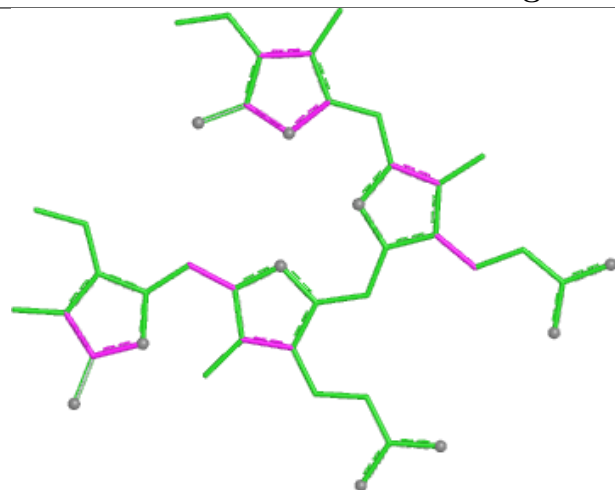


Rings

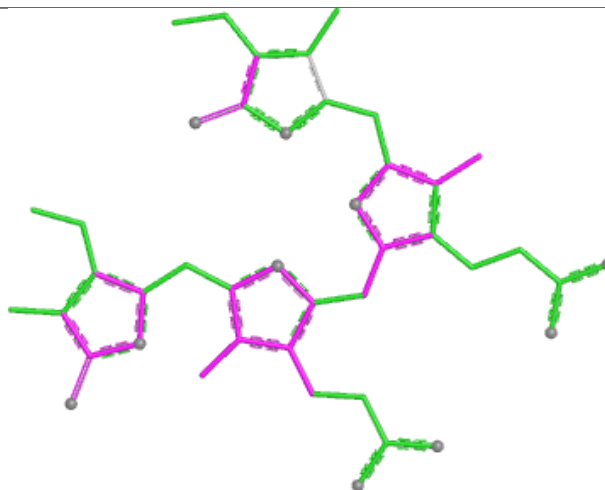




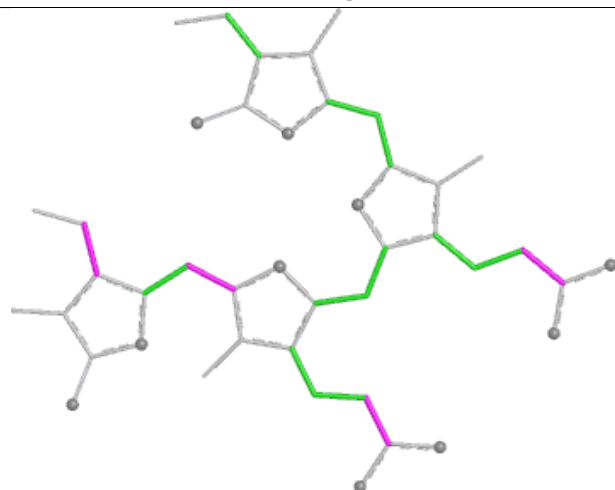
Ligand PEB I 167



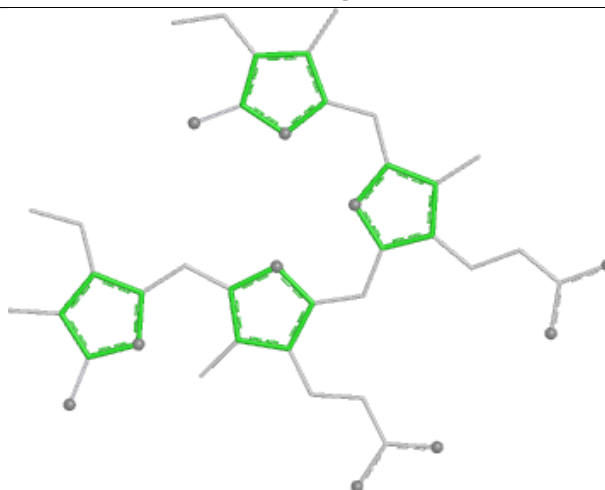
Bond lengths



Bond angles

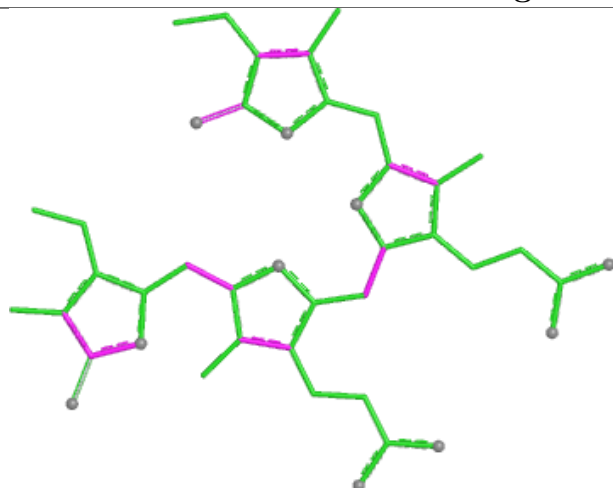


Torsions

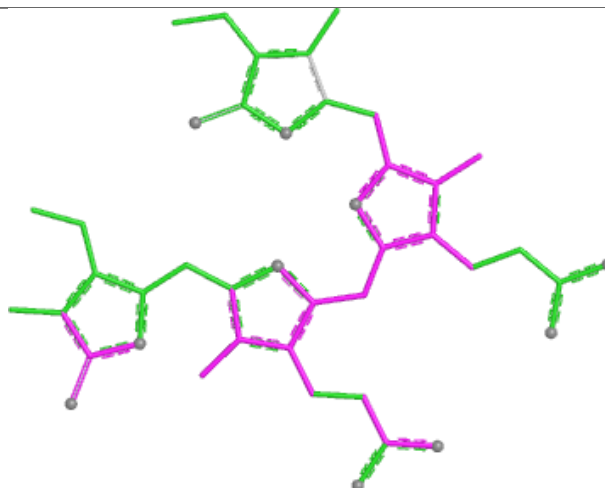


Rings

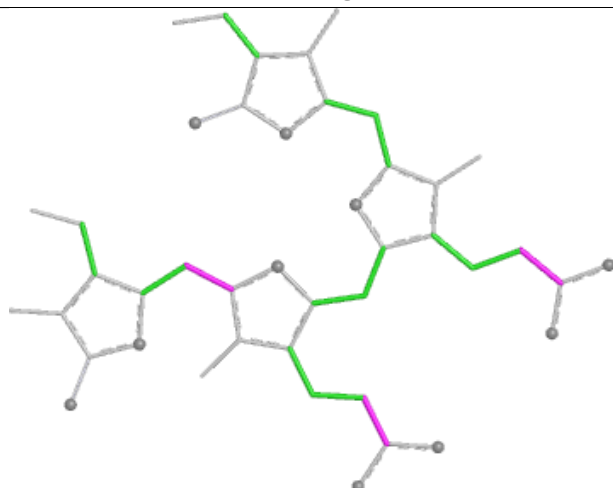
Ligand PEB D 167



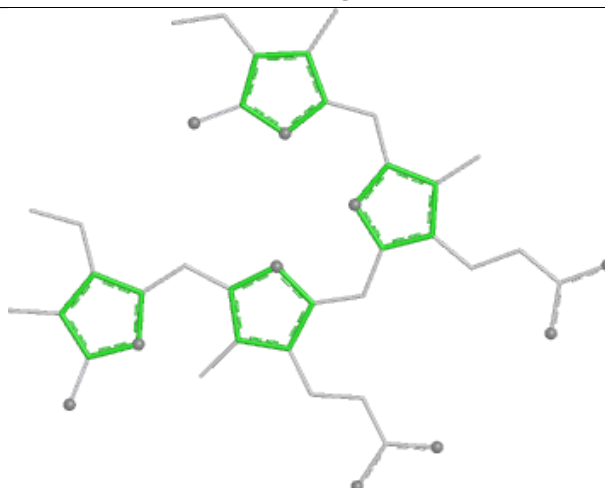
Bond lengths



Bond angles

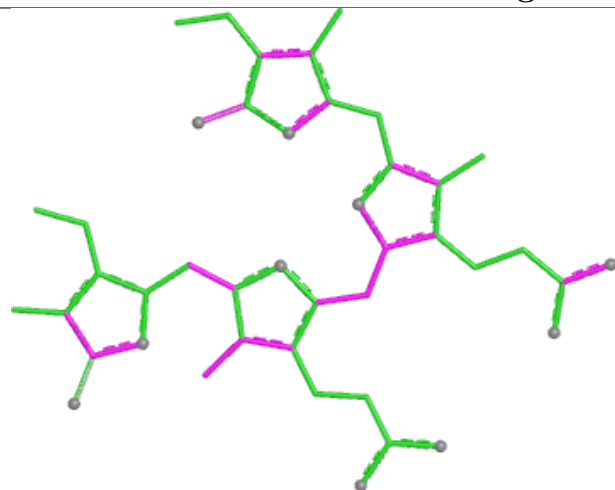


Torsions

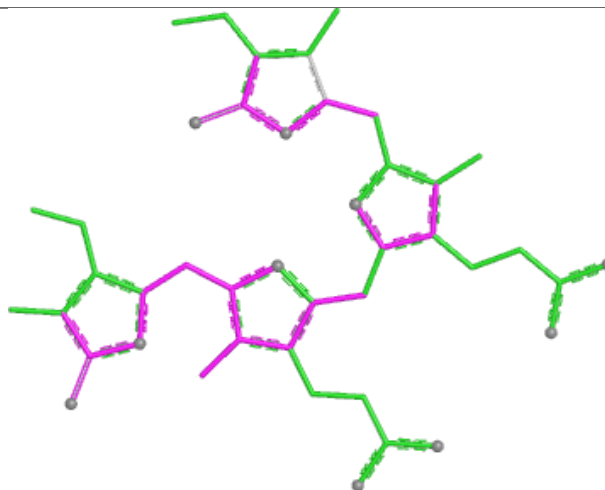


Rings

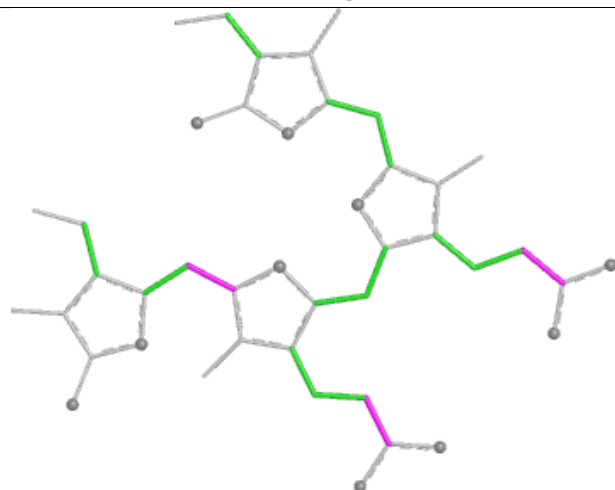
Ligand PEB P 186



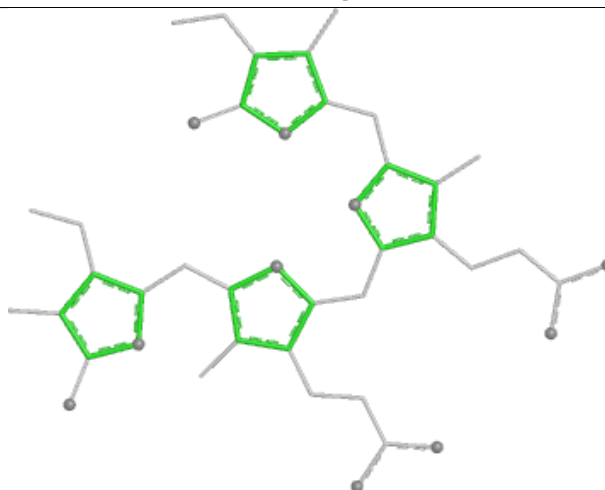
Bond lengths



Bond angles

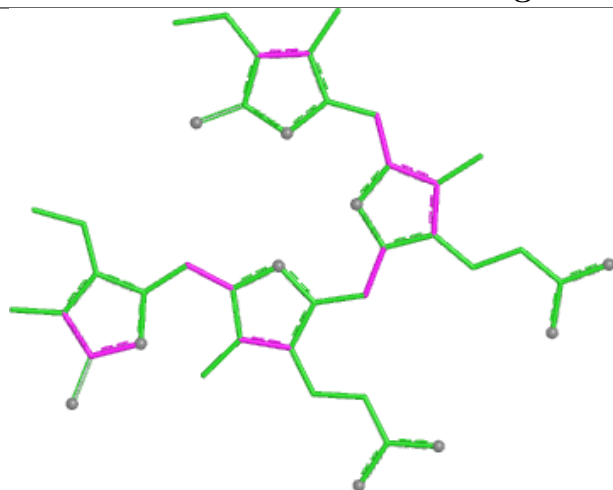


Torsions

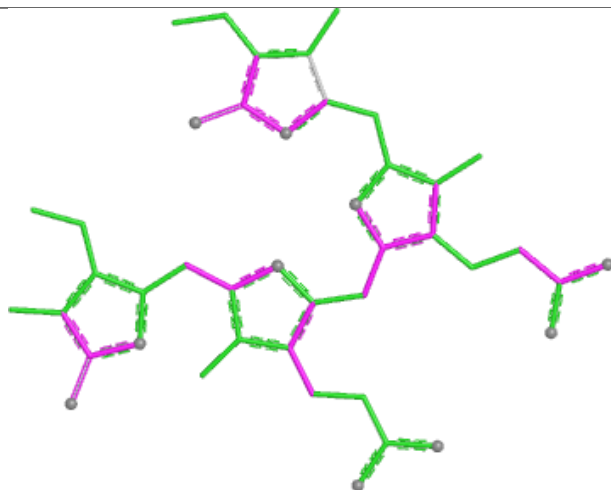


Rings

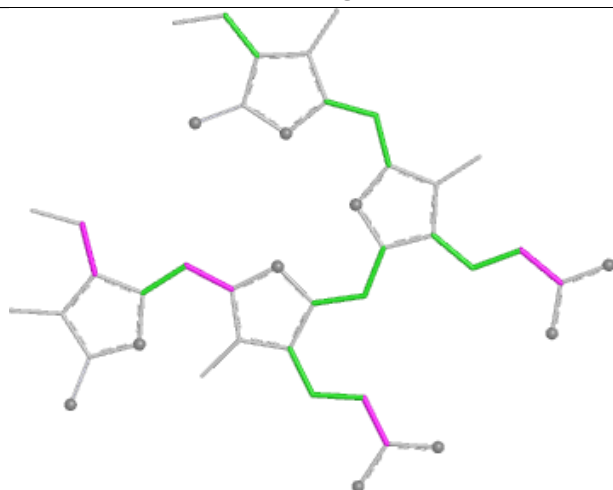
Ligand PEB A 167



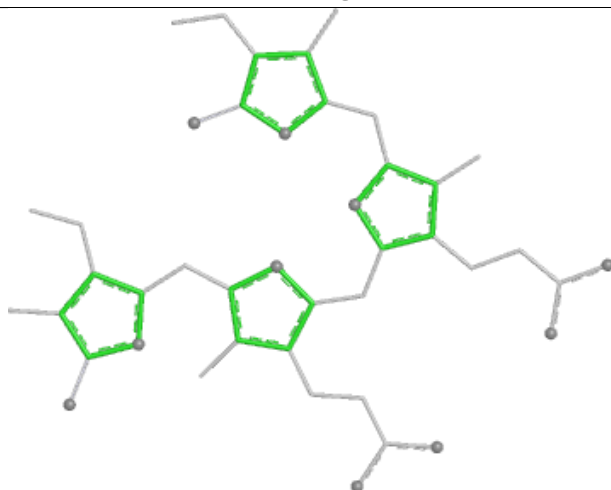
Bond lengths



Bond angles

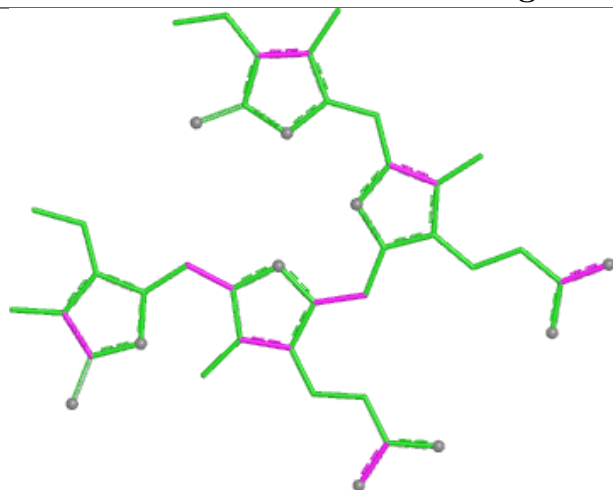


Torsions

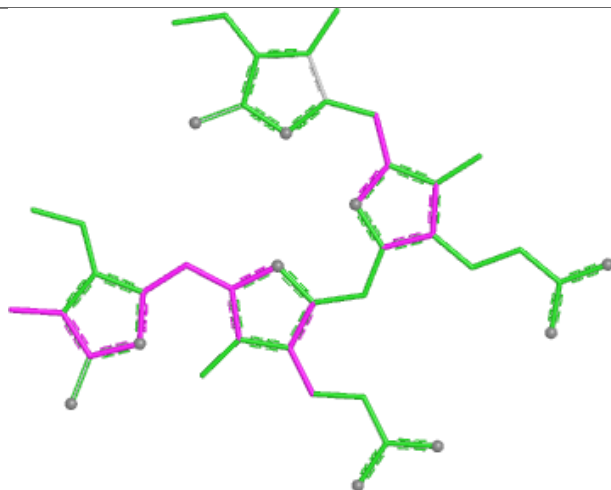


Rings

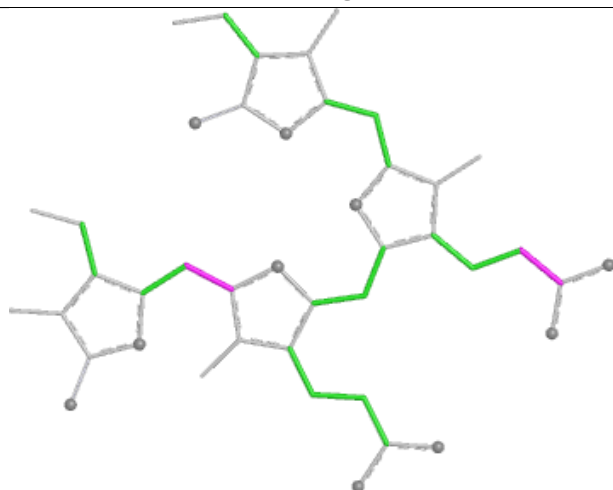
Ligand PEB J 166



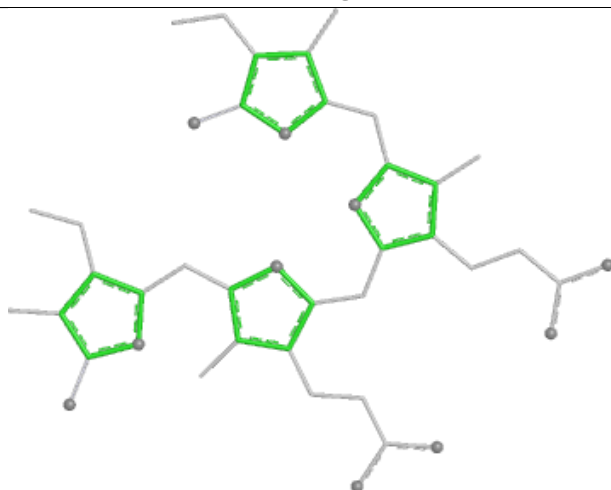
Bond lengths



Bond angles

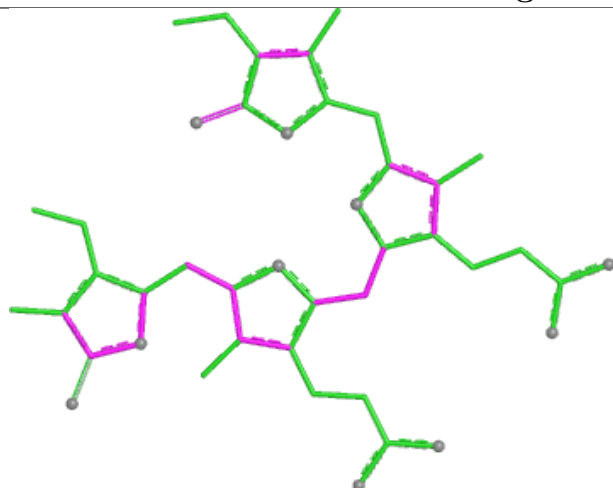


Torsions

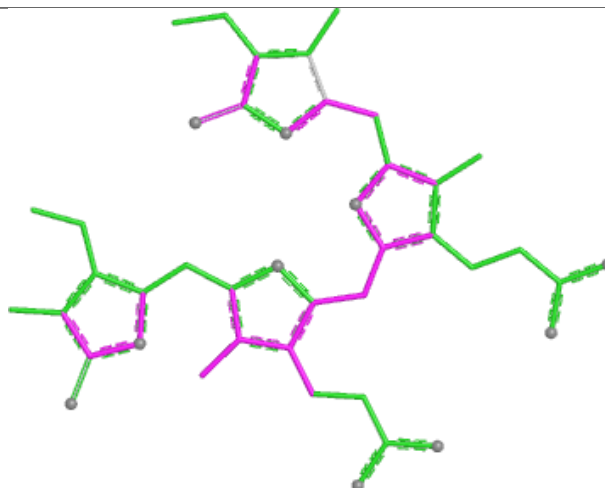


Rings

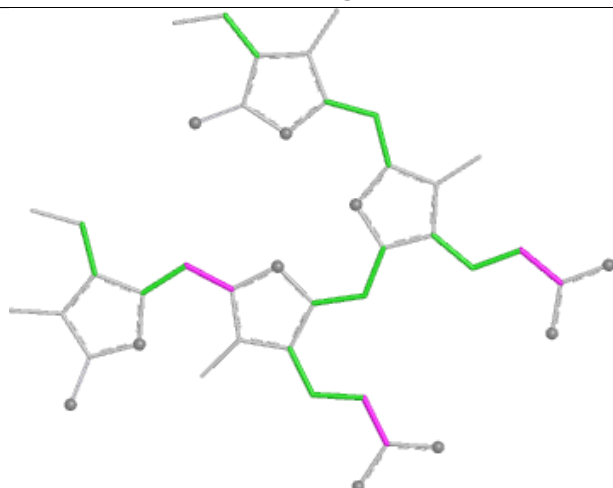
Ligand PEB F 167



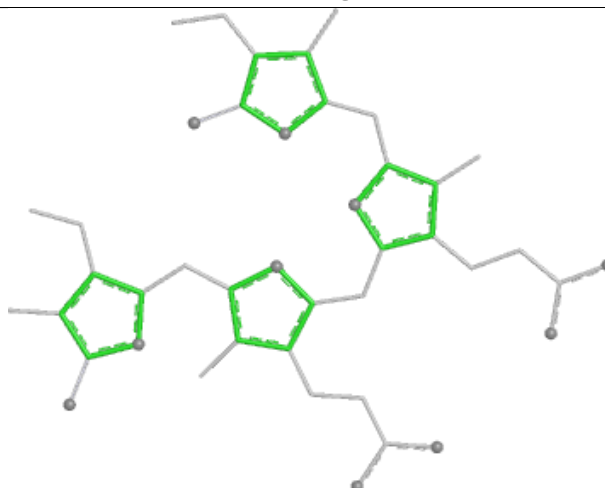
Bond lengths



Bond angles

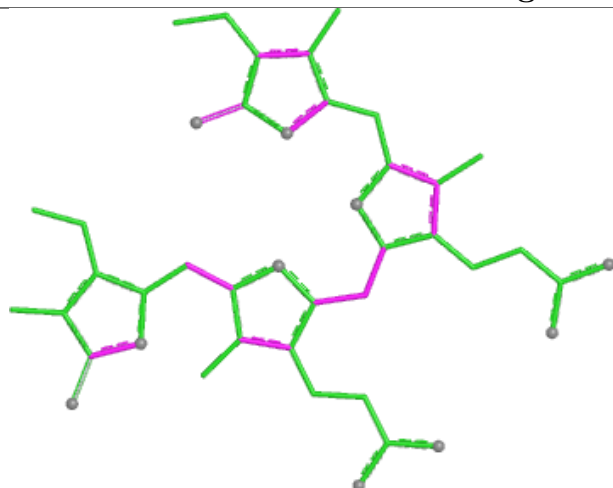


Torsions

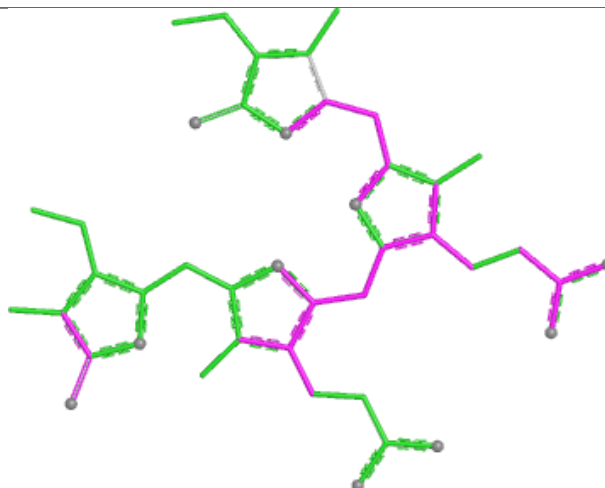


Rings

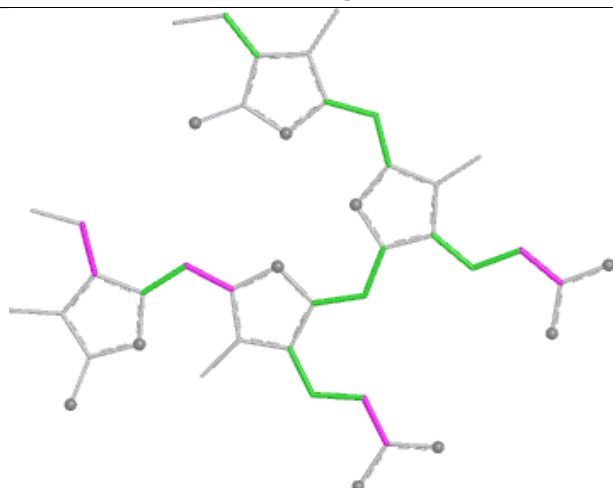
Ligand PEB S 187



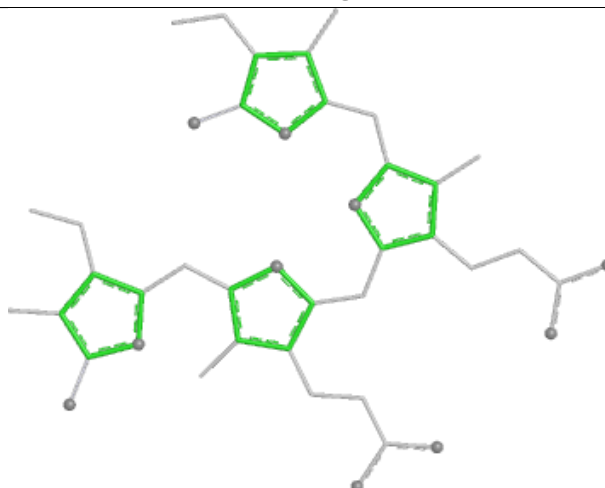
Bond lengths



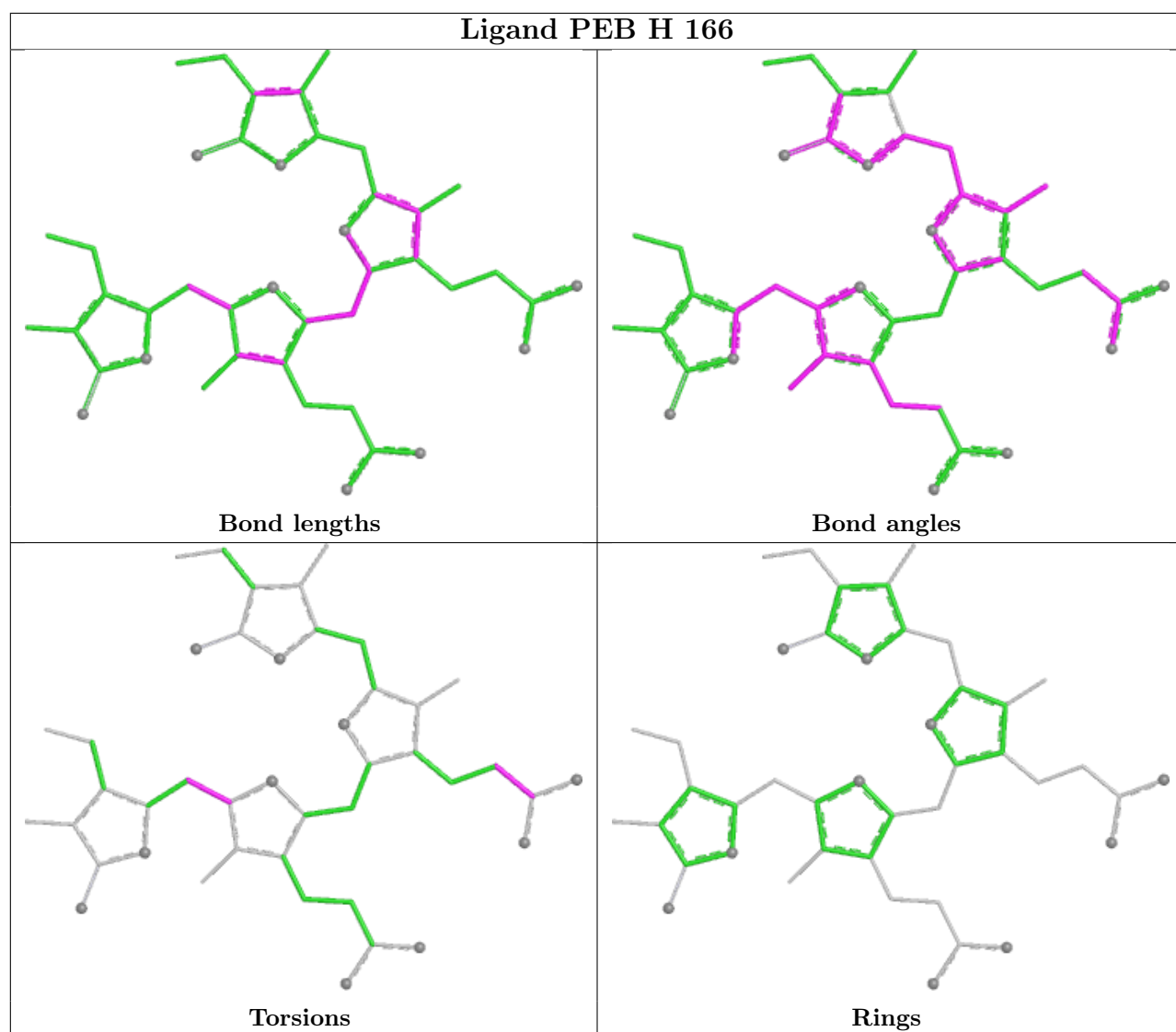
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	23	GLY	5.8
2	U	28[A]	PHE	5.2
2	T	24	ALA	5.1
2	X	150	GLY	4.2
2	T	28[A]	PHE	3.8
2	T	184[A]	SER	3.8
2	U	24	ALA	3.7
2	O	150	GLY	3.6
2	Q	22	MET	3.3
2	S	150	GLY	3.3
2	V	184[A]	SER	3.2
1	E	69	SER	3.1
2	S	28[A]	PHE	3.0
2	M	24	ALA	3.0
2	R	150	GLY	3.0
2	U	22	MET	3.0
2	T	25	LEU	2.9
2	Q	28[A]	PHE	2.9
2	X	28[A]	PHE	2.9
2	P	28[A]	PHE	2.9
2	R	28[A]	PHE	2.9
2	T	183	LEU	2.8
2	O	184	SER	2.8
2	T	168	LEU	2.7
2	U	25	LEU	2.5
2	W	28[A]	PHE	2.5
2	V	150	GLY	2.5
1	B	61[A]	GLN	2.5
2	Q	24	ALA	2.4
1	H	75	THR	2.4
2	R	183	LEU	2.4
2	T	153	LEU	2.4
2	R	22	MET	2.4
2	P	25	LEU	2.3
2	O	28[A]	PHE	2.3
2	S	184	SER	2.3
2	S	22[A]	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	150	GLY	2.3
1	F	69	SER	2.3
2	R	166	ALA	2.3
2	P	21	ASP	2.3
2	M	28[A]	PHE	2.2
2	W	151	GLY	2.2
2	P	24	ALA	2.2
2	O	109	ASN	2.1
2	N	28	PHE	2.1
2	R	179	VAL	2.1
2	T	160	VAL	2.1
2	U	21	ASP	2.1
1	H	68	ASN	2.1
1	G	69	SER	2.1
2	P	22[A]	MET	2.1
1	H	69	SER	2.0
1	C	114	ARG	2.0
2	R	161	VAL	2.0
2	R	117	ALA	2.0
2	R	134	ALA	2.0
2	R	170	ALA	2.0
2	S	117	ALA	2.0
2	U	4	ALA	2.0
2	Q	25	LEU	2.0
2	U	183	LEU	2.0

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

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

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MEN	O	70	9/10	0.99	0.04	10,10,14,15	0
2	MEN	V	70	9/10	0.99	0.03	9,10,14,15	0
2	MEN	W	70	9/10	0.99	0.04	10,11,13,14	0
2	MEN	X	70	9/10	0.99	0.04	10,11,12,14	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MPD	R	204	8/8	0.76	0.23	10,18,21,21	8
7	MPD	O	204	8/8	0.79	0.20	9,20,24,27	8
7	MPD	Q	204	8/8	0.82	0.15	12,15,16,17	8
7	MPD	B	203	8/8	0.82	0.17	13,13,18,23	8
7	MPD	S	204	8/8	0.83	0.14	15,17,19,20	8
8	MRD	V	204	8/8	0.83	0.13	12,16,19,20	8
7	MPD	P	204	8/8	0.85	0.14	12,15,16,17	8
8	MRD	T	204	8/8	0.86	0.12	12,14,18,23	8
7	MPD	M	204	8/8	0.86	0.14	12,14,16,17	8
5	PI	W	205	5/5	0.87	0.12	19,22,26,29	5
7	MPD	U	204	8/8	0.87	0.16	16,18,27,28	8
5	PI	R	205	5/5	0.88	0.12	21,23,24,25	5
7	MPD	W	204	8/8	0.88	0.14	12,14,16,16	8
7	MPD	X	204	8/8	0.90	0.11	13,15,18,18	8
5	PI	N	204	5/5	0.90	0.10	18,20,21,27	5
5	PI	U	205	5/5	0.90	0.11	17,19,20,25	5
5	PI	P	205	5/5	0.91	0.10	18,18,21,22	5
5	PI	E	203	5/5	0.92	0.09	20,20,22,23	5
5	PI	X	205	5/5	0.92	0.11	20,23,26,28	5
5	PI	J	204	5/5	0.93	0.10	16,19,21,25	5
5	PI	M	205	5/5	0.93	0.09	20,22,23,25	5
5	PI	G	203	5/5	0.93	0.10	18,20,23,24	5
5	PI	I	204	5/5	0.93	0.09	14,16,17,18	5
5	PI	O	205	5/5	0.94	0.10	19,20,22,22	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PI	V	205	5/5	0.94	0.09	17,17,20,23	5
5	PI	A	204	5/5	0.94	0.09	15,16,19,23	5
5	PI	C	204	5/5	0.94	0.09	18,18,23,26	5
5	PI	K	203	5/5	0.95	0.08	15,17,18,21	5
5	PI	L	204	5/5	0.95	0.09	16,18,19,22	5
4	NO3	L	203	4/4	0.95	0.08	13,15,22,24	0
3	PEB	J	167	43/43	0.95	0.07	11,16,22,31	0
3	PEB	R	186	43/43	0.95	0.07	15,18,31,46	0
3	PEB	R	188	43/43	0.95	0.08	12,16,31,43	0
5	PI	F	203	5/5	0.95	0.08	17,18,22,24	5
5	PI	T	205	5/5	0.95	0.07	26,27,29,30	5
3	PEB	U	187	43/43	0.95	0.07	8,12,17,33	0
5	PI	H	203	5/5	0.95	0.10	17,18,20,21	5
4	NO3	A	203	4/4	0.95	0.08	11,15,19,21	0
4	NO3	C	203	4/4	0.95	0.07	16,21,22,23	0
5	PI	B	204	5/5	0.96	0.07	14,14,15,19	5
3	PEB	I	167	43/43	0.96	0.07	9,12,18,25	0
3	PEB	S	186[A]	43/43	0.96	0.07	12,14,26,32	6
3	PEB	S	186[B]	43/43	0.96	0.07	12,14,20,33	6
3	PEB	T	186	43/43	0.96	0.07	14,17,27,44	0
3	PEB	T	187	43/43	0.96	0.07	10,14,23,39	0
3	PEB	T	188	43/43	0.96	0.07	12,15,23,26	0
3	PEB	C	167	43/43	0.96	0.07	12,18,26,32	0
3	PEB	X	188	43/43	0.96	0.07	9,11,16,19	0
3	PEB	K	167	43/43	0.96	0.07	11,14,21,27	0
3	PEB	Q	187	43/43	0.96	0.07	10,12,20,38	0
4	NO3	I	203	4/4	0.96	0.06	13,20,22,22	0
4	NO3	J	203	4/4	0.96	0.07	12,20,20,23	0
3	PEB	E	166	43/43	0.96	0.07	14,18,26,35	0
5	PI	Q	205	5/5	0.96	0.07	22,23,24,25	5
3	PEB	R	187	43/43	0.96	0.06	13,15,23,32	0
5	PI	S	205	5/5	0.96	0.08	18,18,21,22	5
3	PEB	P	186	43/43	0.97	0.06	9,13,24,40	0
5	PI	D	204	5/5	0.97	0.06	13,13,16,16	5
3	PEB	P	187	43/43	0.97	0.06	9,11,18,31	0
3	PEB	P	188	43/43	0.97	0.05	8,10,17,22	0
3	PEB	Q	186	43/43	0.97	0.06	10,13,25,45	0
3	PEB	B	167	43/43	0.97	0.06	9,13,19,26	0
3	PEB	F	166	43/43	0.97	0.05	9,11,14,21	0
3	PEB	F	167	43/43	0.97	0.05	10,12,16,21	0
3	PEB	G	166	43/43	0.97	0.05	8,11,13,18	0
3	PEB	I	166	43/43	0.97	0.06	10,12,17,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEB	C	166	43/43	0.97	0.05	10,12,14,18	0
3	PEB	S	187	43/43	0.97	0.06	11,13,20,33	0
3	PEB	S	188	43/43	0.97	0.05	11,12,17,21	0
3	PEB	J	166	43/43	0.97	0.05	10,11,14,19	0
3	PEB	B	166	43/43	0.97	0.05	9,10,12,21	0
3	PEB	K	166	43/43	0.97	0.06	10,12,14,25	0
3	PEB	U	186	43/43	0.97	0.06	9,13,21,41	0
3	PEB	D	167	43/43	0.97	0.06	9,13,17,24	0
3	PEB	U	188	43/43	0.97	0.06	9,11,18,34	0
3	PEB	V	186	43/43	0.97	0.06	8,11,21,32	0
3	PEB	V	187	43/43	0.97	0.05	10,11,17,26	0
3	PEB	W	186	43/43	0.97	0.06	9,13,21,34	0
6	NA	V	206	1/1	0.97	0.20	25,25,25,25	1
3	PEB	W	187	43/43	0.97	0.06	9,11,19,28	0
3	PEB	W	188	43/43	0.97	0.05	10,12,16,23	0
3	PEB	X	186	43/43	0.97	0.06	9,12,24,36	0
3	PEB	L	167	43/43	0.97	0.06	9,12,17,28	0
3	PEB	M	186	43/43	0.97	0.06	8,11,20,37	0
3	PEB	M	188	43/43	0.97	0.06	8,10,14,18	0
4	NO3	D	203	4/4	0.97	0.07	12,16,19,23	0
3	PEB	N	186	43/43	0.97	0.06	9,13,23,32	0
3	PEB	N	187	43/43	0.97	0.05	9,11,17,27	0
3	PEB	N	188	43/43	0.97	0.05	10,12,17,22	0
3	PEB	O	186	43/43	0.97	0.06	8,12,20,33	0
3	PEB	O	187	43/43	0.97	0.06	10,13,20,25	0
6	NA	A	205	1/1	0.98	0.12	18,18,18,18	0
6	NA	S	206	1/1	0.98	0.17	29,29,29,29	0
3	PEB	H	166	43/43	0.98	0.06	13,16,22,29	0
3	PEB	L	166	43/43	0.98	0.04	8,9,12,18	0
3	PEB	V	188	43/43	0.98	0.04	8,10,14,16	0
3	PEB	O	188	43/43	0.98	0.05	9,11,15,16	0
3	PEB	H	167	43/43	0.98	0.05	11,12,16,21	0
3	PEB	E	167	43/43	0.98	0.05	11,13,16,20	0
3	PEB	M	187	43/43	0.98	0.05	9,10,16,26	0
3	PEB	X	187	43/43	0.98	0.05	9,11,19,29	0
3	PEB	D	166	43/43	0.98	0.05	9,11,15,20	0
3	PEB	A	166	43/43	0.98	0.05	8,9,13,19	0
3	PEB	Q	188	43/43	0.98	0.04	10,13,17,19	0
3	PEB	A	167	43/43	0.98	0.05	9,11,17,27	0
3	PEB	G	167	43/43	0.98	0.05	9,12,16,22	0
6	NA	G	204	1/1	0.99	0.09	16,16,16,16	0
6	NA	H	204	1/1	0.99	0.19	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NA	I	205	1/1	0.99	0.12	20,20,20,20	0
6	NA	J	205	1/1	0.99	0.12	17,17,17,17	0
6	NA	K	204	1/1	0.99	0.13	22,22,22,22	0
6	NA	L	205	1/1	0.99	0.13	17,17,17,17	0
6	NA	N	205	1/1	0.99	0.17	28,28,28,28	0
6	NA	B	205	1/1	0.99	0.16	21,21,21,21	0
6	NA	C	205	1/1	0.99	0.14	19,19,19,19	0
6	NA	W	206	1/1	0.99	0.13	25,25,25,25	0
6	NA	E	204	1/1	0.99	0.12	19,19,19,19	0
6	NA	D	205	1/1	1.00	0.13	18,18,18,18	0
6	NA	F	204	1/1	1.00	0.13	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.